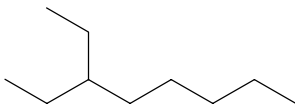
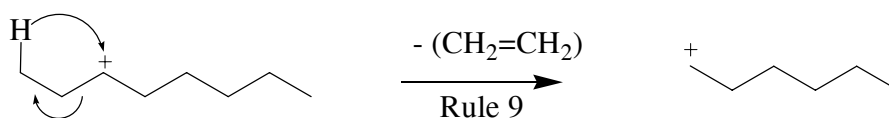
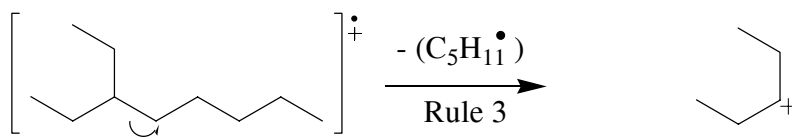
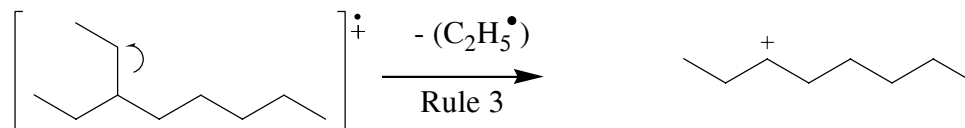
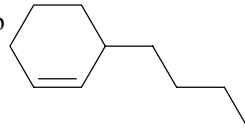
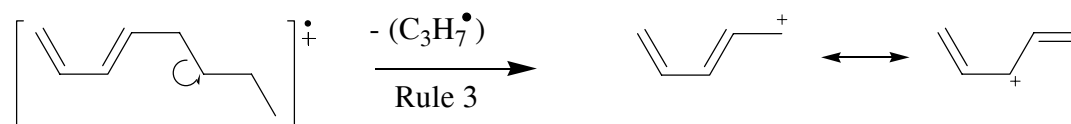
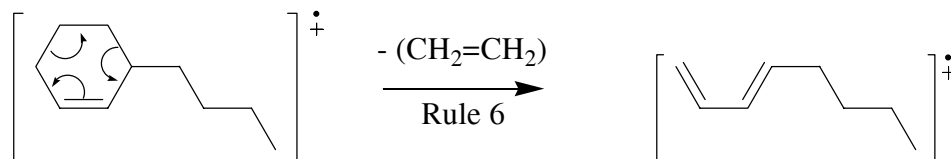
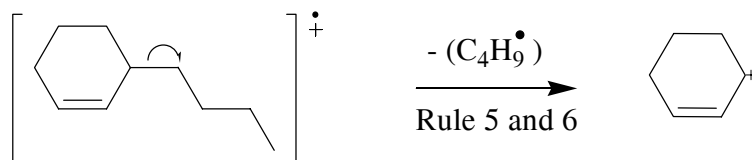
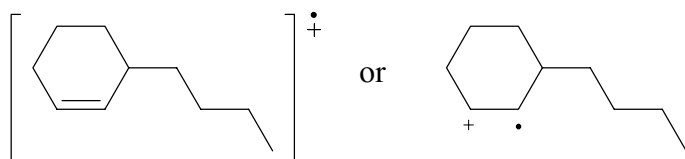
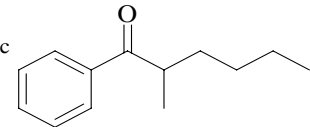


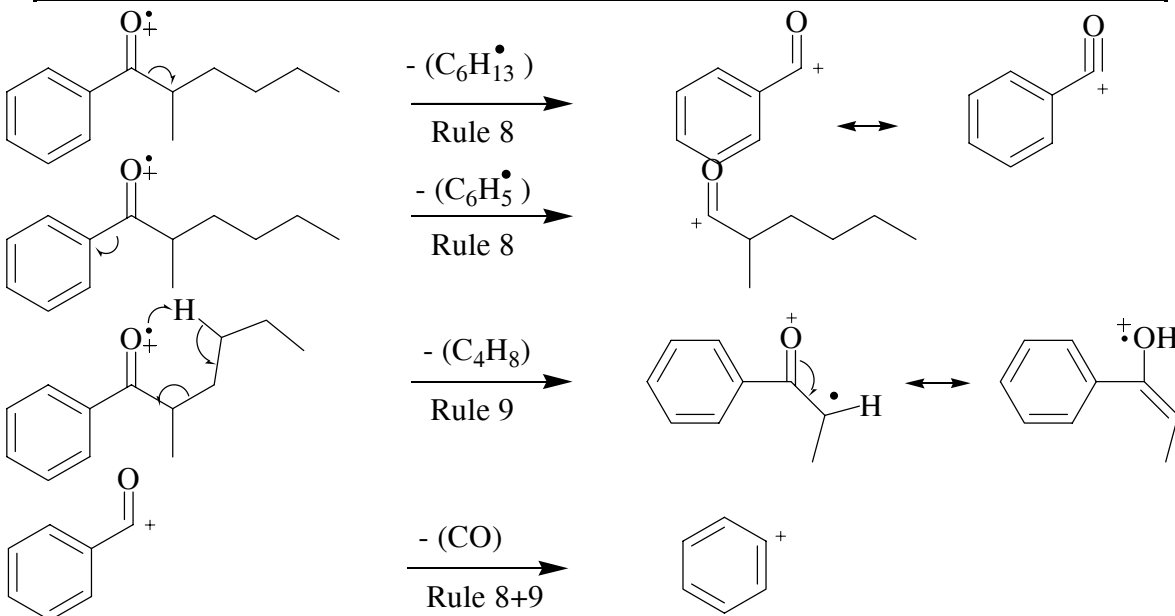
<p>a</p>  <p>3-ethyloctane $C_{10}H_{22}$</p> <p>$C_nH_mX_xN_yO_z$ IHD</p> <p>Index = $(n) - (m/2) - (x/2) + (y/2) + 1 =$ 0</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	22	1.00783	22.17226
	Carbon	10	12.00000	120.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	0	15.9949	0.00000
	Sulfur	0	31.9721	0.00000
Bromine	0	78.9183	0.00000	
Exact Mass				142.17226

