

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082317\
 Data File : BF097992.D
 Acq On : 23 Aug 2017 12:29
 Operator : SJ/JU
 Sample : I4914-04
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 165-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	3.134	176	178	189	rBV	27923	57648	1.77%	0.213%
2	4.940	481	485	491	rVB	159668	195591	6.00%	0.721%
3	5.351	550	555	558	rBV	2330587	2256427	69.24%	8.322%
4	6.375	723	729	732	rBV	2657930	2607387	80.01%	9.616%
5	6.504	747	751	755	rBV	2331062	2402740	73.73%	8.861%
6	6.739	787	791	794	rBV	1029692	860621	26.41%	3.174%
7	6.892	813	817	821	rBV	1982978	1772536	54.39%	6.537%
8	7.298	881	886	890	rBV	1561958	1669957	51.24%	6.159%
9	8.022	1004	1009	1012	rBV	1222904	1110191	34.07%	4.094%
10	9.098	1186	1192	1195	rBV	3212302	3258840	100.00%	12.018%
11	9.492	1251	1259	1261	rBV	211409	183288	5.62%	0.676%
12	9.775	1301	1307	1310	rBV	1207242	1152090	35.35%	4.249%
13	9.980	1334	1342	1348	rBV4	45923	84163	2.58%	0.310%
14	10.557	1436	1440	1444	rBV	1576806	1565211	48.03%	5.772%
15	10.680	1458	1461	1463	rBV	41612	35331	1.08%	0.130%
16	10.927	1498	1503	1508	rVB4	31974	56855	1.74%	0.210%
17	11.251	1554	1558	1562	rBV	1235186	1150925	35.32%	4.245%
18	11.645	1622	1625	1632	rBV	48039	65098	2.00%	0.240%
19	11.792	1644	1650	1653	rBV2	133706	238916	7.33%	0.881%
20	11.821	1653	1655	1658	rVB	59596	51503	1.58%	0.190%
21	11.921	1669	1672	1677	rBV5	26152	32645	1.00%	0.120%
22	12.439	1756	1760	1766	rBV3	147178	227559	6.98%	0.839%
23	12.669	1795	1799	1800	rBV3	41829	49324	1.51%	0.182%
24	12.686	1800	1802	1806	rVB2	61377	65023	2.00%	0.240%
25	12.845	1823	1829	1832	rBV	3131735	3248386	99.68%	11.980%
