

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080218\
 Data File : BF107927.D
 Acq On : 2 Aug 2018 23:23
 Operator : JU/SJ
 Sample : J4262-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-03

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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	5.184	480	484	491	rBV	136380	191769	4.54%	0.634%
2	5.295	495	503	513	rVV	34785	104686	2.48%	0.346%
3	5.595	551	554	573	rBV	406819	1127015	26.69%	3.725%
4	6.607	722	726	743	rBV	242852	939056	22.24%	3.104%
5	6.731	743	747	772	rVB	1840602	3020623	71.53%	9.985%
6	6.954	782	785	791	rBV	396851	611334	14.48%	2.021%
7	7.107	807	811	827	rBV2	2542586	3589009	85.00%	11.864%
8	7.219	827	830	847	rVB4	81802	251968	5.97%	0.833%
9	7.525	878	882	894	rBV	1215245	2144815	50.79%	7.090%
10	7.978	953	959	963	rBV3	63662	148989	3.53%	0.493%
11	8.013	963	965	973	rVB4	42023	93947	2.22%	0.311%
12	8.136	983	986	993	rVB	46295	65670	1.56%	0.217%
13	8.236	999	1003	1005	rBV	755547	877690	20.79%	2.901%
14	8.254	1005	1006	1014	rVB	672236	785332	18.60%	2.596%
15	8.548	1046	1056	1057	rBV7	37200	89634	2.12%	0.296%
16	8.583	1059	1062	1071	rVB6	35641	85638	2.03%	0.283%
17	8.901	1112	1116	1121	rBV3	57299	117511	2.78%	0.388%
18	8.948	1121	1124	1133	rVV	141795	241214	5.71%	0.797%
19	9.048	1137	1141	1149	rVB	220166	285945	6.77%	0.945%
