

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080918\
 Data File : BF108045.D
 Acq On : 9 Aug 2018 11:51
 Operator : JU/SJ
 Sample : J4275-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-02-080718-A

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-BF080818.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	5.254	489	496	503	rBV	1072311	1347644	16.73%	2.018%
2	5.637	556	561	564	rBV	6601606	6482843	80.46%	9.710%
3	6.631	723	730	733	rBV	6652133	7075337	87.82%	10.597%
4	6.784	751	756	759	rBV	7217675	6785774	84.22%	10.163%
5	7.013	791	795	799	rVB	2236611	1802620	22.37%	2.700%
6	7.172	817	822	825	rBV	6059260	5117106	63.51%	7.664%
7	7.572	885	890	894	rBV	4312661	4525467	56.17%	6.778%
8	8.295	1009	1013	1017	rBV	2872579	2338143	29.02%	3.502%
9	9.372	1191	1196	1199	rBV	8426566	8056738	100.00%	12.067%
10	9.760	1258	1262	1265	rBV	504911	394926	4.90%	0.591%
11	10.060	1308	1313	1317	rBV	3089346	2658754	33.00%	3.982%
12	10.854	1443	1448	1451	rBV	5212816	4785857	59.40%	7.168%
13	10.948	1461	1464	1470	rVB	67923	87758	1.09%	0.131%
14	11.554	1563	1567	1571	rBV	2914076	2567028	31.86%	3.845%
15	11.895	1621	1625	1629	rBV	65040	89874	1.12%	0.135%
16	12.060	1647	1653	1657	rBV	296751	317363	3.94%	0.475%
17	12.101	1657	1660	1667	rVB	70948	108132	1.34%	0.162%
18	13.007	1811	1814	1821	rVB2	80585	90826	1.13%	0.136%
19	13.148	1833	1838	1841	rBV	7493016	6976385	86.59%	10.449%
20	14.036	1986	1989	2000	rBV2	161067	364178	4.52%	0.545%
21	14.207	2014	2018	2022	rBV	2066332	1990652	24.71%	2.981%
22	14.989	2149	2151	2156	rVB	100541	100000	1.24%	0.150%
23	15.077	2162	2166	2170	rVB	397158	414409	5.14%	0.621%
24	15.360	2211	2214	2218	rVB	116450	135220	1.68%	0.203%
25	15.771	2279	2284	2293	rVB	1464718	1977303	24.54%	2.961%
26	16.260	2364	2367	2372	rVB2	125966	176741	2.19%	0.265%

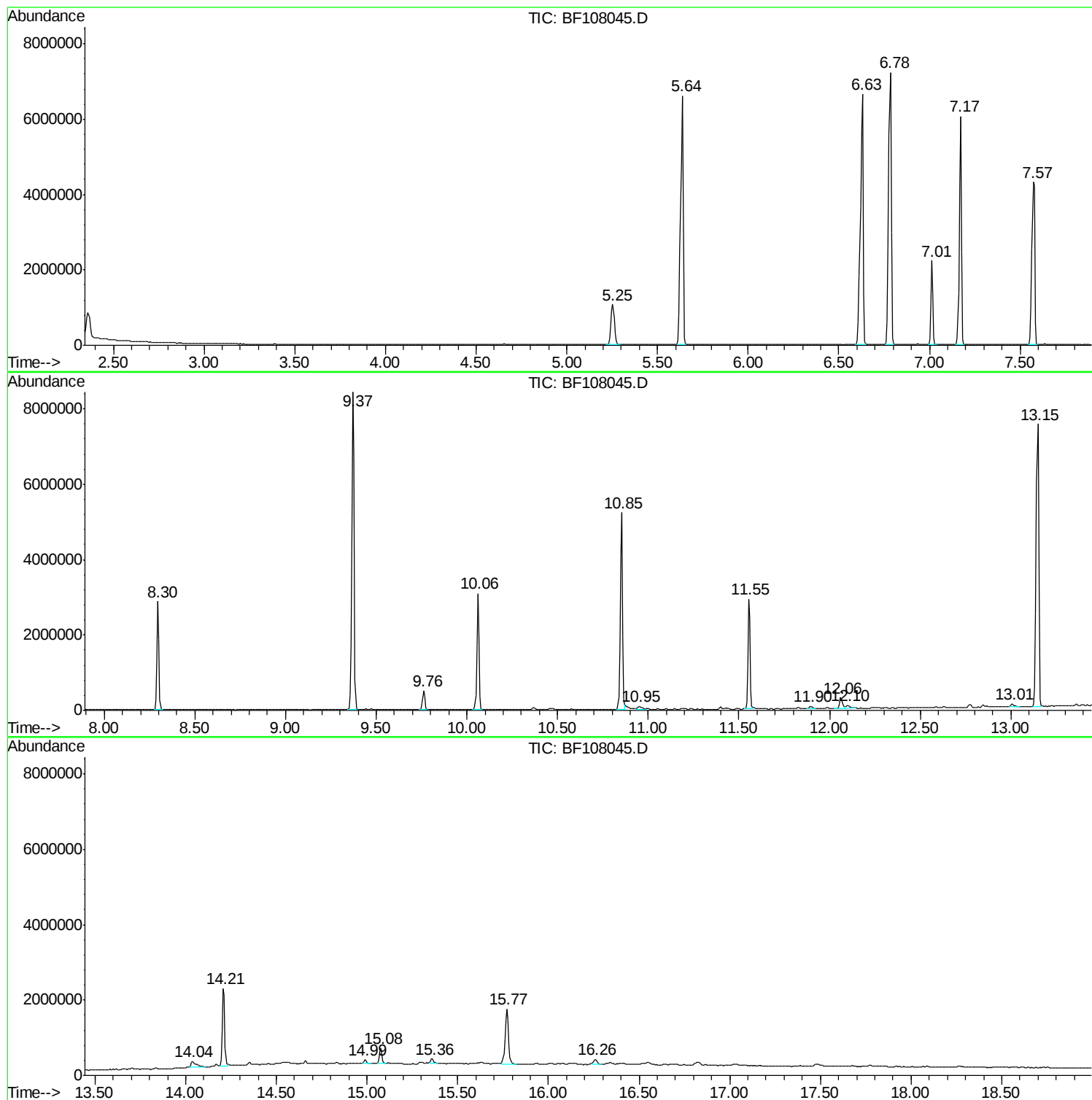