26	13.739	1978	1981	1988	rBV3	154357	201972	6.20%	0.745%
27	13.880	2001	2005	2009	rBV2	1323192	1489793	45.72%	5.494%
28	14.368	2086	2088	2091	rBV2	36429	38378	1.18%	0.142%
29	14.521	2111	2114	2117	rBV	81273	86188	2.64%	0.318%
30	15.098	2206	2212	2222	rVB4	107891	271234	8.32%	1.000%
31	15.298	2242	2246	2251	rVB	512746	629793	19.33%	2.323%

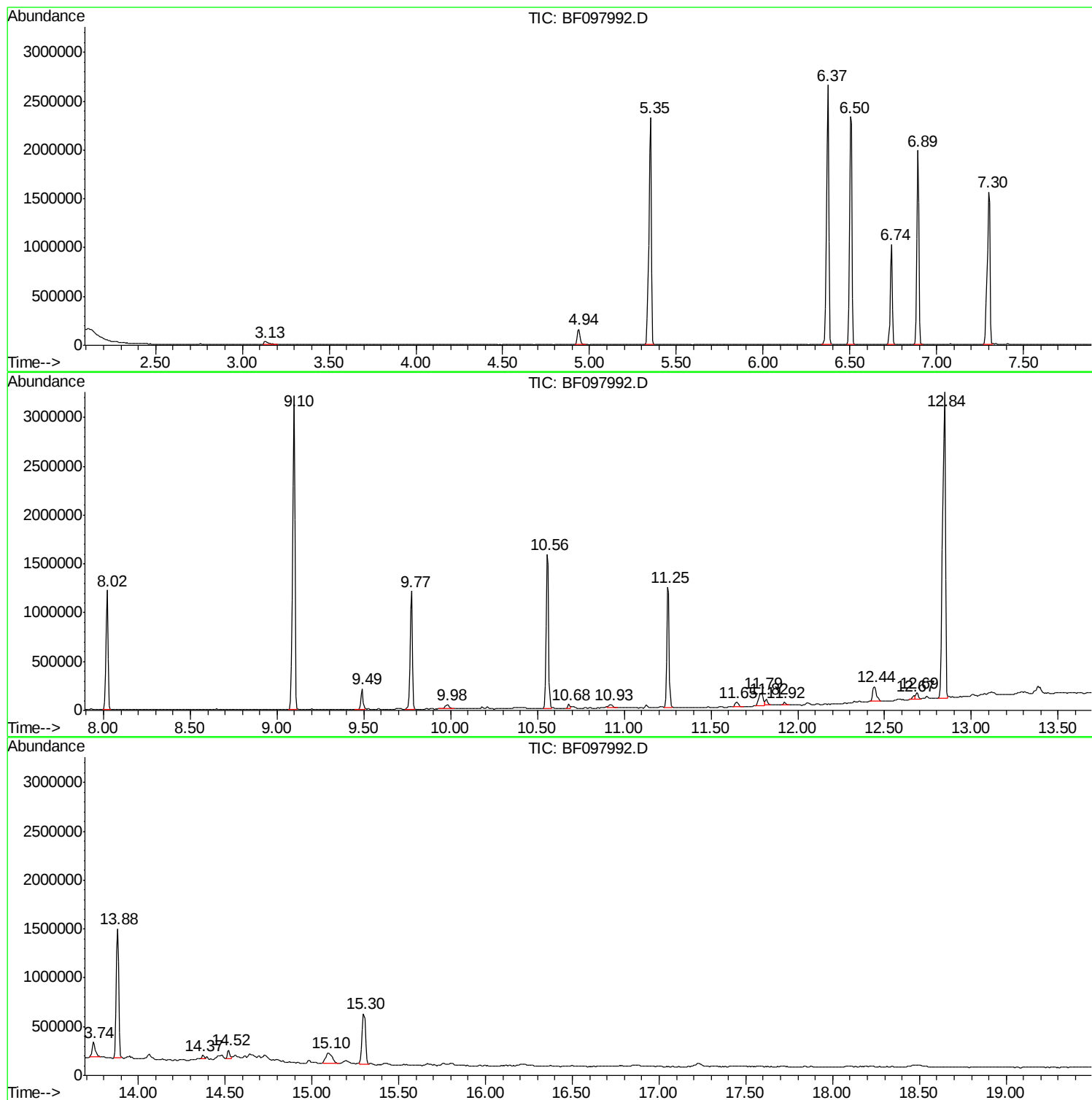
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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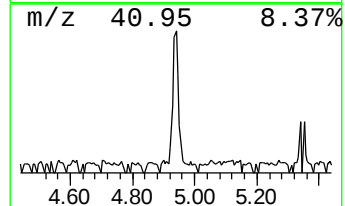
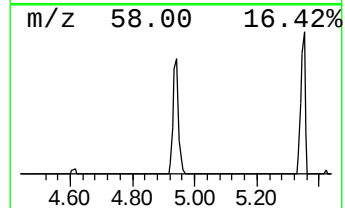
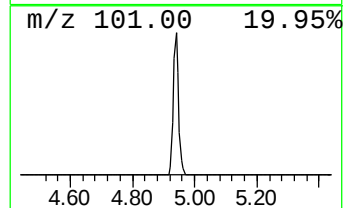
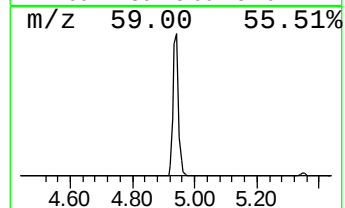
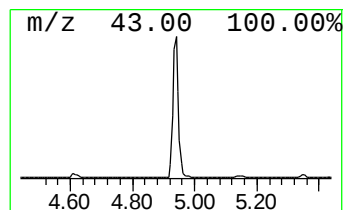
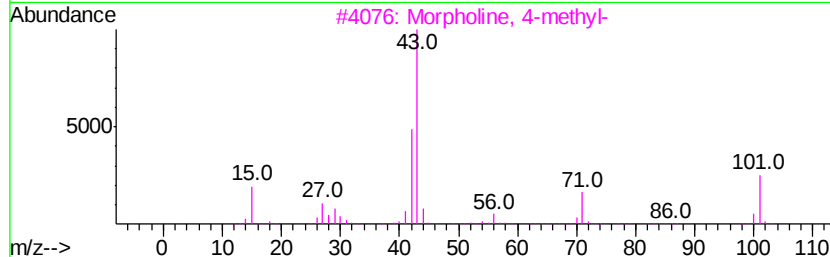
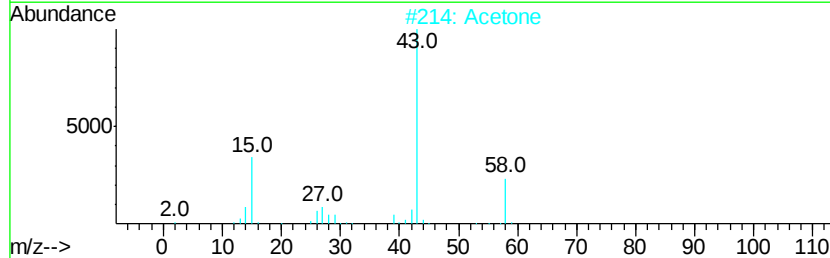
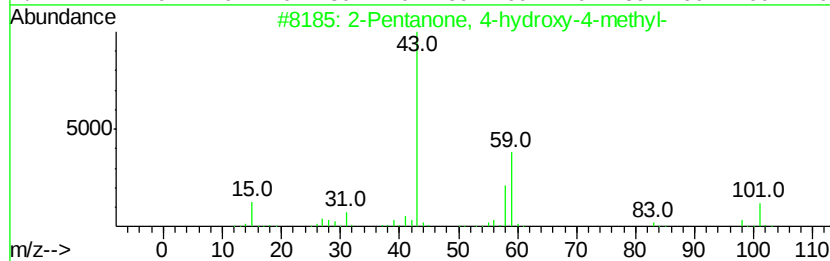
