

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
 Data File : BF090832.D
 Acq On : 26 Oct 2016 2:32
 Operator : UM/SJ
 Sample : H5396-05 2X
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P3-S1

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-BF102116.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	4.956	249	251	262	rBV	231371	301051	14.88%	1.265%
2	5.390	287	289	301	rBV	1376852	1384127	68.42%	5.815%
3	6.430	378	380	383	rBV	1003919	1328578	65.68%	5.582%
4	6.567	389	392	394	rBV	1626935	1739195	85.98%	7.307%
5	6.796	410	412	418	rBV	1070834	1036071	51.22%	4.353%
6	6.956	423	426	428	rBV	1399595	1405587	69.49%	5.905%
7	7.356	459	461	464	rBV	548354	804375	39.76%	3.379%
8	7.470	468	471	477	rVB2	19038	52457	2.59%	0.220%
9	8.087	522	525	527	rBV	1605951	1432165	70.80%	6.017%
10	9.162	617	619	622	rBV	2319061	2022855	100.00%	8.499%
11	9.562	652	654	656	rBV	507957	432970	21.40%	1.819%
12	9.836	676	678	681	rBV	1277326	1443071	71.34%	6.063%
13	9.962	687	689	691	rVB2	24511	22604	1.12%	0.095%
14	10.282	715	717	718	rVB	48097	38713	1.91%	0.163%
15	10.499	733	736	739	rBV	24460	43157	2.13%	0.181%
16	10.625	745	747	750	rBV	843255	858037	42.42%	3.605%
17	10.751	757	758	763	rVB	76701	84127	4.16%	0.353%
18	11.196	796	797	799	rBV2	37657	44106	2.18%	0.185%
19	11.322	806	808	811	rBV	1212522	1184539	58.56%	4.977%
20	11.391	813	814	817	rVB2	41000	41369	2.05%	0.174%
21	11.551	826	828	832	rVV2	17452	29218	1.44%	0.123%
22	11.631	832	835	840	rVB	32817	54553	2.70%	0.229%
23	12.031	866	870	876	rBV	22906	53346	2.64%	0.224%
24	12.374	898	900	903	rBV3	19484	39237	1.94%	0.165%
25	12.431	903	905	906	rVB2	21913	28659	1.42%	0.120%
26	12.465	906	908	912	rBV4	14122	25646	1.27%	0.108%
27	12.534	912	914	917	rBV2	71238	93619	4.63%	0.393%
28	12.579	917	918	921	rVB2	23290	22860	1.13%	0.096%
