

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
 Data File : BF102391.D
 Acq On : 24 Jan 2018 16:03
 Operator : SJ/JU
 Sample : J1250-07
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AB-14(0-2)

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-BF012218.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	4.916	478	481	488	rBV	83937	123668	3.55%	0.380%
2	5.328	545	551	554	rBV	3026923	3259579	93.59%	10.007%
3	6.357	721	726	738	rVB	2773881	3482905	100.00%	10.692%
4	6.487	743	748	751	rBV	3507454	3361625	96.52%	10.320%
5	6.710	783	786	793	rBV	919963	805041	23.11%	2.471%
6	6.869	809	813	816	rBV	2895609	2528823	72.61%	7.763%
7	7.281	878	883	886	rBV	2115864	2169982	62.30%	6.662%
8	7.992	1001	1004	1008	rBV	1195727	1079139	30.98%	3.313%
9	8.551	1096	1099	1103	rBV	349844	302931	8.70%	0.930%
10	8.769	1128	1136	1140	rVB	21235	38938	1.12%	0.120%
11	9.075	1182	1188	1191	rBV	3600422	3422447	98.26%	10.507%
12	9.469	1251	1255	1258	rBV	885441	726514	20.86%	2.230%
13	9.680	1288	1291	1294	rVB	71352	61376	1.76%	0.188%
14	9.745	1298	1302	1306	rBV2	1349677	1210166	34.75%	3.715%
15	10.175	1367	1375	1379	rBV2	117542	213542	6.13%	0.656%
16	10.463	1419	1424	1431	rBV	1633049	1522796	43.72%	4.675%
17	10.539	1432	1437	1440	rBV	1981871	1915515	55.00%	5.880%
18	10.651	1453	1456	1460	rBV	65126	79208	2.27%	0.243%
19	11.098	1524	1532	1535	rBV3	53865	72983	2.10%	0.224%
20	11.127	1535	1537	1542	rVB2	29568	34924	1.00%	0.107%
21	11.233	1551	1555	1558	rBV	1238565	1078690	30.97%	3.311%
22	11.763	1642	1645	1647	rBV2	78487	70090	2.01%	0.215%
23	12.221	1718	1723	1730	rBV10	14973	40332	1.16%	0.124%
24	12.445	1758	1761	1766	rBV	28047	38978	1.12%	0.120%
25	12.821	1820	1825	1828	rBV	2543147	2537153	72.85%	7.789%
26	13.251	1896	1898	1902	rVB4	31872	35564	1.02%	0.109%
27	13.710	1973	1976	1986	rBV	447124	481364	13.82%	1.478%
28	13.868	1999	2003	2007	rVB	834052	752214	21.60%	2.309%
