

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082918\
 Data File : BF108615.D
 Acq On : 29 Aug 2018 20:06
 Operator : JU/SJ
 Sample : J4683-08
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 082718-SIDI-F-U-S

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_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	5.237	489	493	507	rBV	31501	47109	1.10%	0.208%
2	5.631	557	560	584	rBV	415257	896230	20.94%	3.952%
3	6.625	726	729	750	rBV	311063	721098	16.84%	3.180%
4	6.766	750	753	778	rVB	1566899	2056580	48.04%	9.068%
5	7.001	789	793	815	rVB	474566	711636	16.62%	3.138%
6	7.154	815	819	845	rBV	2674833	2900628	67.76%	12.790%
7	7.566	884	889	912	rBV	1918028	2454941	57.35%	10.825%
8	8.284	1007	1011	1035	rBV	592915	876738	20.48%	3.866%
9	9.354	1189	1193	1208	rBV	4204084	4280871	100.00%	18.876%
10	9.742	1256	1259	1279	rBV	177914	228604	5.34%	1.008%
11	10.042	1306	1310	1330	rVB	855097	901056	21.05%	3.973%
12	10.695	1418	1421	1428	rBV	69686	64733	1.51%	0.285%
13	10.836	1441	1445	1458	rBV	1183058	1397909	32.65%	6.164%
14	11.536	1561	1564	1578	rBV	638379	739866	17.28%	3.262%
15	13.124	1829	1834	1843	rBV	2528011	2562048	59.85%	11.297%
16	14.048	1985	1991	2002	rBV4	33590	100155	2.34%	0.442%
17	14.189	2011	2015	2027	rVB	643486	659447	15.40%	2.908%
18	15.024	2153	2157	2161	rBV	71383	80077	1.87%	0.353%
19	15.301	2201	2204	2209	rVB	38667	43079	1.01%	0.190%
20	15.713	2269	2274	2275	rBV	44823	54326	1.27%	0.240%
21	15.748	2275	2280	2294	rVB	426185	640002	14.95%	2.822%
22	16.183	2340	2354	2362	rVB	55231	142260	3.32%	0.627%
23	16.730	2441	2447	2454	rBV	41458	73752	1.72%	0.325%
24	17.377	2552	2557	2564	rVB5	22188	45716	1.07%	0.202%

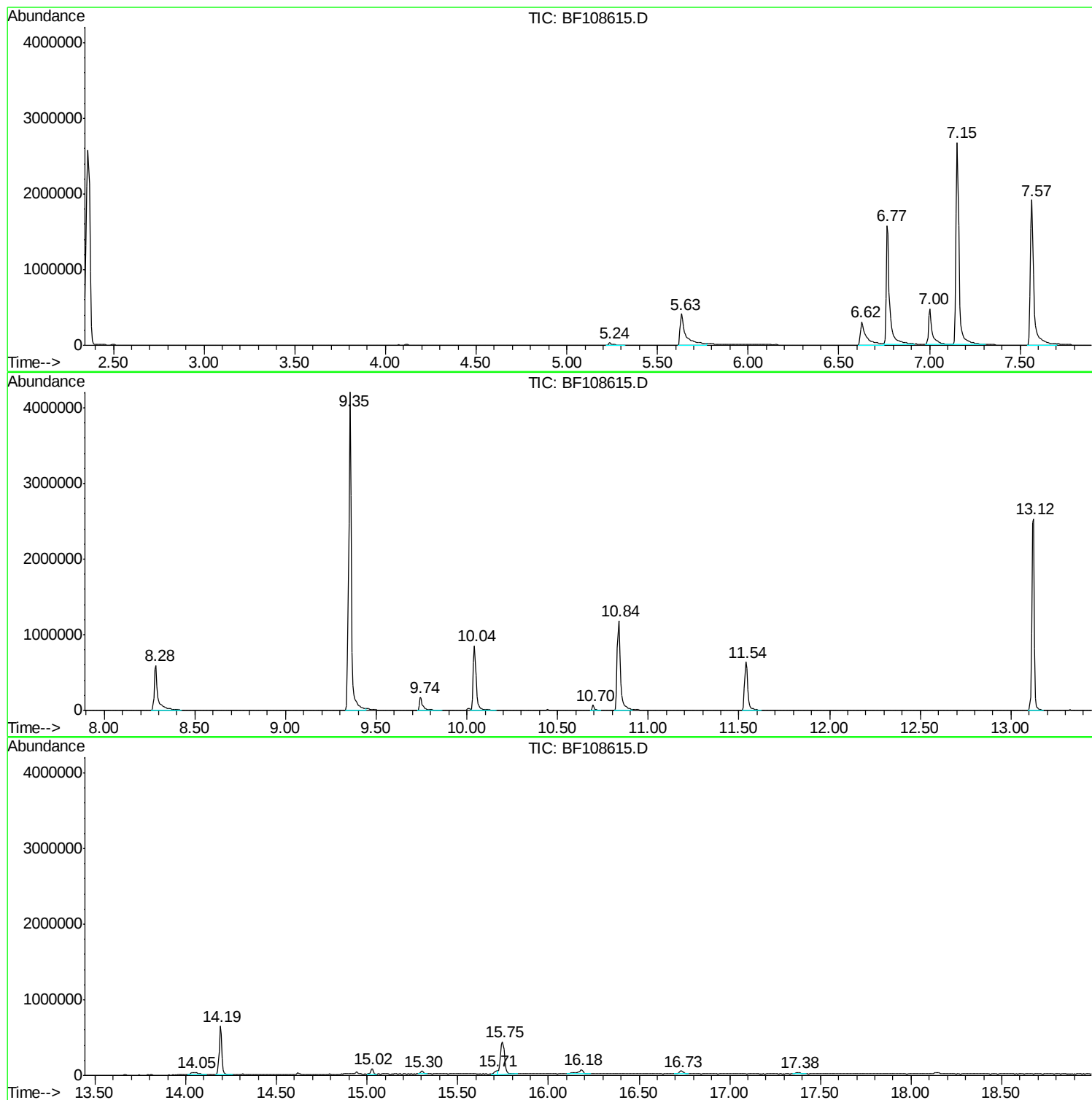
Sum of corrected areas: 22678861

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082918\
Data File : BF108615.D
Acq On : 29 Aug 2018 20:06
Operator : JU/SJ
