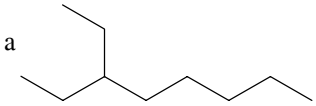
a



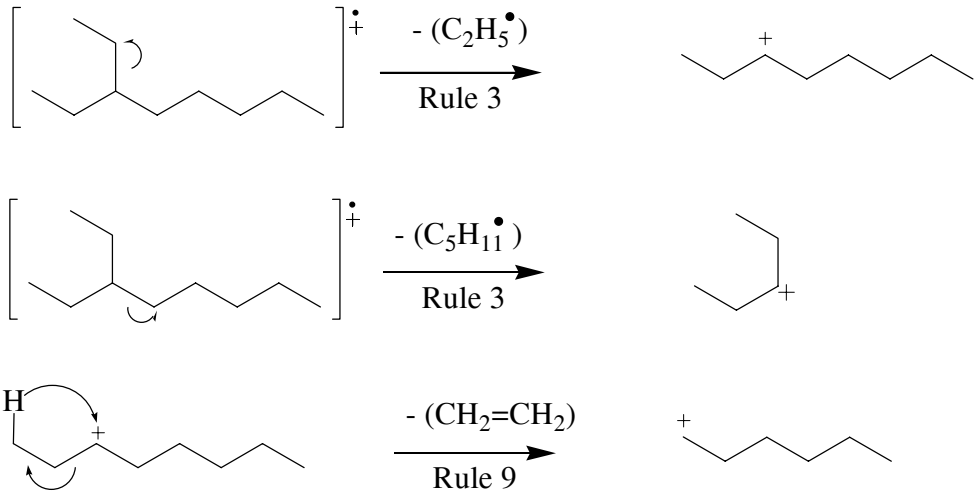
3-ethyloctane
$C_{10}H_{22}$

$C_nH_mX_xN_yO_z$

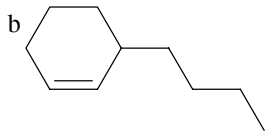
Index = (n) - (m/2) - (x/2) + (y/2) + 1 =

IHD
0

| 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 |




b



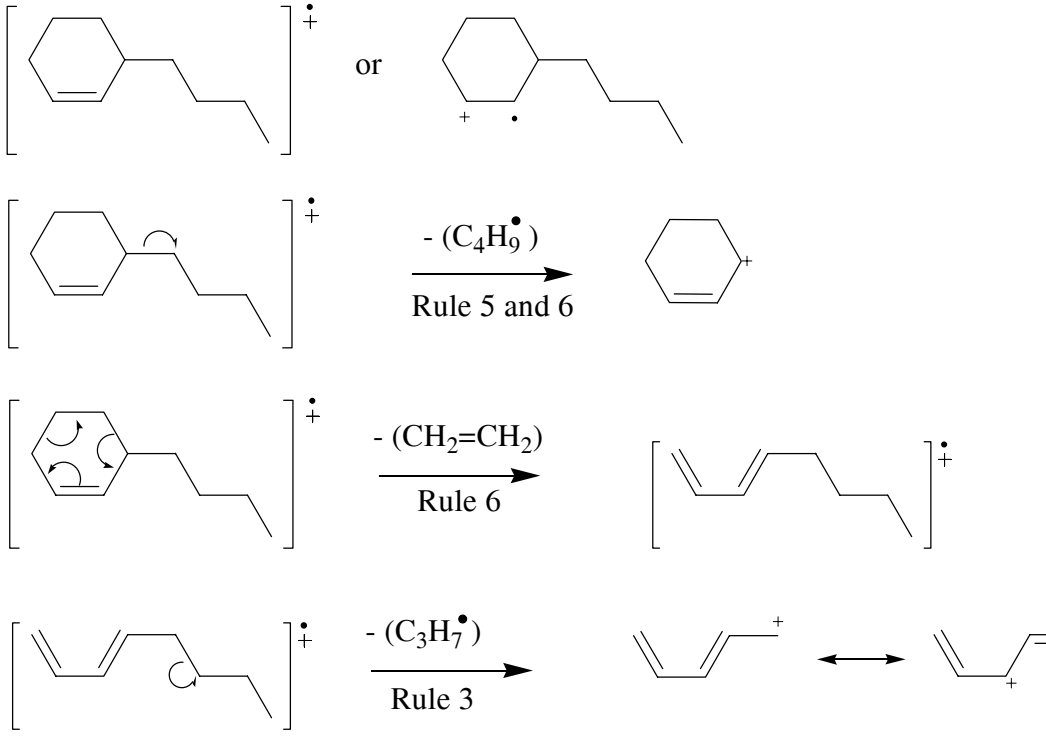
3-butylcyclohex-1-ene
$C_{10}H_{18}$

$C_nH_mX_xN_yO_z$

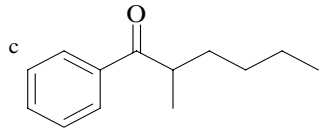
Index = (n) - (m/2) - (x/2) + (y/2) + 1 =

