

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
 Data File : BF090943.D
 Acq On : 31 Oct 2016 22:05
 Operator : UM/SJ
 Sample : H5475-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WOOLSTON-TS-004

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-BF102616.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	4.910	244	247	259	rBV	559151	831518	12.82%	1.084%
2	5.344	282	285	288	rBV	3312251	3413382	52.63%	4.450%
3	6.396	374	377	379	rBV	3326819	3747861	57.79%	4.886%
4	6.510	385	387	390	rBV	2690739	3800416	58.60%	4.954%
5	6.750	406	408	410	rBV	673826	782558	12.07%	1.020%
6	6.899	419	421	424	rBV	2714967	2896967	44.67%	3.776%
7	7.310	454	457	460	rBV	1761664	2155696	33.24%	2.810%
8	8.030	518	520	523	rBV	1277356	1190242	18.35%	1.552%
9	9.116	612	615	617	rBV	4276415	4592504	70.82%	5.987%
10	9.505	647	649	652	rBV	748576	657975	10.15%	0.858%
11	9.779	671	673	676	rBV	1036471	1176868	18.15%	1.534%
12	10.225	710	712	714	rVB	91577	74347	1.15%	0.097%
13	10.568	740	742	745	rVB2	1815560	2597682	40.06%	3.386%
14	10.693	752	753	760	rBV	114610	169192	2.61%	0.221%
15	10.819	762	764	768	rVB	187066	198287	3.06%	0.258%
16	10.933	772	774	777	rBV	155453	192450	2.97%	0.251%
17	11.139	791	792	794	rBV	51796	67891	1.05%	0.089%
18	11.265	801	803	805	rBV	1346198	1157152	17.84%	1.508%
19	11.333	805	809	811	rVB3	83492	110964	1.71%	0.145%
20	11.813	848	851	854	rBV3	44875	124072	1.91%	0.162%
21	11.871	854	856	858	rVV	72596	105670	1.63%	0.138%
22	11.985	862	866	870	rBV5	64595	218169	3.36%	0.284%
23	12.248	887	889	893	rVB	77556	128314	1.98%	0.167%
24	12.316	893	895	898	rVB	119586	127780	1.97%	0.167%
25	12.408	901	903	906	rVB2	108874	117796	1.82%	0.154%
26	12.545	910	915	918	rBV2	112339	185089	2.85%	0.241%
27	12.739	930	932	936	rVB3	64658	92935	1.43%	0.121%
28	12.853	939	942	944	rBV	3799437	3425658	52.82%	4.466%
29	13.071	958	961	965	rBV2	368954	757000	11.67%	0.987%
30	13.276	977	979	980	rVV	106156	93193	1.44%	0.121%
31	13.299	980	981	984	rVB	78588	97418	1.50%	0.127%
32	13.436	989	993	995	rBV2	62980	139537	2.15%	0.182%
33	13.551	1001	1003	1005	rVB	155908	125756	1.94%	0.164%
34	13.711	1014	1017	1018	rBV	39205	66658	1.03%	0.087%

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Integrator: RTE

Smoothing : ON

Sampling : 1

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35	13.756	1018	1021	1024	rVV	1226628	1615832	24.92%	2.106%
36	13.814	1024	1026	1028	rVB	79657	110199	1.70%	0.144%
37	13.894	1030	1033	1036	rBV	800882	1071356	16.52%	1.397%
38	14.008	1041	1043	1047	rVV5	37176	76955	1.19%	0.100%
39	14.076	1047	1049	1052	rVV	198424	235760	3.64%	0.307%
40	14.202	1058	1060	1062	rBV	207792	190117	2.93%	0.248%
41	14.385	1074	1076	1079	rBV	1137431	1394982	21.51%	1.818%
42	14.442	1079	1081	1083	rVV	295096	350645	5.41%	0.457%
43	14.511	1085	1087	1090	rVV	124901	184730	2.85%	0.241%
44	14.625	1094	1097	1098	rVV2	60835	137795	2.12%	0.180%
45	14.659	1098	1100	1102	rVV2	189766	368752	5.69%	0.481%
46	14.739	1105	1107	1111	rVV	366887	634202	9.78%	0.827%
47	14.808	1111	1113	1117	rVB	389159	504806	7.78%	0.658%
48	15.014	1126	1131	1133	rBV2	831534	1500106	23.13%	1.956%
49	15.071	1133	1136	1138	rVV	1115891	1507829	23.25%	1.966%
50	15.151	1141	1143	1145	rBV	102048	144153	2.22%	0.188%
51	15.299	1153	1156	1158	rBV	731204	905416	13.96%	1.180%
52	15.368	1161	1162	1165	rVV	81518	127720	1.97%	0.166%
53	15.425	1165	1167	1170	rVB	141678	204800	3.16%	0.267%
54	15.528	1173	1176	1178	rBV	306425	483249	7.45%	0.630%
55	15.642	1183	1186	1190	rVB	298710	566087	8.73%	0.738%
56	15.734	1192	1194	1196	rBV	220621	352275	5.43%	0.459%
57	15.779	1196	1198	1202	rVV	350305	707731	10.91%	0.923%
58	15.848	1202	1204	1208	rVV	1086424	1876785	28.94%	2.447%
59	15.928	1208	1211	1214	rVV2	211587	499205	7.70%	0.651%
60	15.985	1214	1216	1222	rVV	231806	413842	6.38%	0.539%
61	16.077	1222	1224	1227	rVB3	162726	269957	4.16%	0.352%
62	16.397	1249	1252	1254	rBV3	121985	259409	4.00%	0.338%
63	16.465	1256	1258	1262	rVV2	113114	241084	3.72%	0.314%
64	16.568	1264	1267	1270	rVV2	213495	486341	7.50%	0.634%
65	16.637	1270	1273	1279	rVV2	671376	1556301	24.00%	2.029%
66	16.740	1279	1282	1285	rVV	212902	398927	6.15%	0.520%
67	16.797	1285	1287	1292	rVB2	127797	299528	4.62%	0.390%
68	16.922	1293	1298	1304	rVB2	1059920	2480651	38.25%	3.234%
69	17.037	1304	1308	1314	rVB	344250	736406	11.36%	0.960%
70	17.185	1316	1321	1323	rBV2	710785	1677502	25.87%	2.187%
71	17.254	1323	1327	1333	rVB2	2653788	6485192	100.00%	8.454%

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72	17.368	1333	1337	1342	rBV	574488	1533549	23.65%	1.999%
73	17.482	1342	1347	1353	rVB	1201106	2989266	46.09%	3.897%
74	17.585	1353	1356	1359	rBV	429583	860867	13.27%	1.122%
75	17.642	1359	1361	1364	rBV	76977	147682	2.28%	0.193%
76	17.814	1373	1376	1379	rBV2	113356	267381	4.12%	0.349%
77	17.940	1383	1387	1389	rVV	238934	672333	10.37%	0.876%
78	18.031	1389	1395	1399	rVB4	393867	1636499	25.23%	2.133%
79	18.180	1406	1408	1412	rVB4	61887	109804	1.69%	0.143%
80	18.340	1419	1422	1424	rBV2	70957	152570	2.35%	0.199%
81	18.877	1464	1469	1477	rVB3	258452	916573	14.13%	1.195%
82	19.037	1477	1483	1491	rVB3	202862	749557	11.56%	0.977%

