

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031219\
 Data File : BF113017.D
 Acq On : 12 Mar 2019 21:58
 Operator : JU/SJ
 Sample : K1847-16
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-7B-C-3-031119

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-BF022719.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	5.346	549	554	569	rBV	2697479	2819925	88.73%	8.922%
2	6.369	723	728	731	rBV	3252378	2955715	93.00%	9.352%
3	6.498	746	750	754	rBV	3191902	3050287	95.97%	9.651%
4	6.728	786	789	793	rBV	1103823	1008521	31.73%	3.191%
5	6.887	812	816	820	rBV	2747006	2321327	73.04%	7.345%
6	7.287	880	884	898	rBV	1774021	1943529	61.15%	6.149%
7	8.010	1004	1007	1032	rBV	1139476	1273693	40.08%	4.030%
8	9.086	1186	1190	1205	rBV	3210430	3178261	100.00%	10.056%
9	9.481	1253	1257	1269	rBV	215479	217812	6.85%	0.689%
10	9.763	1301	1305	1319	rBV	1417615	1359948	42.79%	4.303%
11	10.545	1434	1438	1453	rBV	2078076	2153216	67.75%	6.813%
12	11.239	1552	1556	1567	rBV	1315476	1401408	44.09%	4.434%
13	11.775	1644	1647	1657	rBV	330988	385276	12.12%	1.219%
14	11.851	1657	1660	1663	rBV	32626	35186	1.11%	0.111%
15	12.445	1757	1761	1768	rBV	310261	289413	9.11%	0.916%
16	12.563	1778	1781	1794	rBV4	52706	96006	3.02%	0.304%
17	12.669	1794	1799	1803	rBV	262757	294005	9.25%	0.930%
18	12.822	1820	1825	1833	rVB	2628109	2638080	83.00%	8.347%
19	12.998	1853	1855	1859	rVB	42105	40130	1.26%	0.127%
20	13.063	1864	1866	1870	rVV2	40852	41256	1.30%	0.131%
21	13.104	1870	1873	1878	rVV	31932	33277	1.05%	0.105%
22	13.404	1918	1924	1926	rBV2	34415	39416	1.24%	0.125%
23	13.616	1956	1960	1962	rBV3	24025	32858	1.03%	0.104%
24	13.721	1974	1978	1992	rVB2	347310	480602	15.12%	1.521%
25	13.863	1997	2002	2005	rBV	1343271	1460913	45.97%	4.622%
26	13.969	2017	2020	2025	rVB2	31686	39572	1.25%	0.125%