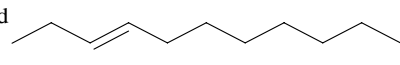


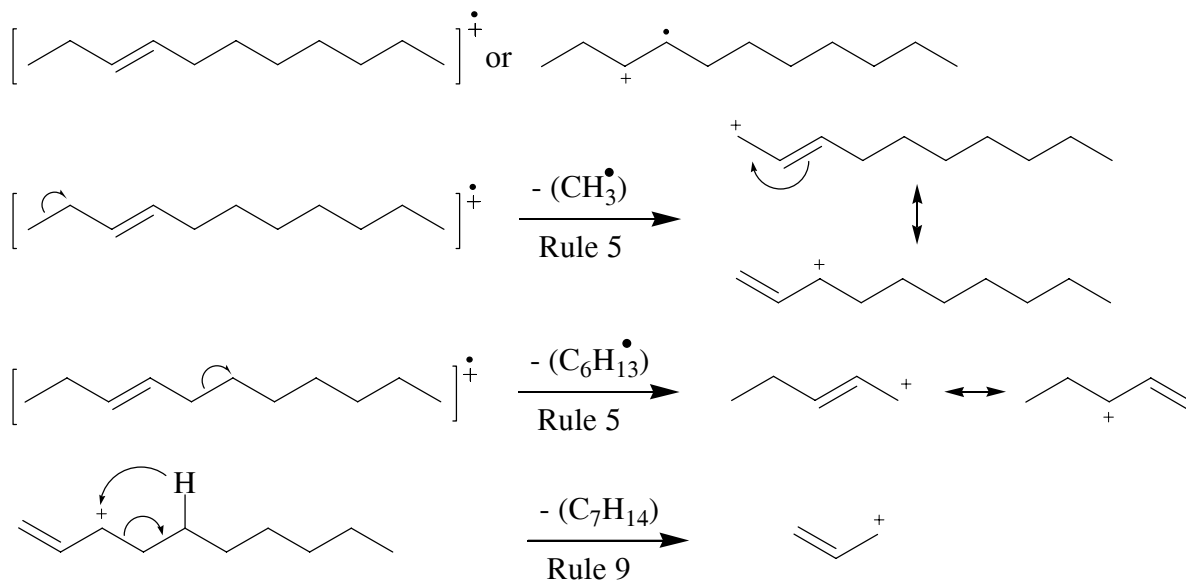
<p>b</p>  <p>3-butylcyclohex-1-ene $C_{10}H_{18}$</p> <p>$C_nH_mX_xN_yO_z$ IHD</p> <p>Index = $(n) - (m/2) - (x/2) + (y/2) + 1 =$ 2</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	18	1.00783	18.14094
	Carbon	10	12.00000	120.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	0	15.9949	0.00000
	Sulfur	0	31.9721	0.00000
Bromine	0	78.9183	0.00000	
Exact Mass				138.14094

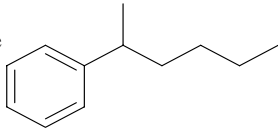


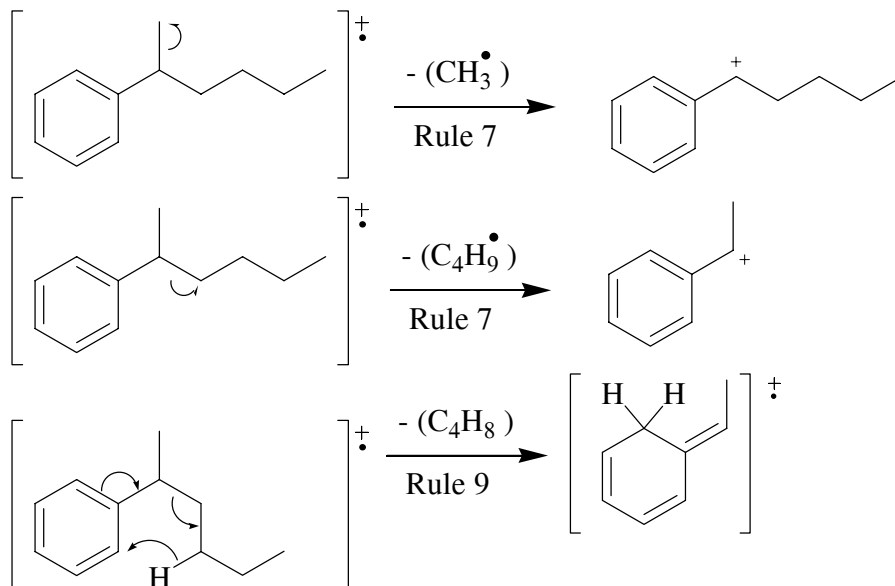
 <p>2-methyl-1-phenylhexan-1-one C₁₃H₁₈O</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 5</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	18	1.00783	18.14094
	Carbon	13	12.00000	156.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	1	15.9949	15.99490
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
			Exact Mass	190.13584