IHD
2

| 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 |



c

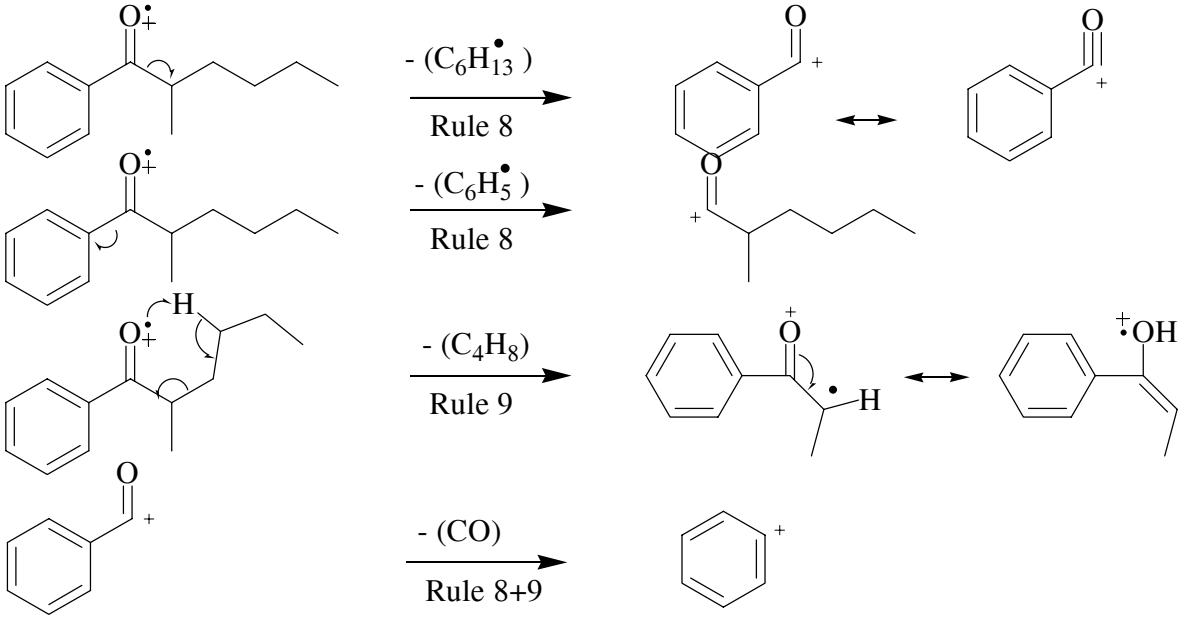


2-methyl-1-phenylhexan-1-one
$C_{13}H_{18}O$

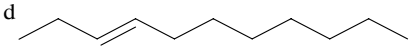
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 5

| 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 |




d

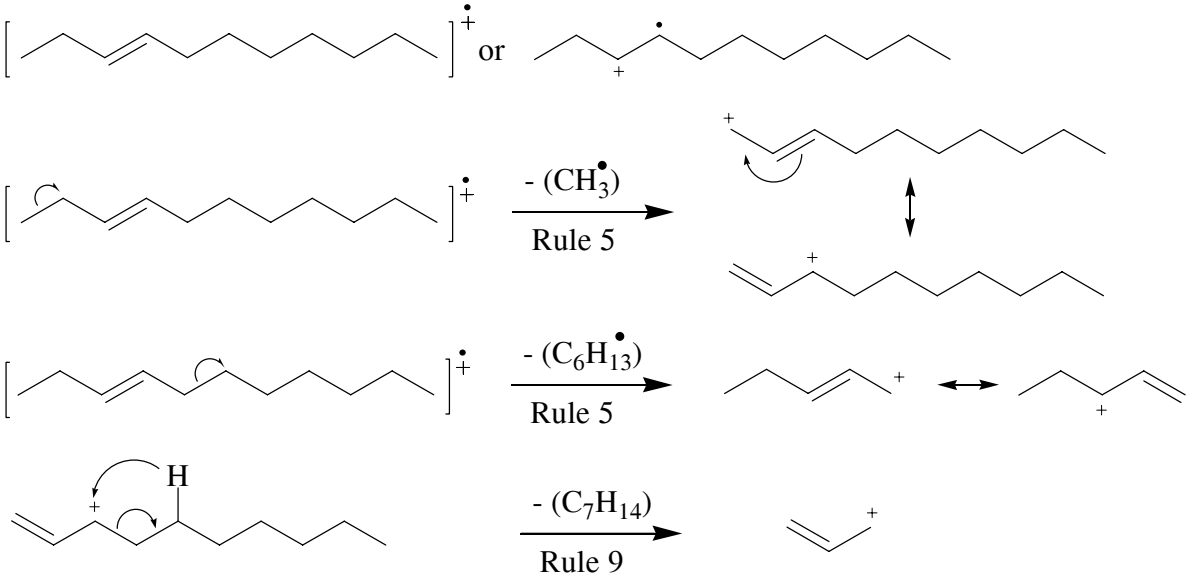


(*E*)-undec-3-ene
$C_{11}H_{22}$

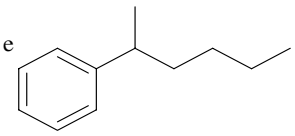
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 1

| 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 |



e

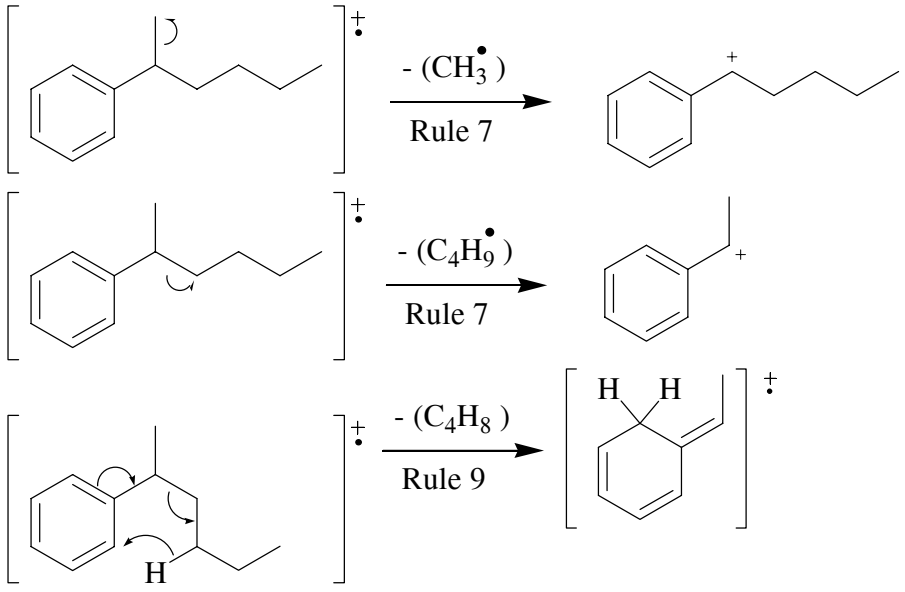


1-(hexan-2-yl)benzene
$C_{12}H_{18}$

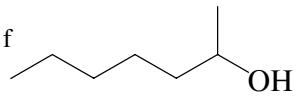
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 4