27	14.045	2030	2033	2038	rVB2	52504	52534	1.65%	0.166%
28	14.345	2081	2084	2087	rBV3	70132	83074	2.61%	0.263%
29	14.645	2131	2135	2140	rBV	66440	101363	3.19%	0.321%
30	14.710	2144	2146	2154	rVB3	43667	58823	1.85%	0.186%
31	14.874	2170	2174	2177	rBV	124360	184757	5.81%	0.585%
32	14.957	2185	2188	2194	rBV3	61479	95809	3.01%	0.303%
33	15.151	2218	2221	2227	rVB	75766	97189	3.06%	0.308%
34	15.210	2227	2231	2236	rBV	86087	125241	3.94%	0.396%

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Integrator: RTE
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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 >
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35	15.268	2237	2241	2246	rBV	794047	1022678	32.18%	3.236%
36	15.721	2314	2318	2322	rVB	43827	57782	1.82%	0.183%
37	15.774	2323	2327	2340	rVB	46337	136405	4.29%	0.432%

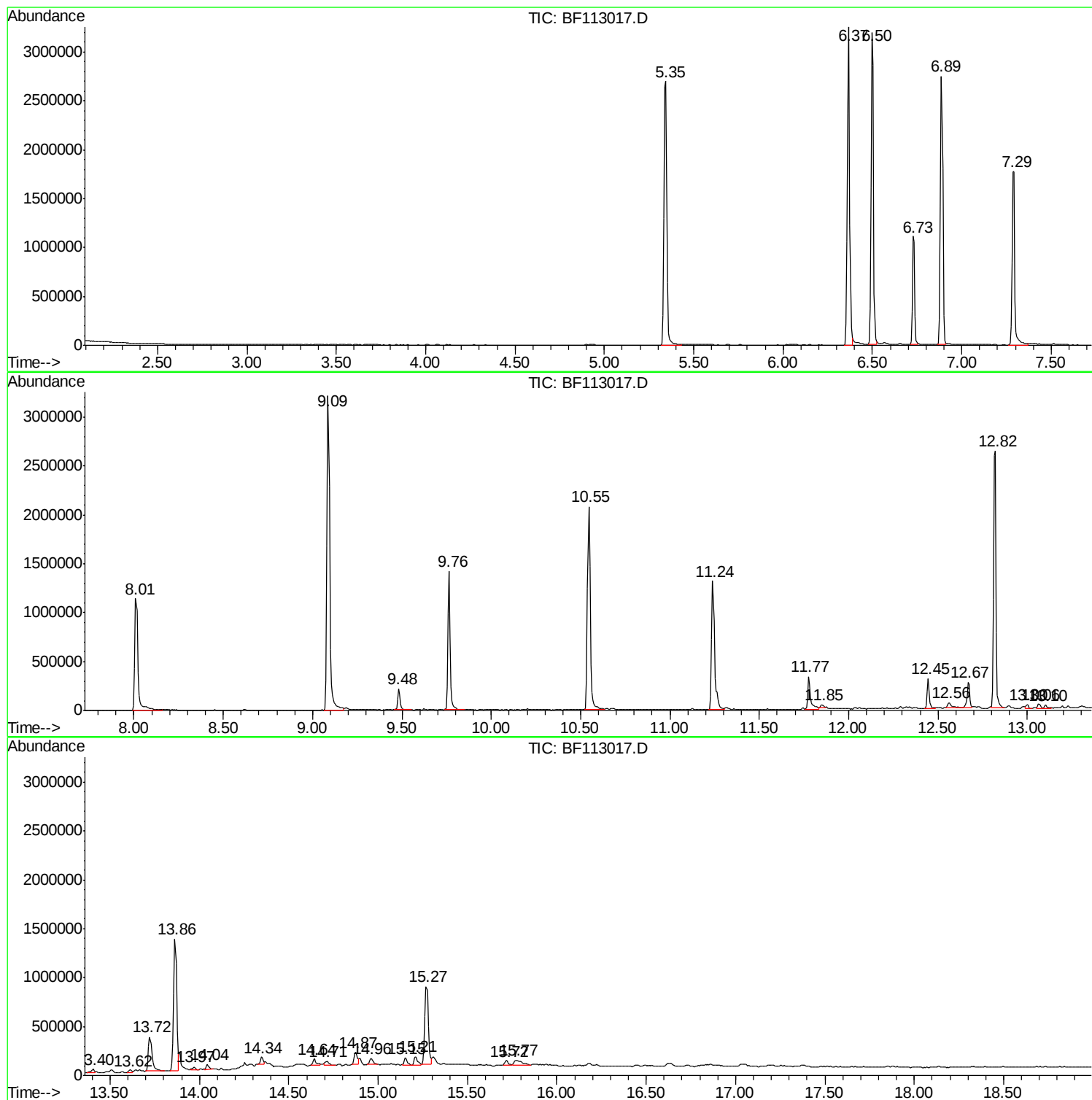
