ChemACE Users Manual

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January 30, 2011

ChemACE Beta Test Version

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1. ChemACE Methodology

The **Chem**ical **A**ssessment **C**lustering **E**ngine (ChemACE) is designed to cluster a list of chemicals based on structure using predefined similarity rules. The ChemACE methodology is based on logic implemented in the Analog Identification Methodology (AIM) tool (http://aim.epa.gov) that identifies analogs based on the presence of common fragments using a tiered approach.

In AIM, the first tier search strategy referred to as 'Pass 1' consists of matching all the same fragments (and ring systems) between the query chemical and chosen analogs and is based on an extensive fragment list. If analogs were not found during Pass 1, a second pass (Pass 2) would commence to identify analogs using a smaller, less restrictive list of possible fragments. The final Pass 3 allows simple substitutions.

ChemACE is designed cluster chemicals that are analogs of one another using the same fragment generation system found in AIM, but uses a more complex method for identifying analogs for the clustering exercises that is based on advanced queries in multidimensional space and by allowing users to design rules to modify the approach. Below, operation of ChemACE will be described in detail.

2. ChemACE Download/Set-Up

ChemACE is a self-extracting file. Once it is downloaded and saved to diskette or hard drive, execute (double-click) the file to install the program (if you selected "Run" and not "Save" at the download prompt, it should install automatically). Note: The ChemACE installation program includes a version of the Java Runtime Environment (JRE).

3. Creating a Chemical Input File

Prior to operating ChemACE, the user needs to identify or create a chemical inventory input file. Input files must be in simple tab delimited text format and must be formatted so that :

- The first row must contain column headings
- Each chemical (and its corresponding information) is entered on its own line
- The first column contains a representation of chemical structure using SMILES format (for more information see http://www.epa.gov/ncct/dsstox/MoreonSMILES.html)
- The second column contains a chemical identifier that can be any combination of numbers and characters, and

- No more than 5 additional (optional) columns (e.g., columns containing of information may be carried over to the output file. Any additional columns beyond that present in the input file will not be displayed in the output report

Creation of an input file is most easily done in Microsoft EXCEL or ACCESS followed by export of the table into a text (.txt) delimited file. A depiction of a table (as it would look in Microsoft EXCEL) is shown below in Figure 1.

Figure 1: Sample Input File

	Column 1	Column 2	Column 3	Column 4	Column 5	Column 6	Column 7
Header	SMILES	Unique ID	Attribute 1	Attribute 2	Attribute 3	Attribute 4	Attribute 5
Data 1	CCOC	500-01-2	Optional	Optional	Optional	Optional	Optional
Data 2	CC(=O)OCC	500-02-3	Optional	Optional	Optional	Optional	Optional
Data 3	CC(=O)OCCC	500-03-4	Optional	Optional	Optional	Optional	Optional
Data 4	CCOCCCCC	500-01-5	Optional	Optional	Optional	Optional	Optional

- The 'Header' for columns 1 and 2 will not show up in the output.
- Column two must reflect a unique identifier for the chemical.
- If attribute data are not to be included (shown above at columns 3-7), then these columns (including the heading) can be left blank. Conversely, the header is required for inclusion of attribute data.
- Proper formatting is required since ChemACE ignores rows that are not compatible with the formatting requirements or which contain incorrect/incompatible SMILES notations.

Two example input files (SampleDataFile.txt and Advanced example.txt) are provided in the ChemACE program folder under the "input" folder as reference. Users are advised to refer to these files when creating their input files. The former "SampleDataFile.txt" file represents a basic input file and the later "Advanced Example.txt" file represents an input file containing attributes. The "Advanced Example.txt" input file was included to 1) demonstrate the use of Data fields within ChemACE and 2) to demonstrate the clustering results of all of the current user options (including those on the advanced tab).

Special Note: Long text fields, especially those with no natural breaking points, may wrap unpredictably in the output file in this version of ChemACE.

4. ChemACE Model Interface

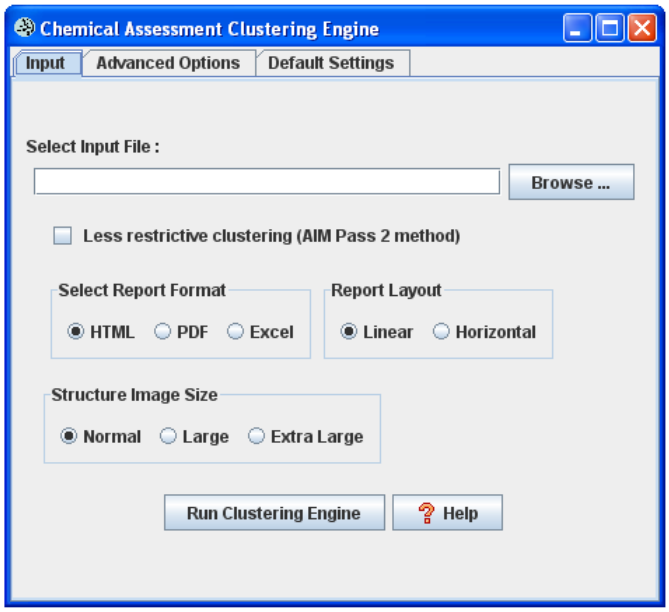
If standard set-up procedures were followed, a shortcut for ChemACE [ ] should be present on the user's desktop. Otherwise, the program should be available in the 'Start' menu under 'Programs'. Either double-click on the desktop icon or navigate the start menu and select the ChemACE program, which has a similar icon (shown above) adjacent to the name, to open the program.

The first screen to appear contains information that should be acknowledged by all users and is related to the operation of the program. Once the user has read this information, the user can click on the 'OK' button at the bottom of the screen to proceed to the actual program.

4.A Input Tab

The default screen that comes up (see Figure 2) displays the 'Input' tab with tab headings for 'Advanced Options' and 'Default Settings'. To navigate to another screen, select the tab heading for the screen to be accessed.

Figure 2: Initial Input Screen



The 'Help' button at the button of the screen allows access to this 'Tutorial' document.

4.A.1. Select the chemical inventory to be clustered

From the 'Input' interface (see Figure 2), click on the 'Browse' button under the 'Selected Input File' heading. A window will appear that allows the user to navigate through the computer files of the computer they are using. Navigate and select the file you wish to use by highlighting it, and then press the 'Select' button.

Special Note: If the data source you select is incompatible with the ChemACE program, the output will be blank; no warning message is displayed.

4.A.2. Select Report Format

ChemACE provides a user with the ability to customize the output report under the 'Input' tab shown in Figure 2 above. Alternatively, the user can refer to the 'Default Settings' tab to establish output report preferences for every run. To see a description of the various options for the report, refer to **Section 4.c** below.

4.A.3. Run the clustering tool with no remapping or exclusion rules.

Click the 'Run Clustering Engine' button. The completed report will open automatically in the selected format. Generation of the report may take a few minutes depending on the number of chemicals runs and depending on whether the output format includes structures (i.e., HTML and Adobe PDF formats).

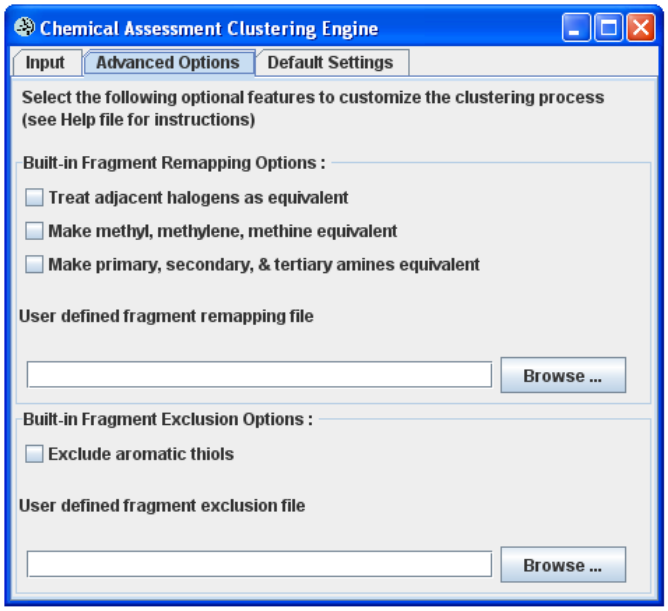
4.A.3. Run clustering tool with reduced fragments (less restrictive).

As in the AIM tool, ChemACE allows user to cluster compounds based on a reduced fragment list referred to as 'Less Restrictive Clustering (AIM Pass 2 Method). Pass 2 removes approximately one half of the fragments from consideration during fragment matching. The user should click the check-box for 'less restrictive clustering' under the input file field to implement this rule.

4.B Advanced Options Tab

ChemACE was designed to mimic the AIM Methodology with pass 1 and 2 logic embedded in ChemACE's general clustering rules. However, ChemACE also allows the user to manually enhance and even customize the clustering process by using "exclusion rules" for specific fragments, or fragment types and enabling remapping, which allows user to define different fragments as the same during the clustering process. These additional remapping and exclusion functions are carried out under the 'Advanced Options' tab and are shown below in Figure 3.

Figure 3: Advanced Options Tab



4.B.1. Predefined Remapping and/or Exclusion Rules.

Check-boxes representing predefined exclusions and remapping are available under the 'Advanced Options' tab; a brief identification and description of each is below.

- Treat adjacent halogens as equivalent - represents a remapping operation, which allows F to be substituted for Cl, Cl for Br, Br for I.
- Make methyl, methylene, methine equivalent- represents a remapping operation, which makes the identified groups equivalent.
- Primary, secondary & tertiary amines - represents a remapping operation, which makes the identified groups equivalent.
- Exclude aromatic thiols – represent an exclusion operation, which removes thiols from consideration.

4.B.2. User Defined Re-Mapping and Exclusion Rules

In addition to the predefined exclusion/remap operations above, the advanced tab allows user to create their own custom clustering rules; these can be used to make clustering either more or less restrictive. These are described in more detail, below.

When re-mapping and exclusion rules are created, the user should keep in mind the following.

- Rules are to be created in text documents (.txt) separate from the ChemACE program.

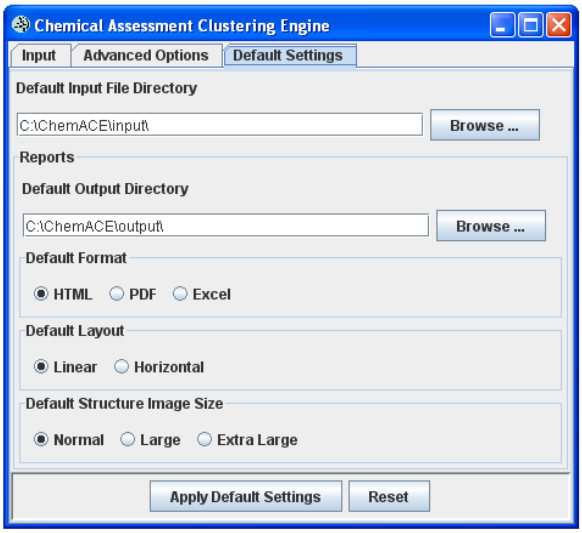
- Remapping and exclusion rules should be separated into individual text files. ChemACE has separate input fields for remapping and exclusion rules and treats the rules differently.
- Lines that start with '#' or '//' are not read by the program, but benefit users by allowing comments about the nature of the rule to be included with the rule text document.
- A fragment should be defined in a rule in only one way. If a fragment is defined in both a remapping and an exclusion rule or if a fragment is modified by a selected pre-programmed rule and is defined in a user-created rule, the program will get confused and may output a single compound multiple times. For example, you cannot require ChemACE to exclude Cl under a user defined rule, and then initiate the default rule to make all halogens equivalent at the same time.

Example remapping and exclusion rules can be found within the 'config' folder of the ChemACE program folder (created during instillation at C:/ChemACE/config) under the map or exclude folders, respectively. These example documents include added instructions and explanation. Also, the advanced example provides an additional column with information about clustering tendencies that may be useful in experimenting with the use and/or creation of remapping and exclusion rules. A complete list of fragment numbers used by ChemACE is required to create remapping and exclusion files, and can be found under Appendix A on page 12 of this document.

4.C Default Setting Tab

ChemACE provides users with the ability to customize the output report for different purposes. The user can specify the output format under the 'Input' tab each time they perform a cluster operation (see Figure 2). However, if the user wants to establish universal default output setting, changes should be made to the 'Default Settings' tab. The user also has the option to select a default input and output file directory.

Figure 4: Default Settings Tab



Listed below are the available fields for output format as seen on both the Input tab (Figure 2) and the Default Settings tab (Figure 4) followed by a brief description.

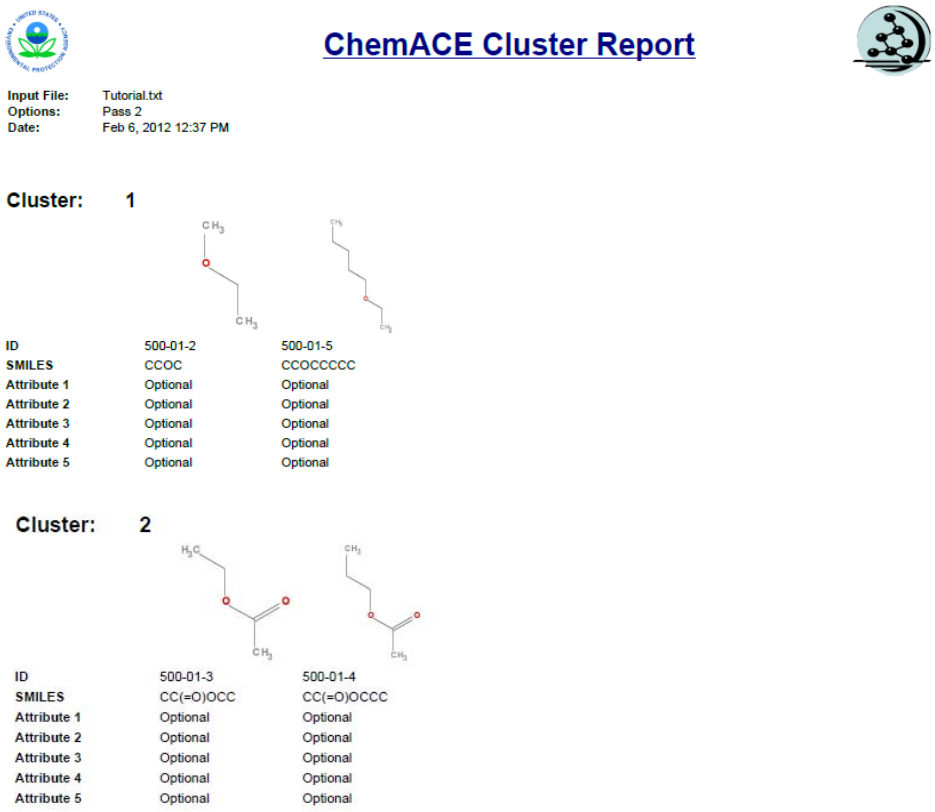
- Report format/Default Format – The user has the option to output the cluster results in HTML, Adobe PDF, or Microsoft EXCEL file formats. HTML or PDF files include structures; Excel does not include structures.
- Report Layout/Default Layout – The user has the option to output the clustering results in a horizontal or vertical layout for Adobe PDF and HTML outputs. The horizontal layout accommodates up to six structures per row.
- Structure Image size/Default Structure Image Size – The user can select the size of the structure from pre-define sizes to be displayed in the HTML or Adobe PDF documents. The user should consider the molecular size of the compounds in their data source when selecting the size of the output structure.

The settings tab allows users to save their preferences so that they appear by default each time ChemACE starts. By hitting the 'Apply' button, the setting choices selected on the screen will be saved as the default for future clustering runs.

5. ChemACE Output Report

Depicted below are sample outputs (created from data shown in Figure 1 table). HTML and Adobe PDF outputs are identical except for their file format and, thus, separate sample outputs are not displayed for these file formats.

Figure 5: PDF and HTML Output Using Horizontal Layout



ChemACE Cluster Report

Input File: Tutorial.txt
Options: Pass 2
Date: Feb 6, 2012 12:37 PM

Cluster: 1

ID	500-01-2	500-01-5
SMILES	CCOC	CCOCCCCC
Attribute 1	Optional	Optional
Attribute 2	Optional	Optional
Attribute 3	Optional	Optional
Attribute 4	Optional	Optional
Attribute 5	Optional	Optional

Cluster: 2

ID	500-01-3	500-01-4
SMILES	CC(=O)OCC	CC(=O)OCCC
Attribute 1	Optional	Optional
Attribute 2	Optional	Optional
Attribute 3	Optional	Optional
Attribute 4	Optional	Optional
Attribute 5	Optional	Optional

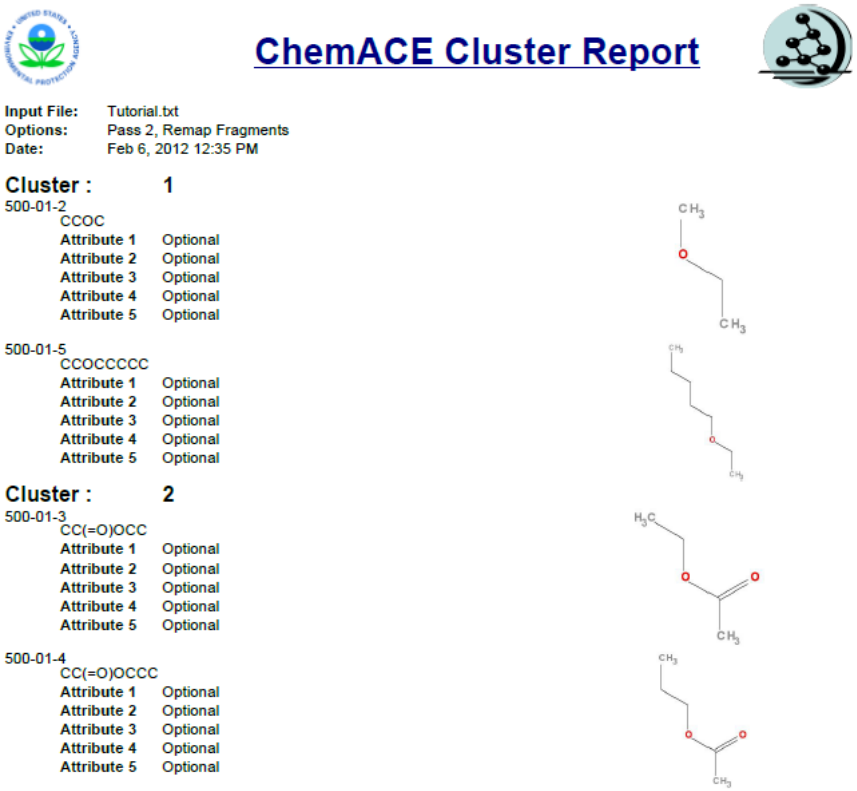
The above horizontal output (Figure 5) differs from the vertical output (Figure 6, below) only by how cluster data are shown.