| 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 |




f

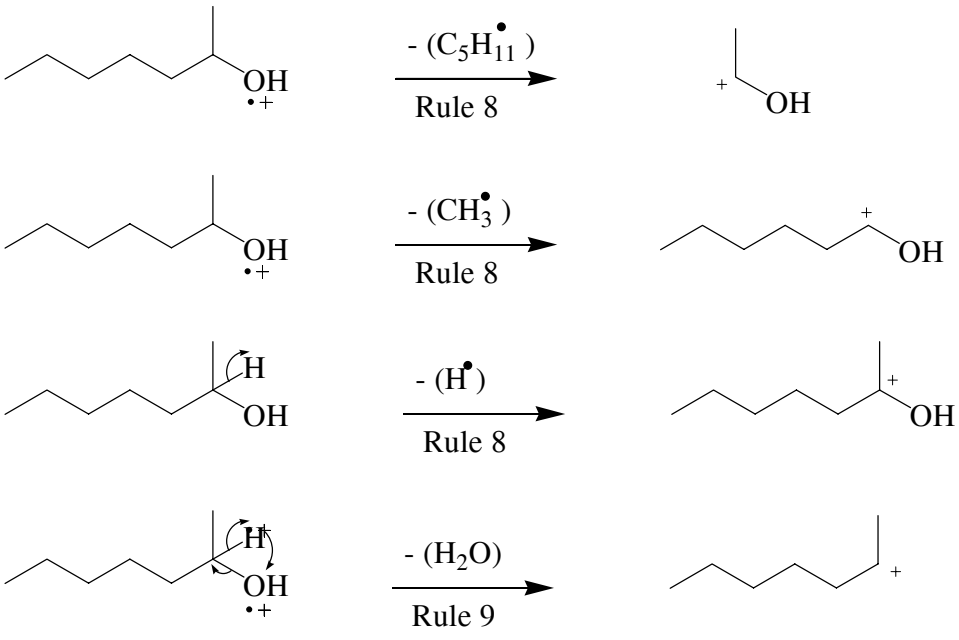


heptan-2-ol
$C_7H_{16}O$

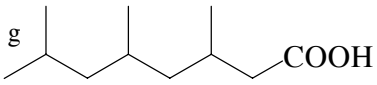
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0

| 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 |



g

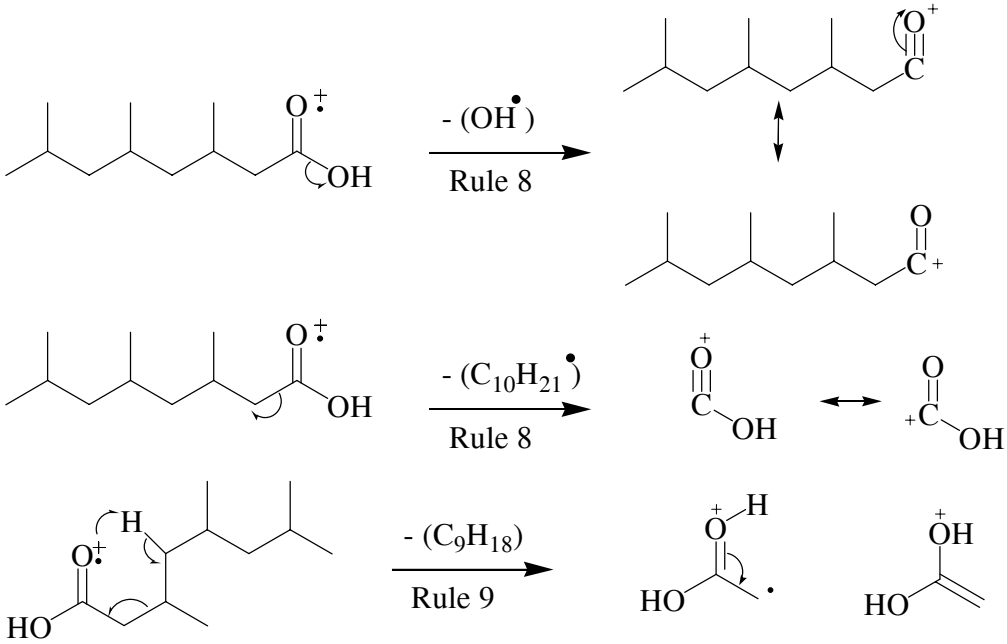



3,5,7-trimethyloctanoic acid
$C_{11}H_{22}O_2$

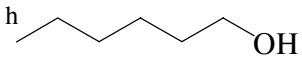
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 1

| 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 |




h

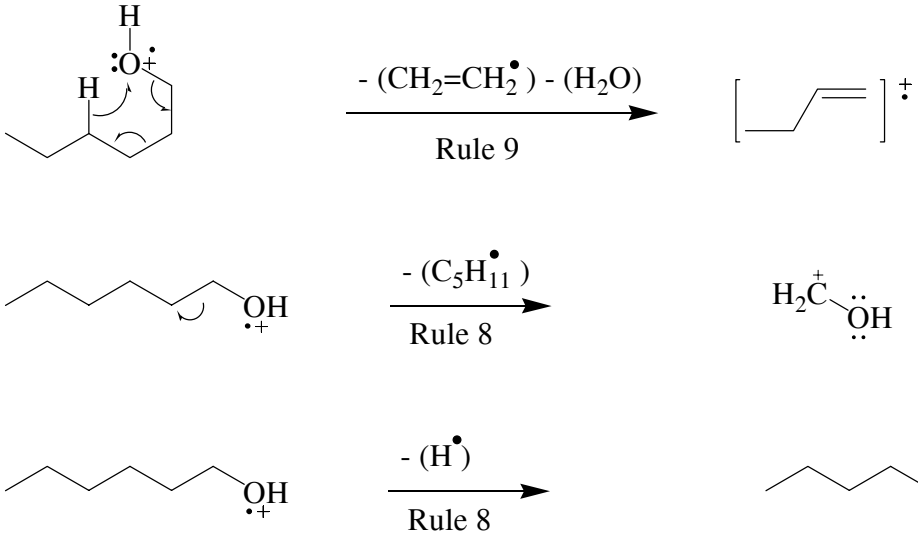



hexan-1-ol
$C_6H_{14}O$

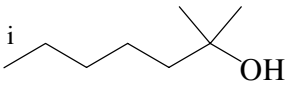
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0

