

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062417\
 Data File : BF096192.D
 Acq On : 24 Jun 2017 16:09
 Operator : SJ/MA
 Sample : I3851-11
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G-35-0-1.5

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-BF060517.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	1.546	7	10	26	rBV	106944	198801	13.53%	1.640%
2	4.416	494	498	521	rBV	55645	163185	11.11%	1.346%
3	5.151	619	623	651	rBV	387495	1077135	73.32%	8.885%
4	6.845	907	911	921	rBV	458721	977299	66.52%	8.062%
5	6.922	921	924	945	rVB	748612	1469089	100.00%	12.118%
6	7.263	977	982	995	rBV	241880	344224	23.43%	2.839%
7	7.498	1017	1022	1044	rBV	745177	1003009	68.27%	8.274%
8	8.186	1135	1139	1157	rBV	381950	678038	46.15%	5.593%
9	9.298	1323	1328	1340	rBV	303164	442065	30.09%	3.647%
10	10.480	1523	1529	1536	rBV3	8722	15683	1.07%	0.129%
11	11.074	1625	1630	1642	rBV	1112343	1369075	93.19%	11.293%
12	11.304	1664	1669	1675	rBV3	18073	26378	1.80%	0.218%
13	11.639	1722	1726	1732	rVB5	13569	22513	1.53%	0.186%