- The horizontal output facilitates read-across of clustered chemicals/information
- Vertical output just lists all chemicals/information under cluster headings

Additional information shown in the upper left corner of the output file includes:

- Name of the input file
- The remapping and exclusion rules applied
- The date of the ChemACE run

Figure 6: Adobe PDF and HTML Output Using Vertical Layout



ChemACE Cluster Report

Input File: Tutorial.txt
Options: Pass 2, Remap Fragments
Date: Feb 6, 2012 12:35 PM

Cluster : 1

500-01-2
CCOC
Attribute 1 Optional
Attribute 2 Optional
Attribute 3 Optional
Attribute 4 Optional
Attribute 5 Optional

500-01-5
CCOCCCCC
Attribute 1 Optional
Attribute 2 Optional
Attribute 3 Optional
Attribute 4 Optional
Attribute 5 Optional

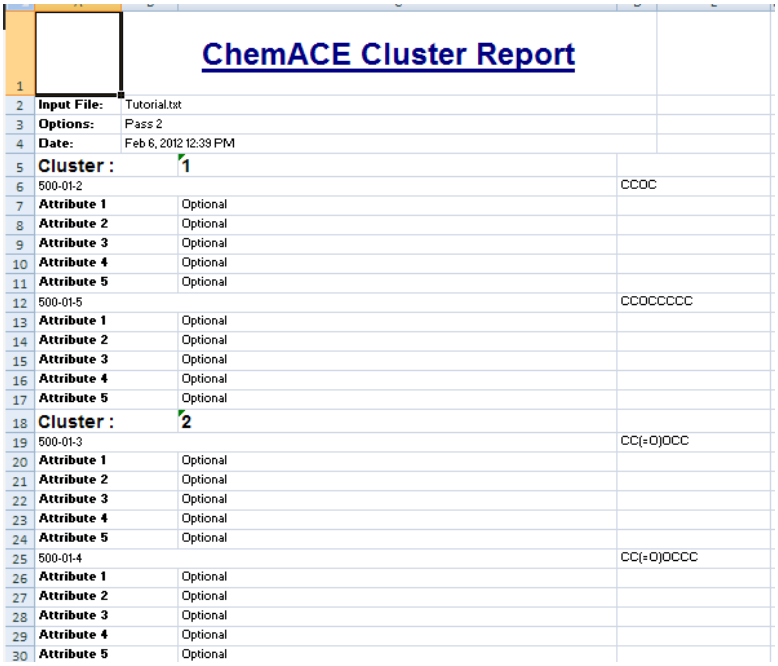
Cluster : 2

500-01-3
CC(=O)OCC
Attribute 1 Optional
Attribute 2 Optional
Attribute 3 Optional
Attribute 4 Optional
Attribute 5 Optional

500-01-4
CC(=O)OCCC
Attribute 1 Optional
Attribute 2 Optional
Attribute 3 Optional
Attribute 4 Optional
Attribute 5 Optional

The below Microsoft EXCEL output (Figure 7) lists data under cluster headings regardless of whether the horizontal or vertical layout is selected. The additional information (similar to Adobe PDF and HTML outputs) shown in the output includes the file name for the input file, an option field that displays some of the remapping and exclusions applied to the cluster run, and the date of the run.

Figure 7: Microsoft EXCEL Output

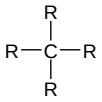
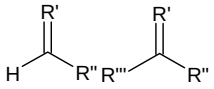
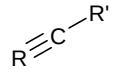
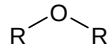
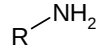
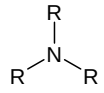
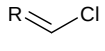


	ChemACE Cluster Report	
Input File:	Tutorial.txt	
Options:	Pass 2	
Date:	Feb 6, 2012 12:39 PM	
Cluster :	1	
500-01-2		CCOC
Attribute 1	Optional	
Attribute 2	Optional	
Attribute 3	Optional	
Attribute 4	Optional	
Attribute 5	Optional	
500-01-5		CCOCCCCC
Attribute 1	Optional	
Attribute 2	Optional	
Attribute 3	Optional	
Attribute 4	Optional	
Attribute 5	Optional	
Cluster :	2	
500-01-3		CC(=O)OCC
Attribute 1	Optional	
Attribute 2	Optional	
Attribute 3	Optional	
Attribute 4	Optional	
Attribute 5	Optional	
500-01-4		CC(=O)OCCC
Attribute 1	Optional	
Attribute 2	Optional	
Attribute 3	Optional	
Attribute 4	Optional	
Attribute 5	Optional	

Note on Chemicals that Could Not be Clustered: After all chemicals that could be grouped together are identified and numbered sequentially, the very last cluster contains all substances that could not be grouped based on structural similarity to other members within the input file. These chemicals are preceded by the title “Not Clustered”. The substances listed under this heading contained sufficient structural diversity from the other chemicals in the list that they could not be grouped using the current clustering parameters.

To minimize the number of chemicals “Not Clustered” it is suggested that users inspect their chemical set and employ the exclusion and remapping options to tailor the clustering logic as appropriate.

Appendix A – ChemACE Chemical Fragment Library

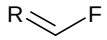
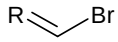
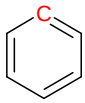
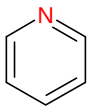
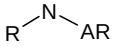
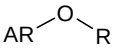
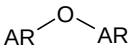
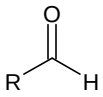
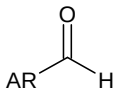
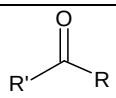
Fragment	Number	Modified Name	General Comments	Structure
-CH3 [aliphatic carbon]	0	Methyl; Primary carbon		
-CH2- [aliphatic carbon]	1	Secondary carbon		
-CH [aliphatic carbon]	2	Tertiary carbon		
C [aliphatic carbon - No H, not tert]	3	Quaternary carbon		
=CH2 [olefinic carbon]	4	Alkene		
=CH- or =C< [olefinc carbon]	5	Vinyl	R's are undefined	
#C [acetylenic carbon]	6	Alkyne		
-OH [hydroxy, aliphatic attach]	7	Hydroxy		
-O- [oxygen, aliphatic attach]	8	Ether		
-NH2 [aliphatic attach]	9	Primary amine		
-NH- [aliphatic attach]	10	Secondary amine		
-N< [aliphatic attach]	11	Tertiary amine		
-CL [chlorine, aliphatic attach]	12	Alkyl chloride		
-CL [chlorine, olefinic attach]	13	Vinyl chloride		
-F [fluorine, aliphatic attach]	14	Alkyl fluoride		

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

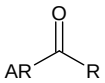
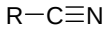
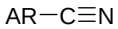
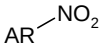
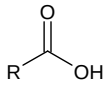
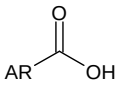
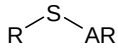
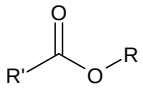
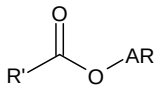
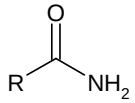
Fragment	Number	Modified Name	General Comments	Structure
-F [fluorine, olefinic attach]	15	Vinyl fluoride		
-Br [bromine, aliphatic attach]	16	Alkyl bromide		
-Br [bromine, olefinic attach]	17	Vinyl bromide		
-I [iodine, aliphatic attach]	18	Alkyl iodide		
Aromatic Carbon	19		Example: Benzene (CAS No. 71-43-2)	 Representative structure
Aromatic Nitrogen	20		Example: Pyridine (CAS No. 110-86-1)	 Representative structure
-CL [chlorine, aromatic attach]	21	Chloro-aromatic		
-Br [bromine, aromatic attach]	22	Bromo-aromatic		
-OH [hydroxy, aromatic attach]	23	Hydroxy-aromatic		
-N [aliphatic N, one aromatic attach]	24	Aryl alkyl amine		
-O- [oxygen, one aromatic attach]	25	Aryl alkyl ether		
-O- [aliphatic O, two aromatic attach]	26	Diaryl ether		
-CHO [aldehyde, aliphatic attach]	27	Alkyl aldehyde		
-CHO [aldehyde, aromatic attach]	28	Aryl aldehyde		
-C(=O)- [carbonyl, aliphatic attach]	29	Alkyl ketone	R' cannot be aromatic	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

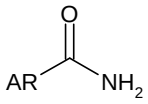
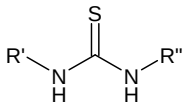
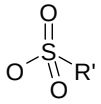
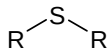
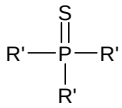
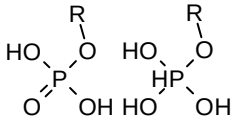
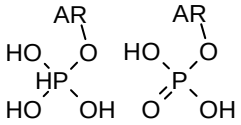
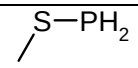
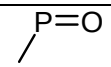
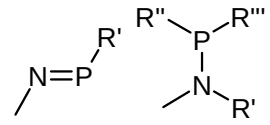
Fragment	Number	Modified Name	General Comments	Structure
-C(=O)- [carbonyl, one aromatic attach]	30	Alkyl aryl ketone		
-C#N [cyano, aliphatic attach]	31	Alkyl nitrile		
-C#N [cyano, aromatic attach]	32	Aryl nitrile		
-NO2 [nitro, aliphatic attach]	33	Alkyl nitro		
-NO2 [nitro, aromatic attach]	34	Aryl nitro		
-COOH [acid, aliphatic attach]	35	Alkyl carboxylic acid		
-COOH [acid, aromatic attach]	36	Aryl carboxylic acid		
-N=O [nitroso]	37		R’ is undefined	
-S- [aliphatic sulfur,one aromatic attach]	38	Alkyl aryl sulfide		
Aromatic Sulfur	39		Example: Thiophene (CAS No. 110-02-1)	 Representative Structure
-C(=O)O [ester, aliphatic attach]	40	Alkyl ester	R’ is undefined	
-C(=O)O [ester, aromatic attach]	41	Aryl ester	R’ is undefined	
-F [fluorine, aromatic attach]	42	Aryl fluoride		
-C(=O)N [aliphatic attach]	43	Alkyl amide		

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-C(=O)N [aromatic attach]	44	Aryl amide		
-NC(=S)N- [thiourea]	45		R's are undefined	
-SH [aliphatic attach]	46	Alkyl thiol		
-SO2-OH [sulfonic], [coef*(1+0.3*(NUM-1))]	47		R' = Alkyl C, Aryl C, N; Cannot be O	
-S- [aliphatic attach]	48	Dialkyl sulfide		
S=P [thio=phosphorus]	49	Thiophosphorus	R' = N, S, O, or C (any combination)	
-O-P [aliphatic attach]	50		R's are undefined	
-O-P [aromatic attach]	51			
-S-P [sulfur, phosphorus attach]	52			
O=P	53			
-N-P [nitrogen, phosphorus attach]	54		R's are undefined	
-I [aromatic attach]	55	Aryl iodide		

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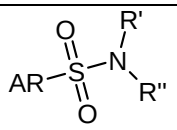
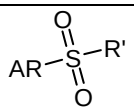
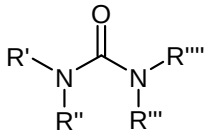
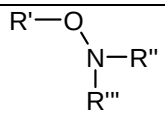
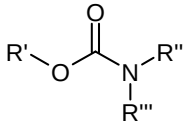
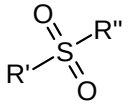
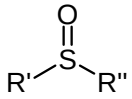
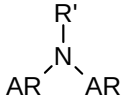
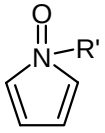
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-SO2-N [aromatic attach]	56	Aryl sulfonamide	R's are undefined	
-SO2- [aromatic attach]	57	Aryl sulfonyl	R' undefined	
-NC(=O)N- [urea]	58	Urea	R's are undefined; Unlikely alternative structure using higher valence Nitrogen (+5)	
-O-N [oxygen, nitrogen attach]	59			
Aromatic Oxygen	60			 Representative Structure
-OC(=O)N [carbamate]	61	Carbamate	R' cannot be H; R'', R''' are undefined	
-SO2- [sulfone, aliphatic attach]	62	Sulfone	R' = O, H, R; R'' is undefined	
-S(=O)- [sulfoxide, aliphatic attach]	63	Sulfoxide	R' = O, H, R; R'' is undefined	
-N- [aliphatic N, two aromatic attach]	64	Diaryl amine		
Aromatic n=O [nitrogen oxide]	65		R' is undefined	

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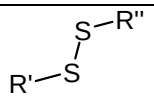
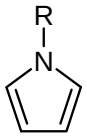
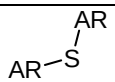
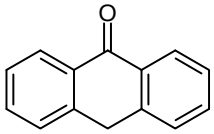
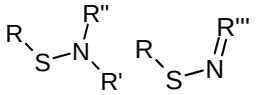
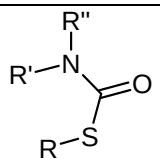
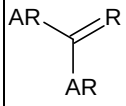
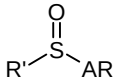
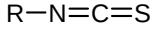
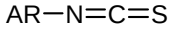
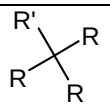
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-SS- [disulfide]	66	Disulfide	R's are undefined	
Aromatic Nitrogen [5-member ring]	67			
-S- [aliphatic S, two aromatic attach]	68			
-C(=O)- [two aromatic attach, in ring]	69			 Representative Structure
-S-N [sulfur, nitrogen attach]	70		R, R' and R'' are undefined R''' = O or N	
-S-C(=O)-N- [Thiocarbamate]	71	Thiocarbamate	R's are undefined	
Olefinic Carbon [two aromatic attach]	72	Diaryl alkene		
-S(=O)- [sulfoxide, aromatic attach]	73		R'=not O	
-N=C=S [isothiocyanate, aliphatic attach]	74			
-N=C=S [isothiocyanate, aromatic attach]	75			
-tert Carbon [3 or more carbon attach]	76		R' cannot be H	

R = Must be an aliphatic carbon attachment

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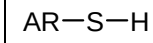
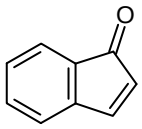
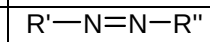
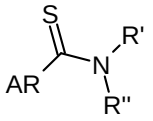
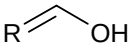
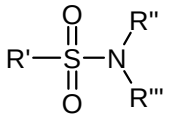
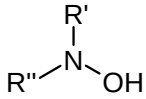
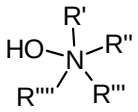
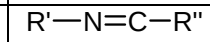
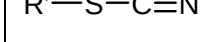
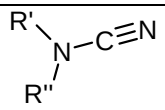
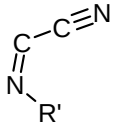
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-SH [thiol, aromatic attach]	77			
Ketone in a ring [olefin, aromatic attach]	78			 Representative structure
-N=N- [Azo]	79		R's are undefined	
-C(=S)N [aromatic attach]	80		R's are undefined	
-OH [alcohol, olefinic attach]	81	Vinyl alcohol		
-SO2-N [aliphatic attach]	82		R' = not O; R", R''' are undefined	
-OH [hydroxy, nitrogen attach]	83		R's are undefined	 
-N=C [aliphatic attach]	84		R's are undefined	
C#N-S [cyano, sulfur attach]	85		R' is undefined	
C#N-N [cyano, nitrogen attach]	86		R's are undefined	
C#N-C=N [cyano, -C=N attach]	87		R' is undefined	

R = Must be an aliphatic carbon attachment

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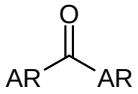
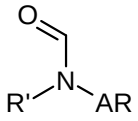
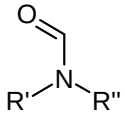
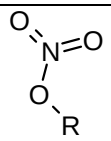
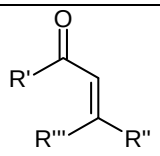
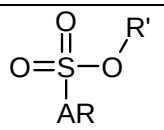
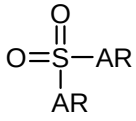
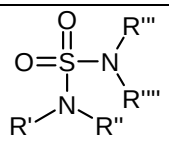
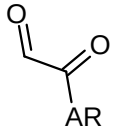
R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

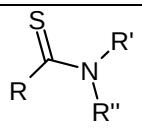
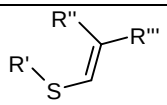
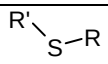
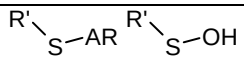
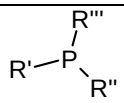
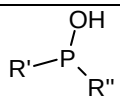
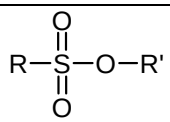
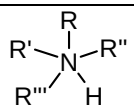
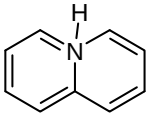
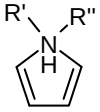
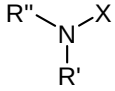
Fragment	Number	Modified Name	General Comments	Structure
Carbonyl, non-cylic, two aromatic attach	88	Diaryl carbonyl		
Aldehyde, [-N-CHO; aromatic attach]	89		R’ is undefined	
Aldehyde, [-N-CHO; aliphatic attach]	90		R’s are undefined	
-ONO2 [aliphatic attach]	91			
-C(=O)- [carbonyl, olefinic attach]	92		R’= not O or H; R’’, R’’’ = undefined	
-SO2-O [sulfonate, aromatic attach]	93	Aryl sulfonate	R’ is undefined	
SO2 [two aromatic attach]	94	Diaryl sulfone		
-N-SO2-N- [sulfamide]	95		R’s are undefined	
-CO-CO [aromatic attach]	96			

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-C(=S)N- [aliphatic attach]	97		R's are undefined	
-S-C= [S to aliphatic, double bonded C]	98		R's are undefined	
-Si- [silicon, aliphat attach (not oxy)]	99		R , R'= not oxygen	
-Si- [silicon, aromatic or oxygen attach]	100		R' is undefined	
>P- [phosphine type]	101		R's are undefined	
-OH [phosphorus attach]	102		R's are undefined	
-SO2-O [sulfonate, aliph att]	103		R = not O; R' is undefined	
>N< [+5 valence; single bonds;no H attach]	104		R's are undefined	
Aromatic nitrogen [fused ring location]	105			 Representative structure
Aromatic nitrogen [+5 valence type; no H]	106			 Representative structure
Halogen {-CL,-Br,-F,-I} [Nitrogen attach]	107		R's are undefined	

R = Must be an aliphatic carbon attachment

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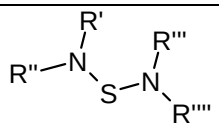
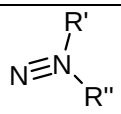
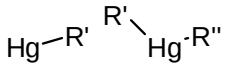
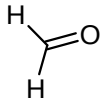
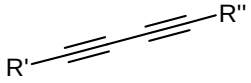
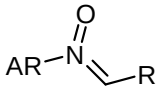
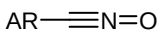
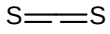
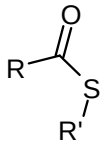
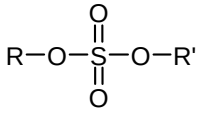
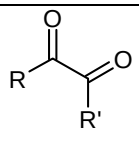
R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

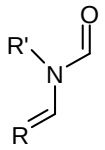
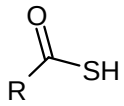
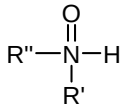
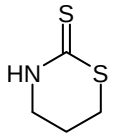
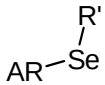
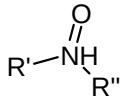
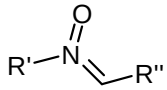
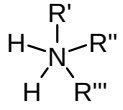
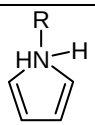
Fragment	Number	Modified Name	General Comments	Structure
-S- [aliphatic sulfur, 2 nitrogen attach]	108		R's are undefined	
N#N {alias: charged =N[+]=N[-] }	109		R's are undefined	
-Hg- [mercury]	110		R's are undefined	
Formaldehyde experimental value - constant	111			
#C [acetylenic carbon-acetylenic attach]	112		R's are undefined	
-N(=O)=C [nitrone, aromatic attach]	113			
-C#N=O [cyanooxide, aromatic attach]	114			
S=C=S [carbon disulfide, experimental]	115			
-C(=O)-S [thioester, aliphatic attach]	116		R,R' = not H; R=not O	
-O-SO2-O- [sulfate, linear]	117		R,R' = not H; R=not O	
-CO-CO [aliphatic attach]	118		R = not H or O; R' is undefined	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

