

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF110417\
 Data File : BF100192.D
 Acq On : 4 Nov 2017 21:24
 Operator : SJ/JU
 Sample : I6313-11
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF017-01

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-BF102317.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	4.387	388	391	404	rBV3	12318	37968	1.53%	0.187%
2	4.987	489	493	518	rBV	213323	407606	16.42%	2.010%
3	5.392	559	562	596	rBV	1306712	1970617	79.37%	9.716%
4	6.416	733	736	754	rBV	1581479	1997173	80.44%	9.847%
5	6.539	754	757	771	rVB	2103972	2060785	83.01%	10.161%
6	6.763	792	795	807	rVB	508221	477737	19.24%	2.356%
7	6.916	818	821	842	rBV	1753268	1637488	65.96%	8.074%
8	7.334	889	892	916	rBV	1114826	1238045	49.87%	6.104%
9	8.045	1010	1013	1038	rBV	714433	683270	27.52%	3.369%
10	9.116	1191	1195	1198	rBV	2786504	2482681	100.00%	12.241%
11	9.516	1260	1263	1276	rBV	215205	188541	7.59%	0.930%
12	9.798	1307	1311	1325	rVB	825646	799140	32.19%	3.940%
13	10.592	1443	1446	1459	rBV	1382863	1392479	56.09%	6.866%
14	11.286	1561	1564	1575	rBV	834569	813322	32.76%	4.010%
15	11.804	1649	1652	1665	rBV	177801	179072	7.21%	0.883%
16	12.586	1782	1785	1796	rBV	73170	91715	3.69%	0.452%
17	12.868	1829	1833	1836	rBV	2446559	2436977	98.16%	12.016%
18	13.739	1978	1981	1990	rBV	208884	217064	8.74%	1.070%
19	13.939	2012	2015	2024	rBV	618718	610403	24.59%	3.010%
20	14.657	2133	2137	2144	rBV2	41507	49496	1.99%	0.244%
