

## Supplementary material

# **New insights into the occurrence of vehicle related compounds in one of Europe's longest rivers**

Juan Escobar-Arnanz<sup>a,\*</sup>, Silvia Royano<sup>a</sup>, Irene Navarro<sup>a</sup>, Adrián de la Torre<sup>a,1</sup>, María Ángeles Martínez<sup>a,1</sup>

\*Corresponding author contact information

Email: [Juan.Escobar@ciemat.es](mailto:Juan.Escobar@ciemat.es)

<sup>a</sup>*Unit of POPs and Emerging Pollutants in Environment, Department of Environment, CIEMAT, Avda. Complutense 40, E-28040 Madrid, Spain Madrid, Spain.*

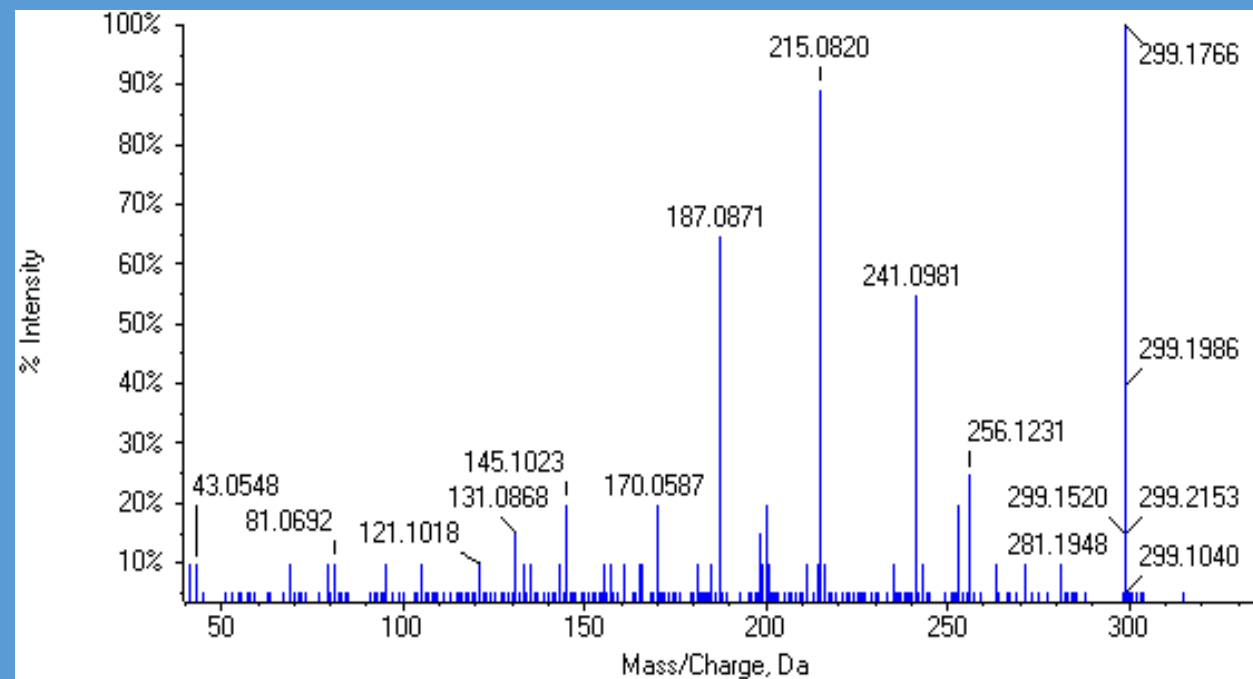
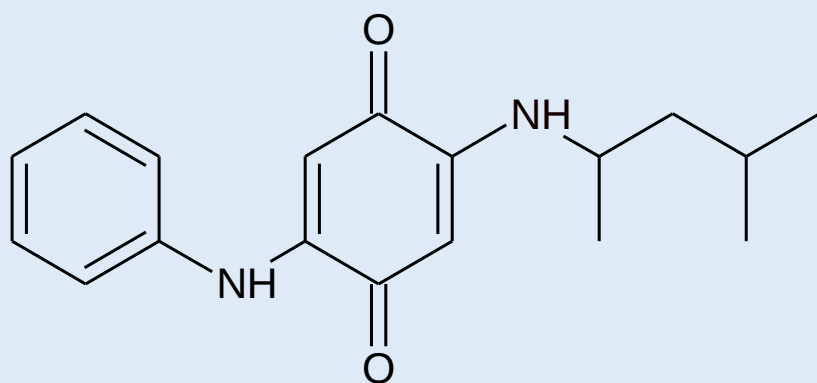
<sup>1</sup>Adrián de la Torre and María Ángeles Martínez share last authorship.

Supplementary material-3

Mass spectral library of detected VRCs

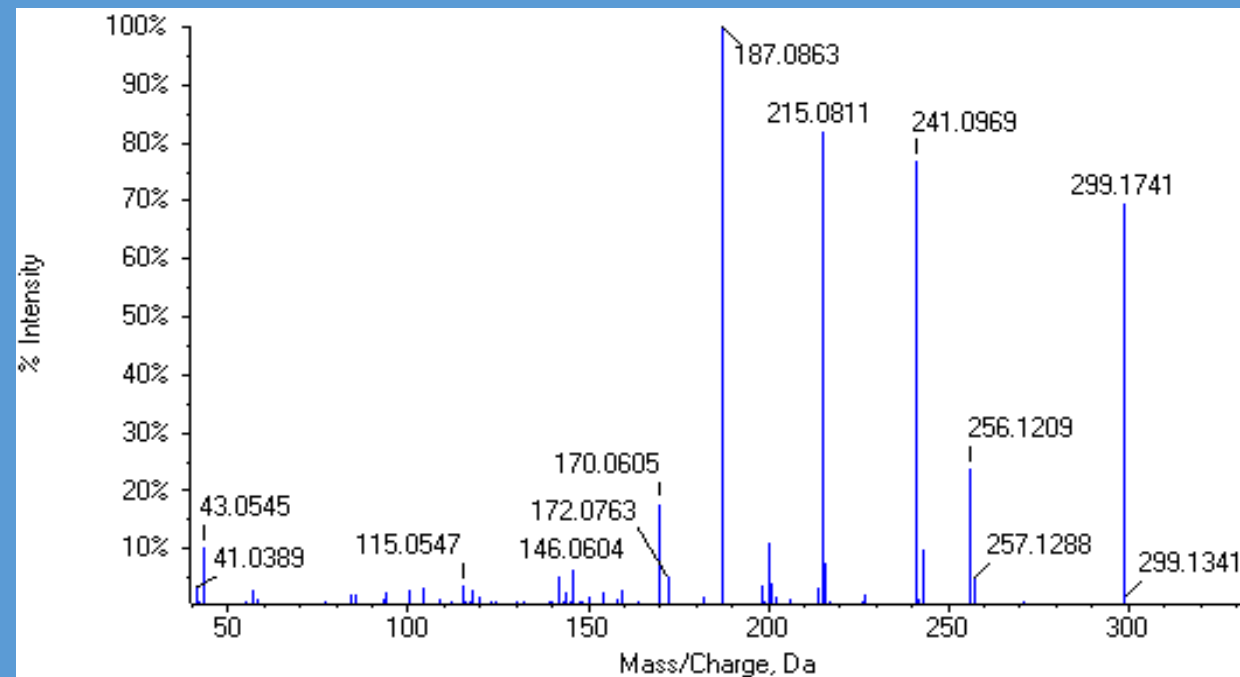
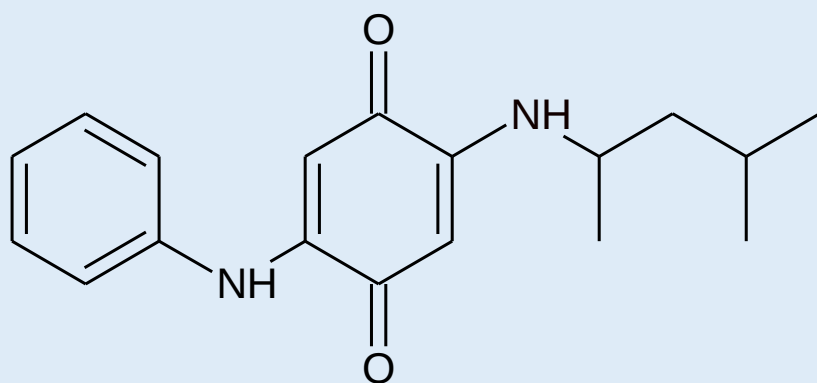
Name: N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine quinone (6PPD-Q)

Identification level: 1



6PPD-Q  
RT: 12.51 min

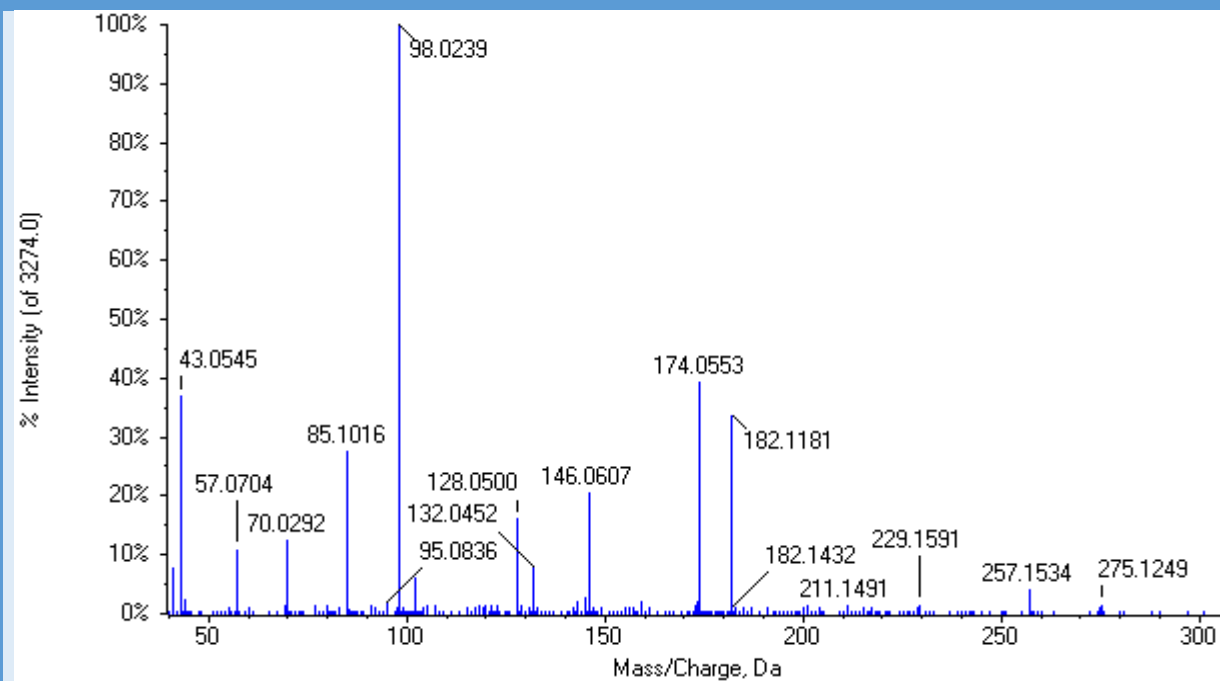
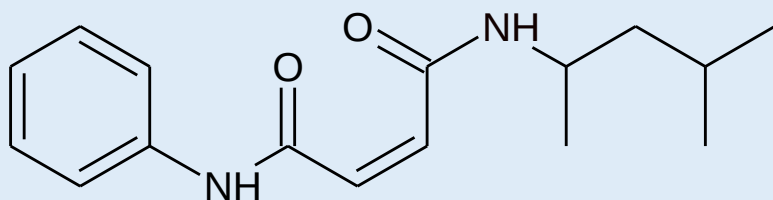
Identification level: 1



6PPD-Q  
RT: 12.51 min

Name: 6PPD TP274

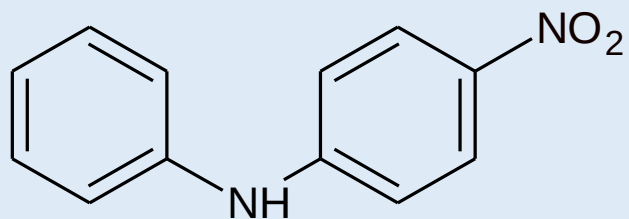
Identification level: 3



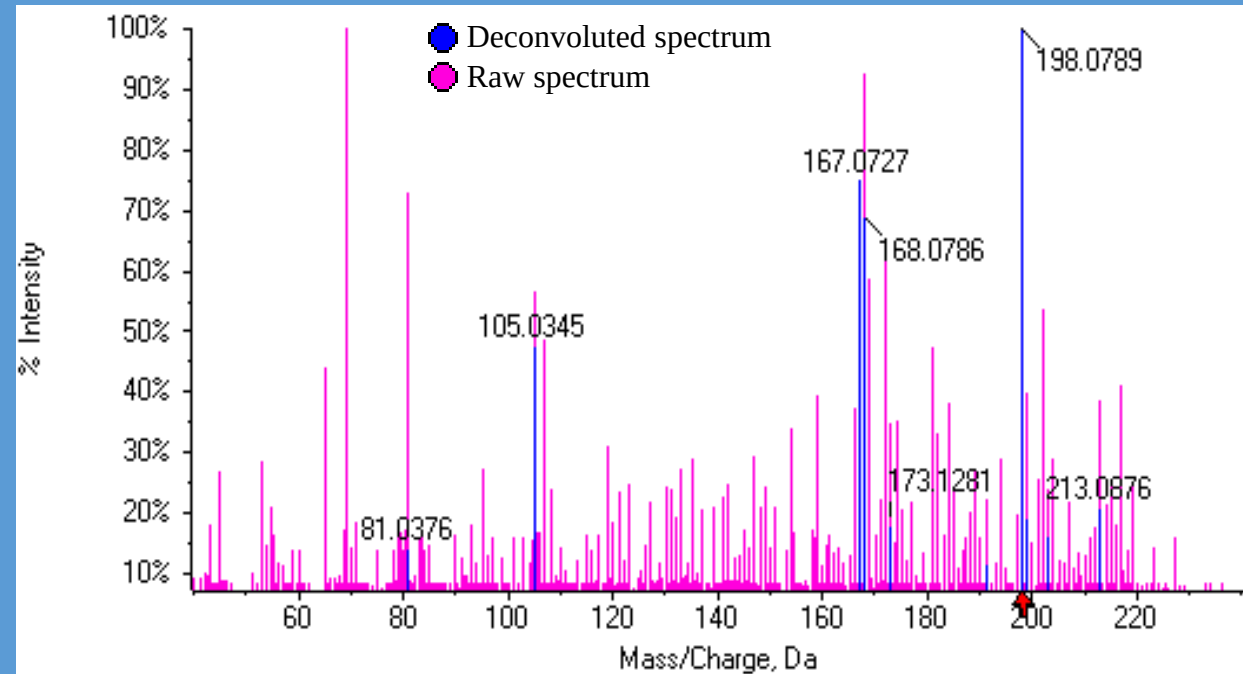
6PPD TP274  
RT: 11.67 min

Name: 4-nitrodiphenylamine (4-NDPA)

Identification level: 2a

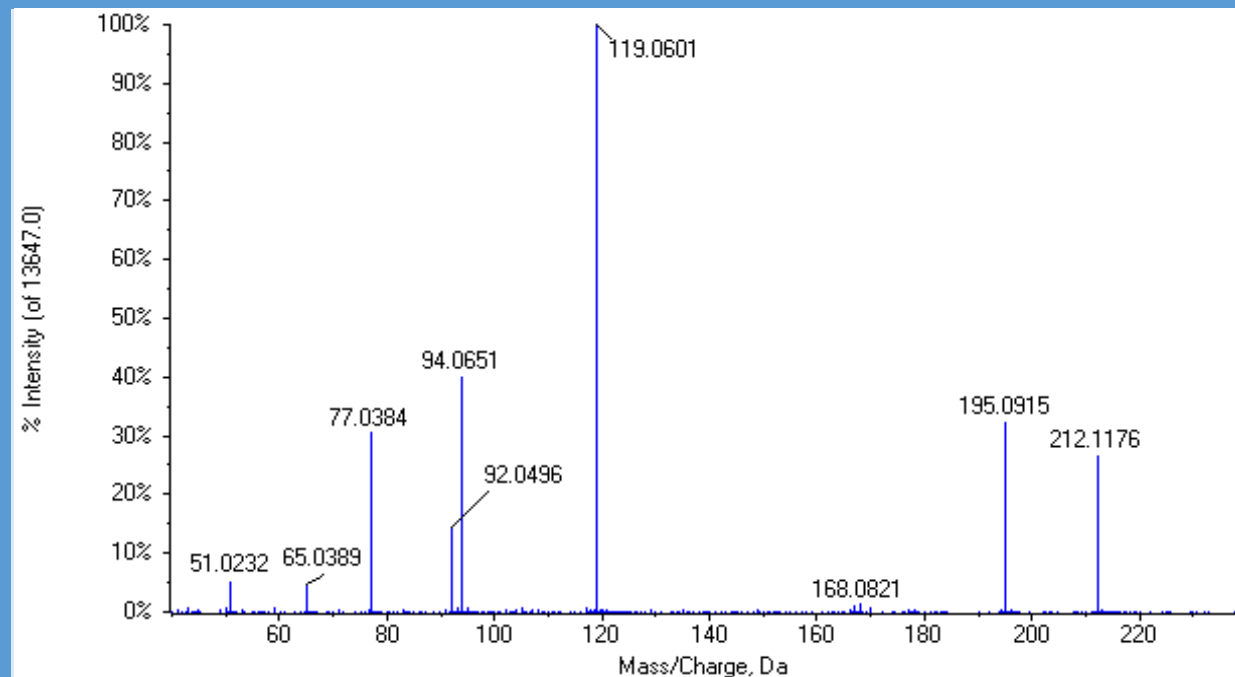
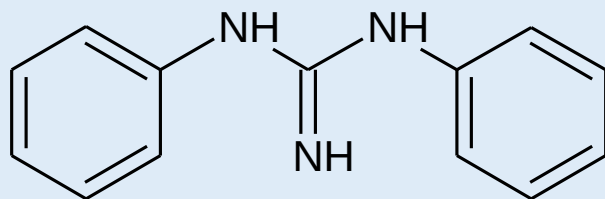


4-NDPA  
RT: 10.86 min



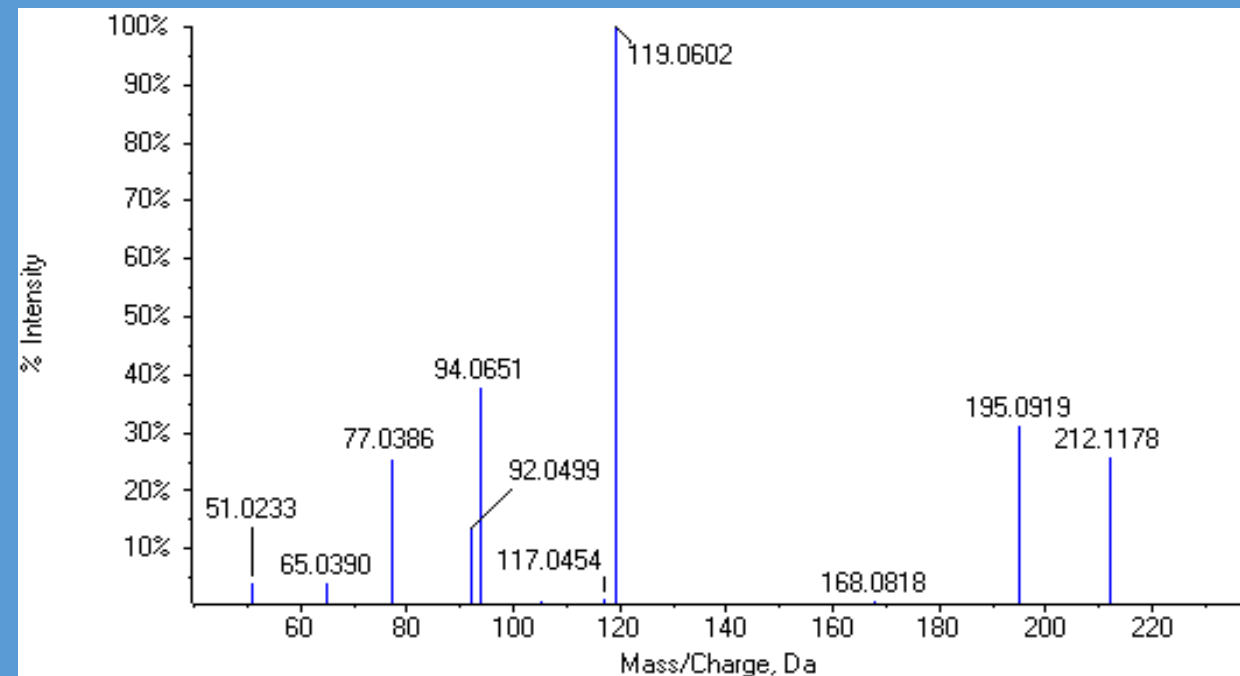
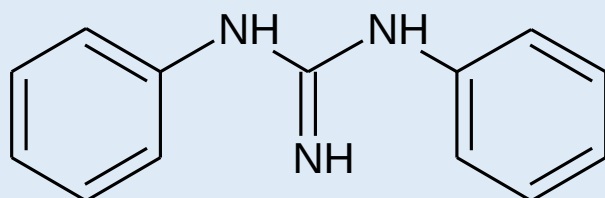
Name: 1,3-diphenyl guanidine (DPG)

Identification level: 1



DPG  
RT: 4.50 min

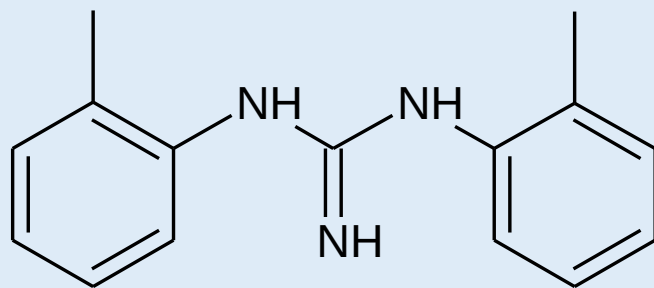
Identification level: 1



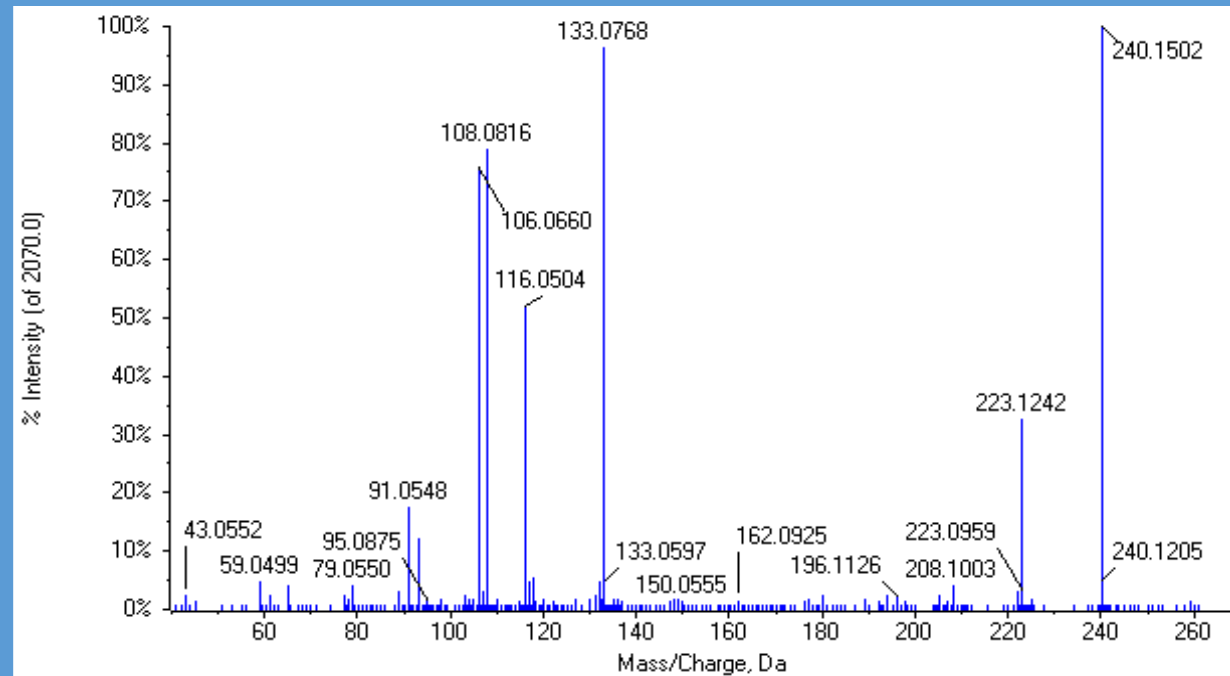
DPG  
RT: 4.50 min

Name: 1,3-Di-o-tolilguanidine (DTG)

