

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
 Data File : BF101975.D
 Acq On : 10 Jan 2018 1:31
 Operator : SJ/JU
 Sample : J1038-03
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

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-BF010918.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	4.928	478	483	488	rVB	208605	261807	5.13%	0.699%
2	5.340	548	553	556	rBV	3108682	2911823	57.00%	7.769%
3	6.363	722	727	737	rVB	1919621	1922859	37.64%	5.131%
4	6.498	745	750	753	rBV	4915935	4727030	92.54%	12.613%
5	6.728	785	789	792	rBV	1702766	1348787	26.40%	3.599%
6	6.887	811	816	819	rVB	4838193	4407623	86.29%	11.760%
7	7.298	880	886	889	rBV	3670065	3668891	71.82%	9.789%
8	7.487	914	918	920	rBV	91506	71060	1.39%	0.190%
9	8.010	1003	1007	1010	rBV	2034106	1629083	31.89%	4.347%
10	8.569	1100	1102	1105	rVB	90930	66157	1.30%	0.177%
11	9.092	1185	1191	1194	rBV	5635643	5108141	100.00%	13.629%
12	9.481	1254	1257	1260	rBV	128563	98328	1.92%	0.262%
13	9.763	1301	1305	1309	rVB	1652541	1327225	25.98%	3.541%
14	10.481	1423	1427	1429	rBV	103962	92701	1.81%	0.247%
15	10.551	1434	1439	1442	rBV	2590207	2301949	45.06%	6.142%
16	10.657	1454	1457	1465	rVB	49085	59727	1.17%	0.159%
17	11.245	1553	1557	1560	rBV	1381981	1101570	21.56%	2.939%
18	11.780	1645	1648	1652	rBV2	130735	129826	2.54%	0.346%
19	12.839	1823	1828	1831	rBV	3682889	3891299	76.18%	10.383%
