

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
 Data File : BF117596.D
 Acq On : 29 Oct 2019 17:38
 Operator : JU
 Sample : K5540-15
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 158-88-(0-1)

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-BF101819.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	5.357	552	556	582	rBV	554051	757369	89.37%	11.146%
2	6.386	727	731	744	rBV	647251	812636	95.89%	11.959%
3	6.504	748	751	759	rVB	896677	847468	100.00%	12.472%
4	6.728	786	789	799	rBV	235066	210726	24.87%	3.101%
5	6.881	812	815	832	rBV	626876	589823	69.60%	8.680%
6	7.292	882	885	916	rBV	396864	503373	59.40%	7.408%
7	8.010	1004	1007	1026	rBV	200768	244060	28.80%	3.592%
8	9.080	1185	1189	1202	rBV	661688	605735	71.48%	8.914%
9	9.480	1254	1257	1270	rBB	64579	67662	7.98%	0.996%
10	9.757	1301	1304	1318	rBB	211547	227849	26.89%	3.353%
11	10.557	1436	1440	1455	rBV	283806	325062	38.36%	4.784%
12	11.251	1554	1558	1569	rBV	170238	204718	24.16%	3.013%
13	11.774	1645	1647	1654	rVB2	30217	32561	3.84%	0.479%
14	12.463	1761	1764	1770	rBV	57207	61387	7.24%	0.903%
15	12.692	1798	1803	1808	rBV	56154	67495	7.96%	0.993%
16	12.827	1822	1826	1833	rBV	485840	411653	48.57%	6.058%
17	13.739	1976	1981	1989	rBV5	43676	90973	10.73%	1.339%
18	13.857	1997	2001	2003	rBV	24059	22823	2.69%	0.336%
19	13.892	2003	2007	2011	rBV2	211824	237339	28.01%	3.493%
20	14.345	2081	2084	2087	rBV3	11908	11944	1.41%	0.176%
21	14.509	2108	2112	2115	rVB	77624	74443	8.78%	1.096%
22	14.645	2133	2135	2139	rVB5	17501	16377	1.93%	0.241%
23	14.927	2180	2183	2185	rBV	28100	33737	3.98%	0.496%
24	14.956	2186	2188	2196	rVB4	37556	43516	5.13%	0.640%
25	15.027	2198	2200	2205	rVB6	9722	13448	1.59%	0.198%
26	15.215	2230	2232	2235	rVB	13263	11296	1.33%	0.166%
