

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123021\
 Data File : BF126414.D
 Acq On : 30 Dec 2021 12:07
 Operator : JU/CG
 Sample : M5223-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DB-19-(40-45)-12-22-21

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126414.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	495	499	505	rVB	58367	75351	1.73%	0.254%
2	5.410	560	565	569	rBV	3605621	4120401	94.81%	13.908%
3	6.428	732	738	741	rBV	3665641	4345771	100.00%	14.669%
4	6.792	797	800	804	rBV	1088534	937243	21.57%	3.164%
5	6.857	808	811	819	rBV	234341	207542	4.78%	0.701%
6	7.357	891	896	899	rBV	2833491	2969670	68.33%	10.024%
7	7.981	997	1002	1010	rBV	62698	90489	2.08%	0.305%
8	8.075	1014	1018	1022	rBV	1372222	1293006	29.75%	4.364%
9	9.157	1197	1202	1205	rBV	4056319	3999661	92.04%	13.500%
10	9.239	1212	1216	1222	rBV2	83438	79302	1.82%	0.268%
11	9.433	1245	1249	1256	rBV	59780	62438	1.44%	0.211%
12	9.833	1310	1317	1320	rBV	1534991	1365448	31.42%	4.609%
13	10.245	1383	1387	1390	rBV2	41774	46672	1.07%	0.158%
14	10.622	1445	1451	1454	rBV	2552141	2420337	55.69%	8.170%
15	10.757	1469	1474	1476	rVB	41642	44402	1.02%	0.150%
16	11.316	1565	1569	1572	rBV	1575303	1313234	30.22%	4.433%
17	11.569	1604	1612	1618	rBV6	33819	72514	1.67%	0.245%
18	11.716	1634	1637	1640	rVB	62819	48886	1.12%	0.165%
19	11.851	1656	1660	1663	rBV	224664	210383	4.84%	0.710%
20	11.880	1663	1665	1668	rVB	115034	94511	2.17%	0.319%
21	12.104	1700	1703	1706	rVB	227333	173918	4.00%	0.587%
22	12.421	1754	1757	1760	rVB2	144195	113556	2.61%	0.383%
