

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091117\
 Data File : BF098424.D
 Acq On : 12 Sep 2017 1:29
 Operator : SJ/JU
 Sample : I5138-10
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EME-UTS-TS007-01

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-BF091117.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	4.857	468	471	485	rBV	483192	809088	10.73%	1.426%
2	5.281	538	543	546	rBV	6396730	6678958	88.57%	11.775%
3	6.328	714	721	736	rBV	5486033	7541227	100.00%	13.295%
4	6.445	736	741	744	rBV	6545612	6672564	88.48%	11.763%
5	6.669	775	779	786	rVB	1818101	1591256	21.10%	2.805%
6	6.822	801	805	809	rBV	4384718	4466733	59.23%	7.875%
7	7.239	870	876	879	rBV	4385352	4504424	59.73%	7.941%
8	7.951	989	997	1000	rBV	2539995	2088177	27.69%	3.681%
9	9.027	1174	1180	1183	rBV	5806876	5218980	69.21%	9.201%
10	9.110	1189	1194	1198	rBV3	106424	114329	1.52%	0.202%
11	9.422	1244	1247	1250	rVB	1271698	1041701	13.81%	1.836%
12	9.639	1281	1284	1288	rVB	97510	80052	1.06%	0.141%
13	9.698	1288	1294	1298	rBV	2318891	2100462	27.85%	3.703%
14	10.416	1411	1416	1423	rBV2	95500	112325	1.49%	0.198%
15	10.492	1424	1429	1432	rBV	3634620	3454988	45.81%	6.091%
16	10.604	1445	1448	1453	rVB3	96134	123397	1.64%	0.218%
17	10.763	1472	1475	1477	rBV2	151059	136529	1.81%	0.241%
18	10.886	1493	1496	1499	rBV	107171	92587	1.23%	0.163%
19	10.957	1501	1508	1513	rBV3	93650	150332	1.99%	0.265%
20	11.068	1522	1527	1532	rVB4	83808	120182	1.59%	0.212%
21	11.180	1541	1546	1549	rBV	2180289	1919893	25.46%	3.385%
22	11.204	1549	1550	1553	rVV	171001	113702	1.51%	0.200%
23	11.251	1553	1558	1561	rVB3	118418	156120	2.07%	0.275%
24	12.021	1685	1689	1692	rBV4	56865	80650	1.07%	0.142%
25	12.263	1726	1730	1732	rBV	229755	234079	3.10%	0.413%
26	12.280	1732	1733	1737	rVB3	143758	112714	1.49%	0.199%
27	12.386	1746	1751	1754	rBV	162579	185338	2.46%	0.327%
28	12.615	1784	1790	1793	rBV	177397	178236	2.36%	0.314%
29	12.762	1811	1815	1818	rBV	3462210	3102892	41.15%	5.470%
30	13.662	1964	1968	1975	rBV2	258075	315618	4.19%	0.556%
31	13.809	1988	1993	1997	rBV	1166610	1242187	16.47%	2.190%
32	14.292	2072	2075	2079	rBV2	84417	100352	1.33%	0.177%
33	14.562	2118	2121	2127	rBV2	132505	143748	1.91%	0.253%
34	14.886	2174	2176	2179	rBV	81874	82992	1.10%	0.146%

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.915	2179	2181	2186	rVB2	70927	81421	1.08%	0.144%
36	15.215	2227	2232	2241	rVB	881570	1138081	15.09%	2.006%
37	15.627	2299	2302	2306	rBV	91032	135315	1.79%	0.239%
38	15.839	2335	2338	2340	rBV4	56759	79705	1.06%	0.141%
39	17.056	2540	2545	2546	rBV3	148963	221895	2.94%	0.391%