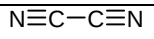
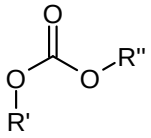
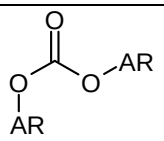
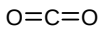
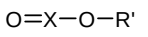
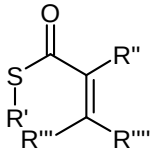
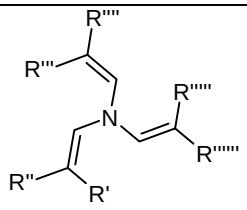
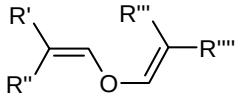
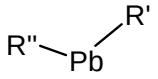
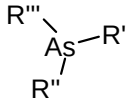
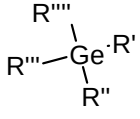
Fragment	Number	Modified Name	General Comments	Structure
Aldehyde, [-N-CHO; olefinic attach]	119		R’ is undefined	
-C(=O)-SH [aliphatic attach]	120			
N=O [nitroso; N+5 valence]	121		R’s are undefined	
N-C(=S)-S [cyclic]	122			 Representative Structure
-Se- [aromatic attach]	123		R’ is undefined	
-N(=O)- [N-oxide +4 type; no H attach]	124		R’s are undefined	
-N(=O)=C [nitrone,aliphatic attach;linear]	125		R’s are undefined	
Aromatic Selenium	126			 Representative Structure
>N< [+5 valence; single bonds; H attach]	127		R’s are undefined	
Aromatic nitrogen [+5 valence; H attach]	128			 Representative Structure

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-C#N [cyano attach]	129			
-OC(=O)O- [carbonate,aliphatic attach]	130		R's are undefined	
-OC(=O)O- [carbonate,aromatic attachs]	131			
O=C=O [carbon dioxide, experimental]	132			
Halogen [mono- or dioxy-type][one/struct]	133		R' is undefined	
-C(=O)-S [thioester, olefinic attach]	134		R' = not H; R'', R''', R'''' are undefined	
-N< [two or three olefinic attach]	135		Rs =undefined	
-O- [oxygen, two olefinic attach]	136		Rs =undefined	
[Pb] (Lead)	137	This entry appears no matter how many R groups are added.	Rs =undefined	
[As] (Arsenic)	138	This entry appears no matter how many R groups are added.	Rs =undefined	
[Ge] (Germanium)	139	This entry appears no matter how many R groups are added.	R's are undefined	

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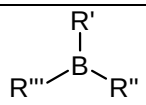
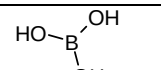
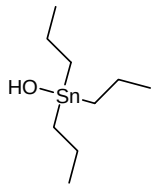
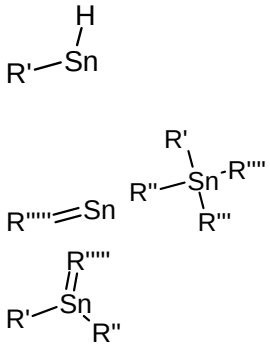
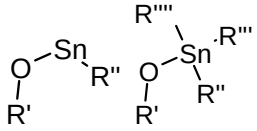
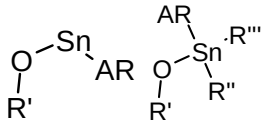
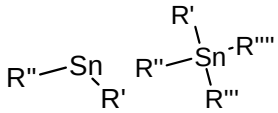
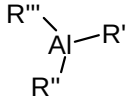
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Boron	140	This entry appears no matter how many R groups are added.	R's are undefined	
-OH { Metal or miscellaneous attach)	141			 Representative structure  Representative structure
Tin [Sn]	142	Sn can be II or IV valence	R', R'', R''', R'''' = not O, X or AR	
Tin [Sn] { oxygen attach }	143	Sn can be II or IV valence	R' = not H; R'', R''', R'''' = not OH or X or AR	
Tin [Sn] { oxygen and aromatic attach }	144	Sn can be II or IV valence	R' = not H; R'', R'''' are undefined	
Tin [Sn] { halogen or -OH attach }	145	Sn can be II or IV valence	R' = X, O R'',R''',R'''' are not X if R' is X	
Aluminum [Al]	146		R's are undefined	

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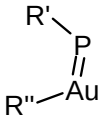
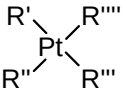
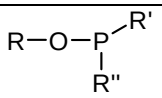
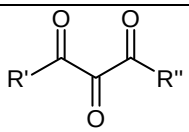
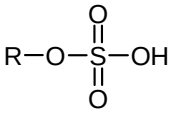
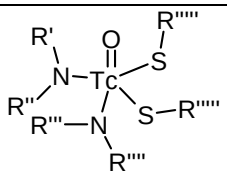
Fragment	Number	Modified Name	General Comments	Structure
Gold [Au]=P { Phosphorus attach }	147		R's are undefined	
Platinum [Pt] { halogen & nitrogen attach}	148		R'= halogen or $N(R)_2$; R'', R''', R'''' are undefined	
-O-P [phosphine phosphorus attach]	149		R's are undefined	
-C(=O)- [di-carbonyl attach]	150		R's are undefined	
SO2(-OH)-O [sulfonic]	151			
Technetium [Tc](-S)(-S)(-N)(-N)	152			
Krypton [Measured]	153			Kr
Argon [Measured]	154			Ar
Neon [Measured]	155			Ne
Xenon [Measured]	156			Xe
Radon [Measured]	157			Rn
Helium [Measured]	158			He
O=O [oxygen; experimental]	159			O=O
[H][H] { Hydrogen gas; experimental }	160			H—H

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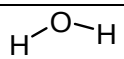
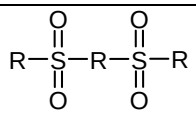
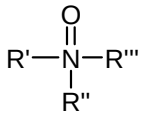
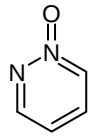
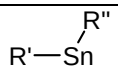
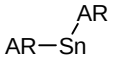
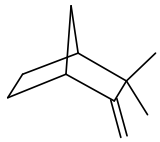
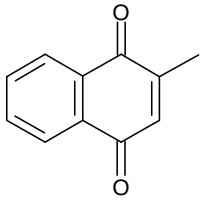
Fragment	Number	Modified Name	General Comments	Structure
O [oxygen,no attach; water, experimental]	161			
N#N [Nitrogen gas, experimental]	162			
-SO2- [additional sulfone,aliphat attach]	163			
N=O [nitroso; N+5 valence; single bonds]	164		R's are undefined	
Mercury [Measured]	165			Hg
Aromatic n=O [nitrogen oxide,nitrogen att]	166			 Representative Structure
Tin [Sn] { divalent; carbon attach }	167		R',R''= C	
Tin [Sn] { divalent; aromatic attach }	168			
	169			
	170			
Ring aliphatic Carbon	171		Representative structure = Camphene (CAS No. 79-92-5)	 Representative structure
Ring olefinic Carbon	172		Representative structure = 2-Methyl-1,4-Naphthoquinone (CAS No. 58-27-5)	 Representative structure

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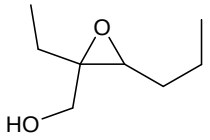
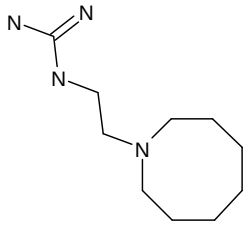
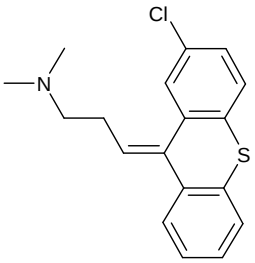
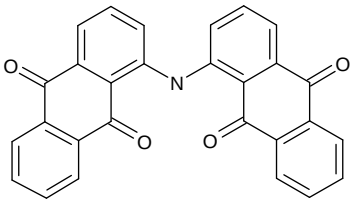
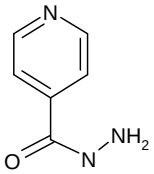
Fragment	Number	Modified Name	General Comments	Structure
Ring aliphatic Oxygen	173		Representative structure = 2,3-epoxy-2-ethyl-1-hexanol (CAS No. 78-72-8)	 Representative structure
Ring aliphatic Nitrogen	174		Representative structure = Guanethidine (CAS No. 55-65-2)	 Representative structure
Ring aliphatic Sulfur	175		Representative structure = Chlorprothixene (CAS No. 113-59-7)	 Representative structure
Ring Carbonyl	176		Representative structure = Anthrimide (CAS No. 82-22-4)	 Representative structure
Aliphatic N-N hydrazine type	178		Representative structure = Isoniazid (CAS No. 54-85-3)	 Representative structure
Sodium [Na]	179			Na
Potassium [K]	180			K
Lithium [Li]	181			Li

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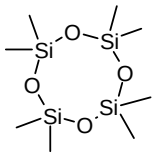
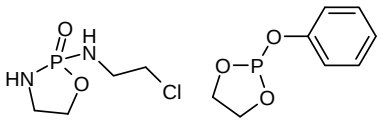
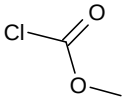
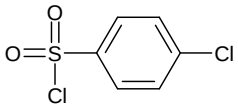
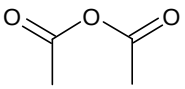
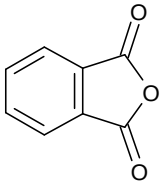
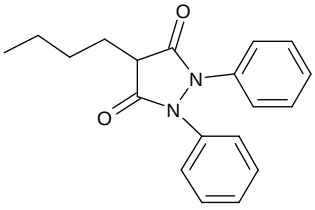
Fragment	Number	Modified Name	General Comments	Structure
Ring Silicon	182		Representative structure = Octamethylcyclotetrasiloxane (CAS No. 556-67-2)	 Representative structure
Ring Phosphorus	183		Representative structure = 2-Phenoxy-1,3,2-dioxaphospholane (CAS No. 1077-05-0)	 Representative structure
Class - Acetyl Halide	200		Representative structure = Methyl chloroformate (CAS No. 79-22-1)	 Representative structures
Class - Sulfur Halide	201		Representative structure = 4-Chloro-benzenesulfonyl chloride (CAS No. 98-60-2)	 Representative structure
Class - Linear Anhydride	202		Representative structure = Acetic anhydride (CAS No. 108-24-7)	 Representative structure
Class - Cyclic Anhydride	203		Representative structure = Phthalic anhydride (CAS No. 85-44-9)	 Representative structure
Class - Nitrogen-Nitrogen	204		Representative structure = Phenylbutazone (CAS No. 50-33-9)	 Representative structure

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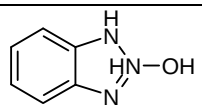
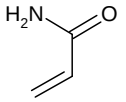
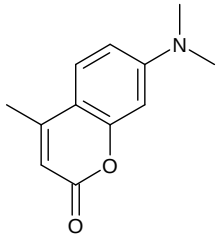
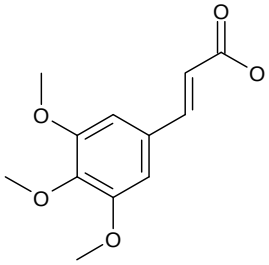
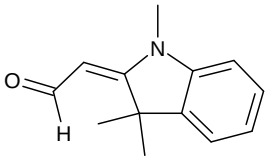
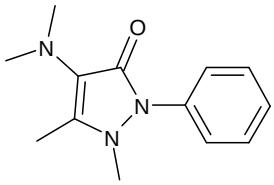
Fragment	Number	Modified Name	General Comments	Structure
Class - aromatic Nitrogen-O-	205			 Representative structure
Class - Acrylamide	206		Representative structure = Acrylamide (CAS No. 76-06-1)	 Representative structure
Class - Acrylate	207		Representative structure = 7-Dimethylamino-4-methylcoumarin (CAS No. 87-04-1)	 Representative structure
Class - Acid-olefin	208		Representative structure = 3,4,5-Trimethoxycinnamic acid (CAS No. 90-50-6)	 Representative structure
Class - Aldehyde-olefin	209		Representative structure = Tribasenaldehyde (CAS No. 84-83-3)	 Representative structure
Class - Vinyl Amine	210		Representative structure = Aminopyrine (CAS No. 58-15-1)	 Representative structure

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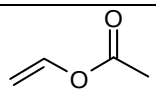
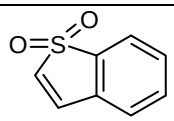
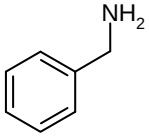
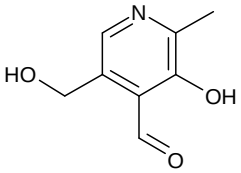
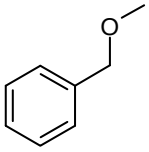
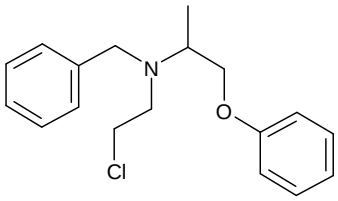
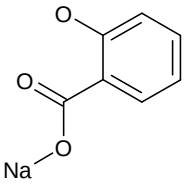
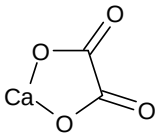
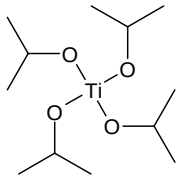
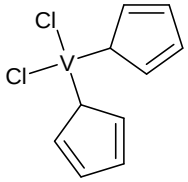
Fragment	Number	Modified Name	General Comments	Structure
Class - Vinyl Ether	211		Representative structure = Paracotin (CAS No. 91-89-4)	 Representative structure
Class - Vinyl sulfone/sulfoxide	212		Representative structure = Benzo(B)thiophene-S,S-dioxide (CAS No. 825-44-5)	 Representative structure
Class - Benzyl amine - NH2	213		Representative structure = Benzylamine (CAS No. 100-46-9)	 Representative structure
Class - Benzyl alcohol	214		Representative structure = Pyridoxal (CAS No. 66-72-8)	 Representative structure
Class - Benzyl ether type	215		Representative structure = Benzyl methyl ether (CAS No. 538-86-3)	 Representative structure
Class - Benzyl amine -NH- , >N-	216		Representative structure = Phenoxybenzamine (CAS No. 59-96-1)	 Representative structure
	217			
	218			

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Group Ia	219		Structures containing the following elements: Li, Na, K, Rb, Cs, and Fr. Representative structure = Sodium salicylate (CAS No. 54-21-7)	 Representative structure
Group IIa	220		Structures containing the following elements: Be, Mg, Ca, Sr, Ba, and Ra. Representative structure = Calcium oxalate (CAS No. 563-72-4)	 Representative structure
Group IIIb	221		Structures containing the following elements: Sc, Y. Representative structure = Scandium trichloride (CAS No. 10361-84-9)	$ScCl_3$ Representative structure
Group IVb	222		Structures containing the following elements: Ti, Zr, Hf, Rf. Representative structure = Titanium isopropylate (CAS No. 546-68-9)	 Representative structure
Group Vb	223		Structures containing the following elements: V, Nb, Ta, Db. Representative structure = Vanadocene dichloride (CAS No. 12083-48-6)	 Representative structure

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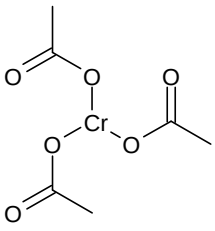
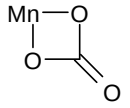
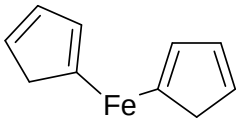
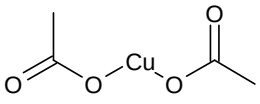
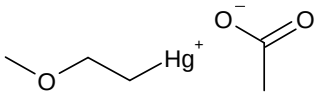
Fragment	Number	Modified Name	General Comments	Structure
Group VIb	224		Structures containing the following elements: Cr, Mo, W, and Sg. Representative structure = Chromic acetate (CAS No. 1066-30-4)	 Representative structure
Group VIIb	225		Structures containing the following elements: Mn, Tc, Re, and Bh. Representative structure = Manganese carbonate (CAS No. 598-62-9)	 Representative structure
Group VIII	226		Structures containing the following elements: Fe, Ru, Os, Hs. Representative structure = Ferrocene (CAS No. 102-54-5)	 Representative structure
Group Ib	227		Structures containing the following elements: Cu, Ag, Au, and Rg. Representative structure = Cupric acetate (CAS No. 142-71-2)	 Representative structure
Group IIb	228		Structures containing the following elements: Zn, Cd, Hg, and Cn. Representative structure = (Methoxyethyl)mercuric acetate (CAS No. 151-38-2)	 Representative structure

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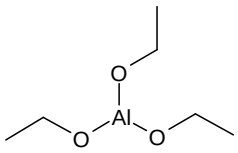
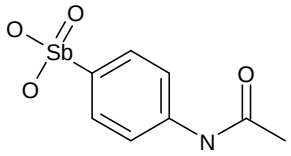
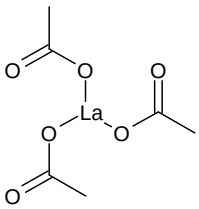
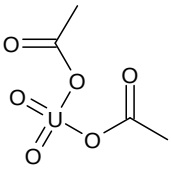
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Group IIIa	229		Structures containing the following elements: B, Al, Ga, In, Tl. Representative structure = Aluminum ethoxide (CAS No. 555-75-9).	 Representative structure
Group IVa	230		Structures containing the following elements: Ge, Sn, Pb, Fl. Representative structure = Trimethyltin hydroxide (CAS No. 56-24-6)	 Representative structure
Group Va	231		Structures containing the following elements: Sb and Bi (does not include As, P, N). Representative structure = Stibacetin (CAS No. 138-31-8)	 Representative structure
Group Lanthanides	232		Structures containing the following elements: La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu. Representative structure = Acetic acid, lanthanum(3) salt (CAS No. 917-70-4)	 Representative structure
Group Actinides	233		Structures containing the following elements: Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr. Representative structure = Uranyl	 Representative structure

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Fragment	Number	Modified Name	General Comments	Structure
			acetate (CAS No. 541-09-3)	
Group Noble Gases	234		Structures containing the following elements: He, Ne, Ar, Ar, Kr, Xe, Rn. Representative structure = Xenon fluoride (CAS No. 13693-09-9)	XeF_6 Representative structure

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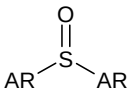
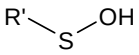
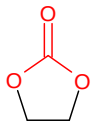
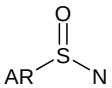
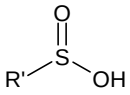
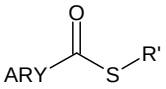
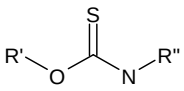
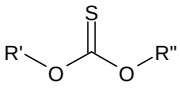
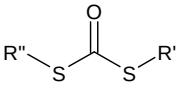
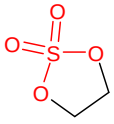
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
NO2-N [nitro, nitrogen attach]	0E	Nitro amine	R' is undefined	
-ONO2 [aromatic attach]	1E	Aryl nitrate		
-S(=O)- [two aromatic attach]	2E	Diaryl sulfoxide		
-OH [hydroxy, sulfur (no oxide) attach]	3E			
-OC(=O)O- [carbonate,cyclic]	4E	Cyclic carbonate	Example: 1,3-Dioxolan-2-one (CAS No. 96-49-1)	 Representative structure
-S(=O)-N- [aromatic attach]	5E	Aryl sulfinamide		
-S(=O)-OH	6E	Sulfinic acid	R' = C, N, S	
-C(=O)-S [thioester, aromatic attach]	7E	Aryl thioester	R' cannot be H	
-O-C(=S)-N- [thiocarbamate]	8E	Thiocarbamate	R's are undefined	
-O-C(=S)-O- [thiocarbonate]	9E	Thiocarbonate	R', R" = C, H, X, N, S	
-S-C(=O)-S [dithioester]	10E	Diothioester	R', R'' = Aryl C, Alkyl C, N, S	
-O-SO2-O- [sulfate, cyclic]	11E	Cyclic sulfate		 Representative structure

