

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
 Data File : BF108517.D
 Acq On : 27 Aug 2018 18:15
 Operator : JU/SJ
 Sample : J4538-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VSS4

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	5.242	490	494	501	rBV	81846	96511	3.56%	0.328%
2	5.625	555	559	563	rBV	2133932	2110675	77.88%	7.183%
3	6.625	724	729	732	rBV	2238105	2265413	83.59%	7.709%
4	6.772	749	754	757	rBV	2575878	2290318	84.51%	7.794%
5	7.001	789	793	796	rBV	845745	760576	28.06%	2.588%
6	7.154	815	819	823	rBV	2069162	1808806	66.74%	6.155%
7	7.560	883	888	891	rBV	1604172	1464624	54.04%	4.984%
8	8.283	1007	1011	1014	rBV	1116513	943707	34.82%	3.211%
9	9.354	1189	1193	1202	rVB	3178506	2710196	100.00%	9.223%
10	9.742	1256	1259	1265	rBV	173127	147604	5.45%	0.502%
11	10.042	1305	1310	1320	rVB	1198632	1067379	39.38%	3.632%
12	10.836	1441	1445	1453	rBV	1612232	1406340	51.89%	4.786%
13	11.460	1548	1551	1555	rBV3	41395	44727	1.65%	0.152%
14	11.536	1561	1564	1567	rBV	1063481	951034	35.09%	3.236%
15	11.566	1567	1569	1572	rVB	67478	57480	2.12%	0.196%
16	12.042	1647	1650	1655	rBV	109560	106294	3.92%	0.362%
17	13.124	1830	1834	1837	rBV	2109915	1848820	68.22%	6.292%
18	13.554	1904	1907	1911	rVB	60112	45419	1.68%	0.155%
19	13.795	1944	1948	1954	rVB	79629	78528	2.90%	0.267%
20	14.001	1980	1983	1985	rBV	42548	38457	1.42%	0.131%
21	14.030	1985	1988	1998	rVV3	93651	192120	7.09%	0.654%
22	14.124	2001	2004	2011	rVB3	28230	33704	1.24%	0.115%
23	14.189	2011	2015	2019	rBV	847634	794343	29.31%	2.703%
24	14.624	2086	2089	2093	rVB	111299	100616	3.71%	0.342%
25	14.677	2093	2098	2104	rBV3	54693	114807	4.24%	0.391%
26	14.948	2140	2144	2148	rVB	62407	72111	2.66%	0.245%
27	15.036	2155	2159	2162	rVB	93528	103020	3.80%	0.351%
28	15.112	2167	2172	2179	rVB	369707	403294	14.88%	1.372%
29	15.312	2202	2206	2211	rVB	348325	414747	15.30%	1.411%
30	15.377	2212	2217	2229	rBV2	217031	654976	24.17%	2.229%
31	15.748	2271	2280	2286	rBV	537262	823742	30.39%	2.803%
32	15.871	2298	2301	2304	rVB3	51126	57344	2.12%	0.195%
33	15.948	2309	2314	2319	rVB	154733	218638	8.07%	0.744%
34	16.195	2350	2356	2363	rVB	613420	1040243	38.38%	3.540%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

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

35	16.330	2369	2379	2386	rBV5	73422	288148	10.63%	0.981%
36	16.471	2397	2403	2407	rBV	121372	229058	8.45%	0.779%
37	16.512	2407	2410	2416	rVB2	52371	102185	3.77%	0.348%
38	16.748	2445	2450	2455	rVB3	57931	101784	3.76%	0.346%
39	17.071	2500	2505	2512	rVB	141391	292516	10.79%	0.995%
40	17.395	2550	2560	2573	rBV	198516	566885	20.92%	1.929%
41	17.571	2581	2590	2608	rBV7	137709	636834	23.50%	2.167%
42	18.012	2657	2665	2681	rBV7	228106	1039847	38.37%	3.539%
43	18.218	2697	2700	2708	rVB3	87733	176733	6.52%	0.601%
44	18.406	2728	2732	2739	rVB6	65306	148414	5.48%	0.505%
45	18.536	2743	2754	2761	rBV5	133739	450316	16.62%	1.532%
46	18.953	2820	2825	2828	rBV6	41346	86058	3.18%	0.293%

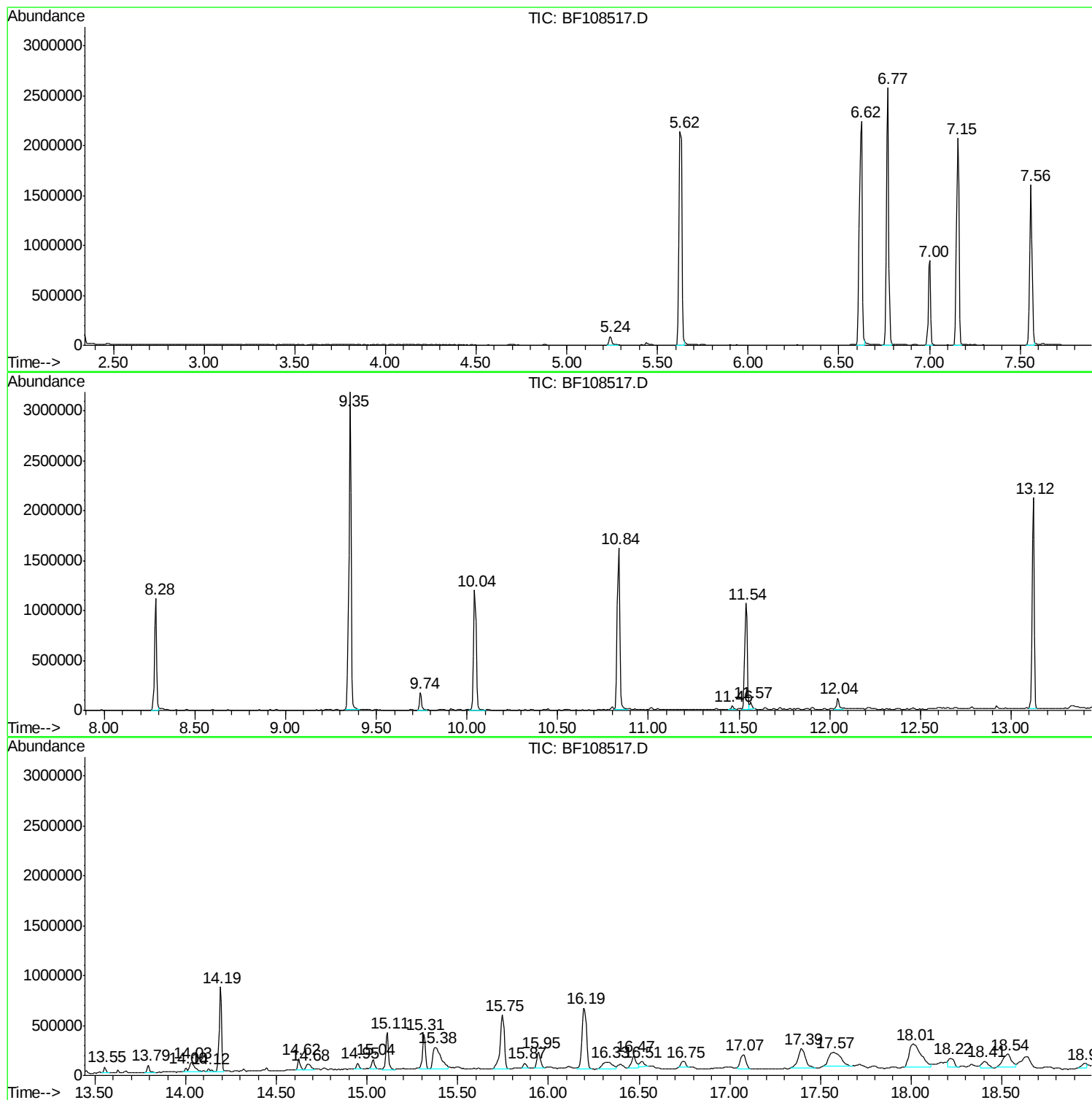
Sum of corrected areas: 29385391

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
VSS4

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\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

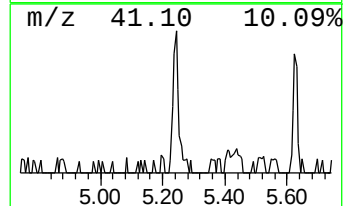
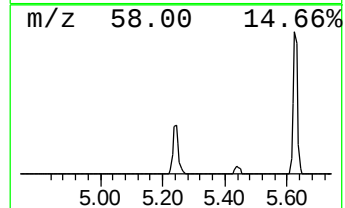
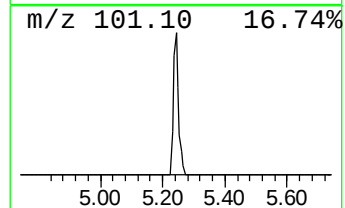
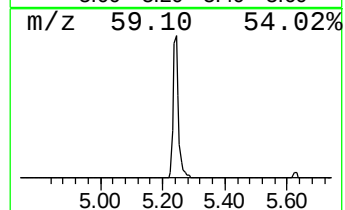
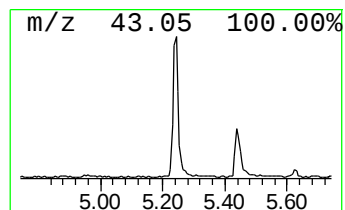
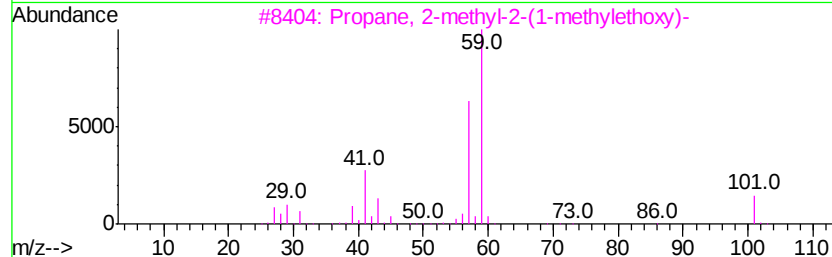
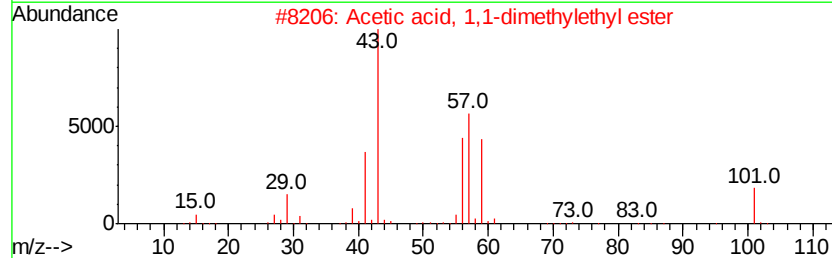
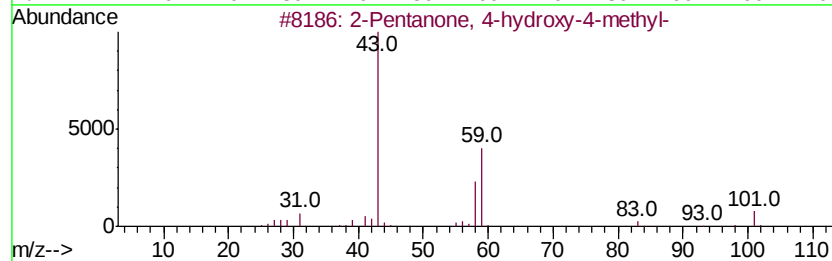
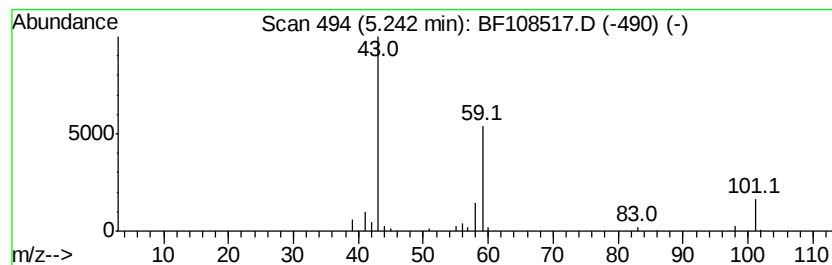
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	2.54 ng	96511	1,4-Dichlorobenzene-d4	7.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

