

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM072618\
 Data File : BM016087.D
 Acq On : 27 Jul 2018 00:13
 Operator : SJ/JU
 Sample : J4160-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 072418-TIPC-F-U-B

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	5.722	408	414	426	rBV	548368	835565	20.18%	3.723%
2	7.363	687	693	706	rBV	364392	606535	14.65%	2.702%
3	7.728	749	755	770	rBV	1117722	1811358	43.74%	8.070%
4	8.204	830	836	848	rBB	311943	508772	12.28%	2.267%
5	8.528	884	891	904	rBB	1682329	2644288	63.85%	11.781%
6	9.392	1031	1038	1051	rBV	1239662	2043498	49.34%	9.105%
7	11.022	1309	1315	1324	rBV	346960	590800	14.27%	2.632%
8	13.457	1722	1729	1742	rVB	3011625	4080490	98.53%	18.180%
9	14.280	1864	1869	1878	rBB	196106	263569	6.36%	1.174%
10	14.833	1954	1963	1971	rVB2	453236	712761	17.21%	3.176%
11	16.098	2174	2178	2183	rVB	69123	76376	1.84%	0.340%
12	16.315	2209	2215	2227	rBV	1437005	1940801	46.86%	8.647%
13	17.562	2421	2427	2436	rBV	519291	724215	17.49%	3.227%
14	18.403	2566	2570	2574	rBV	68868	86775	2.10%	0.387%
15	20.133	2858	2864	2869	rBV	3663817	4141549	100.00%	18.452%
16	21.350	3067	3071	3080	rBV9	32541	75215	1.82%	0.335%
17	21.680	3122	3127	3133	rBV	543780	672562	16.24%	2.997%
18	24.044	3523	3529	3537	rVB2	322631	629752	15.21%	2.806%