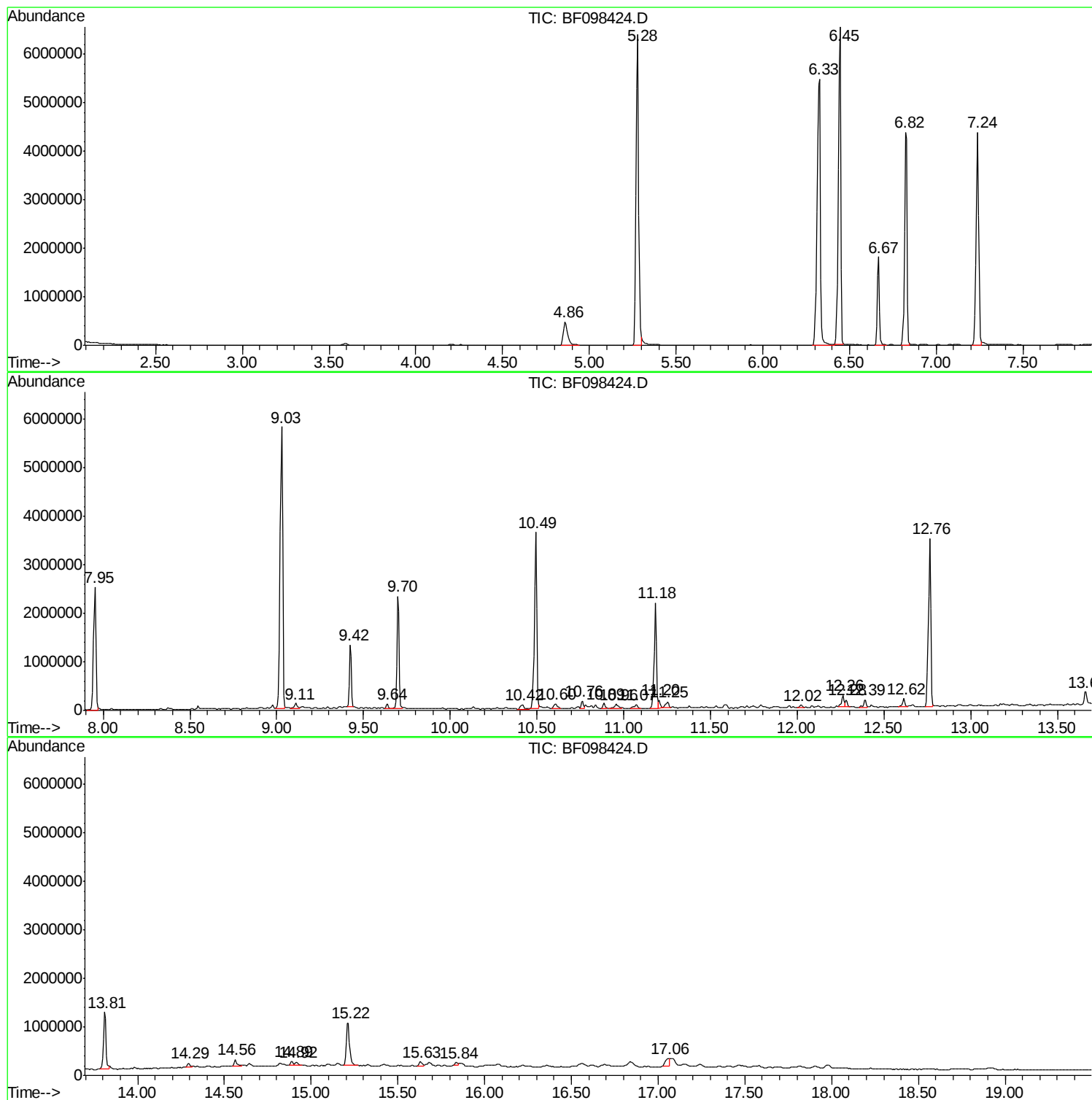
Sum of corrected areas: 56723229

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

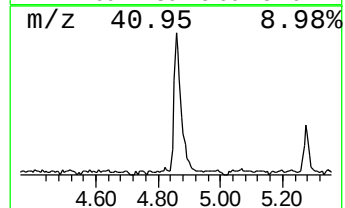
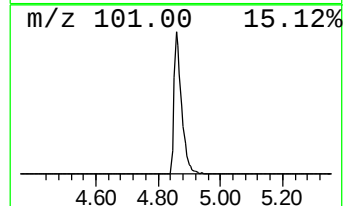
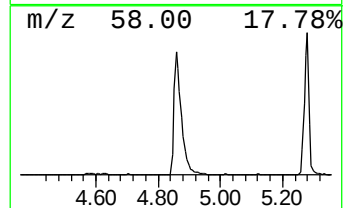
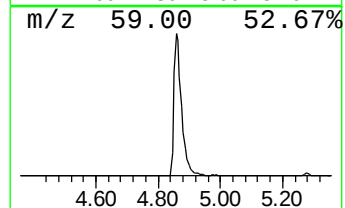
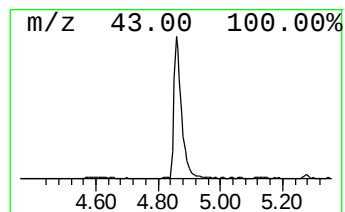
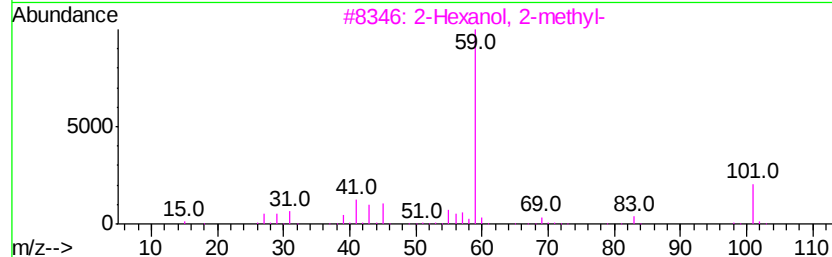
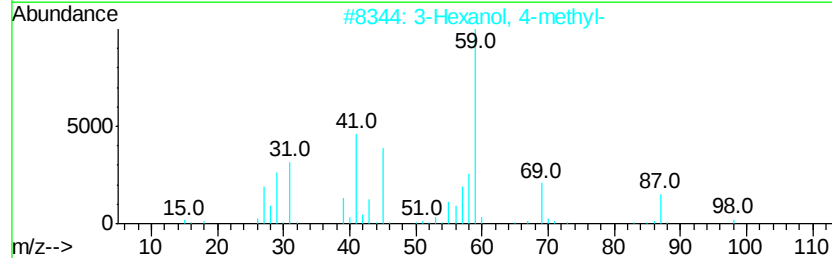
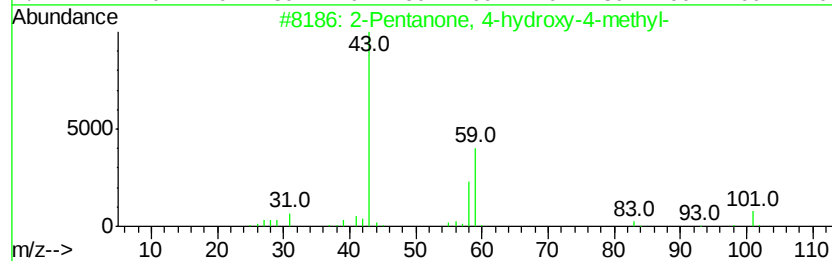
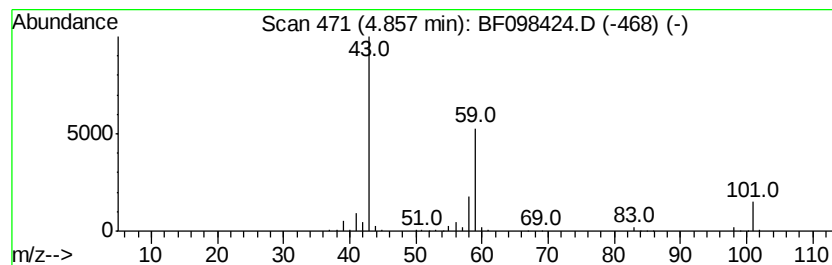
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
4.86	10.17 ng	809088	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

