

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
 Data File : BF092700.D
 Acq On : 1 Feb 2017 00:03
 Operator : SJ/MA
 Sample : I1596-07
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-05

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-BF013017.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	5.127	264	266	269	rBV	691507	859667	15.14%	2.020%
2	5.561	301	304	306	rBV	2828023	2925463	51.52%	6.874%
3	6.590	391	394	396	rBV	1386818	1946641	34.28%	4.574%
4	6.716	402	405	408	rBV	4022880	3992929	70.32%	9.383%
5	6.944	422	425	427	rBV	1257216	1076554	18.96%	2.530%
6	7.104	436	439	441	rBV	3860139	3740363	65.87%	8.789%
7	7.150	441	443	445	rVB	60828	64583	1.14%	0.152%
8	7.287	452	455	457	rBV2	49684	72754	1.28%	0.171%
9	7.470	467	471	472	rBV	33930	66534	1.17%	0.156%
10	7.516	472	475	477	rVV	3254702	3473936	61.18%	8.163%
11	7.893	505	508	511	rBV	352534	373495	6.58%	0.878%
12	8.236	536	538	540	rBV	1635342	1434374	25.26%	3.371%
13	8.602	567	570	573	rBV5	27706	87547	1.54%	0.206%
14	8.659	573	575	576	rBV	151773	214744	3.78%	0.505%
15	8.773	583	585	586	rBV	114124	101951	1.80%	0.240%
16	8.865	590	593	594	rBV2	39842	58319	1.03%	0.137%
17	8.967	598	602	607	rBV5	74725	202508	3.57%	0.476%