14	11.774	1745	1749	1755	rBV	100848	137445	9.36%	1.134%
15	11.816	1755	1756	1760	rVB2	19578	17913	1.22%	0.148%
16	11.969	1778	1782	1789	rVB6	14194	25346	1.73%	0.209%
17	12.116	1802	1807	1812	rBV2	331880	425580	28.97%	3.511%
18	12.163	1812	1815	1820	rVB2	34254	46944	3.20%	0.387%
19	12.498	1866	1872	1875	rBV6	8958	16194	1.10%	0.134%
20	12.669	1898	1901	1907	rVB4	11373	23673	1.61%	0.195%
21	12.974	1949	1953	1957	rVB	42751	46950	3.20%	0.387%
22	13.021	1957	1961	1965	rBV6	10144	16931	1.15%	0.140%
23	13.333	2010	2014	2018	rBV3	22284	32651	2.22%	0.269%
24	13.421	2024	2029	2043	rBV	254954	437335	29.77%	3.608%
25	13.668	2068	2071	2075	rBV2	12266	19598	1.33%	0.162%
26	13.745	2080	2084	2086	rBV2	42360	61310	4.17%	0.506%
27	14.427	2196	2200	2205	rBV4	27113	35271	2.40%	0.291%
28	14.474	2205	2208	2210	rVV	30140	30617	2.08%	0.253%
29	14.510	2210	2214	2219	rVV	301785	405838	27.63%	3.348%
30	14.551	2219	2221	2228	rVB	42207	57054	3.88%	0.471%
31	14.645	2235	2237	2244	rBV2	12787	20233	1.38%	0.167%
