

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
 Data File : BF097075.D
 Acq On : 26 Jul 2017 15:07
 Operator : SJ/JU
 Sample : I4443-06 5X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-M7-BASE

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	4.622	462	465	477	rVB	48668	65092	6.27%	0.438%
2	5.092	541	545	559	rBV	621339	732538	70.55%	4.926%
3	5.228	565	568	575	rVB	50197	53565	5.16%	0.360%
4	6.151	720	725	738	rBV	796090	849254	81.79%	5.711%
5	6.263	741	744	751	rVV	892411	820347	79.00%	5.517%
6	6.492	780	783	790	rBV	828390	698736	67.29%	4.699%
7	6.651	806	810	816	rBV	615898	583121	56.16%	3.921%
8	7.057	876	879	890	rBV	446494	389482	37.51%	2.619%
9	7.551	956	963	966	rBV4	6427	14745	1.42%	0.099%
10	7.781	997	1002	1005	rBV	1054137	978005	94.18%	6.577%
11	7.810	1005	1007	1014	rVB	65668	69823	6.72%	0.470%
12	8.857	1180	1185	1188	rBV	868133	724703	69.79%	4.873%
13	9.257	1249	1253	1256	rBV	73252	64942	6.25%	0.437%
14	9.351	1267	1269	1276	rVB2	18851	19331	1.86%	0.130%
15	9.469	1286	1289	1294	rBV3	8841	12248	1.18%	0.082%
16	9.522	1294	1298	1302	rBV	1104894	1038391	100.00%	6.983%
17	9.957	1367	1372	1374	rBV	97960	88300	8.50%	0.594%
18	10.198	1407	1413	1416	rBV3	8204	12534	1.21%	0.084%
19	10.310	1428	1432	1437	rBV	414946	374367	36.05%	2.517%
20	10.533	1467	1470	1472	rBV3	15719	14631	1.41%	0.098%
21	10.704	1495	1499	1502	rBV3	20859	21211	2.04%	0.143%
22	10.998	1545	1549	1553	rBV	1170431	1010902	97.35%	6.798%
23	11.498	1630	1634	1639	rBV7	10464	22438	2.16%	0.151%
24	11.557	1639	1644	1654	rVV	247932	264060	25.43%	1.776%
25	12.245	1753	1761	1762	rBV	247050	328938	31.68%	2.212%
26	12.263	1762	1764	1773	rVV	334820	652905	62.88%	4.391%
27	12.339	1774	1777	1788	rVB	155999	207609	19.99%	1.396%
28	12.504	1803	1805	1808	rBV2	23470	19092	1.84%	0.128%
29	12.580	1814	1818	1822	rVB	583379	517466	49.83%	3.480%
30	12.816	1854	1858	1860	rBV2	39058	46298	4.46%	0.311%
31	13.292	1936	1939	1943	rVB	132881	116777	11.25%	0.785%
32	13.498	1970	1974	1979	rBV	290301	332188	31.99%	2.234%
33	13.551	1980	1983	1989	rVV2	48100	63322	6.10%	0.426%
34	13.621	1991	1995	1999	rVV	648491	585253	56.36%	3.936%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.663	2000	2002	2006	rBV5	12005	12779	1.23%	0.086%
36	13.821	2026	2029	2032	rBV	46488	48386	4.66%	0.325%
37	13.939	2046	2049	2053	rVB	108671	94768	9.13%	0.637%
38	14.127	2077	2081	2087	rBV	244281	291436	28.07%	1.960%
39	14.180	2087	2090	2092	rVB2	30102	29022	2.79%	0.195%
40	14.239	2099	2100	2104	rBV3	18585	27343	2.63%	0.184%
41	14.539	2148	2151	2156	rBV	190404	185150	17.83%	1.245%
42	14.727	2177	2183	2187	rVB2	103067	137498	13.24%	0.925%
43	14.810	2194	2197	2201	rBV5	27764	52291	5.04%	0.352%
44	14.974	2218	2225	2230	rVB	519295	591538	56.97%	3.978%
45	15.192	2259	2262	2267	rVB3	42015	59613	5.74%	0.401%
46	15.392	2292	2296	2299	rBV2	40734	56246	5.42%	0.378%
47	15.433	2300	2303	2308	rVV5	42488	60765	5.85%	0.409%
48	15.486	2308	2312	2316	rBV	73427	106329	10.24%	0.715%
49	15.586	2327	2329	2340	rVB10	47227	80762	7.78%	0.543%
50	16.151	2424	2425	2426	rBV	23020	14463	1.39%	0.097%
51	16.427	2469	2472	2479	rVB2	66540	119641	11.52%	0.805%
52	16.727	2517	2523	2532	rVB3	216964	449731	43.31%	3.024%
53	16.845	2539	2543	2550	rBV4	38697	71533	6.89%	0.481%
54	16.933	2551	2558	2567	rBV3	196825	458628	44.17%	3.084%
55	17.056	2578	2579	2586	rVB7	23559	21385	2.06%	0.144%
56	17.133	2589	2592	2600	rVB10	42503	74675	7.19%	0.502%
57	17.198	2601	2603	2606	rBV4	22437	34050	3.28%	0.229%

