

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101219\
 Data File : BF117388.D
 Acq On : 13 Oct 2019 00:10
 Operator : JU
 Sample : K5316-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-11

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-BF091319.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	5.416	562	566	586	rBV	622302	746431	75.10%	8.570%
2	6.439	736	740	758	rBV	717733	856432	86.17%	9.833%
3	6.569	758	762	774	rVB	954048	871886	87.73%	10.011%
4	6.792	797	800	813	rVB	238636	224687	22.61%	2.580%
5	6.951	823	827	843	rBV	669645	644406	64.84%	7.399%
6	7.357	893	896	913	rBV	407050	504751	50.79%	5.795%
7	8.075	1015	1018	1039	rBV	201064	298880	30.07%	3.432%
8	9.151	1197	1201	1224	rBV	989166	993026	99.92%	11.402%
9	9.545	1265	1268	1282	rBV	77924	90849	9.14%	1.043%
10	9.827	1313	1316	1327	rBV	349368	367344	36.96%	4.218%
11	10.622	1447	1451	1467	rBV	505159	563132	56.66%	6.466%
12	11.322	1566	1570	1579	rBV	321954	369385	37.17%	4.241%
13	11.386	1579	1581	1590	rVB3	11561	12493	1.26%	0.143%
14	11.839	1654	1658	1668	rBV3	14605	23744	2.39%	0.273%
15	12.539	1774	1777	1784	rBV	18279	19640	1.98%	0.225%
16	12.763	1809	1815	1821	rBV	21409	29315	2.95%	0.337%
17	12.898	1834	1838	1842	rBV	1090718	993867	100.00%	11.411%
18	13.792	1986	1990	2006	rBV2	104170	220924	22.23%	2.537%
19	13.963	2015	2019	2027	rBV	305305	317633	31.96%	3.647%
20	14.110	2039	2044	2047	rBV2	10786	13276	1.34%	0.152%
21	14.410	2092	2095	2098	rBV2	14155	15478	1.56%	0.178%
22	14.710	2143	2146	2149	rBV2	25678	24828	2.50%	0.285%
23	15.039	2198	2202	2206	rVB2	26871	32906	3.31%	0.378%
24	15.115	2210	2215	2219	rBV7	6093	11400	1.15%	0.131%
25	15.357	2253	2256	2260	rBV5	7515	11242	1.13%	0.129%
26	15.415	2260	2266	2275	rBV	208292	319952	32.19%	3.674%
