

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\
 Data File : BF096882.D
 Acq On : 19 Jul 2017 20:56
 Operator : SJ/JU
 Sample : I4280-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-01-071817-A

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-BF071317.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	2.057	7	12	21	rVB2	43422	98568	3.60%	0.458%
2	4.757	467	471	480	rVB	194204	285070	10.42%	1.325%
3	5.193	541	545	549	rBV	2195767	2424855	88.60%	11.270%
4	6.239	718	723	734	rBV	2451893	2736763	100.00%	12.720%
5	6.357	739	743	746	rBV	2464800	2433027	88.90%	11.308%
6	6.587	778	782	786	rBV	856855	679762	24.84%	3.159%
7	6.745	804	809	812	rBV	2048230	1848795	67.55%	8.593%
8	7.151	873	878	881	rBV	1449153	1422895	51.99%	6.613%
9	7.869	996	1000	1003	rBV	1041051	836621	30.57%	3.889%
10	8.951	1178	1184	1187	rBV	2479450	2304648	84.21%	10.712%
11	9.045	1197	1200	1203	rVB	33560	28225	1.03%	0.131%
12	9.339	1247	1250	1256	rVB	308602	274371	10.03%	1.275%
13	9.569	1286	1289	1293	rBV	42747	34732	1.27%	0.161%
14	9.616	1293	1297	1301	rBV	932245	803838	29.37%	3.736%