| 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 |



i

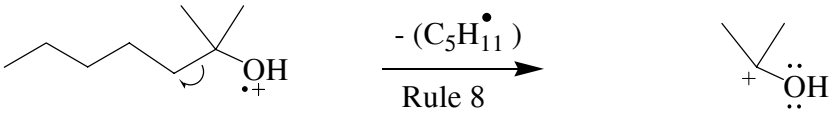


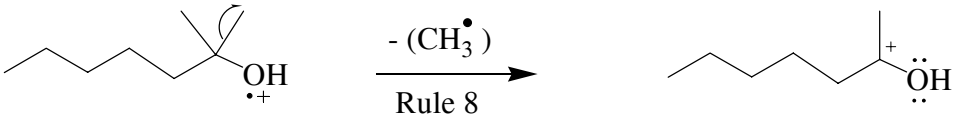
2-methylheptan-2-ol
$C_8H_{18}O$

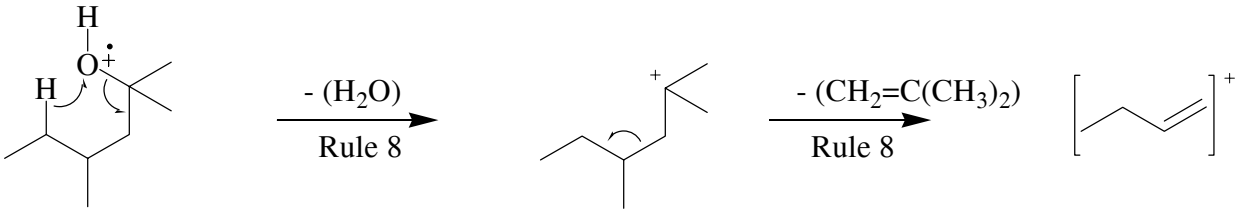
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0

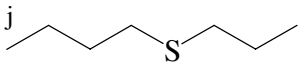
| Atom Type | # of Atoms | Mass | Total Mass |
|---|---|---|---|
| Hydrogen | 18 | 1.00783 | 18.14094 |
| Carbon | 8 | 12.00000 | 96.00000 |
| Nitrogen | 0 | 14.0031 | 0.00000 |
| Oxygen | 1 | 15.9949 | 15.99490 |
| Sulfur | 0 | 31.9721 | 0.00000 |
| Bromine | 0 | 78.9183 | 0.00000 |
| | | Exact Mass | 130.13584 |




j

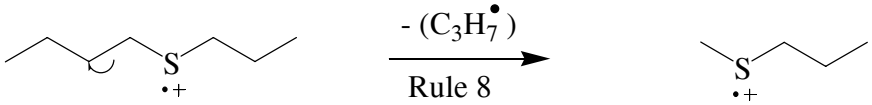


butyl(propyl)sulfane
$C_7H_{16}S$

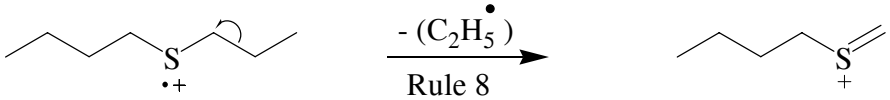
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0

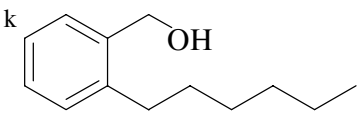
| Atom Type | # of Atoms | Mass | Total Mass |
|---|---|---|---|
| Hydrogen | 16 | 1.00783 | 16.12528 |
| Carbon | 7 | 12.00000 | 84.00000 |
| Nitrogen | 0 | 14.0031 | 0.00000 |
| Oxygen | 0 | 15.9949 | 0.00000 |
| Sulfur | 1 | 31.9721 | 31.97210 |
| Bromine | 0 | 78.9183 | 0.00000 |
| | | Exact Mass | 132.09738 |