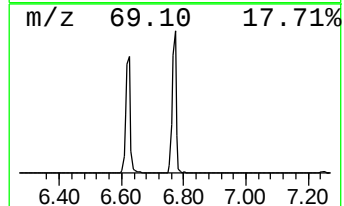
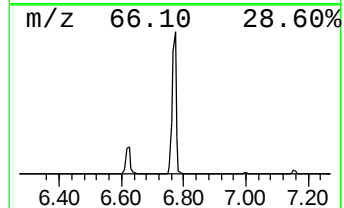
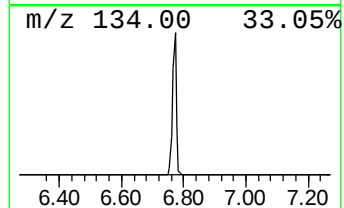
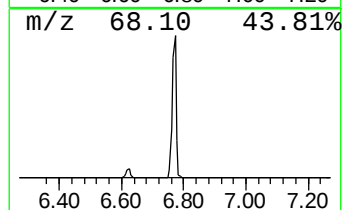
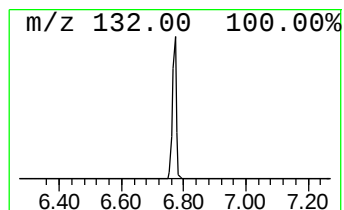
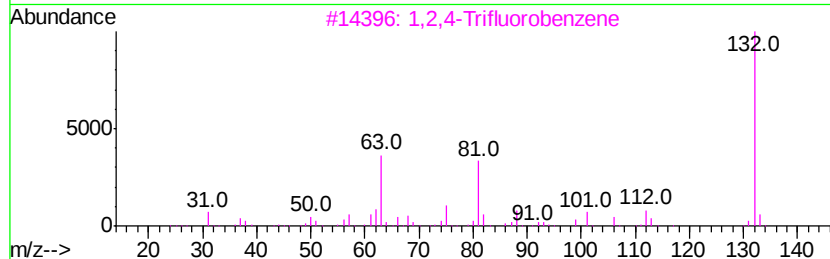
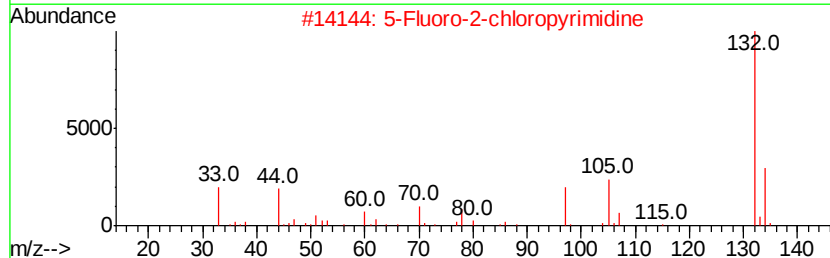
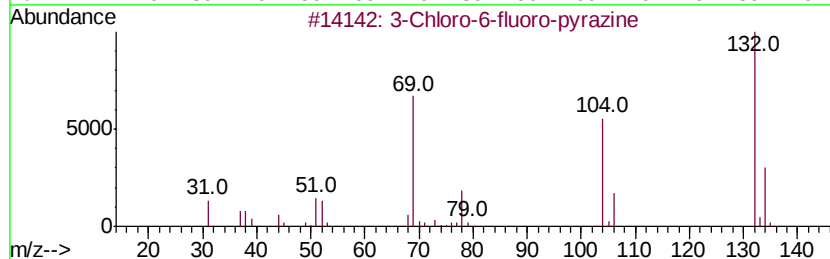
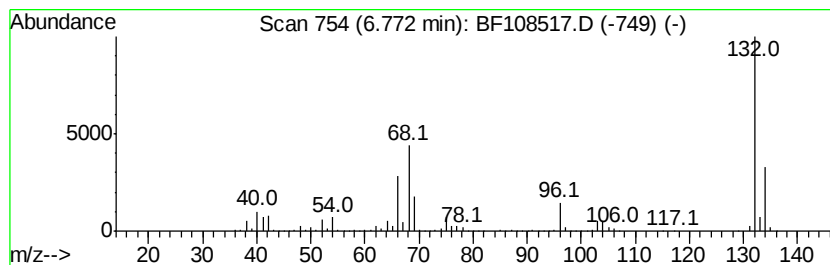
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	60.23 ng	2290320	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	16
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	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\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

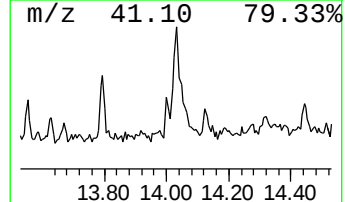
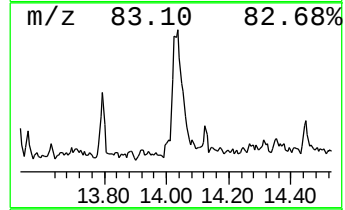
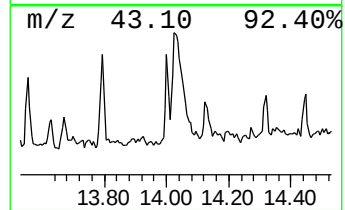
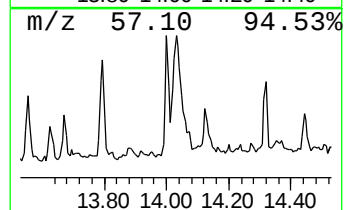
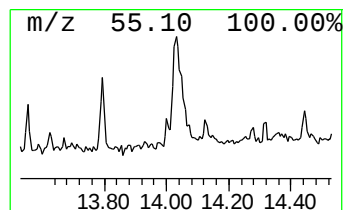
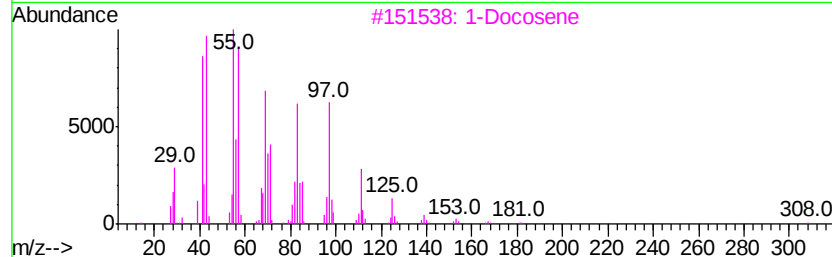
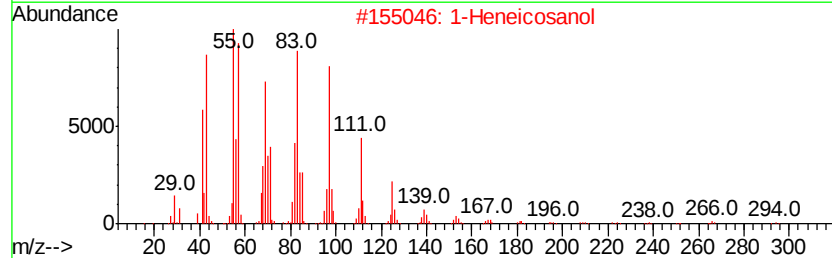
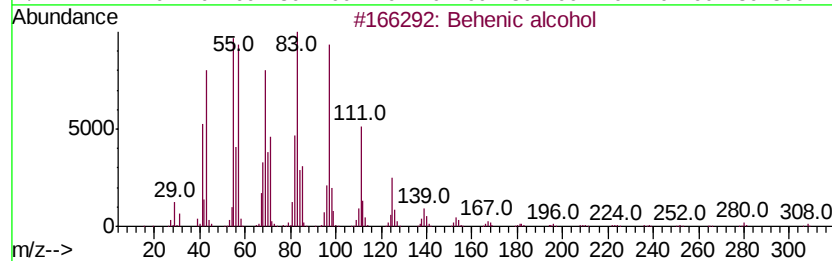
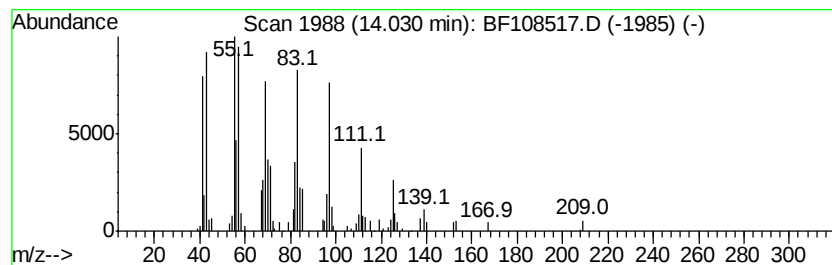
Instrument :
BNA_F
ClientSampleId :
VSS4

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 Behenic alcohol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.03	4.84 ng	192120	Chrysene-d12	14.19	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	90
3	1-Docosene	308	C22H44	001599-67-3	76
4	Octacosyl heptafluorobutyrte	606	C32H57F7O2	1000351-83-6	70
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

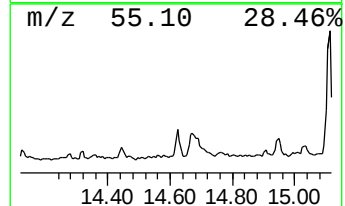
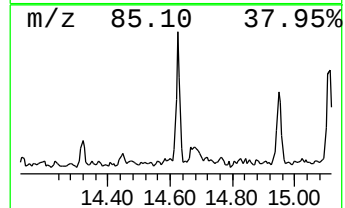
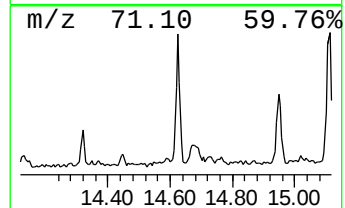
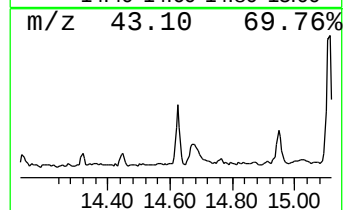
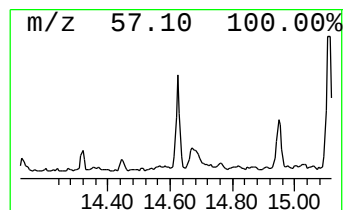
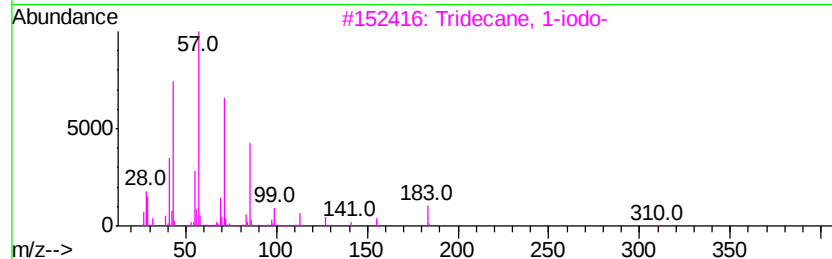
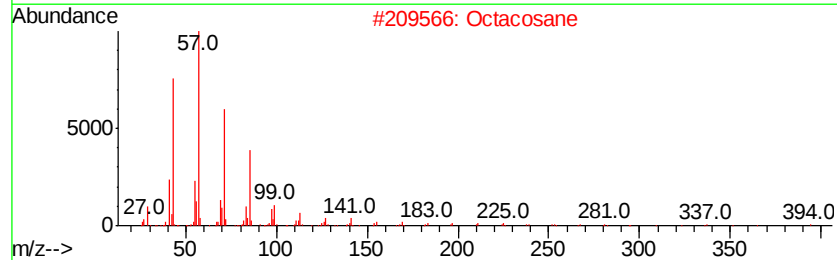
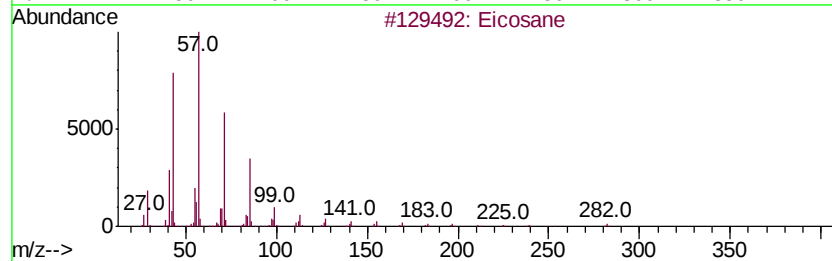
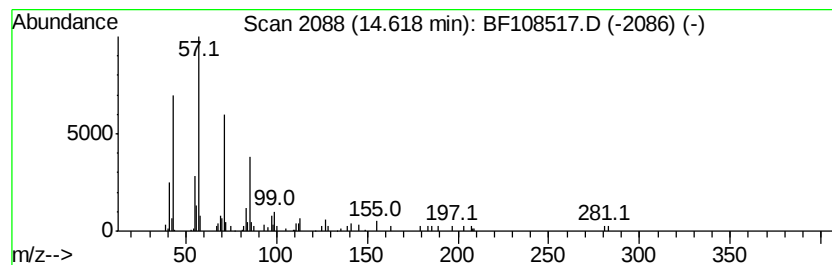
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.53 ng	100616	Chrysene-d12	14.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	96
2	Octacosane		394	C28H58	000630-02-4	91
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	91
4	Heptadecane		240	C17H36	000629-78-7	91
5	Tetracosane		338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