27	15.821	2331	2335	2340	rVB2	23294	32066	3.23%	0.368%
28	15.909	2343	2350	2353	rBV8	16205	38465	3.87%	0.442%
29	16.309	2412	2418	2422	rBV4	12376	20123	2.02%	0.231%
30	16.874	2509	2514	2516	rBV5	9618	16008	1.61%	0.184%
31	17.539	2616	2627	2629	rBV8	8522	25024	2.52%	0.287%

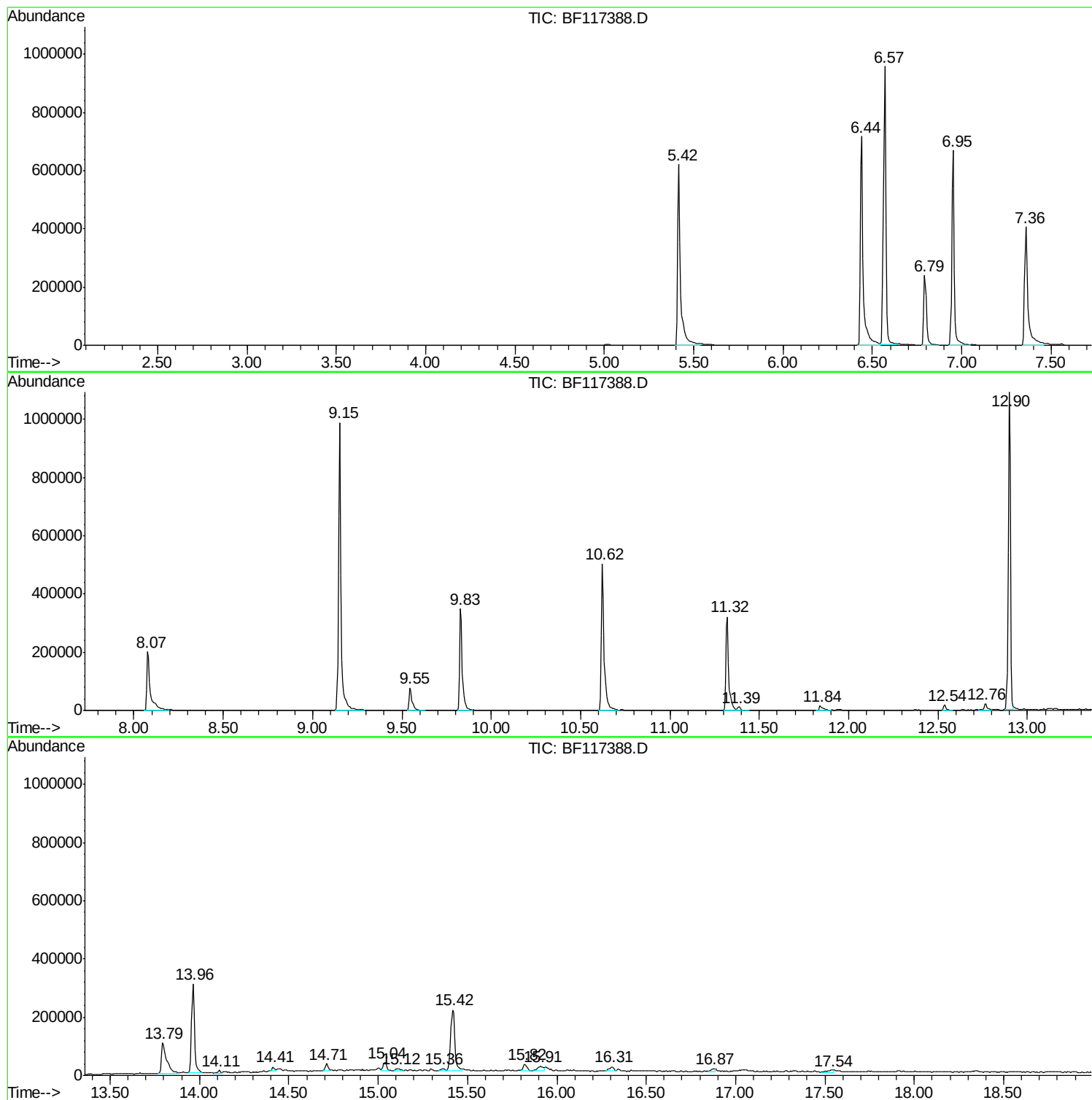
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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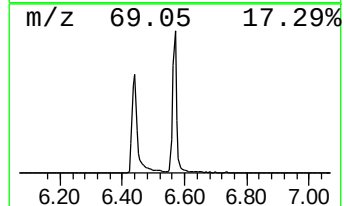
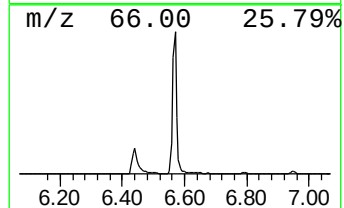
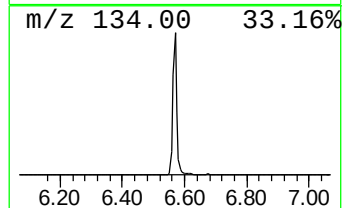
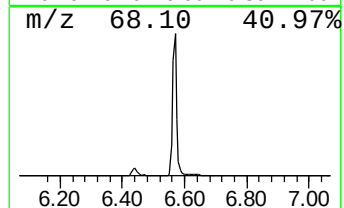
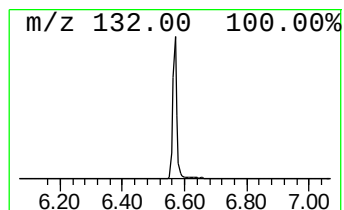
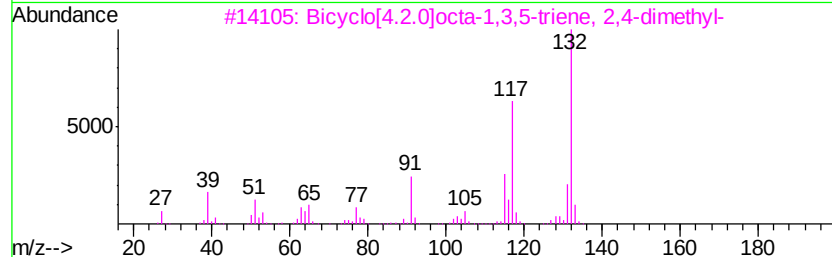
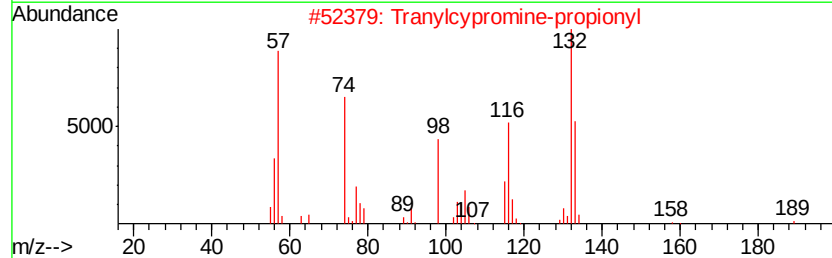
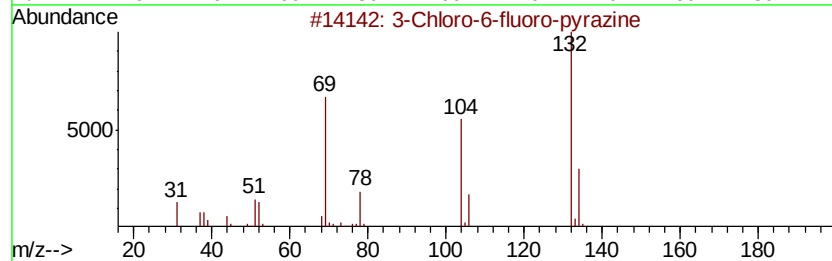
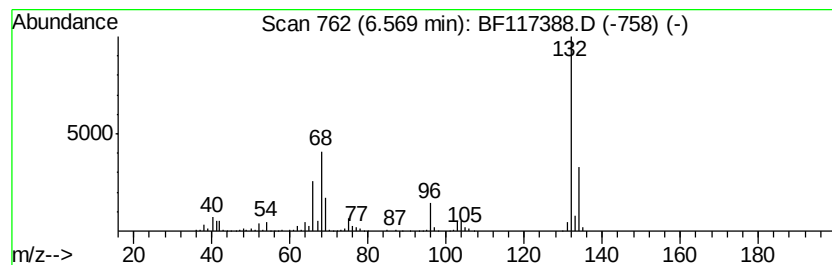
