

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081618\
 Data File : BF108217.D
 Acq On : 17 Aug 2018 1:25
 Operator : JU/SJ
 Sample : J4502-01
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LGS-CONCRETE

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	3.855	253	258	264	rBV	33285	48112	1.28%	0.148%
2	4.666	390	396	400	rBV	1978538	2164337	57.66%	6.656%
3	5.260	491	497	500	rBV	2129465	2544200	67.78%	7.824%
4	5.643	558	562	565	rBV	2460730	2109737	56.21%	6.488%
5	6.631	725	730	733	rBV	2948749	2909982	77.52%	8.949%
6	6.784	752	756	759	rBV	3029626	2628728	70.03%	8.084%
7	7.013	792	795	799	rBV	1094723	942854	25.12%	2.900%
8	7.172	818	822	825	rBV	3086268	2581023	68.76%	7.937%
9	7.578	886	891	894	rBV	2152203	2088110	55.63%	6.422%
10	8.295	1009	1013	1017	rBV	1233013	1155577	30.79%	3.554%
11	9.372	1191	1196	1199	rBV	4336097	3753633	100.00%	11.543%
12	9.760	1258	1262	1267	rBV	147626	121579	3.24%	0.374%
13	10.060	1309	1313	1323	rBV	1423876	1253646	33.40%	3.855%
14	10.848	1444	1447	1460	rBV	547909	535970	14.28%	1.648%
15	11.554	1563	1567	1571	rBV	1356604	1194938	31.83%	3.675%
16	13.019	1813	1816	1819	rVB	45076	41487	1.11%	0.128%
17	13.142	1833	1837	1840	rBV	4125284	3659213	97.48%	11.253%
18	14.030	1984	1988	1999	rBV2	141519	273087	7.28%	0.840%
19	14.207	2014	2018	2022	rBV	1375115	1266805	33.75%	3.896%
20	14.654	2089	2094	2096	rBV2	52398	83385	2.22%	0.256%
21	14.966	2143	2147	2154	rBV3	80325	126844	3.38%	0.390%