27	15.280	2240	2243	2246	rVV	19441	26224	3.09%	0.386%
28	15.333	2247	2252	2264	rVB	118037	192533	22.72%	2.833%
29	15.715	2315	2317	2323	rVB4	20686	23516	2.77%	0.346%
30	16.356	2421	2426	2430	rBV8	10777	14513	1.71%	0.214%
31	16.798	2499	2501	2506	rVB6	9647	12968	1.53%	0.191%

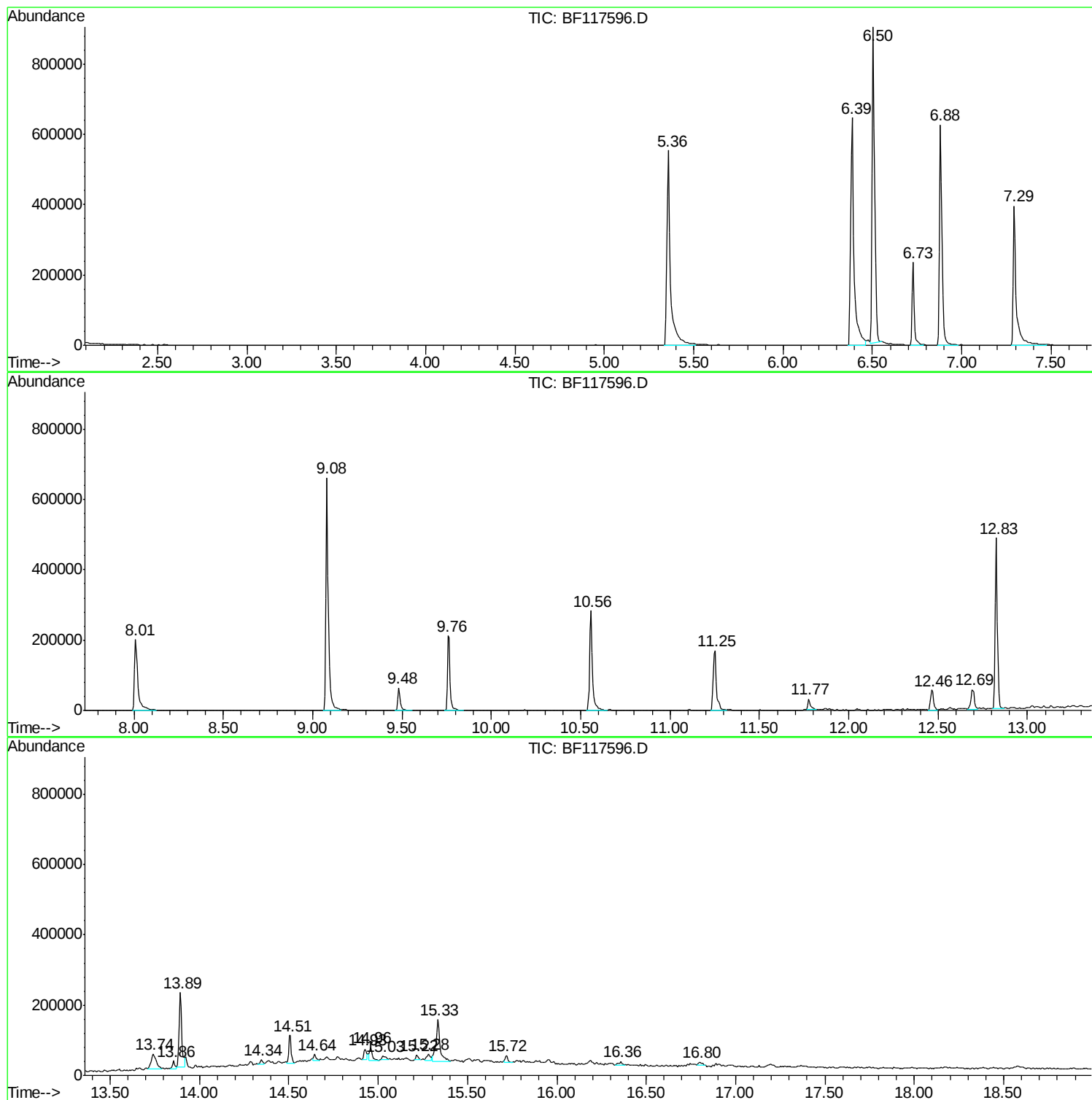
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ClientSampled :
158-88-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.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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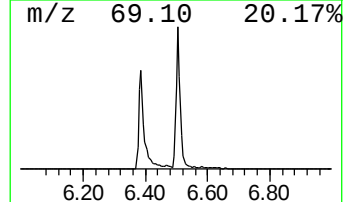
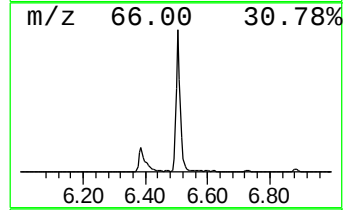
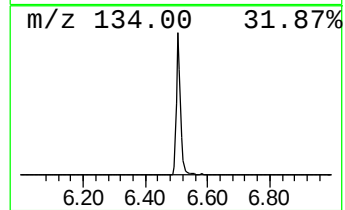
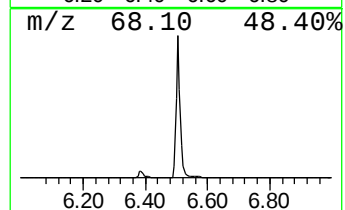
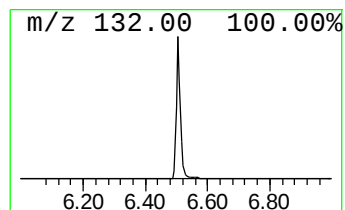
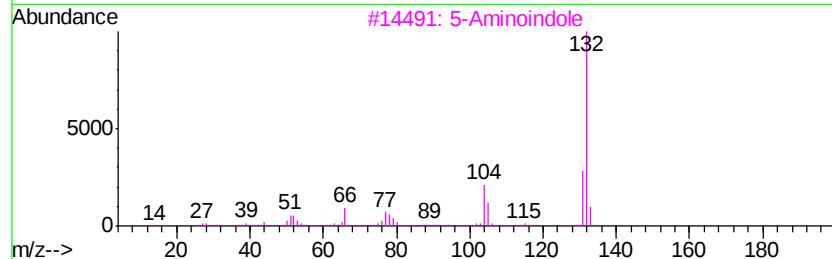
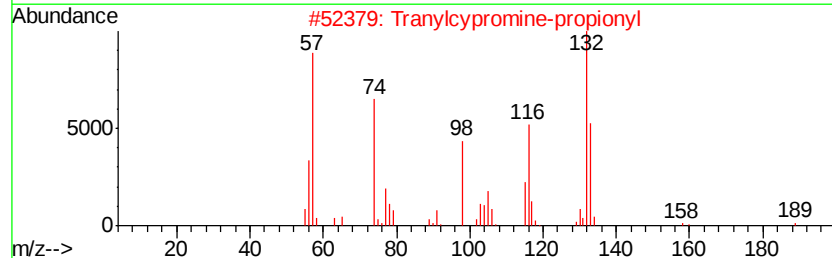