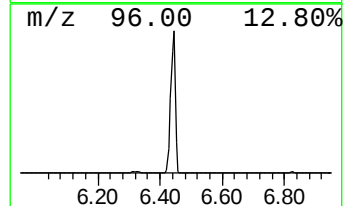
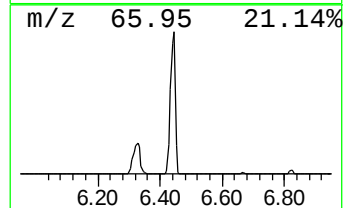
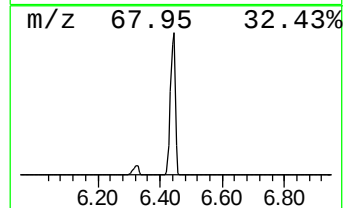
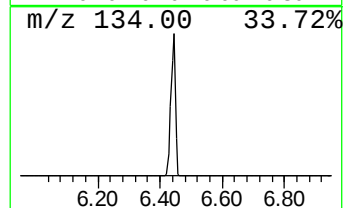
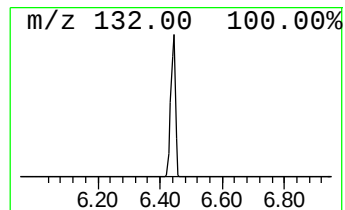
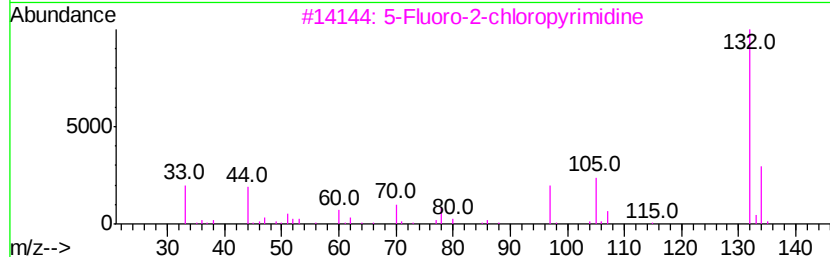
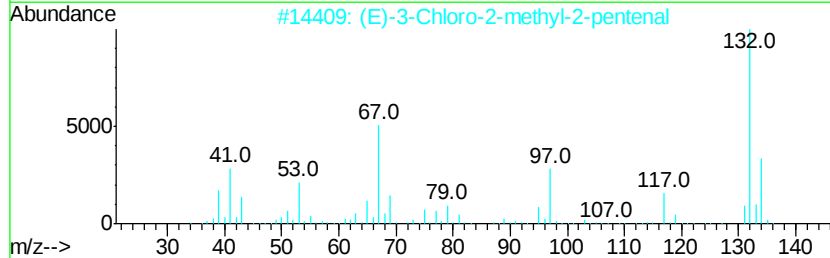
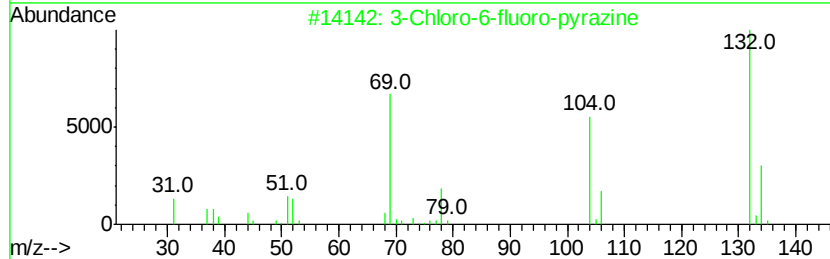
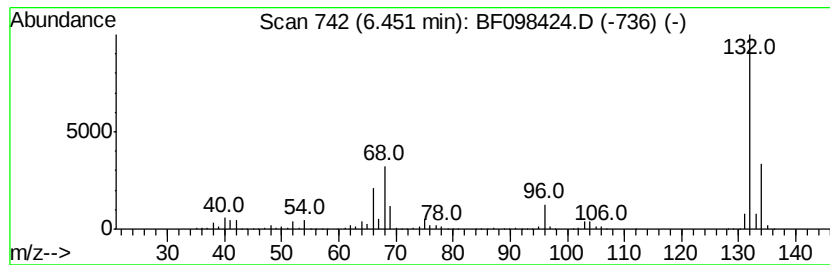
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	83.87 ng	6672560	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