29	12.716	924	930	931	rBV5	17633	59904	2.96%	0.252%
30	12.796	931	937	945	rBV	1327018	1837507	90.84%	7.720%
31	12.911	945	947	950	rBV	1537991	1353132	66.89%	5.685%
32	13.048	957	959	962	rVB	40796	41179	2.04%	0.173%
33	13.151	967	968	970	rVB2	31610	29747	1.47%	0.125%
34	13.379	986	988	989	rBV2	16547	24862	1.23%	0.104%

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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

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35	13.414	989	991	994	rVB3	35569	60651	3.00%	0.255%
36	13.494	996	998	1001	rVB2	31571	37812	1.87%	0.159%
37	13.562	1002	1004	1006	rBV2	15103	23802	1.18%	0.100%
38	13.608	1006	1008	1011	rBV2	37896	35711	1.77%	0.150%
39	13.711	1015	1017	1018	rBV	19699	22947	1.13%	0.096%
40	13.768	1018	1022	1024	rBV2	25965	50767	2.51%	0.213%
41	13.814	1024	1026	1030	rBV2	160682	234696	11.60%	0.986%
42	13.962	1036	1039	1045	rBV	1134157	1200780	59.36%	5.045%
43	14.454	1079	1082	1087	rBV	200973	331830	16.40%	1.394%
44	14.980	1126	1128	1132	rBV	50120	87488	4.32%	0.368%
45	15.060	1133	1135	1141	rBV2	94569	247627	12.24%	1.040%
46	15.380	1161	1163	1166	rBV	616145	884681	43.73%	3.717%
47	15.837	1201	1203	1205	rBV	72207	110301	5.45%	0.463%
48	15.883	1205	1207	1211	rVV	66740	125770	6.22%	0.528%
49	15.974	1213	1215	1219	rVB4	61913	103408	5.11%	0.434%
50	17.300	1328	1331	1336	rBV2	94199	239480	11.84%	1.006%
51	17.974	1387	1390	1394	rVB	39481	81538	4.03%	0.343%
52	18.260	1412	1415	1422	rVB2	54952	161334	7.98%	0.678%
53	19.231	1496	1500	1506	rVB4	125972	368365	18.21%	1.548%

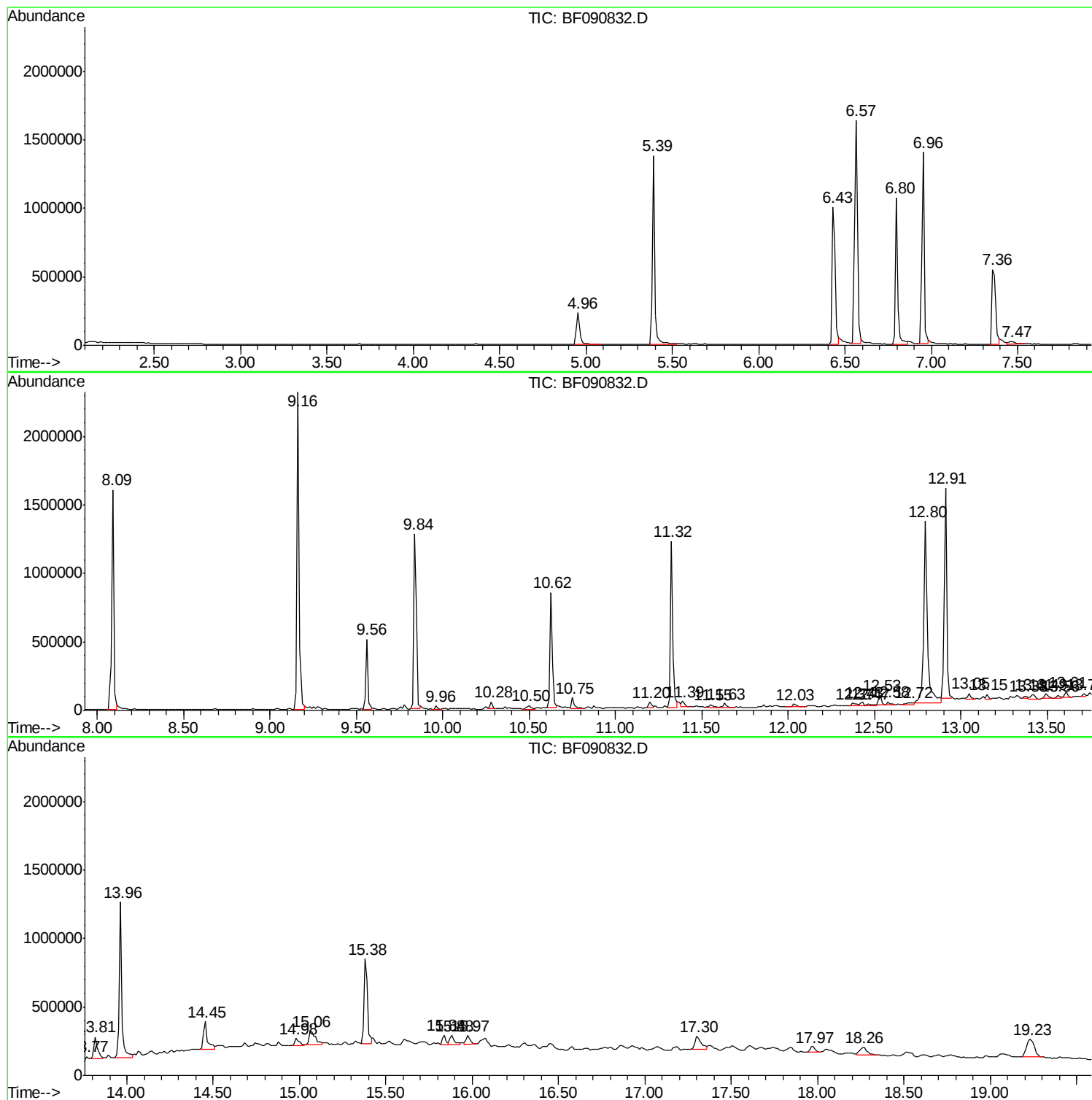
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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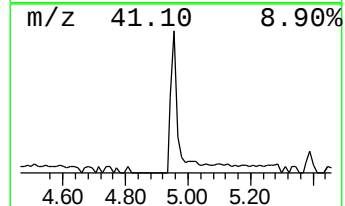
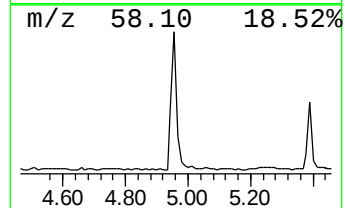
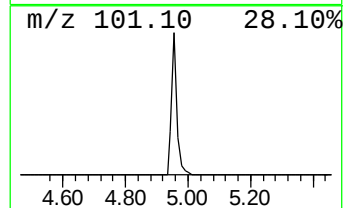
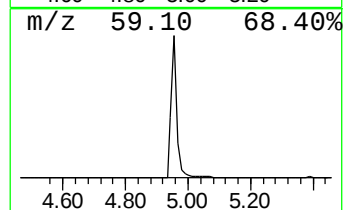