20	9.307	1180	1185	1200	rBV	3480809	4222601	100.00%	13.958%
21	9.407	1200	1202	1211	rVB2	124471	169872	4.02%	0.562%
22	9.483	1211	1215	1219	rBV4	39180	79610	1.89%	0.263%
23	9.648	1239	1243	1245	rBV	38392	48589	1.15%	0.161%
24	9.701	1249	1252	1260	rVV	109508	151211	3.58%	0.500%
25	9.766	1260	1263	1274	rVB5	34078	72644	1.72%	0.240%
26	9.995	1298	1302	1305	rBV	811814	923039	21.86%	3.051%
27	10.024	1305	1307	1321	rVB	154050	195410	4.63%	0.646%
28	10.124	1321	1324	1332	rBV	27663	59016	1.40%	0.195%
29	10.207	1336	1338	1348	rVB3	25024	52982	1.25%	0.175%
30	10.501	1384	1388	1392	rBV	31421	67797	1.61%	0.224%
31	10.548	1392	1396	1402	rVB	62650	95377	2.26%	0.315%
32	10.713	1420	1424	1432	rBV2	47493	85133	2.02%	0.281%
33	10.789	1433	1437	1449	rBV	1646003	2199630	52.09%	7.271%
34	11.019	1473	1476	1481	rVB	36833	42266	1.00%	0.140%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.171	1497	1502	1505	rBV5	61953	119313	2.83%	0.394%
36	11.489	1552	1556	1568	rBV	699583	1084523	25.68%	3.585%
37	11.748	1597	1600	1609	rBV2	40226	69031	1.63%	0.228%
38	11.995	1639	1642	1646	rBV2	90090	113602	2.69%	0.376%
39	12.036	1647	1649	1656	rVB5	35882	59784	1.42%	0.198%
40	13.071	1821	1825	1845	rBV	2979201	3845733	91.07%	12.713%
41	13.948	1972	1974	1980	rBV4	55668	70087	1.66%	0.232%
42	14.142	2003	2007	2017	rBV	682756	950599	22.51%	3.142%
43	15.671	2263	2267	2280	rVB	373813	701712	16.62%	2.320%

