

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
 Data File : BF096496.D
 Acq On : 5 Jul 2017 20:51
 Operator : SJ/MA
 Sample : I4049-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DRUM-1-070317

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-BF070117.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	3.063	164	166	174	rBV2	22807	48640	1.74%	0.206%
2	4.904	474	479	490	rVB	315033	430497	15.39%	1.820%
3	5.328	546	551	554	rBV	2709320	2652995	94.82%	11.216%
4	6.351	720	725	728	rBV	2591372	2797963	100.00%	11.829%
5	6.481	743	747	751	rBV	2766749	2683909	95.92%	11.347%
6	6.710	783	786	790	rVB	816972	641198	22.92%	2.711%
7	6.786	794	799	806	rBV	29829	61310	2.19%	0.259%
8	6.869	809	813	816	rBV	2331257	2011781	71.90%	8.505%
9	7.269	876	881	884	rBV	1578418	1652211	59.05%	6.985%
10	7.375	894	899	902	rBV	38432	40332	1.44%	0.171%
11	7.992	1000	1004	1007	rBV	1088772	848012	30.31%	3.585%
12	9.075	1183	1188	1191	rBV	2878107	2596770	92.81%	10.979%
13	9.463	1251	1254	1257	rBV	396363	302806	10.82%	1.280%
14	9.745	1298	1302	1306	rBV2	900835	769262	27.49%	3.252%
15	9.869	1320	1323	1327	rVB	43172	39500	1.41%	0.167%
16	10.086	1356	1360	1362	rBV	52370	50165	1.79%	0.212%
17	10.416	1411	1416	1421	rBV	49496	62101	2.22%	0.263%