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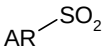
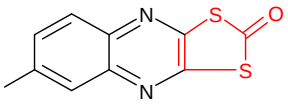
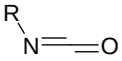
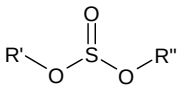
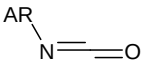
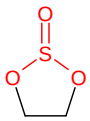
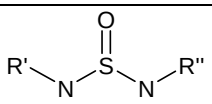
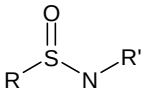
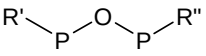
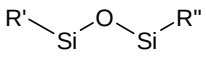
Fragment	Number	Modified Name	General Comments	Structure
-SO-O [sulfonate, aromat att]	12E	Aryl sulfonate		
-SO-O [sulfonate, aliph att]	13E	Alkyl sulfonate		
>P< [phosphonium +5 type]	14E			 Representative structure
-S-C(=O)-S [dithioester, cyclic]	15E	Cyclic dithioester	Example: Oxythioquinox (CAS No. 2439-01-2)	 Representative structure
-N=C=O [isocyanate, aliphatic attach]	16E	Alkyl isocyanate		
-O-SO-O- [sulfite, linear]	17E		R', R'' = Aliphatic C, aromatic C, cannot be H	
-N=C=O [isocyanate, aromatic attach]	18E	Aryl isocyanate		
-O-SO-O- [sulfite, cyclic]	19E	Cyclic sulfite		 Representative structure
-N-SO-N- [sulfamide]	20E	Sulfamide	R', R'' = H, aliphatic C, aromatic C	
-S(=O)-N- [aliphatic attach]	21E	Alkyl sulfonamide	R' = H, aliphatic C, aromatic C	
P-O-P [oxygen, two phosphorus attach]	22E		R', R'' = H, aliphatic C, aromatic C	
-O- [oxygen, two silicon attach, linear]	23E	Siloxane	R', R'' = H, aliphatic C, aromatic C	

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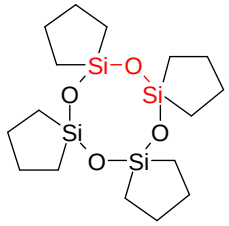
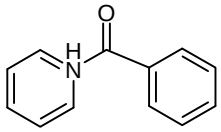
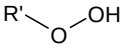
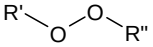
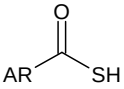
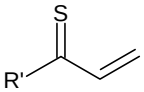
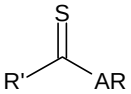
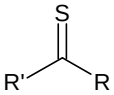
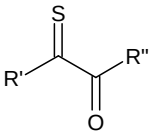
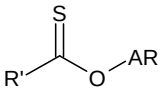
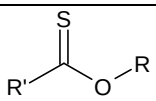
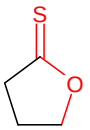
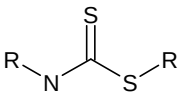
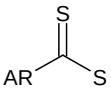
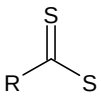
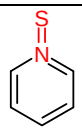
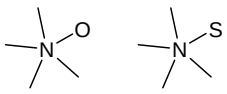
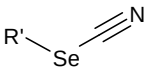
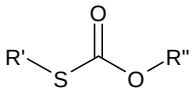
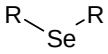
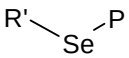
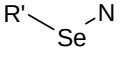
Fragment	Number	Modified Name	General Comments	Structure
-O- [oxygen, two silicon attach, cyclic]	24E	Cyclosiloxane	Example: Tetracyclotetramethylenecyclotetrasiloxane (CAS No. 177-49-1)	 Representative structure
-C(=O)- [aromatic nitrogen,carbon attach]	25E			 Representative structure
-OH [oxygen attach]	26E	Hydroperoxide	R' is undefined	
-O- [oxygen attach]	27E	Peroxide	R's are undefined	
-C(=O)-SH [aromatic attach]	28E			
-C(=S)- [olefinic attach]	29E	Vinyl thione	R' is undefined	
-C(=S)- [aromatic attach]	30E	Aryl thione	R' is undefined	
-C(=S)- [aliphatic attach]	31E	Alkyl thione	R' is undefined	
-C(=S)-C(=O)	32E		R's are undefined	
-C(=S)-O [aromatic attach]	33E	Aryl thionoester	R' is undefined	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

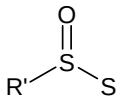
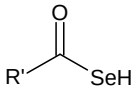
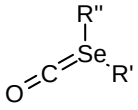
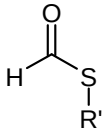
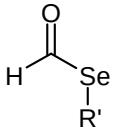
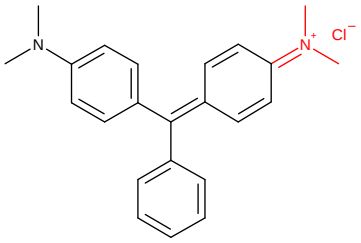
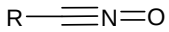
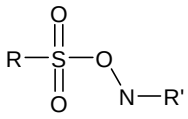
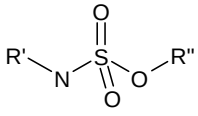
Fragment	Number	Modified Name	General Comments	Structure
-C(=S)-O [aliphatic attach]	34E	Alkyl thionoester	R’ is undefined	
-C(=S)-O [cyclic]	35E	Cyclic thionoester	Example: G-Thiobutyrolactone (CAS No. 39700-44-2)	 Representative structure
N-C(=S)-S [linear]	36E	Dithiocarbamate		
-C(=S)-S [thioester, aromatic attach]	37E			
-C(=S)-S [thioester, aliphatic attach]	38E			
	39E			
Aromatic n=S [nitrogen sulfide]	40E			 Representative structure
{-O- or -S-} to nitrogen (+5 valence)]	41E			
C#N-Se [cyano, selenium attach]	42E	Cyano selenide	R’ is undefined	
-S-C(=O)-O-	43E		R’s are undefined	
-Se- [aliphatic attach]	44E	Alkyl selenide		
-Se- [phosphorus attach]	45E	Phosphorus selenide	R’ is undefined	
-Se- [nitrogen attach]	46E	Nitrogen selenide	R’ is undefined	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

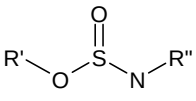
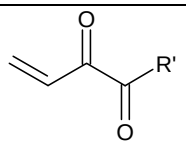
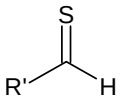
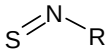
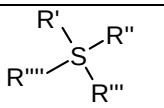
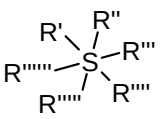
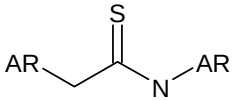
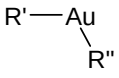
Fragment	Number	Modified Name	General Comments	Structure
-S-S(=O) [sulfur, S(=O) attach]	47E	Thiosulfinic acid	R' is undefined	
-SeH [aliphatic attach]	48E	Alkyl hydrogen selenide		
-SeH [aromatic attach]	49E	Aryl hydrogen selenide		
-C(=O)-SeH	50E			
-C(=O)=Se-	51E		R', R'' are undefined	
CHO-S-	52E		R' is undefined	
CHO-Se-	53E		R' is undefined Se may have 1 or 3 attachments	
=N< [nitrogen +5 valence]	54E			 Representative structure
-C#N=O [cyanooxide, aliphatic attach]	55E	Alkyl cyanooxide		
-SO2-O-N [N-sulfonate, aliph att]	56E		R' is undefined	
-O-SO2-N- [sulfone,N and O attach]	57E		R' is undefined; R" cannot be H	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-O-SO-N- [sulfoxide,N and O attach]	58E		R' cannot be H; R" can be H	
-CO-CO [olefinic attach]	59E		R' is undefined	
S=CH [thioaldehyde type]	60E	Thioaldehyde	R' can be H	
-N=S [aliphatic attach]	61E			
-S [sulfur +4 or +6 valence;miscellaneous]	62E		R's are undefined	 
-C(=S)N- [both aromatic attach]	63E			
Gold [Au]	64E			Au
Bismuth [Bi]	65E			Bi
Calcium [Ca]	66E			Ca
Magnesium [Mg]	67E			Mg
Antimony [Sb]	68E			Sb
Zinc [Zn]	69E			Zn
Gold [Au] { halogen attach }	70E		R' = Halogen; R" can be H	
Platinum [Pt] { halogen attach }	71E		R' = Halogen	
Platinum [Pt]	72E			Pt
Iron [Fe]	74E			Fe

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R', R'', R''', etc. = Defined in General Comments

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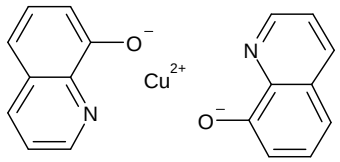
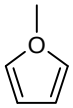
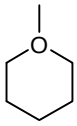
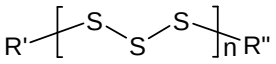
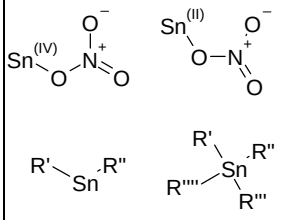
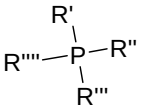
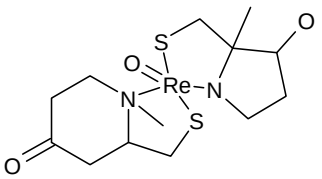
Fragment	Number	Modified Name	General Comments	Structure
Cadmium [Cd]	75E			Cd
Cadmium [Cd] { halogen attach }	76E		R’ = Halogen	
Miscellaneous Metal [Ni,Cu,Zr,Be]	77E		Representative structure = Bis(8-quinolinolato-(N1,O8))copper (CAS No. 10380-28-6)	 Representative structure
Oxygen [aromatic; not +2 valence; misc.]	78E			 Representative structure
Oxygen [aliphatic; not +2 valence; misc]	79E			 Representative structure
-S- [di-,poly- sulfur attach]	80E		R’, R” can be H	
Tin [Sn] { multi-halogen or -ONO2 }	83E		R”, R”” = Halogen only; R’’’, R’’’’ = May be halogen	
[P] Phosphorus {four single bonds}	84E		R’s cannot be H	
Miscellaneous sulfide (=S) or oxide (=O)	85E		Representative structure = Oxorhenium-23	 Representative structure

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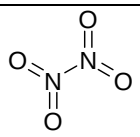
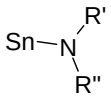
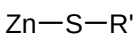
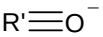
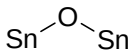
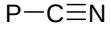
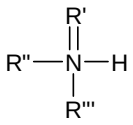
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-NO2 [-NO2 attach]	86E			
Tin [Sn] { nitrogen attach }	87E		Sn can be II or IV valence; R', R" can be H	
[Zn]-S { zinc-sulfur }	88E		R' is undefined; Zn substitution undefined	
Oxygen [#O]	89E		R' is undefined	
[Sn]-O-[Sn] { bis-tin ether }	90E		Sn can be II or IV valence	
-C#N [Phosporus attach]	91E			
=N< [nitrogen +5 valence;hydrogen attach]	92E			

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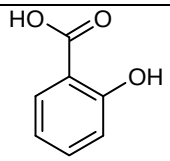
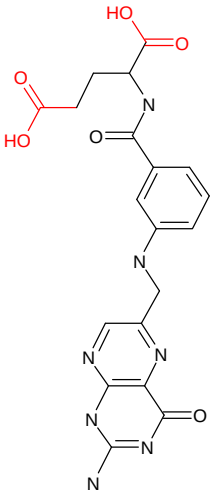
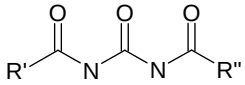
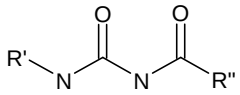
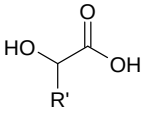
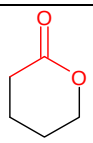
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ortho reaction -> hydroxy/acid correc	0C			 Representative structure
Multi-aliphatic carboxylic acids	1C		Example: Folic acid (CAS No. 59-30-3)	 Representative structure
-CO-N-CO-N-CO- structure correction	2C		R', R" can be H	
-N-CO-N-CO- structure correction	3C		R', R" can be H	
HO-C-COOH (alcohol-acid carbon)	4C	Lactic acid-type correction	R' is undefined	
Cyclic ester correction	5C			 Representative structure

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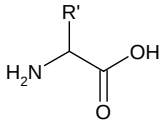
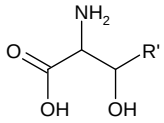
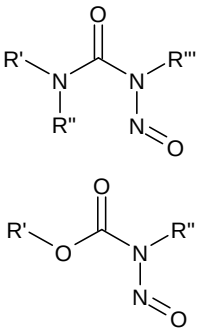
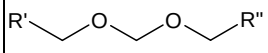
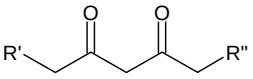
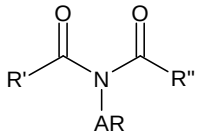
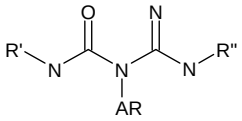
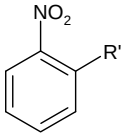
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Amino acid (alpha-position) correction	6C	Alpha-amino acid		
Alcohol - amino acid correction	7C			
Nitroso (urea/carbamate type) correction	8C		R's can be H	
C-O-C-O-C structure correction	9C		R's are undefined	
C-CO-C-CO-C structure correction	10C		R's are undefined	
N-aromatic -CO-N-CO- structure correction	11C		R', R" cannot be H	
Di-N urea/acetamide aromatic correction	12C		R's are undefined	
Ring reaction -> -NO2 with -OH/amino/azo	13C		R' = -OH, -NH2, -N=N- at ortho, meta, or para positions	 Representative structure

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AR = Must be an aromatic carbon attachment

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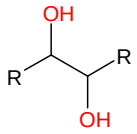
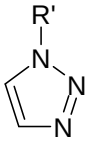
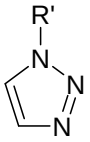
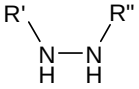
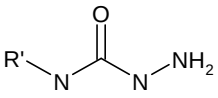
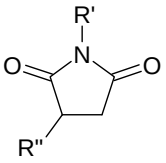
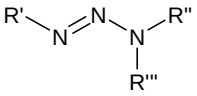
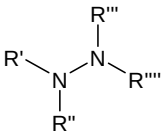
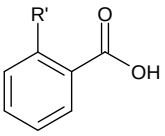
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Multi-alcohol correction	14C		Must be an aliphatic carbon. Cannot be aromatic.	 Representative structure
1,2,3-Triazole correction	15C		R’ can be H	
N-substitution on 123-triazole (at 1-pos)	16C		R’ cannot be H	
-NH-NH- structure correction	17C		R’, R” can be H	
Amino urea correction	18C		R’ can be H	
-CO-N-CO- 5-member ring [not pyrroledione]	19C		R’s are undefined	
-N=N-N- structure correction	20C	Amino diazene correction	R’, R”, R’’’ can be H	
>N-N<- structure correction	21C	Hydrazine – type correction	R’ cannot be H; R”, R’’’, R’’’’ can be H	
Ring reaction -> ortho to aromatic acid	22C	O-substituted benzoic acid	R’ is undefined	

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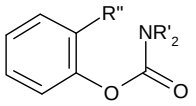
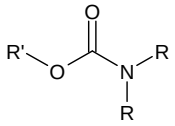
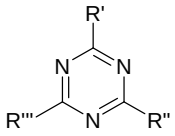
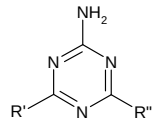
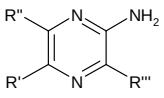
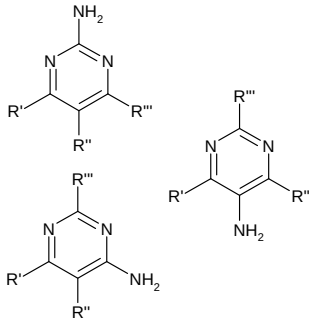
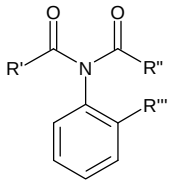
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring reaction->ortho to O-phenyl carbamate	23C		R’ can be H; R”= Undefined	
di-N-aliphatic substitution [carbamate]	24C	N-dialkyl carbamate	R’ cannot be H	
sym-Triazine ring correction	25C		R’s are undefined	
Amino triazine/pyrazine/pyrimidine correc.	26C		R’s are undefined	 Amino triazine  Amino pyrazine  Amino pyrimidine
Ortho-substituted N-phenyl CO-N-CO correc.	27C		R’, R” can be H; R’’’ can be X	

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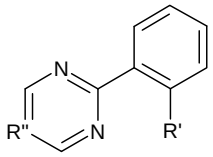
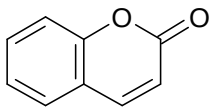
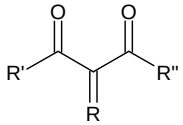
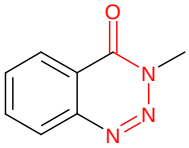
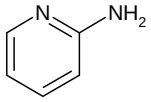
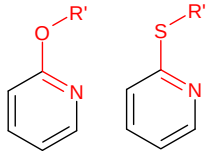
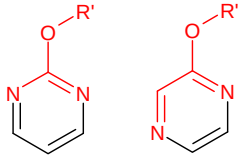
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ortho-substituted aromatic at ncn location	28C		R’ = C, X; R” = C or N	
Cyclic ester [olefinic type] correction	29C		Representative structure = Coumarin (CAS No. 91-64-5)	 Representative structure
Di-ketone [CO-C-CO..olefinic C] correction	30C		R’s are undefined	
N=N-N-CO-aromatic structure correction	31C		Example: 3-Methylbenzotriazin-4-one (CAS No. 22305-44-8)	 Representative structure
Ortho-Amino pyridine correction	32C			
Ortho-Alkyloxy(thio) to 1 aromat nitrogen	33C		R’ cannot be H	 Representative structures
o-Alkyloxy to 2 aromat nitrogens/pyrazine	34C		R’ cannot be H	 Representative structures

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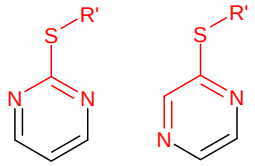
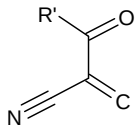
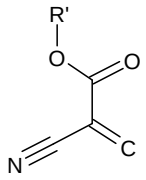
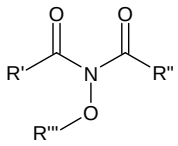
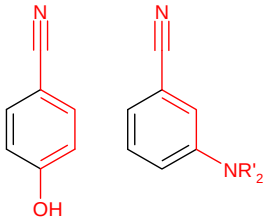
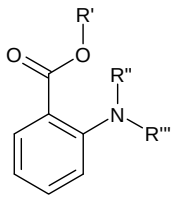
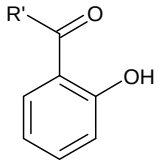
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
o-Alkylthio to 2 arom nitrogens/pyrazine	35C		R’ cannot be H	 Representative structures
=C-(C#N)-CO- structure correction	36C		R’ can be H	
=C-(C#N)-CO-O- structure correction	37C		R’ can be H	
Oxygen-substitution at N on -CO-N-CO-	38C		R’, R”, R’’’ can be H	
Ring reaction -> cyano & phenol or -N	39C		Can be ortho, meta, para positions; R’ can be H	 Representative structures
Ortho-Amino [N-subst]/ester correction	40C		R’ cannot be H; R”, R’’’ can be H	
Ortho-Hydroxy to misc. -C(=O)- correction	41C		R’ can be H	

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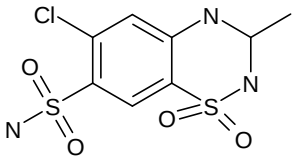
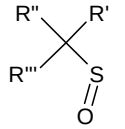
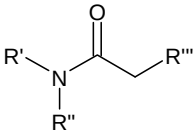
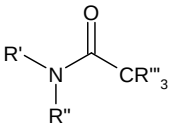
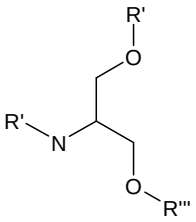
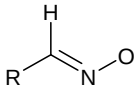
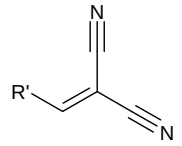
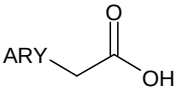
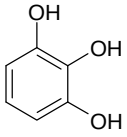
Fragments containing “C” or “X” are not used in Pass 2