Sample : J4683-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082718-SIDI-F-U-S

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\BF082918\
Data File : BF108615.D
Acq On : 29 Aug 2018 20:06
Operator : JU/SJ
Sample : J4683-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082718-SIDI-F-U-S

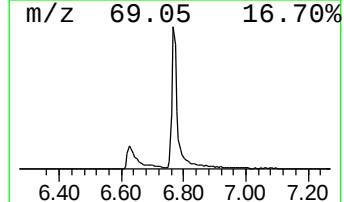
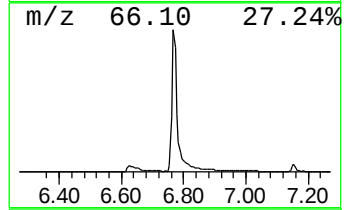
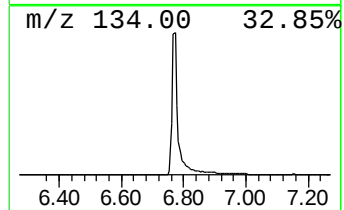
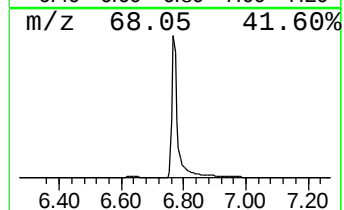
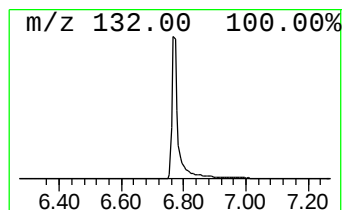
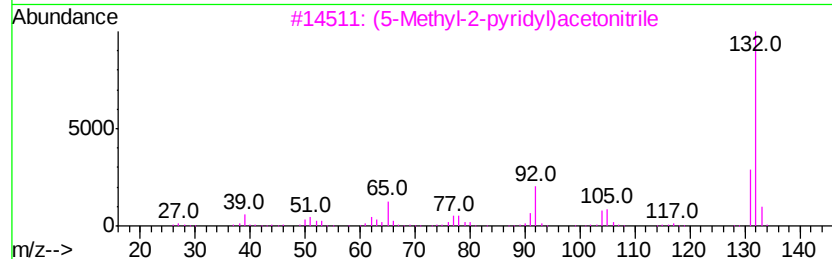
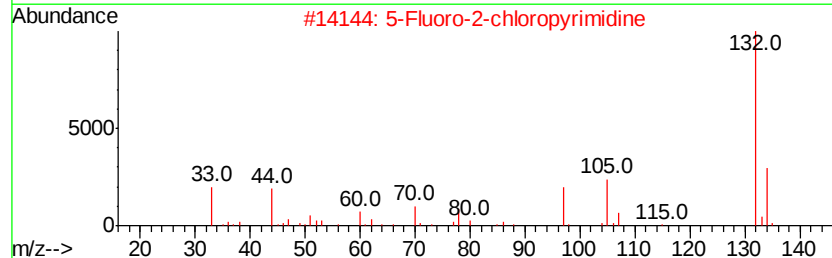
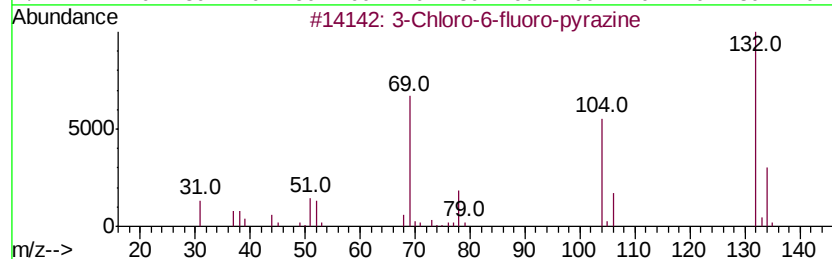
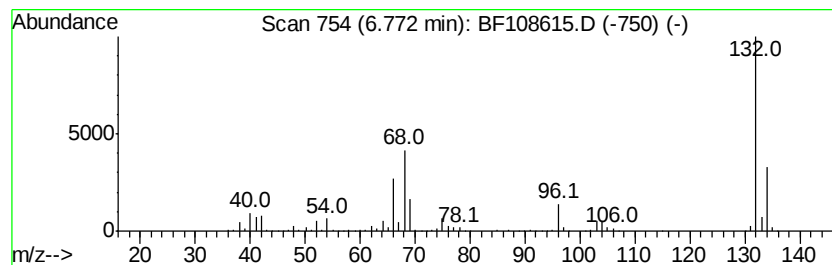
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	57.80 ng	2056580	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082918\
Data File : BF108615.D
Acq On : 29 Aug 2018 20:06
Operator : JU/SJ
Sample : J4683-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

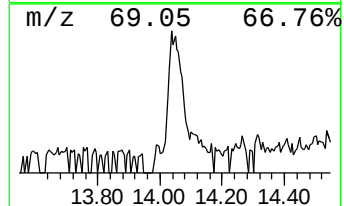