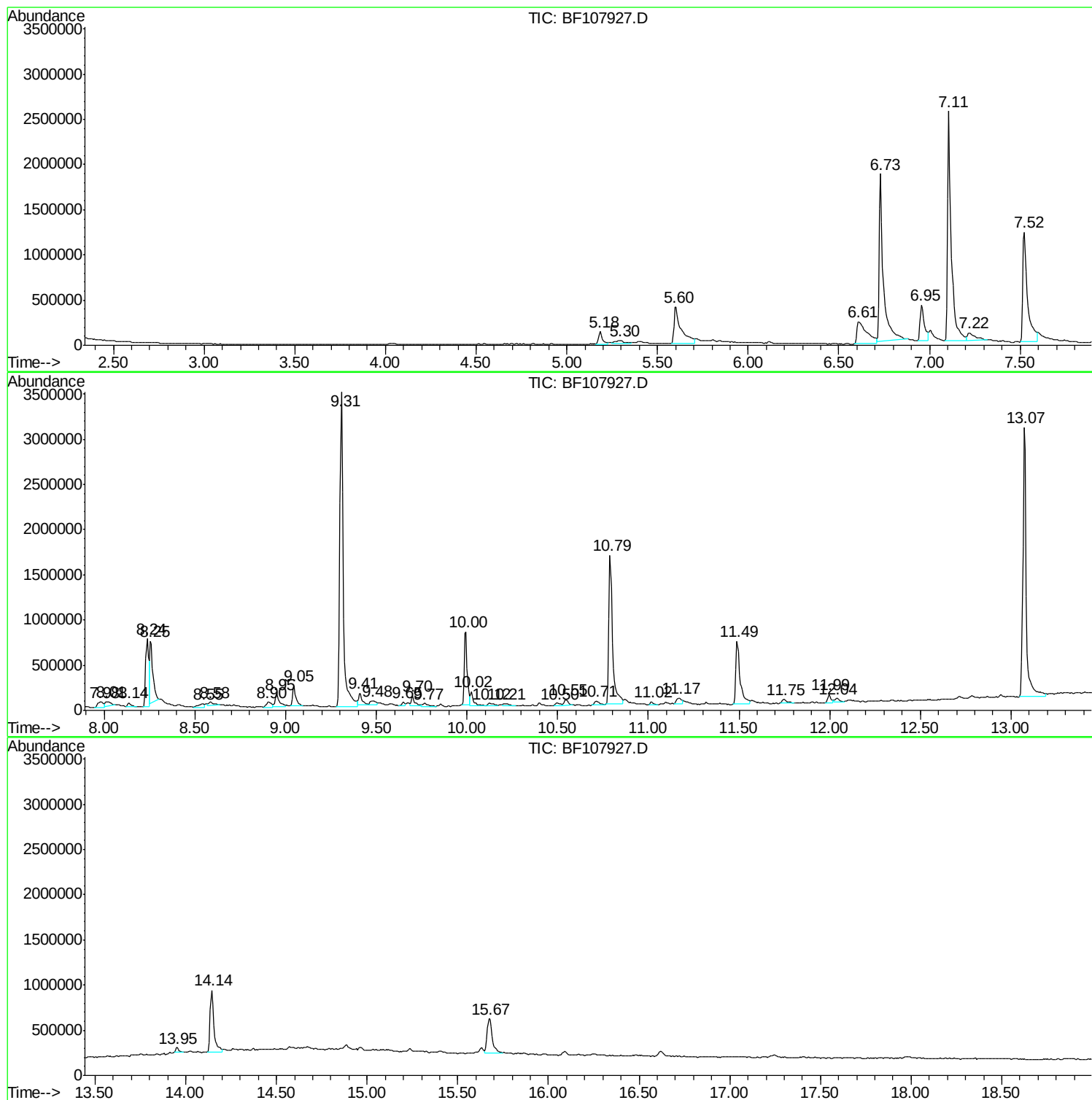
Sum of corrected areas: 30251406

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

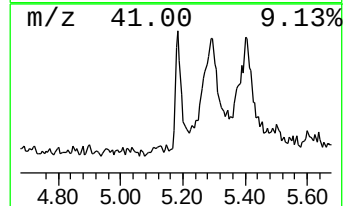
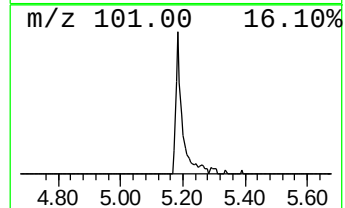
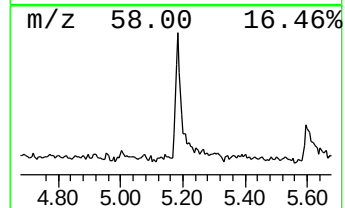
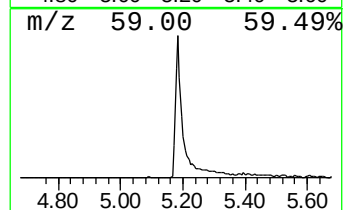
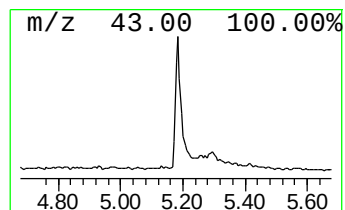
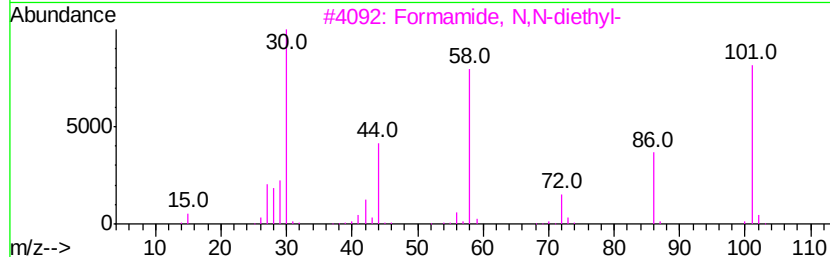
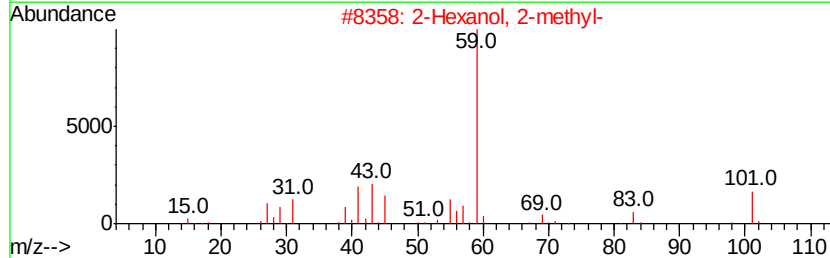
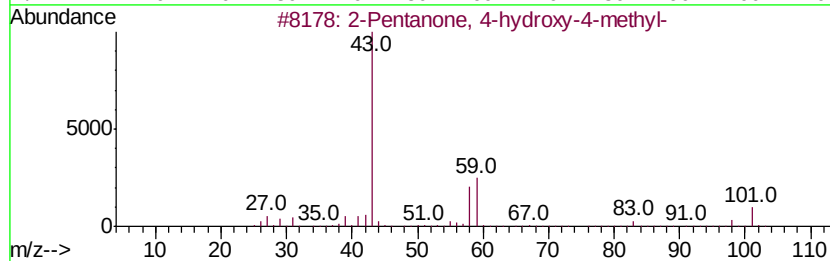
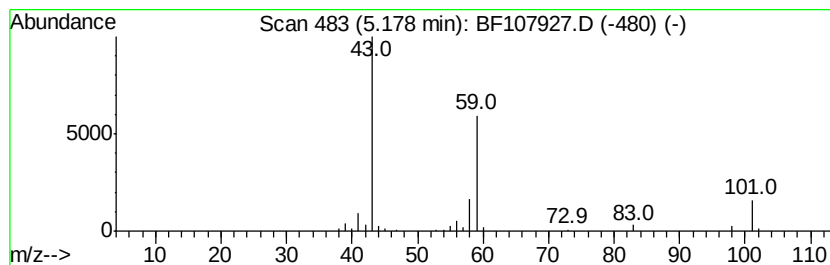
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	6.27 ng	191769	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

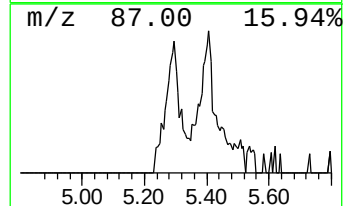
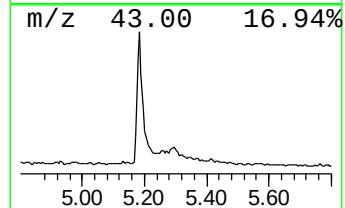
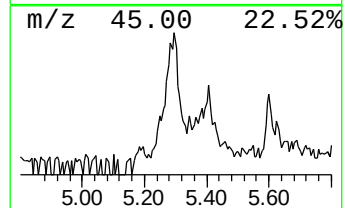
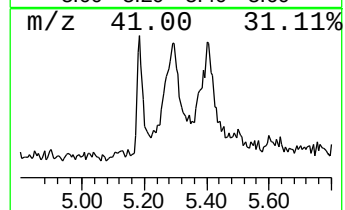
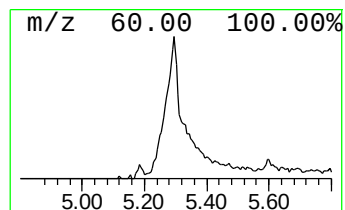
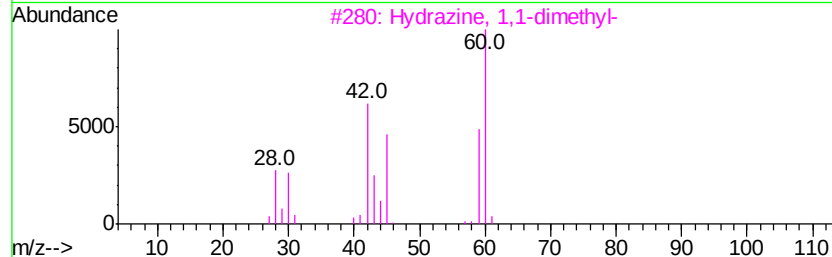
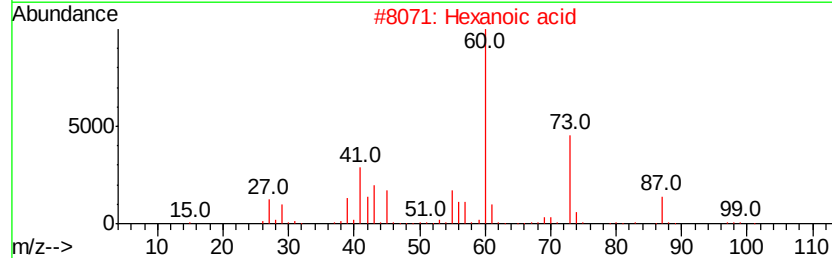
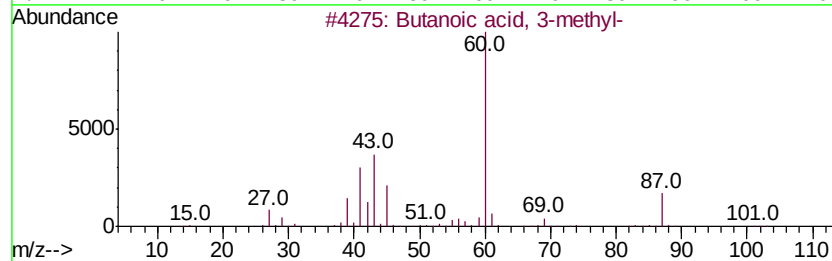
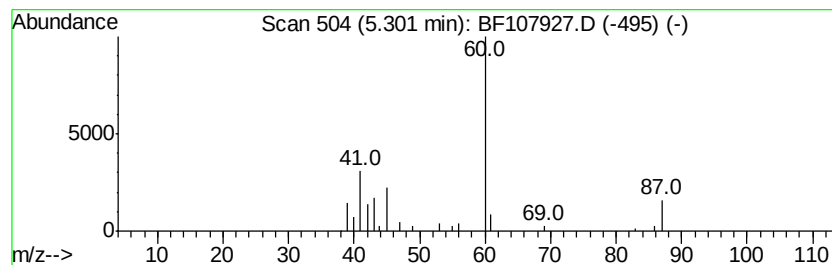
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.30	3.42 ng	104686	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2		Hexanoic acid	116	C6H12O2	000142-62-1	50
3		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4		1-Pentanamine	87	C5H13N	000110-58-7	9
5		Pentanoic acid	102	C5H10O2	000109-52-4	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