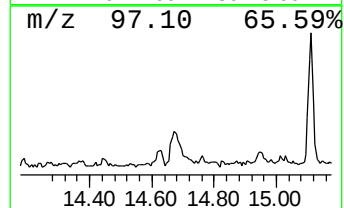
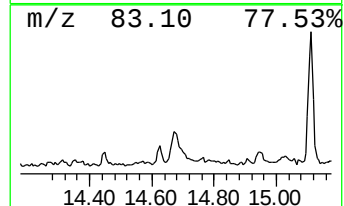
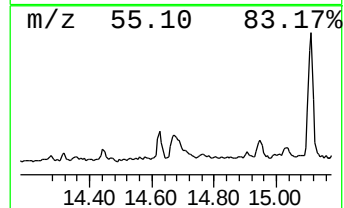
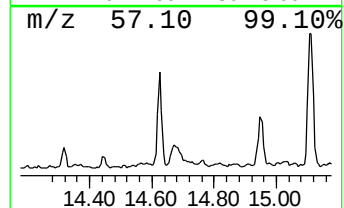
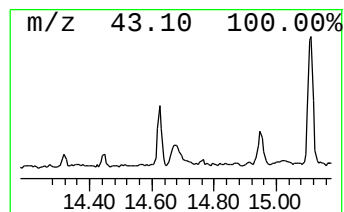
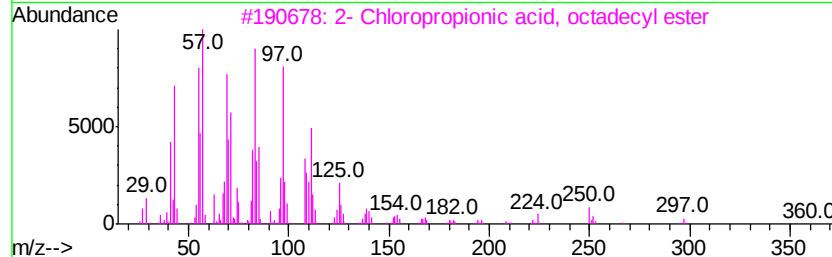
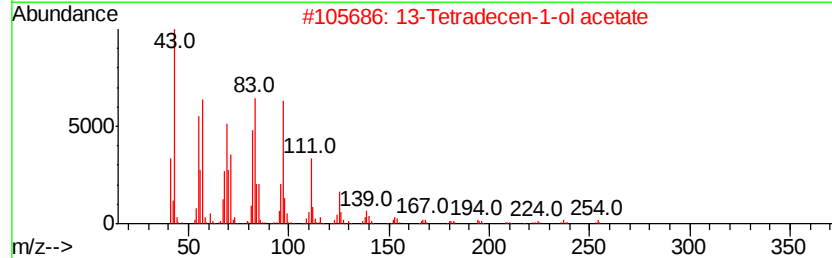
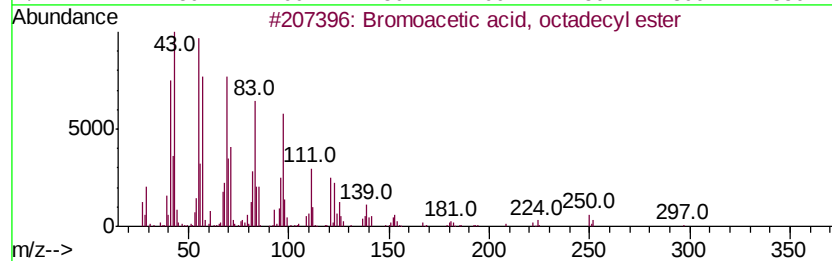
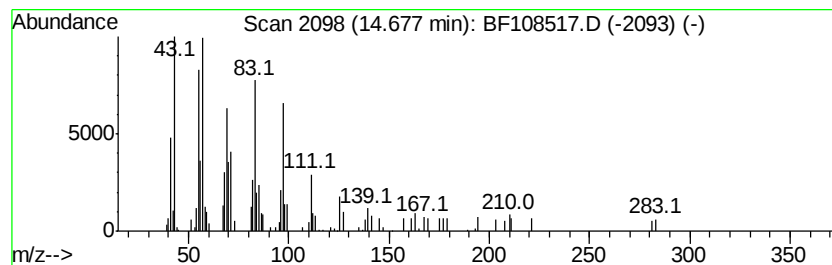
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Bromoacetic acid, octadecyl... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	2.89 ng	114807	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	91
3		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
4		Behenic alcohol	326	C22H46O	000661-19-8	87
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

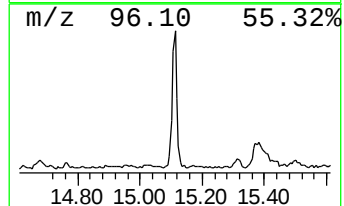
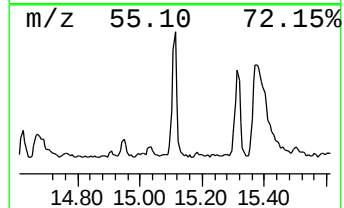
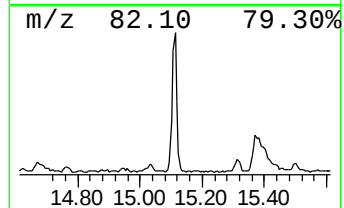
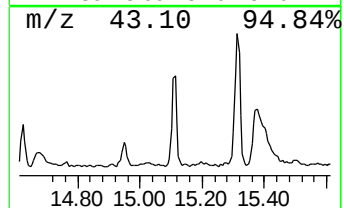
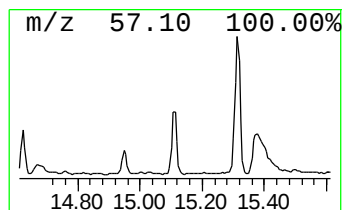
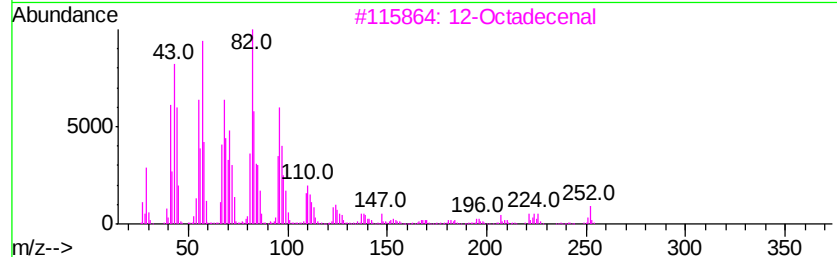
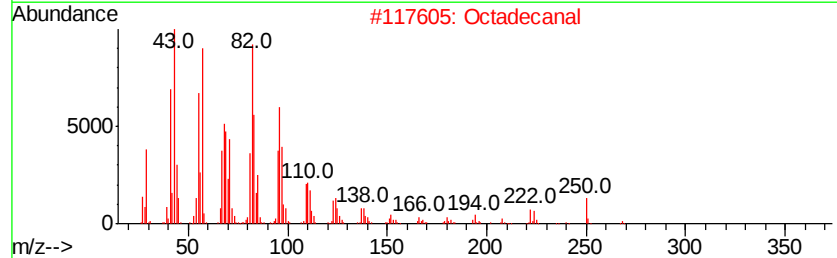
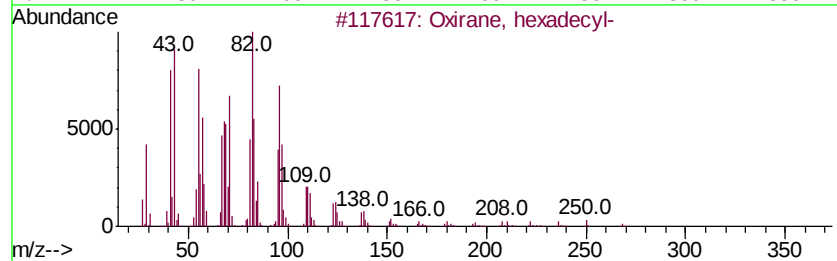
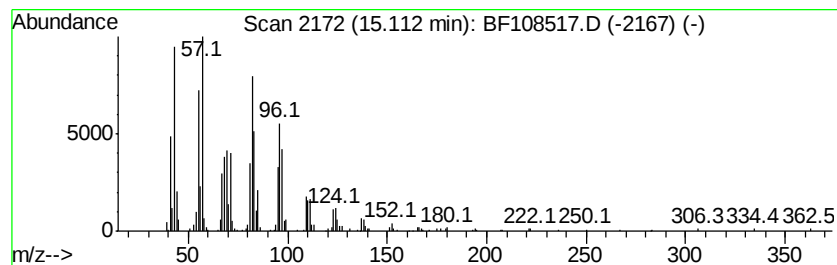
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.11	9.79 ng	403294	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Octadecanal	268	C18H36O	000638-66-4	91
3		12-Octadecenal	266	C18H34O	056554-91-7	90
4		13-Octadecenal	266	C18H34O	056554-90-6	90
5		1,13-Tetradecadiene	194	C14H26	021964-49-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