32	15.162	2322	2325	2329	rVB2	19831	23462	1.60%	0.194%
33	15.327	2350	2353	2357	rBV3	11962	17848	1.21%	0.147%
34	15.374	2358	2361	2364	rBV3	11075	15251	1.04%	0.126%

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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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.539	2387	2389	2395	rVB7	25238	37116	2.53%	0.306%
36	15.774	2426	2429	2433	rBV3	22650	25889	1.76%	0.214%
37	16.145	2488	2492	2495	rBV2	18199	29710	2.02%	0.245%
38	16.345	2520	2526	2533	rBV	101493	148193	10.09%	1.222%
39	16.651	2574	2578	2585	rBV	130216	171960	11.71%	1.418%
40	16.898	2615	2620	2626	rBV	888252	1074977	73.17%	8.867%
41	18.162	2832	2835	2840	rBV6	38247	70430	4.79%	0.581%
42	18.250	2846	2850	2855	rBV2	325584	444019	30.22%	3.663%
43	19.292	3024	3027	3031	rBV	148876	158828	10.81%	1.310%
44	19.933	3133	3136	3141	rBV	218711	261682	17.81%	2.159%

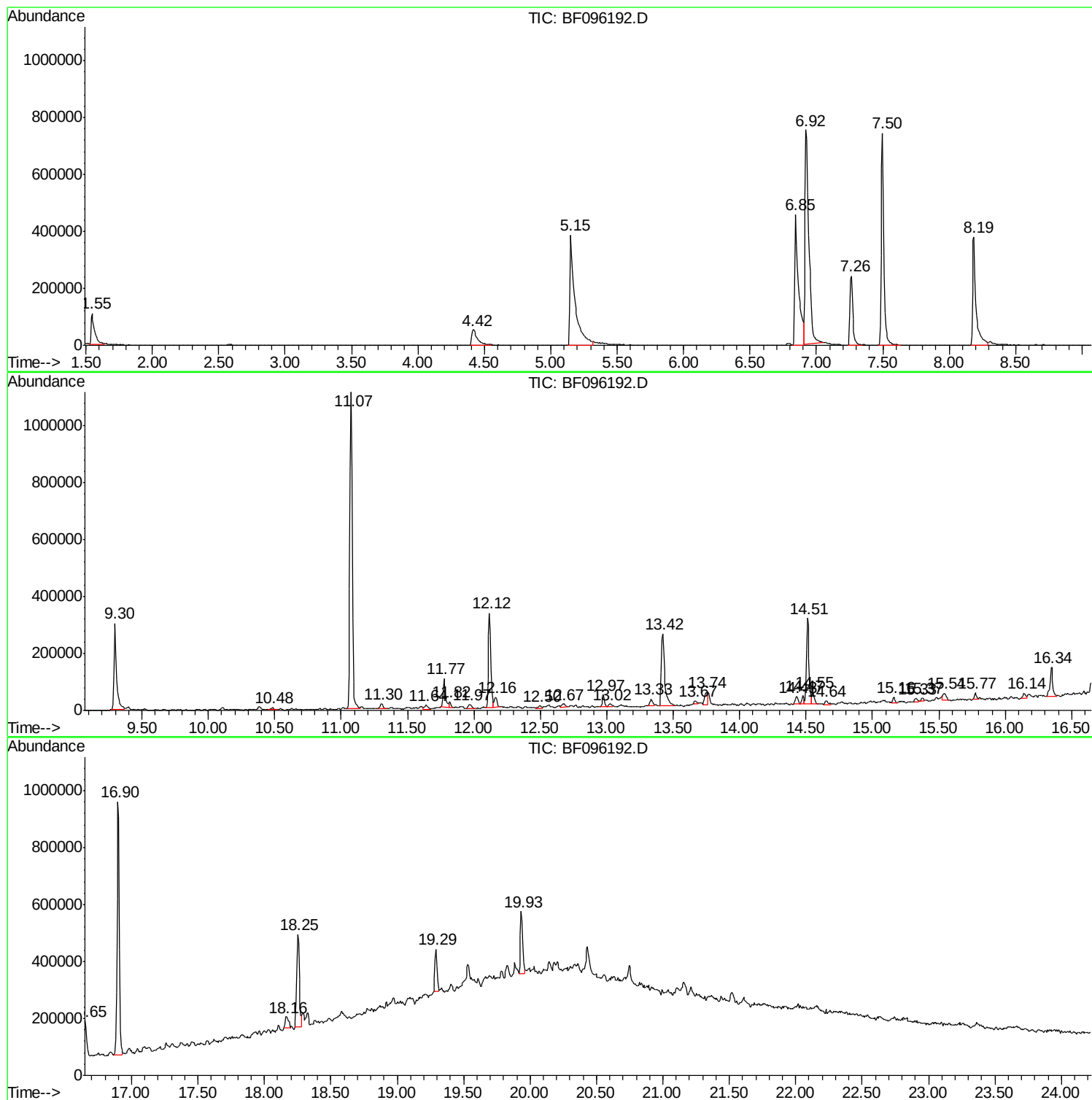
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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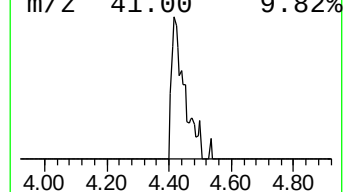