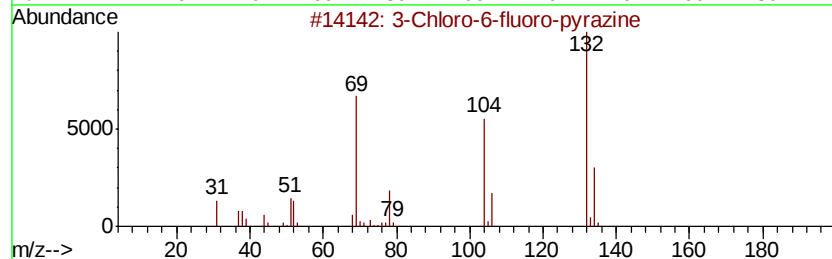
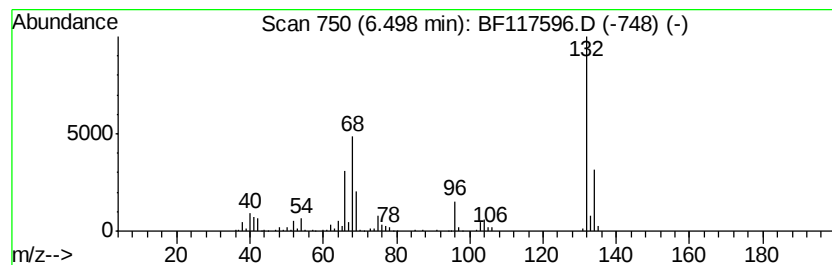
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	80.43 ng	847468	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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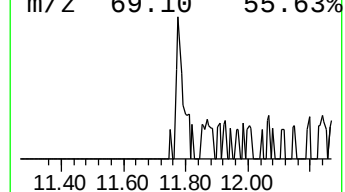
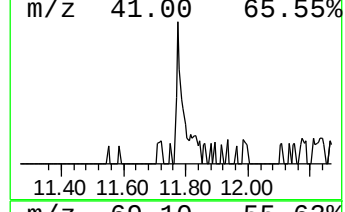
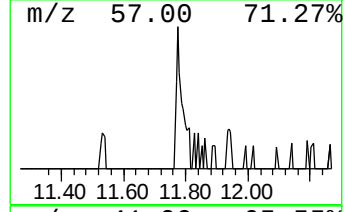
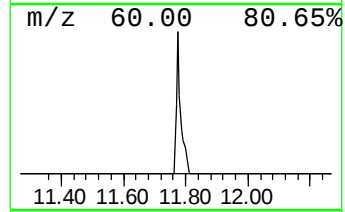
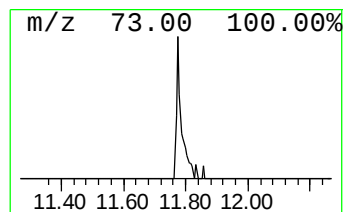
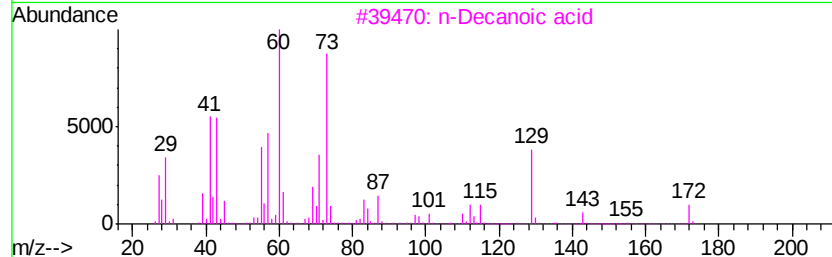
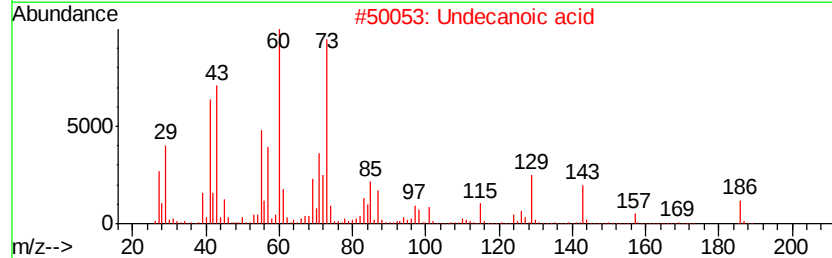
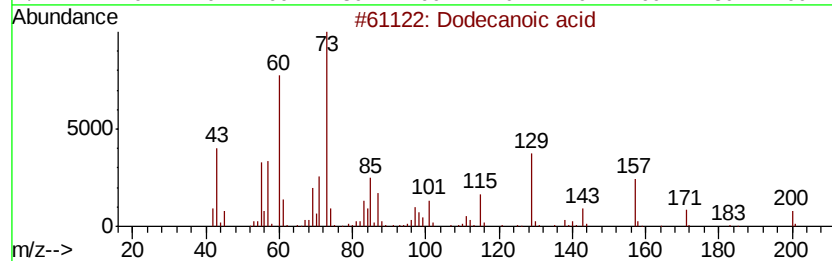
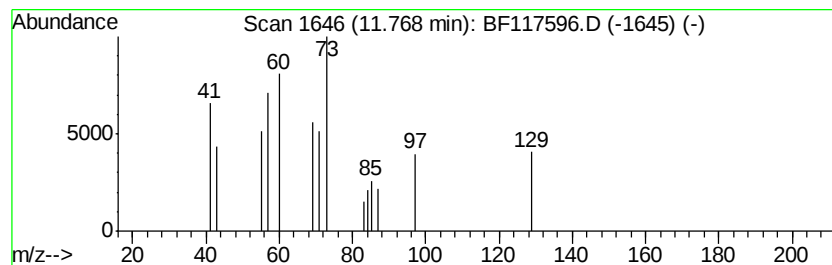
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Peak Number 3 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.77	3.18 ng	32561	Phenanthrene-d10		11.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	50
2			Undecanoic acid	186	C11H22O2	000112-37-8	47