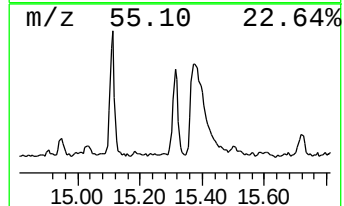
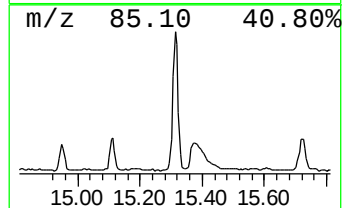
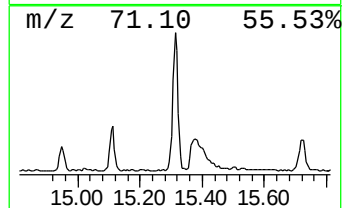
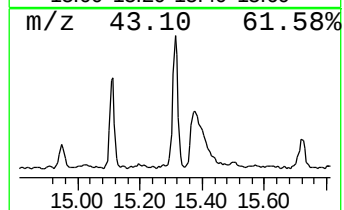
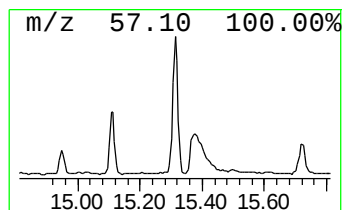
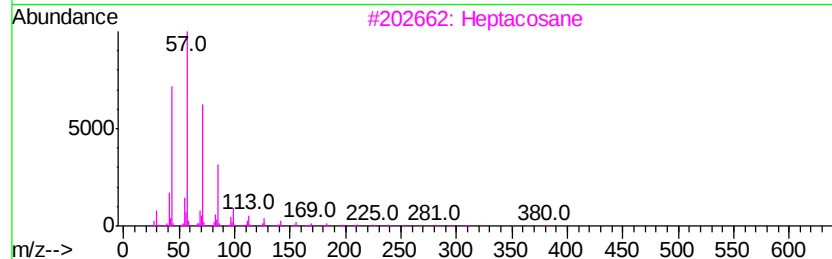
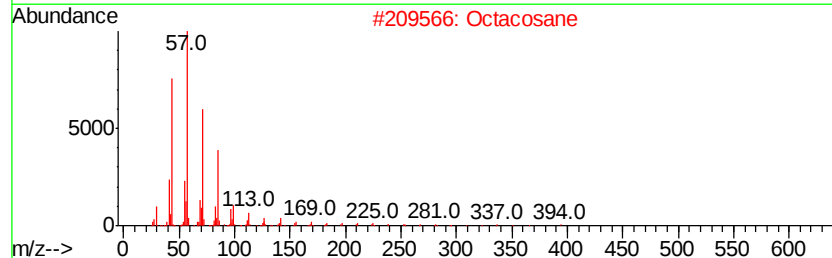
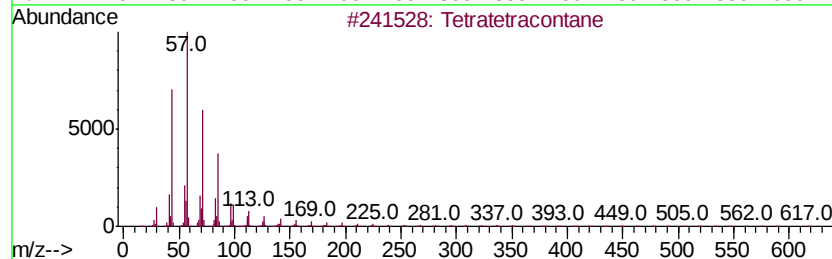
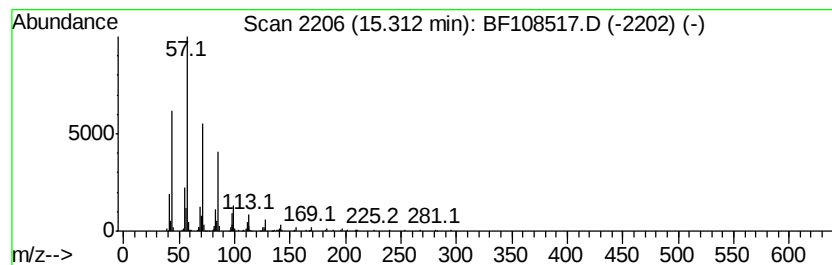
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	10.07 ng	414747	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

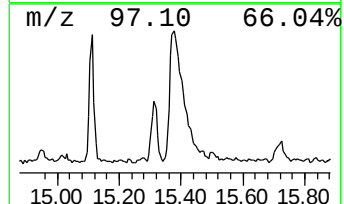
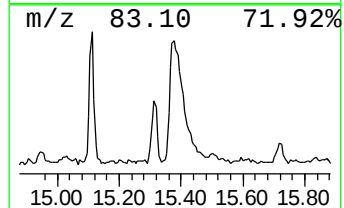
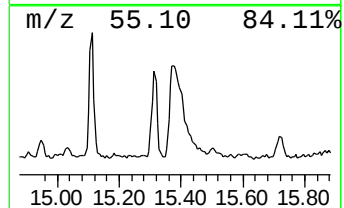
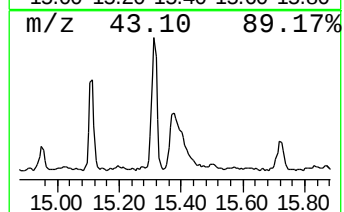
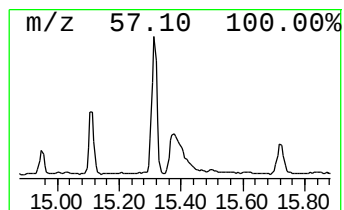
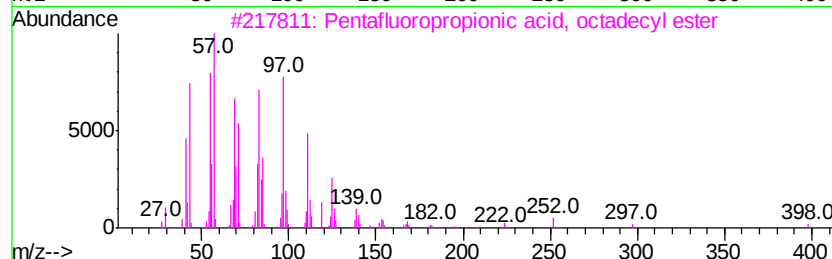
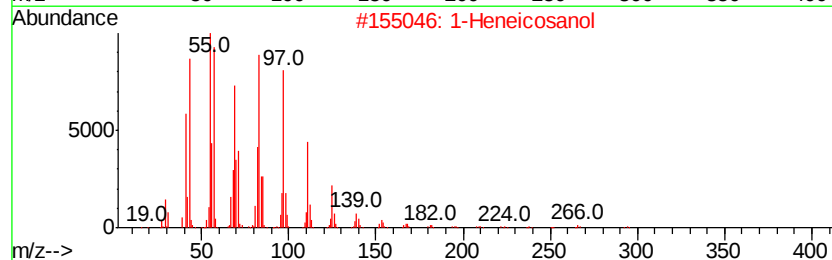
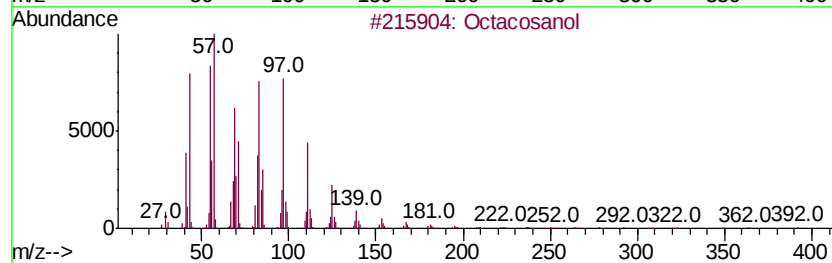
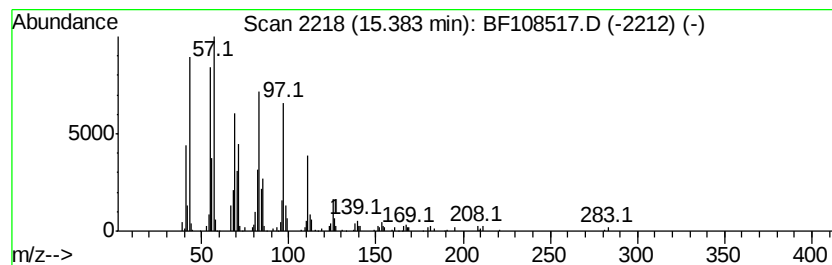
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	15.90 ng	654976	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Pentafluoropropionic acid, octadecyl...	416	C21H37F5O2	959261-25-7	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Heptafluorobutyric acid, n-octadecyl...	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

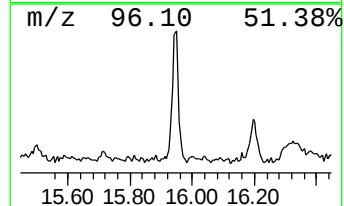
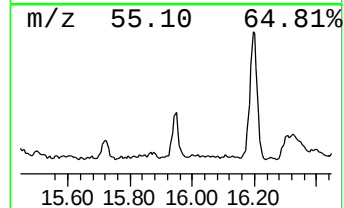
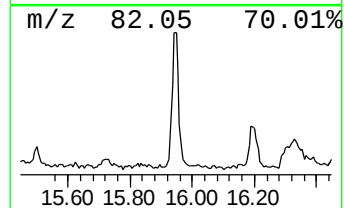
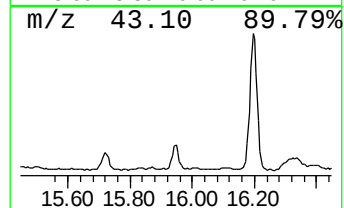
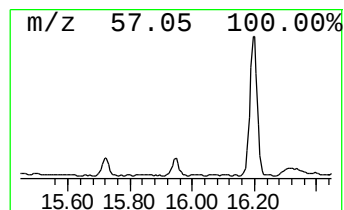
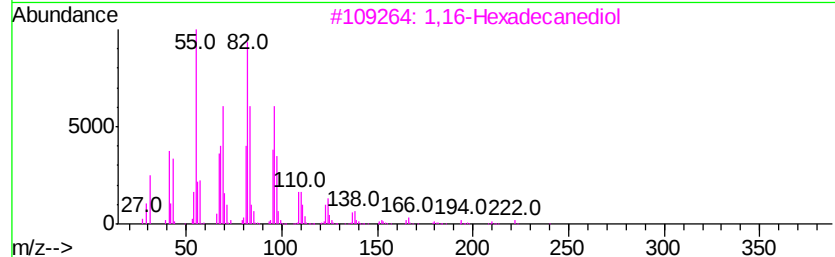
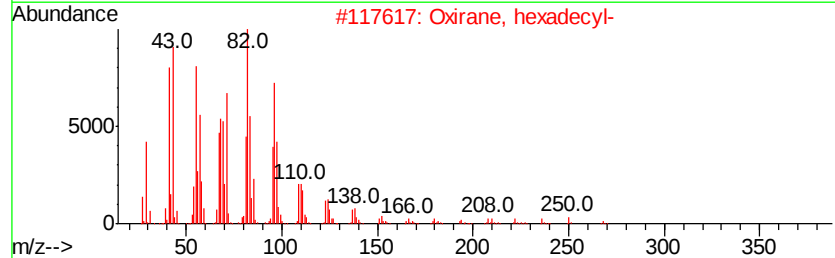
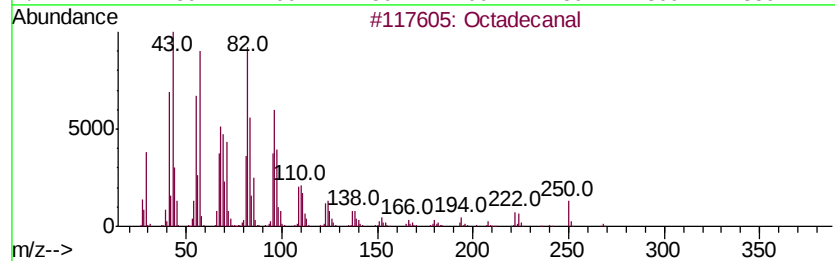
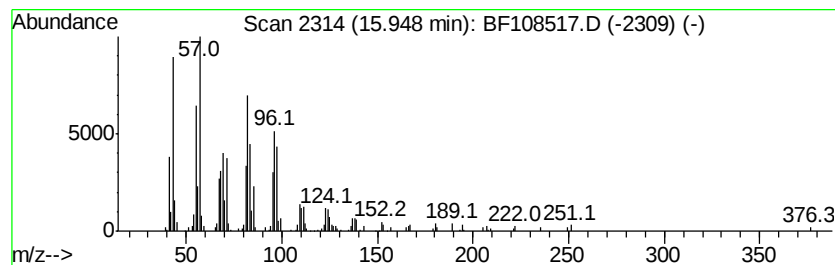
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	5.31 ng	218638	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	83
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
3		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	81
4		1,19-Eicosadiene	278	C20H38	014811-95-1	81
5		Stearic acid, 9-hexadecenyl este...	507	C34H66O2	022393-91-5	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