15	10.069	1371	1374	1377	rVB	58472	46962	1.72%	0.218%
16	10.286	1406	1411	1414	rBV	20737	30592	1.12%	0.142%
17	10.404	1426	1431	1434	rBV	1141794	1062846	38.84%	4.940%
18	10.539	1451	1454	1462	rBV	66558	75966	2.78%	0.353%
19	10.986	1526	1530	1533	rBV	46428	36199	1.32%	0.168%
20	11.092	1544	1548	1551	rBV	791559	660576	24.14%	3.070%
21	11.116	1551	1552	1557	rVB	45736	27499	1.00%	0.128%
22	11.410	1598	1602	1606	rBV	32091	30319	1.11%	0.141%
23	12.298	1750	1753	1758	rVB	90805	82035	3.00%	0.381%
24	12.521	1786	1791	1794	rBV	79181	82022	3.00%	0.381%
25	12.680	1813	1818	1821	rBV	1564539	1547764	56.55%	7.194%
26	12.857	1845	1848	1851	rVB3	26135	31479	1.15%	0.146%
27	12.921	1851	1859	1863	rBV8	28796	62336	2.28%	0.290%
28	13.468	1948	1952	1956	rBV4	19450	41562	1.52%	0.193%
29	13.586	1969	1972	1978	rVB2	93062	112466	4.11%	0.523%
30	13.721	1990	1995	1998	rBV	574190	613596	22.42%	2.852%
31	15.092	2224	2228	2231	rBV	414915	455491	16.64%	2.117%
32	15.709	2330	2333	2339	rVB2	106859	172110	6.29%	0.800%
33	16.086	2394	2397	2406	rVB2	66838	131240	4.80%	0.610%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CL-01-071817-A