29	15.292	2241	2245	2252	rVB	580591	758488	21.78%	2.328%
30	15.939	2352	2355	2364	rVB3	130770	236346	6.79%	0.726%
31	16.351	2421	2425	2429	rVB2	80638	133075	3.82%	0.409%

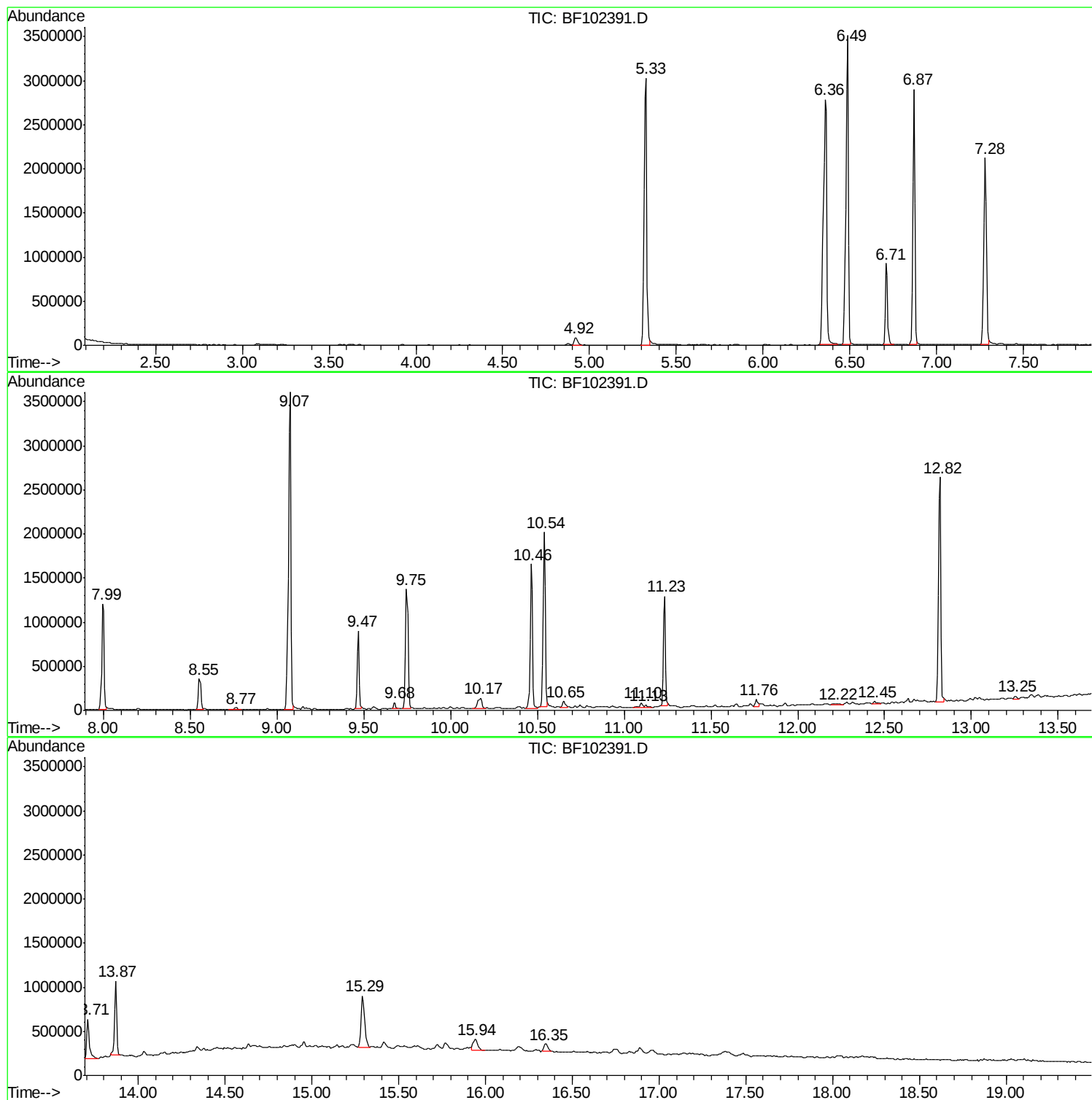
Sum of corrected areas: 32574396

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

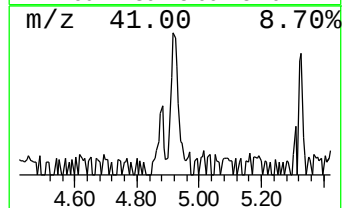
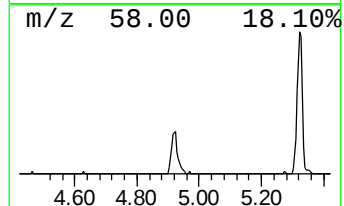
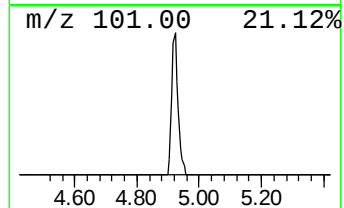
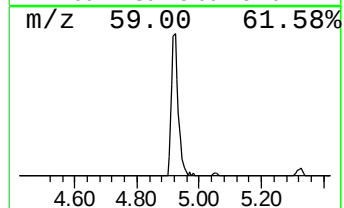
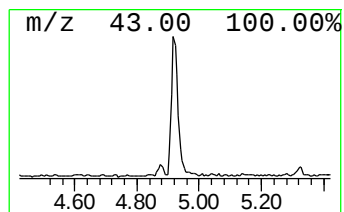
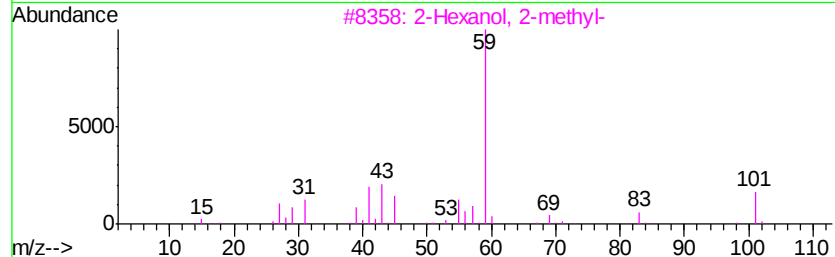
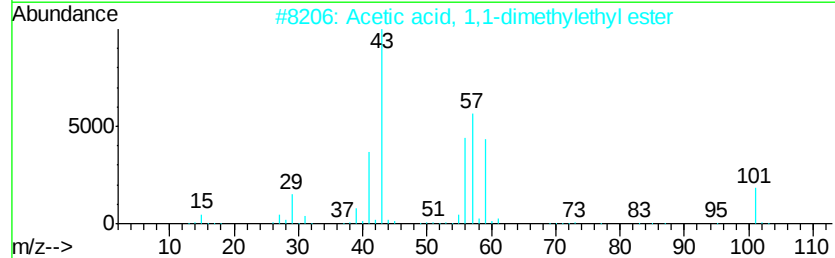
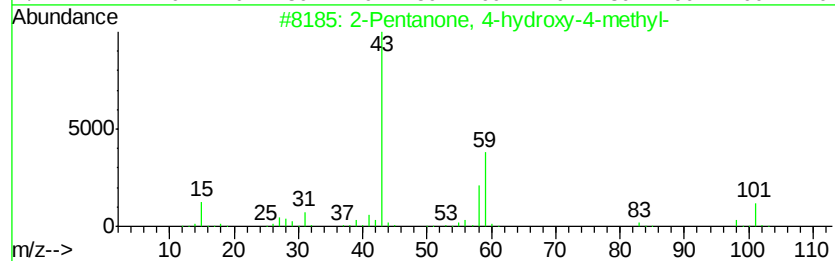
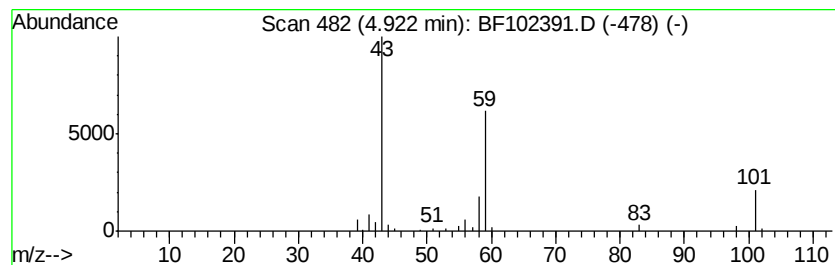
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.07 ng	123668	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

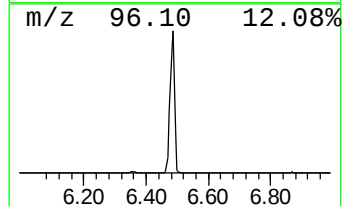
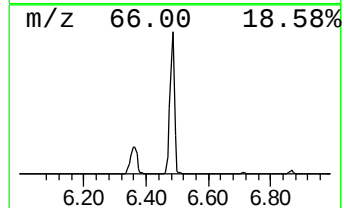
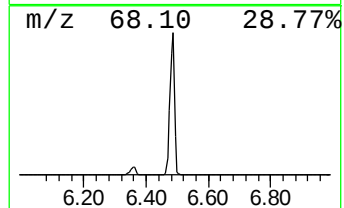