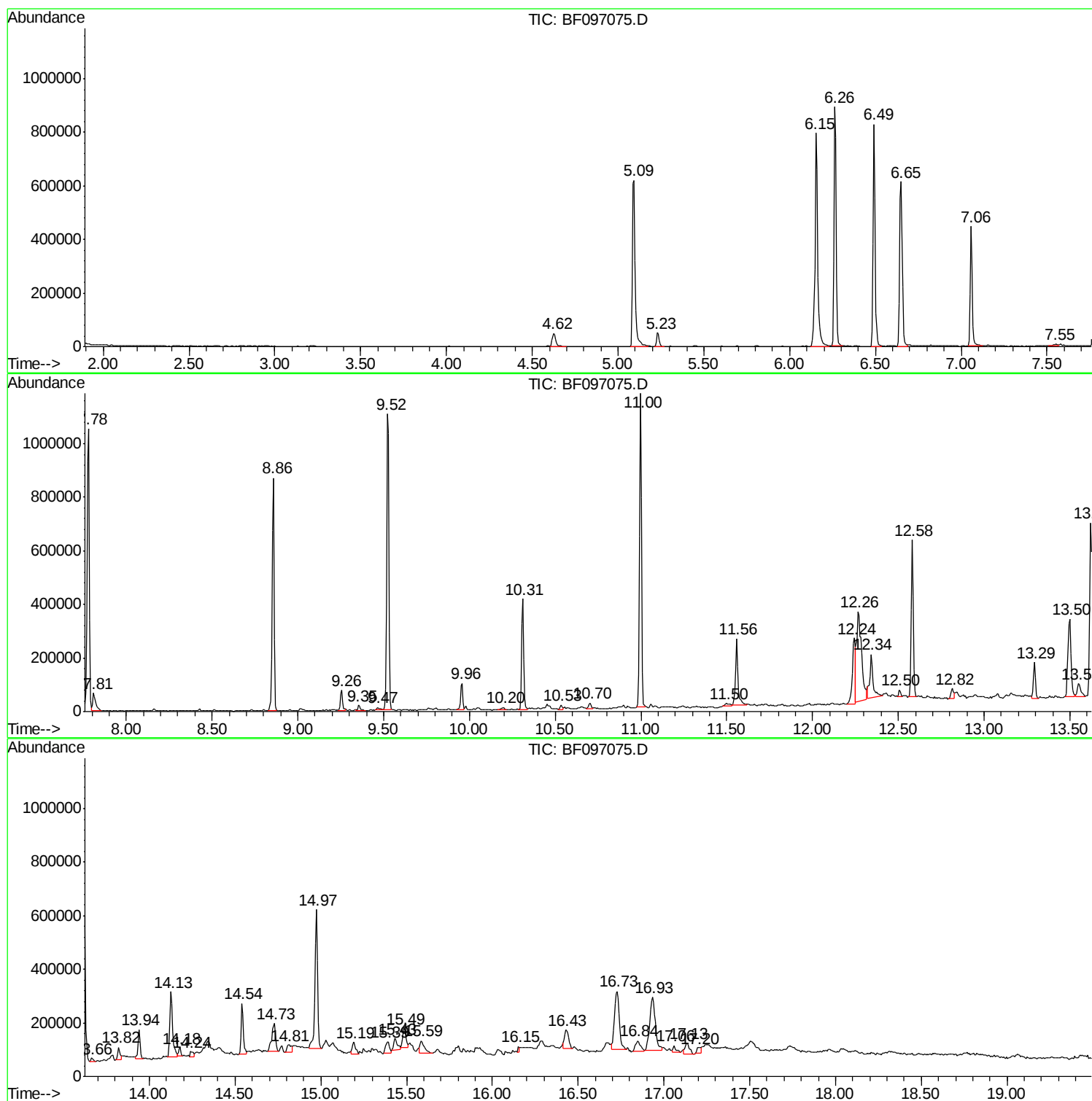
Sum of corrected areas: 14870646

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
E2-M7-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

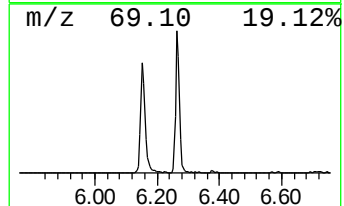