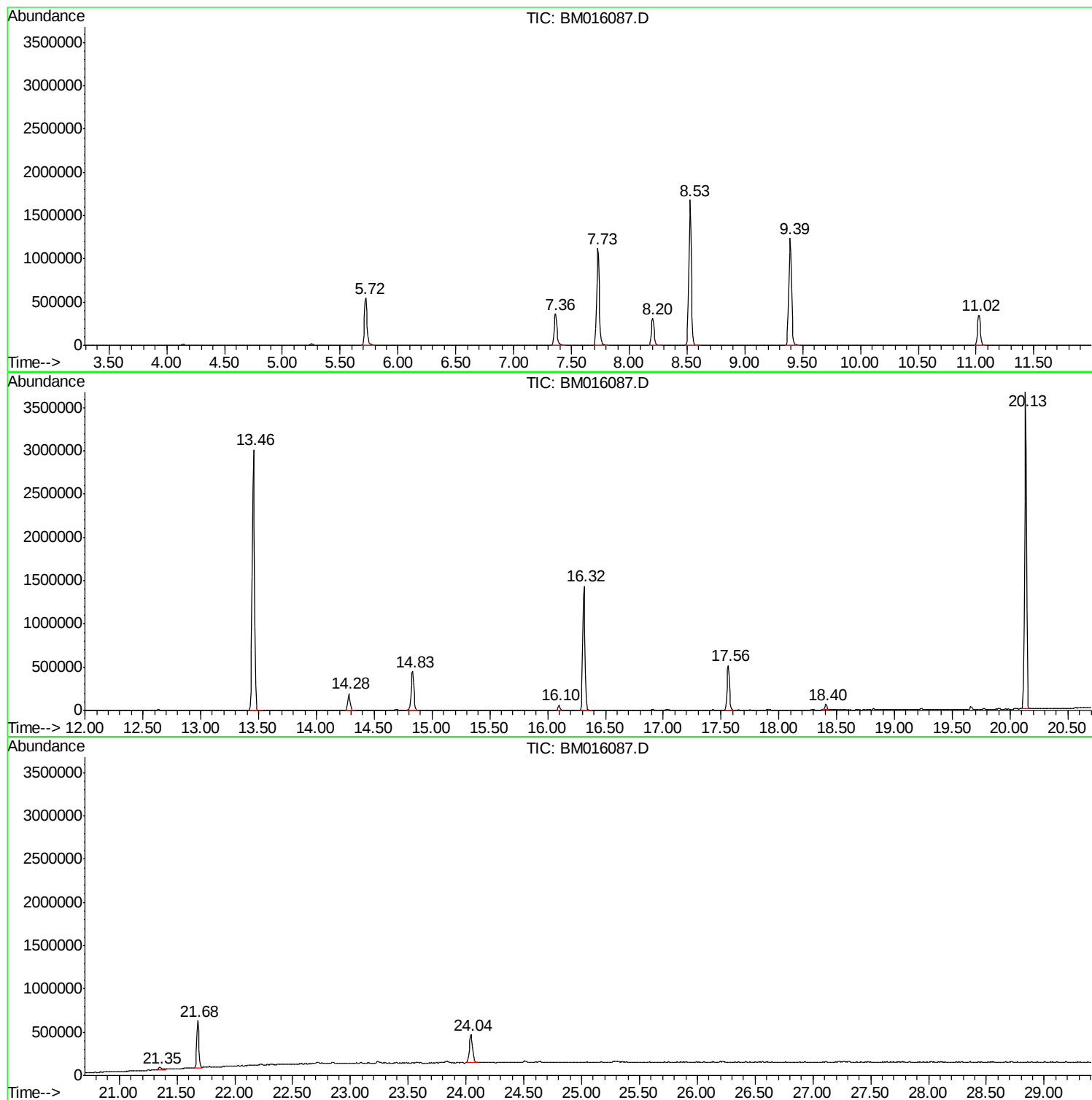
Sum of corrected areas: 22444881

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM072618\
Data File : BM016087.D
Acq On : 27 Jul 2018 00:13
Operator : SJ/JU
Sample : J4160-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
072418-TIPC-F-U-B

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\BM072618\
Data File : BM016087.D
Acq On : 27 Jul 2018 00:13
Operator : SJ/JU
Sample : J4160-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
072418-TIPC-F-U-B

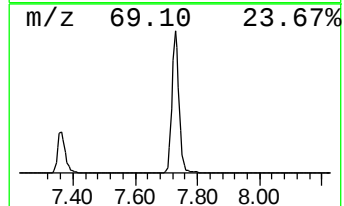
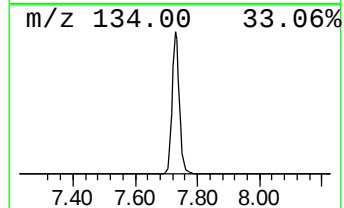