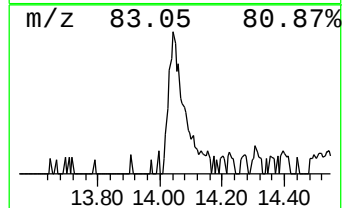
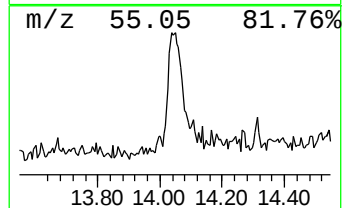
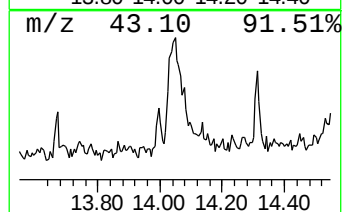
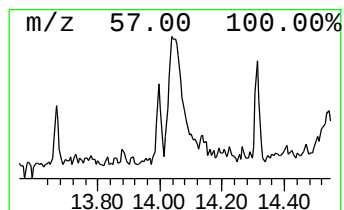
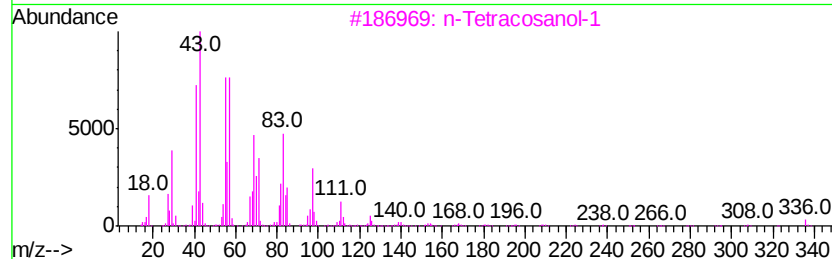
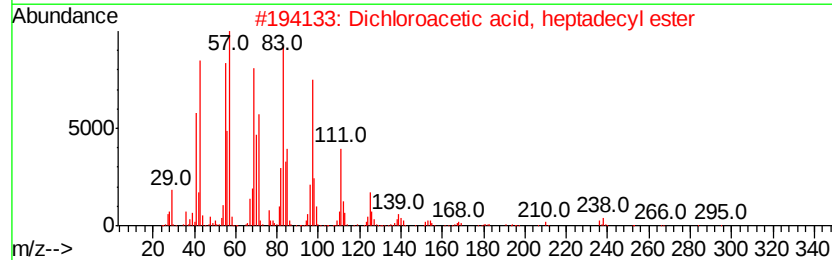
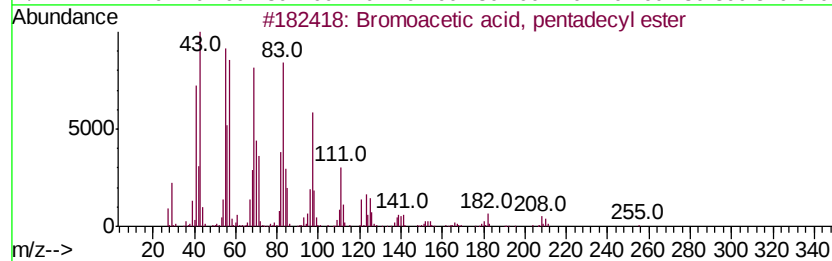
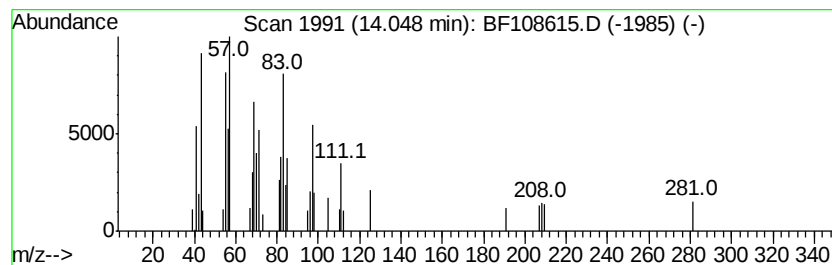
Instrument :
BNA_F
ClientSampleId :
082718-SIDI-F-U-S

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 3 Bromoacetic acid, pentadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.05	3.04 ng	100155	Chrysene-d12	14.19		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	87
4		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	87
5		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082918\
Data File : BF108615.D
Acq On : 29 Aug 2018 20:06
Operator : JU/SJ
Sample : J4683-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082718-SIDI-F-U-S

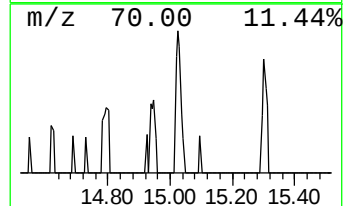
