

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041718\
 Data File : BF104582.D
 Acq On : 18 Apr 2018 00:34
 Operator : JU/SJ
 Sample : J2387-04
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20180242-COMPOSITE-D

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:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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	5.028	496	500	507	rVB	128528	182537	4.90%	0.581%
2	5.428	562	568	571	rBV	3191887	3630913	97.52%	11.554%
3	6.081	676	679	688	rBV	31061	46061	1.24%	0.147%
4	6.445	735	741	744	rBV	3103333	3723118	100.00%	11.847%
5	6.575	758	763	767	rBV	3358801	3694947	99.24%	11.758%
6	6.804	798	802	805	rBV	1122608	872322	23.43%	2.776%
7	6.963	824	829	832	rBV	3129747	2848777	76.52%	9.065%
8	7.375	893	899	901	rBV	2186832	2367740	63.60%	7.534%
9	8.086	1016	1020	1024	rBV	1387595	1122537	30.15%	3.572%
10	9.163	1198	1203	1206	rBV	3709072	3649188	98.01%	11.612%
11	9.557	1266	1270	1273	rBV	298913	245223	6.59%	0.780%
12	9.769	1301	1306	1310	rBV	95719	76615	2.06%	0.244%
13	9.845	1315	1319	1323	rVV	1175931	1114773	29.94%	3.547%
14	10.269	1388	1391	1394	rVB	120022	87905	2.36%	0.280%
15	10.486	1422	1428	1431	rBV	30289	38721	1.04%	0.123%
16	10.633	1449	1453	1456	rBV	2112132	1945504	52.25%	6.191%
17	10.739	1469	1471	1479	rVB	95337	97445	2.62%	0.310%
18	11.192	1544	1548	1550	rBV	44060	38293	1.03%	0.122%
19	11.327	1568	1571	1575	rBV	978897	926524	24.89%	2.948%
20	12.921	1837	1842	1845	rBV	2757513	2619254	70.35%	8.335%
21	13.774	1982	1987	1990	rBV	48998	61006	1.64%	0.194%
22	13.810	1990	1993	2003	rVB	386876	398708	10.71%	1.269%