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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

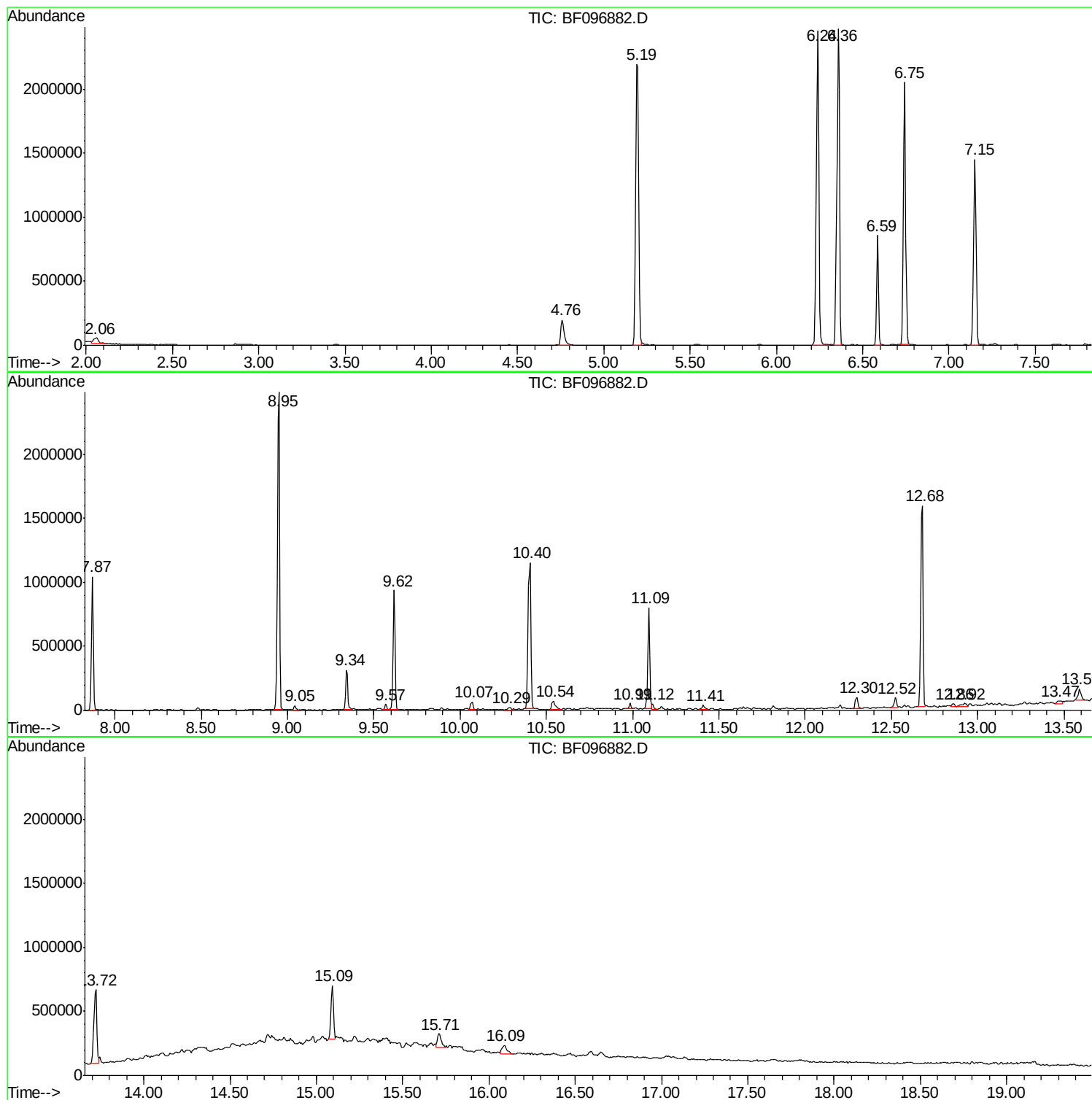
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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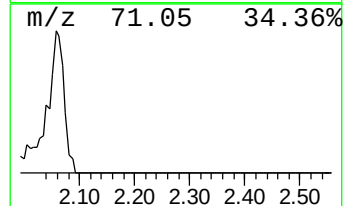
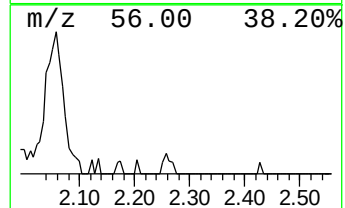
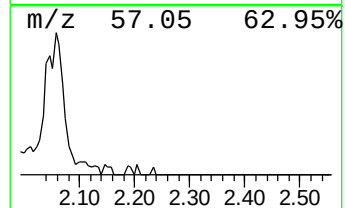
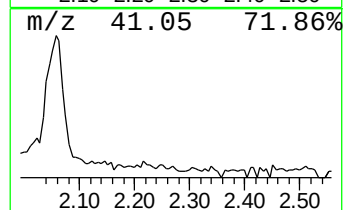
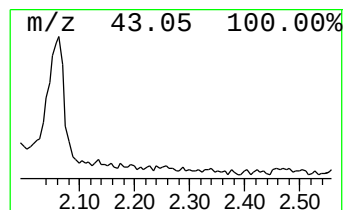
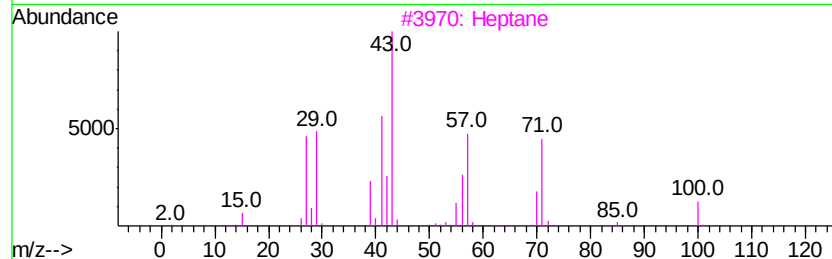
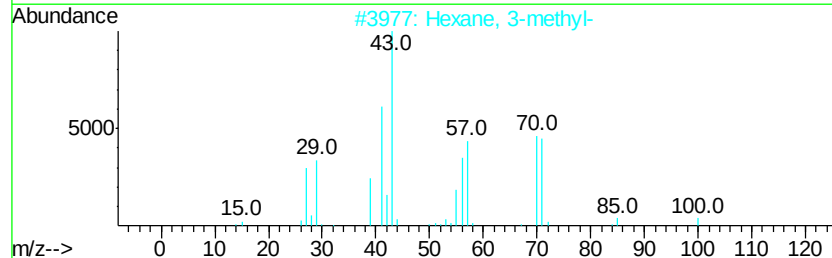
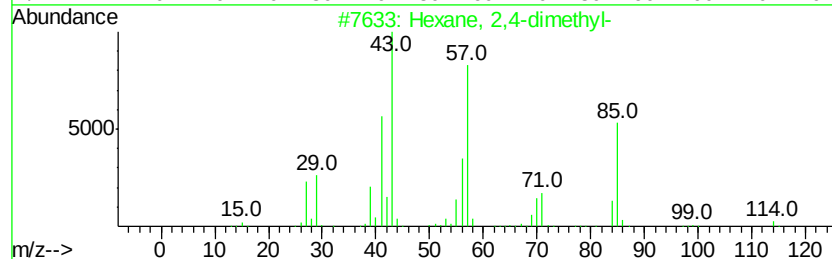
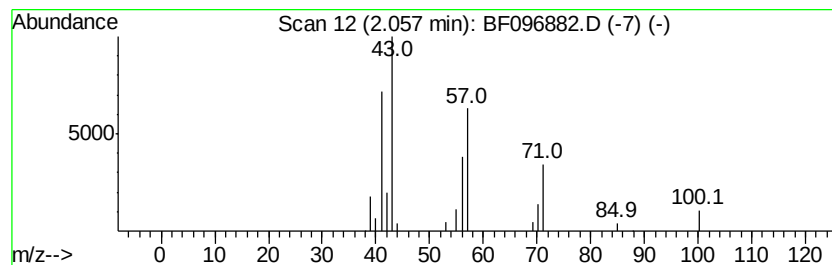
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexane, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	2.90 ng	98568	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
2		Hexane, 3-methyl-	100	C7H16	000589-34-4	64
3		Heptane	100	C7H16	000142-82-5	59
4		Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	40
5		Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	36



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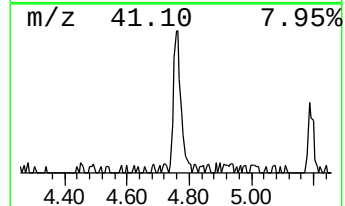