23	12.457	1760	1763	1767	rVB	89824	78925	1.82%	0.266%
24	12.551	1776	1779	1785	rVB3	30786	45810	1.05%	0.155%
25	12.633	1790	1793	1798	rBV3	41285	62805	1.45%	0.212%
26	12.904	1834	1839	1843	rBV	3081895	3292763	75.77%	11.114%
27	13.815	1990	1994	2002	rBV4	113345	279312	6.43%	0.943%
28	13.951	2013	2017	2021	rVB	946677	878182	20.21%	2.964%
29	14.280	2070	2073	2077	rBV	123236	114951	2.65%	0.388%
30	14.809	2159	2163	2167	rVB	41908	43905	1.01%	0.148%
31	15.392	2257	2262	2267	rBV2	607994	744827	17.14%	2.514%

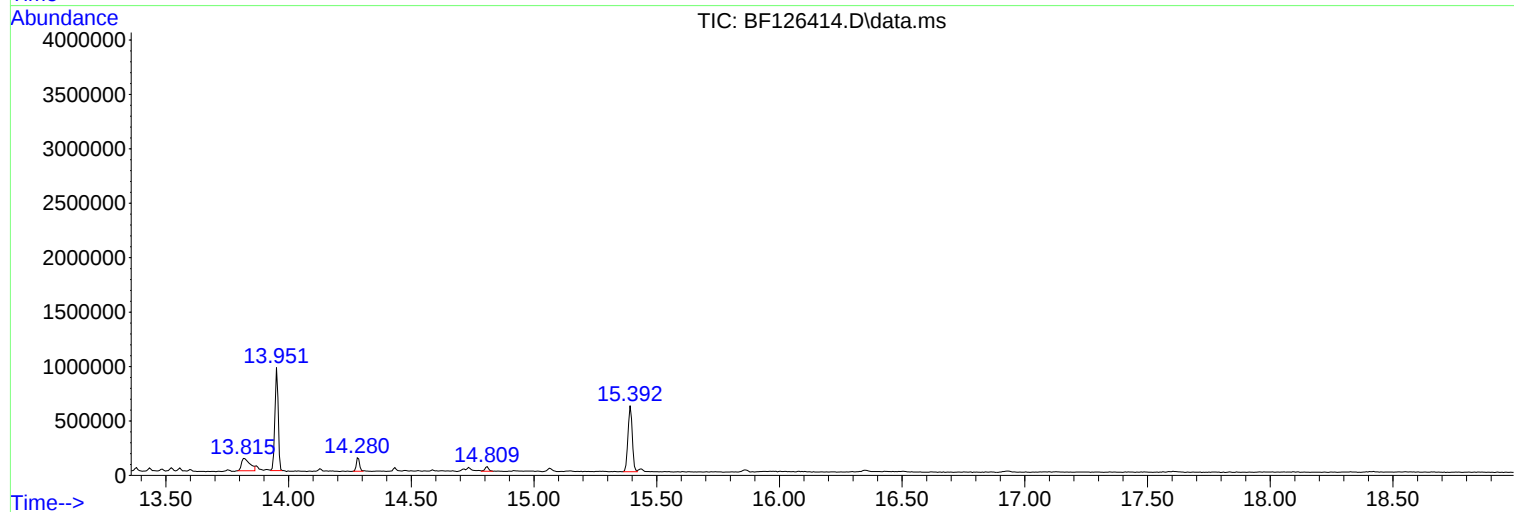
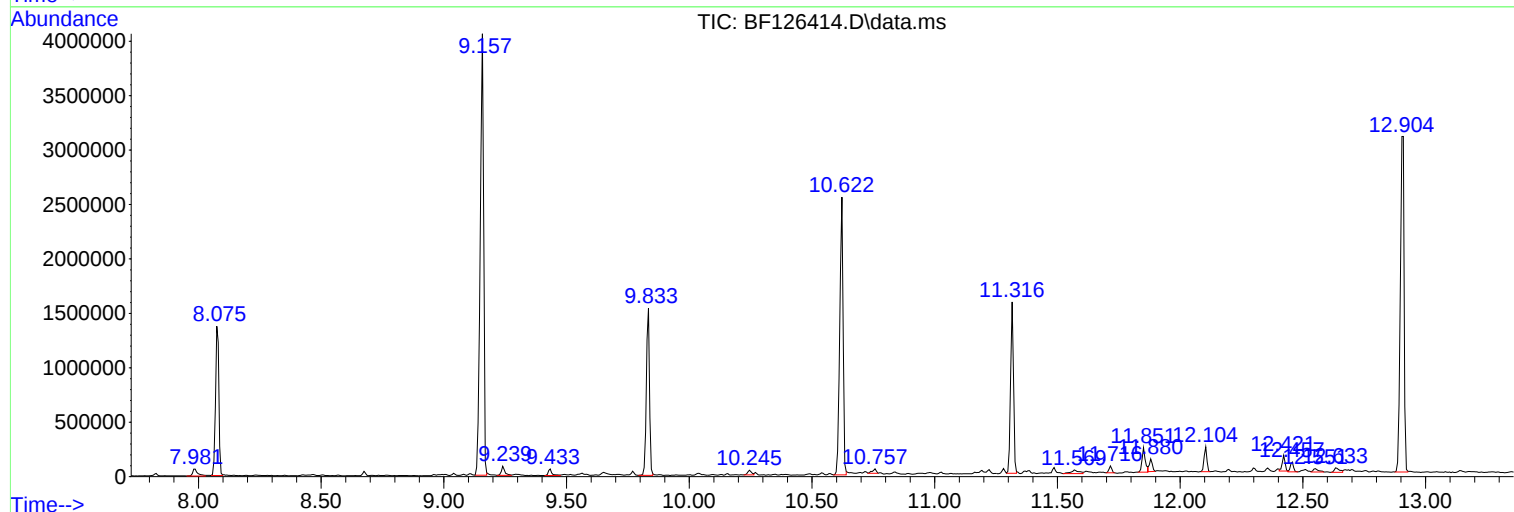
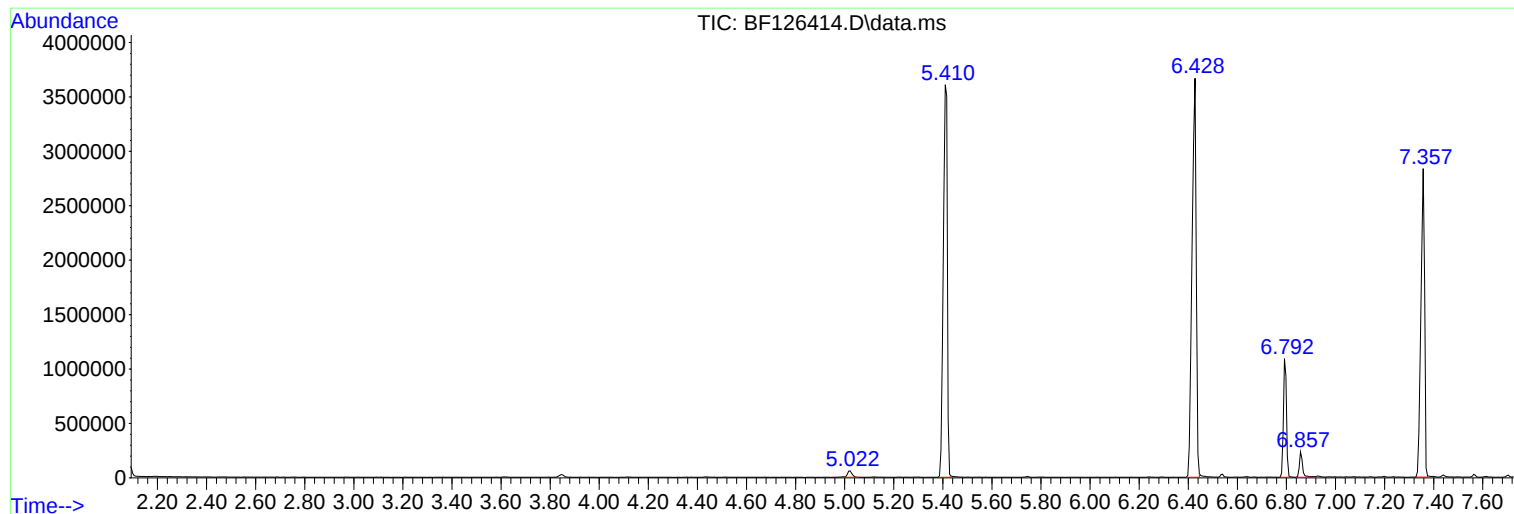
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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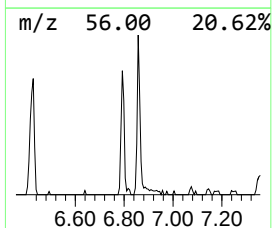