Identification level: 1

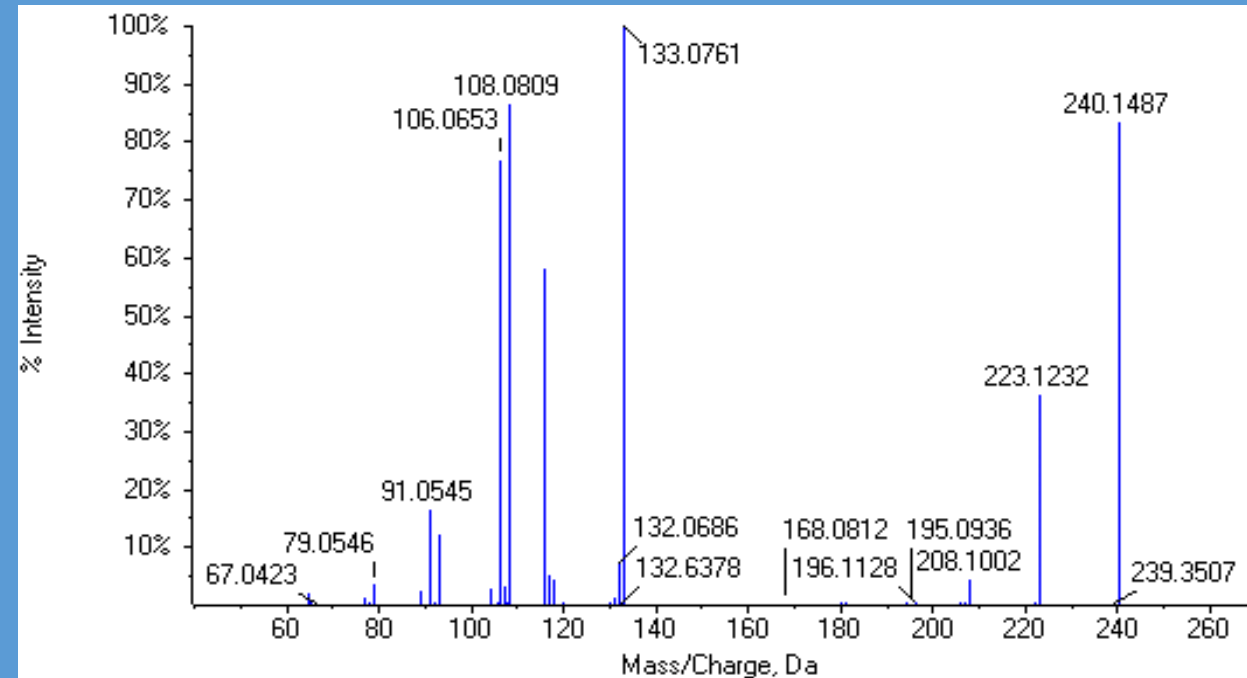
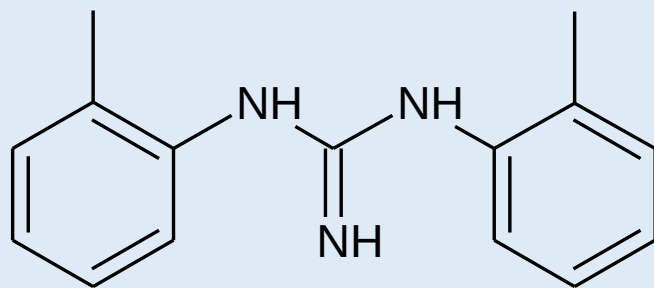


DTG  
RT: 5.70 min





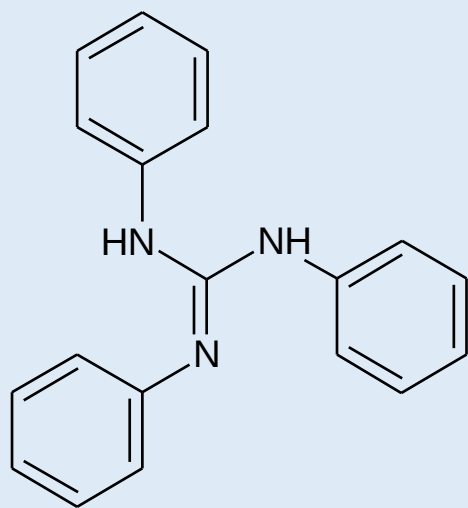
Identification level: 1



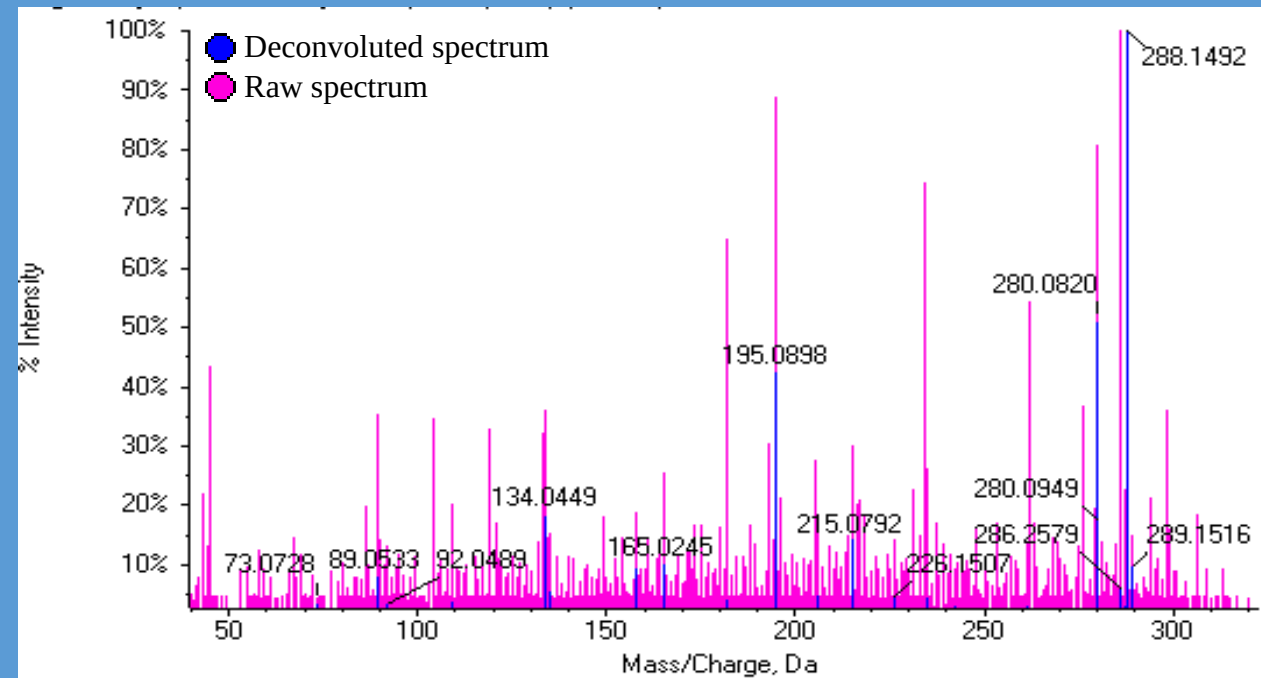
DTG  
RT: 5.70 min

Name: 1,2,3-Triphenylguanidine (123-TPG)

Identification level: 3

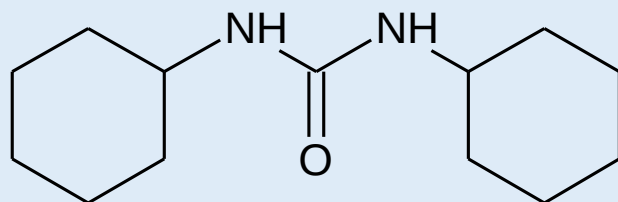


123-TPG  
RT: 7.56 min

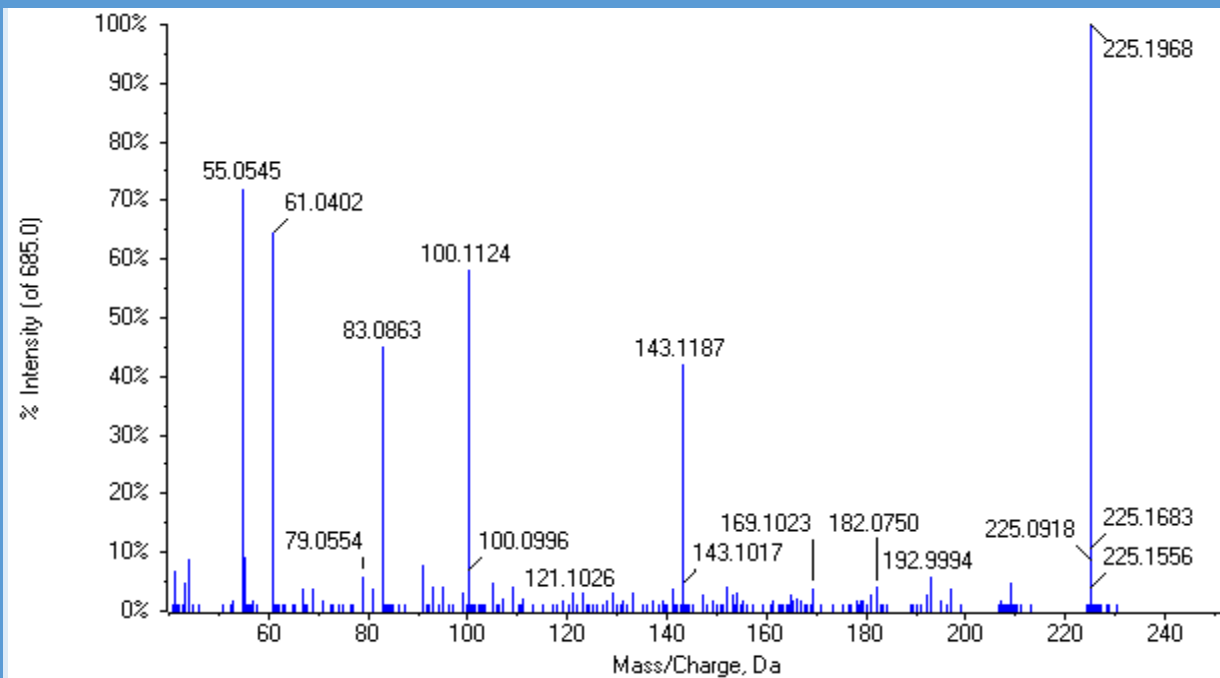


Name: 1,3-Dicyclohexylurea (DCU)

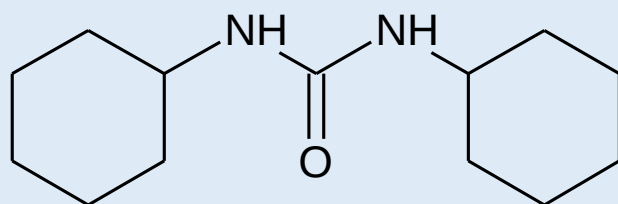
Identification level: 1



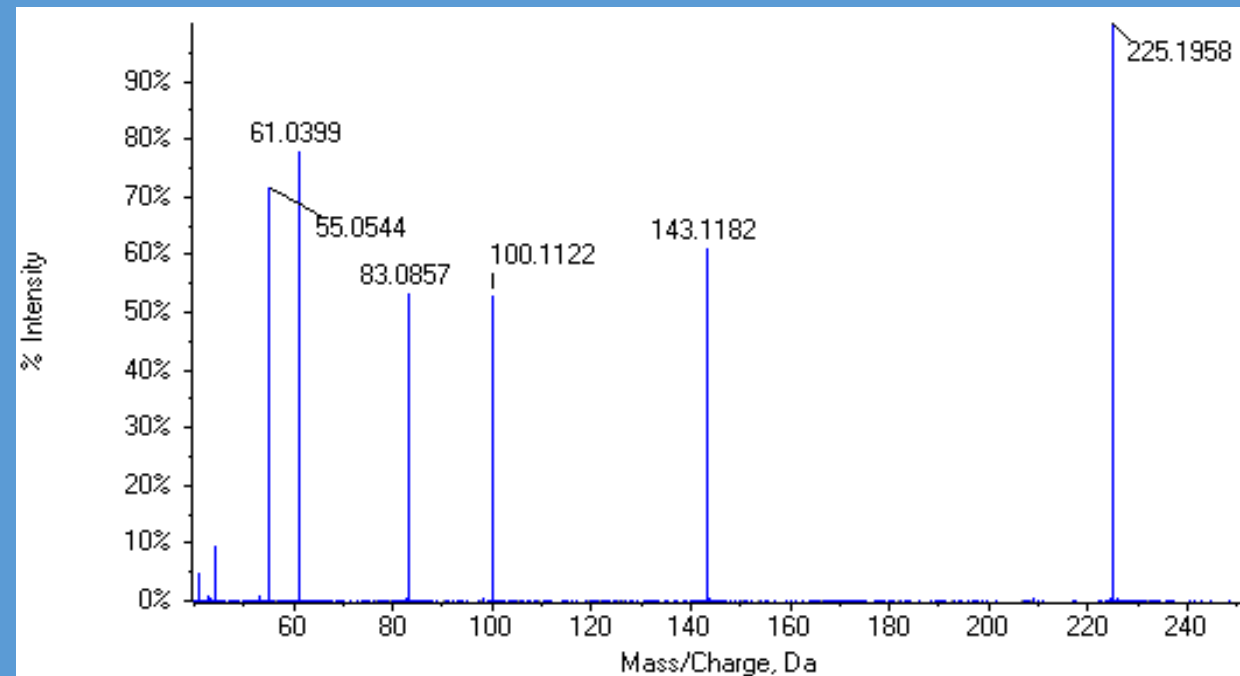
DCU  
RT: 10.23 min



Identification level: 1

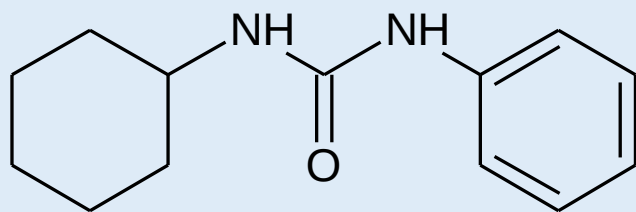


DCU  
RT: 10.23 min

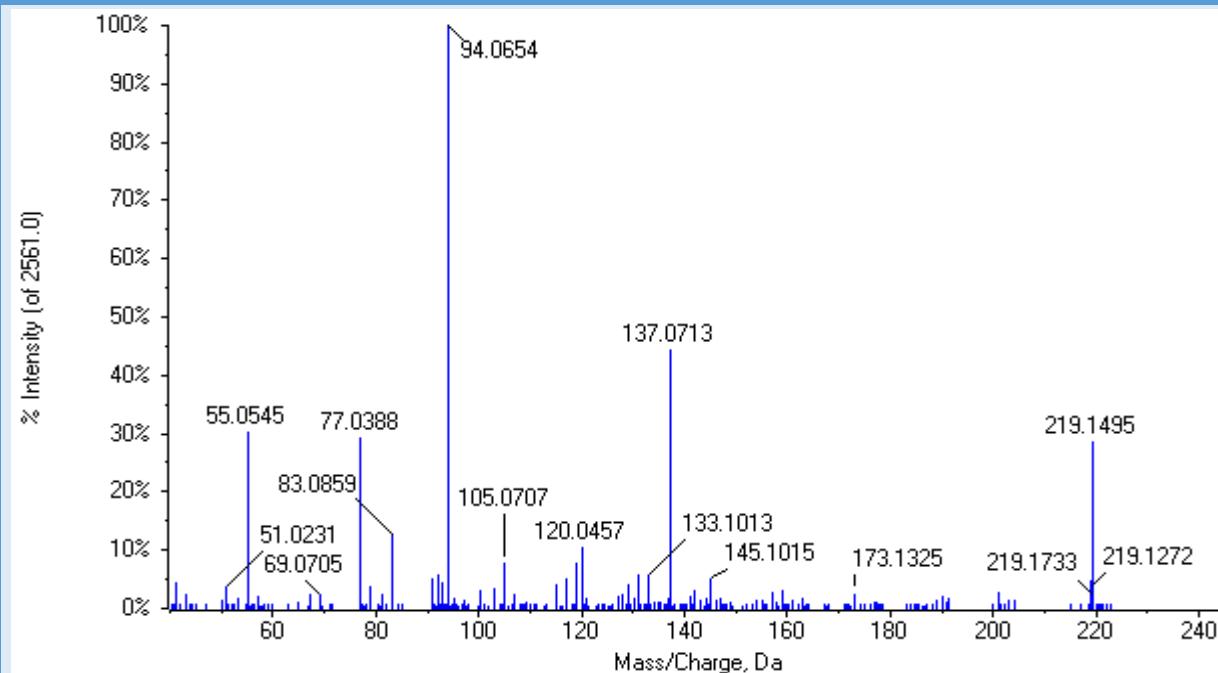


Name: 1-cyclohexyl-3-phenylurea (CPU)

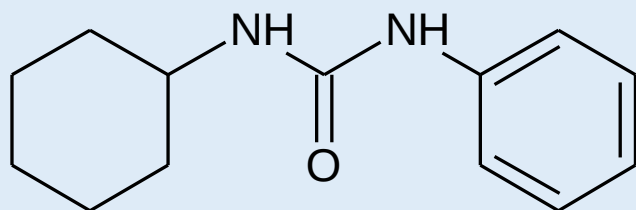
Identification level: 1



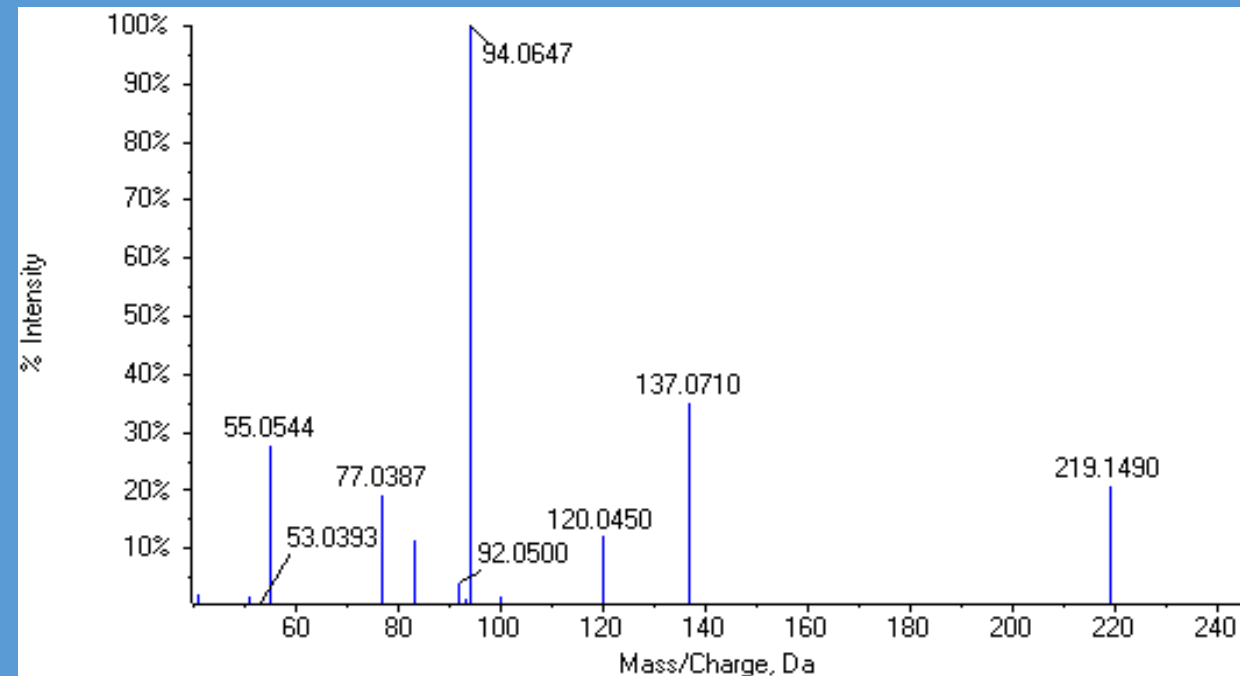
CPU  
RT: 9.45 min



Identification level: 1

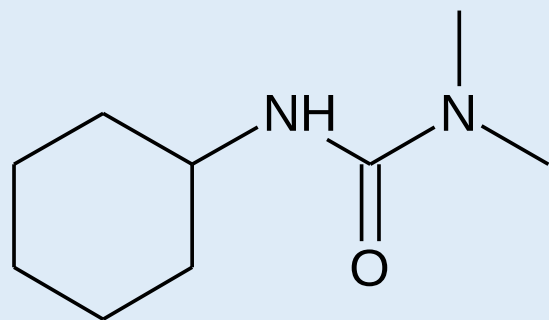


CPU  
RT: 9.45 min

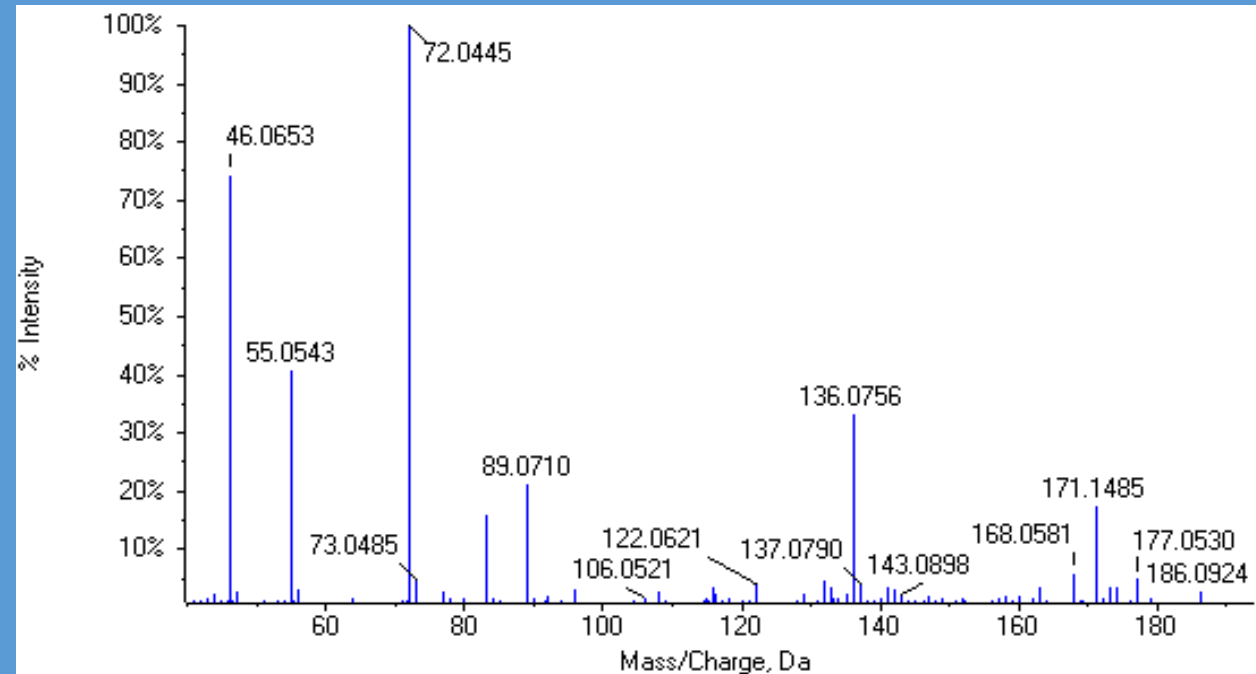


Name: 3-cyclohexyl-1,1-dimethylurea (C-DMU)

Identification level: 2a

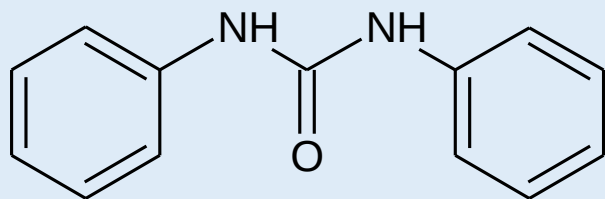


C-DMU  
RT: 6.99 min

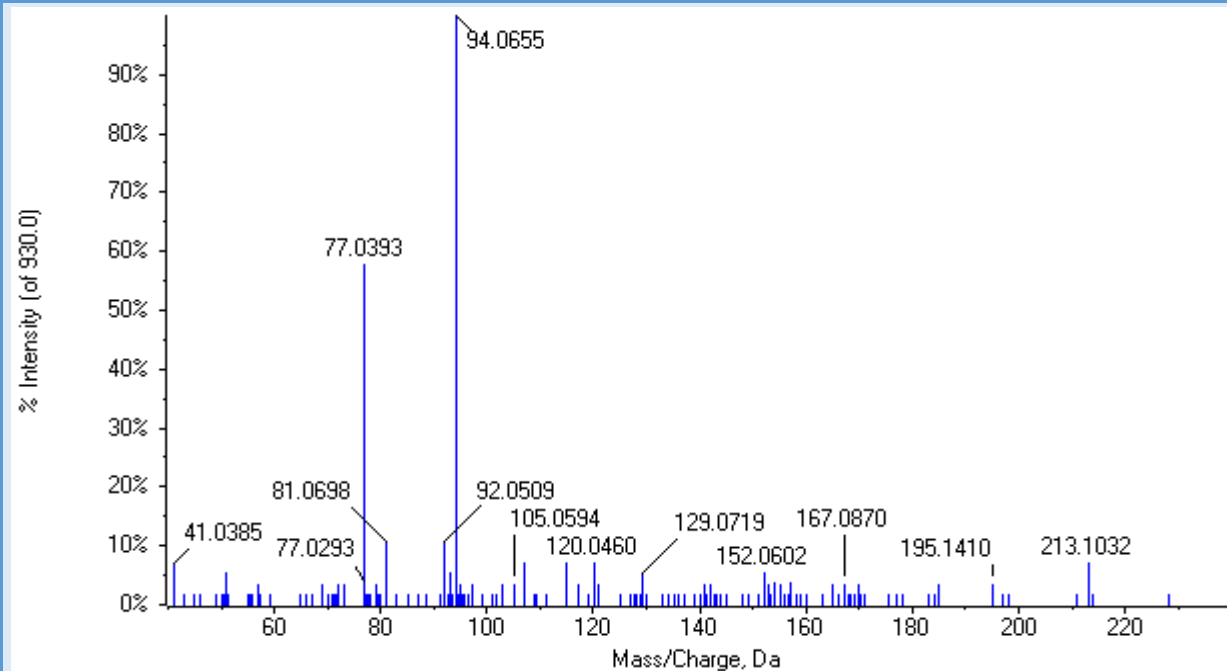


Name: 1,3-Diphenylurea (DPU)

