

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
 Data File : BF102618.D
 Acq On : 30 Jan 2018 00:53
 Operator : SJ/JU
 Sample : J1353-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EPE-106-5(20-22)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	478	482	490	rBV	100752	153171	3.75%	0.500%
2	5.334	547	552	571	rBV	3586164	3839807	93.96%	12.532%
3	6.363	722	727	744	rBV	3398896	4086564	100.00%	13.337%
4	6.487	744	748	751	rBV	3878681	3629229	88.81%	11.845%
5	6.710	783	786	795	rBV	1156212	1017353	24.90%	3.320%
6	6.869	809	813	816	rBV	3193850	2907384	71.14%	9.489%
7	7.281	879	883	896	rBV	2253217	2364788	57.87%	7.718%
8	7.992	1001	1004	1023	rBV	1329712	1384139	33.87%	4.517%
9	9.069	1183	1187	1198	rBV	3507486	3341028	81.76%	10.904%
10	9.469	1249	1255	1263	rBV	285511	305932	7.49%	0.998%
11	9.675	1286	1290	1294	rBV	80679	65642	1.61%	0.214%
12	9.745	1298	1302	1311	rVV	1164309	1153870	28.24%	3.766%
13	10.169	1372	1374	1377	rVB	99336	84282	2.06%	0.275%
14	10.539	1433	1437	1452	rBV	1499934	1591262	38.94%	5.193%
15	10.645	1452	1455	1459	rVV	102371	93171	2.28%	0.304%
16	11.092	1528	1531	1533	rBV	62195	48104	1.18%	0.157%
17	11.233	1551	1555	1566	rBV	913032	893645	21.87%	2.917%
18	12.816	1820	1824	1828	rBV	1958600	1896797	46.42%	6.191%
19	13.710	1973	1976	1985	rBV	64190	100231	2.45%	0.327%
20	13.874	2000	2004	2012	rBV	757505	783750	19.18%	2.558%
21	14.698	2141	2144	2148	rVB	47160	51092	1.25%	0.167%
22	15.310	2243	2248	2258	rBV	585433	848422	20.76%	2.769%