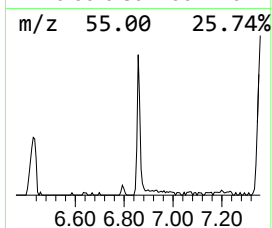
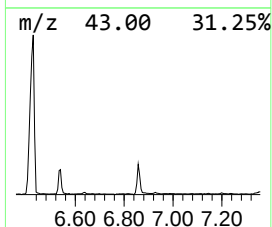
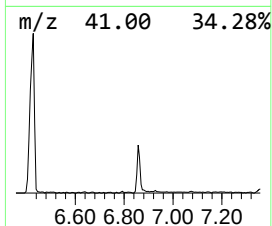
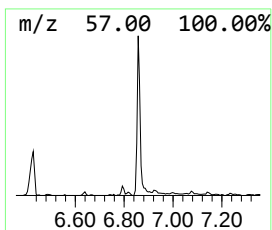
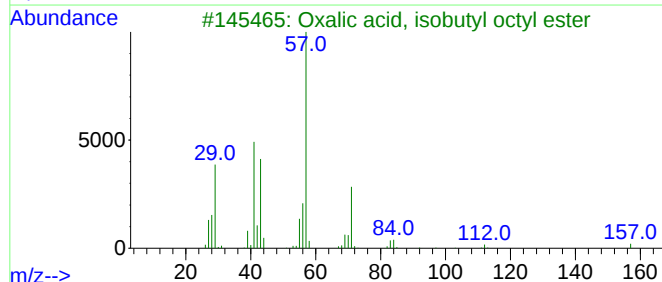
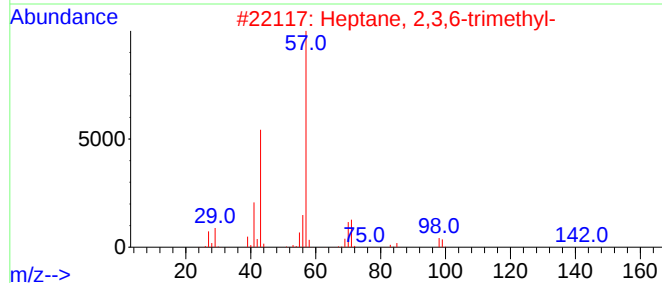
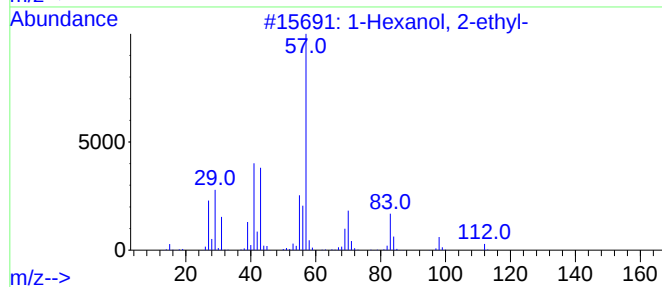
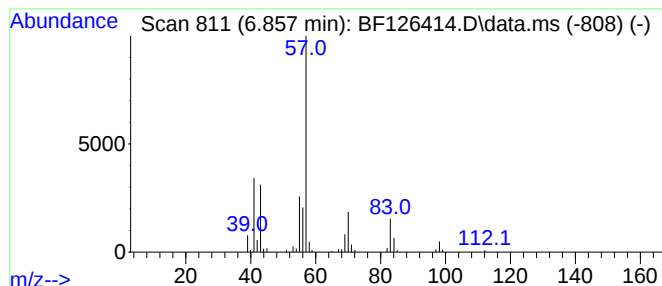
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.857	4.43 ng	207542	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	53
3			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
4			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	42
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	42



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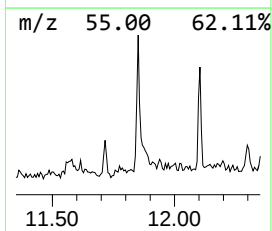
