

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062018\
 Data File : BF106641.D
 Acq On : 21 Jun 2018 1:03
 Operator : JU/SJ
 Sample : J3575-14
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-11-S

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-BF061918.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	5.201	483	487	495	rVB	138594	166874	8.98%	0.977%
2	5.607	552	556	560	rBV	1940287	1730954	93.11%	10.131%
3	6.607	721	726	741	rBV	1841471	1798318	96.73%	10.525%
4	6.736	744	748	752	rBV	1830029	1806351	97.17%	10.572%
5	6.960	782	786	789	rBV	670303	518665	27.90%	3.036%
6	7.119	808	813	816	rBV	1502053	1396742	75.13%	8.175%
7	7.525	877	882	885	rBV	1289907	1174268	63.17%	6.873%
8	8.242	1000	1004	1007	rBV	773667	626218	33.68%	3.665%
9	9.313	1182	1186	1190	rBV	1979517	1859046	100.00%	10.880%
10	9.707	1249	1253	1259	rBV	272495	226826	12.20%	1.328%
11	9.913	1283	1288	1290	rBV	39962	33483	1.80%	0.196%
12	10.001	1299	1303	1307	rBV	771854	646384	34.77%	3.783%
13	10.413	1370	1373	1376	rVB	51881	41173	2.21%	0.241%
14	10.713	1421	1424	1427	rBV	26456	21629	1.16%	0.127%
15	10.795	1434	1438	1441	rBV	1272074	1115603	60.01%	6.529%
16	10.883	1450	1453	1458	rVB	44062	43244	2.33%	0.253%
17	11.489	1553	1556	1560	rBV	588531	566457	30.47%	3.315%
18	12.936	1797	1802	1804	rBV	28078	30455	1.64%	0.178%
19	13.077	1822	1826	1829	rBV	1911124	1643231	88.39%	9.617%
20	13.954	1972	1975	1985	rBV	147201	164260	8.84%	0.961%
21	14.142	2002	2007	2010	rBV	751071	697263	37.51%	4.081%
22	14.277	2027	2030	2034	rBV4	20656	24444	1.31%	0.143%
23	14.595	2081	2084	2090	rBV5	38775	57969	3.12%	0.339%
24	14.989	2148	2151	2155	rVB	82988	80952	4.35%	0.474%
25	15.671	2262	2267	2273	rBV	439204	615630	33.12%	3.603%