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	77.61 ng	871886	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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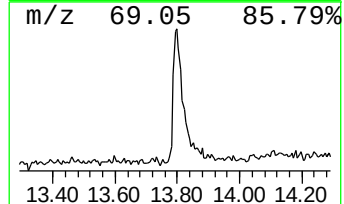
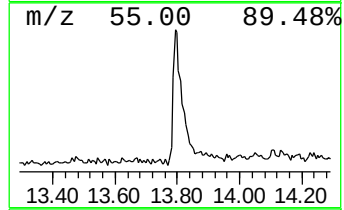
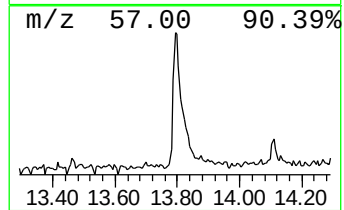
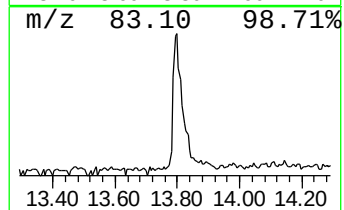
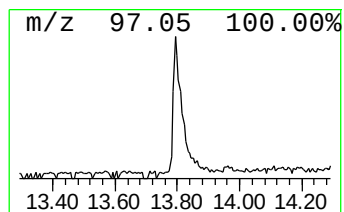
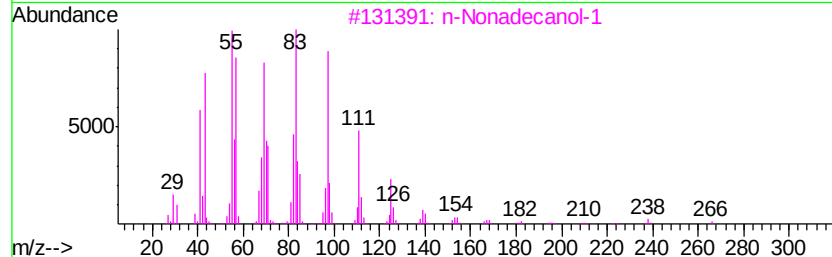
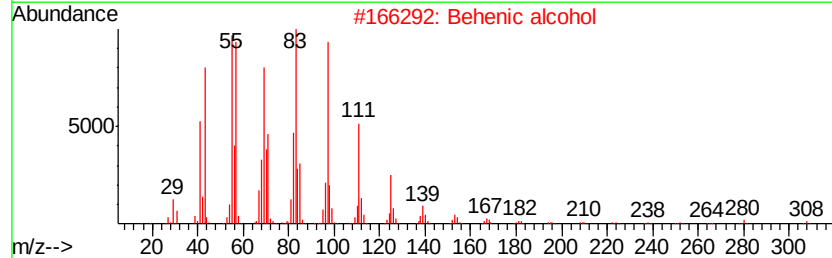
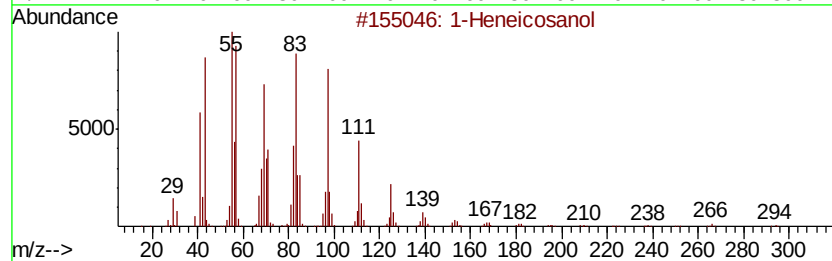
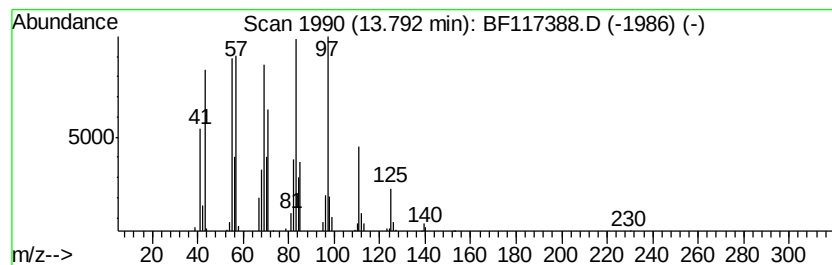
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Peak Number 3 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	13.91 ng	220924	Chrysene-d12	13.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	Behenic alcohol	326 C22H46O	000661-19-8	94
3	n-Nonadecanol-1	284 C19H40O	001454-84-8	94
4	1-Heptacosanol	396 C27H56O	002004-39-9	91
5	n-Tetracosanol-1	354 C24H50O	000506-51-4	91



