

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
 Data File : BF108847.D
 Acq On : 7 Sep 2018 2:08
 Operator : JU/SJ
 Sample : J4803-14
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q2-I6

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-BF090518.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	4.931	438	441	450	rVB	125488	143062	4.17%	0.429%
2	5.349	507	512	515	rBV	3140568	2987113	86.98%	8.964%
3	6.366	680	685	688	rBV	3458448	3077736	89.62%	9.236%
4	6.501	704	708	711	rBV	3579543	3146456	91.62%	9.442%
5	6.566	716	719	725	rVB	108070	95299	2.78%	0.286%
6	6.737	744	748	751	rBV	1429099	1168204	34.02%	3.506%
7	6.890	770	774	778	rBV	2861698	2575338	74.99%	7.728%
8	7.290	838	842	845	rBV	2237593	1968294	57.31%	5.906%
9	8.013	961	965	969	rBV	1579460	1387464	40.40%	4.164%
10	9.089	1144	1148	1151	rBV	4116694	3434170	100.00%	10.305%
11	9.484	1211	1215	1218	rBV	1178200	885022	25.77%	2.656%
12	9.766	1259	1263	1266	rBV	1673553	1377644	40.12%	4.134%
13	10.542	1392	1395	1399	rBV	1750285	1641356	47.79%	4.925%
14	11.242	1510	1514	1517	rBV	1421971	1248157	36.35%	3.745%
15	11.783	1602	1606	1615	rBV2	215738	282351	8.22%	0.847%
16	12.342	1696	1701	1709	rBV8	40374	96511	2.81%	0.290%
17	12.560	1736	1738	1751	rBV7	36364	66276	1.93%	0.199%
18	12.672	1754	1757	1762	rVB	40032	42349	1.23%	0.127%
19	12.825	1779	1783	1786	rBV	3318817	3047624	88.74%	9.145%
20	13.724	1933	1936	1948	rBV	600769	742200	21.61%	2.227%
21	13.866	1956	1960	1963	rBV	1648884	1516206	44.15%	4.550%
22	14.360	2042	2044	2053	rVB2	80304	114858	3.34%	0.345%
23	14.624	2086	2089	2092	rBV	153110	153806	4.48%	0.462%