18	10.533	1432	1436	1439	rBV	1211769	1133726	40.52%	4.793%
19	10.633	1450	1453	1456	rBV	105262	84772	3.03%	0.358%
20	10.663	1456	1458	1459	rVV	67697	52640	1.88%	0.223%
21	10.680	1459	1461	1468	rVB	107791	100389	3.59%	0.424%
22	11.110	1532	1534	1537	rBV	53676	54112	1.93%	0.229%
23	11.145	1537	1540	1545	rVB	144984	140818	5.03%	0.595%
24	11.227	1550	1554	1557	rVV	633881	548821	19.62%	2.320%
25	11.492	1597	1599	1603	rBV	64269	62405	2.23%	0.264%
26	11.798	1648	1651	1655	rBV	126719	117899	4.21%	0.498%
27	11.839	1655	1658	1660	rBV3	54130	71366	2.55%	0.302%
28	12.010	1685	1687	1689	rVB2	61077	43323	1.55%	0.183%
29	12.227	1722	1724	1729	rVB	160797	172061	6.15%	0.727%
30	12.445	1758	1761	1764	rBV	172148	201241	7.19%	0.851%
31	12.480	1764	1767	1770	rBV2	131467	197292	7.05%	0.834%
32	12.816	1821	1824	1831	rBV2	1531585	1761388	62.95%	7.447%
33	13.868	2000	2003	2006	rVB	1260457	1221077	43.64%	5.163%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

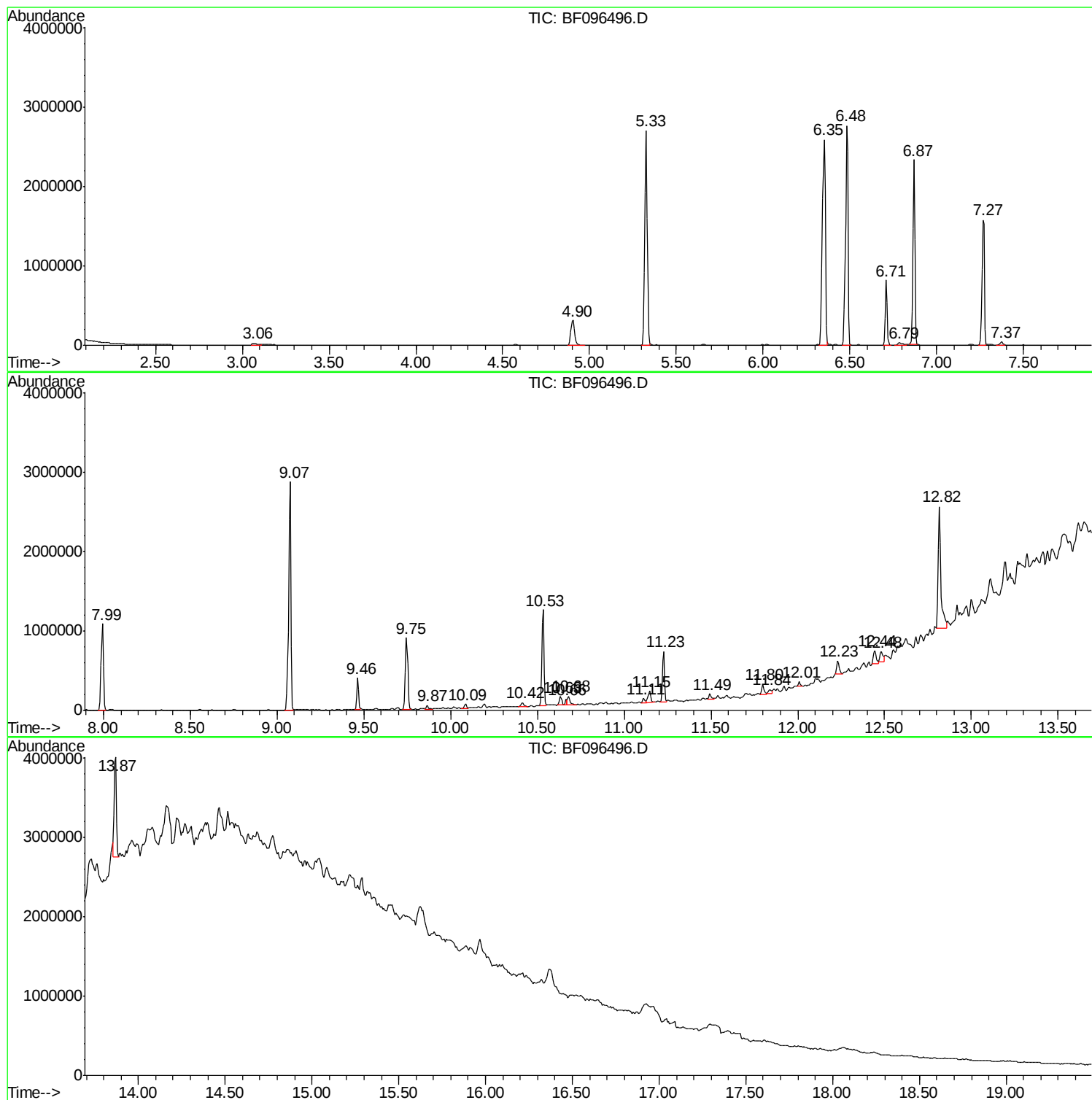
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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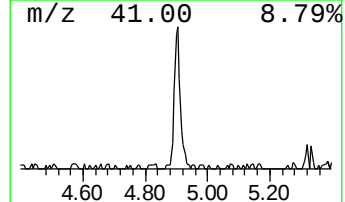
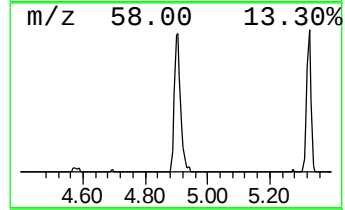
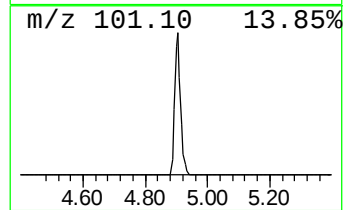