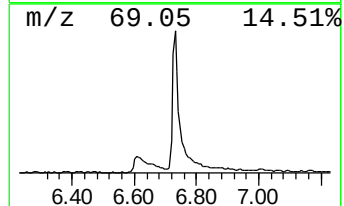
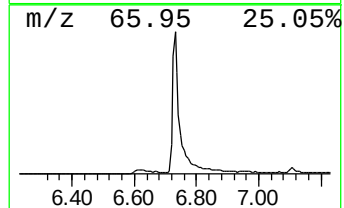
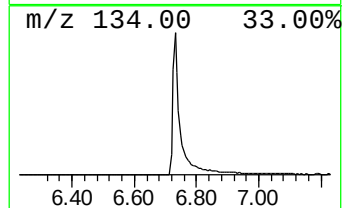
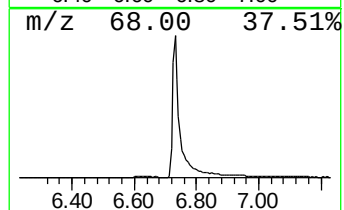
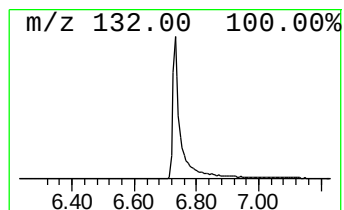
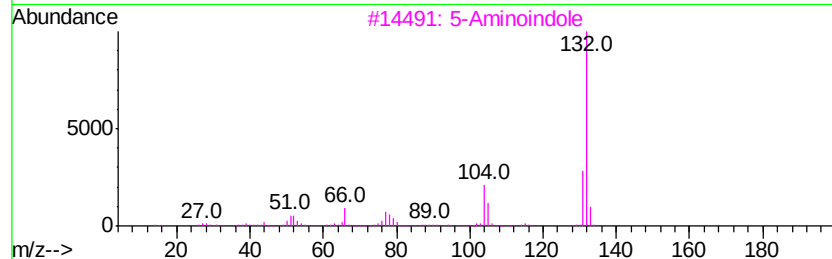
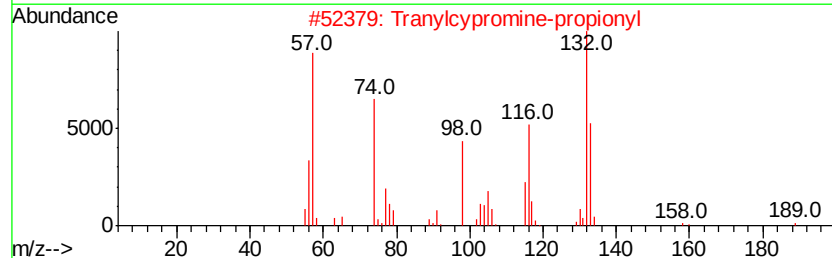
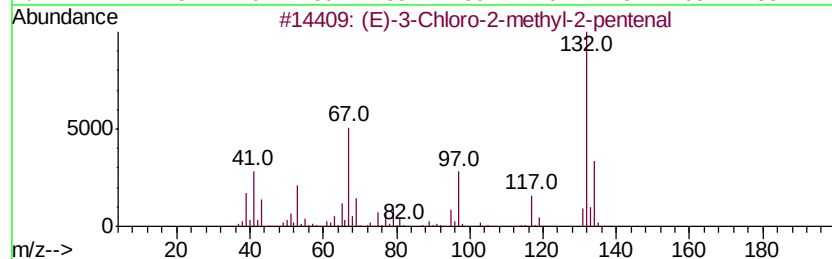
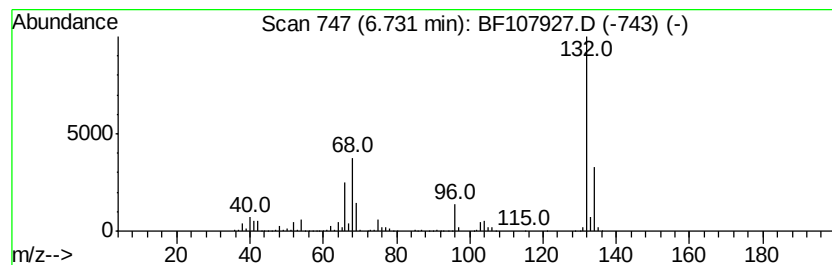
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	98.82 ng	3020620	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

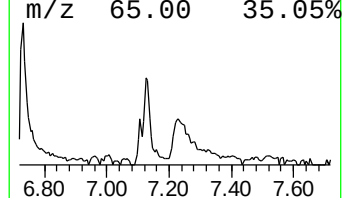
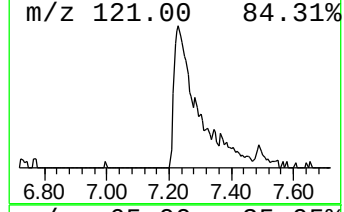
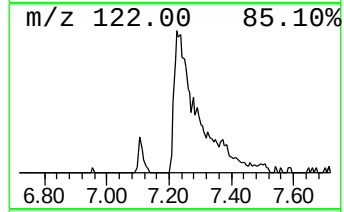
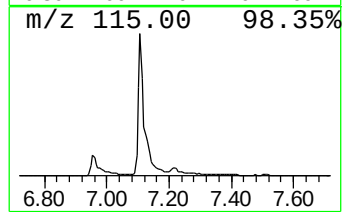
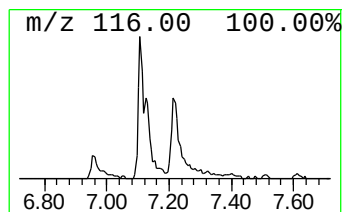
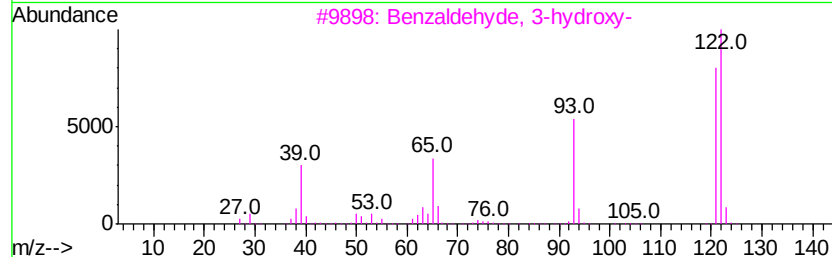
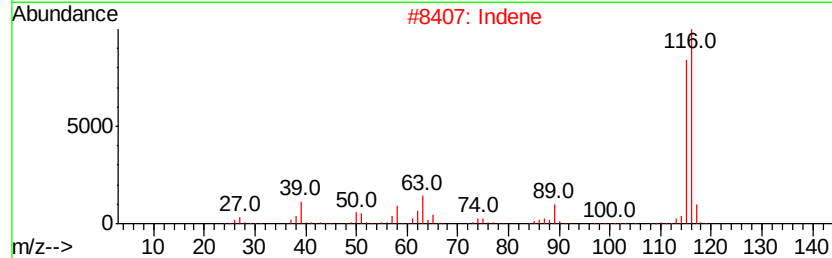
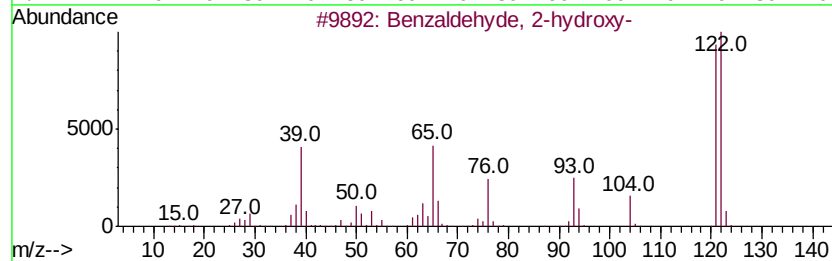
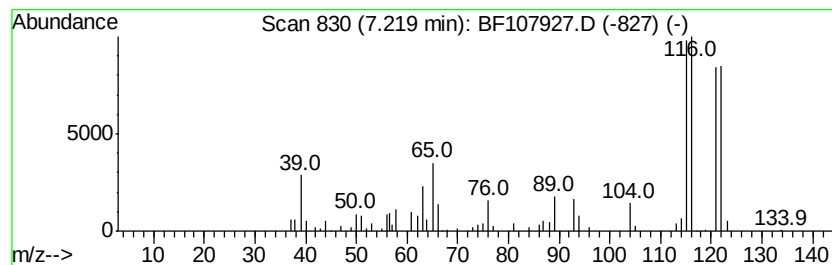
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzaldehyde, 2-hydroxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	8.24 ng	251968	1,4-Dichlorobenzene-d4	6.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzaldehyd, 2-hydroxy-	122	C7H6O2	000090-02-8	95
2		Indene	116	C9H8	000095-13-6	83
3		Benzaldehyd, 3-hydroxy-	122	C7H6O2	000100-83-4	43
4		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	41