21	15.398	2259	2263	2277	rVB	309115	452320	18.22%	2.230%
22	15.751	2318	2323	2328	rBV4	18900	29757	1.20%	0.147%
23	16.227	2399	2404	2412	rVB5	14694	27862	1.12%	0.137%

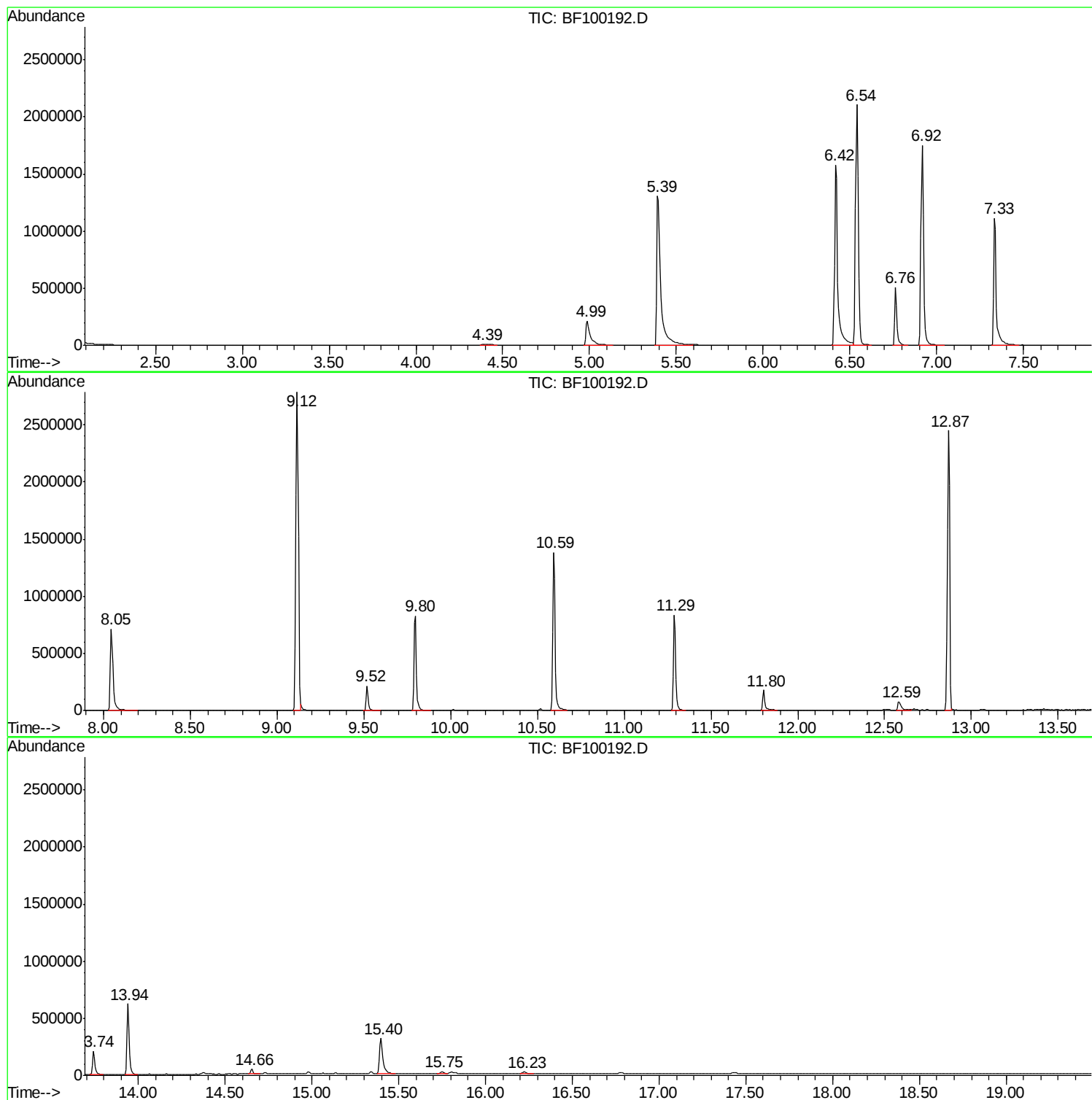
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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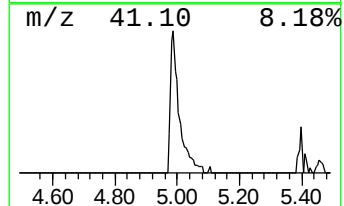
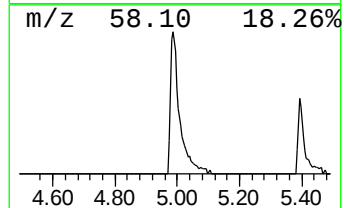
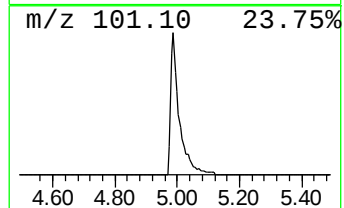
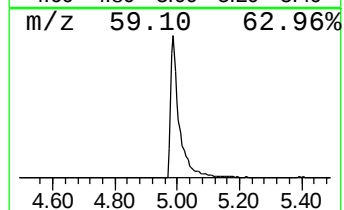
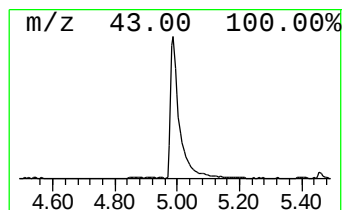
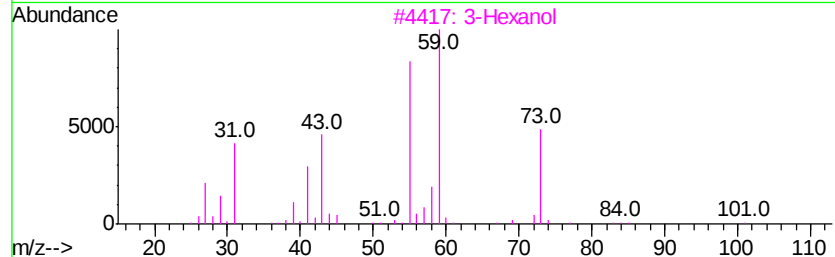
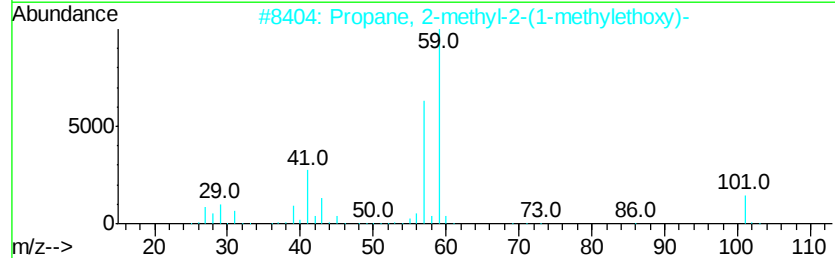
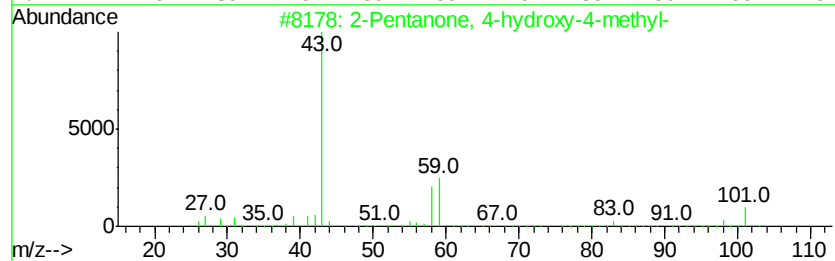
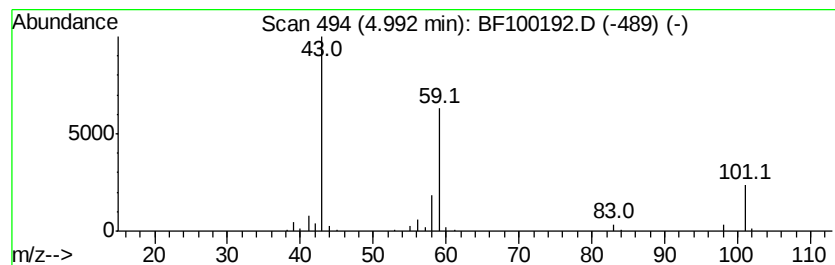