20	13.733	1976	1980	1987	rBV	312882	323664	6.34%	0.864%
21	13.880	2001	2005	2009	rBV	1411936	1223064	23.94%	3.263%
22	15.304	2242	2247	2251	rBV	664656	806264	15.78%	2.151%

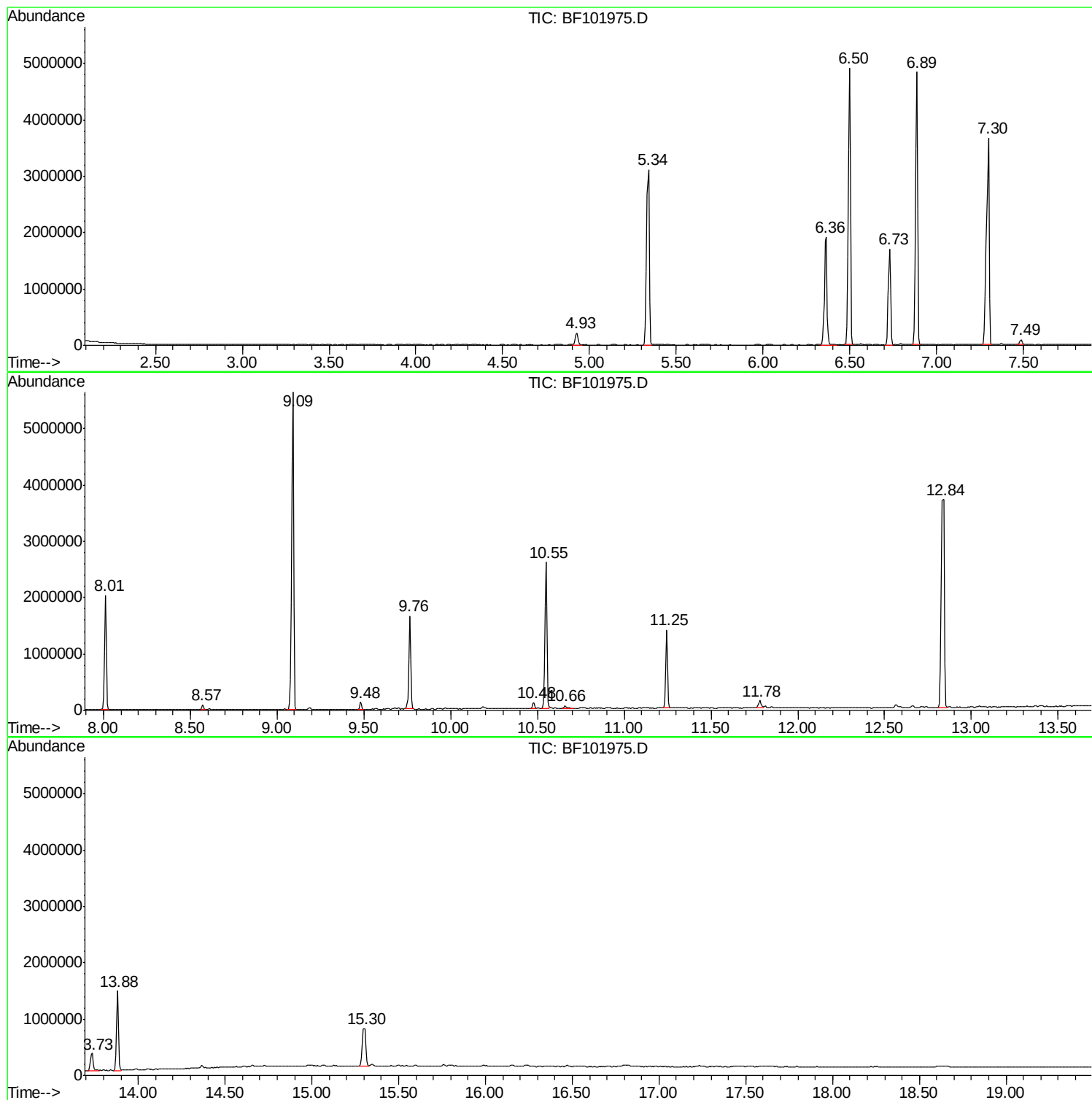
Sum of corrected areas: 37478878

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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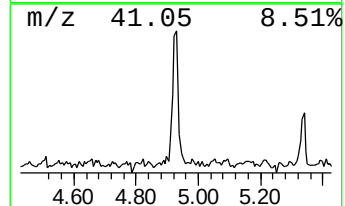
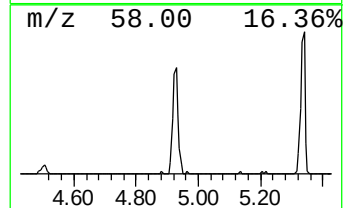
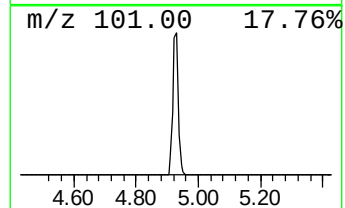
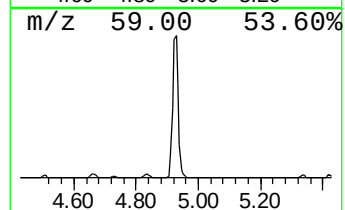
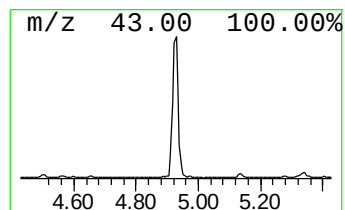
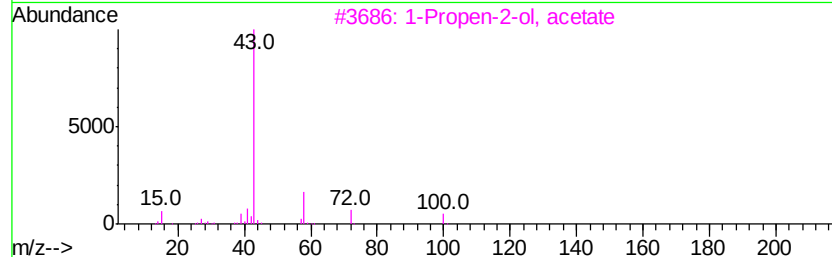
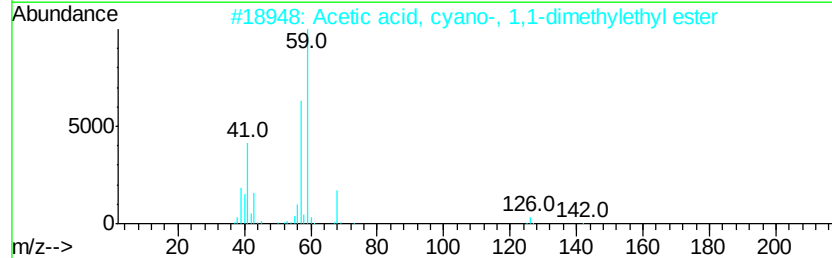
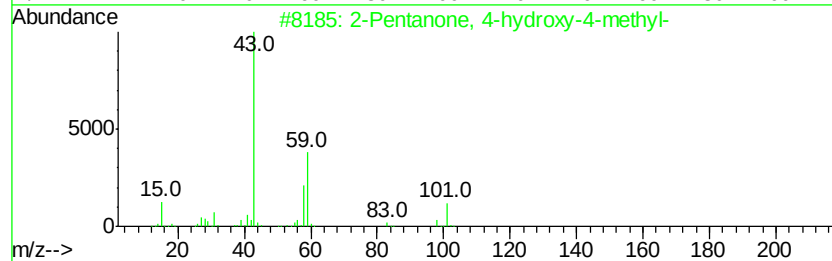
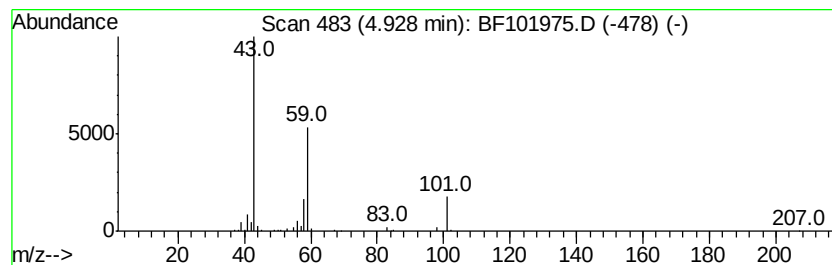