5		1,3-Benzodioxole	122	C7H6O2	000274-09-9	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

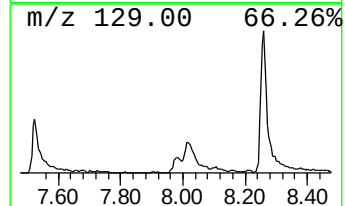
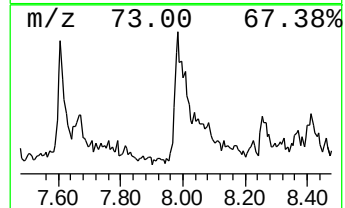
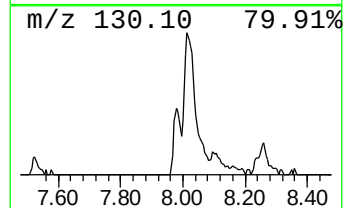
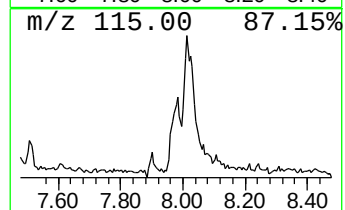
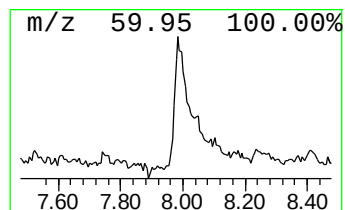
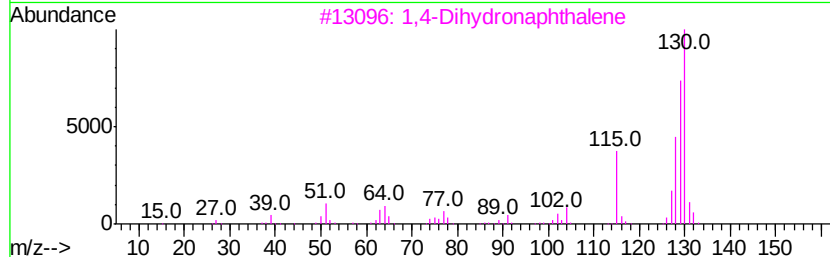
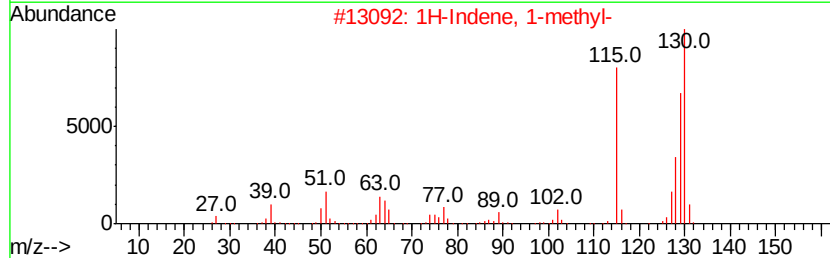
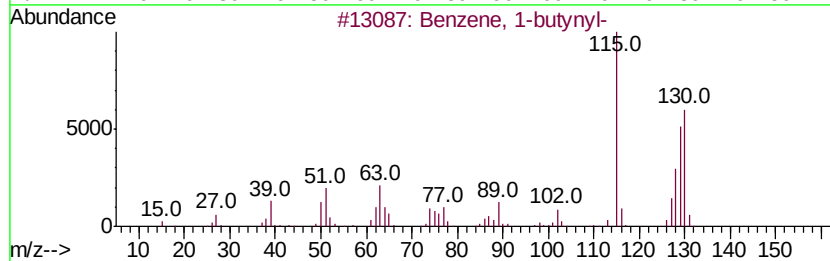
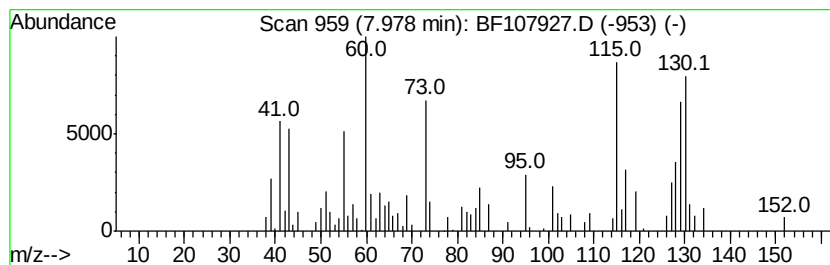
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1-butylnyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.98	3.40 ng	148989	Naphthalene-d8	8.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-butylnyl-	130	C10H10	000622-76-4	50
2		1H-Indene, 1-methyl-	130	C10H10	000767-59-9	50
3		1,4-Dihydronaphthalene	130	C10H10	000612-17-9	46
4		Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	45
5		Tetracyclo[5.3.0.0<2,6>.0<3,10>]...	130	C10H10	034324-40-8	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

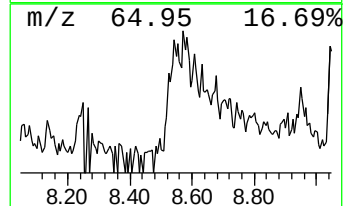
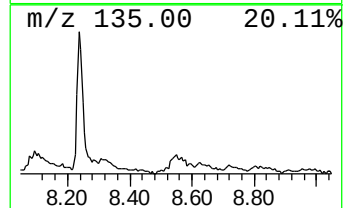
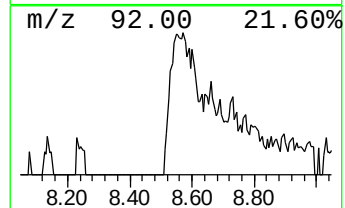
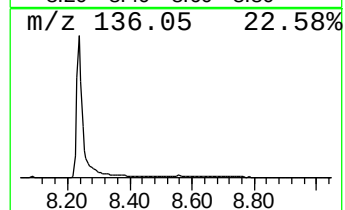
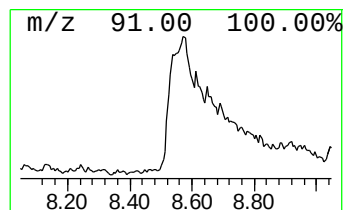
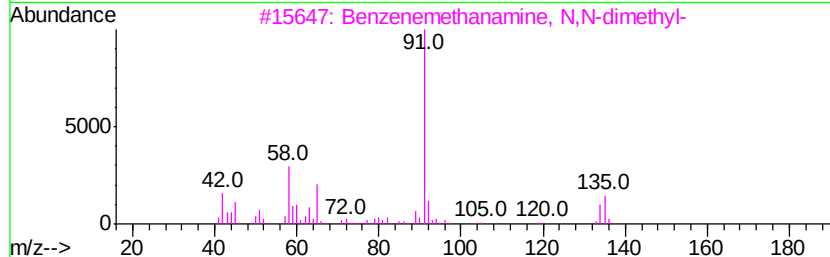
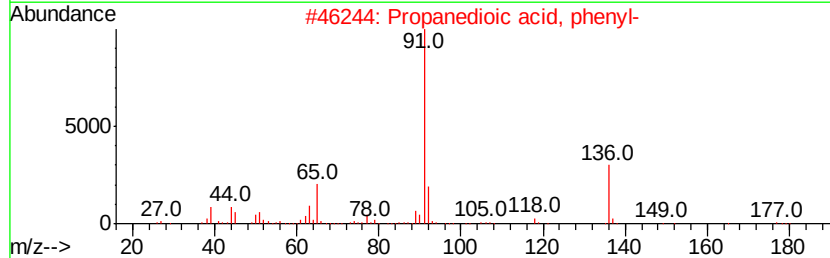
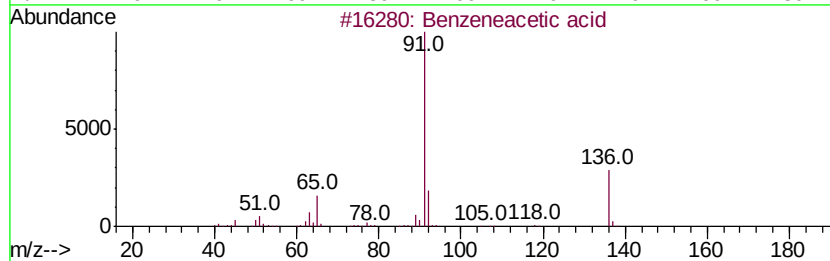
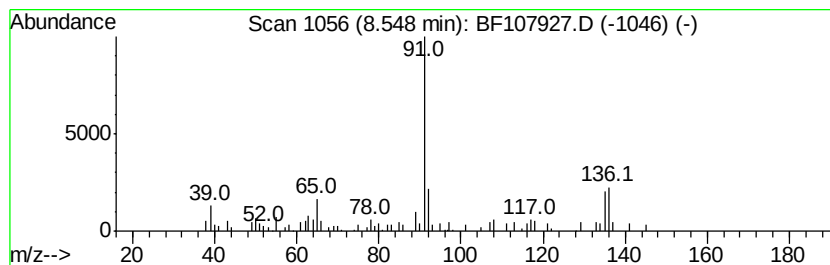