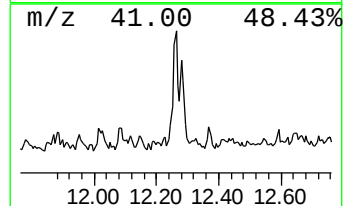
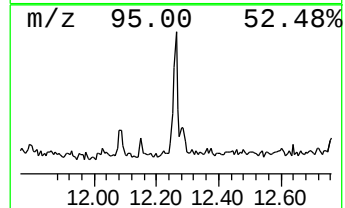
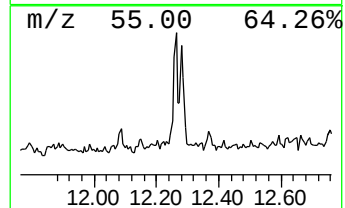
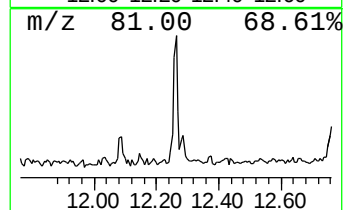
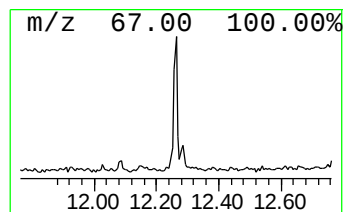
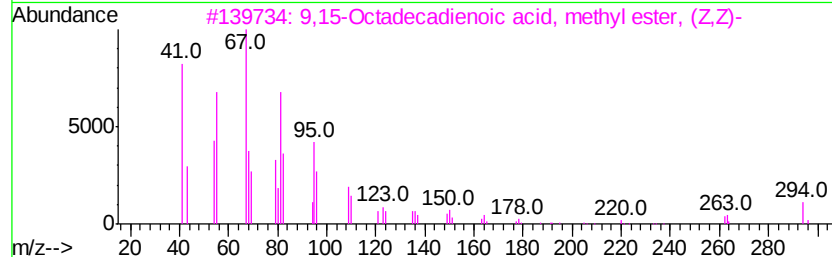
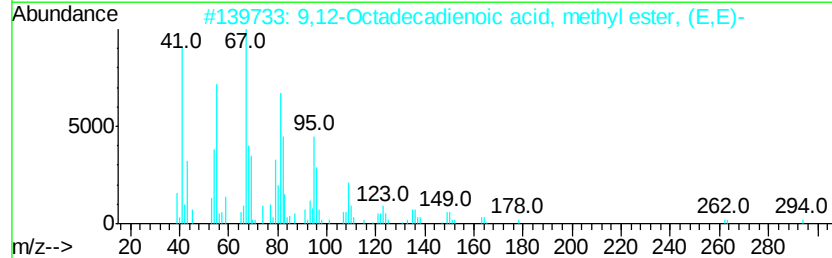
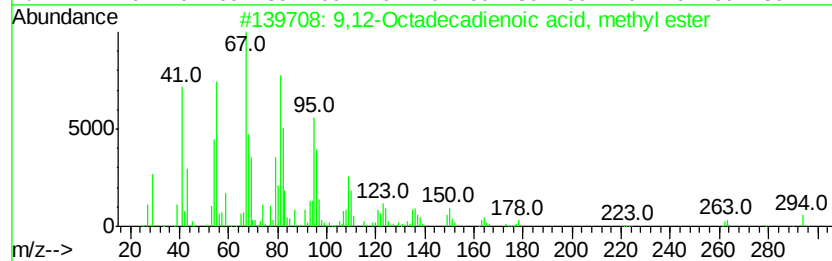
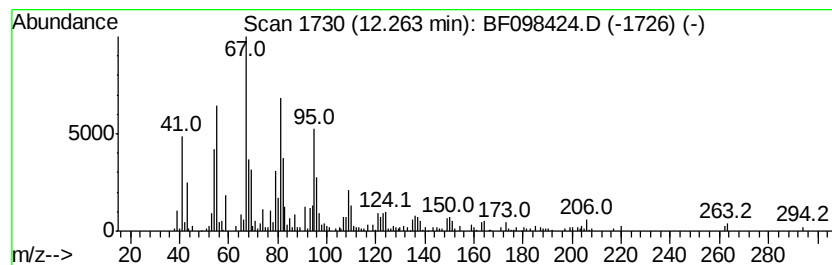
Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.26	2.44 ng	234079	Phenanthrene-d10	11.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,15-Octadecadienoic acid, methv...	294	C19H34O2	017309-05-6	98
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	90