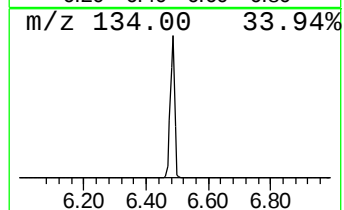
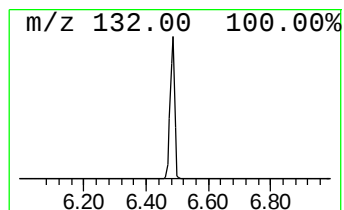
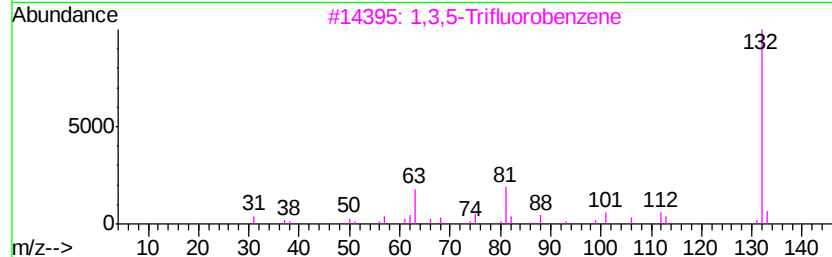
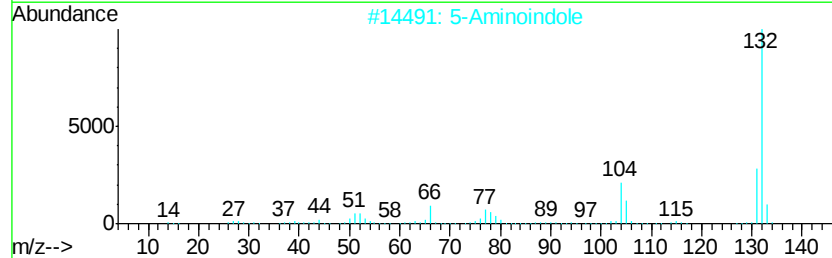
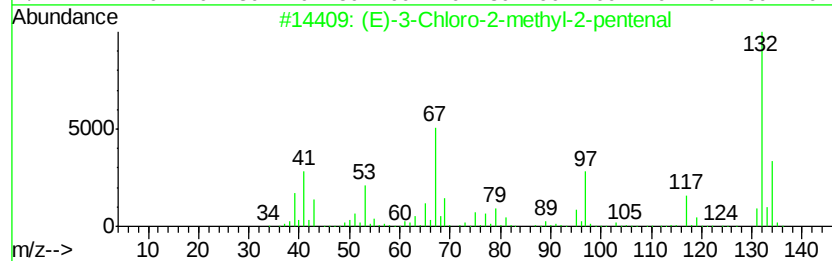
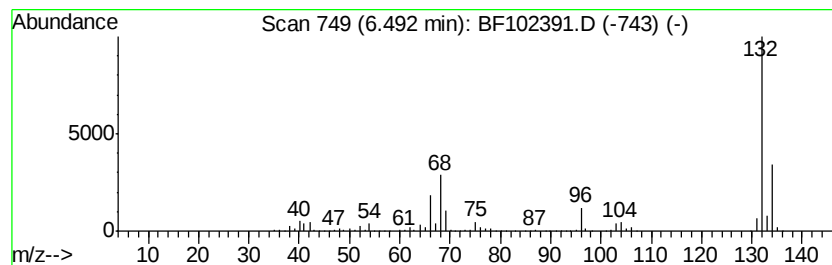
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	83.51 ng	3361630	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

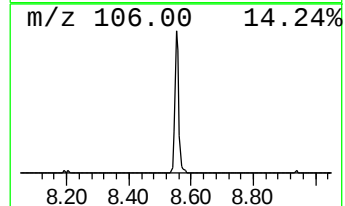
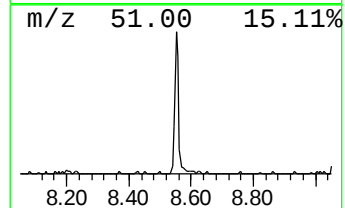
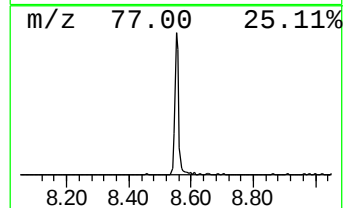
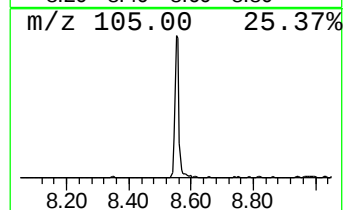
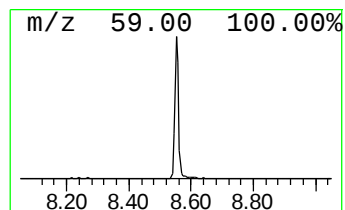
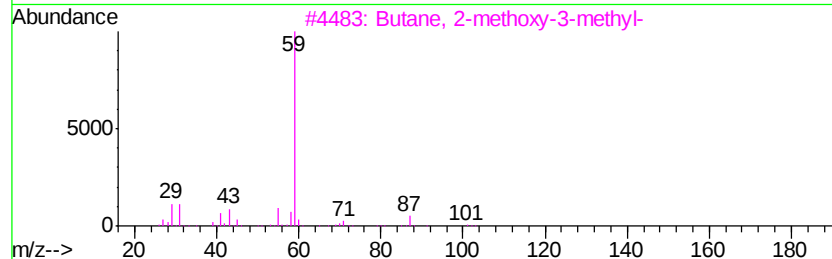
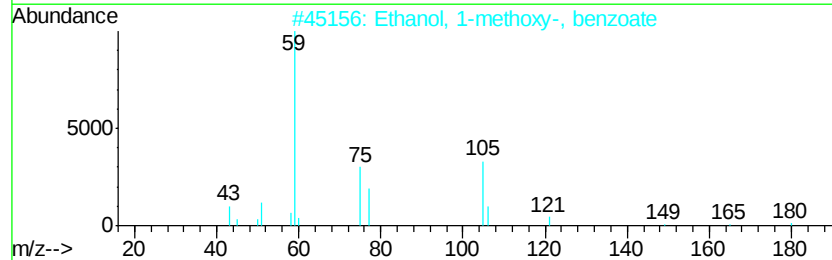
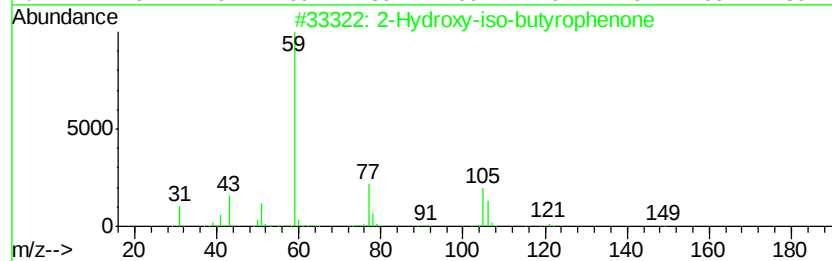
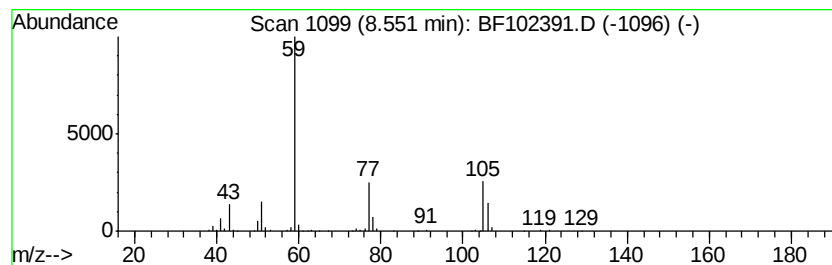
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.55	5.61 ng	302931	Napthalene-d8	7.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90	
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56	