22	15.771	2278	2284	2291	rVB	707120	983990	26.21%	3.026%
23	16.230	2360	2362	2372	rVB4	30601	50141	1.34%	0.154%

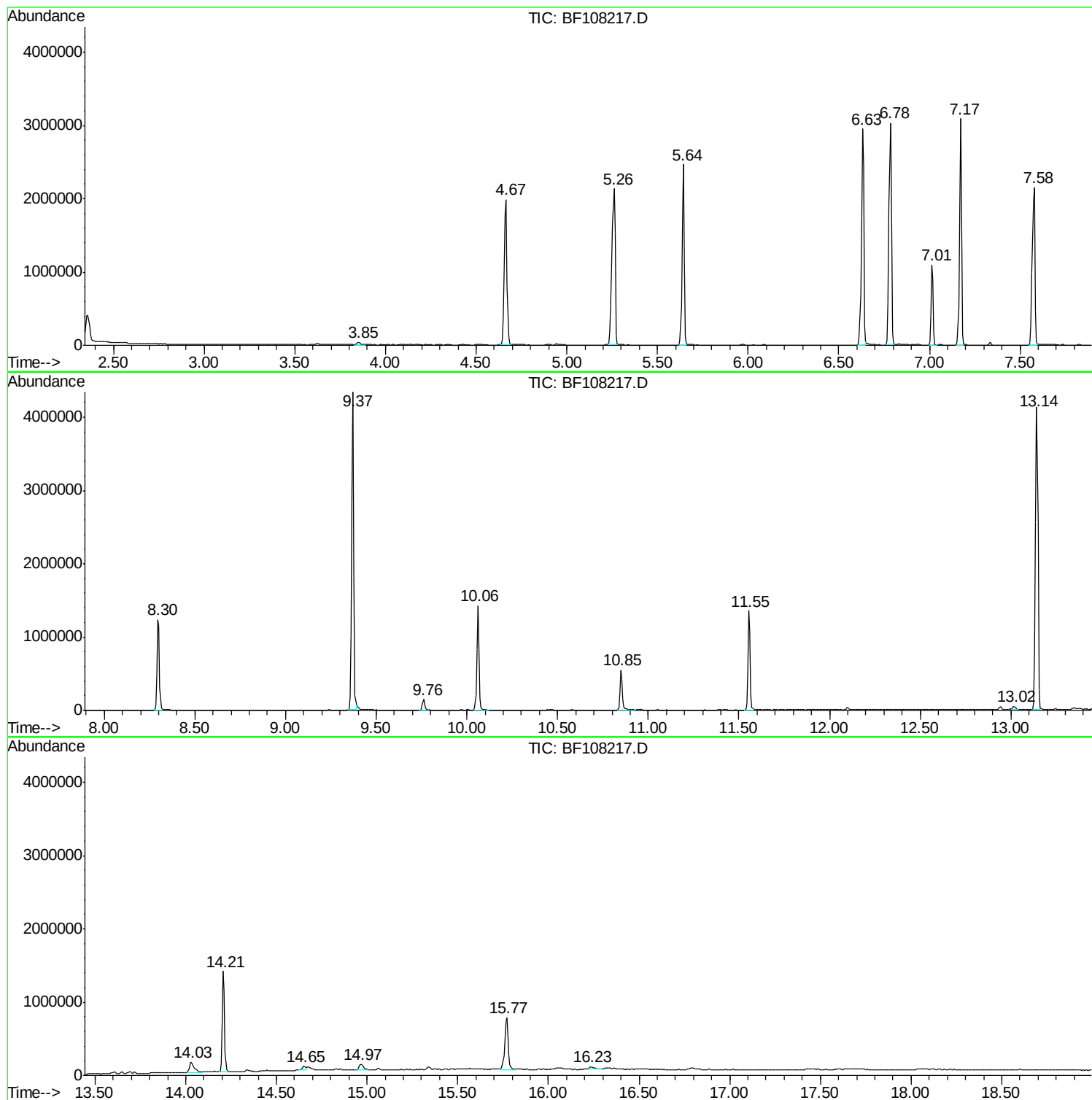
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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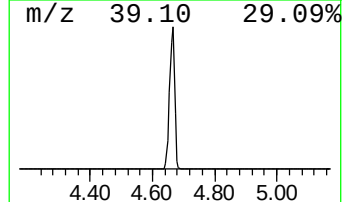
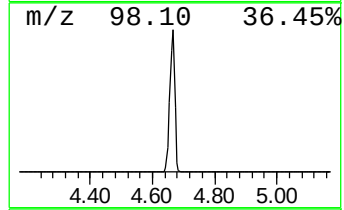
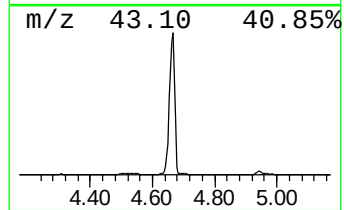
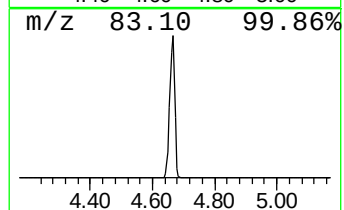
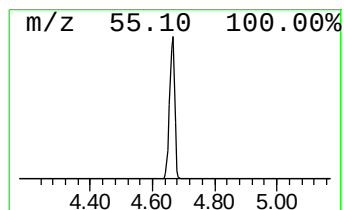
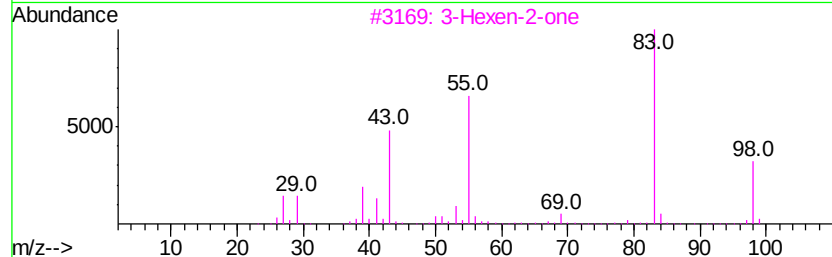
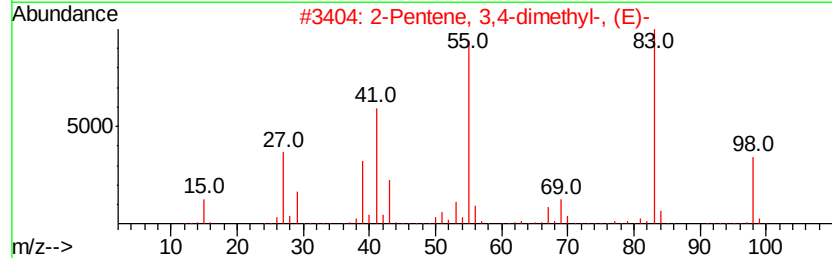
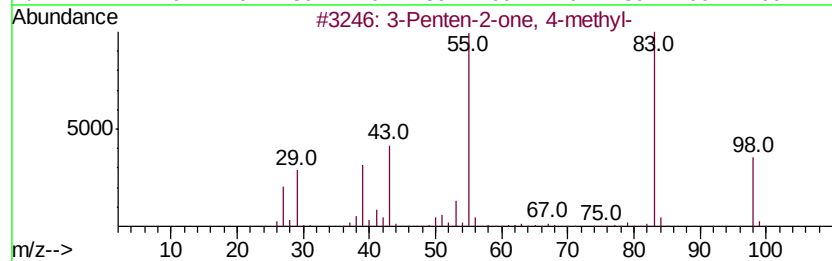
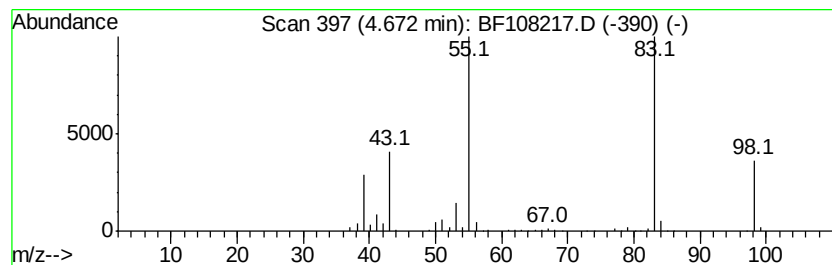
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	45.91 ng	2164340	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		3-Hexen-2-one	98	C6H10O	000763-93-9	87