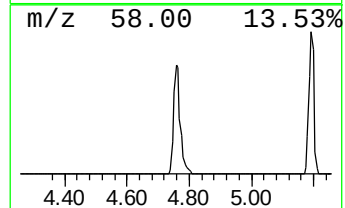
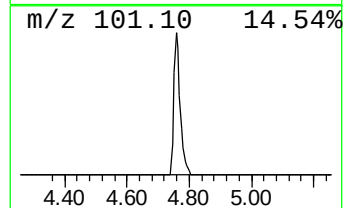
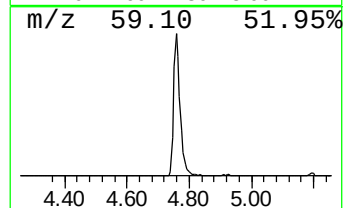
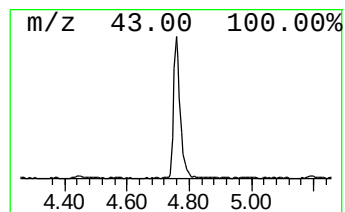
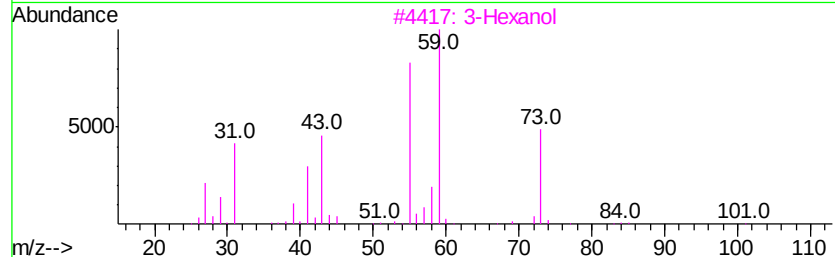
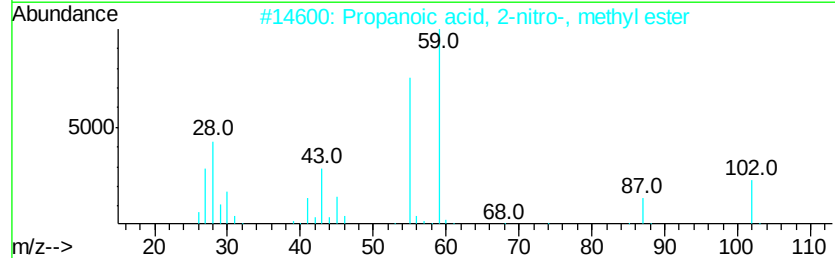
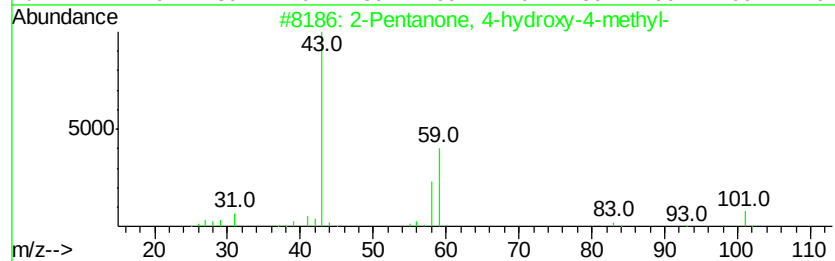
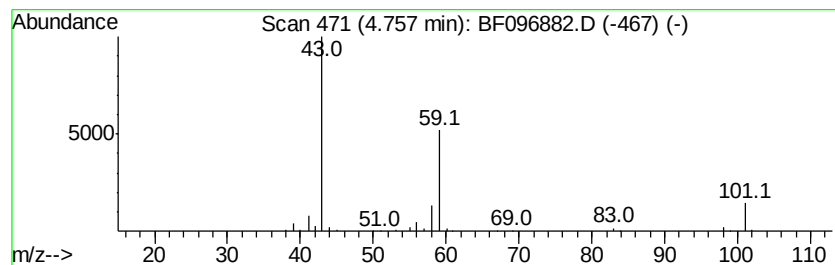
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	8.39 ng	285070	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
3		3-Hexanol	102	C6H14O	000623-37-0	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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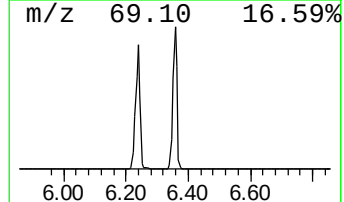
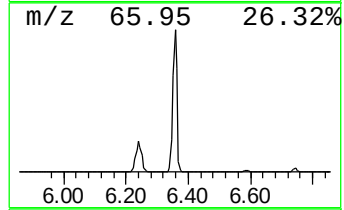
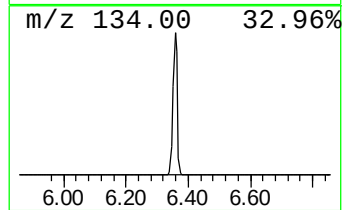
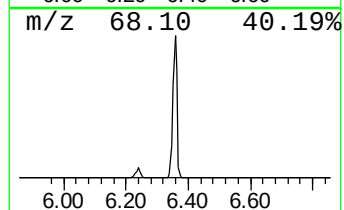
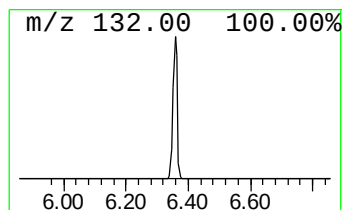
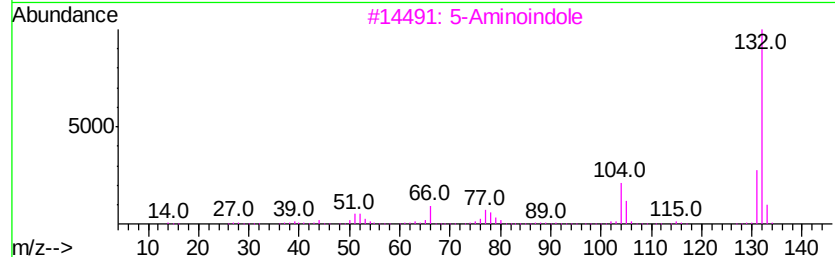
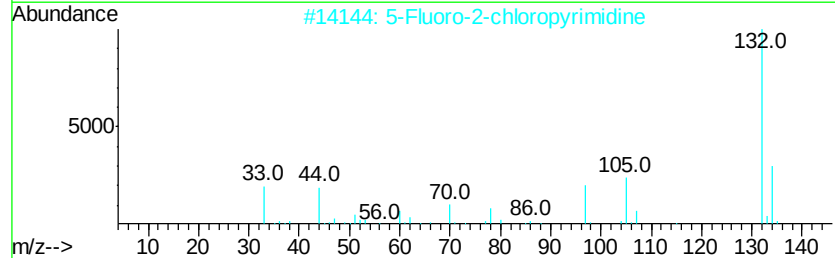
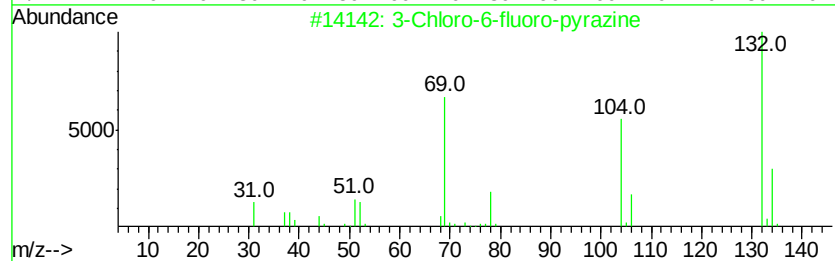
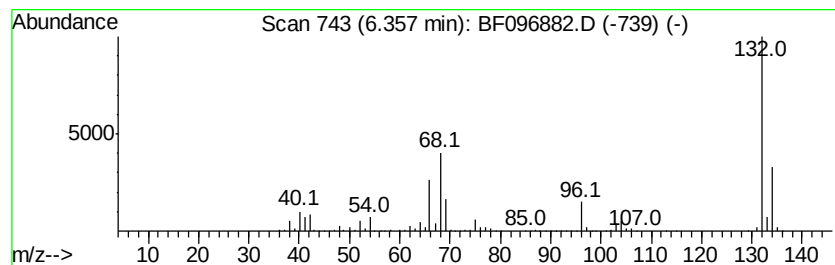
