

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
 Data File : BF091646.D
 Acq On : 15 Dec 2016 23:27
 Operator : UM/SJ
 Sample : H6007-16
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-12-10-15

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-BF120916.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	4.967	249	252	258	rBV	1918611	3078667	41.38%	4.459%
2	5.390	286	289	292	rVB	5781406	7439260	100.00%	10.774%
3	6.430	377	380	383	rVB	5566571	7073174	95.08%	10.244%
4	6.556	388	391	394	rBV	6817357	6963727	93.61%	10.086%
5	6.613	394	396	398	rVB	184361	165386	2.22%	0.240%
6	6.784	408	411	413	rBV	2065897	1730234	23.26%	2.506%
7	6.853	414	417	419	rBV2	67975	93103	1.25%	0.135%
8	6.944	422	425	427	rBV	6347632	6441576	86.59%	9.329%
9	7.356	457	461	463	rBV	5004530	6188466	83.19%	8.963%
10	7.447	466	469	473	rVB	58306	88440	1.19%	0.128%
11	8.065	521	523	526	rBV	1740268	2179191	29.29%	3.156%
12	9.150	615	618	620	rBV	7155254	6650735	89.40%	9.632%
13	9.539	650	652	655	rBV	934929	1162403	15.63%	1.684%
14	9.825	674	677	679	rBV	2301051	2008149	26.99%	2.908%
15	10.259	711	715	717	rBV2	96057	166874	2.24%	0.242%
16	10.613	743	746	748	rBV	4097853	4178704	56.17%	6.052%
17	10.739	754	757	761	rVB	126424	196137	2.64%	0.284%
18	11.185	791	796	797	rBV	130468	136572	1.84%	0.198%
19	11.299	804	806	810	rVV2	1337883	1697228	22.81%	2.458%
