

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111317\
 Data File : BF100523.D
 Acq On : 14 Nov 2017 4:33
 Operator : SJ/JU
 Sample : I6301-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-02-110917-A

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-BF110817.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	2.193	14	18	23	rVB	20124	28510	1.01%	0.111%
2	5.116	511	515	526	rBV	467237	585983	20.73%	2.275%
3	5.510	577	582	585	rBV	2690666	2699341	95.50%	10.479%
4	6.516	747	753	764	rBV	2655529	2826539	100.00%	10.973%
5	6.657	773	777	781	rBV	2648548	2715325	96.07%	10.541%
6	6.892	813	817	820	rBV	952673	791026	27.99%	3.071%
7	7.045	839	843	847	rVB	2270310	2069257	73.21%	8.033%
8	7.451	907	912	915	rBV	1820856	1719945	60.85%	6.677%
9	8.175	1031	1035	1037	rBV	1080717	987274	34.93%	3.833%
10	8.722	1122	1128	1132	rBV	278627	220627	7.81%	0.857%
11	9.245	1212	1217	1220	rBV	2982381	2594386	91.79%	10.072%
12	9.633	1280	1283	1287	rBV	479598	394042	13.94%	1.530%
13	9.786	1304	1309	1313	rBV	26690	29103	1.03%	0.113%
14	9.928	1329	1333	1336	rVB	1122365	926182	32.77%	3.596%
15	10.639	1450	1454	1457	rBV	747752	591281	20.92%	2.295%
16	10.716	1463	1467	1470	rBV	1438128	1262788	44.68%	4.902%
17	10.833	1482	1487	1490	rBV	40240	45208	1.60%	0.176%
18	11.298	1563	1566	1573	rVB4	27961	40765	1.44%	0.158%
19	11.410	1582	1585	1588	rBV	819598	754520	26.69%	2.929%
20	11.433	1588	1589	1593	rVB	80195	58887	2.08%	0.229%
21	11.927	1667	1673	1679	rBV3	39636	69148	2.45%	0.268%
22	12.621	1788	1791	1794	rBV	198653	178424	6.31%	0.693%
23	12.663	1794	1798	1801	rVV	89339	77781	2.75%	0.302%
24	12.851	1824	1830	1834	rBV	179268	207295	7.33%	0.805%
25	12.998	1850	1855	1858	rBV	1856648	1704849	60.32%	6.618%
26	13.068	1864	1867	1871	rBV3	20564	36142	1.28%	0.140%
27	13.180	1884	1886	1889	rVB2	50099	39586	1.40%	0.154%
28	13.245	1895	1897	1900	rBV	32085	30305	1.07%	0.118%
29	13.286	1900	1904	1906	rBV2	28990	34187	1.21%	0.133%
30	13.886	2002	2006	2012	rVB2	88798	108326	3.83%	0.421%
31	14.051	2027	2034	2037	rBV	907241	954440	33.77%	3.705%
32	14.074	2037	2038	2044	rVB	130545	88349	3.13%	0.343%
33	15.092	2208	2211	2219	rVB	94943	176679	6.25%	0.686%
34	15.462	2272	2274	2281	rVB	64845	74428	2.63%	0.289%

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-02-110917-A

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.527	2281	2285	2296	rVB	427540	637959	22.57%	2.477%
----	--------	------	------	------	-----	--------	--------	--------	--------

