

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
 Data File : BM016286.D
 Acq On : 09 Aug 2018 17:54
 Operator : SJ/JU
 Sample : J4369-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-35

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_M\METHODS\8270-BM072318.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	3.787	80	85	93	rVB2	17828	28634	1.07%	0.205%
2	5.187	316	323	334	rBV	42232	66120	2.46%	0.474%
3	5.669	399	405	421	rVB	347769	555104	20.66%	3.976%
4	7.310	679	684	698	rBV	183746	332683	12.38%	2.383%
5	7.663	738	744	755	rBV	743888	1213155	45.14%	8.690%
6	8.134	818	824	831	rBV	163599	271601	10.11%	1.946%
7	8.451	871	878	891	rVB	741810	1203015	44.76%	8.618%
8	8.904	944	955	959	rBV2	52010	111630	4.15%	0.800%
9	9.322	1019	1026	1032	rBV	526898	901715	33.55%	6.459%
10	9.569	1054	1068	1074	rBV2	51823	145475	5.41%	1.042%
11	9.710	1084	1092	1098	rBV2	39222	67020	2.49%	0.480%
12	9.781	1098	1104	1109	rVB3	20003	32314	1.20%	0.231%
13	10.945	1294	1302	1311	rBV	176747	302771	11.27%	2.169%
14	13.227	1683	1690	1704	rBV7	11019	32429	1.21%	0.232%