20	11.608	831	833	835	rBV	140532	119175	1.60%	0.173%
21	11.836	851	853	855	rBV2	95958	116054	1.56%	0.168%
22	11.916	858	860	865	rVB3	52685	86504	1.16%	0.125%
23	12.511	910	912	914	rBV	389087	350666	4.71%	0.508%
24	12.739	929	932	934	rBV	303512	389530	5.24%	0.564%
25	12.888	943	945	948	rBV	4840546	4861893	65.35%	7.042%
26	13.174	968	970	974	rBV2	51038	89389	1.20%	0.129%
27	13.379	985	988	991	rBV	394316	522341	7.02%	0.757%
28	13.791	1021	1024	1028	rBV2	236681	331265	4.45%	0.480%
29	13.939	1034	1037	1038	rBV	1199991	1752988	23.56%	2.539%
30	13.962	1038	1039	1042	rVB	131963	113771	1.53%	0.165%
31	14.660	1098	1100	1104	rVB2	130556	215811	2.90%	0.313%
32	14.785	1109	1111	1113	rVB2	73379	85785	1.15%	0.124%
33	14.945	1122	1125	1129	rBV	106916	214402	2.88%	0.311%
34	15.220	1147	1149	1151	rBV	64886	91510	1.23%	0.133%

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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-BF120916.M
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35	15.277	1152	1154	1157	rBV	71199	118907	1.60%	0.172%
36	15.345	1157	1160	1163	rVB	837480	1077146	14.48%	1.560%
37	15.482	1170	1172	1175	rVB	84839	102229	1.37%	0.148%
38	15.791	1197	1199	1201	rBV2	47206	79129	1.06%	0.115%
39	15.837	1201	1203	1207	rBV4	53533	158278	2.13%	0.229%
40	16.008	1215	1218	1224	rVB2	88502	225413	3.03%	0.326%