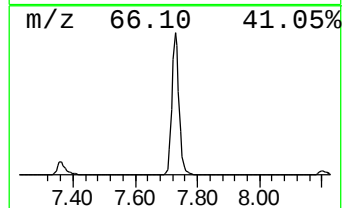
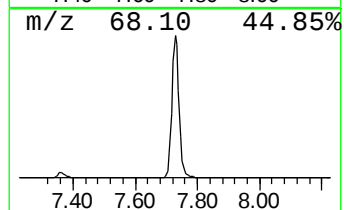
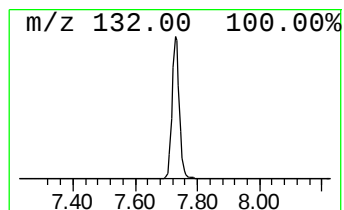
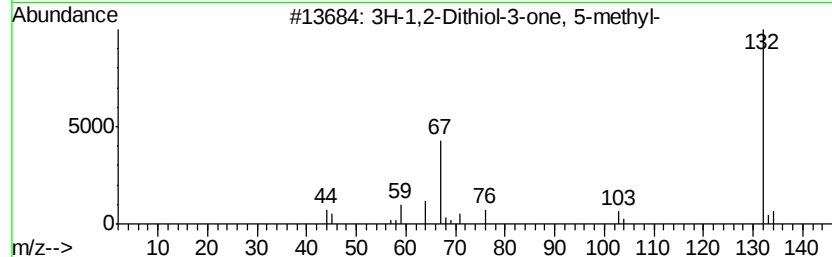
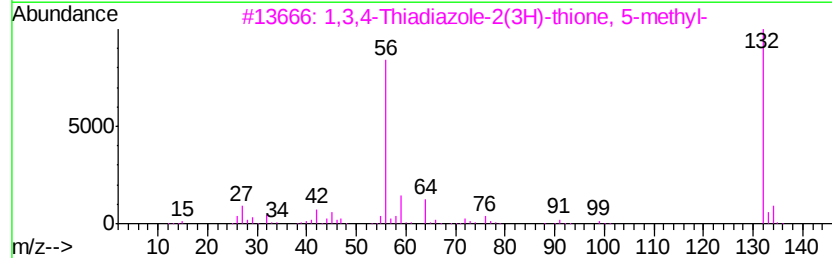
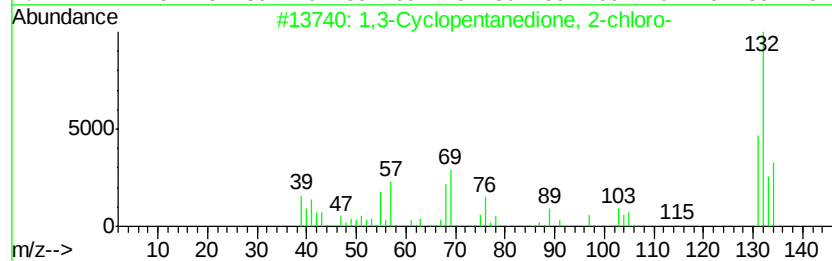
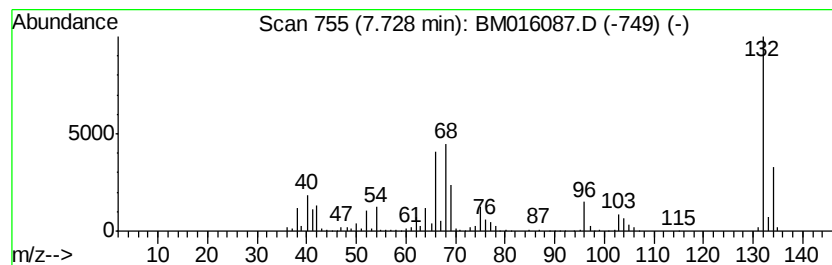
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	71.21 ng	1811360	1,4-Dichlorobenzene-d4	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM072618\
Data File : BM016087.D
Acq On : 27 Jul 2018 00:13
Operator : SJ/JU
Sample : J4160-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
072418-TIPC-F-U-B