15	13.386	1708	1717	1726	rVV	1256294	1787966	66.53%	12.808%
16	14.222	1854	1859	1864	rVB	62483	88702	3.30%	0.635%
17	14.580	1910	1920	1923	rBV4	14225	28757	1.07%	0.206%
18	14.769	1944	1952	1959	rVB2	242149	375765	13.98%	2.692%
19	16.257	2199	2205	2217	rBV	1112672	1538069	57.23%	11.018%
20	16.492	2241	2245	2251	rBV7	21298	37470	1.39%	0.268%
21	17.310	2379	2384	2388	rVB	20531	34558	1.29%	0.248%
22	17.504	2412	2417	2424	rBV	302820	441023	16.41%	3.159%
23	18.357	2557	2562	2570	rBV2	163133	250231	9.31%	1.792%
24	19.615	2772	2776	2782	rBV	84012	131393	4.89%	0.941%
25	20.080	2850	2855	2861	rBV	2239752	2687475	100.00%	19.251%
26	21.298	3059	3062	3072	rBV2	150743	219772	8.18%	1.574%
27	21.633	3115	3119	3125	rVB	438259	525889	19.57%	3.767%
28	23.974	3512	3517	3524	rVB2	288221	549208	20.44%	3.934%

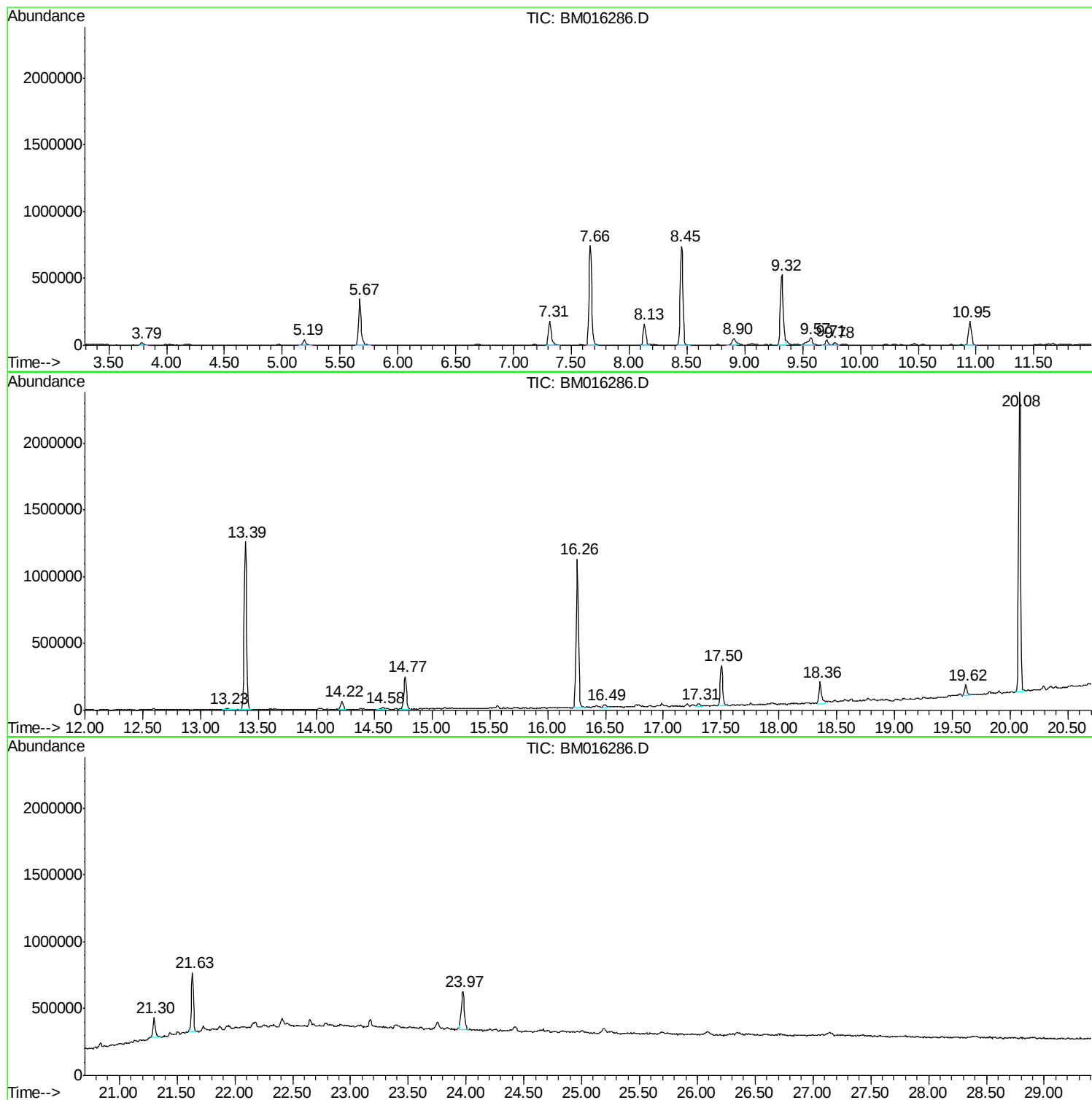
Sum of corrected areas: 13959944

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

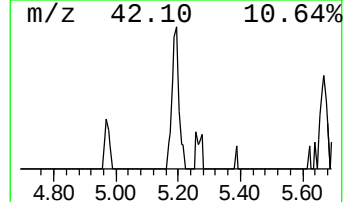
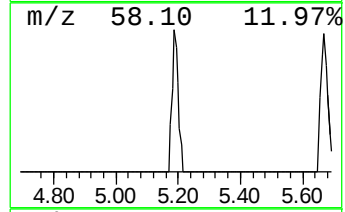
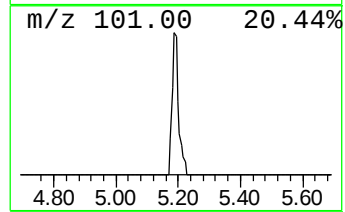
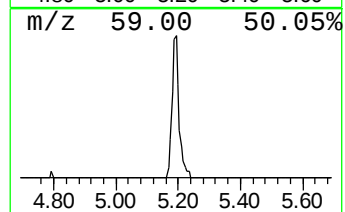
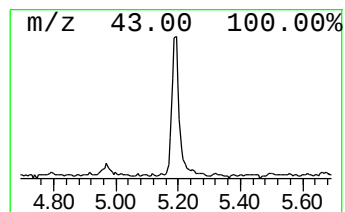