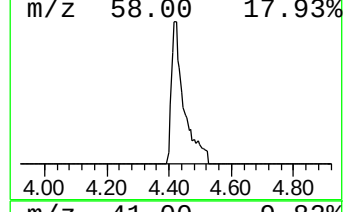
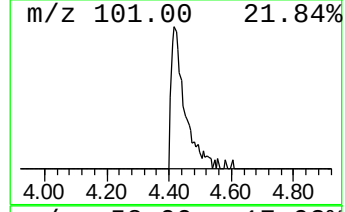
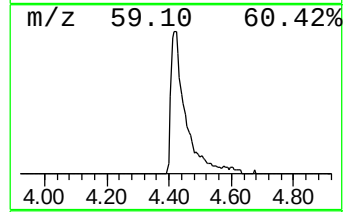
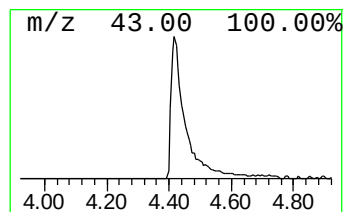
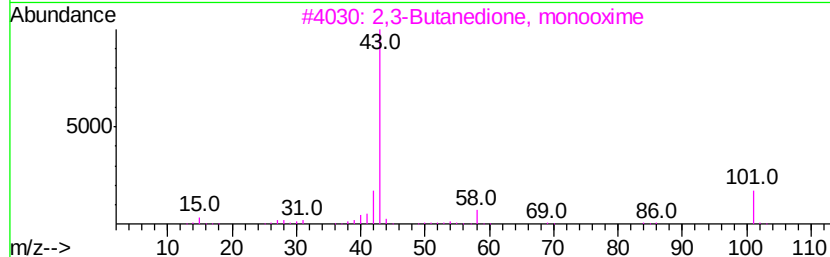
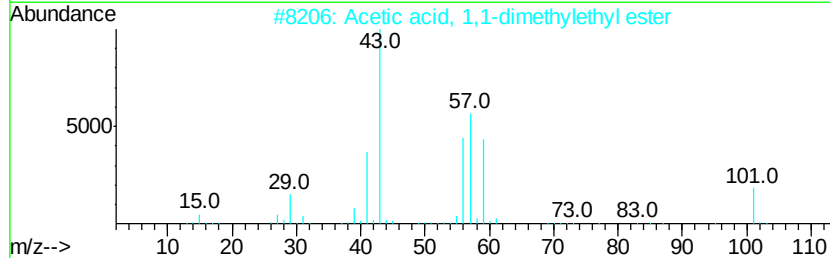
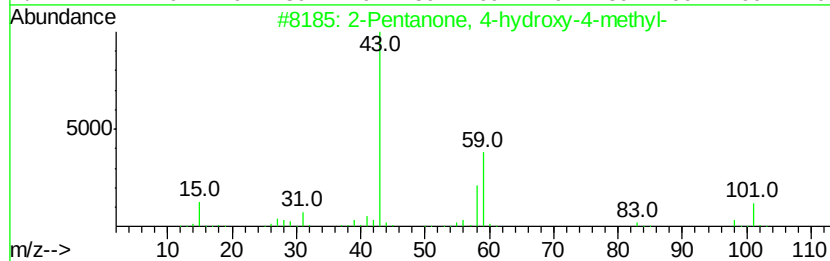
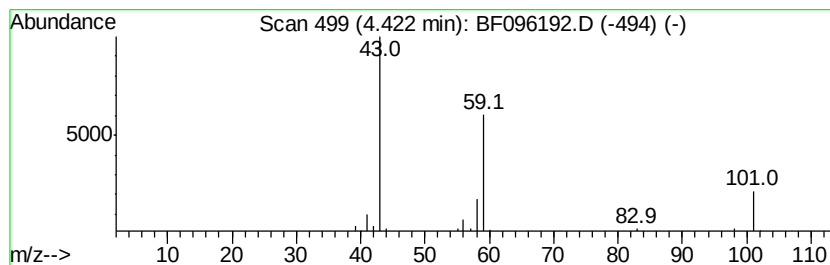
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	9.48 ng	163185	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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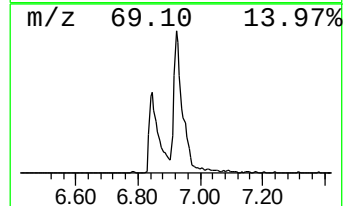
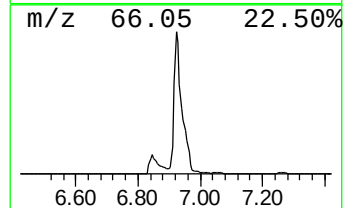
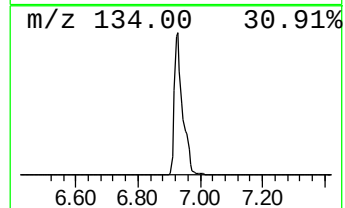
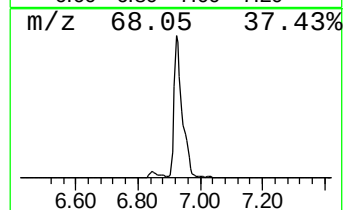
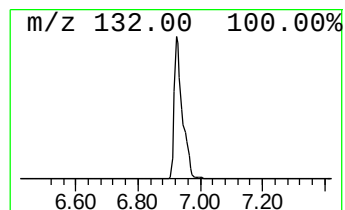
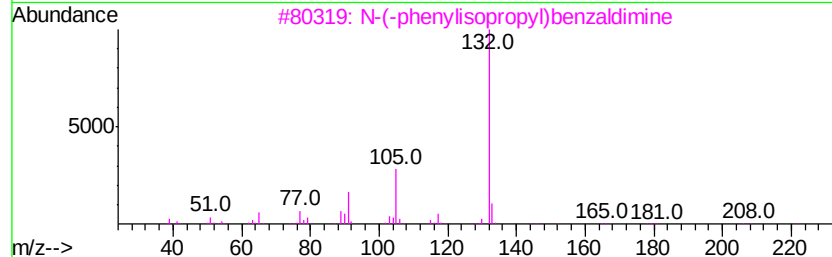
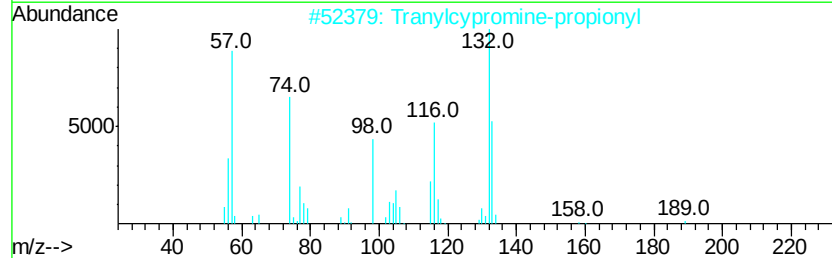
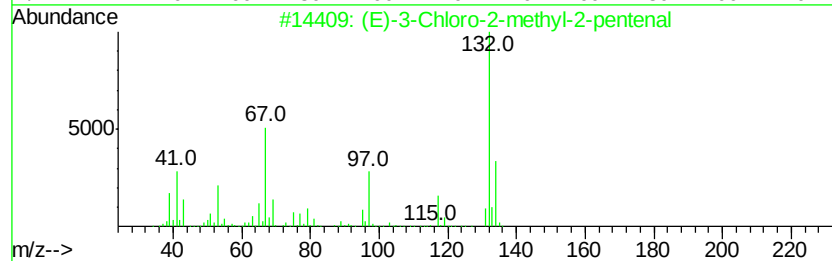
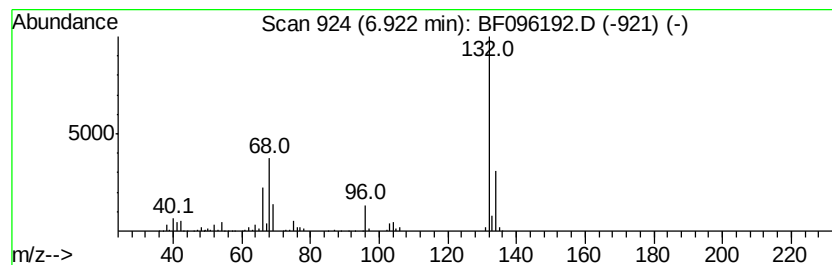