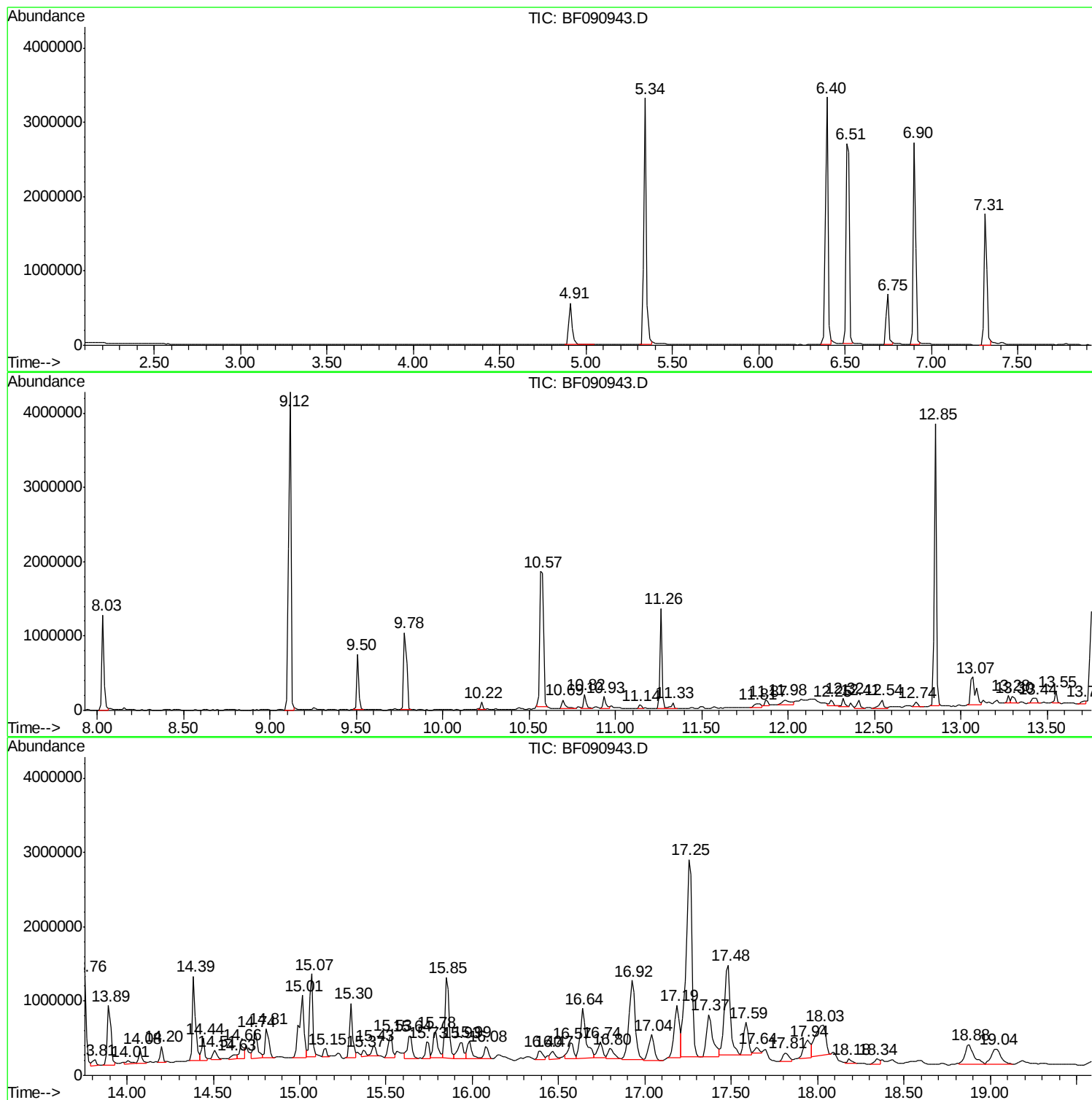
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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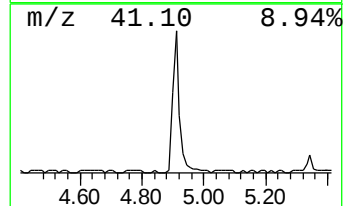
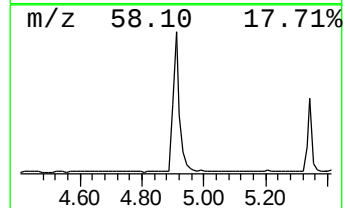
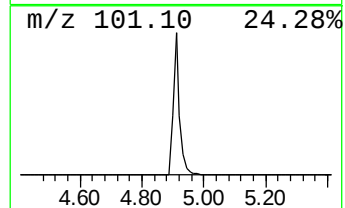
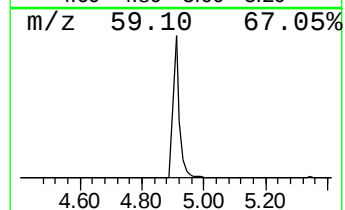
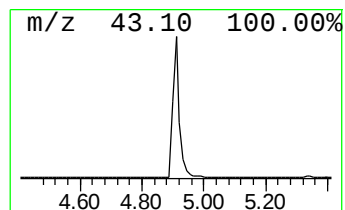
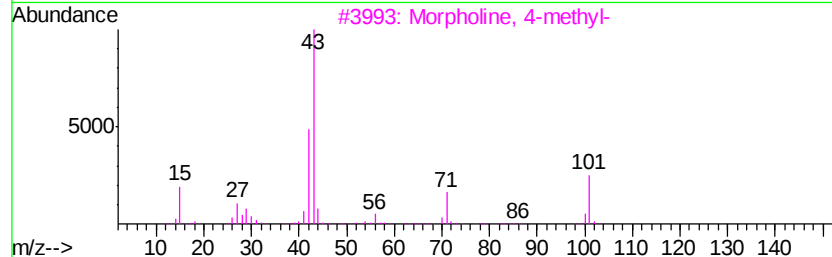
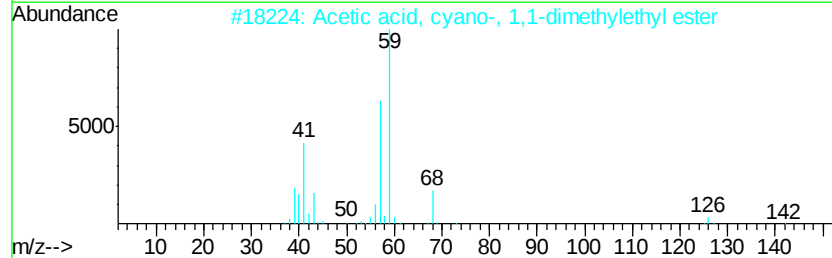
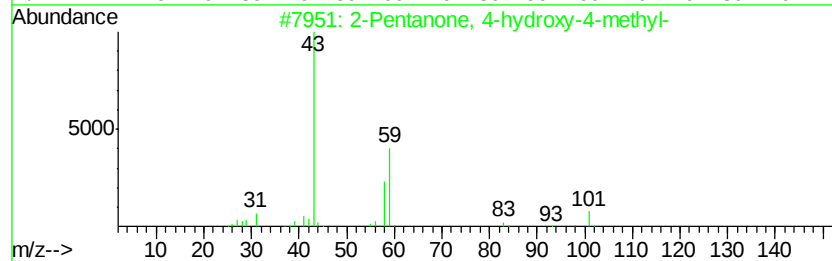
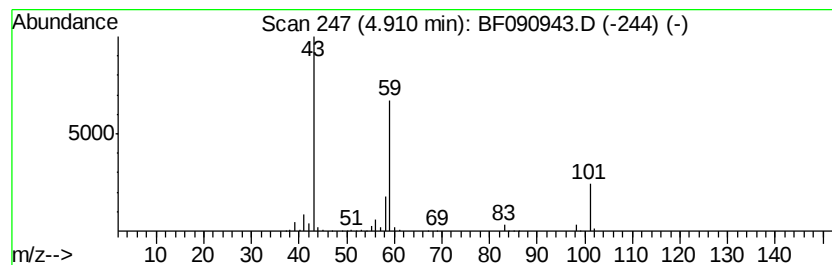
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	21.25 ng	831518	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Acetone	58	C3H6O	000067-64-1	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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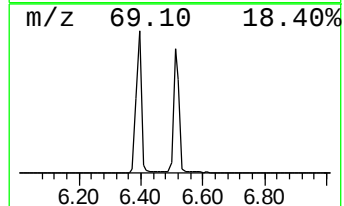
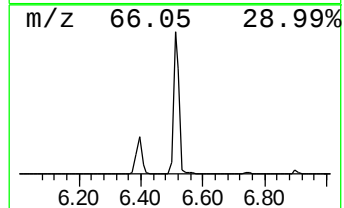
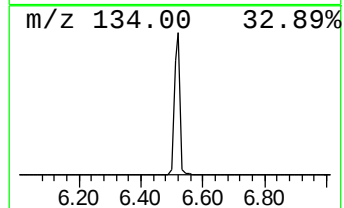
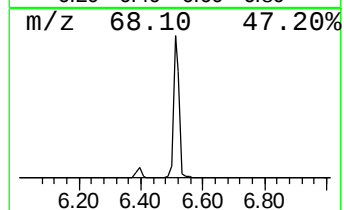
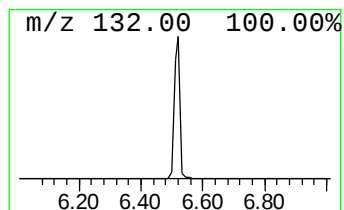
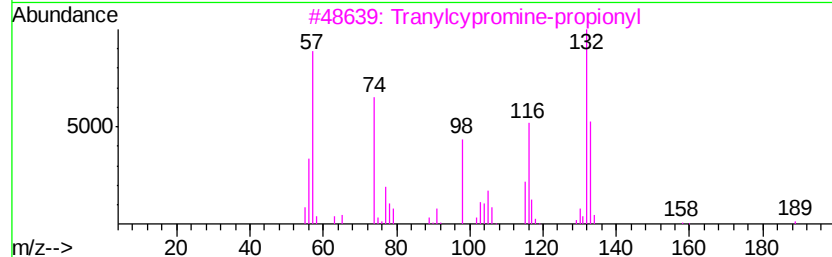
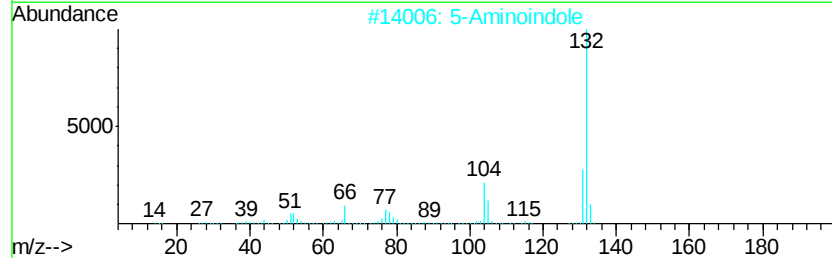
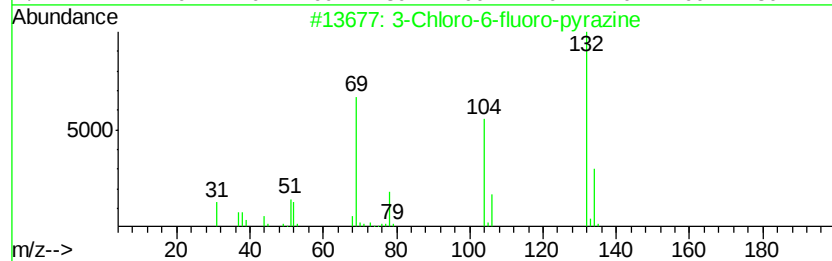
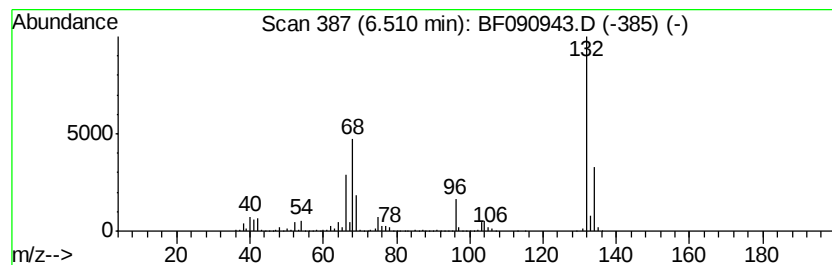
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	97.13 ng	3800420	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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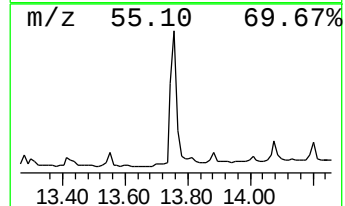
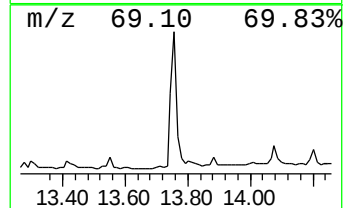
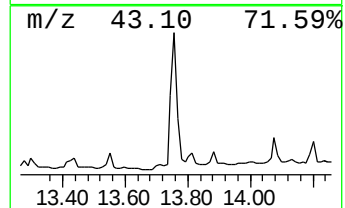
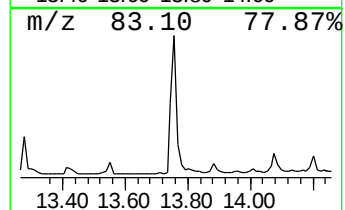
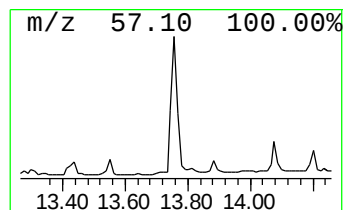
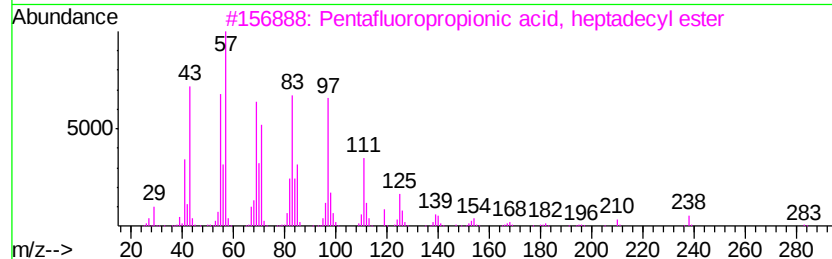
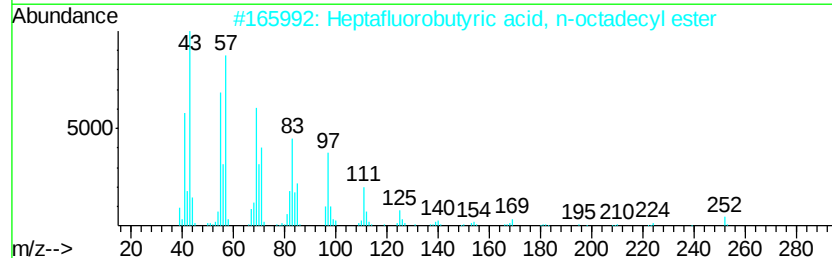
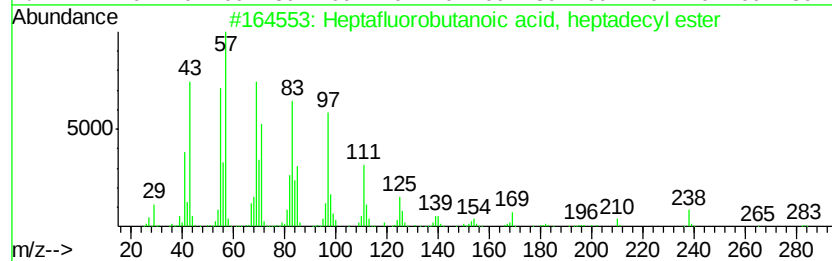
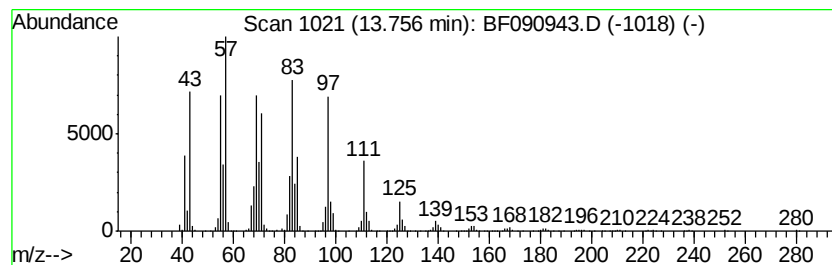
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptafluorobutanoic acid, h... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	30.16 ng	1615830	Chrysene-d12	13.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
4			1-Docosene	308	C22H44	001599-67-3	87
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	83