24	14.724	2103	2106	2109	rVB	308579	278800	8.12%	0.837%
25	14.971	2146	2148	2152	rBV2	51226	56944	1.66%	0.171%
26	15.271	2194	2199	2205	rBV	1386300	1605207	46.74%	4.817%
27	15.777	2282	2285	2294	rBV3	98286	186012	5.42%	0.558%

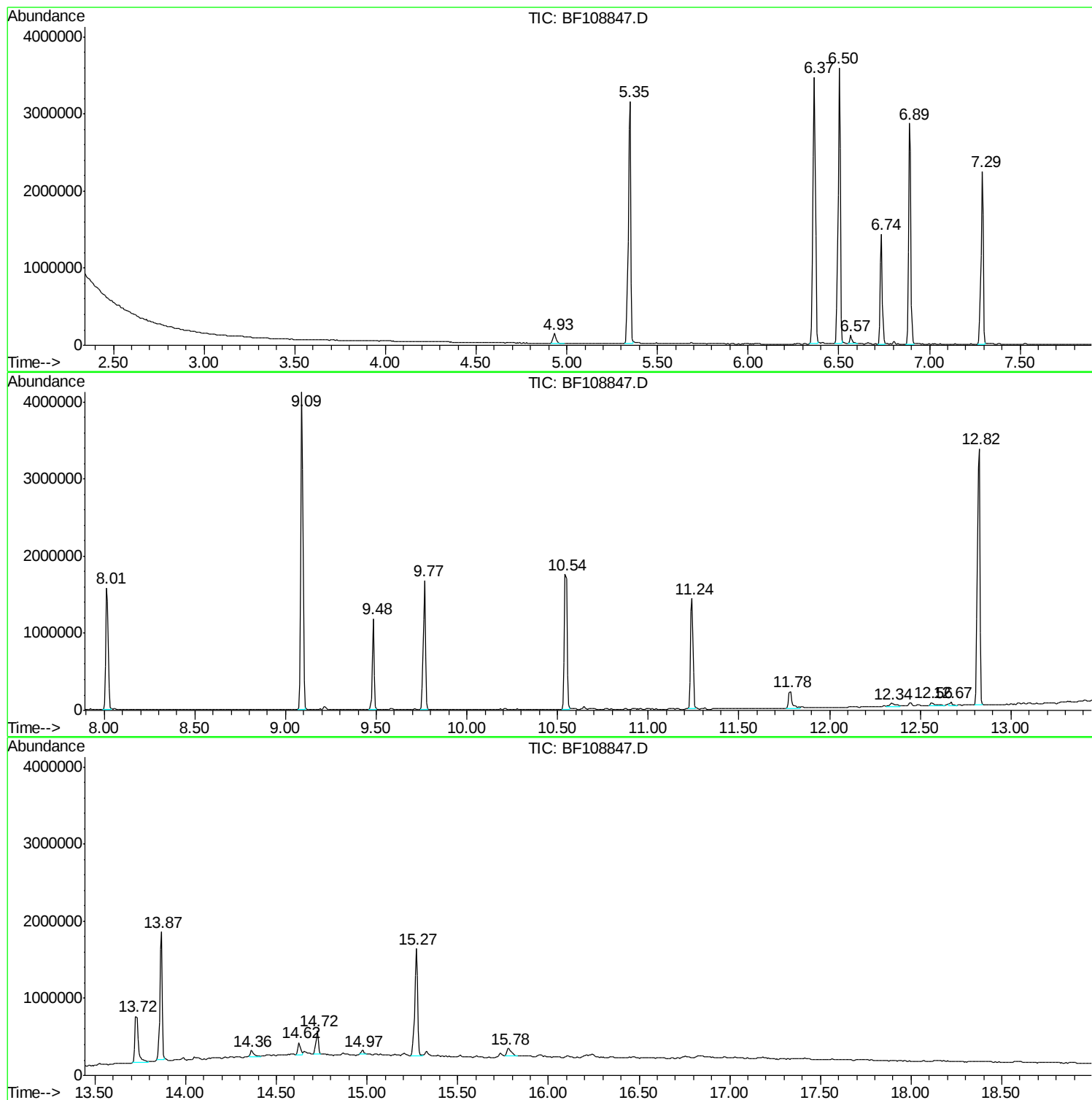
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ClientSampled :
EP1-Q2-I6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.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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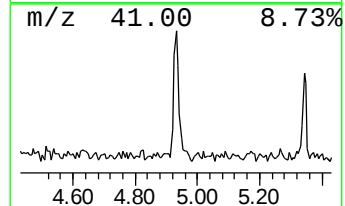
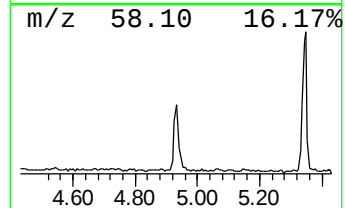
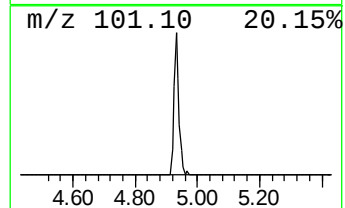
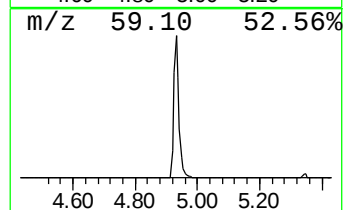
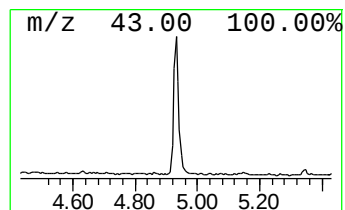
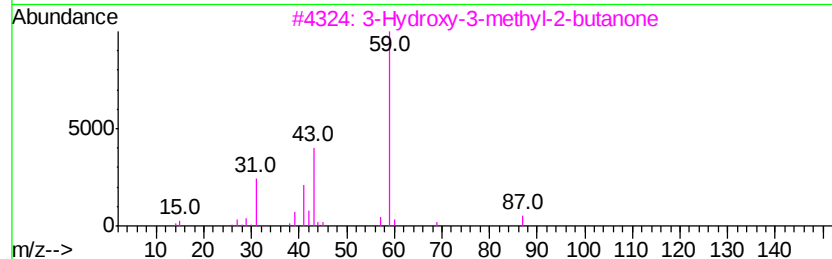
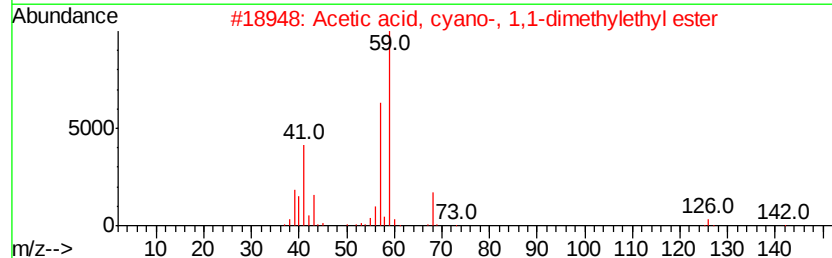