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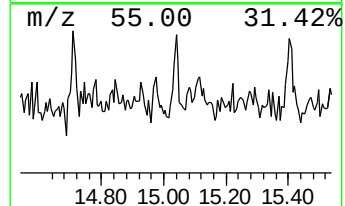
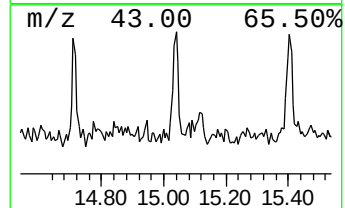
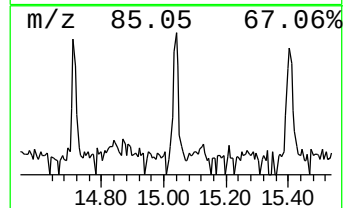
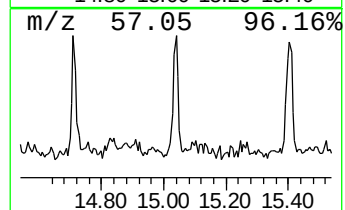
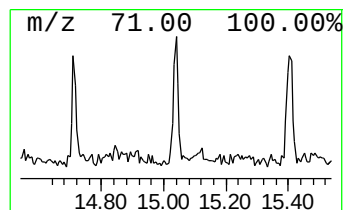
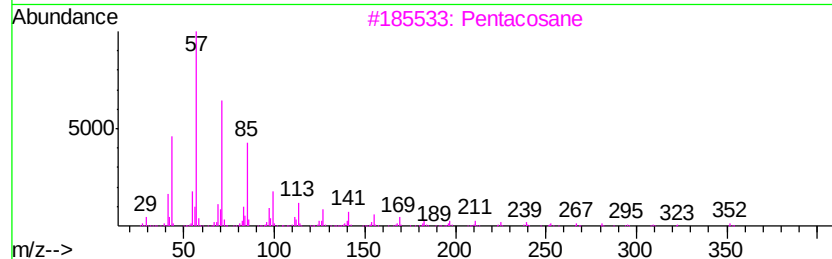
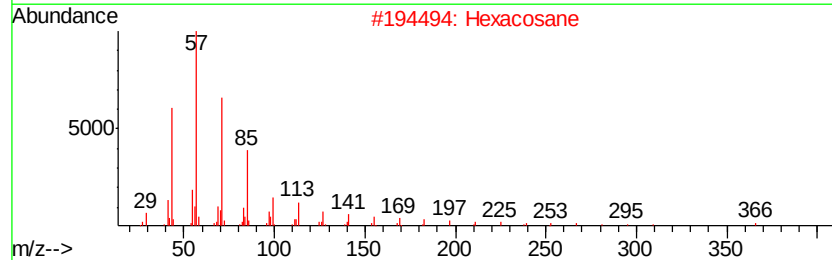
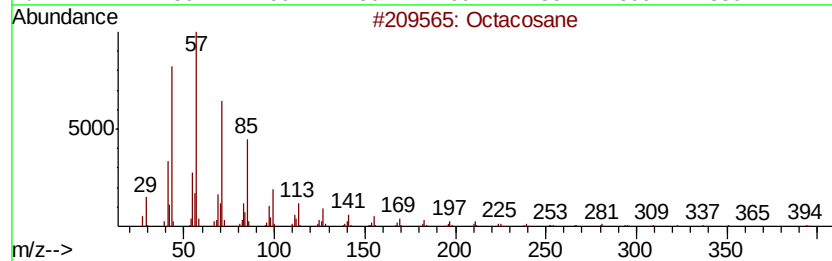
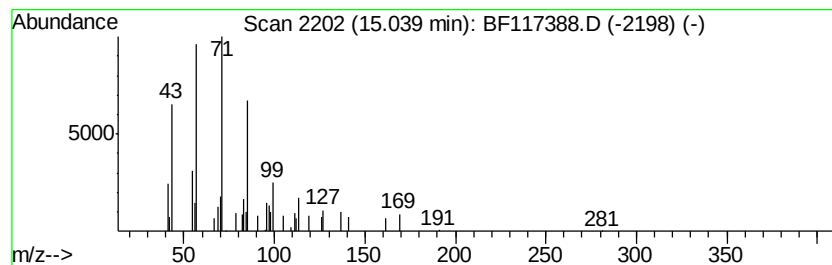
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Peak Number 4 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.04	2.06 ng	32906	Perylene-d12		15.42
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentacosane	352	C25H52	000629-99-2	90
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Heptacosane	380	C27H56	000593-49-7	86



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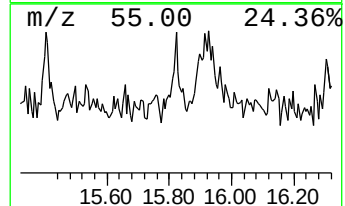
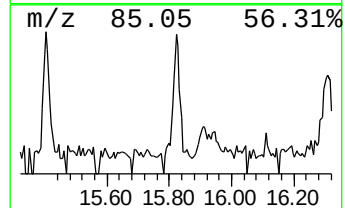