18	9.082	607	612	615	rVB6	57145	129397	2.28%	0.304%
19	9.162	615	619	623	rBV7	42108	173160	3.05%	0.407%
20	9.242	623	626	627	rVB2	88012	102408	1.80%	0.241%
21	9.276	627	629	630	rBV	95478	97718	1.72%	0.230%
22	9.322	630	633	635	rBV	5032602	5678492	100.00%	13.344%
23	9.482	645	647	648	rBV2	37092	64438	1.13%	0.151%
24	9.505	648	649	651	rVB2	84252	74057	1.30%	0.174%
25	9.539	651	652	655	rVB2	80361	80867	1.42%	0.190%
26	9.607	656	658	660	rBV3	59768	84963	1.50%	0.200%
27	9.653	660	662	664	rVV2	112231	144348	2.54%	0.339%
28	9.710	665	667	669	rVV	138099	157179	2.77%	0.369%
29	9.813	673	676	677	rVV2	68773	117662	2.07%	0.276%
30	9.848	677	679	682	rVB	84324	97984	1.73%	0.230%
31	9.996	690	692	695	rVB	1702418	1582667	27.87%	3.719%
32	10.053	695	697	699	rBV2	32028	66494	1.17%	0.156%
33	10.259	711	715	717	rBV3	98802	182244	3.21%	0.428%
34	10.293	717	718	720	rVV2	73703	79041	1.39%	0.186%

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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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35	10.430	728	730	734	rVB3	58298	91607	1.61%	0.215%
36	10.682	750	752	755	rVB3	59784	85392	1.50%	0.201%
37	10.739	755	757	759	rBV2	85469	139888	2.46%	0.329%
38	10.796	759	762	764	rBV	2784929	3031739	53.39%	7.124%