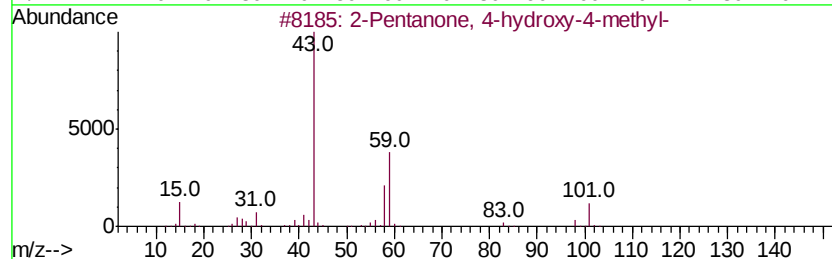
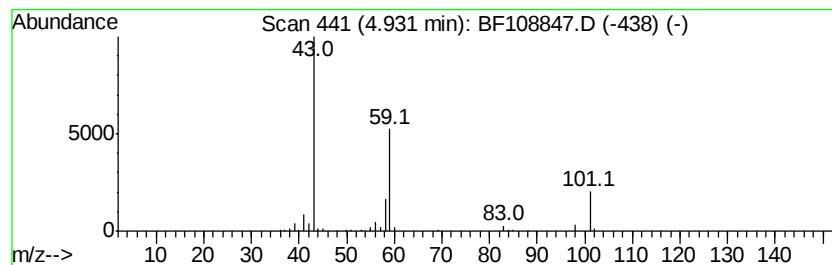
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.45 ng	143062	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	45
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4			2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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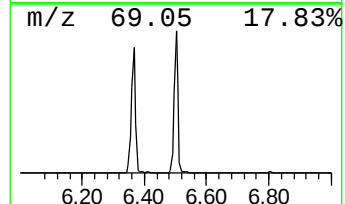
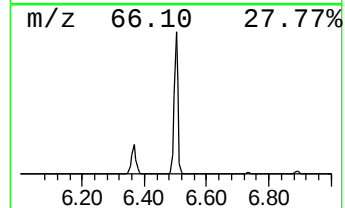
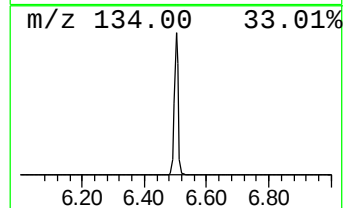
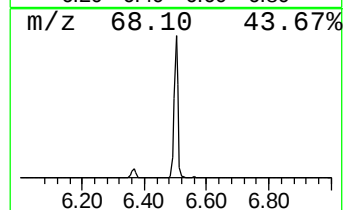
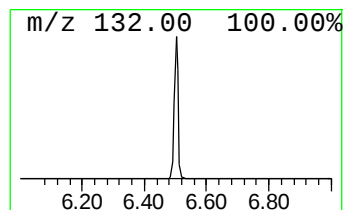
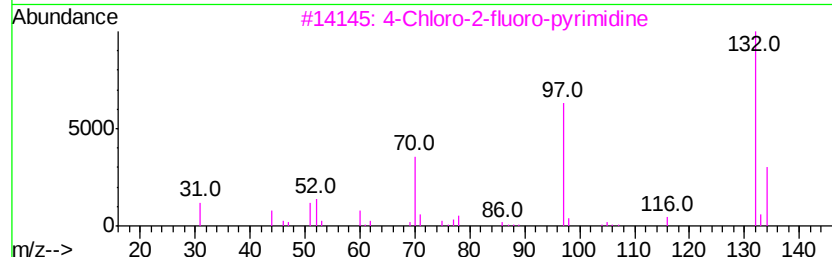
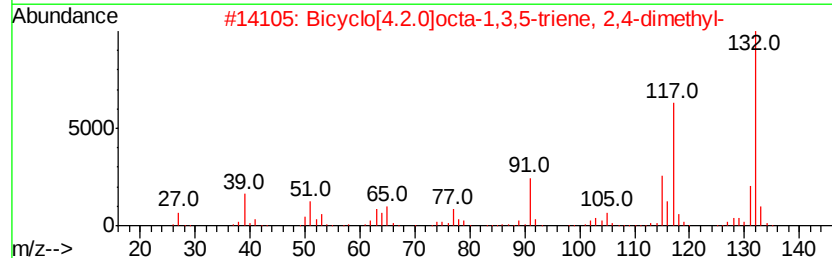
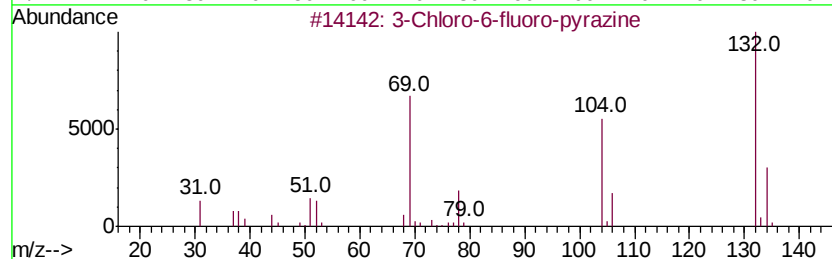
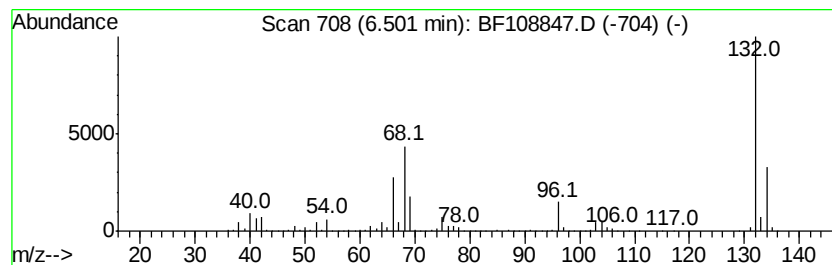
