m/z, comp (1) (2)	Substructure, neighbor	Prop (3)	Abnd (4)	Spcf (5)
m/z 71 (38%) (6)		10% (7)	33%	
C_4H_7O, 71.0496 (8)		29 (9)	35	62
	$-(CH_2)_3-CO-$: CH_2 70%; -O- 25%, CH_2 20%	15+ (10)	32	50
	C_3H_7-CO-: CH_2 35%; -O- 25% (12)	7 (11)	60	60
C_5H_{11}, 71.0860 (13)		20	35	84
	$-CO-CH_2-CO-$, cyc-$CH_2CH(O-)CH(O-)$- (14) (15)	30	30	45
C_4H_9N, 71.0734	$-(CH_2)_4N(-)-$, $(CH_3)_2NCH_2CH_2-$, arN-C_3H_7, $H_2N(CH_2)_4-$, cycN (16) (17)	6	22	61
also C_3H_3S, 70.9959; $C_3H_7N_2$, 71.0607; $C_2H_3N_2O$, 71.0244; C_2HNO_2, 71.0006; C_2N_2F, 71.0044 (18)				
m/z, 72 (26%)		8%	19%	
C_4H_8O, 72.0575		22	16	63
	$C_2H_5-CO-CH_2-$, $CH_3-CO-CH(CH_3)-$: CH_2 75%	7	50+	85
	HO-cyc (20), CH_3O-cyc (19), $C_2H_5OCH_2CH_2-$ (21)			

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1 nominal mass of the singly charged ion in daltons

2 elemental composition

3 proportion of this entry out of the total entries of this type

4 average abundance (maximum 99)

5 specificity of this explanation for the peak vs. other probable explanations (maximum 99)

6 proportion of data-base spectra with mass 71 of ≥1% abundance

7 proportion of data-base spectra with an "important" peak at mass 71

8 for the substructure Y_L-$(CH_2)_3$-CO-Y_R, 70% of the Y_L neighbors are CH_2 groups and 25% of Y_R are ethers

9 proportion of mass 71 ions assigned as $C_4H_7O^+$

10 proportion of $C_4H_7O^+$ assignments from compounds containing $-(CH_2)_3-CO-$

11 "+" indicates that the proportion for compounds of molecular weight >236 is larger by >25% (absolute) vs. the proportion for others

12 butyryl or isobutyryl

13 no substructures indicated for hydrocarbons because of high tendency to rearrange

14 substituent at each end of substructure

15 -O-CH-CH-O-
H_2C
(cyclic)

16 most common substructures yielding $C_4H_9N^+$; data are averages for all

17 e.g., pyrollidinyl

18 less common compositions found for mass 71 peaks

19 methoxycycloalkyl

formation of the indicated ion can involve H transfer

20 to the substructure shown, and can also involve H transfer

21 from the substructure shown

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Mass Spectral Correlations

Second Edition

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Advances in Chemistry Series

M. Joan Comstock, *Series Editor*

In Mass Spectral Correlations; McLafferty, F., el al.;
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FOREWORD

ADVANCES IN CHEMISTRY SERIES was founded in 1949 by the American Chemical Society as an outlet for symposia and collections of data in special areas of topical interest that could not be accommodated in the Society's journals. It provides a medium for symposia that would otherwise be fragmented, their papers distributed among several journals or not published at all. Papers are reviewed critically according to ACS editorial standards and receive the careful attention and processing characteristic of ACS publications. Volumes in the ADVANCES IN CHEMISTRY SERIES maintain the integrity of the symposia on which they are based; however, verbatim reproductions of previously published papers are not accepted. Papers may include reports of research as well as reviews since symposia may embrace both types of presentation.

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INTRODUCTION

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INTRODUCTION

Since the First Edition of this book appeared in 1963 (1), mass spectrometry has become a widely accepted technique for molecular structure determination. Particularly impressive is the extensive use of gas chromatography/mass spectrometry resulting from its unique analytical applicability to complex mixtures. Identification of scores of components, even at the subnanogram level, is possible, but requires interpretation of the individual spectra. Literally thousands of papers have now appeared correlating mass spectra with structure for a wide variety of compounds (2), but these emphasize the spectral patterns or decomposition pathways to be expected for a specific type of molecular structure. However, in determining the structure of an unknown compound the situation is reversed; it is from the known prominent ions in the unknown spectrum that the probable structures must be ascertained. This similar problem in other fields of spectroscopy has led to charts or tables indicating the prominent functional group or other structural features which are found at particular wavelengths. Possibly the best known is the "Colthup chart" (3) of infrared spectroscopy, whose wide utility led to the original suggestion for this tabulation (4).

Extended use of the First Edition has led to a number of suggestions for improvements as well as additional correlations. A real motivation was supplied by the availability of a reference file containing mass spectra of ten times as many compounds as the original file. Correlating these spectra was only possible with computer assistance, but this had the advantage of yielding much more extensive and accurate statistical data. This compilation lists more than 3,000 structures corresponding to 1,500 elemental compositions, several times the numbers of the First Edition.

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Format of the Correlations

The tabulation lists the most probable elemental compositions and substructures corresponding to specific m/z values of singly charged ions found in electron ionization (~70 eV) mass spectra. Under each m/z value (starting at 12) are listed the most probable elemental compositions and their exact masses; for most compositions the common substructure assignments are given, and for some of these common neighboring groups are listed. Other data are the proportion of total entries represented by a specific entry and the weighted average of peak abundances for the entry. The degree of ambiguity in classifying the entry is indicated by the value for its specificity. Most entries resulted from the computer-assisted procedure described below, after which other correlations (such as peaks from skeletal rearrangements) were added using the First Edition and other tabulations (2).

Preparation of the Correlations

These data have been taken from a collection of electron-ionization mass spectra of 32,830 different compounds (5) whose structures are coded in Wiswesser Line Notation (WLN) (6). The correlations utilized a DEC PDP-11/45 computer system with GT-40 CRT display and DIVA 58 Mbyte disk system. The spectral data with the compound name, molecular formula, molecular weight, and WLN were stored on the disk as one file. To facilitate structure manipulation, the WLNs were decoded into a connection table showing the individual units and their connections to other units using a computer program similar to the one described by Hyde et al. (6). The WLN connection table preserves the linear connectivity information, and so is particularly useful in assigning specific substructures to fragment ions. The computer-assisted correlation of spectral peaks with structure involves four major steps: the selection of significant peaks from individual spectra, assignment of all possible elemental compositions, assignment of substructures, and statistical tabulation of the results. The following is a brief description of each step in the process.

Selection of Significant Peaks. The abundances of major peaks in each spectrum are first corrected for isotopic contributions estimated from the elemen-

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tal formula of the compound. Using the peak selection procedures developed for the Probability Based Matching System (7), the peaks are then assigned uniqueness (U) and abundance (A) values; these are based on the occurrence probability of peaks in the data base (5), shown in Figure 1. From each spectrum the 15 to 26 peaks (more for compounds of higher molecular weight) of highest (U + A) values are selected (7) as the "condensed spectrum" and written on a separate disk file.

Assignment of Elemental Compositions. This program uses the molecular formula as the upper bound to determine the numbers and kinds of elements possible in each peak of the condensed spectrum. Improbable compositions exceeding bonding limitations (e.g., $C_2H_8^+$) or with a much higher degree of unsaturation than the molecule (e.g., C_7H^+ from C_8H_{18}) are eliminated to generate the list of possible elemental compositions. These data are mapped according to their heteroatom content so that ions with specific heteroatom compositions are grouped together. For example, an organic compound with one oxygen and one nitrogen atom will have four groups: one with only carbon and hydrogen atoms, one with these plus an oxygen, one with these plus a nitrogen, and one with these and an oxygen and a nitrogen. This step facilitates the substructure assignment by enabling the programs to start from specific heteroatom centers in the molecule and determine all possible substructures for all ions with the same heteroatom compositions.

Assignment of Substructures. Because of the high tendency for rearrangement accompanying the formation of hydrocarbon ions (2), specific substructures are assigned only to peaks with elemental compositions containing one or more heteroatoms. Given a particular heteroatom composition, the program labels their locations in the connection table description of the structures. Starting from each identified heteroatom location, a neighbor unit connected to it is added and the elemental composition comprising the units computed. This composition is compared against the assigned composition; if it is identical (the number of hydrogen atoms is allowed to differ by ±2) the substructure is stored as a possible assignment for the composition. In addition, all the neighbor units connected to the terminals of the substructure are saved. All paths from the same heteroatom center in the molecular graph are explored to assign all possible substructures. This process is repeated starting

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from all other heteroatom centers in the structure, if any, for a particular heteroatom composition. When a composition has more than one heteroatom, all possible combinations of heteroatom centers in the structure are considered by taking them one at a time in assigning substructural possibilities.

Scoring of Substructure Probabilities. This procedure often results in multiple substructure assignments for a possible elemental composition of a peak. For heteroatom-containing ions, the probability that an assignment is correct is estimated by a scoring system whose rules are summarized in Table I. These rules, based on the most common types of ion fragmentations (2), compare the difference in number of hydrogen atoms between the assigned elemental composition and substructure, the type of ion (odd- or even-electron), the type of bond cleavage, the number of bonds cleaved, and the bond environment. The two substructures with the highest score are retained as the most probable assignments to the fragment.

For hydrocarbon ions, the compositions, but not structures, were correlated; the score for each is based on a comparison of its composition and rings-plus-double-bonds (r + db) value (2) with that of the largest hydrocarbon fragment in the structure. A score of full, half, or eighth credit is assigned if the r + db value of the proposed composition is less than that of the largest hydrocarbon fragment by ≤ 1.5, ≤ 2.5, or >2.5, respectively. Further, the neutral lost from largest hydrocarbon fragment in forming the ion is considered; if the ratio of the r + db value of the neutral to its number of carbons is 0.57-0.66, this score is halved; it is one-quarter if this ratio is >0.66. All scores are further halved if the r + db value of the fragment ion is less than 4. Only the hydrocarbon composition of highest score is retained.

Tabulation of Results. The file for each m/z value containing the results of previous steps (relative abundance, elemental composition, substructures, and neighbor units) is read to compile the following correlations: the occurrence of a significant peak at the particular m/z value as a percentage of the total number of spectra examined; the occurrence of a particular elemental composition as a percentage of the total number of significant peaks observed at that m/z value; the occurrence of a particular substructure as a percentage of the total number of iso-

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Table I. Pathway Probabilities for Heteroatom Ion Formation

H atom loss[a]	Ion type[b]	Formed by	Score
0	$OE^{+\cdot}$	Cleavage of 2 ring bonds	Full
0	$OE^{+\cdot}$	Other	Half
0	EE^{+}	α-cleavage[c]	Full
0	EE^{+}	Other	Half
±1	$OE^{+\cdot}$	Any	Full
±1	EE^{+}	Only one bond cleaved	Half
+1	EE^{+}	α-cleavage plus a second α-cleavage or cleavage of a hetero-atom bond	Full
+1	EE^{+}	Other	Half
-2	$OE^{+\cdot}$, EE^{+}	Only one bond cleaved	Quarter
±2	$OE^{+\cdot}$, EE^{+}	Other	Half

[a]Number of hydrogen atoms in the assigned composition minus the number in the possible substructure.
[b]$OE^{+\cdot}$, EE^{+}: odd- and even-electron ions.
[c]For a carbon attached to O, N, S, or P, cleavage of another bond to that carbon.

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mers observed with that elemental composition; and the occurrence of a particular neighbor at a particular terminal of a substructure as a percentage of all neighbors found at that terminal. The specificity of an elemental composition or substructure assignment is the reciprocal of the number of possible assignments stored; the specificity of an entry is then the average of these individual values.

Explanatory Notes

For each m/z value the most common elemental composition assignments of singly-charged non-metastable ions are listed. For each of these the most probable substructure assignments are illustrated, and for some common substructures the common neighboring groups are listed. In contrast to the First Edition (loc. cit.), the mechanism for fragment ion formation is now shown. The entries are ranked according to the product of their proportion and abundance values. None of the listings is exhaustive; the entries only indicate the most probable assignments. Structures in parentheses are illustrative of the preceding entry; "etc" indicates that isomeric ions are commonly formed by similar pathways. The user must remember that there is a finite possibility that the correct assignment for a peak in an individual unknown spectrum is not represented in this compilation.

The number of hydrogen atoms in the listed substructure may actually differ from that of the indicated elemental composition; the computer correlation considered that the rearrangement of as many as two hydrogen atoms to or from the substructure during its formation was possible.

Proportion: The percent value in parenthesis following the nominal m/z heading indicates the proportion of reference spectra in the data base which have a peak at this nominal mass of abundance equal to or greater than 1% (Figure 1). The value on the same line in the Proportion column is the percentage of reference spectra having a peak at this mass whose abundance and "uniqueness" were sufficiently significant to be used in the correlations (those peaks selected as significant by the Probability Based Matching algorithm - see above). For the elemental composition subheadings (those followed by an exact mass value) the entry in the Proportion column indicates the percentage of the entries of this nominal mass which were determined to have this elemental

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composition. For the substructure entries (non-underlined data in the Proportion column) the values are the percentage of the elemental composition entries which were assigned to the particular substructure shown. The percentage values following the colon after the substructure indicate the entries for a particular "neighbor" group (see below) adjacent to the substructure relative to the total number of neighbor entries at the designated location of that substructure. All these proportion values have been adjusted for multiple assignment possibilities (see Specificity below) so that the total of all entries (including those not listed here) should equal 100%.

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Neighbors: Following the colon after each substructure are listed the most abundant neighbors in descending order of proportion; the percentage values are given only if the data were statistically significant (less accurate values are rounded to the nearest 5%). The horizontal dashes in the substructure indicate bonds; those which are incompletely substituted are the positions holding neighboring groups. The symbol "(-)" indicates a free bond to an undesignated neighboring group from the immediately preceding atom not in parentheses; this symbol at the left of the substructure (or following "cyc") is a free bond to the preceeding group. The symbol "$(-)_2$" indicates two such single bonds, not a double bond, which is indicated as "=". The neighbors for each of these positions, left to right, are listed together, separated by semicolons; the proportion of a particular pair of neighbors occurring simultaneously is indicated by neighboring groups separated by a colon, listed at the end of the neighbor data. Thus "$-CH_2-CO-$: CH_2 50%, CH 25%; -O- 40%; CH_2:-O- 25%" indicates for the $-CH_2-CO-$ substructure that 50% occur as $-CH_2CH_2-CO-$, 25% as $-CH(-)CH_2-CO-$, 40% as $-CH_2-CO-O-$, and 25% as $-CH_2CH_2-CO-O-$.

Abundance: The average (weighted for Specificity, below) of the abundances of the peaks are given as a percentage value in the second column.

Specificity: A particular peak can have more than one assignment of both elemental composition and substructure identity; for example, m/z 43 in $C_3H_7-CO-CH_3$ could be $C_3H_7^+$ and/or $C_2H_3O^+$, or $C_2H_3O^+$ in $CH_3-CO-OCH=CH_2$ could be CH_3-CO^+ or $CH_2=CHO^+$. The specificity is 100% if only one assignment is made, 50% for each assignment if two are made, and so forth.

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The Specificity column shows the average percentage of the assignments for the indicated entries.

High molecular weight data (+ and - signs): The statistics were taken in two sets to ascertain the effect of molecular weight on the results. If the proportion or abundance values for the compounds of molecular weight above 236 were more than 25% (absolute) greater than those of the lower molecular weight set, a "+" follows the weighted average shown; if the value for the lower molecular weight set is more than 25% (absolute) greater than the higher, a "-" follows the weighted average value.

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Literature Cited

1. McLafferty, F. W., "Mass Spectral Correlations," Advances in Chemistry Series No. 40, American Chemical Society, Washington, DC (1963).
2. McLafferty, F. W., "Interpretation of Mass Spectra," Third Edition, University Science Books, Mill Valley, CA (1980).
3. Colthup, N. B., J. Opt. Soc. Am. (1950), 40, 397.
4. McLafferty, F. W. and Gohlke, R. S., Anal. Chem. (1959), 31, 1160.
5. Stenhagen, E., Abrahamsson, S., and F. W. McLafferty, "Registry of Mass Spectral Data," extended version on magnetic tape, Wiley, New York (1978).
6. Hyde, E., Mathews, F. W., Thomson, L. H., and Wiswesser, W. J., J. Chem. Doc. (1967), 7, 200.
7. Pesyna, G. M., Venkataraghavan, R., Dayringer, H. E., and McLafferty, F. W., Anal. Chem. (1976), 48, 1362.

Publication Date: May 5, 1982 | doi: 10.1021/ba-1982-0040.pr001

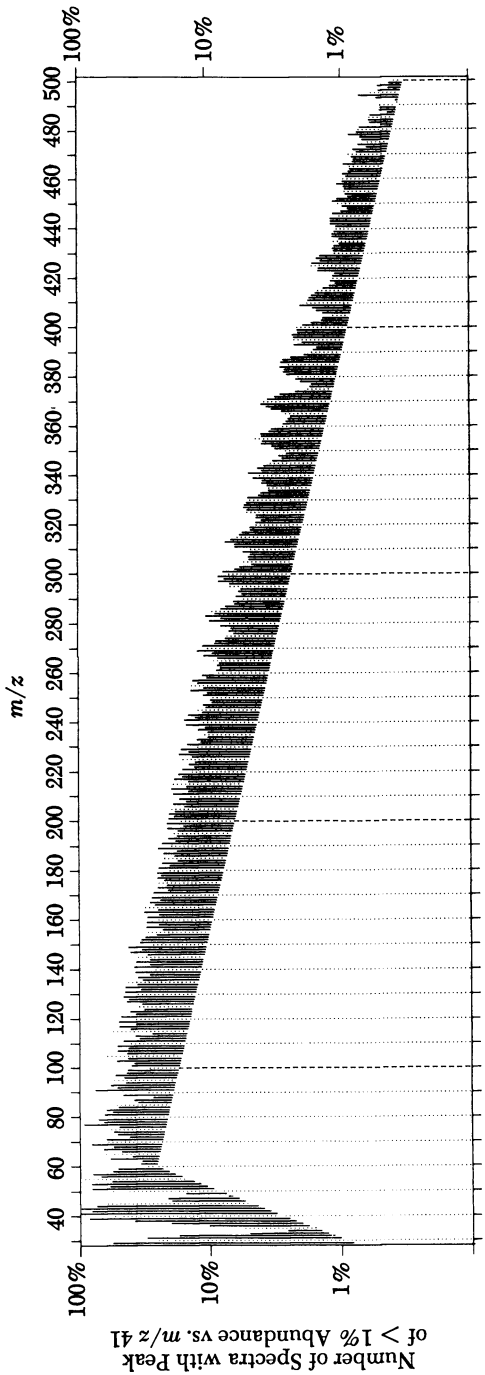

Figure 1. Mass spectra of 29,041 different compounds containing only the elements H, C, N, O, F, Si, P, S, Cl, Br, and I in natural isotopic abundances.

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MASS SPECTRAL DATA

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 12				
C, 12.0000	small molecules			
m/z 13				
CH, 13.0018	small molecules			
m/z 14				
CH_2, 14.0156				
N, 14.0031				
m/z 15				
CH_3, 15.0235	CH_3-Y*			
m/z 16				
O, 15.9949				
H_2N, 16.0187				
m/z 17				
HO, 17.0027				
H_3N, 17.0265				
m/z 18				
H_2O, 18.0106	data not meaningful, as water is ubiquitous in inlet systems			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 19				
F, 18.9984				
H_3O, 19.0184				
m/z 20-23 uncommon				
m/z 24				
C_2, 24.0000	highly unsatd hc			
B_2H_2, 24.0343				
m/z 25				
C_2H, 25.0078	highly unsatd hc			
B_2H_3, 25.0421				
m/z 26				
C_2H_2, 26.0156	ar/unsatd hc			
CN, 26.0031	NC-R, $RCHN_2$			
B_2H_4, 26.0499				
m/z 27				
C_2H_3, 27.0235	CH_2=CH-Y*, other hc			
CH_4B, 27.0406	CH_3BH-, higher boron alkyls			
B_2H_5, 27.0577				

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 28				
N_2, 28.0061	N_2 gas is a common contaminant			
C_2H_4, 28.0313	hc			
CH_2N, 28.0187	aziridines, $(CH_3)_2N$-, other amines			
CO, 27.9949	lactones, etc			
m/z 29 (34%)		2%	51%	
CHO, 29.0027		40	63	73
	$-CH_2O-$	40	85	60
C_2H_5, 29.0391		17	60	75
CH_3N, 29.0265		15	38	75
	$-CH_2N(-)-$, $-CH_2NH-$	40	40	80
m/z 30 (15%)		5%	25%	
CH_4N, 30.0343		28	33	74
	$-CH_2NH-$: CH_2 50%; C=O 30%, CH_2 30%	25	50	65
	H_2NCH_2-: CH_2 70%, CH 17%	15	70	75
CH_2O, 30.0105	CH_3O-, $-CH_2O-$, $HOCH_2-$	33	17	76
also NO, 29.9979 ($-NO_2$, $-N(-)NO$, $-O-NO$); H_2N_2, 30.0216; H_2Si, 30.9921				
m/z 31 (19%)		4%	29%	
CH_3O, 31.0184		48	32	80
	$HOCH_2-$: CH 45%, CH_2 33%, C 13%	36	35	80
	$-CH_2O-$: CH_2 47%, CH_3 42%; C=O 61%	31	33	67

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
CH_3O-:	C=O 59%	13	28	46
CF, 30.9984		11	21	82
F-C(-)$_2$-:	F, Cl	63	18	90
F-ar-, F-C(-)=		24	32	40
HNO, 31.0057		4	25	67
-O-N(-)-		55	28	46
CH_5N, 31.0421		3	18	85
CH_3NH-:	C=O 35%	40	20	75
m/z 32				
Data unreliable because oxygen is a common contaminant				
S, 31.9721; O_2, 31.9898; CH_4O, 32.0262				
m/z 33 (3%)		4%	4%	
CH_5O, 33.0340; HS, 32.9802; CH_2F, 33.0140; H_2P, 32.9894				
m/z 34 (2%)		3%	2%	
H_2S, 33.9880 (can be impurity)		50	2	99
m/z 35 (4%)		2%	4%	
Cl, 34.9688 Cl:	Y*	72	4	99
H_2NF, 35.0171		1	3	99
m/z 36 (6%)		3%	13%	
HCl, 35.9766 (can be impurity)		20	10	99

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 37 (12%)		2%	9%	
C_3H, 37.0078		85	8	99
m/z 38 (23%)		3%	17%	
C_3H_2, 38.0156	unsatd hc	58	15	89
C_2N, 38.0030	arN, ar-N(-)-, ar-NH-	22	13	66
m/z 39 (50%)		4%	37%	
C_3H_3, 39.0235	$HC{\equiv}CCH_2$-, ar, etc	57	38	96
C_2HN, 39.0108	arN, unsatd R-CN	20	24	75
m/z 40 (34%)		4%	19%	
C_3H_4, 40.0313	diunsatd/cyc hc	31	15	78
C_2O, 39.9949	ar(CO), R-CO-, etc	21	21	60
C_2H_2N, 40.0186	arN, imines, unsatd amines, etc	17	19	58
CN_2, 40.0060	arN_2	7	20	53
m/z 41 (60%)		6%	52%	
C_3H_5, 41.0391	$CH_2{=}CHCH_2$-, other hc	32	69	87
C_2HO, 41.0027	$-CH_2-CO-$, $-CH(-)-CO-$, $-C(-)_2-CO-$, ar-OH, etc	26	52	74
C_2H_3N, 41.0265	arN, $NC-CH_2$-, $-CH_2CH_2N(-)$,			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	$CH_2CH(-)NH-$	13	38	65
CHN_2, 41.0138	arN_2, $arN-NH_2$, etc	3	24	52
m/z 42 (49%)		14%	28%	
C_2H_2O, 42.0105		25	24	62
	$-CH_2-CO-$: CH_2 60%, CH_3 15%; O 40%,			
	CH_2 30%	23	32	48
	CH_3-CO-: -O- 30%, CH_2 20%, -N(-)- 15%,			
	-NH- 12%	15	15	52
	also $-CH(-)-CO-$, $CH_2CH(-)O-$, $-CH_2CH_2O-$, $=CH-CO-$			
C_3H_6, 42.0469	$CH_2=CH-CH_2-$, $cycC_3H_5-$, hc	22	22	75
C_2H_4N, 42.0343	$CH_3N=CH-$, arN, cycN,			
	aziridinyl, etc	16	31	60
CH_2N_2, 42.0216	arN_2, H_2N-arN, $CH_3N=N-$	5	35	56
CNO, 41.9979	-NH-CO-, -N(-)-CO-, HO-arN,			
	OCN-, etc	5	28	48
N_3, 42.0090	-NH-N=N-, -N(-)N=N-	1	31	69
m/z 43 (59%)		9%	72%	
C_2H_3O, 43.0184		40	78	74
	CH_3-CO-: -O- 28%, CH 19%, CH_2 13%,			
	-NH- 10%	35	88	60
	$-CH_2-CO-$: CH_2 60%, CO 21%; -O- 53%,			
	CH_2 23%	21	77	60
	$-CH(OH)CH_2-$: CH_2 67%; CH_2 78%	10	72	65
	$-CH_2CH_2O-$: CH_2 65%, CH_3 20%; CO 53%,			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
CH_2 25-%	8	68	47
$-CH_2C(-)_2O-$, $-CH(CH_3)O-$, $-CH_2OCH_2-$	12	75	70
C_3H_7, 43.0547	18	79	87
C_2H_5N, 43.0421	7	52	60
cycN, $-CH_2CH_2N(-)-$, C_2H_5NH-, $-CH_2CH(-)NH-$, $-CH(CH_3)N(-)-$, $-CH_2CH_2NH-$, $-CH_2N(CH_3)-$	52	72	52
CHNO, 43.0057 $-NH-CO-$, $-N(-)-CO-$, H_2N-CO-	5	56	61
CH_3N_2, 43.0295 $arN-NH_2$, $-N(-)N(-)CH_2-$, $-N=NCH_3$, $-N=NCH_2-$	3	53	66
also HN_3, 43.0168; C_2F, 42.9984; CP, 42.9738			
m/z 44 (45%)	10%	33%	
C_2H_4O, 44.0262	25	24	66
CH_3-CO-: -NH- 32%, -O- 20%, N 17%	23	21	58
C_2H_5O-, $HOCH_2CH_2-$, $-CH_2CH_2O-$, HO-cyc, $H-CO-CH_2-$	37	23	52
C_2H_6N, 44.0499	13	43	63
$CH_3CH(NH_2)-$, CH_3NHCH_2-: CH_2 75%	12	88	75
$-CH_2NHCH_2-$: CH_2 50%, CH 30%; CH_2:CH_2 30%	7	55	88
$(CH_3)_2N-$: -CH=, ar, C=O, -S-	6	35	50
cyc-$CH_2N(CH_3)-$, $-CH_2CH_2NH-$, $-CH_2CH(NH_2)-$, $-CH_2CH_2N(-)-$, $-CH_2N(CH_3)-$, $H_2NCH_2CH_2-$	34	30	62
CH_2NO, 44.0135	9	30	69
$-NH-CO-$: ar 30%, CH_2 20%; N 22%,			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	-NH- 17%, -O- 15%	41	25	65
	H_2N-CO-: CH_2 35%, -NH- 20%, ar 15%	22	43	79
	HO-arN, H-CO-NH-, -N(-)-CO-, ON-ar, ON-CH=	21	30	58
CO_2, 43.9898	(also from thermal decomp)	9	30	60
	HO-CO-: CH 30%, ar 25%, CH_2 25%	42	40	60
	-O-CO-: CH_3 55%; CH 28%, ar 20%, CH_2 20%	45	25	52
CH_4N_2, 44.0373		3	40	58
	-N(CH_3)N(-)-	25	50+	80
	-N(-)N(-)CH_2-	17+	35	40
	CH_3N=N-, -N-CH=N-, H_2N-$NHCH_2$-, H_2N-arN, H_2NC(-)=N-, cyc-$CH_2N(NH_2)$-	30	45-	60
also C_2HF, 44.0062; N_2O, 44.0009; CS, 43.9724				
m/z 45 (45%)		9%	30%	
C_2H_5O, 45.0340		22	36	66
	CH_3OCH_2-: CH 47%, CH_2 28%	15	59	75
	CH_3CHOH-: CH_2 62%, CH 28%, C=O 6%	8	70	70
	-CH_2OCH_2-: CH_2 76%, CH_3 15%; CH_2:CH_2 55%	12	39	56
	-CH(CH_3)O-: CH_3 50%, -O- 33%, CH_2 42%, C=O 38%	5	43	76
	-CH_2CHOH-, $HOCH_2CH_2$-, $HOC(-)_2CH_2$-, $HOCH_2CH$(-)-	18	30	63
	CH_3CH_2O-, -CH_2CH_2O-, CH_3CH(-)-O-	16	25	43
CHO_2, 44.9976		18	27	70
	-CO-O-: CH_2 40%, CH 15%, ar 15%; Si 39%+, CH_2 28%-, CH_3 25%	54+	20	58