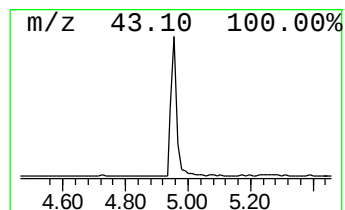
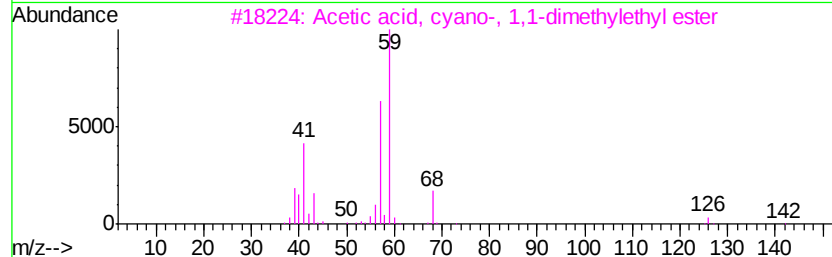
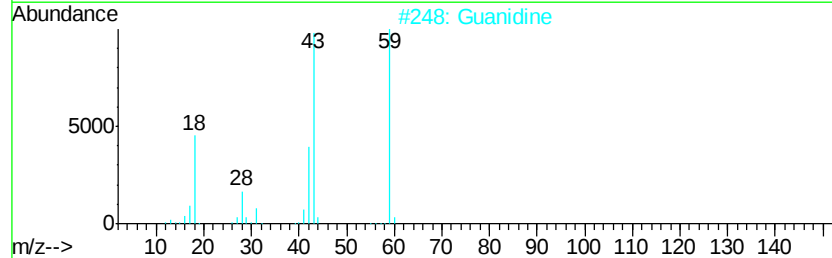
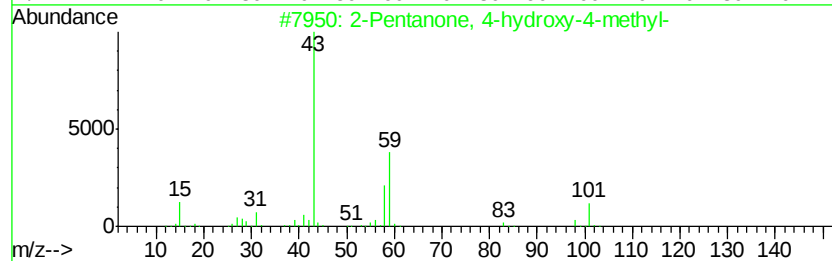
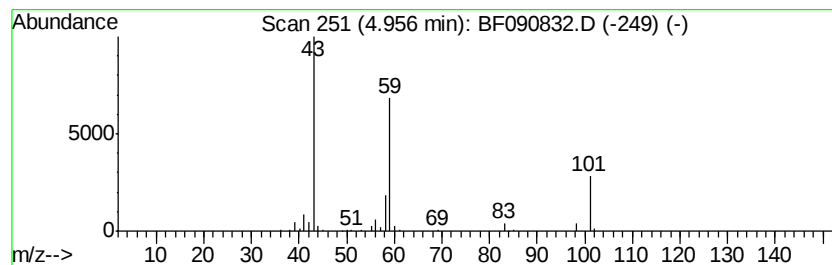
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	5.81 ng	301051	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	43
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Acetone	58	C3H6O	000067-64-1	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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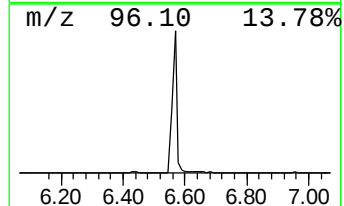
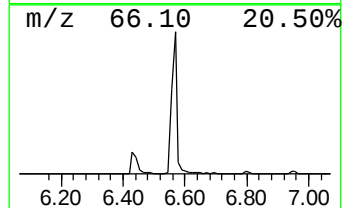
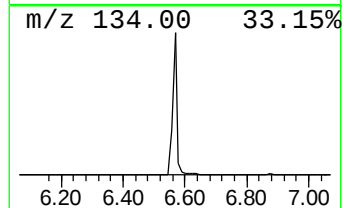
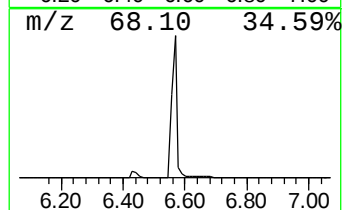
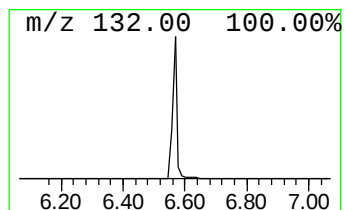
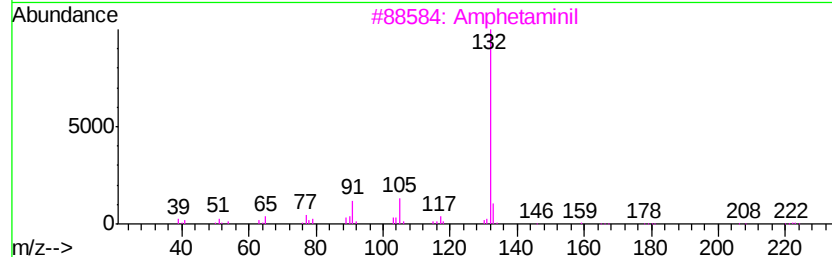
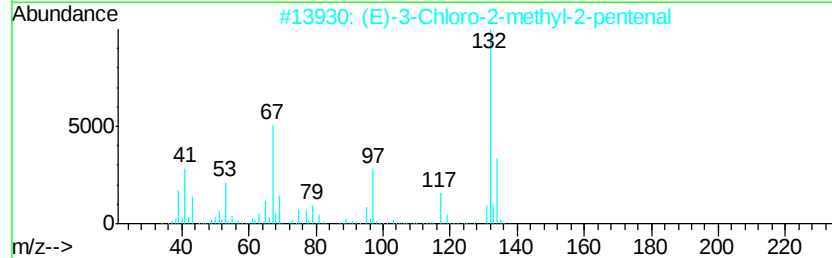
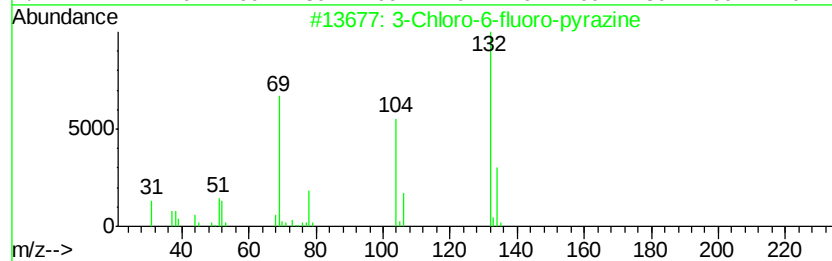
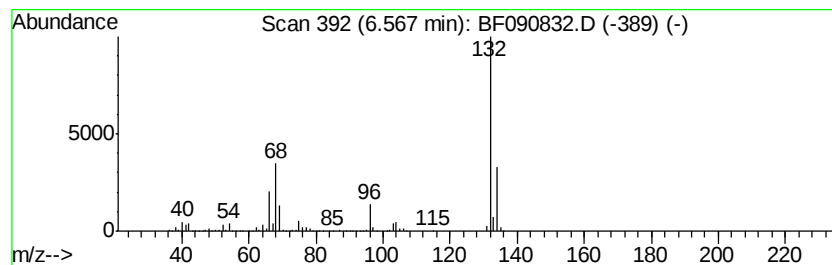
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	33.57 ng	1739200	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Xenon	132	Xe	007440-63-3	9



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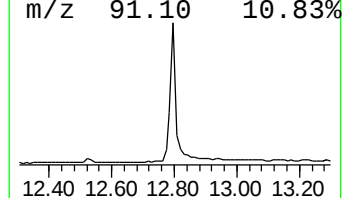
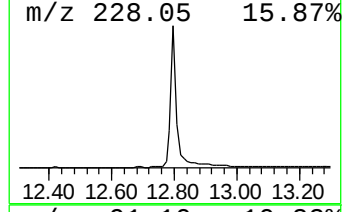
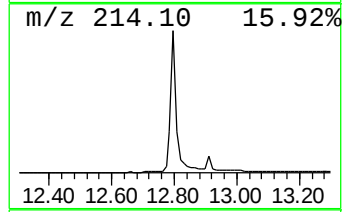
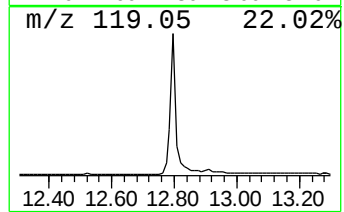
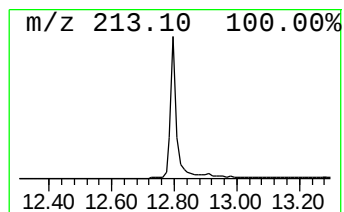
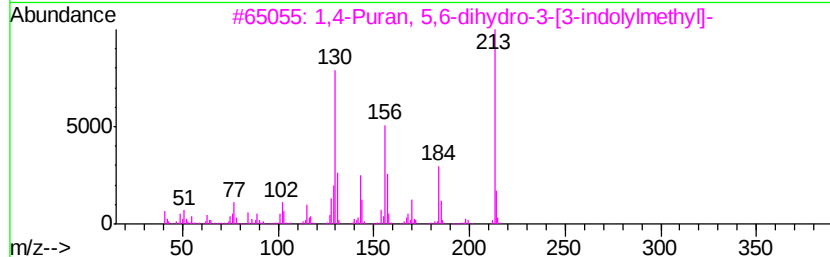
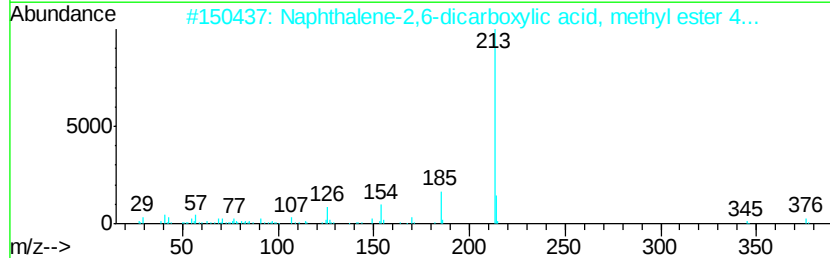
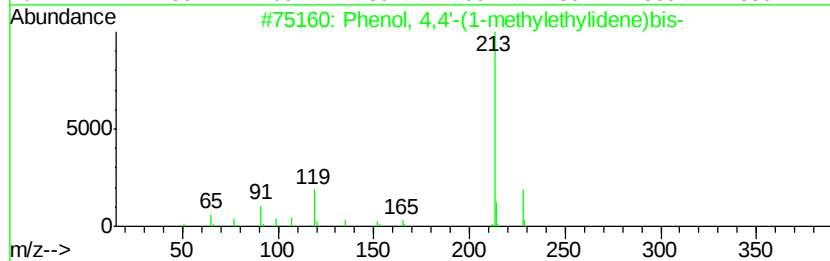
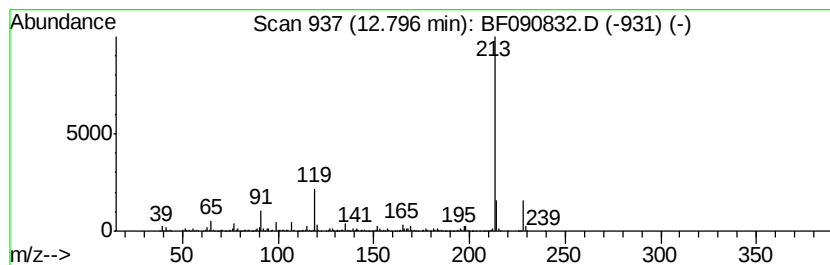
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	30.61 ng	1837510	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97	
2	Naphthalene-2,6-dicarboxylic aci...	376	C24H24O4	1000189-60-8	40	
3	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	40	
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	40	
5	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	38	