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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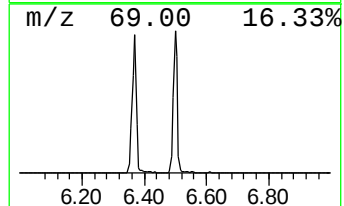
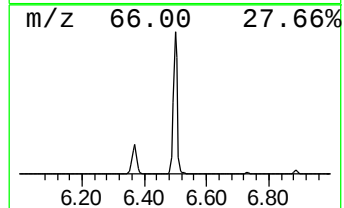
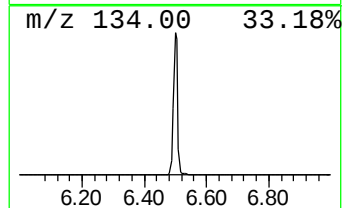
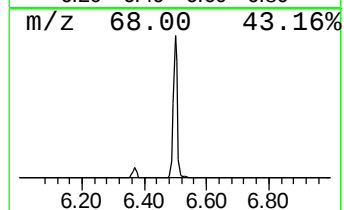
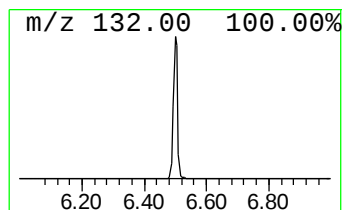
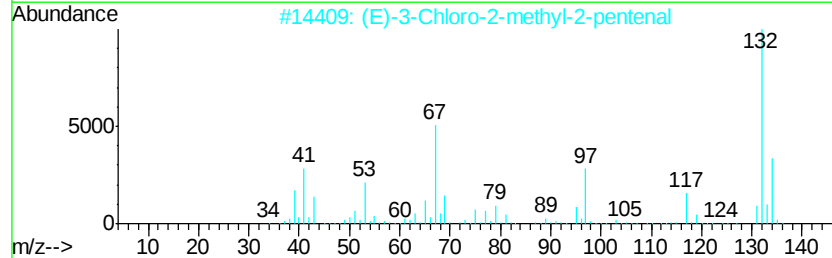
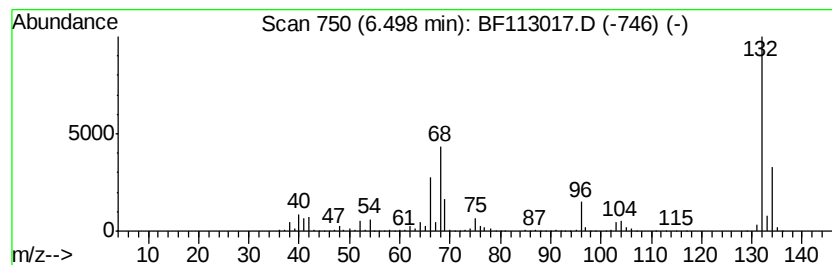
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	60.49 ng	3050290	1,4-Dichlorobenzene-d4	6.73

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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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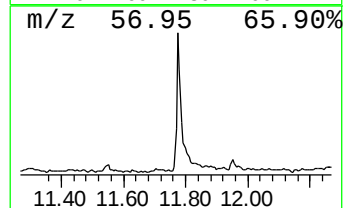
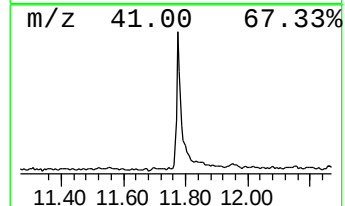
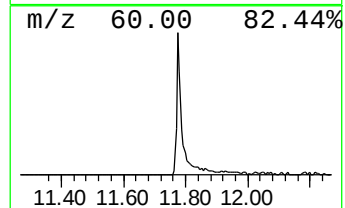
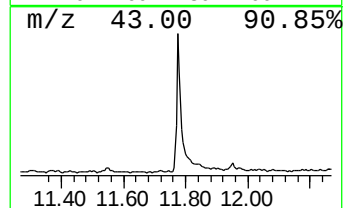
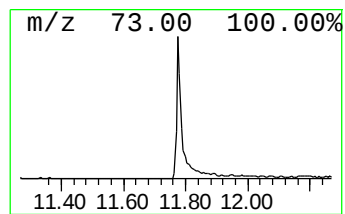
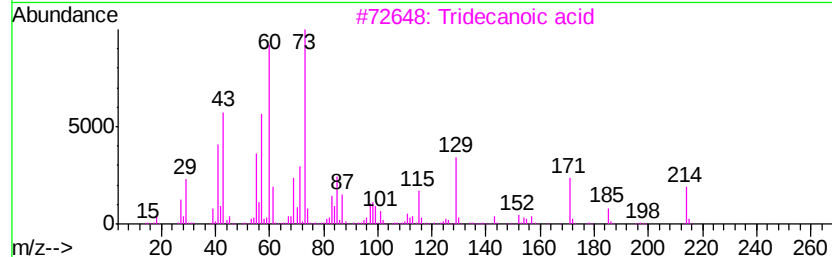