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	HOOC-: CH_2 50%, CH 20%, ar 17%, C 8%	29-	33	68
	$-OC(-)_2O-$, $-OCH_2O-$, -OCH(-)O-	10	30	55
CHS, 44.9799		7	24	86
	arS	56	19	87
	$-SCH_2-$: CH_2 45%, CH 25%; CH_2 55%, CH 20%	23	36	52
	ar-S-	8	19	45
C_2H_7N, 45.0578	($C_2H_6N^+$ usually larger)	4	18	81
	$(CH_3)_2N-$: CH_2 30%, C=O 25%, -C= 15%	53	20	85
	$H_2NCH_2CH_2-$: CH_2 70%, NH 5%, CH 5%	13	18	76
	$H_2NCH(CH_3)-$, $-CH(NH_2)CH_2-$, CH_3CH_2NH-	25	13	85
CH_3NO, 45.0215	H_2N-CO-, -NH-CO-, ONCH-	3	22	63
C_2H_2F, 45.0140	CHF=CH-, $CH_3CF(-)-$, -CF=CHF-	1	21	72
CH_5N_2, 45.0452		1	21	65
m/z 46 (12%)		7%	9%	
NO_2, 45.9928	nitrates, ar-NO_2, R-ONO	6	34	94
CH_2O_2, 46.0054		18	5	82
C_2H_6O, 46.0418		16	7	79
CH_2S, 45.9880	$-CH_2S-$, etc	7	10	75
NS, 45.9754	S=N-	1	27	78

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 47 (13%)		8%	10%	
CH_3S, 46.9959	$HSCH_2$-, $-CH_2S$-, CH_3S-	12	9	82
CH_3O_2, 47.0133	-OCH(-)O-, HO-CO-	8	11	86
also CCl, 46.9688; C_2H_7O, 47.0496 (CH_3O-Y*-CH_3, polyalcohols/ethers); C_2H_4F, 47.0297 (CH_3CHF-); PO, 46.9687; CH_4P, 47.0051; COF, 46.9933 (F-CO-); FSi, 47.9749				
m/z 48 (4%)		6%	3%	
CH_4S, 48.0037		6	8	80
CH_3S-: CH_2 50%, CH 20%, C=O 8%		40	20	73
$-CH_2S$-: CH_2 35%, CH 12%, CH_2 40%, CH 12%		35	5	70
CHCl, 47.9766		9	3	89
H_2NO_2, 48.0084	-ONO, $-NO_2$	4	3	95
H_2NS, 47.9910		1	16	70
also CH_4O_2, 48.0211; OS, 47.9673; HOP, 47.9765				
m/z 49 (9%)		5%	6%	
C_4H, 49.0078		61	5	98
CH_2Cl, 48.9844		12	12	85
$ClCH_2$-: CH_2 35%, CH 30%, C=O 10%		45	16	67
$ClC(-)_2$-		20+	13	84
ClCH(-)-: Cl 25%, CH_3 20%, CH_2 20%		17	5	80
HOS, 48.9751	O=S(-)-: CH_2 35%, O 35%	1	3	99

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
H_2OP, 48.9843	O=P(-)$_2$-: CH_3 40%, O 15%, S 15%	1	12	99
also H_2FSi, 48.9809; NCl, 48.9718; CH_2OF, 49.0089				
m/z 50 (35%)		5%	17%	
C_4H_2, 50.0156	ar	63	16	95
C_3N, 50.0030	arN	7	17	63
CF_2, 49.9968	-CF_2- etc	5	13	89
CH_3Cl, 49.9923		1	47	78
	$ClCH_2$-: C=O 45%, -C=C- 45%	70-	57	75
m/z 51 (48%)		11%	20%	
C_4H_3, 51.0235	ar	45	18	89
C_3HN, 51.0108	arN, ar-N(-)-	21	21	68
CHF_2, 51.0046		2	36	88
	CHF_2-: CX_2 35%, C=O 30%	25	80	82
	-CF_2-	50	23	78
also FS, 50.9708; HFP, 50.9800				
m/z 52 (35%)		5%	19%	
C_3H_2N, 52.0186	arN, ar-NH_2	20	15	51
C_3O, 51.9949	ar-CO-, ar(C=O), ar-O-, etc	19	18	63
C_4H_4, 52.0313	ar, unsatd hc	19	13	69
C_2N_2, 52.0060	arN_2	11	20	51

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 53 (49%)		8%	20%	
C_4H_5, 53.0391	polyunsatd hc	31	18	88
C_3HO, 53.0027	ar(C=O), arO, ar-O-, cyc-CO-, cyc-O-	22	21	67
C_3H_3N, 53.0265	arN, ar-NH_2, cycN, etc	11	18	58
C_2HN_2, 53.0138	arN_2, $cycN_2$, etc	4	18	48
m/z 54 (34%)		5%	24%	
C_4H_6, 54.0469		34	25	81
C_3H_2O, 54.0105	ar(CO), R-CO-, etc	20	23	60
C_3H_4N, 54.0343	NC-CH_2CH_2-, ar(NH), imines (-CH_2CH_2C(=NH)-)	11	24	51
$C_2H_2N_2$, 54.0216	arN_2, etc	5	18	46
also C_2NO, 53.9979 (arNO); CN_3, 54.0090 (arN_3)				
m/z 55 (55%)		10%	46%	
C_4H_7, 55.0547	H_2C=C(CH_3)CH_2-, CH_3CH=$CHCH_2$-, other hc	34	55	88
C_3H_3O, 55.0184		29	48	74
	cyc-CH_2CH_2-CO-: CH_2 50%, CH 15%; CH_2 40%, -O- 30%	38	56	72
	CH_2=CH-CO-, -CH=CH-CO-	6	53	68
	also -CH=$CHCH_2O$-, $HOCH_2C{\equiv}C$-, ar-OCH_3, etc			
C_3H_5N, 55.0421	substd/cyc amines,			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	$NC-CH_2CH_2-$, $CN-CH_2CH_2-$, arN	8	31	61
C_2HNO, 55.0057	$-CH_2-CO-N(-)-$, $-CH_2N(-)-CO-$, $OCN-CH_2-$, $-NHCH(-)-CO-$, etc	3	28	45
$C_2H_3N_2$, 55.0295	arN_2, $arN-NHCH_3$, cyc/substd diamines	2	26	52
also CHN_3, 55.0168 (arN_3)				
m/z 56 (42%)		11%	28%	
C_4H_8, 56.0626	$H-C_4H_8-Y^*$, $H-C_4H_8-R-Y^*$, $H-R-CH_2C(CH_3)=CH_2$ etc, hc	30	31	78
C_3H_4O, 56.0262	substd/cyc ketones/ethers, etc	24	26	62
C_3H_6N, 56.0499	cyc/subst amines ($cyc-CH_2CH_2CH(NH_2)-$)	11	29	57
C_2H_2NO, 56.0135	cyc/subst amides ($-N(CH_3)-CO-$), $OCN-CH_2-$, ar-NO, etc	6	27	53
C_2O_2, 55.9898	$-CH_2O-CO-$, $-CH_2-CO-O-$, $-CO-CO-$, etc	4	24	42
also $C_2H_4N_2$, 56.0373 (arN_2, $C_2H_5N(-)N(-)-$, etc); CN_2O, 56.0009; CH_2N_3, 56.0246 (arN_3)				
m/z 57 (48%)		11%	43%	
C_3H_5O, 57.0340		27	40	64
	$-CH_2CH_2OCH_2-$: CH_2 68%, OH 23%; CH_2 72%, CH 18%	8	68	85
	$-CH_2CH_2-CO-$: CH_2 35%, -O- 20%; CH_2 30%,			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
-O- 20%	13	35	50
C_2H_5-CO-: CH_2 33%, -O- 21%	7	76	57
$-CH_2CH_2CH(OH)-$ (cycloalkanols),			
$-CH(CH_2OH)CH_2-$, cycO	10	60	80
$-(CH_2)_3O-$, $CH_3CH(-)-CO-$	13	25	50
C_4H_9, 57.0704	24	55	85
C_2HO_2, 56.9976	8	36	53
$-CH_2O-CO-$: CH_2 35%, CH_3 27%; CH 30%	38	33	50
$-CH_2-CO-O$: CH_2 45%, CH_3 18%; CH_3 47%	27	35	48
-CO-CO-	6	50	60
$-C(-)_2O-CO-$, cyc-CH(OH)-CO-,			
$-C(-)_2-CO-O-$, cyc-CH(-COOH)-	10	65	45
C_3H_7N, 57.0577 $-(CH_2)_3N(-)-$,			
$-CH_2CH_2N(CH_3)-$, $CH_3N=CHCH_2-$, $-(CH_2)_3NH-$,			
$-CH_2CH_2N(-)CH_2-$, $-C(CH_3)_2N(-)-$	8	27	60
C_2H_3NO, 57.0214	5	23	55
also $C_2H_5N_2$, 57.0451; CHN_2O, 57.0087; CH_3N_3, 57.0325; C_2H_2P, 56.9894			
m/z 58 (34%)	6%	32%	
C_3H_8N, 58.0656	16	57	74
$(CH_3)_2NCH_2-$: CH_2 65%, CH 20%	31	95	86
$-CH_2N(C_2H_5)-$: CH_3 50%; C=O 60%	8	40	73
cyc-$CH_2N(CH_3)CH_2-$: CH_2:CH_2 50%	6	63+	70
other cycN	12	38	55
$C_2H_5NHCH_2-$, $C_2H_5CH(NH_2)-$, $(CH_3)_2C(NH_2)-$, $CH_3NHCH(CH_3)-$	7	80	70
C_3H_6O, 58.0418	25	28	68

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	CH_3-CO-CH_2-: CH_2 55%, C=O 25%, CH 10%	10	47+	75
	-CH_2-CO-CH_2-	6	55	94
	HO-cyc (cycloalkanols)	12	30	58
	$CH_3OCH_2CH_2$-, HO$(CH_2)_3$-, -CH_2CH_2-CO-, C_3H_7O-	11	35	55
$C_2H_2O_2$, 58.0054	CH_3O-CO-, -CH_2-CO-O-	9	23	55
C_2H_4NO, 58.0292	CH_3NH-CO-, -N(CH_3)-CO-	7	23	62
CH_2N_2O, 58.0165	-O-arN_2, HO-arN_2, -NH-CO-N(-)-	2	25	61
also C_2H_2S, 57.9880; $C_2H_6N_2$, 58.0529; CNO_2, 57.9928; CNS, 57.9754				
m/z 59 (31%)		13%	23%	
$C_2H_3O_2$, 59.0133		27	22	77
	CH_3O-CO-: CH_2 50%, CH 20%, ar 9%	60	23	75
	-CO-OCH_2-: CH_2 41%, CH 24%, ar 13%; CH_3 40%, CH_2 35%, CH 15%	9	17	60
	-CH(OH)CH_2O-: CH_3 70%; CH_2 50%, ar 25%	2	38	65
C_3H_7O, 59.0496		16	28	70
	-$C(CH_3)_2O$-	8	45	60
	$C_2H_5OCH_2$-: CH_2 30%, C=O 25%, CH 25%	5	45	55
	$C_2H_5CH(OH)$-: CH_2 60%, CH 15%	4	75	65
	$(CH_3)_2C(OH)$-: CH_2 55%, CH 20%	4	70	85
	-$CH_2CH_2OCH_2$-, -$CH_2CH_2CH_2O$-, -$CH(CH_3)OCH_2$-	15	20	55
C_2H_5NO, 59.0370		4	24	69
	H_2N-CO-CH_2: CH_2 80%, CH 15%	12	84	99
	CH_3-CO-NH-: CH 40%, CH_2 30%	15	19	55

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
HO-N=CHCH$_2$-	2	90	99
cyc-C(=N-OH)-CH$_2$-	4	25	99
cyc-CH(NH$_2$)-CH(OH)-	3	50	99
cyc-N(CH$_3$)-CO-, CH$_3$O-N=CH-, -CH$_2$NH-CO-	17	10	75
C$_2$H$_3$S, 58.9959	3	20	75
cyc-S-CH(CH$_3$)-: C; -O-, S	23+	42+	90
-CH(CH$_3$)S-	15	11	80
-CH=CH-S-	4	23-	65
-CH$_2$CH$_2$S-, -CH$_2$SCH$_2$-, CH$_3$SCH(-)-	20	12	80
C$_3$H$_9$N, 59.0734 (C$_3$H$_8$N usually larger)	3	7	77
H$_2$NCH$_2$CH$_2$CH$_2$-: CH$_2$ 80%	16	9	76
(CH$_3$)$_2$NCH$_2$-, C(CH$_3$)$_2$NH-, -CH$_2$N(C$_2$H$_5$)-, (CH$_3$)$_2$CHNH-	30	10	70
CHNO$_2$, 59.0006 O$_2$NCH$_2$-, -O-CO-N(-)-, -O-CO-NH-	1	20	60
C$_3$H$_4$F, 59.0297 cyc-CHFCH$_2$CH$_2$-, cyc-CH$_2$CHFCH$_2$-	1	20	80
m/z 60 (19%)	6%	20%	
C$_2$H$_4$O$_2$, 60.0211	27	22	79
HO-CO-CH$_2$-: CH$_2$ 60%, CH 12%	18	45	76
-O-CO-CH$_2$-: CH$_2$:CH$_2$ 25%	11	22	74
cyc-CH(OH)CH(OH)-	10	35	76
C$_3$H$_8$O, 60.0575 cyc-CH(CH$_3$)CH$_2$O-, cyc-CH$_2$CH(OH)CH$_2$-, etc	11	16	62
C$_2$H$_6$NO, 60.0448	6	28	72
CH$_3$-CO-NH-: CH$_2$ 40%, CH 40%	35	24	77
HOCH$_2$CH(NH$_2$)-: CH$_2$ 40%, C=O 40%	5	55	75

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	$-CH(CH_2OH)NH-$: C=O; C=O	3	70	55
	$(CH_3)_2N-O-$	4	55	95
C_2H_4S, 60.0037		5	20	74
	$-CH_2CH_2S-$: CH_2; CH_2	25	38	73
CHOP, 59.9765 arP		1	20+	70
m/z 61 (21%)		5%	16%	
$C_2H_5O_2$, 61.0289		21	16	80
	$CH_3-CO-O-$: CH_2 65%, CH 30%	17	13	60
	$HO-CO-CH_2-$, CH_3O-CO-: CH_2, CH	20	21	73
	cyc-CH(OH)CH(OH)-	13	18	85
	also $CH_3OCH(-)O-$, $-OC(-)(CH_3)O-$			
C_5H, 61.0078		24	10	90
C_2H_5S, 61.0115		9	28	80
	CH_3SCH_2-: CH_2 80%	12	75	80
	$-CH_2SCH_2-$	35+	35	80
	$CH_3CH(SH)-$, $-CH(CH_3)S-$, $-CH_2CH_2S-$, C_2H_5S-	25	25	55
C_2H_2Cl, 60.9844	$-CH_2CHCl-$, ClCH=CH-, Cl-cyc	5	19	93
C_2H_6P, 61.0207	$(CH_3)_2P-$ (abnd 100%), etc	1	70	64
also CH_2OP, 60.9843 (-P-CO-); CH_5N_2O, 61.0400 ($H_2N-CO-NH-$); C_2H_2OF, 61.0089 (FCH_2-CO-); C_3H_6F, 61.0453 ($(CH_3)_2CF-$)				
m/z 62 (20%)		5%	10%	
C_5H_2, 62.0156		53	9	94

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_4N, 62.0030	arN, ar-N(-)-	11	11	75
C_2H_3Cl, 61.9923		4	16	90
C_2H_7P, 62.0285	$(CH_3)_2P$-: -CO-; C_2H_5PH-	1	50	72
C_2H_6S, 62.0193	C_2H_5S-	2	13	79
CH_4NO_2, 62.0241	H_2N-CO-O-	1	20	96
C_2F_2, 61.9968		2	7	83
$C_2H_6O_2$, 62.0367		1	10	84
also CH_2OS, 61.9829; CH_4NS, 62.0067; H_2N_2S, 61.9940; CHNCl, 61.9796 (Cl-arN)				
m/z 63 (35%)		8%	18%	
C_5H_3, 63.0235		56	16	88
C_4HN, 63.0108	arN	10	16	72
C_2H_4Cl, 63.0001		3	34	79
	$ClCH_2CH_2$-: O 35%, C=O 15%, CH_2 15%	38	42	65
	$ClCH(CH_3)$-: C=O 30%, CH_2 20%, CH 20%	11	54	43
COCl, 62.9637	Cl-CO-: O 40%, CH_2 15%	1	41	97
CH_3OS, 62.9908	$-CH_2S(=O)$-, CH_3OS-, $CH_3S(=O)$-	1	36	74
C_2HF_2, 63.0046	CHF=CF-, -CF(-)CF(-)-	1	27	90
CFS, 62.9708	cyc-CF(-)S- etc	1	26	99
also CH_3O_3, 63.0082	$(-C(-O-)_3$, $O=C(-O-)_2)$			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 64 (24%)		7%	12%	
C_5H_4, 64.0313	ar	46	9	82
C_4H_2N, 64.0186	arN, ar-N(-)-, etc	10	11	50
C_3N_2, 64.0060	arN_2	5	12	43
C_4O, 63.9949	ar(C=O), ar-CO-, arO	5	9	50
$C_2H_2F_2$, 64.0124	$-CH_2CF_2-$, etc	2	26	84
S_2, 63.9448	disulfides	1	33	81
CH_4OS, 63.9986	CH_3O-S-	1	23	79
SO_2, 63.9622	(could be impurity)	1	21	99
also C_2H_5Cl, 64.0079; HO_2P, 63.9714; CHFS, 63.9786; CNF_2, 63.9998				
m/z 65 (43%)		8%	19%	
C_5H_5, 65.0391	unsatd hc, ar	34	17	77
C_4H_3N, 65.0265	arN, ar-NH_2, ar-NH-	17	19	58
C_4HO, 65.0027	ar-CO-, ar(C=O), arO, ar-O-, ar-OH	13	18	58
C_3HN_2, 65.0138	arN_2, ar-N=N-, arN-N(-)-, ar-CH=N-NH-	4	23	48
H_2O_2P, 64.9792	$O=P(OH)(-R)_2$, $O=P(O-)_3$, etc	1	27	70
$C_2H_3F_2$, 65.0203	CH_3CF_2-, -CHF-CF(-)-,			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
ar-F_2, etc	1	44-	75
also HO_2S, 64.9700; H_2ClSi, 64.9513; $CHNF_2$, 65.0076			
m/z 66 (29%)	7%	13%	
C_5H_6, 66.0469 ar, CH_3-pyridines	26	11	84
C_4H_2O, 66.0105 ar-CO-, ar-O-, ar-OH etc	17	10	62
C_4H_4N, 66.0343 arN (pyrrolyl-, N-R-pyrrolyl)	12	11	50
$C_3H_2N_2$, 66.0216 arN_2 (pyrazolyl), ar-CH=N-NH-	6	12	42
C_3NO, 65.9979 ar(NH-CO-), arN-OH, arON etc	4	11	47
H_2S_2, 65.9604 -S-S-	1	39	55
C_2N_3, 66.0090 arN_3 etc	1	13	35
CFCl, 65.9672 -CClF-, ClFC=	1	11	99
m/z 67 (40%)	11%	34%	
C_5H_7, 67.0547 polyunsatd/cyc hc	43	38	95
C_4H_3O, 67.0184 substd ketones, furyl, ar(C-O), etc	17	35	73
C_4H_5N, 67.0421 pyrrolyl, cyc imines, substd amines, etc	7	22	58
$C_3H_3N_2$, 67.0295 arN_2 (imidazoyl, etc), cyc hydrazone	3	20	42
C_3HNO, 67.0057 ar(-NH-CO-), arN-OH, arN-CO-, etc	2	20	42

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
also C_2N_3, 67.0168 (arN_3); CHFCl, 66.9750 (FClCH-); $CHOF_2$, 66.9995 ($-CF_2O-$); ClS, 66.9412; OFS, 66.9657				
m/z 68 (33%)		6%	27%	
C_5H_8, 68.0626	cyclopentyl, cyc/unsatd hc	37	28	84
C_4H_4O, 68.0262	subst/cyc -CO-/-O-	20	29	59
C_4H_6N, 68.0499	subst/cyc amines/imines, nitriles	8	23	50
C_3H_2NO, 68.0135	arN-OH, ar(NO) (isoxazolyl), ar-O-, ar(N-CO), $NC-CH_2-CO-$	4	24	42
$C_3H_4N_2$, 68.0373	arN_2 (pyrimidinyl, etc), $arN-NH_2$, etc	4	17	49
C_3O_2, 67.9898	ar-CO-O-, ar(C=O)-O-, substd/unsatd -CO-O-, etc	3	23	46
also C_2N_2O, 68.0009 (NarNH-CO-, etc); $C_2H_2N_3$, 68.0246 (arN_3, arN_2-NH-); C_4HF, 68.0062; CN_4, 68.0120 (arN_4)				
m/z 69 (49%)		12%	35%	
C_5H_9, 69.0704	$CH_2=CHC(CH_3)_2-$, cyclopentyl, other unsatd/cyc hc	28	35	90
C_4H_5O, 69.0340		20	33	66
	$cyc-CH(CH_3)CH_2-CO-$, $cyc-CH_2CH(CH_3)-CO-$, $cyc-CH_2CH_2CH(-CO-)-$, $cyc-(CH_2)_3-CO-$, etc	25+	35	72
	$CH_3CH=CH-CO-$, other C_3H_5-CO-, $CH_3-CO-CH=CH-$	5	55	60

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	also $CH_3C{\equiv}CCH(OH)$-, cyc/unsatd/subst -O-/OH			
C_3HO_2, 68.9976	unsatd/cyc/ar -CO-/-O-/-OH (-CH=CH-CO-, etc)	7	33	56
CF_3, 68.9952	CF_3-, polyfluoro/haloalkanes	3	63	73
C_3H_3NO, 69.0214	-CH=CH-CO-NH-, HO-arN, OarN, ar-NO, etc	4	21	48
C_4H_7N, 69.0577	$NC(CH_2)_3$-, arN, substd/cyc amines	4	19	57
	also $C_3H_5N_2$, 69.0451 (unsatd/ar amines/imines/azo); C_2HN_2O, 69.0087; $C_2H_3N_3$, 69.0325 (arN_3); C_3HS, 68.9802 (arS); CHN_4, 69.0198 (arN_4)			
m/z 70 (37%)		8%	28%	
C_5H_{10}, 70.0782	H-C_5H_{10}-Y*, H-C_5H_{10}-R-Y*, H-R-$CH(CH_3)C(CH_3)=CH_2$ etc, hc	25	27	82
C_4H_6O, 70.0418	cyc/substd ketones/-O-/-OH	21	27	59
C_4H_8N, 70.0656	cyc/subst amines (pyrrolidinyl, $CH_3N=CHCH_2CH_2$-, aziridinyl-CH_2-, cyc-$CH_2CH(CH_3)CH(NH_2)$-, etc)	12	30	58
$C_3H_2O_2$, 70.0054	-CH_2O-CO-CH_2-, -$CH_2CH(-)$-CO-O-, 4-pyrones, -CH_2CH_2O-CO-, -CO-CH_2-CO-, HO-ar(C=O), etc	6	25	43
C_3H_4NO, 70.0292	-CH_2CH_2-CO-NH-, cyc-$N(C_2H_5)$-CO-, $CH_3C(CN)(OH)$-, H_2N-CO-CH=CH-, NCO-$CH(CH_3)$-, OCN-C_2H_4-, -$CH(CH_3)$-CO-NH-, etc	4	27	44