Identification level: 2a



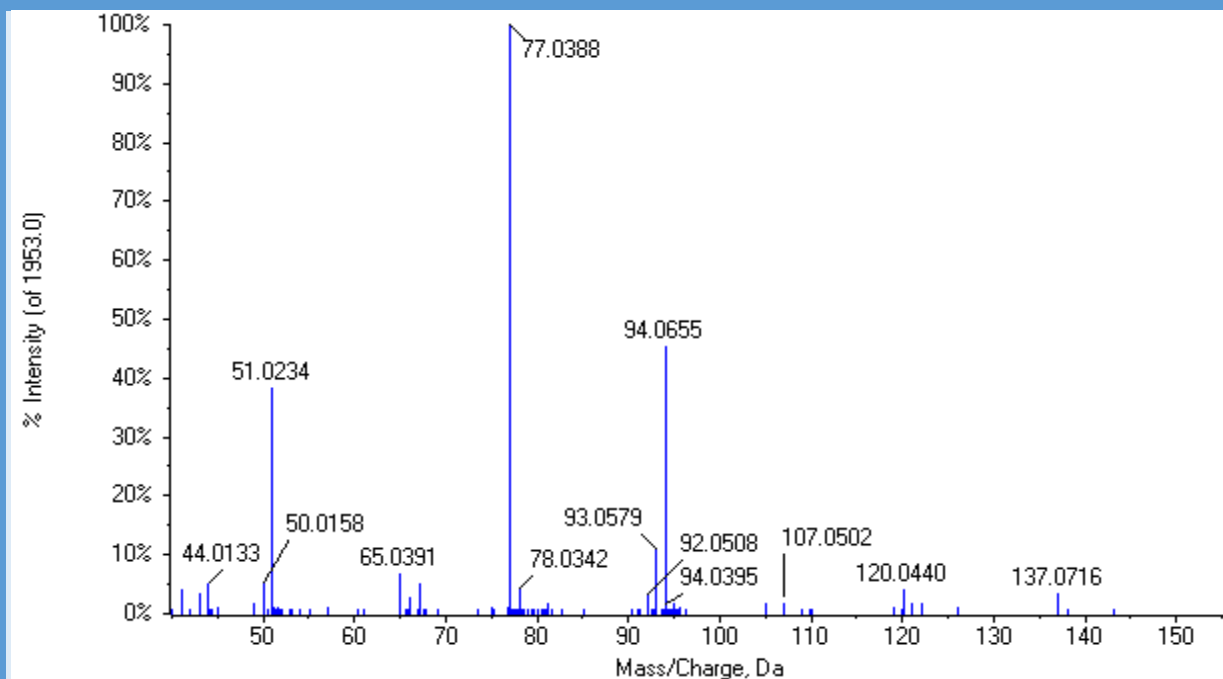
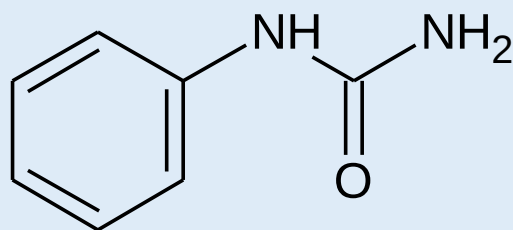
DPU  
RT: 8.63 min





Name: Phenylurea (PU)

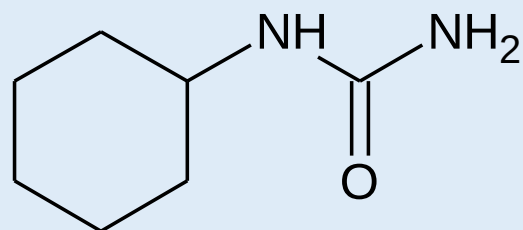
Identification level: 3



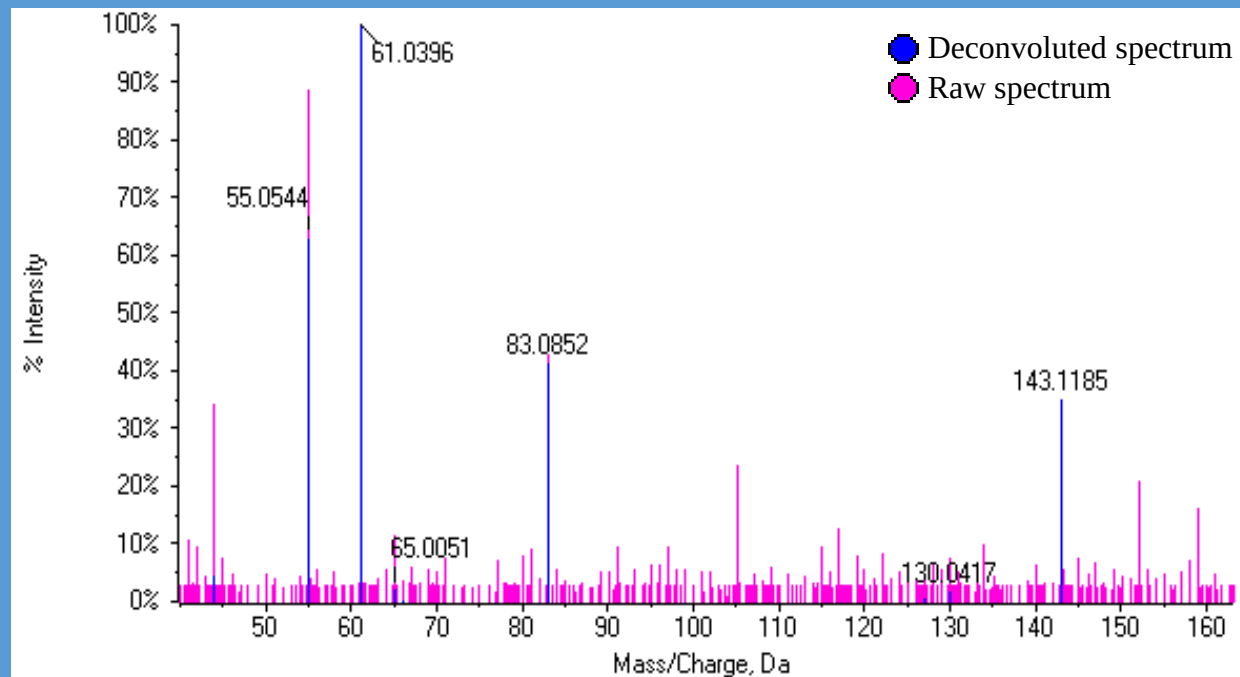
PU  
RT: 3.54 min

Name: Cyclohexylurea (CHU)

Identification level: 3

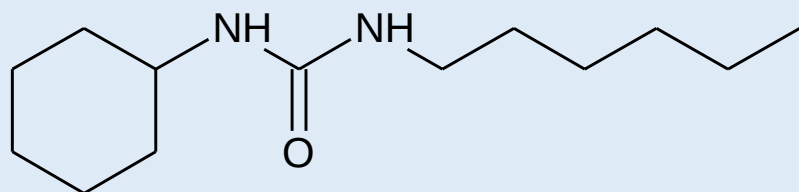


CHU  
RT: 5.15 min

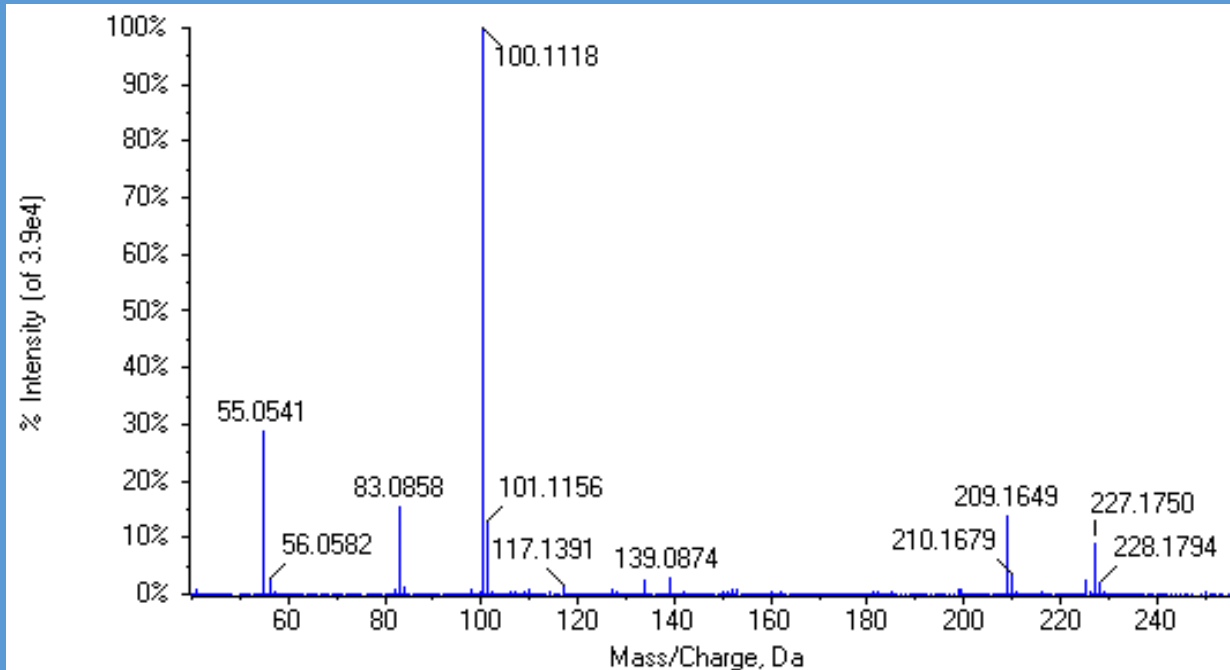


Name: N-Hexyl-N'-cyclohexylurea

Identification level: 4

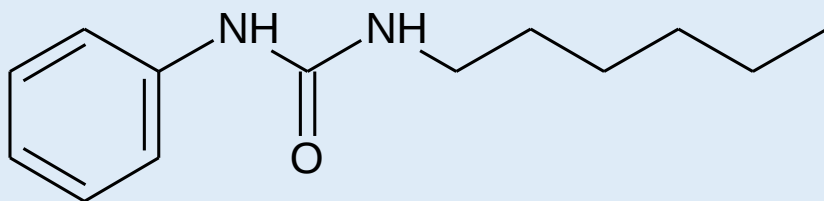


N-Hexyl-N'-cyclohexylurea  
RT: 3.75 min

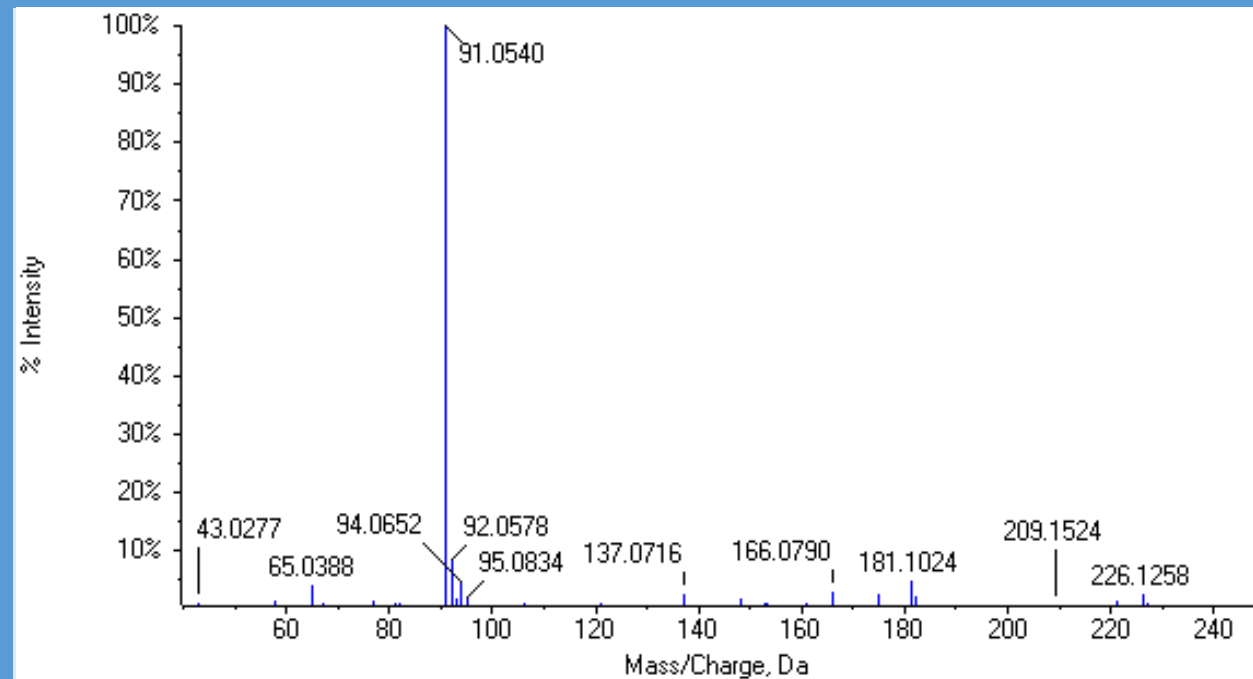


Name: N-Hexyl-N'-phenylurea

Identification level: 4

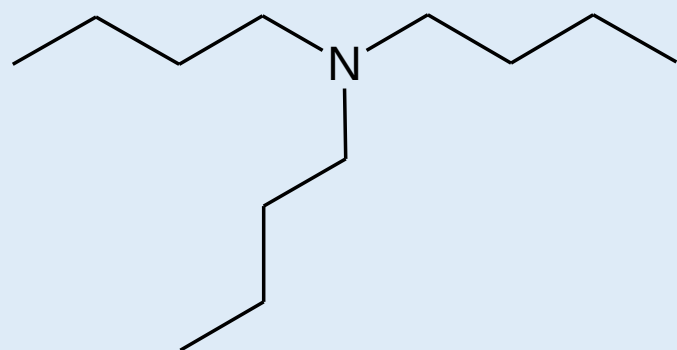


N-Hexyl-N'-phenylurea  
RT: 10.46 min

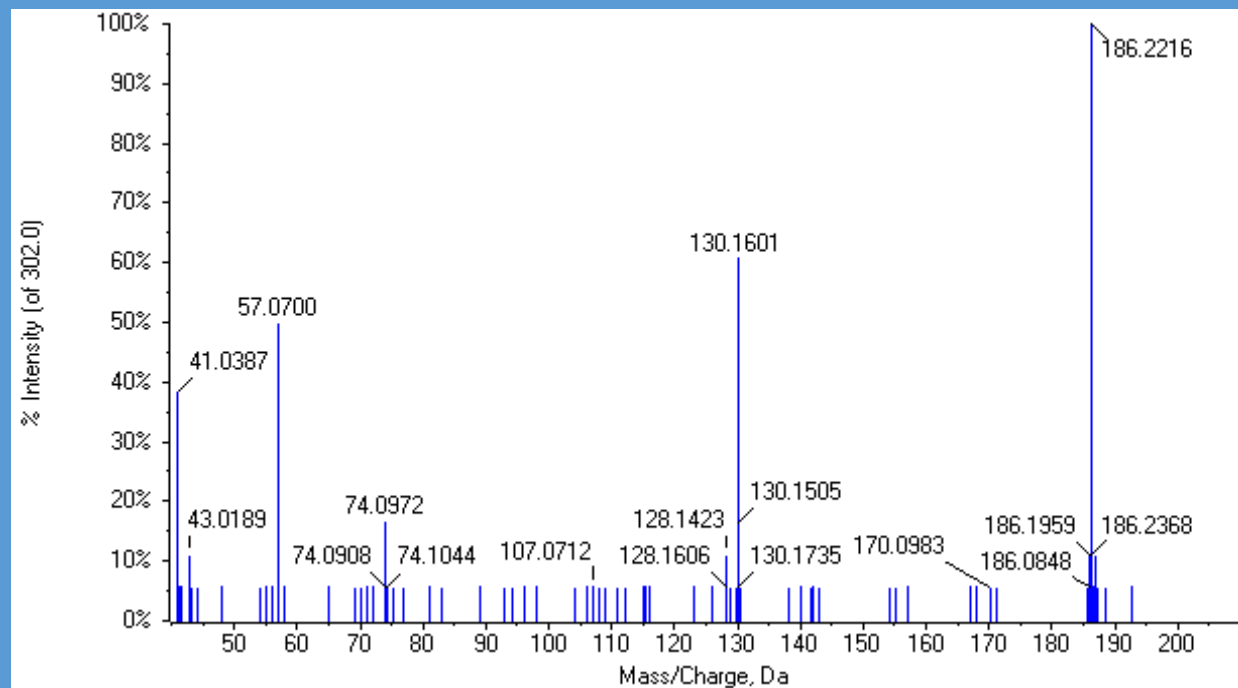


Name: Tributylamine (TBA)

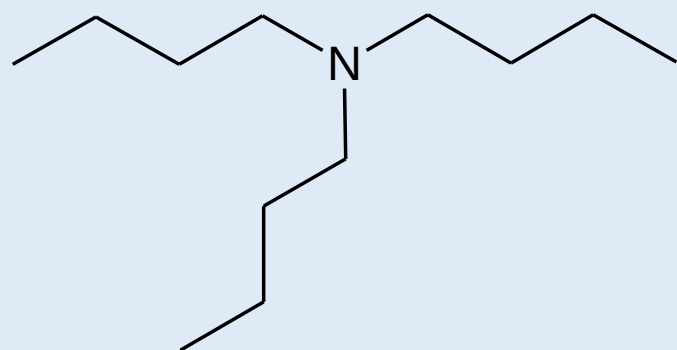
Identification level: 1



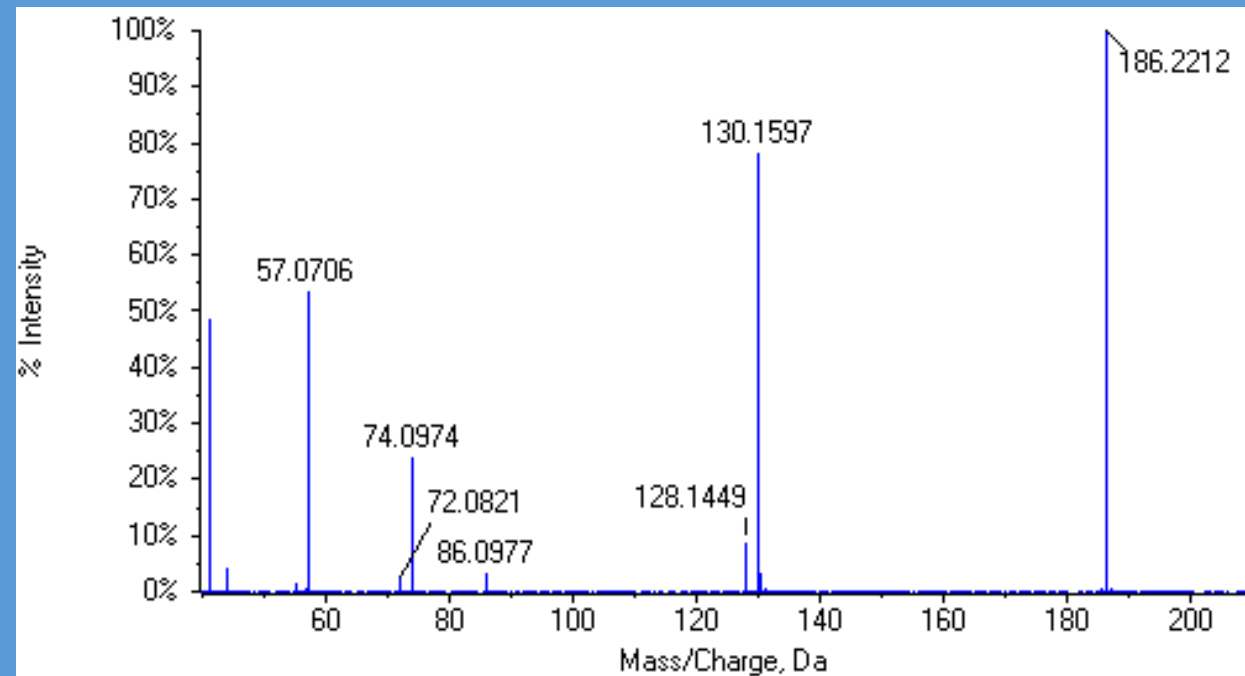
TBA  
RT: 5.92 min



Identification level: 1

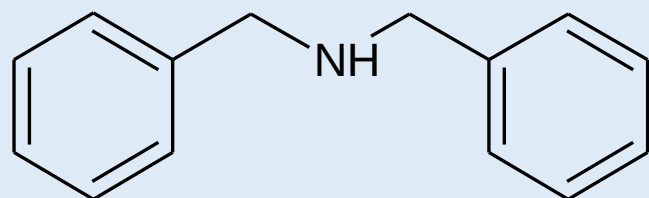


TBA  
RT: 5.92 min

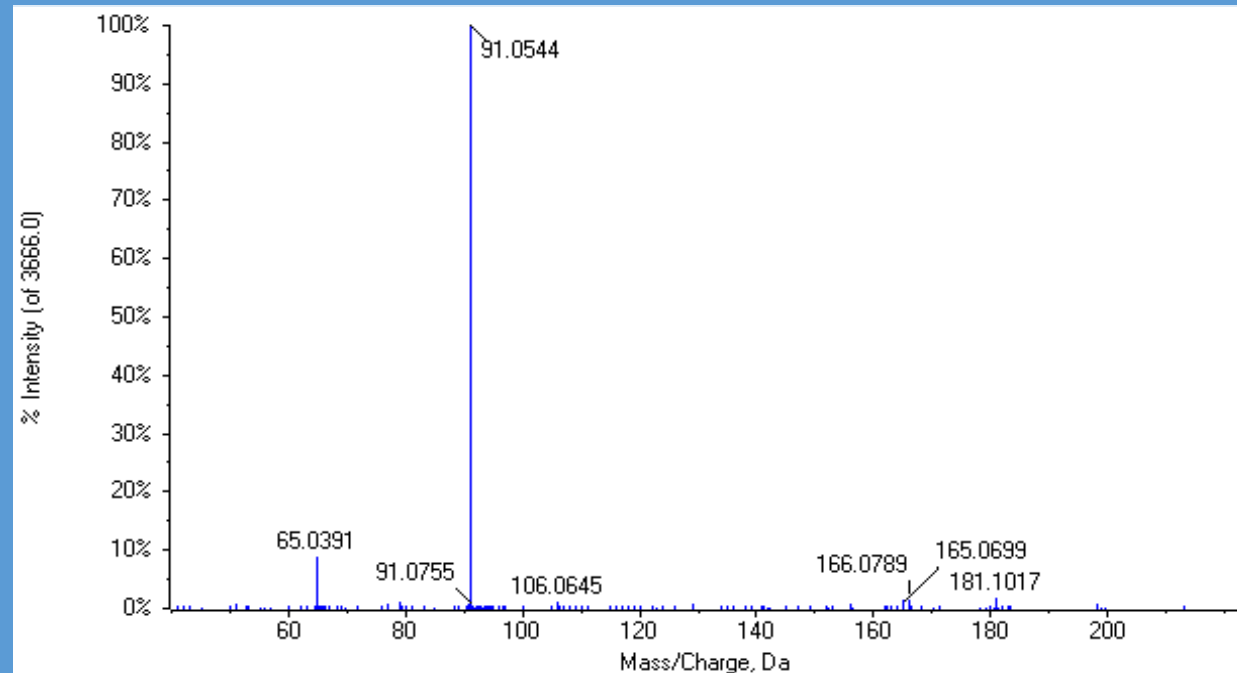


Name: Dibenzylamine (DBA)

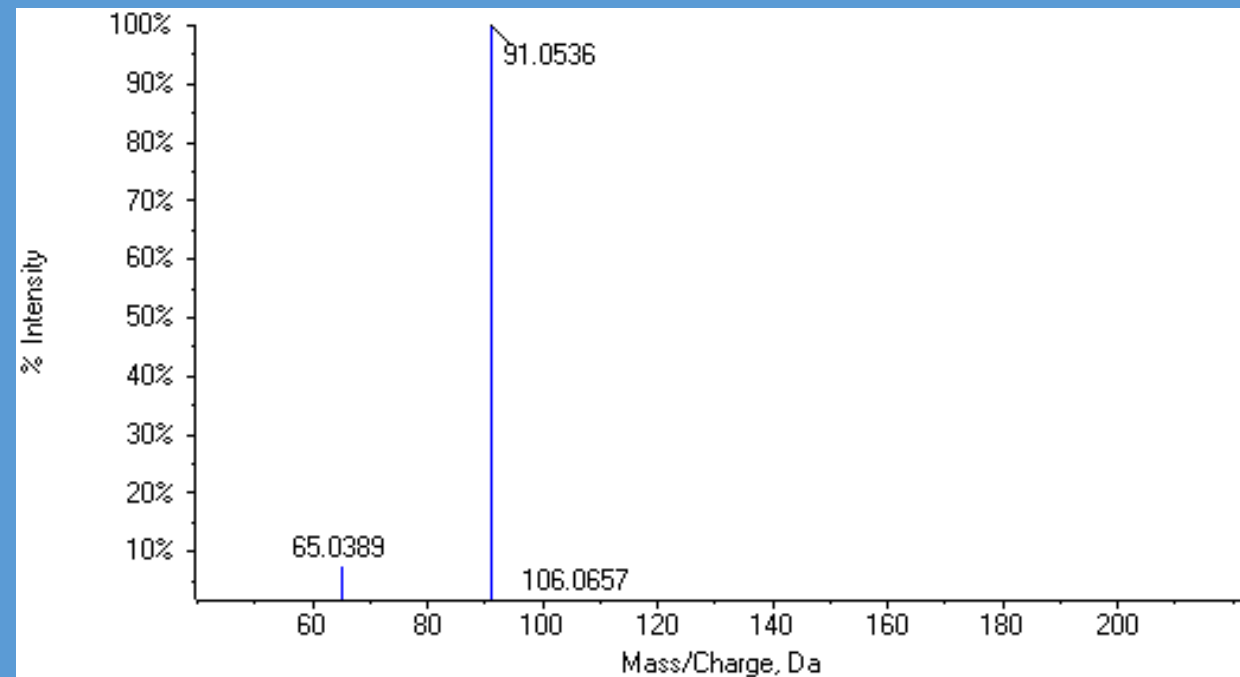
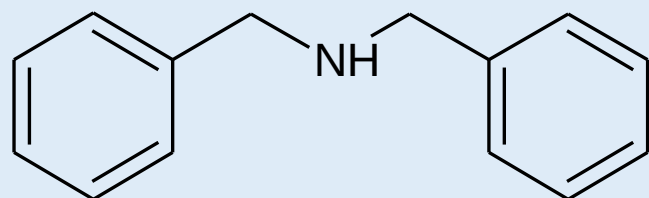
Identification level: 1