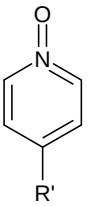
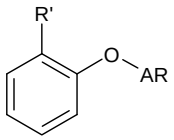
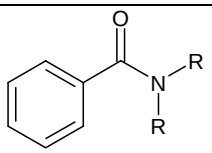
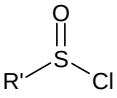
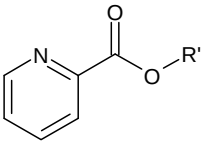
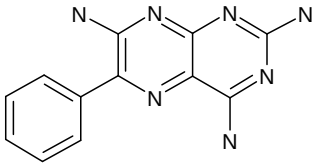
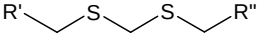
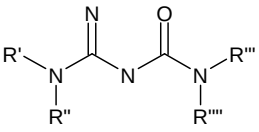
Fragment	Number	Modified Name	General Comments	Structure
Di Aromatic-SO2-N correction	42C		Representative structure = 3-Methylhydrochlorothiazide (CAS No. 890-67-5)	 Representative structure
SO-C(polyhalo) structure correction	43C		R', R" = Must be X; R"' can be X	
Mono-halo acetamide [-N-CO-C-halo]	44C		R', R" can be H; R"' = X	
Poly-halo acetamide [-N-CO-C-polyhalo]	45C		R', R" can be H; R"' = X (at least 2)	
-N-C-(C-OH)-C-OH structure correction	46C		R', R", R"' can be H	
-CH=N-OH [oxime,aliphatic attach] corr.	47C	Alkyl oxime correction		
C=C-(C#N)-C#N [dicyano] correction	48C		R' is undefined	
Aromatic-C[-C or -H]-COOH correction	49C			
Ring reaction -> 1,2,3-trihydroxy	50C			

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Aromatic n-oxide rx with NO2/C#N/amino	51C		R’ = Nitro, cyano, amino; in ortho, meta, or para position	 Representative structure
Ortho-subst on di-aromatic ether (non-cyl)	52C			
Di-N-sub(alph carbon) aromatic carboxamide	53C			
Halo-sulfo [SO-halo] correction	54C			
Pyridine ester [2-position] correction	55C		R’ is undefined	
Arom nitrogens-> Amino (fused ring) correc	56C		Representative structure = 2,4,7-Triamino-6-Phenyl-p-teridine (CAS No. 396-01-0)	 Representative structure
C-S-C-S-C structure correction	57C		R’ , R” are undefined	
Amidino urea (-N-C(=N)-N-CO-N-) correction	58C	Amidino urea correction	R’, R”, R”’, R”” can be H	

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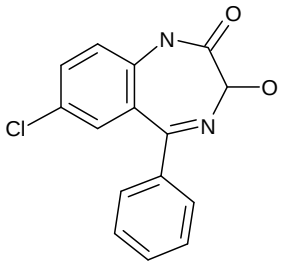
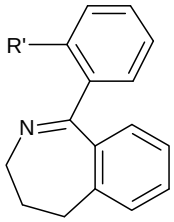
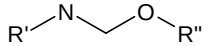
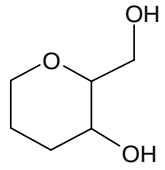
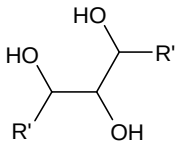
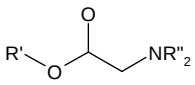
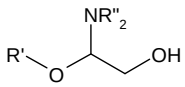
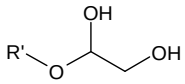
R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
N=C< di-aromatic (or cyclic) correction	59C		Representative structure = Oxazepam (CAS No. 604-75-1)	 Representative structure
Ortho-substitutes on N=C< attached aromats	60C		R' = Aliphatic, Halogen; Structure must contain 7-membered ring with C=N and fused aromatic ring, in addition to ortho-substituted aromatic.	 Representative structure
-N-C-O- structure correction	61C		R' cannot be H; R" is undefined	
HO-CH-C(-O-)-CH-OH structure correction	62C		More than likely cyclic	 Representative structure
HO-CH-C(-OH)-CH-OH structure correction	63C		R', R" can be H; Structure may be cyclic	
-O-C(-OH)-C-N- structure correction	64C		R' cannot be H; R" can be H	
-O-C(-N-)-C-OH structure correction	65C		R' cannot be H; R" can be H	
-O-C(-OH)-C-OH structure correction	66C		R' cannot be H	

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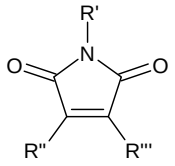
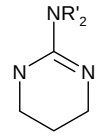
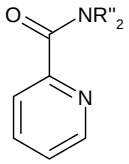
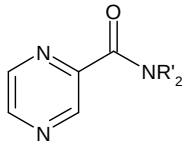
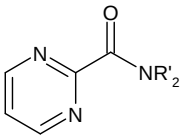
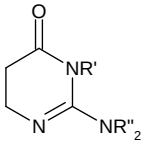
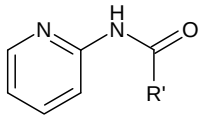
R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Pyrrole-2,5-dione ring correction	67C		R’ is undefined	
-N-C(-amino)=N- aliphatic ring correction	68C		R’ can be H	 Representative structure
Carboxamide ortho to aromatic nitrogen	69C		R’ can be H	 Representative structure
Pyrazine/Pyrimidine (2-posit)/ carboxamide	70C		R’ can be H	 Carboxamide pyrazine  2-carboxamide pyrimidine
-CO-N-C(-amino)=N aliphatic ring correc.	71C		R’, R” can be H	 Representative structure
Ring reaction (pyridine) -> -NH-C(=O)-	72C		Can be ortho, meta, para substitution; R’ cannot be H	 Representative structure

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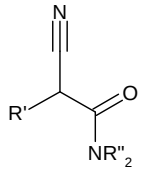
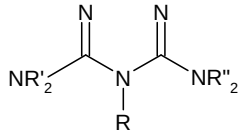
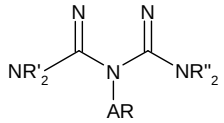
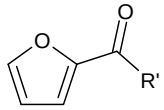
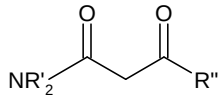
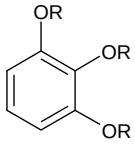
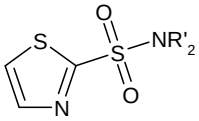
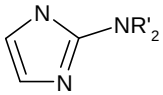
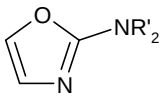
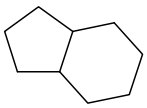
AR = Must be an aromatic carbon attachment

R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
C-(C#N)-C(=O)N structure correction	73C		R', R" can be H	
-Biguanide (aliphatic attach) correction	74C	Alkyl biguanide	R', R" can be H	
-Biguanide (aromatic attach) correction	75C	Aryl biguanide	R', R" can be H	
Furan -> carbonyl (at 2-position) correct.	76C		R' can be H	
C-(C(=O)-)-C(=O)N structure correction	77C		R', R" can be H	
Ring reaction -> 1,2,3-trialkyloxy	78C			
Thiazole -> 2-sulfonamide correction	79C			
Imidazole type -> 2-amino type correction	80C		R' can be H	
Oxazole type -> 2-amino type correction	81C		R' can be H	
Fused aliphatic ring unit correction	82C			 Representative structure

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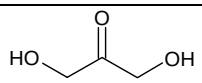
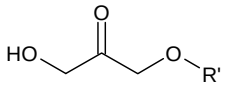
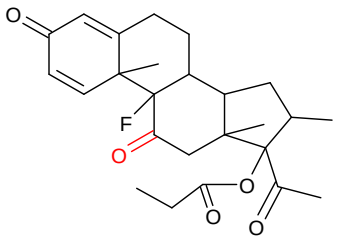
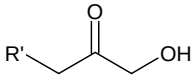
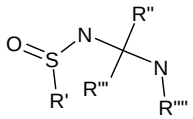
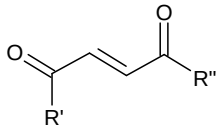
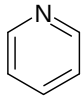
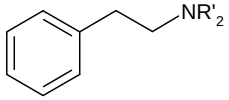
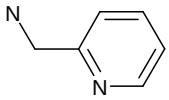
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
HO-C-C(=O)-C-OH structure correction	83C			
HO-C-C(=O)-C-O- structure correction	84C		R’ cannot be H	
Internal aliphatic fused-ring ketone cor.	85C		Representative structure = Clobetasone-17-propionate-des-cl (CAS No. 4351-59-1)	 Representative structure
-C-C(=O)-C-OH structure correction	86C		R’ can be H	
substituted carbon on [-SO-N-C-N-] corr.	87C		R’, R”” can be H; R”, R”’ is undefined	
-C(=O)-C=C-C(=O)- [aliphatic attachs] cor.	88C		R’s are undefined	
Pyridine ring (non-fused) correction	89C			
Benzene to -C-C-N- correction	90C		R’ can be H	
Methyl/ethylamine to aromatic (Nar ring)	91C		Representative structure = 2-Pyridinemethaneamine (CAS No. 3731-51-9); Methyl or ethylamine attached to an aromatic ring containing nitrogen.	 Representative structure

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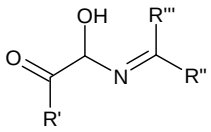
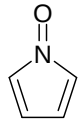
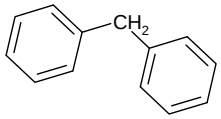
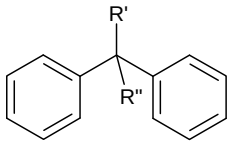
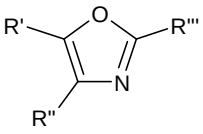
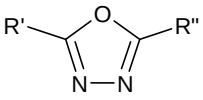
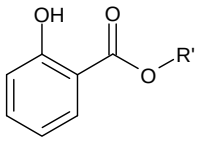
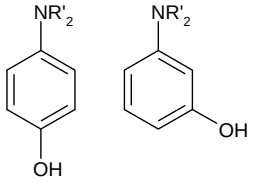
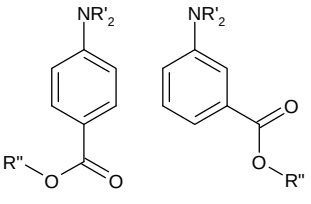
R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-CO-C(-OH)-N=C structure correction	92C		R’, R”, R’’’ can be H	
Non-fused n=O aromatic ring correction	93C			 Representative structure
-CH2- (aliphatic), 2 phenyl attach correc	94C		Substitution on the phenyls	
>C< (aliphatic), 2 phenyl attach correc	95C	Diphenyl alkane correction	R’, R” can be H; no aromatic attach	
Oxazole ring (non-fused) correction	96C		R’, R”, R’’’ is undefined	
1,3,4-Oxadiazole ring correction	97C		R’s are undefined	
Ring reaction -> -OH ortho to ester	98C		R’ cannot be H	
Ring reaction -> -N< / -OH (non-ortho)	99C		R’ can be H	
Ring reaction -> -N< / ester (non-ortho)	100C		R’ can be H; R” cannot be H	

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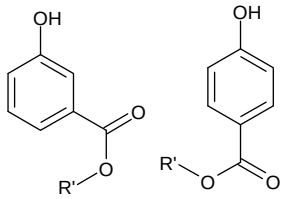
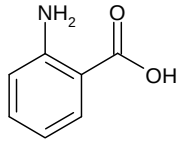
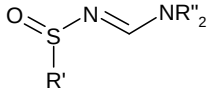
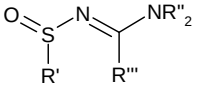
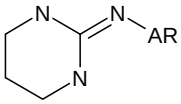
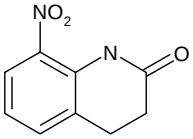
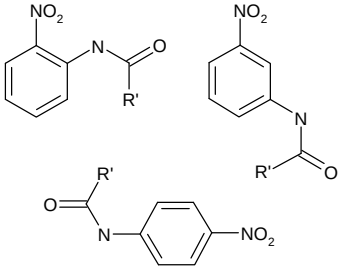
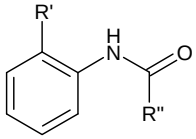
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring react -> -OH(mono)/ester (non-ortho)	101C		R’ cannot be H	
Ring reaction-> -NH2 ortho to acid (COOH)	102C			
-SO-N=C-N- [thiadiazine type] correction	103C	Thiadiazine-type correction	R’, R” can be H	
substituted carbon on [-SO-N=C-N-] corr.	104C		R’, R” can be H; R’’’ cannot be H	
Guanidine [N-C(=N-)-N](2-arom,cyclic type)	105C		Does not have to 6-membered ring.	 Representative structure
Ring reaction -> NO2/-NC(=O) [cyclic]	106C			 Representative structure
Ring reaction -> NO2/-NC(=O) [non-cyclic]	107C		R’ cannot be H	
Ring reaction -> ortho to -NHC(=O) type	108C		R’, R” cannot be H	

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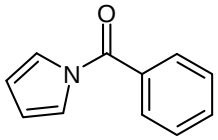
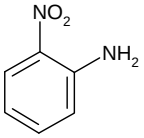
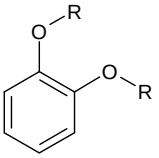
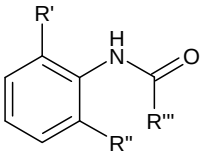
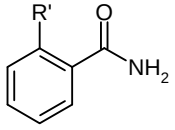
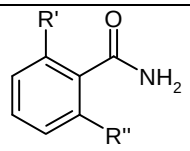
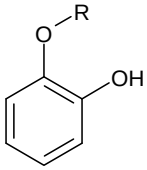
Fragment	Number	Modified Name	General Comments	Structure
Ring reaction -> NSO2- with an ester	109C			 Representative structure
Ring reaction -> -NH2 ortho to -NO2(mono)	110C			
Ring reaction -> 1,2-dialkyloxy	111C			
Ring reaction -> di-ortho to -NHC(=O)	112C		R', R'', R''' cannot be H	
Ring reaction -> ortho to -C(=O)NH-	113C			 Representative structure
Ring reaction -> di-ortho to -C(=O)NH-	114C			 Representative structure
Ring reaction -> alkyloxy ortho to -OH	115C		Substitution can be ortho, meta, or para	

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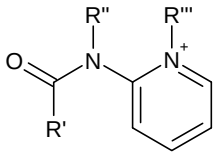
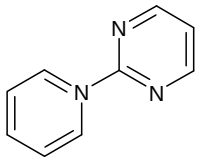
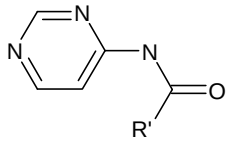
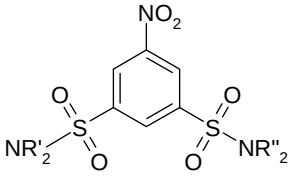
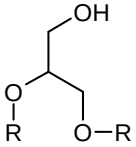
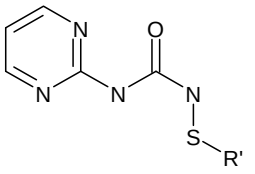
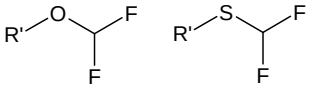
Fragment	Number	Modified Name	General Comments	Structure
Ring Rx (1+ aromatic n) -> >N(C(=O)-)-	116C		R', R", R''' cannot be H	
Extended aromatic nitrogen at ncn position	117C		Can be 5- or 6- member aromatics	 Representative structure
Ring Rx (2+ aromatic n) -> -NHC(=O)-	118C		R' cannot be H; 2-N's can be positioned anywhere on the ring.	 Representative structure
Ring Reaction -> di-SO2-N / -NO2	119C		R', R" can be H	
-O-C(-C-HO)-C-O- structure correction	120C			
-N-CO-N-S at aromatic ncn carbon	121C		R' is undefined	 Representative structure
-O-C(F)F or -S-C(F)F correction	122C		R' is undefined	

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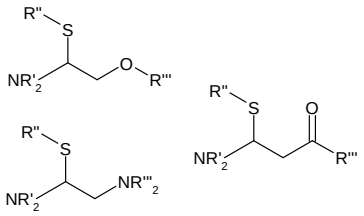
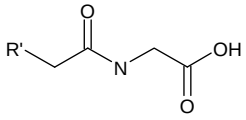
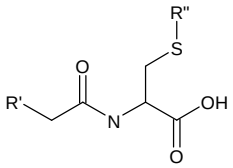
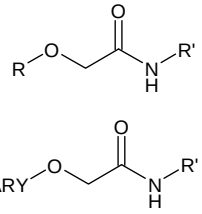
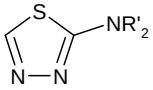
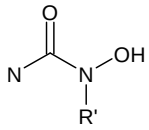
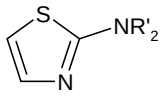
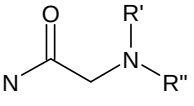
Fragment	Number	Modified Name	General Comments	Structure
>N-C(-S-)-C-{O,N,CO} correction	123C		R’, R”, R’’’ can be H	
C-C(=O)N-C-COOH structure correction	124C		R’ can be H	
C-C(=O)N-C(-COOH)-C-S- correction	125C		R’ can be H; R” cannot be H	
Aryloxy (or -C-O)-C-C(=O)NH- correction	126C		R’ can be H	
1,3,4-Thiadiazole ring (non-fused)	127C	1,3,4-Thiadiazole		
Ring Reaction: amino-type thiadiazole	128C		R’ can be H	
tertiary-N-hydroxy urea correction	129C		R’ can be OH	
Ring Reaction: amino-type thiazole	130C		R’ can be H	
N-CO-C-N< [C or H attach] correction	131C		R’, R” can be C or H	

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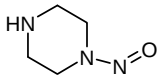
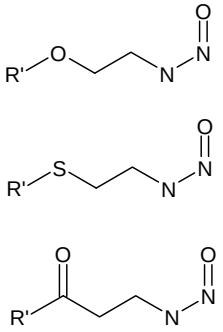
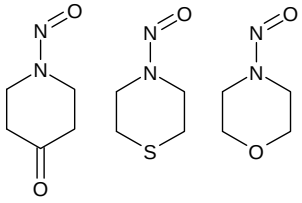
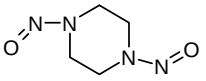
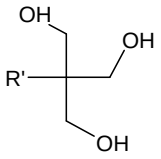
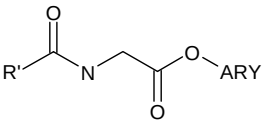
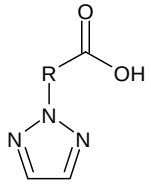
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-C(-N-N=O [cyclic]) -C-N- correction	132C			 Representative structure
N-Nitroso [linear] -C-C- { O,S, or CO} cor	133C		R' can be H	
N-Nitroso [cyclic] -C-C- { O,S, or CO} cor	134C			 Representative structures
-C(-N-N=O [cyclic]) -C-N-N=O correction	135C			 Representative structure
-C(-C-OH)(-C-OH)-C-OH structure correct.	136C		R' can be H	
-CO-NH-C-CO-O-aromatic structure correc.	137C		R' can be H	
1,2,3-Triazole / -COOH (aliphatic) react.	138C		Aliphatic chain can be greater than 1 carbon.	