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.92 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	85.36 ng	1469090	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	12
4		Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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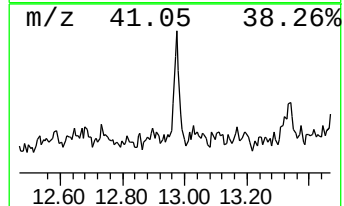
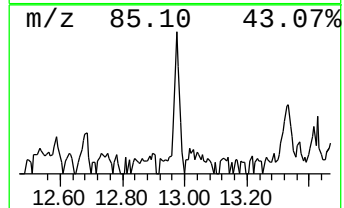
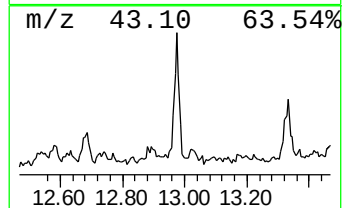
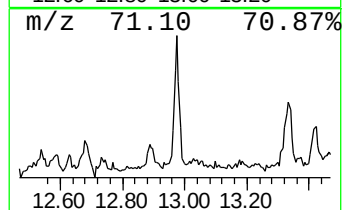
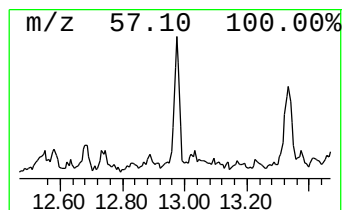
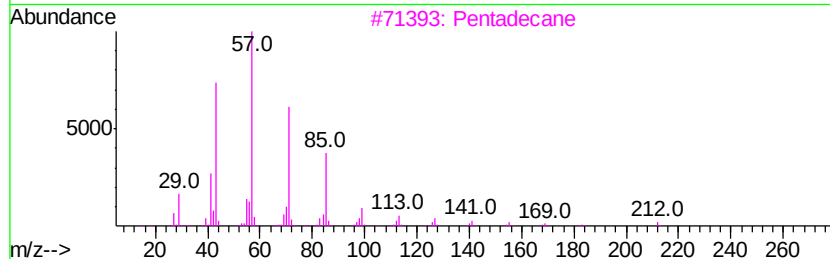
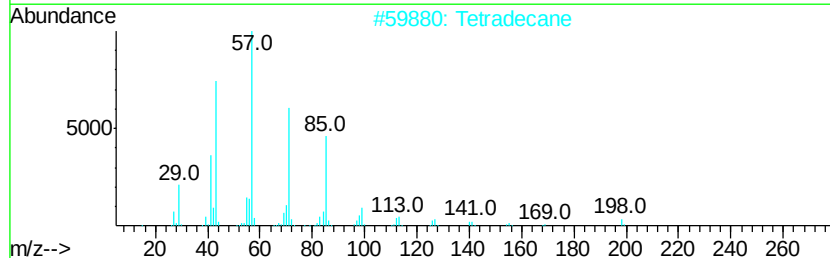
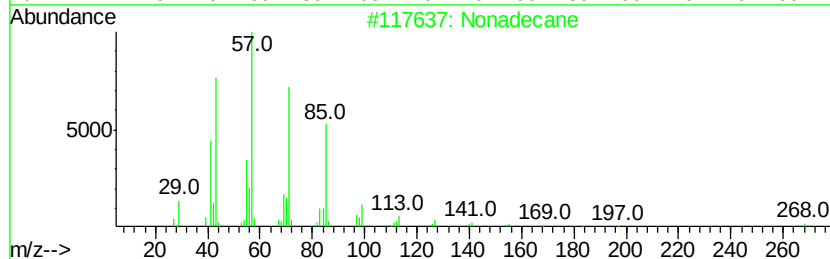
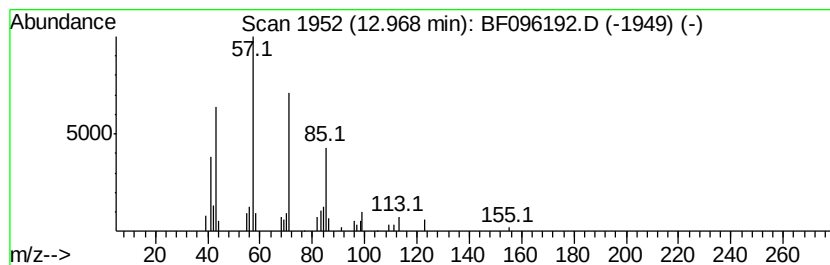
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	2.21 ng	46950	Acenaphthene-d10	12.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	90
2	Tetradecane		198	C14H30	000629-59-4	86
3	Pentadecane		212	C15H32	000629-62-9	86
4	Tritetracontane		605	C43H88	007098-21-7	86
5	Tetratetracontane		619	C44H90	007098-22-8	86



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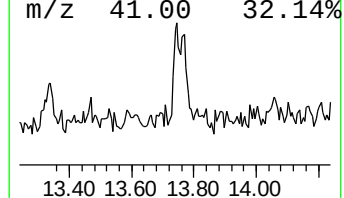