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	53.87 ng	3146460	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	16
2	Bicyclo[4.2.0]octa-1,3,5-triene,...			132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9



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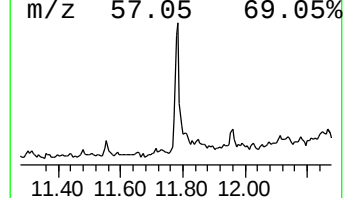
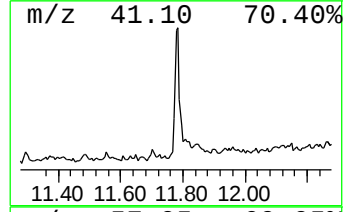
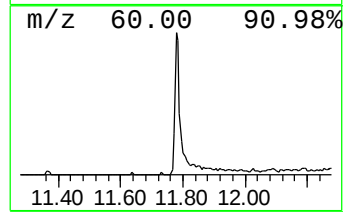
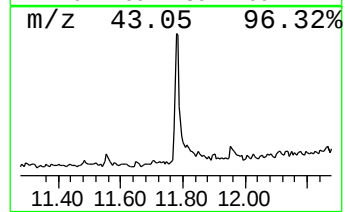
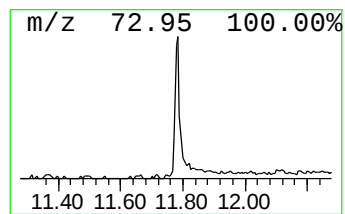
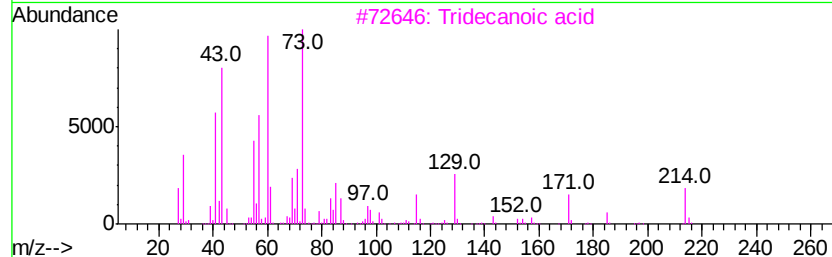
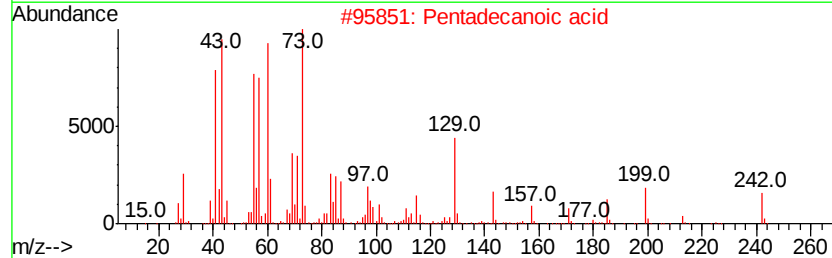
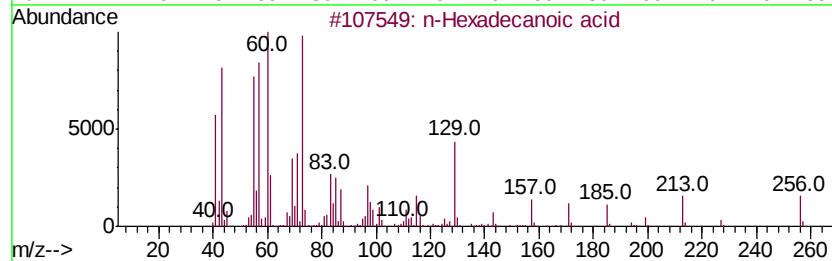
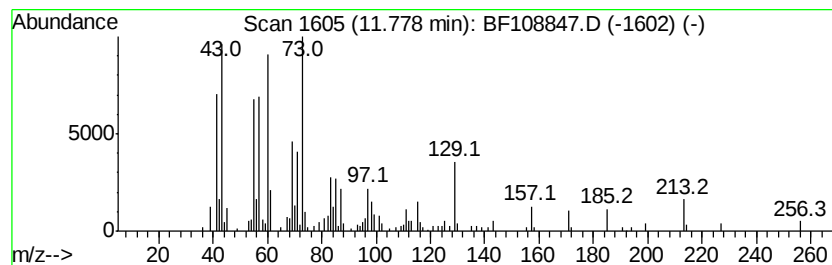
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 Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.78	4.52 ng	282351	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	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20