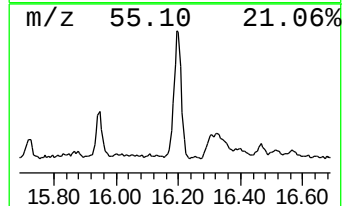
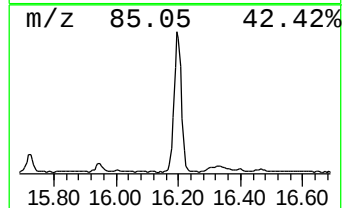
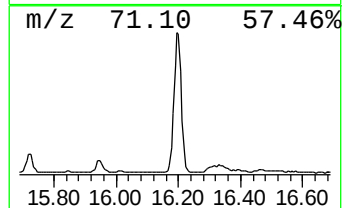
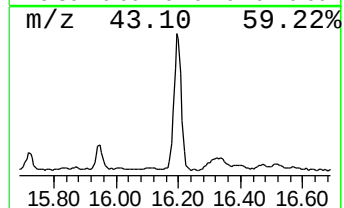
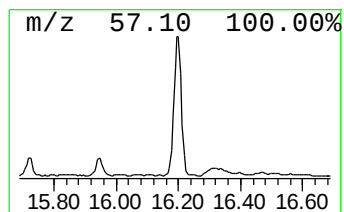
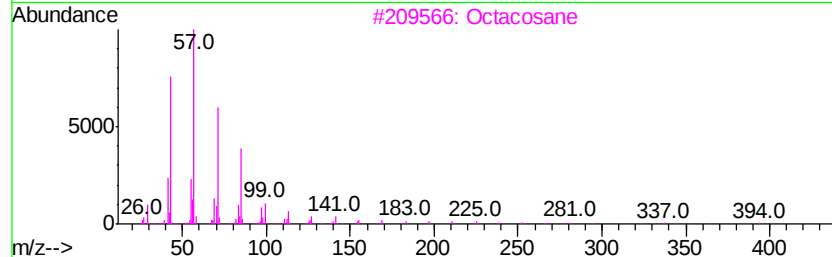
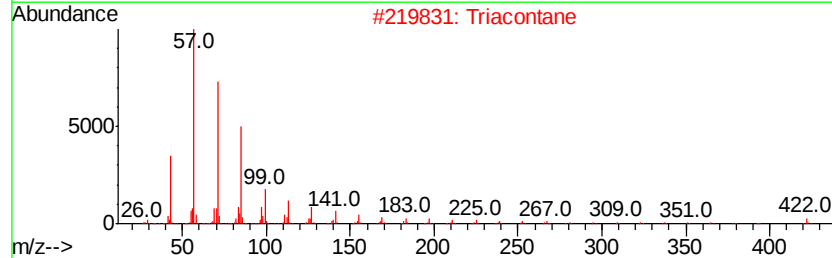
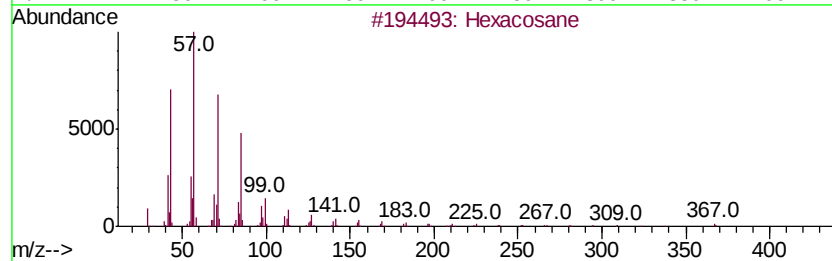
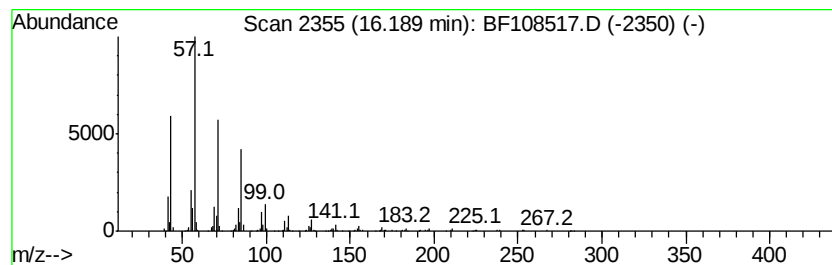
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	25.26 ng	1040240	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Triacontane	422	C30H62	000638-68-6	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

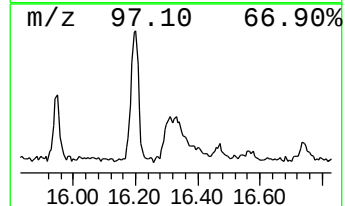
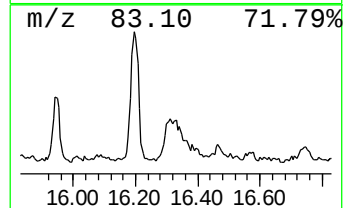
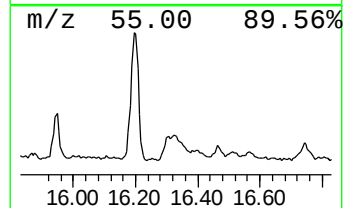
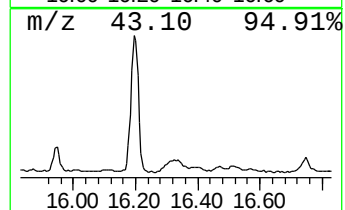
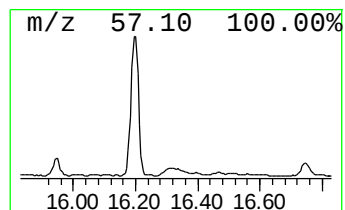
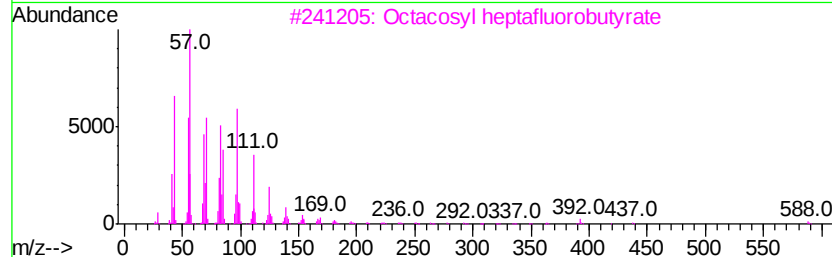
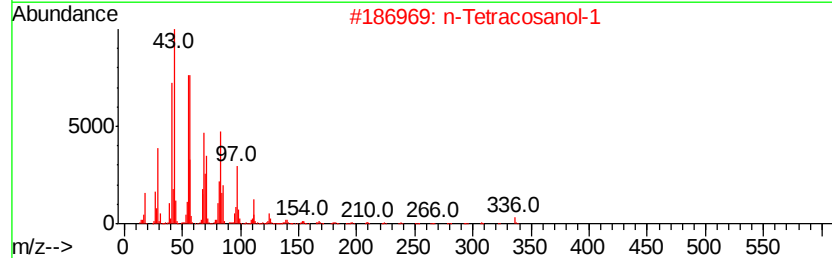
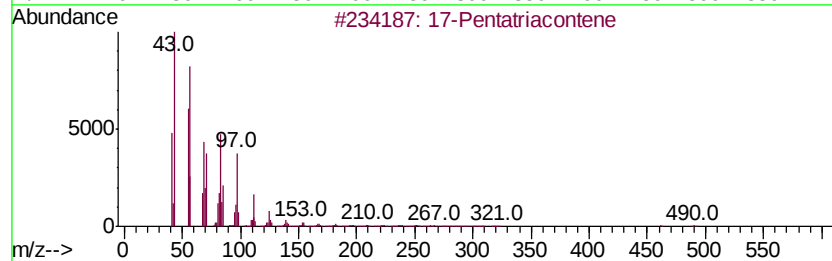
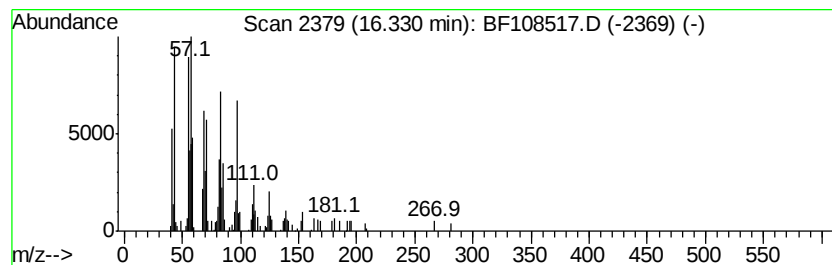
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 17-Pentatriacontene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	7.00 ng	288148	Perylene-d12	15.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	64
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	60
3			Octacosyl heptafluorobutvrate	606	C32H57F7O2	1000351-83-6	60
4			1-Hexacosanol	382	C26H54O	000506-52-5	60
5			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

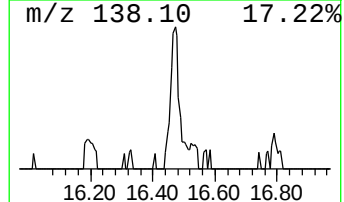
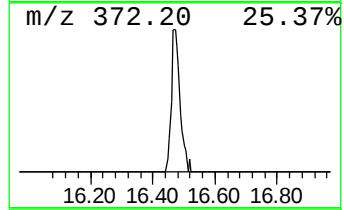
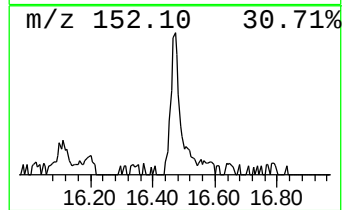
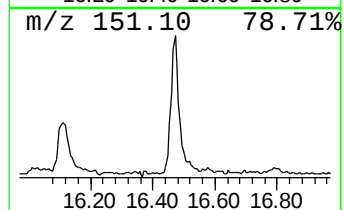
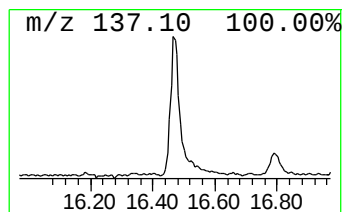
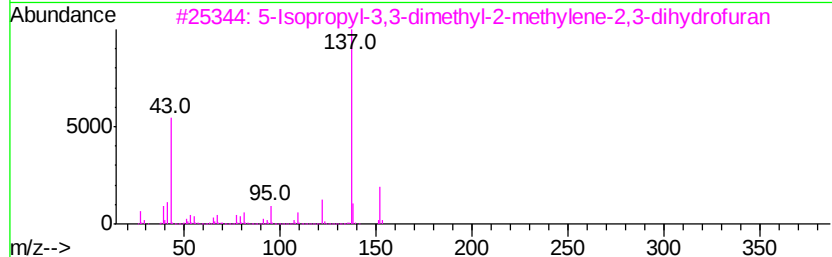
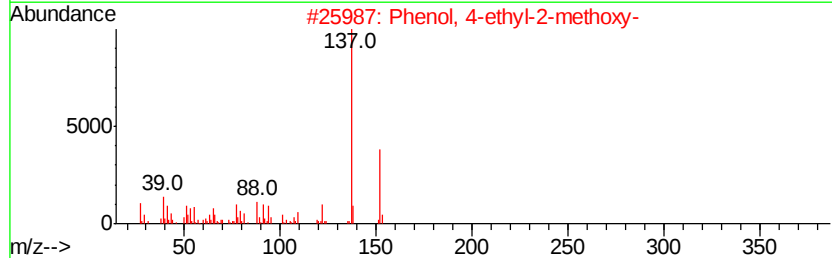
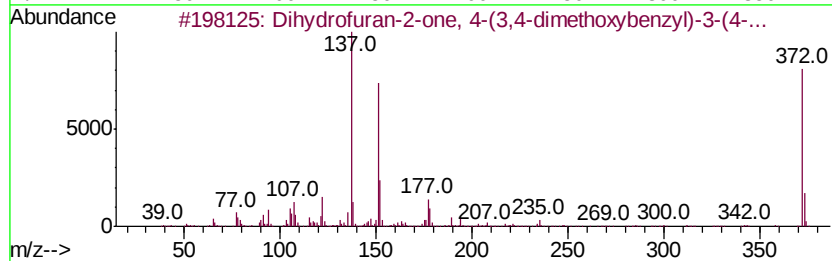
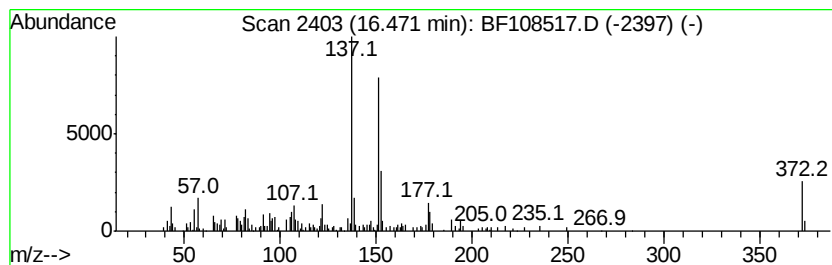
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Dihydrofuran-2-one, 4-(3,4-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	5.56 ng	229058	Perylene-d12	15.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dihydrofuran-2-one, 4-(3,4-dimet...	372	C21H24O6	1000295-41-7	95
2			Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	002785-89-9	41
3			5-Isopropyl-3,3-dimethyl-2-methyl...	152	C10H16O	081250-44-4	38
4			O-Methoxy-.alpha.-methylbenzyl a...	152	C9H12O2	013513-82-1	38
5			3,4-Dimethoxyphenylacetone	194	C11H14O3	000776-99-8	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