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

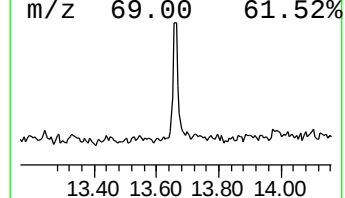
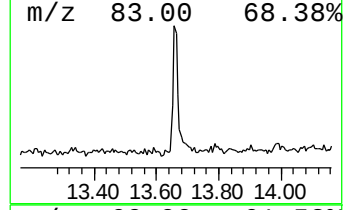
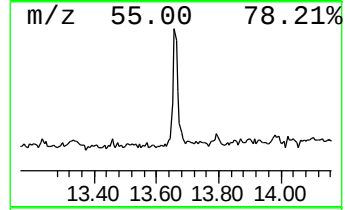
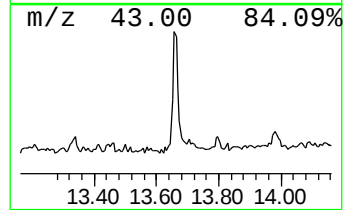
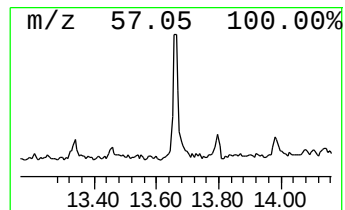
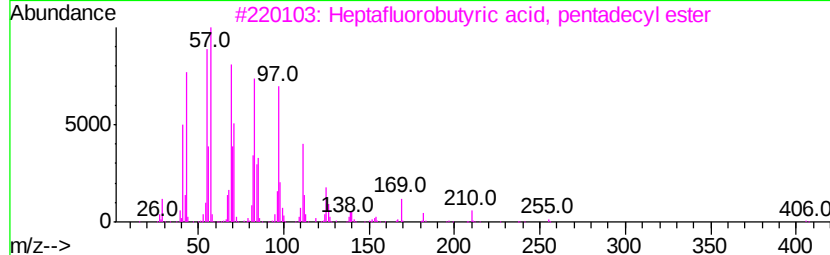
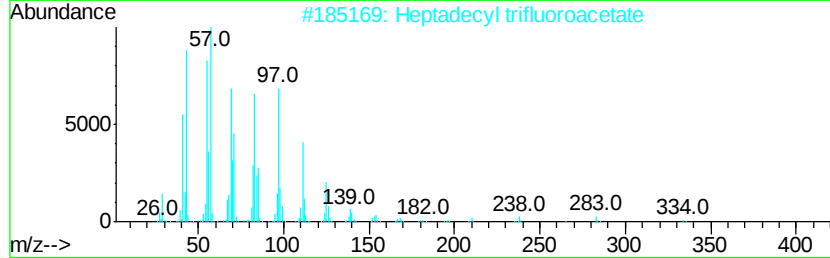
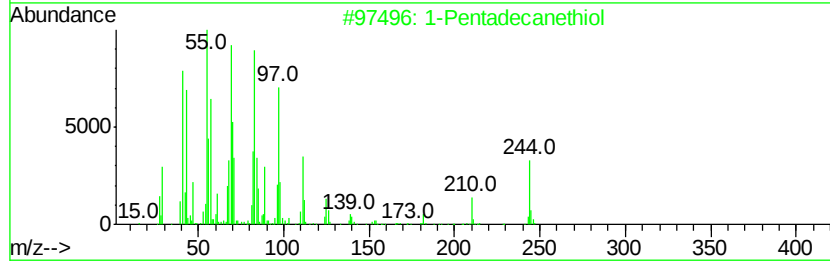
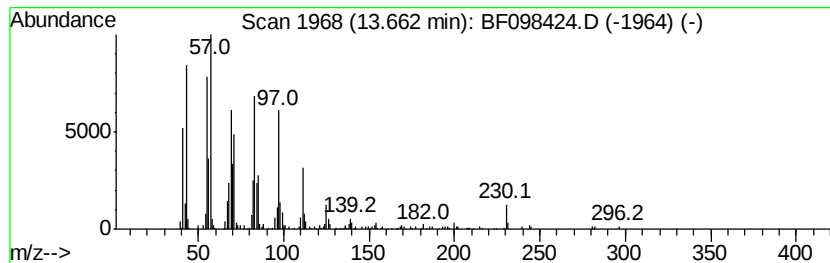
Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Pentadecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.66	5.08 ng	315618	Chrysene-d12	13.81		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	94
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Heptafluorobutvric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