41	16.260	1238	1240	1244	rVB4	54450	96974	1.30%	0.140%
42	16.408	1250	1253	1257	rVB	115034	208562	2.80%	0.302%

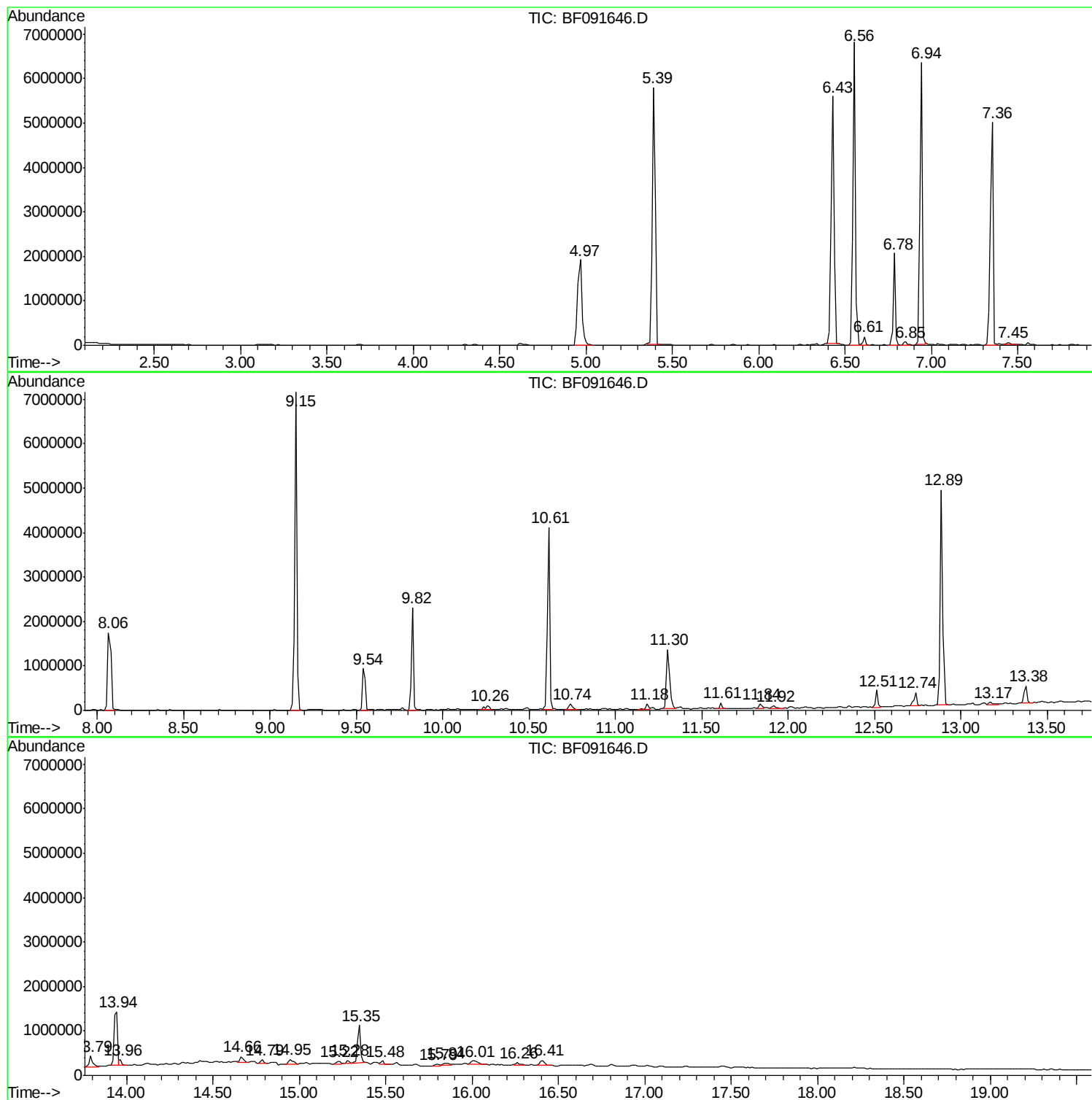
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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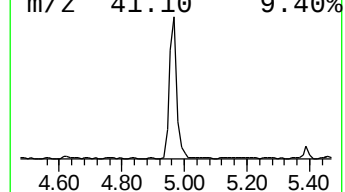
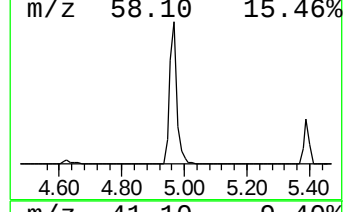
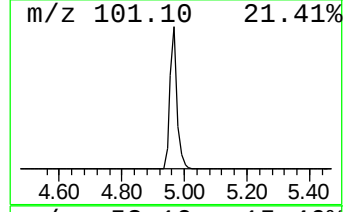
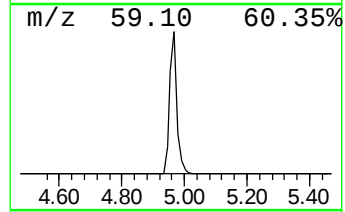
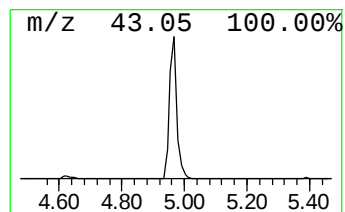
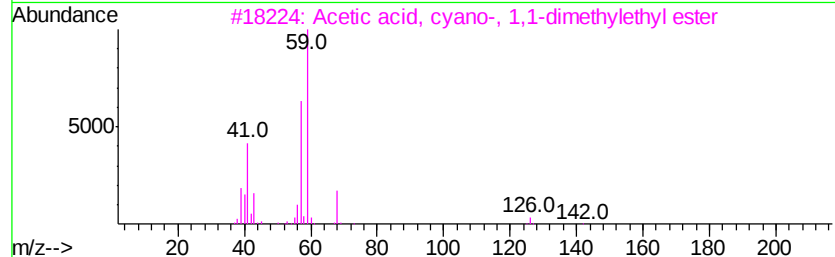
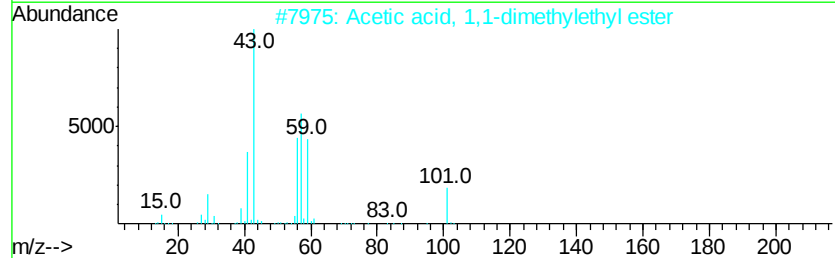
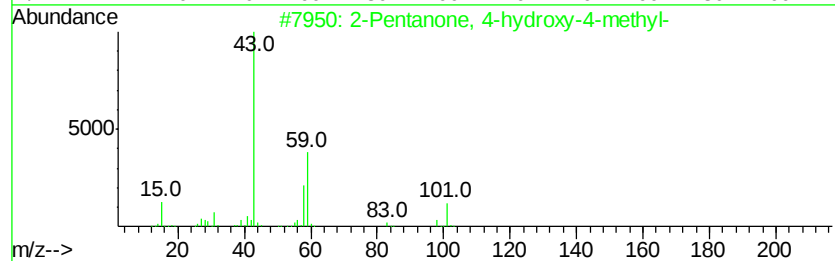
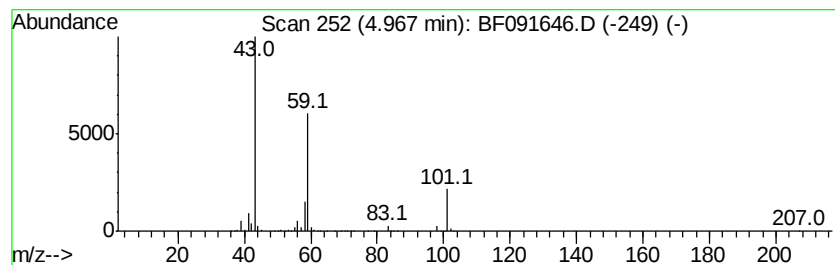
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.97	35.59 ng	3078670	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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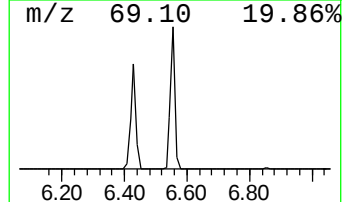
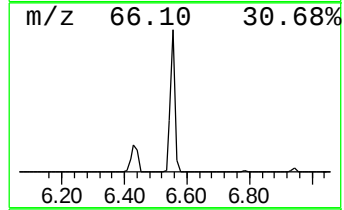
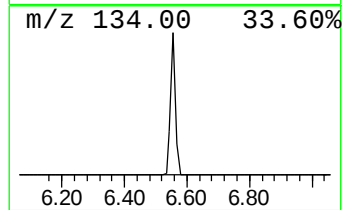
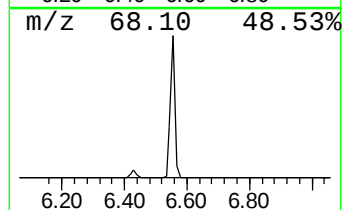
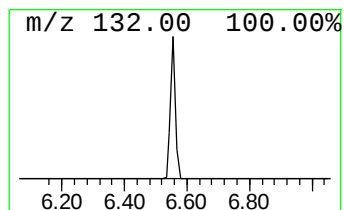
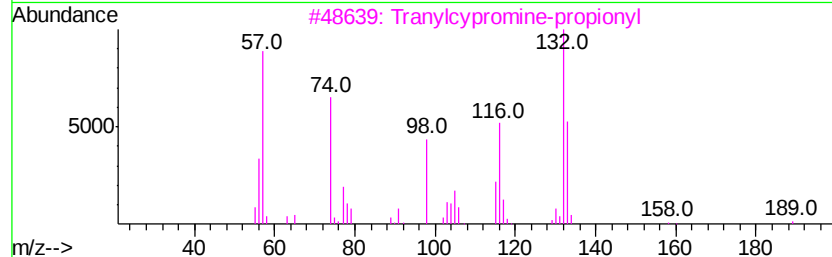
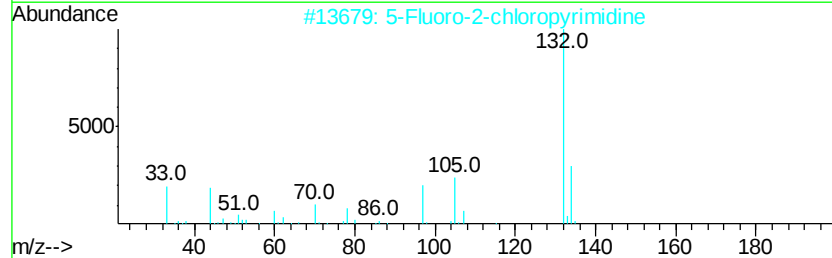
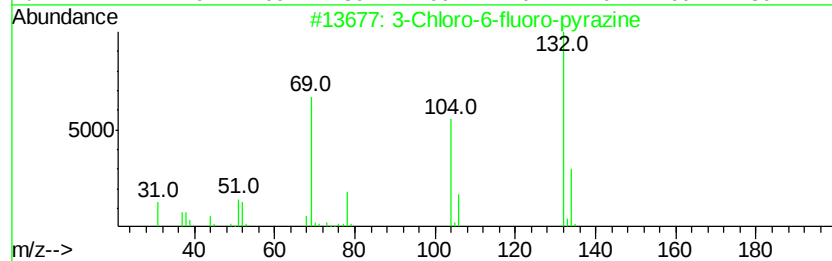
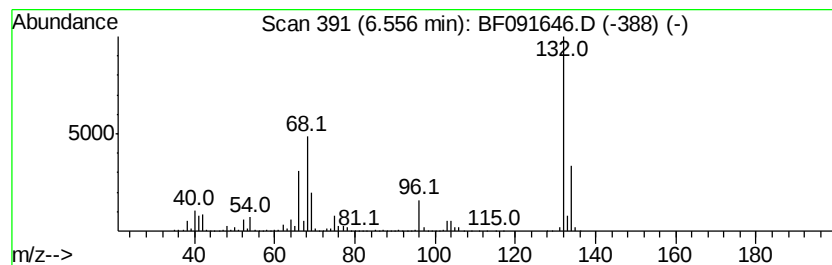
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	80.49 ng	6963730	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10	
5	5-Aminoindole	132	C8H8N2	005192-03-0	10	