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	3.88 ng	261807	1,4-Dichlorobenzene-d4	6.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10	
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	



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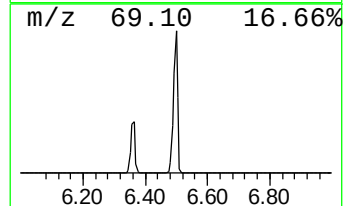
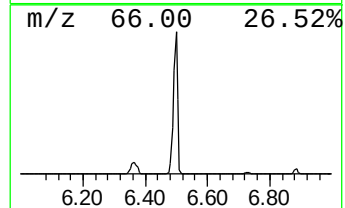
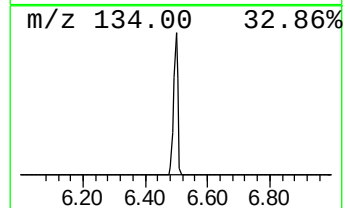
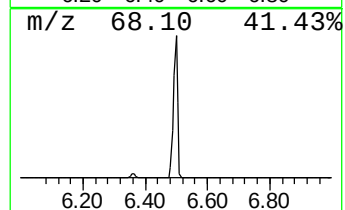
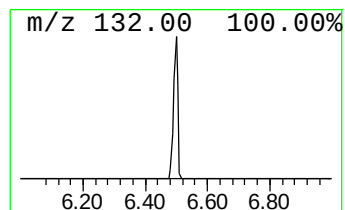
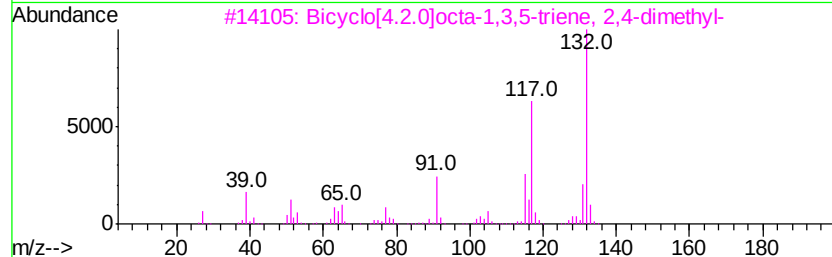
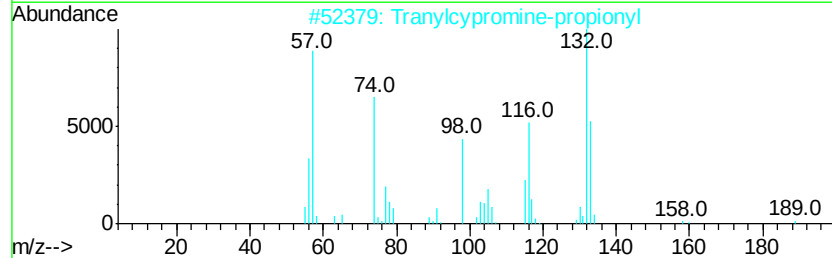
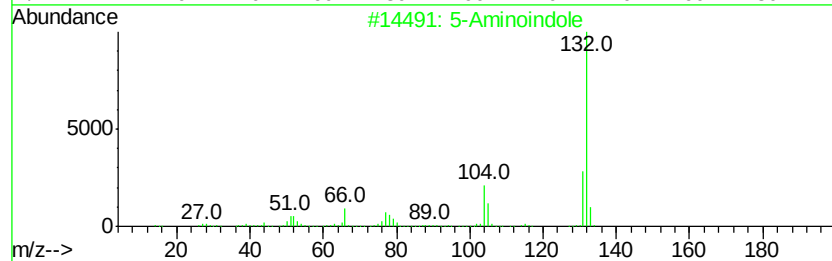
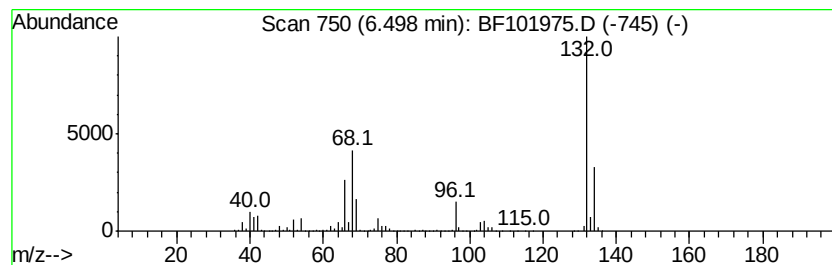