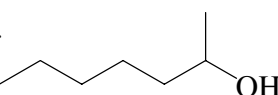


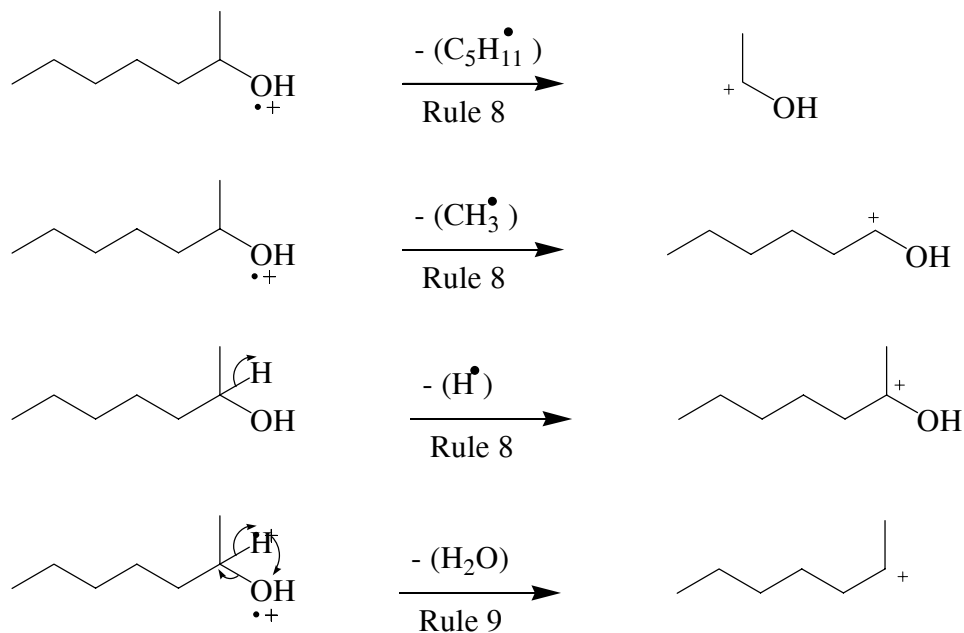
 <p>(E)-undec-3-ene C₁₁H₂₂</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 1</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	22	1.00783	22.17226
	Carbon	11	12.00000	132.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	0	15.9949	0.00000
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
			Exact Mass	154.17226

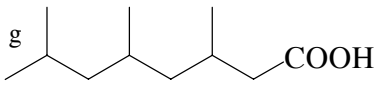


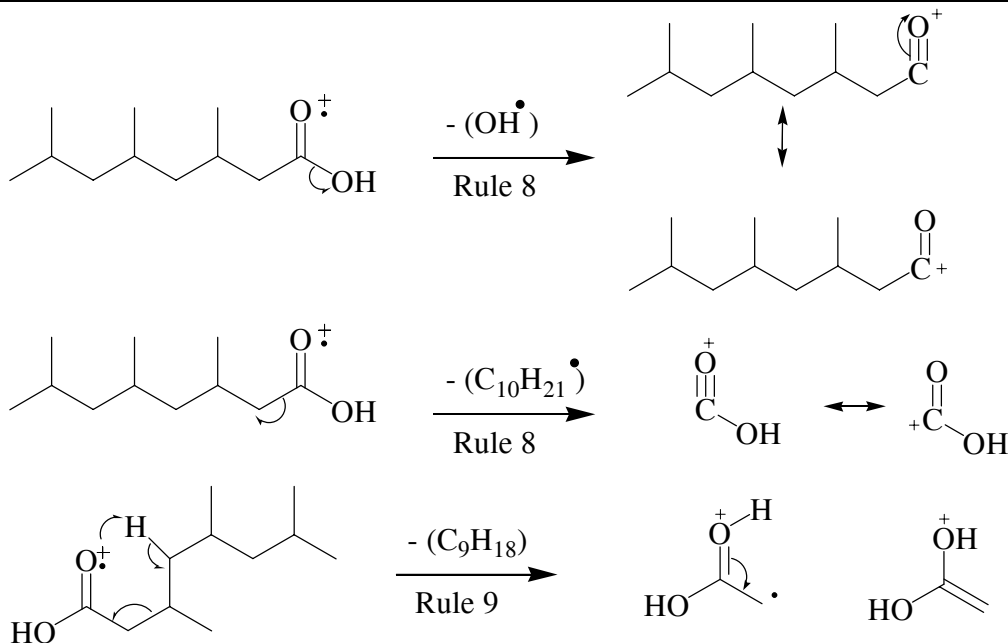
<p>e</p>  <p>1-(hexan-2-yl)benzene C₁₂H₁₈</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 4</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	18	1.00783	18.14094
	Carbon	12	12.00000	144.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	0	15.9949	0.00000
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
Exact Mass				162.14094

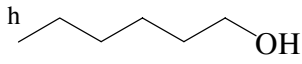


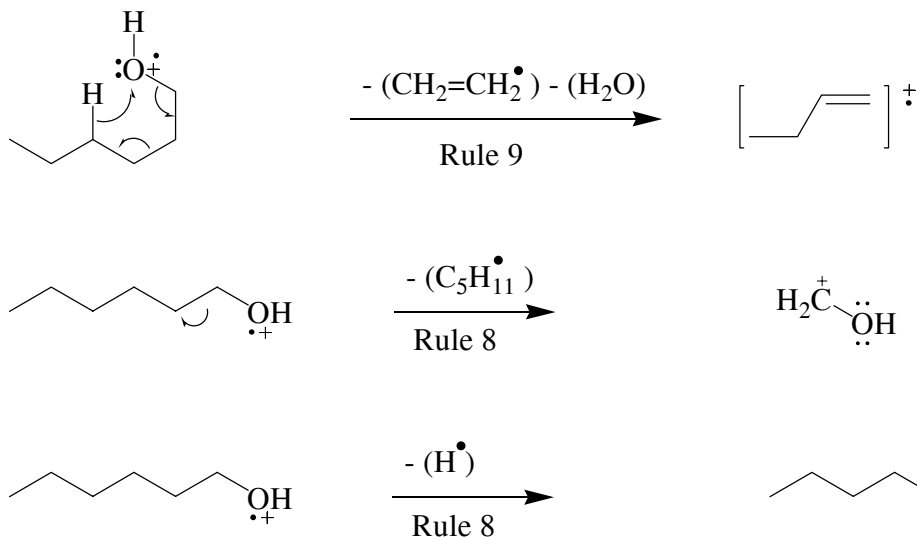
<p>f</p>  <p>heptan-2-ol C₇H₁₆O</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	16	1.00783	16.12528
	Carbon	7	12.00000	84.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	1	15.9949	15.99490
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
Exact Mass				116.12018