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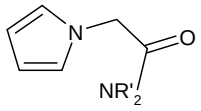
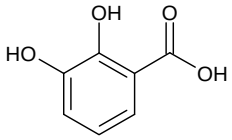
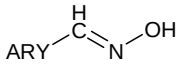
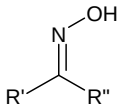
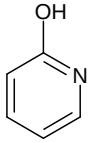
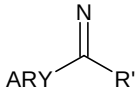
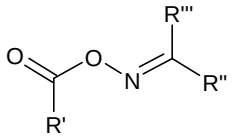
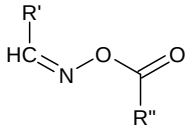
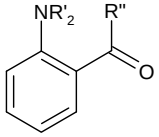
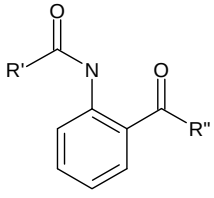
R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

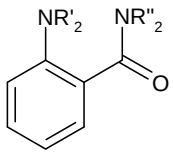
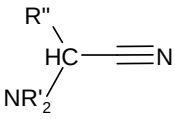
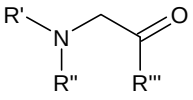
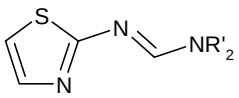
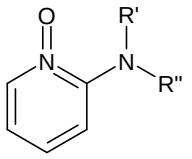
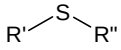
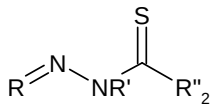
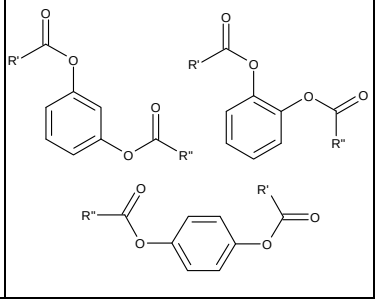
Fragment	Number	Modified Name	General Comments	Structure
Aromatic nitrogen-C-CO-N< structure corr.	139C			 Representative structure
Ring reaction -> -COOH & -OH ortho to -OH	140C			
-CH=N-OH [oxime,aromatic attach] corre.	141C	Aryl oxime correction		
>C=N-OH [ketoxime] correction	142C	Ketoxime correction	R', R" cannot be H	
Ring rx -> -OH ortho to aromatic nitrogen	143C			
>C=NH [ketimine, aromatic attach] correc	144C	Aryl ketimine	R' = Aromatic or alkyl C; cannot be H	
>C=N-O-CO- structure correction	145C		R', R" can be H; R''' cannot be H	
-CH=N-O-CO- structure correction	146C		R' cannot be H; R" can be H	
Ring reaction -> ortho amino / ketone	147C		R' can be H; R" = Aromatic or aliphatic attachment	
Ring reaction -> ortho -NC(=O) / ketone	148C		R' cannot be H; R" = Aromatic or aliphatic attachment	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring reaction -> ortho amino-type/-C(=O)N	149C		R’, R” can be H	
-N-CH-C#N [aminomethylcyano] correction	150C	Aminomethylcyano correction	R’, R” can be H	
-N-C-C(=O)-carbon structure correction	151C		R’ can be H; R”, R’’’ cannot be H	
Ring reaction -> 2-thiazole-type / -N=C-N	152C		R’ can be H	
Ring reaction -> amino-type ortho to n=O	154C		R’, R” can be H	 Representative structure
Sulfur halide structure correction	155C		R’ = Halogen; R” is undefined	
=NNC(=S)N- [thiosemicarbazone] correct.	156C	Thiosemicarbazone correction	R’, R” can be H	
Ring reaction -> -O-CO / -O-CO	157C			

R = Must be an aliphatic carbon attachment

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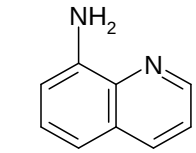
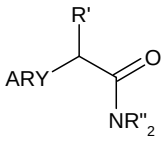
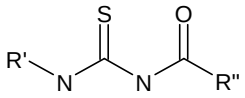
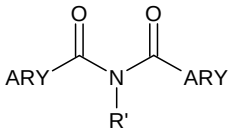
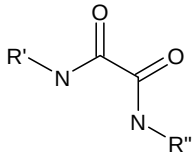
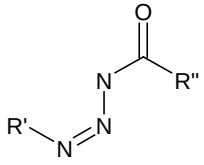
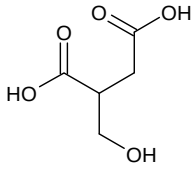
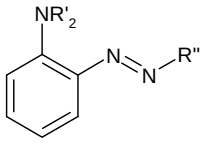
R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Fused ring reaction: c-c(-N<)-c[fused]-n	158C		Representative structure = 8-Aminoquinoline (CAS No. 578-66-5)	 Representative structure
aromatic-CH(-CO-N)-{-N	159C		R’ = -N, -OH, -C=O; R” can be H	
-N-C(=S)-N-C(=O)- structure correction	160C		R’, R” can be H	
aromatic-CO-N-CO-aromatic [linear] correc	161C		R’ can be H	
-N-CO-CO-N- structure correction	162C		R’, R” can be H	
N=N-N-CO-aliphatic structure correction	163C		R’, R” can be H	
HOOC-C-(C-COOH)(C-OH) structure correction	164C			
Ring reaction -> amino-type ortho to Azo	165C		R’, R” can be H	

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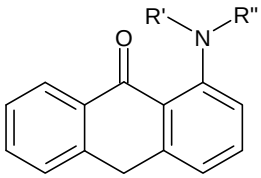
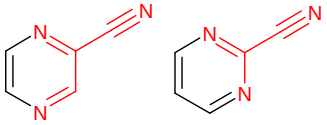
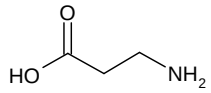
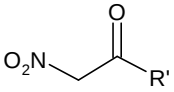
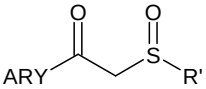
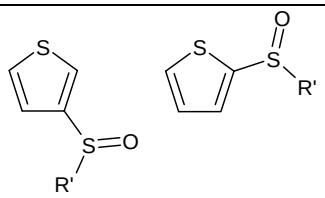
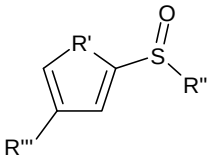
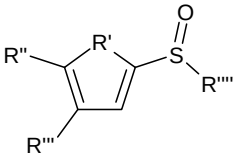
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring rx -> amino / cyclic C(=O)->aromatic	166C		R', R" can be H	
ortho-Cyano to 2 aromat nitrogens/pyrazine	167C			
Amino acid (non-alpha carbon type) corr.	168C		Amino is on beta-carbon in representative structure.	 Representative structure
C-(NO2)-CO- structure correction	169C		R' can be H	
aromatic-CO-C-S(=O)-structure correct.	170C		R' can be H	
Ring rx: aromatic Sulfur / -S(=O)-C	171C		R' cannot be H	
Ring rx: -SO-C with NO2/C#N/OH/amino (5R)	172C		R' = O or S, only; R" cannot be H; R''' = Nitro, cyano, hydroxy, or amino group (in any ring position)	
Ring rx:-SO-C with di-NO2/C#N/OH/amino(5R)	173C		R' = O or S, only; R",R''' = Nitro, cyano, hydroxy, or amino group (in any ring position); R"" cannot be H;	

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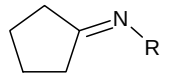
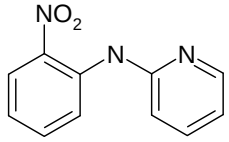
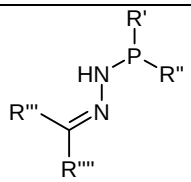
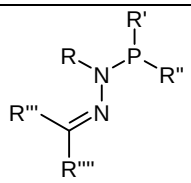
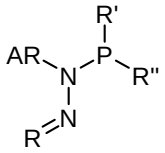
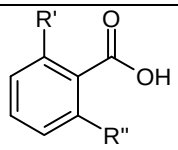
Fragments containing "C" or "X" are not used in Pass 2

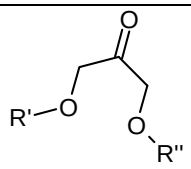
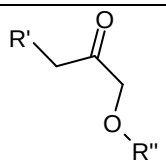
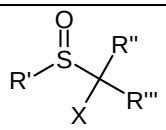
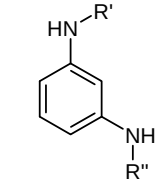
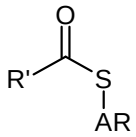
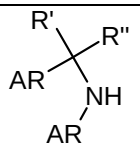
Fragment	Number	Modified Name	General Comments	Structure
>C=N-C [cyclic-type imine, ali carbon att]	174C			 Representative structure
Ortho rx: (-NO2/-N-) on diarylamine(o-Nar)	175C			
=N-NH-P structure correction	176C		R's are undefined	
=N-N(-aliphatic)-P structure correction	177C		R's are undefined	
=N-N(-aromatic)-P structure correction	178C		P may have 3 or 5 substituents	
Ring reaction -> di-ortho to aromatic acid	179C			 Representative structure

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-O-C-CO-C-O- structure correction	180C		R', R'' and other substitution undefined	
-C-CO-C-O- structure correction	181C		R' , R'' and other substitution undefined	
SO-C(halo) structure correction	182C		R' undefined; R'' and R''' not X or other halogen	
Ring rx -> -NH & -NH (phenyl,non-ortho)	183C			 Representative structure
-C(=O)-S-aromatic correction	184C		R' is undefined	
aromatic-C-N-aromatic correction	185C		R' and R'' are undefined	

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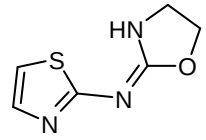
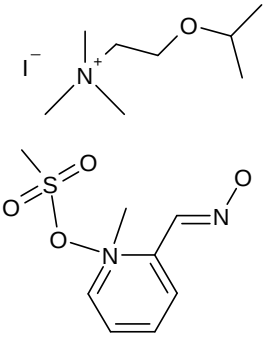
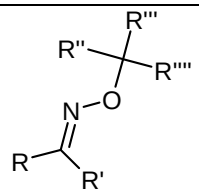
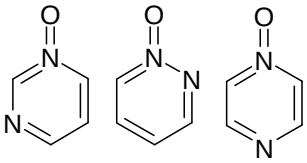
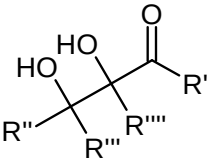
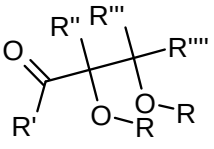
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring rx -> 2-thiazole-type / -CH=N-OH	186C			 Representative structure
Reaction: nitrogen[+5] / polar group	187C		Representative structures = Isopropoxyethyl trimethyl ammonium iodide (CAS No. 21949-06-4) and 2-[(Hydroxyimino)methyl] -1-methyl-pyridinium (CAS No. 154-97-2)	 Representative structures
aliph-C=N-O-carbon(aliphat) [iminoxy] cor.	188C		Rs are undefined	
Ring reaction -> n=O / aromatic nitrogen	189C			
HO-C-C(-OH)-C(=O)- structure correction	190C		Rs are undefined	
-O-C-C(-O-)-C(=O)- structure correction	191C		Rs are undefined	

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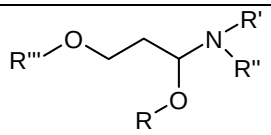
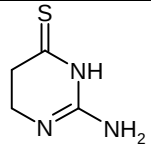
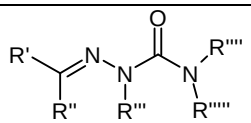
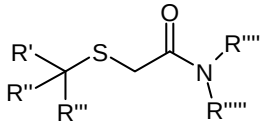
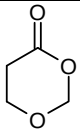
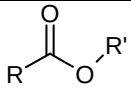
Fragment	Number	Modified Name	General Comments	Structure
-O-C-C(-N-)-O- structure correction	192C		R’ , R’’, R’’’ and other substitution undefined	
-C(=S)-N-C(-amino)=N aliphatic ring correc	193C			 Representative structure
C=NN-CO-N- [semicarbazone] correction	194C		R’s are undefined	
-C-S-C-CO-N- structure correction	195C		R’ , R’’, R’’’ and other substitution undefined	
-CO-O-C-{-O-,-N-} [on cyclic ester] correc	196C			 Representative structure
C(=O)-O-{Na,K,Li} [coef*(1+0.5*(NUM-1))]	197C		R’ = Na, K, Li	

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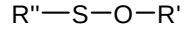
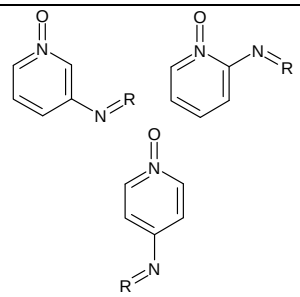
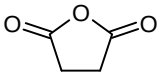
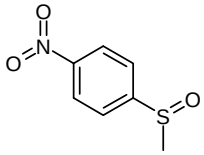
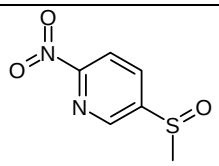
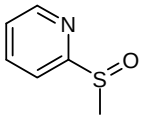
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
S-O-{Na,K,Li} [coef*(1+0.3*(NUM-1))]	198C		R’ = Na, K, Li R’’ is undefined	
Aromatic n-oxide rx with misc -N< / -N=	199C			
Cyclic ester [di-carbonyl type] correction	200C			 Representative structure
Ph Ring rx: -SO-C with NO2/C#N/OH/amino	201C			 Representative structure
Nar Ring rx: -SO-C with NO2/C#N/OH/amino	202C			 Representative structure
Ring rx: -SO-C with 1 aromatic nitrogen	203C			 Representative structure

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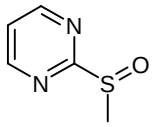
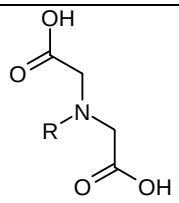
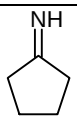
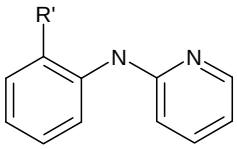
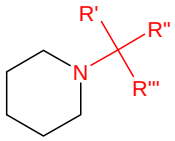
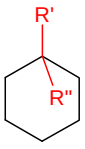
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring rx: -SO-C with 2+ aromatic nitrogens	204C			 Representative structure
HOOC-C-N-C-COOH structure correction	205C			
>C=NH [cyclic ketimine, aliphat attachs]	206C			 Representative structure
Ortho rx: (to -N-) on diarylamine(o-Nar)	207C		R’ cannot be H.	
Ring -N- to quat carbon-type correction	208C		R’, R”, R’’’ cannot be H	 Representative structure
Quaternary carbon(cyclic,2 halogen attach)	209C		R’, R” = Halogen	 Representative structure

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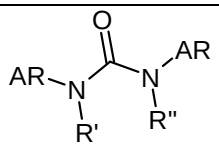
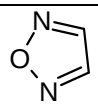
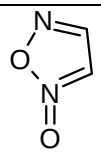
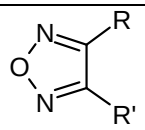
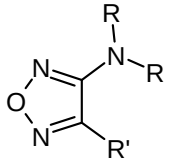
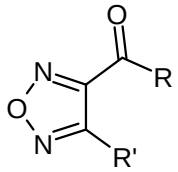
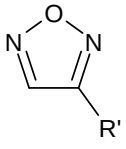
Fragment	Number	Modified Name	General Comments	Structure
Urea (N & N'-disubstituted; diaryl) correc	210C		R's are undefined	
1,2,5-Oxadiazole ring correction	211C			
1,2,5-Oxadiazole n-oxide ring correction	212C			
Aliph carbon subst. on 1,2,5-oxadiazole	213C		R' is undefined	
Amino-type subst on 1,2,5-oxadiazole ring	214C		R' is undefined	
Carbonyl subst. on 1,2,5-oxadiazole ring	215C		R' is undefined	
-S(=O) subst. on 1,2,5-oxadiazole ring	216C		R' = -S(=O)-Armoatic or –SO2-C-	

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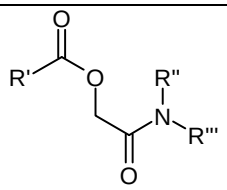
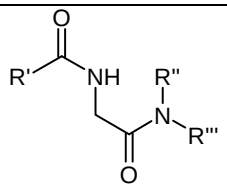
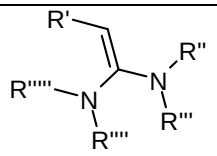
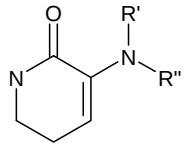
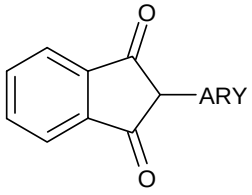
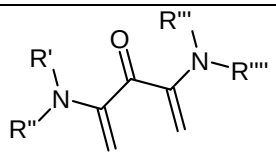
Fragment	Number	Modified Name	General Comments	Structure
-C(=O)-O-C-C(=O)-N- correction	217C		Rs are undefined	
-CO-N-C-CO-N- (linear C;aliphatic) corr.	218C		Rs are undefined	
C=C(-N-)-N- correction	219C		Rs are undefined	
C=C(-N-)-C(=O)- correction	220C		R', R" can be H; Must be 5- or 6-membered cyclic	 Representative structure
cyclic C(CO-Car)(CO-Car)-Car correction	221C			
-N-C-C(=O)-C-N- [olefinic carbons] corr.	222C		Rs are undefined	

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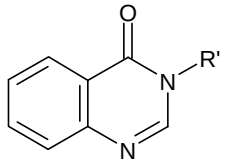
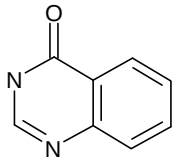
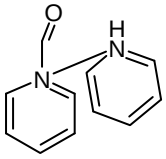
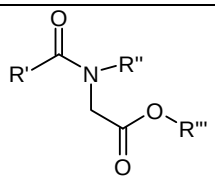
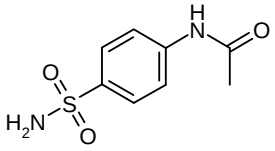
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Pyrimidin-4-one type ring [arom att;N-sub]	223C		R’ cannot be H; Fused aromatic can be 5- or 6-membered.	 Representative structure
Pyrimidin-4-one type ring [aromatic att]	224C		Fused aromatic can be 5- or 6-membered.	 Representative structure
carbon-C(=O)-aromatic N - aromatic N cor.	225C			 Representative structure
-O-CO-C-N-CO- [no aromatic attach] cor.	226C		R’, R’’, R’’’ cannot be aromatic	
Ring reaction: -NH-CO with -SO2-N	227C			 Representative structure

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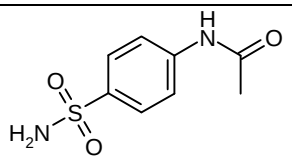
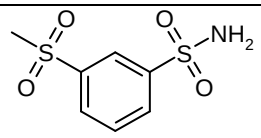
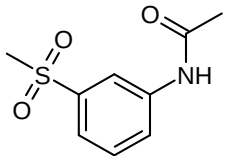
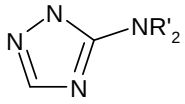
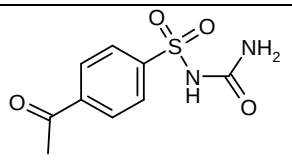
Fragments containing “C” or “X” are not used in Pass 2

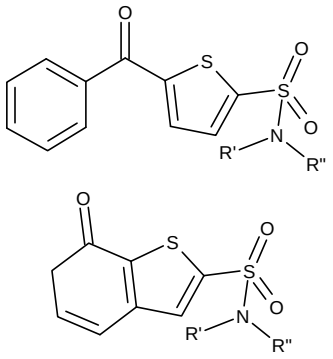
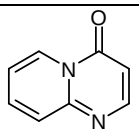
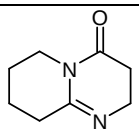
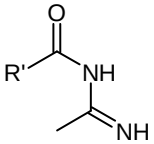
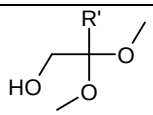
Fragment	Number	Modified Name	General Comments	Structure
Ring reaction: -N-CO with -SO2-N	228C			 Representative structure
Ring reaction: -SO2-C with -SO2-N/-N-CO	229C			 Representative structure  Representative structure
Additional amino-type triazole correction	230C		R' Can be H; Has to be 1,2,4 – triazole, no amine on N	
Ring rx: -SO2-N with SO-Car/-CO-C [6 mem]	231C			 Representative structure