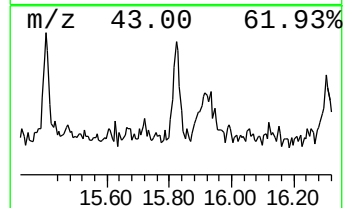
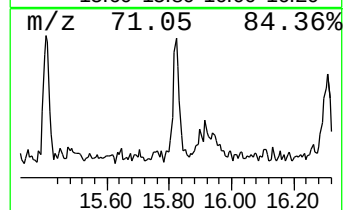
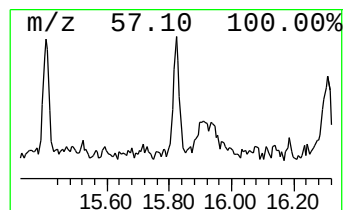
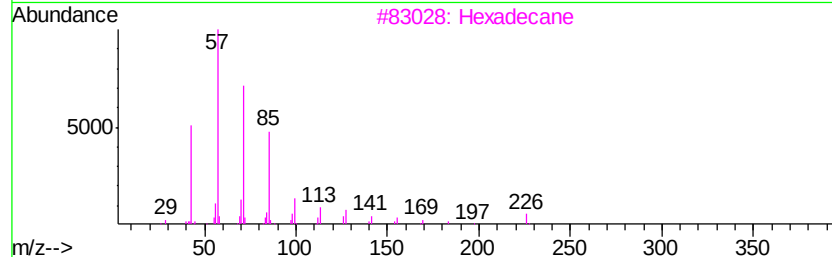
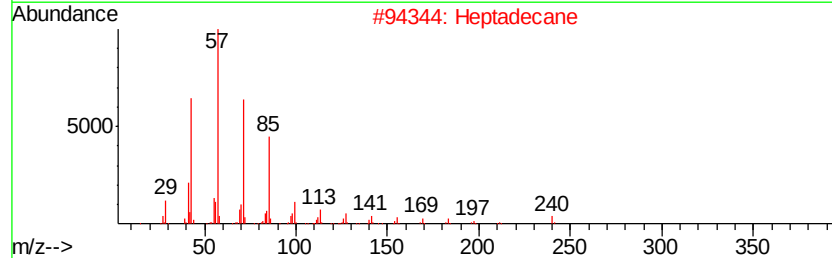
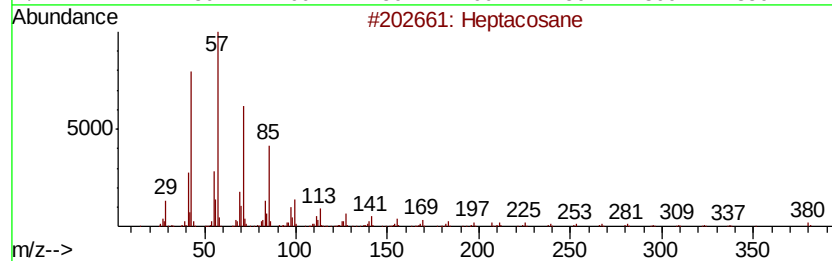
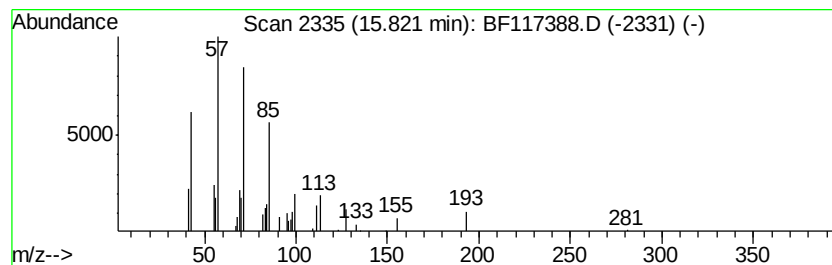
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Peak Number 5 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.82	2.00 ng	32066	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	72
2	Heptadecane	240	C17H36	000629-78-7	72
3	Hexadecane	226	C16H34	000544-76-3	72
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
5	Octacosane	394	C28H58	000630-02-4	64



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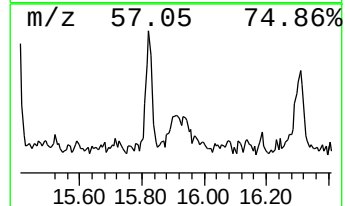
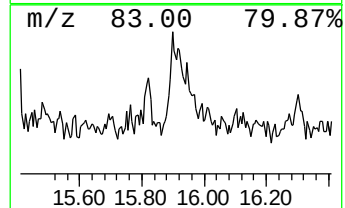
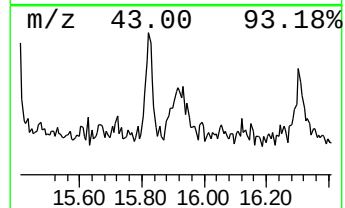
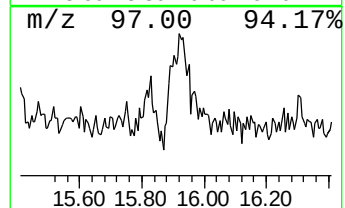