23	13.974	2017	2021	2025	rBV	980333	832044	22.35%	2.648%
24	14.451	2098	2102	2107	rBV2	28083	39593	1.06%	0.126%
25	14.821	2162	2165	2169	rVB	56572	55901	1.50%	0.178%
26	15.439	2265	2270	2283	rVB	494177	640286	17.20%	2.037%
27	15.939	2350	2355	2361	rBV3	42806	70005	1.88%	0.223%

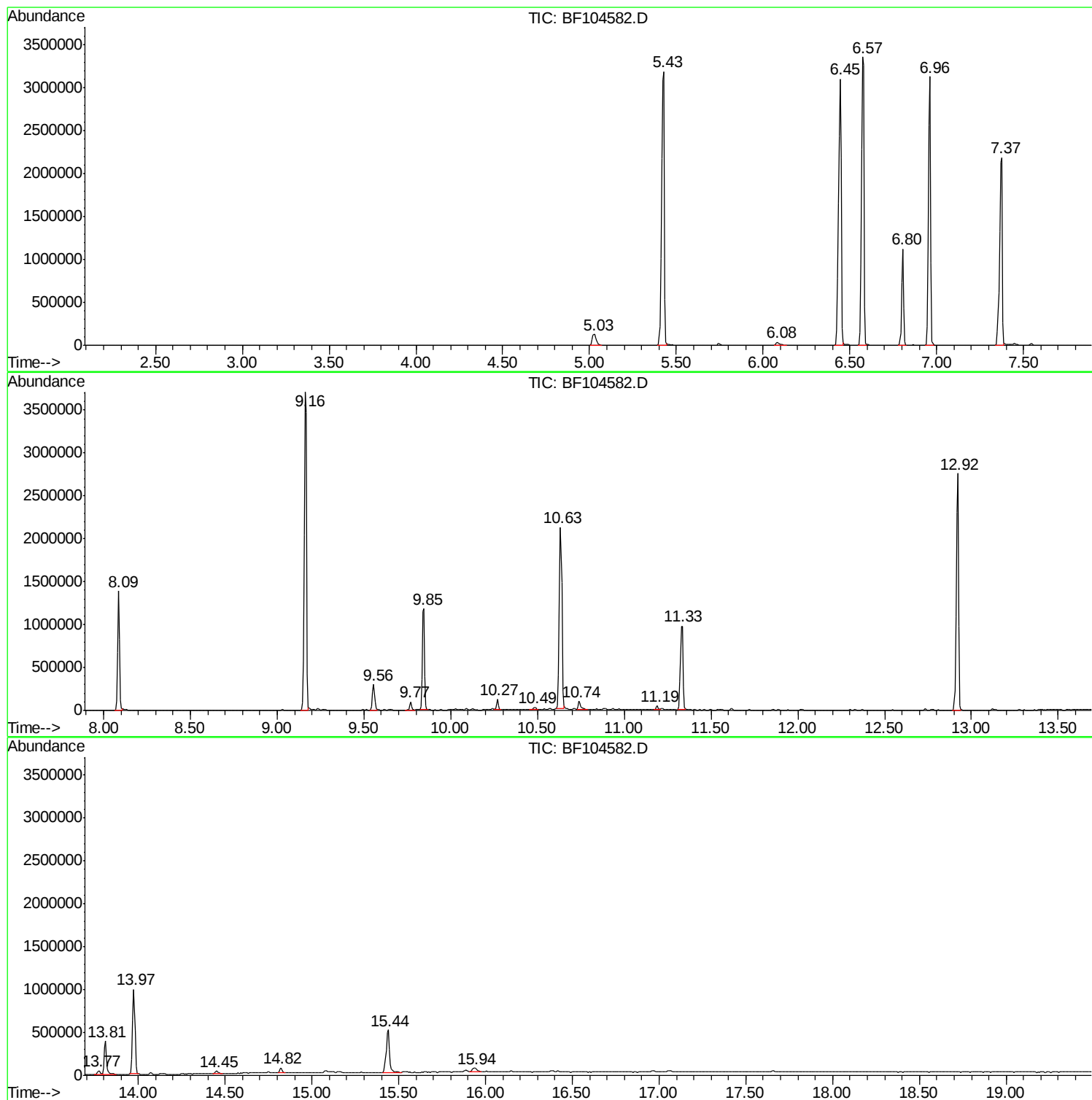
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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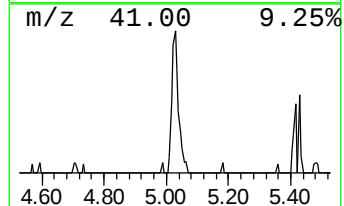
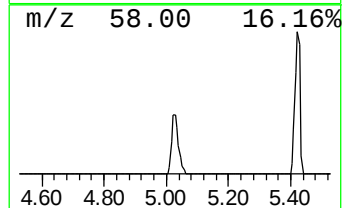
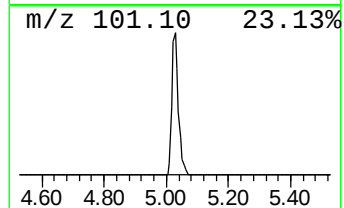
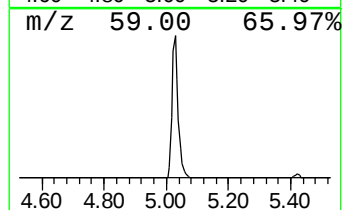
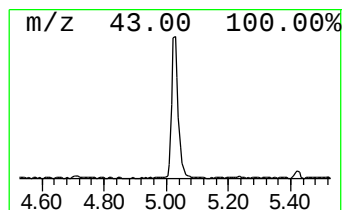
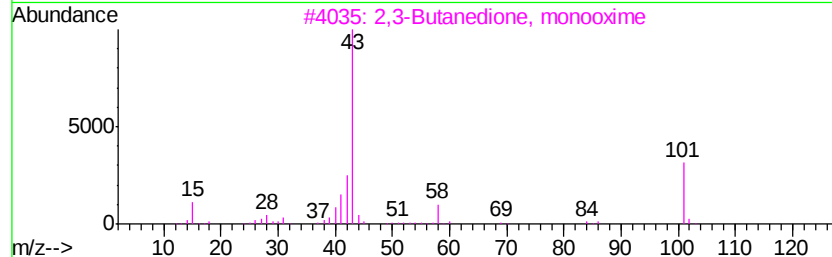
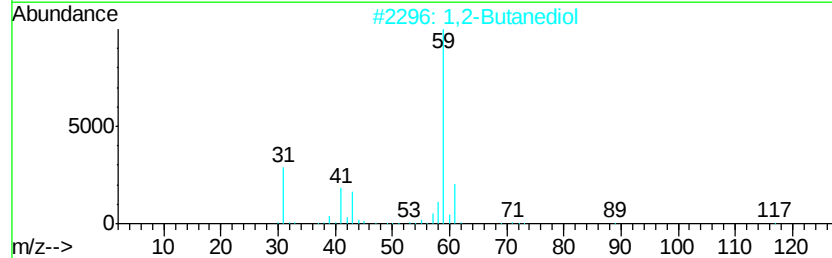
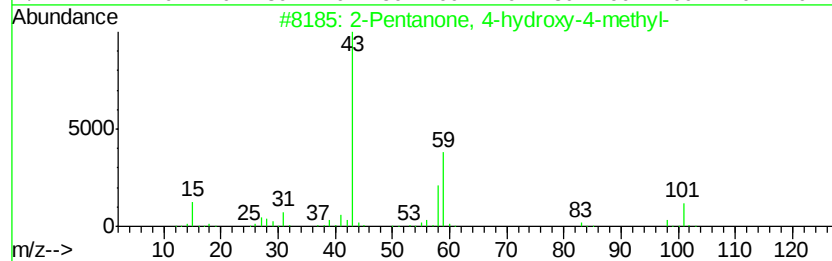
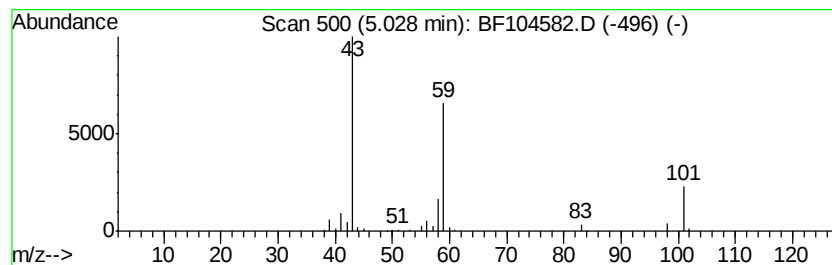