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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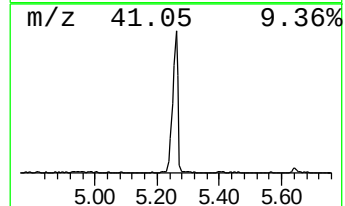
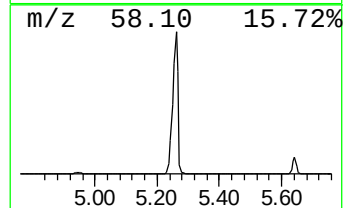
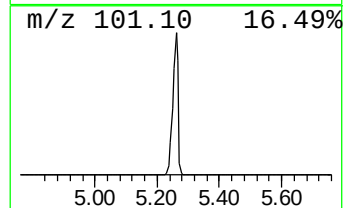
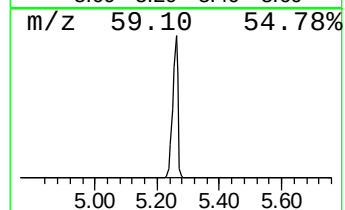
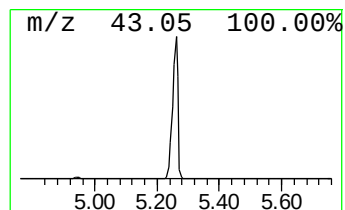
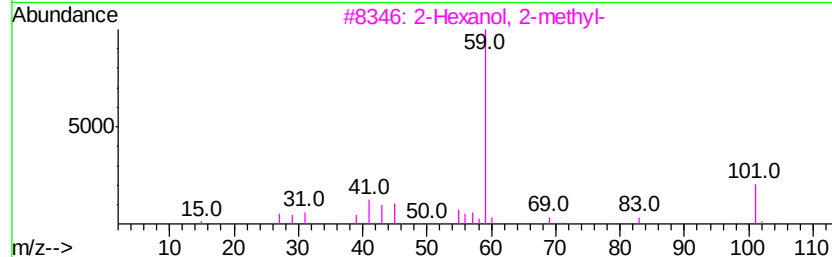
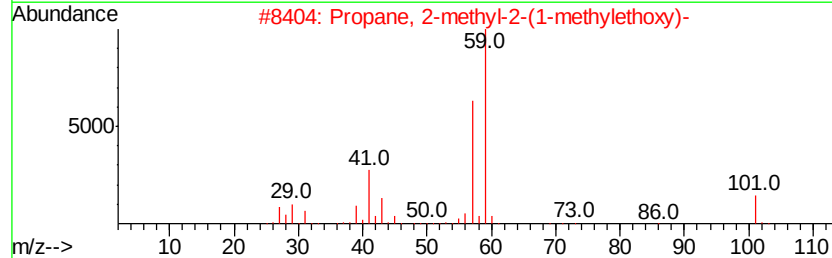
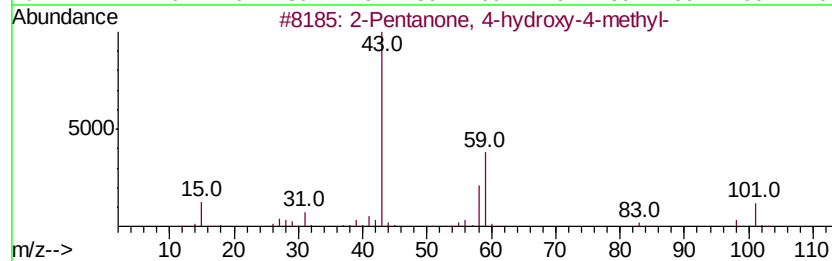
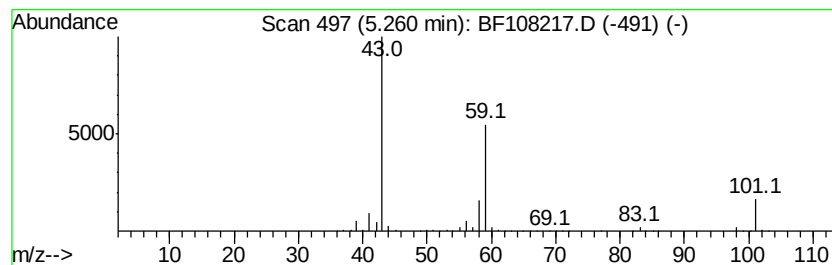
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	53.97 ng	2544200	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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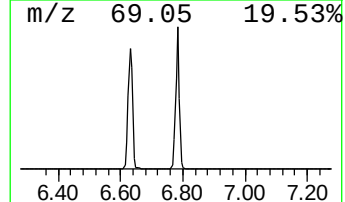
