

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121217\
 Data File : BF101349.D
 Acq On : 13 Dec 2017 00:02
 Operator : SJ/JU
 Sample : I6822-05
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(8-10)

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:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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	5.057	502	505	517	rBV	62849	104513	7.27%	0.861%
2	5.451	568	572	575	rBV	1367172	1351364	94.03%	11.129%
3	6.469	740	745	759	rBV	1291037	1424254	99.10%	11.729%
4	6.598	762	767	770	rBV	1646862	1437226	100.00%	11.836%
5	6.822	802	805	812	rBB	333481	265837	18.50%	2.189%
6	6.981	828	832	835	rBV	1213513	1033256	71.89%	8.509%
7	7.392	897	902	905	rBV	874630	822891	57.26%	6.777%
8	8.104	1020	1023	1029	rBV	403763	343779	23.92%	2.831%
9	9.180	1201	1206	1209	rBV	1466728	1252731	87.16%	10.317%
10	9.575	1268	1273	1276	rBV	166989	136919	9.53%	1.128%
11	9.780	1304	1308	1313	rVB2	26680	25296	1.76%	0.208%
12	9.863	1318	1322	1326	rBV	397339	343338	23.89%	2.827%
13	10.280	1386	1393	1396	rBV	35376	36619	2.55%	0.302%
14	10.663	1453	1458	1461	rBV	802638	817472	56.88%	6.732%
15	10.757	1471	1474	1478	rVB	25402	27347	1.90%	0.225%
16	10.963	1502	1509	1511	rBV6	9327	18010	1.25%	0.148%
17	11.204	1547	1550	1554	rBV3	19199	26172	1.82%	0.216%
18	11.357	1572	1576	1578	rBV	418685	364026	25.33%	2.998%
19	11.380	1578	1580	1584	rVB	81401	68486	4.77%	0.564%
20	11.968	1678	1680	1683	rBV2	26871	31947	2.22%	0.263%
21	12.574	1780	1783	1786	rBV	116261	94854	6.60%	0.781%
22	12.804	1817	1822	1829	rBV	115944	153863	10.71%	1.267%
23	12.945	1842	1846	1849	rBV	1091095	974542	67.81%	8.026%
24	13.827	1993	1996	2003	rVB3	75294	89487	6.23%	0.737%
25	14.010	2022	2027	2029	rBV2	371701	373284	25.97%	3.074%
26	14.033	2029	2031	2034	rVB	61197	47184	3.28%	0.389%
27	15.057	2201	2205	2213	rVB	43770	91946	6.40%	0.757%
28	15.357	2253	2256	2262	rVB	30812	47641	3.31%	0.392%
29	15.421	2264	2267	2272	rVB	42176	49850	3.47%	0.411%
30	15.486	2273	2278	2282	rBV	199177	238422	16.59%	1.963%