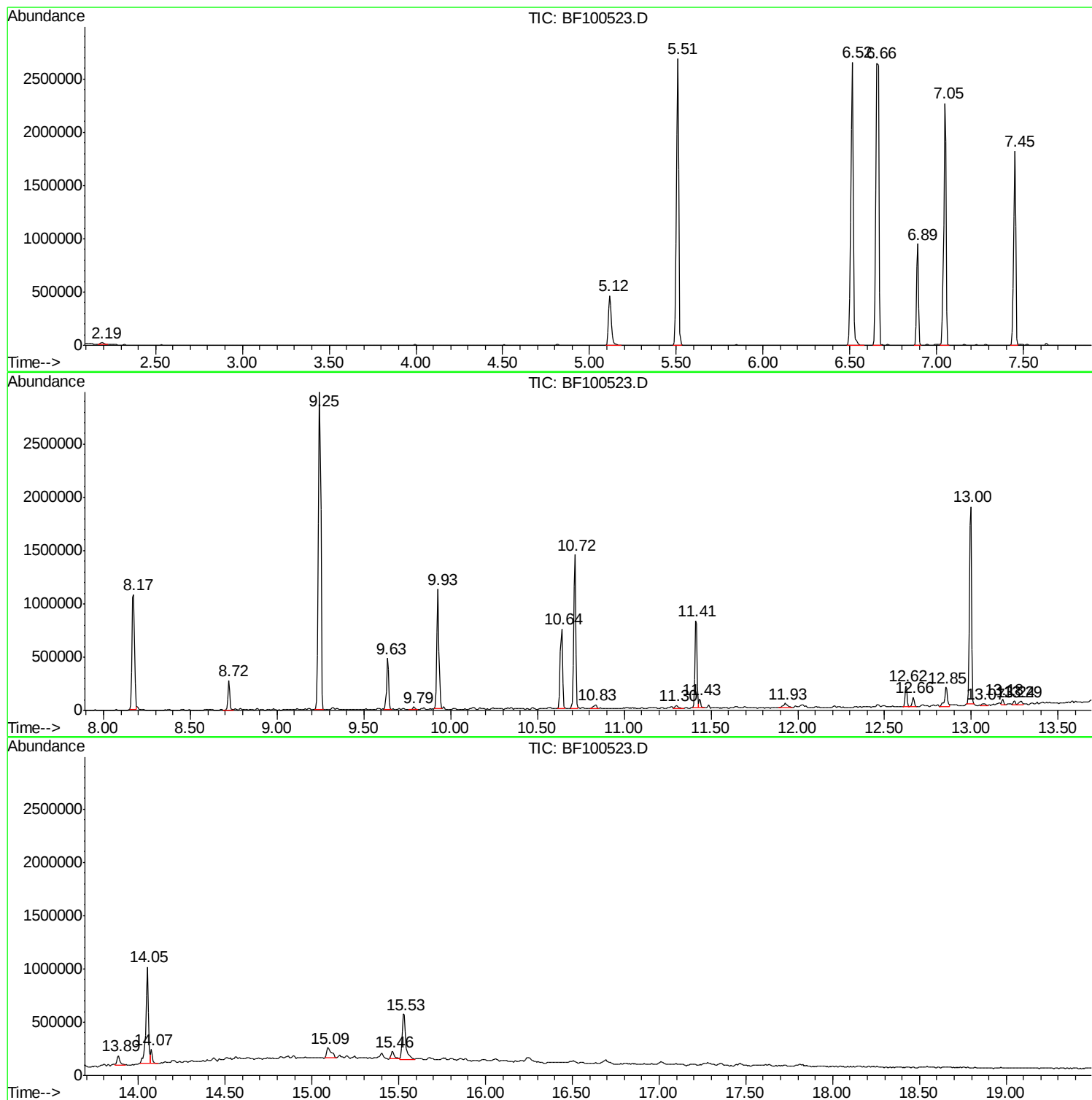
Sum of corrected areas: 25758887

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-02-110917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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\SV0ASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
JC-02-110917-A