k



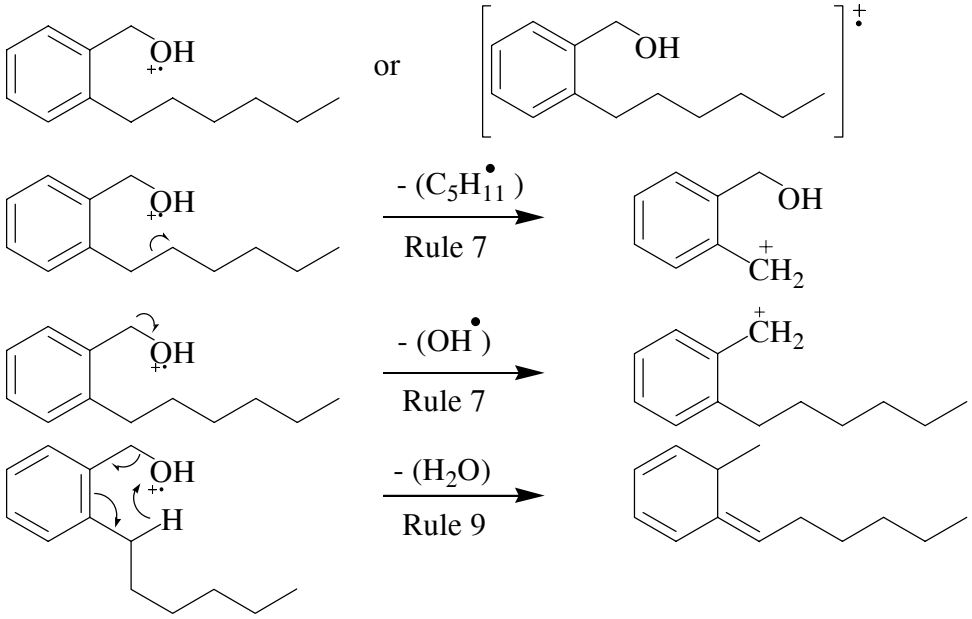
(2-hexylphenyl)methanol

$C_{13}H_{20}O$

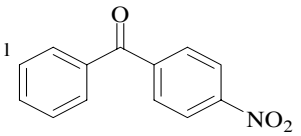
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 4