Sum of corrected areas: 66767078

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108045.D
Acq On : 9 Aug 2018 11:51
Operator : JU/SJ
Sample : J4275-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-080718-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.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\BF080918\
Data File : BF108045.D
Acq On : 9 Aug 2018 11:51
Operator : JU/SJ
Sample : J4275-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-080718-A

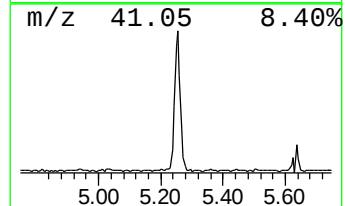
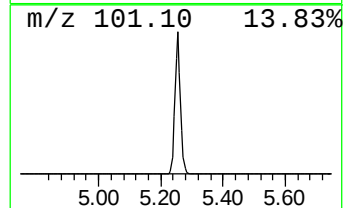
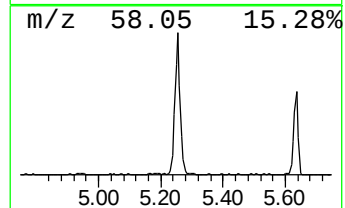
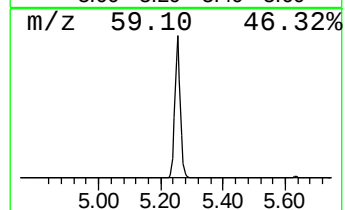
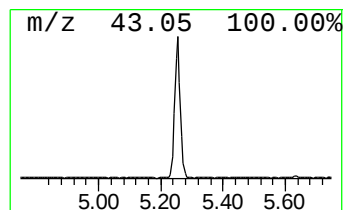
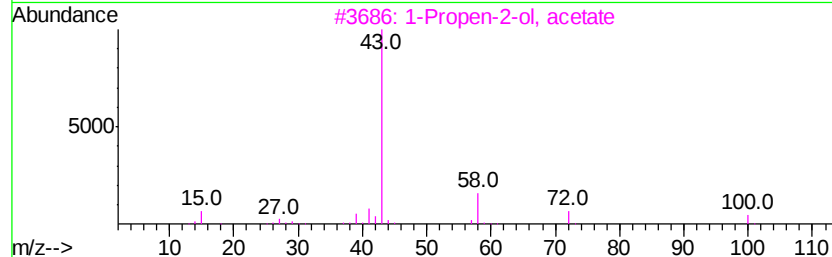
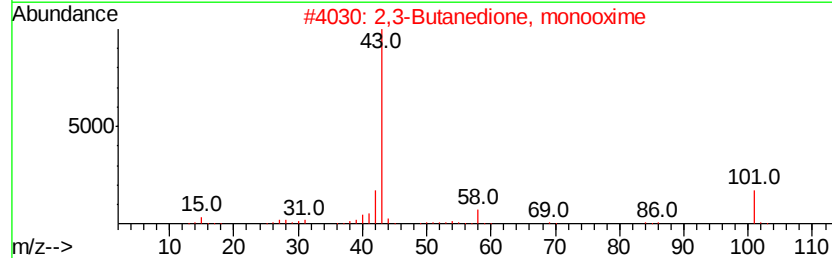
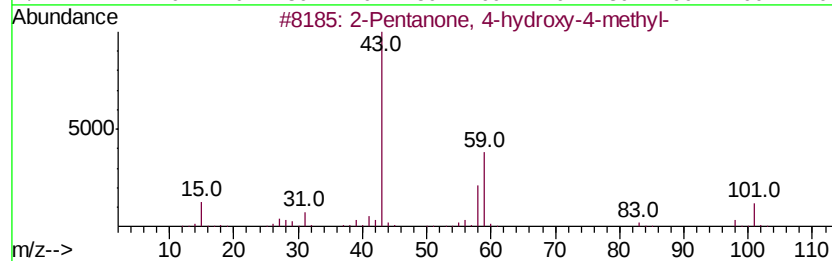
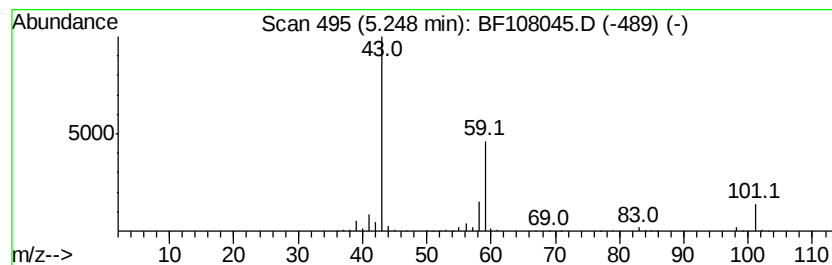