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_3H_6N_2$, 70.0529	C_3H_7-N=N-, arN_2, $cycN_2$, etc	3	28	46
also $C_2H_2N_2O$, 70.0165 (HO-arN_2); C_2NO_2, 69.9928 (-CO-NH-CO-); $C_2H_4N_3$, 70.0403				
m/z 71 (38%)		10%	33%	
C_4H_7O, 71.0496		29	35	62
	$-(CH_2)_3-CO-$: CH_2 70%; -O- 25%, CH_2 20%	15+	32	50
	C_3H_7-CO-: CH_2 35%; -O- 25%	7	60	60
	$-(CH_2)_4O-$, tetrahydrofuryl-, 1,2-epoxybutyl-, $-(CH_2)_3CH(OH)-$, $-(CH_2)_3OCH_2-$, $-CH_2CH_2CH(CH_2OH)-$, $-CH_2CH_2OCH_2CH_2-$	22	30	75
C_5H_{11}, 71.0860		20	35	84
$C_3H_3O_2$, 71.0133		11	30	49
	$-CH_2CH_2-CO-O-$, $-CH_2-CO-OCH_2-$	30	35	50
	$-CH_2CH_2O-CO-$, $-CH(CH_3)-CO-O-$, $-CO-CH_2-CO-$, cyc-$CH_2CH(O-)CH(O-)-$	30	30	45
C_4H_9N, 71.0734	$-(CH_2)_4N(-)-$, $(CH_3)_2NCH_2CH_2-$, $arN-C_3H_7$, $H_2N(CH_2)_4-$, $cycN$	6	22	61
C_3H_5NO, 71.0370		3	21	40
also C_3H_3S, 70.9959; $C_3H_7N_2$, 71.0607; $C_2H_3N_2O$, 71.0244; C_2HNO_2, 71.0006; C_2N_2F, 71.0044				
m/z, 72 (26%)		8%	19%	
C_4H_8O, 72.0575		22	16	63
	$C_2H_5-CO-CH_2-$, $CH_3-CO-CH(CH_3)-$: CH_2 75%	7	50+	85
	HO-cyc, CH_3O-cyc, $C_2H_5OCH_2CH_2-$, $CH_3OCH_2CH_2CH_2-$	10	25	50

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$C_3H_4O_2$, 72.0211	C_2H_5O-CO-, CH_3O-CO-CH_2-	13	15	56
C_3H_6NO, 72.0448		8	33	60
	$(CH_3)_2N$-CO-: -NH-, ar, -N(-)-	16	75	81
	CH_3-CO-$NHCH_2$-: CH_2 70%	18	25	80
	C_2H_5NH-CO-: -NH-, C	3	53	56
	H_2N-CO-CH_2CH_2-: CH_2, CH	3	33	50
also HON=$CHCH_2CH_2$-				
$C_4H_{10}N$, 72.0812		10	26	64
	$C_3H_7NHCH_2$-, $C_3H_7CH(NH_2)$-, $(CH_3)_2NCH(CH_3)$-, etc	20	65	65
	-$CH(C_3H_7)NH$-, -$CH_2N(C_3H_7)$-, etc	5	85	90
	$(C_2H_5)_2N$-, C_3H_7NHCH(-)-, C_4H_9NH-, C_4H_9N(-)-	10	33	55
$C_2H_2NO_2$, 72.0084	-CH(-CO-OH)NH-, -N(CH_3)-CO-O-, -$CH(NH_2)$-CO-O-, -CH_2O-CO-NH	3	21	50
$C_2H_4N_2O$, 72.0322	-N(CH_3)-CO-N(-)-	2	24	55
also $C_3H_8N_2$, 72.0686; C_2H_2NS, 71.9910 ($SCNCH_2$-); C_3H_5P, 72.0129				
m/z 73 (32%)		14%	38+%	
$C_3H_5O_2$, 73.0289		21	30	67
	-CH_2CH_2-CO-O-: CH_2 60%; Si 50%	7	60+	46
	HO-CO-CH_2CH_2-: CH_2 55%, CH 16%, S 12%	7	48	66
	C_2H_5O-CO-: CH_2 55%, CH 18%	12	19	73
	CH_3O-CO-CH_2- (also m/z 74): CH_2 37%, CH 34%	5	26	41
	CH_3-CO-OCH_2-: CH_2 50%, CH 30%	7	20+	65
	-$CH_2OCH_2CH_2O$-, cyc-CH_2CH_2OCH(-)-O-, -$CH_2CH(OH)CH(OH)$-	10	45	75

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_4H_9O, 73.0653		12	34	63
	$-(CH_2)_4O-$: CH_2 75%; Si 50%	13+	34	57
	$C_2H_5CH(OCH_3)-$: CH_2 80%	5	80+	90
	$CH_3(CH_2)_3O-$: C=O 80%	6	19	40
	C_2H_5-CO- (also m/z 72): CH_2 80%	5	20+	94
	$C_2H_5CH_2CH(OH)-$, $(CH_3)_2CH(OH)-$, $-(CH_2)_3OCH_2-$, $(CH_3)_2CHOCH_2-$, $C_2H_5CH_2OCH_2-$, $C_2H_5C(CH_3)(OH)-$, cyc-$C(CH_3)(C_2H_5)O-$	20	40	65
C_3H_7NO, 73.0526		4	35	70
	$CH_3-CO-NH-CH_2-$ (also m/z 72): CH_2 85%	19	34	85
	$-CH_2CH=NOCH_3$, $CH_3C(=NOCH_3)-$			
	$-CH_2CH(=NOCH_3)-$: CH_2; C=O	9	80	99
	$-CH_2CH_2C(=N-OH)-$: CH_2 50%; CH_2 50%	5	75	99
	$CH_3-CO-N(CH_3)-$	3	55-	55
	$C_2H_5-CO-NH-$	2	30	99
	$(CH_3)_2C=N-O-$, $-CH(OCH_3)-CH(-NH-)-$, $-CH_2-CO-NH-CH_2-$, $CH_3NHCH_2CH(-)-O-$	10	80	80
$C_2H_3NO_2$, 73.0163		3	35	68
	$-NHCH_2-CO-O-$: C=O; Si	13	80	76
	$-NHCH(-)-CO-O-$, $-N(-)-CH_2-CO-O-$	15+	50+	80
	$HO-CO-CH(NH_2)-$: CH_2	10	14	80
	$ar-CH=C(NO_2)-$	5	10	59
C_2HO_3, 72.9925		2	28	70
	$-OCH_2-CO-O-$: CH_2, ar, Si; Si, CH_2	10	73	53
	$-OCH(-)-CO-O-$, $-OC(-)_2-CO-O-$, $HOCH(-)-CO-O-$	22	55+	50
	$-CO-CO-O-$: ar, $-O-$; Si, CH_2	5	50-	60
C_3H_9Si, 73.0373	$(CH_3)_3Si-$, $-CH_2Si(CH_3)_2-$	1	44	80
$C_2H_5N_2O$, 73.0400		1	23	70

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	O=N-N(C_2H_5)-: CH_2	16-	45-	80
also $C_3H_9N_2$, 73.0764	((CH_3)$_2$N-N(CH_3)-)			
m/z 74 (34%)		5%	27%	
$C_3H_6O_2$, 74.0367		30	43	84
	CH_3O-CO-CH_2-: CH_2 70%, CH 13%	51+	63	84
	CH_3O-CO-CH=: =CH-	3	31	95
	HO-CO-CH(CH_3)-: CH_2 70%, -NH- 20%	2	60	75
	cyc-CH(OH)CH(OCH_3)-	2	50	45
C_6H_2, 74.0156		23	13	92
$C_2H_4NO_2$, 74.0241		5	20	81
	HO-CO-CH(NH_2)-: CH_2 75%, CH 20%	30	40	77
	-CH_2O-CO-N(-)-	2	70	58
$C_4H_{10}O$, 74.0731	CH_3O-cyc, cycO, HO-cyc	5	18	69
$C_2H_2O_3$, 74.0003	cyc-OCH(O-)CH(OH)-, -OC(OCH_3)O-, -OC(-OCH_2-)O-	3	23	55
C_3H_6S, 74.0193	cyc-SC(CH_3)$_2$-, -(CH_2)$_3$S-, -$CH_2CH_2SCH_2$-	3	39	64
C_3H_8NO, 74.0605	-CH(OH)CH($NHCH_3$)-, -CH(OH)CH(CH_3)NH-, CH_3CH(OH)CH(NH_2)-	2	46	60
also C_5N, 74.0030 (arN); C_3F_2, 73.9968 (F_2-ar); $CH_2N_2O_2$, 74.0114 (ONNH-CO-); C_2H_4NS, 74.0067 (arNS); CH_2N_2S, 73.9940 (H_2N-arNS, -S-arN_2); C_3H_3Cl, 73.9923 (Cl-ar)				
m/z 75 (36%)		8%	30%	
C_6H_3, 75.0235		30	20	88
$C_3H_7O_2$, 75.0445		13	30	80

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m/z, comp — Substructure, neighbor	Prop	Abnd	Spcf
CH_3O-CO-CH_2-: CH_2 65%, CH 15%	24+	22	93
$(CH_3O)_2$CH-: CH_2 70%, CH 20%	6	75-	80
C_2H_5-CO-O: CH_2 70%, CH 20%	6	29	74
$HOC_2H_4OCH_2$-, $HOC_2H_4CH(OH)$-, $CH_3OCH_2CH(OH)$ etc	9	22	85
CH_3-CO-OCH_2- also $C_2H_5OCH(-)O$-	2	42	70
C_5HN, 75.0108 arN	9	19	74
C_2H_7OSi, 75.0165 -$Si(CH_3)_2$-O-, $(CH_3)_2Si(OH)$-	3	75	96
C_3H_4Cl, 75.0001	4	31	71
C_3H_7S, 75.0271	3	42	66
$C_2H_5SCH_2$-, $CH_3SCH(CH_3)$- also C_3H_7S-	20	95	55
$C_2H_5NO_2$, 75.0319 HO-CO-$CH(NH_2)$-, -$NHCH_2$-CO-O-, NH_2-CO-OCH_2-	3	28	78
$C_2H_3O_3$, 75.0082 cyc-CH(-O-)-CO-O-, -OCH-CO-O-	2	27	55

also C_2H_3OS, 74.9908; C_3HF_2, 75.0046 (ar-F_2); C_3H_9NO, 75.0683($CH_3CH(OH)CH(NH_2)$-); C_2OCl, 74.9637; $C_2H_7N_2O$, 75.0556 (CH_3-CO-NH-NH-); C_4H_8F, 75.0610

m/z 76 (30%)	10%	13%	
C_6H_4, 76.0313	38	10	86
C_5H_2N, 76.0186 arN	10	13	61
C_5O, 75.9949 ar(CO), arO	6	21	63

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_4N_2, 76.0060	arN_2	4	16	49
C_3H_5Cl, 76.0079	ClC_3H_6-	2	19	82
C_3H_8S, 76.0350	C_3H_7S-	2	12	72
CS_2, 75.9448	arS_2, -S-C(=S)-, pyrolysis product	1	21	90
$C_2H_4O_3$, 76.0160	CH_3O-CO-O-, HO-CO-CH(OH)-, -CH(OH)-CO-O	1	12	55
also $C_3H_2F_2$, 76.0124; $H_2N_3O_2$, 76.0144				
m/z 77 (55%)		18%	29%	
C_6H_5, 77.0391	phenyl-Y, Y-phenyl-Y'	41	27	86
C_5H_3N, 77.0265	arN, ar-N(-)-	10	30	56
C_5HO, 77.0027	ar-CO-, etc	6	26	60
C_4HN_2, 77.0138	arN_2, arN-N(-)-, etc	2	26	40
$C_3H_3F_2$, 77.0203	$-C_2H_4CF_2$-, CF_2=$CHCH_2$-, etc	1	57	80
C_3H_6Cl, 77.0157	C_2H_5CHCl-, etc	1	26	71
CH_2O_2P, 76.9792	$CH_3OP(=O)(-)$-, etc	1	24	70
m/z 78 (39%)		7%	18%	
C_6H_6, 78.0469	phenyl	42	15	83
C_5H_4N, 78.0343	pyridyl-, other arN, ar-NH-	11	21	51

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_5H_2O, 78.0105	ar-CO-, arO	7	22	56
$C_4H_2N_2$, 78.0216	arN_2, ar-N=N-	5	20	43
C_4NO, 77.9979	arN-CO-, ar-NO, arNO, etc	2	19	36
CH_2S_2, 77.9604	$-CH_2-S-S-$, $-SCH_2S-$, SCH(-)S-	1	44	88
also C_3N_3, 78.0090; C_2OF_2, 77.9917 ($-CF_2-CO-$)				
m/z 79 (43%)		11%	30%	
C_6H_7, 79.0547		32	34	89
C_5H_3O, 79.0184	ar-O-, $ar-CH_2OH$, subst cyc(C=O), etc	14	27	66
C_5H_5N, 79.0421	arN, subst cyc-NH-, etc	10	21	55
$C_4H_3N_2$, 79.0295	arN_2, etc	3	20	38
C_4HNO, 79.0057	arN-CO-, arNO, ar-NO, etc	2	20	34
CH_4O_2P, 78.9949	$CH_3OP(=O)(-)_2$, $CH_3P(=O)(-)O-$	1	34	85
CH_3O_2S, 78.9857	$CH_3OS(=O)-$, $-CH_2OS(=O)-$	1	42	78
Br, 78.9183		2	14	93
also CH_3S_2, 78.9683 (CH_3-S-S-); C_2H_4OCl, 78.9950 ($ClCH_2OCH_2-$, $ClCH_2CH(OH)-$); C_2HFCl, 78.9750; O_3P, 78.9585 (-OPH(=O)O-, -OP(-)(=O)O-)				
m/z 80 (28%)		8%	17%	
C_6H_8, 80.0626	cyclohexenes, etc	29	18	91

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_5H_4O, 80.0262	arO, etc	13	16	61
C_5H_6N, 80.0499	arN (pyridyl, pyrrolyl-CH_2-), ar-NH_2, subst cycloalkanones	9	15	57
C_4H_2NO, 80.0135	arN-OH, ar(N-CO-), ar-NO, etc	4	15	44
$C_4H_4N_2$, 80.0373	arN_2, arN-NH_2	4	14	44
$C_3H_2N_3$, 80.0246	arN_3, arN_2-NH-	2	15	36
C_4O_2, 79.9898	ar-COOH, -CO-C≡C-CO-, ar-CO-O-	2	14	42
HBr, 79.9261	(can be impurity)	2	9	96
C_3N_2O, 80.0009	arN_2-O-, arN_2(C=O), etc	1	12	42
also CH_4O_2S, 79.9935 ($CH_3OS(=O)$-); HO_3P, 79.9663 (-OPH(=O)O-); CH_4S_2, 79.9761 (CH_3S-S-)				
m/z 81 (39%)		6%	36%	
C_6H_9, 81.0704	polyisoprenes, polyunsatd/cyc hc	33	46	92
C_5H_5O, 81.0340		19	40	67
	furyl-CH_2-: -O- 49%, -S- 28%, CH_2 11%	3	94-	55
	unsatd/subst hc-CO-	25	40	75
	ar-OH, subst/unsatd/cyc hc-OH	10	25	70
C_5H_7N, 81.0577	arN (CH_3-pyrrolyl etc), unsatd/cyc/substd imine/amine, ar amine	6	23	60

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_4H_3NO, 81.0214	Nar(C=O), NarO, unsatd methoxime, unsatd oxyamine, etc	3	25	48
C_4HO_2, 80.9976	subst/cyc-O-CO-, arO_2, -O-ar-O-, etc	3	13	47
also $C_4H_5N_2$, 81.0451 (arN_2, etc); C_3HN_2O, 81.0087; $C_3H_3N_3$, 81.0325 (arN_3, etc); C_2F_3, 80.9952; H_2O_3P, 80.9741 (-OP(=O)O-, etc); C_4HS, 80.9802 (arS); C_5H_2F 81.0140 (ar-F); $C_2H_3OF_2$ (CH_3OCF_2-); C_2H_3FCl, 80.9907 ($-CH_2CFCl-$, $-CH_2CHFCl$)				
m/z 82 (33%)		7%	29%	
C_6H_{10}, 82.0782	cyclohexyl, subst/unsatd hc	30	32	84
C_5H_6O, 82.0148	furyl-CH_2-, ketones, cyc-OH, cycO, etc	17	29	57
C_5H_8N, 82.0656	pyrrolizidinyl, cyc/substd/unsatd amines/imines, NC-C_4H_8-	7	29	53
C_4H_4NO, 82.0292	unsatd ketoamines ($CH_3NHC(-)=CH-CO-$), arNO (CH_3-isoxazolyl), arN(C=O), subst/cyc aminoethers, etc	4	25	46
$C_4H_2O_2$, 82.0054	$ar(C=O)_2$, HO-CO-C≡CCH_2-, ar-CO-OH, unsatd-CO-O-	4	23	49
$C_4H_6N_2$, 82.0529	arN_2 (pyrimidinyl-CH_2-), unsatd amines	2	27	49
also $C_3H_2N_2O$, 82.0165; $C_3H_4N_3$, 82.0403 (triazinyl);				

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_3NO_2, 81.9928; C_4H_2S, 81.9880; CCl_2, 81.9376; $C_2H_2N_4$, 82.0276 (arN_4); C_2HF_3, 82.0030; CF_2S, 81.9692				
m/z 83 (38%)		10%	34%	
C_6H_{11}, 83.0860	cyclohexyl, $CH_3CH=CHC(CH_3)_2$- etc	29	33	89
C_5H_7O, 83.0496	cyc ketones (-$CH_2C(CH_3)_2$-CO- etc), lactones, cyc/subst/unsatd -O-/-OH/-CO- (($CH_3)_2C$=CH-CO-)	22	29	69
$C_4H_3O_2$, 83.0133	diketones, ketoesters, ar-CO-OCH_3, subst/cyc -O-/-OH/-CO- (HO-furyl-)	6	28	50
C_5H_9N, 83.0734	$NC(CH_2)_4$-, cyc/substd amines (piperidyl)	4	29	57
C_4H_5NO, 83.0370	unsatd/cyc -NH-/-NH_2/C=O/-OH/-O-/-CH=N-OH (cyc-NH-CO-CH=$C(CH_3)$-, -CH=$C(CH_3)$NH-CO-, H_2N-CO-$C(CH_3)$=CH-)	4	24	50
$CHCl_2$, 82.9454	$CHCl_2$, -CCl_2-	2	54	88
$C_4H_7N_2$, 83.0607	-CH=CHC(CH_3)=NNH- etc	2	37	57

also $C_3H_3N_2O$, 83.0244 ($arN_2(C=O)$, arN_2-OH, etc); C_3HNO_2, 83.0006; $C_3H_5N_3$, 83.0481; C_5H_4F, 83.0297; C_4H_3S, 82.9959 (thiophenyl-); $C_2H_2F_3$, 83.0108; FO_2S, 82.9603 (F-S(=O)O-)

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m/z, comp — Substructure, neighbor	Prop	Abnd	Spcf
m/z 84 (81%)	12%	19%	
C_5H_8O, 84.0575 cyc/subst ketones (2-R-cyclopentanones), cyc/substd/unsatd -O-/-OH	21	18	57
C_6H_{12}, 84.0938 H-C_6H_{12}-Y*, H-C_6H_{12}-R-Y*, etc	23	14	77
$C_4H_4O_2$, 84.0211 beta diketones, CH_3-4-pyrones, substd/cyc -O-CO-, HO-CO-	10	19	50
$C_5H_{10}N$, 84.0812 cyc/subst amines (2-piperidynl, N-CH_3-pyrrolidinyl, cyc-$CH_2CH_2CH(NHC_2H_5)$- etc)	7	25	54
C_4H_6NO, 84.0448 subst/cyc amides (-$CH_2CH(NH$-CO-CH_3, -$CH_2CH_2CH_2$-CO-NH-), -$CH_2CH_2CH(NH_2)$-CO-, -$CH(NH_2)CH_2CH_2$-CO-, OCN-C_3H_6, etc	6	22	45
$C_4H_8N_2$, 84.0686 C_4H_9-N=N-, -$(CH_2)_3C(-)$=N-NH-, -N(-)$(CH_2)_3N(-)$-, arN_2 etc	2	28	49
$C_3H_4N_2O$, 84.0322 HO-arN, -CH(-)NH-CO-NHCH(-)-, H_2N-CO-arN, $N_2ar(C=O)$, etc	2	23	48
$C_3H_2NO_2$, 84.0084 -N(-CO-CH_3)-CO-, -$C(NH_2)$=CH-CO-O-, HO-CO-arN, ar-NO_2	2	19	42
also C_3O_3, 83.9847 (-O-CO-CH_2-CO-)			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 85 (33%)		14%	20%	
C_5H_9O, 85.0653		22	20	66
	$-(CH_2)_4-CO-$: CH_2 70%; -O- 27%	17+	25	63
	C_4H_9-CO-: CH_2 35%; $-CH(-)_2$ 30%	6	40	65
	cycO (tetrahydropyryl-), $-(CH_2)_5O-$, $-(CH_2)_4CH(-)O-$, $-(CH_2)_3OCH_2CH_2-$, $C_3H_7C(-)(CH_2OH)-$, $-(CH_2)_4OCH_2-$	16	32	65
C_6H_{13}, 85.1017		19	17	85
$C_4H_5O_2$, 85.0289		15	19	58
	$CH_3-CO-CH_2-CO-$	4	60	82
	gamma-lactones	2	90	81
	$-(CH_2)_3-CO-O-$, $-CH_2CH_2-CO-OCH_2-$, $-CH_2CH_2O-CO-CH_2-$, 2-(methylethylene ketal)-, $-CH_2CH(O-)CH_2CH(O-)-$, $-O(CH_2)_3-CO-$	20	20	60
$C_5H_{11}N$, 85.0890	$(CH_3)_2N(CH_2)_3-$, $-(CH_2)_5N(-)-$, arN-C_4H_9, $C_4H_9CH=N-$	4	12	63
also C_4H_7NO, 85.0526; $C_3H_3NO_2$, 85.0163; C_3HO_3, 84.9925; $CClF_2$, 84.9656; $C_4H_9N_2$, 85.0764 ($cycN_2$, $(CH_3)_2N-N=CH-CH_2-$); C_4H_5S, 85.0115 (cycS)				
m/z 86 (22%)		6%	18%	
$C_5H_{12}N$, 86.0968		8	36	62
	$(C_2H_5)_2NCH_2-$, $C_4H_9NHCH_2-$, $C_3H_7N(CH_3)CH_2-$, $C_4H_9CH(NH_2)-$, $(CH_3)_2NC(CH_3)_2-$, etc	15	75	70
	$-CH_2N(C_4H_9)-$, $-CH(CH_3)N(CH_3)CH(CH_3)-$, $-CH_2CH_2N(C_2H_5)CH_2-$	8	55	60

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_4H_6O_2$, 86.0367	1-dioxolanyl(-)-cyc-CH_2-	14	16	54
$C_5H_{10}O$, 86.0731		13	17	53
	C_3H_7-CO-CH_2-, C_2H_5-CO-CH(CH_3)-,			
	Y*-$C_5H_{10}O$-	7	20	63
C_4H_8NO, 86.0605	H_2N-CO-CH_2CH(CH_3)-,			
	CH_3NH-cyc-OH	8	24	57
$C_3H_4NO_2$, 86.0241	-CH(-CO-OCH_3)-NH-,			
	-CH(NH_2)-CO-OCH_2-	4	27	44
also $C_3H_6N_2O$, 86.0478 (-NH-CO-NH-); $C_3H_2O_3$, 86.0003; $C_4H_{10}N_2$, 86.0842 ((CH_3)$_2$NN=CH-CH_2-); $C_2H_4N_3O$, 86.0351 (H_2N-CO-NH-N=CH-)				
m/z 87 (23%)		7%	21%	
$C_4H_7O_2$, 87.0445		25	26	62
	CH_3O-CO-CH_2CH_2-: CH_2 55%, -CH= 15%	12	34	35
	CH_3O-CO-CH(-)-CH_2-: CH_2 70%; CH_2 55%	5	50	58
	CH_3O-CO-CH=CH-: CH_2	3	53-	99
	-O-CO(CH_2)$_3$-, HO-CO-(CH_2)$_3$-,			
	-CO-O(CH_2)$_3$-, -CH_2O-CO-(CH_2)$_2$-,			
	-CO-(CH_2)$_3$-O-, CH_3-dioxolanyl-,			
	CH_3CO-O(CH_2)$_2$-	2	23	55
$C_5H_{11}O$, 87.0809		11	22	60
	HOC(C_2H_5)$_2$-, HOC(C_3H_7)(CH_3)-,			
	HOCH(C_4H_9)-	11	50-	80
	$C_4H_9OCH_2$-, $C_2H_5OC(CH_3)_2$-,			
	$CH_3OCH(C_3H_7)$-	7	20-	70
	-(CH_2)$_5$-O-, -(CH_2)$_4$$OCH_2$-, -($CH_2$)$_3$O($CH_2$)$_2$-,			
	-CH(OH)(CH_2)$_4$-, -CH_2C(OH)(-)C_3H_6-	16	35	40