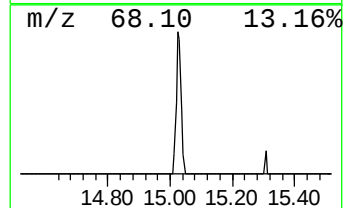
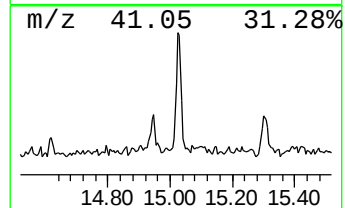
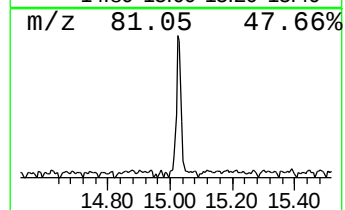
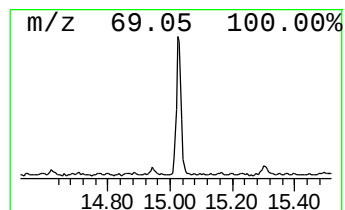
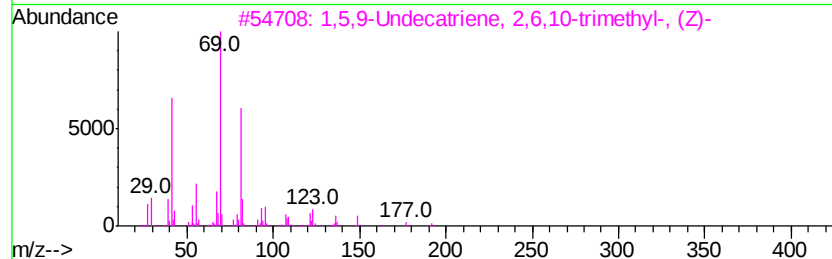
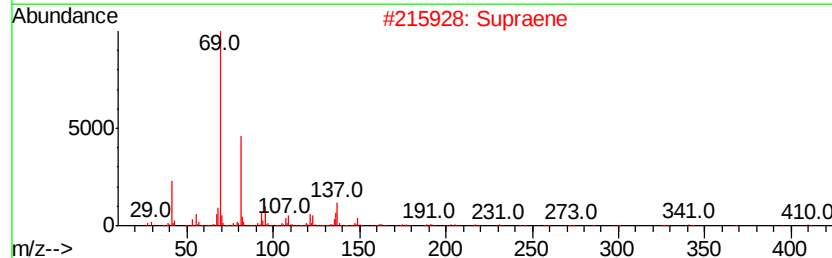
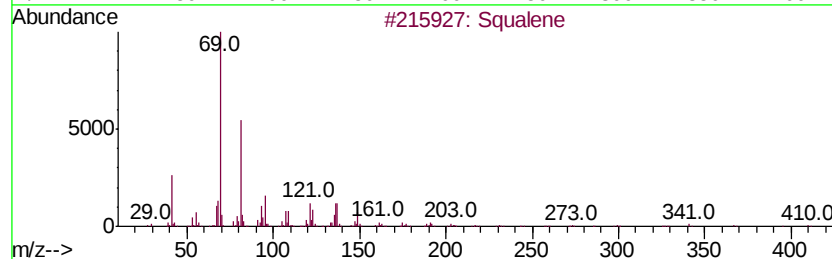
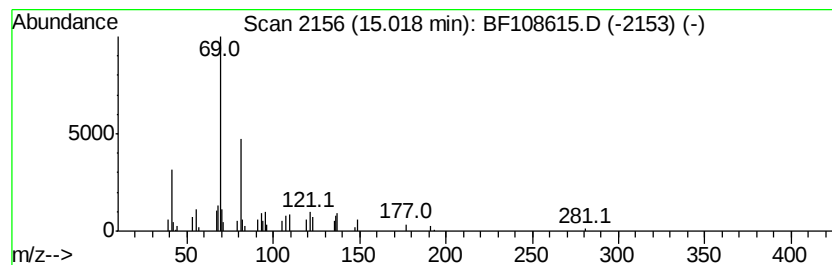
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.50 ng	80077	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene		410	C30H50	000111-02-4	91
2	Supraene		410	C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...		192	C14H24	062951-96-6	80
4	trans-Farnesol		222	C15H26O	000106-28-5	72
5	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082918\
Data File : BF108615.D
Acq On : 29 Aug 2018 20:06
Operator : JU/SJ
Sample : J4683-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082718-SIDI-F-U-S

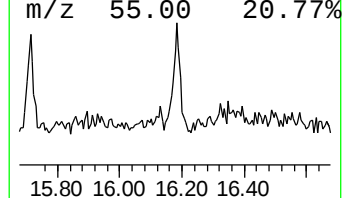
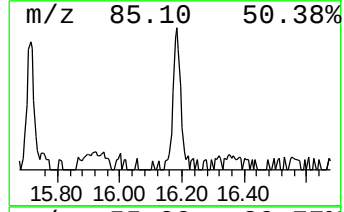