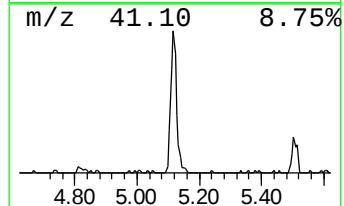
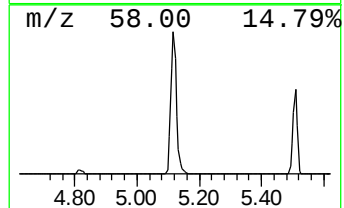
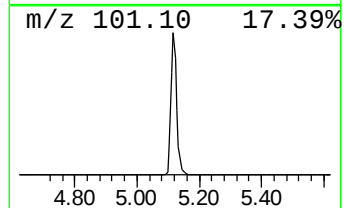
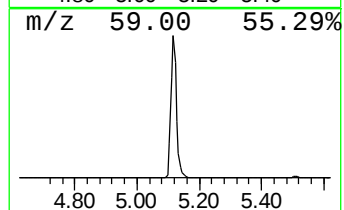
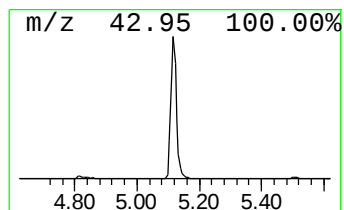
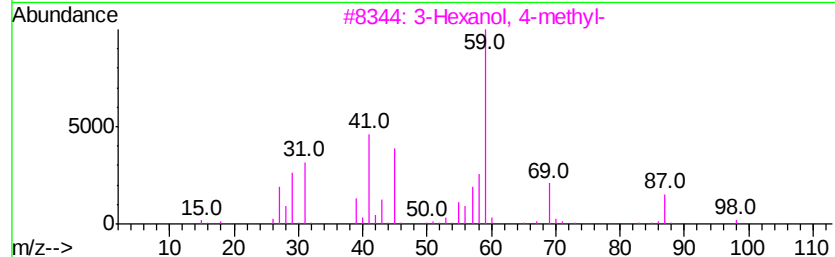
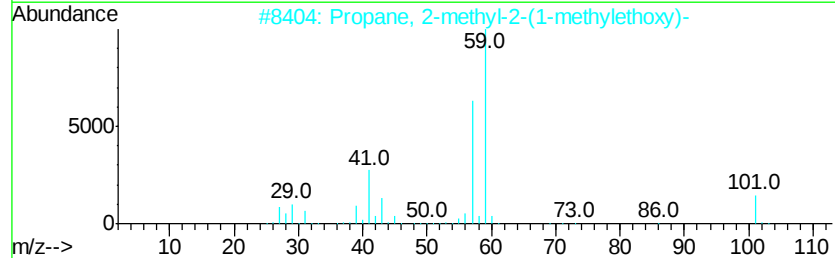
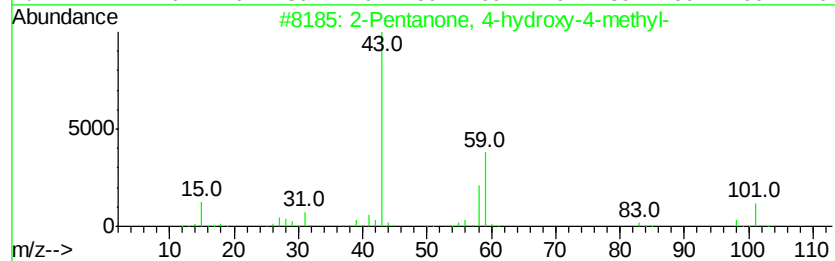
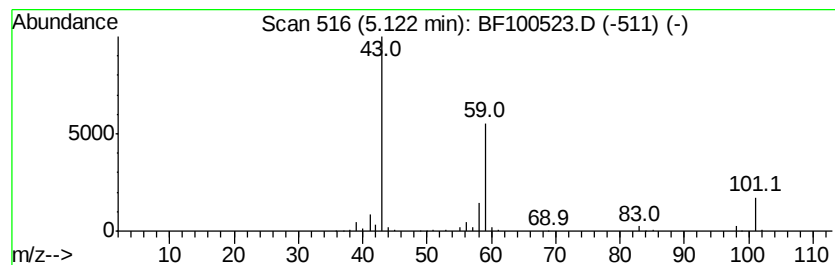
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.12	14.82 ng	585983	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-02-110917-A