DBA  
RT: 5.11 min



Identification level: 1

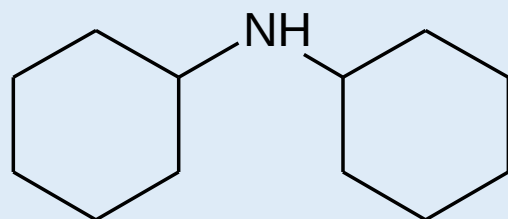


DBA  
RT: 5.11 min

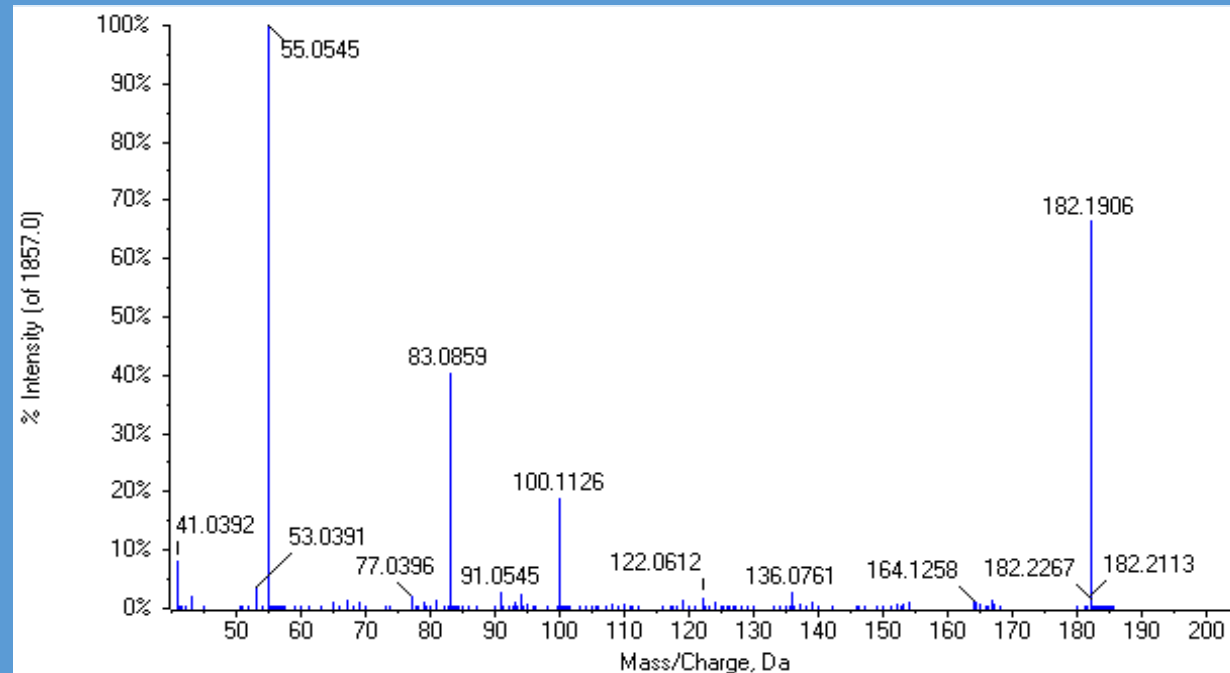


Name: Dicyclohexylamine (DCA)

Identification level: 2a

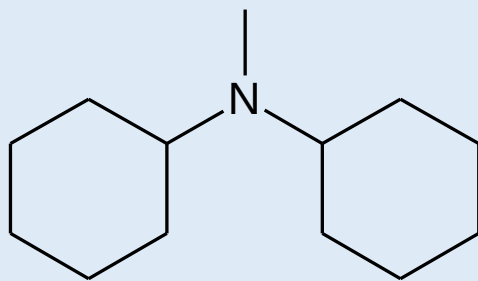


DCA  
RT: 5.42 min

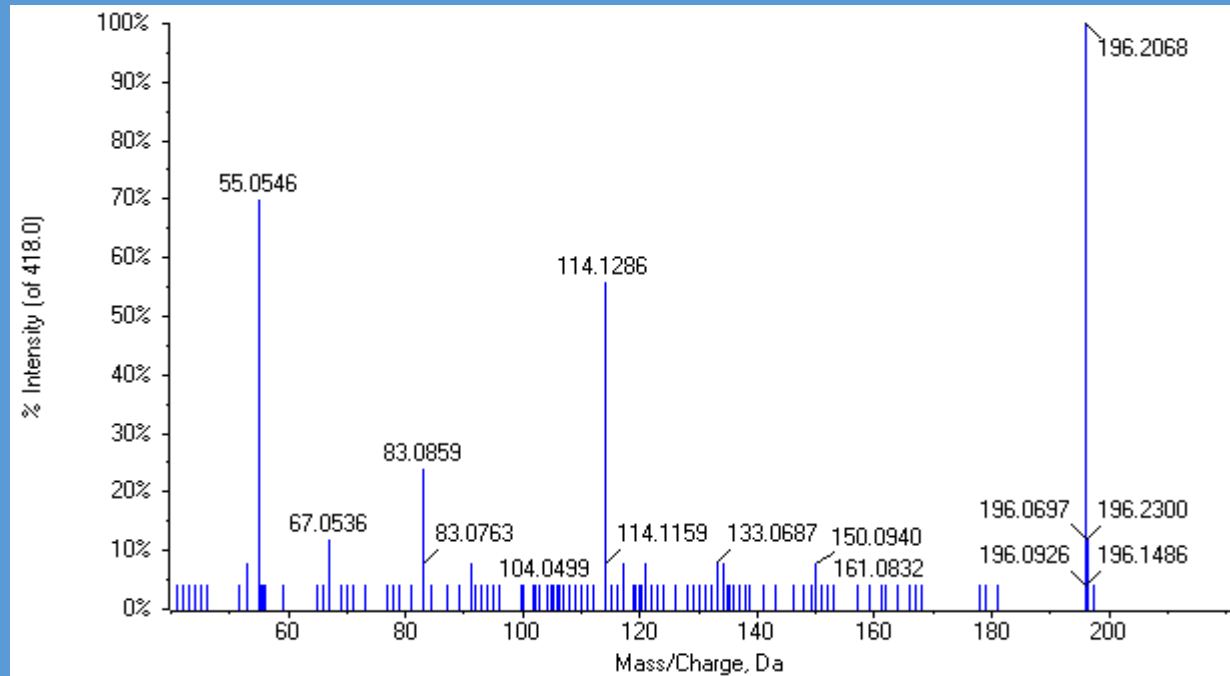


Name: N-methyldicyclohexylamine (M-DCA)

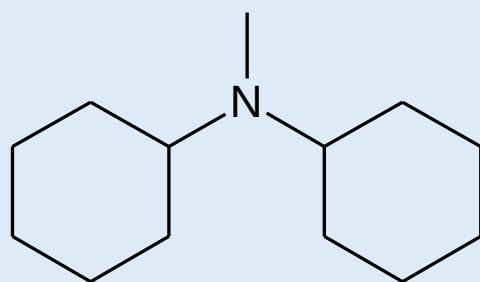
Identification level: 1



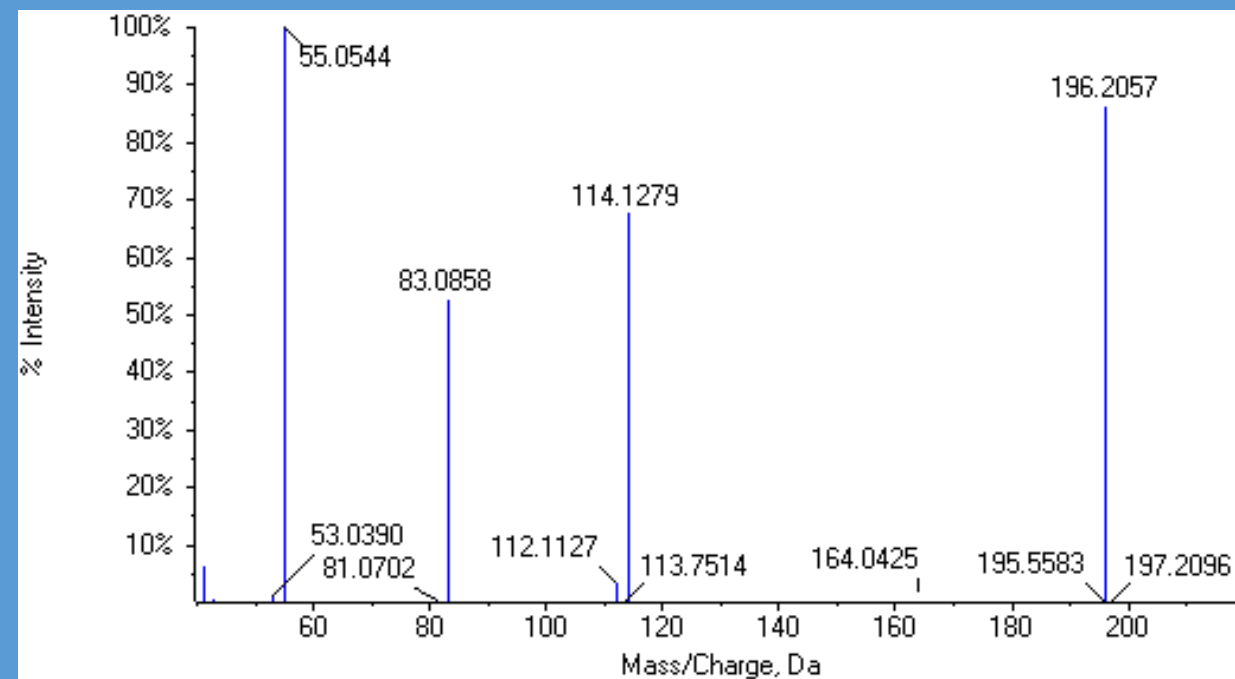
M-DCA  
RT: 5.17 min



Identification level: 1

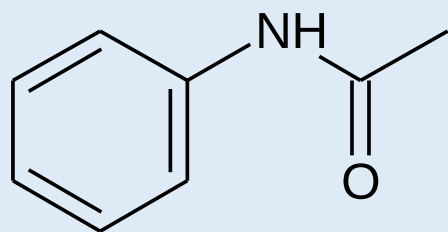


M-DCA  
RT: 5.17 min

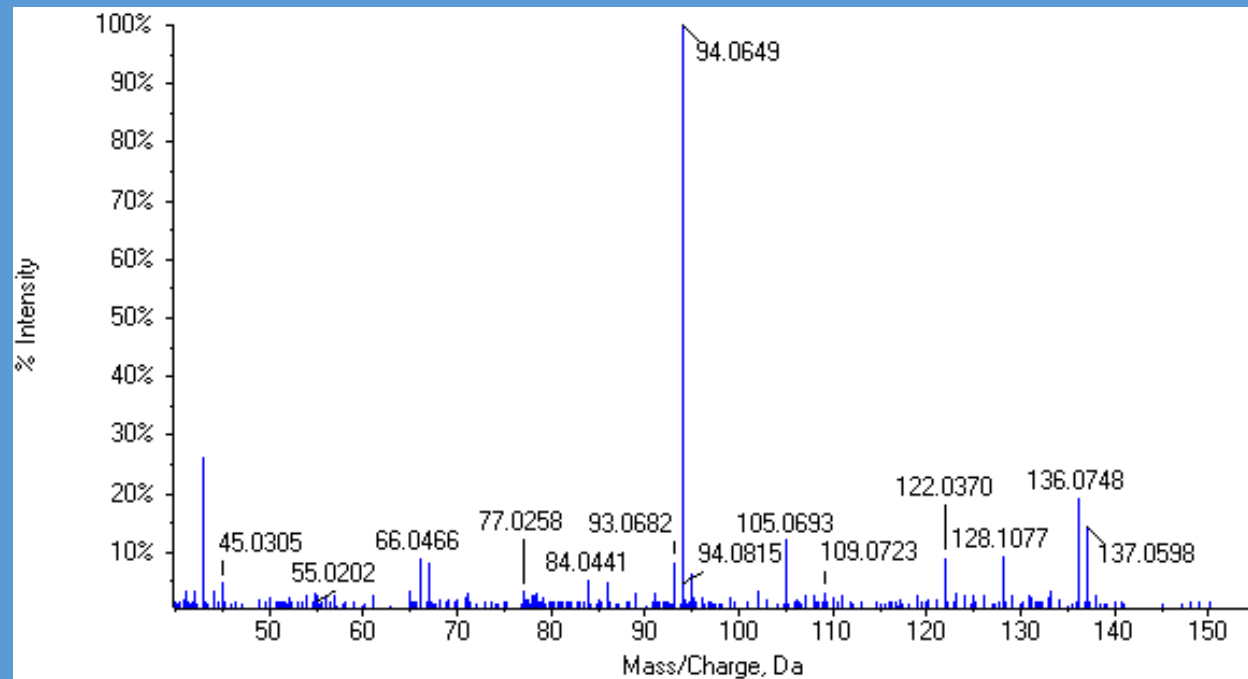


Name: Acetanilide

Identification level: 2a

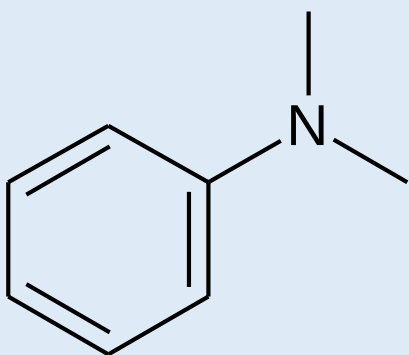


Acetanilide  
RT: 4.73 min

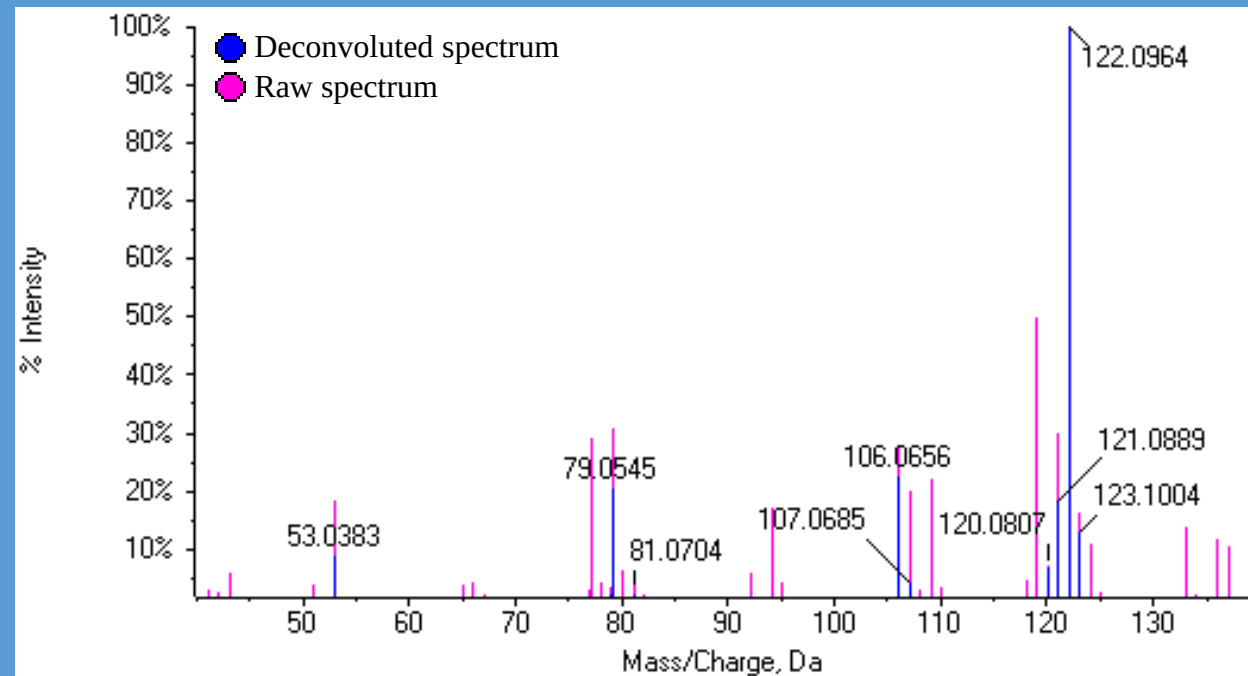


Name: N,N-Dimethylaniline

Identification level: 2a

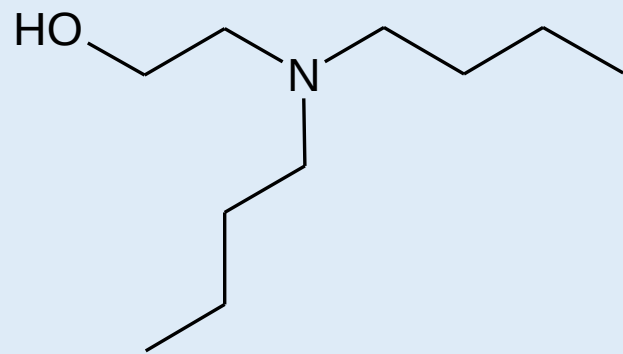


N,N-Dimethylaniline  
RT: 2.21 min

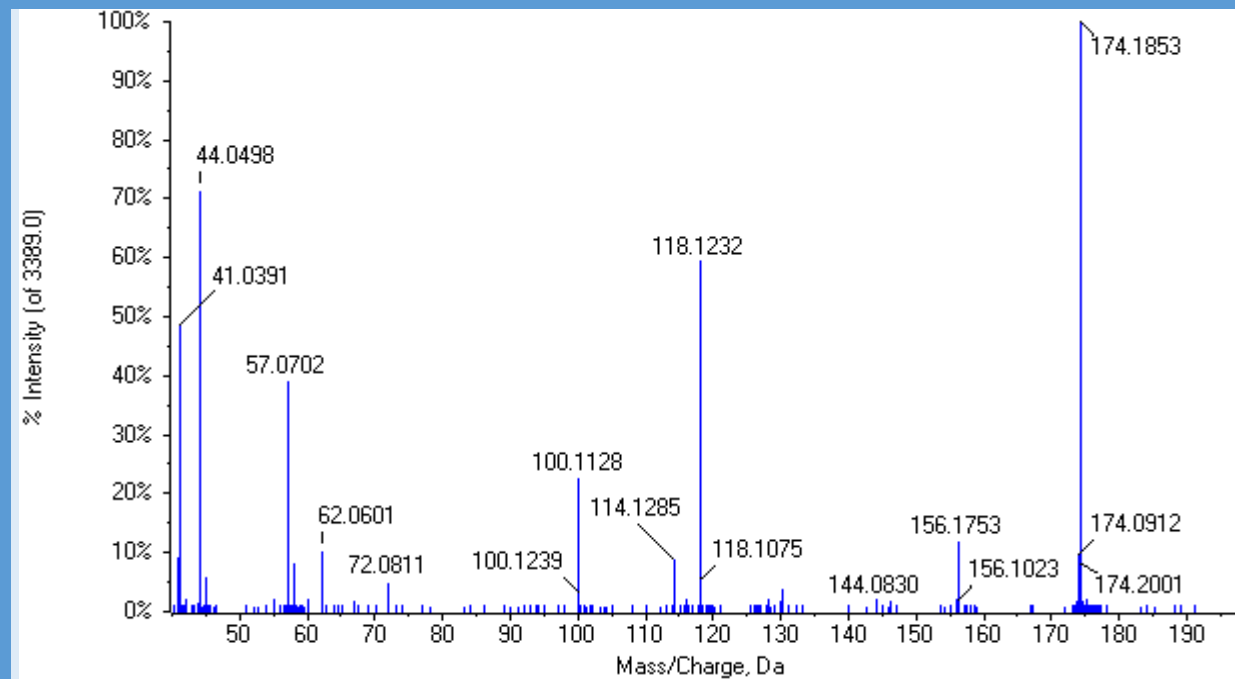


Name: 2-N-dibutylaminoethanol (2-DBAE)

Identification level: 3

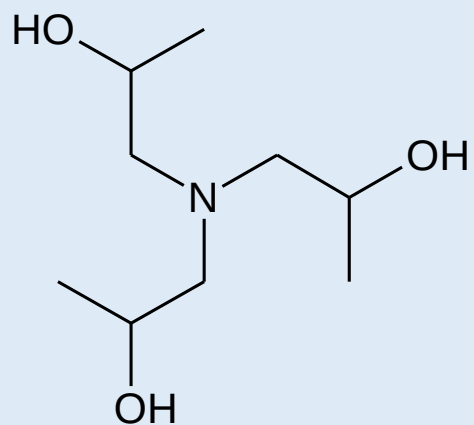


2-DBAE  
RT: 3.40 min

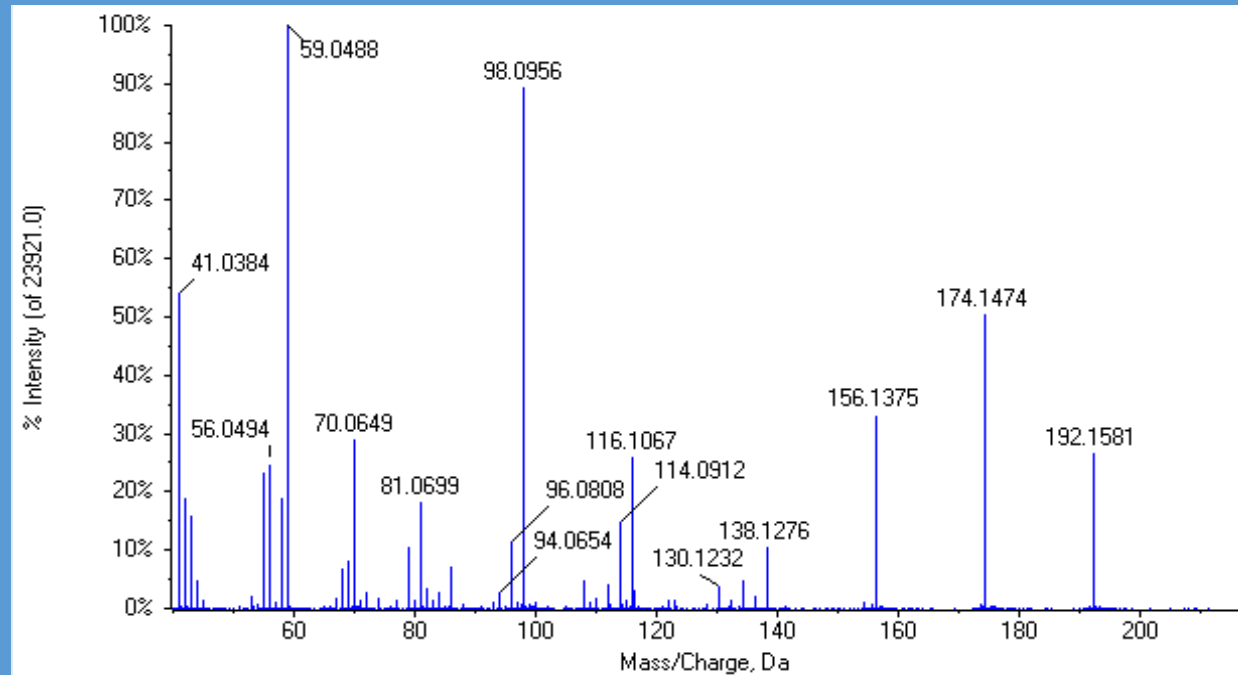


Name: Triisopropanolamine (TIPA)

Identification level: 2a

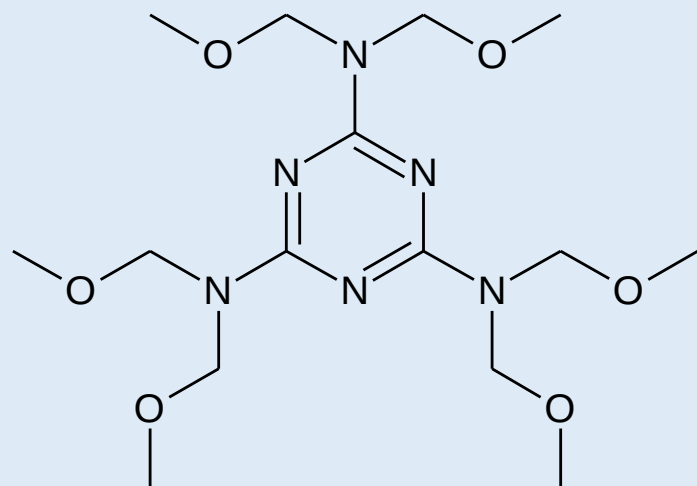


TIPA  
RT: 1.09 min

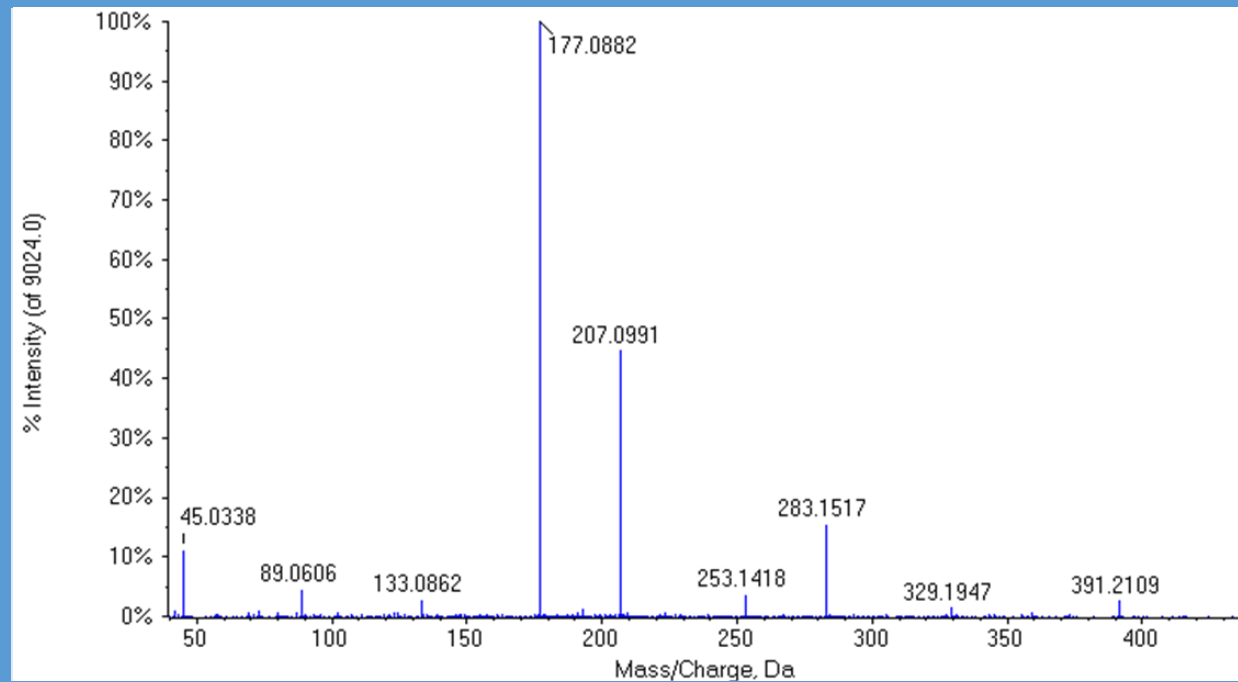


Name: Hexa(methoxymethyl)melamine (HMMM)