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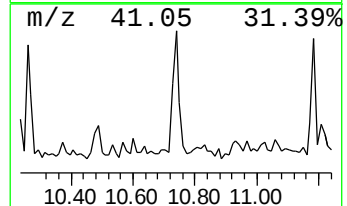
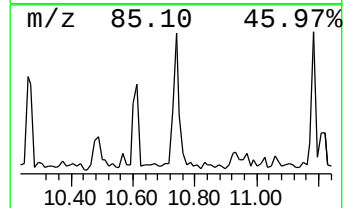
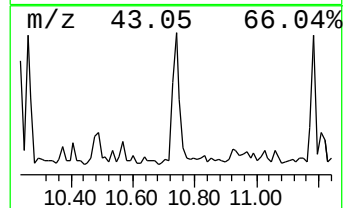
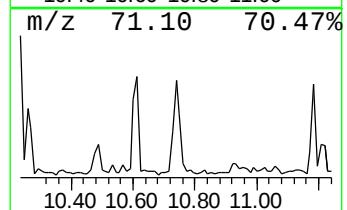
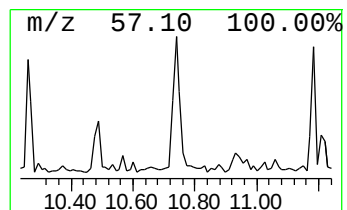
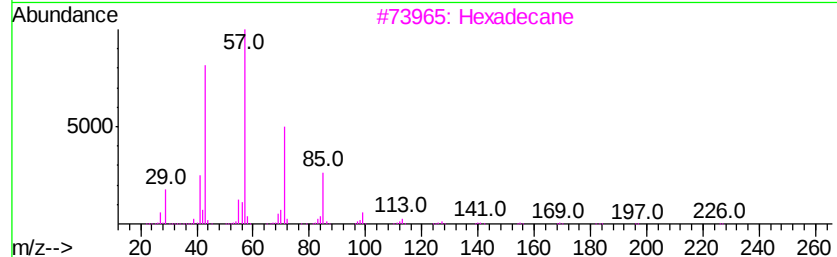
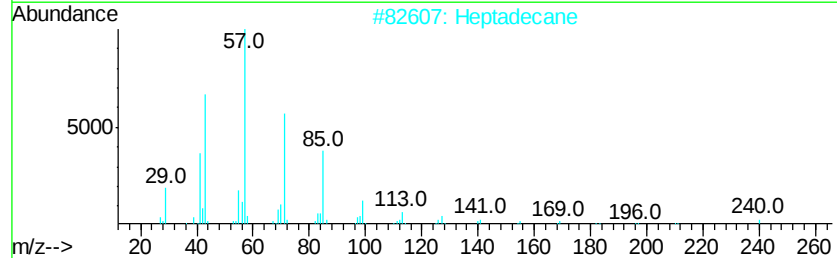
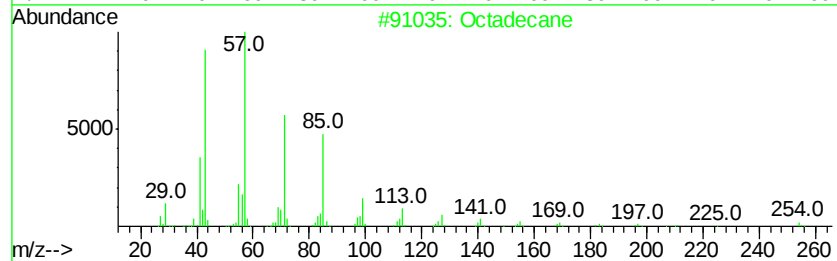
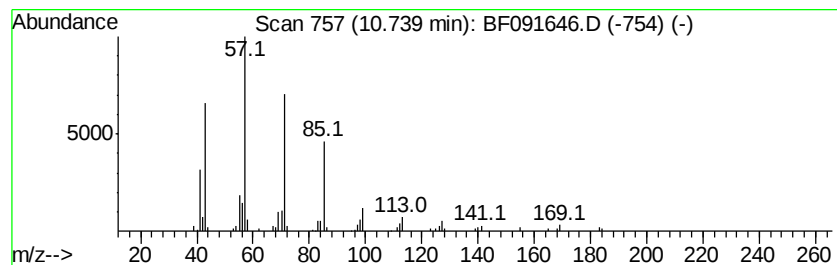
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.31 ng	196137	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Hexadecane	226	C16H34	000544-76-3	90
4		Pentadecane	212	C15H32	000629-62-9	90
5		Tetradecane	198	C14H30	000629-59-4	86



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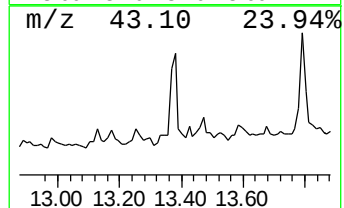
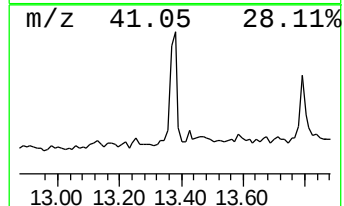
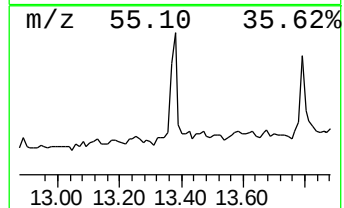
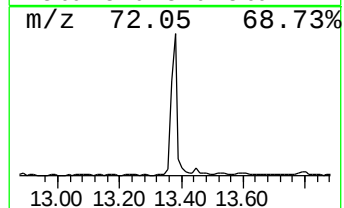
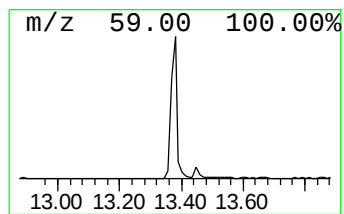
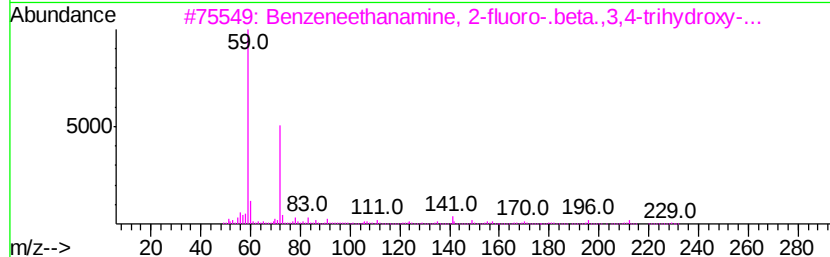
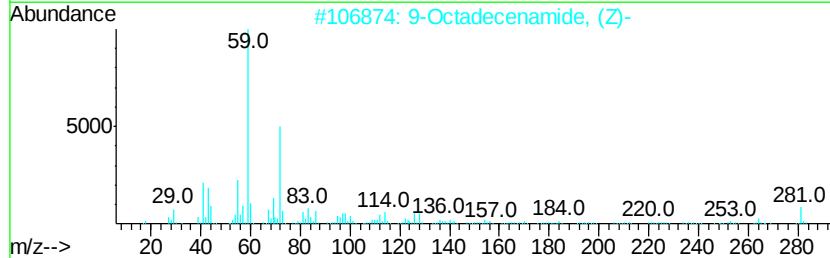
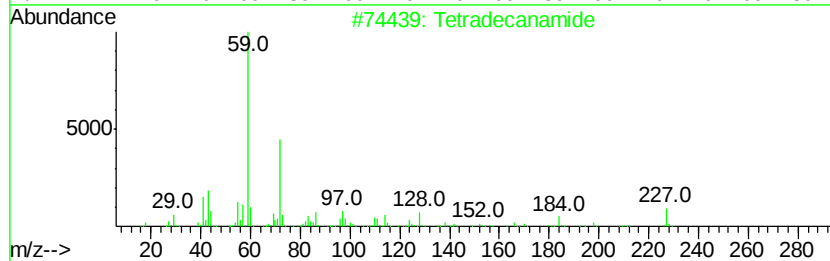
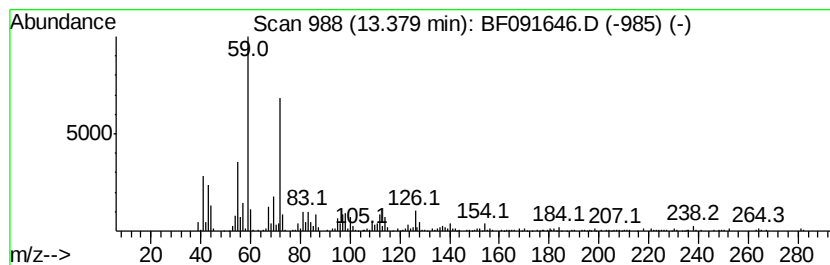
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.38	5.96 ng	522341	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	Nonanamide	157	C9H19NO	001120-07-6	50



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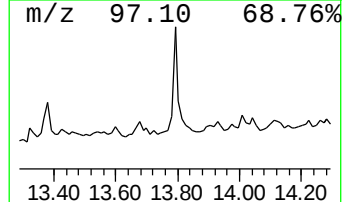