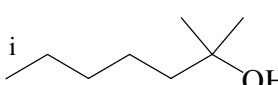


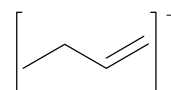
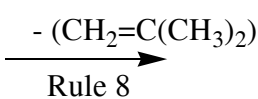
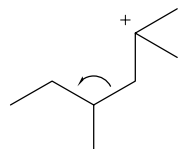
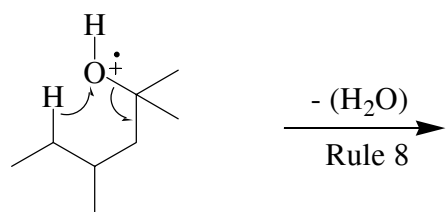
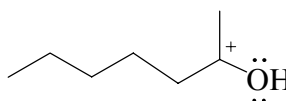
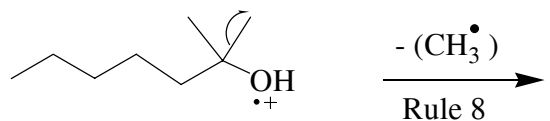
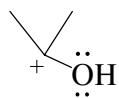
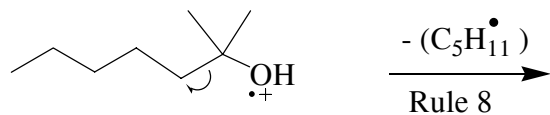
<p>g</p>  <p>3,5,7-trimethyloctanoic acid C₁₁H₂₂O₂</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 1</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	22	1.00783	22.17226
	Carbon	11	12.00000	132.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	2	15.9949	31.98980
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
Exact Mass				186.16206

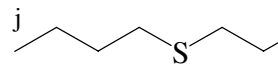


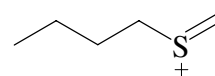
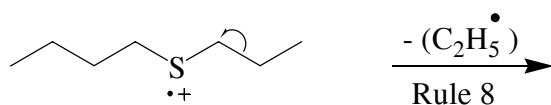
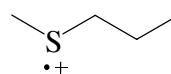
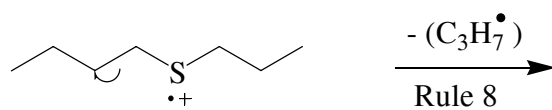
<p>h</p>  <p>hexan-1-ol C₆H₁₄O</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	14	1.00783	14.10962
	Carbon	6	12.00000	72.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	1	15.9949	15.99490
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
Exact Mass				102.10452

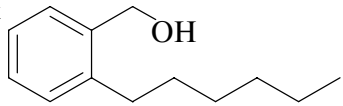


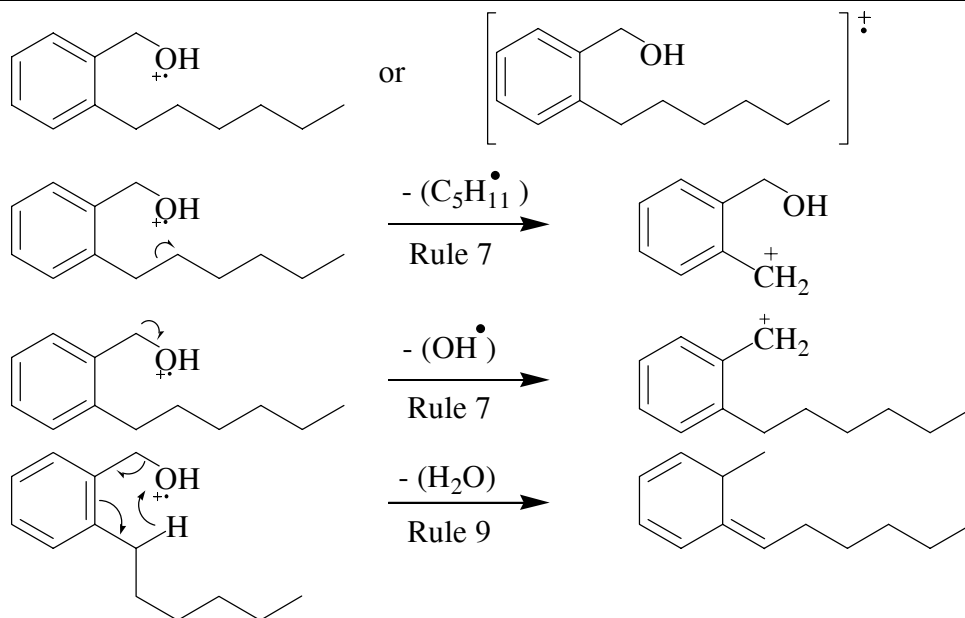
<p>i</p>  <p>2-methylheptan-2-ol C₈H₁₈O</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	18	1.00783	18.14094
	Carbon	8	12.00000	96.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	1	15.9949	15.99490
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
			Exact Mass	130.13584