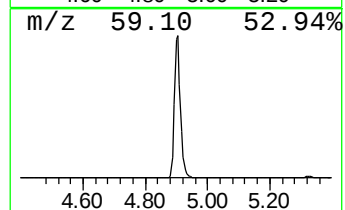
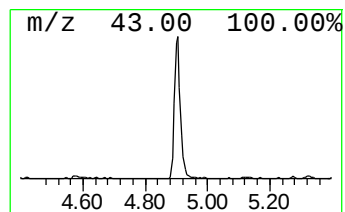
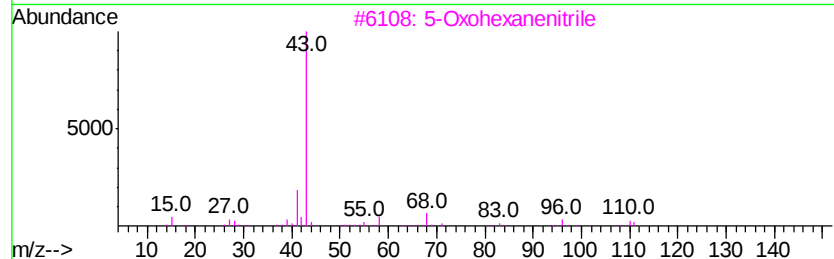
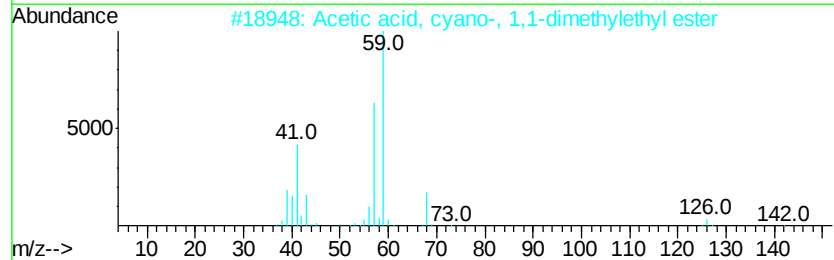
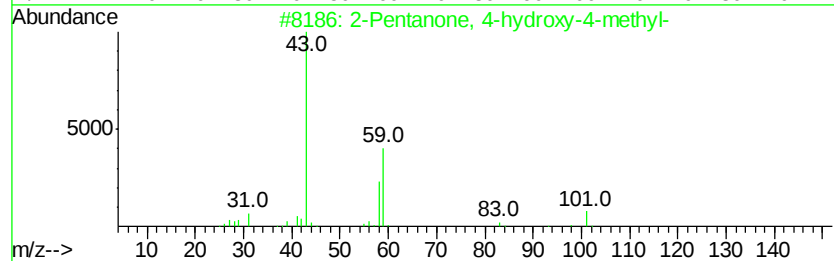
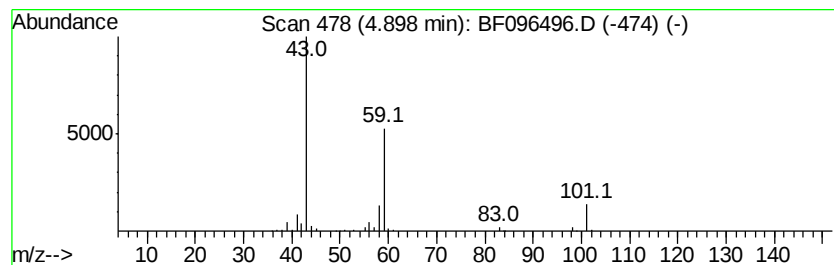
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	13.43 ng	430497	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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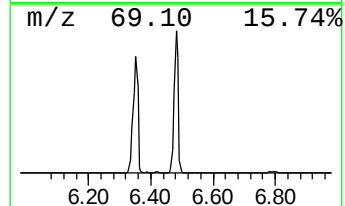
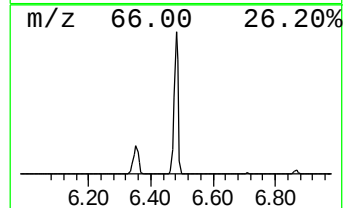
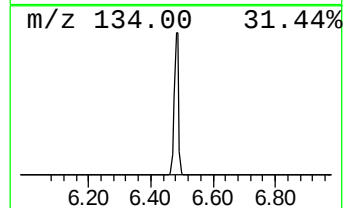
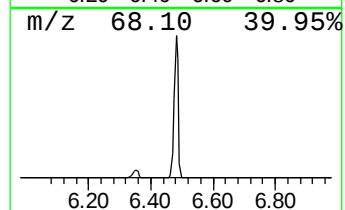
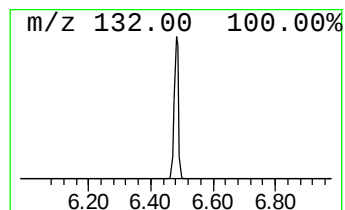
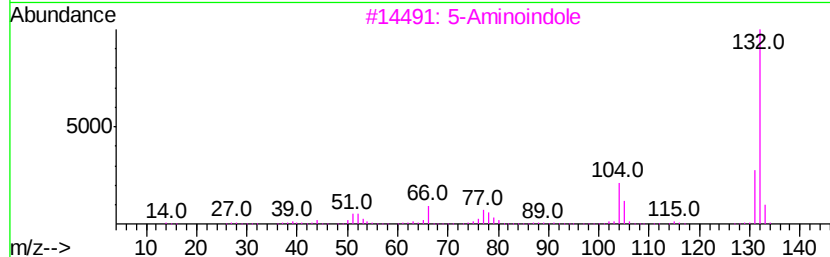
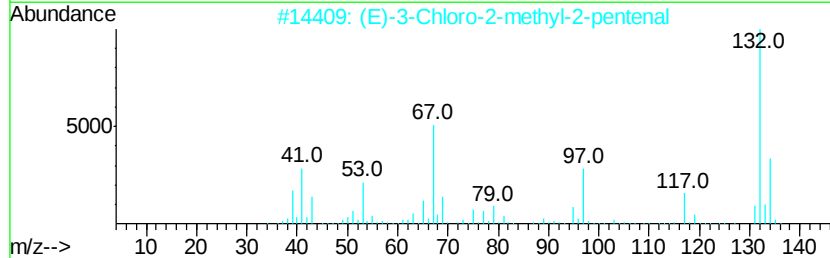
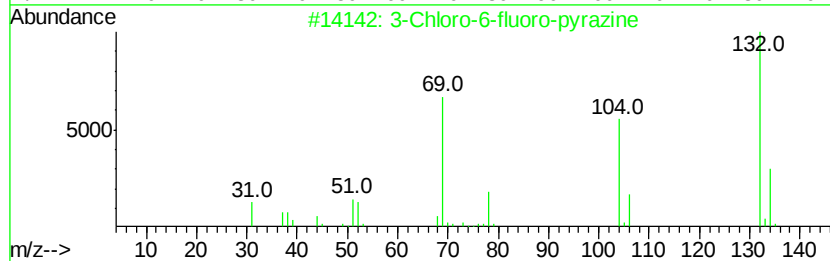
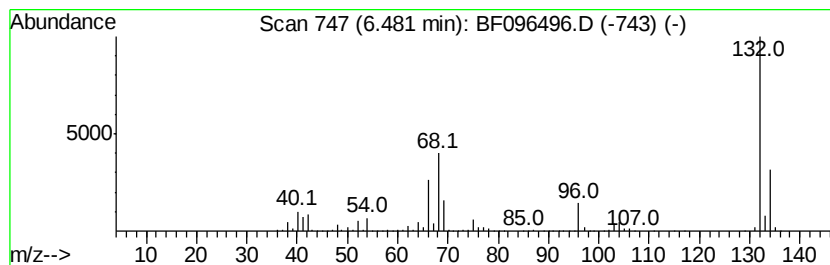
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	83.72 ng	2683910	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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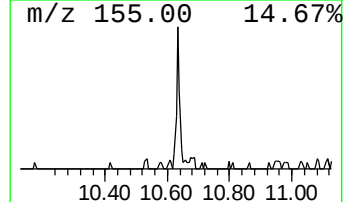
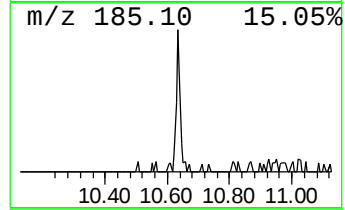
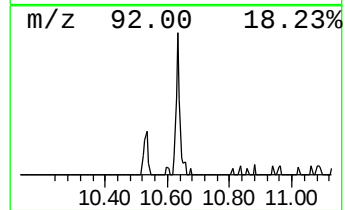
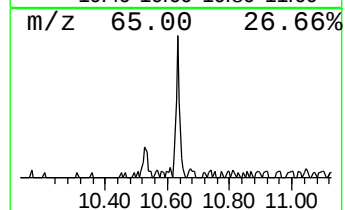
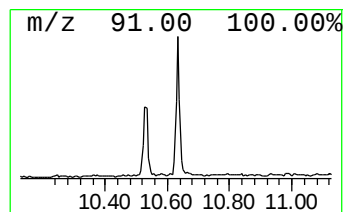
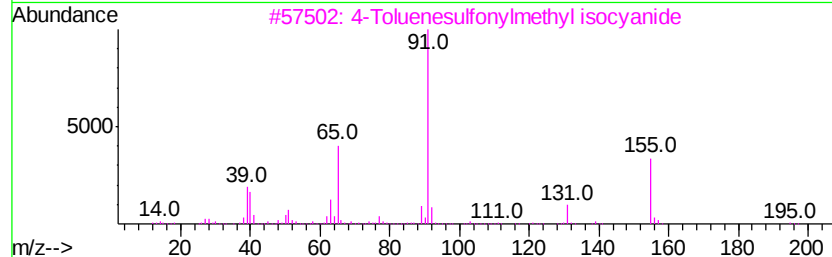