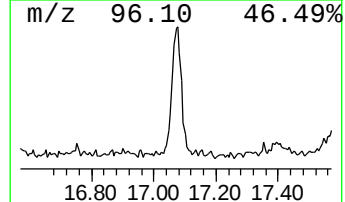
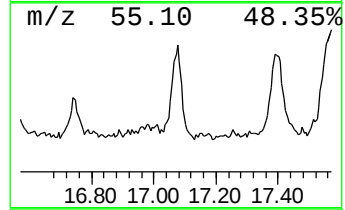
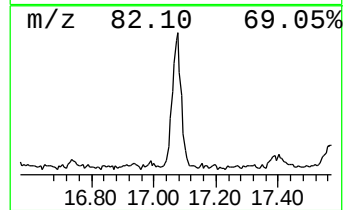
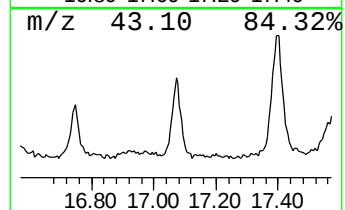
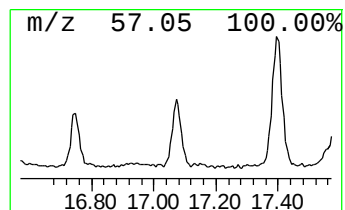
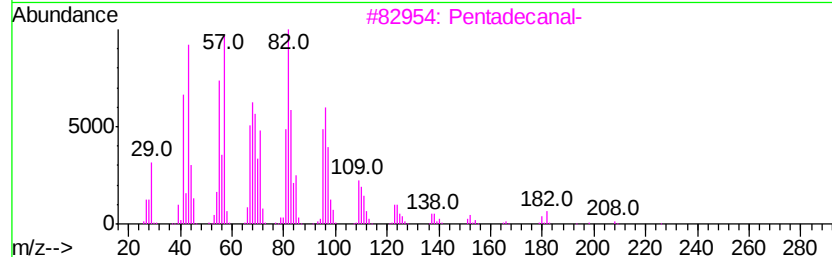
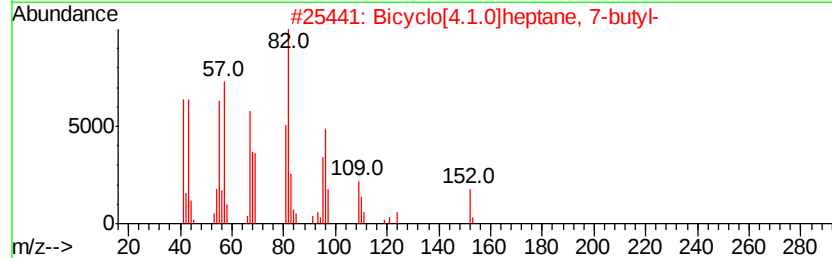
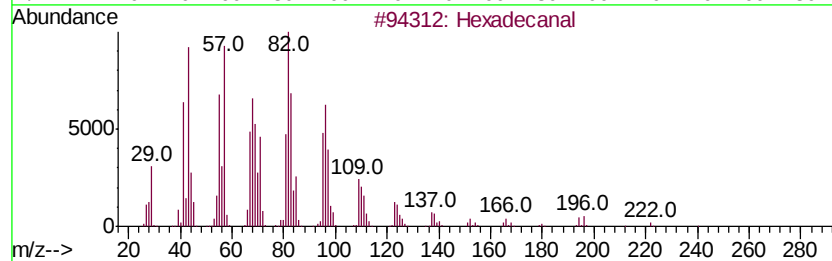
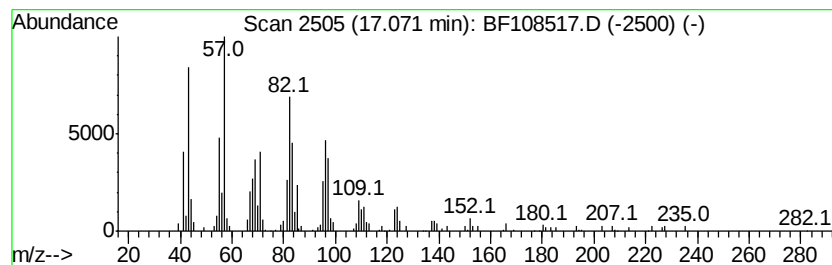
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.07	7.10 ng	292516	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanal	240	C16H32O	000629-80-1	64
2		Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	43
3		Pentadecanal-	226	C15H30O	002765-11-9	43
4		7-Azabicyclo[4.1.0]heptane, 1-me...	111	C7H13N	025022-25-7	38
5		17-Pentatriacontene	491	C35H70	006971-40-0	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

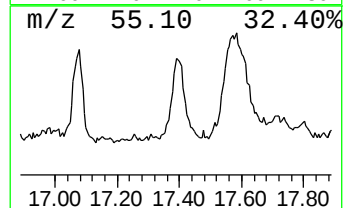
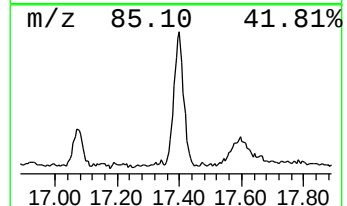
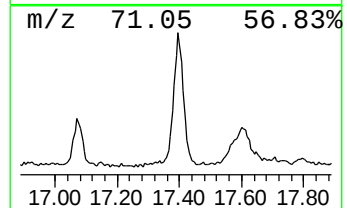
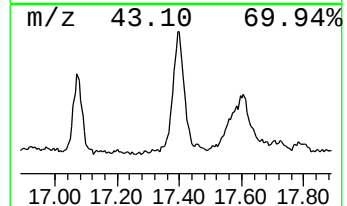
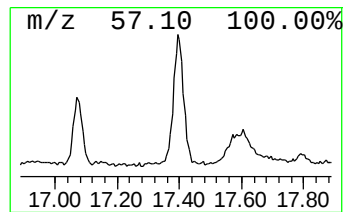
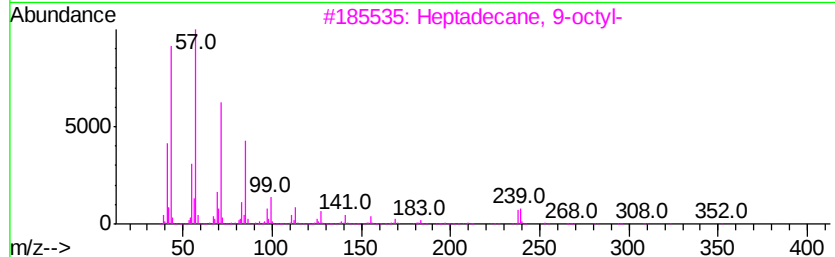
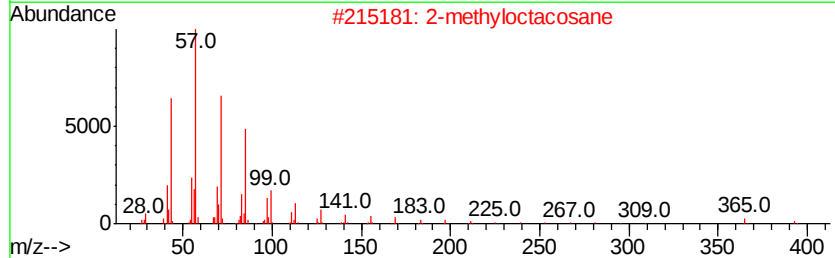
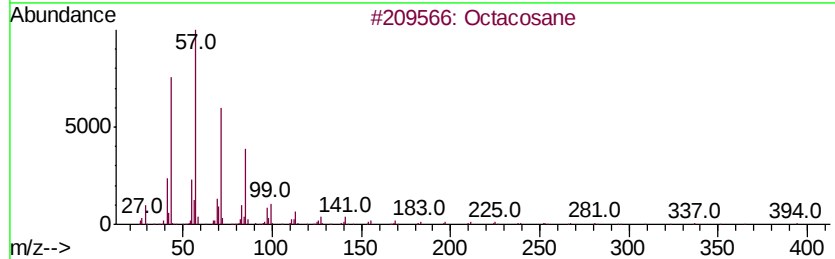
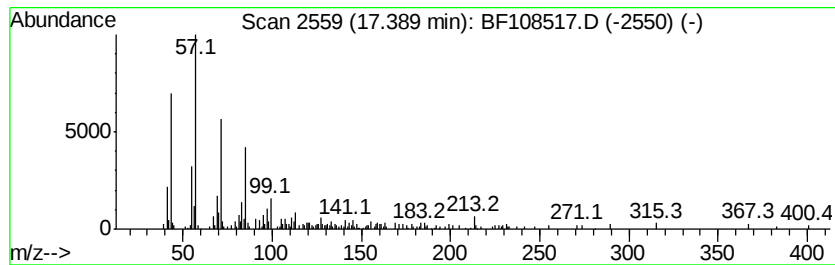
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	13.76 ng	566885	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		2-methyloctacosane	408	C29H60	1000376-72-8	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Hentriacontane	437	C31H64	000630-04-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