39	10.899	770	771	776	rVB3	62760	102003	1.80%	0.240%
40	11.208	795	798	799	rBV2	42434	61635	1.09%	0.145%
41	11.368	808	812	813	rBV2	147530	330518	5.82%	0.777%
42	11.493	820	823	825	rBV	1470152	1539892	27.12%	3.619%
43	13.082	959	962	964	rBV	4448945	4940677	87.01%	11.610%
44	14.122	1051	1053	1056	rVB	1199256	1295136	22.81%	3.043%
45	15.597	1179	1182	1189	rVB	874401	1196075	21.06%	2.811%
46	16.054	1219	1222	1226	rVB	37954	76990	1.36%	0.181%
47	16.557	1264	1266	1269	rVB	32958	58718	1.03%	0.138%

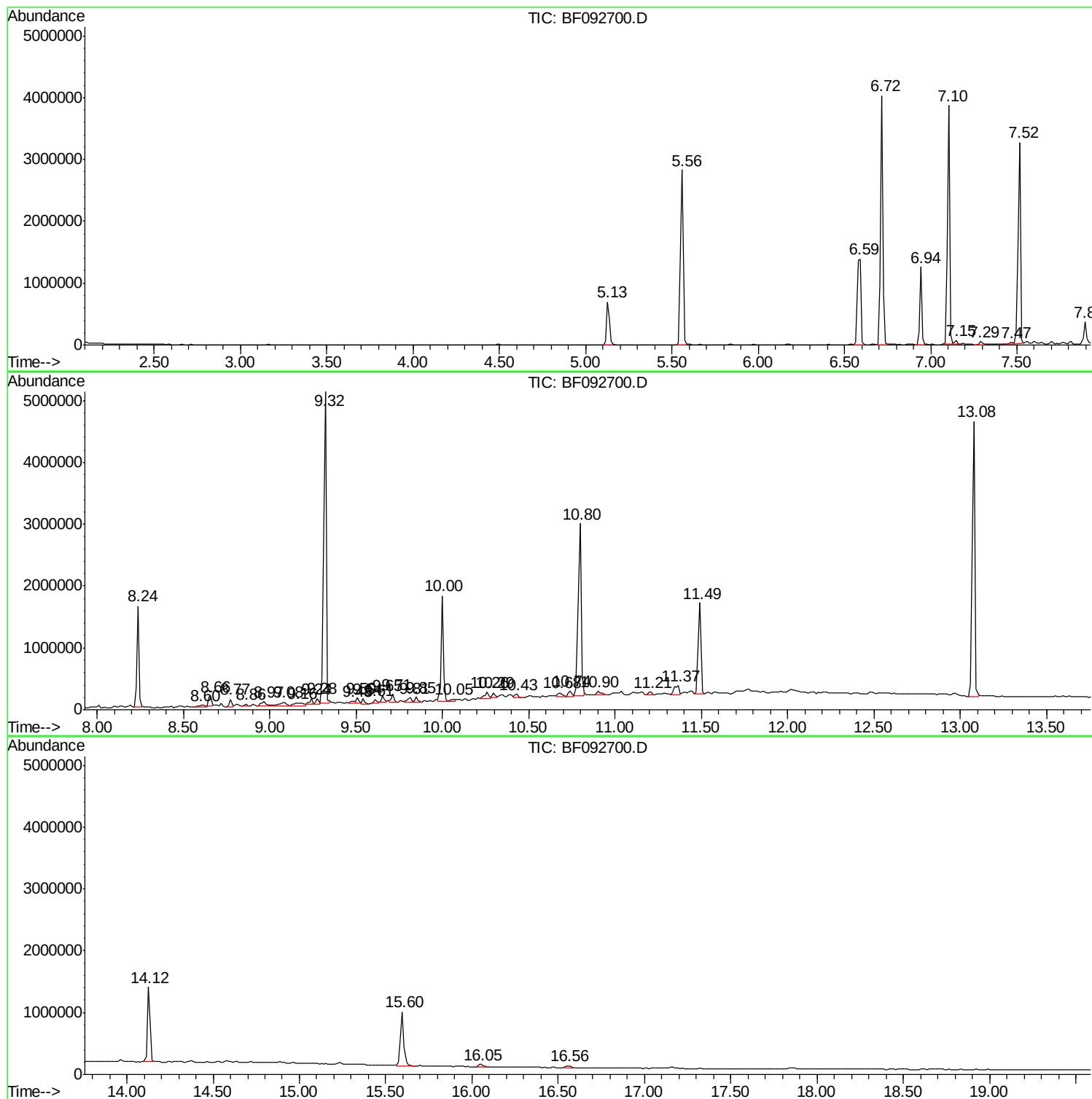
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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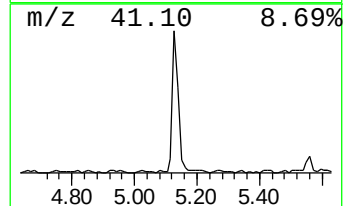
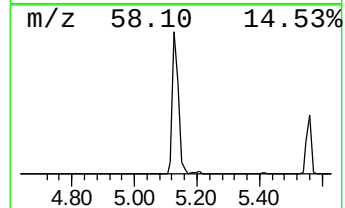
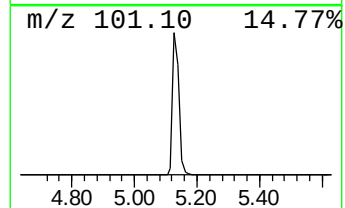
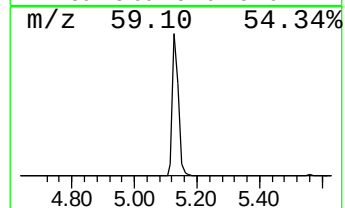
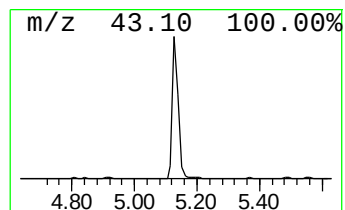
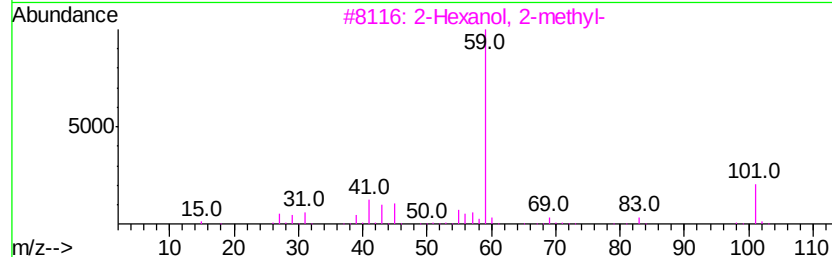
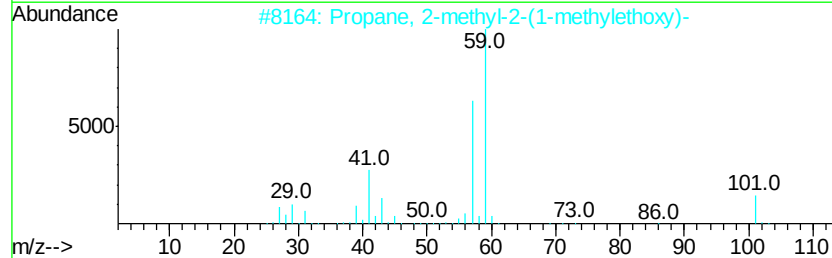
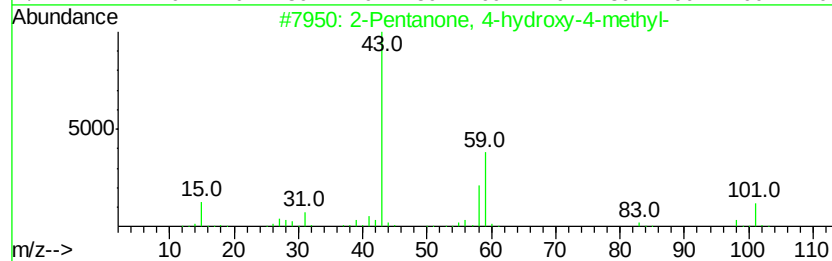
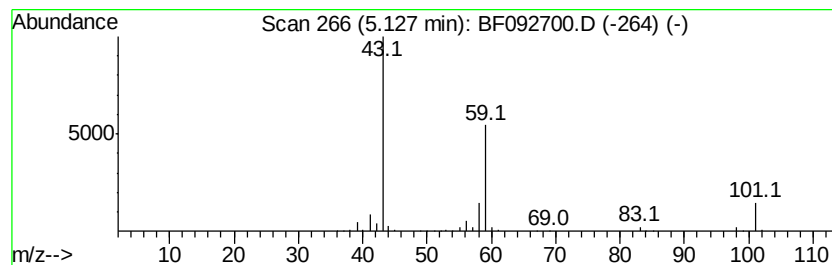
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.		
5.13	15.97 ng	859667	1,4-Dichlorobenzene-d4	6.94		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32	