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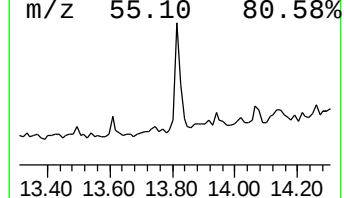
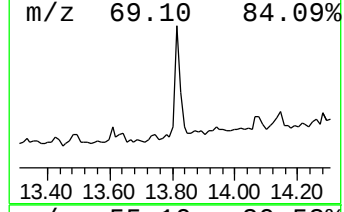
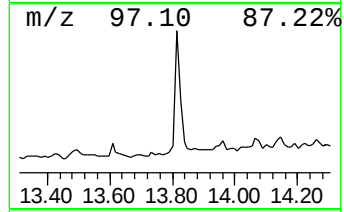
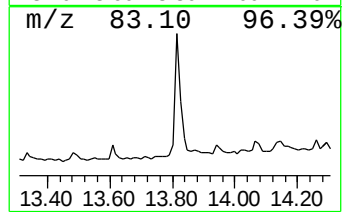
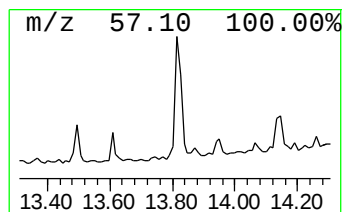
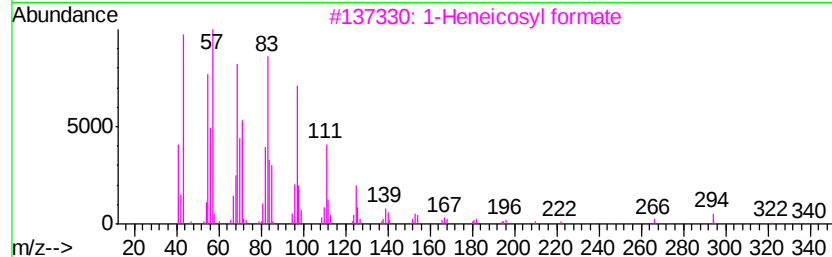
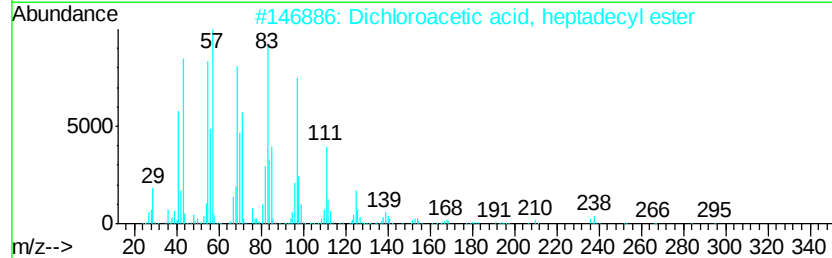
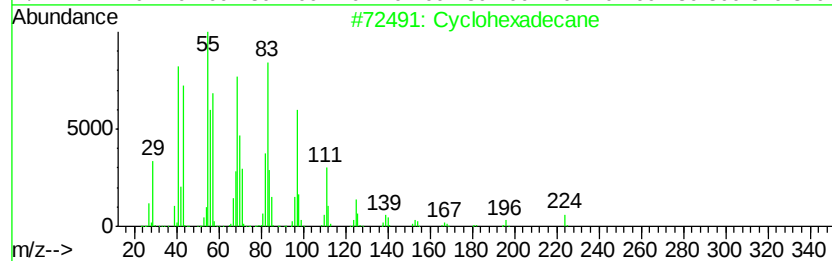
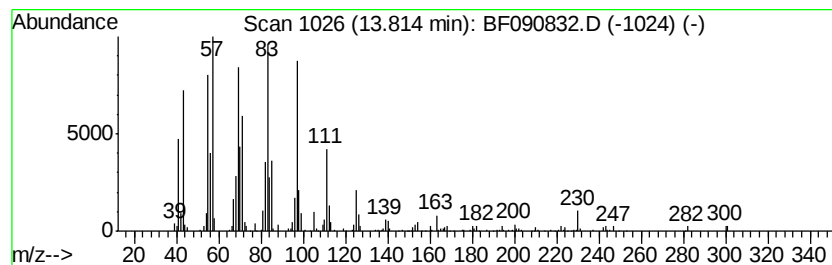
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.91 ng	234696	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	98
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



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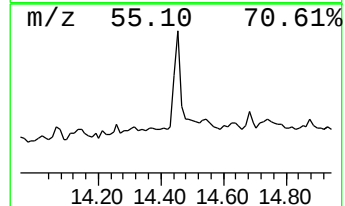
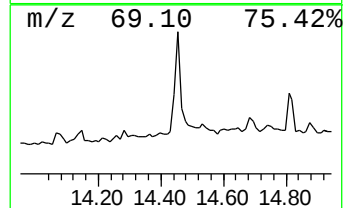
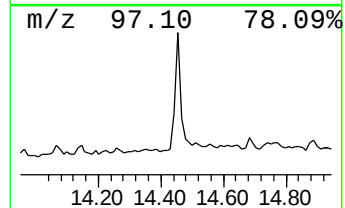
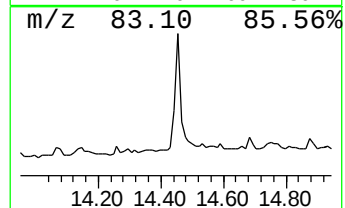
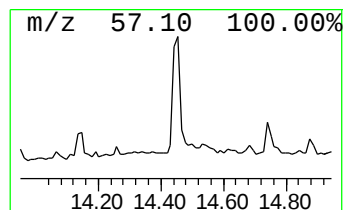
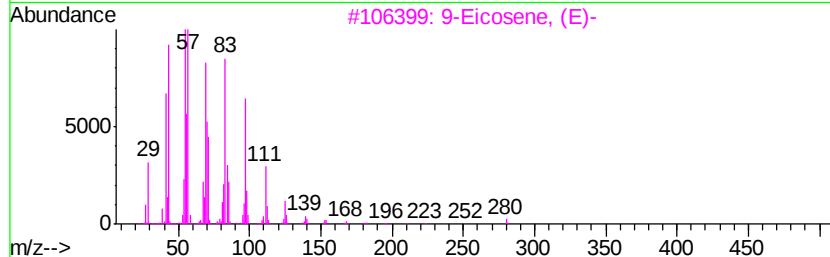
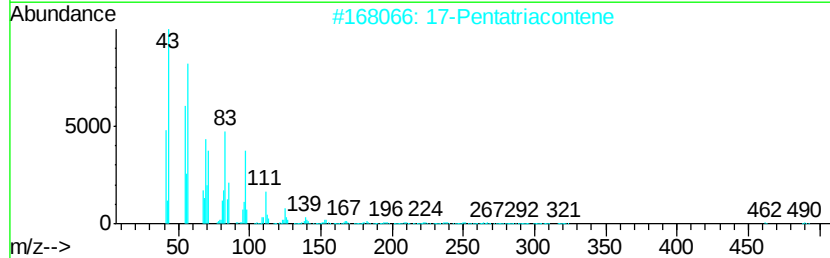
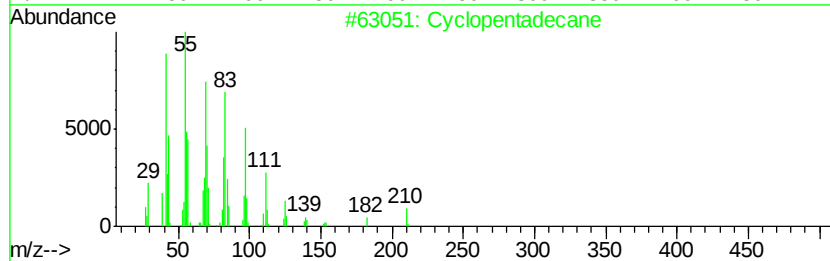
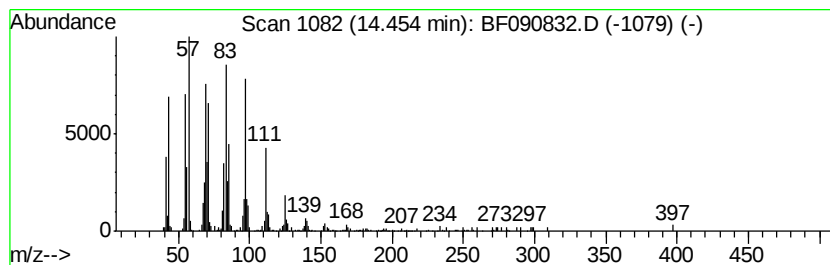
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	5.53 ng	331830	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentadecane	210	C15H30	000295-48-7	94
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	90
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5		1-Tetracosanol	354	C24H50O	000506-51-4	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102516\
Data File : BF090832.D
Acq On : 26 Oct 2016 2:32
Operator : UM/SJ
Sample : H5396-05 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P3-S1

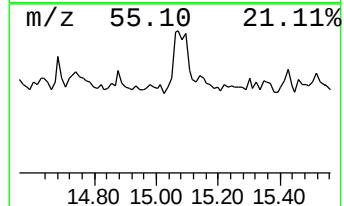
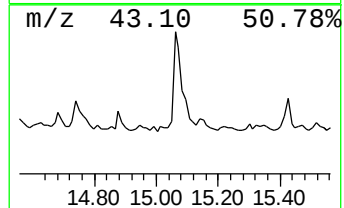
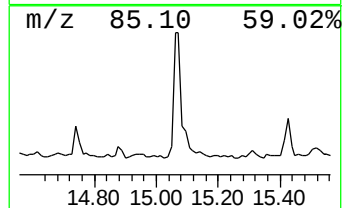
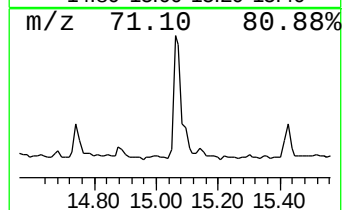
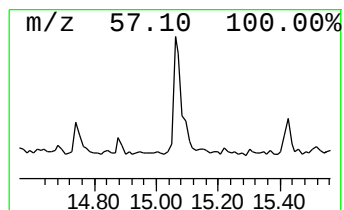
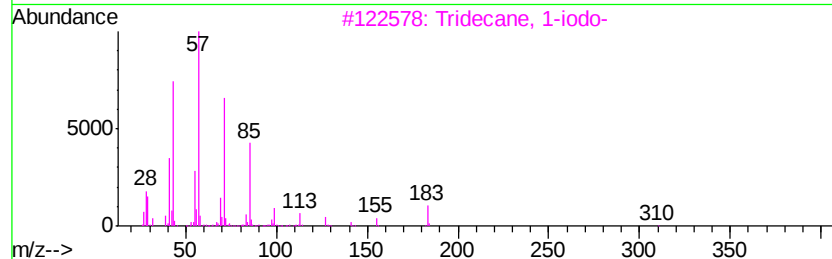