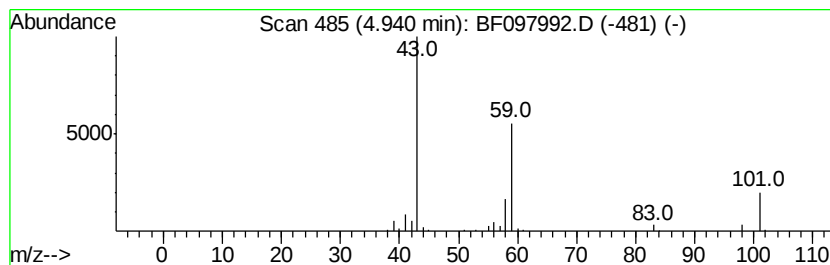
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.94	4.55 ng	195591	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetone	58	C3H6O	000067-64-1	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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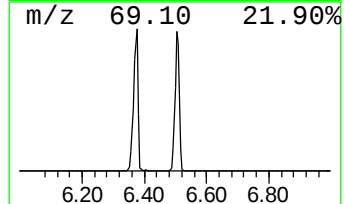
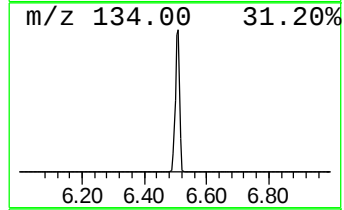
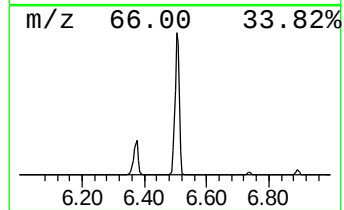
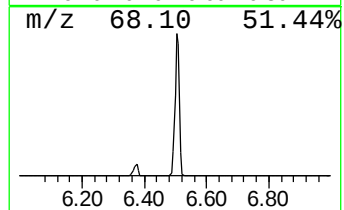
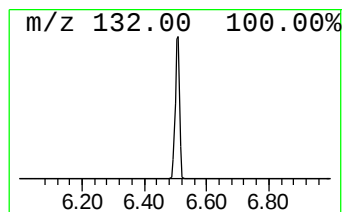
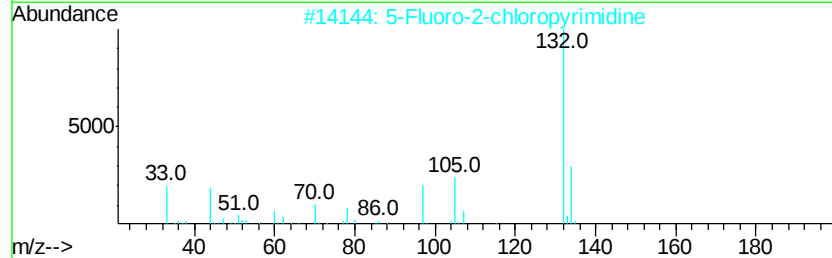
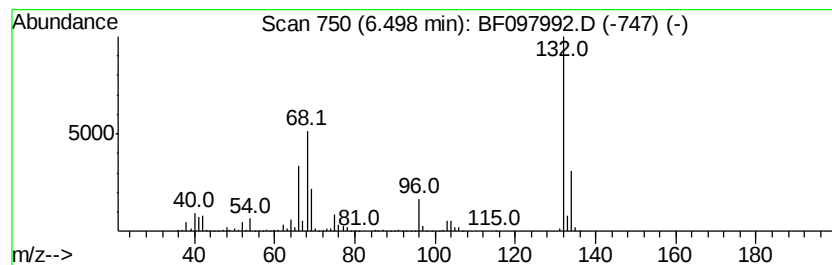
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	55.84 ng	2402740	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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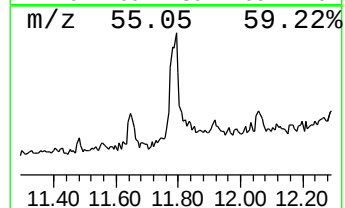
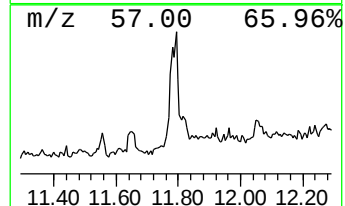