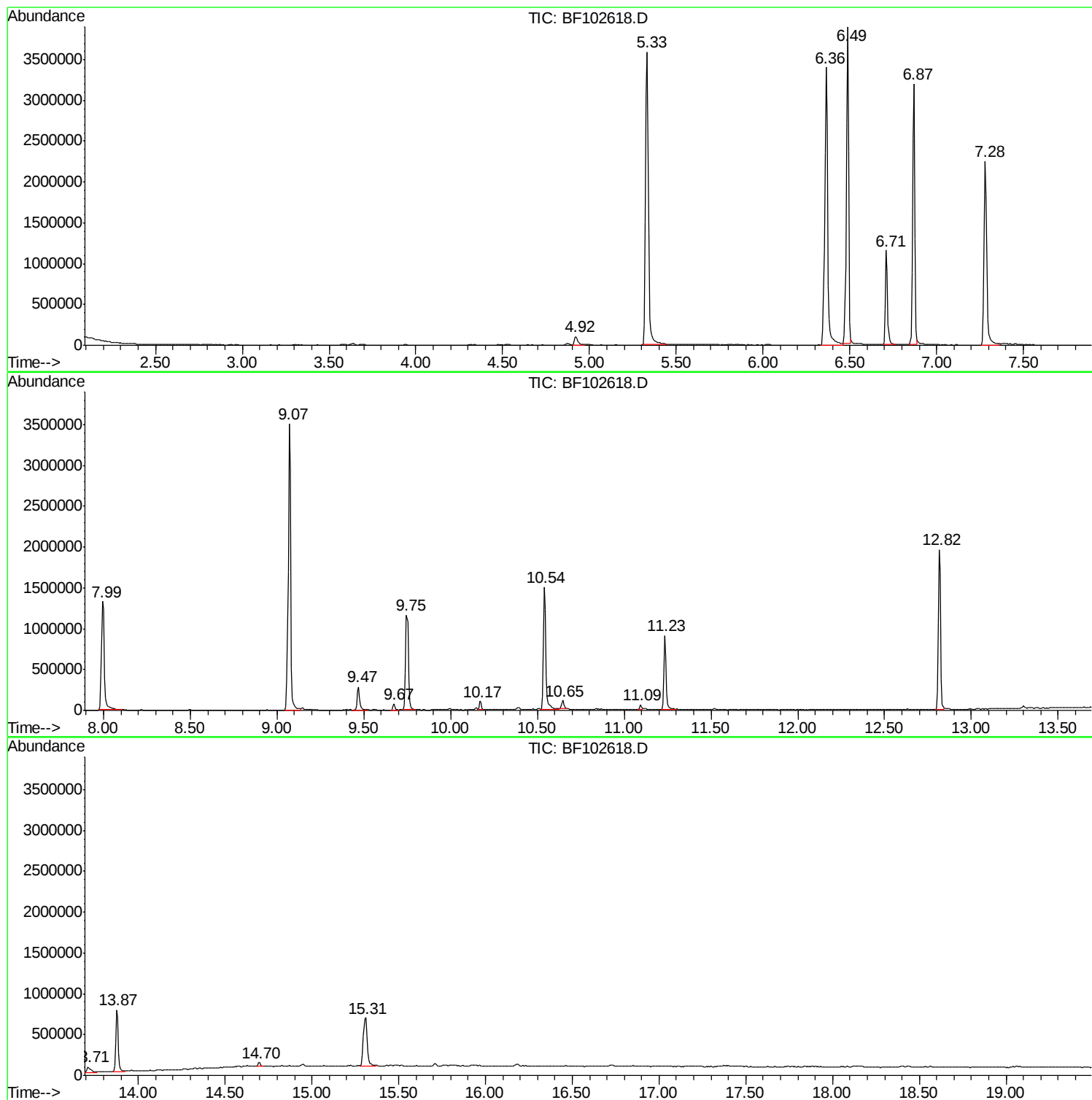
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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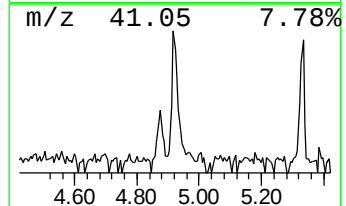
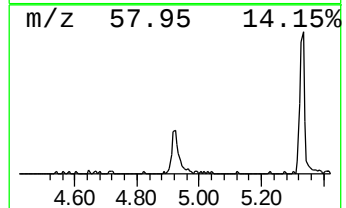
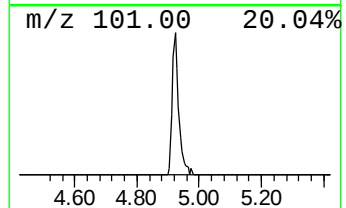
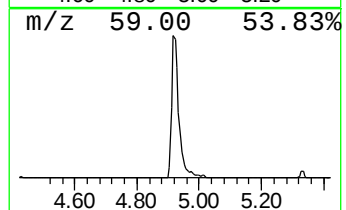
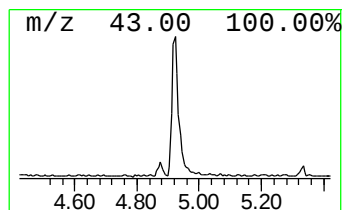
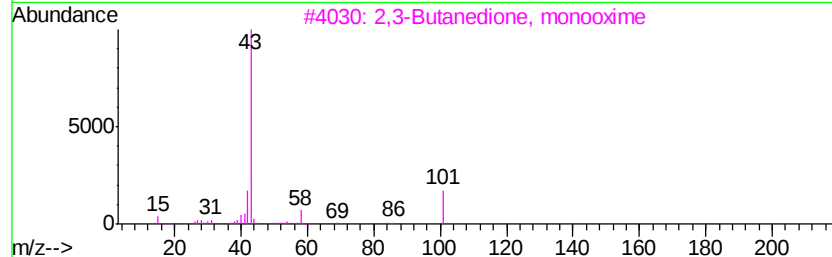
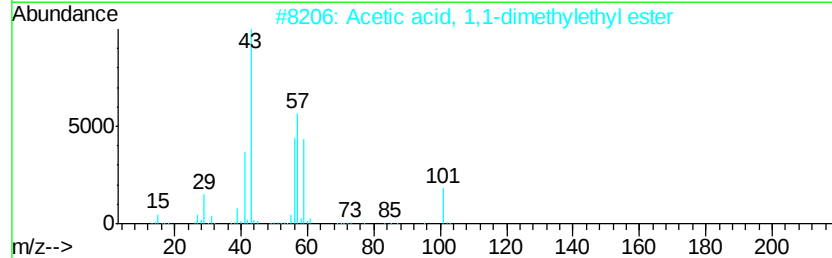
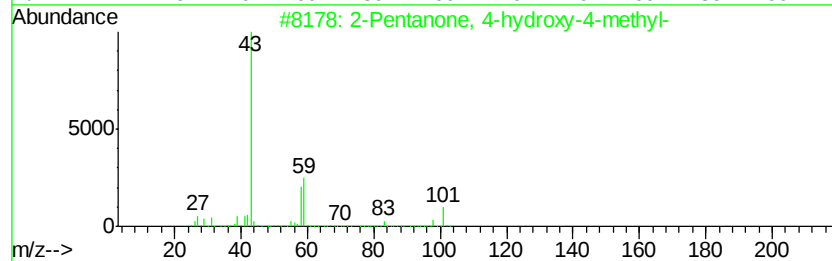
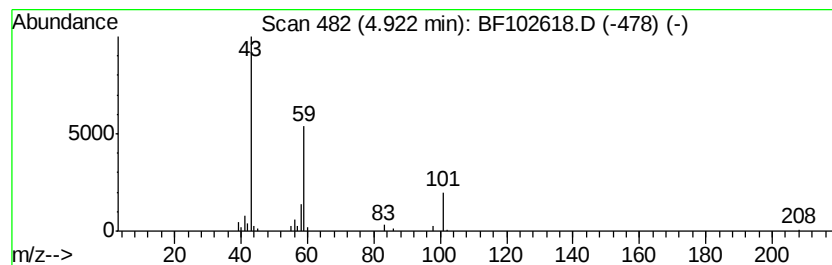
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.01 ng	153171	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			3-Hexanol	102	C6H14O	000623-37-0	28



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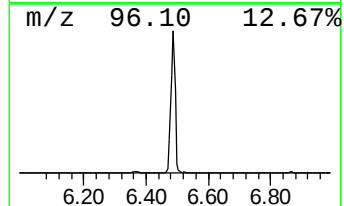