Identification level: 1

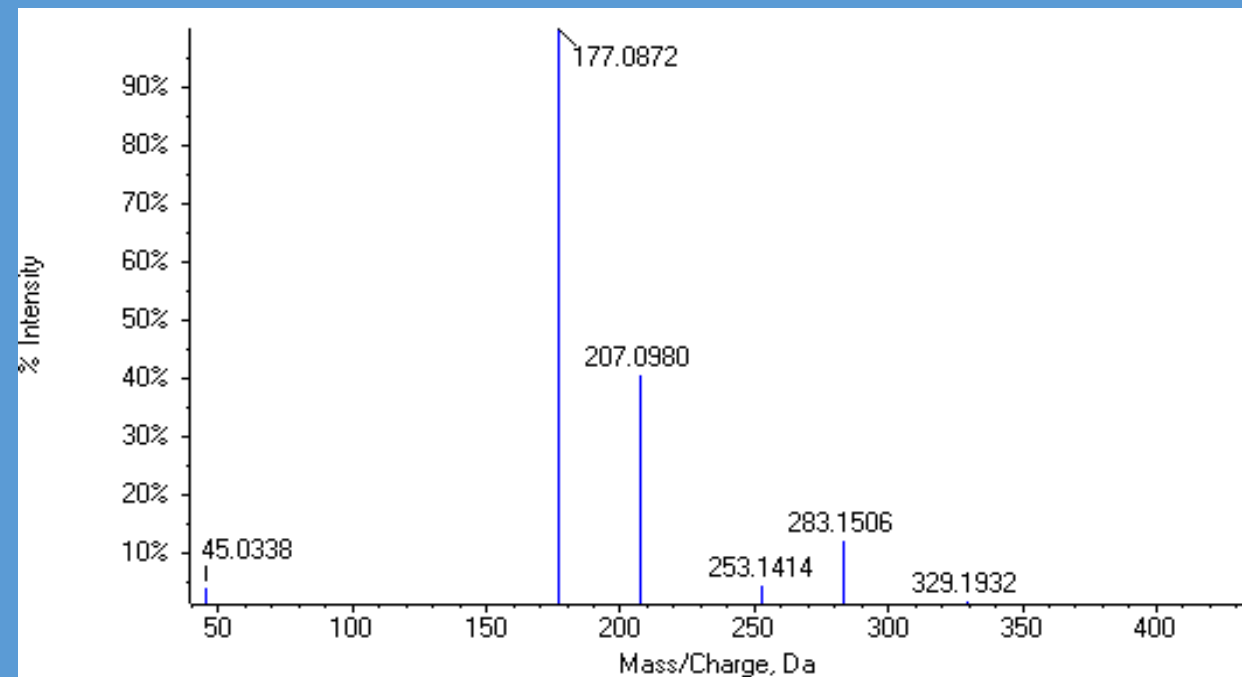
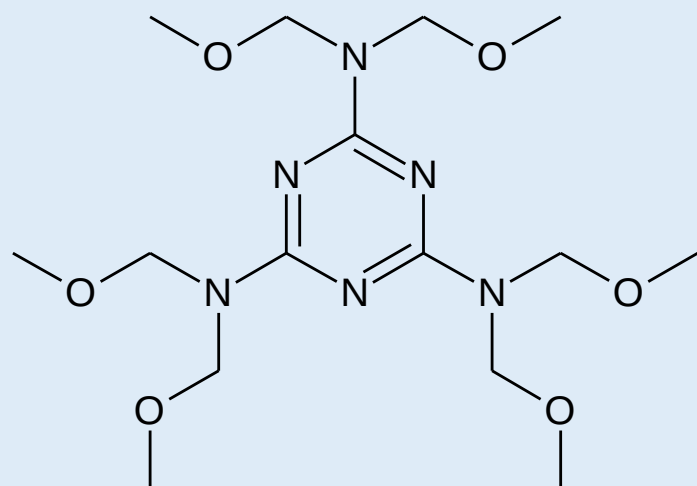


HMMM  
RT: 8.97 min





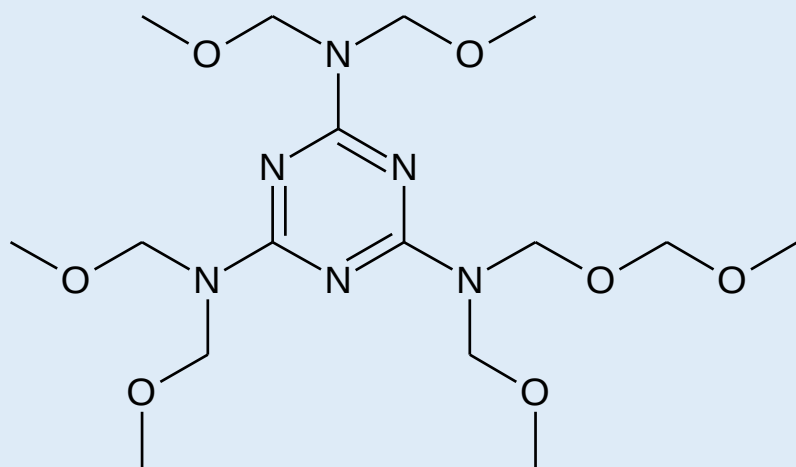
Identification level: 1



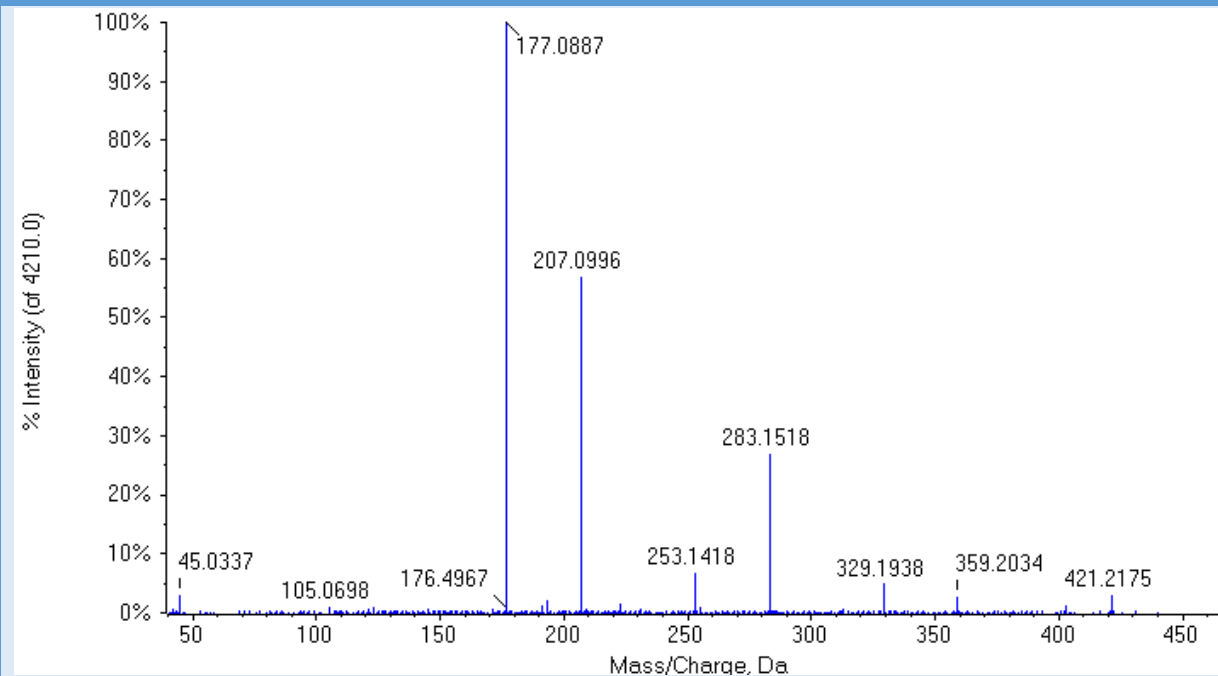
HMMM  
RT: 8.97 min

Name: diformylated-Hexa(methoxymethyl)melamine (d-HMMM)

Identification level: 2a

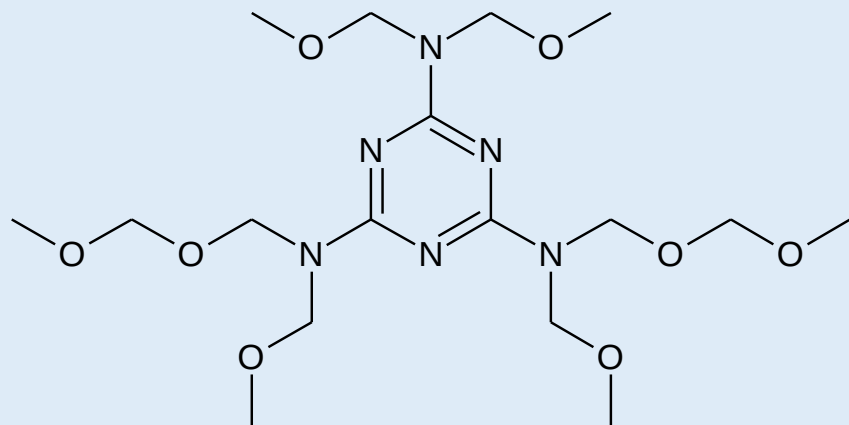


d-HMMM  
RT: 8.97 min

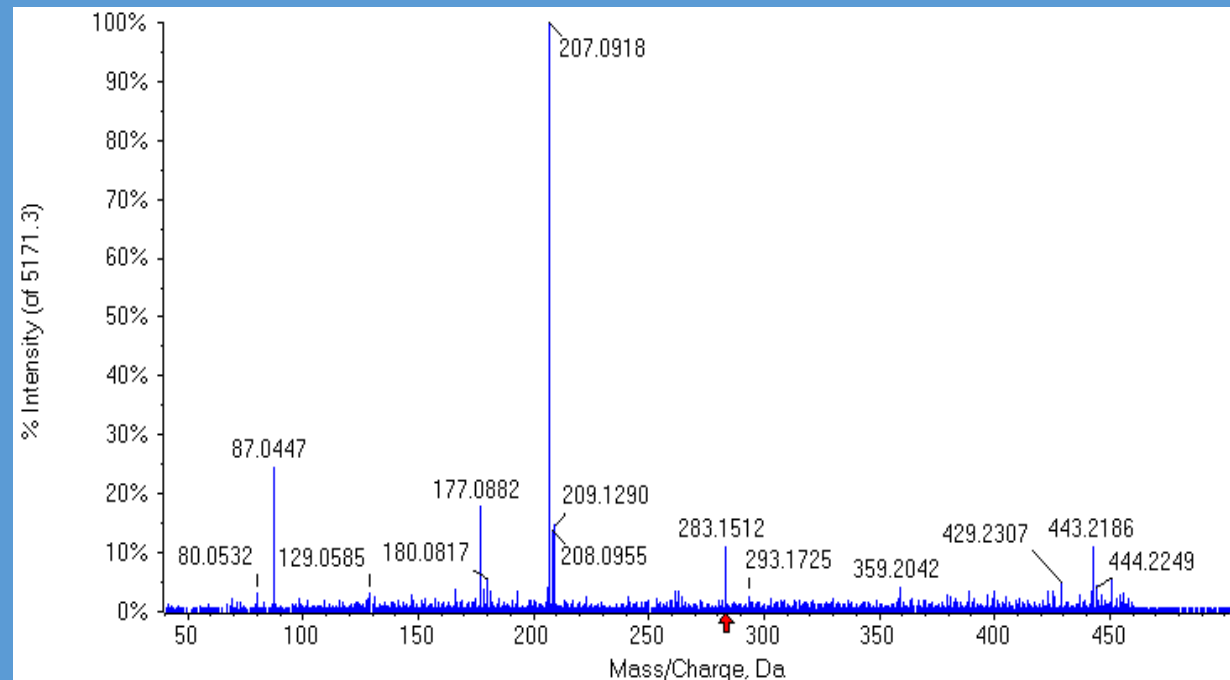


Name: double diformylated-HMMM (dd-HMMM)

Identification level: 3

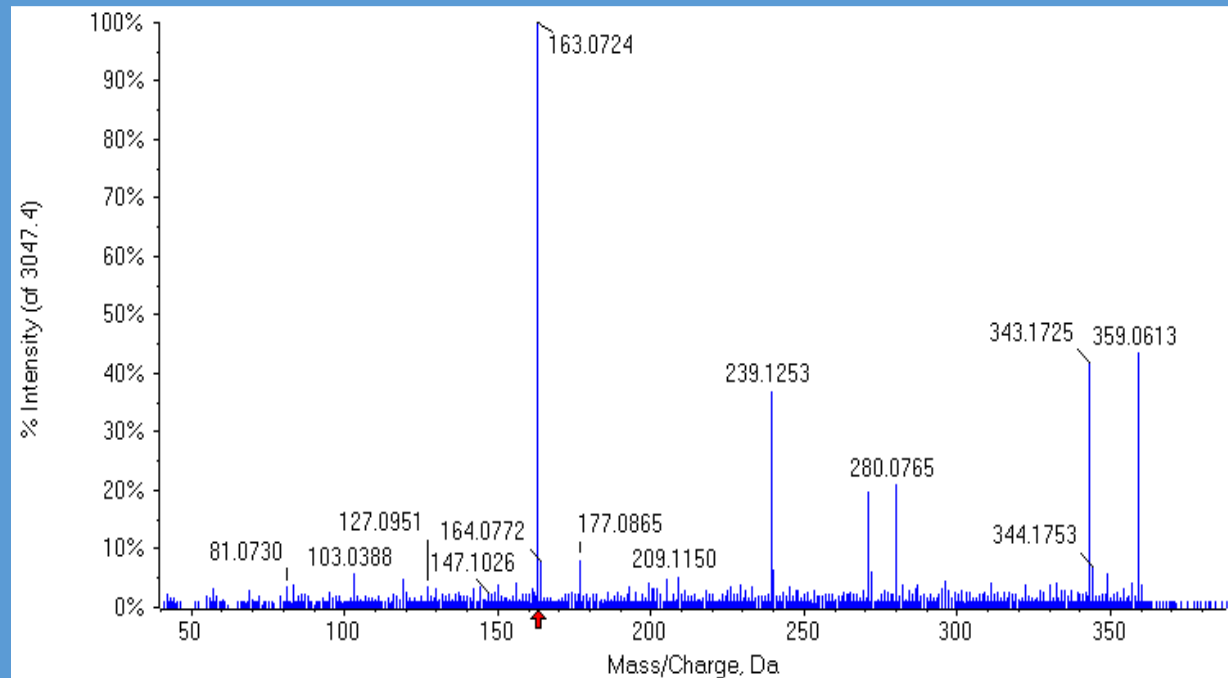
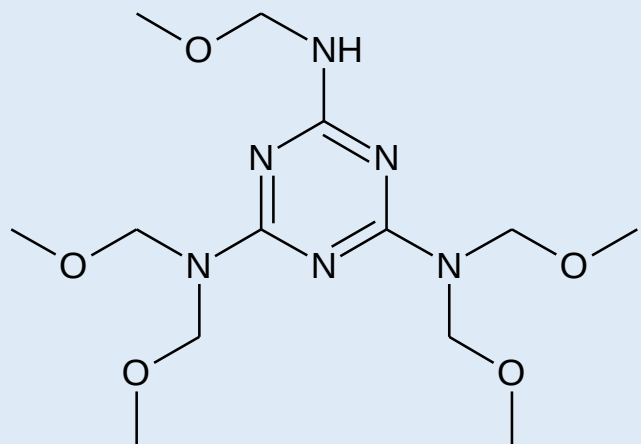


dd-HMMM  
RT: 9.83 min



Name: Penta(methoxymethyl)melamine (PMMM)

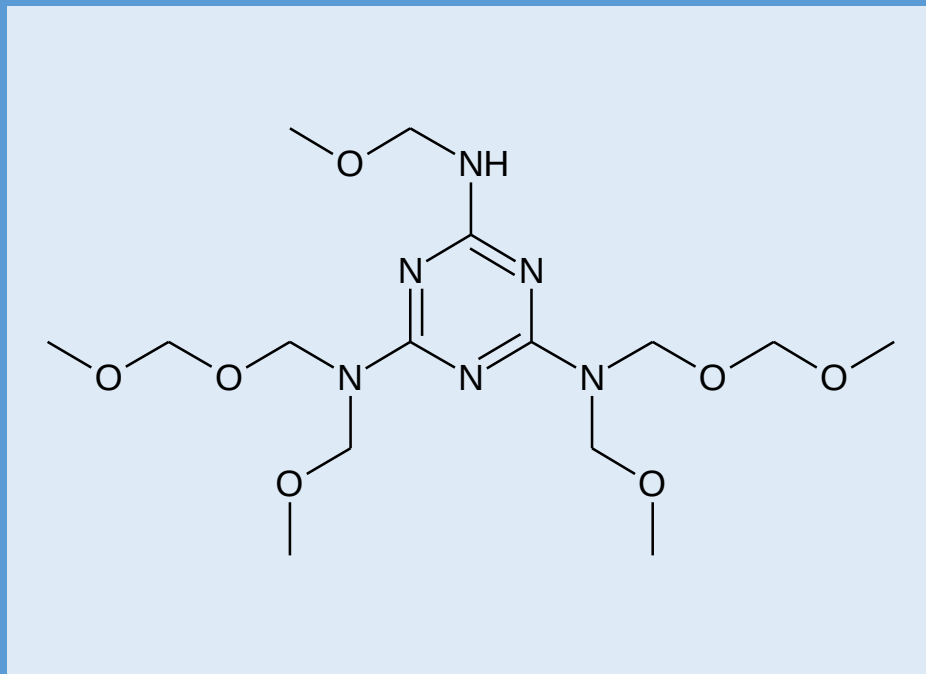
Identification level: 3



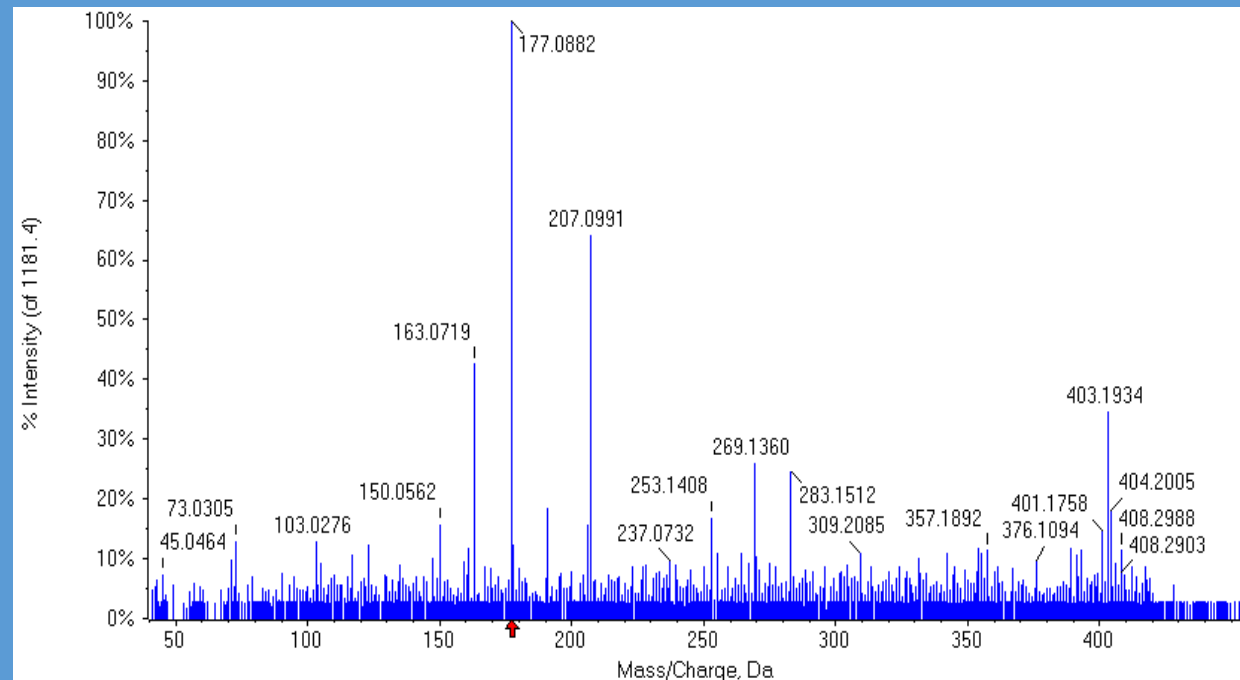
PMMM  
RT: 7.55 min

Name: double diformylated-PMMM (dd-PMMM)

Identification level: 3

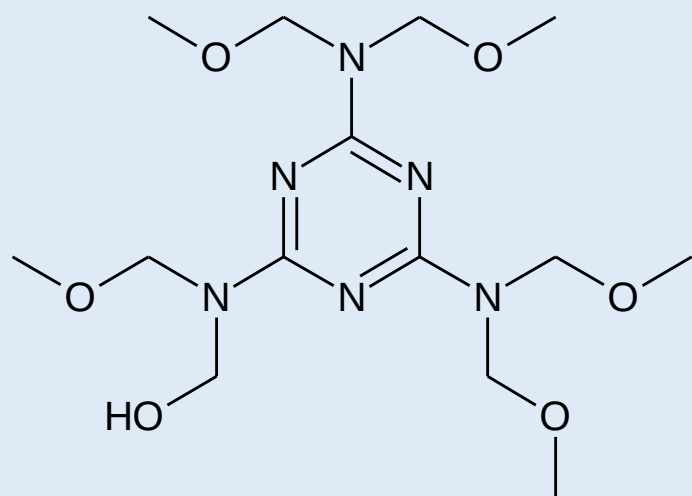


dd-PMMM  
RT: 8.31 min

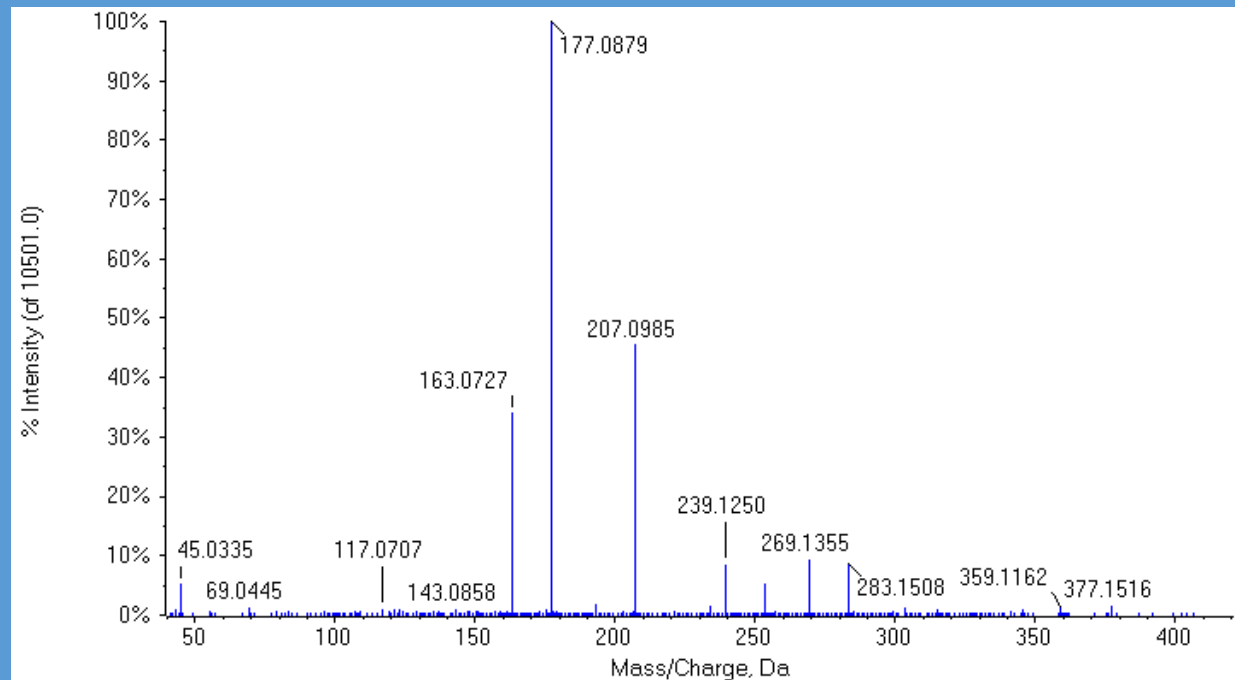


Name: Hexamethylolmelamine pentamethyl ether (HMPE)