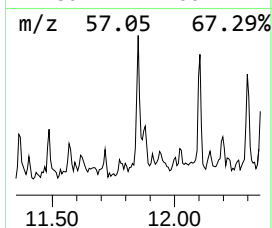
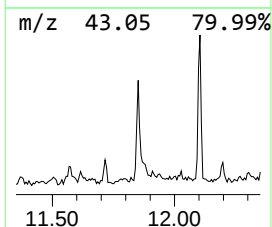
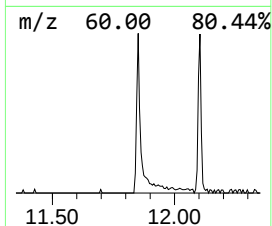
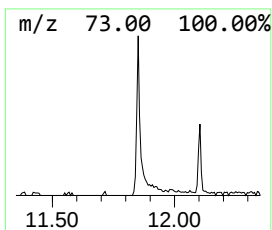
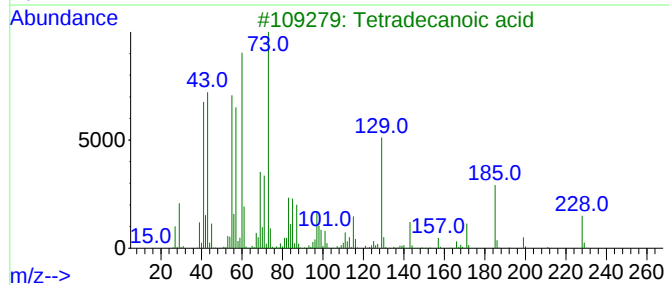
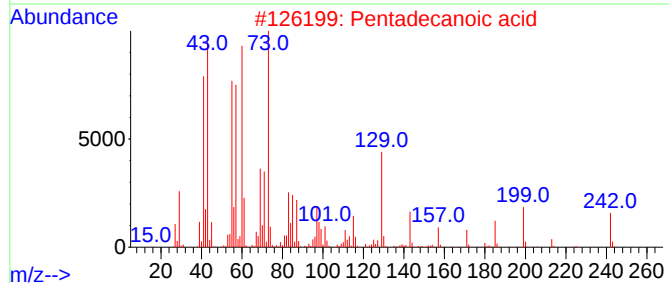
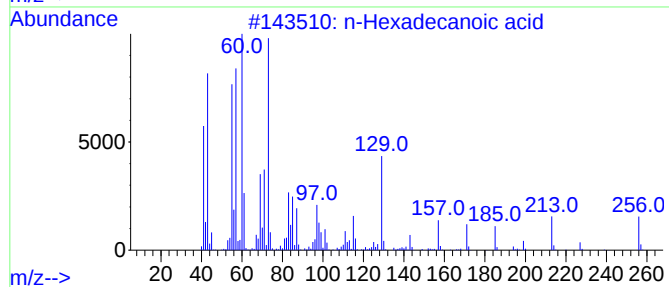
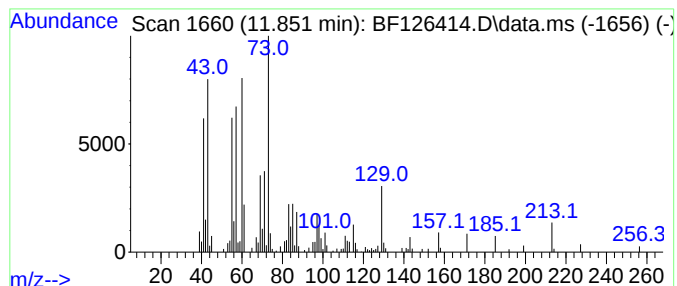
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	3.20 ng	210383	Phenanthrene-d10	11.316

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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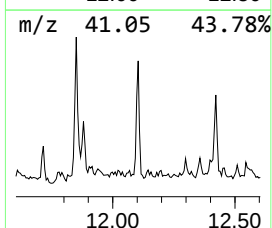
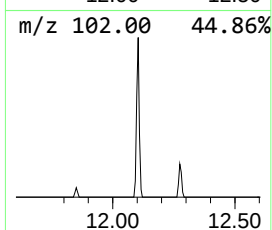
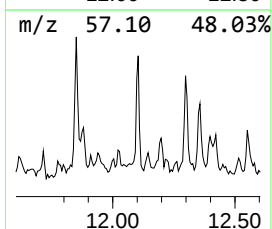
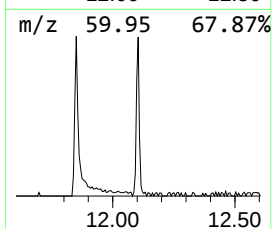
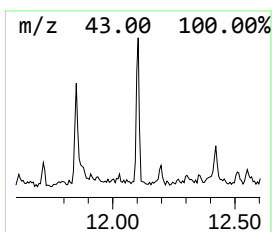
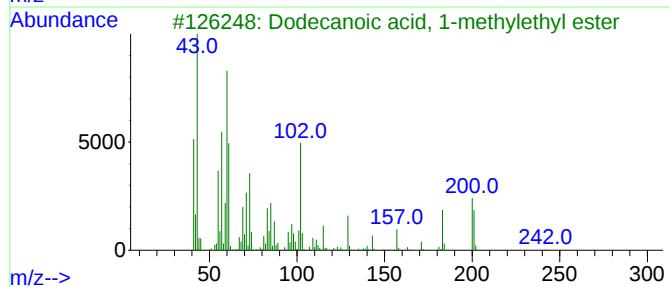