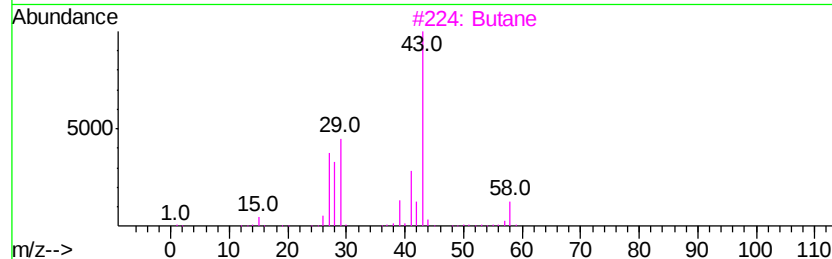
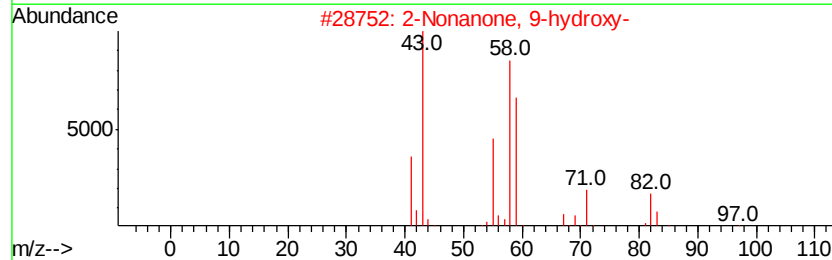
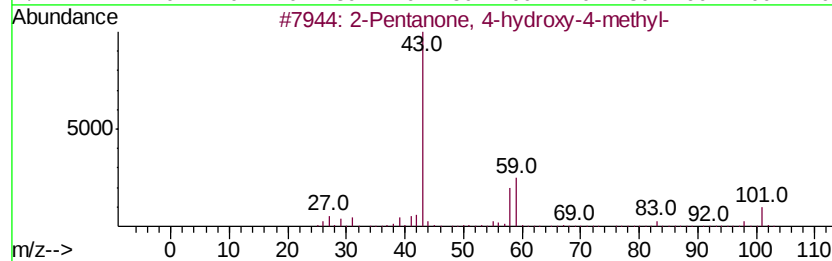
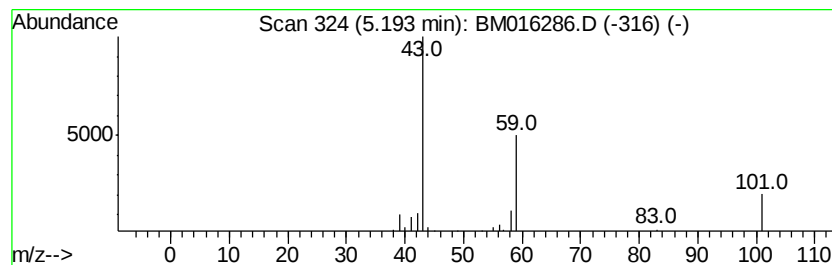
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.87 ng	66120	1,4-Dichlorobenzene-d4	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
3		Butane	58	C4H10	000106-97-8	16
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		Propylamine	59	C3H9N	000107-10-8	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

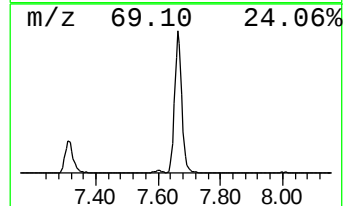
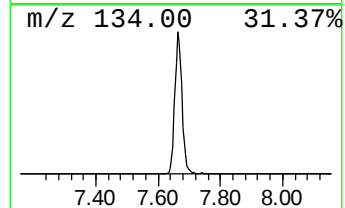
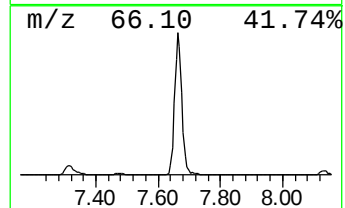
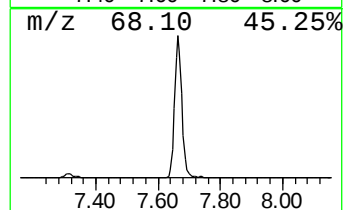
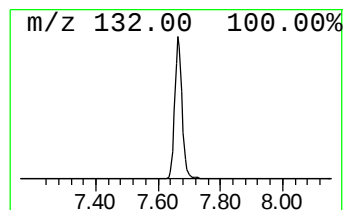
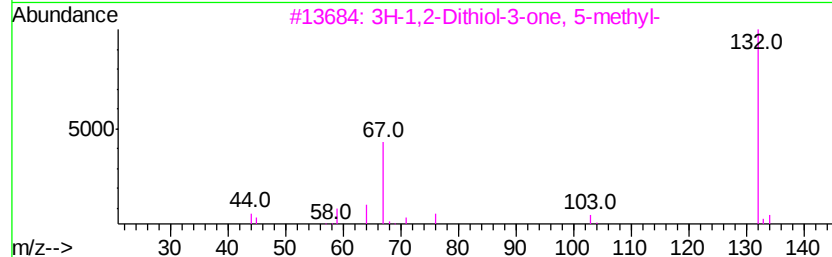
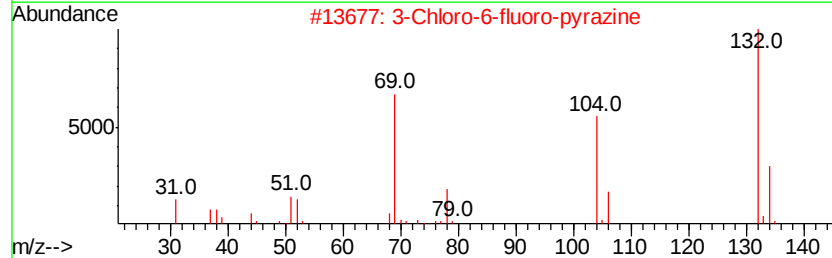
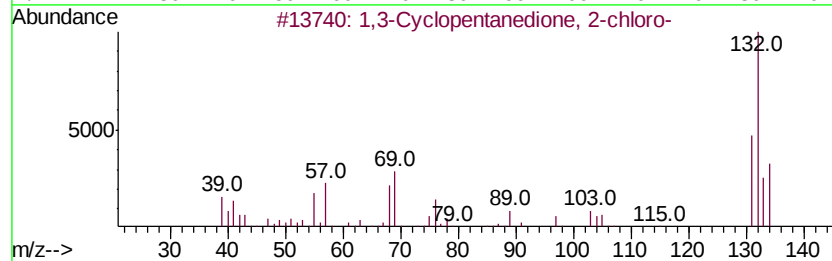
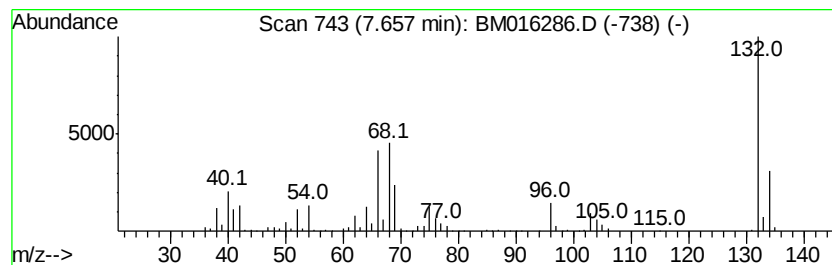
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	89.33 ng	1213160	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

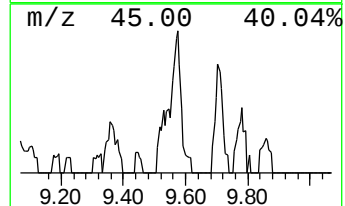
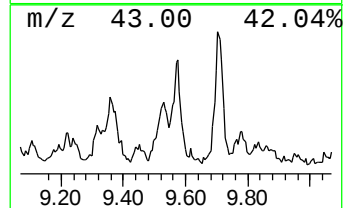
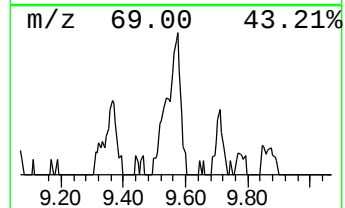