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

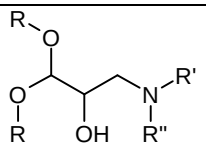
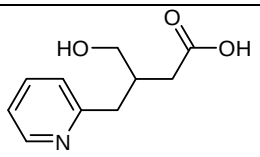
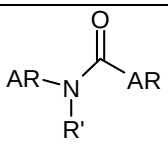
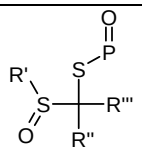
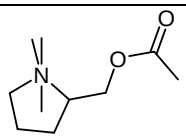
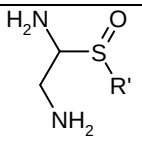
Fragment	Number	Modified Name	General Comments	Structure
Ring rx: -SO2-N with SO-Car/-CO-C [5 mem]	232C		R', R" can be H	
C=C-C(=N-C)-N-C(=O)- [fused ring type]	233C			 Representative structure
-C-C(=N-C)-N-C(=O)- [fused ring type]	234C			 Representative structure
-CO-N-C(=NH)-C correction	235C		R' is undefined	
C-O-C(-C-OH)-O-C correction	236C		R' undefined Ether methyl group may be substituted and alcohol can be secondary or tertiary	 Representative structure

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

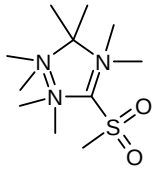
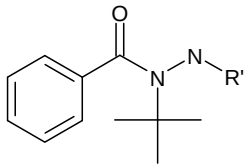
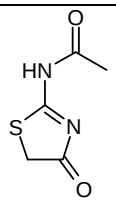
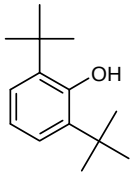
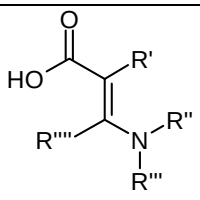
Fragment	Number	Modified Name	General Comments	Structure
N-C-C(-OH)-C(-O-)(-O-) correction	237C		R', R" can be H	
C[-C-O][C-CO-O][C-Caromatic-Naromatic]	238C			 Representative structure
Caromatic-N-C(=O)-Caromatic correction	239C		R' is undefined	
-P(=O)-S-C-S(=O) correction	240C			
Reaction: nitrogen[+5] / ester	241C			 Representative structure
>N-C(-S(=O)-)-C-{O,N,CO} correction	242C		R' cannot be H	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring rx: -SO2-C with 3+ arom nitrogens(5R)	243C			 Representative structure
Car-C(=O)-N(>C	244C		R’ can be H	
-S-C[cyclic](=N-C(=O))-N-C(=O) correction	245C			 Representative structure
Ring rx: -OH / di-ortho;sec- or t- carbon	246C			 Representative structure
Amino acid (olefin; non-alpha carbon type)	247C		Rs are undefined	

R = Must be an aliphatic carbon attachment

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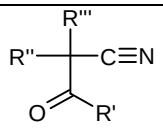
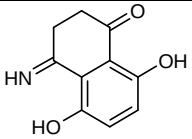
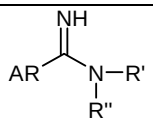
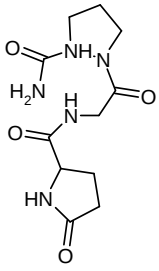
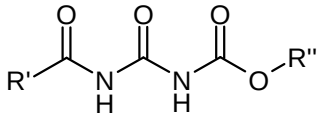
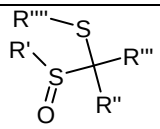
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-C-(C#N)-CO- structure correction	248C		Rs are undefined	
>C(=NH) [ketimine,cyclic,aromatic attach]	249C			 Representative structure
-C(=NH)-N [aromatic attach] correction	250C		Rs are undefined	
multi: -CO-N-C-CO-N- (cyclic C;aliphatic)	251C			 Representative structure
-O-CO-N-CO-N-CO- structure correction	252C		Rs are undefined	
C-S-C-S(=O)- structure correction	253C		Rs are undefined	

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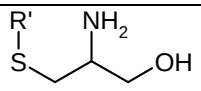
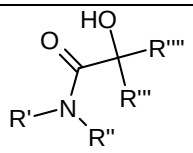
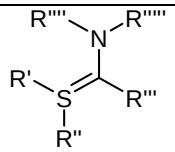
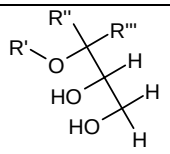
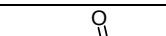
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-S-C-C(-N-)-C-OH structure correction	254C		R’ and other substitution undefined	
-N-CO-C-OH [linear CO;>C	255C		R’ and R’’ are undefined; R’’’ and R’’’’ cannot be H	
>S=C(-N-) structure correction	256C		R’s are undefined	
-C-N=C-N-C- [cyclic] structure correction	257C			 Representative structure
HO-CH2-CH(-OH)-C-O- [linear-type] correc.	258C		R’s are undefined	
Azide correction N=N#N	259C		R’ is undefined	
Special cyclic ester (large ring;olefin)	260C		Minimum amount of double bonds and carbons shown in Rep. Structure	 Representative structure

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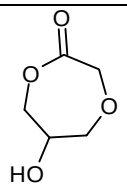
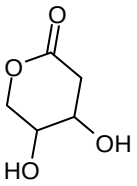
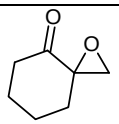
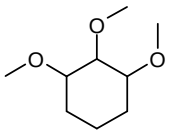
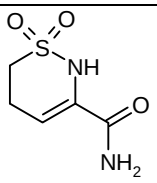
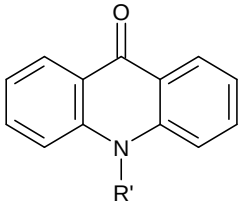
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
O-C-C(-OH)-C-O-C(=O)-C (cyclic ester part)	261C			 Representative structure  Representative structure
Epoxide - Cyclic Ketone enhancement	262C			 Representative structure
-C(-O-C)(-C-O-C)(-C-O-C) {cyclic type}	263C			 Representative structure
C=C(-N-SO2-)({-N-;-C(=O)-N}) [cyclic]	264C			 Representative structure
Fused ketone ring (di-aromatic + nitrogen)	265C		R' can be H	

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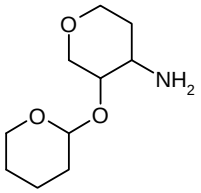
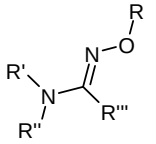
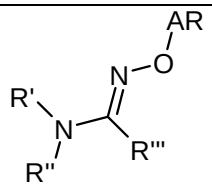
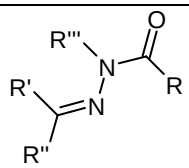
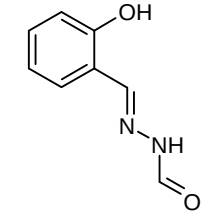
R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
N-C-C--O--C-O-C [di-cyclic ether type]	266C			 Representative structure
N-C=N-O-carbon(aliphatic) [iminoxy] corr.	267C		R's are undefined	
N-C=N-O-carbon(aromatic) [iminoxy] corr.	268C		R's are undefined	
C=N-N-CO-carbon [acyl hydrazone]	269C		R's are undefined	
Ring rx: -OH ortho to -C=N-N-CO-	270C			 Representative structure

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AR = Must be an aromatic carbon attachment

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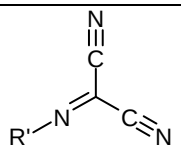
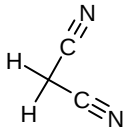
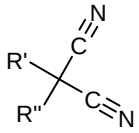
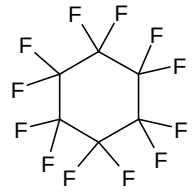
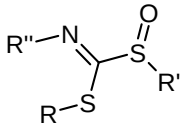
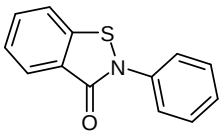
Fragments containing "C" or "X" are not used in Pass 2

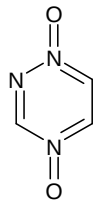
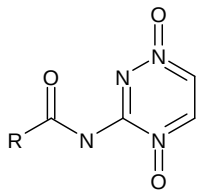
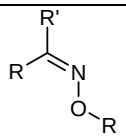
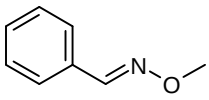
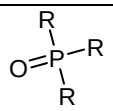
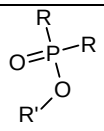
Fragment	Number	Modified Name	General Comments	Structure
N=C-(C#N)-C#N [dicyano] correction	271C		R’ is undefined	
CH2-(C#N)-C#N [dicyano] measured corr.	272C			
-C-(C#N)-C#N [dicyano] correction	273C		R’ and R’’ is undefined	
MultiQuat carbon(cyclic,2 fluorine attach)	274C		Representative structure = Perfluorocyclohexane (CAS No. 355-68-0)	 Representative structure
C-S-C(=N-)-S(=O)- structure correction	275C		R’s are undefined	
aromat-N(-CO-aromat)(-S-aromat)[cyclic]	276C			 Representative structure

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2

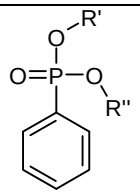
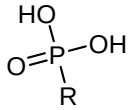
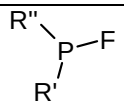
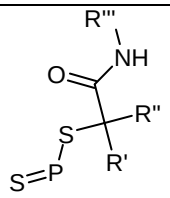
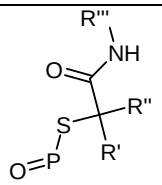
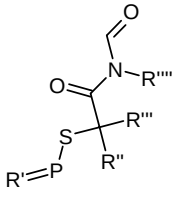
Fragment	Number	Modified Name	General Comments	Structure
Excessive n=O ring correction (type 1)	277C			
Excessive n=O ring correction (type 2)	278C			
aliph-C=N-O-carbon(aliphat) [iminoxy] cor.	279C		R' is undefined	
aliph-CH=N-O-carbon(aliphat) [iminoxy] cor	280C			 Representative structure
O=P(carbon)(carbon)(carbon) correction	281C			
O=P(carbon)(carbon)(oxygen) correction	282C			

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

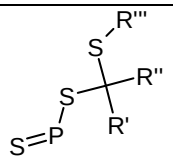
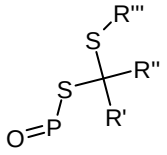
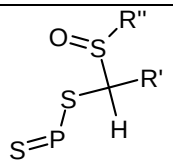
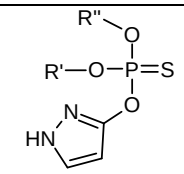
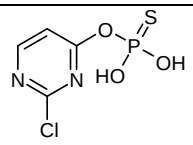
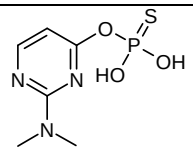
Fragment	Number	Modified Name	General Comments	Structure
O=P(oxygen)(oxygen)(-CH2-phenyl) correct	283C		R's are undefined	
O=P(-OH)(-OH)(aliphatic carbon) correction	284C			
Phosphorus-Fluorine correction	285C		R's are undefined	
S=P-S-C-C(=O)-N- correction	286C		R's are undefined	
O=P-S-C-C(=O)-N- correction	287C		R's are undefined	
{O,S}=P-S-C-C(=O)-N-C(=O) correction	288C		R' = O or S; R'',R''',R'''' = undefined	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

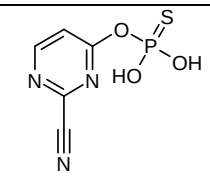
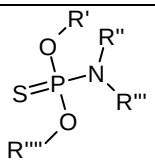
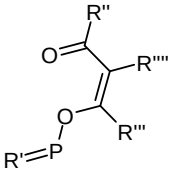
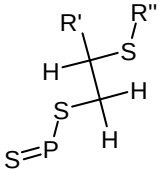
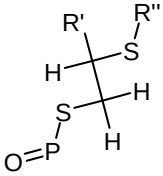
Fragment	Number	Modified Name	General Comments	Structure
S=P-S-C-S- correction	289C		R's are undefined	
O=P-S-C-S- correction	290C		R's are undefined	
S=P-S-C-S- unhindered S(=O) correction	291C		R's are undefined	
Ring rx: S=P(O)(O)O- / 5-mem (2+ nitrogen)	292C			 Representative structure
Ring rx: S=P(O)(O)O / aromat N + halogen	293C			 Representative structure
Ring rx: S=P(O)(O)O / aromat N + amino	294C			 Representative structure

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

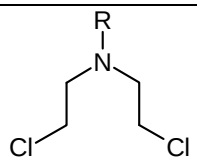
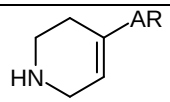
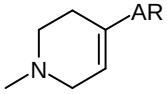
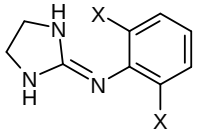
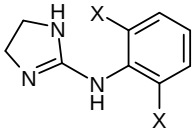
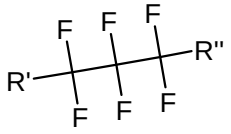
Fragment	Number	Modified Name	General Comments	Structure
Ring rx: S=P(O)(O)O / cyano (nitrile)	295C			 Representative structure
S=P(-O)(-O)-N- correction	296C		Rs cannot be H	
{O,S}=P-O-C=C-C(=O)-{O,N} correction	297C		R= O or S; R''= O or N; R''' and R'''' are undefined	
S=P-S-CH2-CH-S- correction	298C		Rs are not defined	
O=P-S-CH2-CH-S- correction	299C		Rs are not defined	

R = Must be an aliphatic carbon attachment

AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
CL-CH-CH2-N-CH2-CH-CL correction	300C			
Tetrahydropyridine (NH-type) aromat-attach	301C			 Representative structure
Tetrahydropyridine (-N-type) aromat-attach	302C			 Representative structure
di-ortho-halo -c-N=C(-NH)-NH- correction	303C			 Representative structure
di-ortho-halo -c-NH-C(=N)-NH- correction	304C			 Representative structure
-CF2(-CF2)(-CF2) (linear -CF2- core)	305C			
-Hg- [mercury]	310C			Hg

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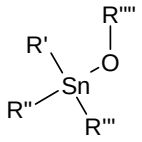
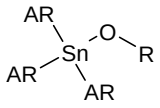
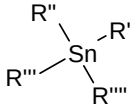
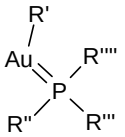
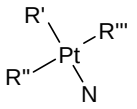
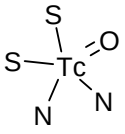
AR = Must be an aromatic carbon attachment

R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
[Pb] (Lead)	311C			Pb
[As] (Arsenic)	312C			As
[Ge] (Germanium)	313C			Ge
Tin [Sn]	314C			Sn
Tin [Sn] { oxygen attach }	315C		R', R", R''' Can be H; R'''' Cannot be H	
Tin [Sn] { oxygen and aromatic attach }	316C		Must have at least one aromatic attachment.	
Tin [Sn] { halogen or -OH attach }	317C		R' = Hydroxy, Halogen; R", R''', R'''' can be H	
Aluminum [Al]	318C			Al
Gold [Au]=P { Phosphorus attach }	319C		R's can be H	
Platinum [Pt] { halogen & nitrogen attach}	320C		R' = Halogen; R", R''' can be H	
Technetium [Tc](-S)(-S)(-N)(-N)	321C			
Krypton [Measured]	322C			Kr
Argon [Measured]	323C			Ar
Neon [Measured]	324C			Ne
Xenon [Measured]	325C			Xe

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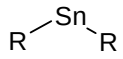
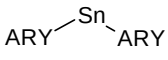
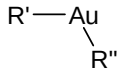
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Radon [Measured]	326C			Rn
Helium [Measured]	327C			He
Mercury [Measured]	328C			Hg
Tin [Sn] { divalent; carbon attach }	329C			
Tin [Sn] { divalent; aromatic attach }	330C			
Sodium [Na]	331C			Na
Potassium [K]	332C			K
Lithium [Li]	333C			Li
Gold [Au]	334C			Au
Bismuth [Bi]	335C			Bi
Calcium [Ca]	336C			Ca
Magnesium [Mg]	337C			Mg
Antimony [Sb]	338C			Sb
Zinc [Zn]	339C			Zn
Gold [Au] { halogen attach }	340C		R' = Halogen; R" can be H	
Platinum [Pt] { halogen attach }	341C		R' = Halogen	
Platinum [Pt]	342C			Pt
Iron [Fe]	343C			Fe
Cadmium [Cd]	344C			Cd
Cadmium [Cd] { halogen attach }	345C		R' = Halogen	

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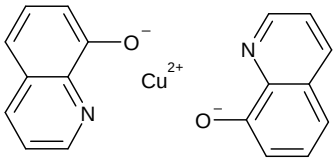
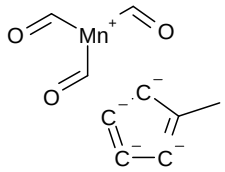
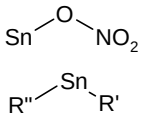
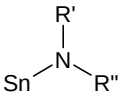
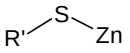
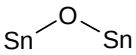
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Miscellaneous Metal [Ni,Cu,Zr,Be]	346C		Representative structure = Bis(8-quinolinolato-(N1,O8))copper (CAS No. 10380-28-6)	 Representative structure
Miscellaneous Elements (Value Unknown)	347C		Representative structure= Methylcyclopentadienyl manganese (CAS No. 12108-13-3)	 Representative structure
Tin [Sn] { multi-halogen or -ONO2 }	348C		R', R" = Halogen (must have at least two)	
Tin [Sn] { nitrogen attach }	349C		R', R" can be H	
[Zn]-S { zinc-sulfur }	350C		R' can be H	
[Sn]-O-[Sn] { bis-tin ether }	351C			
	352C			
[He]	353C			He
[Ne]	354C			Ne
[Ar]	355C			Ar
[Kr]	356C			Kr
[Xe]	357C			Xe
[Rn]	358C			Rn
[At]	359C			At
[Po]	360C			Po
[Bi]	361C			Bi
[Ga]	362C			Ga

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Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
[In]	363C			In
[Tl]	364C			Tl
[Cu]	365C			Cu
[Ag]	366C			Ag
[Ni]	367C			Ni
[Pd]	368C			Pd
[Co]	369C			Co
[Rh]	370C			Rh
[Ir]	371C			Ir
[Ru]	372C			Ru
[Os]	373C			Os
[Mn]	374C			Mn
[Tc]	375C			Tc
[Re]	376C			Re
[Cr]	377C			Cr
[Mo]	378C			Mo
[W]	379C			W
[V]	380C			V
[Nb]	381C			Nb
[Ta]	382C			Ta
[Ti]	383C			Ti
[Zr]	384C			Zr
[Hf]	385C			Hf
[Sc]	386C			Sc
[Y]	387C			Y
[La]	388C			La

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Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
[Ce]	389C			Ce
[Pr]	390C			Pr
[Nd]	391C			Nd
[Pm]	392C			Pm
[Sm]	393C			Sm
[Eu]	394C			Eu
[Gd]	395C			Gd
[Tb]	396C			Tb
[Dy]	397C			Dy
[Ho]	398C			Ho
[Er]	399C			Er
[Tm]	400C			Tm
[Yb]	401C			Yb
[Lu]	402C			Lu
[Ac]	403C			Ac
[Th]	404C			Th
[Pa]	405C			Pa
[U]	406C			U
[Np]	407C			Np
[Pu]	408C			Pu
[Am]	409C			Am
[Cm]	410C			Cm
[Bk]	411C			Bk
[Cf]	412C			Cf
[Es]	413C			Es
[Fm]	414C			Fm