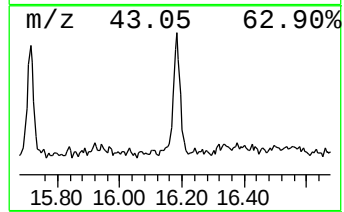
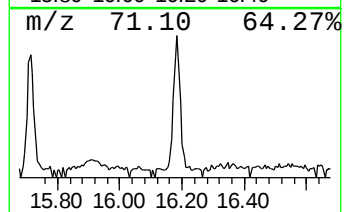
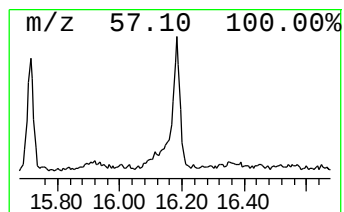
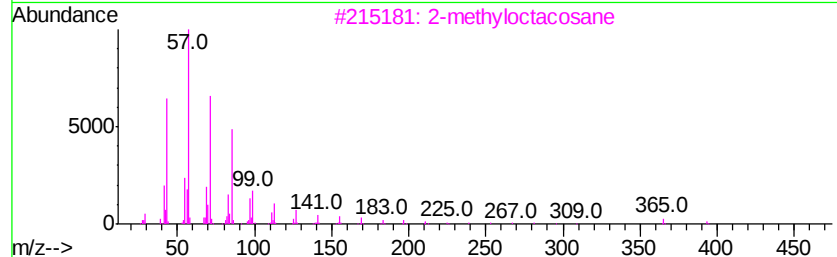
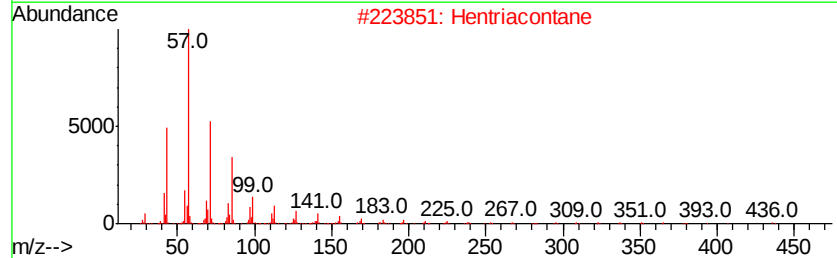
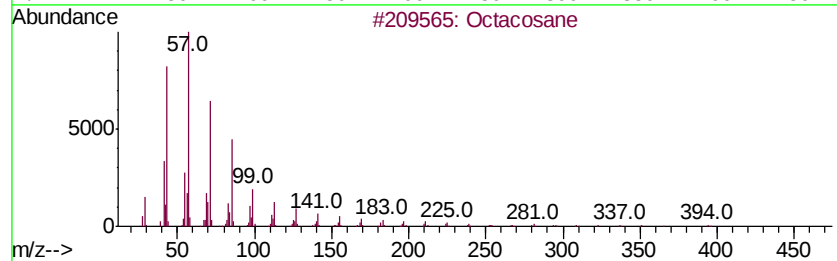
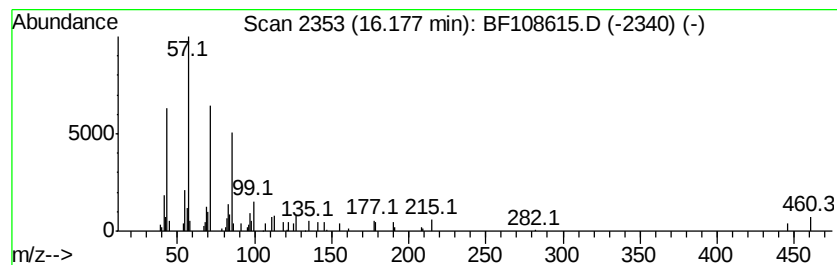
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	4.45 ng	142260	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Hentriacontane		437	C31H64	000630-04-6	87
3	2-methyloctacosane		408	C29H60	1000376-72-8	86
4	Heneicosane		296	C21H44	000629-94-7	83
5	Tetracosane		338	C24H50	000646-31-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082918\
Data File : BF108615.D
Acq On : 29 Aug 2018 20:06
Operator : JU/SJ
Sample : J4683-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082718-SIDI-F-U-S

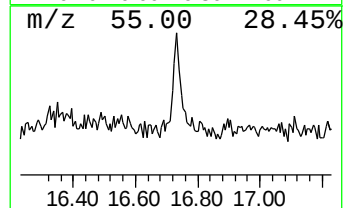
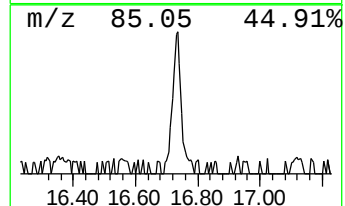
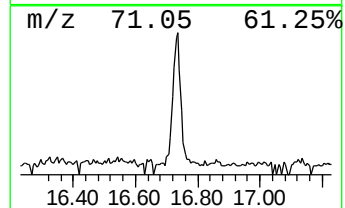
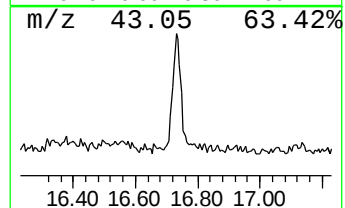