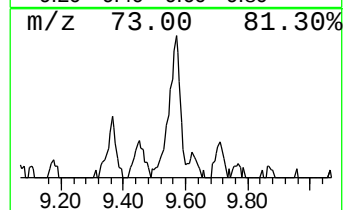
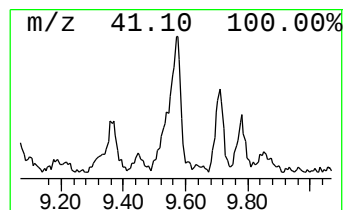
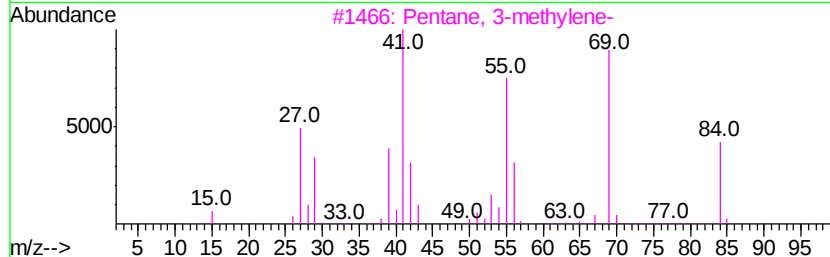
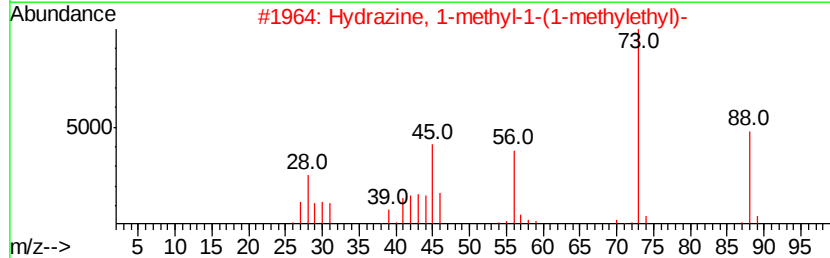
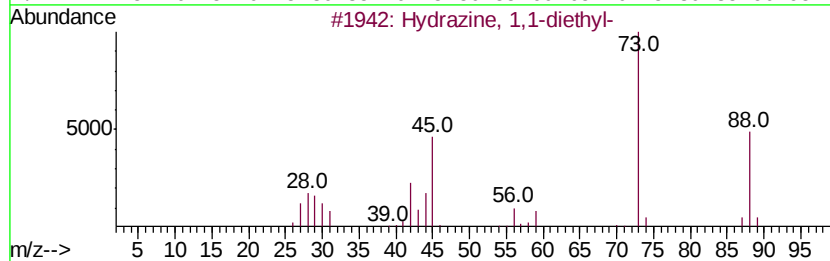
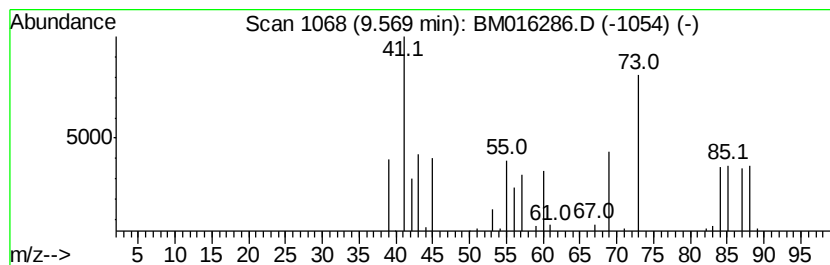
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.57 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	9.61 ng	145475	Naphthalene-d8	10.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrazine, 1,1-diethyl-	88	C4H12N2	000616-40-0	27
2		Hydrazine, 1-methyl-1-(1-methyle...	88	C4H12N2	033668-54-1	25
3		Pentane, 3-methylene-	84	C6H12	000760-21-4	16
4		Furan, 2,5-dihydro-3-methyl-	84	C5H8O	001708-31-2	12
5		Dicyclopropyl carbinol	112	C7H12O	014300-33-5	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

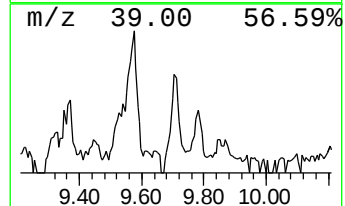
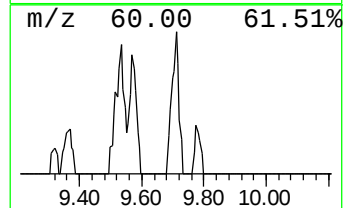
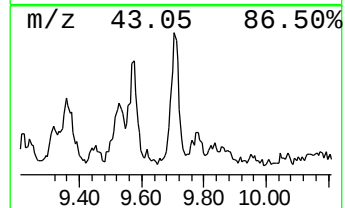
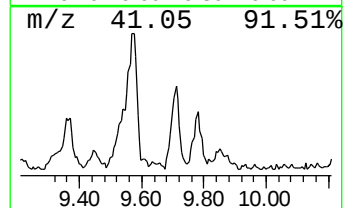
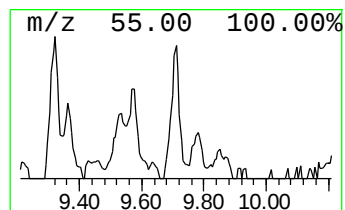
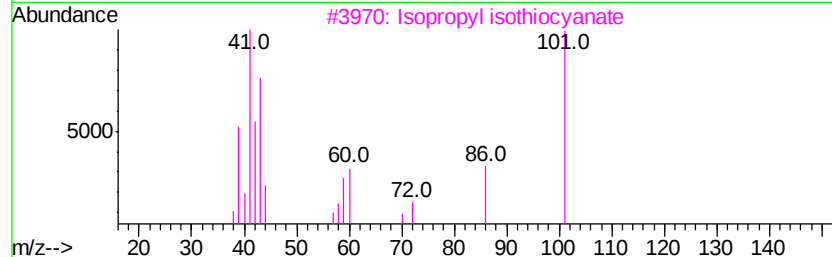
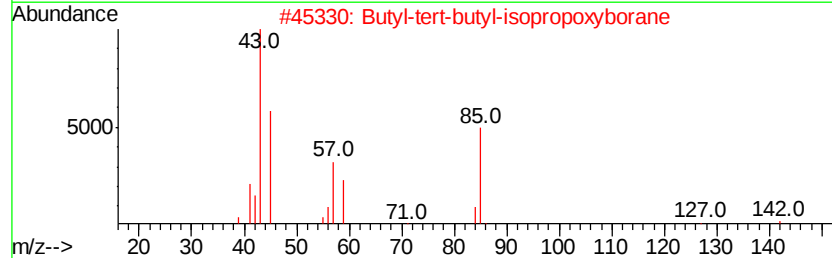
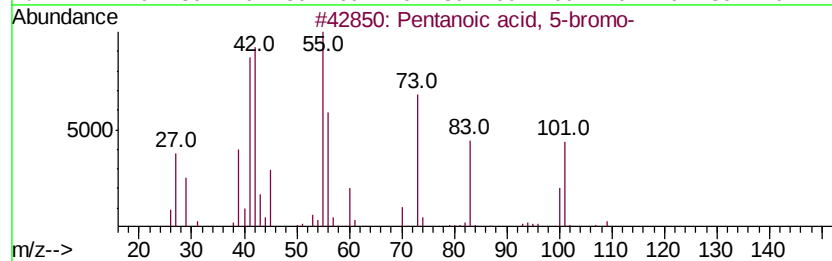