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.99	17.06 ng	407606	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Guanidine	59	CH5N3	000113-00-8	9



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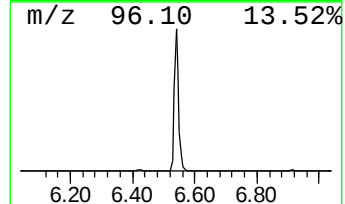
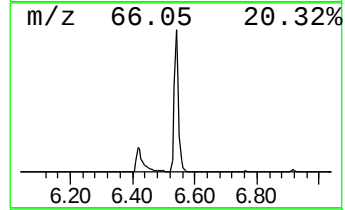
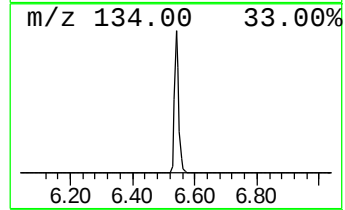
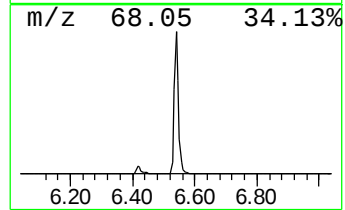
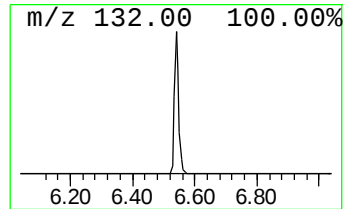
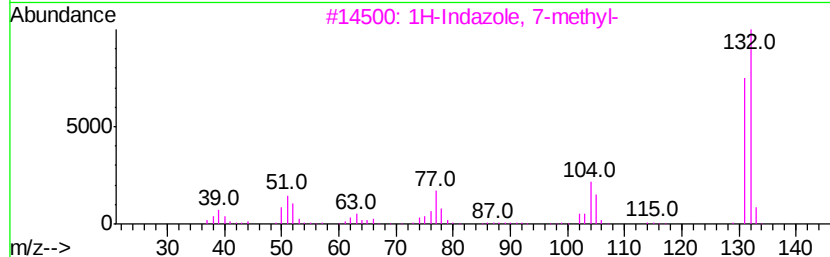
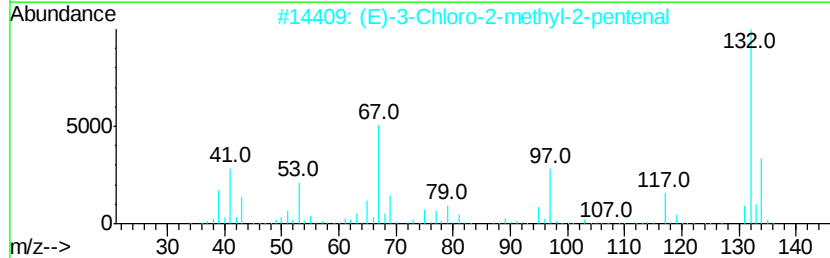
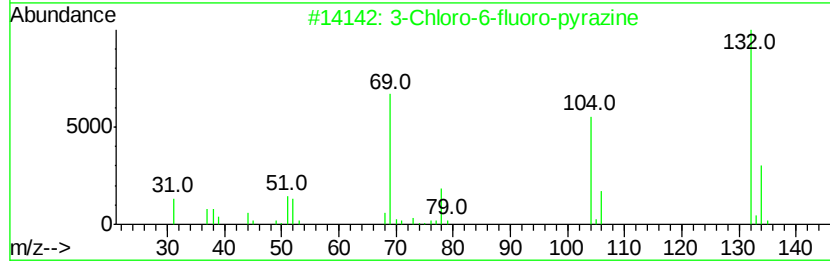
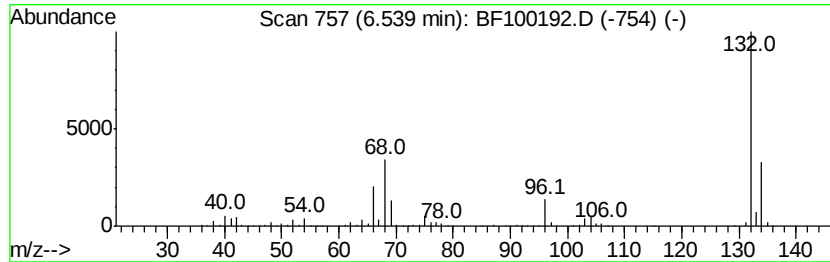
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	86.27 ng	2060790	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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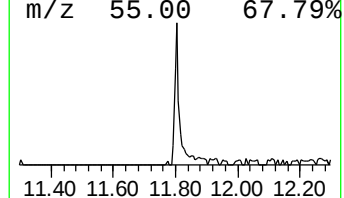