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
C_4H_9NO, 87.0683	4	25	74
$CH_3ON{=}C(CH_3)CH_2$-: CH_2	8	90	99
$(CH_3)_2N$-CO-CH_2-	2	99+	99
CH_3CO-NH$(CH_2)_2$-, C_3H_7CO-NH-, CH_3CO-N(CH_3)-CH_2-	28	18	85
$C_3H_3O_3$, 87.0082 -CO-CH_2CO-O-, -CO-CH(-)-CO-O-, -CO-O-CH_2CH_2O-, -CH(O-)-CH(OH)-CH(O-)-, -CH(OH)CH_2O-CO-, -CH(C_2H_5)O-CO-, -$(CH)_3$(-)(OH)(O-)-O-	4	19	56
C_4H_7S, 87.0271	3	20	83
Thiacyclopentyl-: CH_2	5	99	75
other thiacycloalkanes (cycS)	75	20	70
$C_3H_5NO_2$, 87.0319	3	20	62
-$CH_2C(NH_2)$(COOH)-	7	37-	99
CH_3O-CO-CH(NH_2)-	3	59-	99
CH_3CO-N(-)-CO-, -CH(OH)CH_2N(-)-CO-, -NHCH(-)-CO-OCH_2-, CH_3O-CO-CH_2-NH-, (arN)-CO-OCH_2-, -C(=NOH)-C(OH)(-)-	30	25	75
also $C_5H_{13}N$, 87.1047 ($(C_2H_5)_2NCH_2$-); C_4H_4Cl, 87.0001; $C_3H_7N_2O$, 87.0556; $C_4H_{11}Si$, 0530 ($C_2H_5Si(CH_3)_2$-)			
m/z 88 (17%)	5%	22%	
$C_4H_8O_2$, 88.0524	22	29	66
CH_3O-CO-CH(CH_3)-: CH_2 70%	13	80	92
C_2H_5O-CO-CH_2-: CH_2 55%, C=O 15%, CH 15%	16	52	78
HO-CO-CH(C_2H_5)-, HO-CO-C$(CH_3)_2$-	4	30	75
cyc-CH(OCH_3)CH(OCH_3)-	2	56	22
also $C_2H_5OC(-)(CH_3)O$-			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
C_7H_4, 88.0131 ext/substd ar	16	10	84
$C_3H_6NO_2$, 88.0397	6	26	78
-CH(-CO-OCH_3)-NH-: CH_2 60%, C=O 70%	31	32	80
CH_3O-CO-CH_2NH-: C=O 65%, Si, 15%	9	25	80
also CH_3O-CO-CH(NH_2)-			
$C_3H_4O_3$, 88.0160	4	24	48
-CH(O-)CH(OCH_3)O-	9	67	33
also C_4H_5Cl, 88.0079; $C_5H_{12}O$, 88.0887 (CH_3O-cyc); C_6H_2N, 88.0186 (arN); $C_4H_{10}NO$, 88.0661 ($CH_3OCH_2NHCH(CH_3)$-); C_4H_8S, 88.0350 (-$CH(CH_3)CH_2SCH_2$-); $C_3H_8N_2O$, 88.0635			
m/z 89 (28%)	11%	15%	
C_7H_5, 89.0391 ext-arY, unsatd-ar	36	12	83
C_6H_3N, 89.0265 arN	9	12	61
$C_4H_9O_2$, 89.0602	7	17	78
C_3H_7-CO-O-: CH_2 85%	10	32	74
also $C_3H_7OCH(-)O$-			
$C_3H_5O_3$, 89.0238 CH_3-CO-CO-O-	3	25	67
C_6HO, 89.0027 arO, ar-CO-	5	13	65
C_4H_9S, 89.0428 $C_3H_7SCH_2$-, $C_2H_5SCH(CH_3)$-	2	28	61
$C_3H_7NO_2$, 89.0475 HO-CO-$CH(NH_2)CH_2$-, CH_3O-CO-CH_2NH-, HO-CO-$C(CH_3)(NH_2)$-	2	14	76
C_3H_9OSi, 89.0322 -$CH_2OSi(CH_3)_2$-	1	25	99
also C_3H_5OS, 89.0064 (1,3-oxathiolanyl); C_4H_6Cl,			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
89.0157 ($ClCH{=}C(CH_3)CH_2$-); C_5HN_2, 89.0138 (arN_2)				
m/z 90 (19%)		7%	14%	
C_7H_6, 90.0469		33	12	83
C_6H_4N, 90.0343	arN, ar-NH-	14	11	62
C_6H_2O, 90.0105	ar(CO), arO, ar-O-	7	13	56
$C_5H_2N_2$, 90.0216	arN_2	4	16	43
$C_3H_6O_3$, 90.0316		2	23	76
	CH_3O-CO-CH(OH)-: CH, CH_2	25	70	87
	also C_2H_5O-CO-O-			
$C_3H_8NO_2$, 90.0554	CH_3O-CO-CH_2NH-	1	22	80
also C_4H_7Cl, 90.0235 (C_4H_8Cl-); $C_4H_{10}S$, 90.0506 (C_4H_9S-); C_5NO, 89.9979; $C_4H_{10}O_2$, 90.0680; C_3H_6OS, 90.0142; C_4N_3, 90.0090 (arN_2-N(-)-, arN_3)				
m/z 91 (46%)		11%	38%	
C_7H_7, 91.0547	phenyl-CH_2-Y, phenyl-C(-Y)$_n$, CH_3-phenyl-Y_n, etc	39	44	82
C_6H_5N, 91.0421	cycN-ar, ar-NH-, arN	10	30	58
C_6H_3O, 91.0184	ar-CO-, arO, etc	10	28	56
$C_5H_3N_2$, 91.0295	arN_2, ar-N=N-, etc	2	36	40
C_4H_8Cl, 91.0314		1	46	70
	$Cl(CH_2)_4$-: n-C_nH_{2n+1}	40	40	65
	$C_2H_5CCl(CH_3)$-	8	72	75

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_5HNO, 91.0057	ar-NO, cycN(C=O), arN(C=O), etc	1	25	37
also C_3H_4OCl, 90.9950 (ClC_2H_4-CO-); C_2H_5NOS, 91.0094; $CHNS_2$, 90.9556 (-C(=S)NH-); $C_3H_7O_3$, 91.0394 ($C_2H_5OC(-)(-O-)_2$)				
m/z 92 (31%)		11%	15%	
C_7H_8, 92.0626	phenyl-CH_2- etc	32	13	85
C_6H_4O, 92.0262	arO, ar(C=O), ar-O-, ar-OH	12	13	55
C_6H_6N, 92.0499	pyridyl-CH_2-, ar-NH_2, ar-NH-	8	14	52
$C_5H_4N_2$, 92.0373	arN_2, etc	4	16	43
C_5H_2NO, 92.0135	ar-NO, arN-CO-, etc	3	12	38
also $C_4H_2N_3$, 92.0246; C_4N_2O, 92.0009; C_5O_2, 91.9898; CHBr, 91.9261; $C_3H_8O_3$, 92.0473 ($HOCH_2CH(OH)CH(OH)$-)				
m/z 93 (35%)		8%	34%	
C_7H_9, 93.0704	terpenes, cyclohexenyl-, polyunsatd cyc hc	24	41	89
C_6H_5O, 93.0340	phenyl-O-, HO-phenyl- ar-CO-, ar-O-, subst/cyc(C=O), etc	15	26	66
C_6H_7N, 93.0577	pyridyl-CH_2-, phenyl-NH-, ar-amines, cyc-NH-, CH_3-pyridyl-	8	35	62
$C_5H_5N_2$, 93.0451	CH_3-pyrazinyl-, R_2N-pyridyl-, arN_2, ar-N=N-, arN-NH_2	3	26	46

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_5H_3NO, 93.0214	imidazoyl, arN-CO-, cyclopentadienyl-NO, ar-NO, arN-OH	3	22	45
C_5HO_2, 92.9976	ar-$(O-)_2$, arO-CO-, etc	3	27	42
$C_4H_3N_3$, 93.0325	arN_3, etc	2	22	37
C_4HN_2O, 93.0078	$arN_2(C=O)$, ar-NH-CO-NH-	2	36	41
C_3F_3, 92.9952	unsatd, perhalocarbon	2	22	73
C_3H_6OCl, 93.0106	$ClC_2H_4OCH_2$-, $ClCH_2C(OH)(CH_3)$-, etc	1	50	65
CH_2Br, 92.9339	$BrCH_2$-, cyc-Br	1	24	84
also CH_2O_3P, 92.9741 ($CH_3OP(=O)(-)O-$); C_2H_6ClSi, 93.9922 ($(CH_3)_2SiCl$-)				
m/z 94 (27%)		8%	19%	
C_7H_{10}, 94.0782	polyunsatd/cyc hc	22	17	91
C_6H_6O, 94.0418		19	22	65
	C_6H_5O-: CH_2 55%, C=O 15%	14	56	72
	also ar-OH, $ar-OCH_3$, substd alkanones, cyc-CO-O-, etc			
C_6H_8N, 94.0656	subst amines, imines, etc	7	19	57
C_5H_4NO, 94.0292	pyrrolyl-CO-, HO-arN-, etc	4	17	48
$C_5H_2O_2$, 94.0054	ar(C=O)-CO-, subst esters, etc	4	14	44
$C_5H_6N_2$, 94.0529	arN_2 (CH_3-pyrazinyl-) subst/unsatd $cycN_2$	3	14	44

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
also $C_4H_2N_2O$, 94.0165 ($C_3H_2N_2$-CO-); $C_4H_4N_3$, 94.0403 (ext-arN_3); $C_3H_2N_4$, 94.0276 (ext-arN_4); C_2Cl_2, 93.9376; $C_2H_6S_2$, 93.9917 (C_2H_5S-S-)				
m/z 95 (34%)		17%	26%	
C_7H_{11}, 95.0860	polyunsatd/cyc hc	26	25	92
C_6H_7O, 95.0496	ar or cyc/subst/unsatd oxygen cpds	16	25	67
$C_5H_3O_2$, 95.0133	furyl-CO-, ar(-O-CO-), subst/cyc -CO-OCH_3, etc	5	23	55
C_6H_9N, 95.0734	cyc imine, nitriles, cyc/unsatd amine	3	18	56
C_5H_5NO, 95.0370	pyridyl-O-, ar(N-CO-), subst/cyc-NH-CO-, ar-NO	3	16	48
$C_5H_7N_2$, 95.0607	arN_2, cyc imine	2	24	51
$C_4H_3N_2O$, 95.0244	imidazole-CO-, arN_2-CO-, arN_2-OH, etc	2	20	48
C_4HNO_2, 95.0006	ar$N(CO)_2$, -CO-ar-NH-CO-	1	14	42
also $C_4H_5N_3$, 95.0481 (arN_2-NH_2); C_3HN_3O, 95.0117; C_2HCl_2, 94.9454; $C_3H_3N_4$, 95.0355; CH_4O_3P, 94.9898 ($CH_3OP(=O)O$-); C_6H_4F, 95.0297 (ar-F)				
m/z 96 (28%)		9%	19%	
C_7H_{12}, 96.0938	substd/cyc/unsatd hc	23	19	81
C_6H_8O, 96.0575	R-CO-, substd/cyc ketones, cyc-O-, etc	19	18	60

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_6H_{10}N$, 96.0812	quinolizidinyl, substd/cyc amines, NC-C_5H_{10}-	7	22	58
$C_5H_4O_2$, 96.0211	unsatd esters, etc	5	13	47

also C_5H_6NO, 96.0448; $C_5H_8N_2$, 96.0686 (arN-NH-, etc), $C_4H_2NO_2$, 96.0084 (NHar$(C=O)_2$, etc); $C_4H_4N_2O$, 96.0322 (arN_2-OH etc); $C_4H_6N_3$, 96.0559 (C_2H_5-arN_3); $C_2H_2Cl_2$, 95.9532; $C_3H_4N_4$, 96.0433

m/z 97 (32%)		15%	21%	
C_7H_{13}, 97.1017	CH_3-cyclohexyl etc	23	21	88
C_6H_9O, 97.0653	cyc ketones (cyclopentyl-CO-, cyc-$CH_2CH(C_3H_7)$-CO- etc), epoxycyclohexyl, C_3H_7CH=CH-CO- etc, cyc/subst/unsatd -O-/-OH	21	19	71
$C_5H_5O_2$, 97.0289	cyc/unsatd/subst $C=O/(C=O)_2$/-O-/$(-O-)_2$/-OC(-)$_2$O-(cyclopentadione)	7	21	52
$C_6H_{11}N$, 97.0890	NC$(CH_2)_5$-, CH_3-pyrrolizidinyl-, subst/cyc/unsatd amines	4	18	62
C_5H_7NO, 97.0526	CH_3-oxazoles, cyc/unsatd -N(-)-/-NH-/-N=/C=O/-OH/-O-	3	15	45

also $C_4H_3NO_2$, 97.0163 (-CH=CH-CO-N(-)-CO-, ar-NO_2); $C_4H_5N_2O$, 97.0400 (carbamyl); C_4HO_3, 96.9925; $C_5H_9N_2$, 97.0764; C_5H_5S, 97.0115 (thiophenyl-CH_2-, ar-SCH_3), $C_2H_3Cl_2$, 96.9611; C_2OF_3, 96.9901 (-C_2HF_3-O-, CF_3-CO-)

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m/z, comp — Substructure, neighbor	Prop	Abnd	Spcf
m/z 98 (26%)	10%	19%	
C_7H_{14}, 98.1094 H-C_7H_{14}-Y*, H-C_7H_{14}-R-Y*	22	12	79
$C_6H_{10}O$, 98.0731 2-R-cyclohexanone, R-$(CH_2)_5$-CO-Y, C_2H_5CH=CH-CO-CH_2-, cyc/subst ketones/-O-/-OH, etc	18	20	60
$C_5H_6O_2$, 98.0367 furyl-CH(OH)-, 2,3-$(CH_3)_2$-4-pyrones, substd/cyc esters etc	11	19	53
$C_6H_{12}N$, 98.0968 cyc/substd amines, (piperidine-CH_2-), C_4H_9-CH=NCH_2- etc	6	29	60
C_5H_8NO, 98.0605 cyc amides (valerolactams etc), $(CH_3)_2$NCH=CH-CO-, -$(CH_2)_3$CH(NH_2)-CO-, OCN-C_4H_8-	5	25	50
also $C_4H_4NO_2$, 98.0241 (H_2N-CO-CH=CH-CO-); $C_5H_{10}N_2$, 98.0842 (C_5H_{11}-N=N-); $C_4H_2O_3$, 98.0003 (HO-CO-CH=CH-CO-, HO-CO-ar-CO-); $C_4H_6N_2O$, 98.0478; C_4H_4NS, 98.0065 (thiazole-CH_2-)			
m/z 99 (26%)	9%	17%	
$C_6H_{11}O$, 99.0809	15	15	62
C_5H_{11}-CO-: CH_2 20%, -CH= 18%, -NH- 16%	9	40	65
-$(CH_2)_5$-CO-, -$(CH_2)_5$CH(OH)-, -$(CH_2)_4$CH(OH)CH(-)-, -CH_2CH(C_4H_9)O-	13	20	60
$C_5H_7O_2$, 99.0445 delta- and CH_3-gamma-lactones, -$(CH_2)_4$-CO-O-, CH_3-CO-C_2H_4-CO-, 1-dioxolanyl(-)-cyc-CH_2CH_2-	14	18	60

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_7H_{15}, 99.1173	satd hc	19	10	87
also C_5H_9NO, 99.0319	(OCN-$(CH_2)_4$-); $C_4H_5NO_2$, 99.0319 (arN-CO-OC_2H_5); $C_6H_{13}N$, 99.1047; $C_4H_3O_3$, 99.0082; $C_5H_{11}N_2$, 99.0920 (cycN_2); C_5H_7S, 99.0271 (cycS); C_4H_5NS, 99.0145 (thiazole-CH_2-)			
m/z 100 (18%)		6%	18%	
$C_5H_{10}NO$, 100.0761	$(C_2H_5)_2$N-CO-, -$(CH_2)_4$-NH-CO-, CH_3O-N=C(CH_3)CH(CH_3)-	8	24	62
$C_5H_8O_2$, 100.0524	CH_3O-CO-CH=CH-CH_2-, (CH_3-CO-)$_2$CH-	13	15	59
$C_6H_{14}N$, 100.1125	C_5H_{11}CH(NH_2)-, cyc-CH_2CH(CH_3)C(CH_3)$_2$-N(-)-, -CH_2CH(CH_3)-N(C_2H_5)-CH_2-	7	17	68
$C_6H_{12}O$, 100.0887	C_2H_5-CO-C(CH_3)$_2$-, C_4H_9O-ar	9	11	64
$C_4H_6NO_2$, 100.0397	-CH_2C(=NOCH_3)-CO-, -CH=CHCH_2NH-CO-O-	5	16	54
$C_4H_4O_3$, 100.0160	substd trioxane, HO-CO-C(-)$_2$$CH_2$-CO-	5	15	50
C_8H_4, 100.0313	ar/unsatd hc	7	10	71
$C_5H_{12}N_2$, 100.0998	cyc-CH_2CH_2N($CH_2CH_2CH_2$NH-)-, -CH_2CH_2N(-)(CH_2)$_3$NH-	3	20	59
also $C_4H_8N_2O$, 100.0635	(-NH(CH_2)$_3$N(-)-CO-); $C_3H_4N_2O_2$, 100.0033 (HO-CO-CH(-)NH-CO-); C_2F_4, 99.9936			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 101 (25%)		8%	22%	
$C_5H_9O_2$, 101.0602	C_2H_5O-CO-CH_2CH_2-, C_4H_9O-CO-, cyc-$CH_2CH_2C(OCH_3)_2$-, C_2H_5-dioxolanyl-, -$(CH_2)_3$-CO-O-CH_2-	19	21	60
C_8H_5, 101.0391	-styrenyl-Y_2*, ext-ar	12	11	75
$C_6H_{13}O$, 101.0966	$C_5H_{11}CH(OH)$-, $C_4H_9C(CH_3)(OH)$-, $CH_3CH(-)(CH_2)_3C(-)(OH)$-, cyc-$(CH_2)_3CH(-CH_2CH_2O-)$-	8	13	68
$C_4H_5O_3$, 101.0238	CH_3O-CO-CH_2-CO-, -$O(CH_2)_3$-CO-O-, -CH_2-CO-OCH_2CH_2O-, CH_3O-CO-CH(-)-CO-, cyc-$CH_2CH(-O-)CH(-O-)$-O-	7	29	57
C_7H_3N, 101.0265	ext-arN, NC-phenyl-	6	9	67
$C_4H_7NO_2$, 101.0475	HO-CO-$CH(NH_2)CH_2CH_2$-Y, CH_3O-CO-CH=CH-N(-)-, C_2H_5O-CO-arN	3	18	62
also $C_5H_{11}NO$, 101.0839 (CH_3-CO-NH$(CH_2)_3$-, $(CH_3)_2N(CH_2)_3O$-); C_5H_9S, 101.0428 (CH_3-thiacyclopentyl-); C_4H_5OS, 101.0064 (-CH_2CH_2S-CO-CH_2-); $CFCl_2$, 100.9360; C_4H_6OP, 101.0156 (-phospholane-O-); C_4H_7NS, 101.0299 (SCN-$(CH_2)_3$-); $C_3H_7N_3O$, 101.0586 (H_2N-CO-NH-N=CH-CH_2-)			
m/z 102 (23%)		7%	15%	
C_7H_{12}, 96.0938	phenyl-C(-)=CH-, ext-ar, quinolines	23	12	86

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_7H_4N, 102.0343	ext-arN, phenyl-arN	11	12	61
$C_5H_{10}O_2$, 102.0680	C_2H_5O-CO-CH(CH_3)-, C_3H_7-CO-CH_2-, -$(CH_2)_4$-CO-O-, C_3H_7O-CO-CH(-)-	9	15	69
C_7H_2O, 102.0105	ext-ar(C=O), ext-arO	8	12	71
$C_4H_8NO_2$, 102.0554	C_2H_5O-CO-CH(NH_2)-, C_2H_5O-CO-NHCH_2-, (CH_3-CO-)$_2$N-, C_4H_8-ONO, CH_3O-CO-C(CH_3)(NH_2)-, CH_3-CO-NHCH_2CH(OH)-, -NH$(CH_2)_3$-CO-O-	4	22	65
$C_6H_2N_2$, 102.0216	ext-arN_2, NC-pyridyl-	3	14	43
$C_4H_6O_3$, 102.0316	-CH(OH)CH(OH)CH(OH)CH(-)-, CH_3O-CO-CH(-CH_2OH)-, CH_3-CO-CH(-)-CO-O-	3	11	50
also $C_5H_{12}NO$, 102.0917 ($C_2H_5OCH_2CH_2$CH(NH_2)-); $C_3H_4NO_3$, 102.0190 (cyc-CH(OH)-CH(-NH-CO-)-)				
m/z 103 (32%)		12%	17%	
C_8H_7, 103.0547	phenyl-C_2H_2-, indoles, benzofurans, phenyl-CH(-)-CH(-)-	29	13	85
C_7H_5N, 103.0421	phenyl-arN, phenyl-CH=N-, ext-arN, cyc-CH(phenyl)-N(-)-	10	14	58
C_7H_3O, 103.0184	ext-ar(C=O), Y*-phenyl-CO-Y*, ar-CH=CH-CO-, ext-ar-O-	7	15	64
$C_5H_{11}O_2$, 103.0758	(C_2H_5O)$_2$CH-, C_4H_9OCH(-)O-, C_4H_9-CO-O-, HOCH(CH_3)CH_2OCH(CH_3)-,			

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m/z, comp — Substructure, neighbor	Prop	Abnd	Spcf
$CH_3OCH_2CH_2CH(OCH_3)$-, C_4H_9O-CO-	4	25	68
$C_4H_7O_3$, 103.0394 CH_3O-CO-$CH_2CH(OH)$-, CH_3-CO-CH_2-CO-O-, CH_3O-CO-$CH(OCH_3)$-, cyc-CH_2-$CH(CH_2OH)$-OCH(-)-O-	4	16	64
$C_4H_{11}OSi$, 103.0479 $(CH_3)_3SiOCH_2$-, -CH_2OCH_2-$Si(CH_3)_2$-	2	27	90
$C_6H_3N_2$, 103.0295 ext-arN_2, cyc-NN(phenyl)-, -NH-phenyl-N(-)-	2	13	42
$C_5H_{11}S$, 103.0584 $C_4H_9SCH_2$-, $C_2H_5SC(CH_3)_2$-, -$CH(C_2H_5)SCH(CH_3)$-	1	24	55
also C_5H_8Cl, 103.0314 (cyc-CCl(-)-C(-)(CH_3)-C(-)(CH_3)-); $C_3H_3O_4$, 103.0031 (cyc-CH(OH)-CH(-CO-OH)-O-)			
m/z 104 (26%)	**10%**	**19%**	
C_8H_8, 104.0626 tetralins, indans, phenyl-CH_2CH_2-Y*, o-CH_3-phenyl-CH_2-Y*, phenyl-cycR	27	20	84
C_7H_6N, 104.0499 phenyl-arN, ext-arN, cyc-CH(phenyl)-NH-, phenyl-C(-)=N-, cyc-CH_2N(phenyl)-	13	19	62
C_7H_4O, 104.0262 ext-ar(C=O), cyc-phenyl-CO-, Y-phenyl-CO-, cyc-C(-)(phenyl-O-)	10	19	62
$C_6H_4N_2$, 104.0373 phenyl-arN_2, ext-arN_2	5	17	44
C_6H_2NO, 104.0135 ON-phenyl-	3	14	44

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_4H_8O_3$, 104.0473	HOC_2H_4O-CO-CH_2-, C_3H_7O-CO-O-, CH_3O-CO-CH(OCH_3)-	2	16	73
$C_5H_2N_3$, 104.0246	ext-arN_3	1	25	37
also $C_5H_{12}O_2$, 104.0836; C_4H_8OS, 104.0299	(-$CH_2OCH_2CH_2SCH_2$-, $HOCH_2CH_2SCH_2CH_2$-)			
m/z 105 (38%)		9%	37%	
C_7H_5O, 105.0340		18	47	67
	phenyl-CO-: -O- 25%, CH_2 20%, -NH- 20%, CH 20%	30	83	69
	cyc-CH(phenyl)-O-: -O- 75%, CH_2 15%; CH_2 35%, C=O 25%, CH 25%	5	67	70
	also ext-ar(C=O), -phenyl-CO-, -phenyl-OCH_2-, phenyl-C(-)(OH)-			
C_8H_9, 105.0704	phenyl-CH(CH_3)-, CH_3-phenyl-CH_2-, $(CH_3)_2$-phenyl etc	25	34	80
C_7H_7N, 105.0577	phenyl-N(CH_3)-, -phenyl-CH_2-N(-)-, cyc-CH(phenyl)-NH-, phenyl-arN, CH_3-pyridyl-CH_2-	7	29	56
C_6H_3NO, 105.0214	pyridyl-CO-, -phenyl-NO, ext-arN(C=O)	4	36+	50
$C_6H_5N_2$, 105.0451	phenyl-N=N-, ext-arN_2, arN amines	3	23	45
C_6HO_2, 104.9976	ar/unsatd/cyc C=O/-O-/-OH	2	29	44
$C_3H_5S_2$, 104.9839	(dithietane)	1	55+	87

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_5H_3N_3$, 105.0325	ext-arN_3, pyridyl-N=N- etc	2	23	43
$C_4H_9O_3$, 105.0551	C_2H_5O-CO-CH(OH)-, $(CH_3O)_3C$-, -CH_2-CH(OH)-CH(OH)-CH(OH)-, C_3H_7O-CO-O-, -$CH_2OC(OC_2H_5)O$-, $C_3H_7OCH(-O-)O$-	1	30+	77
C_5HN_2O, 105.0087	NC-pyrrolidonyl-, ar/ext-ar C=O/-OH/-NH-/-N=N- etc	1	26	34
$C_3H_5O_2S$, 105.0013	cyc-CH_2CH(-CO-OH)S-, HO-CO-CH_2SCH_2-, -SCH_2CH_2-CO-O-	1	24	86
also $C_5H_{10}Cl$, 105.0470 ($Cl(CH_2)_5$-, $ClC(C_3H_7)(CH_3)$-); C_4H_9OS, 105.0377 (C_3H_7-CO-S-); C_2H_2Br, 104.9339 (BrCH=CH-)				
m/z 106 (27%)		7%	17%	
C_8H_{10}, 106.0782	CH_3-phenyl-CH_2- etc	21	13	76
C_7H_6O, 106.0418	cyc-CH(phenyl)-O-, HO-phenyl-CH_2-, HO-(CH_3-)phenyl-, substd/cyc ketones	15	13	62
C_7H_8N, 106.0656	CH_3-pyridyl-CH_2-, $(CH_3)_2$-pyridyl-, cyc-CH_2N(phenyl)-, ar-amines	7	28	58
C_6H_4NO, 106.0292	pyridyl-CO-, HO-(CH_3-)-pyridyl-, ar(-NH-CO-)	6	23	55
$C_6H_6N_2$, 106.0529	ext-arN_2	5	13	47
also $C_5H_4N_3$, 106.0403 (arN_3); $C_5H_2N_2O$, 106.0165				

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	(arN_2O, $arN_2(C{=}O)$); $C_3H_6S_2$, 105.9917 ($(CH_3S)_2CH$-); $C_4H_{10}O_3$, 106.0629 (-CH_2CH(OH)CH(OH)CH(OH)-)			
m/z 107 (31%)		15%	24%	
C_7H_7O, 107.0496	CH_3O-phenyl-, HO-phenyl-CH_2-, cyc-CH(phenyl)-O-, substd/cyc/unsatd C=O/-OH ketones	16	27	65
C_8H_{11}, 107.0860	polyunsatd/cyc hc	17	21	85
$C_6H_3O_2$, 107.0133	ar/unsatd/cyc C=O/-O-/-OH	5	16	52
C_6H_5NO, 107.0370	ON-phenyl-, CH_3-pyrrole-CO-	4	16	48
C_7H_9N, 107.0734	CH_3-phenyl-NH-, phenyl-N(CH_3)-, cyc/unsatd amines	4	16	55
$C_5H_5N_3$, 107.0481	ext-arN_3	2	21	42
	also $C_6H_7N_2$, 107.0607 (-NH-phenyl-NH-, $(CH_3)_2$-pyrazinyl-); C_2H_4Br, 106.9496 (BrCH(CH_3)-etc); $C_5H_3N_2O$, 107.0244 (ext-arN_2(C=O))			
m/z 108 (26%)		9%	20%	
C_7H_8O, 108.0575	phenyl-CH_2O-, HO-phenyl-CH_2-, CH_3-phenyl-O-, CH_3O-phenyl-, phenyl-O-Y*-CH_3 (Y* = -CO-O-), cyc/substd/unsatd C=O/-O-/HO-	18	24	61
C_8H_{12}, 108.0938	polyunsatd/cyc hc	17	15	82

