

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
 Data File : BM016354.D
 Acq On : 14 Aug 2018 14:48
 Operator : SJ/JU
 Sample : J4442-31
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1-4

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_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	5.169	315	320	332	rBV	116167	173609	9.74%	1.320%
2	5.646	395	401	414	rBV	777250	1188227	66.65%	9.035%
3	7.287	674	680	695	rBV	793894	1268922	71.18%	9.649%
4	7.645	735	741	757	rBB	896212	1389662	77.95%	10.567%
5	8.116	815	821	830	rBV	179041	285116	15.99%	2.168%
6	8.434	869	875	888	rBB	609457	992008	55.64%	7.543%
7	9.304	1016	1023	1038	rBV	463790	774270	43.43%	5.888%
8	10.928	1293	1299	1313	rBB	205027	341867	19.18%	2.600%
9	13.369	1708	1714	1728	rVB	1003463	1457927	81.78%	11.086%
10	14.204	1848	1856	1864	rBV	62017	89925	5.04%	0.684%
11	14.751	1944	1949	1956	rVB2	278240	408588	22.92%	3.107%
12	16.239	2196	2202	2217	rVB	1012426	1411535	79.18%	10.733%
13	16.427	2224	2234	2239	rBV3	10980	24807	1.39%	0.189%
14	17.492	2409	2415	2421	rBV2	300808	433184	24.30%	3.294%
15	18.339	2554	2559	2564	rBV	79814	105816	5.94%	0.805%
16	19.598	2769	2773	2781	rBV3	27398	42646	2.39%	0.324%
17	20.068	2848	2853	2858	rBV	1586906	1782759	100.00%	13.556%
18	21.292	3057	3061	3068	rBV2	60338	101920	5.72%	0.775%
19	21.621	3113	3117	3123	rBV	355663	440587	24.71%	3.350%
20	23.950	3507	3513	3519	rBV	229276	437393	24.53%	3.326%

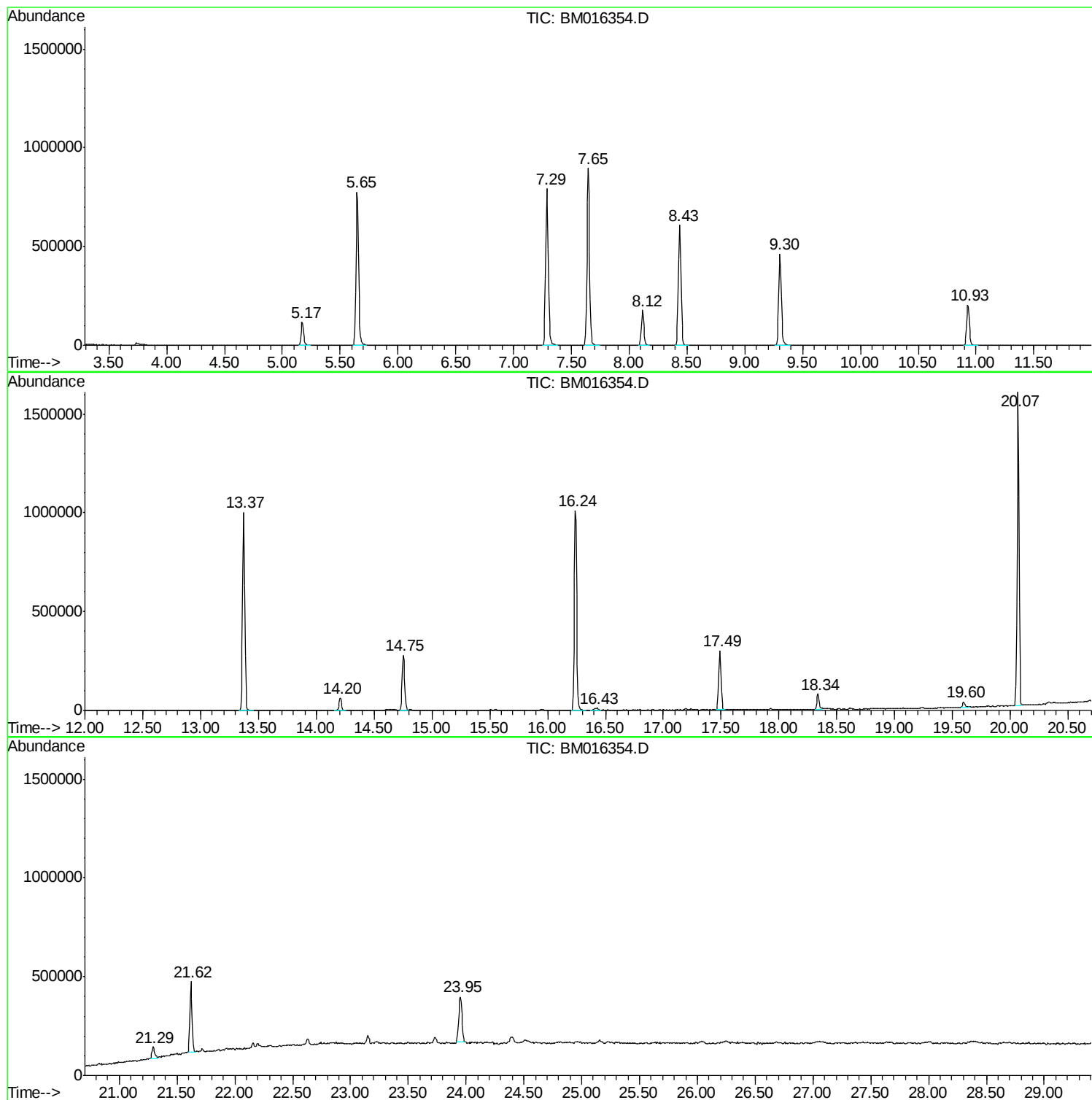
Sum of corrected areas: 13150768

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016354.D
Acq On : 14 Aug 2018 14:48
Operator : SJ/JU
Sample : J4442-31
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampled :
SP-1-4

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\BM081418\
Data File : BM016354.D
Acq On : 14 Aug 2018 14:48
Operator : SJ/JU
Sample : J4442-31
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1-4

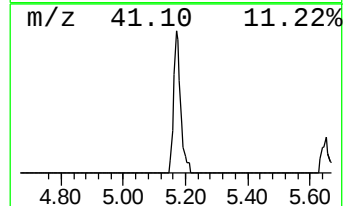
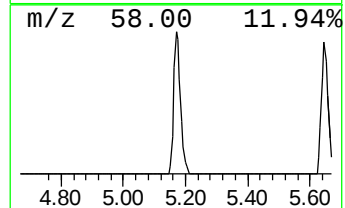
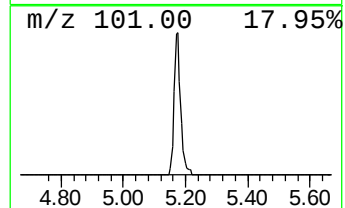
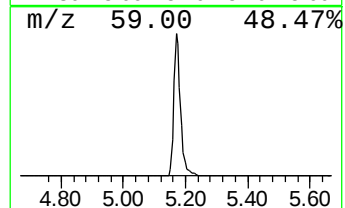
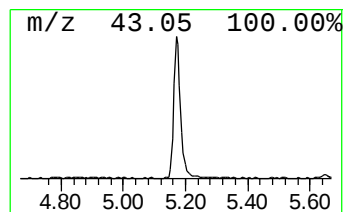
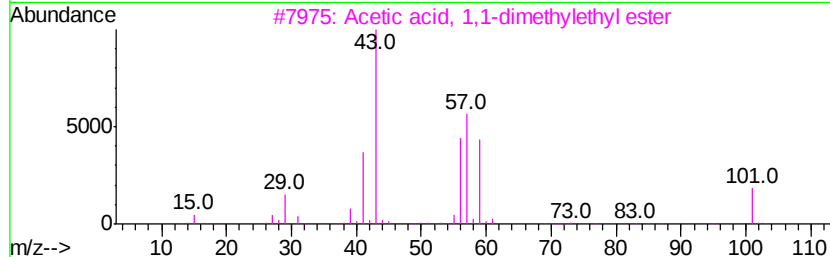
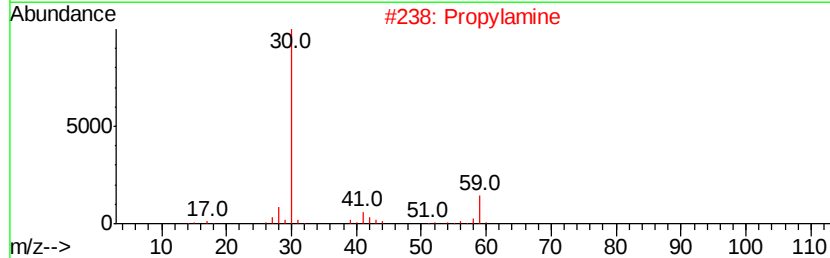
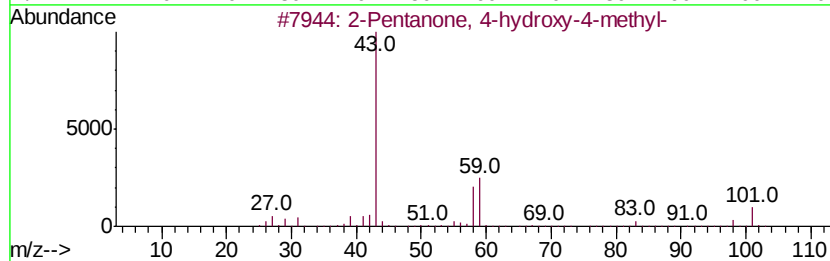
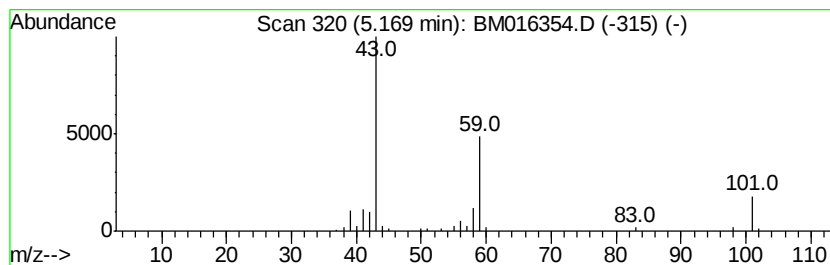
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.18 ng	173609	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propylamine	59	C3H9N	000107-10-8	42
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