| 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 |




l



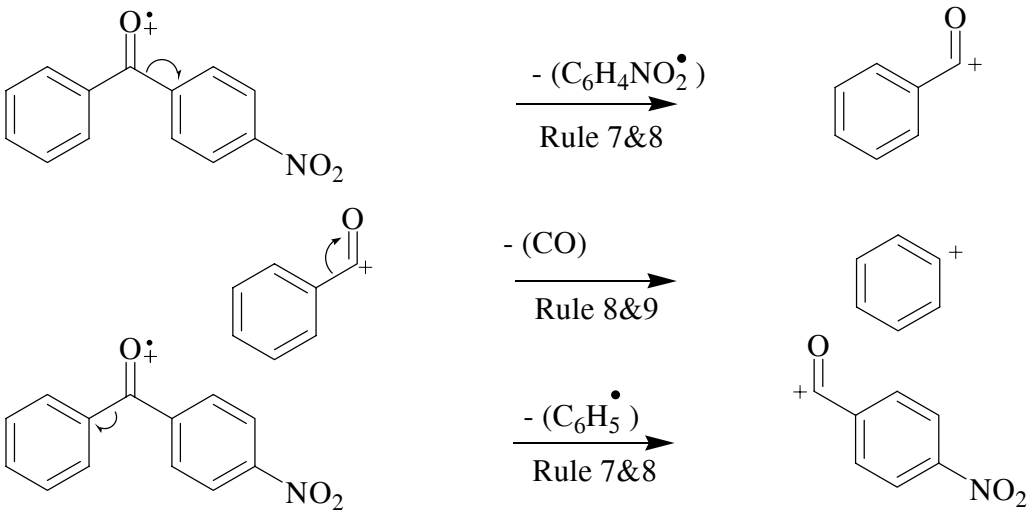
(4-nitrophenyl)(phenyl)methanone

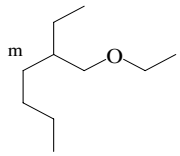
$C_{13}H_9NO_3$

$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 10

| 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 |



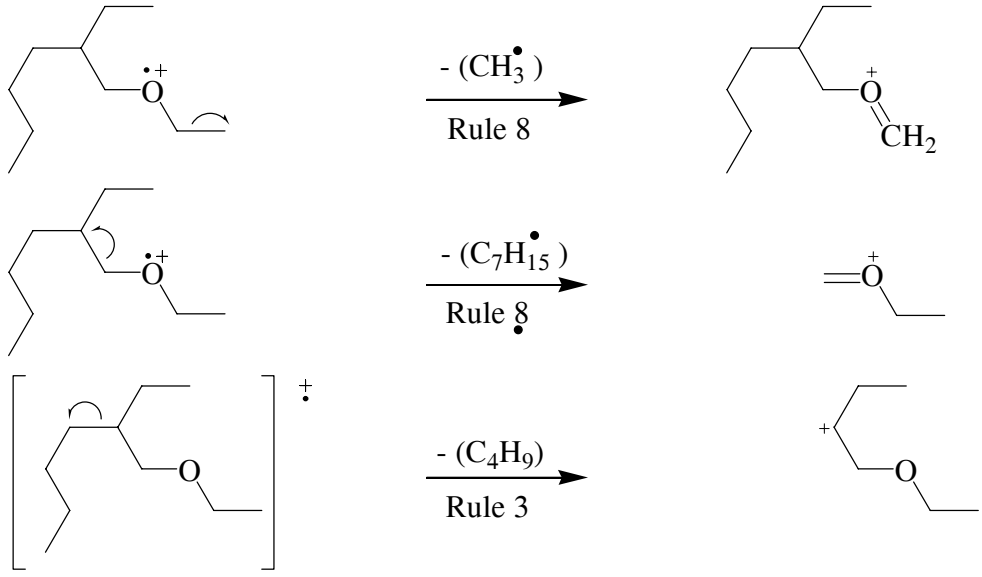


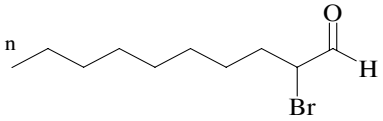
3-(ethoxymethyl)heptane
$C_{10}H_{22}O$

$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0

| 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 |



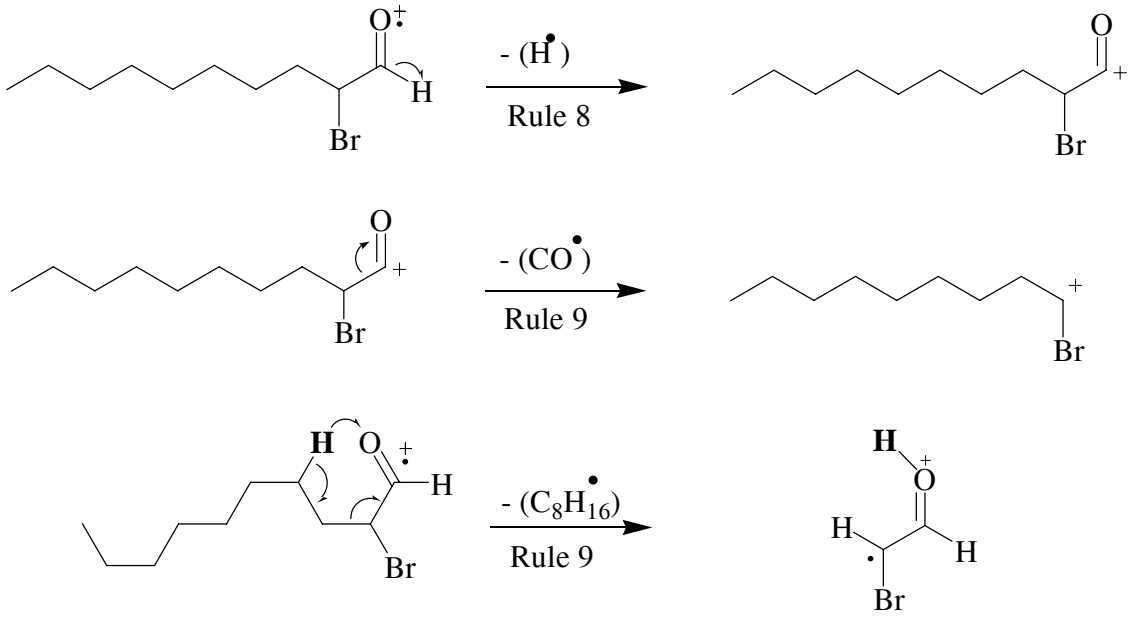



2-bromodecanal
$C_{10}H_{19}BrO$

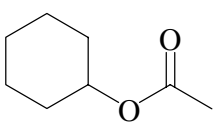
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 1

| 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 |



o



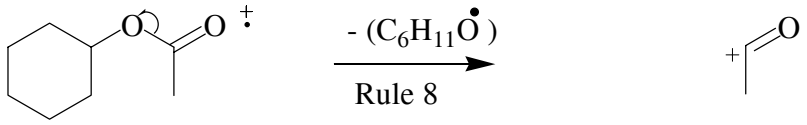
cyclohexyl acetate

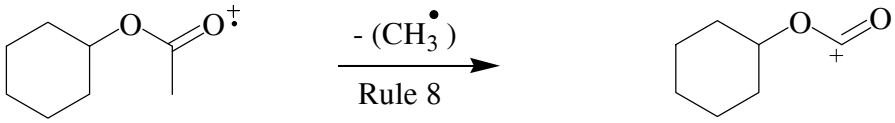
$C_8H_{14}O_2$

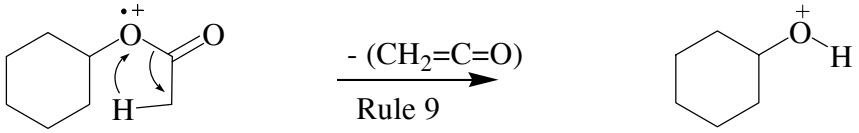
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 2

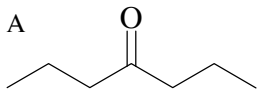
| Atom Type | # of Atoms | Mass | Total Mass |
|---|---|---|---|
| Hydrogen | 14 | 1.00783 | 14.10962 |
| Carbon | 8 | 12.00000 | 96.00000 |
| Nitrogen | 0 | 14.0031 | 0.00000 |
| Oxygen | 2 | 15.9949 | 31.98980 |
| Sulfur | 0 | 31.9721 | 0.00000 |
| Bromine | 0 | 78.9183 | 0.00000 |
| | | Exact Mass | 142.09942 |



A



4-Heptanone
$C_7H_{14}O$
Exact Mass: 114.1045
IHD = 1, match with (k)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 71 | 114 | 99 / C6H11O | 15 / CH3 | |
| | | 86 / C5H10 | 28 / C2H4 | R |
| | | 71 / C4H7O | 43 / C3H7 | |
| | | 58 / C3H5O | 56 / C4H8 | R |
| | | 43 / C3H7 | 71 / C4H7O | |

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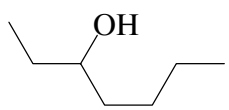
B



3-Heptanol
$C_7H_{16}O$
Exact Mass: 116.1201
IHD = 0, match with (m)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 59 | 116 by CI | 115 / C7H15O | 1 / H | |
| | | 98 / C7H14 | 18 / H2O | R |
| | | 87 / C5H11O | 29 / C2H5 | |
| | | 69 / C5H9 | 18 / H2O, 29 / C2H5 | R |
| | | 59 / C3H7O | 57 / C4H9 | |
| | | 45 / C2H5O | 71 / C5H11 | |
| | | 43 / C3H7 | 73 / C4H9O | |
| | | 41 / C4H5 | 18 / H2O, 57 / C4H9 | R |

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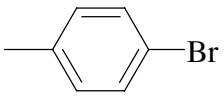
C



4-Bromotoluene
$C_7H_7Br$
Exact Mass: 169.9731
IHD = 4, match with (v)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 91 | 170 | 91 / C7H7 | 79 / Br | Tropylium Ion |
| | | 75 / C6H3 | 80 / HBr, 16 / CH4 | R |
| | | 65 / C5H5 | 79 / Br, 26 / C2H2 | R |
| | | 50 / C4H2 | 120 / C7H5Br | |
| | | 39 / C3H2 | 131 / C4H5Br | |

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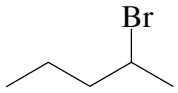
D



2-Bromopentane
$C_5H_{11}Br$
Exact Mass: 150.0044
IHD = 0, match with (r)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 71 | 150 | 121 / C3H6Br | 29 / C2H5 | |
| | | 107 / C2H4Br | 43 / C3H7 | |
| | | 71 / C5H11 | 79 / Br | |
| | | 55 / C4H7 | 80 / HBr, 16 / CH4 | R |
| | | 43 / C3H7 | C2H4Br | |