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
$C_6H_4O_2$, 108.0211 $(HO-)_2$phenyl-, cyc/subtd/unsatd/ar C=O/-O-/HO-	7	18	46
C_6H_6NO, 108.0448 CH_3O-pyridyl-, H_2N-phenyl-O-, -NH-phenyl-O-, substd/cyc -NH-CO-/-OH/-O- etc	4	20	50
$C_7H_{10}N$, 108.0812 cyc/substd/unsatd amines	4	17	57
$C_6H_8N_2$, 108.0686 $(CH_3)_2$-pyrazinyl-, phenyl-NHNH-, arN-NH- etc	3	17	46

also $C_5H_4N_2O$, 108.0322 (-N-ar-NH-CO- etc); $C_5H_2NO_2$, 108.0084 (-O-ar-NH-CO-, O_2N-ar); $C_5H_6N_3$, 108.0559 (pyridyl-NHNH-, H_2N-(CH_3-)pyrimidinyl-); $C_4H_2N_3O$, 108.0195 (H_2N-pyrimidinyl-O-); $C_4H_4N_4$, 108.0433 (ext-arN_4): C_6H_4S, 108.0037 (arS); C_6H_5P, 108.0129 (ar-P)

m/z 109 (31%)	14%	23%	
C_8H_{13}, 109.1017 polyunsatd/cyc hc	20	19	89
C_7H_9O, 109.0653 1-decalones, cyc/substd/unsatd ketones	14	21	65
$C_6H_5O_2$, 109.0289 HO-phenyl-O-, CH_3-furyl-CO-	6	19	49
C_6H_7NO, 109.0526 -O-pyridyl-CH_2-, CH_3O-pyridyl-, H_2N-phenyl-O-, HO-phenyl-NH-	3	27	48
$C_7H_{11}N$, 109.0890 cyc/unsatd imines/amines	3	13	56

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_5H_3NO_2$, 109.0163	ar-NO_2, arN-CO-OH, -O-ar-NH-CO-	2	24	51
also C_6H_5S, 109.0152 (phenyl-S-); $C_5H_5N_2O$, 109.0400 (CH_3-pyrimidinyl-O-); C_5HO_3, 108.9925 (-O-ar-O-CO-); $C_4H_3N_3O$, 109.0274 (H_2N-CO-imidazolyl); $C_3H_3Cl_2$, 108.9611; $C_6H_9N_2$, 109.0764 (arN-NH-); $C_5H_7N_3$, 109.0637 (H_2N-(CH_3)-pyrimidinyl)				
m/z 110 (25%)		7%	20%	
$C_7H_{10}O$, 110.0731	substd/cyc/unsatd ketones	17	20	60
C_8H_{14}, 110.1094	substd/cyc/unsatd hc	20	13	82
$C_7H_{12}N$, 110.0968	substd/cyc amines, NC-C_6H_{12}-	7	26	63
$C_6H_6O_2$, 110.0367	HO-phenyl-O-, $(HO)_2$-phenyl-, substd/cyc $(C=O)_2$/C=O/-O-	7	22	46
C_6H_8NO, 110.0605	oxazoles, cyc/substd/unsatd C=O/N/-CO-N-/C=N-OH, ar-CO-NH-	4	24	41
$C_5H_4NO_2$, 110.0241	pyrrolinedione-CH_2-, maleimidyl-CH_2-, cyc C=O/-N-CO-/-O-	2	23	47
also $C_5H_2O_3$, 110.0003 (ar C=O/-O-/-CO-O-); $C_5H_6N_2O$, 110.0478 (arN_2-O-); $C_6H_{10}N_2$, 110.0842; C_6H_6S, 110.0193 (phenyl-S-); $C_4H_4N_3O$, 110.0352 (N_2ar(C=O)-NH_2); $C_4H_2N_2O_2$, 110.0114 (pyrazine-(-O-)$_2$- C_6H_3Cl, 109.9923 (Cl-phenyl-); $C_2H_7O_3P$, 110.0132 (($CH_3O)_2$-P(=O)-)				

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 111 (28%)		10%	20%	
C_8H_{15}, 111.1173	$(CH_3)_2$-cyclohexyl- etc	23	18	86
$C_7H_{11}O$, 111.0809	cyclohexyl-CO-, $C_4H_9CH{=}CH{-}CO$-, substd/cyc/unsatd -CO-/-O-/-OH	18	19	69
$C_6H_7O_2$, 111.0445	-CO-C_4H_8-CO- (adipates), CH_3O-CO-CH=CHCH=CH-, cyc/unsatd C=O/$(C{=}O)_2$/-O-/-OH, ar-$(OR)_2$	8	23	54
C_6H_9NO, 111.0683	cyc/unsatd amines/imines/C=O/-O-	3	21	47
$C_7H_{13}N$, 111.1047	substd/cyc/unsatd amines, NC-C_6H_{12}-	3	16	62
$C_5H_3O_3$, 111.0082	HO-pyrone-, furanoate, -CO-C(OH)=C(CH_3)-CO-	3	14	57
C_6H_7S, 111.0271	$(CH_3)_2$-thiophenyl-, thiophenyl-CH(CH_3)-, ar-S-	2	31	73
$C_5H_5NO_2$, 111.0319	pyrollyl-CO-O-, H_2N-CO-C(CH_3)=CH-CO-, ar-OCH_2-CO-NH-	2	20	54

also $C_5H_7N_2O$, 111.0556 (cyc-carbamate, arN_2-OH); $C_6H_{11}N_2$, 111.0920 (ar-N=CHN$(CH_3)_2$, cyc imines); C_6H_4Cl, 111.0001 (Cl-phenyl-); $C_4H_3N_2O_2$, 111.0193 (-NH-CO-NH-CO-); $C_4H_5N_3O$, 111.0430 (HO-arN_2-NH_2); $C_3H_5Cl_2$, 110.9767; C_2HOCl_2, 110.9403 (Cl_2CH-CO-, -CCl_2-CO-)

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 112 (21%)		6%	18%	
C_8H_{16}, 112.1251	H-C_8H_{16}-Y*, H-C_8H_{16}-R-Y*	19	9	82
$C_7H_{12}O$, 112.0887	2-R-cyclohexanone-CH_3, R-$(CH_2)_6$-CO-Y, C_3H_7CH=CH-CO-CH_2-, cyc/subst/unsatd -CO-/-O-/-OH	12	18	61
$C_6H_8O_2$, 112.0524	furyl-$CH(OCH_3)$-, cyc diketones, cyc/substd/unsatd -CO-O-/-CO-OH/-O-	10	20	54
$C_7H_{14}N$, 112.1125	cyc/substd/unsatd amines (cyclohexyl-NH-CH_2-)	6	25	63
$C_6H_{10}NO$, 112.0761	cyc-$CH_2CH(N(C_2H_5)$-CO-$CH_3)$-, lactams, other cyc/unsatd amides, cyc HO-N=CH-, OCN-C_5H_{10}-	5	18	56
$C_5H_4O_3$, 112.0160	furyl-CO-O-, ar(C=O)-CO-OH, HO-CO-$C(CH_3)$=CH-CO-, ketoesters	3	26	53
also $C_5H_6NO_2$, 112.0397 (ketoamides); C_5H_6NS, 112.0223 (arNS); $C_6H_{12}N_2$, 112.0998 (-N=N-, aminoimines); $C_5H_8N_2O$, 112.0635 (aminoamides); C_6H_8S, 112.0350 (CH_3-thiophenyl-CH_2-); $C_4H_4N_2O_2$, 112.0271 (-CH(-)-CO-NH-CO-NH-CH(-)-)				
m/z 113 (23%)		6%	21%	
C_8H_{17}, 113.1329	satd hc	19	12	87
$C_7H_{13}O$, 113.0966	C_6H_{13}-CO-,			

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	cyc-$CH(OH)CH_2CH(C_3H_7)$-, $-(CH_2)_6$-CO-, CH_3O-cyclohexyl-	14	30+	71
$C_6H_9O_2$, 113.0602	CH_3O-CO-CH=CH-CH_2CH_2-, C_3H_7-CO-CH_2-CO-, -CH(OH)-$(CH_2)_4$-CO-	11	16	60
$C_5H_5O_3$, 113.0238	furyl-CO-O-, CH_3O-CO-CH=CH-CO-, cyc C=O/-OH/-O-	5	19	57
$C_6H_{11}NO$, 113.0839	cycC=N-OH, pyrrolidinyl-CO-CH_2-, cycN -OH/-O-	3	25+	57
C_6H_9S, 113.0428	thiabicycloalkane	2	29	66
$C_5H_7NO_2$, 113.0475	NC-$CH(CH_3)$-CO-O-CH_2-, CH_3-succinimidyl-, glutarimidyl-	2	22	52

also $C_7H_{15}N$, 113.1203 (cycN); C_8H_3N, 113.0264 (ext-arN); $C_6H_{13}N_2$, 113.1077 ($cycN_2$); $C_5H_9N_2O$, 113.0713 (pentanolactam-NH-); C_5H_7NS, 113.0301 (CH_3-thiazolyl-CH_2-); $C_4H_5N_2O_2$, 113.0349 (cyc(-N-CO-N-CO-)); C_4HO_4, 112.9874 (cyc-CH(-CO-O-)-CH(-CO-O-)-); C_5H_5OS, 113.0064 (CH_3O-thiophenyl-, CH_3S-furyl-, ar-SO-)

m/z 114 (17%)		11%	10%	
$C_6H_{10}O_2$, 114.0680	cyc-$CH(-CH_2-)(CH_2)_3$-CO-O-, CH_3O-CO-CH=$C(CH_3)CH_2$-, CH_3O-CO-C_4H_8-Y*	14	12	61
$C_7H_{16}N$, 114.1281	$(C_3H_7)_2NCH_2$- etc	11	15	64
$C_5H_6O_3$, 114.0316	HO-CO-$(CH_2)_3$-CO-	7	11	48

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_6H_{12}NO$, 114.0917	CH_3-CO-NH-CH(C_3H_7)-, C_4H_9-COCH(-)NH-, $C_4H_9N(CH_3)$-CO-	5	17	56
also $C_7H_{14}O$, 114.1044	(C_5H_{11}-CO-CH_2-); $C_5H_8NO_2$, 114.0554 (CH_3-CO-CH_2-N(-CO-CH_3)-); $C_6H_{14}N_2$, 114.1155 (C_2H_5-imidazolidinyl-CH_2-); $C_4H_6N_2O_2$, 114.0427 (-CH(-)-CO-NH-CO-NH-CH(-)-)			
m/z 115 (34%)		7%	27%	
C_9H_7, 115.0547		28	24	87
$C_6H_{11}O_2$, 115.0758	CH_3O-CO-$(CH_2)_4$-, C_3H_7CH=CH-CO-O-, CH_3O-CO-$CH_2C(CH_3)_2$-, $(CH_3)_2$-1,3-dioxanyl-	7	28	62
$C_5H_7O_3$, 115.0394	CH_3O-CO-CH_2CH_2-CO-, C_2H_5O-CO-CH_2-CO-, CH_3-CO-CH(-)-CO-OCH_2-, -CO-CH_2CH(CH_3)-O-CO-	5	38	55
$C_7H_{17}N$, 115.1359	$C_3H_7NHCH(C_3H_7)$-; and C_8H_5N, 115.0421 ext-arN (indolyl-), pyrrolyl-ar	7	22	60
$C_7H_{15}O$, 115.1122	$C_6H_{13}CH(OH)$-, $C_5H_{11}OCH(CH_3)$-, $(CH_3)_3C$-O-Y*-$C(CH_3)_2$-; and C_8H_3O, 115.0184 ext-ar(-CO-CH_2-), ext-ar-CO- etc	7	20	63
also $C_7H_3N_2$, 115.0295	(indazolyl-); $C_6H_{11}S$, 115.0584 (cyc-$CH_2CH_2CH(SC_3H_7)$-) $C_5H_9NO_2$, 115.0632 (cyc-N(-CH_2CH(-)CH_3)-CO-OCH_2-); $C_6H_{13}NO$, 115.0996 (($C_2H_5)_2$N-CO-CH_2-); $C_4H_5NO_3$, 115.0268 (cyc-C(OH)(CH_3)-CO-NH-CO-); $C_4H_3O_4$, 115.0031			

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	(HO-CO-CH_2-C(-)(-CO-OH)-); C_5H_9NS, 115.0458 (SCN-$(CH_2)_4$-)			
m/z 116 (25%)		7%	16%	
C_9H_8, 116.0626	phenyl-C_3H_3(-)-, ext-ar	24	10	87
C_8H_6N, 116.0499	indolyl, ext-arN, NC-phenyl-CH_2-, phenyl-arN	11	15	60
$C_5H_8O_3$, 116.0473	CH_3O-CO-CH_2-CO-CH_2-, CH_3O-CO-CH(-CO-CH_3)-, CH_3O-CO-CH_2-CO-CH(-)-	4	24	64
C_8H_4O, 115.9898	ext-ar(C=O), ext-ar-CO-	7	11	64
$C_6H_{12}O_2$, 116.0836	CH_3O-CO-CH(C_3H_7)-, -C(C_2H_5)$_2$-CO-O-, C_3H_7O-CO-CH(CH_3)-, (C_2H_5O)$_2$C(CH_3)-	6	13	62
$C_7H_4N_2$, 116.0373	ext-arN_2 (benzimidazoles), phenyl-arN_2	3	12	49
also $C_5H_{10}NO_2$, 116.0710 (CH_3O-CO-CH_2CH_2CH(NH_2)-); $C_4H_4O_4$, 116.0109 ((HO)$_2$-ar(-O-CO-), CH_3O-CO-C(-)$_2$-CO-O-); $C_4H_6NO_3$, 116.0346 (-C(CH_3)(OH)-CO-NH-CO-); $C_4H_4S_2$, 115.9761 (thiophenyl-S-, arS_2); $C_4H_8N_2O_2$, 116.0584 (-CH_2NH-CO-CH_2NH-CO-); $C_4H_8O_2Si$, 116.0193 ((CH_3)$_3$SiO-CO-)			
m/z 117 (30%)		11%	20%	
C_9H_9, 117.0704	CH_2=CH-phenyl-CH_2-, phenyl-CH=CH-CH_2-, indanyl- etc	24	17	83

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_8H_7N, 117.0577	CH_3-phenyl-CH=N-, ext-arN, cyc-CH_2CH(-)-N(phenyl)-, phenyl-arN	9	16	61
C_8H_5O, 117.0340	ext-ar(C=O), HO-ext-ar, ext-ar-CO-	6	16	63
$C_5H_9O_3$, 117.0551	-$CH_2O(CH_2)_3$-CO-O-, CH_3O-CO-CH_2-CO-CH_2-, -CH(-CHO-)-$OC(CH_3)_2$-O-, CH_3O-CO-CH_2CH(OCH_3)-	4	18	67
$C_7H_5N_2$, 117.0451	ext-arN_2, phenyl-arN_2	2	15	46
$C_6H_{13}O_2$, 117.0915	C_5H_{11}-CO-O-, $CH_3OCH(CH_3)CH(CH_3)CH(OH)$-, -$CH_2O$-$(CH_2)_4$-$OCH_2$-, $C_3H_7OCH(OC_2H_5)$-	2	12	61
also $C_6H_{13}S$, 117.0741 ($C_4H_9SCH(CH_3)$-); $C_5H_{13}OSi$, 117.0635 ($(CH_3)_3SiOCH(CH_3)$-, $C_3H_7OSi(CH_3)_2$-); CCl_3, 116.9064; C_7H_3NO, 117.0214 (ext-arN(C=O), ext-arN-CO-); C_5H_9OS, 117.0377 (CH_3-1,3-oxathiane); C_2HF_3Cl, 116.9718 ($CF_3C(-)Cl$-)				
m/z 118 (23%)		6%	18%	
C_9H_{10}, 118.0782	phenyl-C_3H_5(-)-, tetralins, -CH_2phenyl-C_2H_4-	22	15	81
C_8H_8N, 118,0656	phenyl-cyc-amine (-$CH(CH_3)$-N(phenyl)-), phenyl-$C(=NCH_3)$-, phenyl-CH=NCH_2-	10	17	61
C_8H_6O, 118.0418	phenyl-CH_2-CO-, -CH(phenyl)-CH(-)-O-, ext-ar(-CO-CH_2-)	9	19	59

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_7H_6N_2$, 118.0529	ext-ar-N_2, phenyl-arN_2, phenyl-C(-N-)=N-	6	17	54
C_7H_4NO, 118.0292	cyc-N(phenyl)-CO-, -phenyl-CH=N-O-, HO-ext-arN, o-H_2N-CO-phenyl-	4	18	56

also $C_7H_2O_2$, 118.0054 (ext-ar(C=O)-O-, ar-CO-O-, ar-$(C=O)_2$-); $C_6H_4N_3$, 118.0403 (ext-arN_3); $C_5H_{10}O_3$, 118.0629 (HO-CO-C(OH)(C_3H_7)-, C_4H_9O-CO-O-, HOC_3H_6O-CO-CH_2-); $C_6H_2N_2O$, 118.0165 (NC-pyridyl-O-); $C_4H_6O_4$, 118.0265 (HO-CO-C(-)(CH_3)-); $C_4H_8NO_3$, 118.0503 (cyc-CH(OH)-CH(OH)-N(CH_3)-CO-, H_2N-CO-$OCH_2CH(OH)CH_2$-); $C_5H_{12}NO_2$, 118.0867 (C_4H_9NH-CO-O-, C_4H_9O-CO-NH-)

m/z 119 (30%)		12%	21%	
C_9H_{11}, 119.0860	phenyl-C(CH_3)$_2$-, (CH_3)$_3$-phenyl- etc	22	17	79
C_8H_7O, 119.0496	CH_3-phenyl-CO-, dihydrobenzofurans, -CH_2CH(phenyl)-O-, substd/cyc/unsatd ketones	10	20	60
C_7H_5NO, 119.0370	H_2N-phenyl-CO-, phenyl-NH-CO-, cyc-N(phenyl)-CO-, ext-ar(-NH-CO-)	6	21	59
$C_7H_3O_2$, 119.0133	ar$(C=O)_2$, -phenyl-CO-O-, phenyl-ar(-O-CO-)	4	21	54
C_8H_9N, 119.0734	benzo-$NHCH_2$-, phenyl-CH=N-CH_2-, phenyl-$CH_2CH(NH_2)$-, cyc-CH_2CH(phenyl)N(-)-	5	13	54

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_7H_7N_2$, 119.0607	CH_3-phenyl-N=N-, phenyl-CH=N-NH-, CH_3CH=CH-pyrazyl-	3	19	43
also $C_6H_5N_3$, 119.0481 (arN_3); $C_6H_3N_2O$, 119.0244 (imidazolidone-ar, HO-ext-arN_2); $C_5H_3N_4$, 119.0355 (ext-arN_4); C_2F_5, 118.9920				
m/z 120 (24%)		7%	19%	
C_9H_{12}, 120.0938	$(CH_3)_2$-phenyl-CH_2- etc	17	14	73
C_8H_8O, 120.0575	phenyl-CO-CH_2-, cyc-CH_2CH(phenyl)-O-, substd/cyc ketones	12	18	58
$C_8H_{10}N$, 120.0812	$(CH_3)_3$-pyridyl-, $H_2NCH(CH_2$-phenyl)-, ar/unsatd/cyc/substd amines	6	30	64
C_7H_6NO, 120.0448	H_2N-phenyl-CO-, phenyl-NH-CO-, HO(CH_3-)pyridyl-CH_2-	7	25	56
$C_7H_4O_2$, 120.0211	HO-phenyl-CO-, HO-CO-phenyl-, -phenyl-CO-O-, -phenyl-O-CO-, ext-ar(-O-CO-) (dihydrocoumarins)	6	23	53
$C_7H_8N_2$, 120.0686	C_3H_7-pyrazines, phenyl-CH=N-NH-, ar-amines	3	23	43
$C_6H_4N_2O$, 120.0322	ar(-NH-CO-NH-), ext-arN_2O	3	18	55
also $C_5H_4N_4$, 120.0433 (ext-arN_4); $C_6H_6N_3$, 120.0559 (ext-arN_3); $C_6H_2NO_2$, 120.0084 (ext-ar(-CO-NH-CO-), -pyridyl-CO-O-, -CO-NH-ar-CO-); $C_5H_2N_3O$, 120.0195				

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	(ext-arN$_3$(C=O)); C_3H_5Br, 119.9574 (cyc-CH_2CH(-)CHBr-); C_2HOBr, 119.9210 (=CBr-CO-, arBr(OH))			
m/z 121 (30%)		11%	24%	
C_9H_{13}, 121.1017	polyunsatd/cyc hc	20	27	85
C_8H_9O, 121.0653	cyc-CH(-)CH(phenyl)O-, phenyl-C(-)(OCH_3)-, phenyl-CHY*-Y-OCH_3, substd/cyc/unsatd C=O/-O-/-OH	13	27	62
$C_7H_5O_2$, 121.0289	HO-phenyl-CO-, CH_3(-CH_2-)furyl-CO-, furyl-CH=CH-CO-, -O-phenyl-CH_2O-, substd/cyc C=O/-O-	11	30	58
C_7H_7NO, 121.0526	phenyl-CH=N-O-, phenyl-NH-CO-, cyc/unsatd/substd amines/C=O/-O-/-OH	4	14	52
$C_8H_{11}N$, 121.0890	$(CH_3)_2$phenyl-NH-, ar-amines	3	13	55
	also $C_6H_3NO_2$, 121.0163 (O_2N-phenyl-, ar/arN C=O/-NH/-O-/OH); $C_6H_5N_2O$, 121.0400 (pyrazones, HO-phenyl-N=N-); $C_7H_9N_2$, 121.0764 ($(CH_3)_2$N-pyridyl-, pyrazines); $C_5H_3N_3O$, 121.0274 (HO-ext-arN$_3$-); C_7H_5S, 121.0115 (cyc-CH(phenyl)-S-, arS); $C_6H_7N_3$, 121.0637 (ext-arN$_3$); C_2H_2BrO, 120.9289 ($BrCH_2$-CO-)			
m/z 122 (23%)		7%	17%	
$C_8H_{10}O$, 122.0731	C_2H_5O-phenyl-, phenyl-O-Y*-C_2H_5, cyc/substd/unsatd ketones/-OH	14	19	60

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
C_9H_{14}, 122.1095	polyunsatd/cyc hc	16	13	81
$C_7H_6O_2$, 122.0367	CH_3O-(HO-)phenyl-, (HO-)$_2$phenyl-CH_2-, cyc/substd C=O/-O-	11	14	54
C_7H_8NO, 122.0605	ext-ar(NH)(C=O), CH_3O-phenyl-NH-, substd/cyc amines/C=O/-O-	4	18	48
$C_8H_{12}N$, 122.0968	cyc/substd/unsatd amines	4	18	59
$C_6H_4NO_2$, 122.0241	pyridone-CO-, HO-CO-pyridyl-, H-CO-pyrrolyl-CH_2O-, O_2N-phenyl-	3	23	50
also $C_6H_2O_3$, 122.0003; $C_6H_6N_2O$, 122.0478 (HO-(CH_3-)$_2$-pyrazinyl-); $C_7H_{10}N_2$, 122.0842 ((CH_3)$_2$pyrazinyl-CH_2-); $C_5H_4N_3O$, 122.0352 (HO-ext-arN_3-); $C_5H_2N_2O_2$, 122.0114; C_7H_6S, 122.0193 (ext-arS)				
m/z 123 (25%)		9%	22%	
C_9H_{15}, 123.1173	polyunsatd/cyc hc	20	17	88
$C_8H_{11}O$, 123.0809	cyc/substd/unsatd C=O/-OH	14	20	64
$C_7H_7O_2$, 123.0445	phenyl-CO-O-, HO-phenyl-CO(OH)-, phenyl-C(-)(-O-)$_2$, ar/unsatd/cyc C=O/-OH/-O-	9	21	54
$C_6H_3O_3$, 123.0082	ar/unsatd/cyc -CO-O-/-CO-/-O-/-OH	3	17	55
$C_6H_5NO_2$, 123.0319	O_2N-phenyl-,			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
HO-(CH_3)-pyridonyl-	3	18	45
C_7H_9NO, 123.0683 CH_3O-phenyl-NH-, ar-CH_2CH(-CO-NH_2)-, CH_3O-(H_2N-)-phenyl-	2	21	45
also $C_8H_{13}N$, 123.1047 (cyc/unsatd amines); C_7H_7S, 123.0271 (phenyl-SCH_2-, CH_3S-phenyl-); $C_6H_7N_2O$, 123.0556 (CH_3-pyrimidinyl-OCH_2-, CH_3O-(CH_3-)-pyrazinyl-); $C_5H_5N_3O$, 123.0430			
m/z 124 (19%)	**6%**	**22%**	
$C_8H_{12}O$, 124.0887 substd/cyc/unsatd ketones	14	18	60
C_9H_{16}, 124.1251 substd/cyc/unsatd hc	15	10	83
$C_7H_8O_2$, 124.0524 CH_3O-phenyl-O-, $(HO)_2$-phenyl-CH_2-, cyc/substd/unsatd C=O/-O-	8	24	48
$C_8H_{14}N$, 124.1125 substd/cyc amines, NC-C_7H_{14}-	6	30	60
C_7H_8S, 124.0350 CH_3-phenyl-S-	2	59	71
$C_7H_{10}NO$, 124.0761 oxazoles, cyc/substd amines/-O-/C=N-OH	3	24	40
$C_6H_6NO_2$, 124.0397 furyl-CO-$CH(NH_2)$-, maleimides, cyc/unsatd, amines/C=O/-O-	3	17	48
$C_6H_4O_3$, 124.0160 unsatd/ar C=O/-O-/-OH	3	13	44
also $C_6H_8N_2O$, 124.0635; C_6H_6NS, 124.0223 (pyridyl-SCH_2-, CH_3S-pyridyl-, arS-NH-); $C_5H_4N_2O_2$, 124.0271 (O_2N-pyridyl-, CH_3-pyrazinyl-(-O-)$_2$-			

m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
m/z 125 (22%)	6%	20%	
C_9H_{17}, 125.1329 cyc/unsatd hc	21	19	87
$C_8H_{13}O$, 125.0966 cyclohexyl-CH_2-CO-, -C_7H_{14}-CO-, cyc/unsatd/substd -CO-/-O-/-OH; and C_9HO, 125.0027 ext-ar(C=O)	11	16	66
$C_7H_9O_2$, 125.0602 -CO-C_5H_{10}-CO-, cyc/unsatd C=O/-O-/-OH, ar-$(OCH_3)_2$	8	19	58
$C_6H_5O_3$, 125.0238 CH_3O-pyrone-, furanoates etc	4	15	56
C_7H_9S, 125.0428 C_3H_7-thiophenyl-, ar-SR	2	20	72
$C_6H_7NO_2$, 125.0475 ar-NH-CO-OR, furyl-CO-$NHCH_2$-, CH_3-ar-NO_2	2	20	55
also $C_7H_{11}NO$, 125.0839 (arN-O-); $C_8H_{15}N$, 125.1203; $C_6H_9N_2O$, 125.0713 (cyc carbamates); C_7H_6Cl, 125.0157 (Cl-phenyl-CH_2-); C_6H_7NS, 125.0301 (arN-S-); $C_7H_{13}N_2$, 125.1077 (cyc imines); C_5HO_4, 124.9874 (-CH_2O-CO-C≡C-CO-O-, $(-O)_2$ar-CO-); C_6H_4NCl, 125.0031 (Cl-ar-NH-)			
m/z 126 (20%)	6%	20%	
C_9H_{18}, 126.1407 H-C_9H_{18}-Y*, H-C_9H_{18}-R-Y*; and $C_{10}H_6$, 126.0469 naphthyl	20	11	85
$C_8H_{14}O$, 126.1044 2-R-cyclopentanone-C_3H_7, R-$(CH_2)_7$-CO-Y, cyc/substd/unsatd -CO-/-O-/-OH; and C_9H_2O, 126.0105			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
ext-ar(C=O)	11	21	62
$C_7H_{10}O_2$, 126.0680 cyc/substd/unsatd -CO-/-CO-O-/-O- etc	7	19	52
$C_8H_{16}N$, 126.1281 cyc/substd/unsatd amines; and C_9H_4N, 126.0343 substd quinolines	5	17	60
$C_7H_{12}NO$, 126.0917 cyc-C_5H_9-N(-CO-CH_3)-, cyc/unsatd amides, oximes, isocyanates	4	16	54
$C_6H_6O_3$, 126.0316 cyc/substd/unsatd C=O/-CO-O-/-OH (cyc-CH_2CH_2CH(-CO-)CH(-CO-OH)-, HO-pyrone-CH_2-)	3	23	50
also $C_6H_8NO_2$, 126.0554 (cyc-CO-NR-CO-, ar-NH-CO-OCH_3); $C_7H_{10}S$, 126.0506 (arS); C_6H_8NS, 126.0380 (arNS); $C_7H_{14}N_2$, 126.1155 (unsatd diamines); $C_5H_6N_2O_2$, 126.0427 (unsatd/cyc -NH-CO-N(-)-CO-) $C_6H_{10}N_2O$, 126.0791 (C=N-NH-CO-)			
m/z 127 (26%)	**7%**	**16%**	
$C_{10}H_7$, 127.0547 naphthyl-Y*, ext-ar; and C_9H_{19}, 127.1486 satd hc	25	11	87
$C_7H_{11}O_2$, 127.0758 C_4H_9-CO-CH_2-CO-, CH_3O-(Y*-)cyclohexyl-O-, CH_3O-CO-CH=C(CH_3)CH_2CH_2-	8	14	62
$C_8H_{15}O$, 127.1122 C_7H_{15}-CO-, -CH(OH)-$(CH_2)_7$-; and C_9H_3O, 127.0184 ext-ar(C=O)(-benzofuranonyl-), -O-phenyl-ar-O-	9	14	66