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.25	14.95 ng	1347640	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Acetone	58	C3H6O	000067-64-1	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108045.D
Acq On : 9 Aug 2018 11:51
Operator : JU/SJ
Sample : J4275-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-080718-A

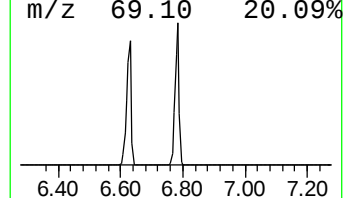
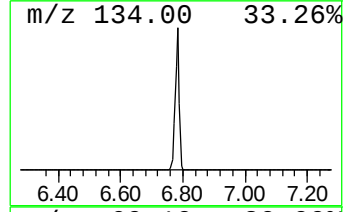
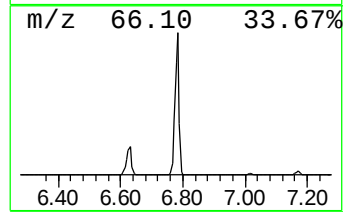
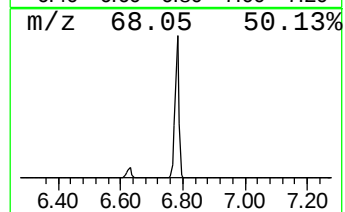
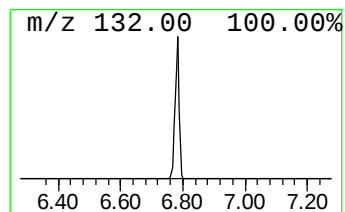
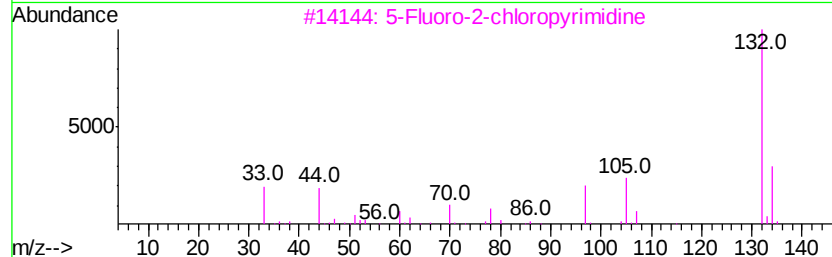
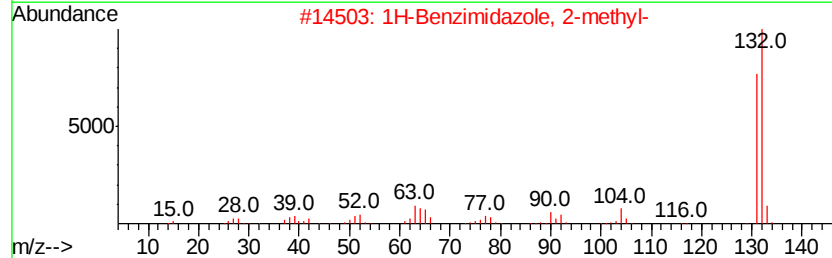
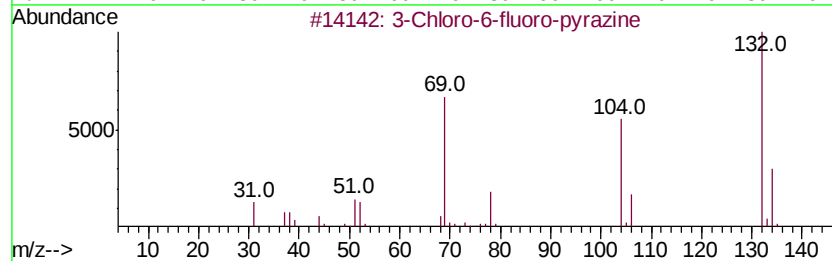
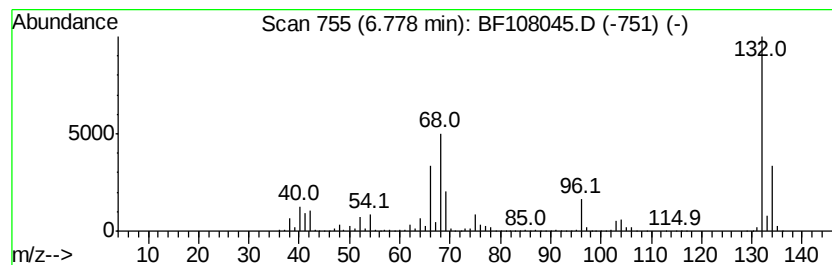
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	75.29 ng	6785770	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108045.D
Acq On : 9 Aug 2018 11:51
Operator : JU/SJ
Sample : J4275-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-080718-A

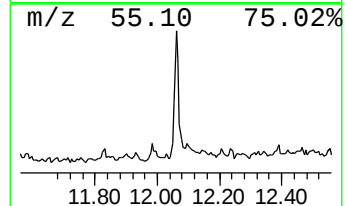