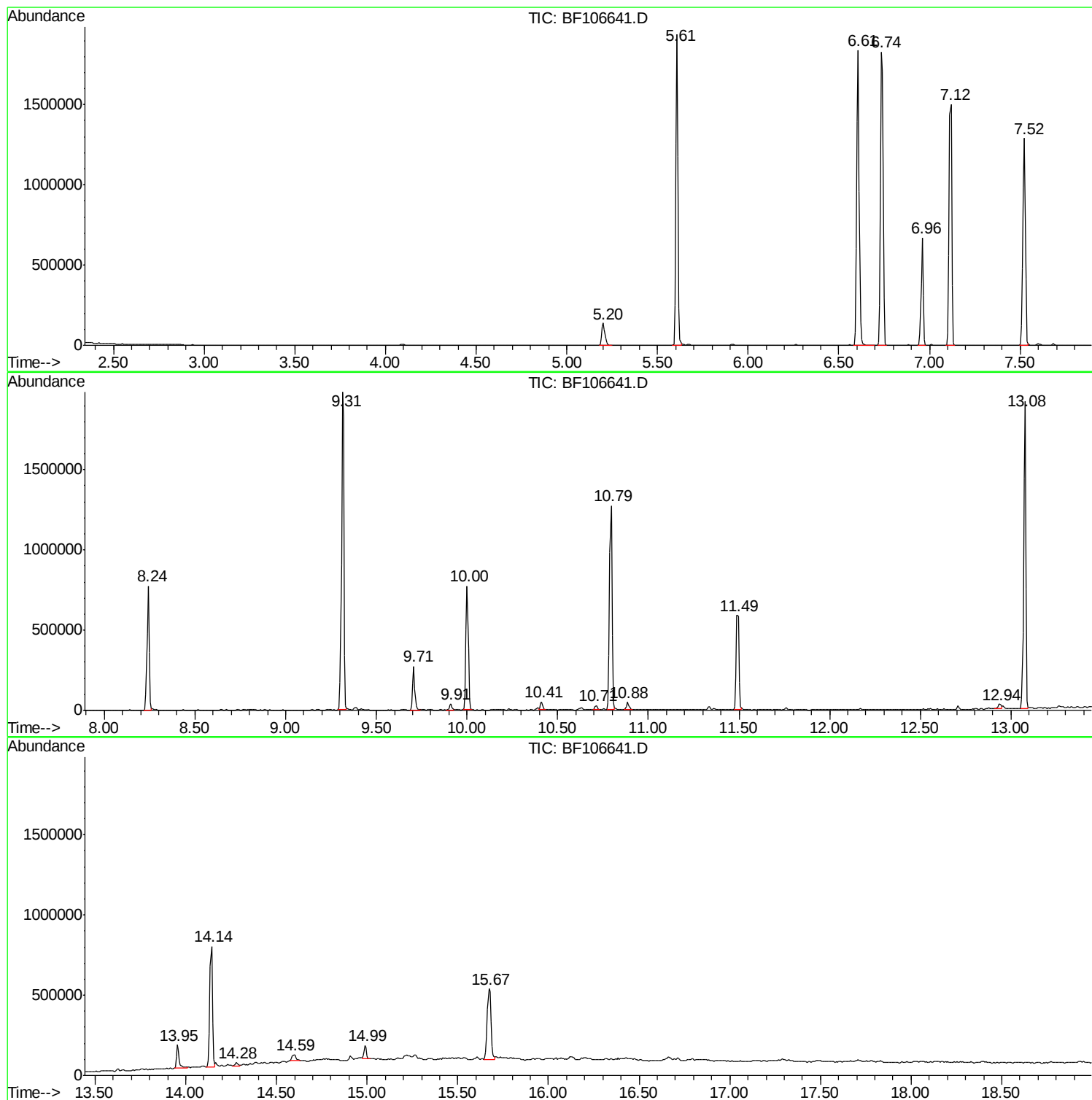
Sum of corrected areas: 17086439

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062018\
Data File : BF106641.D
Acq On : 21 Jun 2018 1:03
Operator : JU/SJ
Sample : J3575-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF062018\
Data File : BF106641.D
Acq On : 21 Jun 2018 1:03
Operator : JU/SJ
Sample : J3575-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-S

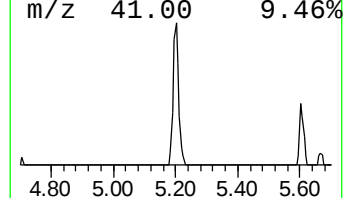
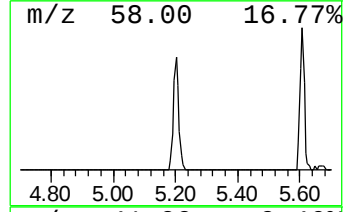
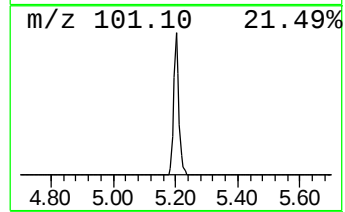
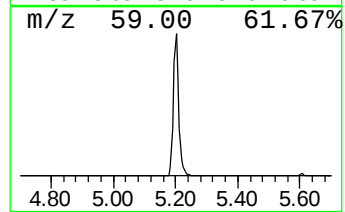
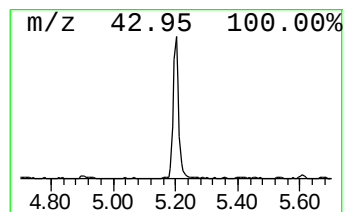
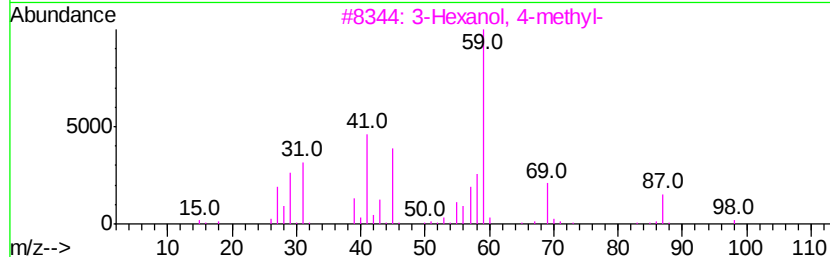
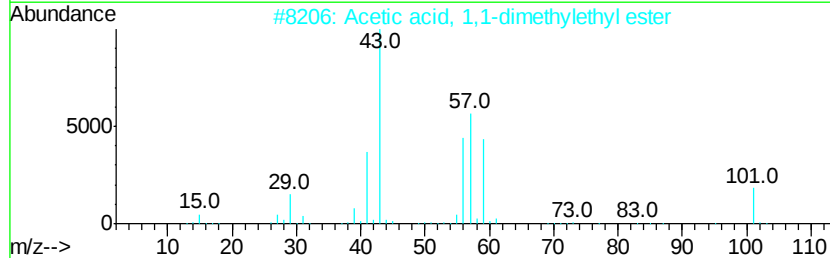
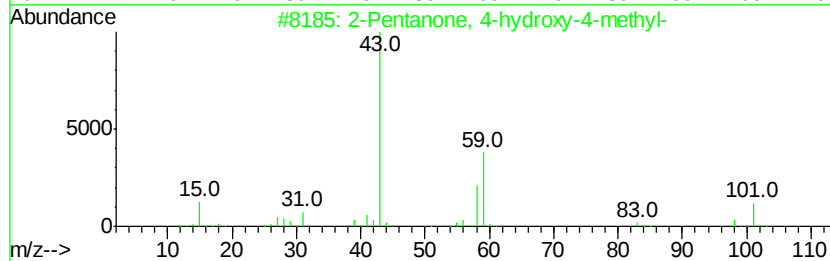
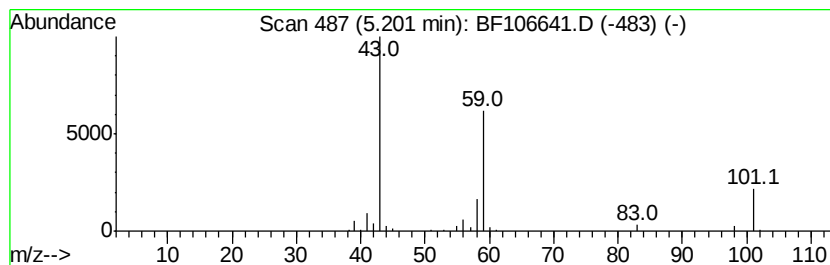