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	4.19 ng	182537	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,2-Butanediol	90	C4H10O2	000584-03-2	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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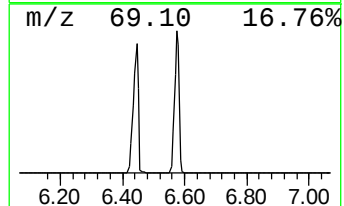
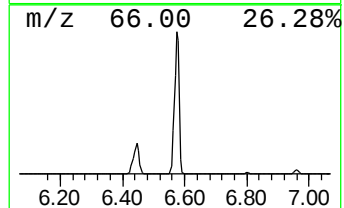
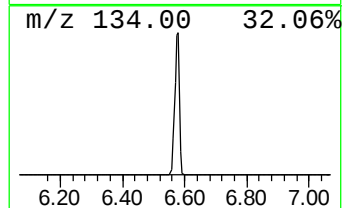
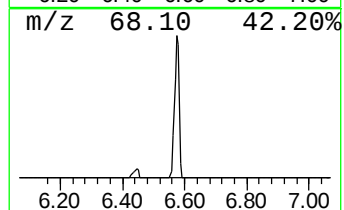
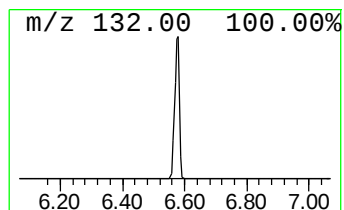
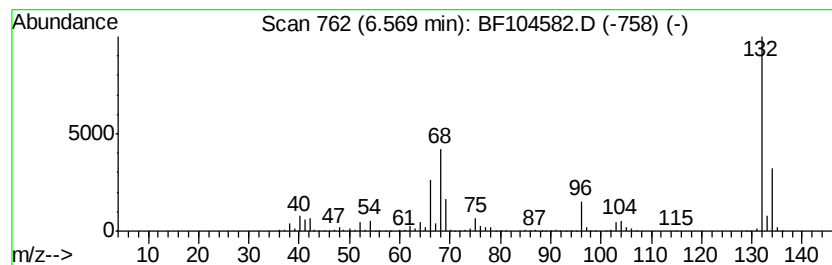
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	84.72 ng	3694950	1,4-Dichlorobenzene-d4	6.80

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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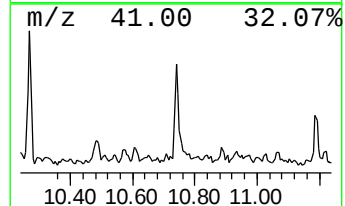
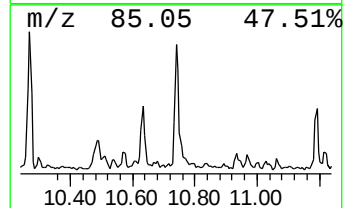