4			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016354.D
Acq On : 14 Aug 2018 14:48
Operator : SJ/JU
Sample : J4442-31
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1-4

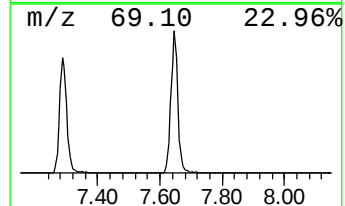
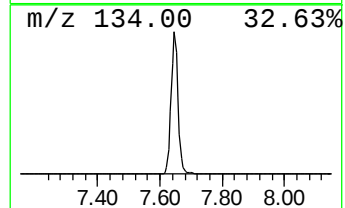
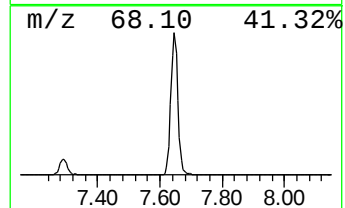
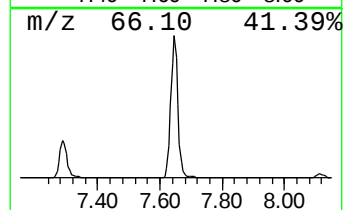
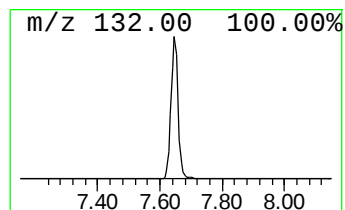
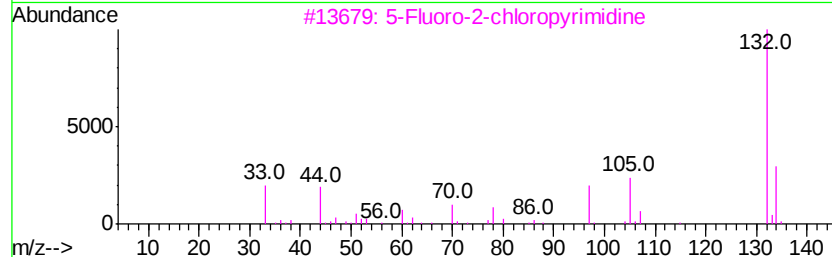
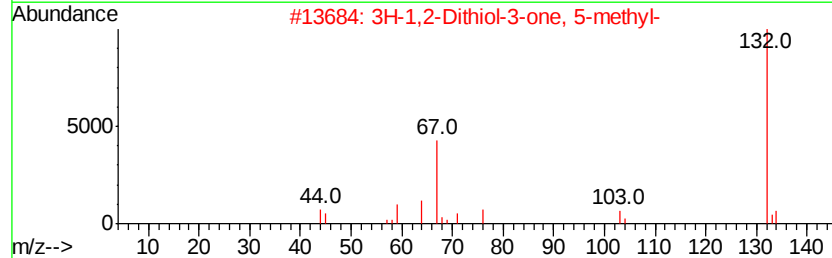
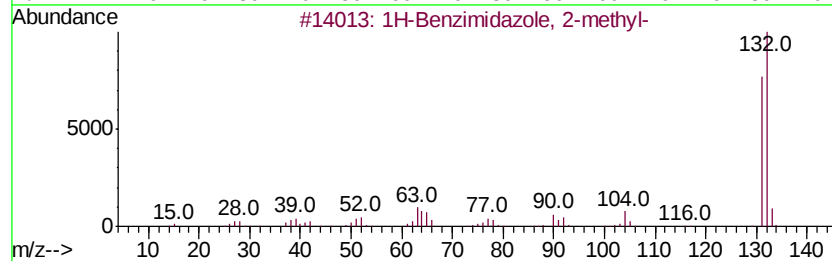
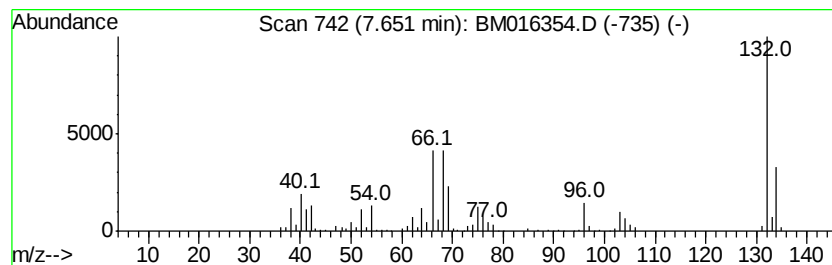
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	97.48 ng	1389660	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016354.D
Acq On : 14 Aug 2018 14:48
Operator : SJ/JU
Sample : J4442-31
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1-4

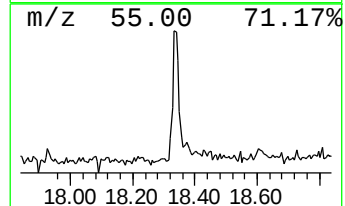