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzeneacetic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.55	2.04 ng	89634	Napthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneacetic acid	136	C8H8O2	000103-82-2	53
2		Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	47
3		Benzenemethanamine, N,N-dimethyl-	135	C9H13N	000103-83-3	43
4		Benzeneacetic acid, heptyl ester	234	C15H22O2	039736-25-9	38
5		2-(1-Adamantyl)-N-benzylglycine	299	C19H25NO2	201992-58-7	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

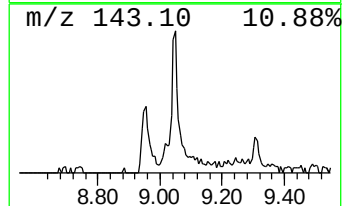
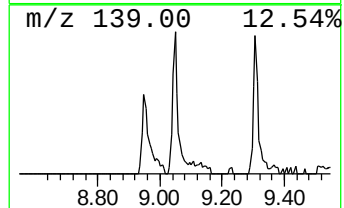
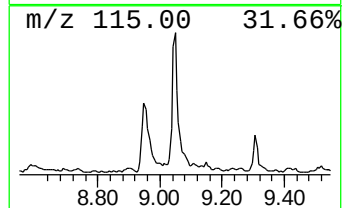
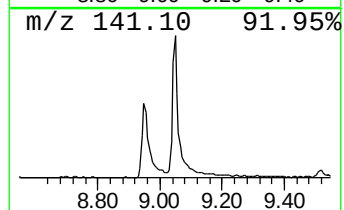
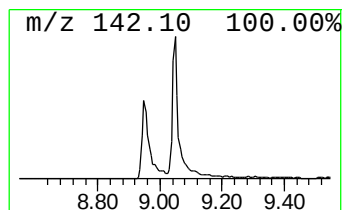
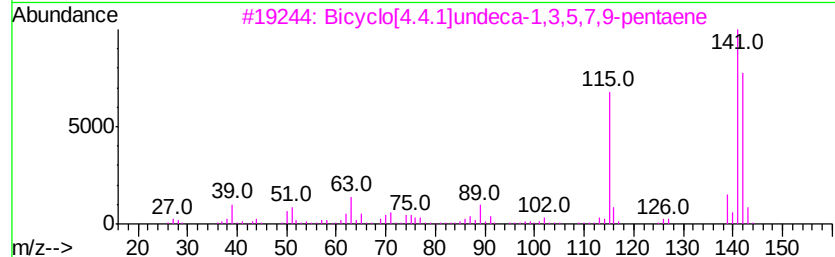
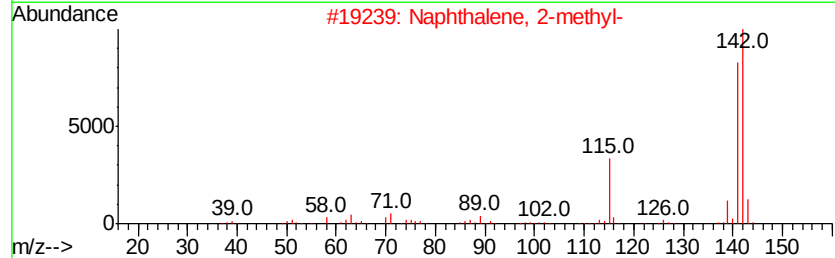
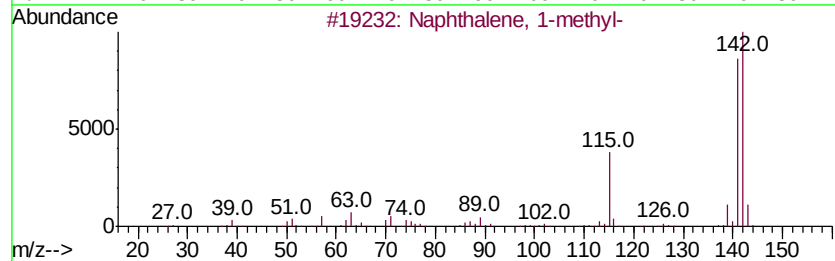
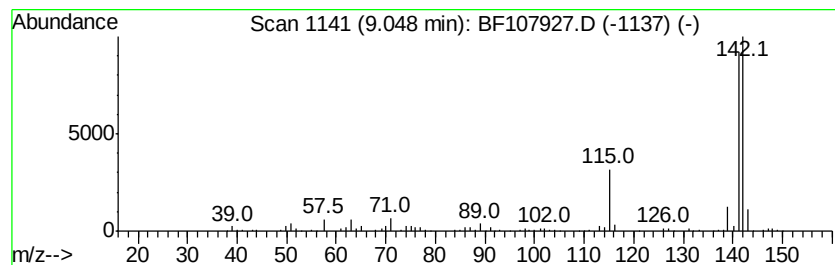
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	6.52 ng	285945	Naphthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
5		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

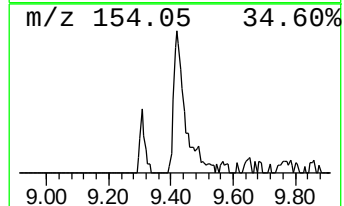
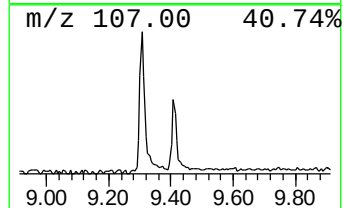
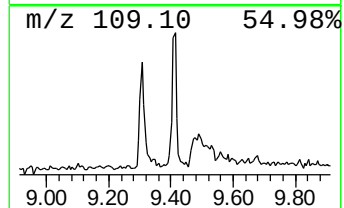
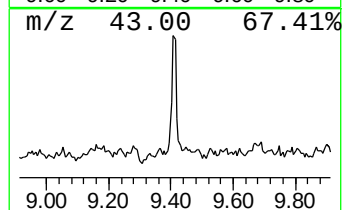
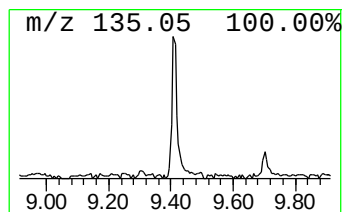
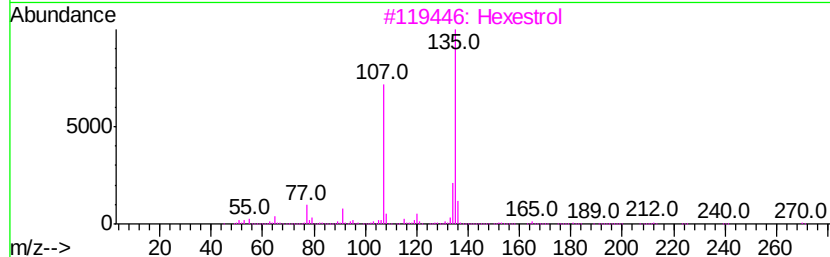
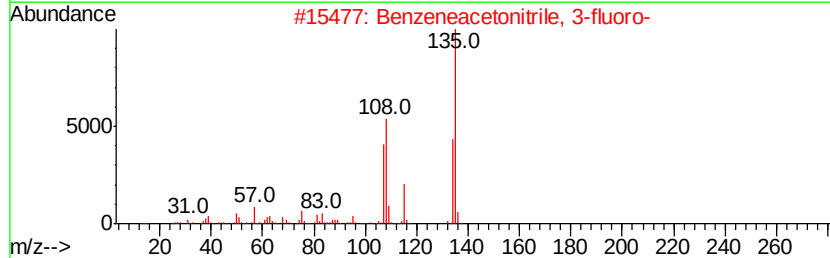