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.20	6.43 ng	166874	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062018\
Data File : BF106641.D
Acq On : 21 Jun 2018 1:03
Operator : JU/SJ
Sample : J3575-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-S

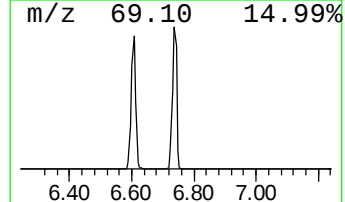
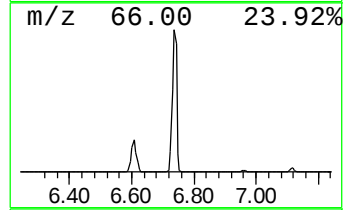
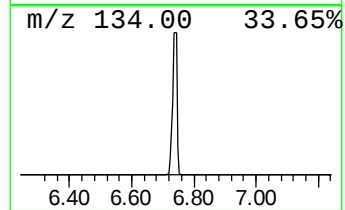
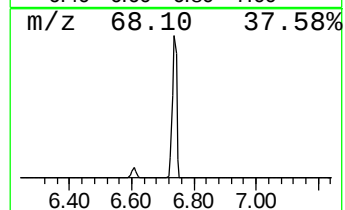
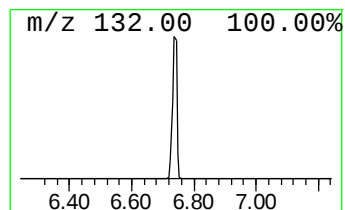
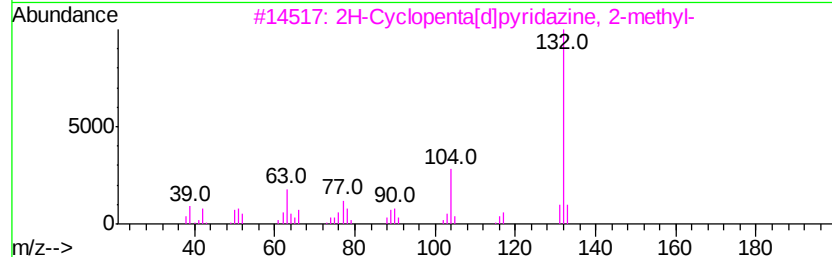
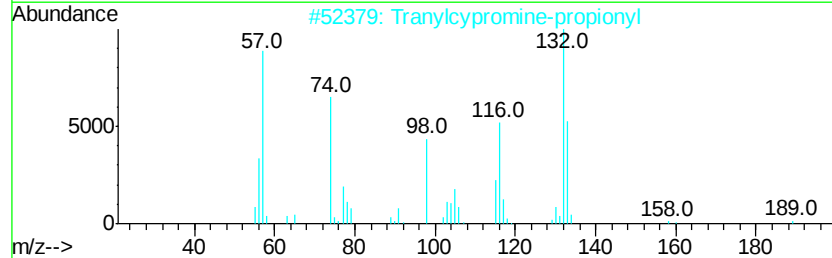
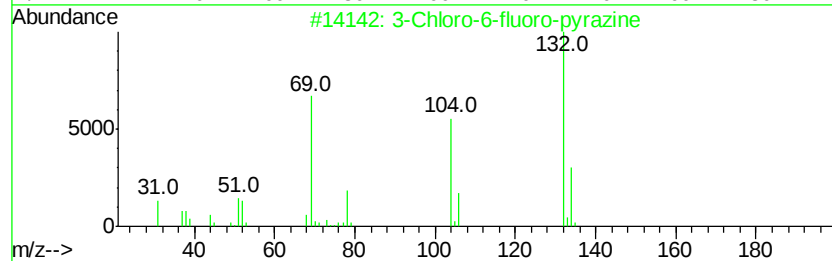
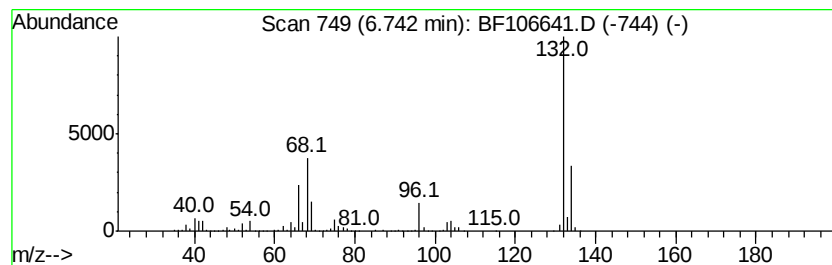
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	69.65 ng	1806350	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062018\
Data File : BF106641.D
Acq On : 21 Jun 2018 1:03
Operator : JU/SJ
Sample : J3575-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-S