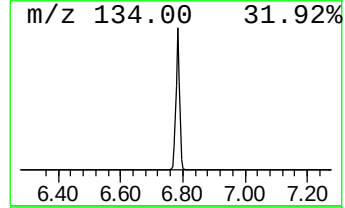
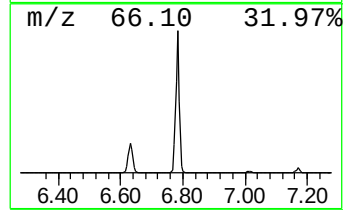
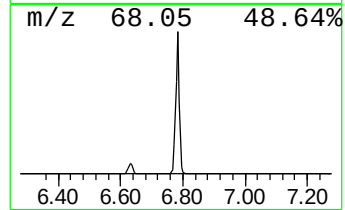
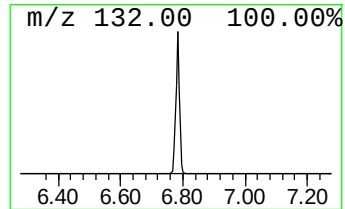
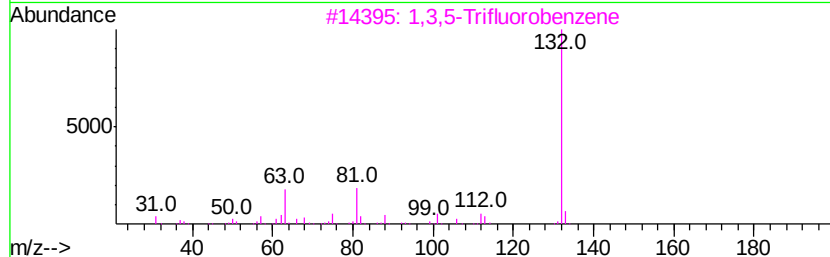
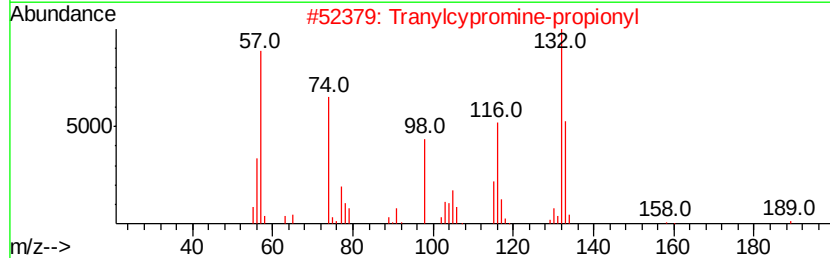
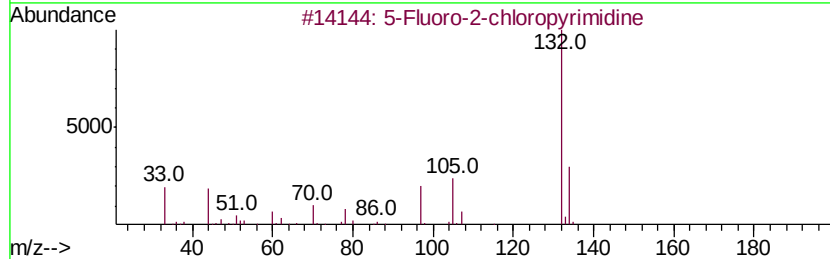
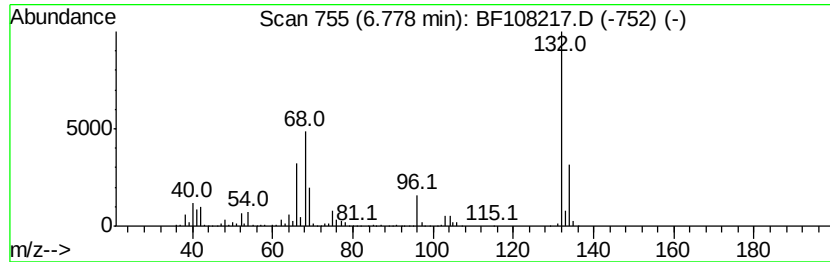
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Peak Number 3 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	55.76 ng	2628730	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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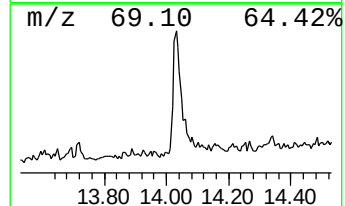
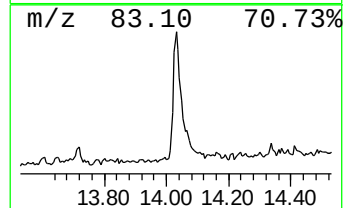
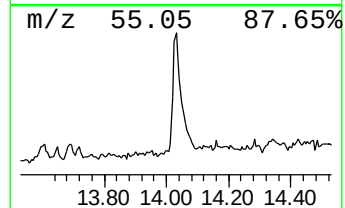