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Instrument :
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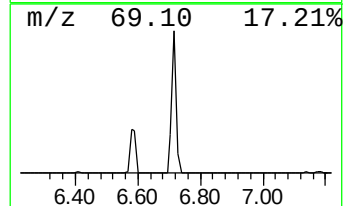
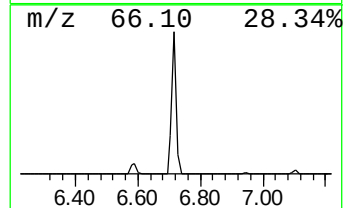
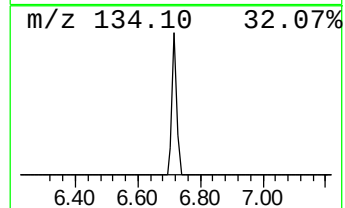
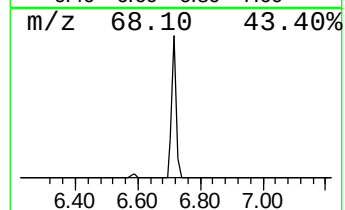
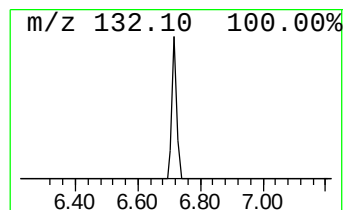
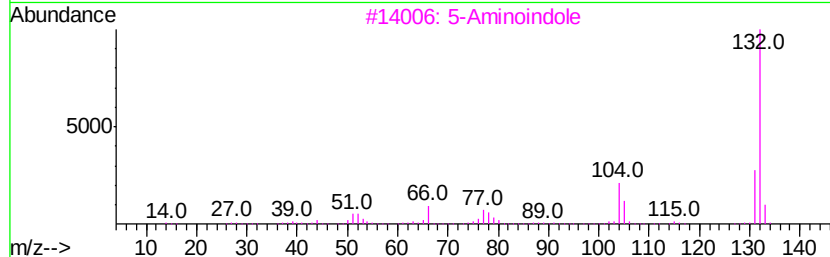
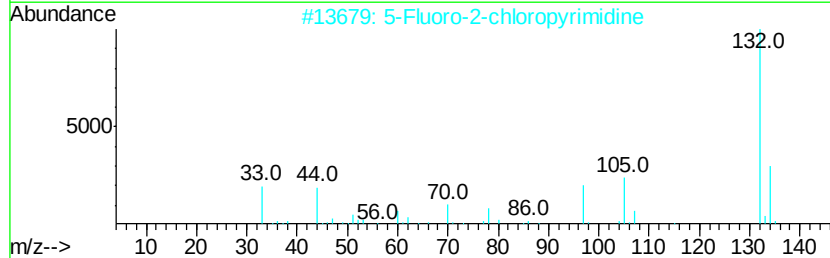
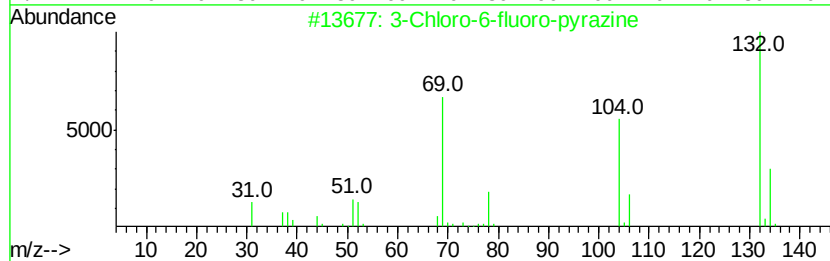
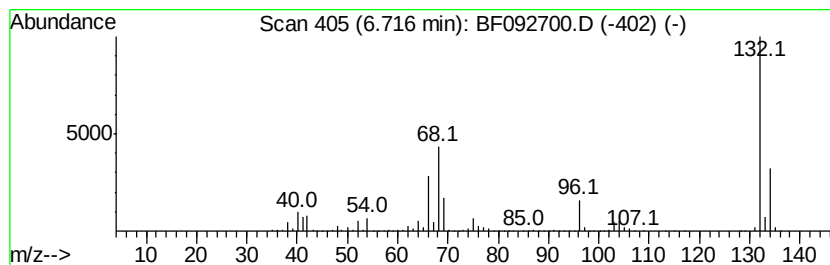
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	74.18 ng	3992930	1,4-Dichlorobenzene-d4	6.94

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		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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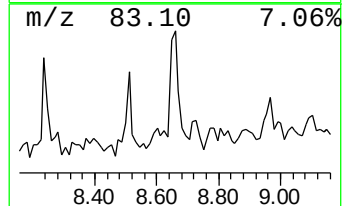
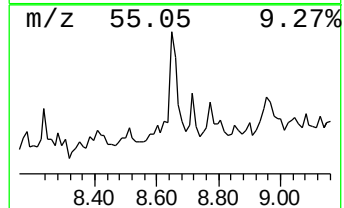
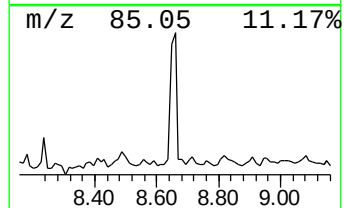
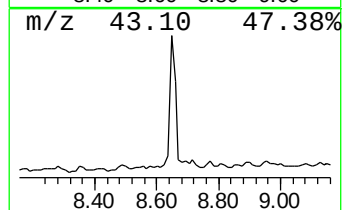
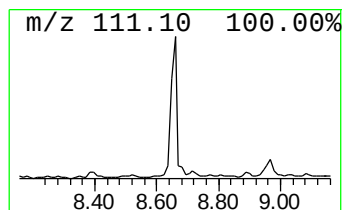
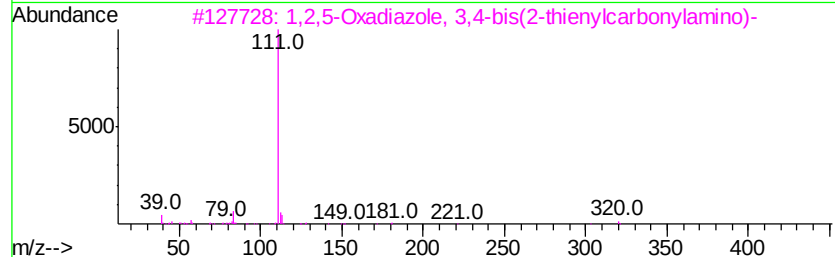
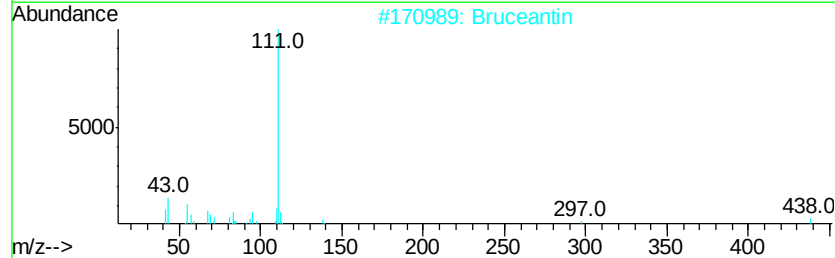
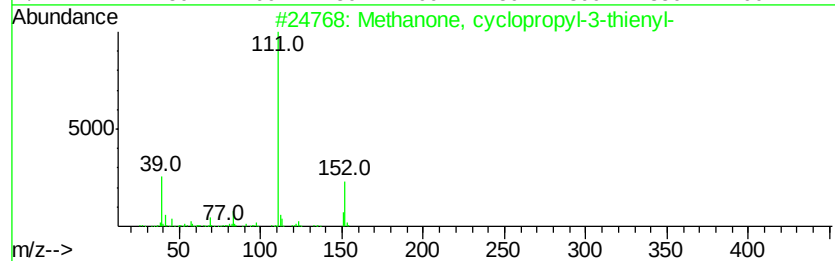
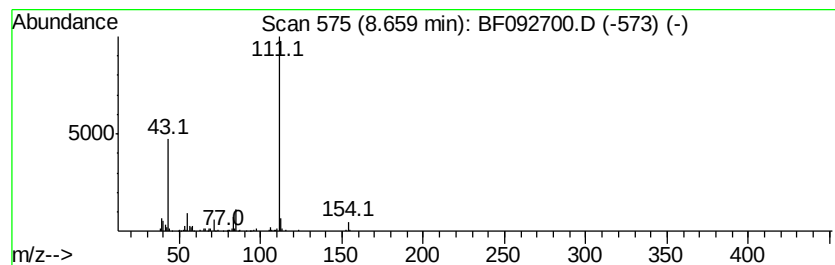