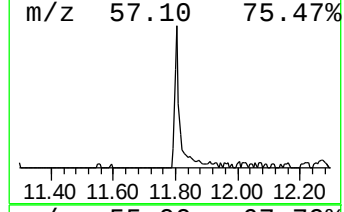
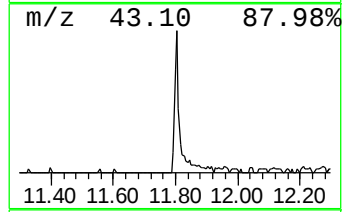
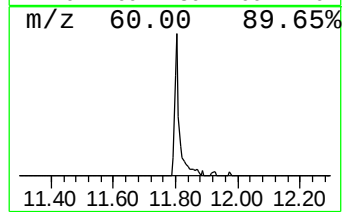
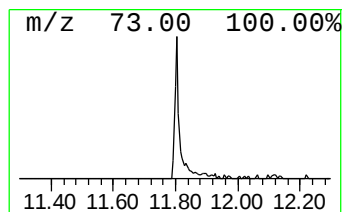
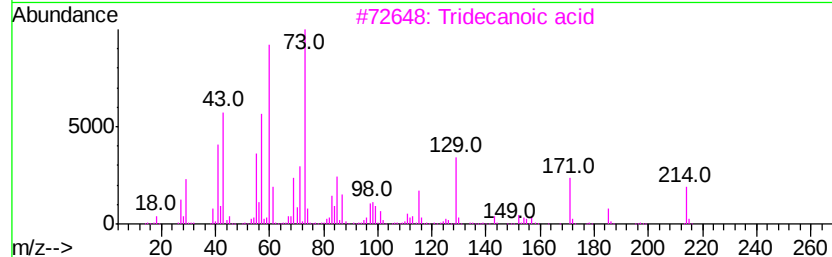
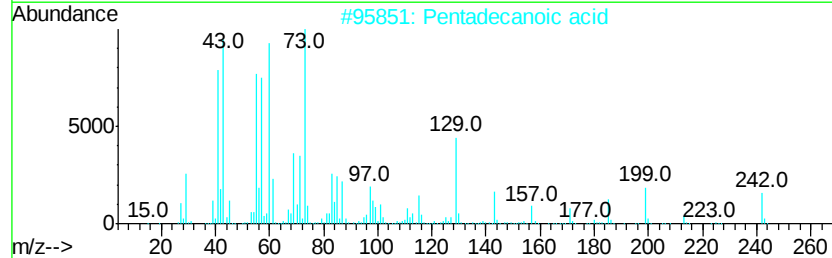
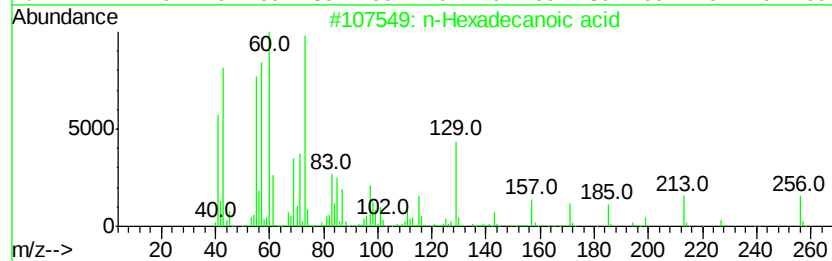
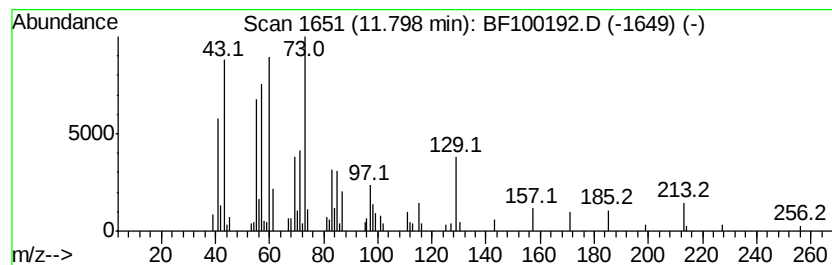
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TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.80	4.40 ng	179072	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20



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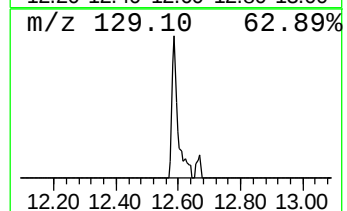
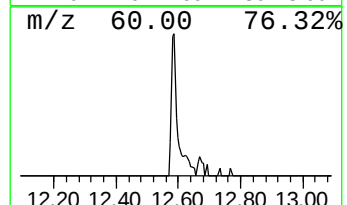