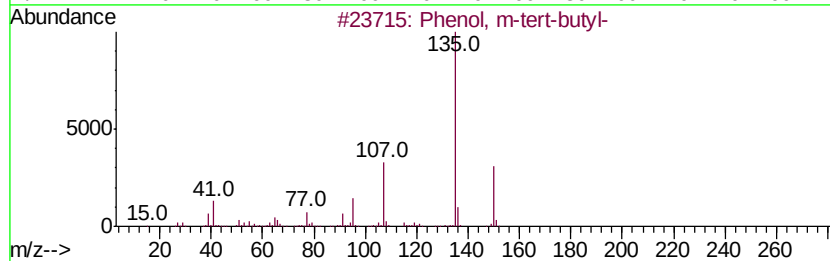
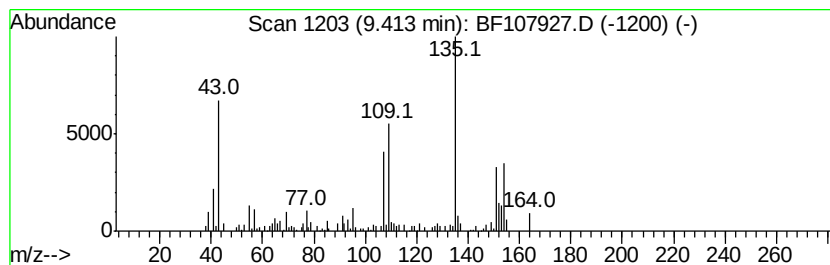
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.41 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	3.68 ng	169872	Acenaphthene-d10	9.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	47
2			Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	47
3			Hexestrol	270	C18H22O2	000084-16-2	43
4			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	38
5			4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

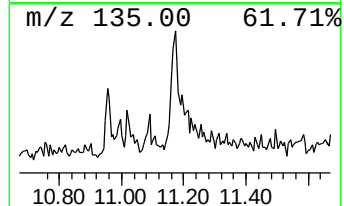
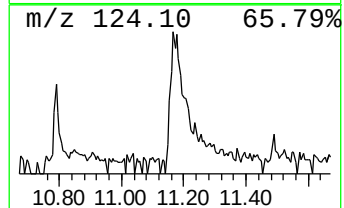
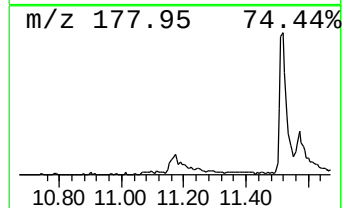
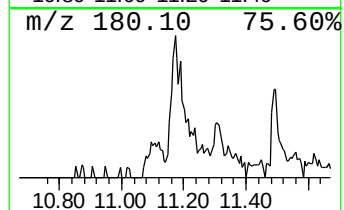
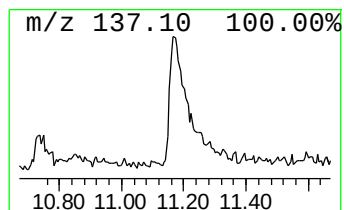
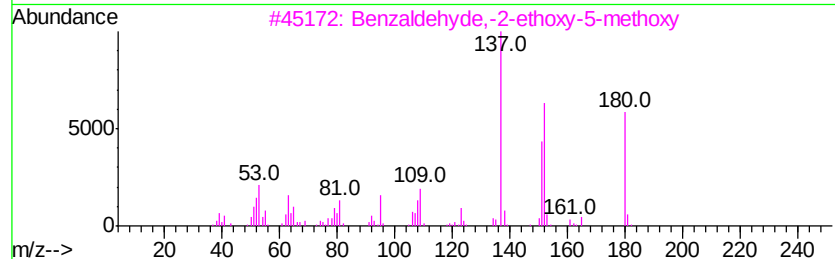
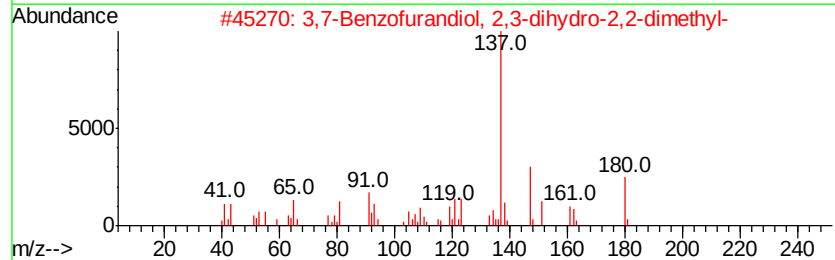
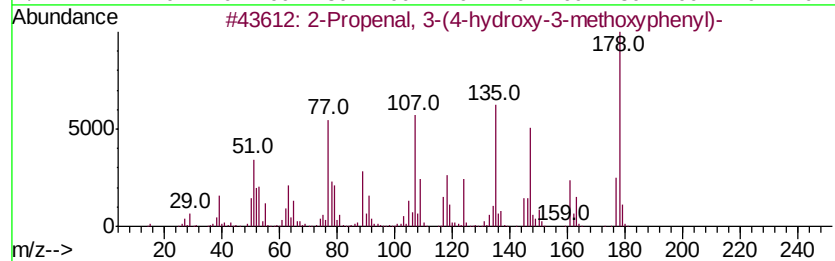
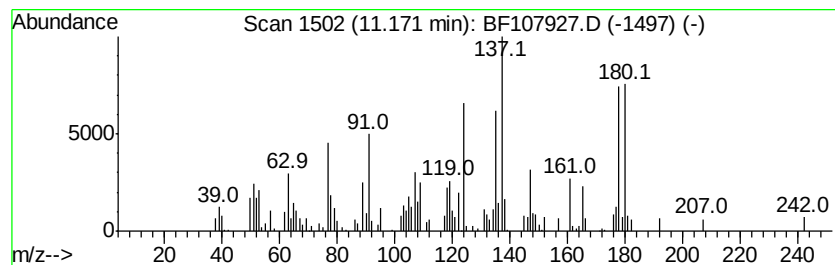
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown11.17 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	2.20 ng	119313	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenal, 3-(4-hydroxy-3-methoxyphenyl)-	178	C10H10O3	000458-36-6	30
2		3,7-Benzofurandiyl, 2,3-dihydro-2,2-dimethyl-	180	C10H12O3	017781-15-6	30
3		Benzaldehyde, -2-ethoxy-5-methoxy	180	C10H12O3	039206-04-7	25
4		6-Methoxycoumaran-7-yl-3-one	180	C9H8O4	204648-65-7	20