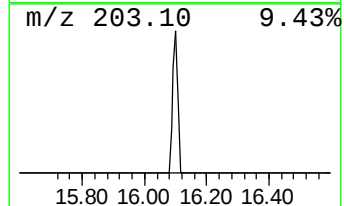
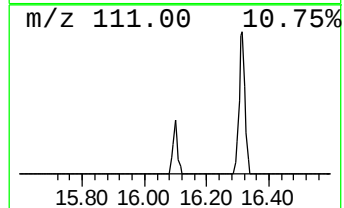
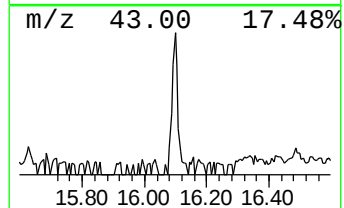
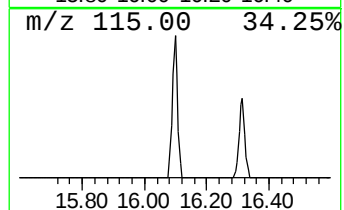
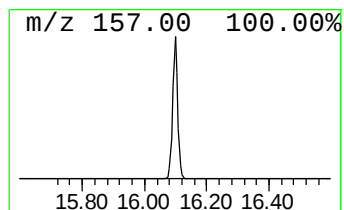
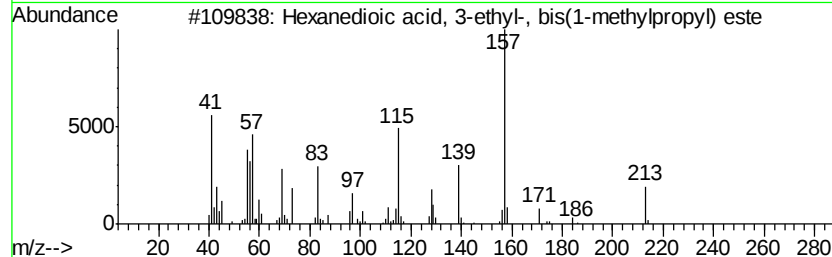
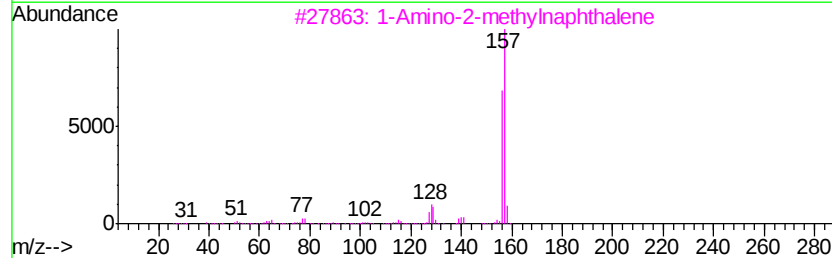
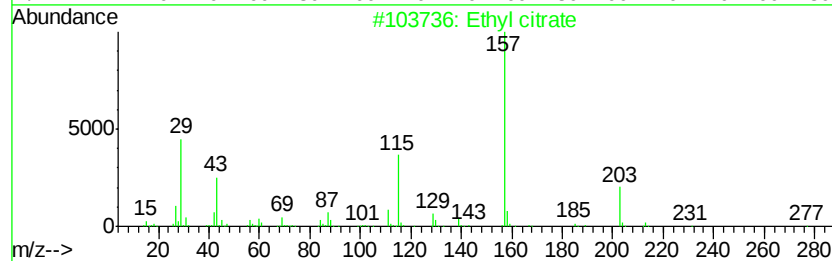
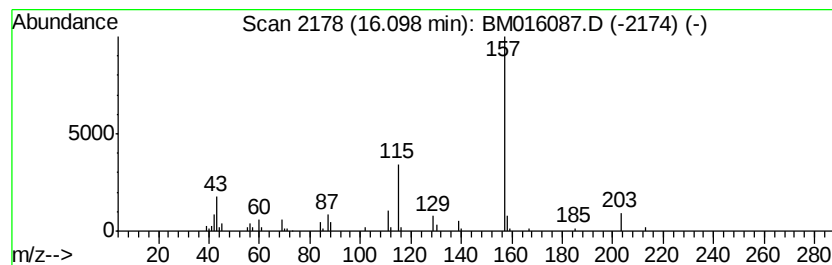
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.14 ng	76376	Acenaphthene-d10	14.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl citrate	276	C12H20O7	000077-93-0	87
2		1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	40
3		Hexanedioic acid, 3-ethyl-, bis(...	286	C16H30O4	057983-54-7	39
4		Pyrimidine, 2-methylthio-4-hydro...	157	C5H7N3OS	001074-41-5	28
5		2-Naphthalenamine, N-methyl-	157	C11H11N	002216-67-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM072618\
Data File : BM016087.D
Acq On : 27 Jul 2018 00:13
Operator : SJ/JU
Sample : J4160-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