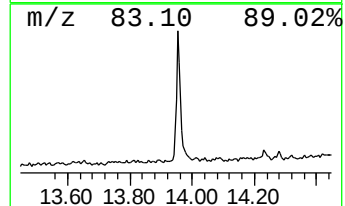
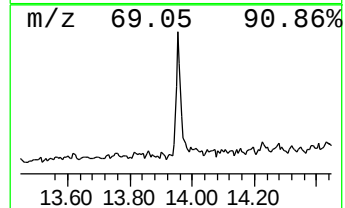
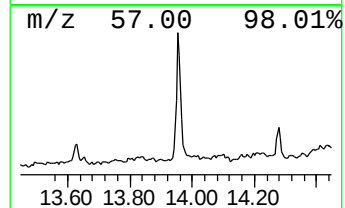
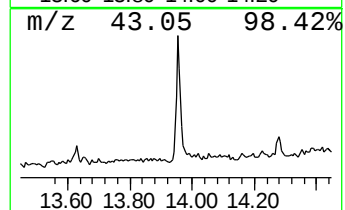
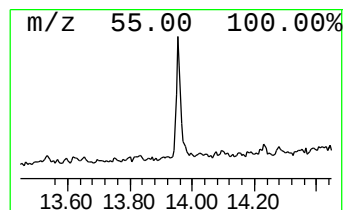
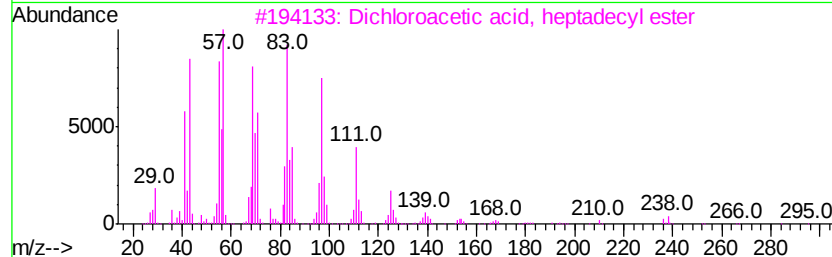
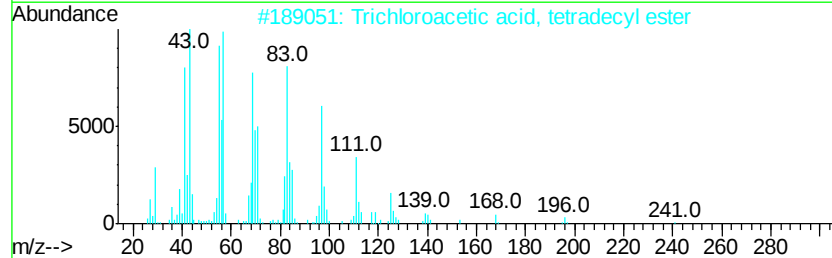
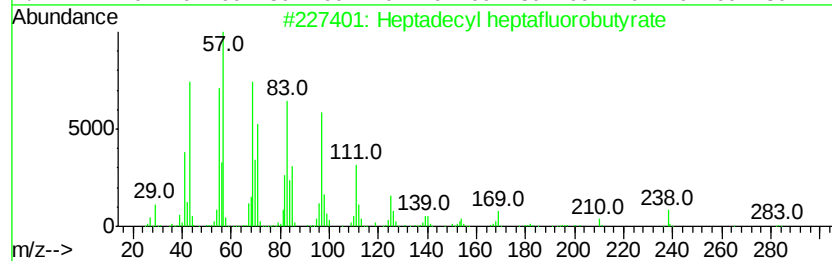
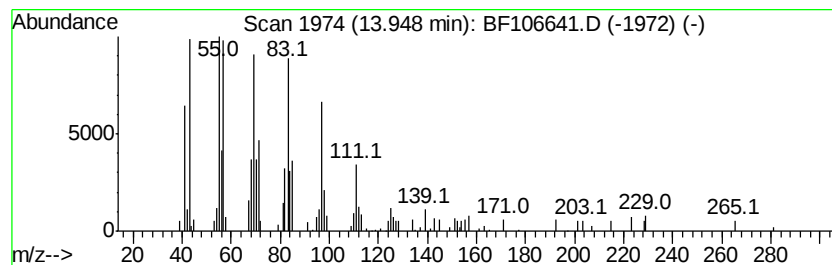
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.71 ng	164260	Chrysene-d12	14.14

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062018\
Data File : BF106641.D
Acq On : 21 Jun 2018 1:03
Operator : JU/SJ
Sample : J3575-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-S

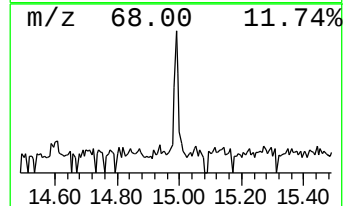
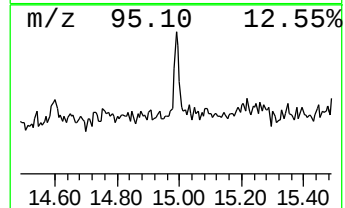
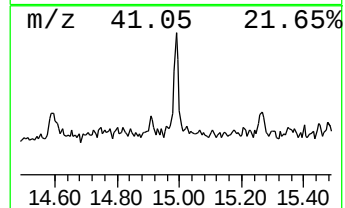
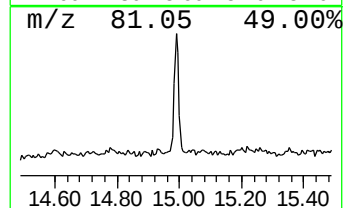