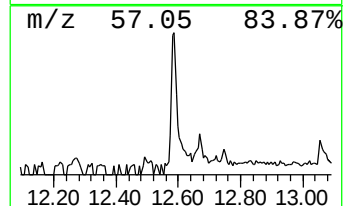
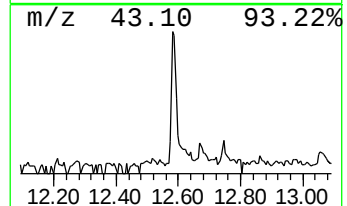
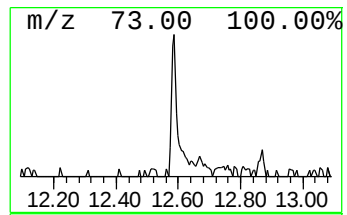
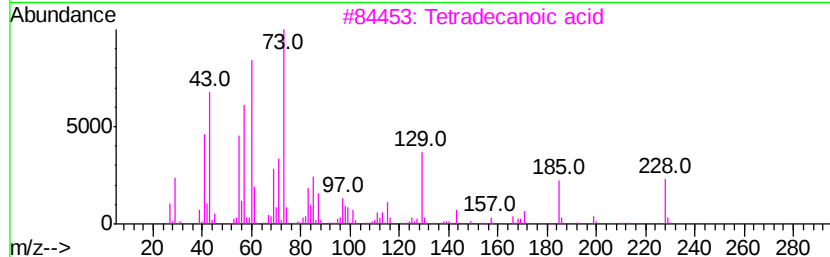
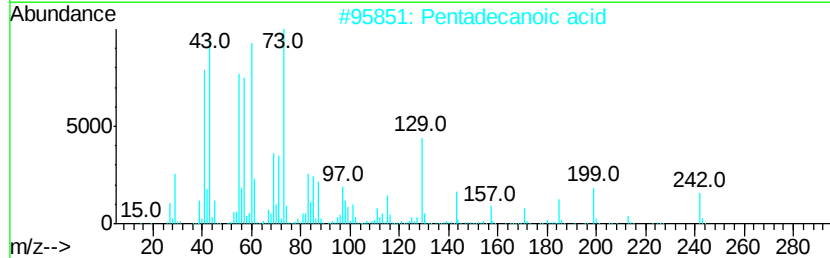
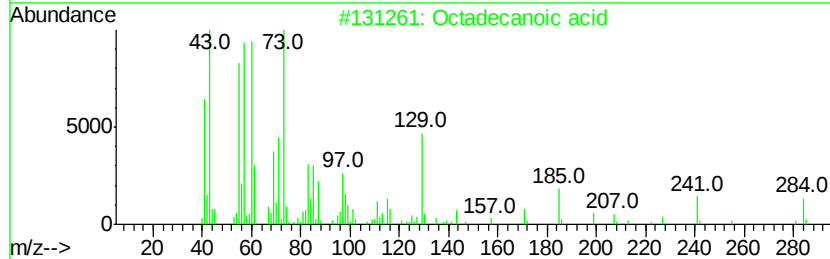
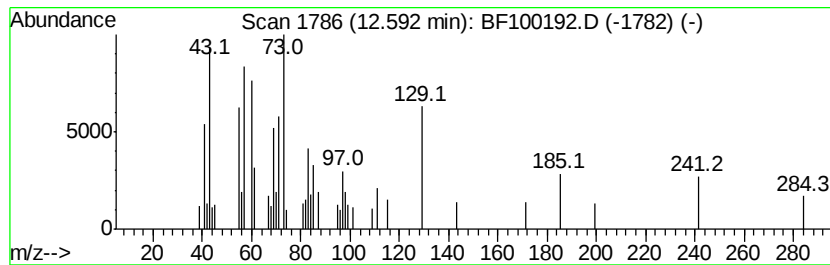
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.59	2.26 ng	91715	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	35
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25



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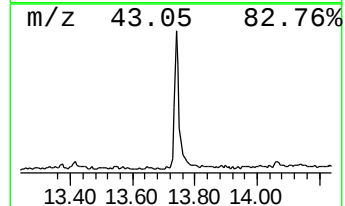
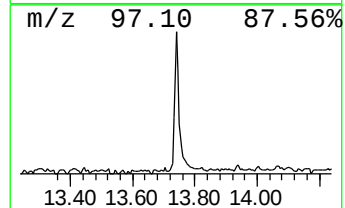
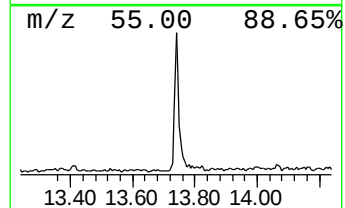
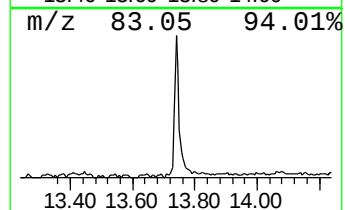