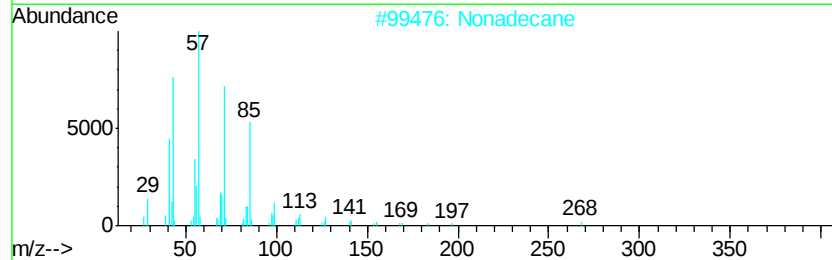
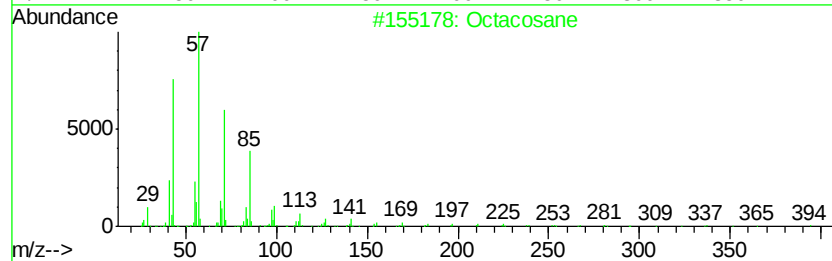
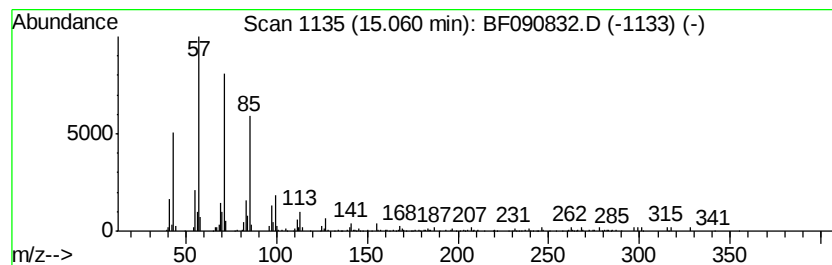
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	5.60 ng	247627	Perylene-d12	15.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Nonadecane		268	C19H40	000629-92-5	87
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	86
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
5	Heptadecane		240	C17H36	000629-78-7	86



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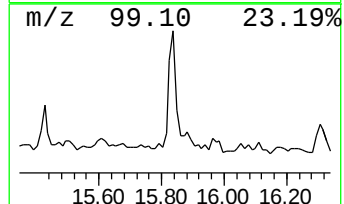
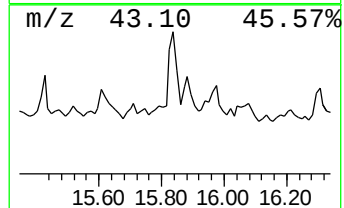
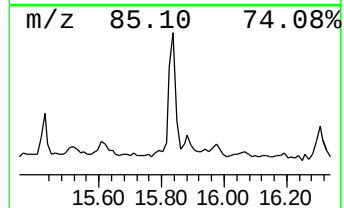
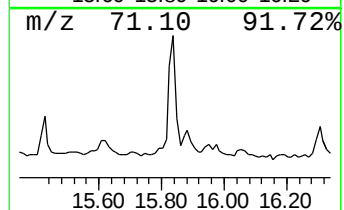
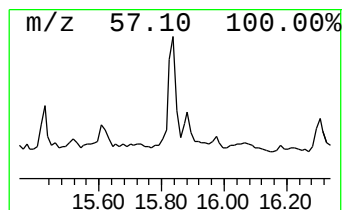
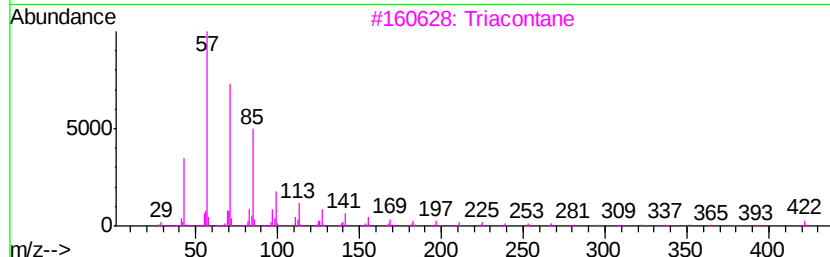
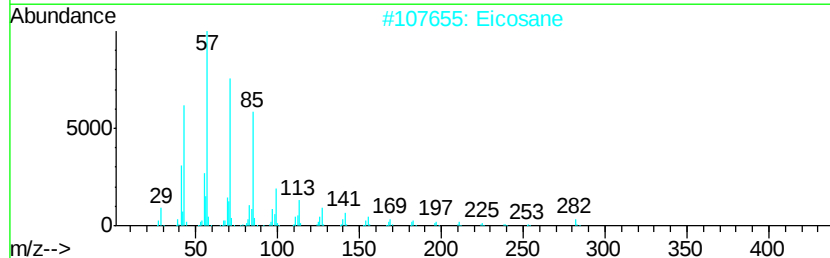
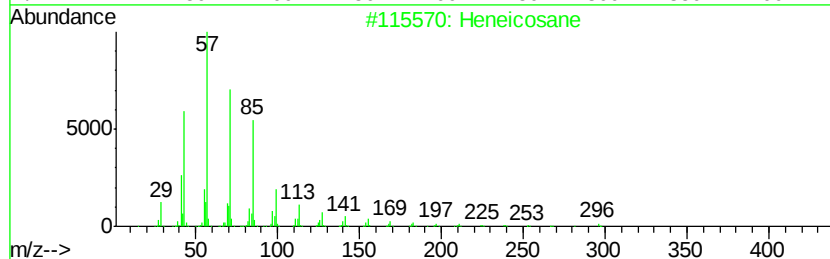
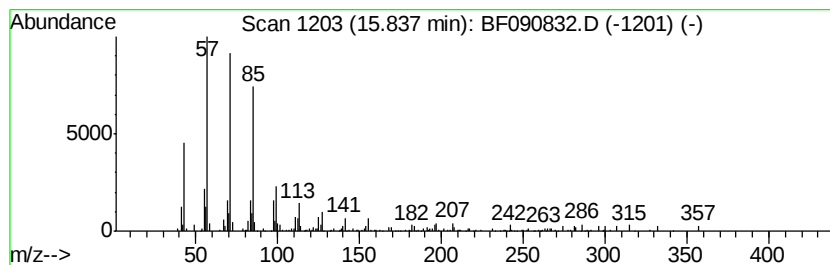
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.49 ng	110301	Perylene-d12	15.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	98
2	Eicosane		282	C20H42	000112-95-8	91
3	Triacontane		422	C30H62	000638-68-6	91
4	Tetracosane		338	C24H50	000646-31-1	86
5	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	83



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Acq On : 26 Oct 2016 2:32
Operator : UM/SJ
Sample : H5396-05 2X
Misc :
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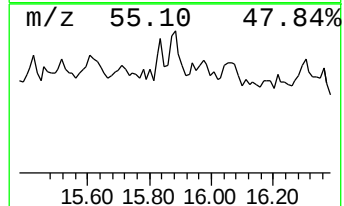
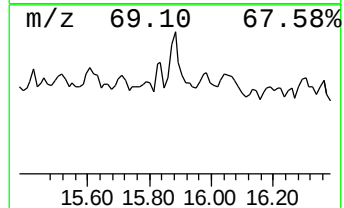
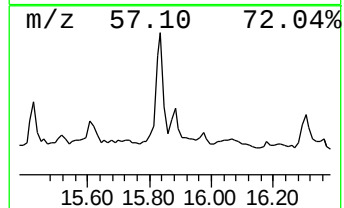
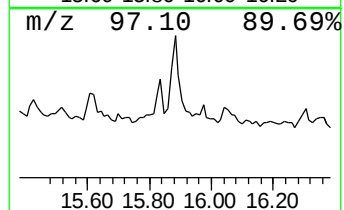
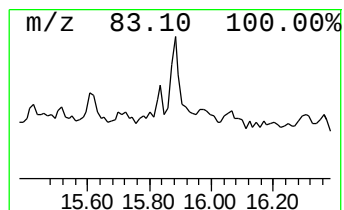
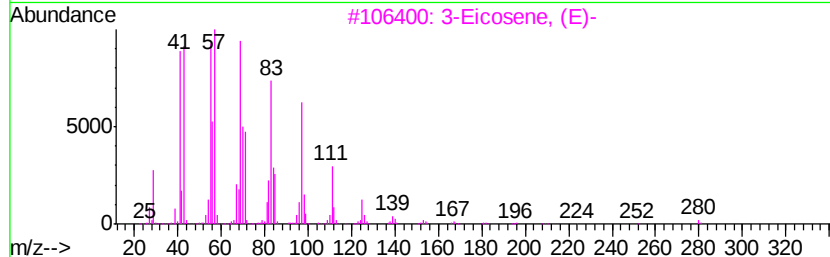
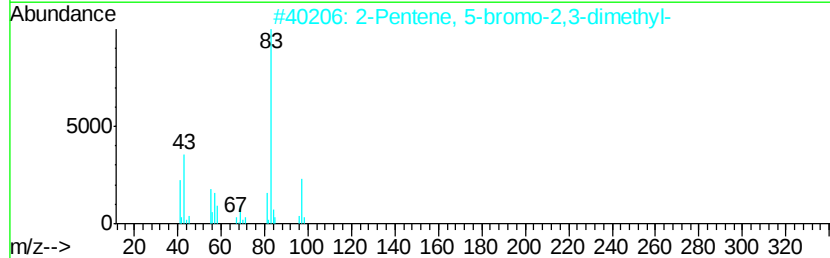
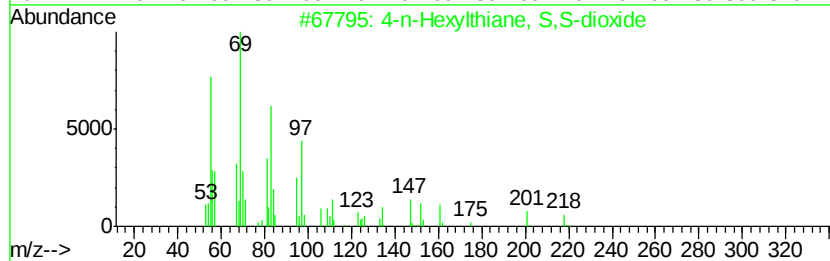
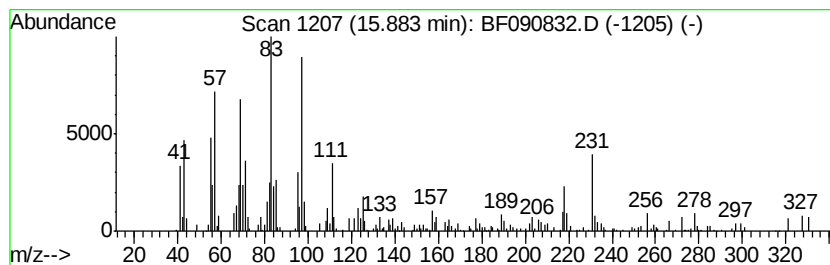