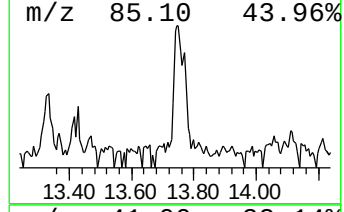
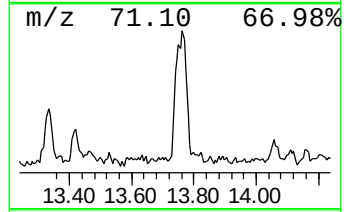
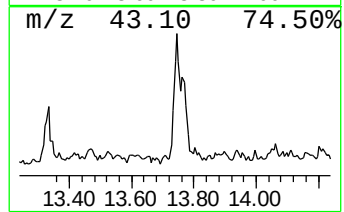
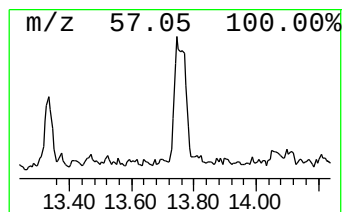
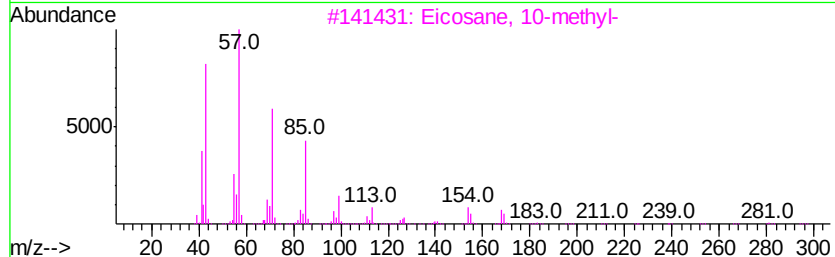
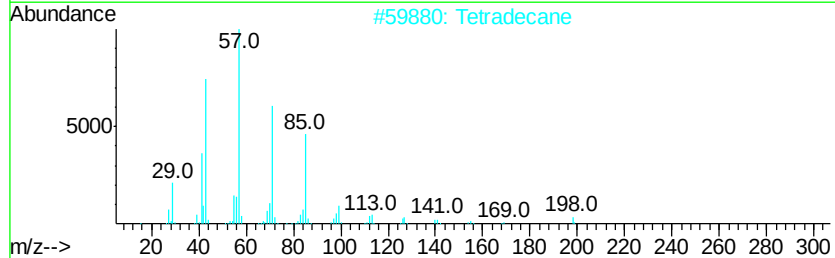
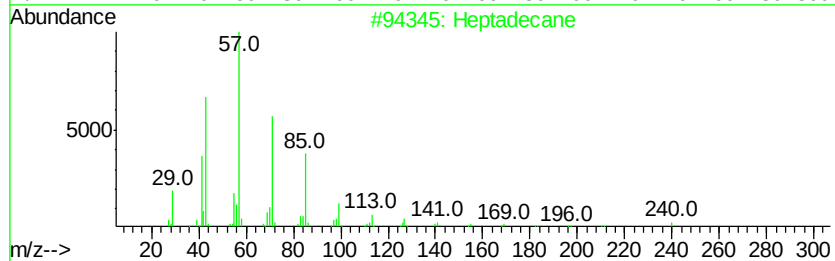
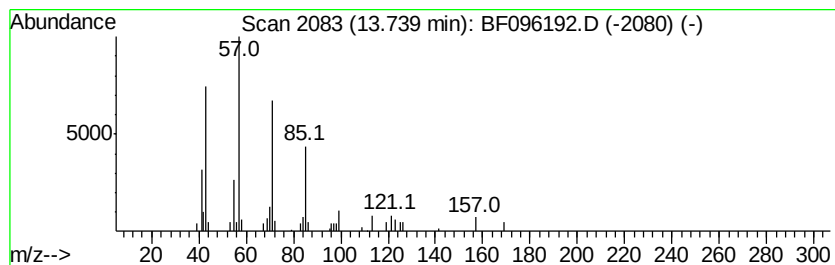
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.74	3.02 ng	61310	Phenanthrene-d10		14.51
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	64
2	Tetradecane	198	C14H30	000629-59-4	64
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	59
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	59
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	59



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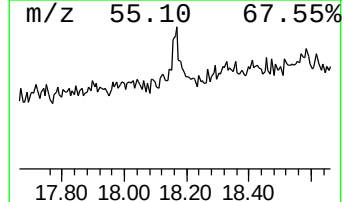
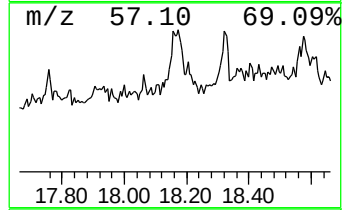
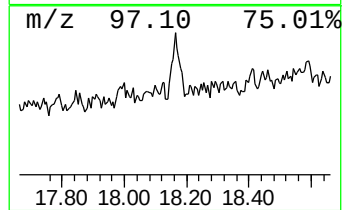
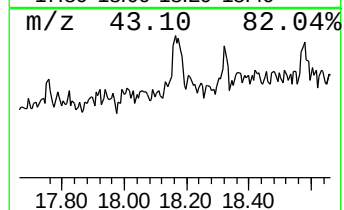
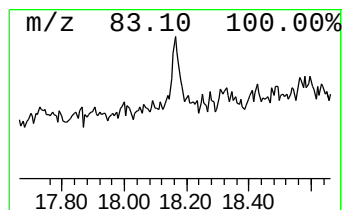
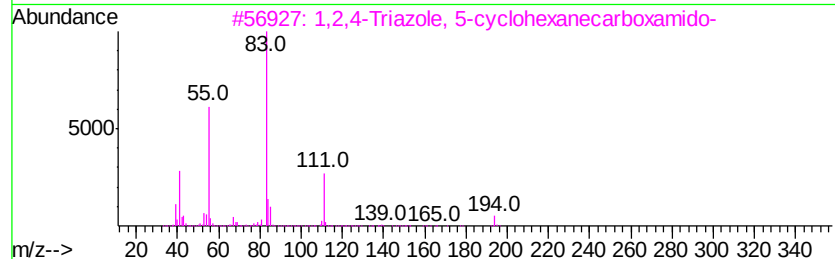
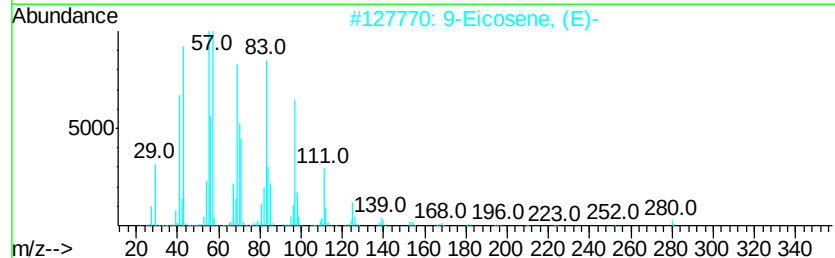