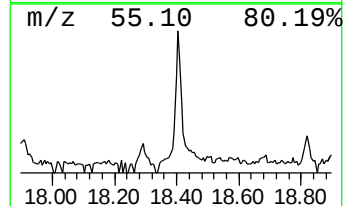
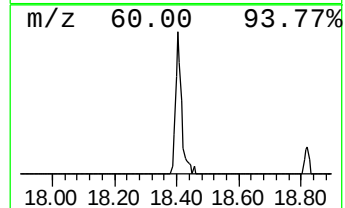
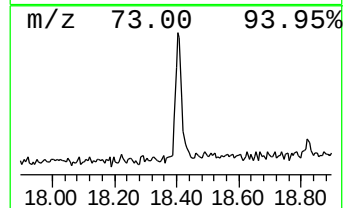
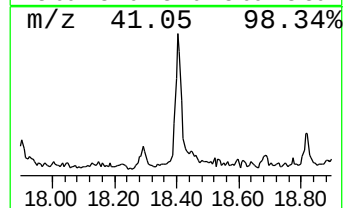
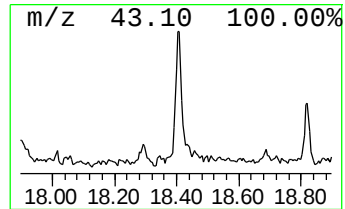
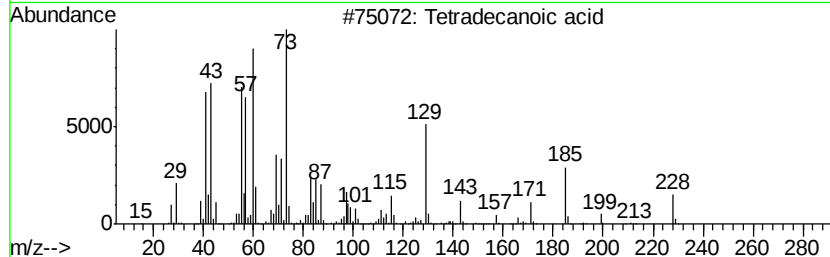
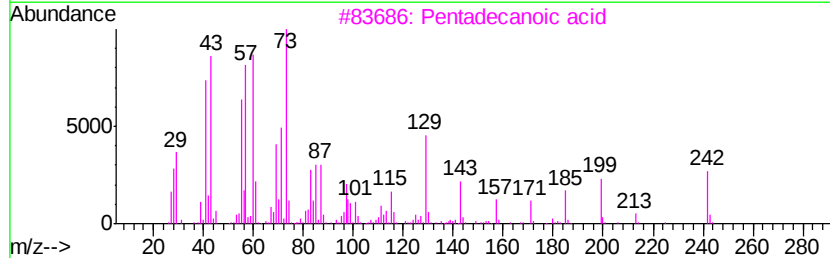
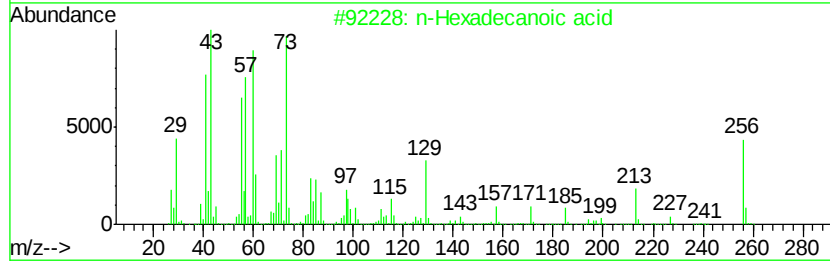
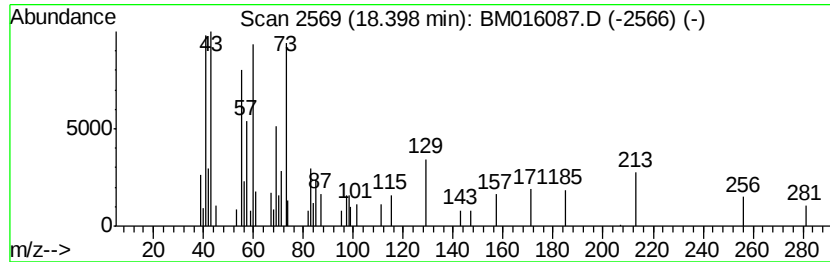
Instrument :
BNA_M
ClientSampleId :
072418-TIPC-F-U-B