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	70.09 ng	4727030	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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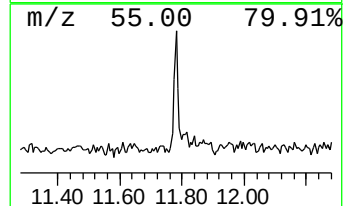
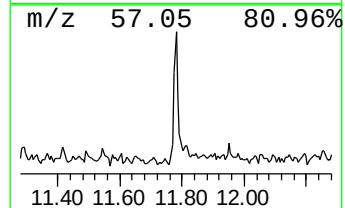
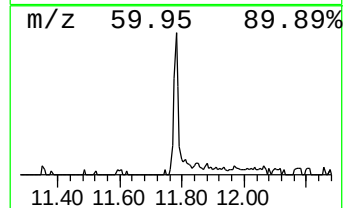
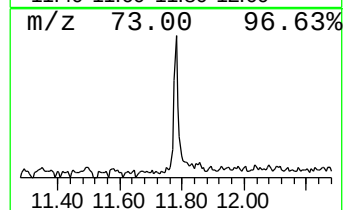
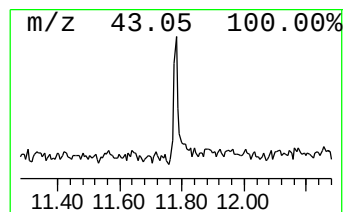
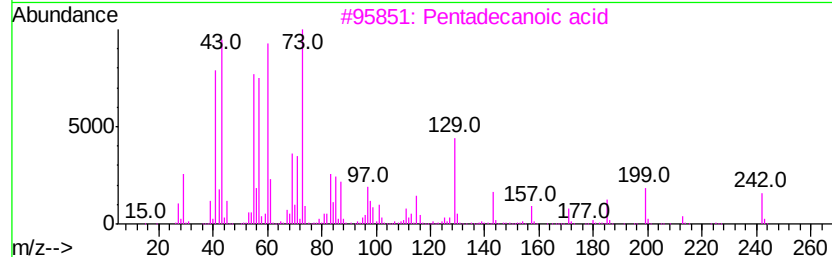
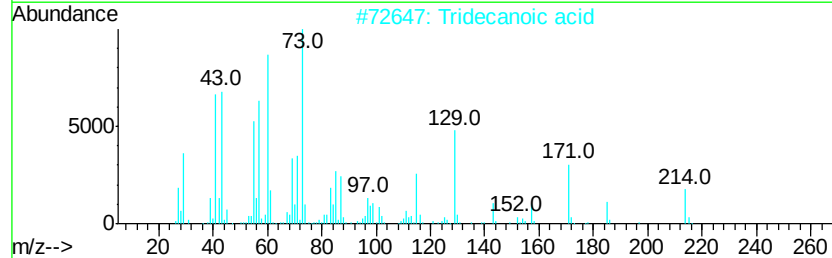
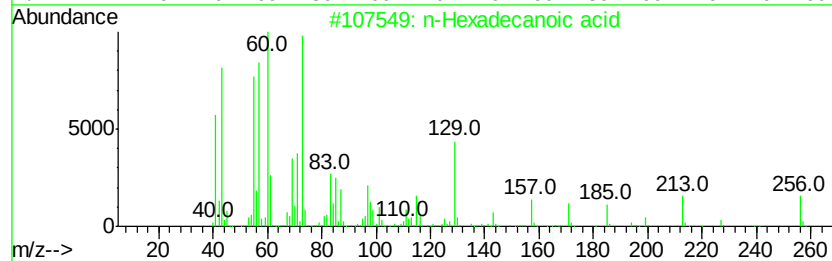
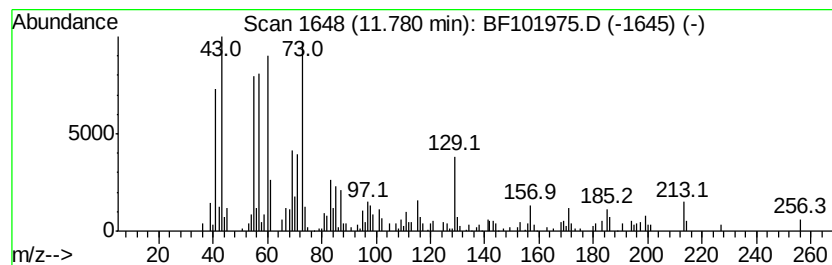
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.36 ng	129826	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	87



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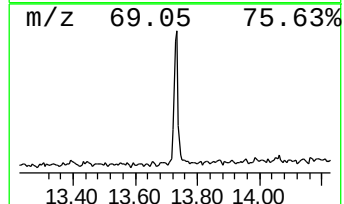