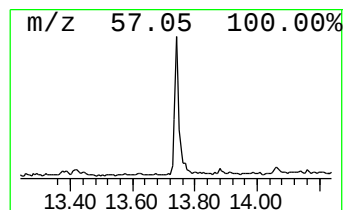
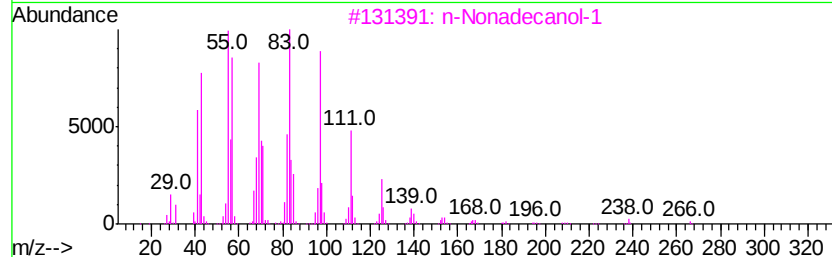
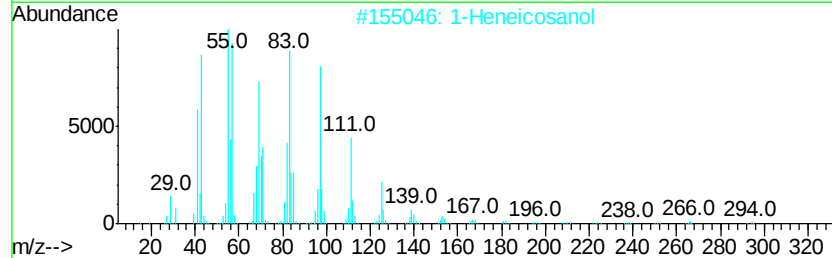
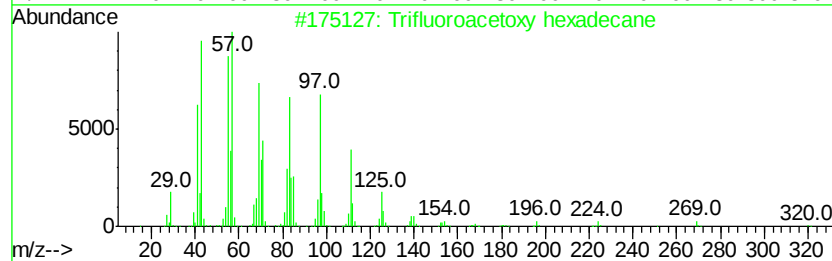
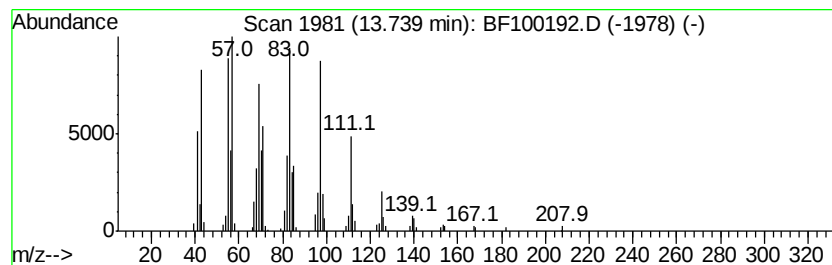
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	7.11 ng	217064	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4		1-Heptacosanol	396	C27H56O	002004-39-9	94
5		Behenic alcohol	326	C22H46O	000661-19-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	17.1	ng	407606	1	6.76	477737	20.0
unknown6.54	6.54	86.3	ng	2060790	1	6.76	477737	20.0
n-Hexadecanoic acid	11.80	4.4	ng	179072	4	11.29	813322	20.0
Octadecanoic acid	12.59	2.3	ng	91715	4	11.29	813322	20.0
Trifluoroacetoxy ...	13.74	7.1	ng	217064	5	13.94	610403	20.0