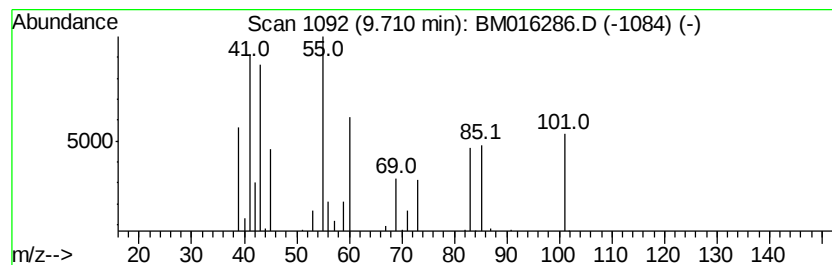
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.71 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.71	4.43 ng	67020	Napthalene-d8	10.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 5-bromo-	180	C5H9BrO2	002067-33-6	17
2		Butyl-tert-butyl-isopropoxyborane	184	C11H25BO	097782-82-6	16
3		Isopropyl isothiocyante	101	C4H7NS	002253-73-8	14
4		Cyclobutanecarboxylic acid, cyclobutyl-	168	C10H16O2	1000282-60-6	12
5		Butanedioic acid, monopropargyl ...	156	C7H8O4	189459-95-8	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

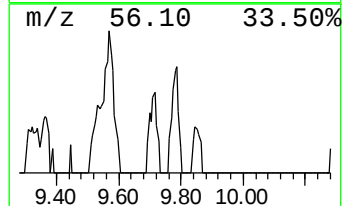
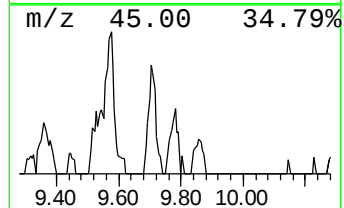
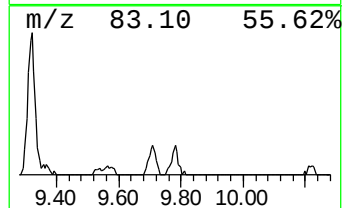
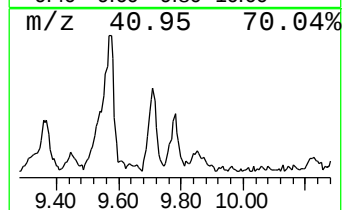
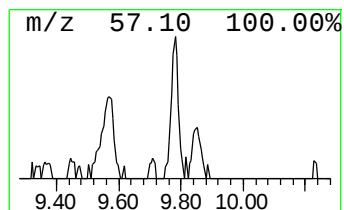
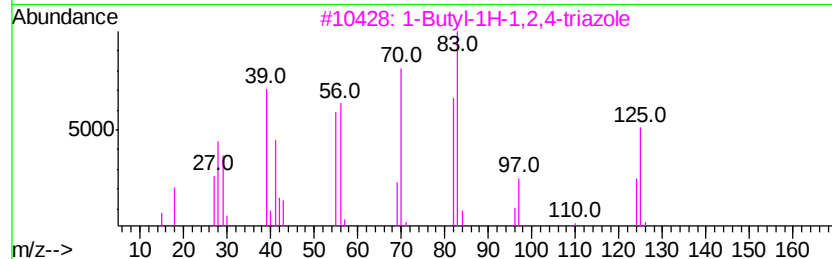
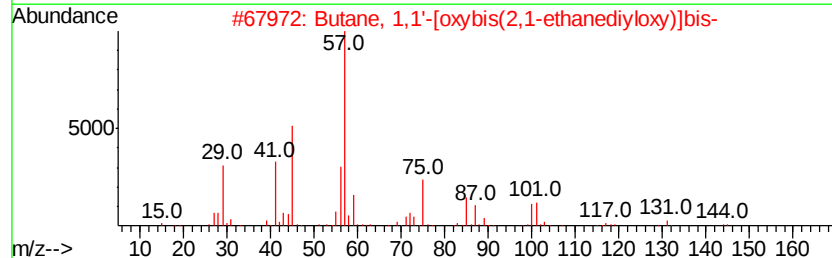
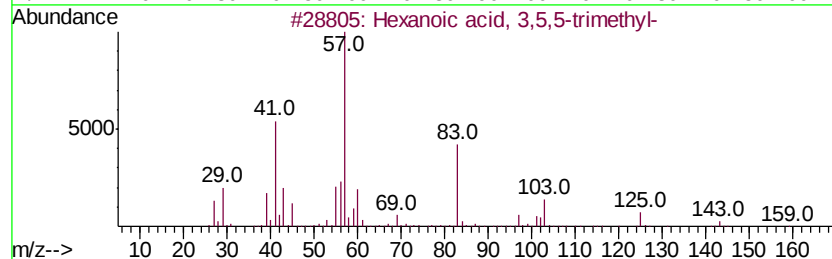
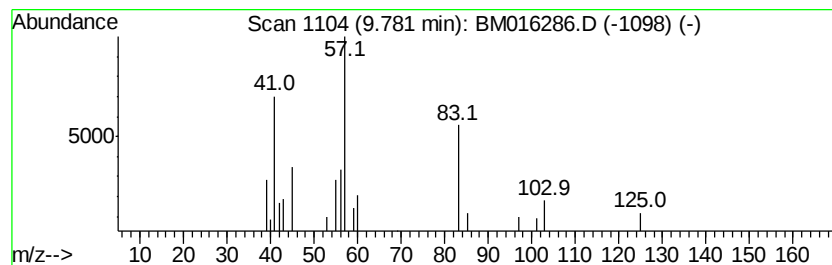
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanoic acid, 3,5,5-trimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.78	2.13 ng	32314	Naphthalene-d8	10.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	78