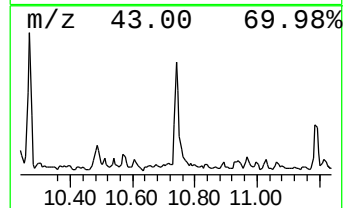
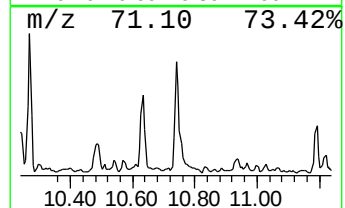
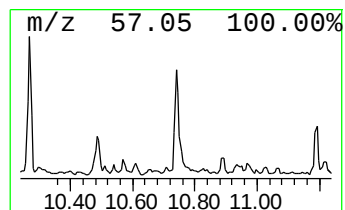
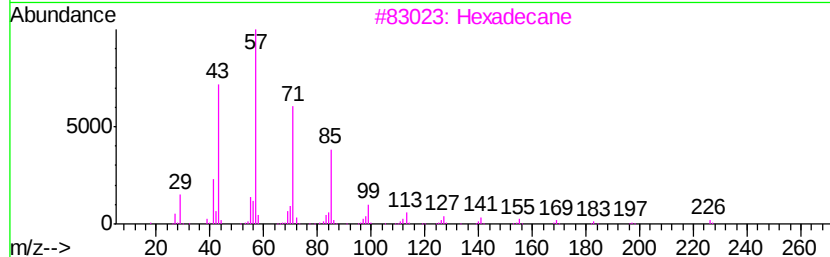
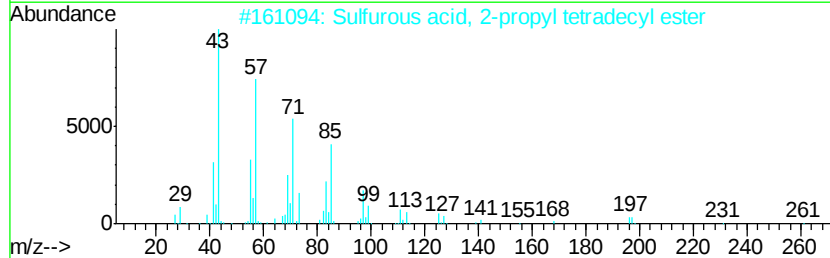
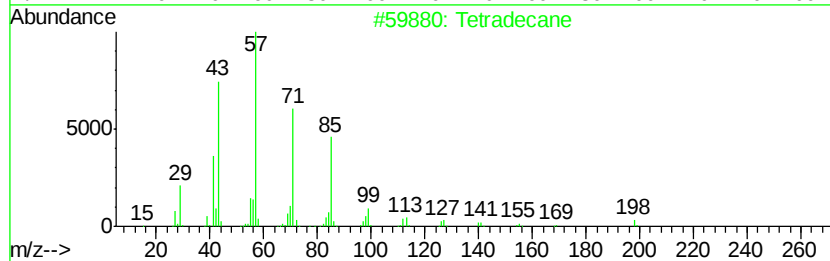
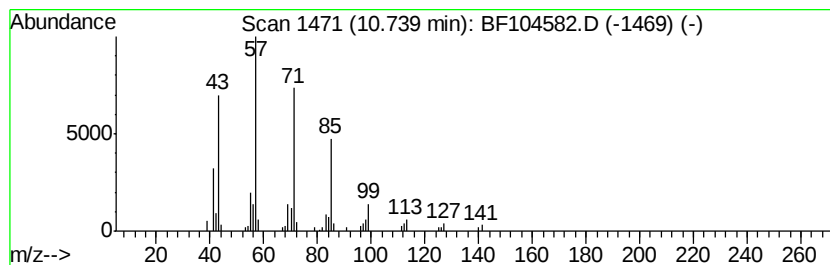
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Peak Number 4 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.10 ng	97445	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	91
2		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	90
3		Hexadecane	226	C16H34	000544-76-3	90
4		Pentadecane	212	C15H32	000629-62-9	86
5		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	86



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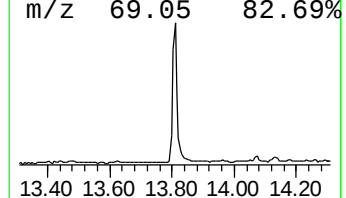