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methanone, cyclopropyl-3-th... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	2.99 ng	214744	Naphthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanone, cvclopropvl-3-thienyl-	152	C8H8OS	113348-25-7	72
2		Bruceantin	548	C28H36O11	041451-75-6	56
3		1,2,5-Oxadiazole, 3,4-bis(2-thie...	320	C12H8N4O3S2	1000294-18-8	45
4		3-Aminopyrazine 1-oxide	111	C4H5N3O	006863-77-0	42
5		Pyridin-2,6-diol, diacetate	195	C9H9NO4	1000153-09-2	38



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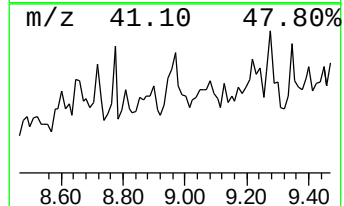
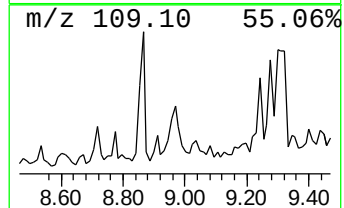
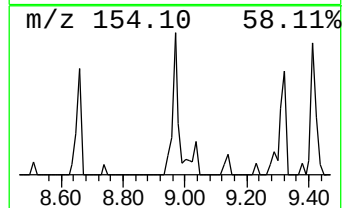
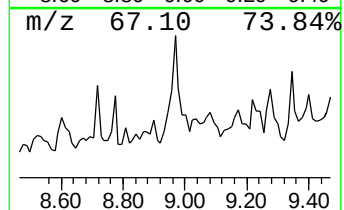
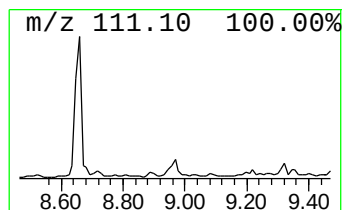
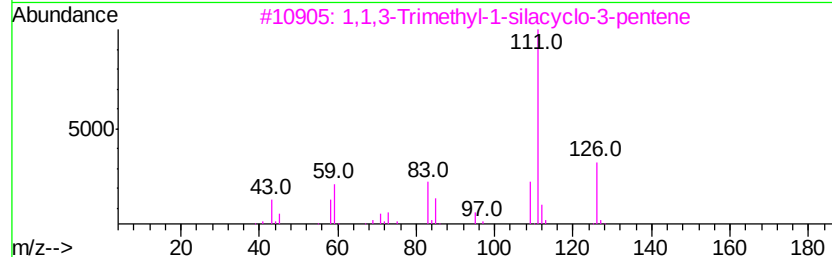
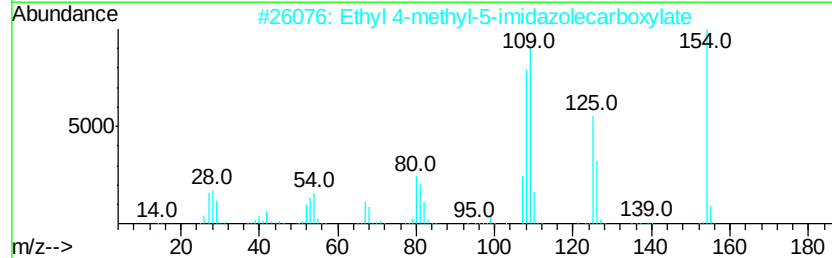
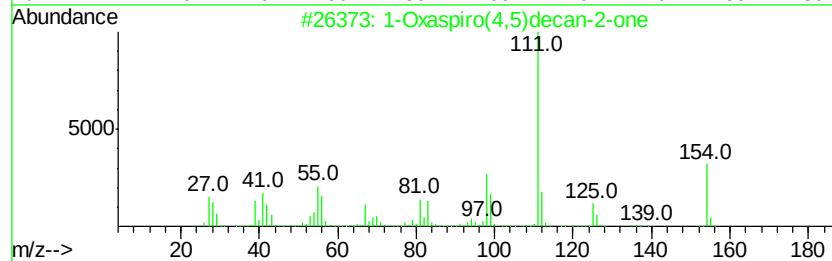
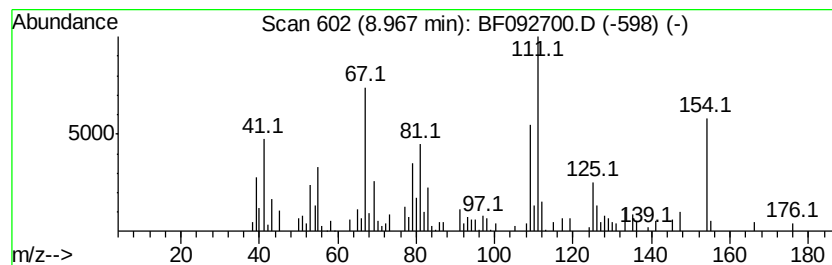
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown8.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	2.82 ng	202508	Napthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Oxaspiro(4,5)decan-2-one	154	C9H14O2	000699-61-6	35
2		Ethyl 4-methyl-5-imidazolecarbox...	154	C7H10N2O2	051605-32-4	30
3		1,1,3-Trimethyl-1-silacyclo-3-pe...	126	C7H14Si	003528-14-1	22
4		3-Octyne, 7-methyl-	124	C9H16	037050-06-9	22