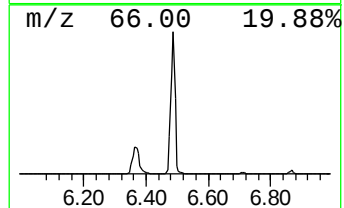
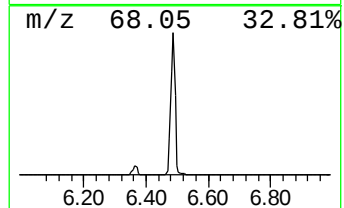
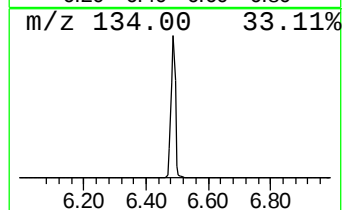
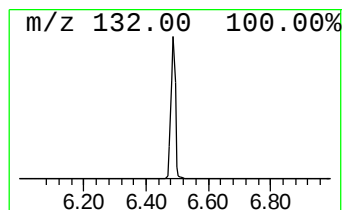
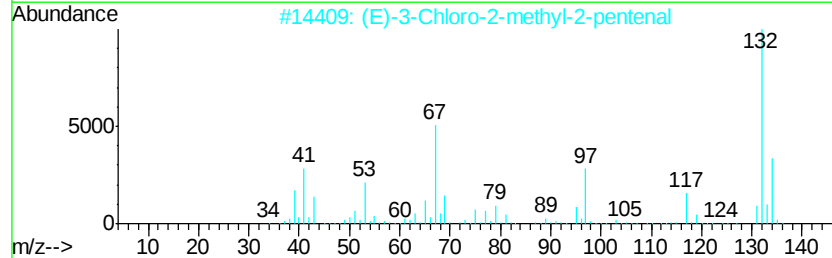
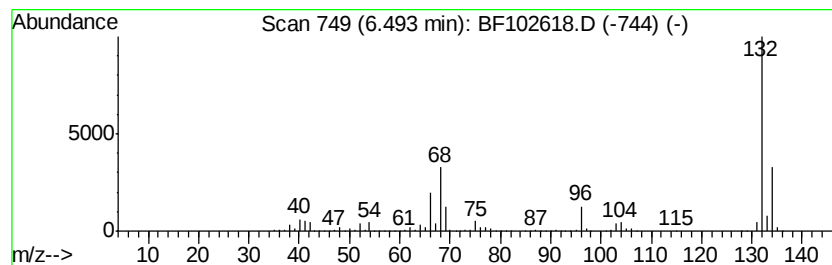
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	71.35 ng	3629230	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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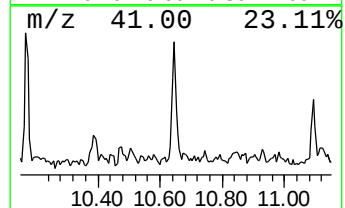
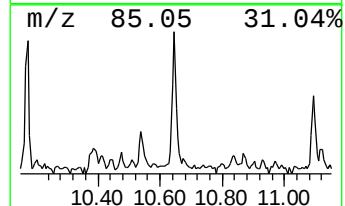
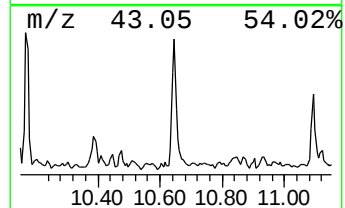
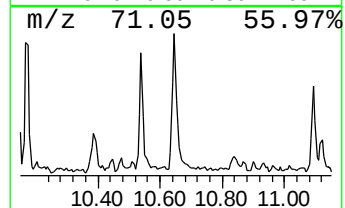
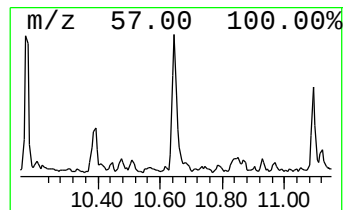
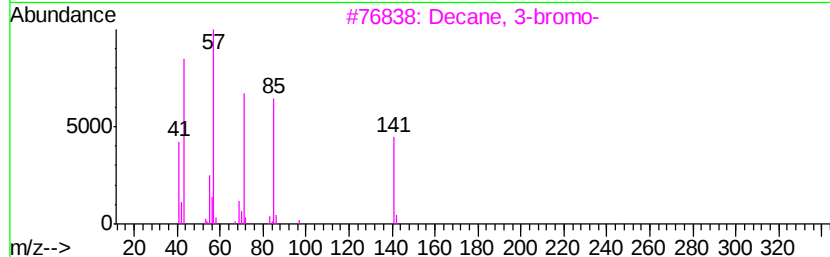
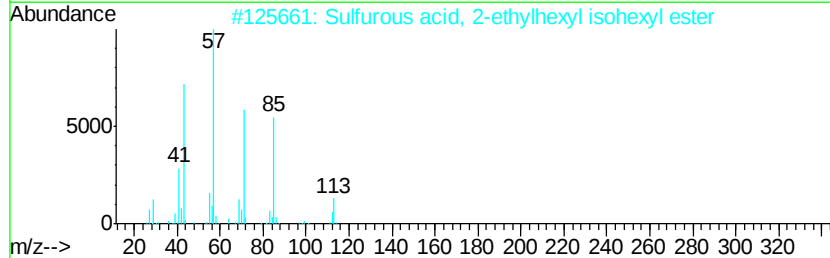