Identification level: 2a

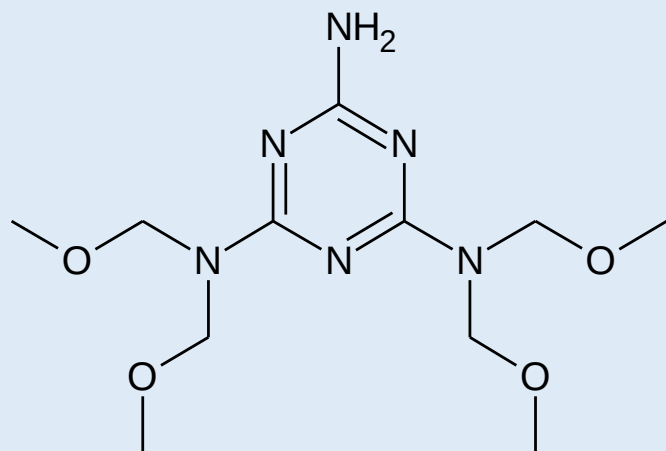


HPME  
RT: 7.43 min

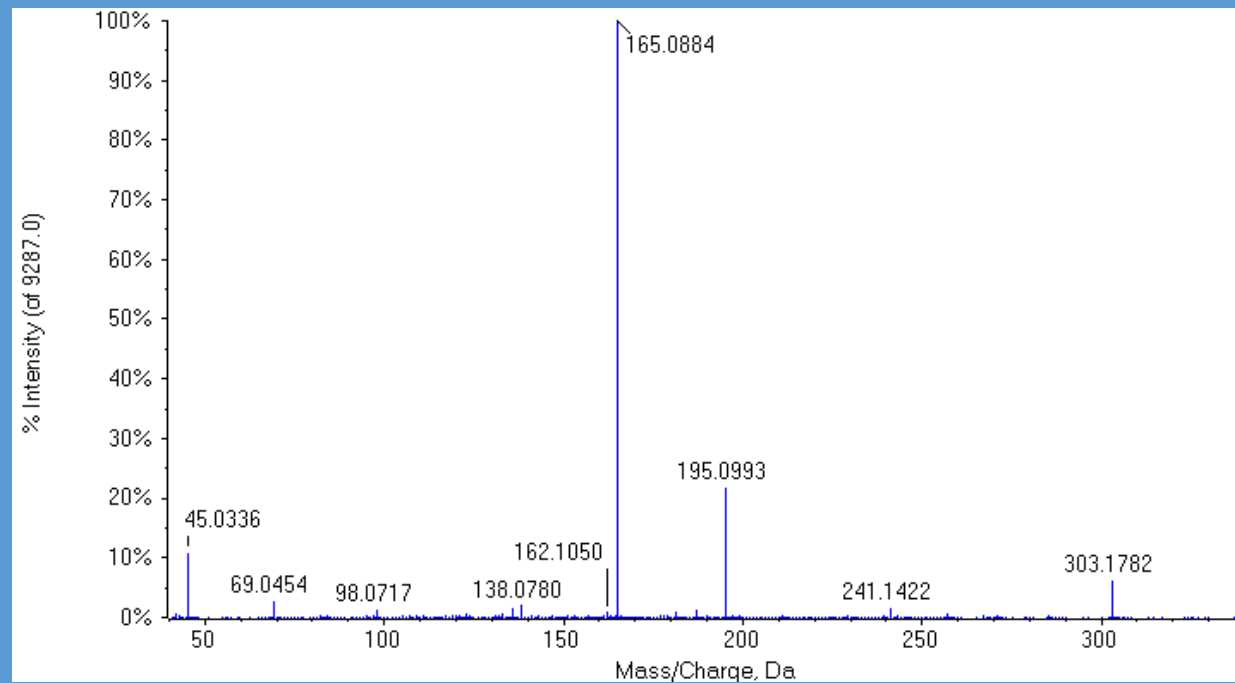


Name: Tetra(methoxymethyl)melamine (TMMM)

Identification level: 2a

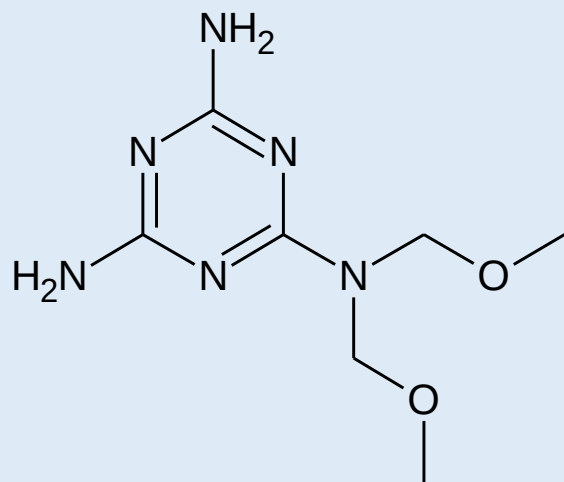


TMMM  
RT: 5.74 min

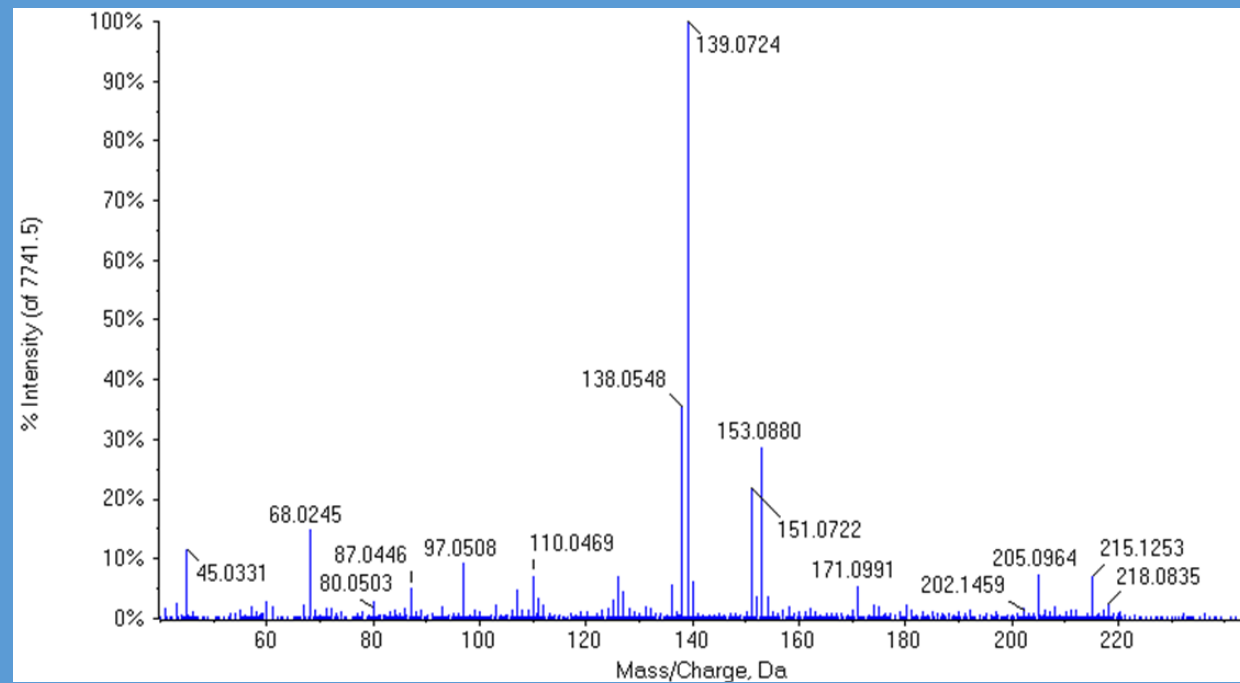


Name: Di(methoxymethyl)melamine (DMMM)

Identification level: 2a



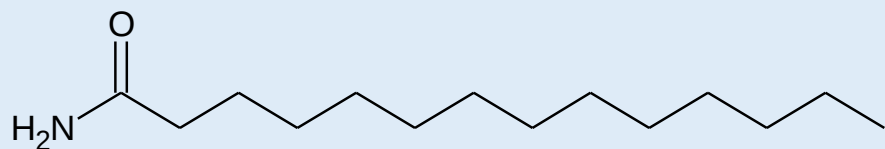
DMMM  
RT: 2.41 min



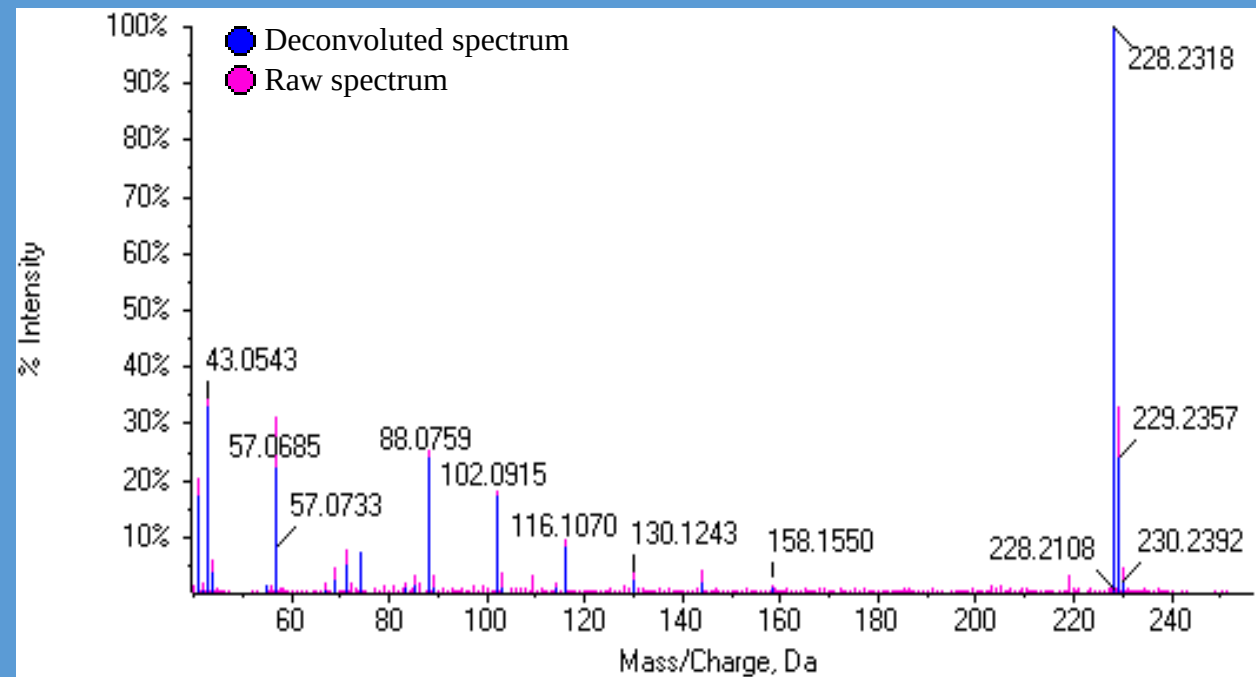


Name: Tetradecamide

Identification level: 2a

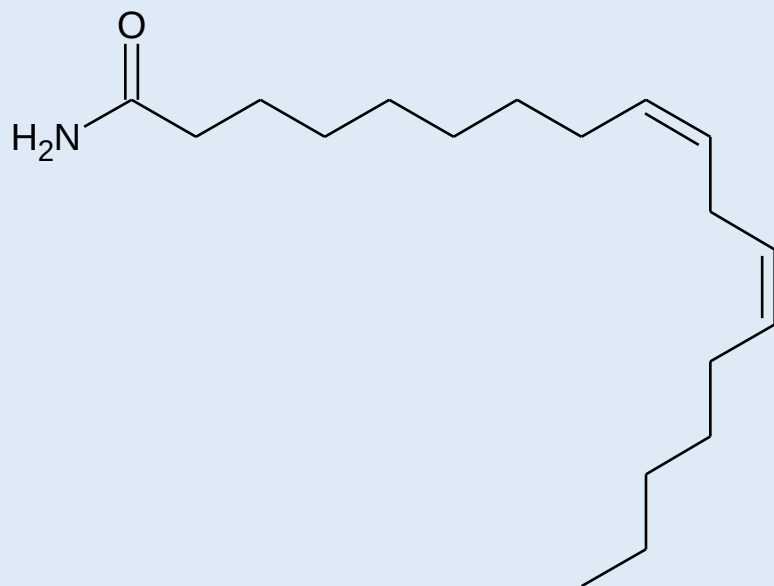


Tetradecamide  
RT: 14.54 min

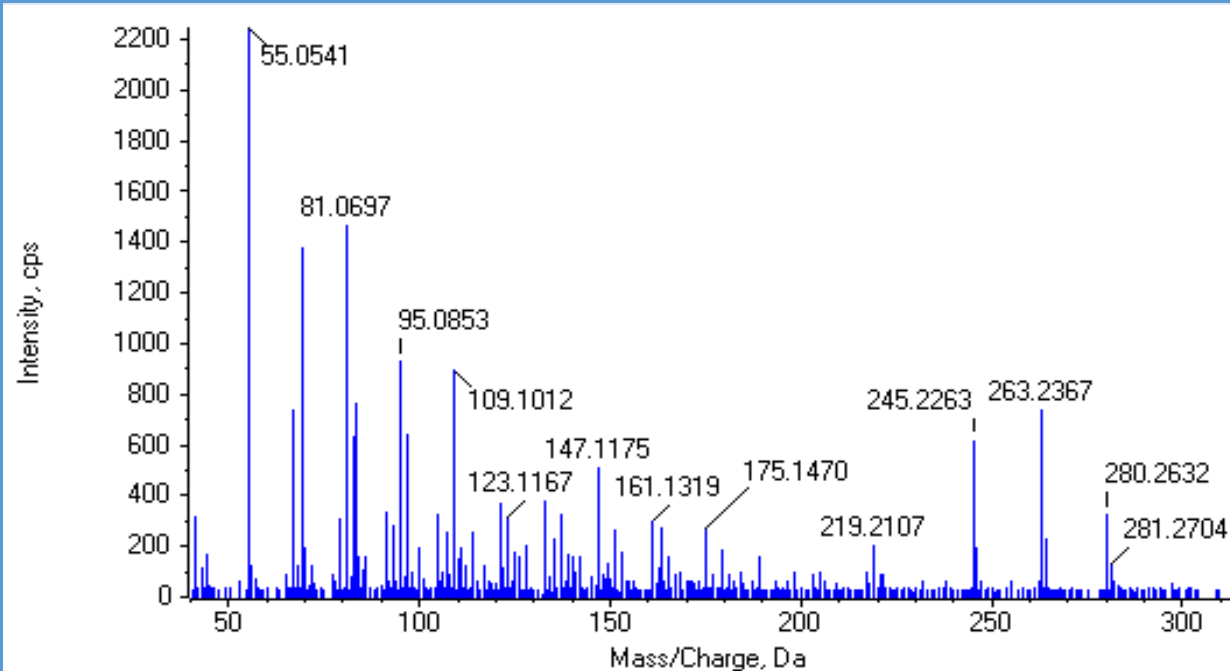


Name: Linoleamide

Identification level: 4

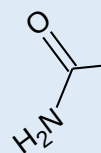


Linoleamide  
RT: 15.17 min

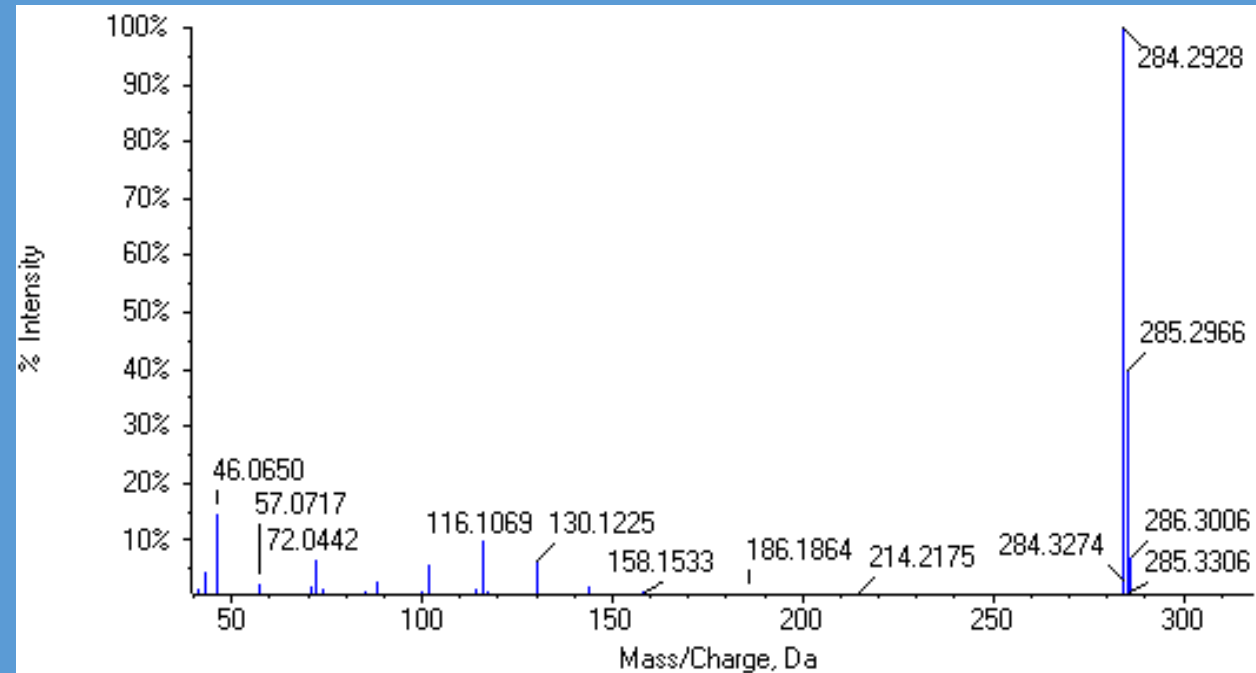


Name: Stereamide

Identification level: 2a

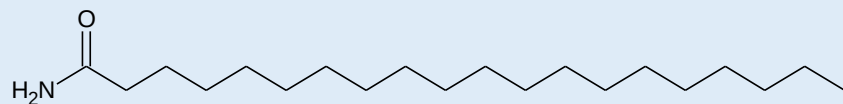


Stereamide  
RT: 16.22 min

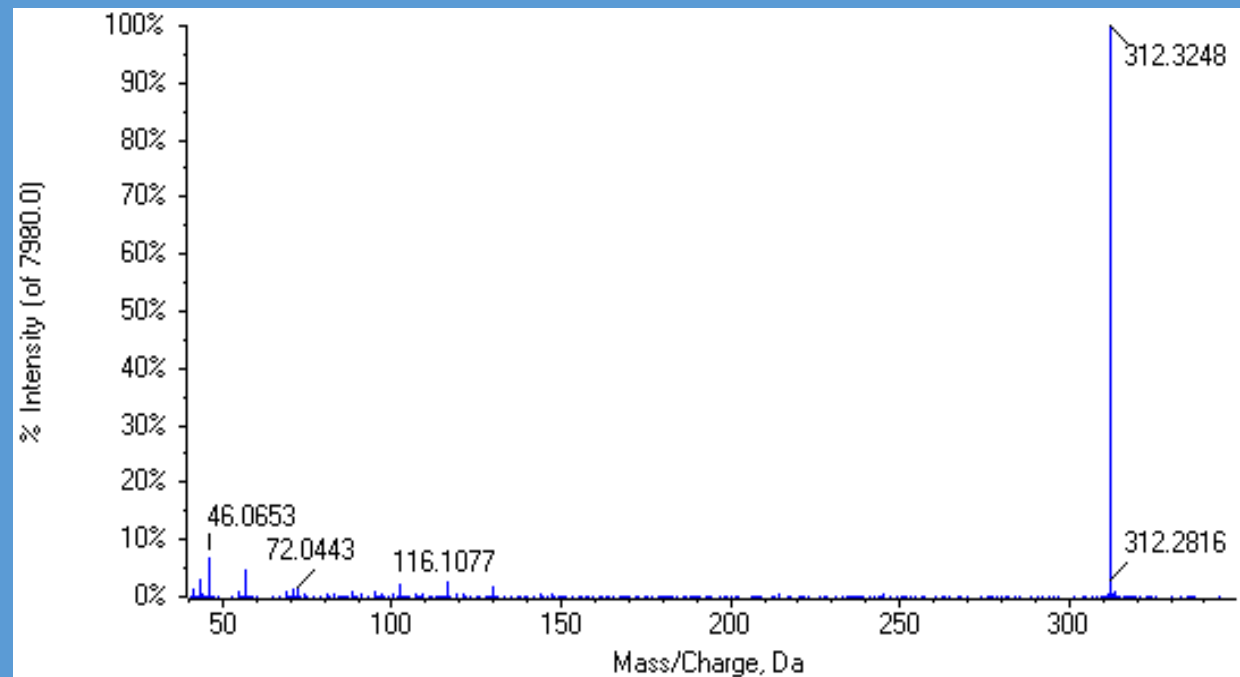


Name: Icosanamide

Identification level: 3

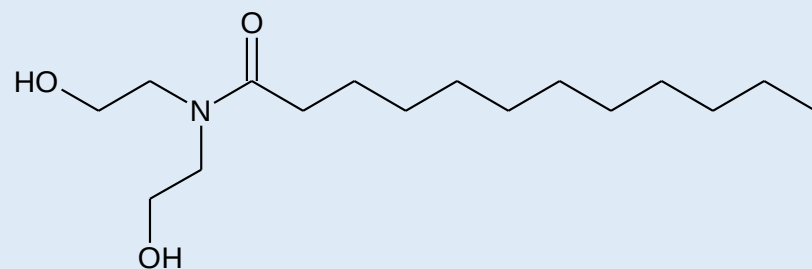


Icosanamide  
RT: 17.03 min

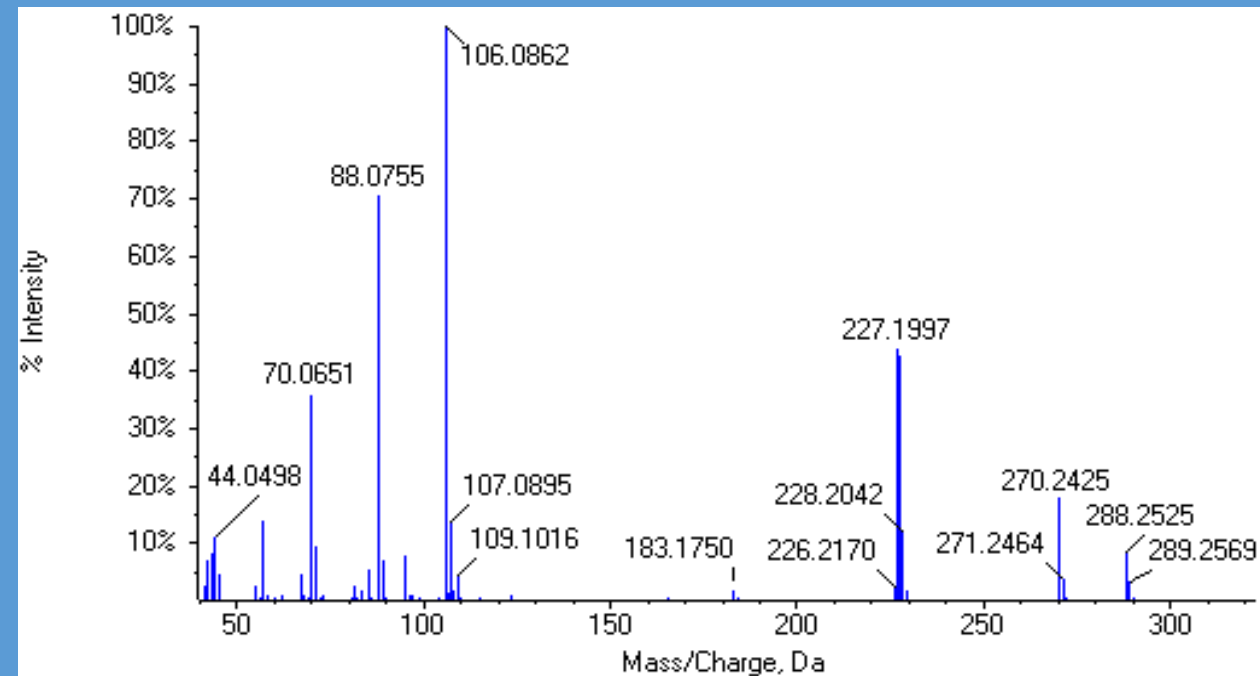


Name: Lauric diethanolamide (Lauric DEA)

Identification level: 2a

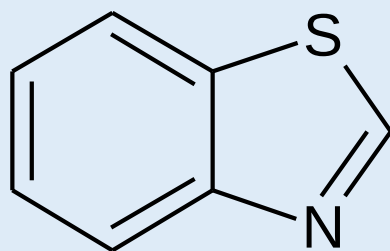


Lauric DEA  
RT: 13.04 min

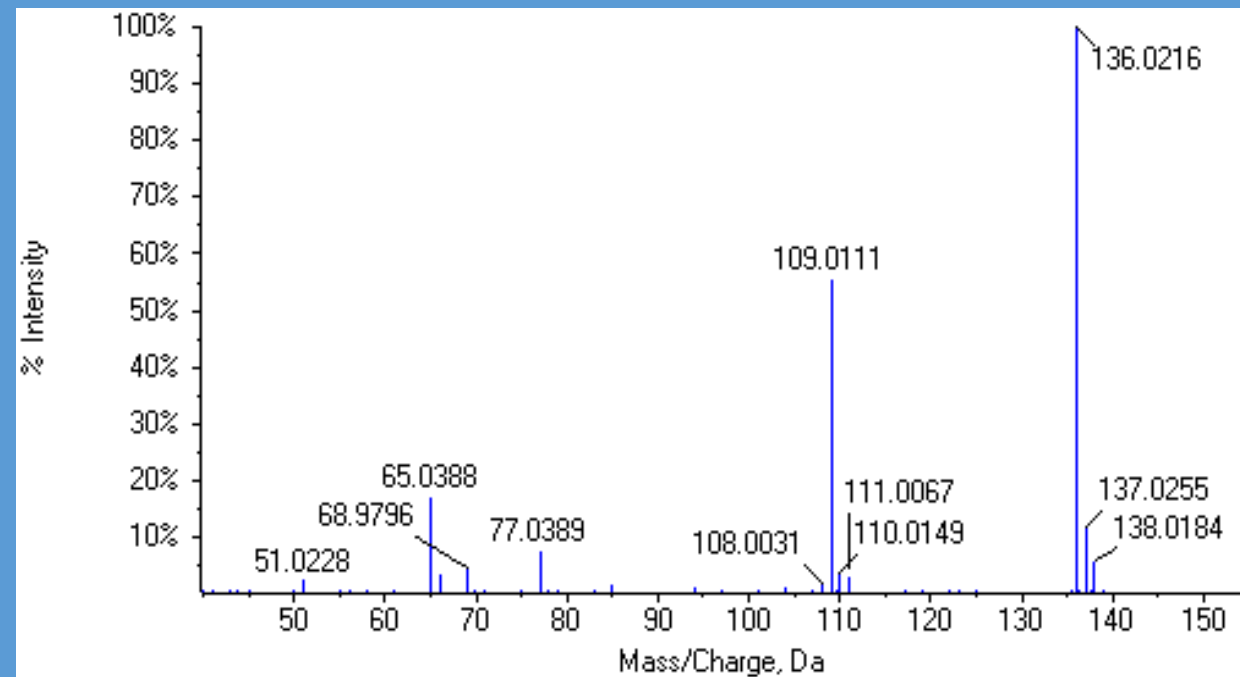


Name: Benzothiazole (BT)