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	71.58 ng	2433030	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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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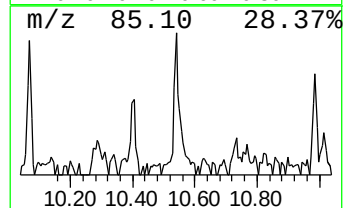
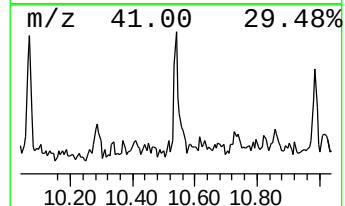
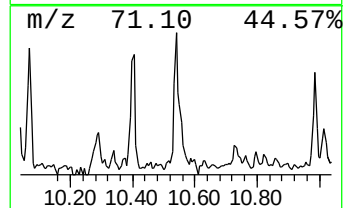
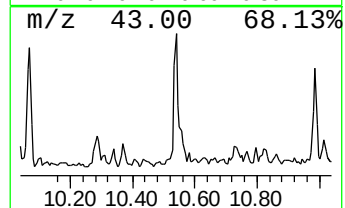
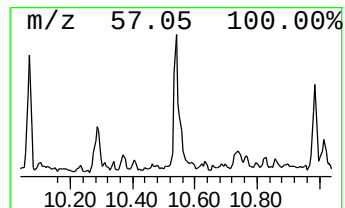
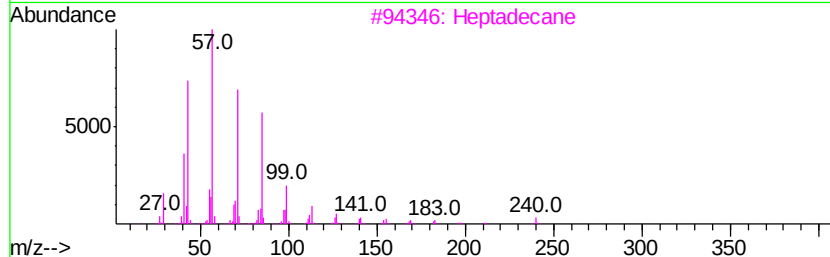
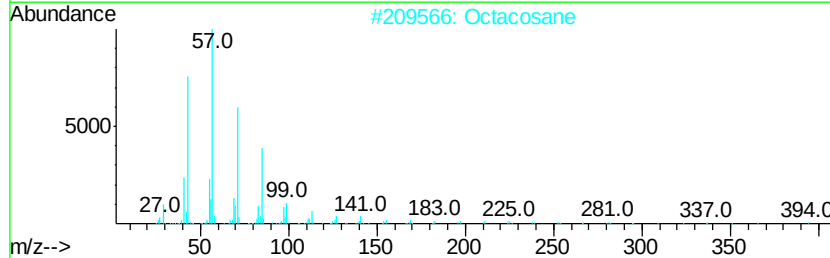
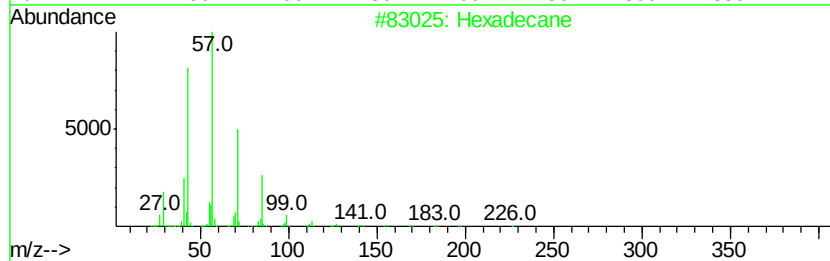
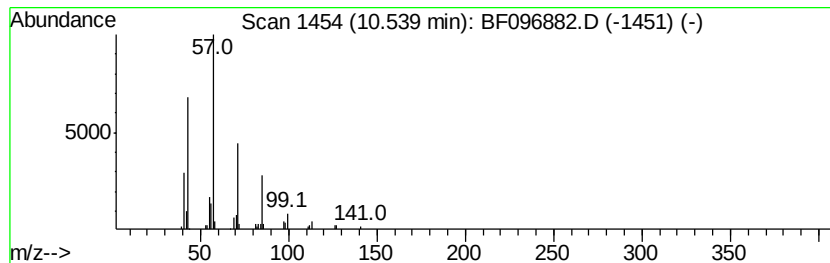
Instrument :
BNA_F
ClientSampleId :
CL-01-071817-A

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.54	2.30 ng	75966	Phenanthrene-d10	11.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Octacosane	394	C28H58	000630-02-4	83
3	Heptadecane	240	C17H36	000629-78-7	80
4	Heneicosane	296	C21H44	000629-94-7	80
5	Eicosane	282	C20H42	000112-95-8	78



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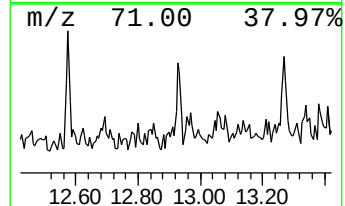
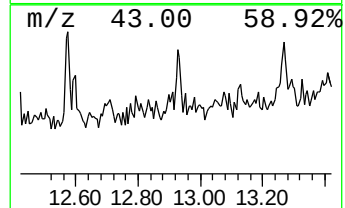
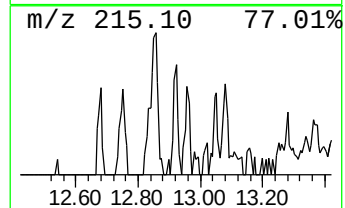
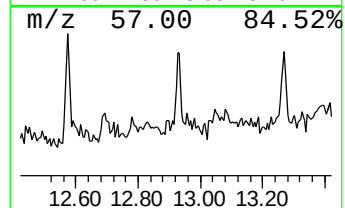