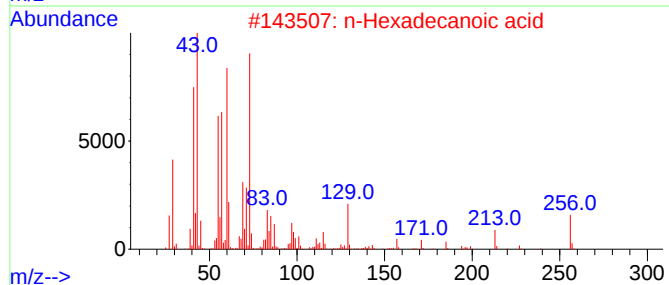
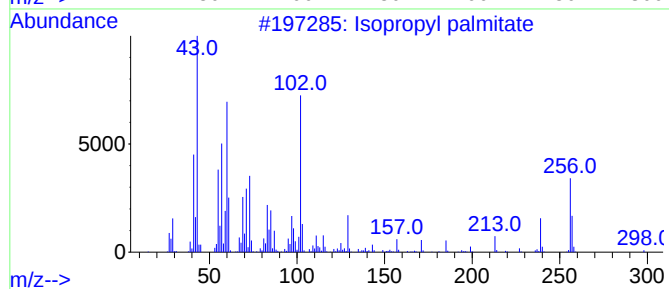
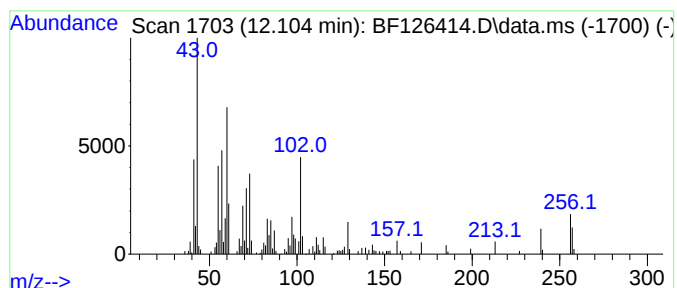
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl palmitate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	2.65 ng	173918	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	50
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	50
5			.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	35



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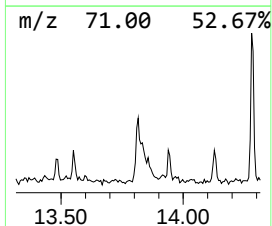
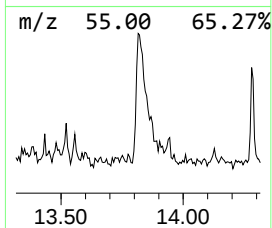
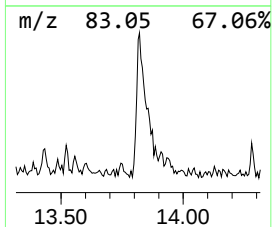
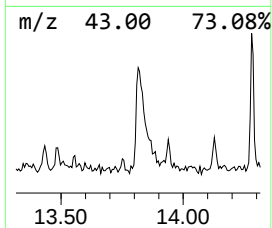
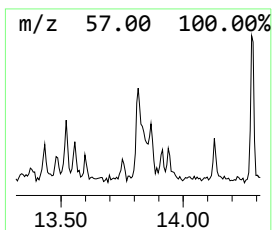
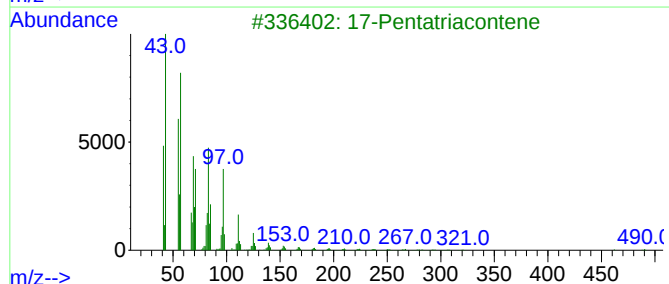
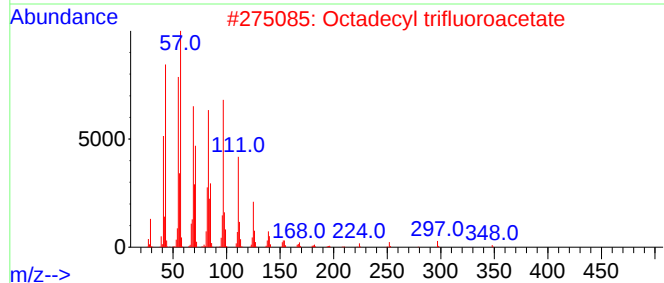