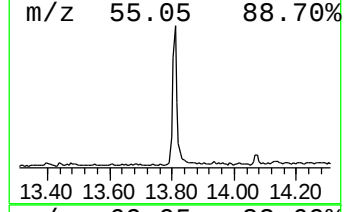
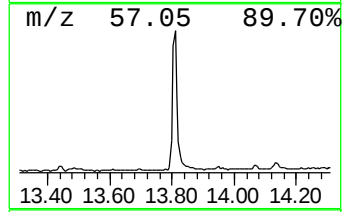
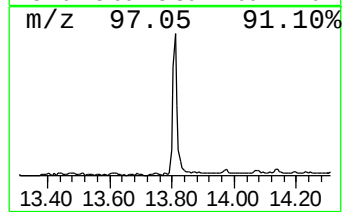
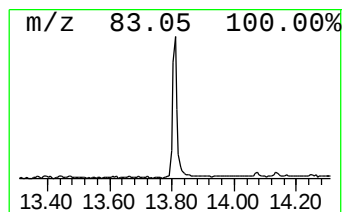
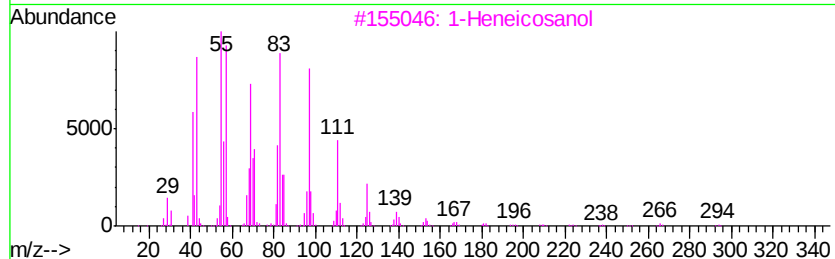
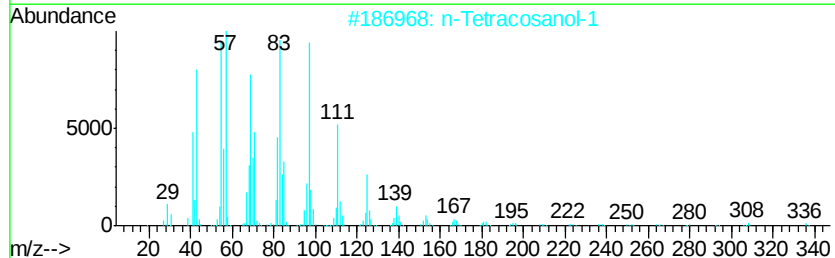
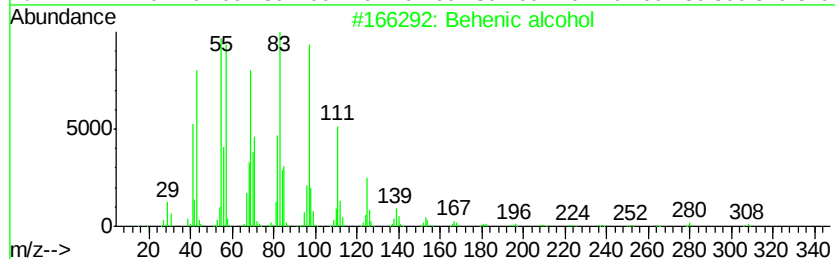
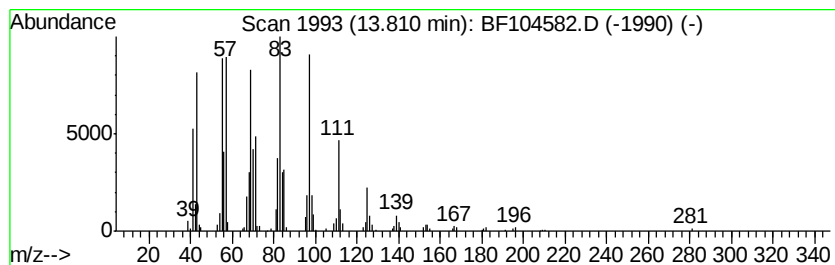
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	9.58 ng	398708	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5		1-Heptacosanol	396	C27H56O	002004-39-9	94



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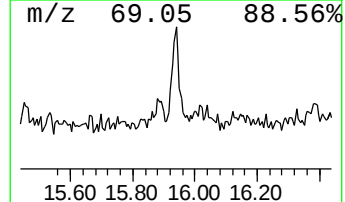
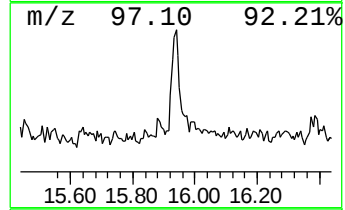
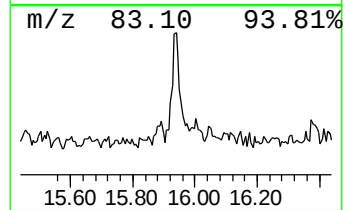
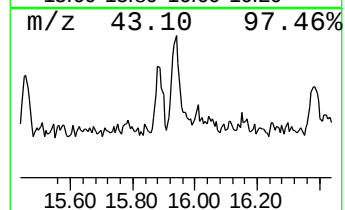
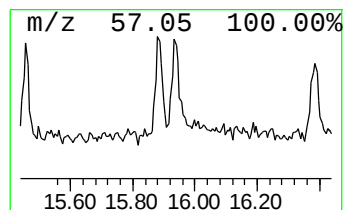
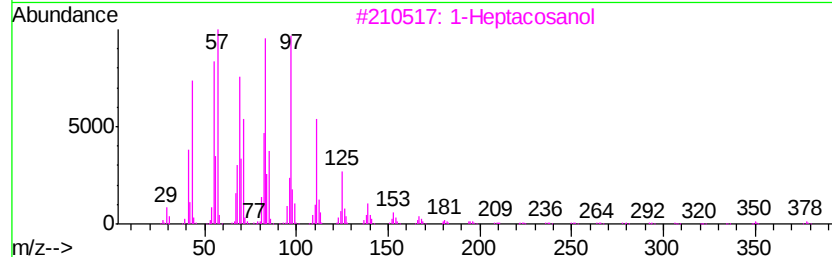