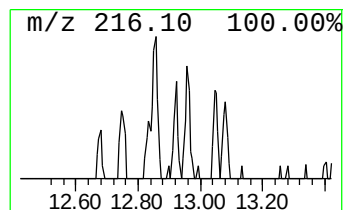
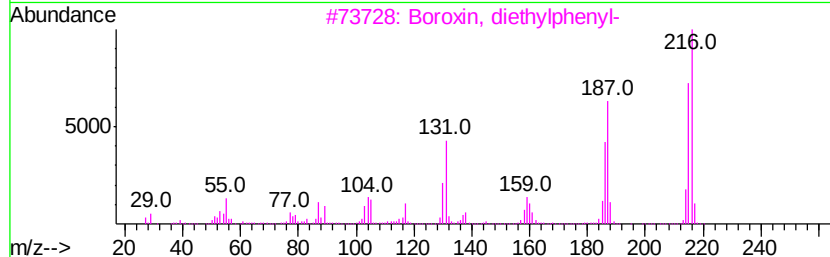
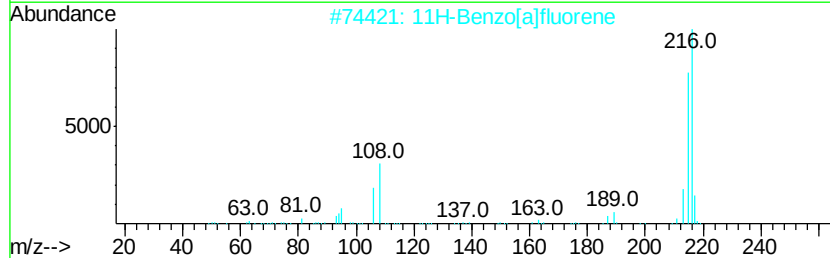
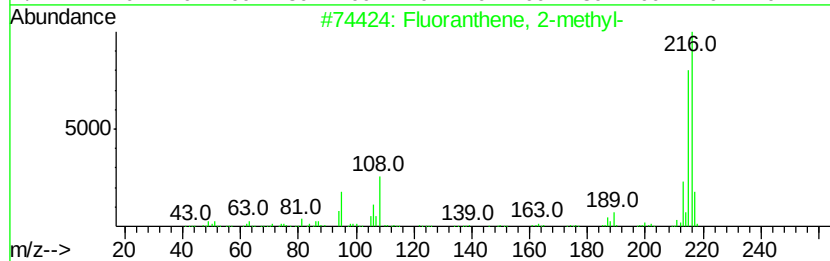
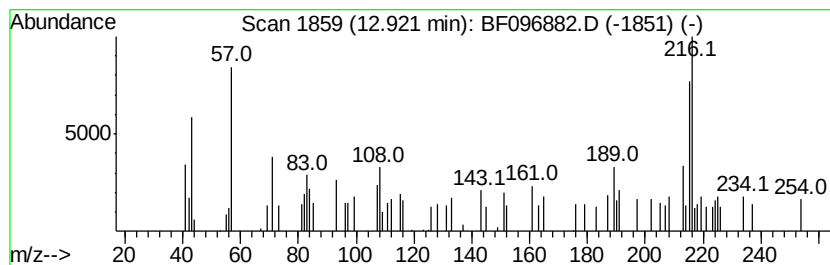
Instrument :
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ClientSampleId :
CL-01-071817-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Fluoranthene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.92	2.03 ng	62336	Chrysene-d12	13.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	50
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	50
3	Boroxin, diethylphenyl-	216	C10H15B3O3	1000151-81-1	50
4	4-Trifluoromethylcinnamic acid	216	C10H7F3O2	002062-26-2	49
5	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	47



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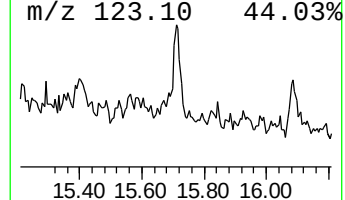
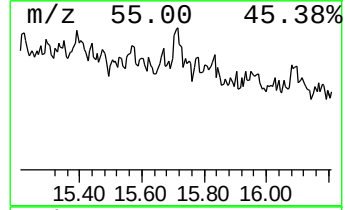
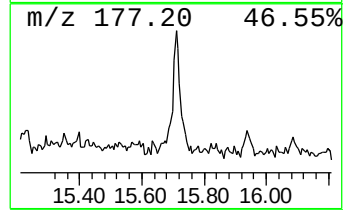
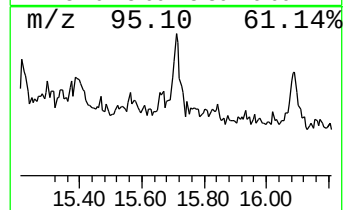
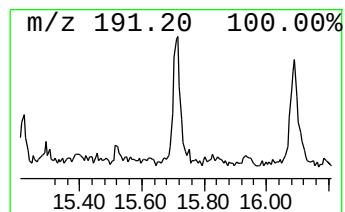
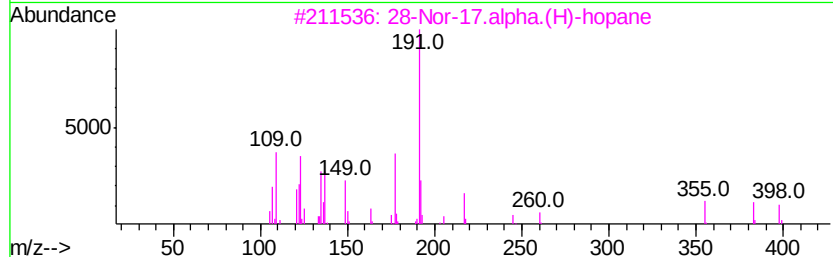
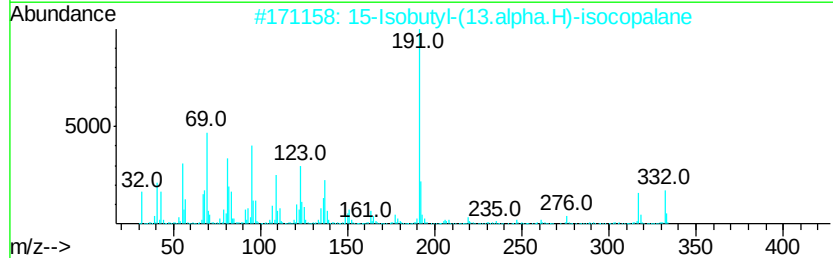