5		3,3,5,5-Tetramethylcyclopentene	124	C9H16	038667-10-6	22



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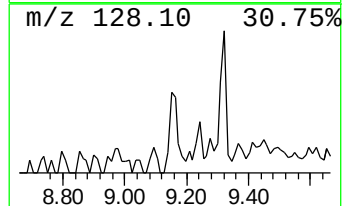
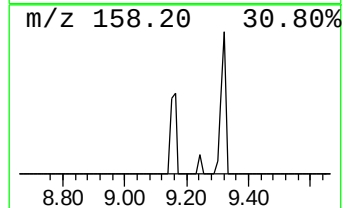
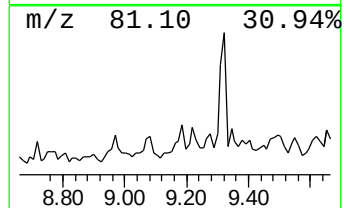
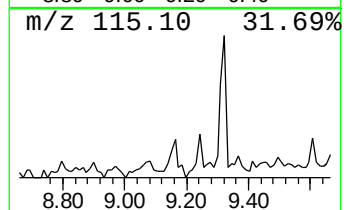
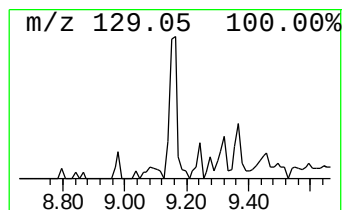
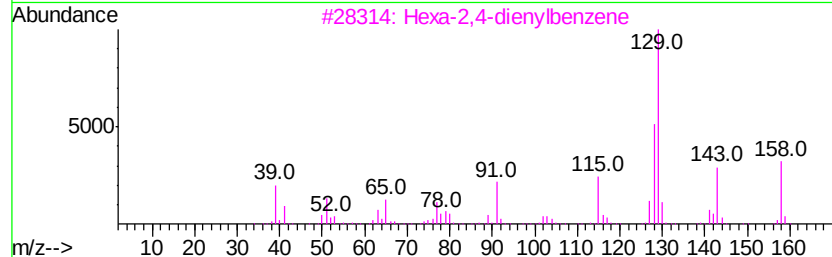
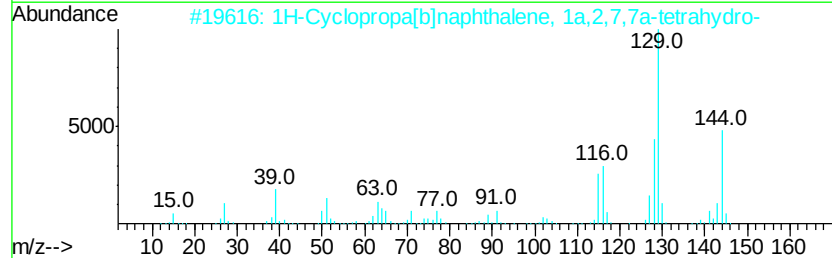
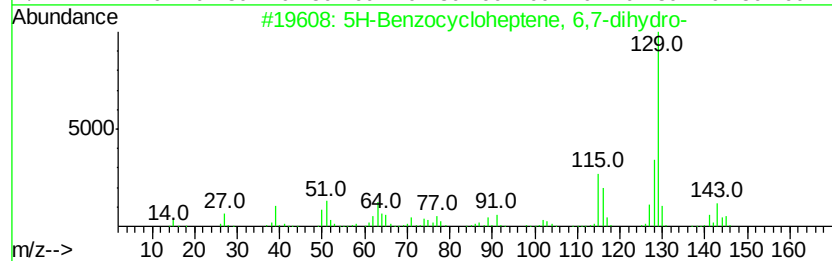
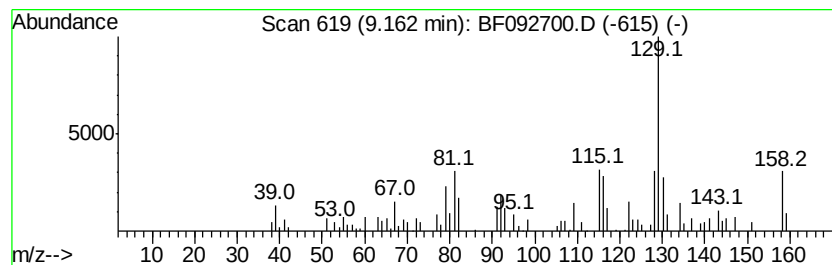
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TIC Integration Parameters: LSCINT.P

Peak Number 6 5H-Benzocycloheptene, 6,7-d... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	2.19 ng	173160	Acenaphthene-d10	10.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	62
2		1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	50
3		Hexa-2,4-dienylbenzene	158	C12H14	079482-86-3	38
4		Naphthalene, 1,2-dihydro-4-methyl-	144	C11H12	004373-13-1	38
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	144	C11H12	071721-26-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013117\
Data File : BF092700.D
Acq On : 1 Feb 2017 00:03
Operator : SJ/MA
Sample : I1596-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