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.88 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	2.84 ng	125770	Perylene-d12	15.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	43		
2	2-Pentene, 5-bromo-2,3-dimethyl-	176	C7H13Br	056312-52-8	38		
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	38		
4	1-Tricosene	322	C23H46	018835-32-0	35		
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	30		



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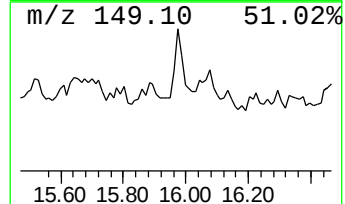
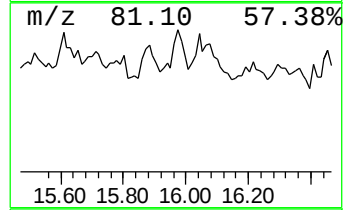
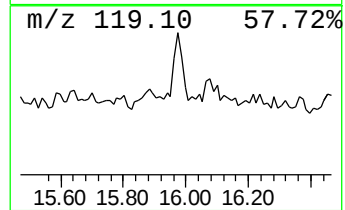
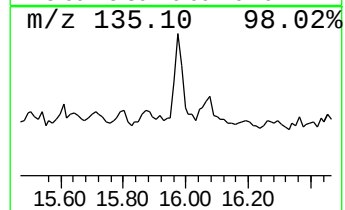
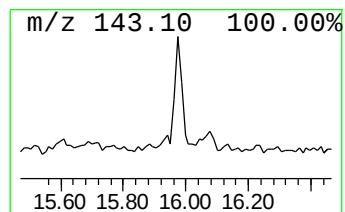
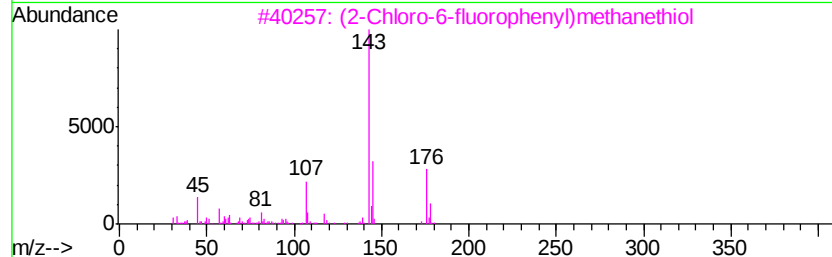
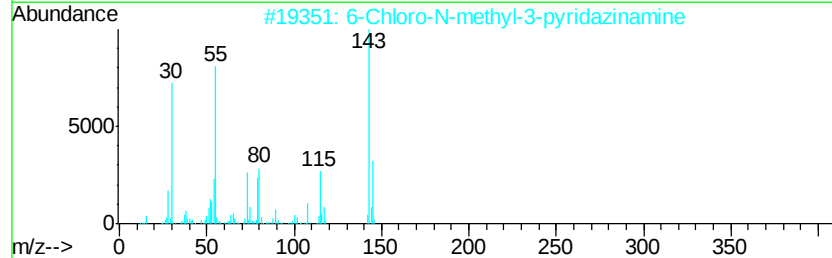
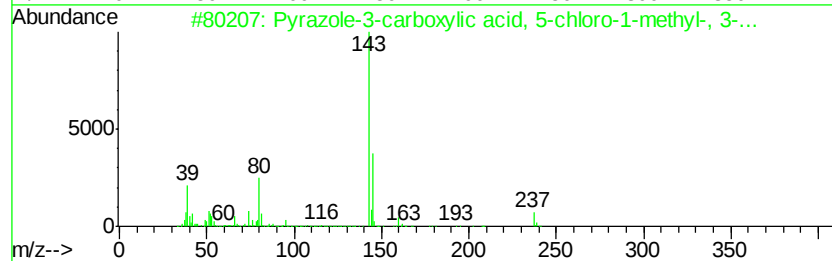
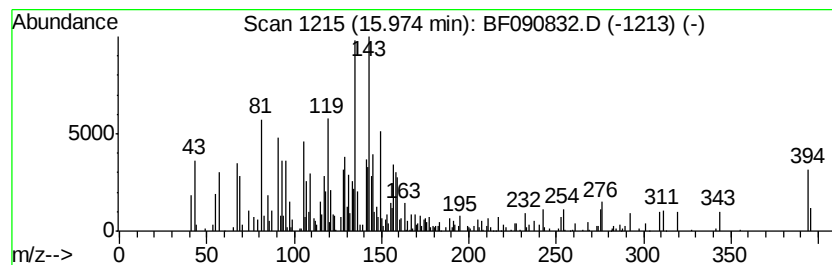
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.97 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.34 ng	103408	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrazole-3-carboxylic acid, 5-ch...	237	C10H8ClN3O2	1000267-97-8	22
2		6-Chloro-N-methyl-3-pyridazinamine	143	C5H6ClN3	014959-32-1	22
3		(2-Chloro-6-fluorophenyl)methane...	176	C7H6ClFS	1000298-15-3	22
4		3-(2-Chloro-4-fluoro-benzyl)-3H-...	277	C14H9ClFN02	1000274-76-5	22
5		m-Aminobenzamidine	135	C7H9N3	003459-66-3	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090832.D
Acq On : 26 Oct 2016 2:32
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Misc :
ALS Vial : 25 Sample Multiplier: 1

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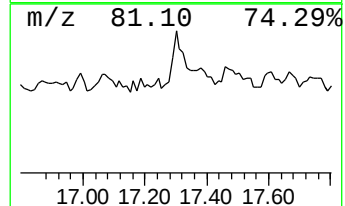
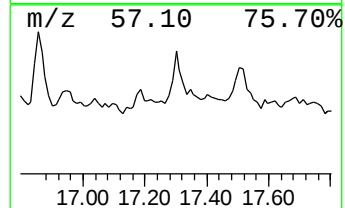
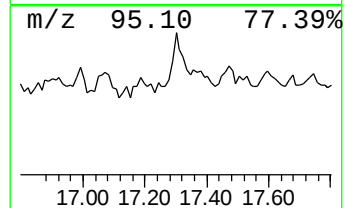
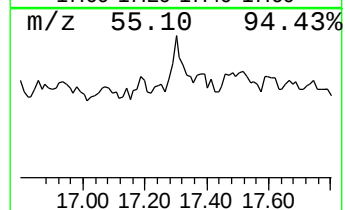
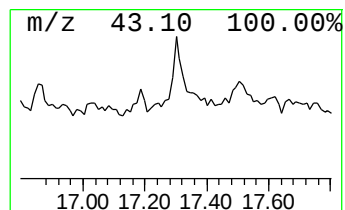
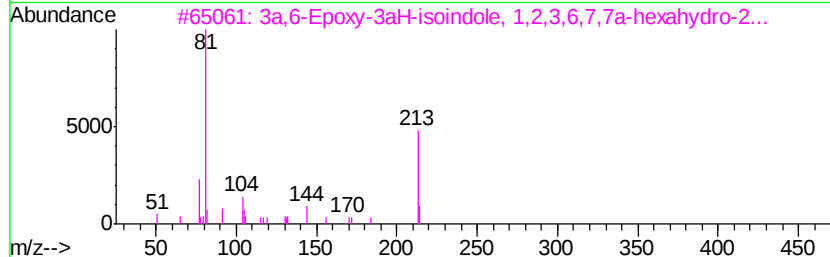
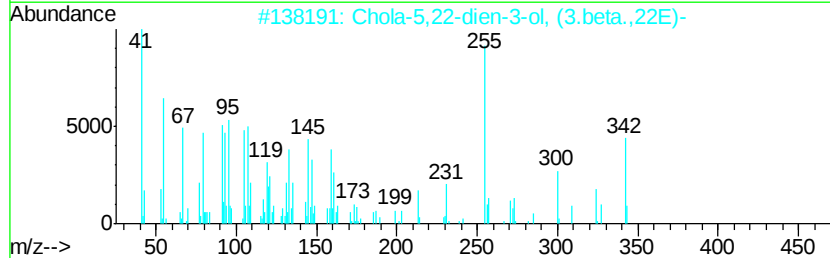
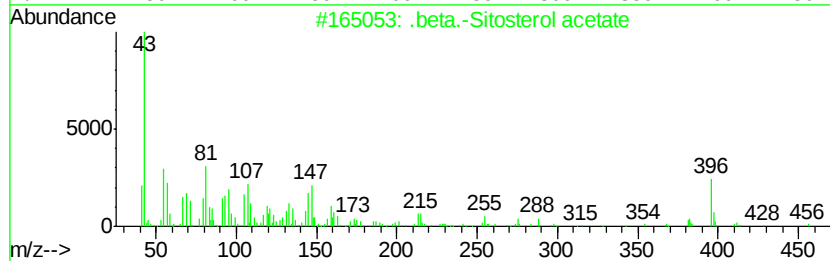