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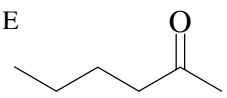
E



2-Hexanone

$C_6H_{12}O$

Exact Mass: 100.0888

IHD = 1, match with (h)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 43 | 100 | 85 / C5H9O | 15 / CH3 | |
| | | 71 / C4H7O | 29 / C2H5 | |
| | | 58 / C4H10 | 42 / C2H2O | R |
| | | 57 / C3H5O | 43 / C3H7 | |
| | | 43 / C3H7 | 57 / C3H5O | |

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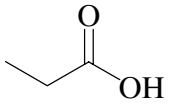
F



Propionic Acid

$C_3H_6O_2$

Exact Mass: 74.0368

IHD = 1, match with(c)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 74 | 74 | 73 / C3H5O2 | 1 / H | |
| | | 57 / C3H5O | 17 / OH | |
| | | 56 / C3H4O | 18 / H2O | R |
| | | 45 / CHO2 | 29 / C2H5 | |

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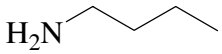
G



butan-1-amine

$C_4H_{11}N$

Exact Mass: 73.0896

IHD = 0, match with (b)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 73 | 73 | 56 / C4H8 | 17 / NH3 | R |
| | | 55 / C4H7 | 18 / NH4 | R |
| | | 44 / C2H6N | 29 / C2H5 | |
| | | 43 / C3H7 | 30 / CH4N | |

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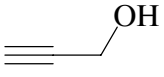
H



prop-2-yn-1-ol

$C_3H_4O$

Exact Mass: 56.0264

IHD = 2, match with (a)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 55 | 56 by CI | 55 / C3H3O | 1 / H | |
| | | 39 / C3H3 | 17 / OH | |
| | | 38 / C3H2 | 18 / H2O | |

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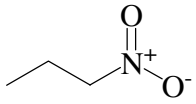
I



1-Nitropropane
$C_3H_7NO_2$
Exact Mass: 89.0477
IHD = 1, match with (d)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 43 | 89 by CI | 90 / C3H8NO2 | Addition of H | |
| | | 72 / C3H6NO | 17 / OH | R |
| | | 43 / C3H7 | 46 / NO2 | |
| | | 42 / C3H6 | 47 / HNO2 | R |

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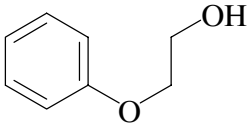
J



2-Phenoxylethanol

$C_8H_{10}O_2$
Exact Mass: 138.0681
IHD = 4, match with (q)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 94 | 138 | 107 / C7H7O | 31 / CH3O | |
| | | 94 / C6H5O | 44 / C2H4O | R |
| | | 77 / C6H5 | 61 / C2H5O2 | |
| | | 66 / C5H6 | 72 C3H5O2 | R |
| | | 51 / C4H3 | 87 / C4H7O2 | |
| | | 39 / C3H2 | 99 / C5H8O2 | |

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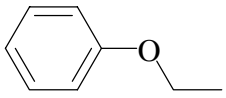
K



Phenetole

$C_8H_{10}O$
Exact Mass: 122.0732
IHD = 4, match with (o)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 94 | 122 | 94 / C6H5O | 28 / C2H4 | R |
| | | 77 / C6H5 | 45 / C2H5O | |
| | | 66 / C5H6 | 56 / C3H4O | |
| | | 51 / C4H3 | 71 / C4H7O | |
| | | 39 / C3H2 | 83 / C5H8O | |

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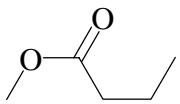
L



Methyl Butyrate

$C_5H_{10}O_2$
Exact Mass: 102.0681
IHD = 1, match with (i)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 43 | 102 | 87 / C4H7O2 | 15 / CH3 | |
| | | 74 / C3H5O2 | 28 / C2H4 | R |
| | | 71 / C4H7O | 31 / CH3O | |
| | | 59 / C2H3O2 | 43 / C3H7 | |
| | | 43 / C3H7 | 59 / C2H3O2 | |

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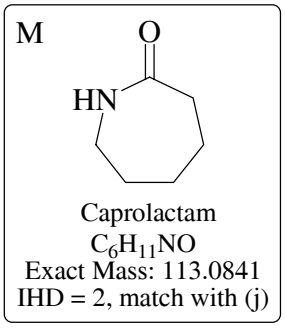


Caprolactam
$C_6H_{11}NO$
Exact Mass: 113.0841
IHD = 2, match with (j)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 113 | 113 | 85 / C5H11N | 28 / CO | R |
| | | 84 / C5H10N | 29 / CHO | |
| | | 56 / C4H8 | 57 / C2H3NO | |
| | | 55 / C4H7 | 58 / C2H4NO | |
| | | 42 / C3H6 | 71 / C3H5NO | R |

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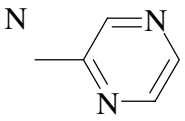


2-methylpyrazine

$C_5H_6N_2$
Exact Mass: 94.0531
IHD =4, match with (e)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 94 | 94 | 67 / C4H5N | 27 / CHN | |
| | | 53 / C3H3N | 41 / C2H3N | |
| | | 42 / C2H4N | 52 / C3H2N | |
| | | 41 / C2H3N | 53 / C3H3N | |
| | | 40 / C2H2N | 54 / C3H4N | |

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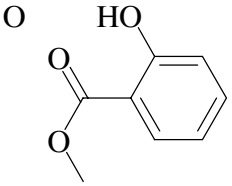