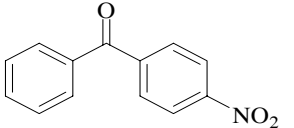


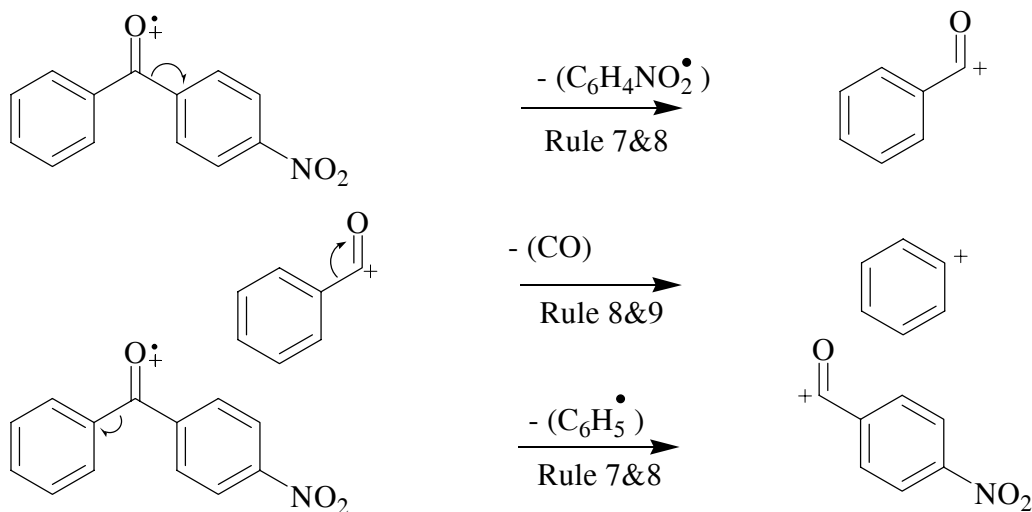
<p>j</p>  <p>butyl(propyl)sulfane C₇H₁₆S</p> <p>C_nH_mX_xN_yO_z IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	16	1.00783	16.12528
	Carbon	7	12.00000	84.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	0	15.9949	0.00000
	Sulfur	1	31.9721	31.97210
	Bromine	0	78.9183	0.00000
			Exact Mass	132.09738

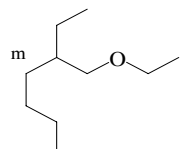


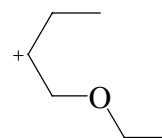
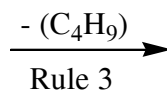
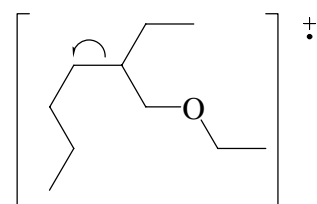
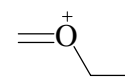
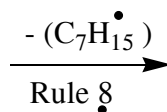
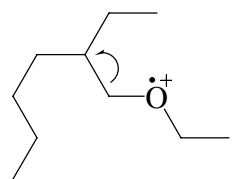
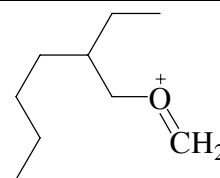
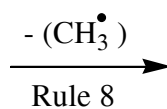
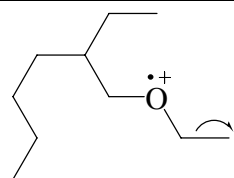
<p>k</p>  <p>(2-hexylphenyl)methanol</p> <p>$C_{13}H_{20}O$</p> <p>$C_nH_mX_xN_yO_z$</p> <p>IHD</p> <p>Index = $(n) - (m/2) - (x/2) + (y/2) + 1 = 4$</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	20	1.00783	20.15660
	Carbon	13	12.00000	156.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	1	15.9949	15.99490
	Sulfur	0	31.9721	0.00000
Bromine	0	78.9183	0.00000	
Exact Mass				192.15150

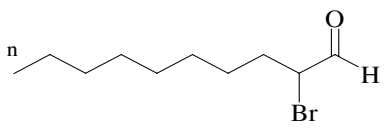


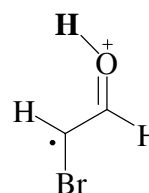
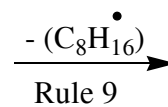
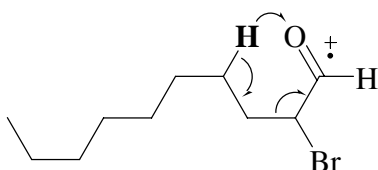
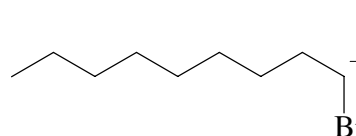
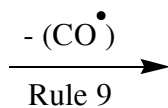
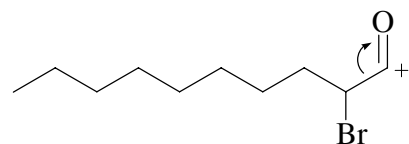
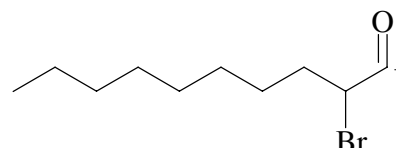
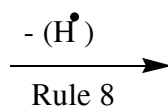
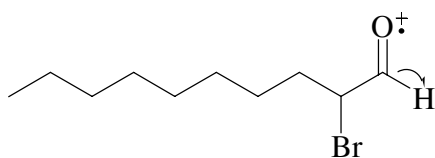
<p>l</p>  <p>(4-nitrophenyl)(phenyl)methanone</p> <p>$C_{13}H_9NO_3$</p> <p>$C_nH_mX_xN_yO_z$</p> <p>IHD</p> <p>Index = $(n) - (m/2) - (x/2) + (y/2) + 1 = 10$</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	9	1.00783	9.07047
	Carbon	13	12.00000	156.00000
	Nitrogen	1	14.0031	14.00310
	Oxygen	3	15.9949	47.98470
	Sulfur	0	31.9721	0.00000
Bromine	0	78.9183	0.00000	
Exact Mass				227.05827