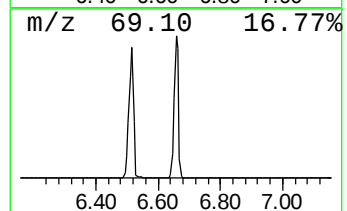
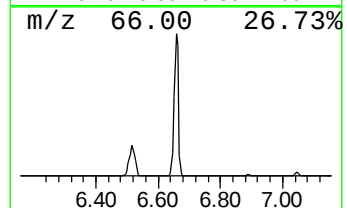
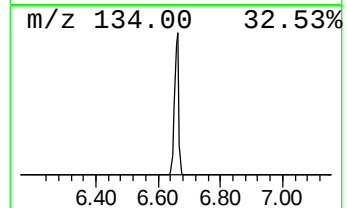
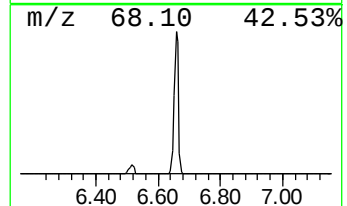
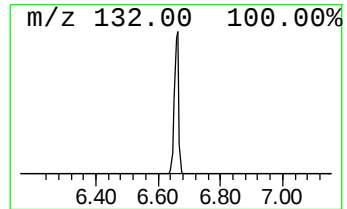
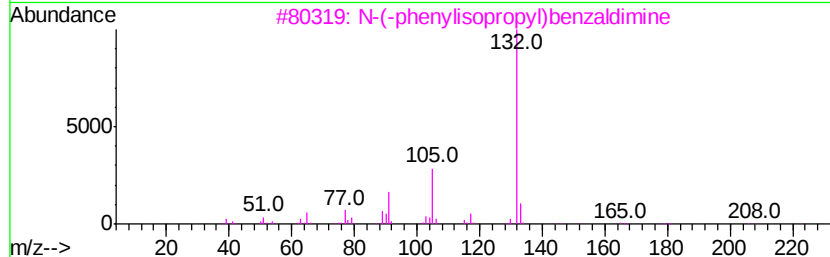
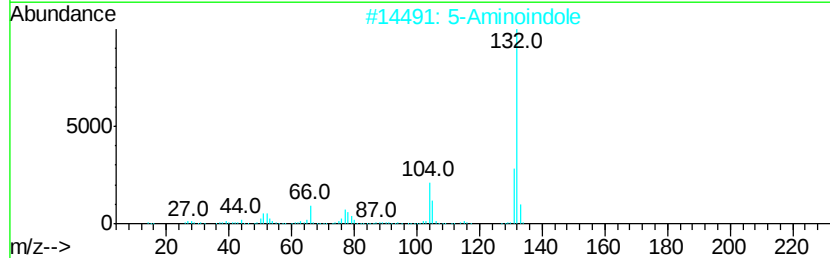
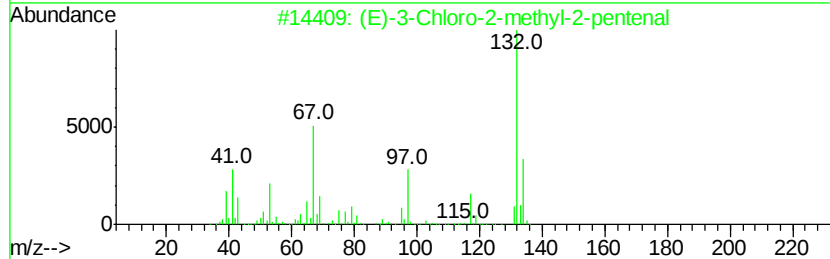
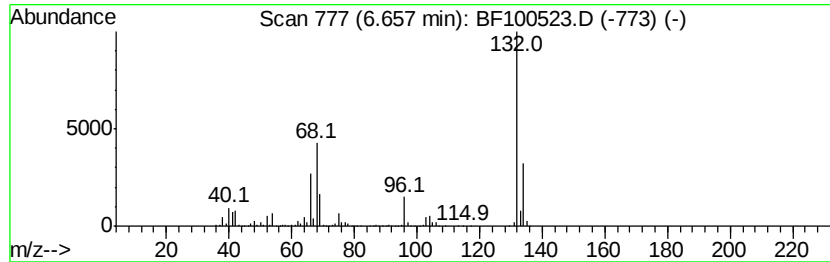
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	68.65 ng	2715330	1,4-Dichlorobenzene-d4	6.89