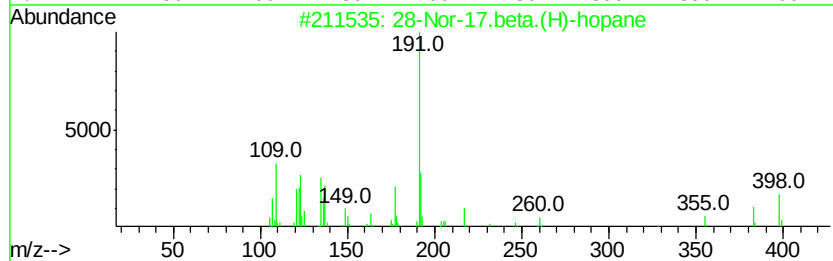
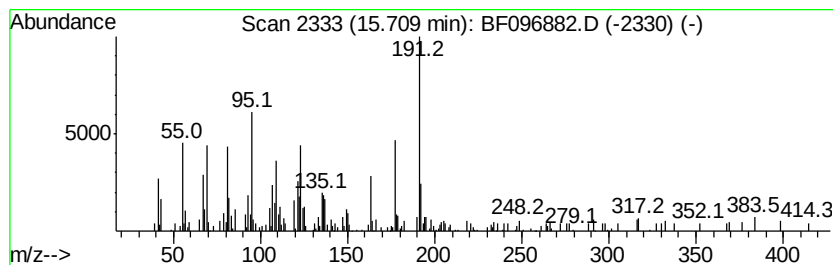
Instrument :
BNA_F
ClientSampleId :
CL-01-071817-A

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 28-Nor-17.beta.(H)-hopane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.71	7.56 ng	172110	Perylene-d12	15.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	83	
2	15-Isobutyl-(13.alpha.H)-isocopa...	332	C24H44	087953-47-7	64	
3	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	62	
4	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43	
5	3-Fluoro-5-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-34-4	25	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096882.D
Acq On : 19 Jul 2017 20:56
Operator : SJ/JU
Sample : I4280-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-071817-A

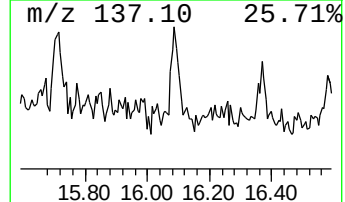
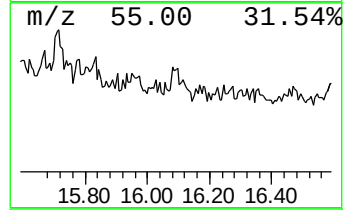
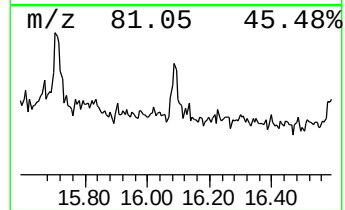
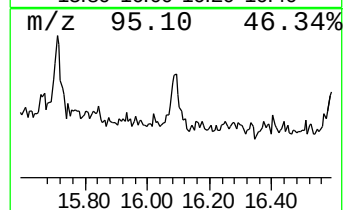
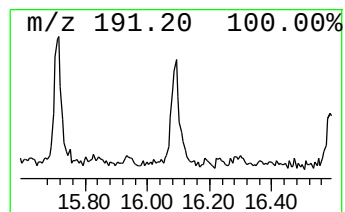
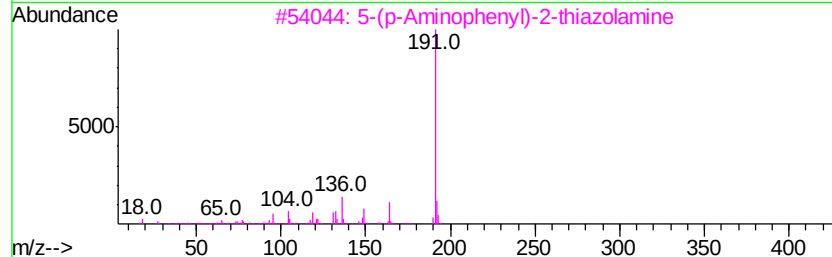
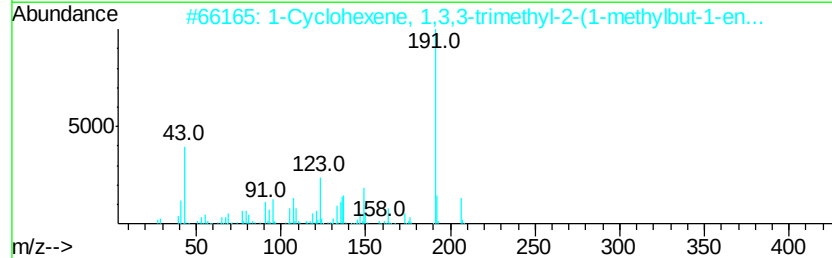