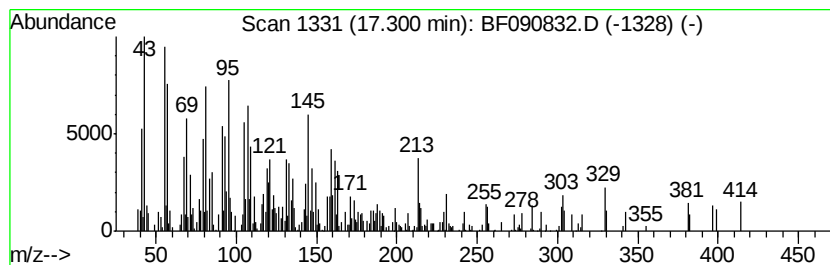
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.30 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	5.41 ng	239480	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	37
2		Chola-5,22-dien-3-ol, (3.beta.,2...	342	C24H38O	057597-08-7	35
3		3a,6-Epoxy-3aH-isoindole, 1,2,3,...	213	C14H15NO	017960-73-5	11
4		Thiazolidin-4-one, 3-(2-furfuryl...	342	C16H10N2O3S2	313966-21-1	10
5		Methanone, (2-furyl)[3-(4-nitrob...	330	C14H10N4O4S	332019-65-5	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102516\
Data File : BF090832.D
Acq On : 26 Oct 2016 2:32
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Misc :
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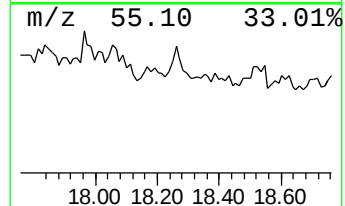
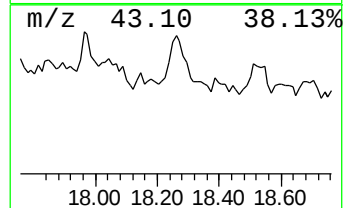
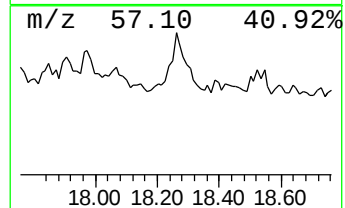
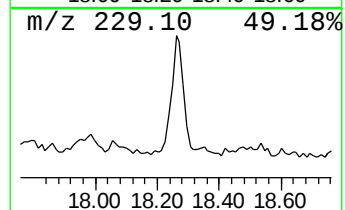
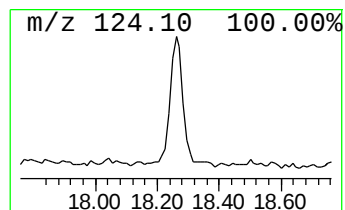
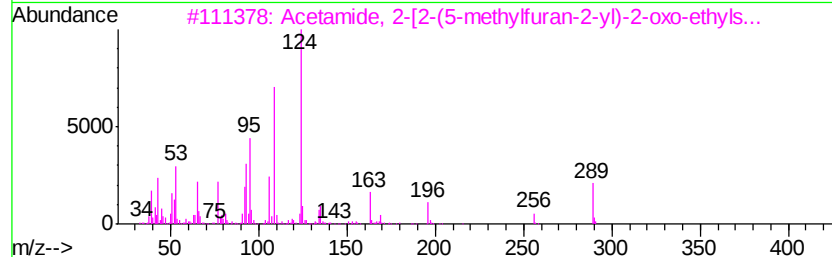
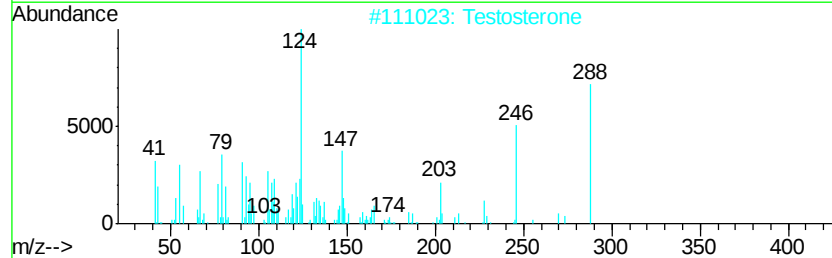
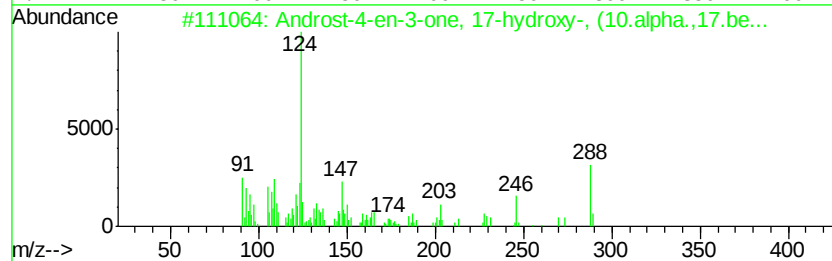
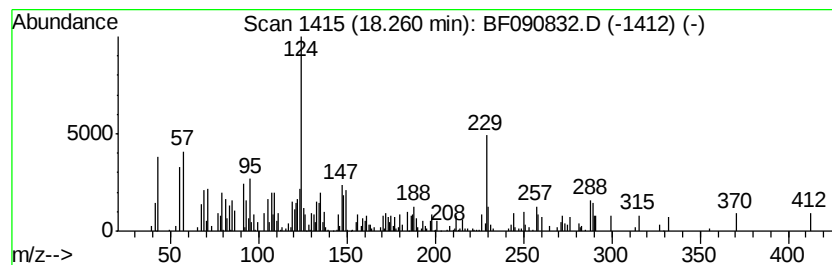
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Androst-4-en-3-one, 17-hydr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	3.65 ng	161334	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Androst-4-en-3-one, 17-hydroxy-, ...	288	C19H28O2	000604-39-7	64
2		Testosterone	288	C19H28O2	000058-22-0	52
3		Acetamide, 2-[2-(5-methylfuran-2-yl)-2-oxo-ethyl]-...	289	C15H15N03S	1000259-79-3	35
4		6-Oxotetrahydropyran-3-carboxylic acid	250	C13H14O5	1000193-75-1	35
5		Hyoscyamine Hydrobromide	289	C17H23NO3	000306-03-6	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102516\
Data File : BF090832.D
Acq On : 26 Oct 2016 2:32
Operator : UM/SJ
Sample : H5396-05 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P3-S1