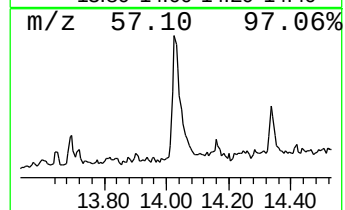
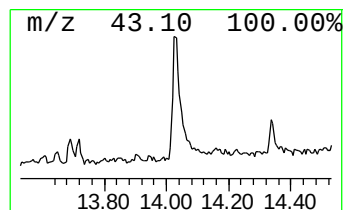
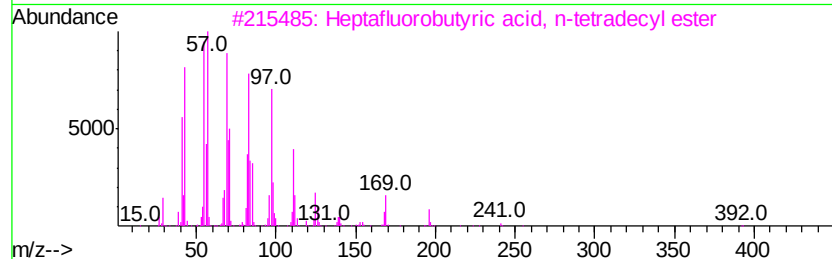
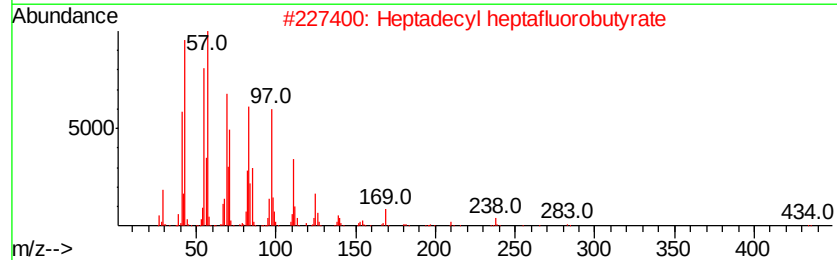
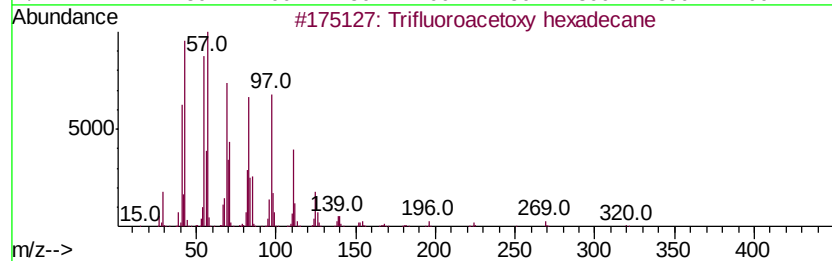
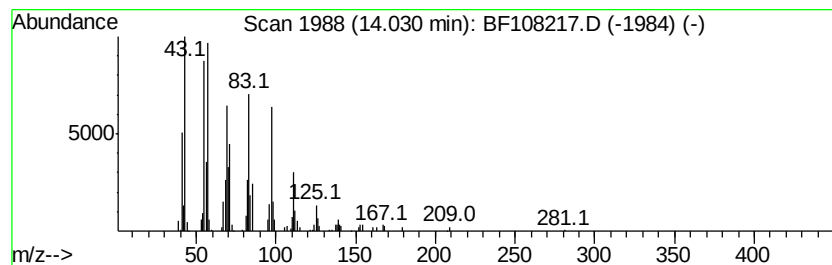
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.03	4.31 ng	273087	Chrysene-d12	14.21		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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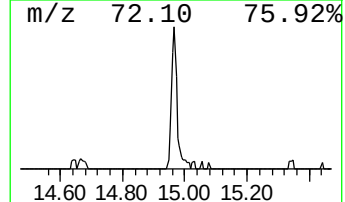
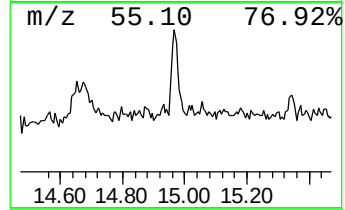
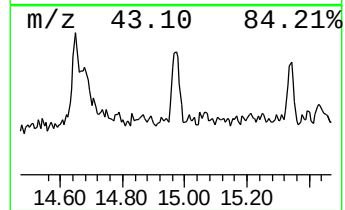
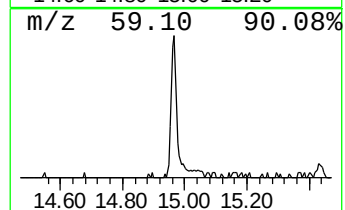
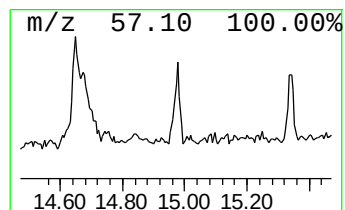
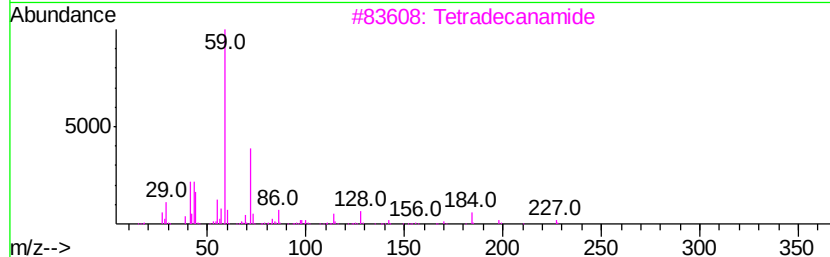
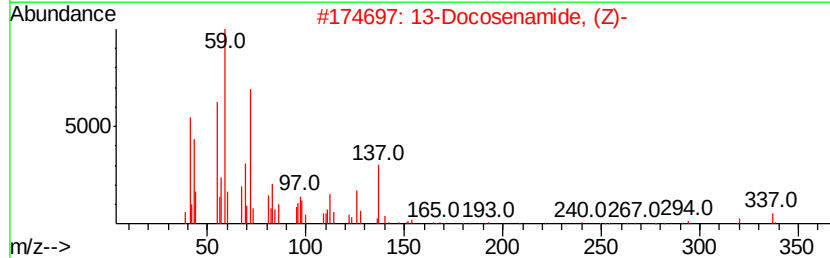