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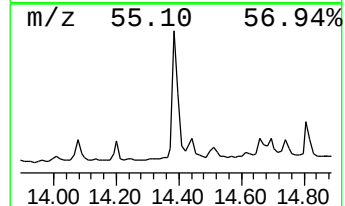
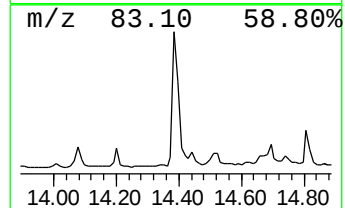
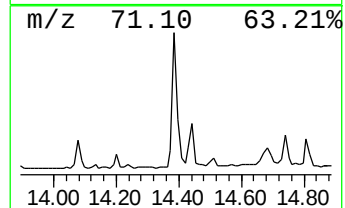
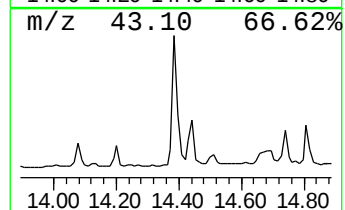
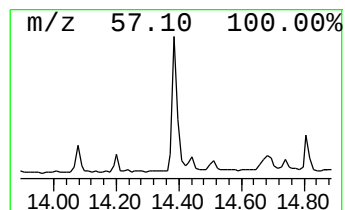
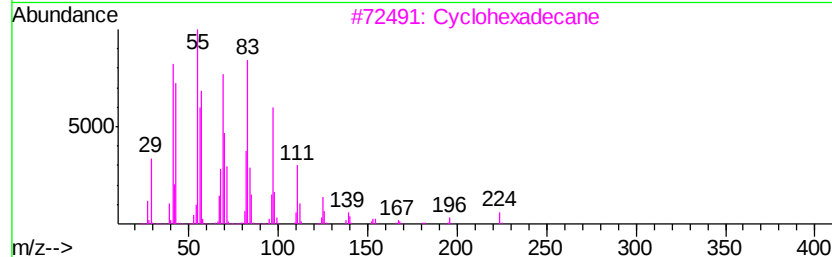
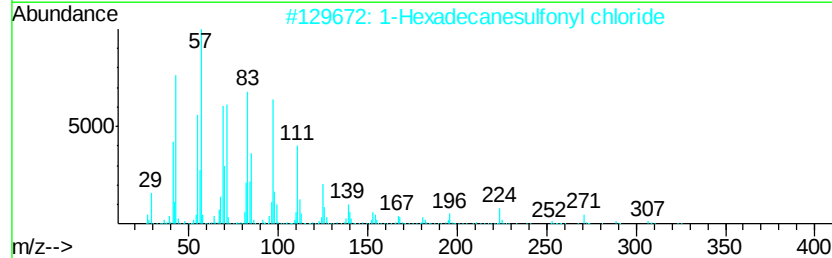
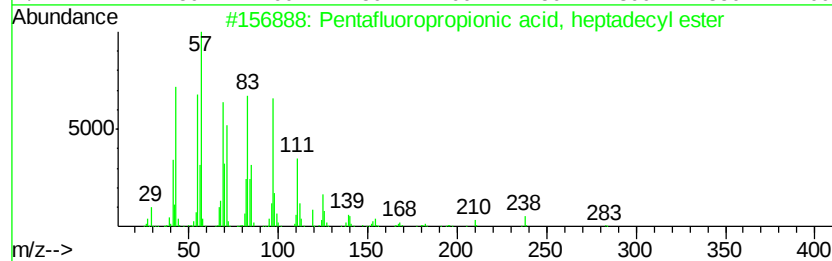
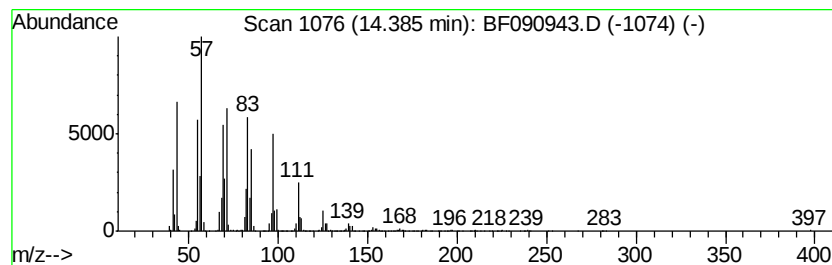
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	26.04 ng	1394980	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
2		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
3		Cyclohexadecane	224	C16H32	000295-65-8	83
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	74
5		17-Pentatriacontene	491	C35H70	006971-40-0	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WOOLSTON-TS-004

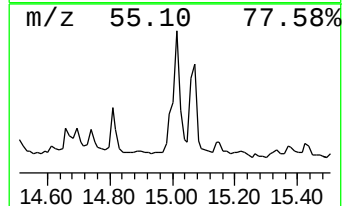
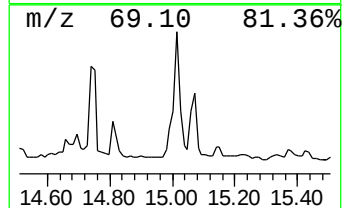
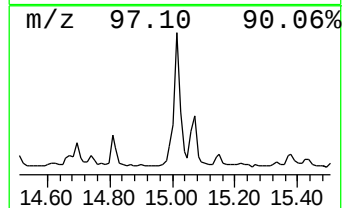
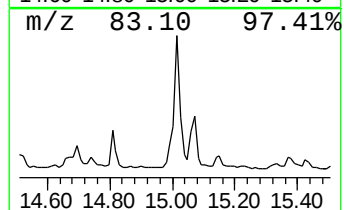
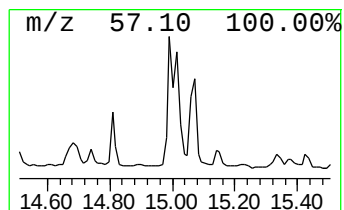
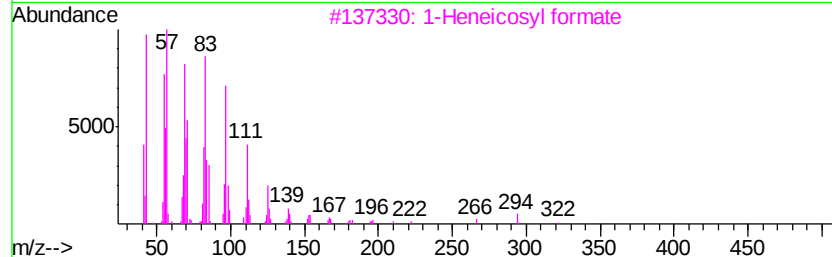
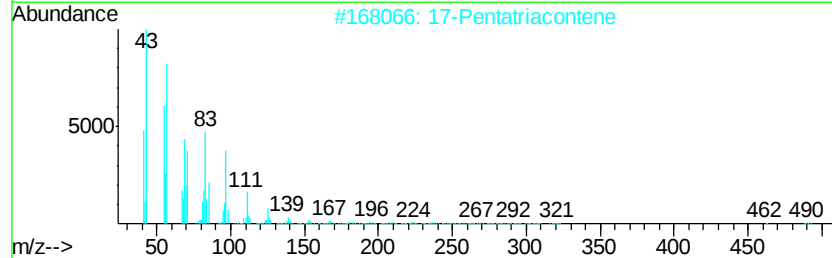
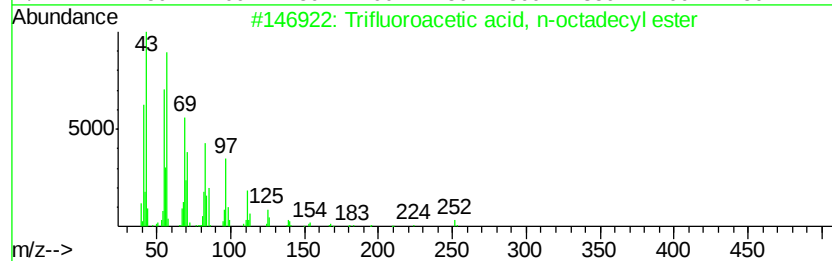
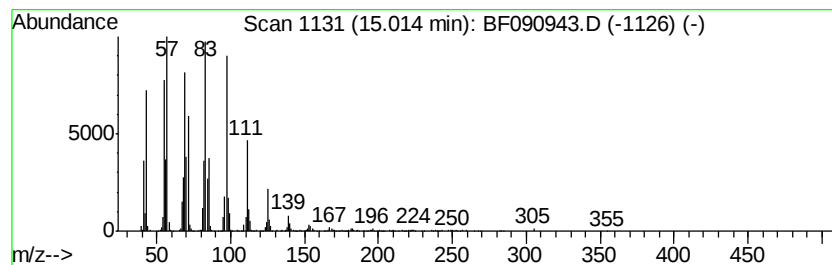
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetic acid, n-oct... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	33.14 ng	1500110	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4		1-Docosene	308	C22H44	001599-67-3	81
5		2-Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WOOLSTON-TS-004

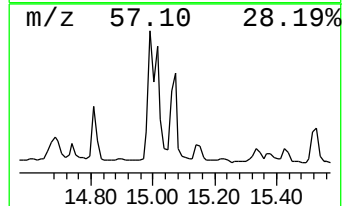
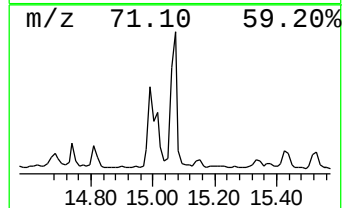
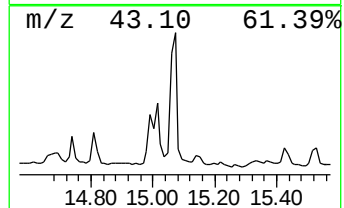
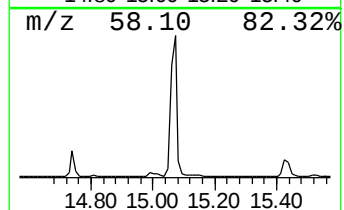
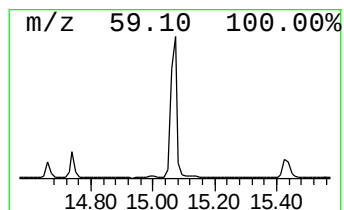
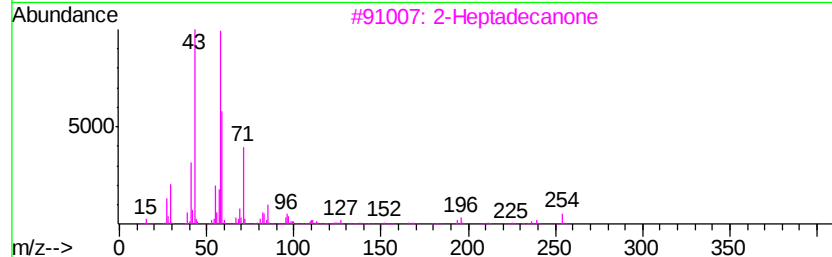
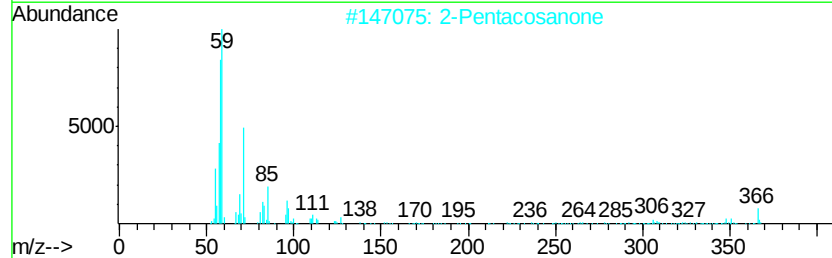
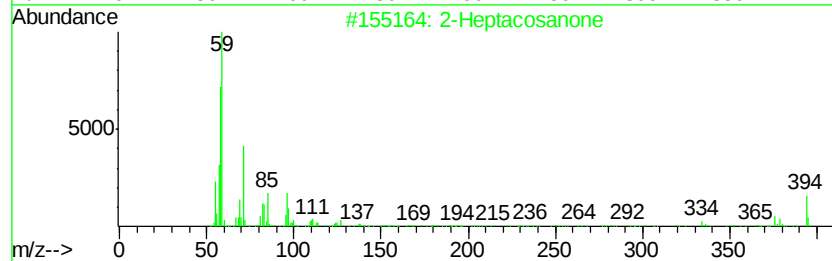
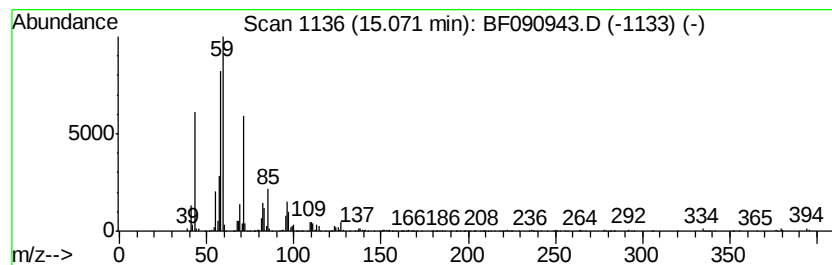
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Heptacosanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	33.31 ng	1507830	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptacosanone	394	C27H54O	007796-19-2	93
2		2-Pentacosanone	366	C25H50O	075207-54-4	91
3		2-Heptadecanone	254	C17H34O	002922-51-2	59
4		2-Nonadecanone	282	C19H38O	000629-66-3	47
5		2-Tetradecanone	212	C14H28O	002345-27-9	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