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		N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-02-110917-A

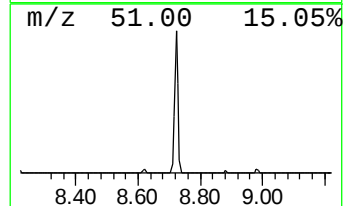
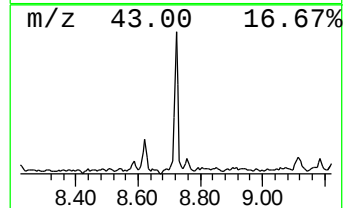
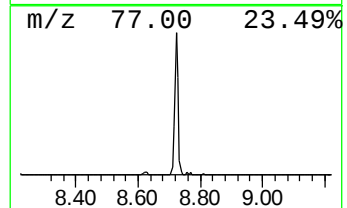
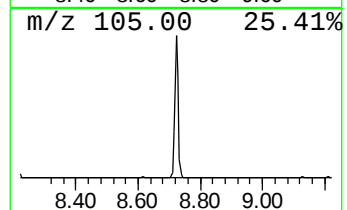
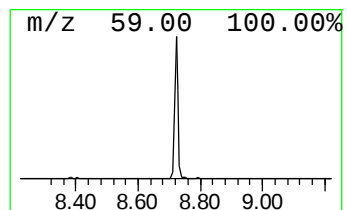
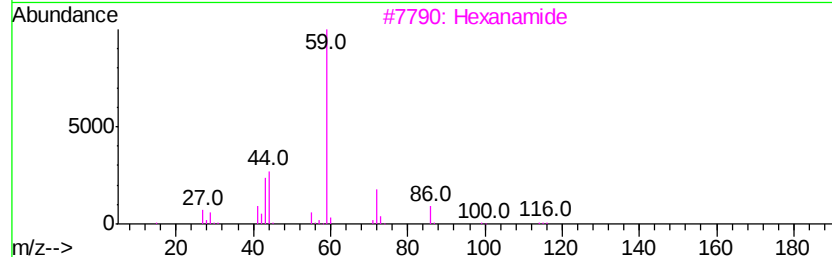
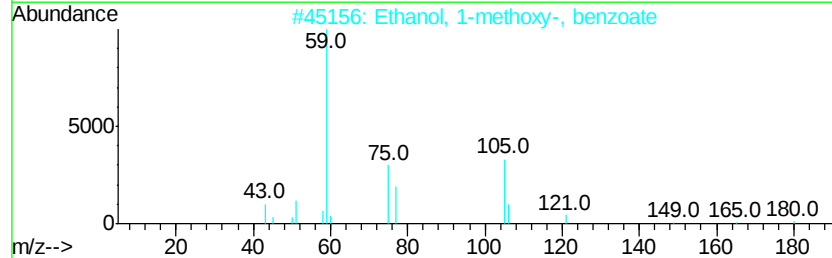
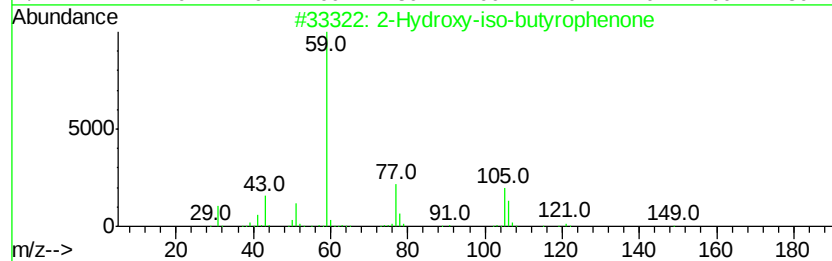
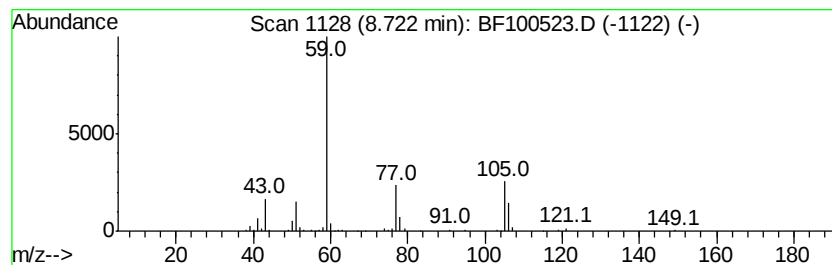
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	4.47 ng	220627	Napthalene-d8	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3		Hexanamide	115	C6H13NO	000628-02-4	9
4		Guanidine	59	CH5N3	000113-00-8	7
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