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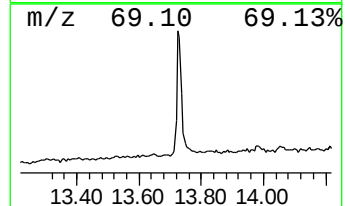
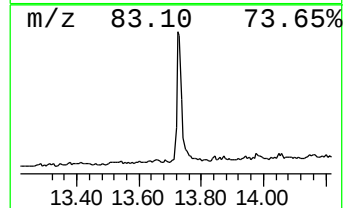
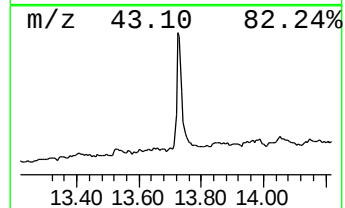
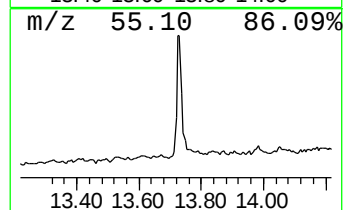
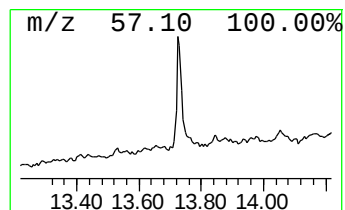
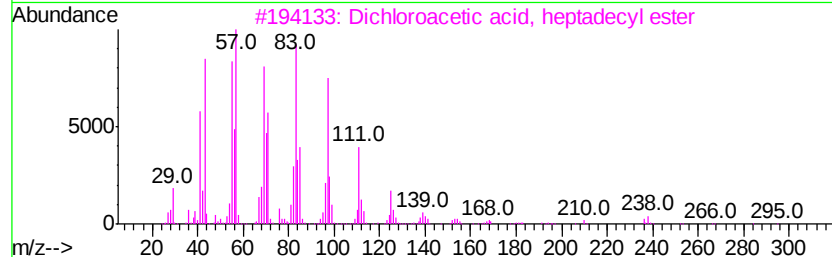
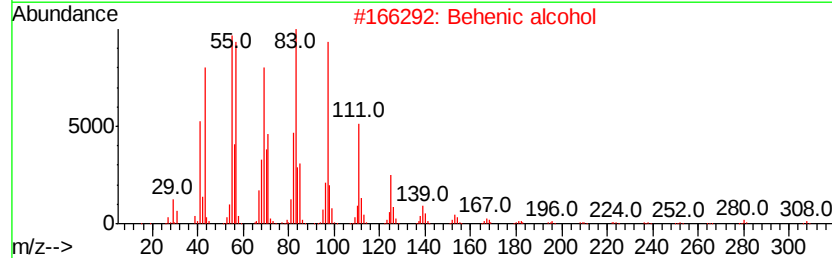
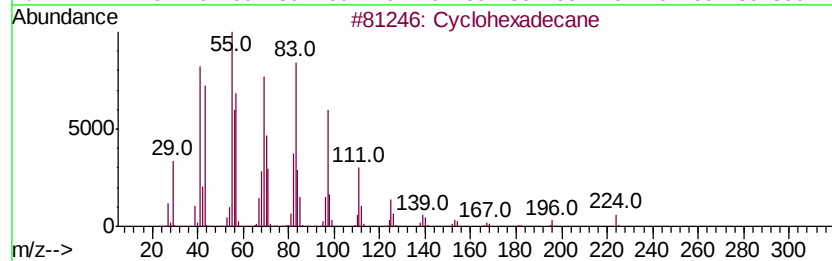
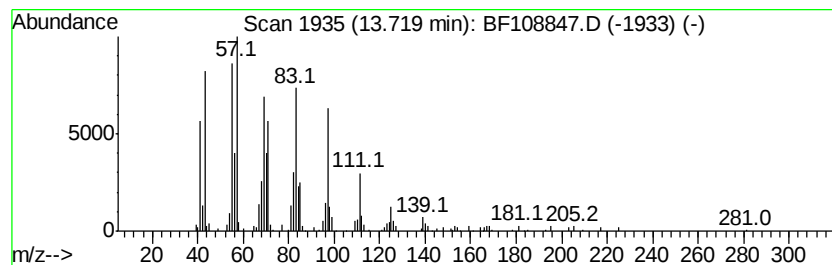
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Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	9.79 ng	742200	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	98
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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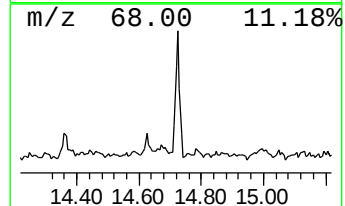