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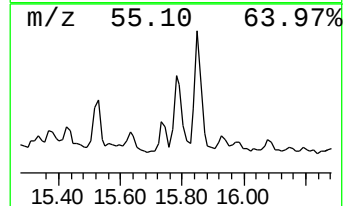
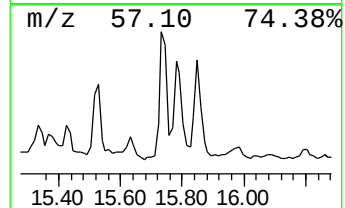
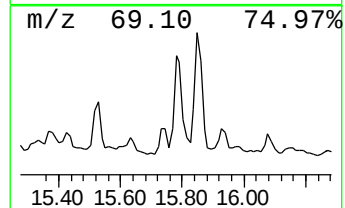
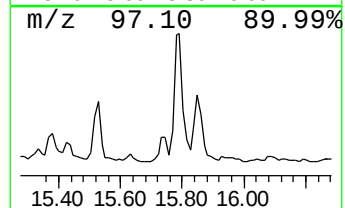
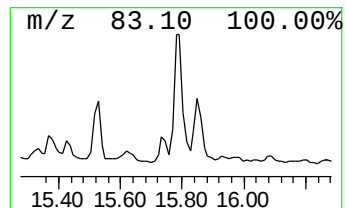
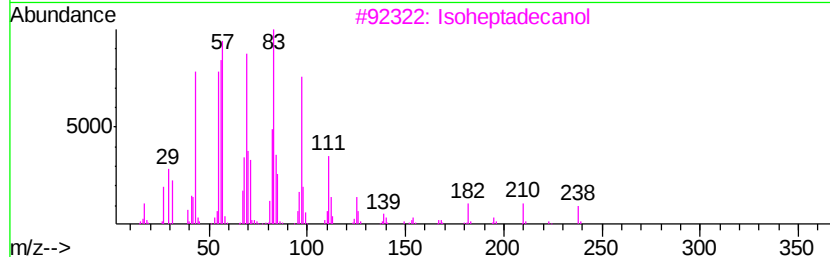
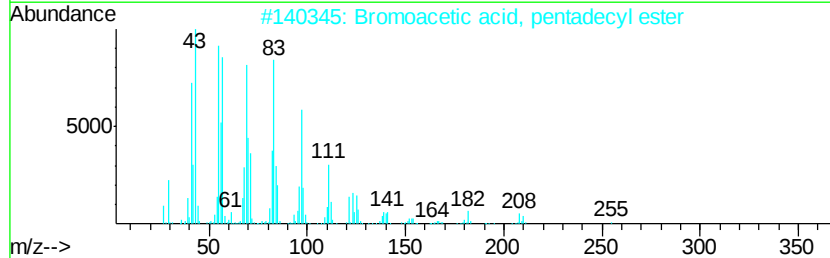
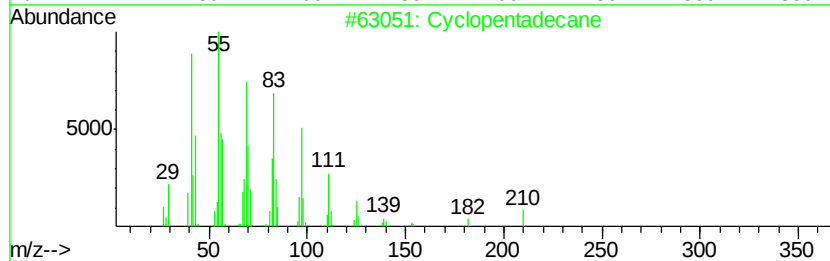
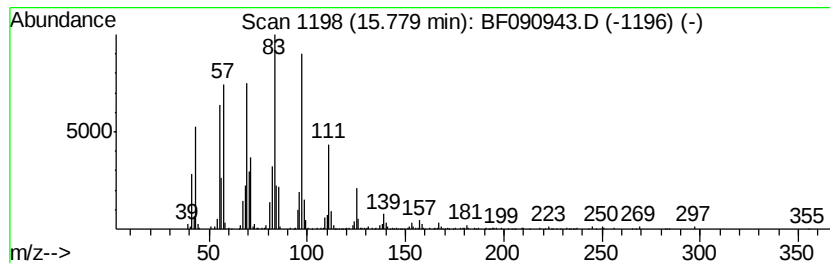
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	15.63 ng	707731	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	86
2		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	53
3		Isoheptadecanol	256	C17H36O	057289-07-3	52
4		1-Eicosanol	298	C20H42O	000629-96-9	49
5		1-Nonadecene	266	C19H38	018435-45-5	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WOOLSTON-TS-004

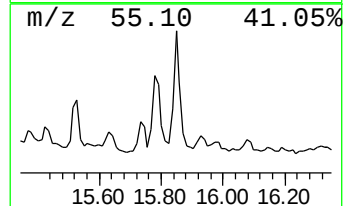
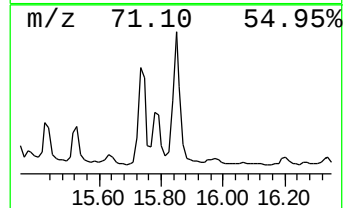
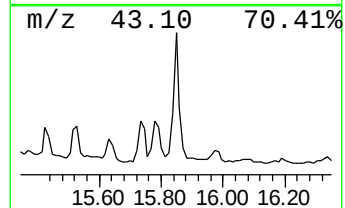
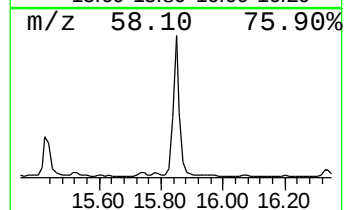
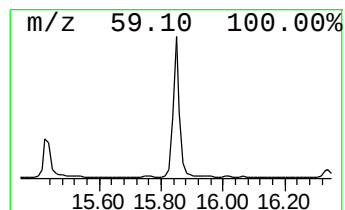
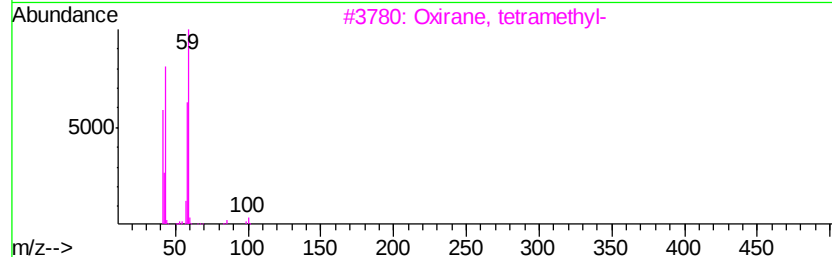
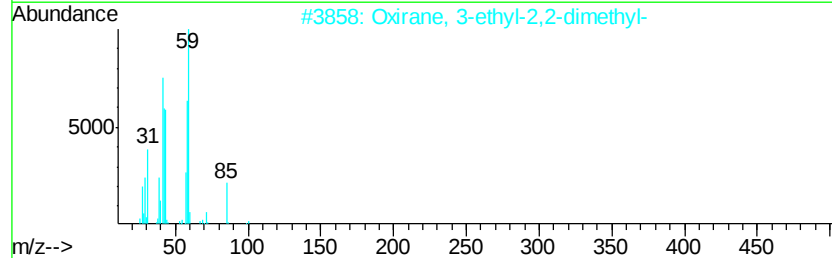
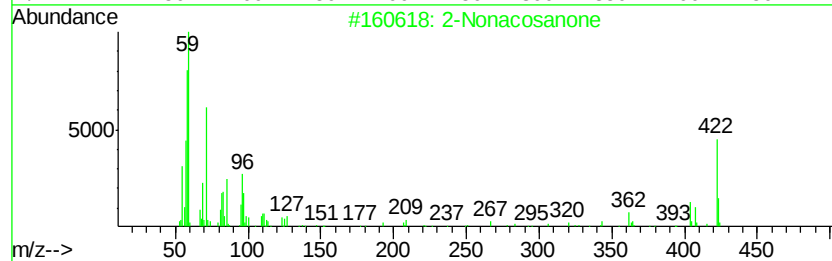
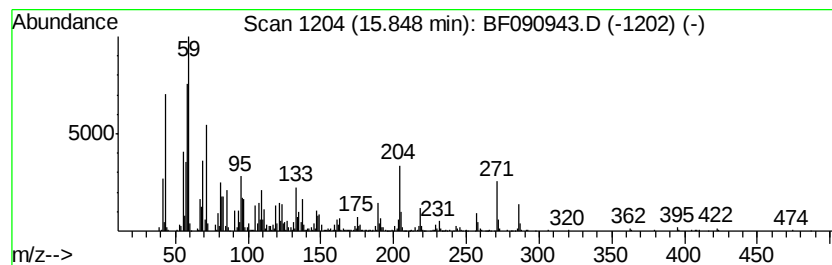
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Nonacosanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	41.46 ng	1876790	Perylene-d12	15.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonacosanone		422	C29H58O	017600-99-6	92
2	Oxirane, 3-ethyl-2,2-dimethyl-		100	C6H12O	001192-22-9	46
3	Oxirane, tetramethyl-		100	C6H12O	005076-20-0	43
4	Bis(2-methoxyethyl) phthalate		282	C14H18O6	000117-82-8	43
5	Butan-1-one, 4-chloro-1-(1,2,3,4...		306	C17H23ClN2O	326033-07-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WOOLSTON-TS-004