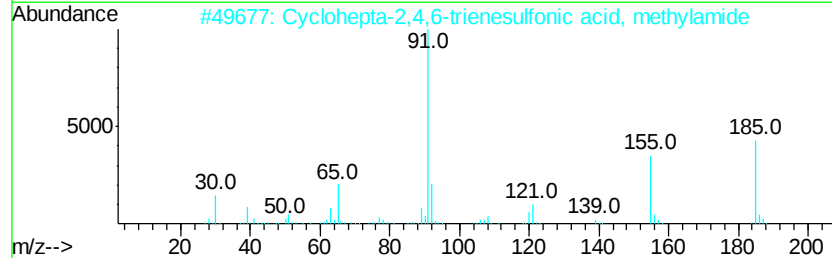
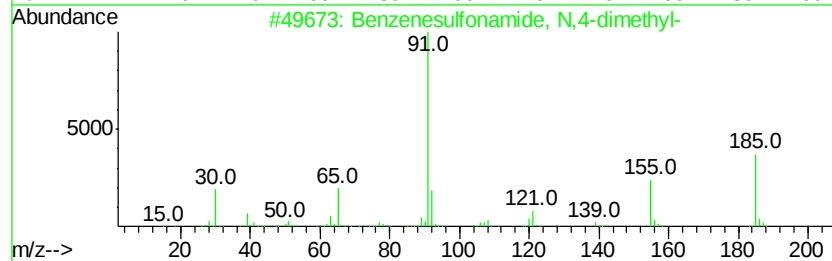
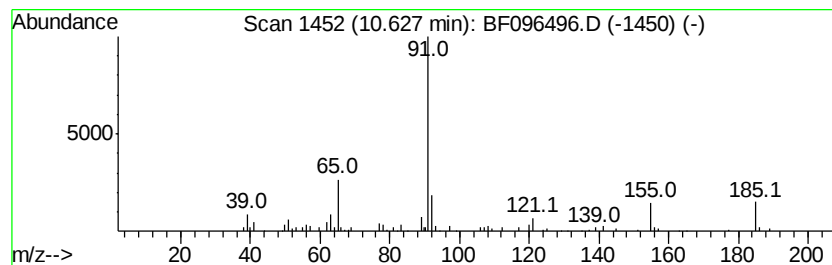
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	3.09 ng	84772	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	90
2		Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	64
3		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	43
4		Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	38
5		3-Benzylsulfanyl-3-fluoro-2-trif...	294	C12H10F4O2S	1000275-92-0	38



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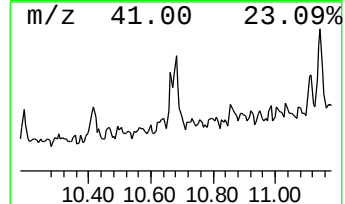
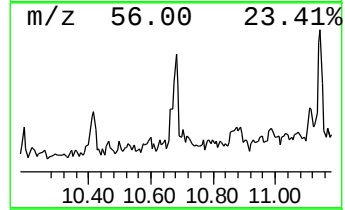
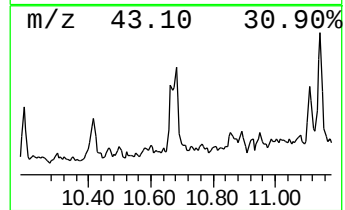
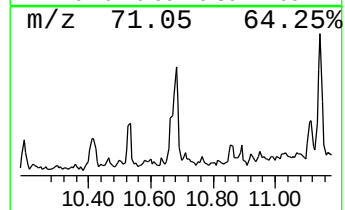
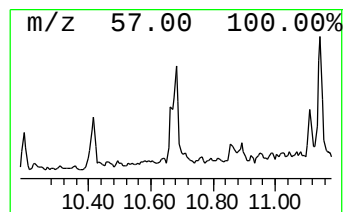
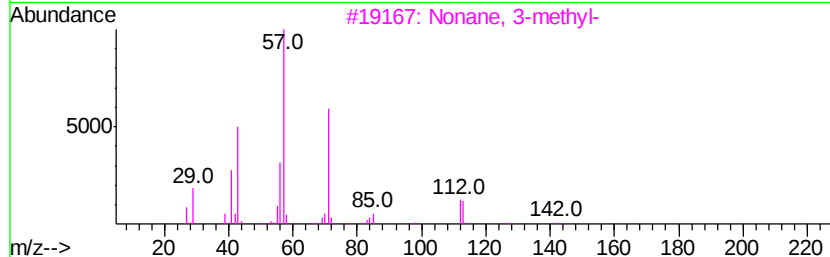
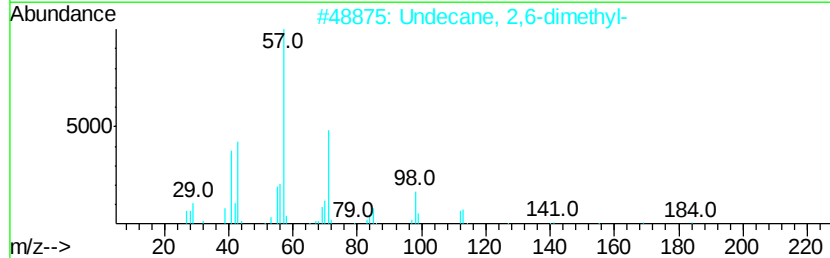
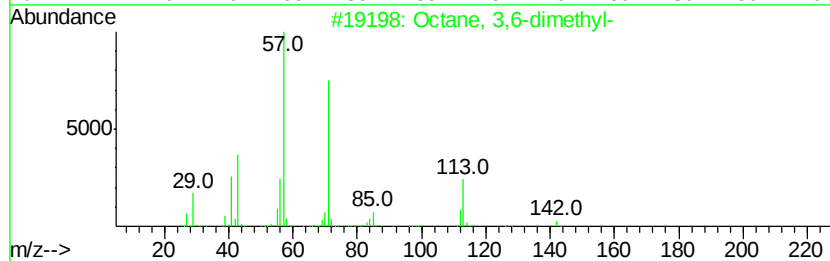
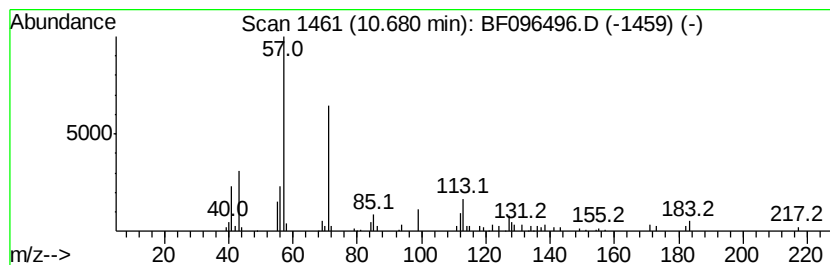
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octane, 3,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	3.66 ng	100389	Phenanthrene-d10	11.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	59
4			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	59