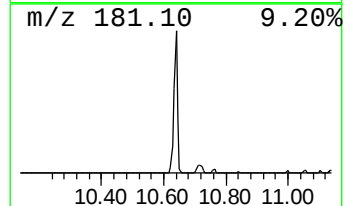
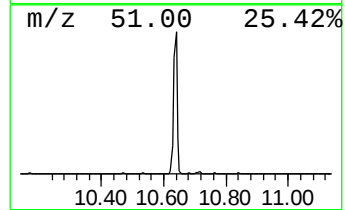
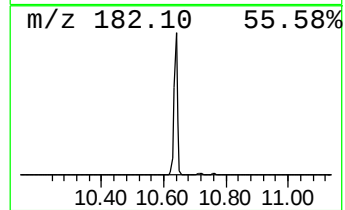
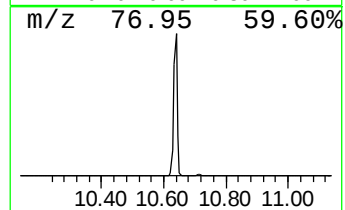
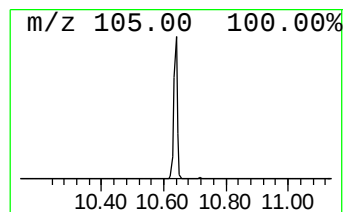
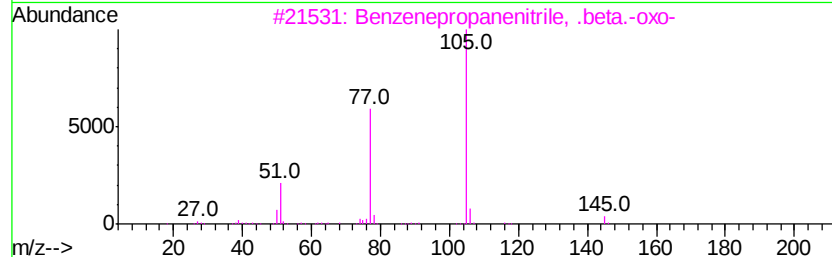
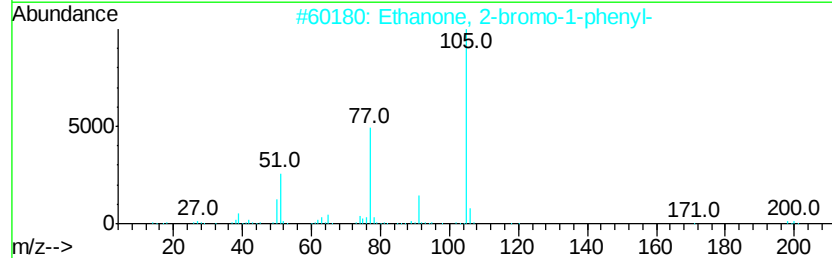
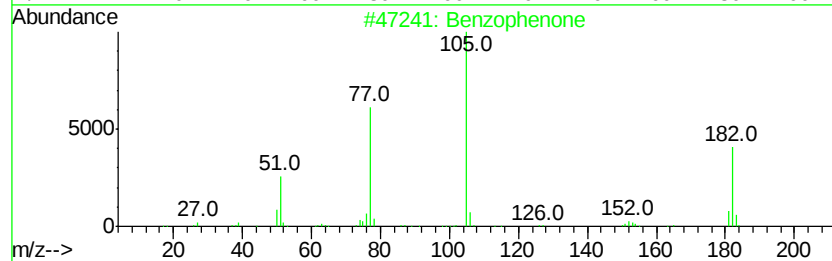
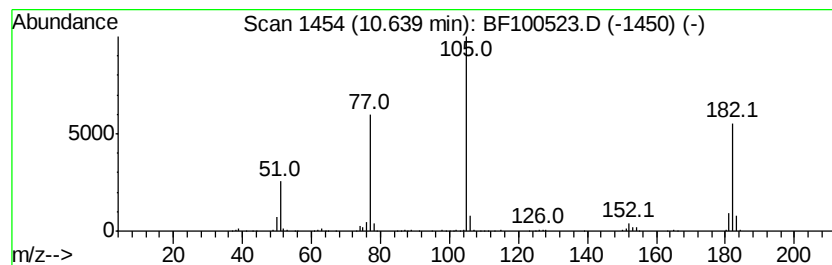
Instrument :
BNA_F
ClientSampleId :
JC-02-110917-A