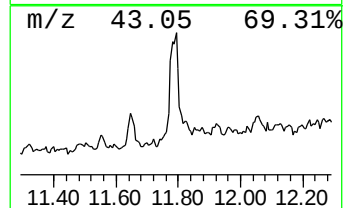
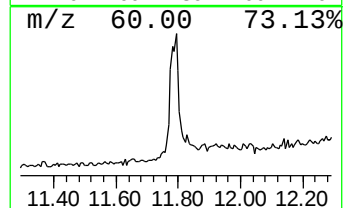
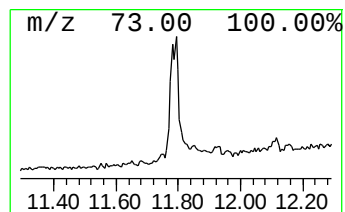
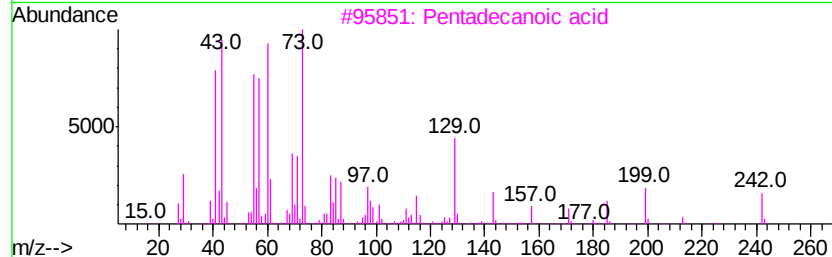
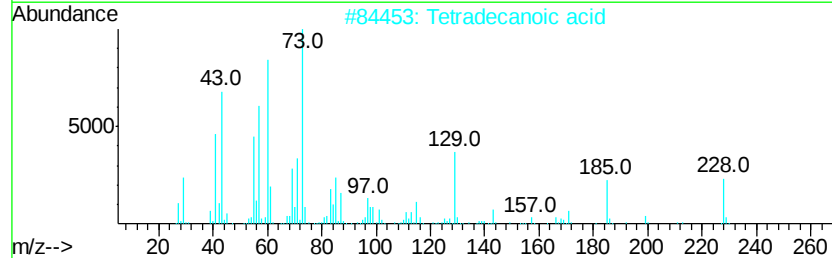
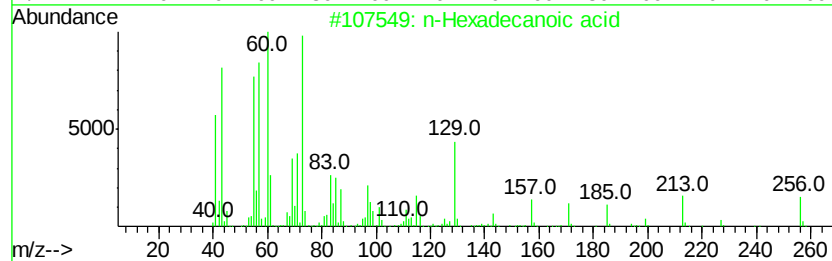
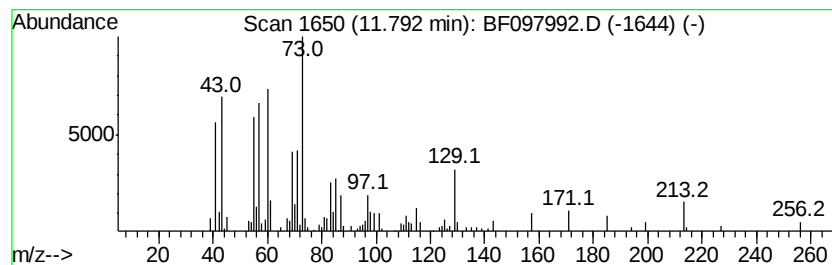
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	4.15 ng	238916	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	35
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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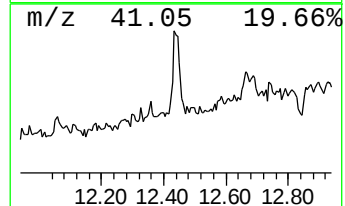
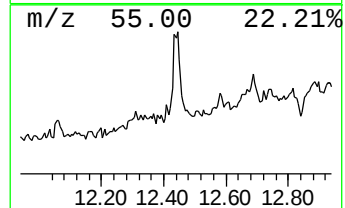
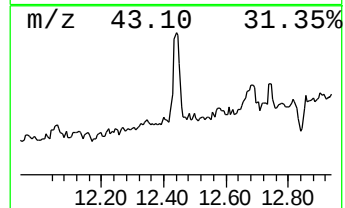
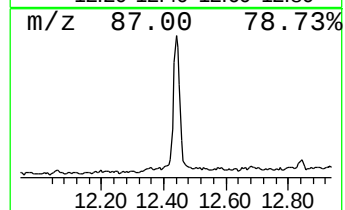
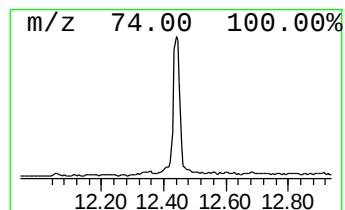
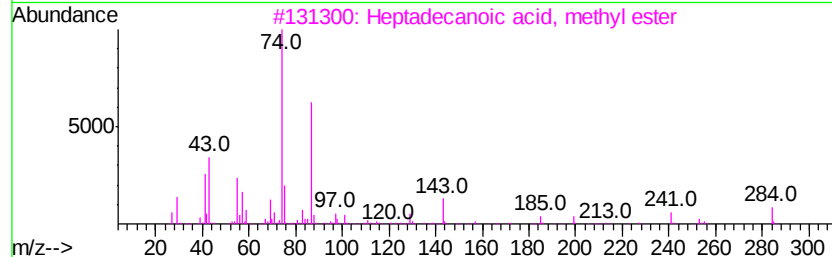
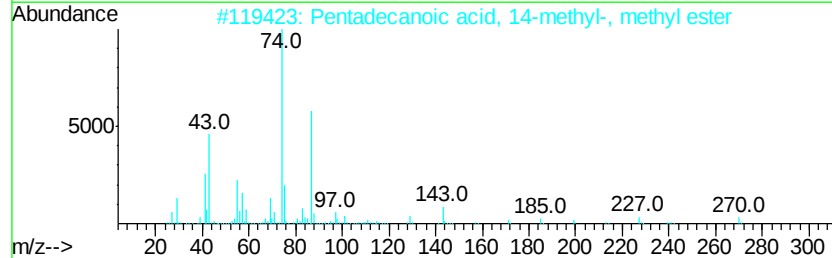