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_6H_7O_3$, 127.0394	ar/cyc/unsatd -O-/-OH/C=O	4	18	58
I, 126.9043	iodo	3	21	68
$C_5H_7N_2O_2$, 127.0505	$-CH_2-CO-NHCH(CH_3)-CO-NH-$, $-C(-)_2-CO-NH-CH_2-CO-NH-CH_2-$	2	30	61
$C_6H_9NO_2$, 127.0632	arN -O-/-OH, $-N(C_2H_5)-CO-C(CH_3)=C(-)-O-$	2	24	62
also C_9H_5N, 127.0421 (ext-arN); $C_7H_{15}N_2$, 127.0295 (ext-arN$_2$); $C_7H_{13}NO$, 127.0196 (piperidyl-CO-CH_2-); $C_7H_{11}S$, 127.0584 (thiabicycloalkane); C_6H_9NS, 127.0457 (C_2H_5-thiazolyl-CH_2-); $C_5H_3O_4$, 127.0031; C_6H_6NCl, 127.0188 (Cl-phenyl-NH-)				
m/z 128 (25%)		8%	17%	
$C_{10}H_8$, 128.0626	ext-ar hc	22	13	85
$C_7H_{12}O_2$, 128.0836	$C_2H_5O-CO-CH=C(CH_3)CH_2-$, $CH_3O-(HO-)-cyclohexyl-$, $C_2H_5O-CO-(CH_2)_4-$, $CH_3O-CO-C(CH_3)_2CH_2CH_2-$	6	17	54
C_9H_6N, 128.0499	quinolinyl, phenyl-arN	8	11	61
C_9H_4O, 128.0262	ext-ar(C=O) (benzofuranonyl-), ext-ar-CO-, phenyl-cyc(C=O)	7	12	58
$C_7H_{14}NO$, 128.1074	$(C_3H_7)_2N-CO-$, $CH_3-CO-NH-CH(C_3H_7)-$, $C_6H_{13}NH-CO-$,			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
cyc-$CH_2CH_2C(CH_3)(OH)CH_2CH_2N(CH_3)$-	3	28	56
$C_6H_8O_3$, 128.0473 CH_3O-CO-$C(OCH_3)$=$CHCH_2$-, CH_3O-CO-$(CH_2)_3$-CO-, C_2H_5O-CO-CH(-CO-CH_3)-	3	20	50
also $C_6H_{10}NO_2$, 128.0710 ($(CH_3)_2NC(OCH_3)$=CH-CO-, cyc-CH_2CH_2CH(-NH-CO-OC_2H_5); $C_8H_{16}O$, 128.1200 (C_6H_{13}-CO-CH_2-); $C_7H_{16}N_2$, 128.1311 ($(C_3H_7)_2C$=N-NH-); $C_8H_4N_2$, 128.0373 (ext-arN_2(-quinoxalinyl)); $C_5H_6NO_3$, 128.0346 (-CH_2CH(NH-CO-CH_3)-CO-O-); C_6H_5OCl, 128.0029 (Cl-phenyl-O-); $C_5H_4O_4$, 128.0109 (-CH_2O-CO-$)_2CH$-)			
m/z 129 (28%)	**10%**	**20%**	
$C_{10}H_9$, 129.0704 indenes, indanes, tetralins etc	21	16	84
$C_7H_{13}O_2$, 129.0915 HO-CO-cyclohexyl-, HO-CO-$(CH_2)_6$-, CH_3-CO-$(CH_2)_5$-, -$(CH_2)_6$-CO-O-	7	20	61
$C_8H_{17}O$, 129.1278 $C_7H_{15}CH$(OH)-, $C_6H_{13}OCH(CH_3)$-; and C_9H_5O, 129.0340 phenyl-CH=C(-)-CO-, -indonyl-O-, cyc-CH_2C(-)(phenyl)-	8	15	64
C_9H_7N, 129.0577 indolyl-CH_2-, 1,2-dihydroquinolinyl-, 2-quinolinyl-	8	14	61
$C_6H_9O_3$, 129.0551 -CO-$(CH_2)_4$-CO-O-, CH_3O-CO-$(CH_3)_2$-CO-, -$C(OCH_3)$=$CHCH_2CH_2$-CO-O-, -$CH_2CH(OH)CH_2O$-CO-CH_2CH_2-	4	19	59

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_8H_5N_2$, 129.0451	ext-arN$_2$ (quinazolinyl, CH_3-benzimidazolyl-)	4	18	53
also C_8H_3NO, 129.0214	(ext-arN-CO-, ext-arN(C=O)); $C_5H_5O_4$, 129.0187 (-O-CO-CH_2CH(OH)CH_2-CO-) $C_6H_{13}N_2O$, 129.1026 (-NH(CH_2)$_3$N(-CO-CH_3)-CH_2-); $C_7H_3N_3$, 129.0325 (ext-arN$_2$-N(-)-); $C_7H_{13}S$, 129.0741 (cyc-CH_2CH_2CH(-SC_4H_9)-)			
m/z 130 (22%)		6%	19%	
$C_{10}H_{10}$, 130.0782	phenyl-C_4H_5(-)-, C_5H_9-phenyl-CH_2-, ext-ar	18	15	83
C_9H_8N, 130.0656	ext-arN (CH_3-indolinyl-, indole-CH_2-), phenyl-arN	9	26	61
C_9H_6O, 130.0418	ext-ar(C=O), -phenyl-CH_2CH(-)-CO-	8	18	65
$C_8H_6N_2$, 130.0529	ext-arN$_2$ (quinazolinyl), phenyl-arN$_2$	5	18	48
C_8H_4NO, 130.0292	NC-phenyl-CO-, ext-arN-CO-, ext-arN-O-	3	23	48
also $C_7H_{14}O_2$, 130.0993	(CH_3O-CO-C(CH_3)(C_3H_7)-); $C_6H_{10}O_3$, 130.0629 (C_2H_5O-CO-CH(-CO-CH_3)-); $C_6H_{12}NO_2$, 130.0866 (CH_3O-CO-(CH_2)$_3$-CH(NH_2)-); $C_5H_8NO_3$, 130.0503 (-N(-CO-O-C_2H_5)-CH_2CH_2O-, -O-CO-CH_2CH_2CH(NH_2)-CO-); $C_6H_{14}N_2O$, 130.1104 ($H_2NCH_2CH_2$N(C_2H_4OH)-CH_2CH_2-); $C_5H_{10}N_2O_2$, 130.0740 ((-CH_2-)$_2$C=N-NH-CO-OCH_3); $C_3H_2N_2O_4$, 130.0013 ((O_2N)$_2$-ar)			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 131 (27%)		10%	20%	
$C_{10}H_{11}$, 131.0860	C_3H_5-phenyl-CH_2-, tetralinyl etc	18	20	82
C_9H_7O, 131.0496	phenyl-CH=CH-CO-, ext-ar(C=O), phenyl-CH(-)CH_2-CO-	11	23	68
C_9H_9N, 131.0734	ext-arN, phenyl-arN	5	14	60
$C_8H_7N_2$, 131.0607	CH_3-indazolyl, phthalazinyl	3	22	57
$C_7H_{15}O_2$, 131.1071	$(C_3H_7O)_2CH$-, C_3H_7-CH(-O-CO-CH_3)-CH_2-; and $C_8H_3O_2$, 131.0133 -O-ar-CO-CH=CH-, ext-ar(C=O)-O-	3	15	56
C_8H_5NO, 131.0370	ext-arN(C=O), phenyl-arNO etc	3	14	47
also $C_6H_{11}O_3$, 131.0707 ($HOCH_2$-(CH_3-)$_2$-dioxetanyl); $C_7H_3N_2O$, 131.0244 (ext-arN$_2$-O-); $C_6H_{11}OS$, 131.0533 ((CH_3)$_2$-1,3-oxathiane); $C_5H_9NO_3$, 131.0581 (CH_3-CO-NH-CH(-CO-O-CH_3)-); $C_6H_{15}OSi$, 131.0791 ((CH_3)$_3$Si-O-CH(C_2H_5)-); C_3F_5, 130.9920				
m/z 132 (21%)		6%	17%	
$C_{10}H_{12}$, 132.0938	tetralins, phenyl-C_4H_7(-)- etc	16	15	80
C_9H_8O, 132.0575	ext-ar(C=O), -CH(CH_3)-C(-)(phenyl)-O-, (CH_3)$_2$-phenyl-CO-	11	17	64

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_9H_{10}N$, 132.0812	cyc-$CH_2CH_2C(NH_2)$(phenyl)-, ar amines/imines, ext-arN	7	24	63
C_8H_6NO, 132.0448	CH_3-phenyl-NH-CO-, HO-ext-arN	6	15	60
$C_8H_8N_2$, 132.0686	phenyl-arN_2	4	16	50
$C_8H_4O_2$, 132.0211	ext-ar$(C=O)_2$, HO-CO-ext-ar, ext-ar(-CO-O-)	4	16	53
$C_5H_8O_4$, 132.0422	$(CH_3O\text{-}CO\text{-})_2CH$-, $(HO\text{-}CO\text{-})_2C(C_2H_5)$-	2	27	63
$C_7H_4N_2O$, 132.0322	ext-arN_2-O- (benzoimidazolyl-O-), ext-arN_2(C=O)	2	18	49
also $C_7H_6N_3$, 132.0559 (ext-arN_3); $C_2F_2Cl_2$, 131.9344				
m/z 133 (27%)		11%	19%	
$C_{10}H_{13}$, 133.1017	CH_3-phenyl-$C(CH_3)_2$-, $(CH_3)_4$-phenyl- etc	17	19	76
C_9H_9O, 133.0653	$(CH_3)_2$-phenyl-CO-, dyhydrobenzopyrans, phenyl-CH_2CH_2-CO-	9	23	61
$C_8H_5O_2$, 133.0289	-phenyl-CO-OCH_2-, -CH_2-phenyl-O-CO-, -CH(OH)-C(-)(phenyl-O-)-	5	23	56
C_8H_7NO, 133.0526	CH_3-phenyl-NH-CO-, phenyl-arON	4	18	55
$C_9H_{11}N$, 133.0890	benzo-cycN	4	11	53

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
$C_8H_9N_2$, 133.0764 $(CH_3)_2$-pyrazinyl-CH=CH-, $(CH_3)_2N$-phenyl-N(-)-	2	23	52
also $C_7H_5N_2O$, 133.0400 (phenyl-ON=N-CH_2-, -phenyl-NHNH-CO-); $C_7H_3NO_2$, 133.0163 (ext-arN(C=O)$_2$); $C_6H_5N_4$, 133.0511 (arN$_4$); C_4H_6Br, 132.9652 ($BrCH_2CH=CHCH_2$-); C_8H_6P, 133.0207 (benzo-cycP); $C_4H_5O_5$, 133.0136 (-CH(OH)-CH(OH)-CH(OH)-CH(OH)-O-)			
m/z 134 (22%)	6%	18%	
$C_{10}H_{14}$, 134.1095 $(CH_3)_3$-phenyl-CH_2-, phenyl-CO-OC_4H_9, etc	17	16	73
$C_8H_6O_2$, 134.0367 CH_3O-CO-phenyl-, ext-ar(-O-CO-), o-HO-phenyl-CH_2-CO-	7	20	54
$C_9H_{10}O$, 134.0731 CH_3O-phenyl-CH_2CH_2-, phenyl-CH_2-CO-CH_2-, cyc/unsatd ketones	9	13	55
C_8H_8NO, 134.0605 CH_3NH-phenyl-CO-, CH_3O-phenyl-CH=N-, CH_3-CO-N(phenyl)-, phenyl-CO-CH=N-	5	19	56
$C_9H_{12}N$, 134.0968 phenyl-N(C_2H_5)CH_2-, $C_2H_5(CH_3)_2$-pyridyl etc	4	20	56
$C_7H_6N_2O$, 134.0478 HO-ext-arN$_2$, ext-arO-NH-, -NH-phenyl-CO-N(-)-	3	20	54
$C_6H_6N_4$, 134.0589 ext-arN$_4$ (purines)	2	30	50
$C_7H_4NO_2$, 134.0241 HO-(CH_3-)pyridyl-CO-, -O-phenyl-CH=N-O-	3	12	56
$C_8H_{10}N_2$, 134.0842 C_2H_5NH-ext-arN,			

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	ar-amines	2	16	46

also $C_6H_4N_3O$, 134.0352 (-NHNH-pyridyl-CO-); $C_5H_2N_4O$, 134.0225 (HO-ext-arN_4); $C_6H_2N_2O_2$, 134.0114; C_7H_4NS, 134.0067 (benzothiazole)

m/z 135 (26%)		10%	23%	
$C_{10}H_{15}$, 135.1173	polyunsatd/cyc hc	13	20	79
$C_8H_7O_2$, 135.0445	HO-(CH_3-)phenyl-CO-, CH_3O-CO-phenyl-, CH_3O-phenyl-CO-	9	19	56
$C_9H_{11}O$, 135.0809	phenyl-OC(CH_3)$_2$-, ar/unsatd/cyc C=O/-O-/-OH	9	17	62
C_8H_9NO, 135.0683	H_2N-CO-phenyl-CH_2-, $HOCH_2$-(CH_3-)pyridyl-CH_2-, phenyl-CO-$NHCH_2$-, H_2N-(CH_3O-)phenyl-	4	17	60
$C_7H_5NO_2$, 135.0319	O_2N-phenyl-CH_2-, H_2N-(HO-)phenyl-CO-	3	23	50
$C_7H_3O_3$, 135.0082	-O-phenyl-CO-O-, ar C=O/-O-/-OH	3	18	50

also $C_9H_{13}N$, 135.1047 (ar-amines); $C_5H_3N_4O$, 135.0304 (ext-arN_3-NH-CO- etc); $C_6H_5N_3O$, 135.0430 (ext-arN_3(C=O)); $C_8H_{11}N_2$, 135.0920 (-CH_2NH-phenyl-NHCH_2-, aminopyridines); $C_6H_3N_2O_2$, 135.0193 (ext-arN_2O(C=O)); $C_7H_7N_2O$, 135.0556 (CH_3NH-CO-pyridyl-, -N(-)-phenyl-NH-CO-); C_4H_8Br, 134.9809 (Br-(CH_2)$_4$-); $C_5H_{11}O_4$, 135.0656 (sugars); $C_7H_9N_3$, 135.0794 (arN_3); $C_6H_7N_4$, 135.0667 (purines); $C_5H_5N_4$, 135.0541 (purine-NH-); $C_5H_5N_5$, 135.0541 (purine-NH-)

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
m/z 136 (20%)	6%	22%	
$C_{10}H_{16}$, 136.1251 polyunsatd/cyc hc	16	22	82
$C_9H_{12}O$, 136.0887 cyc/unsatd/ar HO-C=O/-O-	8	17	57
$C_8H_8O_2$, 136.0524 phenyl-CH_2-CO-O-, ar/unsatd/cyc C=O/-O-/-OH	8	16	50
$C_7H_4O_3$, 136.0160 HO-CO-(HO-)phenyl-, $(HO-)_2$phenyl-CO-, ext-arO(CO)-, cyc/substd/unsatd ketones	4	27	51
$C_7H_6NO_2$, 136.0397 H_2N-(HO-)phenyl-CO-, CH_3-pyridone-CO-, CH_3O-pyridyl-CO-, O_2N-phenyl-CH_2-	4	16	48
$C_9H_{14}N$, 136.1125 cyc/substd/unsatd amines	3	22	67
also $C_8H_{10}NO$, 136.0761 (CH_3O-phenyl-N(CH_3)-, CH_3O-phenyl-CH(NH_2)-; $C_5H_4N_4O$, 136.0382 (HO-ext-arN_4); $C_8H_{12}N_2$, 136.0998 (C_3H_7NH-pyridyl-); C_7H_6NS, 136.0223 (ext-arNS); C_8H_8S, 136.0350 (ext-arS); $C_7H_{10}N_3$, 136.0872 (($CH_3)_2$-pyrimidinyl-$NHCH_2$-); $C_6H_8N_4$, 136.0746 (H_2N-triazinyl-R); $C_5H_6N_5$, 136.0619 (H_2N-purines)			
m/z 137 (22%)	6%	22%	
$C_{10}H_{17}$, 137.1329 decahydronaphthyl	15	15	85
$C_8H_9O_2$, 137.0602 CH_3O-phenyl-CH(OH)-, CH_3-phenyl-CO-O-	9	25	55

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_9H_{13}O$, 137.0966	cyc/unsatd/substd C=O/-O-/-OH	11	16	68
$C_7H_5O_3$, 137.0238	$(HO-)_2$phenyl-CO-, HO-(-O-)phenyl-CH(OH)-	6	26	60
$C_7H_7NO_2$, 137.0475	H_2N-phenyl-CO-O-, phenyl-NH-CO-O-, HO-CO-phenyl-NH-	4	25	59
C_8H_9S, 137.0428	CH_3-phenyl-SCH_2-	2	31	83
$C_8H_{11}NO$, 137.0839	C_2H_5O-(CH_3-)-pyridyl-, CH_3O-(H_2NCH_2-)phenyl-	2	19	50
also $C_9H_{15}N$, 137.1203 (cyc/unsatd amines); C_7H_4NCl, 137.0031 (Cl-ext-arN-, Cl-phenyl-CH=N-); $C_4H_{10}O_3P$, 137.0367 (cyc-CH_2-CH(P(=O)$(OCH_3)_2$)-, $(C_2H_5O)_2P(=O)$-); $C_6H_3NO_3$, 137.0112 (HO-ar-(-O-)-NH-CO-, HO-CO-ar-NH-CO-); $C_7H_9N_2O$, 137.0713			
m/z 138 (17%)		4%	20%	
$C_{10}H_{18}$, 138.1408	cyc/unsatd hc	15	12	84
$C_8H_{10}O_2$, 138.0680	cyc/substd/unsatd C=O/-O-, (-CO-C_6H_{12}-CO-, cycR-O-CO-CH_3), CH_3O-(HO-)(CH_3-)-phenyl-	7	21	56
$C_9H_{14}O$, 138.1044	cyc/substd/unsatd ketones	8	17	57
$C_7H_6O_3$, 138.0316	HO-CO-phenyl-O-, -O-phenyl-O-CO-, etc	6	22	50

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
$C_9H_{16}N$, 138.1281 cyc/substd/unsatd amines, NC-C_8H_{16}-	6	19	61
$C_6H_6N_2O_2$, 138.0427 O_2N-phenyl-NH-, HO-CO-pyridyl-NH-, pyrimidione-C_2H_4-	2	38	48
$C_8H_{12}NO$, 138.0917 cyc/substd/unsatd amines/-O-, -furyl-N-	4	21	47
$C_7H_8NO_2$, 138.0554 cyc/ar/substd/unsatd amines/-O-/-OH/C=O, CH_3O-(HO-)(CH_3-)-pyridyl, ketolactam	3	18	50
also $C_7H_{10}N_2O$, 138.0791 (C_2H_5O-(CH_3-)-pyrimidinyl-)			
m/z 139 (22%)	6%	21%	
$C_{10}H_{19}$, 139.1486 cyc/unsatd hc	22	15	87
$C_9H_{15}O$, 139.1122 2-or 3-C_6H_{13}- cycloalkanone, -C_8H_{16}-CO-, cyc/substd ketones; and $C_{10}H_3O$, 139.0184 ext-ar(C=O)	9	18	66
C_7H_4OCl, 138.9950 Cl-phenyl-CO-	2	88	74
$C_7H_7O_3$, 139.0394 furanoates, ar -CO-O-/-O-	5	23	64
$C_8H_{11}O_2$, 139.0758 ar(C=O)-O-, cyc/unsatd C=O/-O-/-OH	5	16	58
$C_{10}H_5N$, 139.0421 ext-arN $C_9H_{17}N$, 139.1359 cyc/substd amines	4	12	63
$C_6H_3O_4$, 139.0031 HO-CO-furyl-CH_2O-,			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
	HO-CO-furyl-CO-, ar-O-/C=O	2	24	50
also $C_7H_9NO_2$, 139.0632 (arN-CO-O-, ar-NH-CO-O); $C_8H_{13}NO$, 139.0996; $C_6H_7N_2O_2$, 139.0506; $C_8H_{11}S$, 139.0584 (C_4H_9-thiophenyl-); C_7H_7OS, 139.0220 (HO-phenyl-S-CH_2-) C_8H_8Cl, 139.0314 (Cl-phenyl-(C_2H_5)-); $C_9H_3N_2$, 139.0295 (ext-arN_2); $C_6H_5NO_3$, 139.0268 (O_2N-phenyl-O-)			
m/z 140 (17%)		4%	16%	
$C_{10}H_{20}$, 140.1564 H-$C_{10}H_{20}$-Y*; and $C_{11}H_8$, 140.0626 naphthyl-CH_2-		16	8	84
$C_9H_{18}N$, 140.1438 cyc/substd/unsatd amines; and $C_{10}H_6N$, 140.0499 CH_3-quinolinyl, benzoazepinyl		9	12	71
$C_9H_{16}O$, 140.1200 cyc/substd/unsatd -CO-/-O-/-OH; and $C_{10}H_4O$, 140.0262 ext-ar(C=O)		8	11	62
$C_8H_{12}O_2$, 140.0836 cyc/substd/unsatd C=O/-O- etc		5	14	55
$C_8H_{14}NO$, 140.1074 cyc-C_6H_{11}-N(-CO-CH_3)-, cyc/unsatd amides, oximes, HO-amines, isocyanates		4	17	59
$C_7H_8O_3$, 140.0473 cyc/substd/unsatd -O-/C=O/-OH (CH_3O-pyrone-CH_2-)		4	20	60
also $C_7H_{10}NO_2$, 140.0710 (ar-NH-CO-OC_2H_5); $C_7H_{10}NS$, 140.0536 (ar-S-R, arNS); $C_9H_4N_2$, 140.0373 (ext-arN_2); $C_6H_8N_2O_2$, 140.0584 (unsatd amides, carbamates); $C_8H_{12}S$, 140.0662 (arS-R); $C_6H_4O_4$, 140.0109				

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 141 (23%)		6%	19%	
$C_{11}H_9$, 141.0704	naphthyl-CH_2-, ext-ar hc	24	18	90
$C_9H_{17}O$, 141.1278	C_8H_{17}-CO-, -CH(OH)-$(CH_2)_8$-; and $C_{10}H_5O$, 141.0340 -O-phenyl-ar-O-, ext-ar(C=O) etc	8	13	71
$C_8H_{13}O_2$, 141.0915	C_5H_{11}-CO-CH_2-CO-, CH_3O-CO-cyclohexyl(-)-, CH_3O-CO-$(CH_2)_3C{\equiv}CCH_2$-, $C_4H_9C(OCH_3)$=CH-CO-	5	14	60
$C_8H_{13}S$, 141.0741	cyc/substd/unsatd sulfides	2	37	56
$C_7H_9O_3$, 141.0551	ar/cyc/unsatd C=O/-O-/-OH	3	19	54
$C_7H_{11}NO_2$, 141.0788	R-ar(-CO-NH-CO-)-, succinimides	2	30	60
also $C_{10}H_7N$, 141.0577 (ext-arN); $C_9H_5N_2$, 141.0451 (ext-arN-N- etc); $C_6H_5O_4$, 141.0187 (cyc-CH(-CO-O-)-CH(-CO-O-)-); $C_7H_{11}NS$, 141.0614 (arN-S-); C_7H_6OCl, 141.0106 (HO-$(CH_3$-)(Cl-)phenyl-, HO-(Cl-)phenyl-CH_2-); $C_6H_5O_2S$, 141.0013 (phenyl-SO_2-, HO-phenyl-SO-); $C_6H_9N_2O_2$, 141.0662 ($(CH_3)_2$NC(=CH-CO-CH_3)-N(-)-); CH_2I, 140.9199 (iodo-CH_2-)			
m/z 142 (18%)		4%	19%	
$C_{11}H_{10}$, 142.0782	naphthyl-CH_2-, ext-ar hc	19	12	85