3			n-Decanoic acid	172	C10H20O2	000334-48-5	47
4			Lactose	342	C12H22O11	000063-42-3	47
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	38



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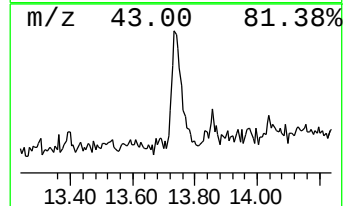
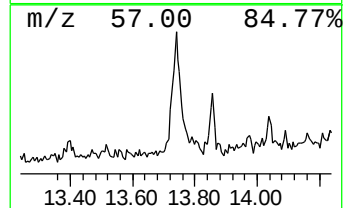
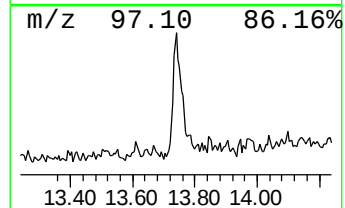
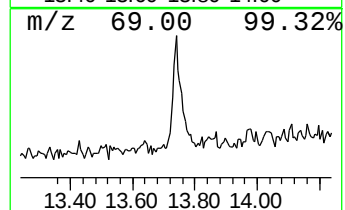
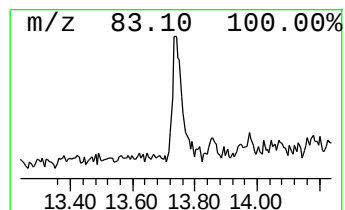
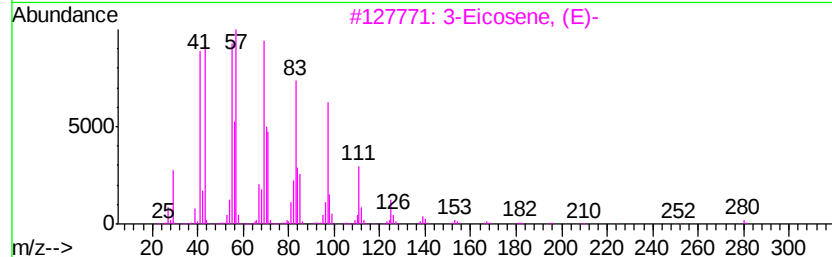
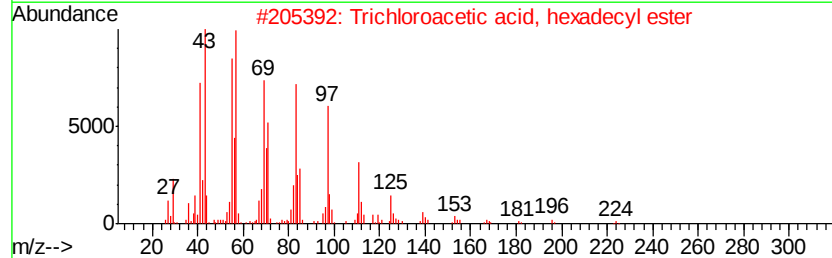
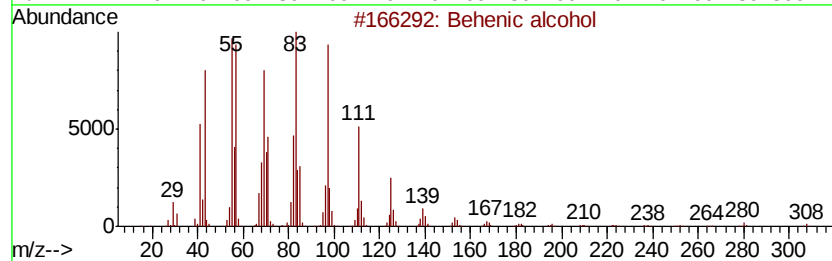
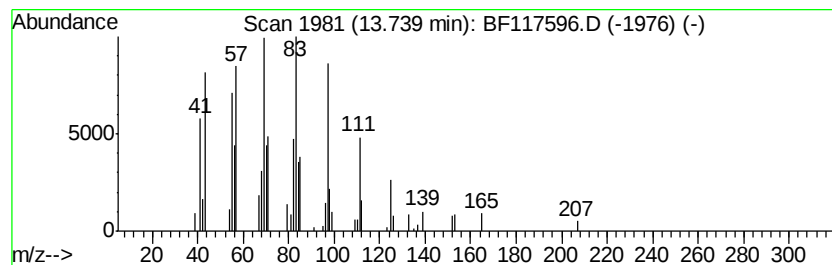
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Peak Number 4 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	7.67 ng	90973	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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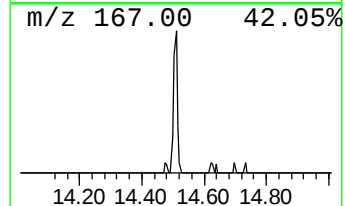