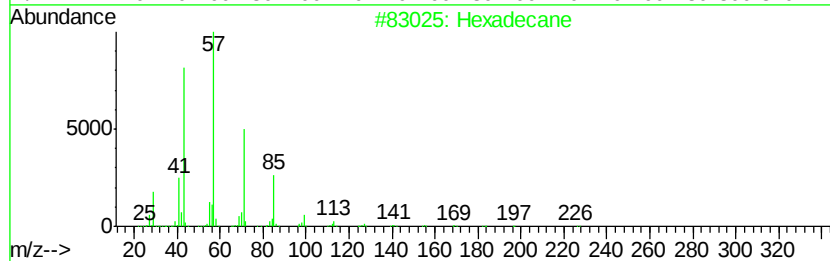
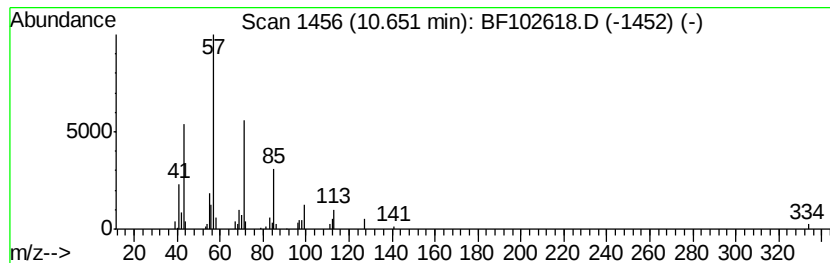
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.09 ng	93171	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	83
2	Sulfurous acid, 2-ethylhexyl iso...		278	C14H30O3S	1000309-19-0	72
3	Decane, 3-bromo-		220	C10H21Br	030571-71-2	64
4	1-Iodoundecane		282	C11H23I	004282-44-4	53
5	Tridecane		184	C13H28	000629-50-5	53



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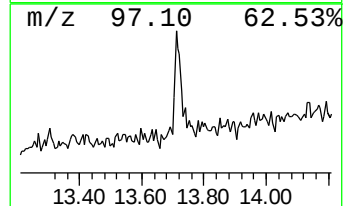
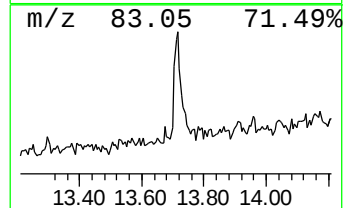
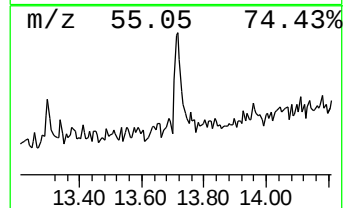
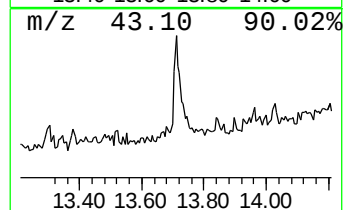
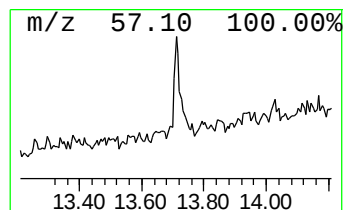
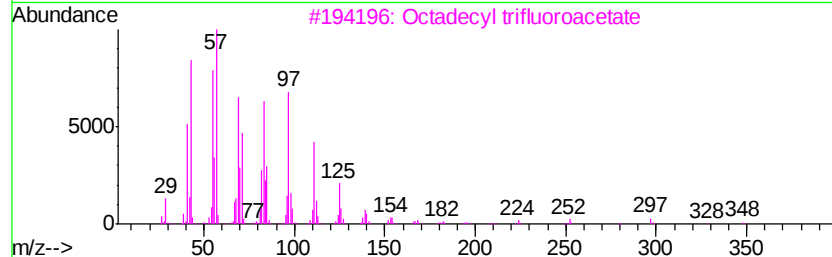