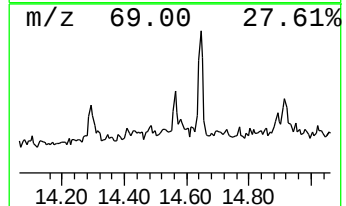
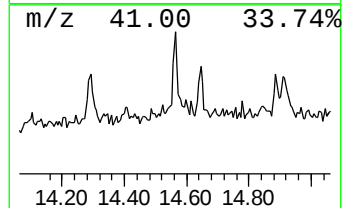
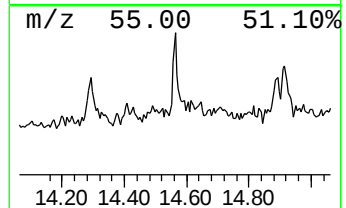
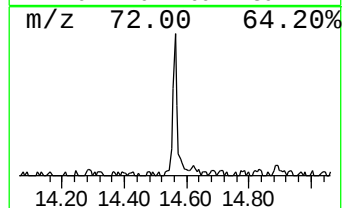
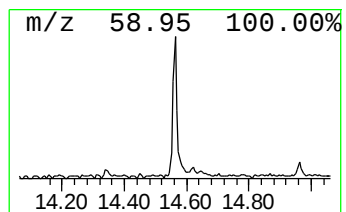
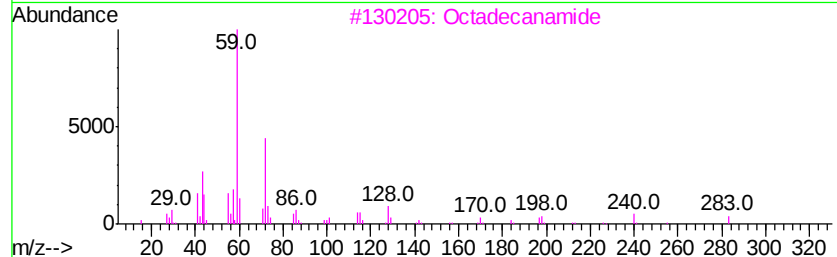
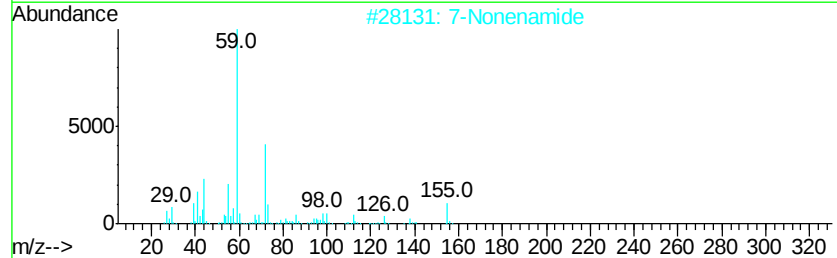
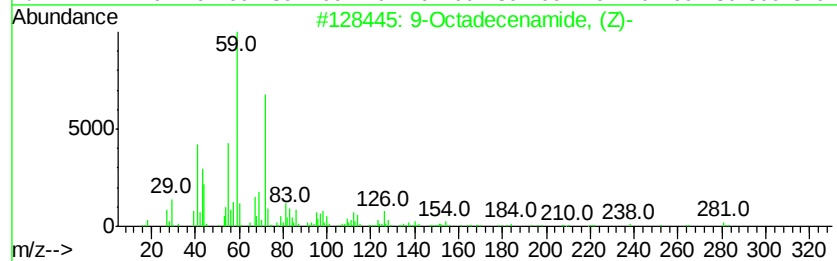
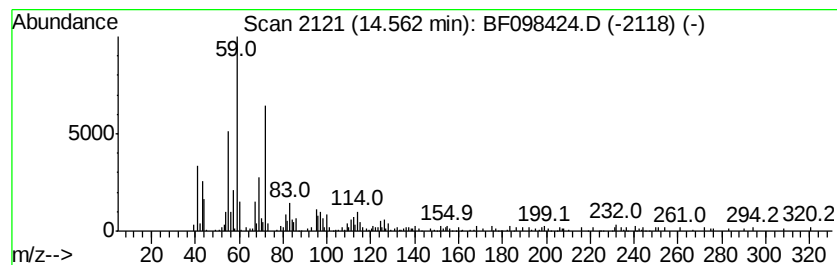
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.53 ng	143748	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		7-Nonenamide	155	C9H17NO	090949-53-4	53
3		Octadecanamide	283	C18H37NO	000124-26-5	50
4		Nonadecanamide	297	C19H39NO	058185-32-3	40
5		7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	38