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.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 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	12.77 ng	591281	Acenaphthene-d10	9.93
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		Ethanone, 2-bromo-1-phenyl-	198 C8H7BrO	000070-11-1 47
3		Benzenepropanenitrile, .beta.-oxo-	145 C9H7NO	000614-16-4 47
4		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
5		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184 C11H8N2O	1000296-76-9 47



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

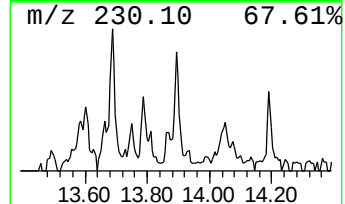
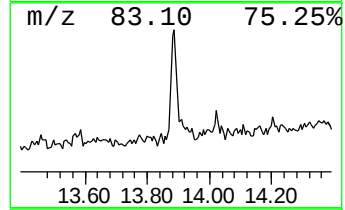
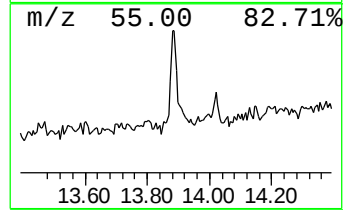
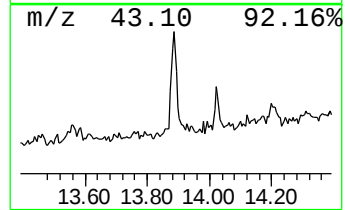
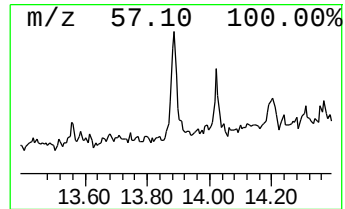
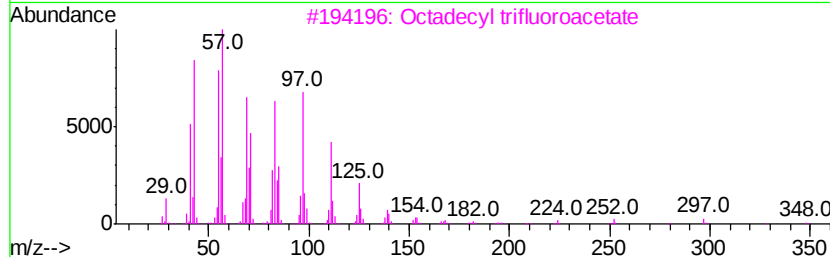
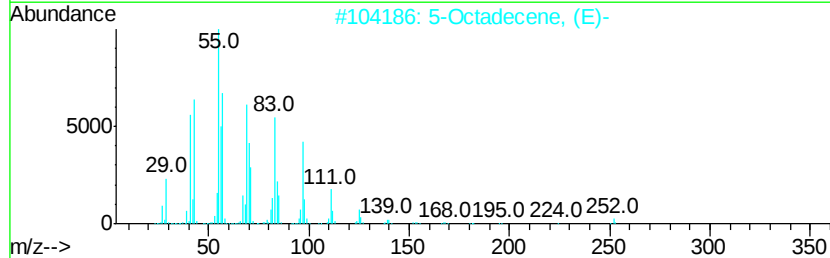
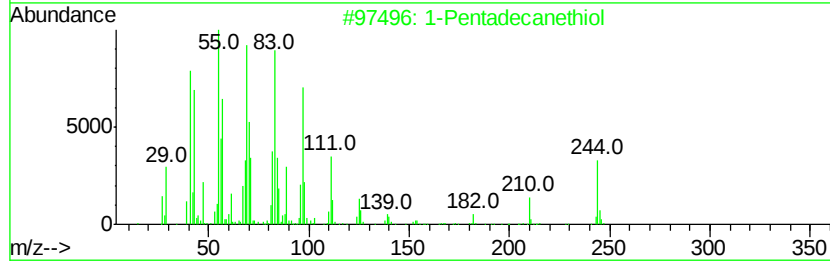