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
$C_{10}H_8N$, 142.0656 ext-arN (CH_3quinolines), naphthyl-NH-, -phenyl-cycN	7	23	68
$C_8H_{14}O_2$, 142.0993 CH_3O-CO-$(CH_2)_6$-, $(CH_3O)_2$-cyclohexyl-	4	14	54
$C_8H_{16}NO$, 142.1230 -$(CH_2)_7$-NH-CO-, CH_3-CO-N(C_5H_{11})CH_2-, HO-(R)-pyrollidinyl-; and C_9H_4NO, 142.0291 ext-arN(C=O) (quinolinonyl), ext-arN-O-	4	21	55
also $C_9H_6N_2$, 142.0529 (ext-arN_2, ext-arN-CH=N-); $C_8H_{18}N_2$, 142.1468 (C_8H_{17}-N(-)-N(-)-); $C_9H_{18}O$, 142.1357 (C_7H_{15}-CO-CH_2-); $C_{10}H_6O$, 142.0418 (ext-arO); $C_7H_{10}O_3$, 142.0629 (CH_3O-CO-C_4H_8-CO-); $C_7H_{12}NO_2$, 142.0866 (CH_3-CO-N(C_4H_9)-CO-); $C_6H_6O_2S$, 142.0091 (HO-phenyl-SO-, phenyl-SO_2-); $C_7H_{12}NS$, 142.0692 (arN-S-); $C_6H_{10}N_2S$, 142.0566 (R-imidazolyl-S-); C_7H_7OCl, 142.0184 (Cl-(CH_3-)phenyl-O-); C_6H_8NOS, 142.0329 (HO-(CH_3-)-pyrrolyl-S-CH_2-); $C_6H_{10}N_2O_2$, 142.0740 (cyc-$CH_2CH(OH)CH(CH_3)$N(-)-CO-N(CH_3)-); $C_6H_6O_4$, 142.0265 (C_2H_5O-CO-C(-)$_2CH_2$-CO-O-)			
m/z 143 (23%)	**6%**	**19%**	
$C_{11}H_{11}$, 143.0860 substd indenes, tetralins etc	18	15	82
$C_{10}H_9N$, 143.0734 naphthyl-NH-, quinolinyl-CH_2-, phenyl-pyrrolyl etc	7	18	66
$C_9H_7N_2$, 143.0607 ext-arN_2 (CH_3-quinoxalinyl-), NC-ext-arN, phenyl-C(-CN)=CH-NH-	6	19	69

m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
$C_9H_{19}O$, 143.1435 $(C_4H_9)_2C(OH)$-, $C_7H_{15}CH(OCH_3)$-	6	14	68
$C_7H_{11}O_3$, 143.0707 CH_3O-CO-C_4H_8-CO-, CH_3O-CO-CH_2CH_2-CH=$C(OCH_3)$-	5	16	63
$C_8H_{15}O_2$, 143.1071 CH_3O-CO-$(CH_2)_6$-, -$(CH_2)_5CH(-)O$-CO-, C_2H_5O-CO-$CH_2CH_2C(-)(C_2H_5)$-; and $C_9H_3O_2$, 143.0133 ext-ar-$(C=O)_2$-, ext-ar$(C=O)_2$	6	13	61
also C_9H_5NO, 143.0370 (phenyl-arN(C=O)); $C_6H_7O_4$, 143.0343 (-$CH(CH_3)$CH(-CO-OCH_3)-CO-O-); $C_6H_{11}N_2O_2$, 143.0818 (-$CH_2CH_2C(-CH_2-)$=N-NH-CO-OCH_3)			
m/z 144 (18%)	5%	22%	
$C_{11}H_{12}$, 144.0938 phenyl-$C_5H_7(-)$-, C_6H_{11}-phenyl-CH_2-, ext-ar	15	13	77
$C_{10}H_{10}N$, 144.0812 ext-arN ($(CH_3)_2$-indolinyl-), phenyl-arN	7	39	67
C_9H_6NO, 144.0448 indole-CO-, phenyl-isoxazolyl-	6	31	58
$C_{10}H_8O$, 144.0575 naphthyl-O-	8	20	63
$C_8H_{16}O_2$, 144.1149 C_2H_5O-CO-$C(C_2H_5)_2$-; and $C_9H_2O_2$, 144.0211 ext-ar$(C=O)_2$	5	17	60
$C_9H_8N_2$, 144.0686 C_2H_5-benzimidazolyl-, phenyl-C(CN)=CH-NH-	4	21	58
also $C_8H_4N_2O$, 144.0322 (HO-quinoxalinyl-); $C_6H_8O_4$,			

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
144.0422	$(-C(-O-CO-C_2H_5)_2)$; $C_7H_{14}NO_2$, 144.0123 $(HO-CO-(CH_2)_5-CH(NH_2)-)$; $C_6H_{10}NO_3$, 144.0659 $(-CH_2CH_2CH(-CO-OCH_3)-NH-CO-)$			
m/z 145 (23%)		9%	20%	
$C_{11}H_{13}$, 145.1017	phenyl-unsatd R, benzo-cycR	17	23	80
$C_{10}H_9O$, 145.0653	CH_3-phenyl-CH=CH-CO-, ext-ar-O-	9	18	64
$C_6H_9O_4$, 145.0500	CH_3O-CO-CH_2-CO-CH_2CH(OH)-, cyc-CH(-CO-OCH_3)-C(-)(-CO-OCH_3)-	3	25	64
C_9H_7NO, 145.0526	quinoline-O-, ext-arN-OH, ext-ar(-NH-CO-)	5	13	61
$C_{10}H_{11}N$, 145.0890	R-ext-arN, R-indolinyl-	4	17	61
$C_8H_5N_2O$, 145.0400	ext-arN(-N-CO-), HO-ext-arN_2-, phenyl-arN_2O	3	15	68
$C_9H_9N_2$, 145.0764	C_2H_5-benzimidazolyl-, phenylpyrazole	2	21	60
also $C_8H_{17}O_2$, 145.1227	$(C_5H_{11}OCH(OC_2H_5)-)$; $C_9H_5O_2$, 145.0289 (-O-ext-ar-CO-); $C_7H_{17}OSi$, 145.0947 $(CH_3)_3SiOCH(C_3H_7)-$, $C_5H_{11}OSi(CH_3)_2-$); $C_7H_3N_3O$, 145.0274 (ext-arN_2-NO); $C_6H_{13}O_2Si$, 145.0584 $(C_3H_7-CO-O-Si(CH_3)_2-)$; $C_6H_{11}NO_3$, 145.0737 (HO-CO-$CH(C_3H_7)$-NH-CO-); $C_6H_3Cl_2$, 144.9611 (Cl_2-phenyl-)			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
m/z 146 (19%)	5%	20%	
$C_{10}H_{10}O$, 146.0731 $(CH_3)_3$phenyl-CO-, phenyl-CH=CH-CO-CH_2-, benzocyclohexanones, cyc-C(C_2H_5)(phenyl)-CO-	8	24	58
$C_{10}H_{12}N$, 146.0968 benzo-cycN, -CH(-CH_2phenyl)NHCH(CH_3)-	6	25	70
$C_{11}H_{14}$, 146.1095 ar/cyc/unsatd hc	12	12	76
C_9H_8NO, 146.0605 HO-benzopyrrolyl-CH_2- etc, phenyl-CH_2CH(-)NH-CO-	5	29	60
$C_9H_6O_2$, 146.0367 HO-phenyl-CH=CH-CO-, phenyl-CH=C(-CO-OH)-, ext-ar$(C=O)_2$, cyc-CO-C(-)(phenyl)-CO-	6	21	65
$C_8H_6N_2O$, 146.0478 ext-arN_2-O-, ext-arN_2(C=O)	2	33	50
$C_8H_4NO_2$, 146.0241 o-CO-phenyl-NH-CO-, ext-arN$(C=O)_2$, HO-CO-benzopyrrolyl, HO-ext-arN(C=O)	2	24	61
$C_9H_{10}N_2$, 146.0842 $(CH_3)_2$N-phenyl-CH=N-, benzo-cycN_2-, H_2NCH_2-ext-arN	3	14	52
also $C_8H_8N_3$, 146.0716 (ext-arN_3); $C_6H_{10}O_4$, 146.0578 ((HO-CO)$_2$-C(C_3H_7)-)			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 147 (25%)		12%	23%	
$C_{11}H_{15}$, 147.1173	$(CH_3)_2$phenylC$(CH_3)_2$-, $(CH_3)_5$phenyl etc	15	23	76
$C_9H_7O_2$, 147.0445	phenyl-CO-CH_2-CO-, HO-phenyl-CO-CH=CH-, CH_3O-benzofuryl-	8	19	65
$C_{10}H_{11}O$, 147.0809	$(CH_3)_3$-phenyl-CO-, CH_3O-phenyl-CH_2CH=CH-, phenyl-CH_2CH(-)CH(OCH_3)-, substd/cyc/unsatd ketones	8	18	63
$C_8H_7N_2O$, 147.0556	oxazolyl-$NHCH_2$-, H_2N-NH-(CH_3-)phenyl-CO-, CH_3O-ext-arN_2	2	32	60
C_9H_9NO, 147.0683	$(CH_3)_2$phenyl-NH-CO-, -phenyl-CO-CH_2CH(NH_2)-, cyc-CH(CH_3)-N(phenyl)-CO-	3	20	54
also $C_{10}H_{13}N$, 147.1047 ($(C_2H_5)_2$N-phenyl-); $C_5H_{15}Si_2O$, 147.0400 (rearr; ≥2 $(CH_3)_3$SiO-groups); $C_8H_5NO_2$, 147.0319 (ext-ar(-CO-N-CO-)); $C_9H_{11}N_2$, 147.0920 ($(CH_3)_2$N-CH=N-phenyl-, ext-arN_2 amines); $C_8H_3O_3$, 147.0082 (-O-benzo-cyc-CH_2O-CO-); $C_7H_3N_2O_2$, 147.0193 (ext-arN_2(C=O)-CO-); C_9H_7S, 147.0271 (benzothiophenyl-CH_2-); $C_7H_5N_3O$, 147.0430 (ext-arN_3(C=O)); $C_7H_7N_4$, 147.0667 (ext-arN_4)			
m/z 148 (21%)		5%	18%	
$C_{11}H_{16}$, 148.1251	$(CH_3)_4$-phenyl-CH_2- etc	13	15	74
$C_9H_8O_2$, 148.0524	CH_3O-CO-CH_2-phenyl-,			

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m/z, comp Substructure, neighbor	Prop	Abnd	Spcf
-phenyl-CH_2-CO-OCH_2-, HO-phenyl-CH=CH-CO-O-	7	21	55
$C_9H_{10}NO$, 148.0761 phenyl-CO-NHCH(CH_3)-, $(CH_3)_2$N-phenyl-CH(OH)-	5	21	57
$C_{10}H_{12}O$, 148.0887 phenyl-CH_2CH_2-CO-CH_2-, cyc/unsatd/ar C=O/-O-/-OH	6	15	62
$C_8H_4O_3$, 148.0160 HO-CO-phenyl-CO-, -CH_2-(HO-)phenyl-CO-O-	3	26	49
$C_8H_6NO_2$, 148.0397 pyridyl-CO-CH_2-CO-, HO-CO-CH_2-pyridyl-, HO-N=CH-CH_2-phenyl-O-	3	21	46

also $C_8H_8N_2O$, 148.0635 (H_2N-NH-(CH_3-)phenyl-CO-); $C_{10}H_{14}N$, 148.1125 (arN, phenyl amines); $C_9H_{12}N_2$, 148.0998 (phenyl diamines); $C_7H_4N_2O_2$, 148.0271 (O_2N-phenyl-CH=N-); $C_6H_2N_3O_2$, 148.0145 (ext-arN_3(C=O)-O-); $C_6H_4N_4O$, 148.0382 (ext-arN_3-NO); $C_7H_8N_4$, 148.0746 (ext-arN_4, $(CH_3)_2$N-ext-arN_3); $C_6H_6N_5$, 148.0620 (purine-NH-CH_2-); $C_8H_{10}N_3$, 148.0872 (phenyl-NHC(=N-NHCH$_3$)-); C_6F_4, 147.9936 (tetrafluorophenyl)

m/z 149 (26%)	9%	19%	
$C_{11}H_{17}$, 149.1329 polyunsatd/cyc hc	12	18	81
$C_9H_9O_2$, 149.0602 phenyl-CH(OH)CH_2-CO-, ar C=O/-O-/-OH	8	16	64
$C_8H_5O_3$, 149.0238 phthalates, HO-CO-phenyl-CO-	5	21	59

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
$C_{10}H_{13}O$, 149.0966	cyc/substd/unsatd/ar C=O/-OH/-O-	7	15	67
$C_8H_7NO_2$, 149.0475	ON-CH_2-phenyl-CO-, arN-CH_2-CO-O-	3	18	51
also $C_9H_{11}NO$, 149.0839 (ar -O-/amines); $C_{10}H_{15}N$, 149.1203 (arN); $C_7H_5N_2O_2$, 149.0349 (ar); $C_9H_{13}N_2$, 149.1077 (C_2H_5NH-phenyl-NHCH$_2$-, pyrazines); $C_6H_3N_3O_2$, 149.0223 (ext-arN_3(C=O)$_2$); C_8H_7NS, 149.0301 (benzothiazole-CH_2-)				
m/z 150 (19%)		5%	20%	
$C_{12}H_6$, 150.0469	ext-ar hc	17	13	84
$C_9H_{10}O_2$, 150.0680	phenyl-CH(-CO-OCH_3)-, cyc/unsatd/ar C=O/-OH/-O-	7	14	59
$C_7H_4NO_3$, 150.0190	O_2N-phenyl-CO-, -O-phenyl-O-CO-NH-	2	60	68
$C_{10}H_{14}O$, 150.1044	cyc/unsatd ketones, phenyl -O-/-OH	5	20	57
$C_8H_6O_3$, 150.0316	phenyl -CO-O-/-OH/CH_3-/-CO-OH/-O-	4	20	53
$C_8H_8NO_2$, 150.0554	CH_3O-CO-NH-phenyl-, ar/cyc/unsatd amines/-CO-O-/C=O/-O-/-CO-NH-	4	24	58
also $C_{10}H_{16}N$, 150.1281 (cyc/substd amines); $C_7H_6N_2O_2$, 150.0427 (HO-CO-ext-arN_2, ON-phenyl-NH-CO-); $C_9H_{12}NO$, 150.0918 ((CH_3)$_2$N-(HO-)(CH_3-)phenyl-); $C_5H_2N_4O_2$, 150.0174 (O_2N-ext-arN_3); $C_7H_6N_2S$,				

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m/z, comp Substructure, neighbor Prop Abnd Spcf

150.0253 (ext-arNS-NH-); C_3F_6, 149.9904; $C_6H_2N_2O_3$, 150.0063 (O_2N-(-N-CO-)$_2$-ar-)

Note: The computer-aided correlations were carried out only for data from m/z 29 to m/z 150, inclusive.

m/z 151

$C_2Cl_2F_3$, 150.9329

$C_9H_{11}O_2$, 151.0758 $(HO)_2$phenyl-$C(CH_3)_2$-

$C_8H_7O_3$, 151.0720 $(CH_3O)_2$phenyl-CH_2, CH_3O-(HO)-phenyl-CO-, CH_3O-CO-phenyl-O-

also IC≡C-, CH_2-CH-(CH_3-)(Cl-)phenyl-, monoterpenones, $C_{12}H_7$

m/z 152

$C_{12}H_8$, 152.0626 -phenyl-phenyl-, phenyl-CH(-)-phenyl

also CH_3O-$C_7H_5O_2$, O_2N-(HO-)phenyl-CH_2-, CH_2=CH-CO-N(cyclohexyl)-, Cl-benzoxazolyl-, aporphine alkaloids

m/z 153

$C_9H_{10}Cl$, 153.0471 Cl-phenyl dvts

$C_{12}H_9$, 153.0704 phenyl-phenyl-, naphthyl-CH=CH-

also BrC_2H_4-CO-O-, $(CH_3O)_2$-phenyl-O-, CH_3O-phenyl-CO-O-, thiophenyl-CO-CH_2-CO-

m/z 154

H-CO-NH-(Cl-)phenyl-, $(phenyl)_2SiCl_2$,

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m/z, comp Substructure, neighbor Prop Abnd Spcf

CF_3-CO-N(C_2H_5)CH_2-, HO-(Cl-)(R-)phenyl-

m/z 155

Cl-(R-)phenyl-O-, Br-phenyl-, HO-(Cl-)phenyl-CO-, (C_2H_5O-)$_2$, P(=O)O-, C_4H_9O-P(=O)(-O-)$_2$, $C_3H_3{}^{81}BrCl$, C_5F_5, $C_3H_2BrF_2$, phenyl-(CH_3O-)PO-, naphthyl-CO-, CH_3-phenyl-SO_2-, C_4H_9O-CO-C_2H_2-CO-, (pyridyl)$_2$-, CH_3-naphthyl-CH_2-, $C_{11}H_{23}$

m/z 156

$C_8H_{17}N(CH_3)CH_2$-, etc, CH_3-quinolinyl-CH_2-, quinolinyl-CH_2CH_2-, Br-pyridyl-, $(C_4H_9)_2N$-CO-

m/z 157

$C_3H_5{}^{81}BrCl$, 156.9244; $C_3H_4BrF_2$, 156.9465; $(C_3H_7)_3Si$-, CH_3-phenyl-pyrazole-

m/z 158

$C_{11}H_{12}N$, 158.0969 (CH_3)$_2$-indole-CH_2-

$C_{12}H_{14}$, 158.1095 -phenyl-cyclohexyl-

m/z 159

$C_7H_5Cl_2$, 158.9768 Cl_2-phenyl-CH_2-, phenyl-CCl_2-
also $C_{12}H_{15}$, C_6H_8Br, CHFI

m/z 160

C_2BrF_3, CH_3O-indole-CH_2-, -Cl_2-phenyl-O-

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In Mass Spectral Correlations; McLafferty, F., el al.;
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m/z, comp Substructure, neighbor Prop Abnd Spcf

m/z 161

$C_{12}H_{17}$, 161.1329; CH_3-benzothiophene-CH_2-, BrC_6H_{10}-, C_3H_5-, CO-N(phenyl)-

m/z 162

$C_6H_4OCl_2$, 161.9639 Cl_2-phenyl-O-
also phenyl-N(C_4H_9)-CH_2-, phenyl-N(-CO-CH_3)CH(CH_3)-

m/z 163

$C_3Cl_2F_3$, 162.9329; $C_{11}H_{15}O$, 163.1122; $C_{10}H_{11}O_2$, $C_9H_7O_3$, $C_{12}H_{19}$, $C^{81}BrCl_2$, $(C_2H_5O)_3Si$-, $C_4H_4ClF_4$, C_3OClF_4, $C_{10}H_{13}ON$

m/z 164

C_6H_{11}-C_6H_9-, C_3H_5-(CH_3O-)phenyl-O-, H-CO-(CH_3O-)phenyl-O-, -fluorene-, berbines

m/z 165

$C_{13}H_9$, 165.0704 phenyl-CH(-)-phenyl-, -(CH_3-)phenyl-phenyl-
also $C_{10}H_{13}O_2$, $C_9H_9O_3$, aporphine alkaloids, $BrCH_2$-CO-OCH(CH_3)-, Cl-phenyl-CH=CH-CO-, Cl-benzofuran-CH_2-, $(C_2H_5O)_2P(=O)C_2H_4$-, C_5Cl_3

m/z 166

$C_{13}H_{10}$, 166.0782 $(phenyl)_2$-C(-)-
also $C_2Cl_3{}^{37}Cl$, -(C_3H_5-)(Cl-)phenyl-O-, carbazole-, O_2N-(HO-)phenyl-CO-, phenyl(-CO-O-)$_2$,

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m/z, comp Substructure, neighbor Prop Abnd Spcf

Cl-phenyl-N(C_3H_5)-

m/z 167

$C_2Cl_3F_2$, 166.9034

$C_{13}H_{11}$, 167.0860 (phenyl)$_2$-CH-, phenyl-CH_2-phenyl-, acenaphthenes

also Cl-phenyl-N(-$CH_2CH{=}CH_2$)-, $C_{10}H_{12}Cl$, Cl-(HO-)phenyl-, C_3H_4-, phenyl(-CO-O-)$_2$

m/z 168

-phenyl-O-phenyl-, (phenyl)$_2$-N-, C_9H_9OCl, O_2N-phenyl-O-, $C_8H_8O_4$, phenyl-NH-CO-, (phenyl)$_2$CH-

m/z 169

$C_{12}H_9O$, 169.0653 phenyl-phenyl-O-, phenyl-O-phenyl-, HO-(phenyl)$_2$-

also C_7H_6Br, 168.9653; $C_9H_{10}OCl$, 169.0420; (phenyl)$_2$N-, Cl-phenyl-Si(CH_3)$_2$-, naphthyl-C_3-, $Cl_2C_2H_3$-CO-OCH(CH_3)-, C_3H_5O-CO-C_4H_8-CO-, Cl-terpenoles, C_3F_7, $ClCH_2$-CO-N(phenyl)-, $C_{12}H_{25}$, -(Br-)(HO-)phenyl-

m/z 170

$C_{12}H_{10}O$, 170.0731 phenyl-phenyl-O-

also (C_5H_{11})$_2$NCH_2-, Br-phenyl-NH-, (pyridyl)$_2$N-, C_3H_7-(Cl-), phenyl-O-

m/z 171

$C_8H_5Cl_2$, 170.9768 -(Cl_2-phenyl)-CH(-)CH_2-,

m/z, comp Substructure, neighbor Prop Abnd Spcf

Cl_2-phenyl-CH=CH-

$C_{12}H_{11}O$, 171.0809 phenyl-phenyl-O-
also -CO-C_7H_{14}-CO-O-, F-phenyl-phenyl-, C_5ClF_4,
CH_3O-phenyl-SO_2-

m/z 172

C_6H_5OBr, 171.9524 Br-phenyl-O-

$C_8H_6Cl_2$, 171.9846 -Cl_2-phenyl-C_2H_3-

m/z 173

$C_8H_7Cl_2$, 172.9924 CH_3-(Cl_2-)phenyl-CH_2-,
Cl_2-phenyl-CH(CH_3)-, Cl_2-phenyl-CH_2CH_2-
also Cl_2-phenyl-CO-, $C_{13}H_{17}$, $CHBr^{81}Br$,
C_2H_5-CO-OCH_2CH(-O-CO-C_2H_5)-

m/z 174

CH_2=$CHCH_2$N(-CO-CH_3)phenyl-, $HBr^{81}BrC$-

m/z 175

$C_7H_5OCl_2$, 174.9717 Cl_2-phenyl-CH(OH)-,
Cl_2-(HO-)phenyl-CH_2-, Cl_2-(HO-)(CH_3-)phenyl-,
Cl-phenyl-OCH_2-

$C_{13}H_{19}$, 175.1486 R_n-phenyl, perhydropyrene
also $C_4Cl_2F_3$, phenyl-Si(Cl)$_2$-,
H_2C=C(Cl)CH_2O-CO-C_2H_4-CO-, $C_{12}H_{15}O$

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 176

$C_{12}H_{16}O$, 176.1201 cyclohexyl-phenyl-O-

m/z 177

$C_{12}H_{17}O$, 177.1279 C_4H_9-(HO-)phenyl-$CH(CH_3)$-,
C_4H_9-(CH_3O-)phenyl-CH_2-
also $C_2H_2{}^{81}BrCl_2$, C_2H_5O-CO-phenyl-CO-, $C_6H_{10}OBr$, CF_2I

m/z 178

$C_{14}H_{10}$, 178.0782 dihydroethanoanthracene,
-(phenyl)$_2$-C_2-
also $C_3Cl_3{}^{37}Cl$, HO-phenyl-$N(C_4H_9)CH_2$-,
phenyl-$CH(CH_3)N(C_2H_4OH)CH_2$-

m/z 179

$C_3Cl_3F_2$, 178.9034

$C_{14}H_{11}$, 179.0860 (phenyl)$_2$-C_2H-
also C_2BrF_4, CH_3O-CO-C_3H_5Br-, $C_2H^{81}BrClF_2$, $C_3HCl_3{}^{37}Cl$,
$C_{11}H_{15}O_2$, Cl_3-phenyl-

m/z 180

$C_9H_{10}NO_3$, 180.0660 O_2N-(HO-)phenyl-$C(CH_3)_2$-

$C_{14}H_{12}$, 180.0938 CH_3-phenyl-CH_2-phenyl-,
C_2H_5-(phenyl-)$_2$-, CH_3-(phenyl-)$_2CH$-, -(phenylCH-)$_2$-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 181