3	Butane, 2-methoxy-3-methyl-	102	C6H14O	062016-49-3	32	
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7	
5	Guanidine	59	CH5N3	000113-00-8	7	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

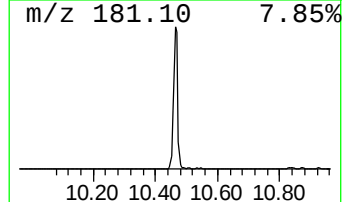
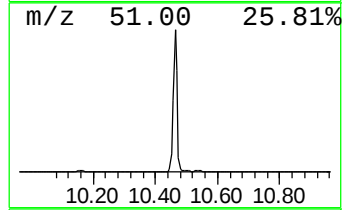
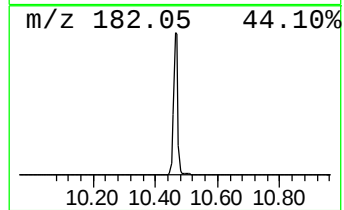
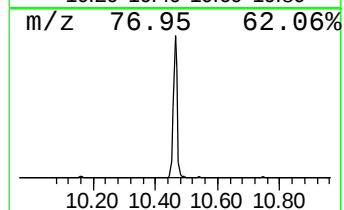
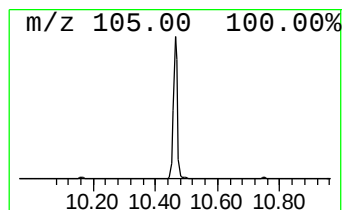
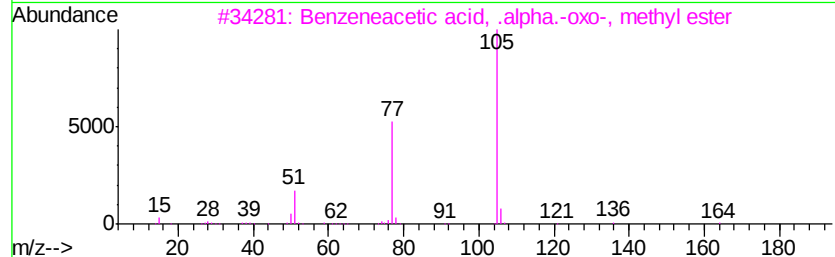
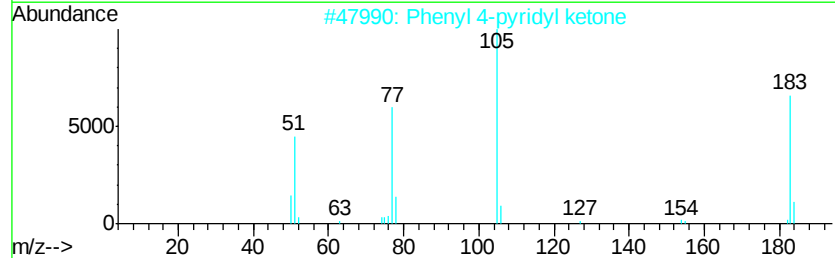
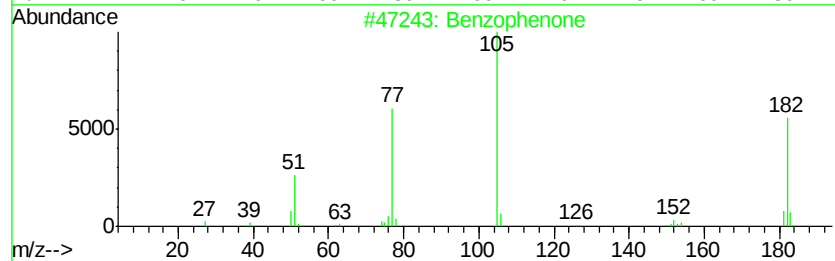
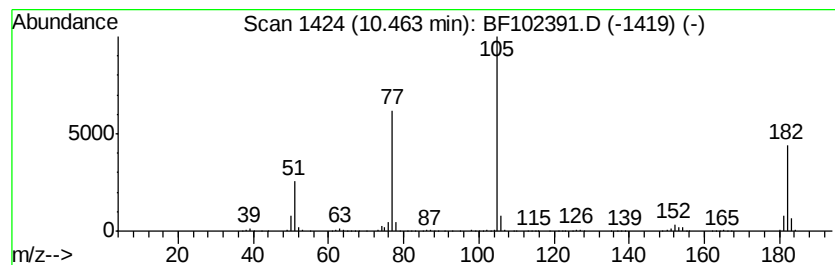
Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	25.17 ng	1522800	Acenaphthene-d10	9.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Phenyl 4-pyridyl ketone	183 C12H9NO	014548-46-0 50
3		Benzeneacetic acid, .alpha.-oxo-...	164 C9H8O3	015206-55-0 49
4		Ethanone, 2-bromo-1-phenyl-	198 C8H7BrO	000070-11-1 47