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

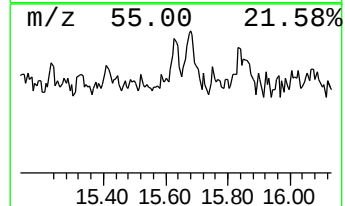
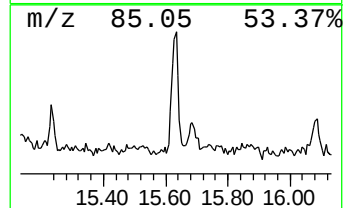
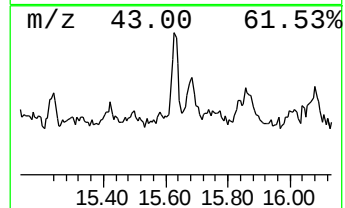
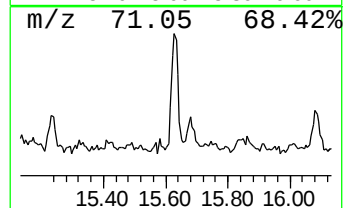
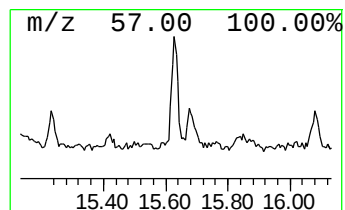
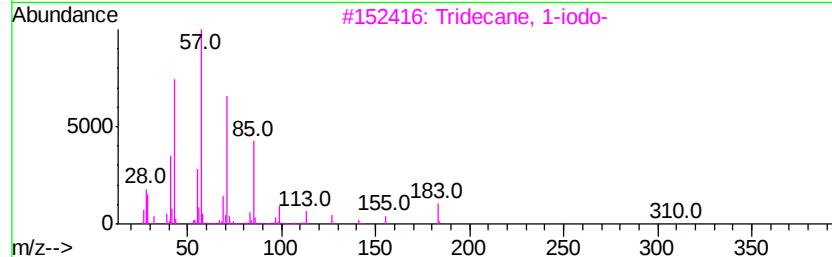
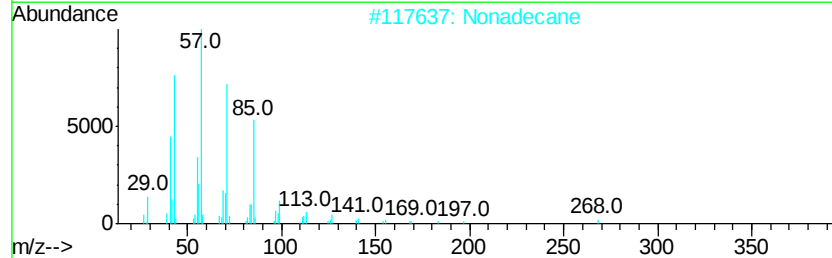
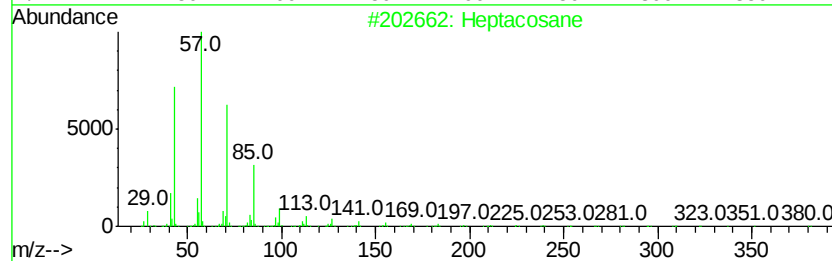
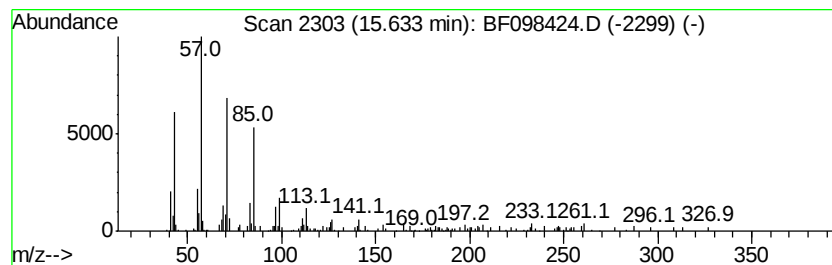
Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	2.38 ng	135315	Perylene-d12	15.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	87
2	Nonadecane	268 C19H40	000629-92-5	81
3	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	80
4	Heptadecane	240 C17H36	000629-78-7	80
5	5-Ethyl-5-methylnonadecane	310 C22H46	1000360-42-7	80