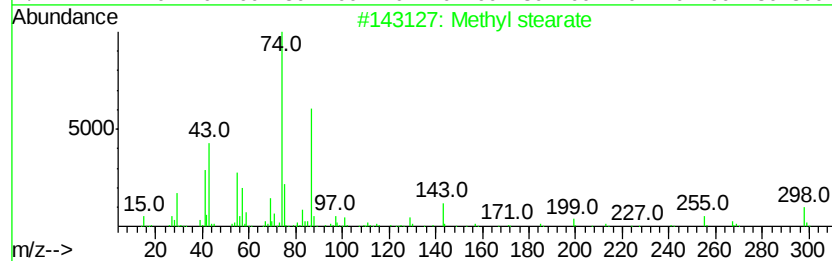
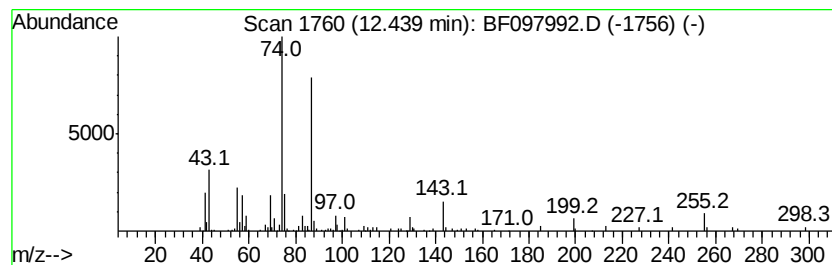
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Peak Number 5 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.44	3.95 ng	227559	Phenanthrene-d10		11.25
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	93
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90



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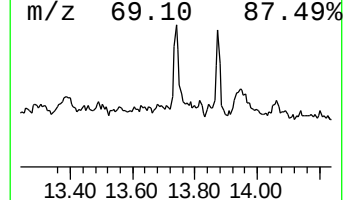
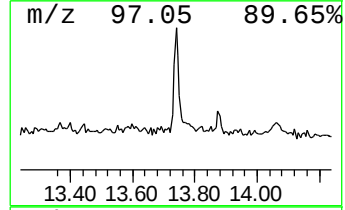
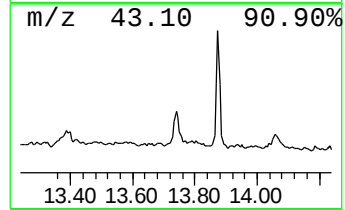
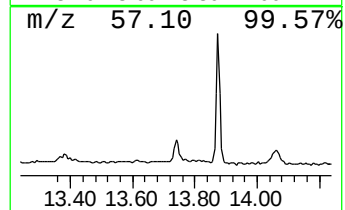
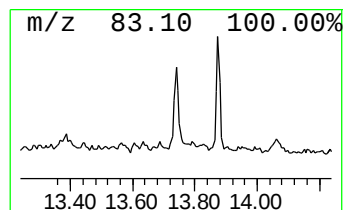
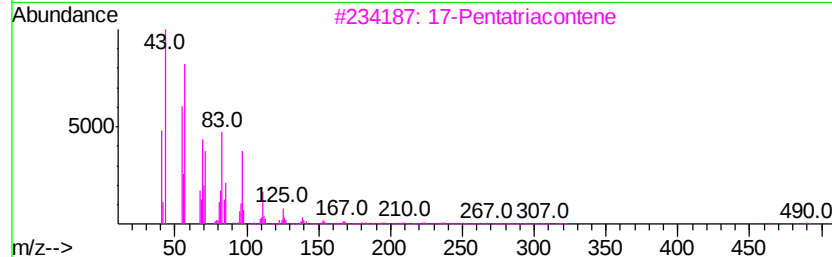
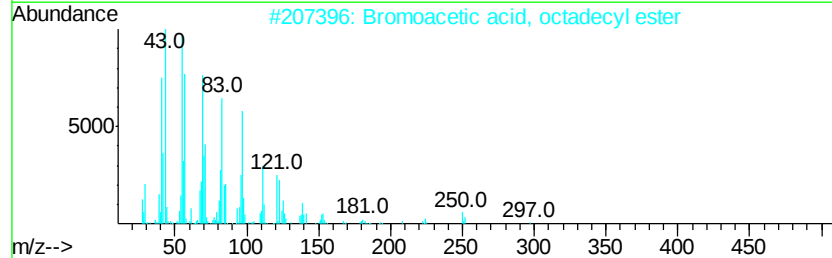
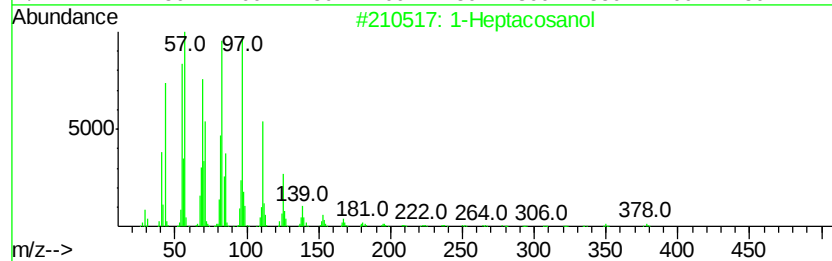
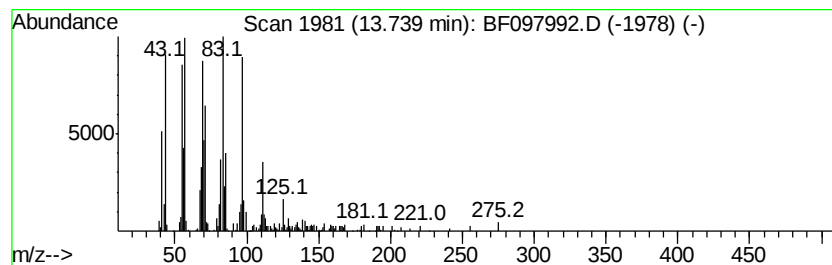