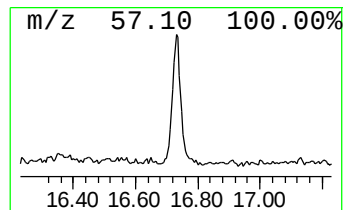
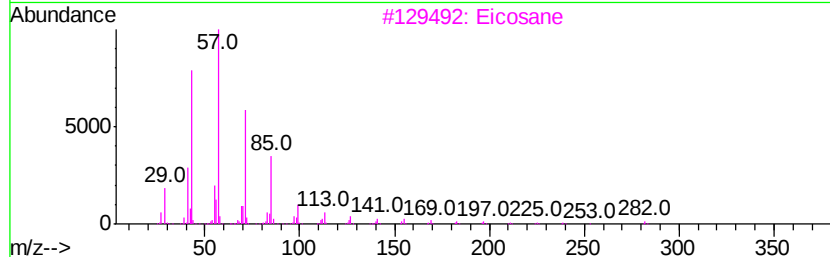
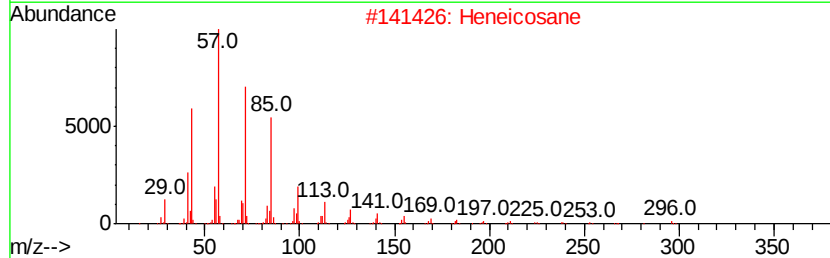
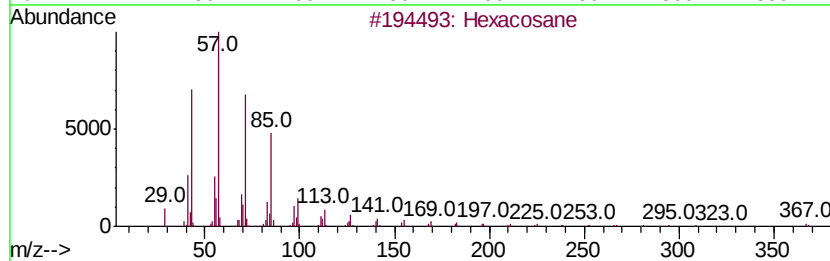
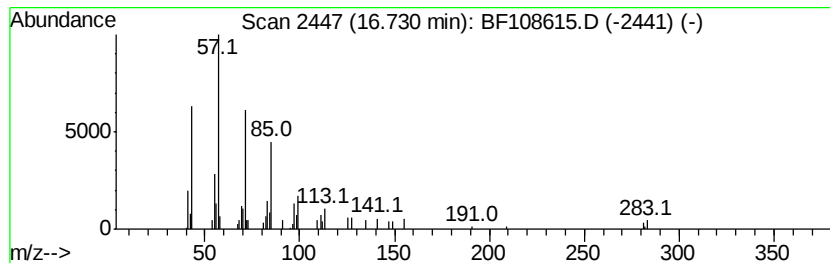
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.30 ng	73752	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Eicosane	282	C20H42	000112-95-8	90
4		Octacosane	394	C28H58	000630-02-4	87
5		Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082918\
Data File : BF108615.D
Acq On : 29 Aug 2018 20:06
Operator : JU/SJ
Sample : J4683-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
082718-SIDI-F-U-S

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
unknown6.77	6.77	57.8	ng	2056580	1	7.00	711636	20.0
Bromoacetic acid,...	14.05	3.0	ng	100155	5	14.19	659447	20.0
Squalene	15.02	2.5	ng	80077	6	15.75	640002	20.0
Octacosane	16.18	4.5	ng	142260	6	15.75	640002	20.0
Hexacosane	16.73	2.3	ng	73752	6	15.75	640002	20.0