5		2,3,5,6-Tetrafluoroanisole	180	C7H4F4O	002324-98-3	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

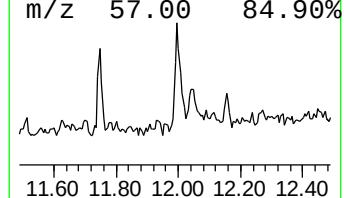
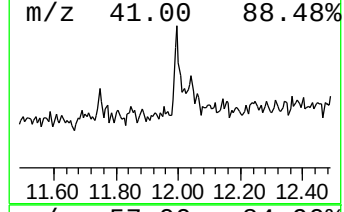
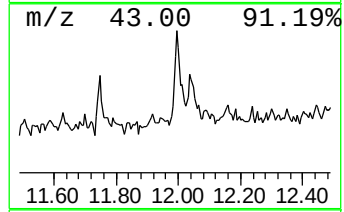
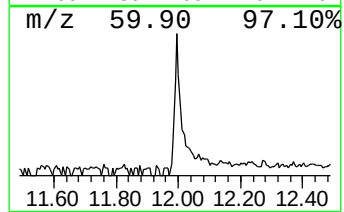
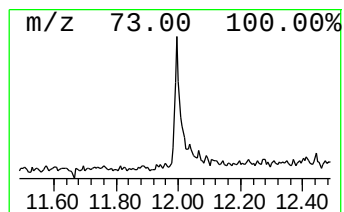
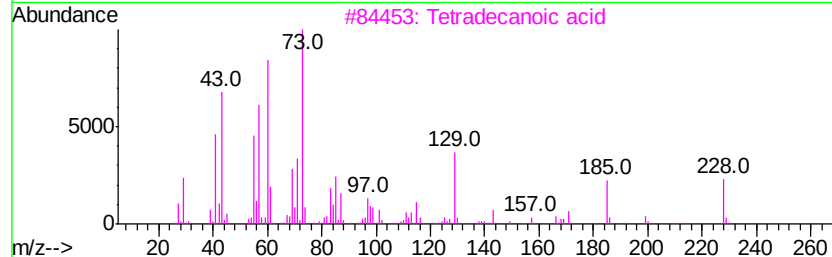
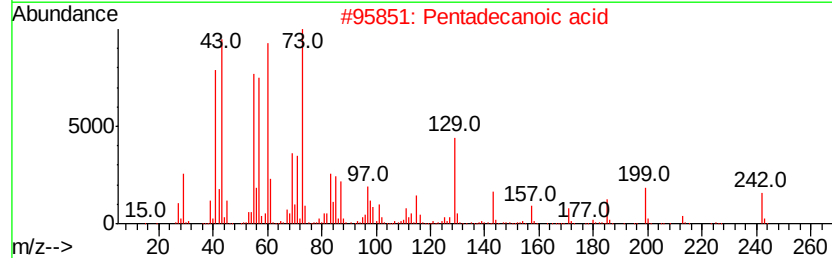
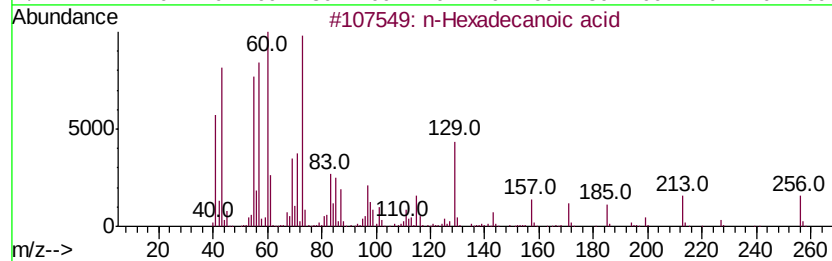
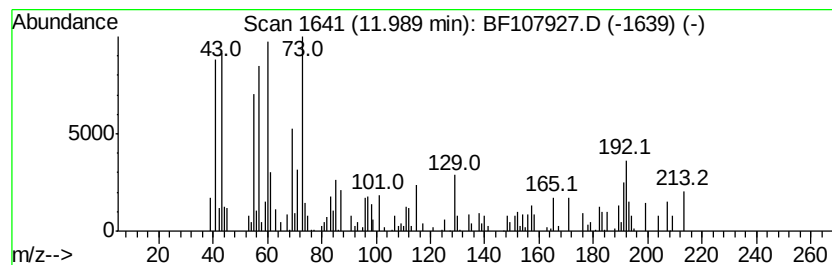
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.09 ng	113602	Phenanthrene-d10	11.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080218\
Data File : BF107927.D
Acq On : 2 Aug 2018 23:23
Operator : JU/SJ
Sample : J4262-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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...	5.18	6.3	ng	191769	1	6.95	611334	20.0
Butanoic acid, 3-...	5.30	3.4	ng	104686	1	6.95	611334	20.0
unknown6.73	6.73	98.8	ng	3020620	1	6.95	611334	20.0
Benzaldehyde, 2-h...	7.22	8.2	ng	251968	1	6.95	611334	20.0
Benzene, 1-butynyl-	7.98	3.4	ng	148989	2	8.24	877690	20.0
Benzeneacetic acid	8.55	2.0	ng	89634	2	8.24	877690	20.0
Naphthalene, 1-me...	9.05	6.5	ng	285945	2	8.24	877690	20.0
unknown9.41	9.41	3.7	ng	169872	3	9.99	923039	20.0
unknown11.17	11.17	2.2	ng	119313	4	11.49	1084520	20.0
n-Hexadecanoic acid	11.99	2.1	ng	113602	4	11.49	1084520	20.0