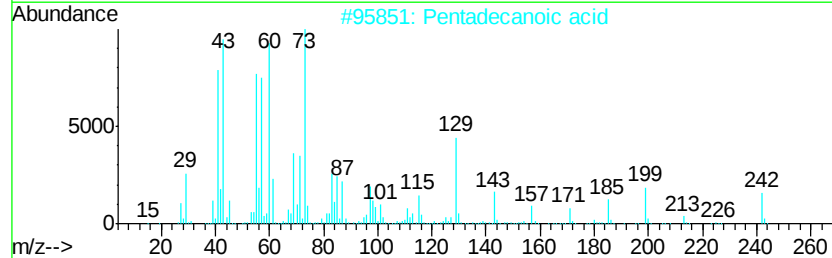
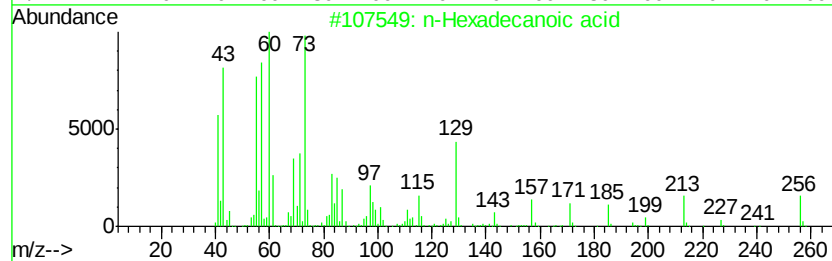
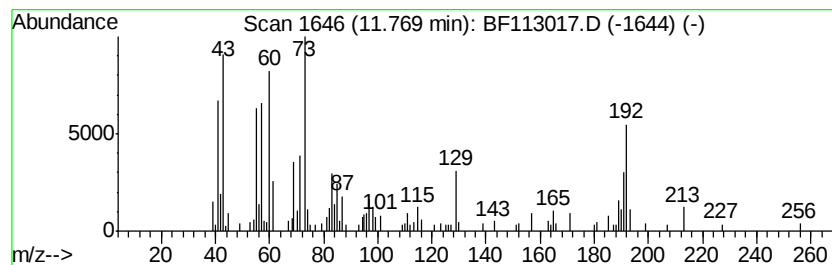
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	5.50 ng	385276	Phenanthrene-d10	11.24	
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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25



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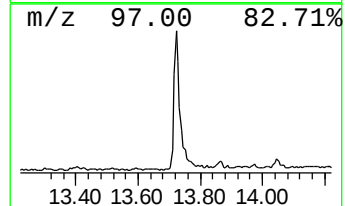
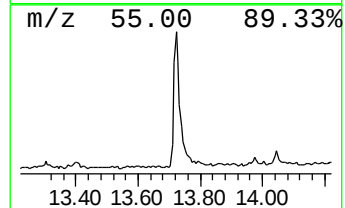
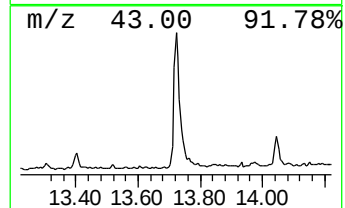
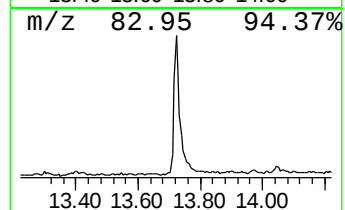
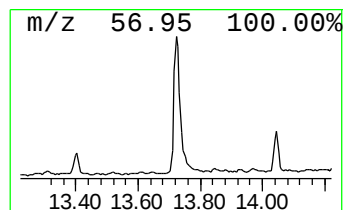
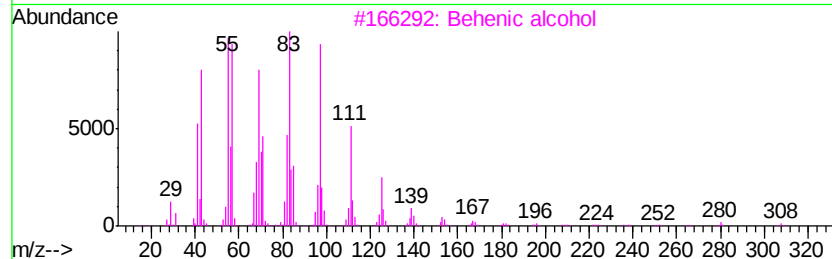
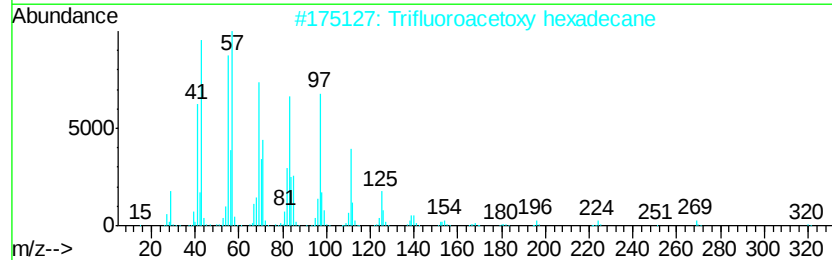
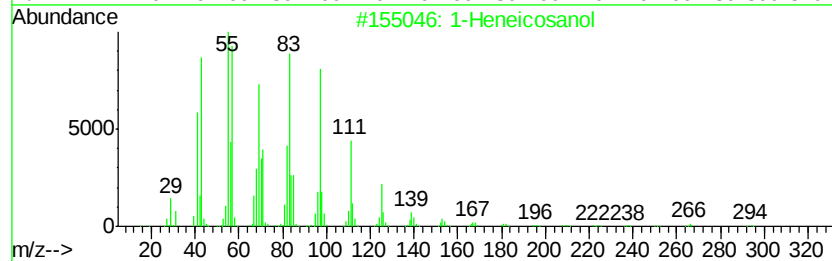
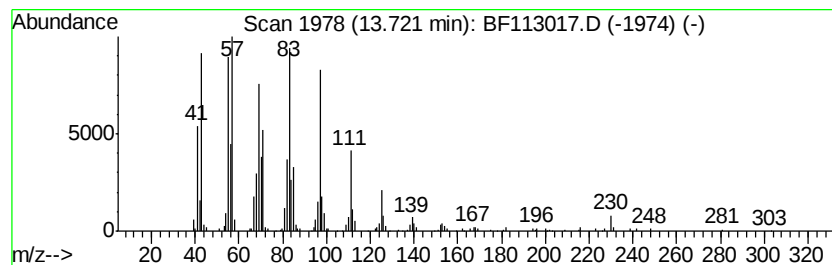
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	6.58 ng	480602	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93