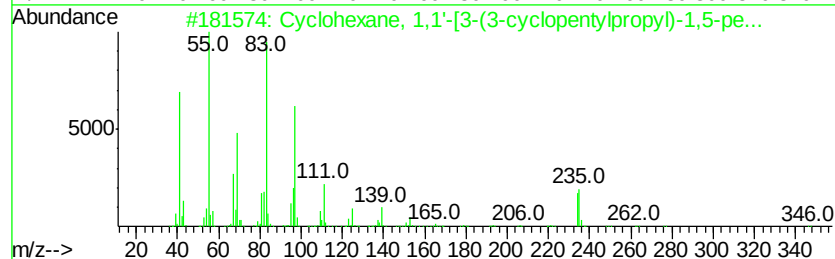
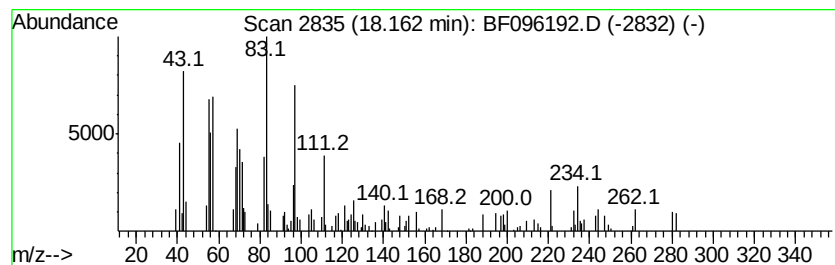
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexane, 1,1'-[3-(3-cyc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	3.17 ng	70430	Chrysene-d12	18.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1'-[3-(3-cyclophen...	346	C25H46	055401-70-2	50
2		9-Eicosene, (E)-	280	C20H40	074685-29-3	46
3		1,2,4-Triazole, 5-cyclohexanecar...	194	C9H14N4O	021051-17-2	42
4		Cyclopentanone, 3-butyl-	140	C9H16O	057283-81-5	41
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062417\
Data File : BF096192.D
Acq On : 24 Jun 2017 16:09
Operator : SJ/MA
Sample : I3851-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

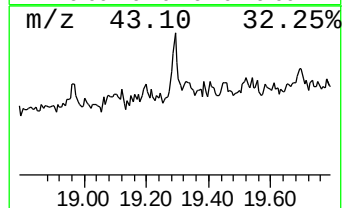
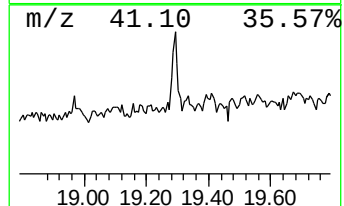
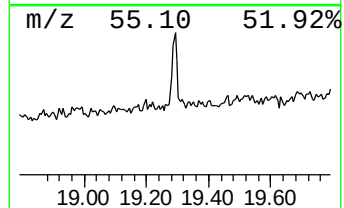
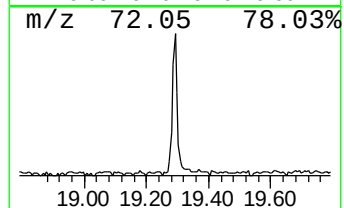
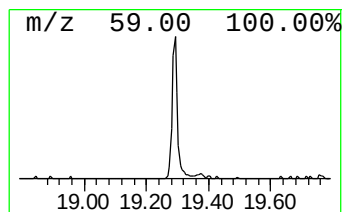
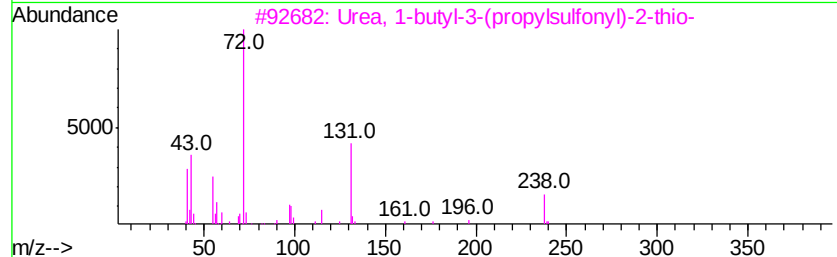
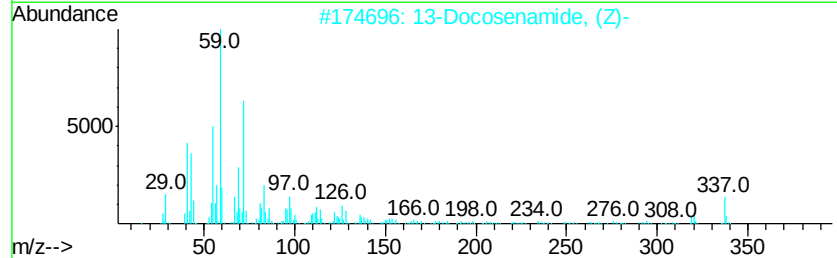