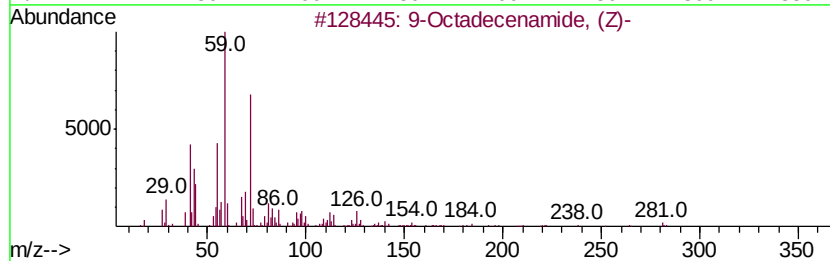
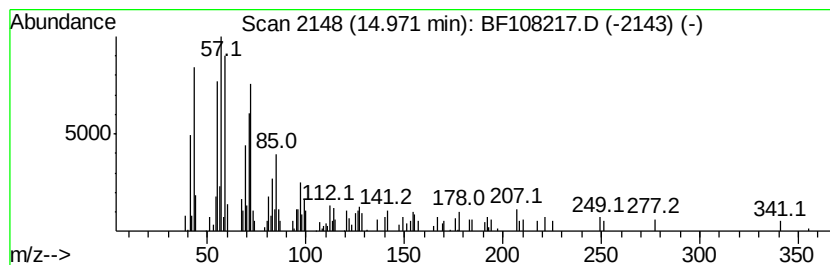
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.97	2.00 ng	126844	Chrysene-d12	14.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
3	Tetradecanamide	227	C14H29NO	000638-58-4	59
4	Octadecanamide	283	C18H37NO	000124-26-5	59
5	3-Hydroxy-3-methyl-butyrac acid,...	132	C5H12N2O2	1000193-80-2	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.67	45.9	ng	2164340	1	7.01	942854	20.0
2-Pentanone, 4-hy...	5.26	54.0	ng	2544200	1	7.01	942854	20.0
unknown6.78	6.78	55.8	ng	2628730	1	7.01	942854	20.0
Trifluoroacetoxy ...	14.03	4.3	ng	273087	5	14.21	1266810	20.0
9-Octadecenamide,...	14.97	2.0	ng	126844	5	14.21	1266810	20.0