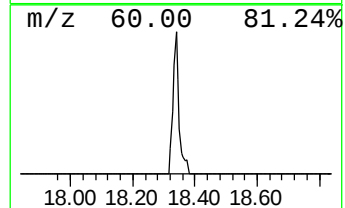
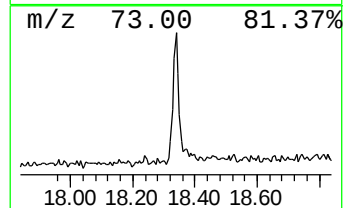
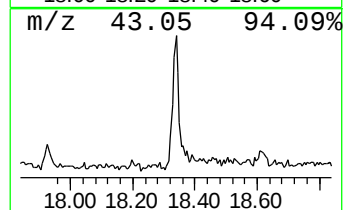
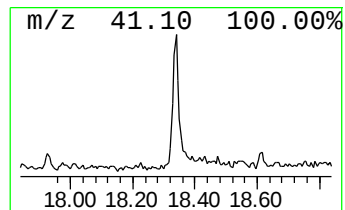
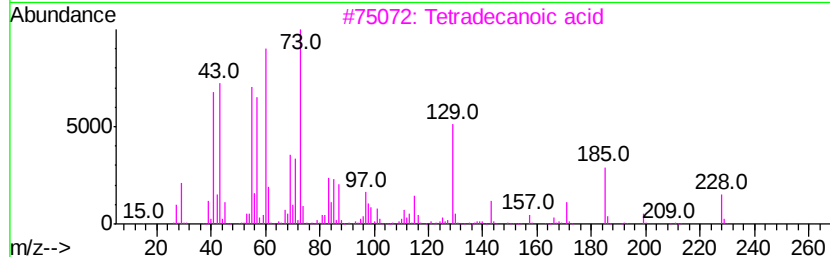
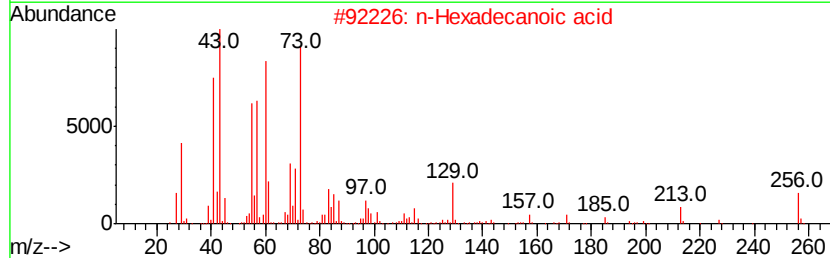
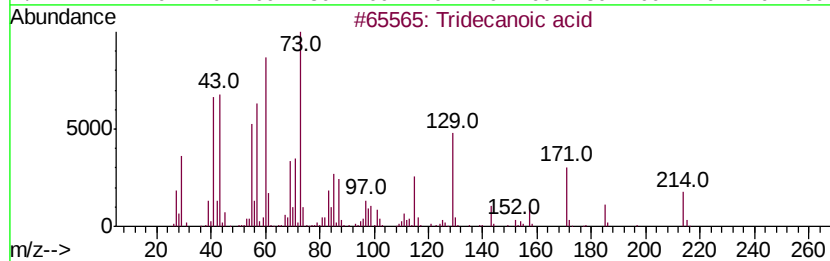
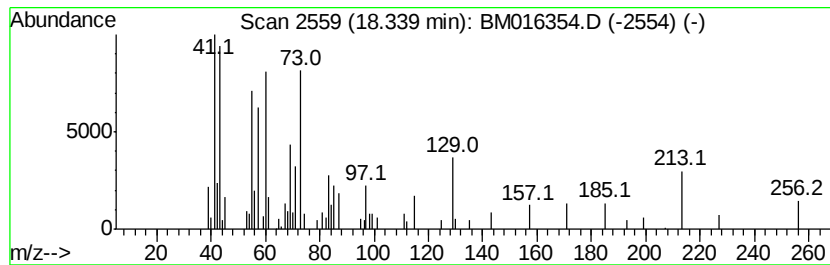
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	4.89 ng	105816	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	76
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016354.D
Acq On : 14 Aug 2018 14:48
Operator : SJ/JU
Sample : J4442-31
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1-4

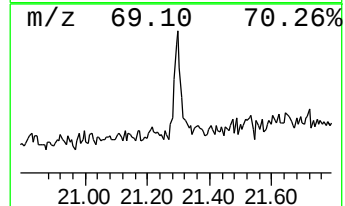
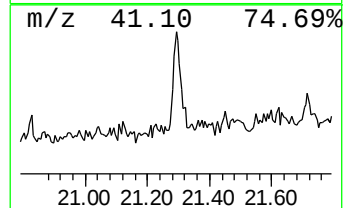
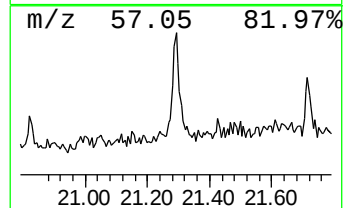
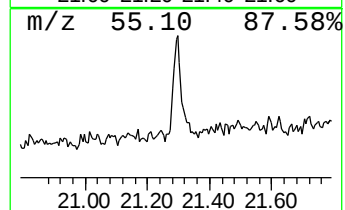
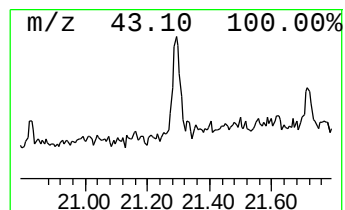