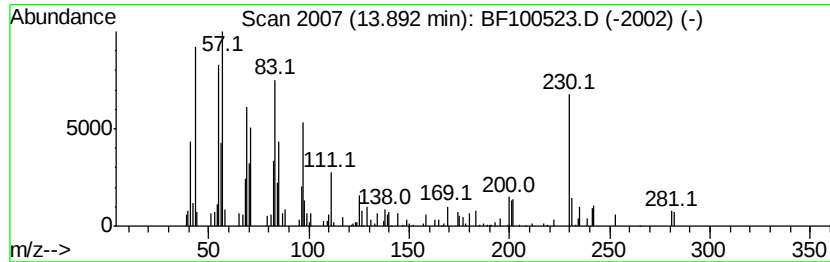
Instrument :
BNA_F
ClientSampleId :
JC-02-110917-A

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Pentadecanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.89	2.27 ng	108326	Chrysene-d12	14.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	94
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	93
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	93
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111317\
Data File : BF100523.D
Acq On : 14 Nov 2017 4:33
Operator : SJ/JU
Sample : I6301-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-02-110917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.12	14.8	ng	585983	1	6.89	791026	20.0
unknown6.66	6.66	68.7	ng	2715330	1	6.89	791026	20.0
2-Hydroxy-iso-but...	8.72	4.5	ng	220627	2	8.17	987274	20.0
Benzophenone	10.64	12.8	ng	591281	3	9.93	926182	20.0
1-Pentadecanethiol	13.89	2.3	ng	108326	5	14.05	954440	20.0