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

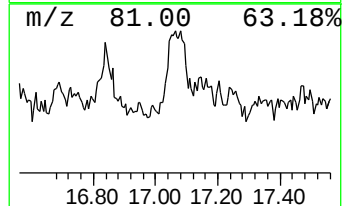
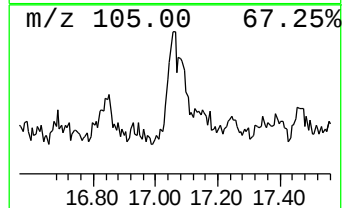
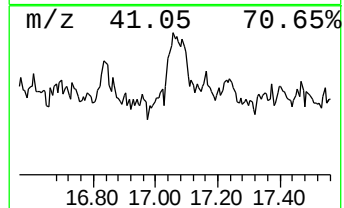
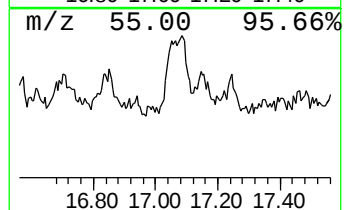
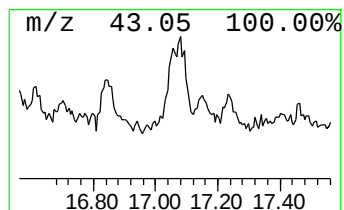
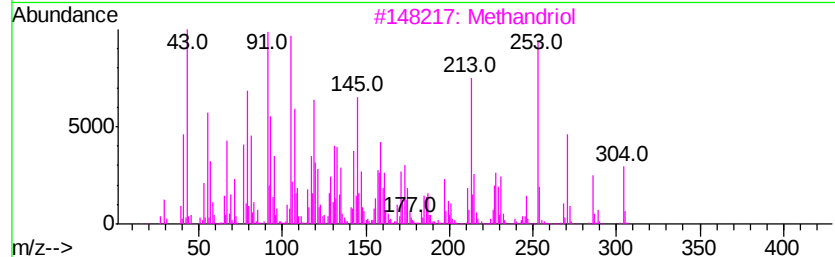
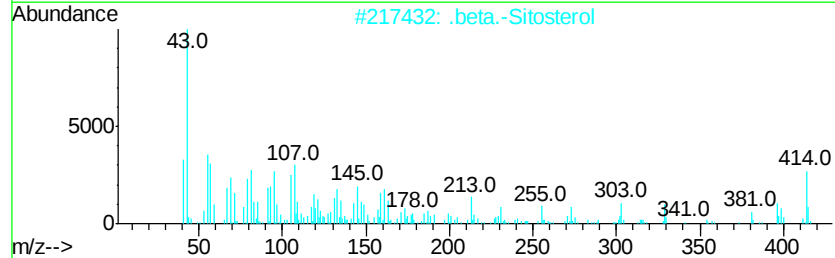
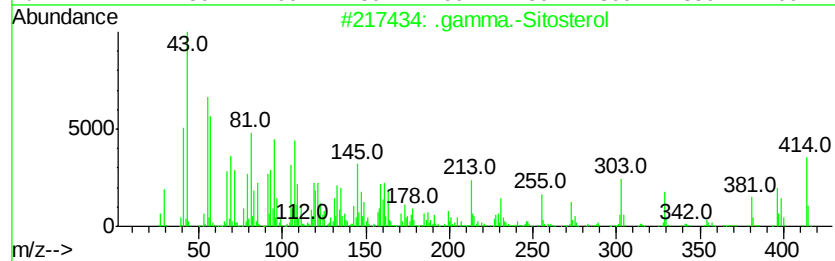
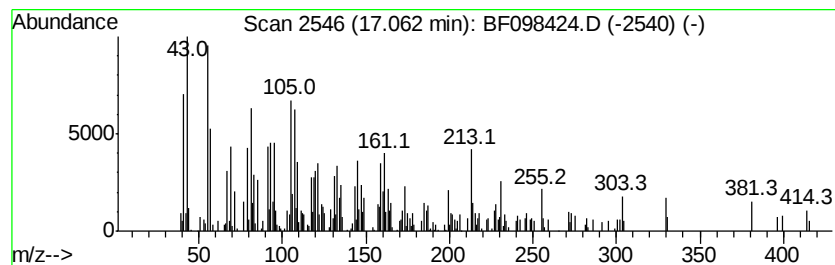
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .gamma.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.06	3.90 ng	221895	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	87
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	70
3		Methandriol	304	C20H32O2	000521-10-8	43
4		Methyl 3-keto-12-acetoxycholanate	446	C27H42O5	189820-40-4	37
5		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	25



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091117\
Data File : BF098424.D
Acq On : 12 Sep 2017 1:29
Operator : SJ/JU
Sample : I5138-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-UTS-TS007-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.86	10.2	ng	809088	1	6.67	1591260	20.0
unknown6.45	6.45	83.9	ng	6672560	1	6.67	1591260	20.0
9,12-Octadecadien...	12.26	2.4	ng	234079	4	11.18	1919890	20.0
1-Pentadecanethiol	13.66	5.1	ng	315618	5	13.81	1242190	20.0
9-Octadecenamide,...	14.56	2.5	ng	143748	6	15.22	1138080	20.0
Heptacosane	15.63	2.4	ng	135315	6	15.22	1138080	20.0
.gamma.-Sitosterol	17.06	3.9	ng	221895	6	15.22	1138080	20.0