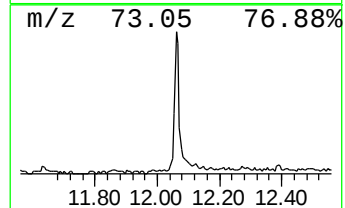
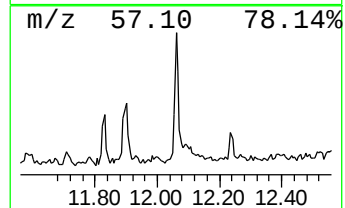
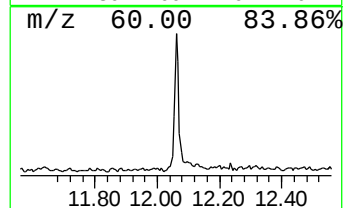
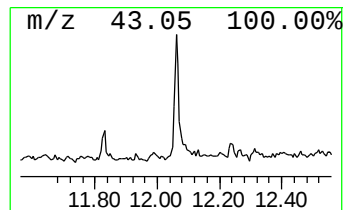
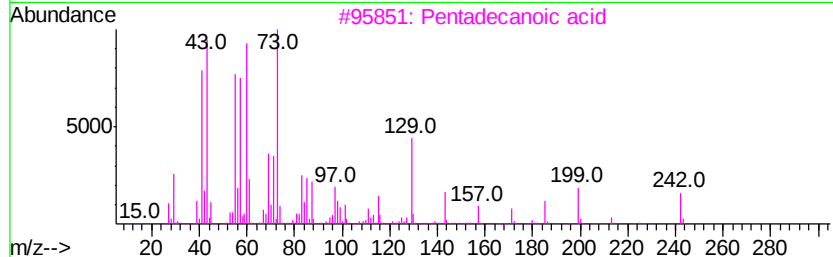
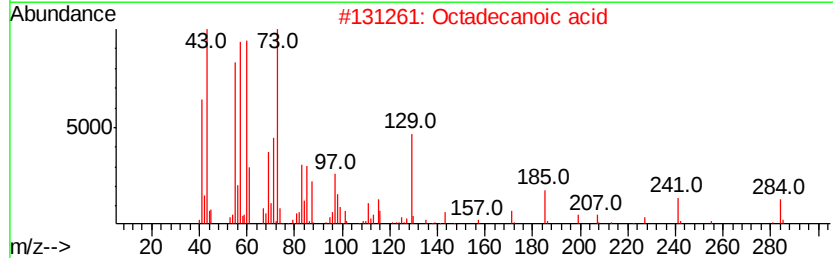
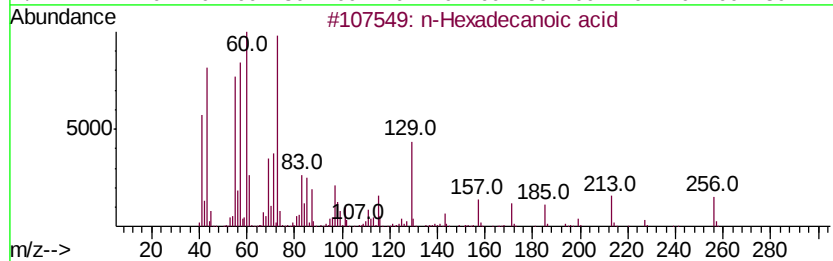
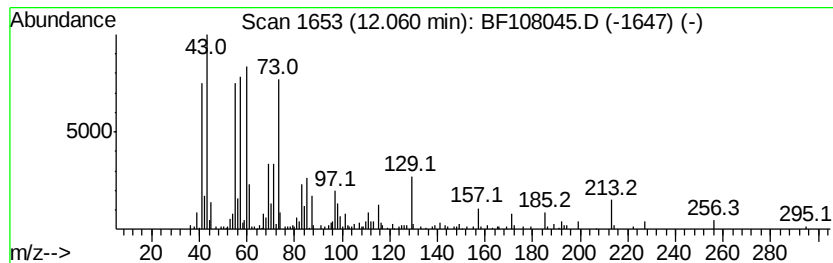
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	2.47 ng	317363	Phenanthrene-d10	11.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Octadecanoic acid	284	C18H36O2	000057-11-4	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108045.D
Acq On : 9 Aug 2018 11:51
Operator : JU/SJ
Sample : J4275-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

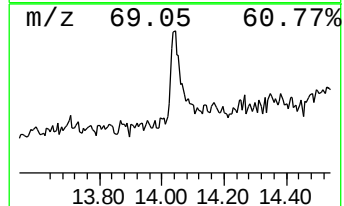
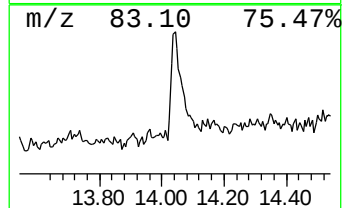
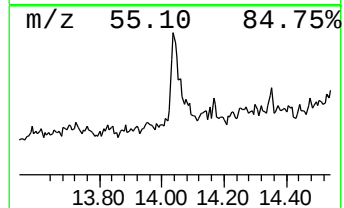
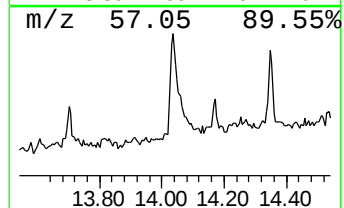
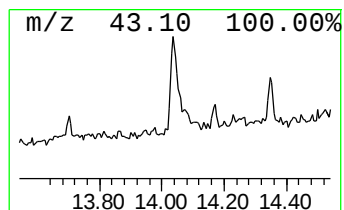
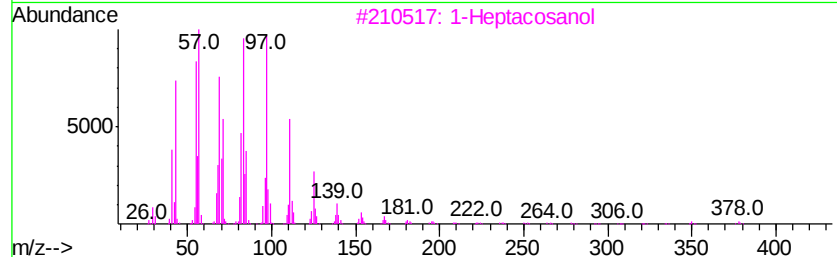