5			Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	58



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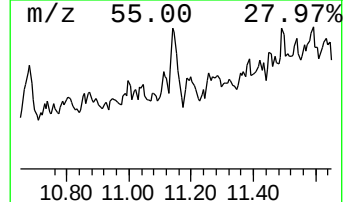
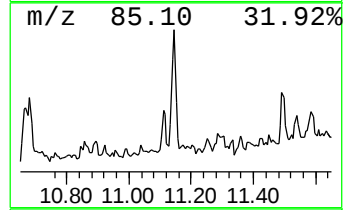
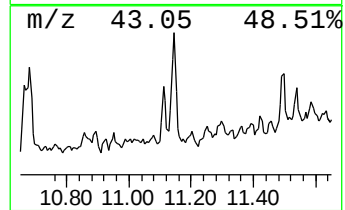
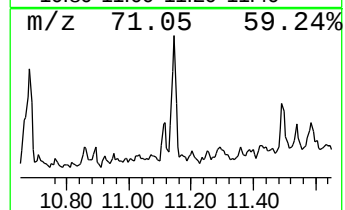
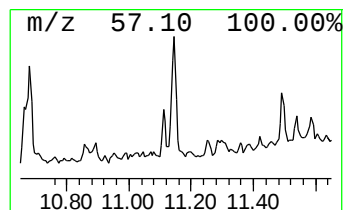
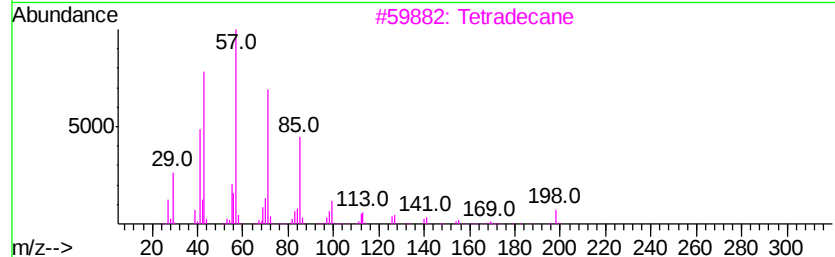
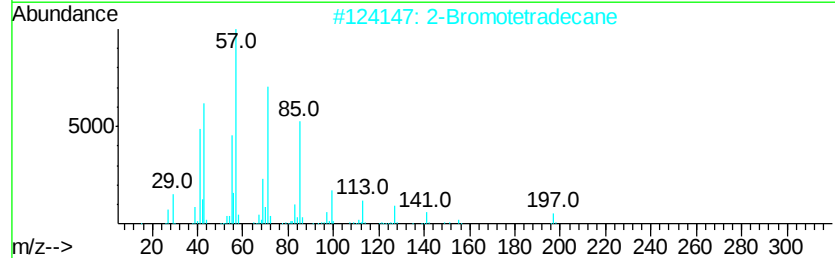
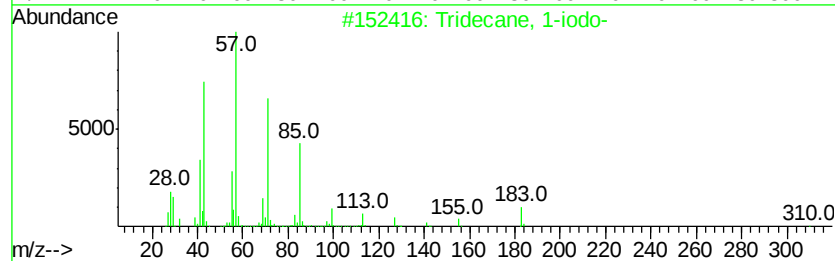
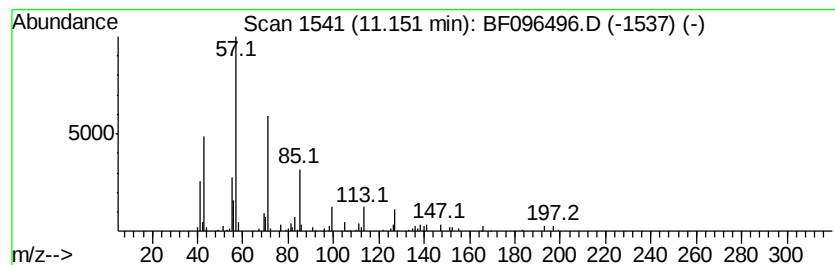
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Peak Number 6 Tridecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.15	5.13 ng	140818	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
3	Tetradecane	198	C14H30	000629-59-4	83
4	Eicosane	282	C20H42	000112-95-8	83
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096496.D
Acq On : 5 Jul 2017 20:51
Operator : SJ/MA
Sample : I4049-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-1-070317

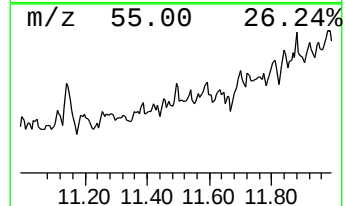
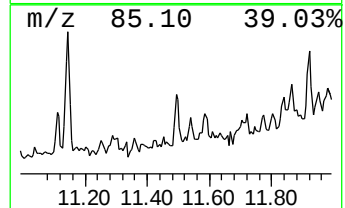
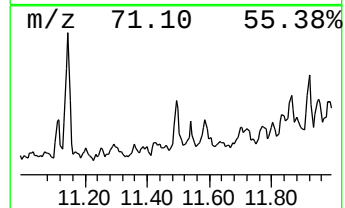
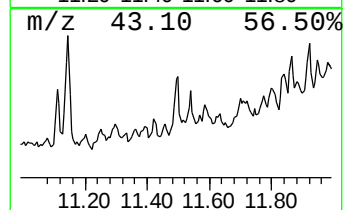
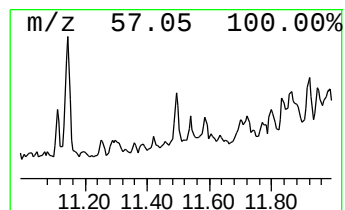
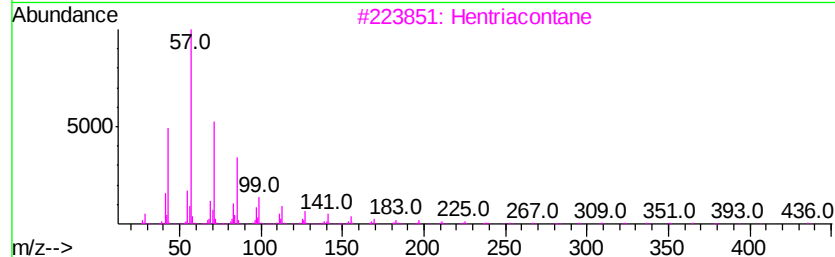
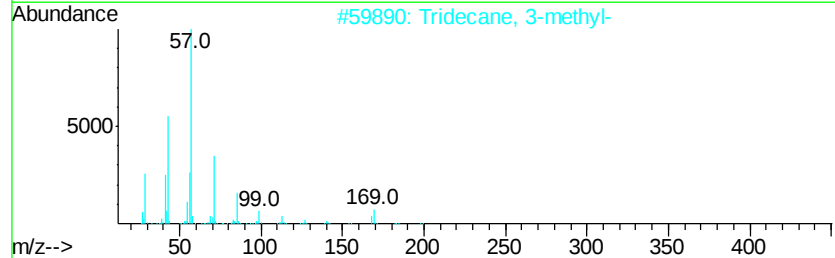