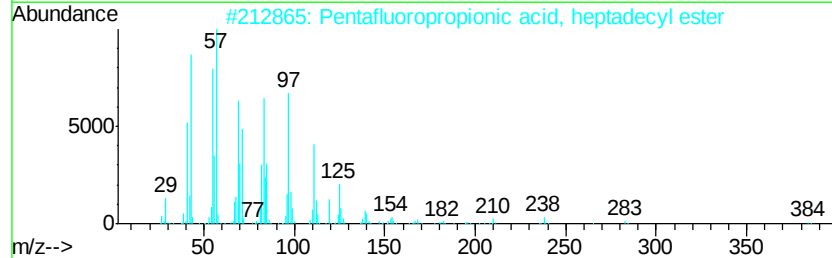
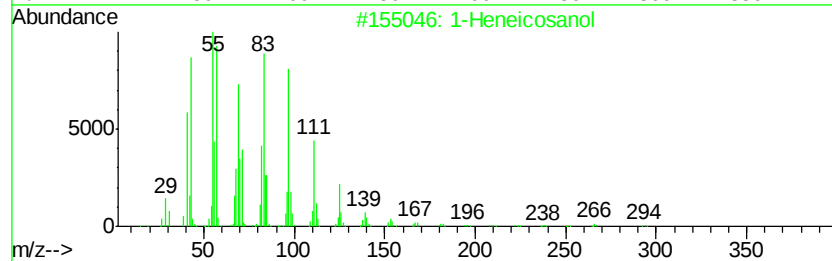
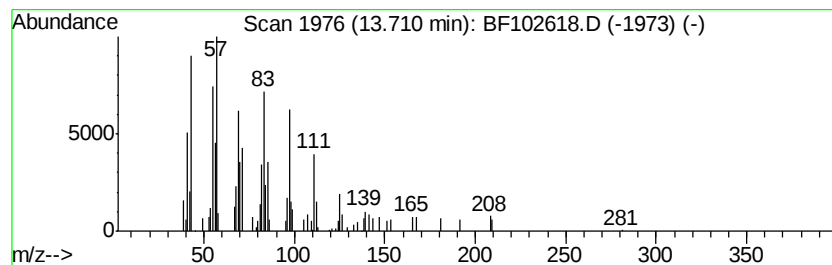
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	2.56 ng	100231	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 95
2		Pentafluoropropionic acid, hepta...	402 C20H35F5O2	959218-78-1 95
3		Octadecyl trifluoroacetate	366 C20H37F3O2	079392-43-1 95
4		Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0 94
5		2- Chloropropionic acid, octadec...	360 C21H41ClO2	088104-31-8 94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	3.0	ng	153171	1	6.71	1017350	20.0
unknown6.49	6.49	71.3	ng	3629230	1	6.71	1017350	20.0
Hexadecane	10.65	2.1	ng	93171	4	11.23	893645	20.0
1-Heneicosanol	13.71	2.6	ng	100231	5	13.87	783750	20.0