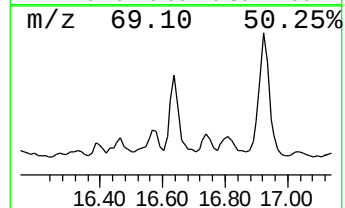
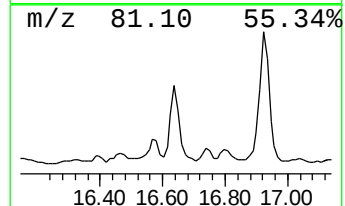
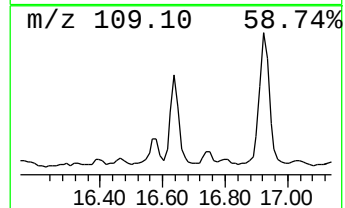
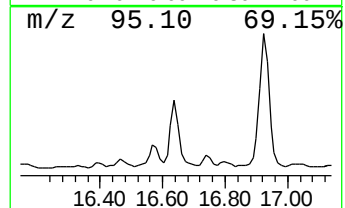
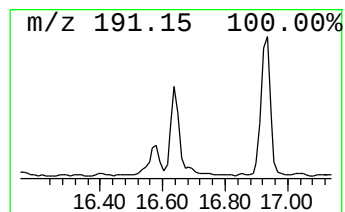
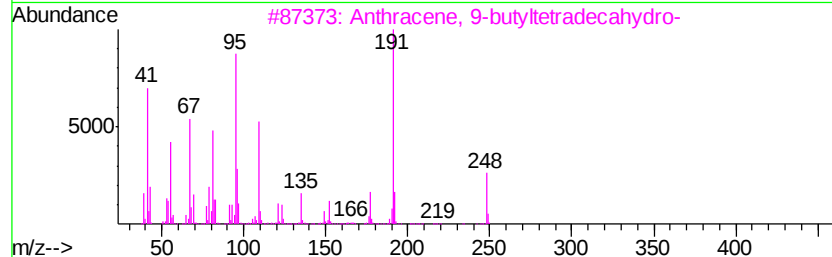
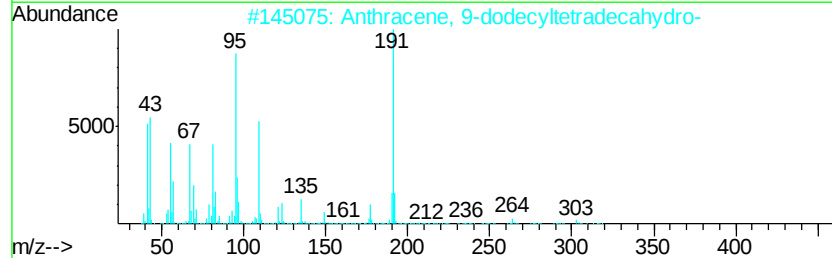
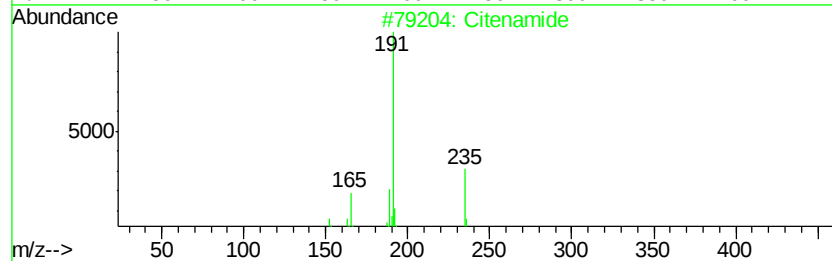
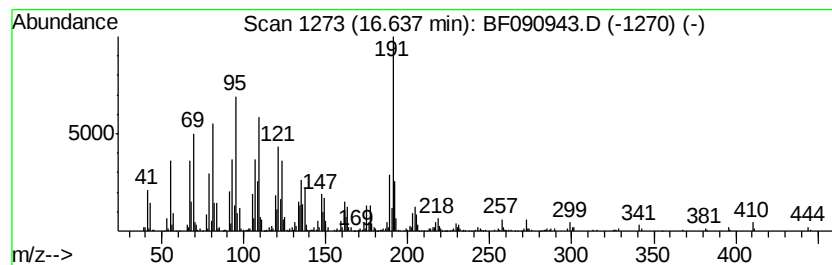
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Citenamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	34.38 ng	1556300	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Citenamide	235	C16H13NO	010423-37-7	72
2		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	50
3		Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	43
4		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	41
5		C(14a)-Homo-27-nor-14.beta.-gamm...	428	C30H52O	024739-08-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
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Misc :
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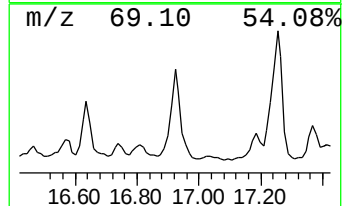
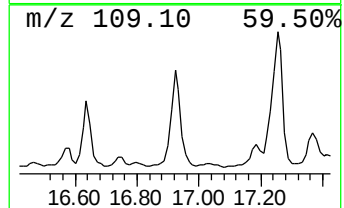
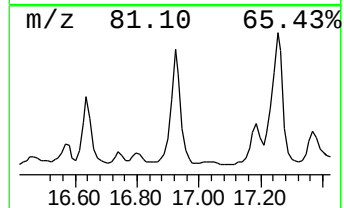
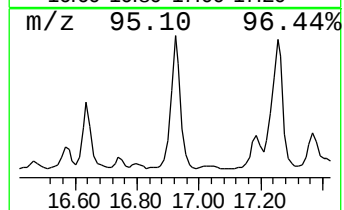
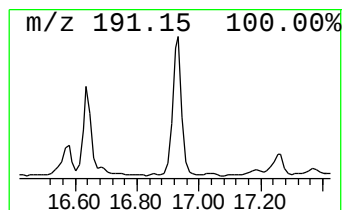
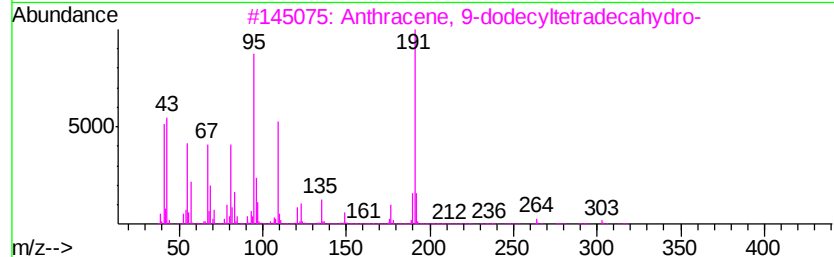
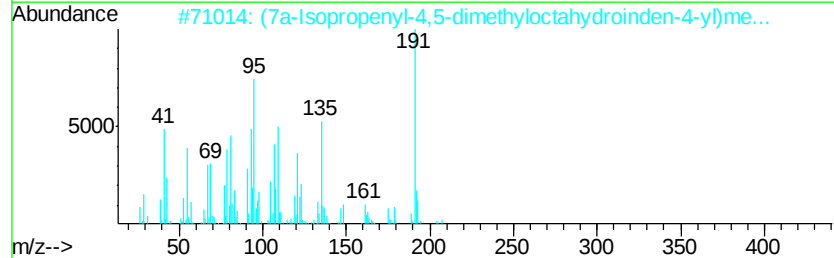
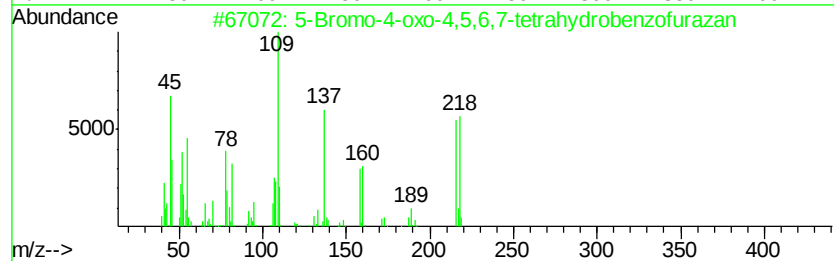
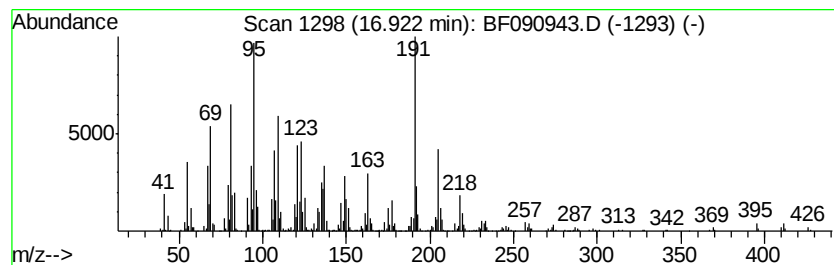
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.92	54.80 ng	2480650	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53
2		(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	53
3		Anthracene, 9-dodecyltetradeca...	360	C26H48	055401-75-7	46
4		2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	44
5		Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WOOLSTON-TS-004

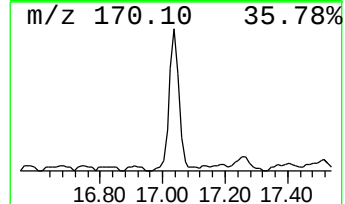
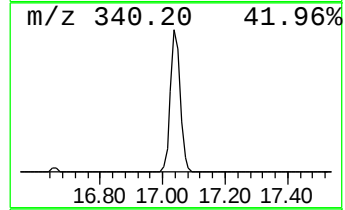
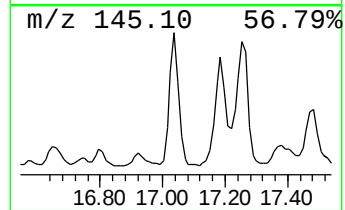
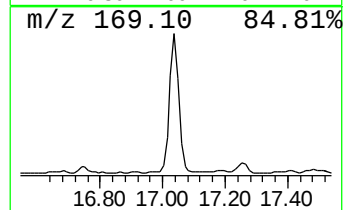
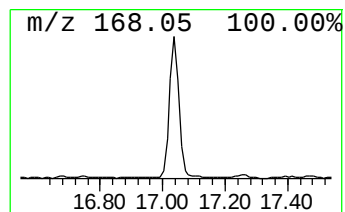
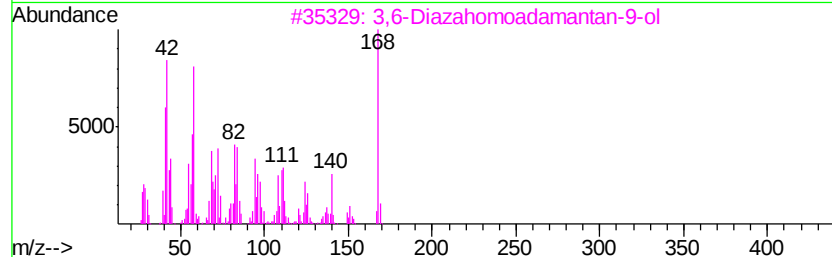
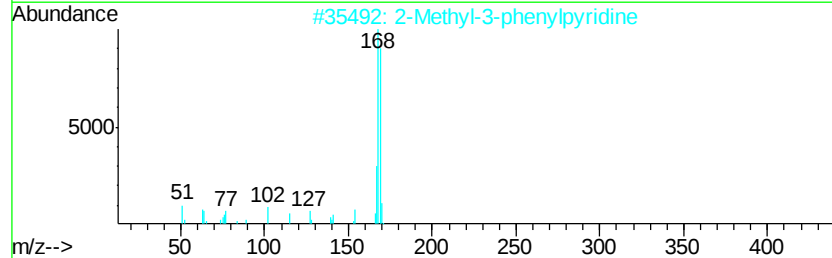
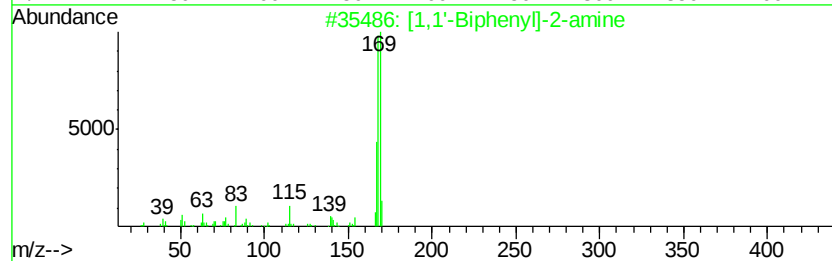
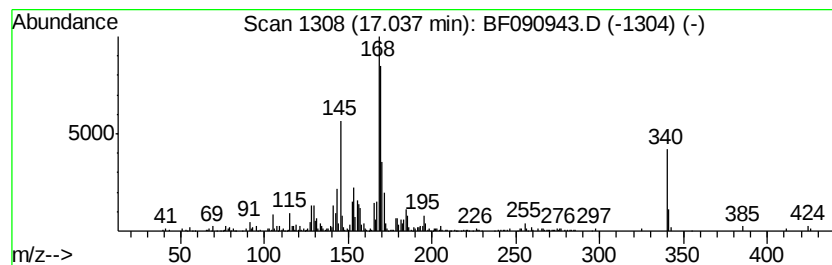
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.04 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	16.27 ng	736406	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	[1,1'-Biphenyl]-2-amine	169	C12H11N	000090-41-5	38
2		2-Methyl-3-phenylpyridine	169	C12H11N	003256-89-1	32
3		3,6-Diazahomoadamantan-9-ol	168	C9H16N2O	138023-21-9	25
4		2-Methyl-2-phenpropionic acid, e...	242	C16H18O2	1000129-24-4	22
5		3-Methyl-5-phenylpyridine	169	C12H11N	010477-94-8	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