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Fragment	Number	Modified Name	General Comments	Structure
[Md]	415C			Md
[No]	416C			No
[Lr]	417C			Lr
[Sr]	418C			Sr
[Ba]	419C			Ba
[Ra]	420C			Ra
[Be]	421C			Be
[Rb]	422C			Rb
[Cs]	423C			Cs
[Fr]	424C			Fr
[Te]	425C			Te

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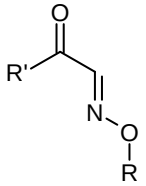
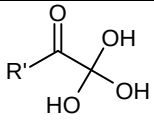
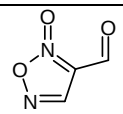
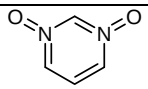
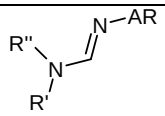
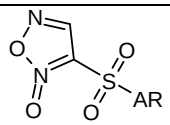
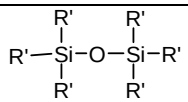
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-C(=O)-C=N-O- structure correction	0X		R’ is undefined	
-C(-OH)(-OH)-C(=O)- structure correction	1X		R’ is undefined	
Carbonyl sub on 1,2,5-oxadiazole n-oxide	2X			 Representative structure
Two or more aromatic n=O in same ring	3X			 Representative structure
Linear >N-C=N-aromatic correction	4X			
-SO-arom sub on 1,2,5-oxadiazole n-oxide	5X			
Linear Si-O-Si correction [coef * NUM - 2]	6X		R’ is undefined	

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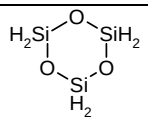
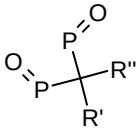
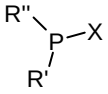
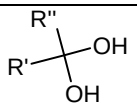
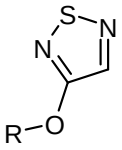
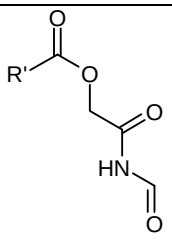
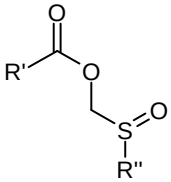
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Cyclic Si-O-Si correction [coef * NUM - 4]	7X			 Representative structure
O=P-C-P=O structure correction	8X			
Phosphorus-halogen correction	9X		R's are undefined	
HO-C-OH (poly-alcohol carbon) correction	10X		R's are undefined	
Ring Rx: thiadiazole / alkyloxy-	11X			
-C(=O)-O-C-C(=O)-N-C(=O)- correction	12X			
-C(=O)-O-C-S(=O)- correction	13X			

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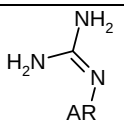
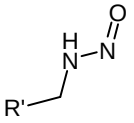
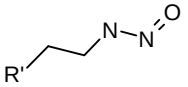
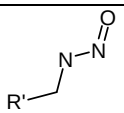
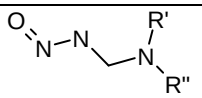
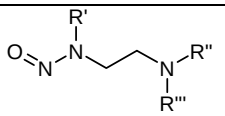
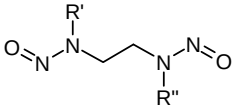
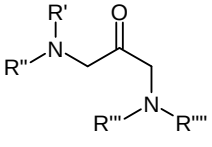
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Guanidine [NC(=N-)N](2-arom,non-cyclic ty)	14X			
N-Nitroso - C - C#N or NO2 correction	15X		R' = C#N or NO_2	
N-Nitroso -C-C- C#N or NO2 correction	16X		R' = C#N or NO_2	
N-Nitroso - C - { O,S, or CO} correction	17X		R' = O, S, C=O	
N-Nitroso - C - Nitrogen correction	18X		R's are undefined	
-C(-N-N=O [linear])-C-N- correction	19X		R's are undefined	
-C(-N-N=O [linear])-C-N-N=O correction	20X		R's are undefined	
-N-C-C(=O)-C-N- correction	21X		R's can be H	

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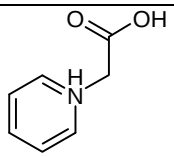
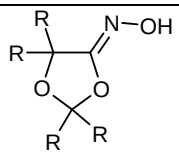
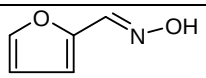
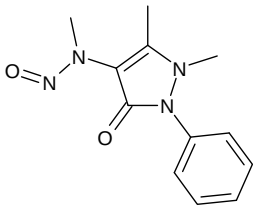
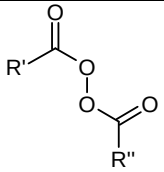
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Aromatic Nitrogen-C-COOH structure correc	22X			 Representative structure
Cyclic ketoxime (>C=N-OH) [aliph attach]	23X			
Ring rx -> -CH=N-OH ortho to arom oxygen	24X			 Representative structure
C=C(-N-N)-C(=O)- correction	25X		Representative structure = CAS No. 73829-38-6	 Representative structure
-C(=O)-O-O-C(=O)- correction	26X		R's are undefined	
>C=NH [ketimine, aliphat attachs] correc	27X			

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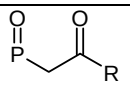
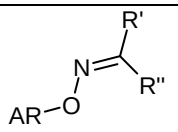
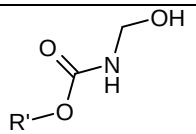
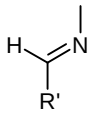
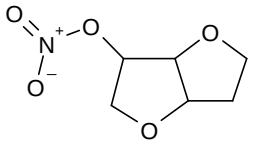
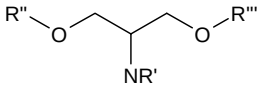
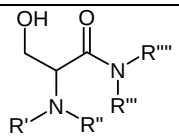
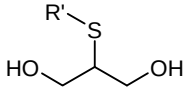
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-P(=O)-C-C(=O)- correction	28X		R's are undefined	
C=N-O-carbon(aromatic) [iminoxy] correc.	29X		R's are undefined	
-O-C(=O)-N-C-OH [linear N] correction	30X		R' undefined	
-CH=N-C [linear imine] correction	31X		R' is undefined	
-O-C(-C-HO)-C-ONO2 structure correction	32X			
-O-C-C(-N-)-C-O- structure correction	33X		R' can be H; R", R''' = Undefined	
HO-C-C(-N-)-C(=O)N- structure correction	34X		R's can be H	
HO-C-C(-S-)-C-OH structure correction	35X		R' is undefined	

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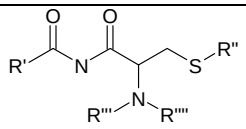
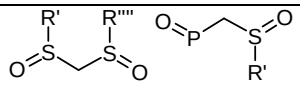
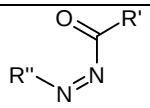
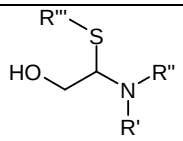
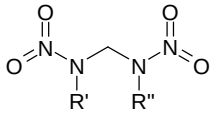
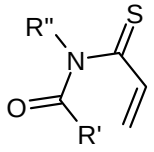
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
CO-N-CO-C(-N-)-C-S structure correction	36X		R's can be H	
-S(=O)-C {-S(=O);-P(=O)} correction	37X		R's are undefined	
-N=N-C(=O)- structure correction	38X		R's are undefined	
-S-C(-N-)-C-OH structure correction	39X		R's are undefined	
NO2-N-C-N-NO2 structure correction	40X		R's are undefined	
-S(=O)-N-S(=O)- structure correction	41X		R's are undefined	

R = Must be an aliphatic carbon attachment

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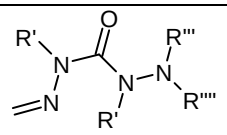
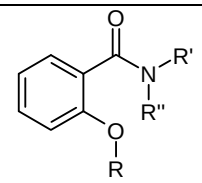
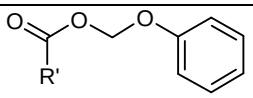
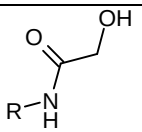
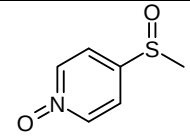
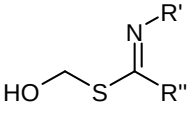
R', R'', R''', etc. = Defined in General Comments

Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
C=NN-CO-N-N- [aminosemicarbazone] correc.	42X		R's are undefined	
Ring rx -> -CO-NH ortho to alkyloxy	43X		R' and R'' undefined	 Representative Structure
aromatic-O-C-O-CO- structure correction	44X			 Representative structure
-N-CO-CH2-OH structure correction	45X		-OH can be attached aromatic, ortho to amide	
Ring reaction -> n=O / -S(=O)-C	46X		Position not defined	 Representative structure
S(-C-O-)(-C=N) structure correction	47X			

R = Must be an aliphatic carbon attachment

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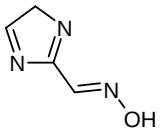
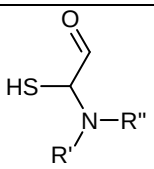
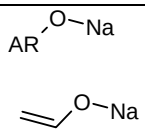
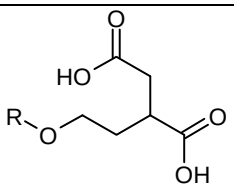
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
{Na,K,Li} [not oxy attach] **questionable!	48X			 Representative structure
Ring rx -> 2-imidazole-type / -C=N-OH	49X			 Representative structure
-C(-S-)(-N-)-C(=O)- correction	50X			
misc-O-{Na,K,Li} [coef*(1+0.5*(NUM-1))]	51X			 Representative structures
HOOC-C-(C-COOH)(C-O-) correction	52X			

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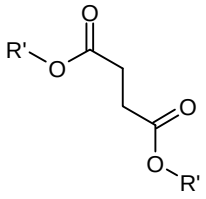
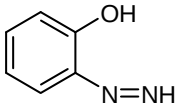
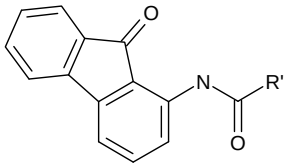
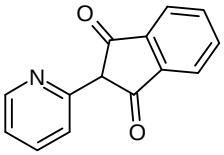
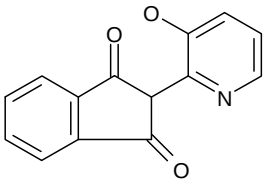
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
MOOC-C-C-COOM {M=metal} correction	53X		R ’= metal	
Ring reaction -> -OH ortho to Azo	54X			 Representative structure
Ring rx -> -NC(=O)/cyclic C(=O)->aromatic	55X		R’ cannot be H	 Representative structure
Ring rx -> nc-C(-CO-aromatic)-CO-C	56X			 Representative structure
Ring rx -> c(OH)c(n)/-C(CO)-CO(or OH) type	57X			

R = Must be an aliphatic carbon attachment

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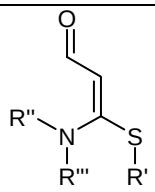
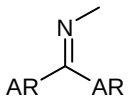
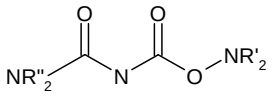
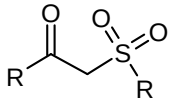
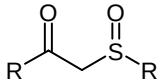
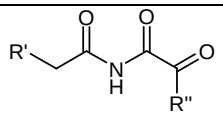
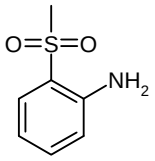
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
C(-S-)(-N-)=C-C(=O)- correction	59X		R's are undefined	
>C=N-C [di-aromatic attached imine] cor.	60X			
N-O-CO-N-CO-N- structure correction	61X		R', R" can be H	
-CO-C-SO2-aliphatic structure correction	62X			
-CO-C-S(=O)-aliphat structure correction	63X			
-C-CO-N-CO-CO- structure correction	64X		R's are undefined	
Ring rx -> amino-type ortho to -SO2-C	65X			 Representative structure

R = Must be an aliphatic carbon attachment

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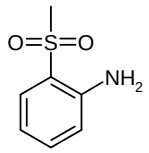
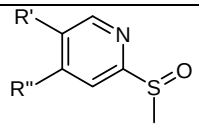
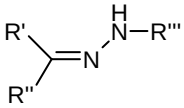
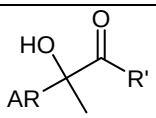
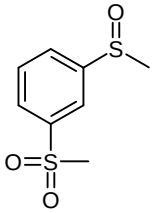
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-S(=O)-to-aromatic nitrogen correction	66X			 Representative structure
Nar Ring rx:-SO-C with di-NO2/C#N/OH/amino	67X		R’ and R’’ = NO2, C#N, OH or Amino	 Representative structure
CH2=N-N- hydrazone correction	68X			
C(-OH)(-C-)(C(=O)-{N,C})-aromatic carbon	69X		R’ = N or C	
Ring rx: -SO-C with -SO2-C	70X			 Representative structure

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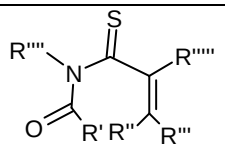
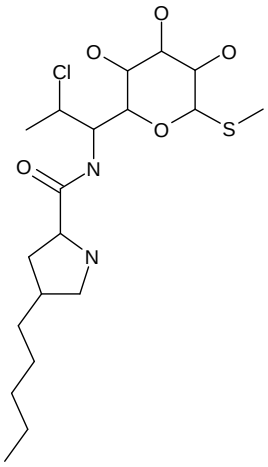
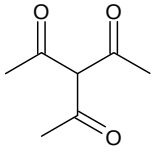
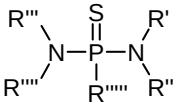
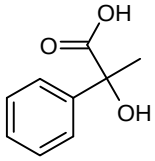
Fragments containing “C” or “X” are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-C(=O)-N-C(=S)-olefinic C correction	71X			
C(-O-)(C-OH)C-N-CO **combination effect**	72X		Representative structure = L-Threo-alpha-D-galacto-octopyryanoside (CAS No. 19096-41-4)	 Representative structure
C-CO-C(-CO-C)-CO-C structure correction	74X			
N-P(=S)-N structure correction	75X		R's are undefined	
C[-C-O][C-CO-O][C-Caromatic] correction	76X		Other substitution undefined	 Representative structure

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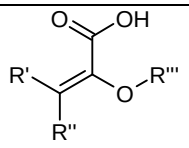
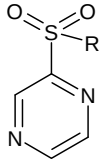
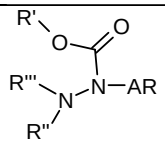
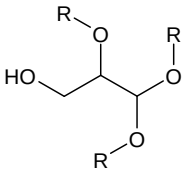
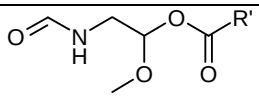
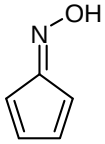
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
C=C(-COOH)-O-C structure correction	77X		R's are undefined	
Ring rx: -SO2-C with 2+ arom nitrogens(6R)	78X			 Representative structure
-N< [aromatic; nitrogen; CO-O attach] cor.	79X		R's are undefined	
HO-C-C(-O-)-C(-O-)(-O-) correction	80X			
C(=O)N-C-C(-O-C)-O-C(=O)- correction	81X			
Cyclic ketoxime(>C=N-OH) [2 olefin attach]	82X			 Representative structure

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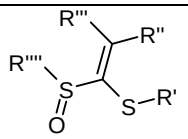
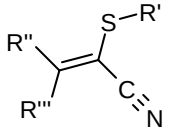
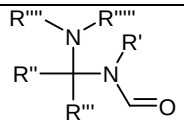
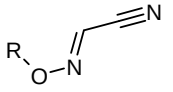
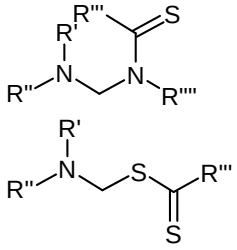
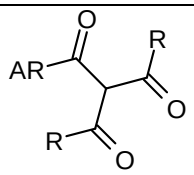
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
C=C(-S)-S(=O)- correction	83X		R's are undefined	
C=C(-S)-C#N correction	84X		R's are undefined	
-N-C-N-CHO [nitrogen/N-aldehyde]correction	85X		R's are undefined	
C(-C#N)=N-O-carbon [iminoxy] correction	86X			
-N-C-NC(=S) or -N-C-SC(=S) correction	87X		R's are undefined	
C-CO-C(-CO-C)-CO-C [aromatic attach type]	88X			

R = Must be an aliphatic carbon attachment

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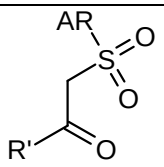
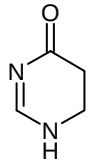
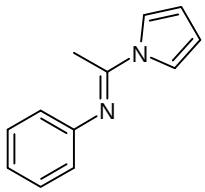
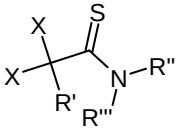
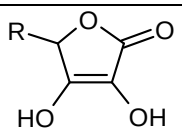
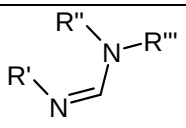
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-CO-C-SO2-aromatic structure correction	89X		R's are undefined	
-C(=O)-N=C(-amino)-N- [cyclic-type]	90X			 Representative structure
aromatic N-C(=N-aromatic)-C imine-type	91X			 Representative structure
-N-C(=S)-C(-polyhalo) correction	92X		X = Halogen	
HO-C=C(-OH)-C(=O)-O- [cyclic] correction	93X			
N-CH=N-OH [oxime-type] correction	94X		R's are undefined	

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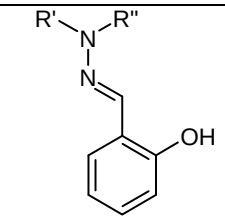
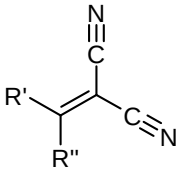
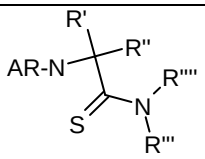
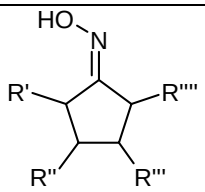
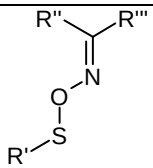
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
Ring rx: -OH ortho to -C=N-N-carbon	95X		R's are undefined	 Representative structure
=C-(C#N)-C#N [dicyano] correction	96X		R's are undefined	
Aromatic nitrogen-C-C(=S)-N< struct corr.	97X		R's are undefined	
Cyclic ketoxime(>C=N-OH) [1 olefin attach]	98X		R's are undefined	
C=N-O-sulfur(aliphatic) [iminoxy] correc	99X		R', R'', R''' undefined	

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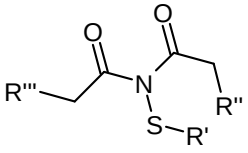
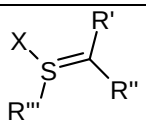
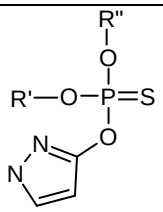
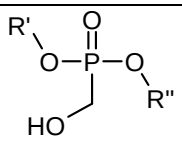
Fragments containing "C" or "X" are not used in Pass 2

Fragment	Number	Modified Name	General Comments	Structure
-S-N(-C(=O)-C)-C(=O)-C struct correction	100X		R’, R’’, R’’’ undefined	
-Sulfur(+4) charged halide-type	101X		R’, R’’, R’’’ undefined	
Ring rx: S=P(O)(O)O- / 5-mem (2 nitrogen)	102X		R’s are undefined	
O=P(-O)(-O)-C-OH correction	103X		R’, R’’ undefined	

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R’, R’’, R’’’, etc. = Defined in General Comments

Fragments containing “C” or “X” are not used in Pass 2