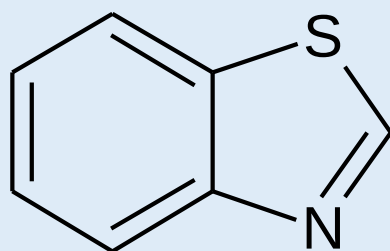
Identification level: 1



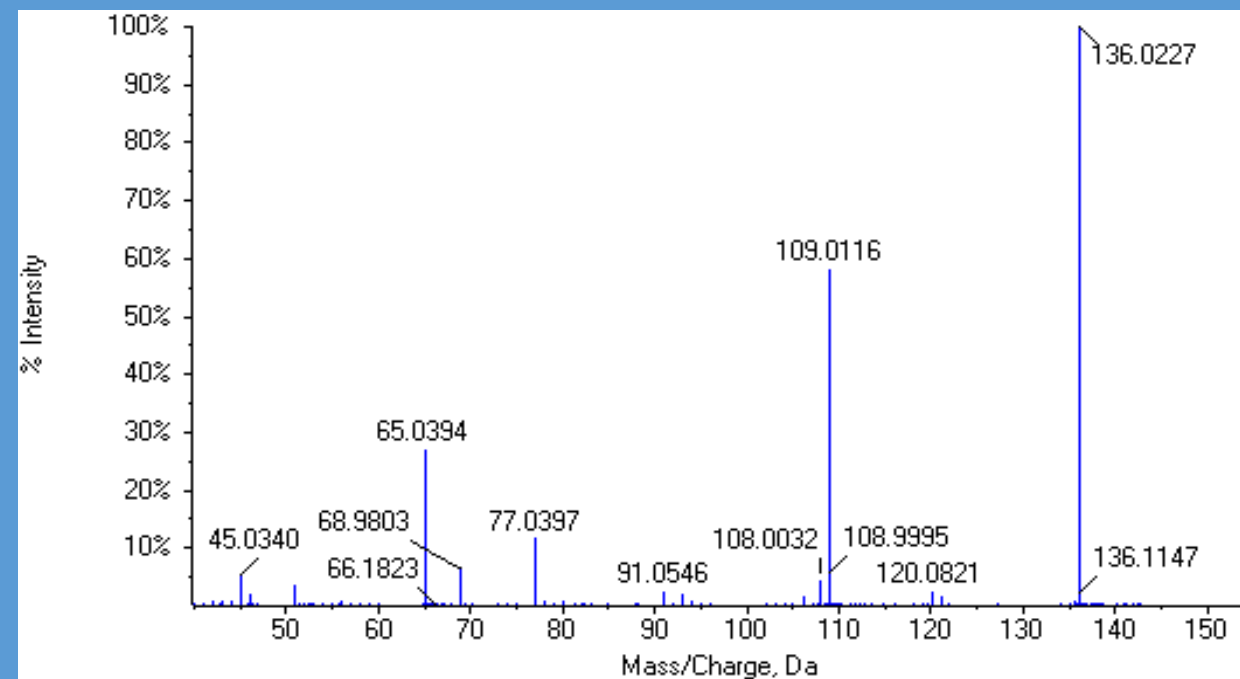
BT  
RT: 7.19 min



Identification level: 1

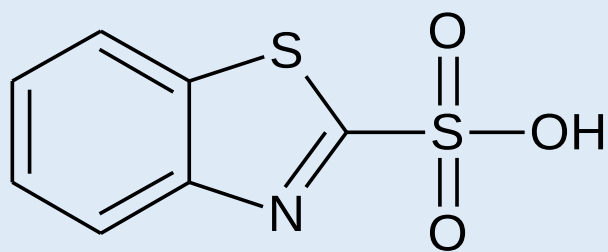


BT  
RT: 7.19 min

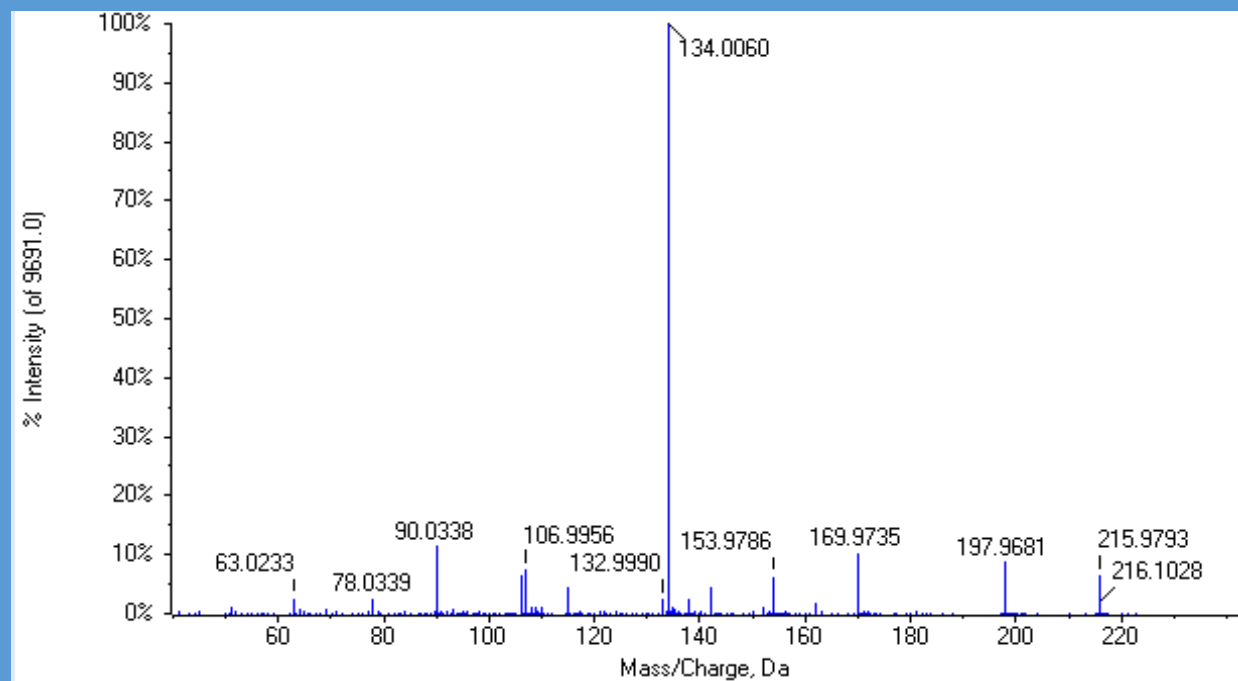


Name: Benzothiazole-2-sulfonic acid (BTSA)

Identification level: 2a



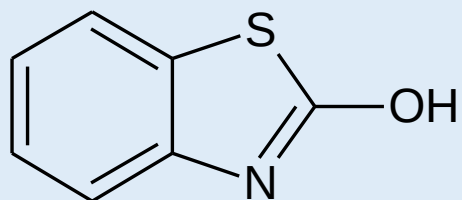
BTSA  
RT: 3.58 min



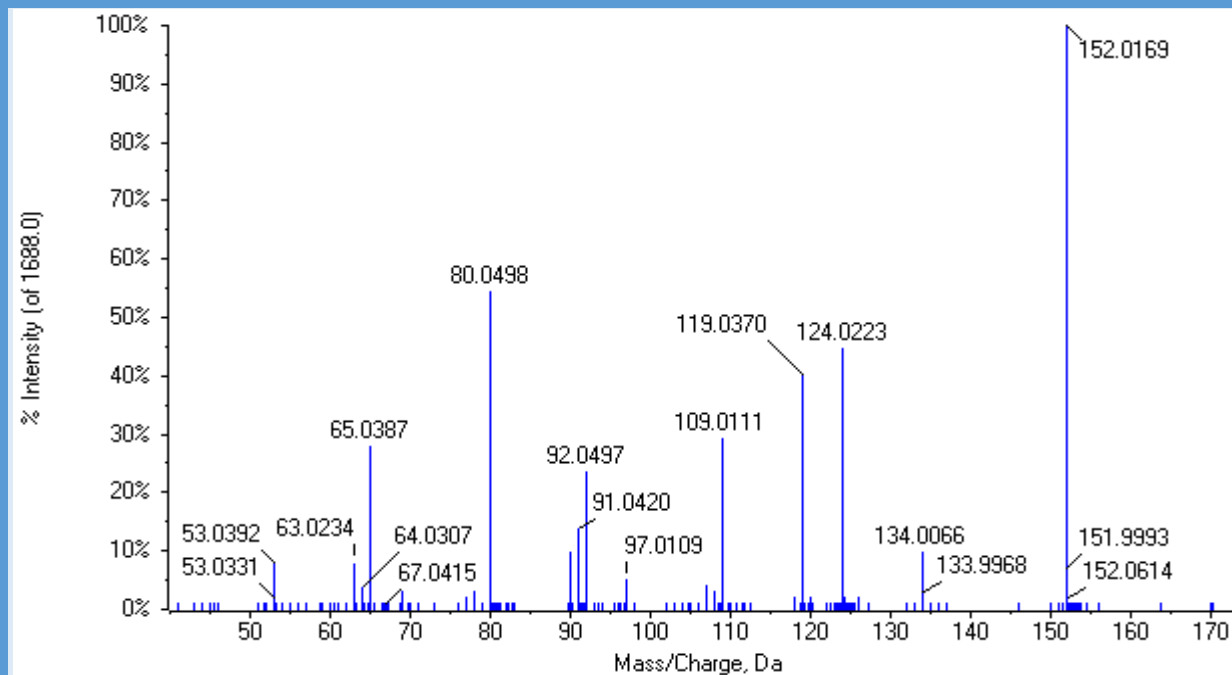


Name: 2-Hydroxybenzothiazole (2-OHBT)

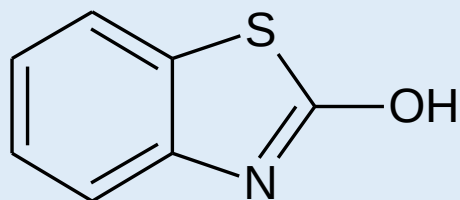
Identification level: 1



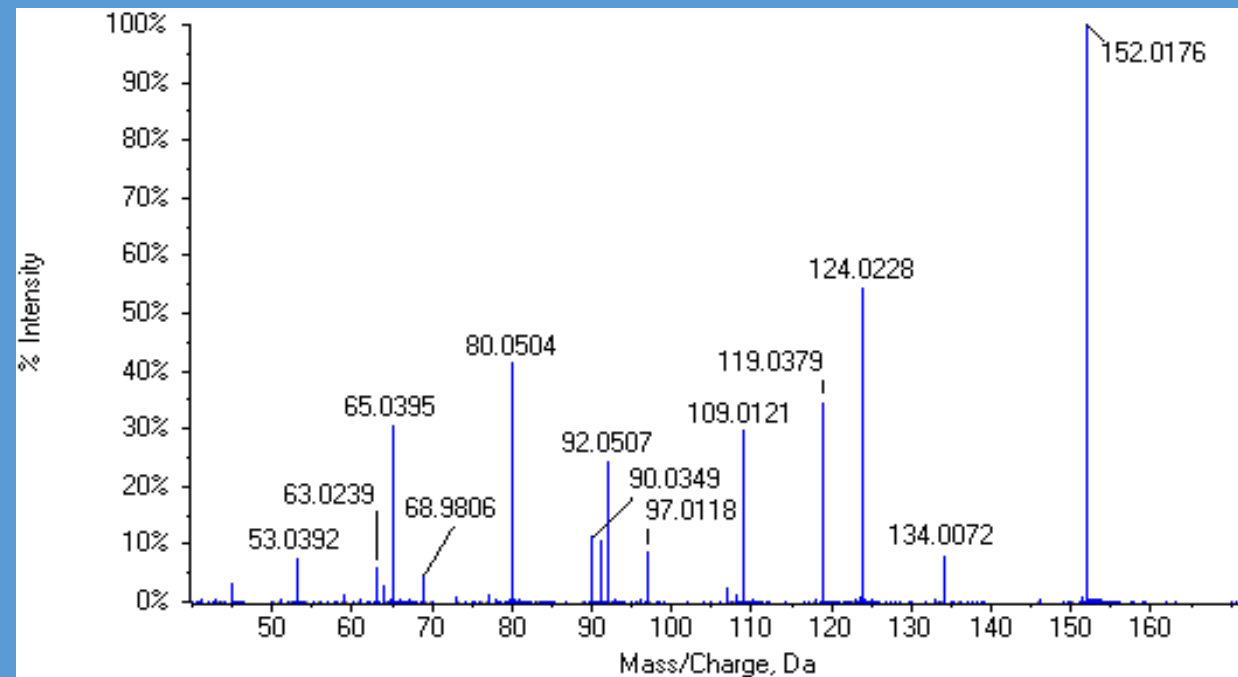
2-OHBT  
RT: 6.57 min



Identification level: 1

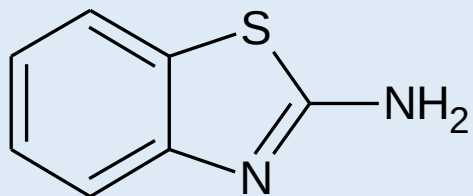


2-OHBT  
RT: 6.57 min

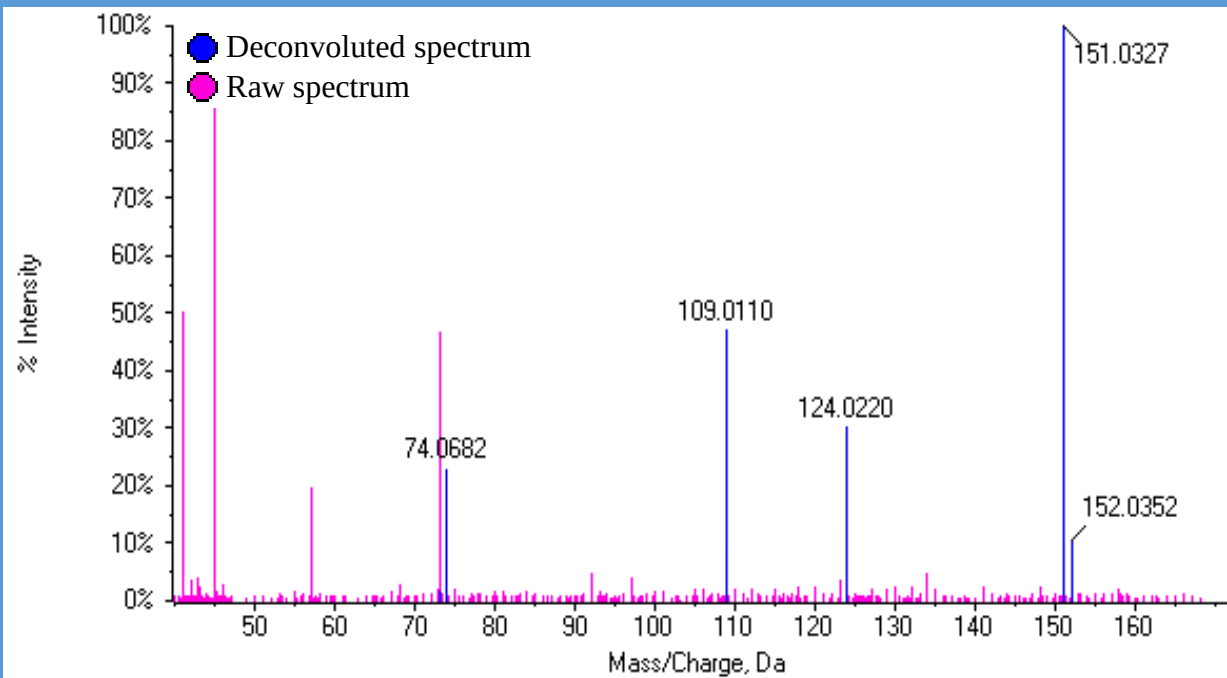


# Name: 2-Aminobenzothiazole (2-ABT)

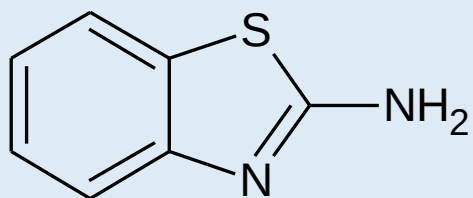
Identification level: 1



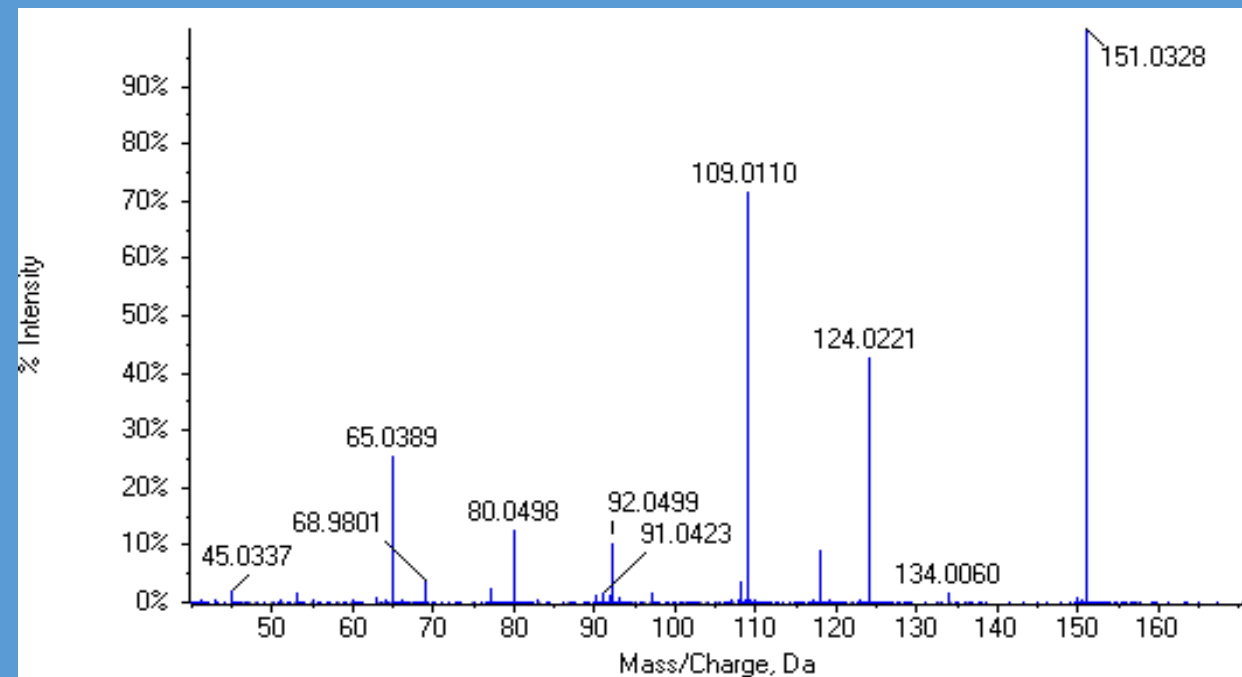
2-ABT  
RT: 3.59 min



Identification level: 1

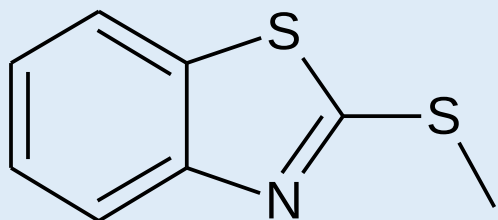


2-ABT  
RT: 3.59 min

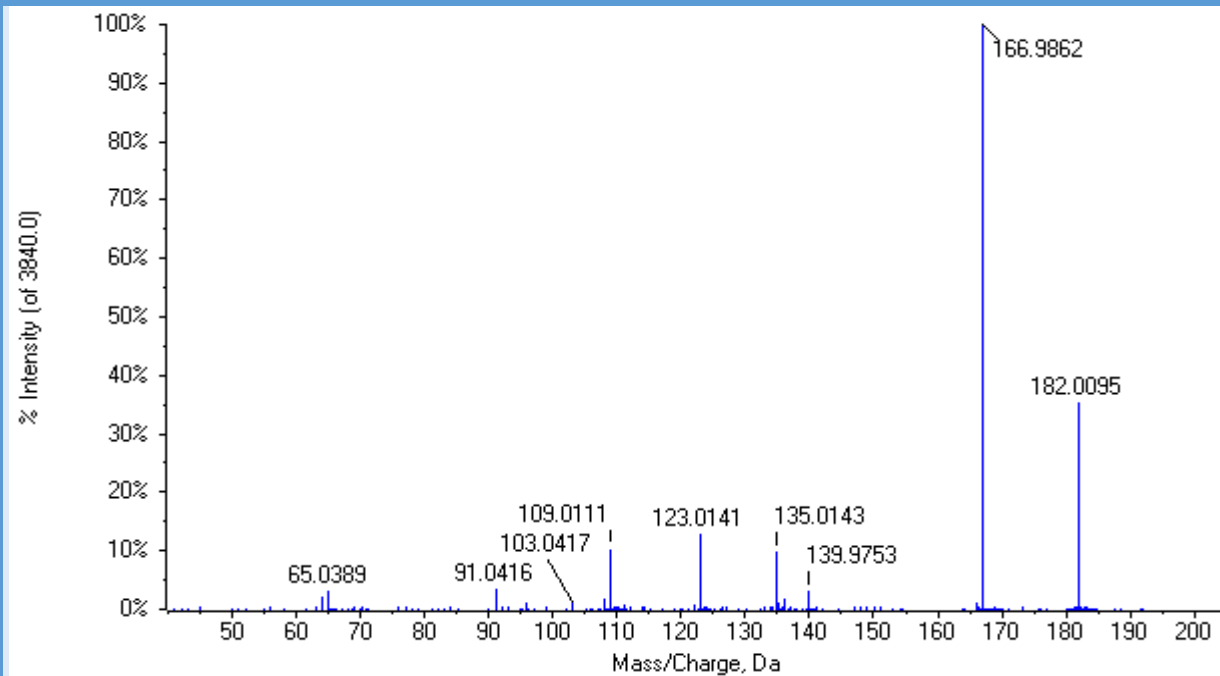


Name: 2-(Methylthio)benzothiazole (MTBT)

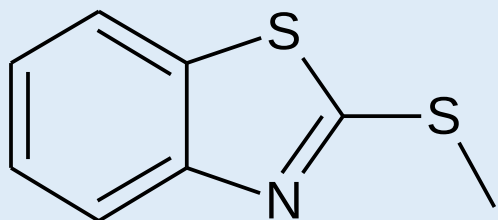
Identification level: 1



MTBT  
RT: 10.10 min

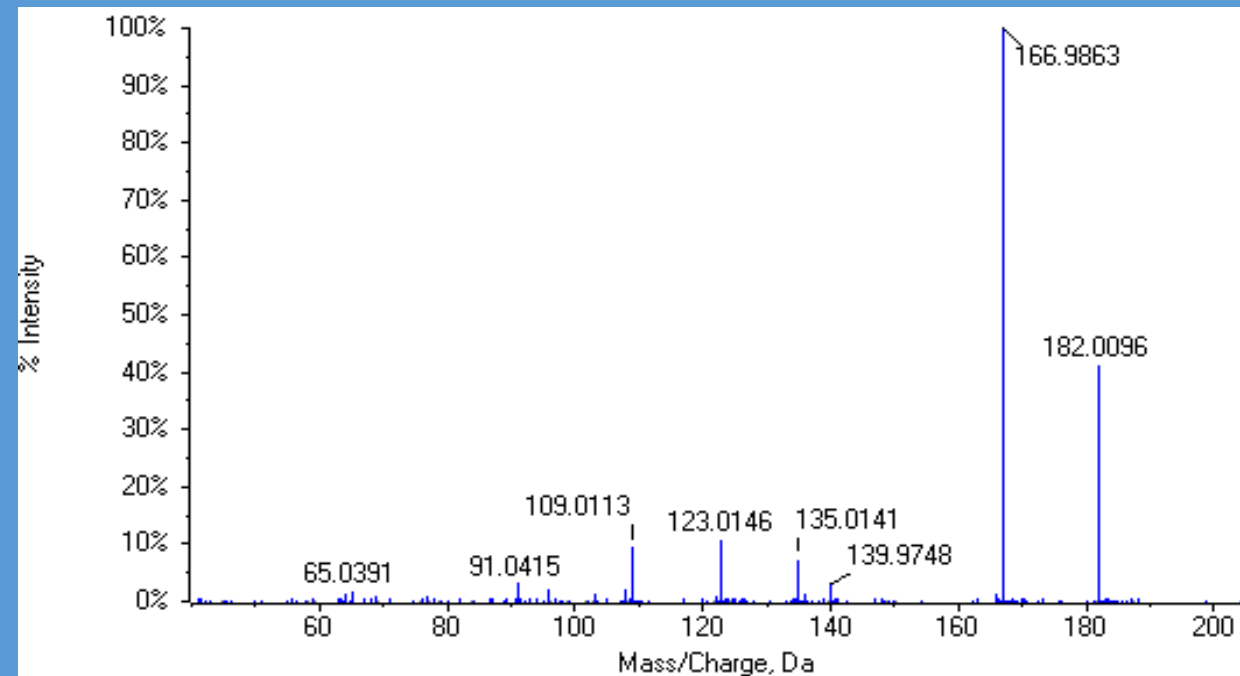


Identification level: 1



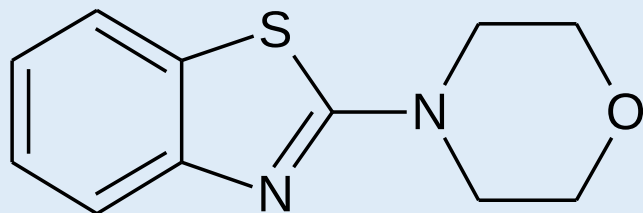
MTBT

RT: 10.10 min

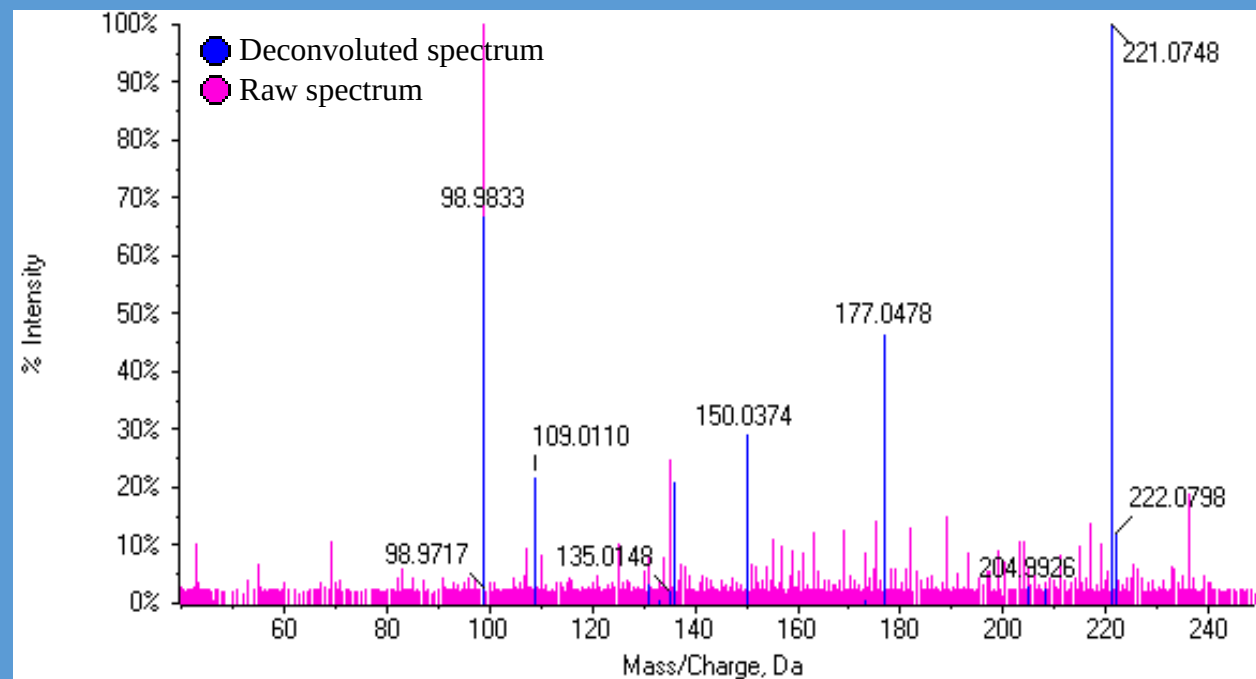


Name: 2-Morpholin-4-yl-benzothiazole (24MOBT)