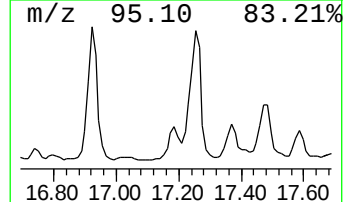
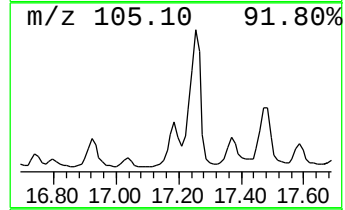
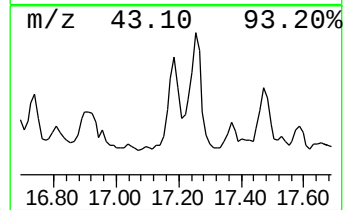
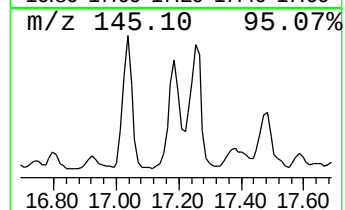
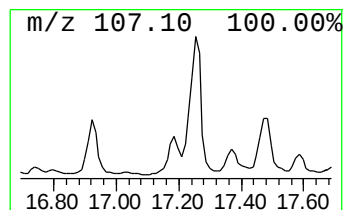
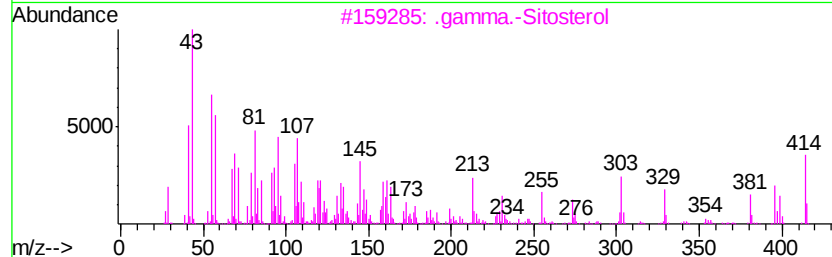
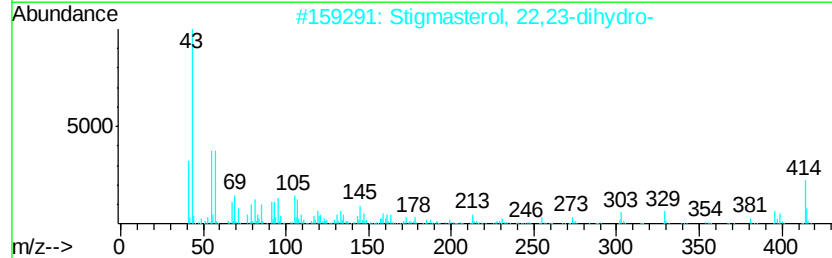
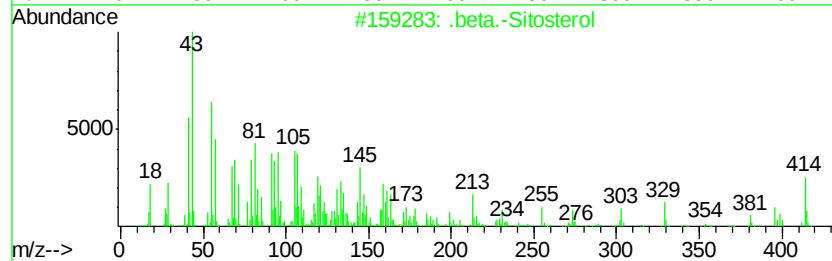
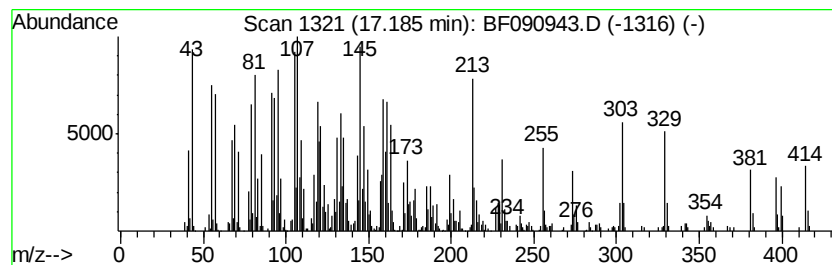
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .beta.-Sitosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.19	37.05 ng	1677500	Perylene-d12	15.30		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2		Stigmasterol, 22,23-dihydro-	414	C29H50O	1000214-20-7	99
3		.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
4		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	30
5		17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

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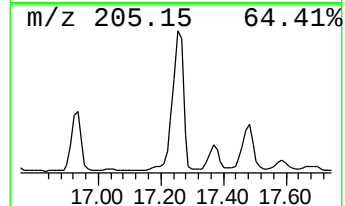
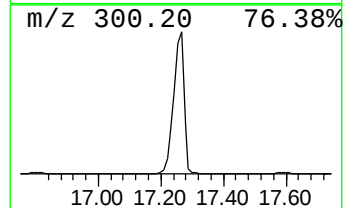
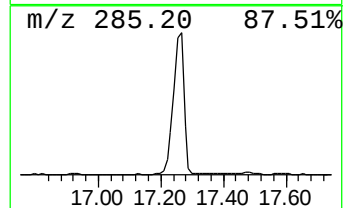
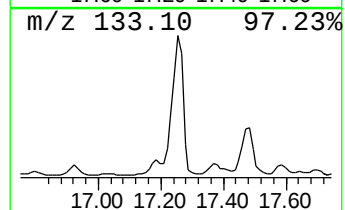
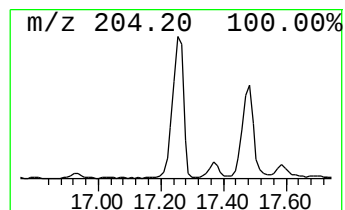
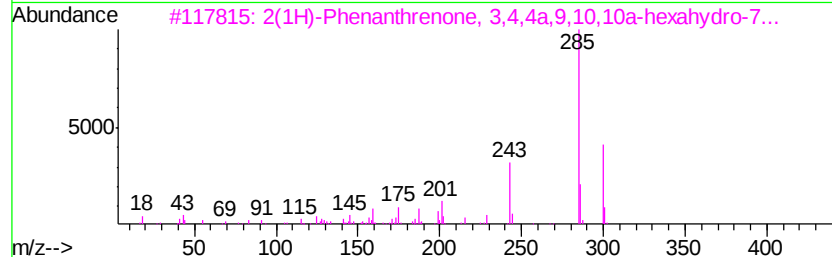
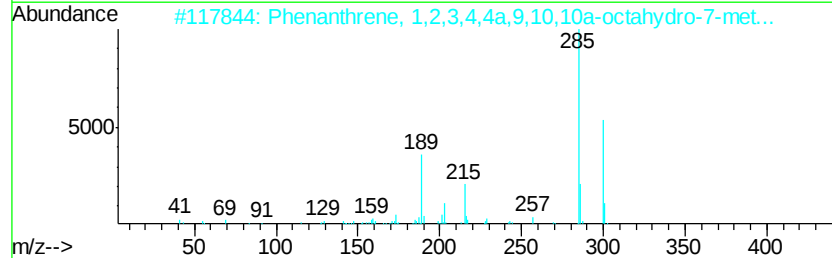
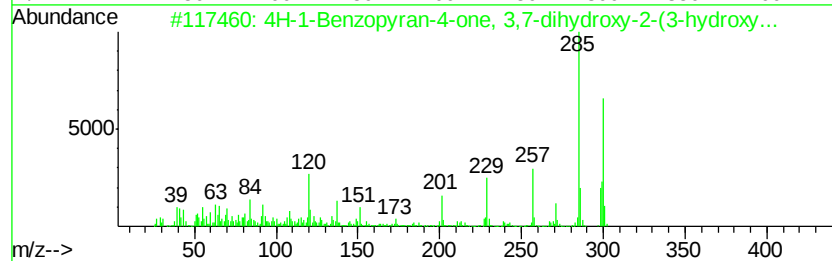
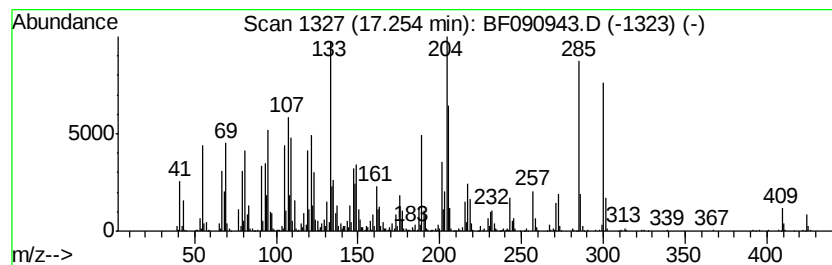
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 4H-1-Benzopyran-4-one, 3,7-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.25	143.25 ng	6485190	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-1-Benzopyran-4-one, 3,7-dihyd...	300	C16H12O6	057396-72-2	52
2		Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	015340-83-7	41
3		2(1H)-Phenanthrenone, 3,4,4a,9,1...	300	C20H28O2	006755-93-7	38
4		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	30
5		9(1H)-Phenanthrenone, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

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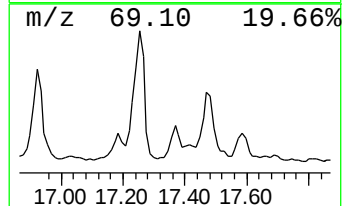
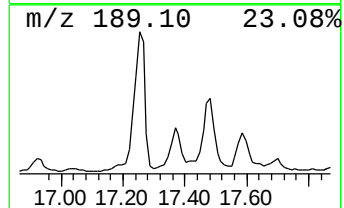
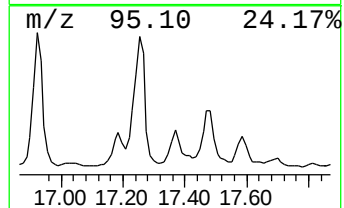
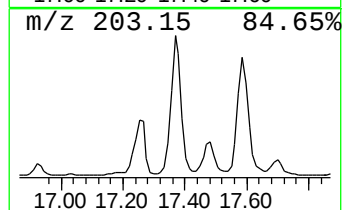
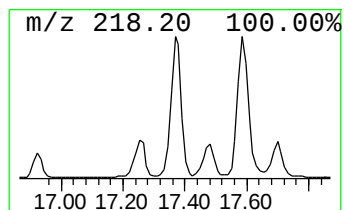
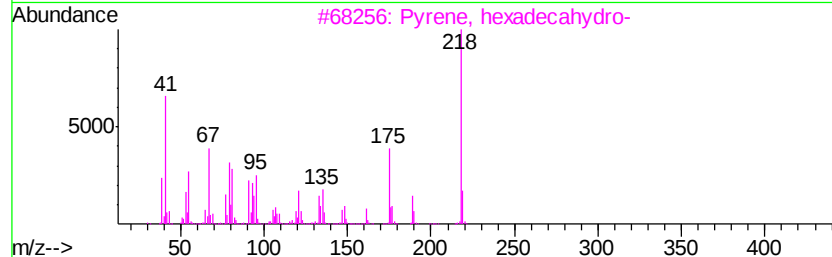
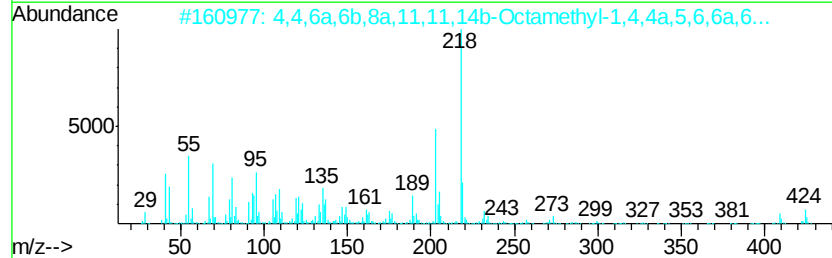
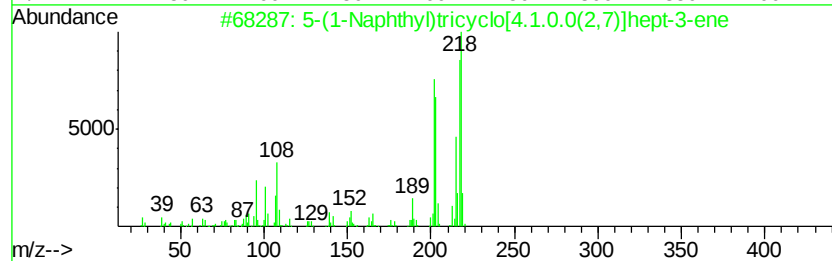
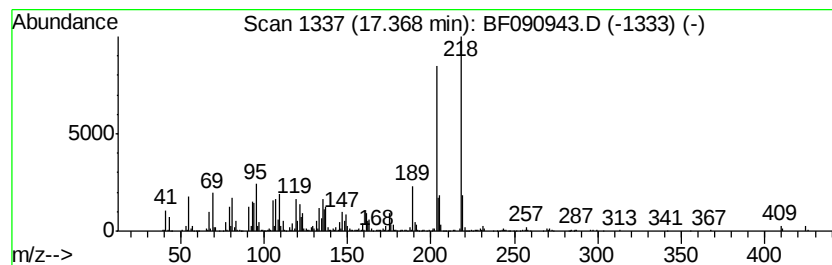
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 5-(1-Naphthyl)tricyclo[4.1.... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	33.88 ng	1533550	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	80
2		4,4,6a,6b,8a,11,11,14b-Octamethy...	424	C30H48O	1000194-62-4	68
3		Pyrene, hexadecahydro-	218	C16H26	002435-85-0	64
4		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	64
5		Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
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Misc :
ALS Vial : 23 Sample Multiplier: 1