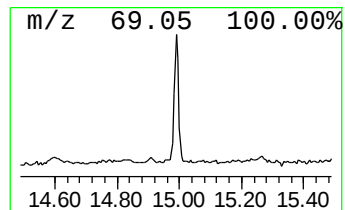
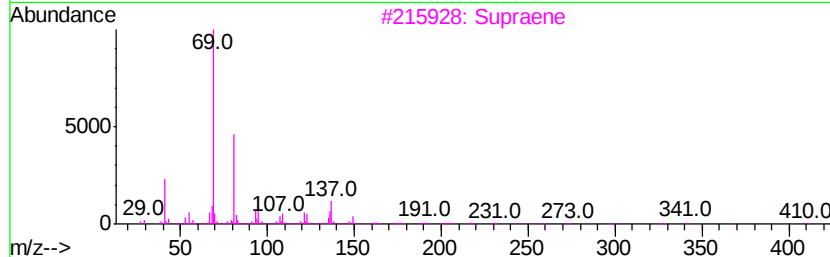
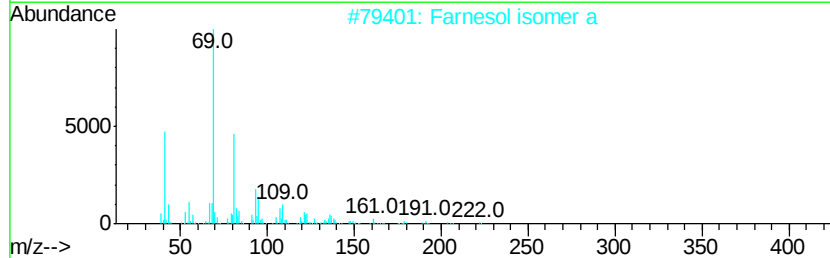
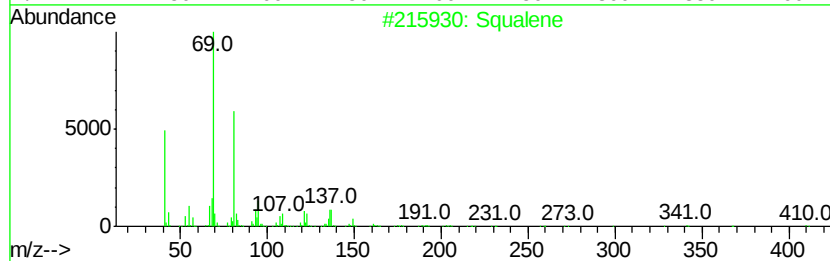
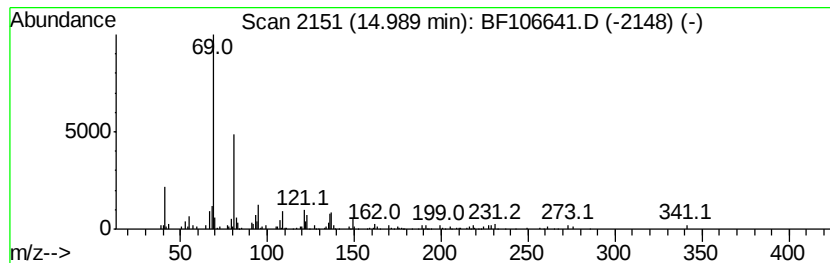
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.63 ng	80952	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	83
2		Farnesol isomer a	222	C15H26O	1000108-92-4	80
3		Supraene	410	C30H50	007683-64-9	74
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
5		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062018\
Data File : BF106641.D
Acq On : 21 Jun 2018 1:03
Operator : JU/SJ
Sample : J3575-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.20	6.4	ng	166874	1	6.96	518665	20.0
unknown6.74	6.74	69.7	ng	1806350	1	6.96	518665	20.0
Heptadecyl heptaf...	13.95	4.7	ng	164260	5	14.14	697263	20.0
Squalene	14.99	2.6	ng	80952	6	15.68	615630	20.0