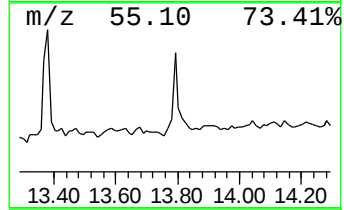
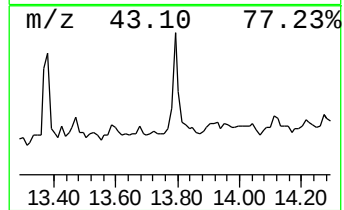
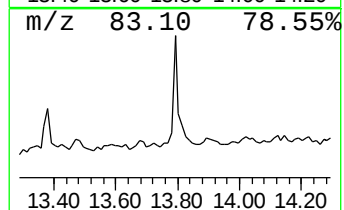
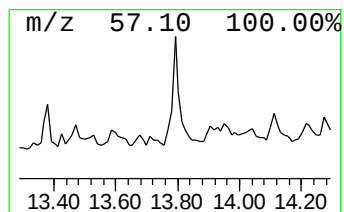
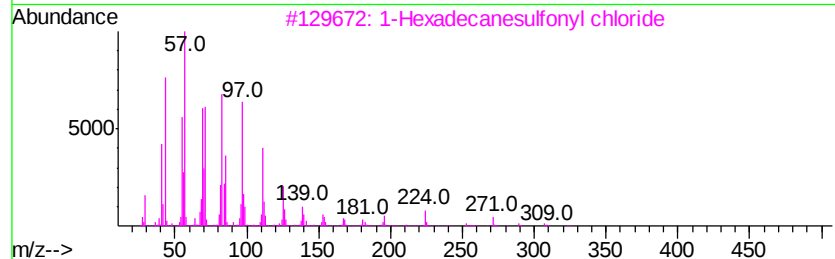
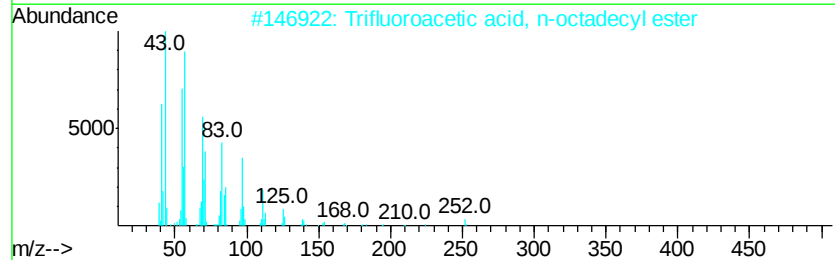
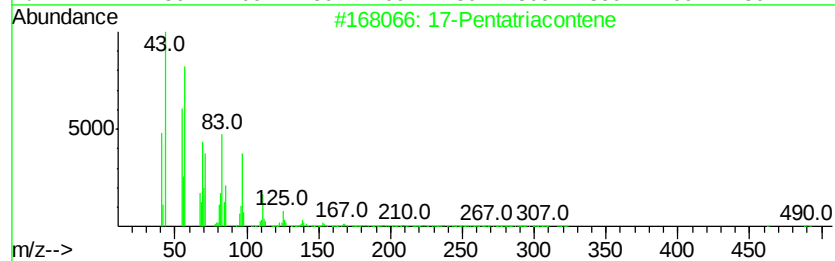
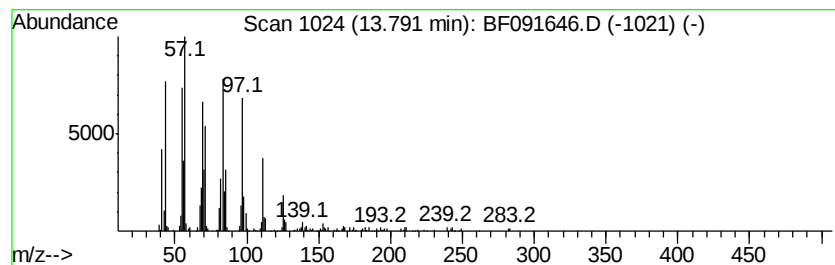
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.78 ng	331265	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	90
5		Cyclopentadecane	210	C15H30	000295-48-7	89



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
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Acq On : 15 Dec 2016 23:27
Operator : UM/SJ
Sample : H6007-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

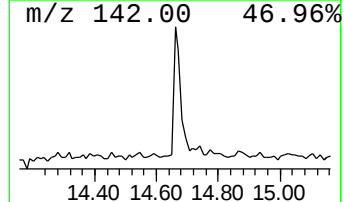
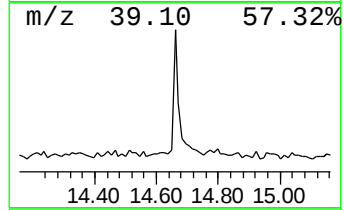
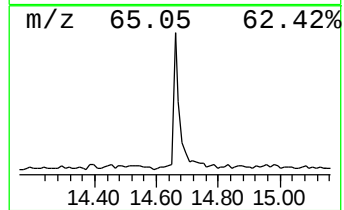
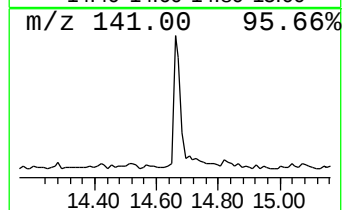
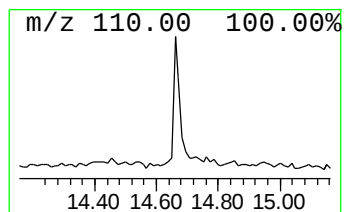
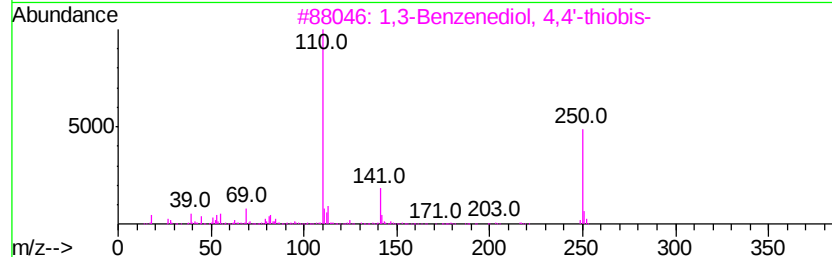
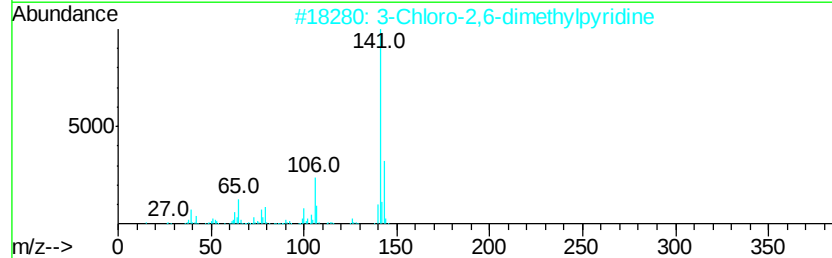
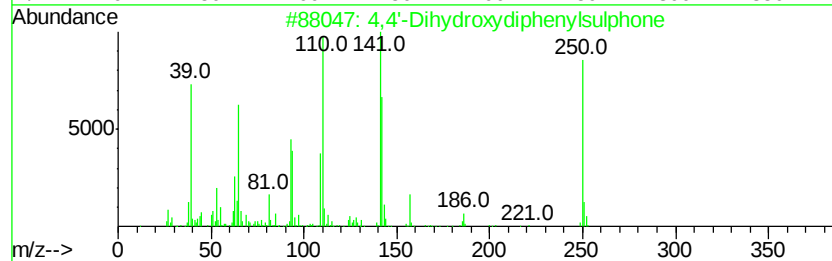
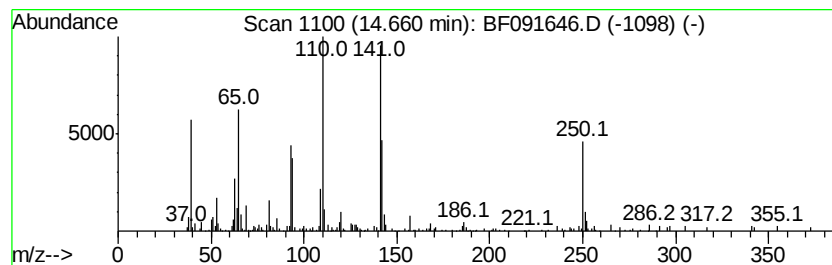
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ClientSampleId :
WC-12-10-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4,4'-Dihydroxydiphenylsulphone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.66	4.01 ng	215811	Perylene-d12	15.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	83