31	16.968	2528	2530	2537	rVB3	19792	31645	2.20%	0.261%
32	17.421	2604	2607	2611	rVB4	11903	18698	1.30%	0.154%

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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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

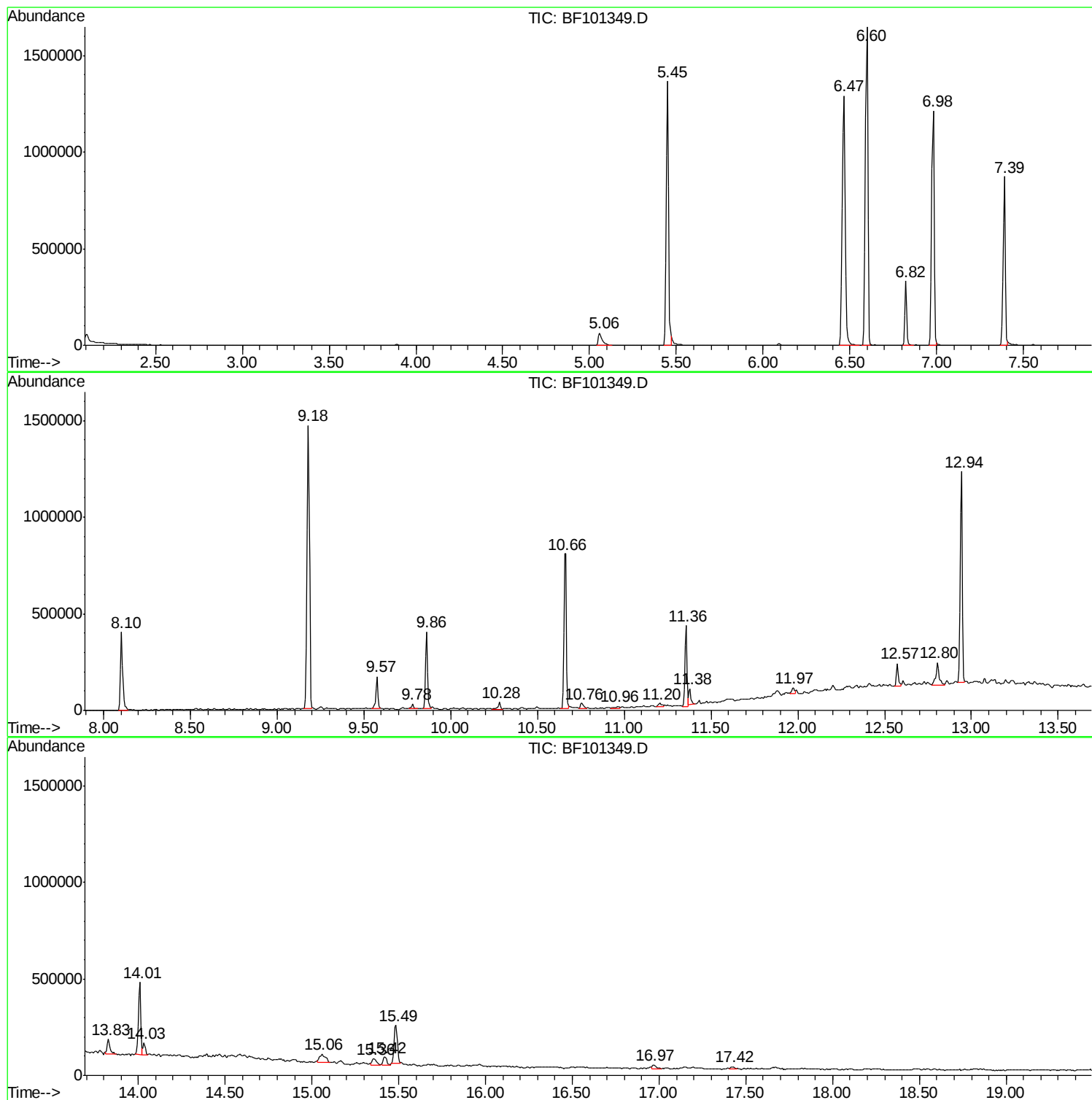
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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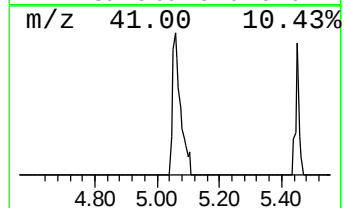
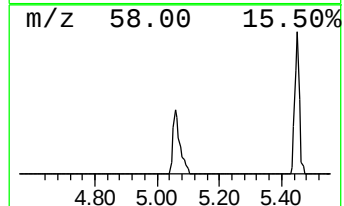
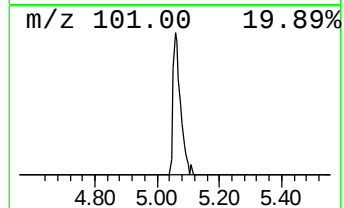
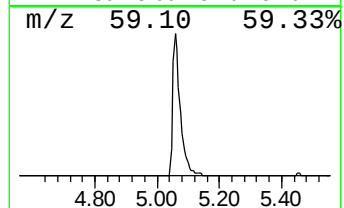
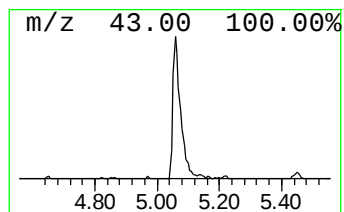
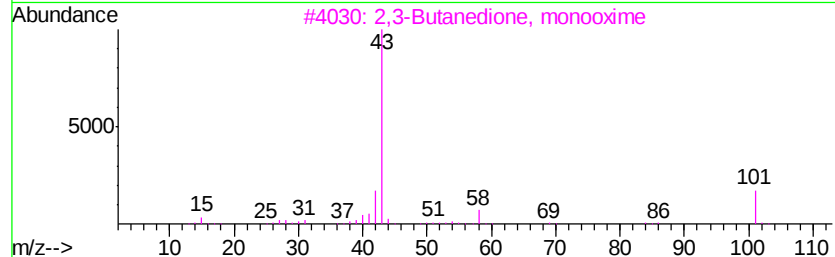
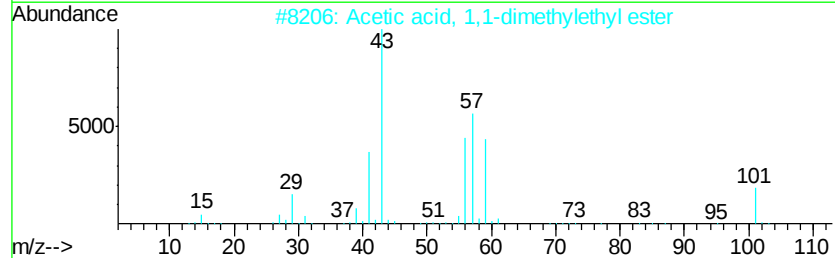
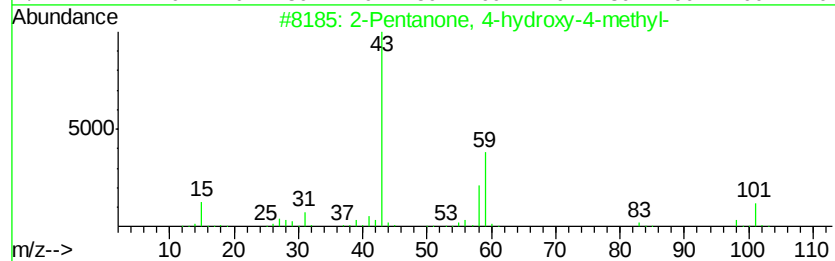
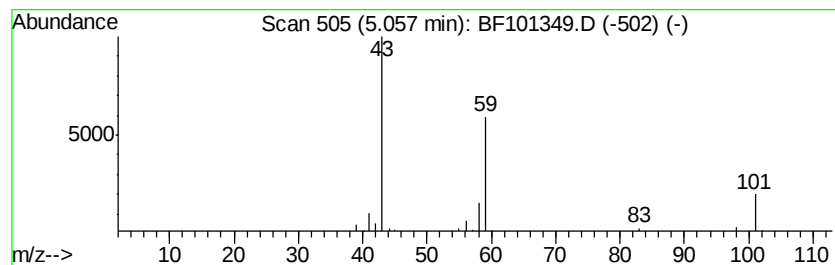
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	7.86 ng	104513	1,4-Dichlorobenzene-d4	6.82

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	25
4			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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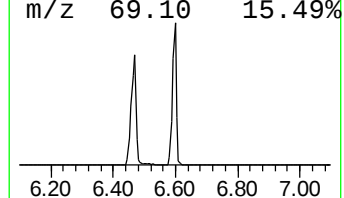