2		Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	12
3		1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	12
4		Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	10
5		2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

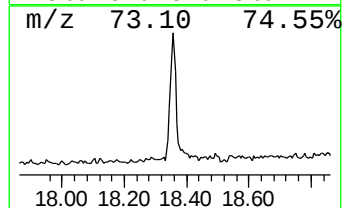
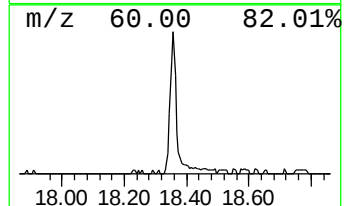
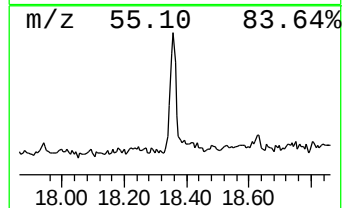
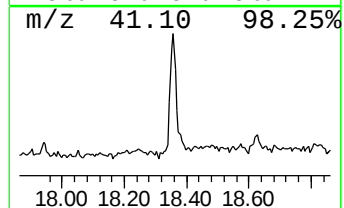
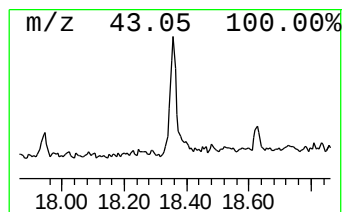
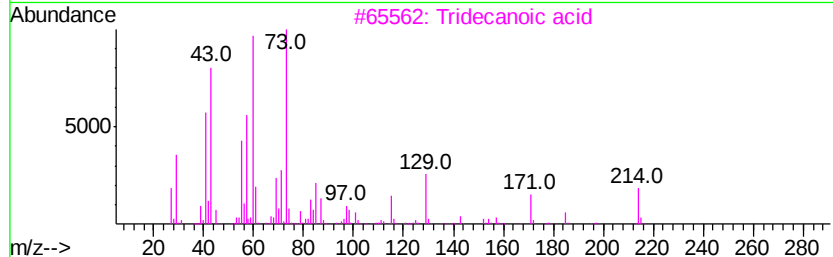
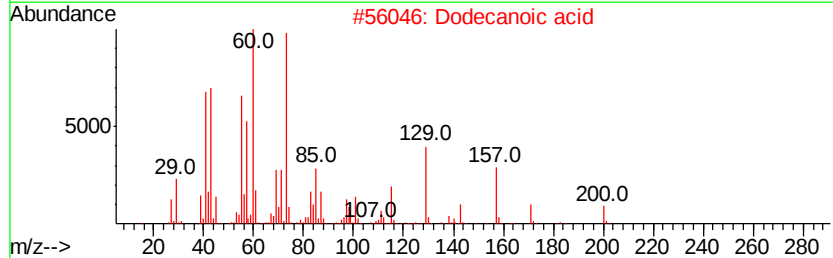
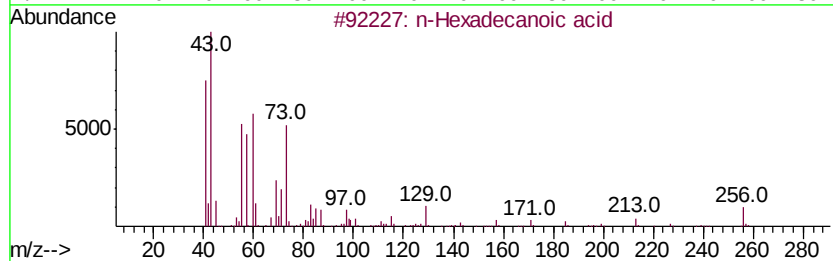
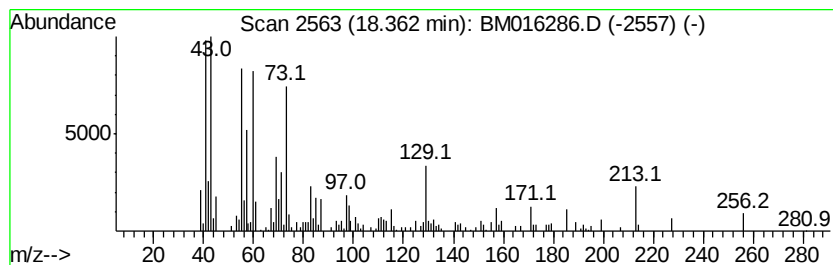
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	11.35 ng	250231	Phenanthrene-d10	17.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Dodecanoic acid	200	C12H24O2	000143-07-7	70
3		Tridecanoic acid	214	C13H26O2	000638-53-9	68
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

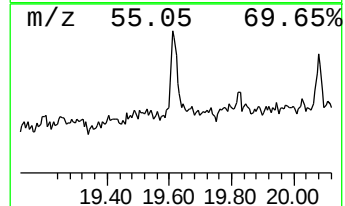
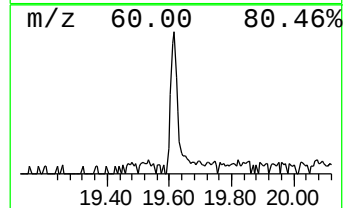
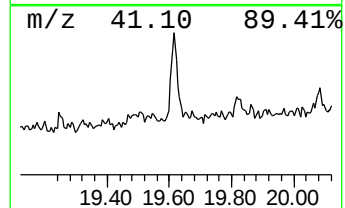