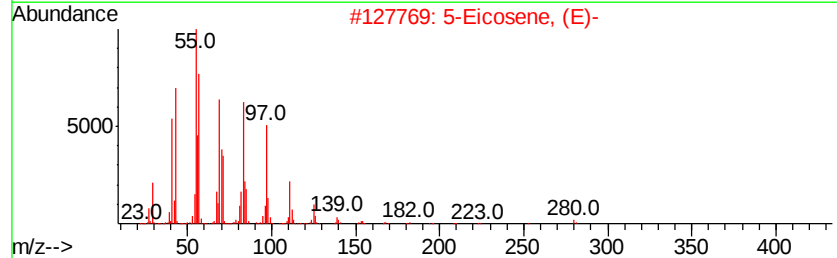
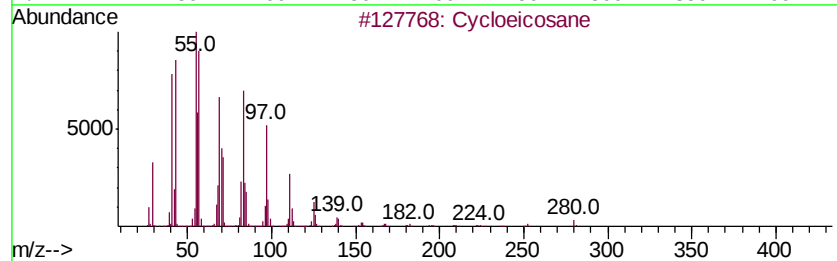
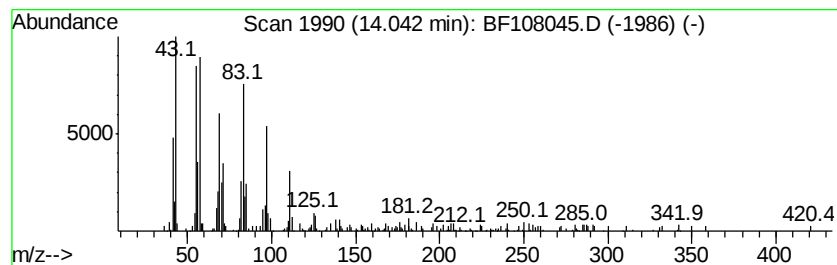
Instrument :
BNA_F
ClientSampleId :
CL-02-080718-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cycloeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	3.66 ng	364178	Chrysene-d12	14.21
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cycloeicosane	280 C20H40	000296-56-0 96
2		5-Eicosene, (E)-	280 C20H40	074685-30-6 95
3		1-Heptacosanol	396 C27H56O	002004-39-9 91
4		Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9 91
5		Heptadecyl heptafluorobutyrate	452 C21H35F7O2	959085-66-6 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108045.D
Acq On : 9 Aug 2018 11:51
Operator : JU/SJ
Sample : J4275-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-080718-A

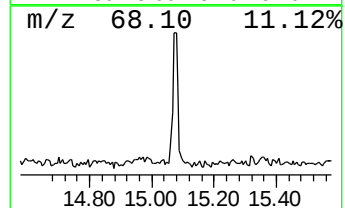
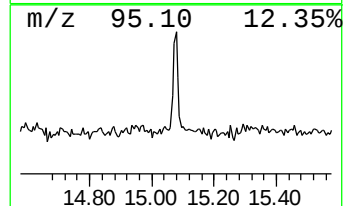
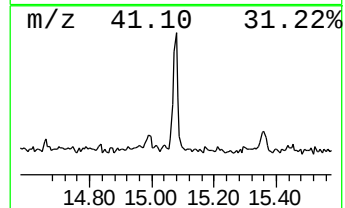