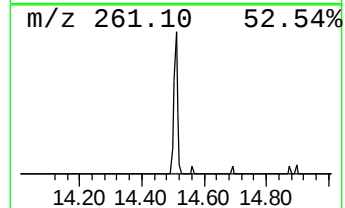
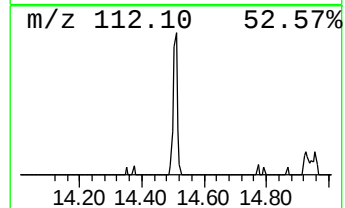
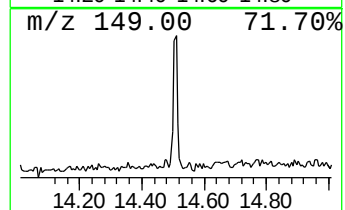
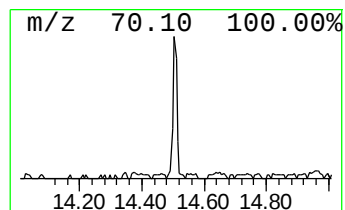
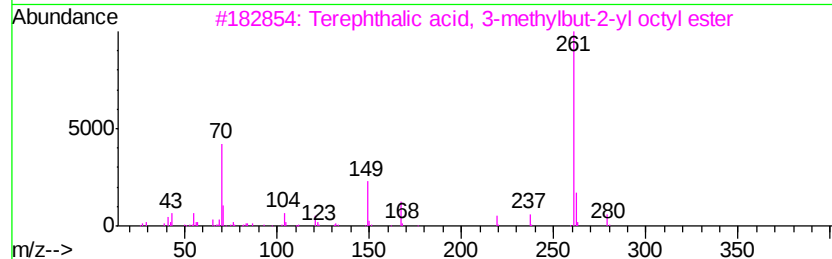
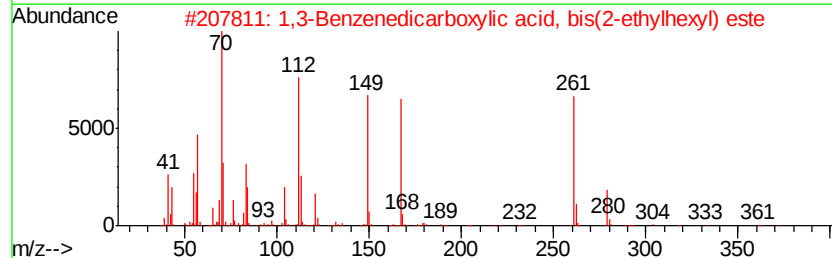
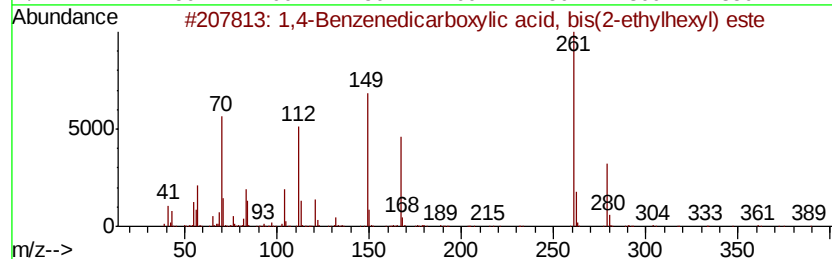
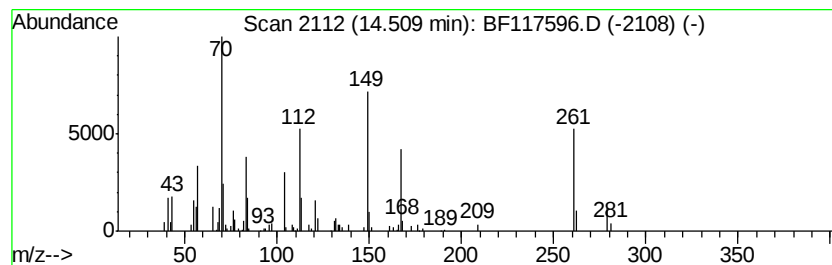
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Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	6.27 ng	74443	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	74
3		Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
4		Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	43
5		Terephthalic acid, 1-cyclopentyl...	374	C23H34O4	1000323-84-1	38



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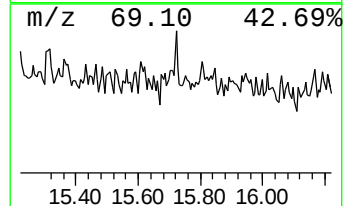
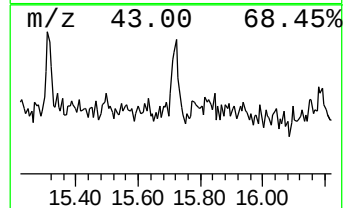
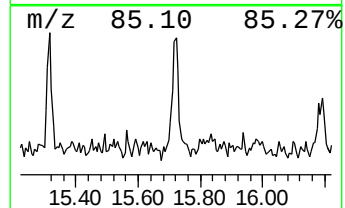