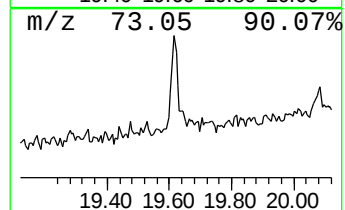
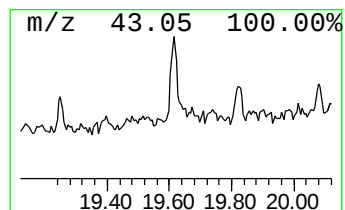
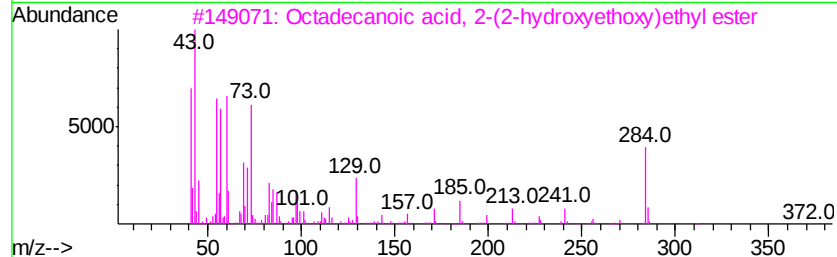
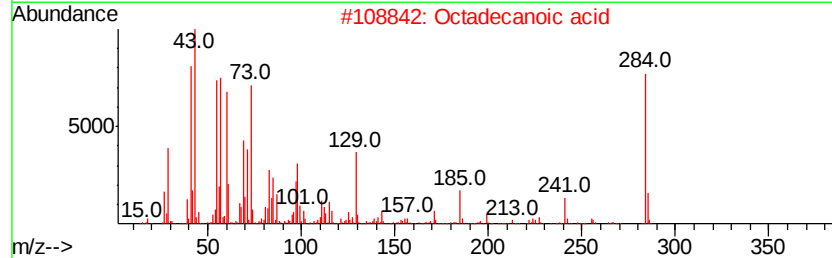
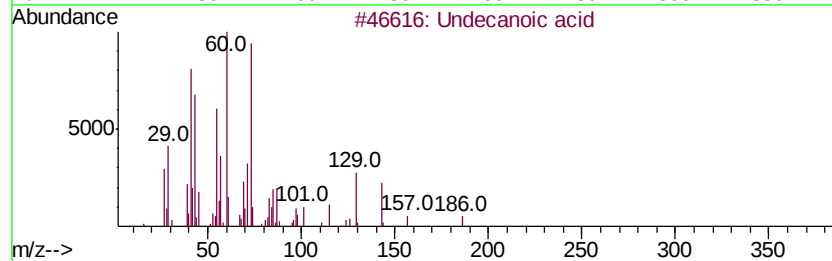
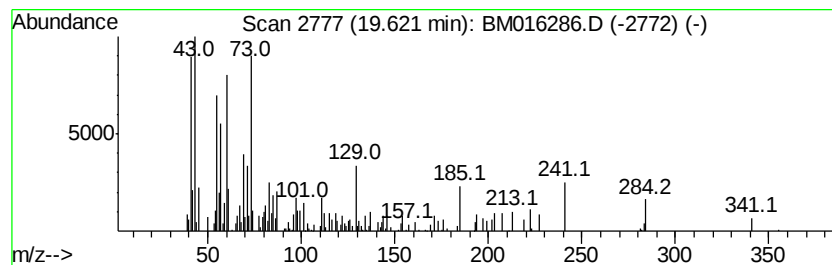
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	5.00 ng	131393	Chrysene-d12	21.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	78
2	Octadecanoic acid		284	C18H36O2	000057-11-4	76
3	Octadecanoic acid, 2-(2-hydroxyve...		372	C22H44O4	000106-11-6	59
4	Dodecanoic acid		200	C12H24O2	000143-07-7	53
5	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

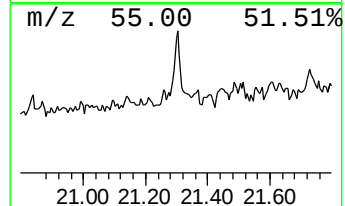
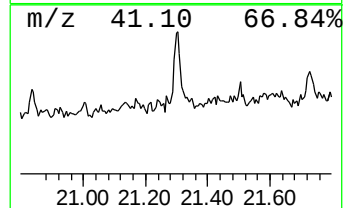
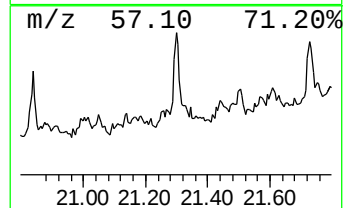
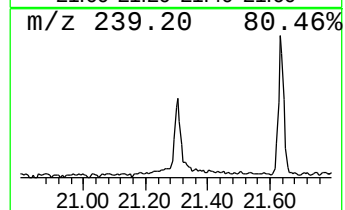
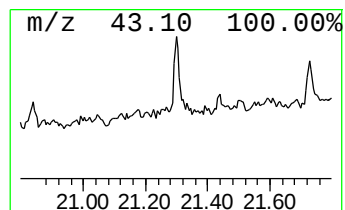
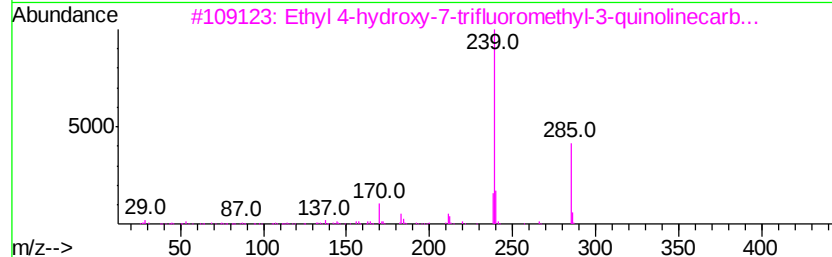
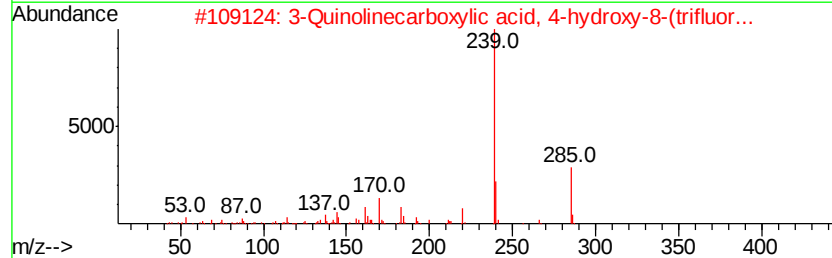
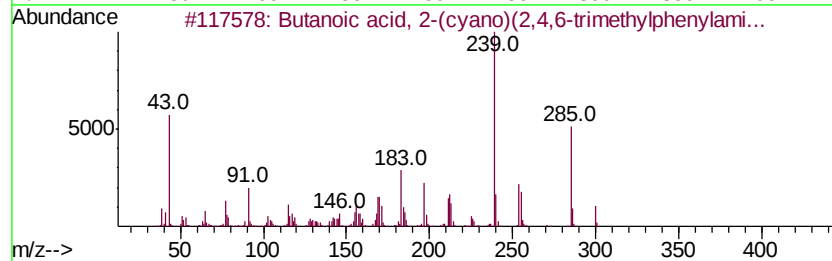
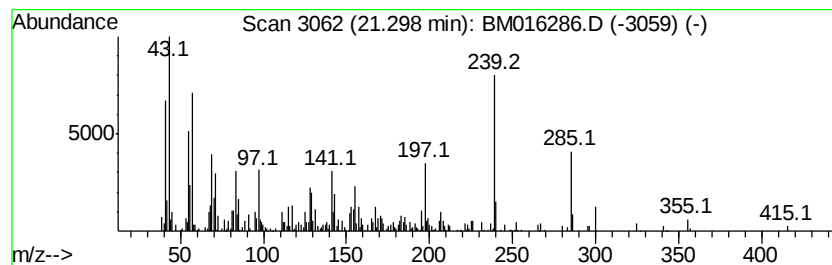
Instrument :
BNA_M
ClientSampleId :