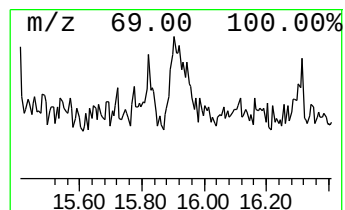
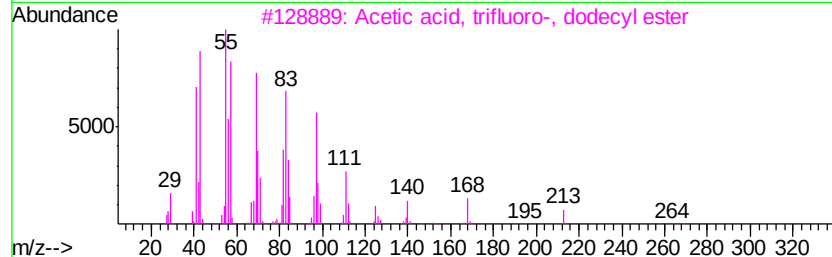
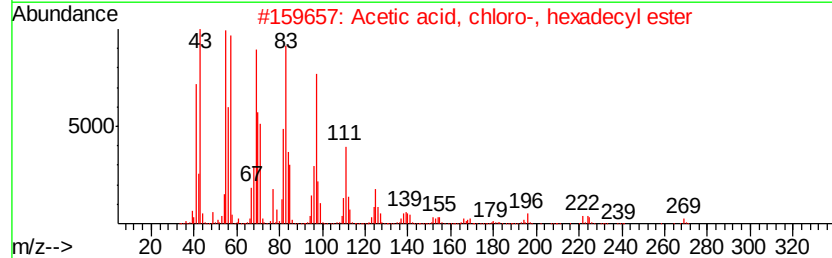
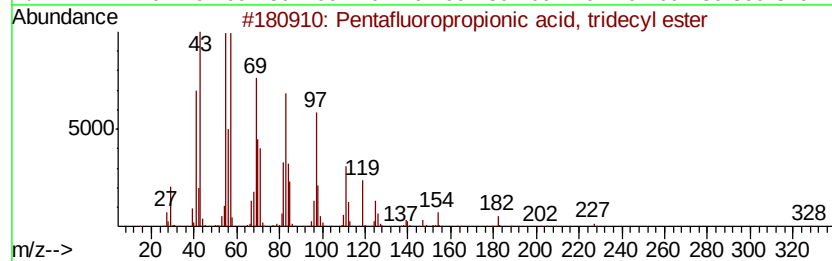
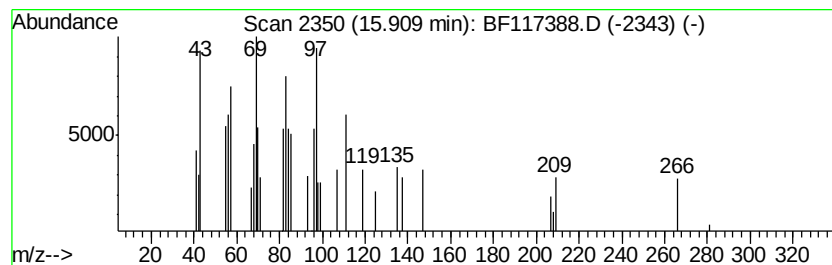
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.40 ng	38465	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, tridecyl...	346	C16H27F5O2	959261-22-4	62
2		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	58
3		Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	58
4		1-Nonadecene	266	C19H38	018435-45-5	53
5		Formic acid, dodecyl ester	214	C13H26O2	028303-42-6	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.57	6.57	77.6	ng	871886	1	6.79	224687	20.0
1-Heneicosanol	13.79	13.9	ng	220924	5	13.96	317633	20.0
Octacosane	15.04	2.1	ng	32906	6	15.42	319952	20.0
Heptacosane	15.82	2.0	ng	32066	6	15.42	319952	20.0
Pentafluoropropio...	15.91	2.4	ng	38465	6	15.42	319952	20.0