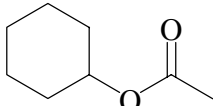


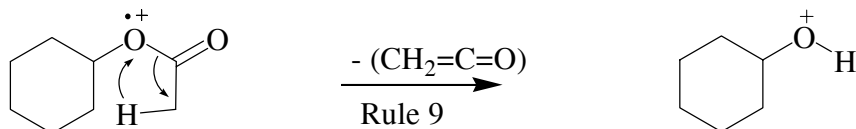
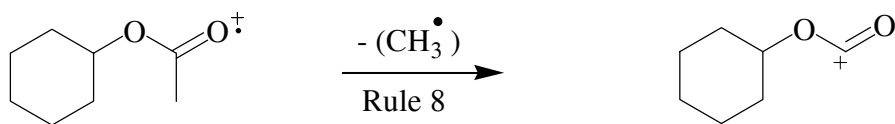
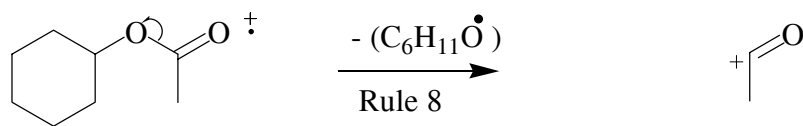
 <p>3-(ethoxymethyl)heptane $C_{10}H_{22}O$ $C_nH_mX_xN_yO_z$ IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	22	1.00783	22.17226
	Carbon	10	12.00000	120.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	1	15.9949	15.99490
	Sulfur	0	31.9721	0.00000
Bromine	0	78.9183	0.00000	
			Exact Mass	158.16716

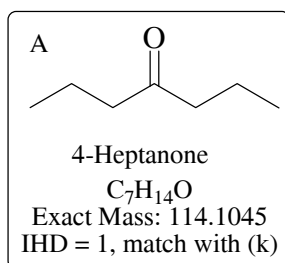


 <p>2-bromodecanal $C_{10}H_{19}BrO$ $C_nH_mX_xN_yO_z$ IHD</p> <p>Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 1</p>	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	19	1.00783	19.14877
	Carbon	10	12.00000	120.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	1	15.9949	15.99490
	Sulfur	0	31.9721	0.00000
Bromine	1	78.9183	78.91830	
			Exact Mass	234.06197

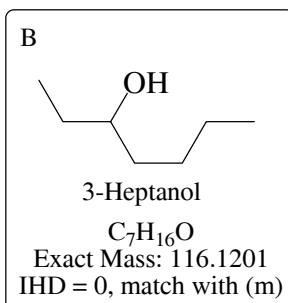


 cyclohexyl acetate $C_8H_{14}O_2$ $C_nH_mX_xN_yO_z$	Atom Type	# of Atoms	Mass	Total Mass
	Hydrogen	14	1.00783	14.10962
	Carbon	8	12.00000	96.00000
	Nitrogen	0	14.0031	0.00000
	Oxygen	2	15.9949	31.98980
	Sulfur	0	31.9721	0.00000
	Bromine	0	78.9183	0.00000
Index = $(n) - (m/2) - (x/2) + (y/2) + 1 =$	IHD		Exact Mass	142.09942
				2

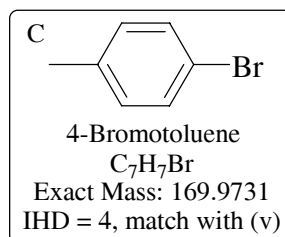




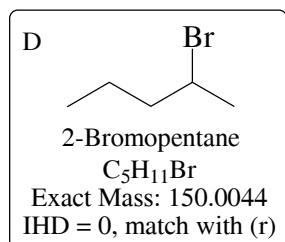
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
71	114	99 / $C_6H_{11}O$	15 / CH_3	
		86 / C_5H_{10}	28 / C_2H_4	R
		71 / C_4H_7O	43 / C_3H_7	
		58 / C_3H_5O	56 / C_4H_8	R
		43 / C_3H_7	71 / C_4H_7O	



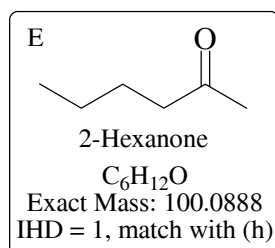
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
59	116 by CI	115 / $C_7H_{15}O$	1 / H	
		98 / C_7H_{14}	18 / H_2O	R
		87 / $C_5H_{11}O$	29 / C_2H_5	
		69 / C_5H_9	18 / H_2O , 29 / C_2H_5	R
		59 / C_3H_7O	57 / C_4H_9	
		45 / C_2H_5O	71 / C_5H_{11}	
		43 / C_3H_7	73 / C_4H_9O	
		41 / C_4H_5	18 / H_2O , 57 / C_4H_9	R



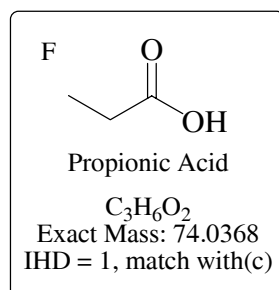
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
91	170	91 / C_7H_7	79 / Br	Tropylium Ion
		75 / C_6H_3	80 / HBr , 16 / CH_4	R
		65 / C_5H_5	79 / Br , 26 / C_2H_2	R
		50 / C_4H_2	120 / C_7H_5Br	
		39 / C_3H_2	131 / C_4H_5Br	