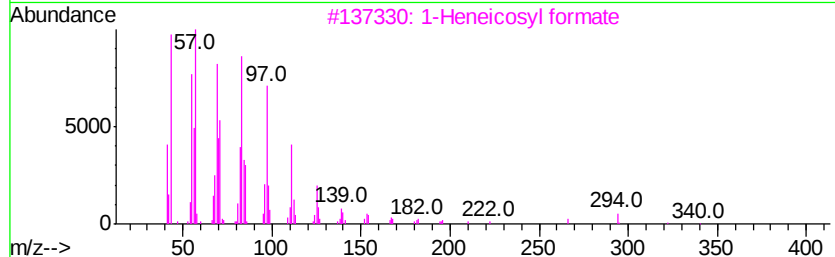
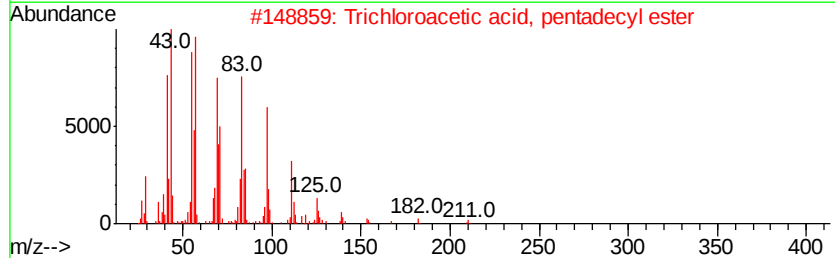
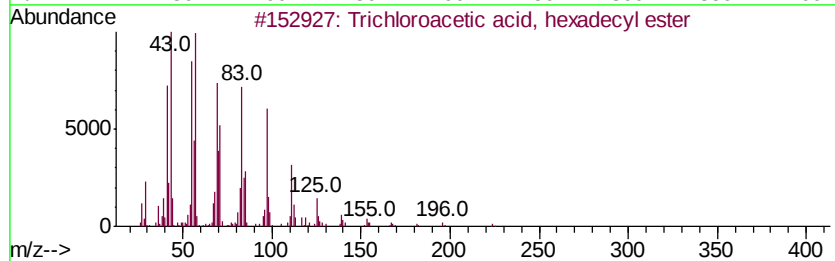
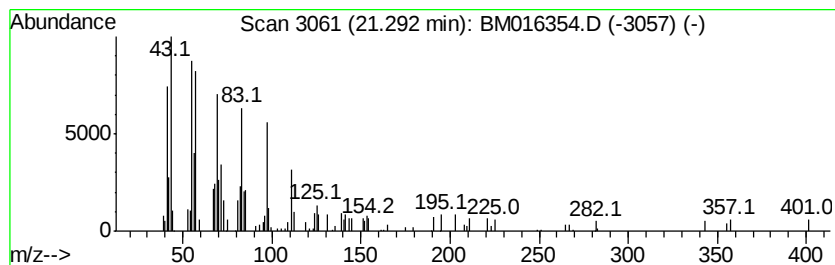
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.63 ng	101920	Chrysene-d12	21.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
5		1-Eicosanol	298	C20H42O	000629-96-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM081418\
Data File : BM016354.D
Acq On : 14 Aug 2018 14:48
Operator : SJ/JU
Sample : J4442-31
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP-1-4

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...	5.17	12.2	ng	173609	1	8.12	285116	20.0
unknown7.65	7.65	97.5	ng	1389660	1	8.12	285116	20.0
Tridecanoic acid	18.34	4.9	ng	105816	4	17.49	433184	20.0
Trichloroacetic a...	21.29	4.6	ng	101920	5	21.62	440587	20.0