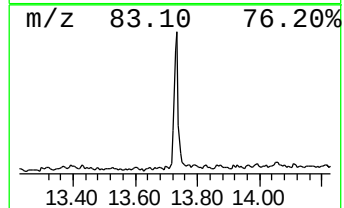
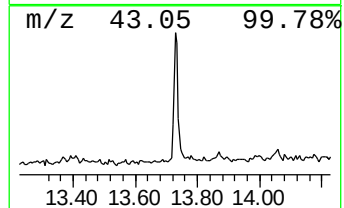
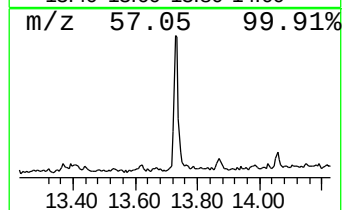
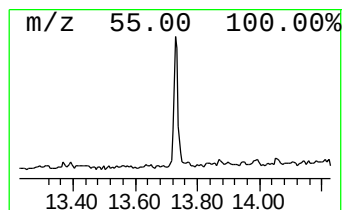
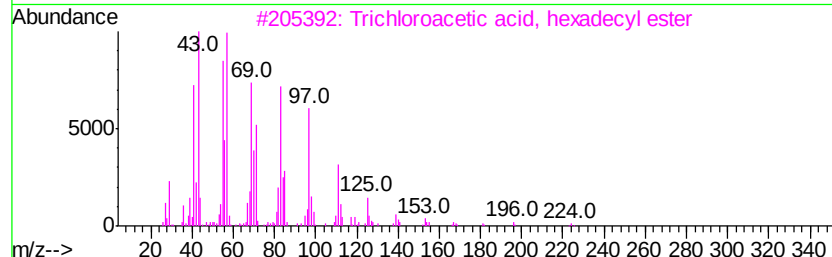
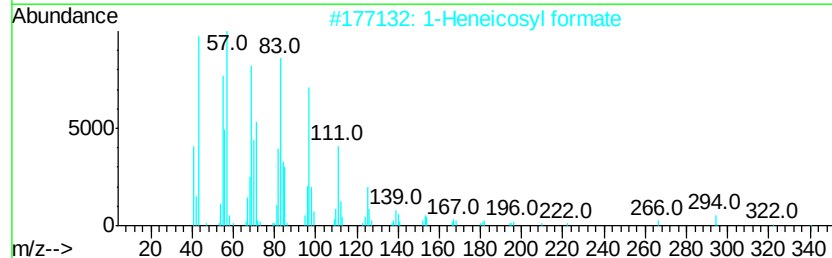
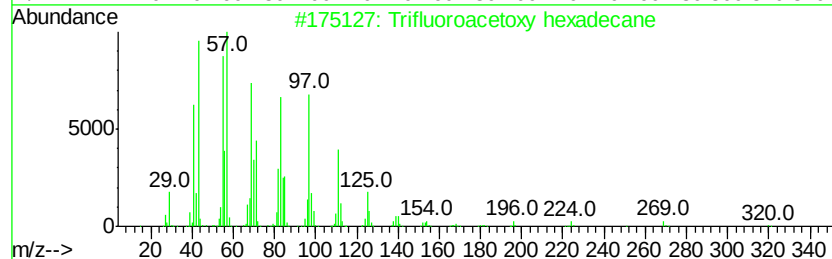
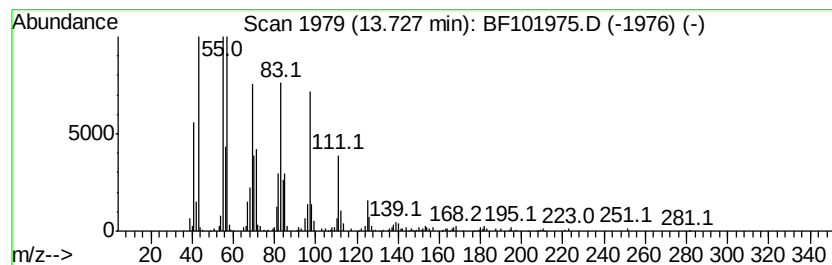
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	5.29 ng	323664	Chrysene-d12	13.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	3.9	ng	261807	1	6.73	1348790	20.0
unknown6.50	6.50	70.1	ng	4727030	1	6.73	1348790	20.0
n-Hexadecanoic acid	11.78	2.4	ng	129826	4	11.25	1101570	20.0
Trifluoroacetoxy ...	13.73	5.3	ng	323664	5	13.88	1223060	20.0