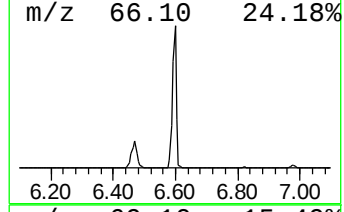
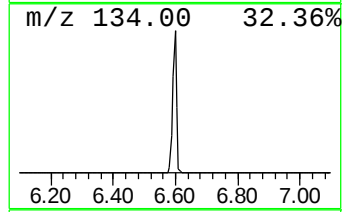
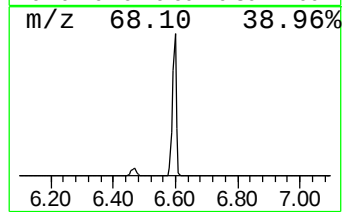
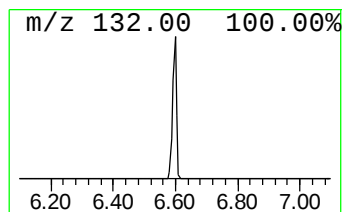
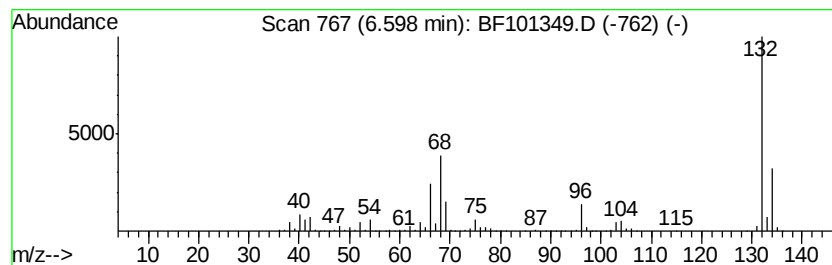
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	108.13 ng	1437230	1,4-Dichlorobenzene-d4	6.82

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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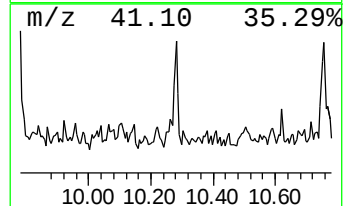
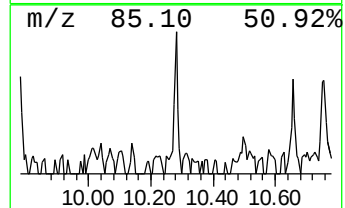
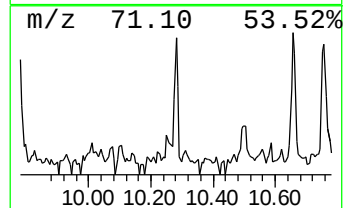
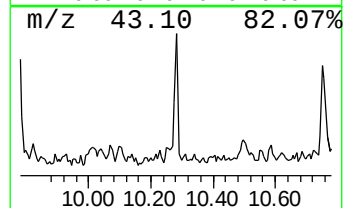
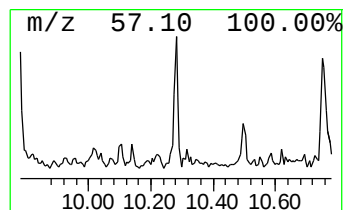
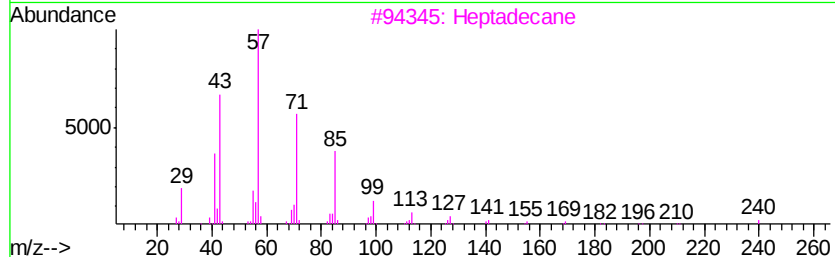
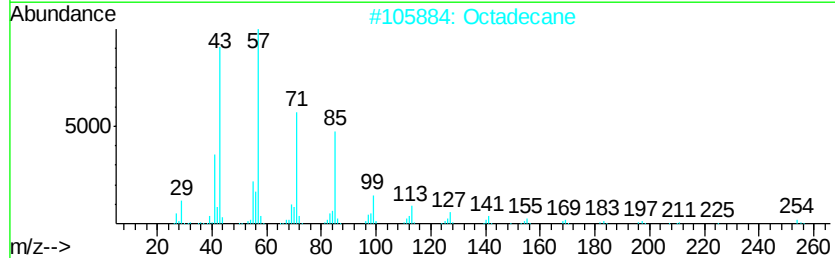
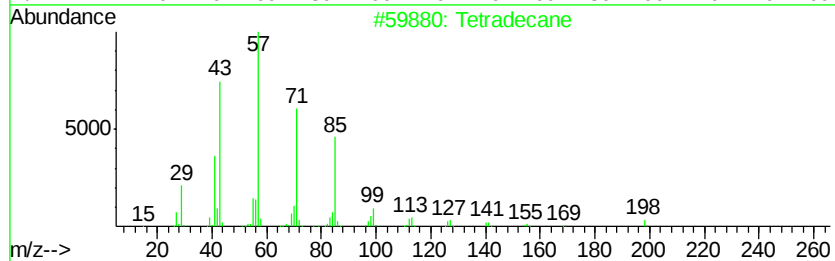
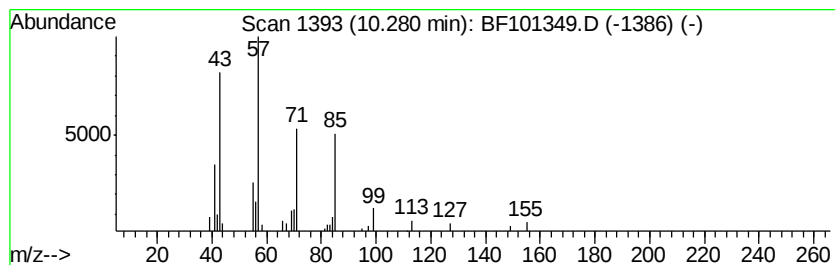
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Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.13 ng	36619	Acenaphthene-d10	9.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	86