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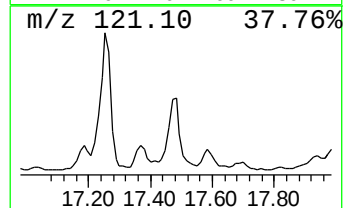
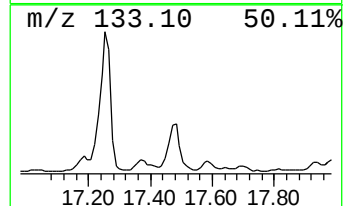
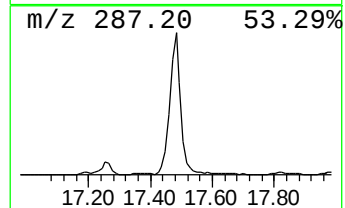
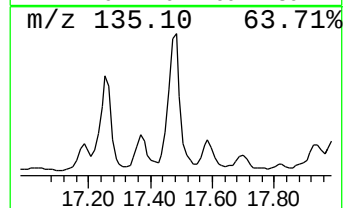
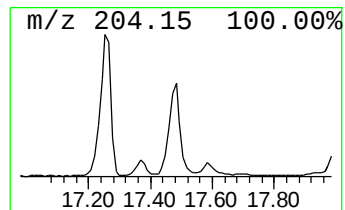
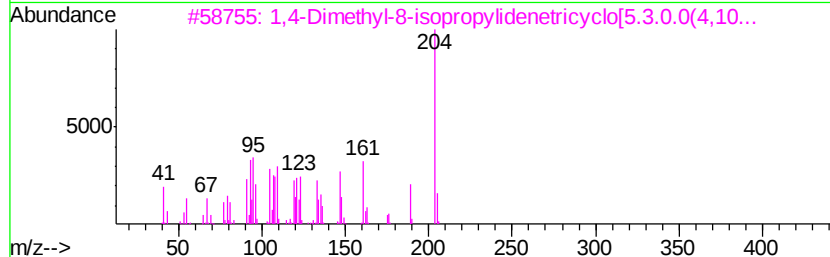
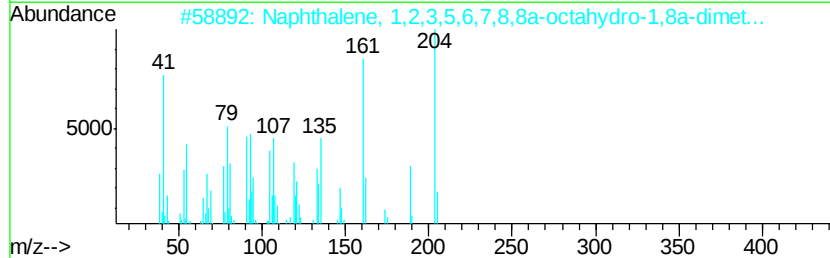
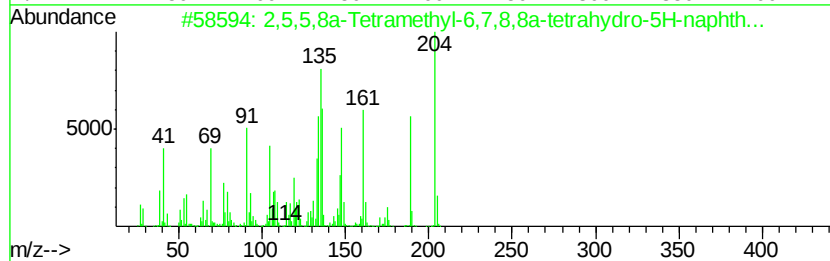
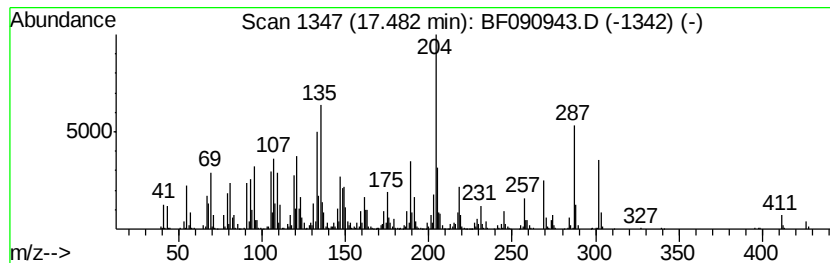
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.48 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.48	66.03 ng	2989270	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H200		124957-09-1	43
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24		004630-07-3	38
3	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24		1000140-07-7	30
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24		137235-51-9	22
5	Naphthalene, decahydro-4a-methyl...	204	C15H24		017066-67-0	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
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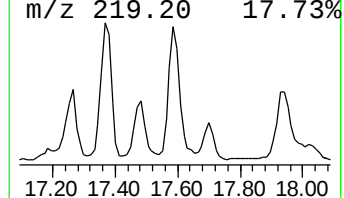
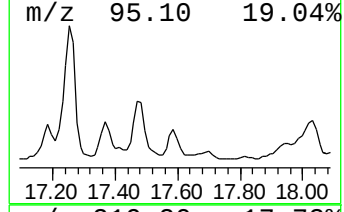
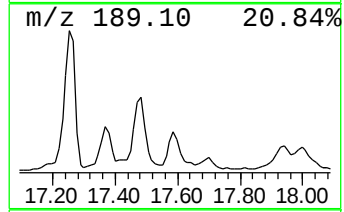
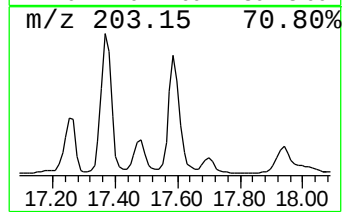
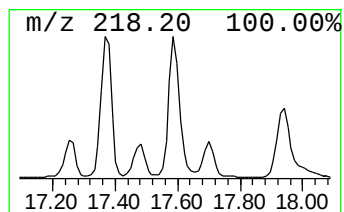
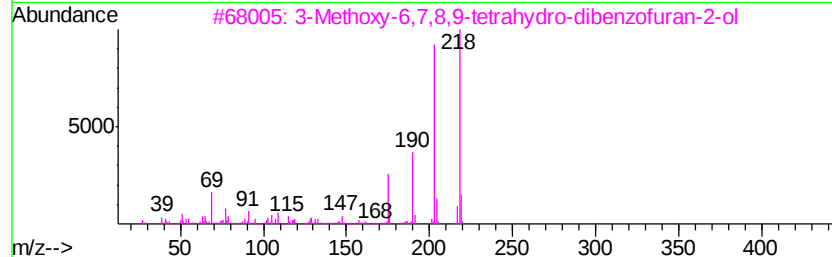
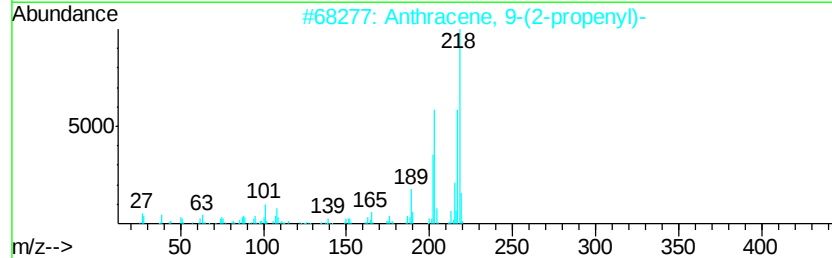
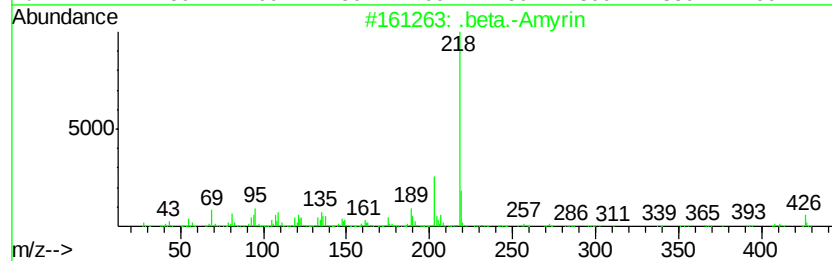
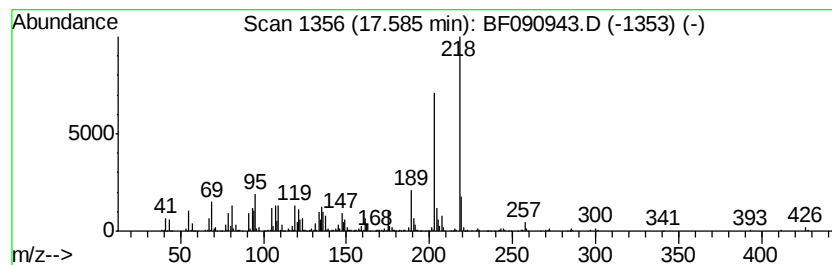
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 .beta.-Amyrin Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.59	19.02 ng	860867	Perylene-d12	15.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Amyrin	426 C30H500	000559-70-6 97
2		Anthracene, 9-(2-propenyl)-	218 C17H14	023707-65-5 64
3		3-Methoxy-6,7,8,9-tetrahydro-dib...	218 C13H14O3	1000186-57-9 62
4		Thieno[2,3-b]pyridine-2-carbonit...	218 C10H10N4S	147992-88-9 59
5		Olean-12-ene	410 C30H50	000471-68-1 58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
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ClientSampleId :
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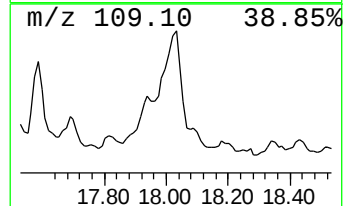
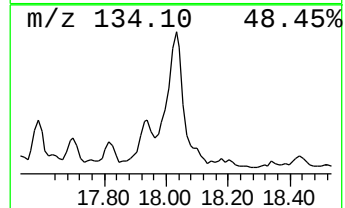
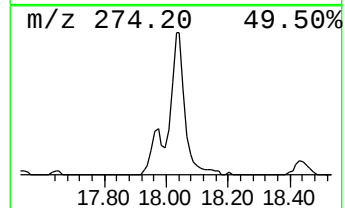
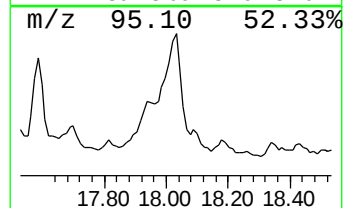
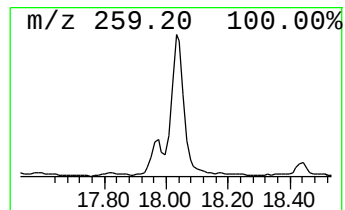
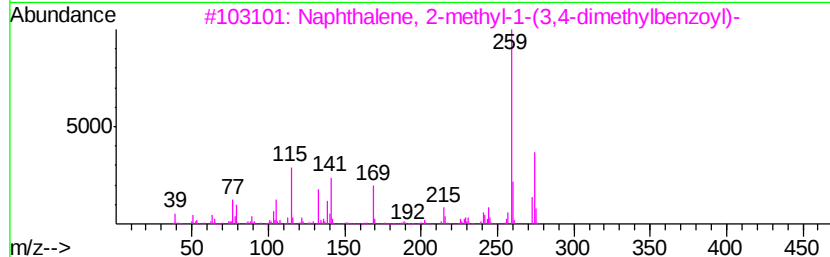
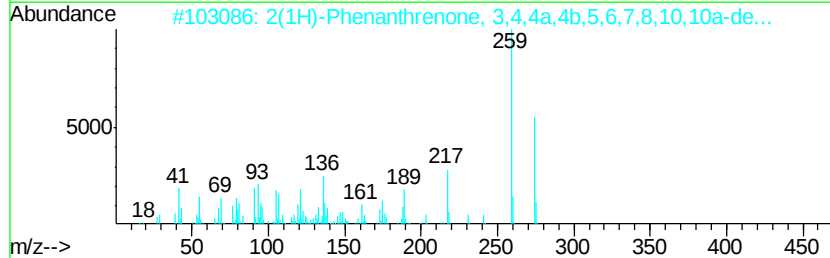
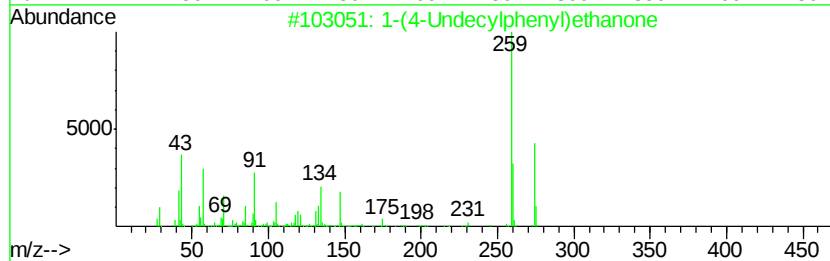
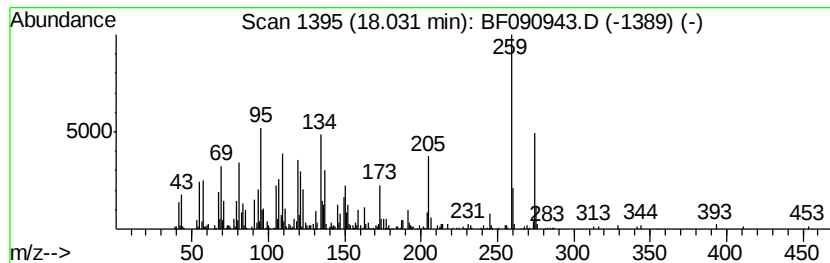
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown18.03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	36.15 ng	1636500	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(4-Undecylphenyl)ethanone	274	C19H30O	1000185-92-4	42
2		2(1H)-Phenanthrenone, 3,4,4a,4b,...	274	C19H30O	007715-44-8	35
3		Naphthalene, 2-methyl-1-(3,4-dim...	274	C20H18O	1000269-03-0	35
4		7H-Furo[3,2-g][1]benzopyran-7-on...	274	C15H14O5	054087-32-0	30
5		10H-Phenoxaphosphine, 2-ethyl-10...	274	C15H15O3P	036360-91-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