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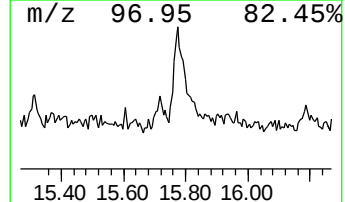
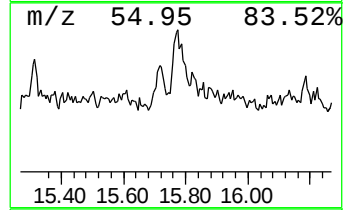
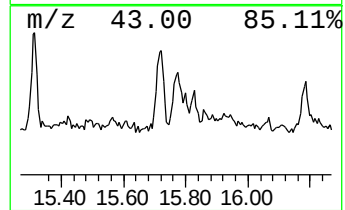
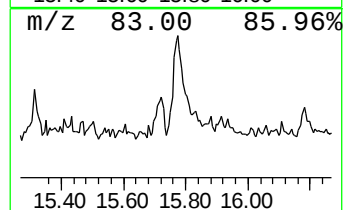
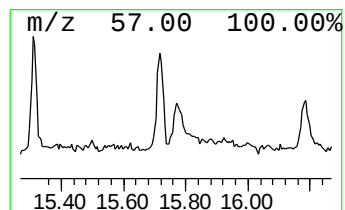
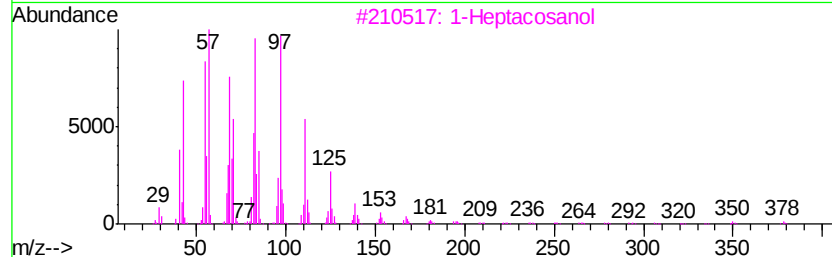
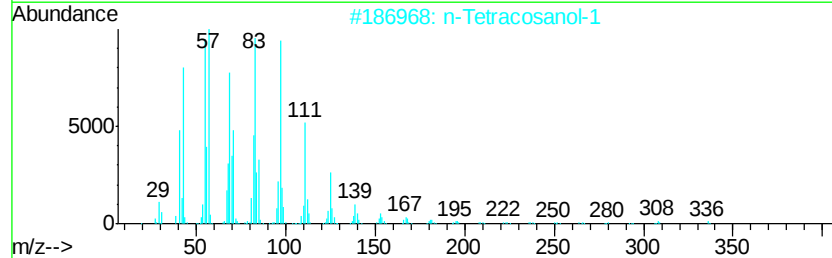
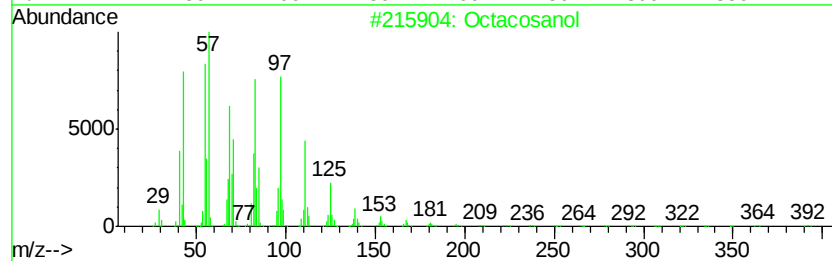
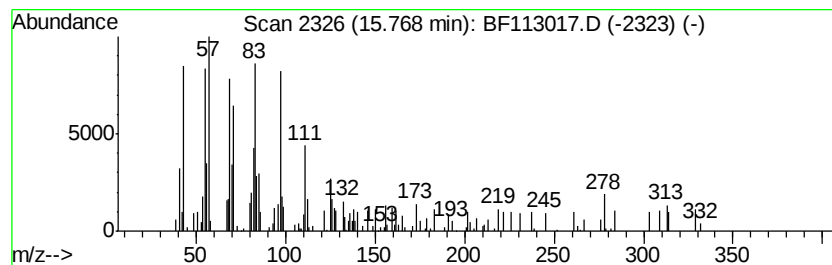
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.77	2.67 ng	136405	Perylene-d12	15.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	1-Heptacosanol	396	C27H56O	002004-39-9	87
4	Behenic alcohol	326	C22H46O	000661-19-8	83
5	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	60.5	ng	3050290	1	6.73	1008520	20.0
n-Hexadecanoic acid	11.77	5.5	ng	385276	4	11.24	1401410	20.0
1-Heneicosanol	13.72	6.6	ng	480602	5	13.86	1460910	20.0
Octacosanol	15.77	2.7	ng	136405	6	15.27	1022680	20.0