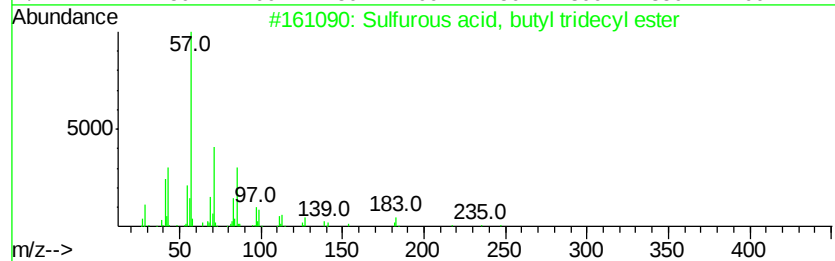
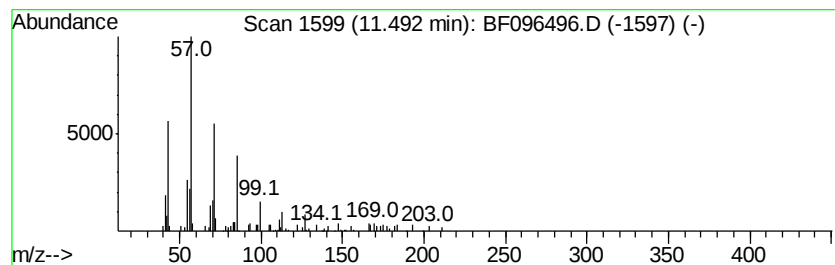
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl tridecyl e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	2.27 ng	62405	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
2		Tridecane, 3-methyl-	198	C14H30	006418-41-3	78
3		Hentriacontane	437	C31H64	000630-04-6	72
4		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	72
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096496.D
Acq On : 5 Jul 2017 20:51
Operator : SJ/MA
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Misc :
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Instrument :
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ClientSampleId :
DRUM-1-070317

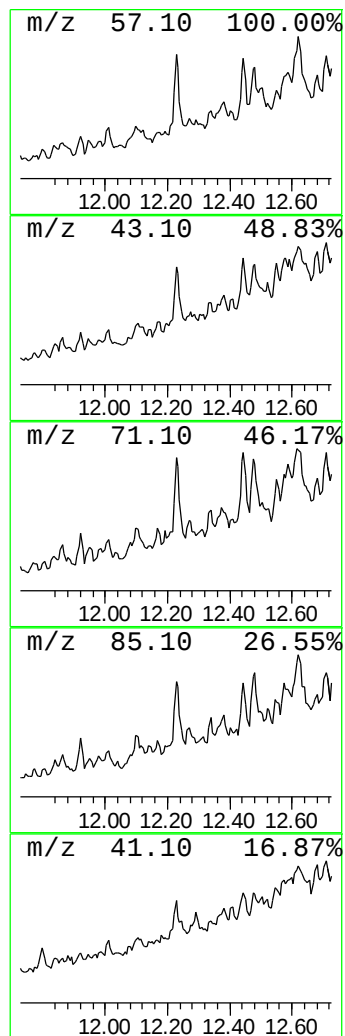
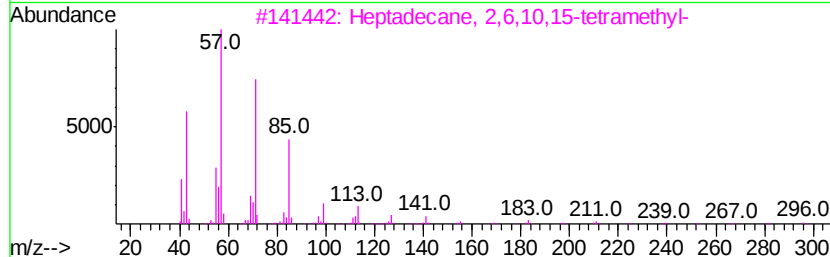
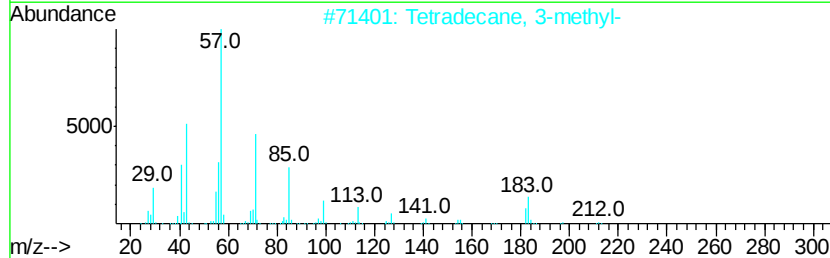
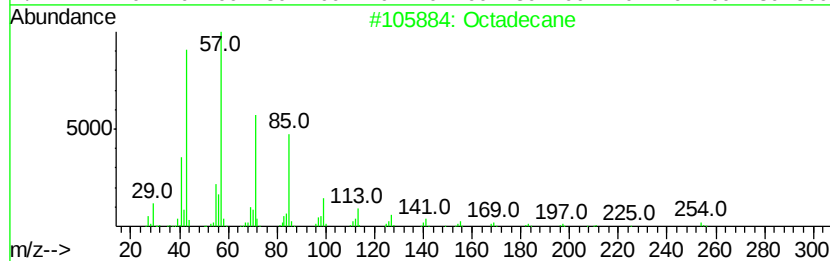
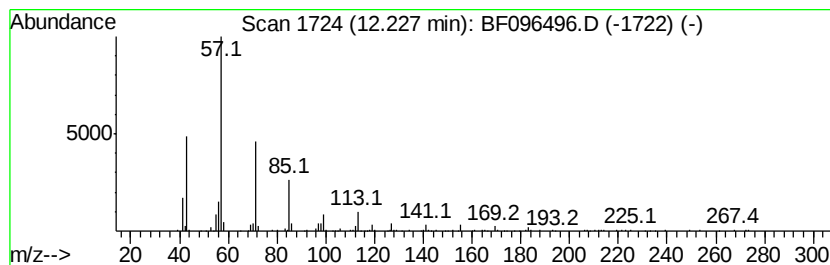
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	6.27 ng	172061	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	86
2		Tetradecane, 3-methyl-	212	C15H32	018435-22-8	86
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4		Heptacosane	380	C27H56	000593-49-7	78