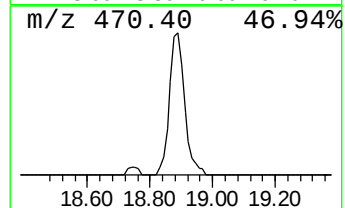
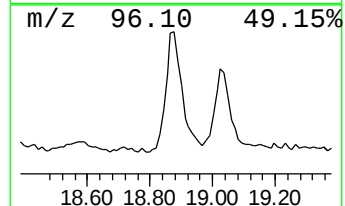
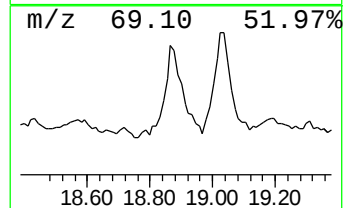
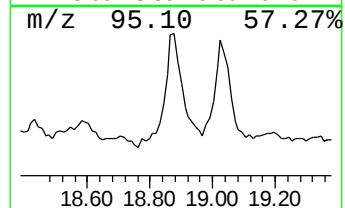
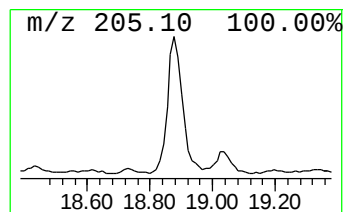
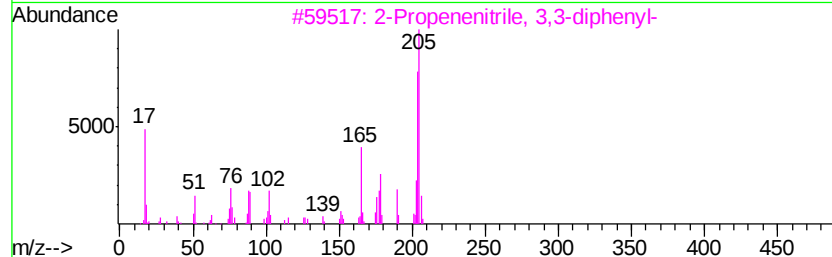
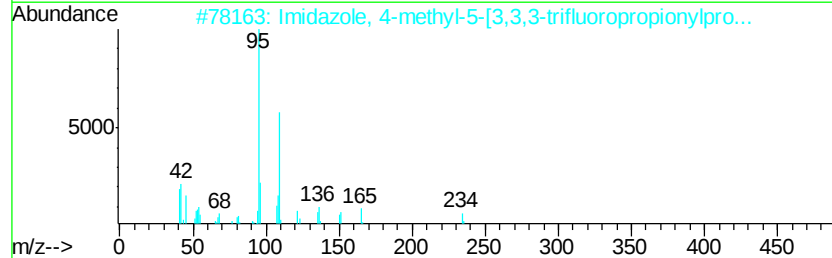
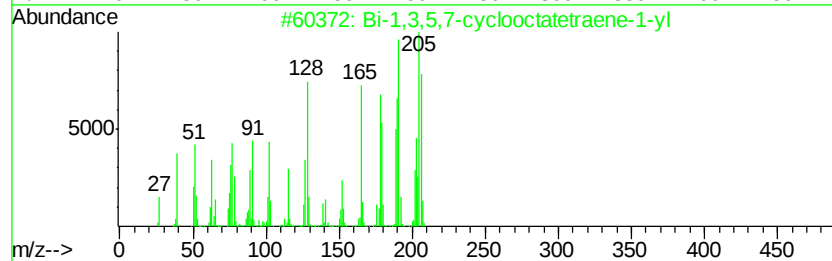
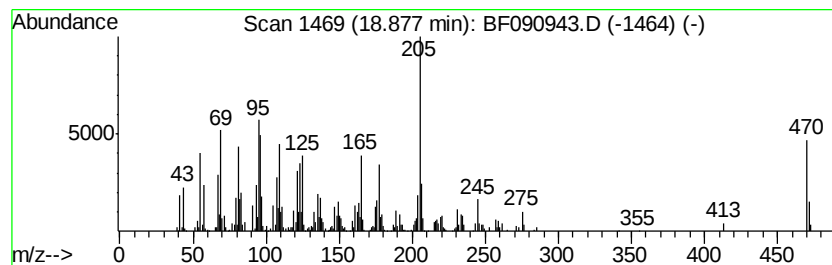
Instrument :
BNA_F
ClientSampleId :
WOOLSTON-TS-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Bi-1,3,5,7-cyclooctatetraen... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.88	20.25 ng	916573	Perylene-d12	15.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Bi-1,3,5,7-cyclooctatetraene-1-yl	206 C16H14	006715-22-6	53
2	Imidazole, 4-methyl-5-[3,3,3-tri...	234 C10H13F3N2O	1000129-15-8	25
3	2-Propenenitrile, 3,3-diphenyl-	205 C15H11N	003531-24-6	22
4	1,1,6,6-Tetramethylspiro[4.4]nonane	180 C13H24	074054-92-5	16
5	2-Amino-4-hydroxy-6,7,8-trimethy...	205 C9H11N5O	013045-86-8	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
Data File : BF090943.D
Acq On : 31 Oct 2016 22:05
Operator : UM/SJ
Sample : H5475-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WOOLSTON-TS-004

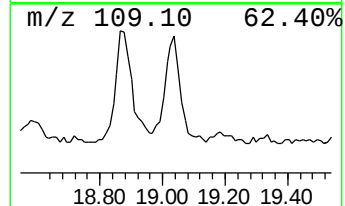
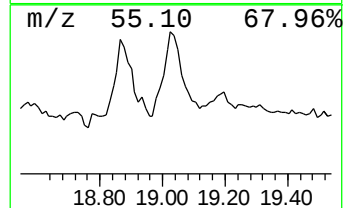
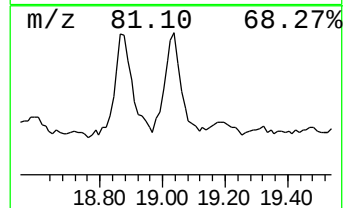
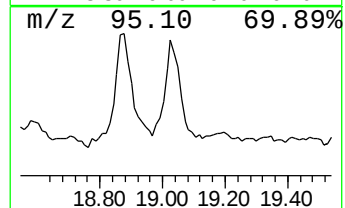
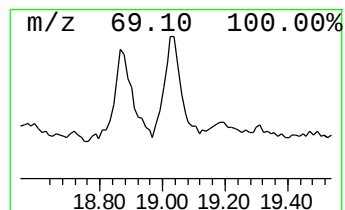
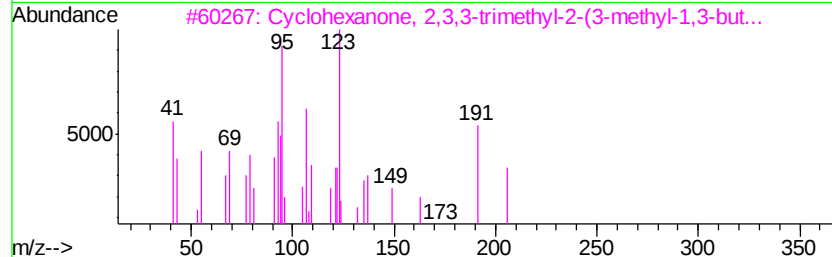
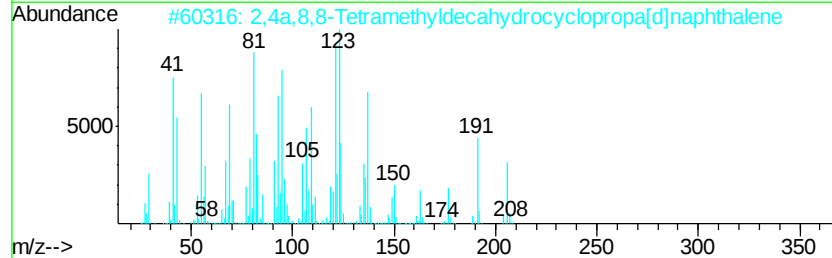
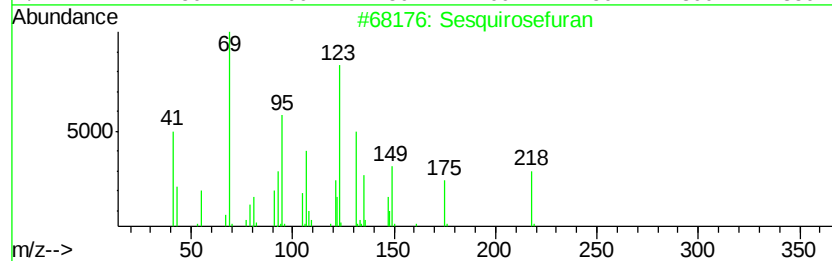
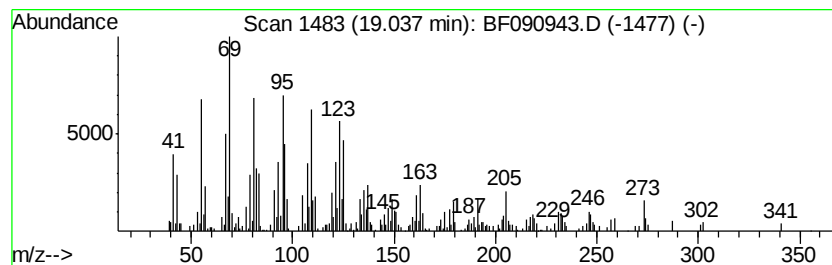
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Sesquirosefuran Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	16.56 ng	749557	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sesquirosefuran	218	C15H22O	039007-93-7	66
2		2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	40
3		Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	35
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	27
5		1,3,3-Trimethyl-2-hydroxymethyl-...	222	C15H26O	1000144-10-7	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103116\
 Data File : BF090943.D
 Acq On : 31 Oct 2016 22:05
 Operator : UM/SJ
 Sample : H5475-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WOOLSTON-TS-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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...	4.91	21.3	ng	831518	1	6.75	782558	20.0
unknown6.51	6.51	97.1	ng	3800420	1	6.75	782558	20.0
Heptafluorobutano...	13.76	30.2	ng	1615830	5	13.89	1071360	20.0
Pentafluoropropio...	14.39	26.0	ng	1394980	5	13.89	1071360	20.0
Trifluoroacetic a...	15.01	33.1	ng	1500110	6	15.30	905416	20.0
2-Heptacosanone	15.07	33.3	ng	1507830	6	15.30	905416	20.0
Cyclopentadecane	15.78	15.6	ng	707731	6	15.30	905416	20.0
2-Nonacosanone	15.85	41.5	ng	1876790	6	15.30	905416	20.0
Citenamide	16.64	34.4	ng	1556300	6	15.30	905416	20.0
5-Bromo-4-oxo-4,5...	16.92	54.8	ng	2480650	6	15.30	905416	20.0
unknown17.04	17.04	16.3	ng	736406	6	15.30	905416	20.0
.beta.-Sitosterol	17.19	37.0	ng	1677500	6	15.30	905416	20.0
4H-1-Benzopyran-4...	17.25	143.3	ng	6485190	6	15.30	905416	20.0
5-(1-Naphthyl)tri...	17.37	33.9	ng	1533550	6	15.30	905416	20.0
unknown17.48	17.48	66.0	ng	2989270	6	15.30	905416	20.0
.beta.-Amyrin	17.59	19.0	ng	860867	6	15.30	905416	20.0
unknown18.03	18.03	36.1	ng	1636500	6	15.30	905416	20.0
Bi-1,3,5,7-cycloo...	18.88	20.3	ng	916573	6	15.30	905416	20.0
Sesquirosefuran	19.04	16.6	ng	749557	6	15.30	905416	20.0