Identification level: 2a

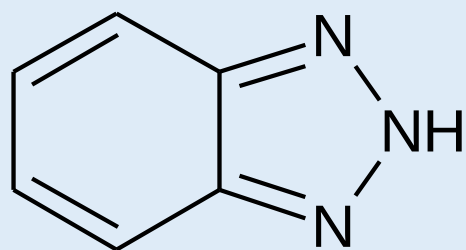


24MOBT  
RT: 8.98 min

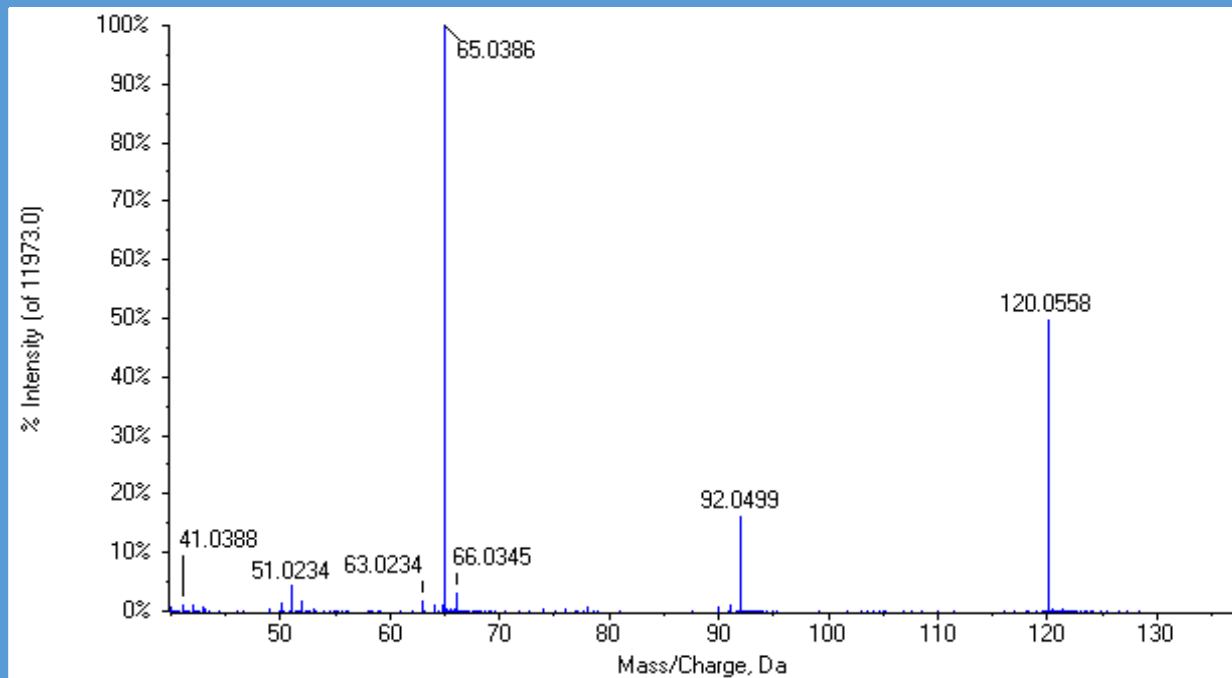


Name: 1H-Benzotriazole (BTR)

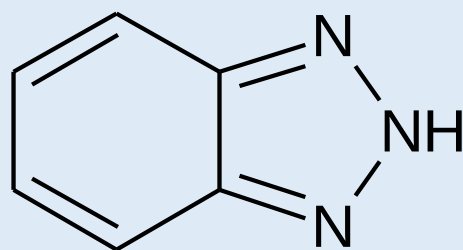
Identification level: 1



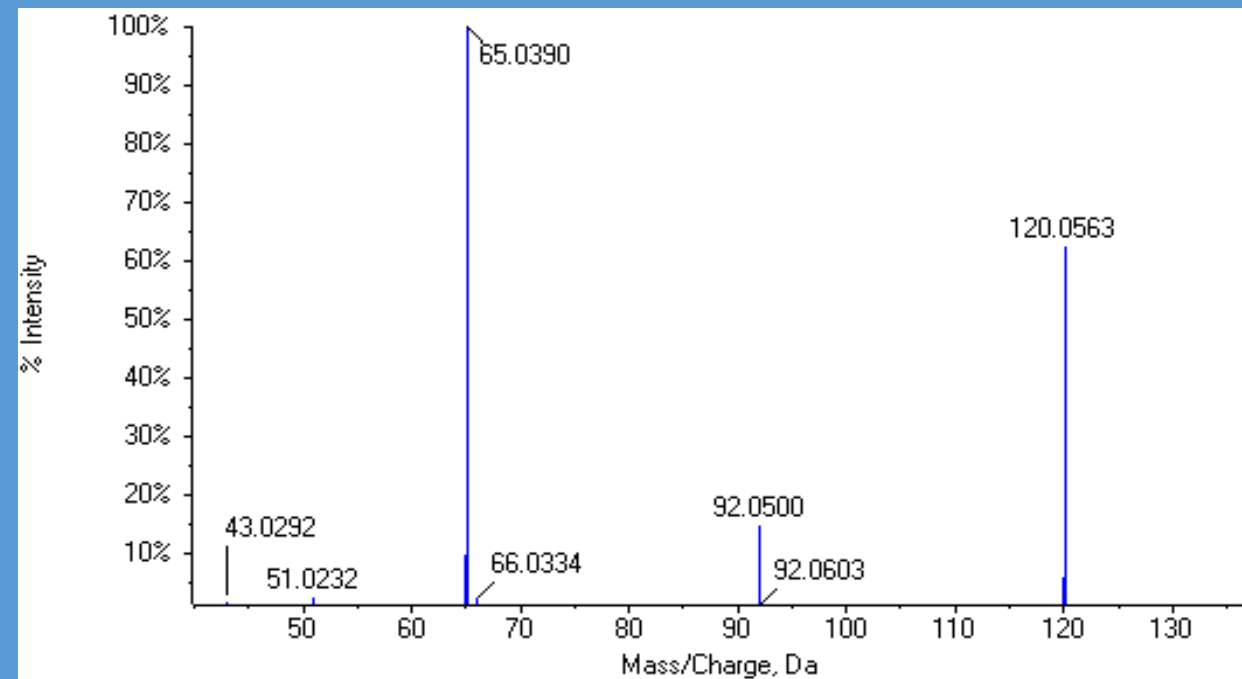
BTR  
RT: 4.21 min





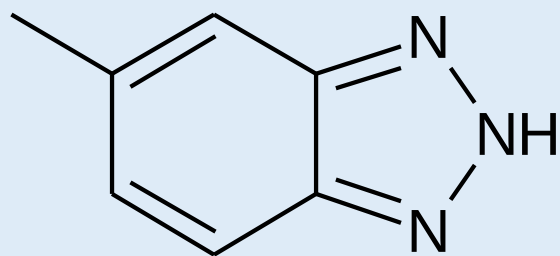


BTR  
RT: 4.21 min

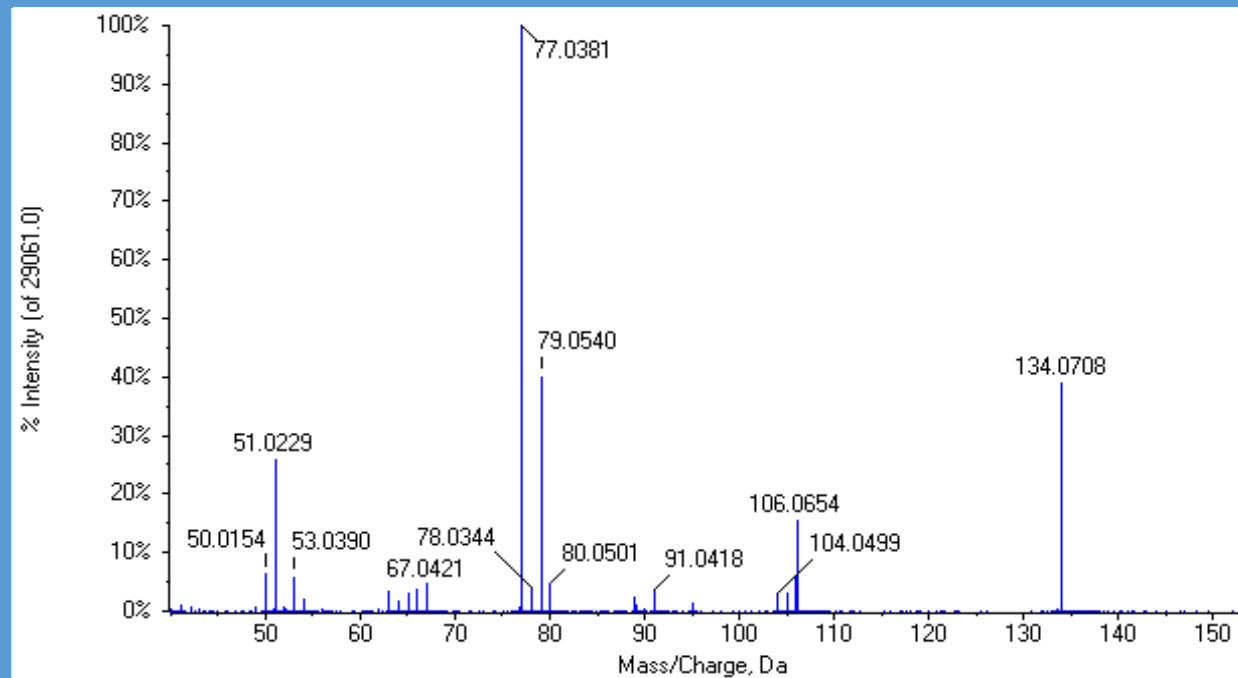


Name: 5-Methyl-1H-benzotriazole (Me-BTR)

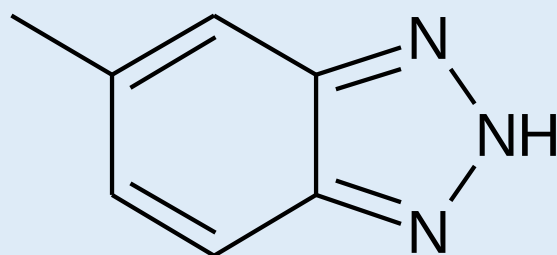
Identification level: 1



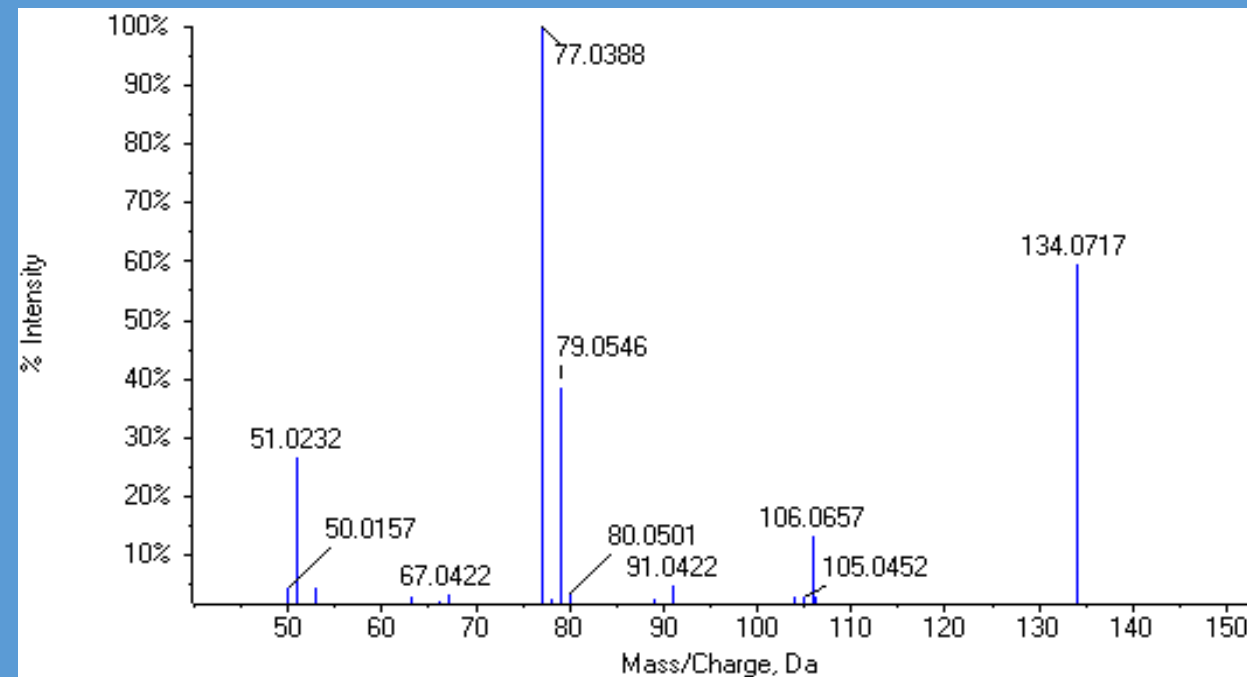
Me-BTR  
RT: 5.90 min



Identification level: 1

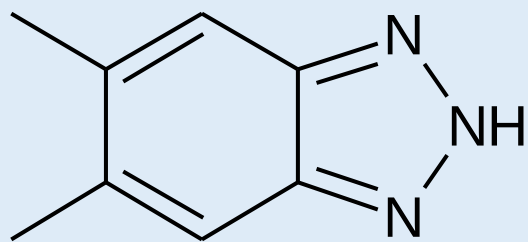


Me-BTR  
RT: 5.90 min

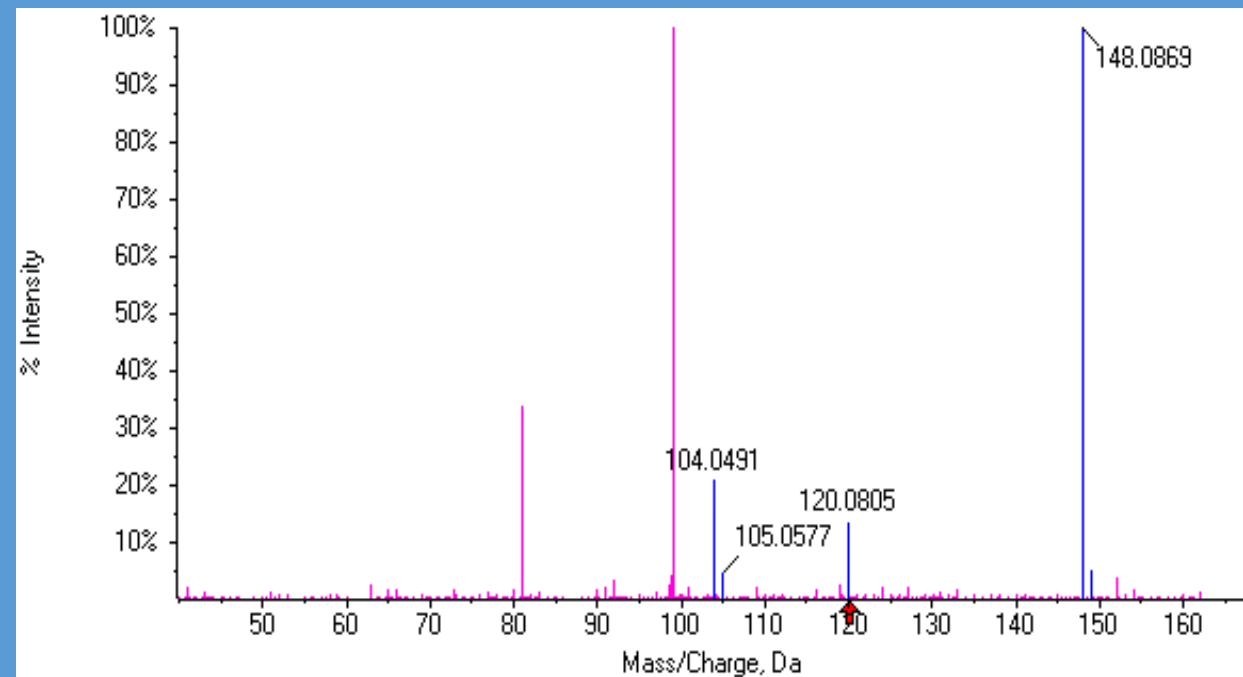


Name: 5,6-Dimethyl benzotriazole (5,6-DiMe-BTR)

Identification level: 4

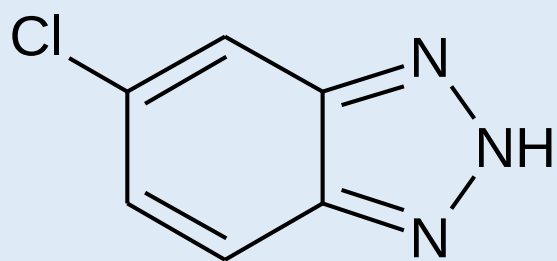


5,6-DiMe-BTR  
RT: 6.82 min

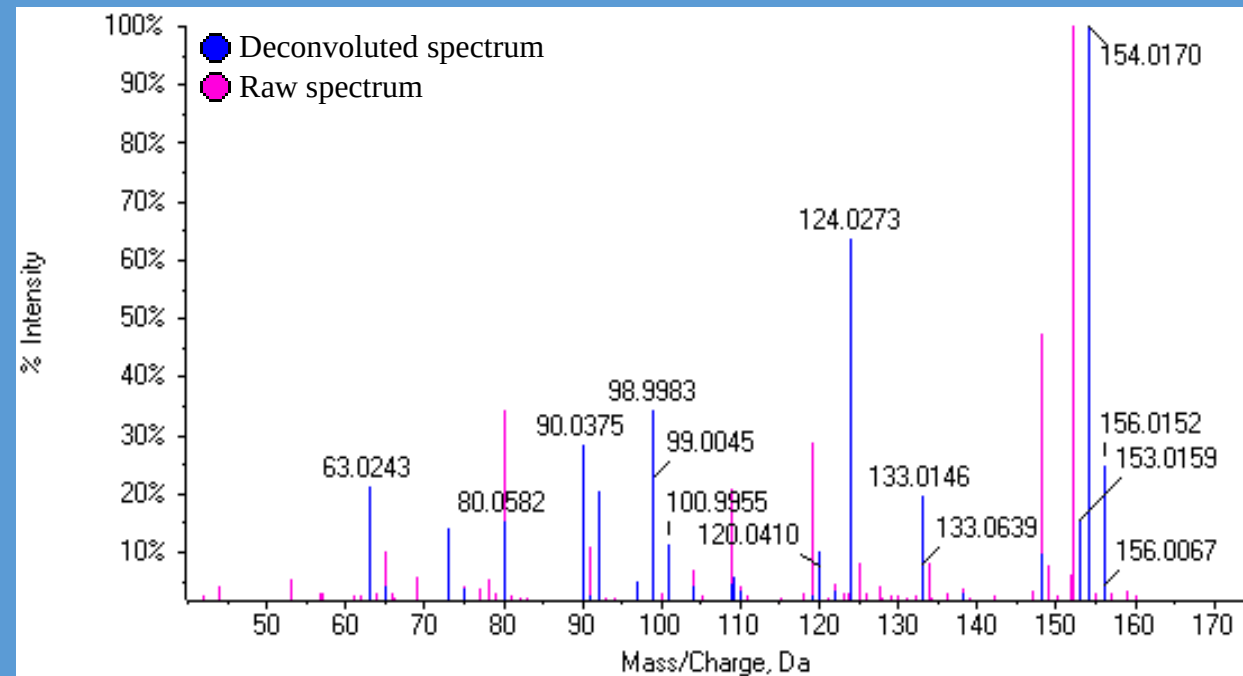


Name: 5-Chlorobenzotriazole (5-Cl-BTR)

Identification level: 4

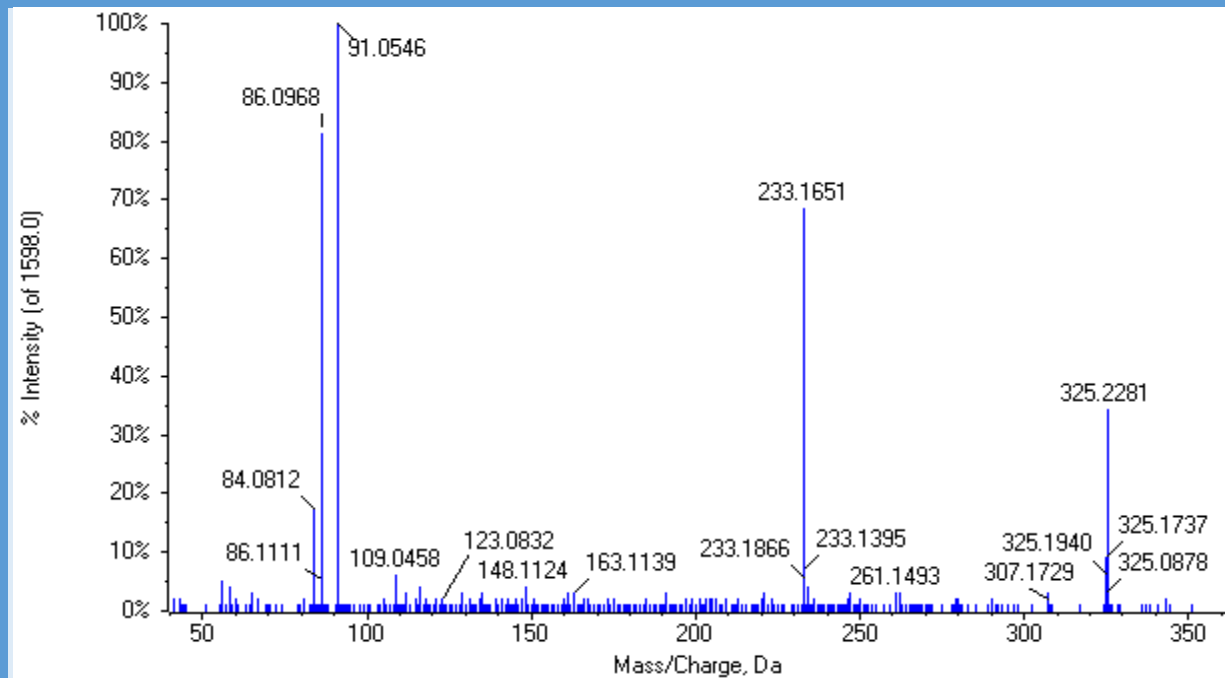
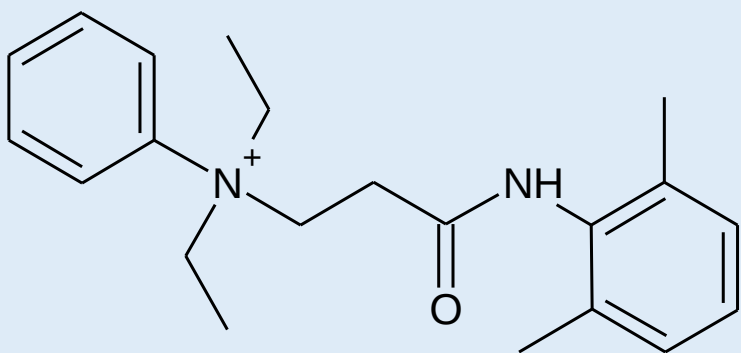


5-Cl-BTR  
RT: 6.82 min



Name: Denatonium benzoate (DB)

Identification level: 2a



DB  
RT: 7.27 min