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096496.D
Acq On : 5 Jul 2017 20:51
Operator : SJ/MA
Sample : I4049-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-1-070317

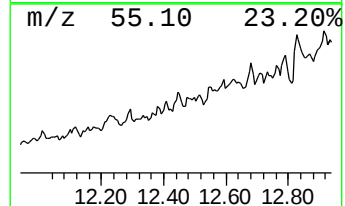
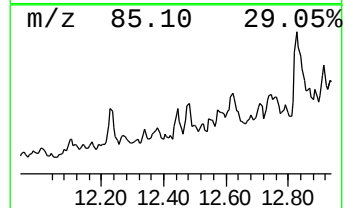
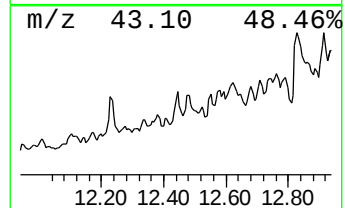
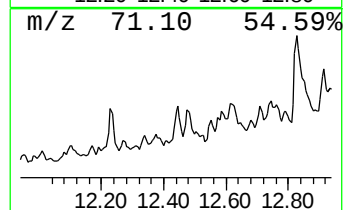
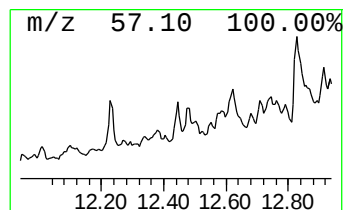
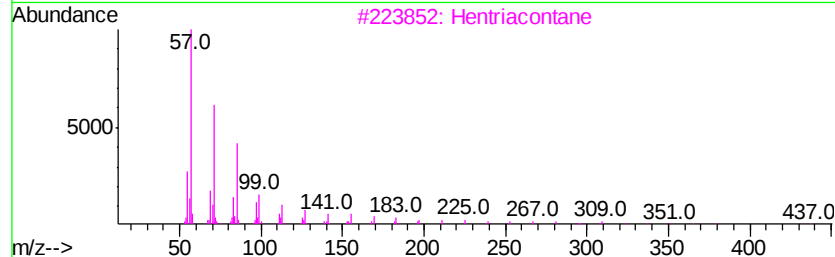
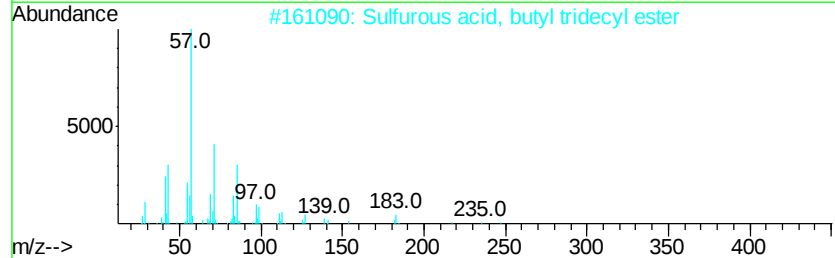
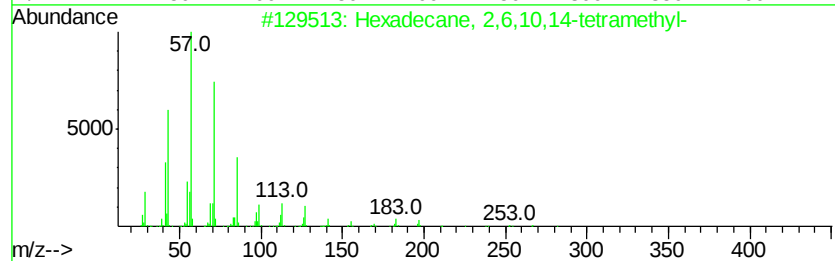
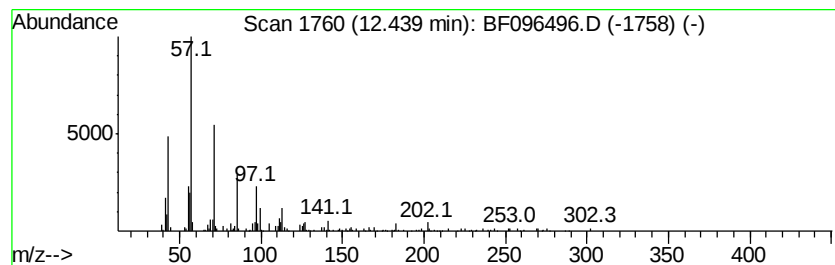
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	7.33 ng	201241	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
2		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	64
3		Hentriacontane	437	C31H64	000630-04-6	64
4		Octadecane, 6-methyl-	268	C19H40	010544-96-4	59
5		2-methyltetracosane	352	C25H52	1000376-72-6	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096496.D
Acq On : 5 Jul 2017 20:51
Operator : SJ/MA
Sample : I4049-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-1-070317

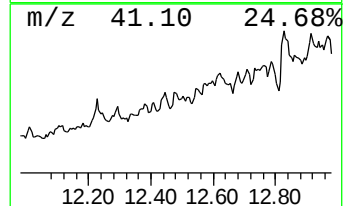
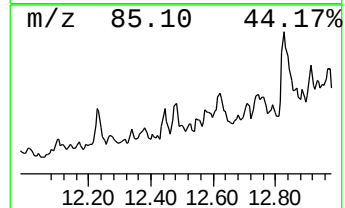
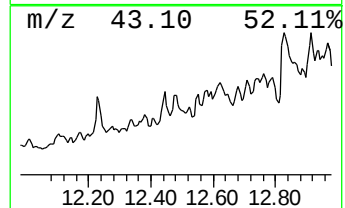
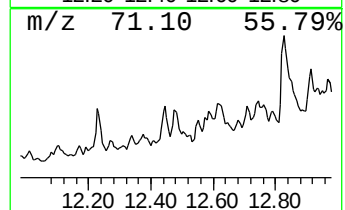
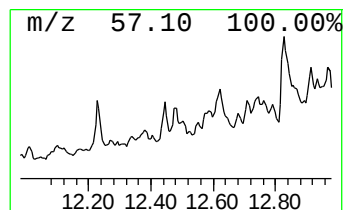