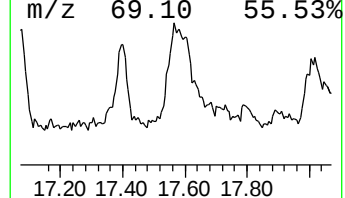
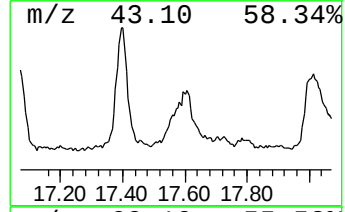
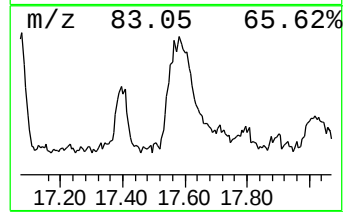
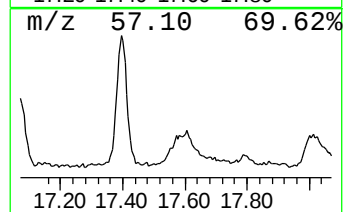
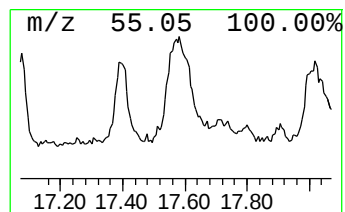
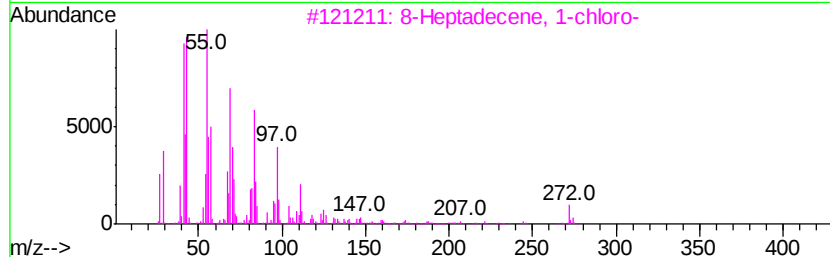
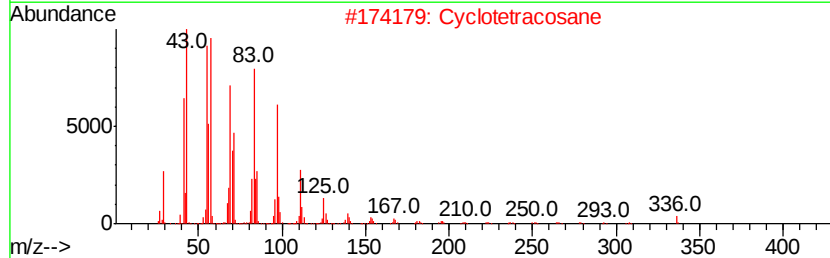
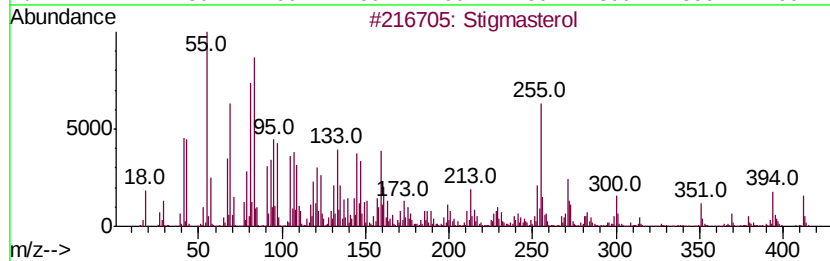
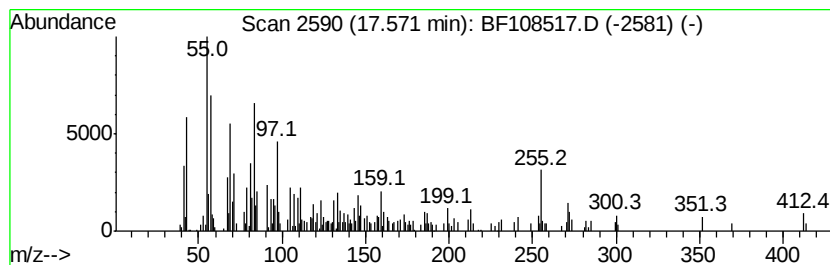
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Stigmasterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	15.46 ng	636834	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmasterol	412	C29H48O	000083-48-7	97
2		Cyclotetracosane	336	C24H48	000297-03-0	49
3		8-Heptadecene, 1-chloro-	272	C17H33Cl	056554-80-4	49
4		Cholesta-22,24-dien-5-ol, 4,4-di...	412	C29H48O	1000128-66-1	47
5		1-Cyclopentyleicosane	350	C25H50	1000357-25-6	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

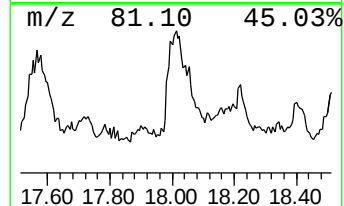
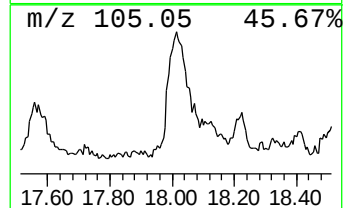
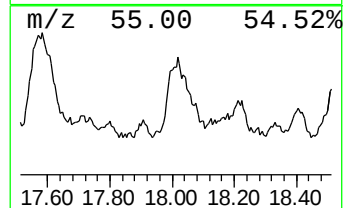
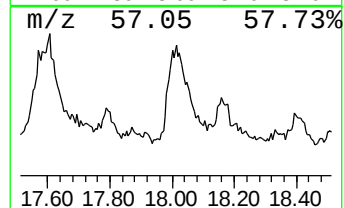
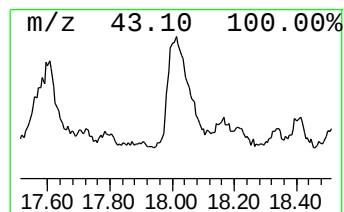
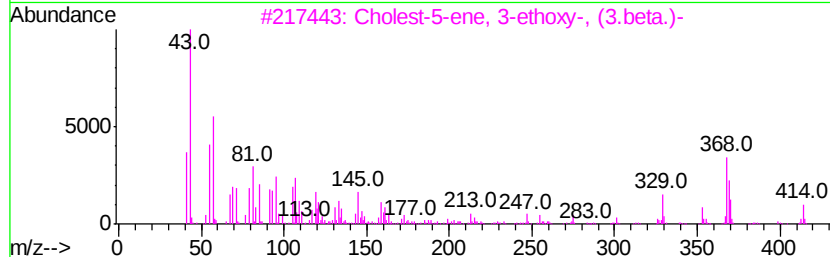
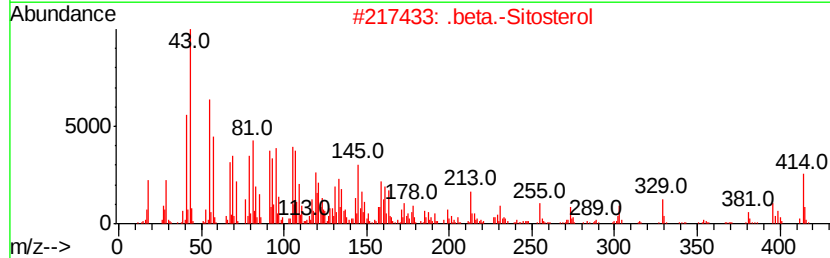
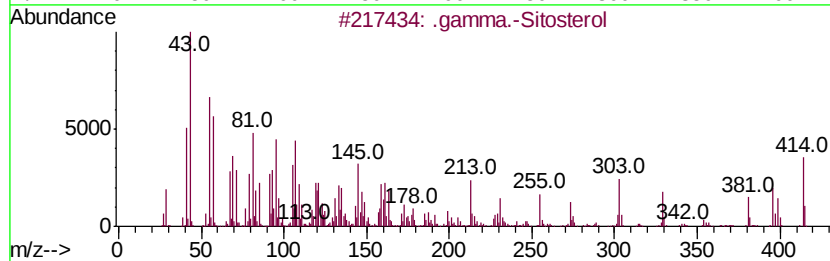
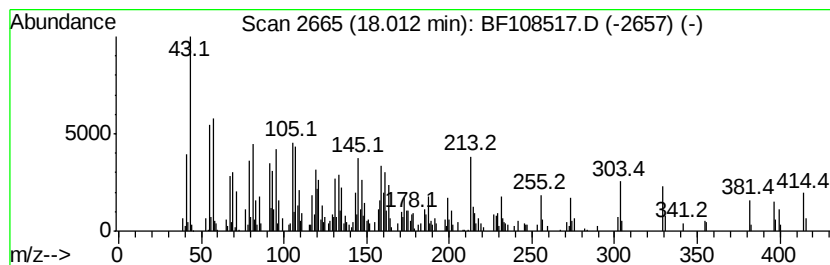
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	25.25 ng	1039850	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	98
3		Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	60
4		Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	37
5		Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

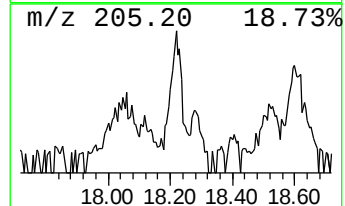
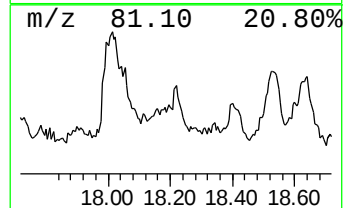
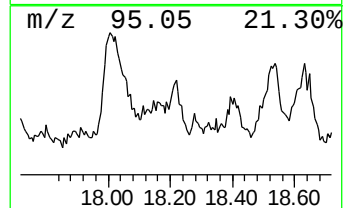
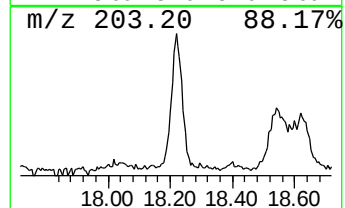
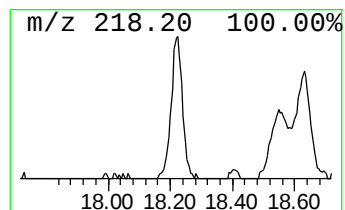
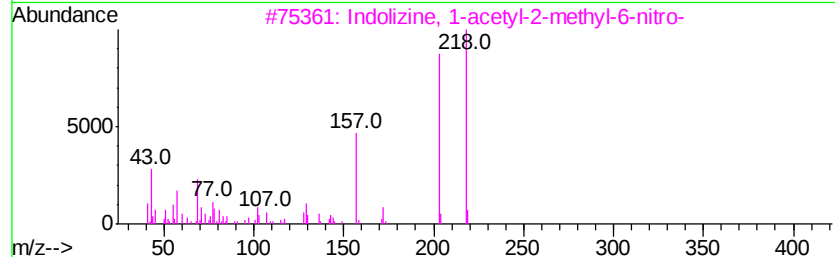
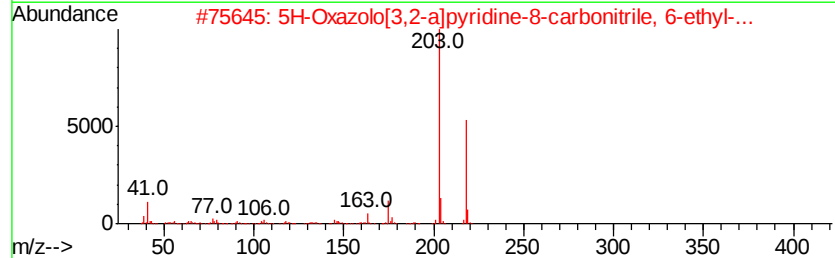
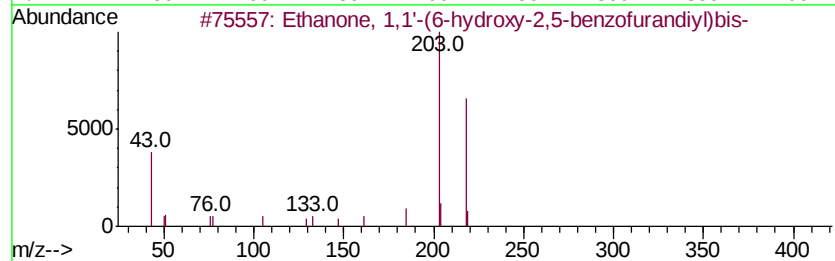
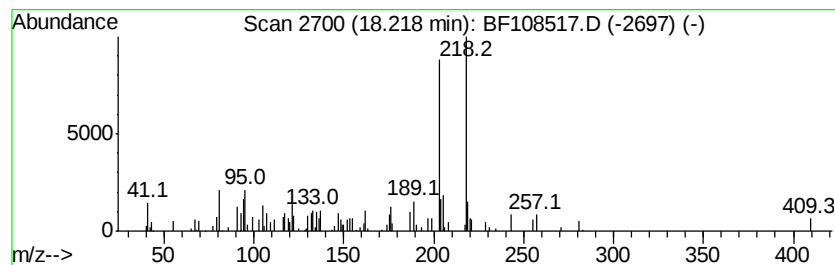
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Ethanone, 1,1'-(6-hydroxy-2... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.22	4.29 ng	176733	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1,1'-(6-hydroxy-2,5-be...	218	C12H10O4	053947-86-7	64
2		5H-Oxazolo[3,2-a]pyridine-8-carb...	218	C12H14N2O2	1000337-58-3	64
3		Indolizine, 1-acetyl-2-methyl-6-...	218	C11H10N2O3	1000071-33-1	64
4		4-Allyl-5-pyridin-3-yl-2,4-dihyd...	218	C10H10N4S	1000300-40-5	64
5		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS4