2		Octadecane	254	C18H38	000593-45-3	86
3		Heptadecane	240	C17H36	000629-78-7	83
4		Pentadecane	212	C15H32	000629-62-9	78
5		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64



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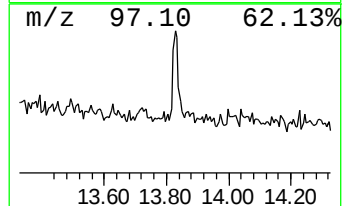
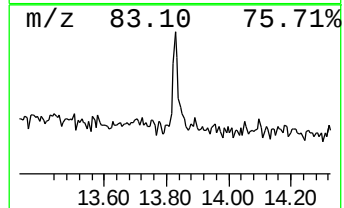
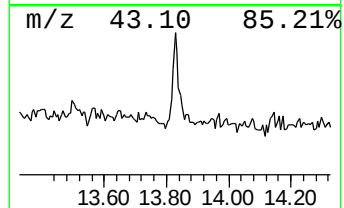
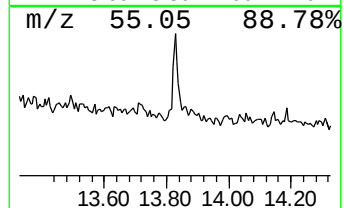
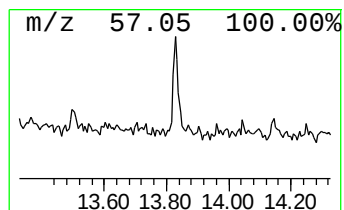
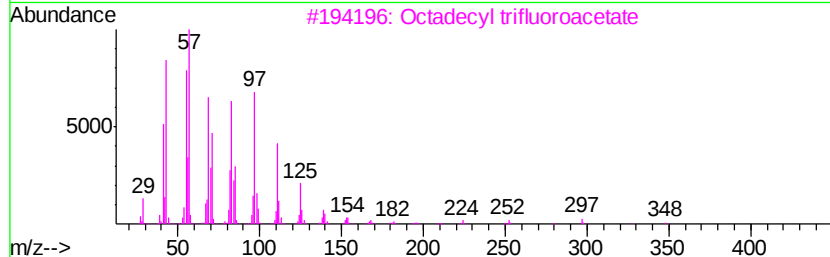
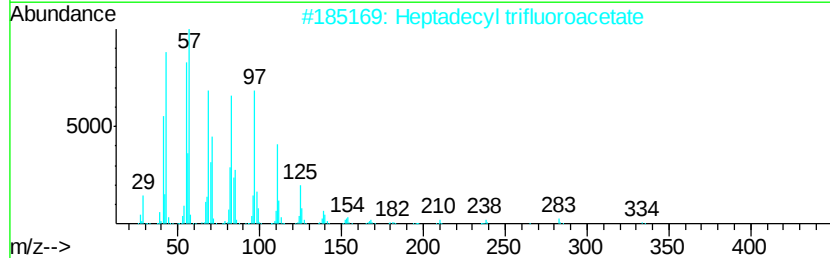
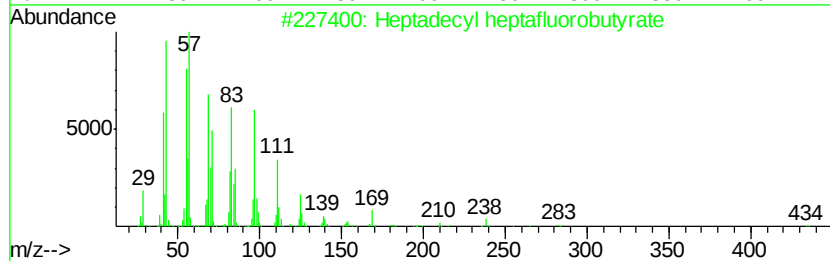
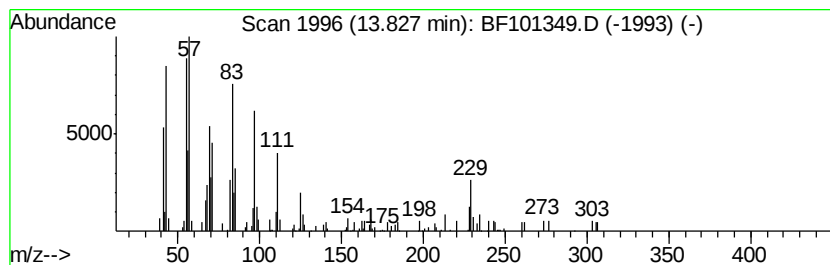
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.79 ng	89487	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
5		Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	7.9	ng	104513	1	6.82	265837	20.0
unknown6.60	6.60	108.1	ng	1437230	1	6.82	265837	20.0
Tetradecane	10.28	2.1	ng	36619	3	9.86	343338	20.0
Heptadecyl heptaf...	13.83	4.8	ng	89487	5	14.01	373284	20.0