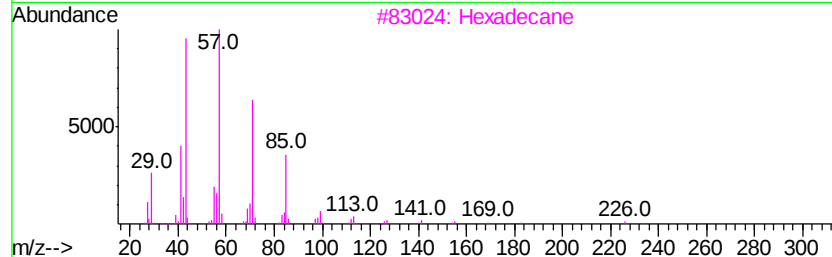
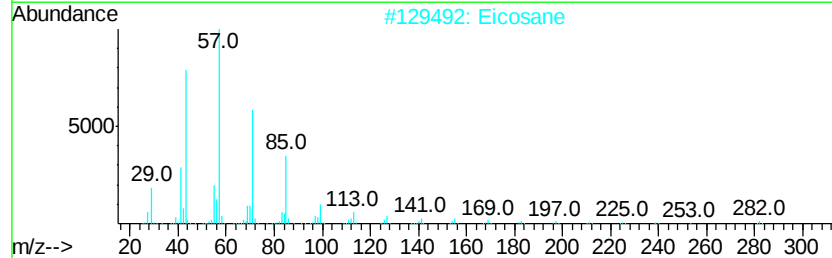
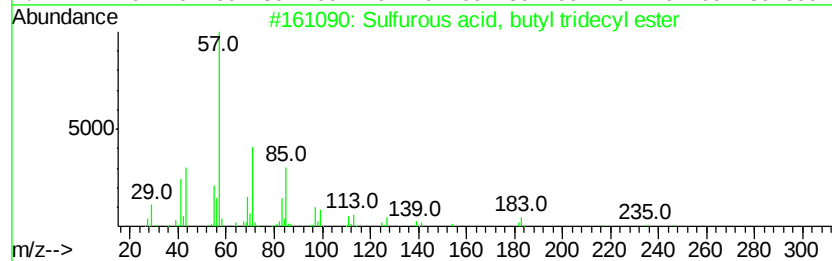
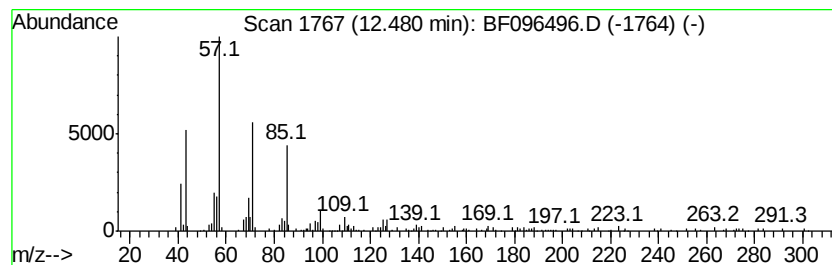
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, butyl dodec... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	7.19 ng	197292	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
2		Eicosane	282	C20H42	000112-95-8	80
3		Hexadecane	226	C16H34	000544-76-3	80
4		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72
5		Pentadecane	212	C15H32	000629-62-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096496.D
Acq On : 5 Jul 2017 20:51
Operator : SJ/MA
Sample : I4049-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.90	13.4	ng	430497	1	6.71	641198	20.0
unknown6.48	6.48	83.7	ng	2683910	1	6.71	641198	20.0
Benzenesulfonamid...	10.63	3.1	ng	84772	4	11.23	548821	20.0
Octane, 3,6-dimet...	10.68	3.7	ng	100389	4	11.23	548821	20.0
Tridecane, 1-iodo-	11.15	5.1	ng	140818	4	11.23	548821	20.0
Sulfurous acid, b...	11.49	2.3	ng	62405	4	11.23	548821	20.0
Octadecane	12.23	6.3	ng	172061	4	11.23	548821	20.0
Hexadecane, 2,6,1...	12.44	7.3	ng	201241	4	11.23	548821	20.0
Sulfurous acid, b...	12.48	7.2	ng	197292	4	11.23	548821	20.0