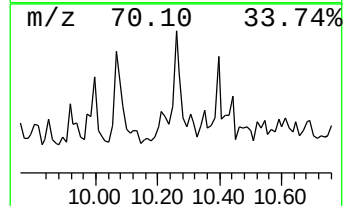
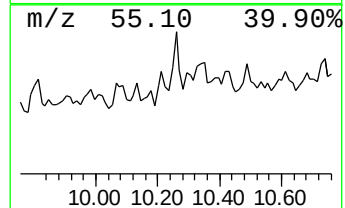
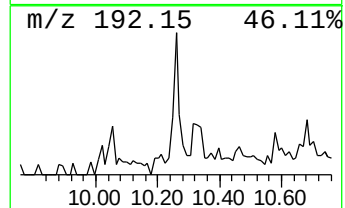
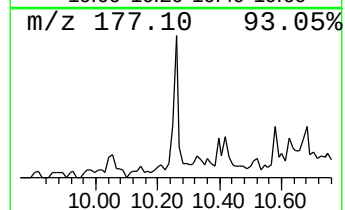
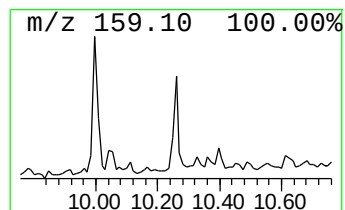
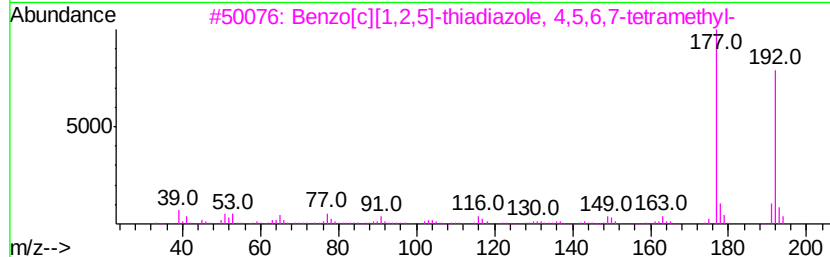
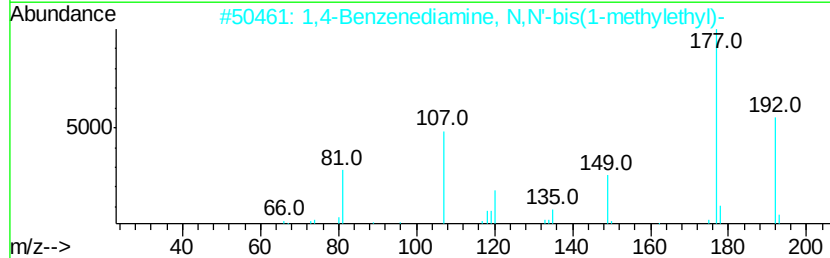
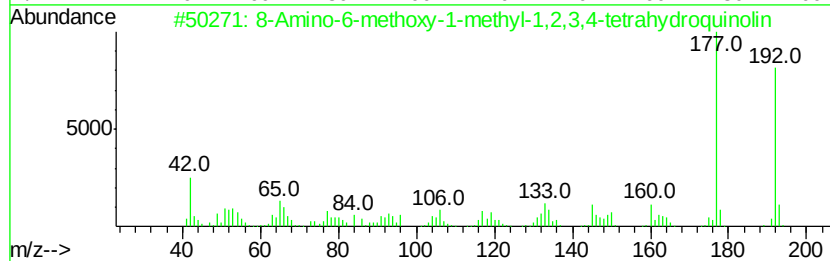
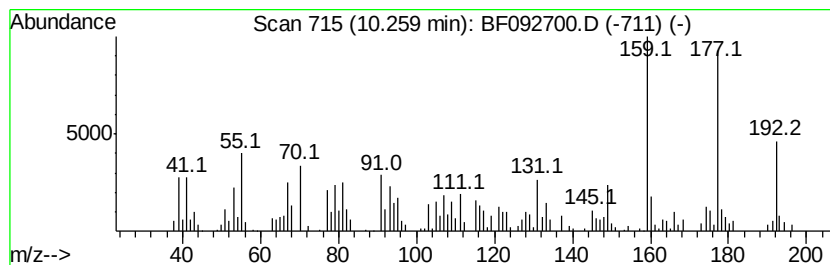
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown10.26 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	2.30 ng	182244	Acenaphthene-d10	10.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Amino-6-methoxy-1-methyl-1,2,3...	192	C11H16N2O	059353-30-9	46		
2	1,4-Benzenediamine, N,N'-bis(1-m...	192	C12H20N2	004251-01-8	43		
3	Benzo[c][1,2,5]-thiadiazole, 4,5...	192	C10H12N2S	106148-64-5	43		
4	5-Ethyl-3,4-dimethyl-1H-pyrano[2...	192	C10H12N2O2	1000296-60-7	41		
5	6-Isopropyl-benzothiazol-2-ylamine	192	C10H12N2S	032895-14-0	38		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013117\
Data File : BF092700.D
Acq On : 1 Feb 2017 00:03
Operator : SJ/MA
Sample : I1596-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

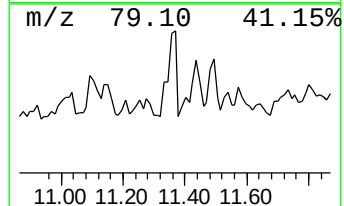
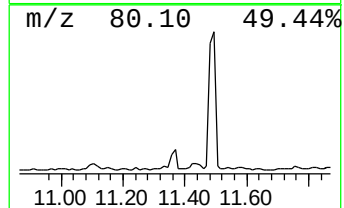
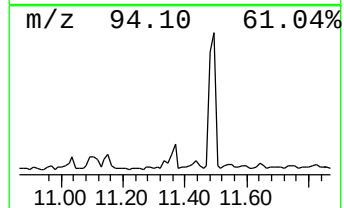