5		1-Butanone, 1-phenyl-	148 C10H12O	000495-40-9 47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

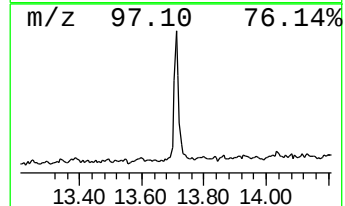
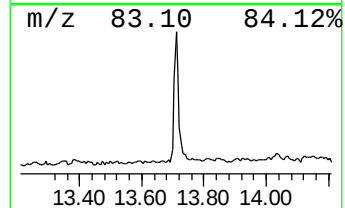
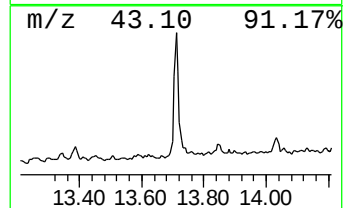
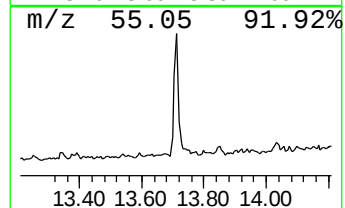
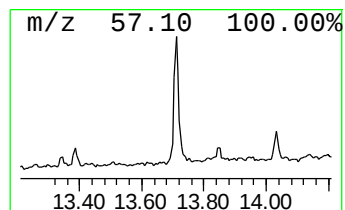
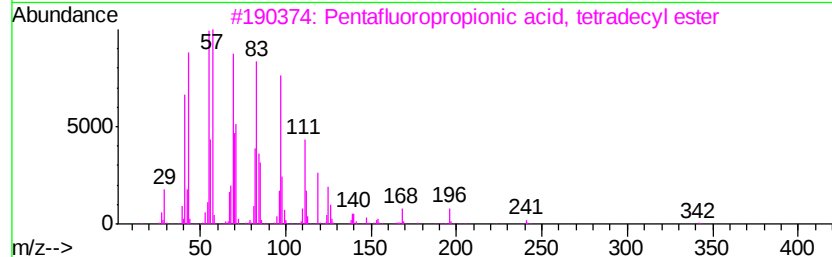
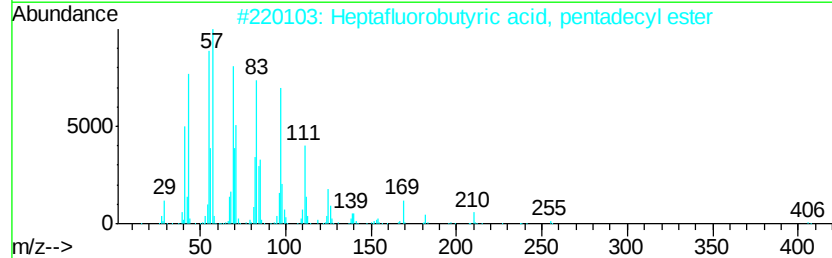
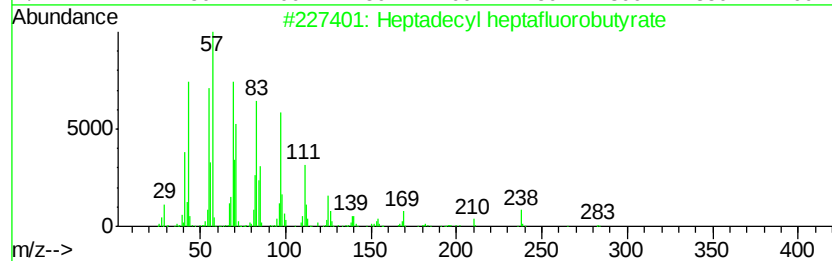
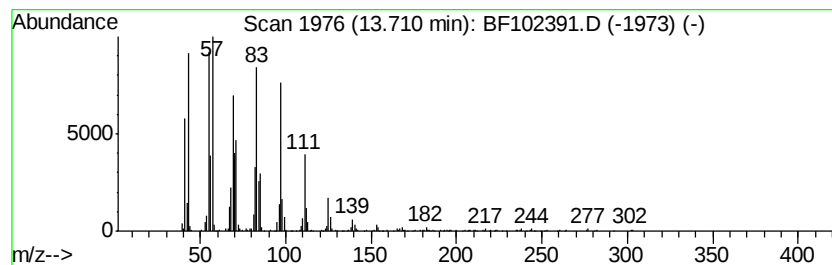
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	12.80 ng	481364	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

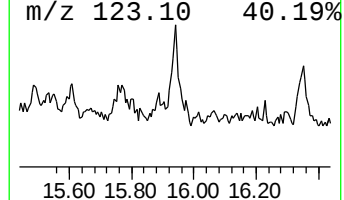
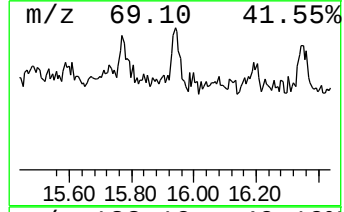
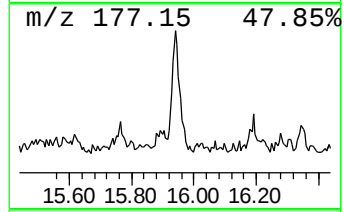
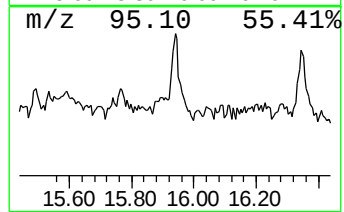
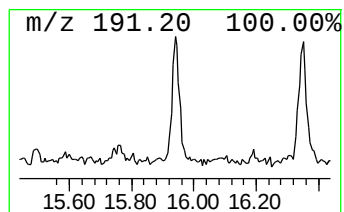
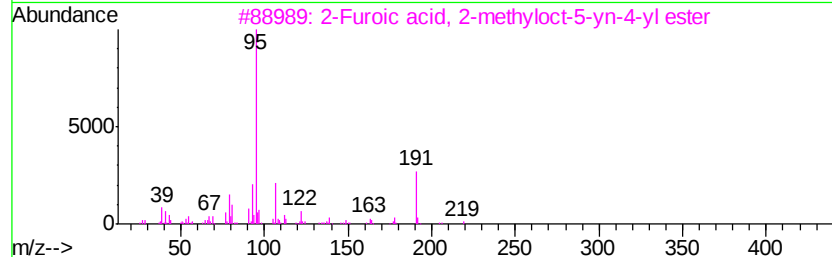
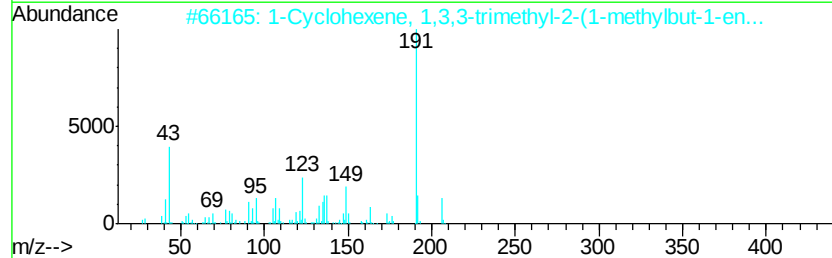
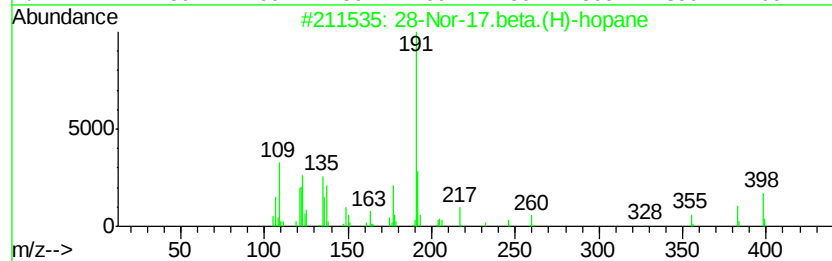
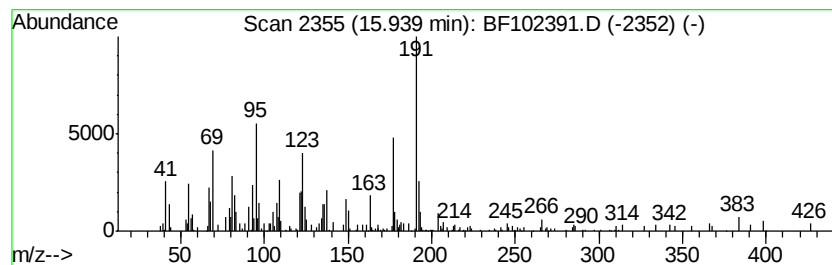
Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 28-Nor-17.beta.(H)-hopane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	6.23 ng	236346	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	28-Nor-17.beta.(H)-hopane	398 C29H50	036728-72-0	68
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206 C14H22O	1000197-08-4	37
3	2-Furoic acid, 2-methyloct-5-yn-...	234 C14H18O3	1000299-23-7	35
4	Anthracene, 9-cyclohexyltetradec...	274 C20H34	055255-70-4	27
5	Anthracene, 9-dodecyltetradecahy...	360 C26H48	055401-75-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

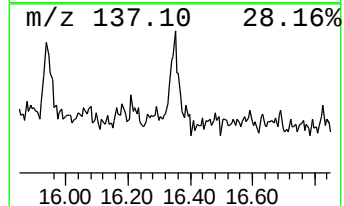
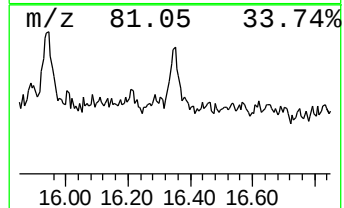
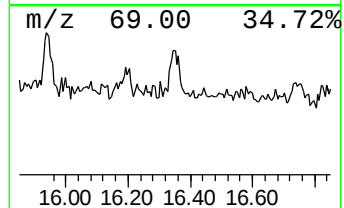
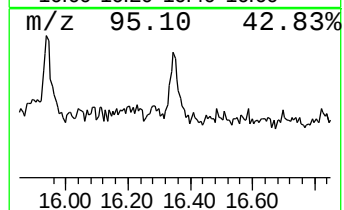
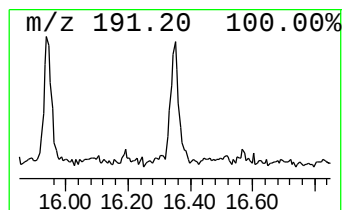
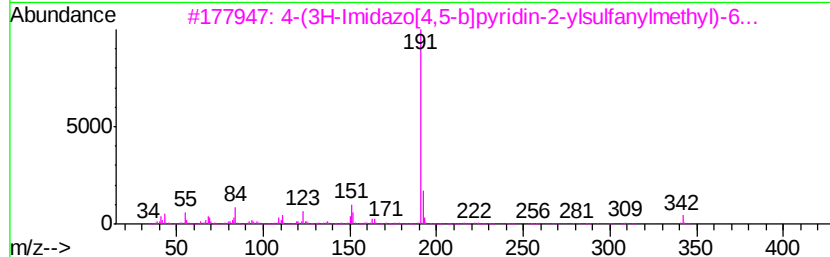
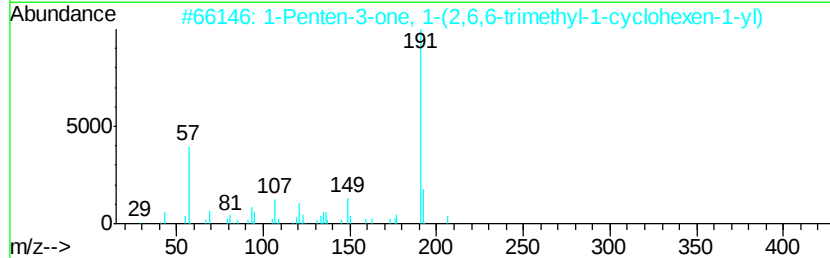
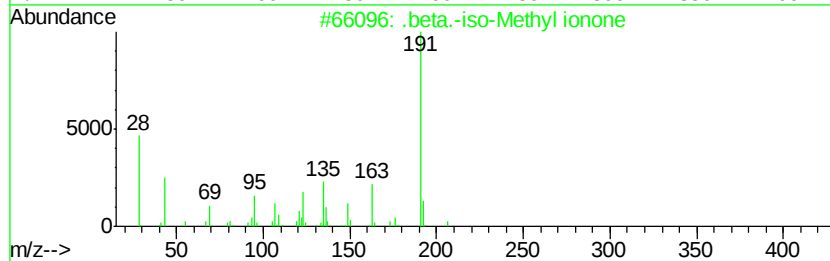
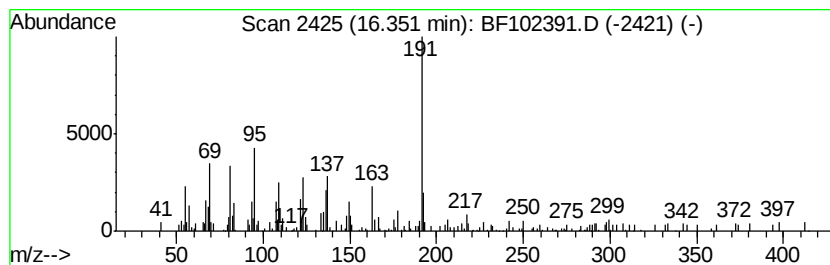
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	3.51 ng	133075	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	41
3		4-(3H-Imidazo[4,5-b]pyridin-2-yl...	342	C15H18N8S	1000276-08-2	35
4		1,2,5,6-Tetraaza-2,4-hexadiene, ...	358	C20H30N4O2	1000188-27-0	35
5		3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102391.D
Acq On : 24 Jan 2018 16:03
Operator : SJ/JU
Sample : J1250-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-14(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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...	4.92	3.1	ng	123668	1	6.71	805041	20.0
unknown6.49	6.49	83.5	ng	3361630	1	6.71	805041	20.0
2-Hydroxy-iso-but...	8.55	5.6	ng	302931	2	7.99	1079140	20.0
Benzophenone	10.46	25.2	ng	1522800	3	9.75	1210170	20.0
Heptadecyl hepta...	13.71	12.8	ng	481364	5	13.87	752214	20.0
28-Nor-17.beta.(H...	15.94	6.2	ng	236346	6	15.29	758488	20.0
.beta.-iso-Methyl...	16.35	3.5	ng	133075	6	15.29	758488	20.0