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Peak Number 6 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.74	2.71 ng	201972	Chrysene-d12		13.89
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74



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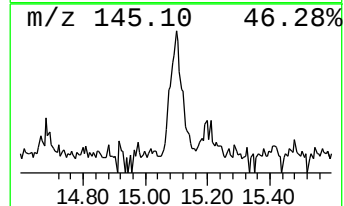
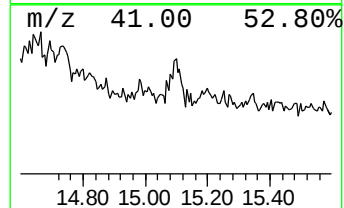
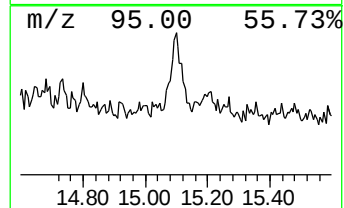
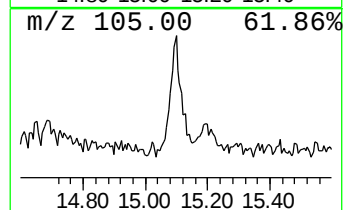
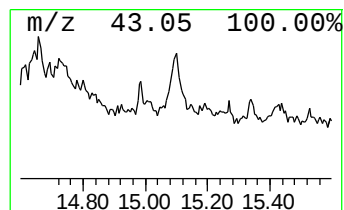
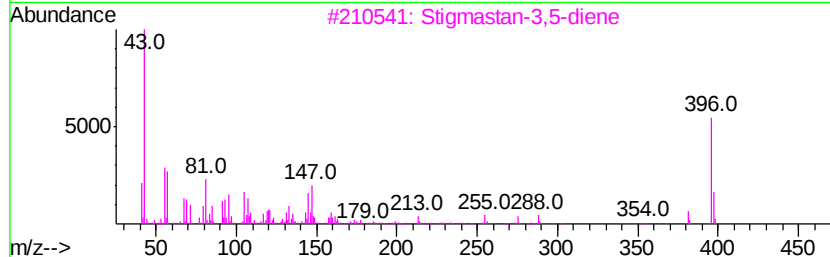
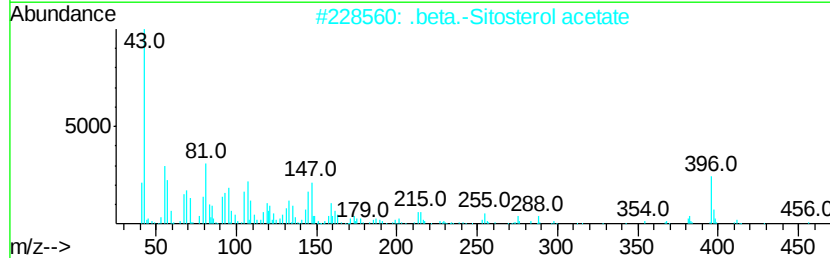
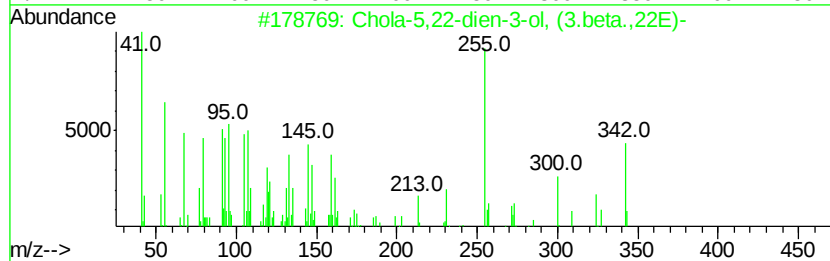
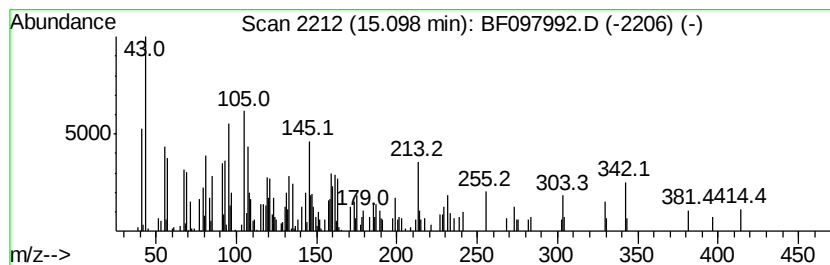
Instrument :
BNA_F
ClientSampleId :
165-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.10 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.10	8.61 ng	271234	Perylene-d12	15.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chola-5,22-dien-3-ol, (3.beta.,2...	342	C24H38O	057597-08-7	42
2	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	38
3	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	37
4	Pren-5-ene-3,12,14,17,20-pentol...	366	C21H34O5	028417-32-5	30
5	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082317\
Data File : BF097992.D
Acq On : 23 Aug 2017 12:29
Operator : SJ/JU
Sample : I4914-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
165-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	4.5	ng	195591	1	6.74	860621	20.0
unknown6.50	6.50	55.8	ng	2402740	1	6.74	860621	20.0
n-Hexadecanoic acid	11.79	4.2	ng	238916	4	11.25	1150930	20.0
Methyl stearate	12.44	4.0	ng	227559	4	11.25	1150930	20.0
1-Heptacosanol	13.74	2.7	ng	201972	5	13.89	1489790	20.0
unknown15.10	15.10	8.6	ng	271234	6	15.30	629793	20.0