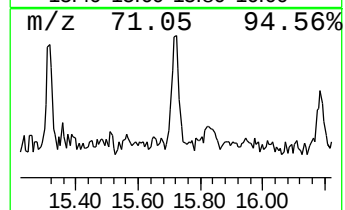
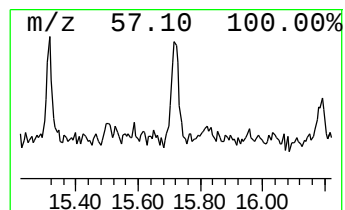
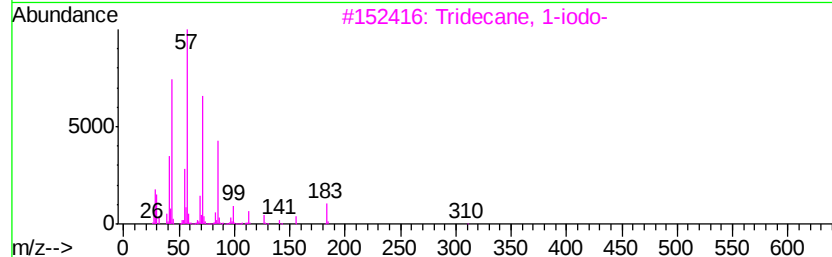
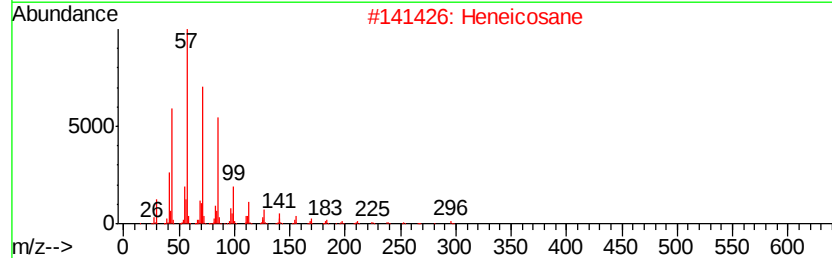
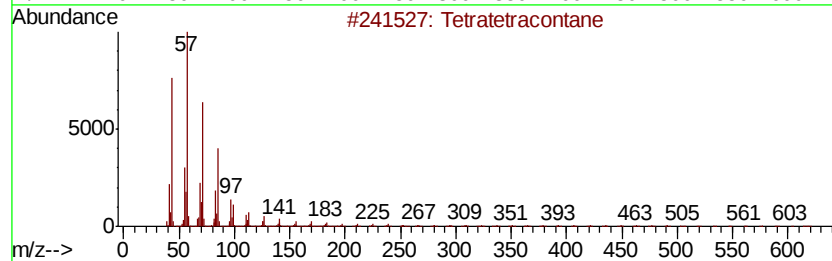
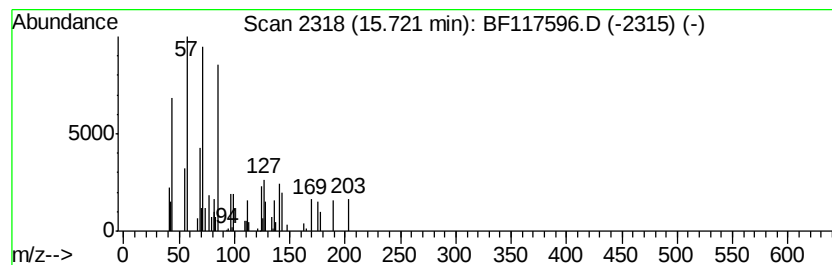
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.44 ng	23516	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	53
2		Heneicosane	296	C21H44	000629-94-7	50
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	50
4		4,4-Dipropylheptane	184	C13H28	017312-72-0	50
5		Decane, 3-bromo-	220	C10H21Br	030571-71-2	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	80.4	ng	847468	1	6.73	210726	20.0
Dodecanoic acid	11.77	3.2	ng	32561	4	11.25	204718	20.0
Behenic alcohol	13.74	7.7	ng	90973	5	13.89	237339	20.0
1,4-Benzenedicarb...	14.51	6.3	ng	74443	5	13.89	237339	20.0
Tetratetracontane	15.72	2.4	ng	23516	6	15.33	192533	20.0