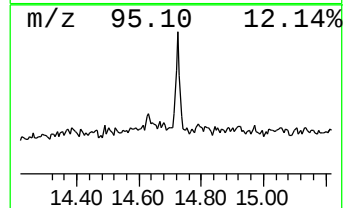
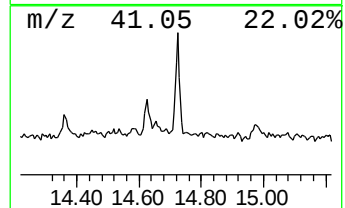
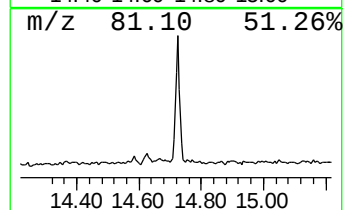
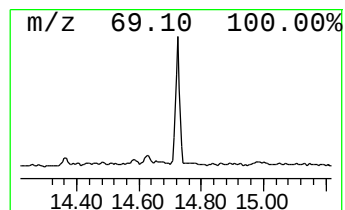
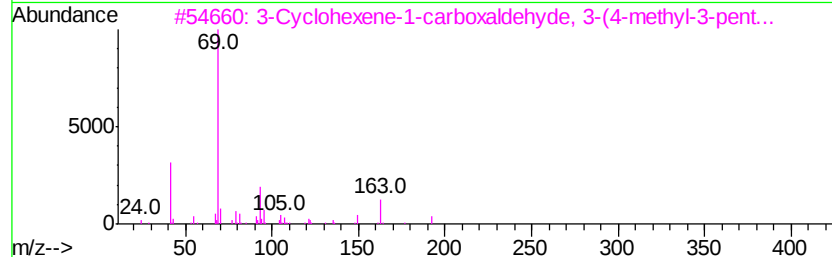
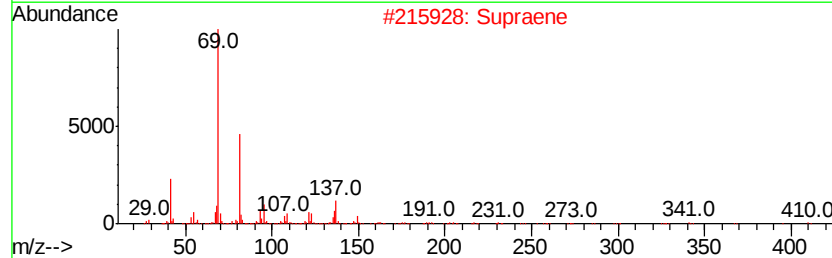
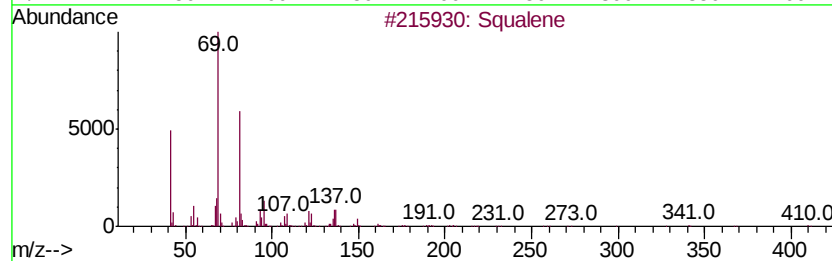
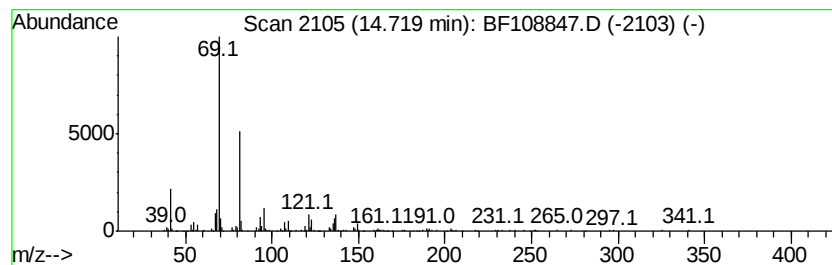
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.47 ng	278800	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	59
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



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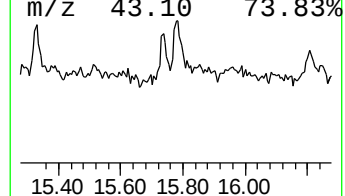
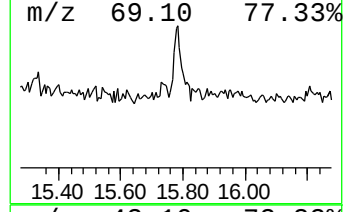
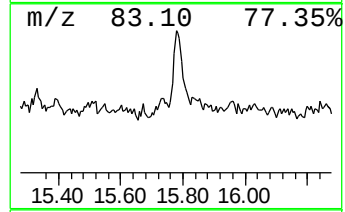
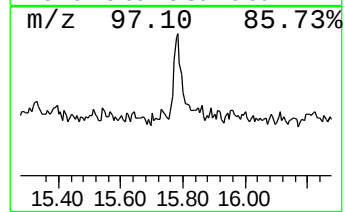
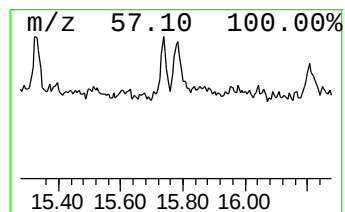