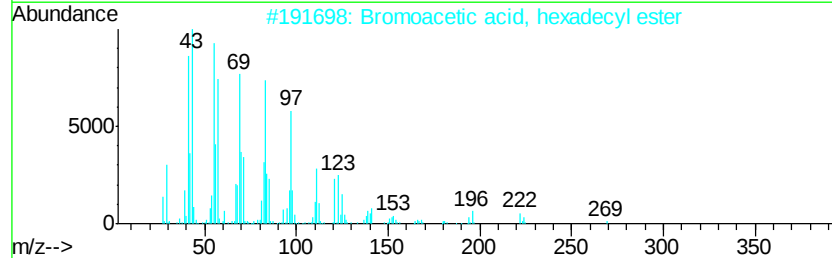
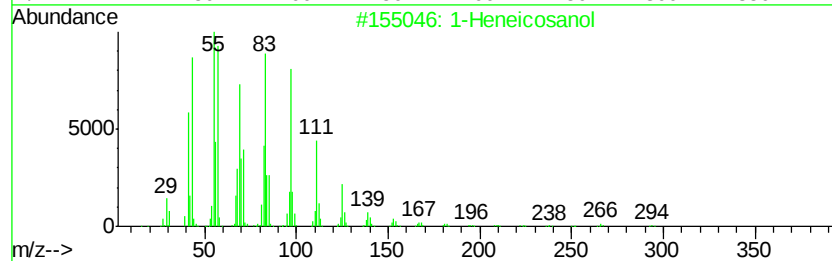
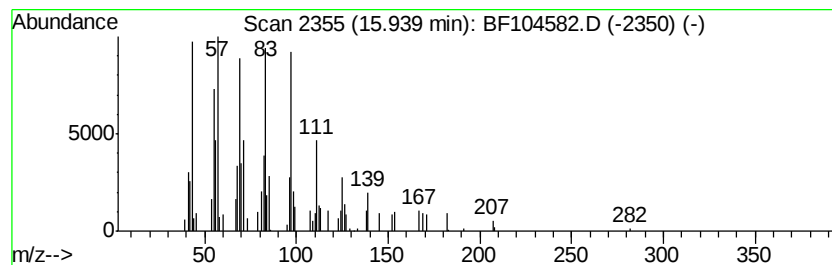
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Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.19 ng	70005	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	91
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
3		1-Heptacosanol	396	C27H56O	002004-39-9	76
4		Heptacosyl acetate	438	C29H58O2	1000351-78-2	76
5		Octacosyl acetate	452	C30H60O2	018206-97-8	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	4.2	ng	182537	1	6.80	872322	20.0
unknown6.57	6.57	84.7	ng	3694950	1	6.80	872322	20.0
Tetradecane	10.74	2.1	ng	97445	4	11.33	926524	20.0
Behenic alcohol	13.81	9.6	ng	398708	5	13.97	832044	20.0
1-Heneicosanol	15.94	2.2	ng	70005	6	15.44	640286	20.0