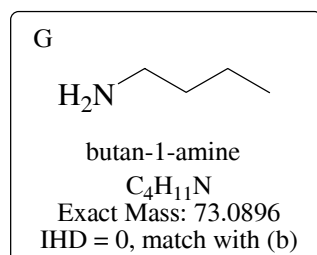
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
71	150	121 / C_3H_6Br	29 / C_2H_5	
		107 / C_2H_4Br	43 / C_3H_7	
		71 / C_5H_{11}	79 / Br	
		55 / C_4H_7	80 / HBr , 16 / CH_4	R
		43 / C_3H_7	C_2H_4Br	



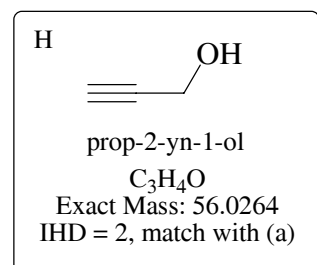
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
43	100	85 / C_5H_9O	15 / CH_3	
		71 / C_4H_7O	29 / C_2H_5	
		58 / C_4H_{10}	42 / C_2H_2O	R
		57 / C_3H_5O	43 / C_3H_7	
		43 / C_3H_7	57 / C_3H_5O	



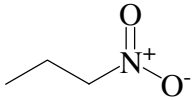
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
74	74	73 / $C_3H_5O_2$	1 / H	
		57 / C_3H_5O	17 / OH	
		56 / C_3H_4O	18 / H_2O	R
		45 / CHO_2	29 / C_2H_5	

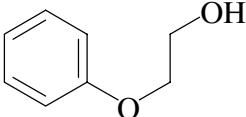


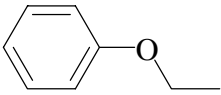
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
73	73	56 / C_4H_8	17 / NH_3	R
		55 / C_4H_7	18 / NH_4	R
		44 / C_2H_6N	29 / C_2H_5	
		43 / C_3H_7	30 / CH_4N	

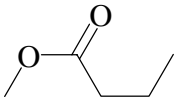


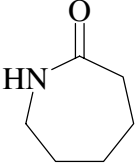
Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
55	56 by CI	55 / C_3H_3O	1 / H	
		39 / C_3H_3	17 / OH	
		38 / C_3H_2	18 / H_2O	

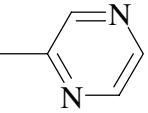
	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
I  1-Nitropropane $C_3H_7NO_2$ Exact Mass: 89.0477 IHD = 1, match with (d)	43	89 by CI	90 / $C_3H_8NO_2$	Addition of H	
			72 / C_3H_6NO	17 / OH	R
			43 / C_3H_7	46 / NO_2	
			42 / C_3H_6	47 / HNO_2	R

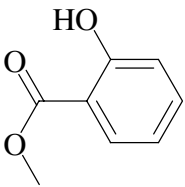
	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
J  2-Phenoxyethanol $C_8H_{10}O_2$ Exact Mass: 138.0681 IHD = 4, match with (q)	94	138	107 / C_7H_7O	31 / CH_3O	
			94 / C_6H_5O	44 / C_2H_4O	R
			77 / C_6H_5	61 / $C_2H_5O_2$	
			66 / C_5H_6	72 / $C_3H_5O_2$	R
			51 / C_4H_3	87 / $C_4H_7O_2$	
			39 / C_3H_2	99 / $C_5H_8O_2$	

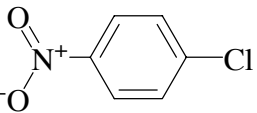
	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
K  Phenetole $C_8H_{10}O$ Exact Mass: 122.0732 IHD = 4, match with (o)	94	122	94 / C_6H_5O	28 / C_2H_4	R
			77 / C_6H_5	45 / C_2H_5O	
			66 / C_5H_6	56 / C_3H_4O	
			51 / C_4H_3	71 / C_4H_7O	
			39 / C_3H_2	83 / C_5H_8O	

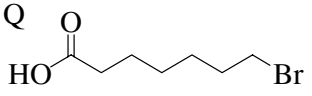
	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
L  Methyl Butyrate $C_5H_{10}O_2$ Exact Mass: 102.0681 IHD = 1, match with (i)	43	102	87 / $C_4H_7O_2$	15 / CH_3	
			74 / $C_3H_5O_2$	28 / C_2H_4	R
			71 / C_4H_7O	31 / CH_3O	
			59 / $C_2H_3O_2$	43 / C_3H_7	
			43 / C_3H_7	59 / $C_2H_3O_2$	

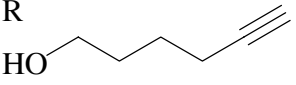
M	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
 <p>Caprolactam C₆H₁₁NO Exact Mass: 113.0841 IHD = 2, match with (j)</p>	113	113	85 / C ₅ H ₁₁ N	28 / CO	R
			84 / C ₅ H ₁₀ N	29 / CHO	
			56 / C ₄ H ₈	57 / C ₂ H ₃ NO	
			55 / C ₄ H ₇	58 / C ₂ H ₄ NO	
			42 / C ₃ H ₆	71 / C ₃ H ₅ NO	R

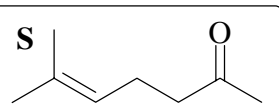
N	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
 <p>2-methylpyrazine C₅H₆N₂ Exact Mass: 94.0531 IHD = 4, match with (e)</p>	94	94	67 / C ₄ H ₅ N	27 / CHN	
			53 / C ₃ H ₃ N	41 / C ₂ H ₃ N	
			42 / C ₂ H ₄ N	52 / C ₃ H ₂ N	
			41 / C ₂ H ₃ N	53 / C ₃ H ₃ N	
			40 / C ₂ H ₂ N	54 / C ₃ H ₄ N	