2	3-Chloro-2,6-dimethylpyridine	141	C7H8ClN	002405-06-3	32
3	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	18
4	Isoindole-1,3-dione, 1,3-dihydro...	345	C20H15N3O3	1000295-36-9	18
5	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
Data File : BF091646.D
Acq On : 15 Dec 2016 23:27
Operator : UM/SJ
Sample : H6007-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-12-10-15

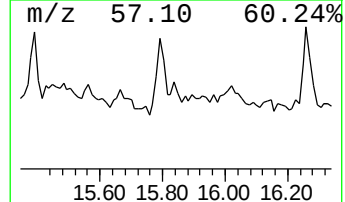
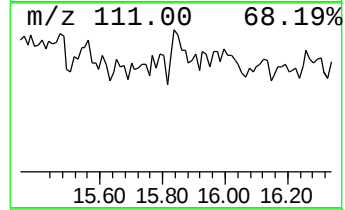
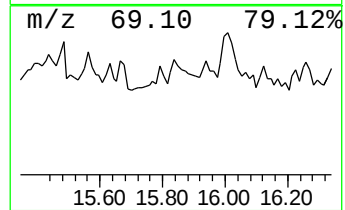
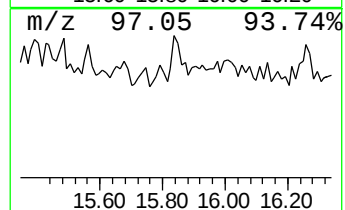
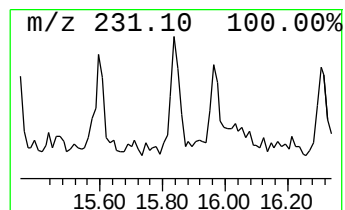
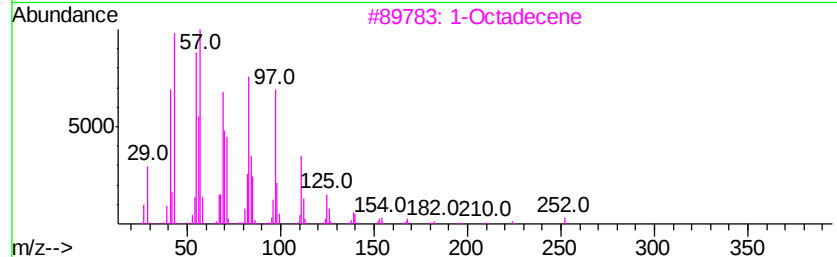
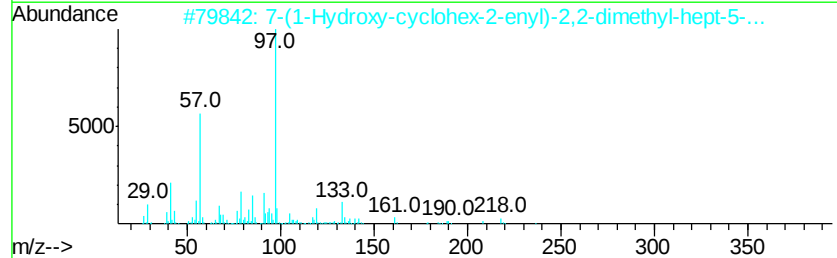
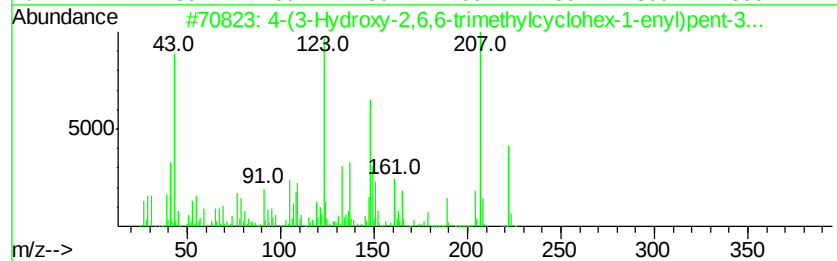
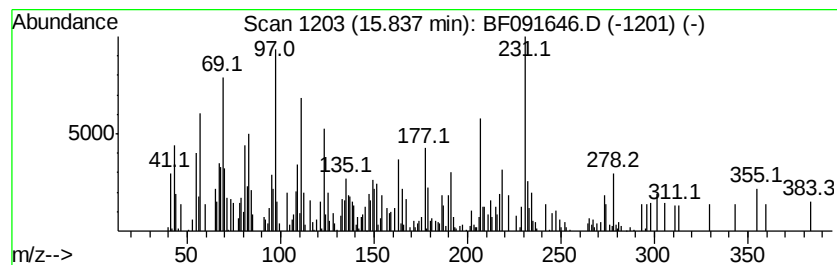
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.84 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.94 ng	158278	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-(3-Hydroxy-2,6,6-trimethylcyclohex-1-enyl)-2,2-dimethylhept-5-enoic acid	222	C14H22O2	097306-57-5	25
2		7-(1-Hydroxy-cyclohex-2-enyl)-2,2-dimethylhept-5-enoic acid	236	C15H24O2	083040-94-2	15
3		1-Octadecene	252	C18H36	000112-88-9	14
4		2-Chloropropionic acid, pentadecyl ester	318	C18H35ClO2	1000292-44-1	14