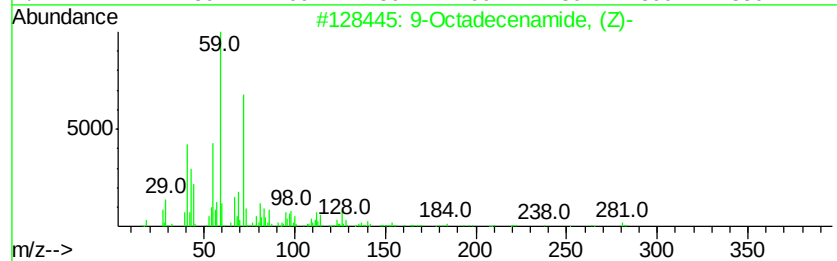
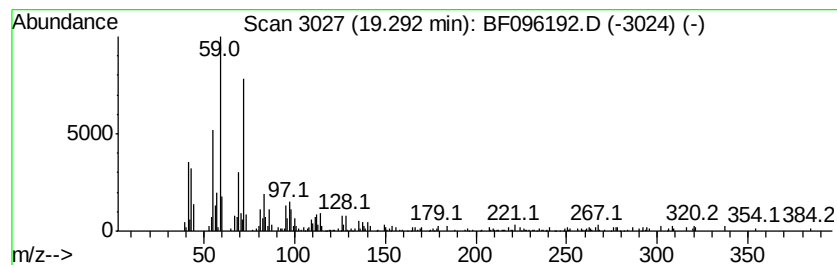
Instrument :
BNA_F
ClientSampleId :
G-35-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.29	12.14 ng	158828	Perylene-d12	19.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	80
3		Urea, 1-butyl-3-(propylsulfonyl)...	238	C8H18N2O2S2	024539-91-1	35
4		2-Butanamine, N,N-dimethyl-	101	C6H15N	000921-04-0	27
5		1,1,3-Trimethyl-1-silacyclobutane	114	C6H14Si	002295-13-8	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062417\
Data File : BF096192.D
Acq On : 24 Jun 2017 16:09
Operator : SJ/MA
Sample : I3851-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-35-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.42	9.5	ng	163185	1	7.26	344224	20.0
unknown6.92	6.92	85.4	ng	1469090	1	7.26	344224	20.0
Nonadecane	12.97	2.2	ng	46950	3	12.12	425580	20.0
Heptadecane	13.74	3.0	ng	61310	4	14.51	405838	20.0
Cyclohexane, 1,1'...	18.16	3.2	ng	70430	5	18.26	444019	20.0
9-Octadecenamide,...	19.29	12.1	ng	158828	6	19.93	261682	20.0