MW-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Butanoic acid, 2-(cyano)(2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.30	8.36 ng	219772	Chrysene-d12	21.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	55
2		3-Quinolinecarboxylic acid, 4-hy...	285	C13H10F3N03	023851-84-5	50
3		Ethyl 4-hydroxy-7-trifluoromethy...	285	C13H10F3N03	000391-02-6	38
4		2-Methyl-1-pyridin-3-yl-3-(2,2,2...	356	C16H15Cl3N2O	1000277-72-3	32
5		Pyrimidine, 2-amino-4-phenyl-6-(...	239	C11H8F3N3	026974-09-4	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080918\
Data File : BM016286.D
Acq On : 09 Aug 2018 17:54
Operator : SJ/JU
Sample : J4369-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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...	5.19	4.9	ng	66120	1	8.13	271601	20.0
unknown7.66	7.66	89.3	ng	1213160	1	8.13	271601	20.0
unknown9.57	9.57	9.6	ng	145475	2	10.95	302771	20.0
unknown9.71	9.71	4.4	ng	67020	2	10.95	302771	20.0
Hexanoic acid, 3,...	9.78	2.1	ng	32314	2	10.95	302771	20.0
n-Hexadecanoic acid	18.36	11.4	ng	250231	4	17.50	441023	20.0
Undecanoic acid	19.62	5.0	ng	131393	5	21.63	525889	20.0
Butanoic acid, 2-...	21.30	8.4	ng	219772	5	21.63	525889	20.0