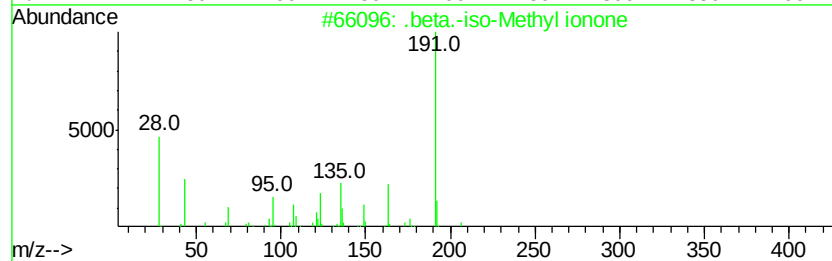
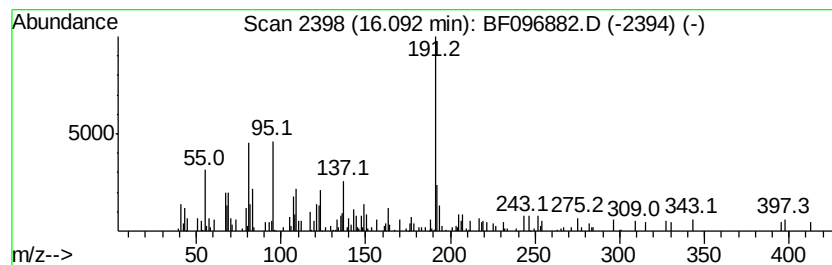
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	5.76 ng	131240	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	50
2		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	43
3		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35
4		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	30
5		2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
Data File : BF096882.D
Acq On : 19 Jul 2017 20:56
Operator : SJ/JU
Sample : I4280-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-071817-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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
Hexane, 2,4-dimet...	2.06	2.9	ng	98568	1	6.59	679762	20.0
2-Pentanone, 4-hy...	4.76	8.4	ng	285070	1	6.59	679762	20.0
unknown6.36	6.36	71.6	ng	2433030	1	6.59	679762	20.0
Hexadecane	10.54	2.3	ng	75966	4	11.09	660576	20.0
Fluoranthene, 2-m...	12.92	2.0	ng	62336	5	13.72	613596	20.0
28-Nor-17.beta.(H...	15.71	7.6	ng	172110	6	15.09	455491	20.0
.beta.-iso-Methyl...	16.09	5.8	ng	131240	6	15.09	455491	20.0