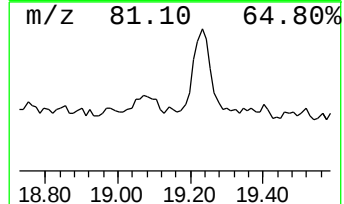
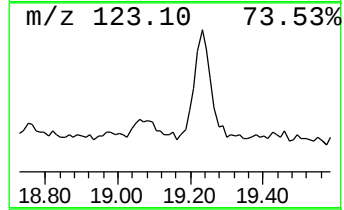
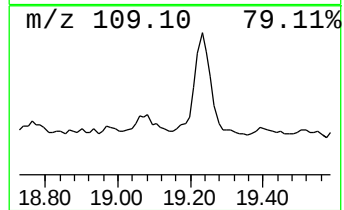
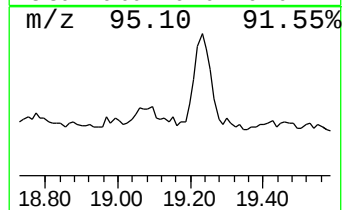
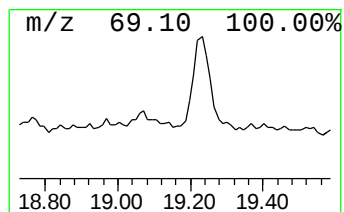
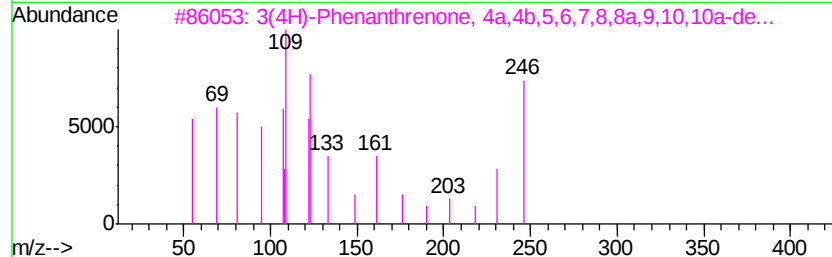
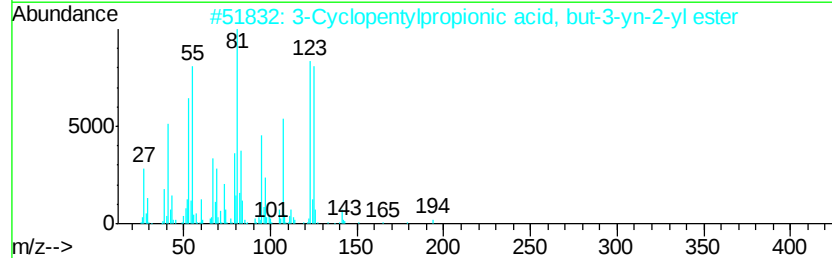
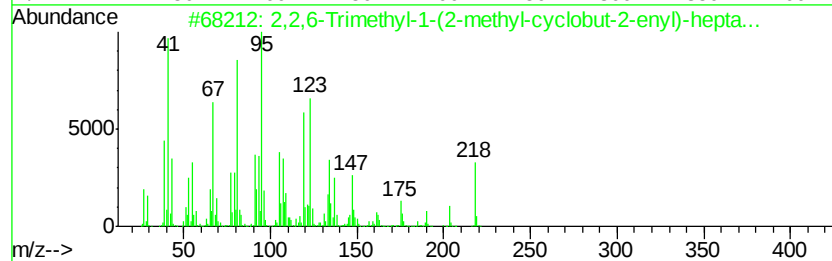
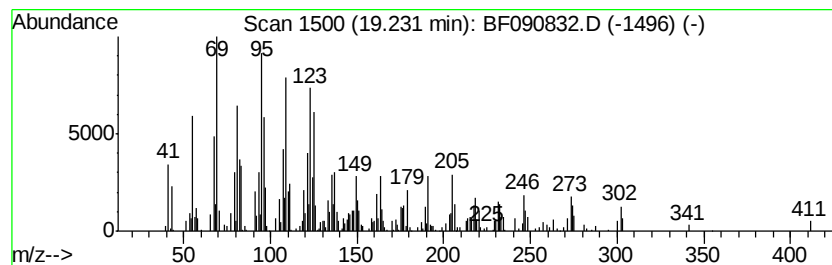
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2,2,6-Trimethyl-1-(2-methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	8.33 ng	368365	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	55
2		3-Cyclopentylpropionic acid, but...	194	C12H18O2	1000292-46-4	51
3		3(4H)-Phenanthrenone, 4a,4b,5,6,...	246	C17H26O	057684-12-5	38
4		1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	30
5		Imidazole, 4-methyl-5-[3,3,3-tri...	234	C10H13F3N2O	1000129-15-8	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102516\
 Data File : BF090832.D
 Acq On : 26 Oct 2016 2:32
 Operator : UM/SJ
 Sample : H5396-05 2X
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P3-S1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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...	4.96	5.8	ng	301051	1	6.80	1036070	20.0
unknown6.57	6.57	33.6	ng	1739200	1	6.80	1036070	20.0
Phenol, 4,4'-(1-m...	12.80	30.6	ng	1837510	5	13.96	1200780	20.0
Cyclohexadecane	13.81	3.9	ng	234696	5	13.96	1200780	20.0
Cyclopentadecane	14.45	5.5	ng	331830	5	13.96	1200780	20.0
Octacosane	15.06	5.6	ng	247627	6	15.38	884681	20.0
Heneicosane	15.84	2.5	ng	110301	6	15.38	884681	20.0
unknown15.88	15.88	2.8	ng	125770	6	15.38	884681	20.0
unknown15.97	15.97	2.3	ng	103408	6	15.38	884681	20.0
unknown17.30	17.30	5.4	ng	239480	6	15.38	884681	20.0
Androst-4-en-3-on...	18.26	3.6	ng	161334	6	15.38	884681	20.0
2,2,6-Trimethyl-1...	19.23	8.3	ng	368365	6	15.38	884681	20.0