Methyl salicylate

$C_8H_8O_3$
Exact Mass: 152.0473
IHD = 5, match with (s)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 152 | 152 | 135 / C8H7O2 | 17 / OH | |
| | | 122 / C7H6O2 | 30 / CH2O | R |
| | | 107 / C7H7O | 45 / CHO2 | R |
| | | 105 / C7H5O | 17 / OH, 30 / CH2O | R |
| | | 92 / C6H4O | 60 / C2H4O2 | R |
| | | 77 / C6H5 | 17 / OH, 58 / C2H2O2 | |
| | | 63 / C5H3 | 89 / C3H5O3 | |
| | | 39 / C3H2 | 113 / C5H6O3 | |

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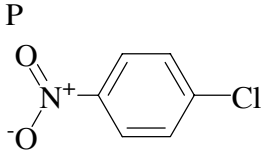
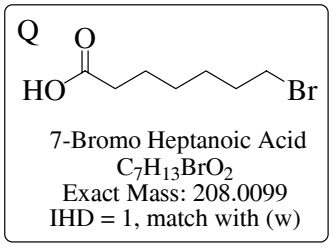



1-Chloro-4-Nitrobenzene
$C_6H_4ClNO_2$
Exact Mass: 156.9931
IHD = 5, match with (t)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 75 or 157 | 157 | 141 / C6H4ClNO | 16 / O | |
| | | 127 / C6H4O | 30 / NO | R |
| | | 111 / C6H4Cl | 46 / NO2 | |
| | | 99 / C5H4Cl | 58 / CNO2 | |
| | | 75 / C6H3 | 46 / NO2, 36 / HCl | R |
| | | 50 / C4H2 | 107 / C2H2ClNO2 | |




7-Bromo Heptanoic Acid
$C_7H_{13}BrO_2$
Exact Mass: 208.0099
IHD = 1, match with (w)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 60 | 208 by CI | 191 / C7H12OBr | 17 / OH | |
| | | 149 / C5H10Br | 59 / C2H3O2 | |
| | | 129 / C7H13O2 | 79 /Br | |
| | | 111 / C7H11O | 79 /Br, 18 / H2O | R |
| | | 83 / C6H11 | 125 / CH2BrO2 | R |
| | | 60 / C2H4O2 | 147 / C5H9Br | R |

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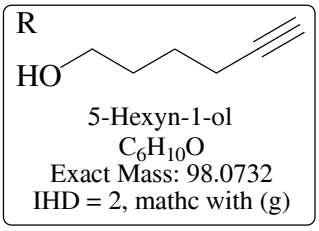


5-Hexyn-1-ol
$C_6H_{10}O$
Exact Mass: 98.0732
IHD = 2, mathc with (g)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 70 | 98 | 97 / C6H9O | 1 / H | |
| | | 83 / C5H7O | 15 / CH3 | |
| | | 79 / C6H7 | 19 / H3O | |
| | | 70 / C4H6O | 28 / C2H4 | |

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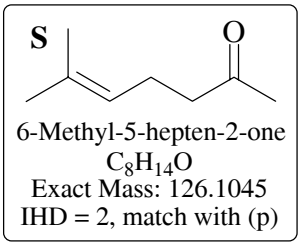


6-Methyl-5-hepten-2-one
$C_8H_{14}O$
Exact Mass: 126.1045
IHD = 2, match with (p)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 43 | 126 | 111 / C7H11O | 15 / CH3 | |
| | | 108 / C8H12 | 18 / H2O | R |
| | | 93 / C7H9 | 33 / CH5O | R |
| | | 83 / C6H11 | 43 / C2H3O | |
| | | 69 / C5H9 | 57 / C3H5O | |
| | | 58 / C3H6O | 68 / C5H8 | R |
| | | 55 / C4H7 | 71 C4H7O | |
| | | 43 / C2H3O | 83 / C6H11 | |

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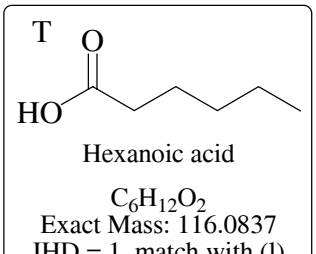


Hexanoic acid
$C_6H_{12}O_2$
Exact Mass: 116.0837
IHD = 1, match with (l)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 60 | 116 by CI | 87 / C4H7O2 | 29 / C2H5 | |
| | | 73 / C3H5O2 | 43 / C3H7 | |
| | | 60 / C2H4O2 | 56 / C4H8 | R |
| | | 45 / CHO2 | 71 / C5H11 | |

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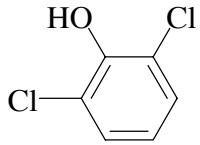
U




2,6-Dichlorophenol

$C_6H_4Cl_2O$
Exact Mass: 161.9639
IHD = 4, match with (u)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 162 | 162 | 126 / C6H3OCl | 36 / HCl | R |
| | | 98 / C5H3Cl | 64 / CHOCl | R |
| | | 63 / C5H3 | 99 / CHOCl2 | |

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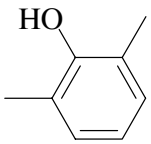
V




2,6-Dimethylphenol
$C_8H_{10}O$
Exact Mass: 122.0732
IHD = 4, match with (n)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 122 | 122 | 121/C8H9O | 1 / H | |
| | | 107/C7H7O | 15 / CH3 | |
| | | 91 / C7H7 | 31 / CH3O | |
| | | 77 / C6H5 | 45 / C2H5O | |
| | | 65 / C5H5 | 57 / C3H5O | |

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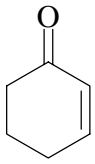
W




2-Cyclohexen-1-one

$C_6H_8O$
Exact Mass: 96.0575
IHD = 3, match with (f)

| Base Peak | Molecular Ion | Fragement Ion | Fragment Loss | Rearrangment |
|---|---|---|---|---|
| 68 | 96 | 68 / C4H4O | 28 / C2H4 | R |
| | | 55 / C3H3O | 41 / C3H5 | |
| | | 53 / C4H5 | 43 / C2H3O | |
| | | 42 / C2H2O | 54 / C4H6 | R |

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