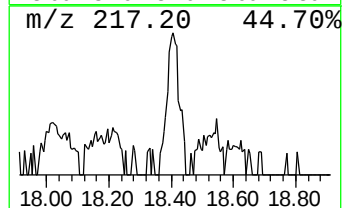
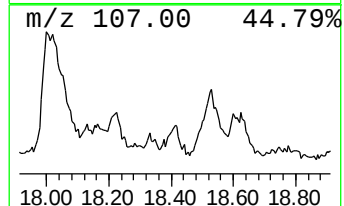
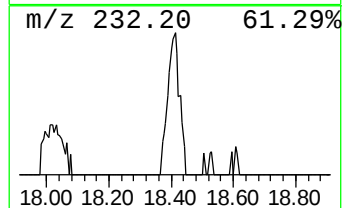
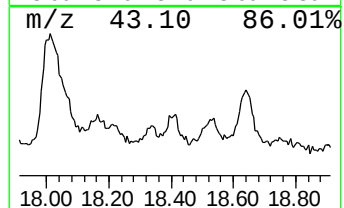
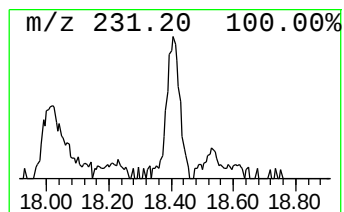
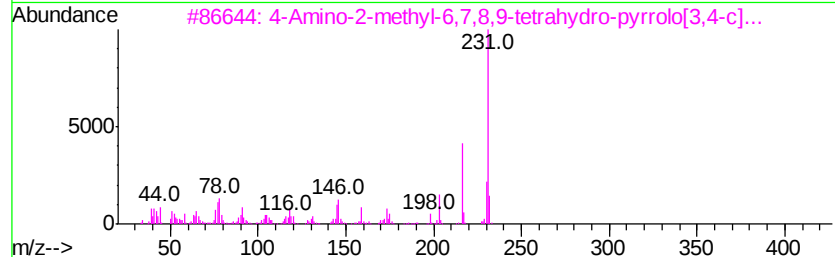
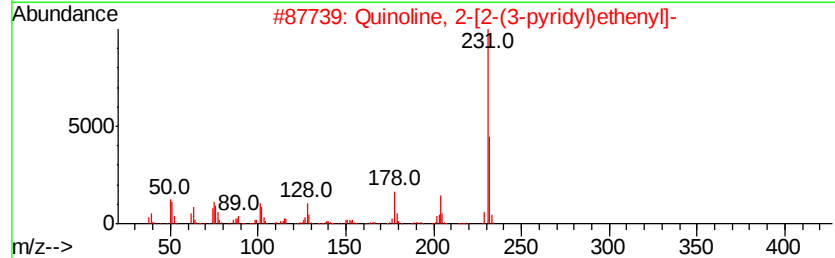
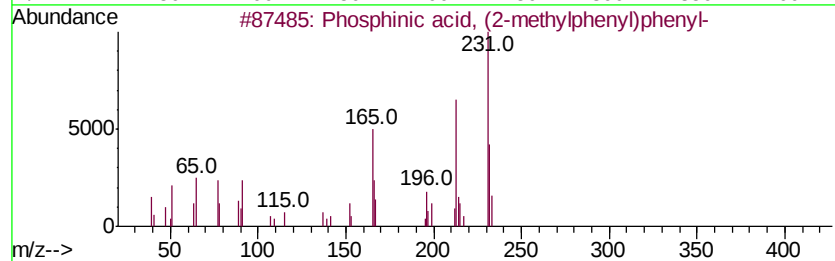
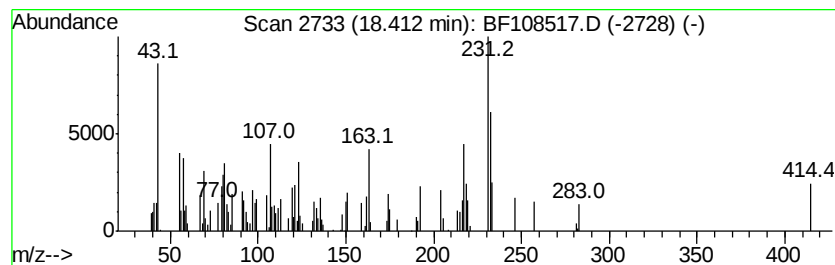
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Phosphinic acid, (2-methylp... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	3.60 ng	148414	Perylene-d12	15.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphinic acid, (2-methylphenyl...	232	C13H13O2P	018593-18-5	38
2			Quinoline, 2-[2-(3-pyridyl)ethen...	232	C16H12N2	001586-51-2	35
3			4-Amino-2-methyl-6,7,8,9-tetrahy...	231	C12H13N3O2	1000300-20-0	25
4			Phosphinic acid, diphenyl-, meth...	232	C13H13O2P	001706-90-7	25
5			Cyclohexanamine, 2-[(phenylethyn...	231	C14H17NS	1000327-34-1	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108517.D
Acq On : 27 Aug 2018 18:15
Operator : JU/SJ
Sample : J4538-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

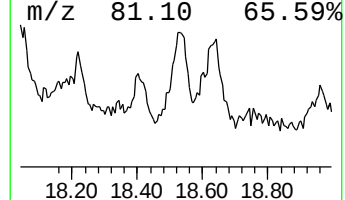
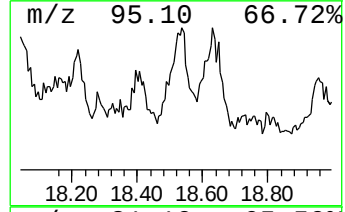
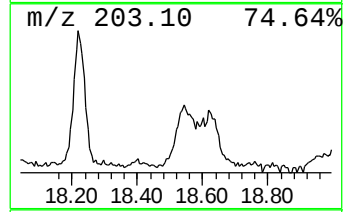
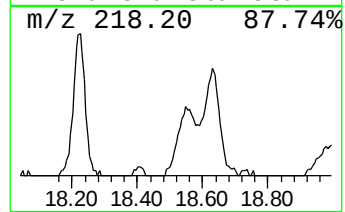
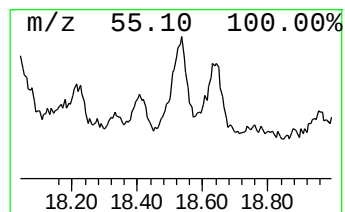
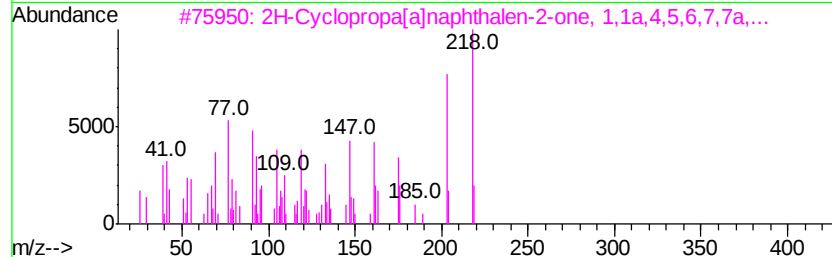
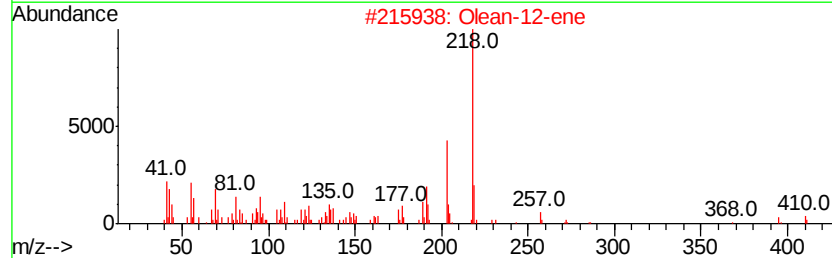
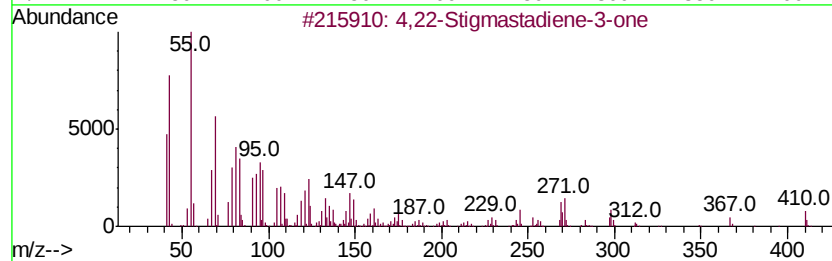
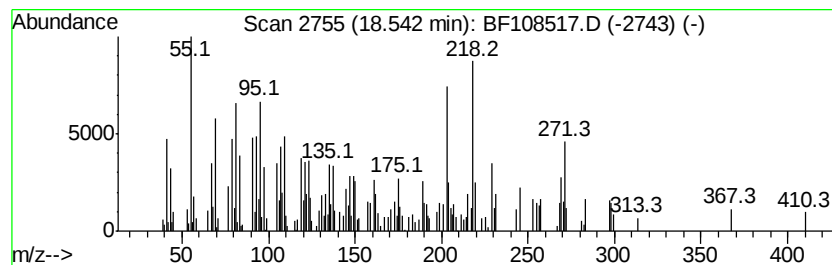
Instrument :
BNA_F
ClientSampleId :
VSS4

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 20 4,22-Stigmastadiene-3-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	10.93 ng	450316	Perylene-d12	15.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	4,22-Stigmastadiene-3-one	410 C29H46O	020817-72-5	94
2	Olean-12-ene	410 C30H50	000471-68-1	83
3	2H-Cyclopropa[alnaphthalen-2-one...	218 C15H22O	006831-17-0	30
4	1,4-Methanoazulene, 7-bromodecah...	282 C15H23Br	024503-54-6	27
5	1,1,6-trimethyl-3-methylene-2-(3...	452 C33H56	1000373-94-5	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
 Data File : BF108517.D
 Acq On : 27 Aug 2018 18:15
 Operator : JU/SJ
 Sample : J4538-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VSS4

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...	5.24	2.5	ng	96511	1	7.00	760576	20.0
unknown6.77	6.77	60.2	ng	2290320	1	7.00	760576	20.0
Behenic alcohol	14.03	4.8	ng	192120	5	14.19	794343	20.0
Eicosane	14.62	2.5	ng	100616	5	14.19	794343	20.0
Bromoacetic acid,...	14.68	2.9	ng	114807	5	14.19	794343	20.0
Oxirane, hexadecyl-	15.11	9.8	ng	403294	6	15.75	823742	20.0
Tetratetracontane	15.31	10.1	ng	414747	6	15.75	823742	20.0
Octacosanol	15.38	15.9	ng	654976	6	15.75	823742	20.0
Octadecanal	15.95	5.3	ng	218638	6	15.75	823742	20.0
Hexacosane	16.19	25.3	ng	1040240	6	15.75	823742	20.0
17-Pentatriacontene	16.33	7.0	ng	288148	6	15.75	823742	20.0
Dihydrofuran-2-on...	16.47	5.6	ng	229058	6	15.75	823742	20.0
Hexadecanal	17.07	7.1	ng	292516	6	15.75	823742	20.0
Octacosane	17.39	13.8	ng	566885	6	15.75	823742	20.0
Stigmasterol	17.57	15.5	ng	636834	6	15.75	823742	20.0
.gamma.-Sitosterol	18.01	25.3	ng	1039850	6	15.75	823742	20.0
Ethanone, 1,1'-(6...	18.22	4.3	ng	176733	6	15.75	823742	20.0
Phosphinic acid, ...	18.41	3.6	ng	148414	6	15.75	823742	20.0
4,22-Stigmastadie...	18.54	10.9	ng	450316	6	15.75	823742	20.0