5		Muco-inositol tri-methaneboronate	252	C9H15B3O6	1000064-40-0	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
Data File : BF091646.D
Acq On : 15 Dec 2016 23:27
Operator : UM/SJ
Sample : H6007-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-12-10-15

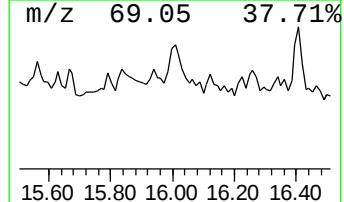
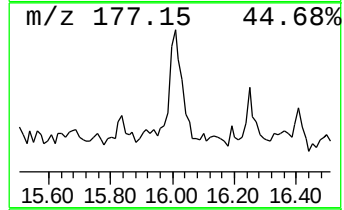
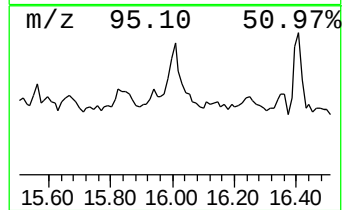
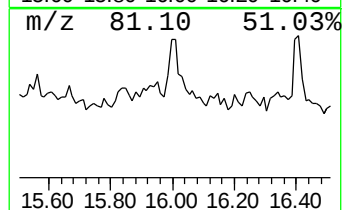
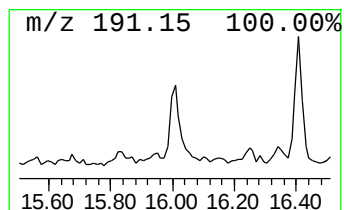
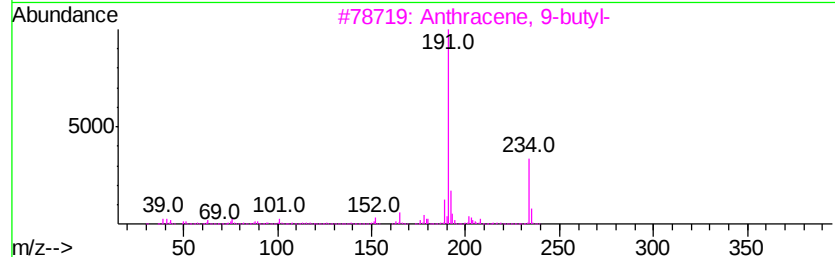
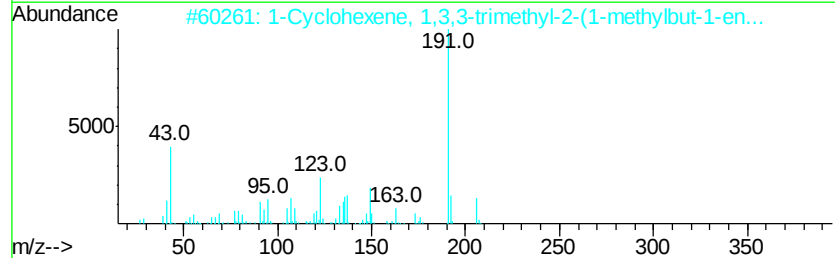
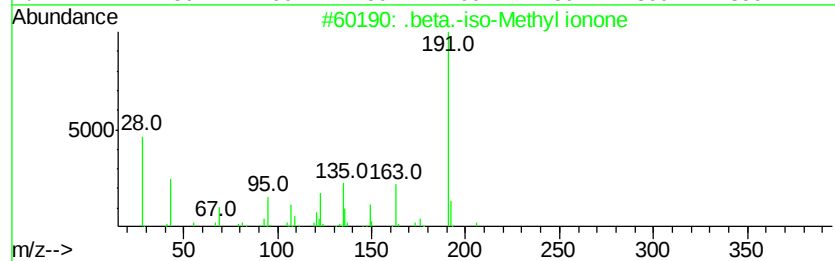
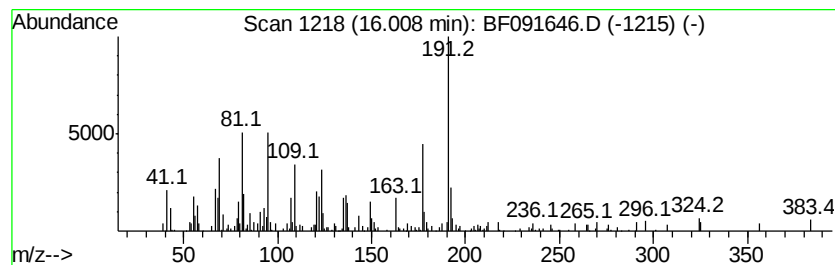
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	4.19 ng	225413	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
2		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	37
3		Anthracene, 9-butyl-	234	C18H18	001498-69-7	27
4		Silane, [4-(1,1-dimethylethyl)ph...	206	C13H22Si	018412-68-5	27
5		5-(7a-Isopropenyl-4,5-dimethyl-o...	290	C20H34O	1000193-54-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
Data File : BF091646.D
Acq On : 15 Dec 2016 23:27
Operator : UM/SJ
Sample : H6007-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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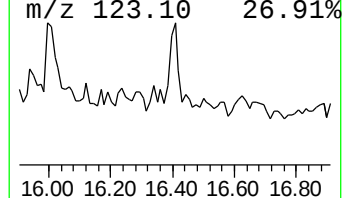
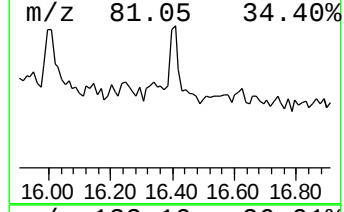
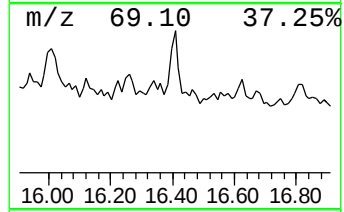