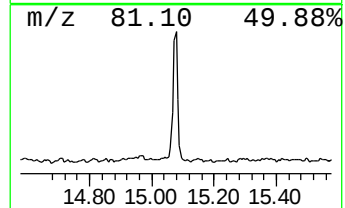
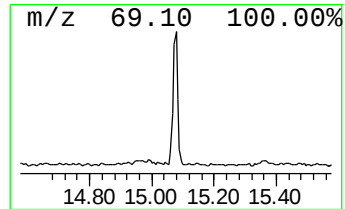
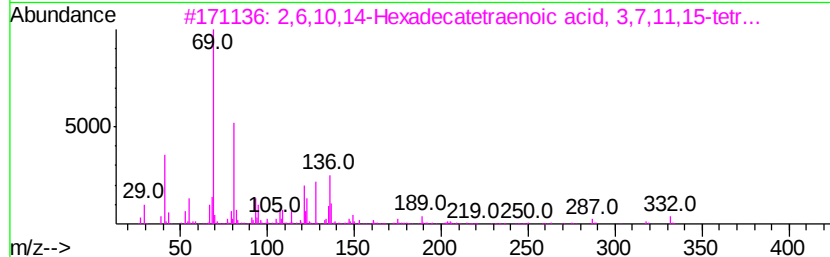
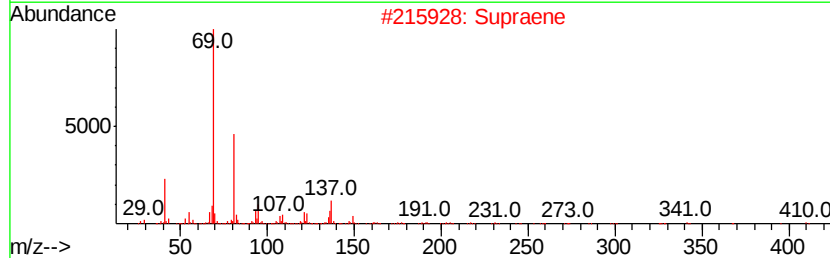
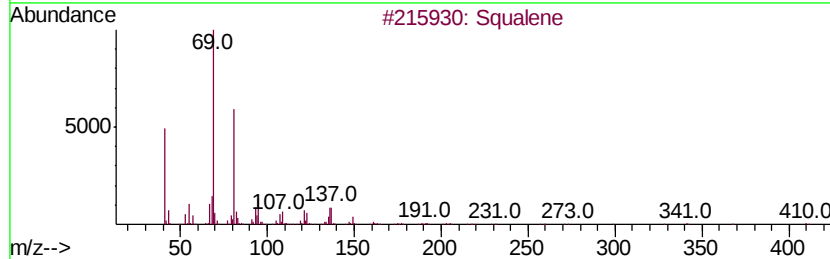
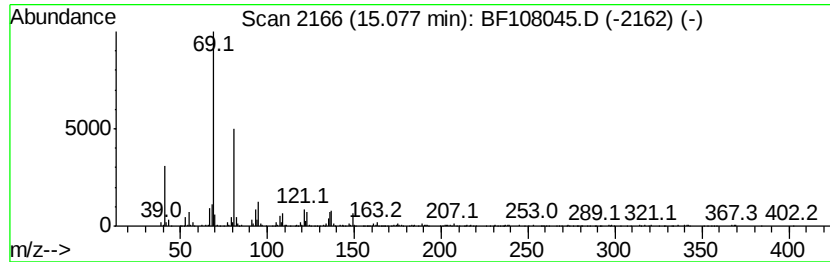
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	4.19 ng	414409	Perylene-d12	15.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
5		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080918\
Data File : BF108045.D
Acq On : 9 Aug 2018 11:51
Operator : JU/SJ
Sample : J4275-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-080718-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.25	14.9	ng	1347640	1	7.01	1802620	20.0
unknown6.78	6.78	75.3	ng	6785770	1	7.01	1802620	20.0
n-Hexadecanoic acid	12.06	2.5	ng	317363	4	11.55	2567030	20.0
Cycloeicosane	14.04	3.7	ng	364178	5	14.21	1990650	20.0
Squalene	15.08	4.2	ng	414409	6	15.77	1977300	20.0