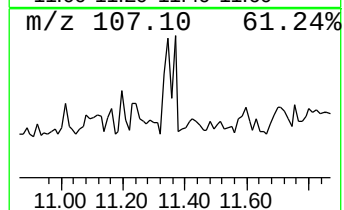
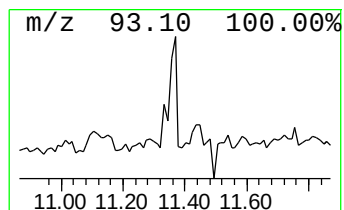
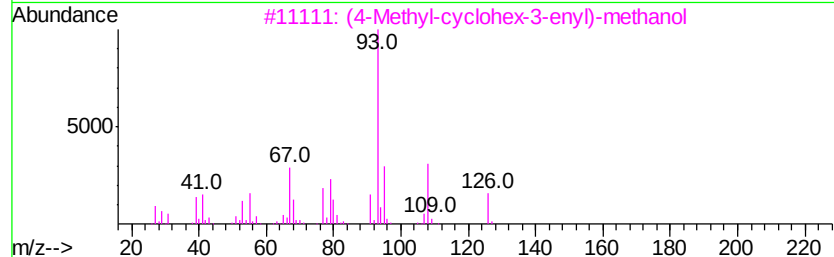
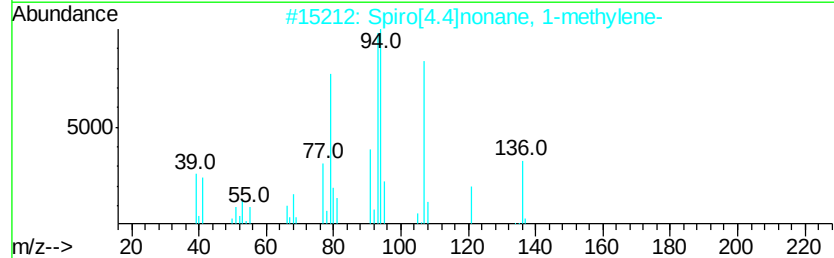
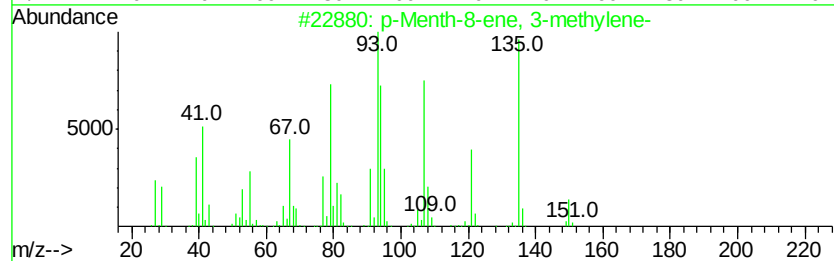
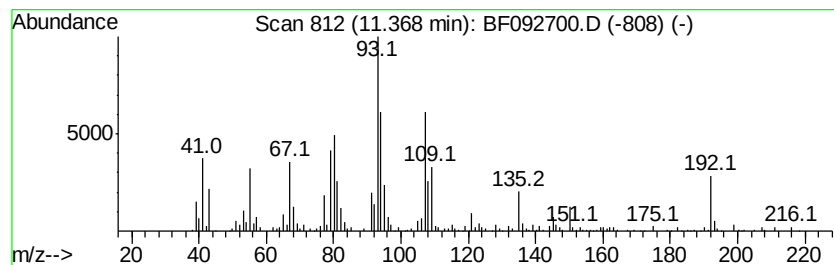
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown11.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.37	4.29 ng	330518	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	p-Menth-8-ene, 3-methylene-	150	C11H18	1000151-25-7	43
2		Spiro[4.4]nonane, 1-methylene-	136	C10H16	019144-06-0	43
3		(4-Methyl-cyclohex-3-enyl)-methanol	126	C8H14O	089690-46-0	35
4		1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	35
5		Bicyclo[3.1.1]hept-2-en-6-one, 2...	150	C10H14O	000473-06-3	35



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Sample : I1596-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	16.0	ng	859667	1	6.94	1076550	20.0
unknown6.72	6.72	74.2	ng	3992930	1	6.94	1076550	20.0
Methanone, cyclop...	8.66	3.0	ng	214744	2	8.24	1434370	20.0
unknown8.97	8.97	2.8	ng	202508	2	8.24	1434370	20.0
5H-Benzocyclohept...	9.16	2.2	ng	173160	3	10.00	1582670	20.0
unknown10.26	10.26	2.3	ng	182244	3	10.00	1582670	20.0
unknown11.37	11.37	4.3	ng	330518	4	11.49	1539890	20.0