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 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	2.40 ng	86775	Phenanthrene-d10	17.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 94
2		Pentadecanoic acid	242 C15H30O2	001002-84-2 72
3		Tetradecanoic acid	228 C14H28O2	000544-63-8 68
4		Tridecanoic acid	214 C13H26O2	000638-53-9 64
5		Dodecanoic acid	200 C12H24O2	000143-07-7 59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM072618\
Data File : BM016087.D
Acq On : 27 Jul 2018 00:13
Operator : SJ/JU
Sample : J4160-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
072418-TIPC-F-U-B

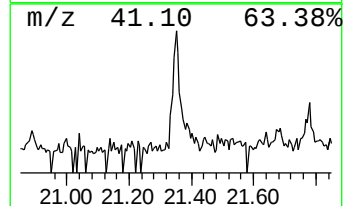
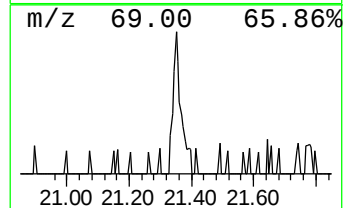
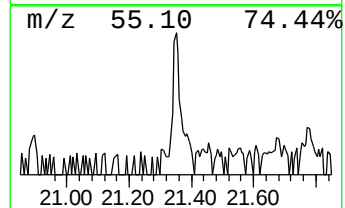
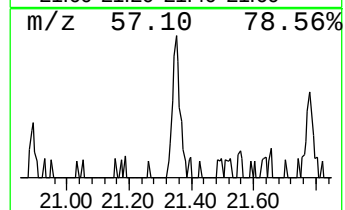
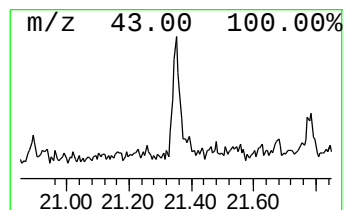
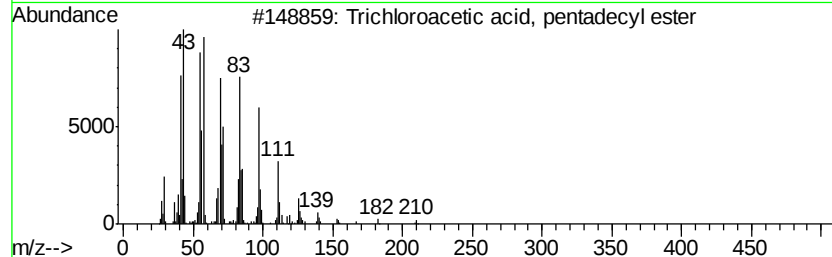
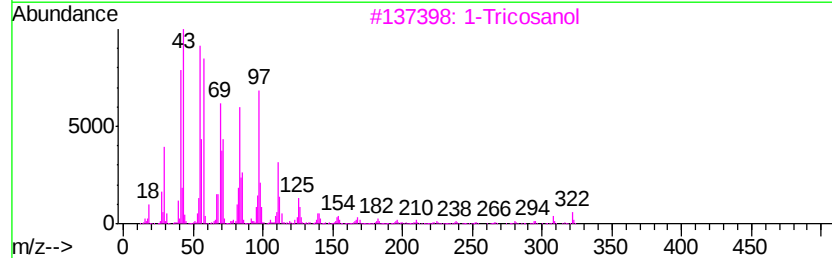
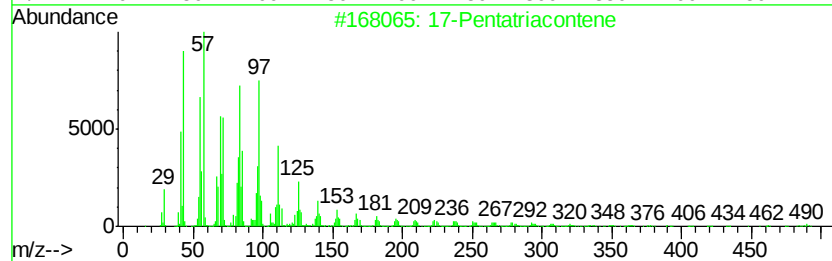
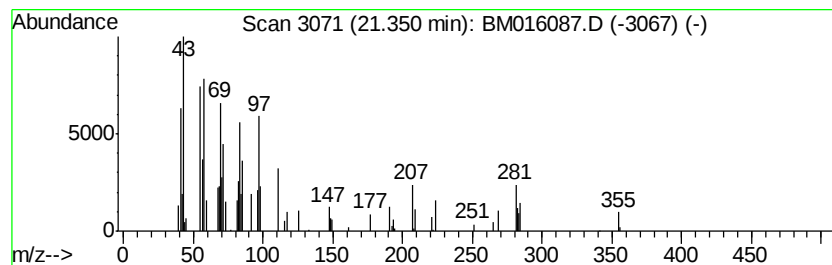
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown21.35 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	2.24 ng	75215	Chrysene-d12	21.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	49
2		1-Tricosanol	340	C23H48O	003133-01-5	49
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	46
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	46
5		Acetic acid, trifluoro-, hexadec...	338	C18H33F3O2	006222-03-3	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM072618\
Data File : BM016087.D
Acq On : 27 Jul 2018 00:13
Operator : SJ/JU
Sample : J4160-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
072418-TIPC-F-U-B

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
unknown7.73	7.73	71.2	ng	1811360	1	8.20	508772	20.0
Ethyl citrate	16.10	2.1	ng	76376	3	14.83	712761	20.0
n-Hexadecanoic acid	18.40	2.4	ng	86775	4	17.56	724215	20.0
unknown21.35	21.35	2.2	ng	75215	5	21.68	672562	20.0