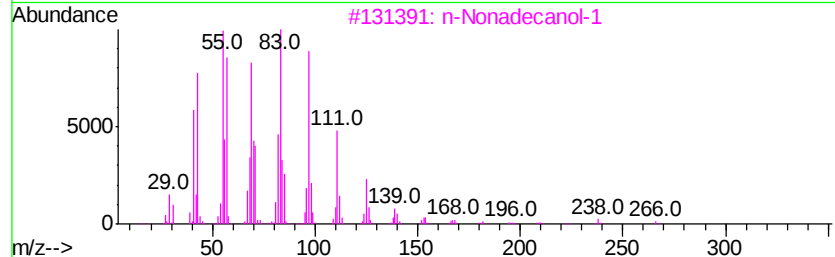
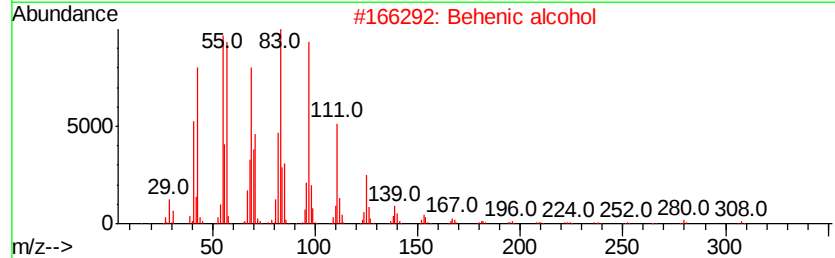
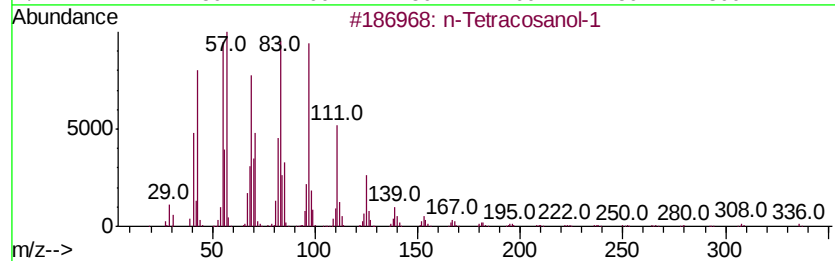
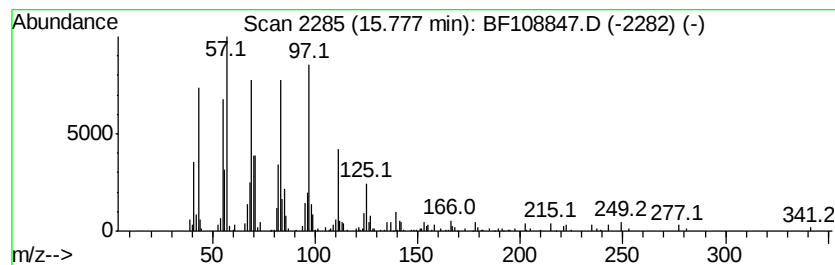
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	2.32 ng	186012	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
Data File : BF108847.D
Acq On : 7 Sep 2018 2:08
Operator : JU/SJ
Sample : J4803-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-I6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.93	2.5	ng	143062	1	6.74	1168200	20.0
unknown6.50	6.50	53.9	ng	3146460	1	6.74	1168200	20.0
n-Hexadecanoic acid	11.78	4.5	ng	282351	4	11.24	1248160	20.0
Cyclohexadecane	13.72	9.8	ng	742200	5	13.87	1516210	20.0
Squalene	14.72	3.5	ng	278800	6	15.27	1605210	20.0
n-Tetracosanol-1	15.78	2.3	ng	186012	6	15.27	1605210	20.0