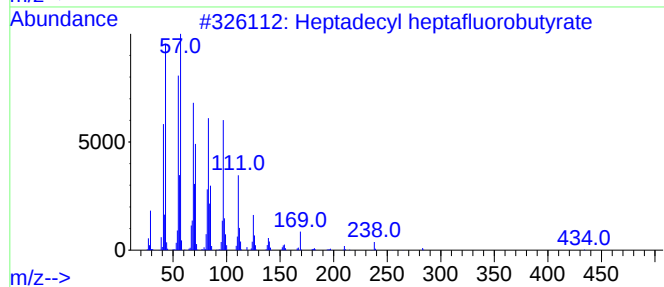
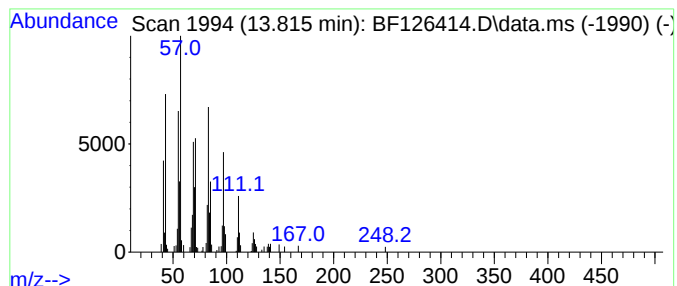
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	6.36 ng	279312	Chrysene-d12	13.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	91
4			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



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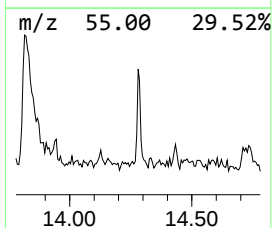
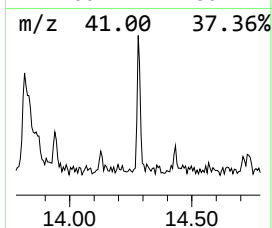
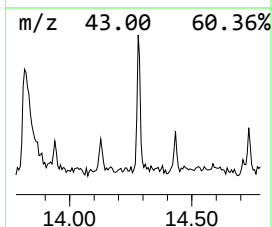
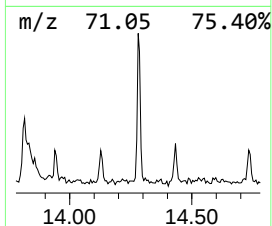
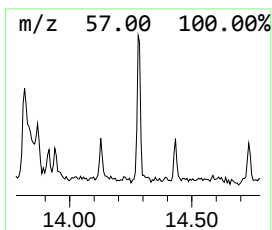
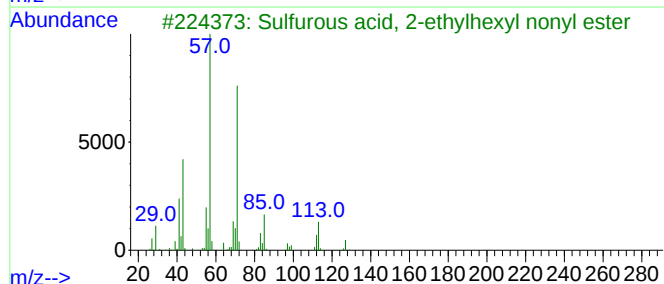
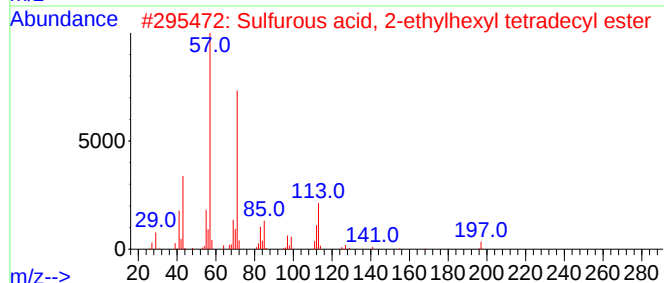
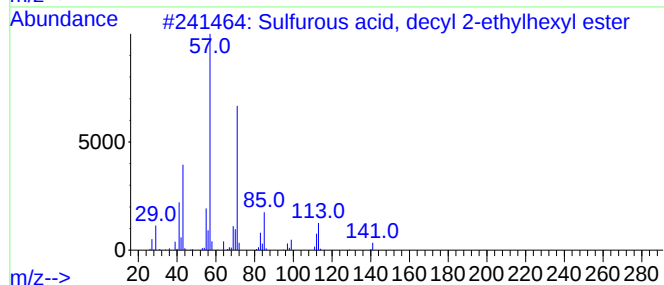
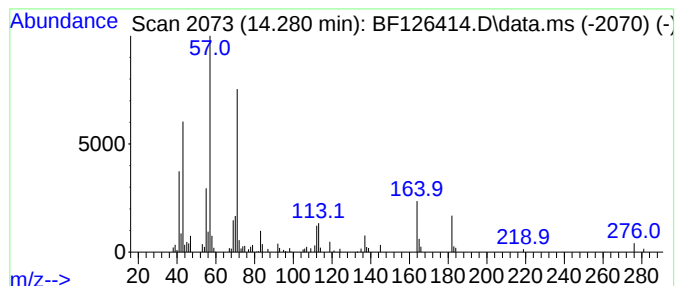
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Peak Number 5 Sulfurous acid, decyl 2-eth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.280	2.62 ng	114951	Chrysene-d12	13.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	58
2			Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	58
3			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	58
4			Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	58
5			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	58



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	6.857	4.4	ng	207542	1	6.792	937243	20.0
n-Hexadecanoic ...	11.851	3.2	ng	210383	4	11.316	1313230	20.0
Isopropyl palmi...	12.104	2.6	ng	173918	4	11.316	1313230	20.0
Heptadecyl hept...	13.815	6.4	ng	279312	5	13.951	878182	20.0
Sulfurous acid,...	14.280	2.6	ng	114951	5	13.951	878182	20.0