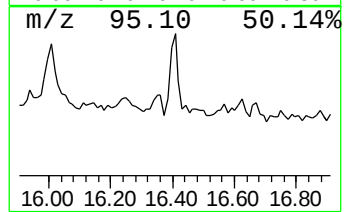
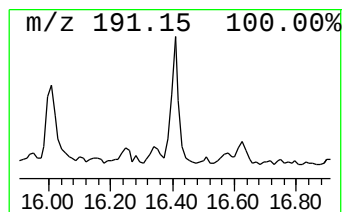
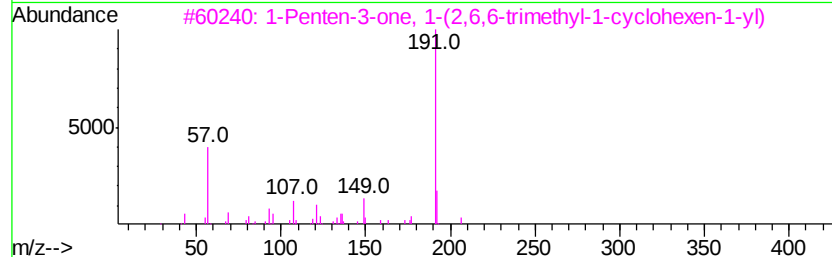
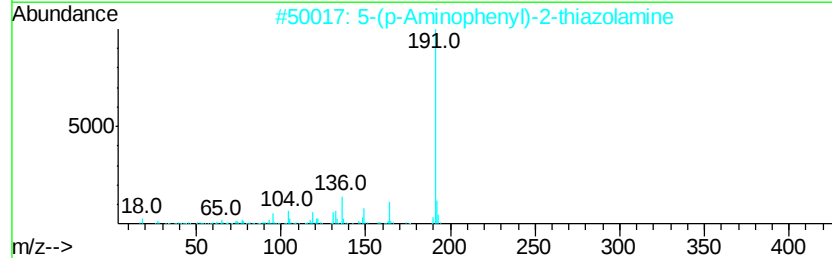
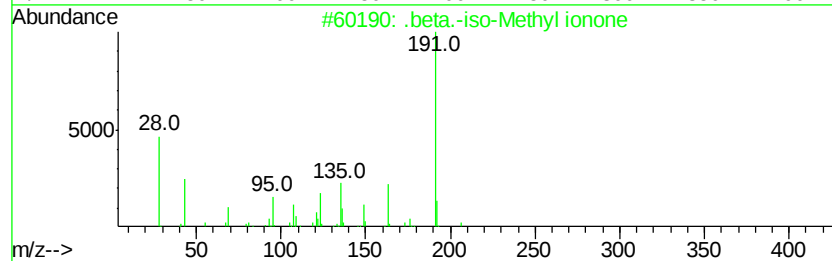
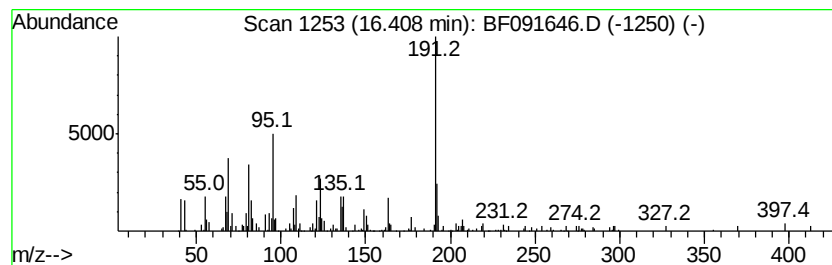
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	3.87 ng	208562	Perylene-d12	15.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
2			5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	49
3			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	46
4			Anthracene, 9-heptyl-	276	C21H24	1000157-50-3	27
5			Anthracene, 9-butyl-	234	C18H18	001498-69-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
Data File : BF091646.D
Acq On : 15 Dec 2016 23:27
Operator : UM/SJ
Sample : H6007-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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...	4.97	35.6	ng	3078670	1	6.78	1730230	20.0
unknown6.56	6.56	80.5	ng	6963730	1	6.78	1730230	20.0
Octadecane	10.74	2.3	ng	196137	4	11.30	1697230	20.0
Tetradecanamide	13.38	6.0	ng	522341	5	13.94	1752990	20.0
17-Pentatriacontene	13.79	3.8	ng	331265	5	13.94	1752990	20.0
4,4'-Dihydroxydip...	14.66	4.0	ng	215811	6	15.35	1077150	20.0
unknown15.84	15.84	2.9	ng	158278	6	15.35	1077150	20.0
unknown16.01	16.01	4.2	ng	225413	6	15.35	1077150	20.0
.beta.-iso-Methyl...	16.41	3.9	ng	208562	6	15.35	1077150	20.0