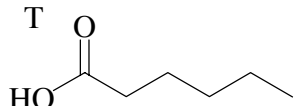
O	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement		
 <p>Methyl salicylate C₈H₈O₃ Exact Mass: 152.0473 IHD = 5, match with (s)</p>	152	152	135 / C ₈ H ₇ O ₂	17 / OH			
			122 / C ₇ H ₆ O ₂	30 / CH ₂ O	R		
			107 / C ₇ H ₇ O	45 / CHO ₂	R		
			105 / C ₇ H ₅ O	17 / OH, 30 / CH ₂ O	R		
			92 / C ₆ H ₄ O	60 / C ₂ H ₄ O ₂	R		
			77 / C ₆ H ₅	17 / OH, 58 / C ₂ H ₂ O ₂			
			63 / C ₅ H ₃	89 / C ₃ H ₅ O ₃			
			39 / C ₃ H ₂	113 / C ₅ H ₆ O ₃			

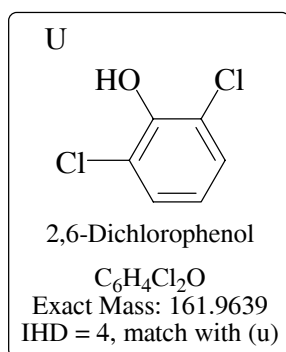
P	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
 <p>1-Chloro-4-Nitrobenzene C₆H₄ClNO₂ Exact Mass: 156.9931 IHD = 5, match with (t)</p>	75 or 157	157	141 / C ₆ H ₄ ClNO	16 / O	
			127 / C ₆ H ₄ O	30 / NO	R
			111 / C ₆ H ₄ Cl	46 / NO ₂	
			99 / C ₅ H ₄ Cl	58 / CNO ₂	
			75 / C ₆ H ₃	46 / NO ₂ , 36 / HCl	R
			50 / C ₄ H ₂	107 / C ₂ H ₂ ClNO ₂	

Q	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangment
 <p>7-Bromo Heptanoic Acid C₇H₁₃BrO₂ Exact Mass: 208.0099 IHD = 1, match with (w)</p>	60	208 by CI	191 / C ₇ H ₁₂ OBr	17 / OH	
			149 / C ₅ H ₁₀ Br	59 / C ₂ H ₃ O ₂	
			129 / C ₇ H ₁₃ O ₂	79 / Br	
			111 / C ₇ H ₁₁ O	79 / Br, 18 / H ₂ O	R
			83 / C ₆ H ₁₁	125 / CH ₂ BrO ₂	R
			60 / C ₂ H ₄ O ₂	147 / C ₅ H ₉ Br	R

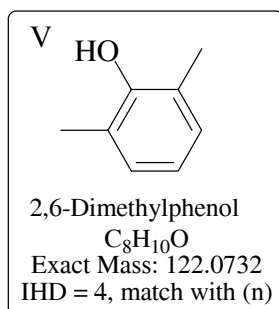
R	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangment
 <p>5-Hexyn-1-ol C₆H₁₀O Exact Mass: 98.0732 IHD = 2, match with (g)</p>	70	98	97 / C ₆ H ₉ O	1 / H	
			83 / C ₅ H ₇ O	15 / CH ₃	
			79 / C ₆ H ₇	19 / H ₃ O	
			70 / C ₄ H ₆ O	28 / C ₂ H ₄	

S	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangment
 <p>6-Methyl-5-hepten-2-one C₈H₁₄O Exact Mass: 126.1045 IHD = 2, match with (p)</p>	43	126	111 / C ₇ H ₁₁ O	15 / CH ₃	
			108 / C ₈ H ₁₂	18 / H ₂ O	R
			93 / C ₇ H ₉	33 / CH ₅ O	R
			83 / C ₆ H ₁₁	43 / C ₂ H ₃ O	
			69 / C ₅ H ₉	57 / C ₃ H ₅ O	
			58 / C ₃ H ₆ O	68 / C ₅ H ₈	R
			55 / C ₄ H ₇	71 C ₄ H ₇ O	
			43 / C ₂ H ₃ O	83 / C ₆ H ₁₁	

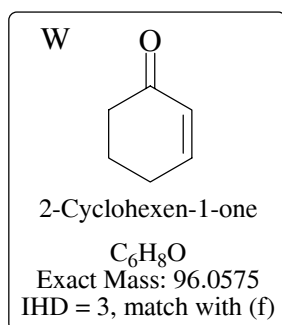
T	Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangment
 <p>Hexanoic acid C₆H₁₂O₂ Exact Mass: 116.0837 IHD = 1, match with (l)</p>	60	116 by CI	87 / C ₄ H ₇ O ₂	29 / C ₂ H ₅	
			73 / C ₃ H ₅ O ₂	43 / C ₃ H ₇	
			60 / C ₂ H ₄ O ₂	56 / C ₄ H ₈	R
			45 / CHO ₂	71 / C ₅ H ₁₁	



Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
162	162	126 / C_6H_3OCl	36 / HCl	R
		98 / C_5H_3Cl	64 / $CHOC_1$	R
		63 / C_5H_3	99 / $CHOC_2$	



Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
122	122	121 / C_8H_9O	1 / H	
		107 / C_7H_7O	15 / CH_3	
		91 / C_7H_7	31 / CH_3O	
		77 / C_6H_5	45 / C_2H_5O	
		65 / C_5H_5	57 / C_3H_5O	



Base Peak	Molecular Ion	Fragment Ion	Fragment Loss	Rearrangement
68	96	68 / C_4H_4O	28 / C_2H_4	R
		55 / C_3H_3O	41 / C_3H_5	
		53 / C_4H_5	43 / C_2H_3O	
		42 / C_2H_2O	54 / C_4H_6	R