C_4F_7, 180.9888; phenyl-phenyl-CH(CH_3)-,
Cl(CH_3H_7-)phenyl-CH(CH_3)-, phenyl-phenyl-NO-

m/z 182

(phenyl)$_2$NCH_2-, (O_2N)$_2$-phenyl-NH-,
phenyl-CH_2-phenyl-NH-

m/z 183

C_7H_4BrO, 182.9446 Br-phenyl-CO-

C_8H_8Br, 182.9810 Br-phenyl-CH(CH_3)-

$C_{13}H_{11}O$, 183.0809 phenyl-O-phenyl-CH_2-, CH_3O-(phenyl)$_2$-,
phenyl-CH_2-phenyl-O-, (phenyl)$_2$-O-CH_2-
also (phenyl)$_2$SiH-, CF_3SSCF_2-

m/z 184

phenyl-CH_2-phenyl-O-, $C_{12}H_{26}N$, (O_2N)$_2$phenyl-O-,
H_2N-(Br-)phenyl-, -ON-phenyl-CO-CH_2-

m/z 185

C_4H_9O-CO-C_4H_8-CO-, $C_2Cl_3{}^{37}ClF$, -Cl-phenyl-OCH_2-CO-O-,
C_3ClF_6, $C_2HBr^{81}Br$, Br-(HO-)(CH_3-)phenyl-

m/z 186

phenyl-O-phenyl-O-, C_4H_9O-CO-C_4H_8-CO-, $C_2H_2Br^{81}Br$,
-Cl-(phenyl)$_2$-

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m/z, comp Substructure, neighbor Prop Abnd Spcf

m/z 187

$C_{14}H_{19}$, Cl_2-phenyl-$C(CH_3)_2$-, $C_2H_3Br^{81}Br$

m/z 189

$C_{14}H_{12}$, 189.1642; $C_8H_7OCl_2$, $C_{13}H_{17}O$,
CH_2=$CHCH_2O$-CO-phenyl-CO-

m/z 190

Cl-(O_2N-)phenyl-, NC-fluorene-

m/z 191

$C_{15}H_{11}$, 191.0860 anthracene-CH_2-, phenanthrene-CH_2-

$C_{14}H_{23}$, 191.1799 tetradecahydroanthracene-

$C_{13}H_{19}O$, 191.1435
also $C_4Cl_3F_2$, C_3H_6ClO-$SiCl_2$-, C_3BrF_4, $CBr^{81}BrF$,
$C_4HCl_3{}^{37}Cl$, $C_3H_4{}^{81}BrCl_2$, C_4ClF_4S, $^{81}BrCl$-phenyl-,
$C_2H_2F_2I$, C_3H_7O-CO-phenyl-CO-

m/z 192

CH_3O-phenyl-$N(C_4H_9)CH_2$-, -Cl_2-phenyl-CCl(-)-

m/z 193

$C_{15}H_{13}$, Cl_3-phenyl-CH_2-, $(C_2H_5O)_3SiOCH_2$-, $C_{12}H_{17}O_2$,
C_2H_5O-CO-C_3H_5Br-, trimellitic anhydride esters

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 194

$C_4Cl_2F_4$, C_2H_5O-CO-phenyl-CO-O-, -(Cl_3-)(HO-)phenyl-

m/z 195

$C_{15}H_{15}$, Cl_3-phenyl-O-, CH_3-phenyl-CO-phenyl-, (CH_3)$_2$-phenyl-O-P(=O)(-O-phenyl-CH_3)-, $C_{12}H_{16}Cl$, CF_3-phenyl-CF_2-, Br-phenyl-C_3H_3-

m/z 196

Cl_3-phenyl-O-, phenyl-CH_2N(phenyl)CH_2-, phenyl-(CH_3-)-2-pyridonyl-

m/z 197

Br-phenyl-C(CH_3)$_2$-, $C_2{}^{81}BrClF_3$, HO-phenyl-CO-phenyl-, HO-(O_2N-)$_2$phenyl-CH_2-, CH_3-phenyl-O-CH_2-, C_4ClF_6, C_4H_9-(Cl-)phenyl-O-CH_2-, Br-CO-$C_2H_3{}^{81}$Br-, (phenyl)$_2$Si(CH_3)-, $C_{15}H_{17}$

m/z 198

(C_6H_{13})$_2$NCH_2-, HO-(O_2N-)$_2$phenylCH_2-, (CH_3)$_2$N-CO-NH-(Cl-)phenyl-

m/z 199

$C_3H_3Br^{81}Br$, Br-(HO-)phenyl-CO-, Cl_2-benzofuran-CH_2-, $C_3HCl_3F_3$

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 200

-Cl-(CH_3-)(phenyl)$_2$-, Y*-$C_3H_4Br^{81}Br$-

m/z 201

$C_3H_5Br^{81}Br$, $C_2HOBr^{81}Br$, Cl-phenyl-CH_2-phenyl-, $C_3Cl_2F_5$, $C_2Cl_4{}^{37}Cl$, $(C_4H_9)_2(CH_3)_2Si_2H$-, $C_{16}H_9$

m/z 202

Hg, -(Cl-)phenyl-O-phenyl-, Cl_2-ext-ar-OCH_3

m/z 203

$Cl_2(CH_3)_3$-phenyl-O-, Cl-phenyl-O-phenyl-, Cl-(HO-)phenyl-phenyl-, Cl-phenyl-phenyl-O-, $C_{15}H_{23}$ (B/C/D rings of cholestane)

m/z 204

phenanthrene-cyc hc, $C_4H_5{}^{81}BrCl_2$, TMS dvts of pyranosides

m/z 205

phenyl -O-/-OH, sesquiterpenones, $C_7H_5{}^{81}BrCl$, C_4H_9O-CO-phenyl-CO-, C_6F_7, C_2H_5O-C_6H_9Br-, Br-phenyl-CF_2-, Br-naphthyl-

m/z 206

C_4H_9-(C_3H_5O-)phenyl-O-, Cl_3-phenyl-CH(-)CH_2-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 207

phenyl C=O/-O-/-OH, Cl_3-phenyl-$CH(CH_3)$-,
methysiloxanes, $CBr^{81}BrCl$, $C_{16}H_{15}$

m/z 208

Pb, 207.9766; OCN-phenyl-CH_2-phenyl-,
phenyl-phenyl-OC_3H_3-

m/z 209

R-(Cl-)phenyl, $C_{12}H_{14}ClO$, $C_4Cl_3{}^{37}ClF$, $C_{15}H_{13}O$,
CH_3-(phenyl-CO-phenyl)-CH_2-, Cl_3-(HO-)-phenyl-,
$C_3{}^{81}BrClF_3$, C_3H_7O-CO-phenyl-CO-O-

m/z 210

O_2N-phenyl-CH=CCl-CO-

m/z 211

HO-phenyl-phenyl-$C(CH_3)_2$-, HO-$(O_2N-)_2$phenyl-$CH(CH_3)$-,
C_3HBrF_5, $(C_4H_9O)_2P(=O)O$-, $C_2H^{81}BrCl_3$, $C_4HCl_3F_3$,
phenyl-phenyl-$Si(CH_3)_2O$-, C_5H_{11}-naphthyl-CH_2-

m/z 212

C_3H_5-(Br-)phenyl-O-, phenyl-O-phenyl-C_3H_6-

m/z 213

$C_4Cl_2F_5$, HO-(Br-)phenyl-$C(CH_3)_2$-, $C_3Cl_4{}^{37}Cl$,
$C_2{}^{81}BrCl_2F_2$, $C_4H_5Br^{81}Br$, $(CF_3)_2$-phenyl-,

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

$Cl(phenyl)_2$-CH=CH-, Δ-5-(HO-) steroid A/B/C rings, $C_6H_{13}O$-CO-C_4H_8-CO-

m/z 215

$C_{16}H_{23}$:Y*-steroid A/B/C rings, $C_4H_7Br^{81}Br$, Cl_2-$(C_2H_5-)_2$phenyl-CH_2-, $Cl_3{}^{81}Cl$-phenyl-, CH_3-benzanthracenyl-

m/z 217

$C_{16}H_{25}$:steroid A/B/C rings, R-phenyl, Cl_2-(CH_3O-)phenyl-$C(CH_3)_2$-, Cl-(CH_3O-)phenyl-phenyl-, CH_3Hg-, $(phenyl-O)_2P$-, $C_3Cl_3F_4$, TMS dvts of furanosides

m/z 218

I-(HO-)phenyl-, $(C_4H_9)_2$NCH(phenyl)-

m/z 219

$C_2Br^{81}BrCl$, C_4F_9, -Cl_2-phenyl-OCH_2-CO-O-, Br-phenyl-SO_2-, ^{81}BrCl-phenyl-R-

m/z 220

Cl-phenyl-O-phenyl-O-, $(CH_3)_2$N-CO-(C_4H_9-)phenyl-, C_4H_9-$(cyclohexyl)_2$-

m/z 221

$C_6H_{17}O_3Si_3$, $(phenyl)_2$-C_5H_7-, Cl_2-$(phenyl)_2$-, $(H_3CO-CO-)_2$phenyl-CO-, C_4ClF_6, Cl_2-$(CH_3O-)_2$phenyl-O-,

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spfc

Cl_3-(C_2H_5-)phenyl-CH_2-, phenyl-CO-CH=C(phenyl)CH_2-, Cl_3-2,3-dihydrobenzofuryl-, Cl_2-phenyl-OCH_2-CO-O-, $C_2H_2Br^{81}BrCl$

m/z 222

C_4BrF_5, $C_5Cl_3F_3$

m/z 223

CH_3Pb, C_3H_7-(phenyl)$_2$-$CH(CH_3)$-, Cl-(C_3H_7-)$_2$phenyl-$CH(CH_3)$-, C_4H_9-(O_2N-)$_2$phenyl-, C_4H_9O-CO-phenyl-CO-O-, $C_4ClF_4S_2$, -(C_3H_7-)(phenyl)$_2$-$CH(CH_3)$-, Cl_3-phenyl-$OCH(CH_3)$-, $C_{10}H_{21}$-cyclohexyl-

m/z 224

-$C_{15}H_{30}CH(C_5H_{11})$-, C_4H_9O-(phenyl)$_2$-, C_6F_8

m/z 225

Cl-(C_4H_9-)(HO)phenyl-$C(CH_3)_2$-, $C_4Cl_4{}^{37}Cl$, $C_3{}^{81}BrCl_2F_2$, C_5H_{11}-naphthyl-$CH(CH_3)$-, HO-(O_2N-)$_2$phenyl-$C(CH_3)_2$-, Br-(C_3H_7-)phenyl-$CH(CH_3)$-, phenyl-O-CO-phenyl-CO-, phenyl-O-phenyl-C_4H_8-, $C_5Cl_2F_5$, $C_{15}H_{31}CH(C_5H_{11})$-

m/z 226

$(C_7H_{15})_2NCH_2$-, $C_{18}H_{10}$, (phenyl)$_2$-O-C_3H_4(OH)-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 227

$C_{18}H_{11}$-, C_4H_9-(HO-)(Br-)phenyl-

m/z 228

$C_{18}H_{12}$, -$C_5H_8Br^{81}Br$-

m/z 229

$Cl_3{}^{37}Cl$-(CH_3-)phenyl-, $C_5H_9Br^{81}Br$-, $C_3H^{81}BrClF_4$, BrHC=$C^{81}BrC(OH)(CH_3)$-, $C_{11}H_{13}Si_3$, Cl_3-phenyl-O-Y-^{37}Cl, $C_4HCl_3{}^{37}ClF_2$, $C_4Cl_3F_4$, $(phenyl)_3$-, $F_3CCClFC(CF_3)(OCH_3)$-

m/z 230

C_6H_{13}-CO-N(phenyl)-C_3H_4-

m/z 231

$(C_4H_9)_2$-phenyl-$C(CH_3)_2$-, ClC_2H_4O-(Cl-)phenyl-$C(CH_3)_2$-, phenyl-$CH(C_{10}H_{21})$-, perhydrobenzanthracene-, ClC_3H_4O-CO-C_2H_4-CO-OC_3H_4-, C_2H_5Hg-, C_5F_9, ICH_2CH(phenyl)-, $Cl_3{}^{37}Cl$-(HO-)phenyl-

m/z 233

disbustd(HO-)steroid A/B/C rings, Cl_3-benzofuran-CH_2-, $(ClC_2H_4O)_2POC_2H_4$-, Br$(phenyl)_2$-, C_7ClF_6, $(phenyl\text{-}O)_2P(=O)$-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 234

-Br^{81}Br-phenyl-

m/z 235

(Cl-phenyl)$_2$CH-, $C_3Cl_3{}^{37}ClF_3$, Br$_2$-phenyl-, ClC_3H_6O-Si(Cl$_2$)OC_2H_4-, (cyclohexyl-C_2H_4-)$_2$CH-, $Cl_3(C_2H_5)_2$-phenyl-

m/z 236

HO-(O$_2$N-)phenyl-C_7H_{14}-, -(Cl$_2$-)-phenyl-O-phenyl-, CH_2=CH-S-(Cl$_3$-)phenyl-Cl$_3$(C_3H_5)-phenyl-O-, -$C_{12}H_{23}$-(C_5H_9)-, -(Br$_2$-)(CH_3-)(HO-)phenyl-, C_7F_8

m/z 237

C_2H_5Pb, C_8H_{17}-thiophenyl-C(CH_3)$_2$-, Cl-(C_3H_7-)$_2$(CH_3-)phenyl-CH(CH_3)-, Cl$_2$-phenyl-O-phenyl-

m/z 238

(CH_3)$_2$Pb

m/z 239

$^{81}BrCl_3$-phenyl-CH_2-, C_5H_{11}-naphthyl-C_3H_6-, phenyl-SiH_2-phenyl-Si(CH_3)$_2$-, $C_{19}H_{11}$, $C_{17}H_{35}$, $C_4H_5{}^{81}BrCl_3$, phenyl-O-phenyl-C_5H_{10}-, $C_{15}H_{31}$-CO-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 240

$C_5Cl_3{}^{37}ClF_2$, $C_{19}H_{12}$, Cl_3-phenyl-OCH_2CH_2O-

m/z 241

$Br^{81}Br$-cyclohexyl-, C_4BrF_6, $C_5Cl_3F_4$,
$ClC_2H_4OC_2H_4O$-phenyl-$C(CH_3)_2$-, benzophenanthrene-CH_2-,
$^{81}BrCl_2$-(HO-)phenyl-, C_4H_9O-CO-C_8H_{16}-CO-,
$C_5HCl_3{}^{37}ClF_2$, $CHBr{=}CBrC(OH)(C_2H_5)$-

m/z 243

Cl_2-$(C_2H_5$-$)_3$-phenyl-CH_2-, Cl_2CH-phenyl-$CCl^{37}Cl$-,
$(phenyl)_3C$-, Cl_3-phenyl-SO_2-, C_6F_9

m/z 244

$(phenyl)_2N$-phenyl-

m/z 245

tetrahydronaphthacene-CH_2-, perhydronaphthacene-,
$(CF_3CH_2O$-$)_2P(=O)$-, C_3H_5O-$(C_4H_9)_2$-phenyl-

m/z 247

$Cl_3{}^{37}Cl$-(HO-)phenyl-O-, C_5ClF_8, $C_4Cl_3{}^{37}ClF_3$

m/z 248

$(C_2H_5)_4$-cyc-Si_3O_3-, -$(phenyl)_2$-C_2Cl_2-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 249

Cl_3-(C_2H_5-)$_2$-phenyl-CH_2-, $Br^{81}Br$-phenyl-CH_2-,
(ClC_3H_6O-)$_2$SiCl-, $C_6Cl_4{}^{37}Cl$, $C_3HCl_5{}^{37}Cl$,
(ClC_2H_4O-)$_2$P(=O)OC_2H_4-, $C_7Cl_2F_5$, (OCN-phenyl-)$_2$CH-

m/z 250

$Br^{81}Br$-(H_2N-)phenyl-

m/z 251

$CBr_2{}^{81}Br$, trisubstd ketosteroids,
Cl-(C_4H_9-)$_2$phenyl-$CH(CH_3)$-,
(phenyl)$_2$-$C(CH_3)_2CH_2C(CH_3)_2$-, $C_3Cl_4{}^{37}ClF_2$,
$Br^{81}Br$-(HO-)phenyl-$C_6H_{11}CH_2CH(C_{10}H_{21})$-

m/z 253

$(CH_3)_3Pb$, Cl_2-phenyl-$C_2H_3{}^{81}Br$-

m/z 254

I_2(iodine)

m/z 255

$C_2HBr^{81}BrCl_2$, CH_3-benzanthracene-CH_2-

m/z 256

$C_6Cl_2F_6$, S_8(255.7766, sulfur)

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 257

$C_{19}H_{29}$, $Cl_3{}^{37}Cl$-(C_2H_5-)phenyl-CH_2-

m/z 259

$Cl_5{}^{37}Cl$-cyclohexyl, $C_5Cl_3{}^{37}ClF_3$, $C_4H_3{}^{81}BrCl_2F_3$,
(CH_3-)$_2$phenyl-CH($C_{11}H_{21}$)-,
ClC_4H_8O-(Cl-)phenyl-C(CH_3)$_2$-

m/z 260

$C_4Cl_5{}^{37}Cl$

m/z 261

$C_4Cl_3F_4S$, $C_5HCl_3F_5$

m/z 262

-(Br^{81}Br-)phenyl-CO-, C_6F_{10}

m/z 263

$Cl_4{}^{37}Cl$-phenyl-CH_2-, Br^{81}Br-phenyl-CH(CH_3)-, $C_2Br_2{}^{81}Br$

m/z 264

$C_2HBr_2{}^{81}Br$, -(CH_3-)cyclohexyl-CH($C_{11}H_{23}$)-

m/z 265

$C_2H_2Br_2{}^{81}Br$, (C_3H_7-)$_2$(phenyl)$_2$-CH(CH_3)-, $C_{17}H_{33}$-CO-,
C_7H_{13}CH($C_{11}H_{23}$)-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 266

$Cl_4{}^{37}Cl$-phenyl-O-, $(CF_3)_2$-triazine-CF_2-, CI_2

m/z 267

C_4H_9-phenyl-O-phenyl-$C(CH_3)_2$-,
ClC_3H_6O-(C_4H_9-)phenyl-$C(CH_3)_2$-, $C_2H_5Pb(CH_3)_2$-, CHI_2,
$C_{17}H_{35}CO$-, $C_4Cl_3F_6$, $(naphthyl)_2$-CH-

m/z 268

$(C_8H_{17})_2N$-CO-, C_8F_9

m/z 269

$C_6H_4BrF_6$, $C_{19}H_{27}O$(Y*$_2$-hydroxyketosteroid),
$Br^{81}Br$Cl-phenyl-, $C_{15}H_{21}Si_2$, C_5F_{11}

m/z 271

$C_{19}H_{27}O$(Y$_2$*-diketosteroid, CF_3Hg, CF_3-$(phenyl)_2$-CF_2-,
Cl_3-phenyl-O-phenyl-

m/z 272

$C_5Cl_5{}^{37}Cl$

m/z 273

$C_{19}H_{29}O$(Y*-hydroxysteroid), Br-(CF_3-)phenyl-CF_2-,
$C_3HBr^{81}BrF_4$

m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 274

C_7F_{10}

m/z 275

$C_5Cl_4{}^{37}ClF_2$, C_4H_9-phenanthrenyl-$C(CH_3)_2$-,
$C_4{}^{81}BrCl_2F_4$, $(CF_3CH_2O)_2P(=O)OCH_2$-,
C_4H_9O-CO-CH_2O-(Cl_2-phenyl)-

m/z 276

-(^{37}Cl-)phenyl-C_2Cl_4-

m/z 277

$CCl_2{}^{37}Cl$-phenyl-CCl_2-, $(C_2H_5)_5$-cyclotrisiloxane-,
$Br^{81}Br$-dihydrobenzofuryl-, $Br^{81}Br$-phenyl-$C(CH_3)_2$-,
dibenzoanthracenyl-

m/z 278

-C_6H_{10}-$CH(C_{13}H_{27})$-

m/z 279

$C_3H_4Br_2{}^{81}Br$, naphthyl-$CH(C_{10}H_{19})$-, $C_5HCl_3{}^{37}ClF_4$

m/z 280

-$(C_9H_{18})CH(C_{10}H_{21})$-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 281

$(CH_3)_7Si_4O_4$-, $CH_3(C_2H_5)_2Pb$, $(C_3H_7$-$)_3(phenyl)_2$-,
$C_9H_5F_8O$, C_6H_{13}-phenyl-O-phenyl-C_2H_4-,
$C_{10}H_{21}CH(C_9H_{19})$-, $Cl_4{}^{37}Cl$-phenyl-S-, C_6F_{11}

m/z 283

$Br^{81}Br$-phenyl-CHCl-

m/z 284

$C_6Cl_5{}^{37}Cl$

m/z 285

tetrahydronaphthyl-$CH(C_{10}H_{21})$-, $C_8H_2F_9O$

m/z 286

phenyl-Bi-, C_8F_{10}

m/z 287

$C_{14}H_{29}CH$(phenyl)-

m/z 291

$C_5H^{81}BrClF_6$, decahydronaphthyl-$CH(C_{10}H_{21})$-

m/z 292

$Br^{81}BrC_3H_5$-phenyl-O-

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf

m/z 293

$Br^{81}Br$-(HO-)phenyl-$C(CH_3)_2$-,
$C_4H_6Br_2{}^{81}Br$-(HO-)phenyl-$C(CH_3)_2$-, $C_4H_6Br_2{}^{81}Br$, C_7F_{11},
$(naphthyl)_2C{=}CHCH_2$-, $(ClC_3H_6O)_2SiCl$-OC_2H_4-

m/z 294

$Br^{81}Br$-(C_3H_5-)phenyl-O-, -$(C_{10}H_{20})$-$CH(C_{10}H_{21})$-

m/z 295

Cl_3-phenyl-$OP(=S)^{37}Cl$-, C_6H_{13}-phenyl-O-phenyl-C_3H_6-,
$(C_2H_5)_3Pb$-, $(C_{10}H_{21})_2CH$-

m/z 297

$C_5Cl_3{}^{37}ClF_5$

m/z 299

C_4H_9-pyrene-$C(CH_3)_2$-

m/z 301

$C_2HBr^{81}Br_2Cl$

m/z 305

C_8F_{11}

m/z 307

(C_5H_{11}-phenyl-)$_2CH$-, $C_5Cl_6{}^{37}Cl$

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 309				
$C_{17}H_{35}CH(C_4H_9)$-				
m/z 311				
Cl_3C-(Cl-)phenyl-$CCl^{37}Cl$-				
m/z 312				
C_7F_{12}				
m/z 313				
$Br_2{}^{81}Br$-phenyl-, $C_5Cl_4{}^{37}ClF_4$				
m/z 315				
$C_3H_3Br^{81}Br_2Cl$				
m/z 317				
C_9F_{11}				
m/z 319				
$C_6Cl_6{}^{37}Cl$, C_6F_{13}				
m/z 324				
$(CF_3CH_2O)_2P(=O)OC_2HF_2(-)$-, C_8F_{12}				

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 325				
	(HO-)(C_4H_9-)(phenyl-)$_2$C(CH_3)-			
m/z 327				
	(C_4H_9O-CO-)$_2C_3H_3$-CO-OC_3H_6-, $Br_2{}^{81}$Br-phenyl-CH_2-			
m/z 329				
	$C_{17}H_{35}$CH(phenyl)-			
m/z 331				
	$C_{21}H_{23}Si_2$, C_7F_{13}			
m/z 337				
	$C_{21}H_{43}$CH(C_2H_5)-			
m/z 341				
	$CCBr_2{}^{81}$Br-phenyl-CH(CH_3)-			
m/z 343				
	$Br_2{}^{81}$Br-(HO-)(CH_3-)phenyl-, C_8F_{13}			
m/z 345				
	$C_2HBr_2{}^{81}Br_2$, I_2-(HO-)phenyl-			
m/z 355				
	silicones, C_9F_{13}			

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m/z, comp	Substructure, neighbor	Prop	Abnd	Spcf
m/z 359				
$C_3H_3Br_2{}^{81}Br_2$				
m/z 367				
$C_{10}F_{13}$				
m/z 368				
-cholestene-				
m/z 369				
C_7F_{15}				
m/z 370				
-cholestane-				
m/z 381				
C_8F_{15}				
above m/z 400				

m/z 405, $C_{10}F_{15}$; m/z 412, C_9F_{16}; m/z 417, $C_{11}F_{15}$; m/z 424, $C_{10}F_{16}$; m/z 429, silicones; m/z 431, C_9F_{15}; m/z 436, $C_{11}F_{16}$; m/z 443, $C_{10}F_{17}$; m/z 447, $C_4Br_3{}^{81}Br_2$; m/z 448, $C_{12}F_{16}$; m/z 455, $C_{11}F_{17}$; m/z 462, $C_{10}F_{18}$; m/z 467, $C_{12}F_{17}$; m/z 469, C_9F_{19}; m/z 474, $C_{11}F_{18}$; m/z 481, $C_{10}F_{19}$; m/z 486, $C_{12}F_{18}$; m/z 493, $C_{11}F_{19}$; m/z 505, $C_{12}F_{19}$; m/z 512, $C_{11}F_{20}$; m/z 517, $C_{13}F_{19}$; m/z 524, $C_{12}F_{20}$; m/z 531, $C_{11}F_{21}$;

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m/z 536, $C_{13}F_{25}$; m/z 543, $C_{12}F_{12}$; m/z 555, $C_{13}F_{21}$;
m/z 562, $C_{12}F_{22}$; m/z 567, $C_{14}F_{21}$; m/z 574, $C_{13}F_{22}$;
m/z 581, $C_{12}F_{23}$; m/z 593; $C_{13}F_{23}$; m/z 605, $C_{14}F_{23}$;
m/z 617, $C_{15}F_{23}$; m/z 631, $C_{13}F_{25}$; m/z 643, $C_{14}F_{25}$.

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Mass spectral correlations

DATE LOANED	BORROWER'S NAME	DATE RETURNED

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ABBREVIATIONS

aliph	aliphatic
ar	aromatic ring
arY	an aromatic (or polyunsaturated) ring containing Y (as indicated) in the ring; ar(C=O) could be quinone, pyrone, etc
ar-Y	a Y-group attached to an aromatic ring
CH_3, CH_2, CH, C	saturated carbon atoms bearing one, two, three, and four substituents, respectively
cleav	cleavage
cntd	continued
corresp	corresponding
cpd	compound
C=O	carbonyl
cyc	a nonaromatic ring; groups listed next can be part of ring
cycR	a nonaromatic cycloalkyl group
cycY	a nonaromatic cyclic group containing Y (as indicated) in the ring
cyc-Y	a Y group attached to an alicyclic ring
decom	decomposition
dvts	derivatives
esp	especially
etc	et cetera (similar or expected structures)
ext-ar	extended aromatic: more than one ring, one is ar; ext-ar(C=O) includes tropolone, benzoquinone, indanone
gp	group
hc	hydrocarbon
mult	multiple
N	nitrogen bearing three substituents
-O-	oxygen (not -OH)
R	hydrocarbon moiety (usually alkyl, can be H)
R*	hydrocarbon moiety plus Y* (see below)
rearr	rearrangement
satd	saturated
slash,/	"and/or"
substd	substituted
TMS	trimethylsilyl
unsatd	unsaturated
X	any halogen atom
Y	a functional group
Y_n	one or more Y groups
Y*	an electronegative functional group: X, $-NO_2$, -CN, -COOR, -COR, -O-CO-R, -OH, -SH, $-SO_2X$, etc
Z	another group or combination of several Ys

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