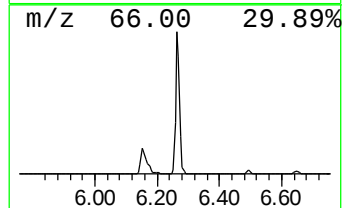
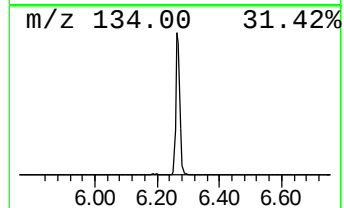
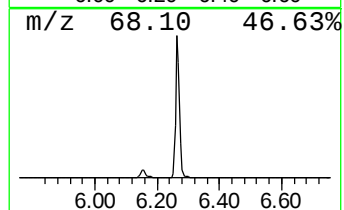
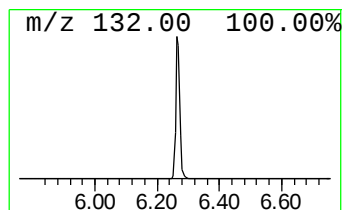
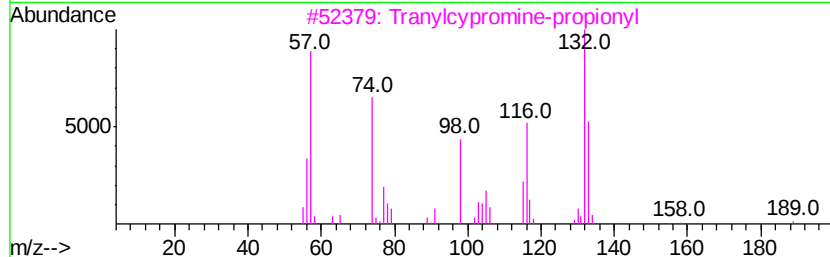
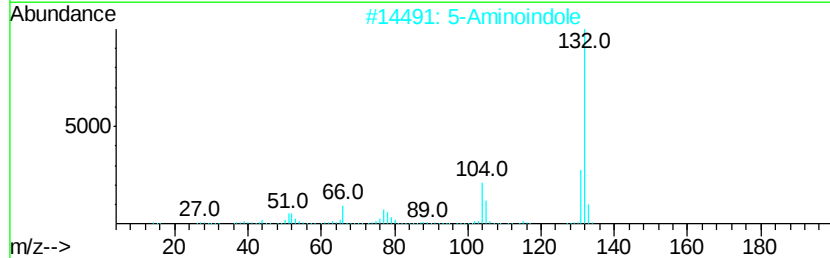
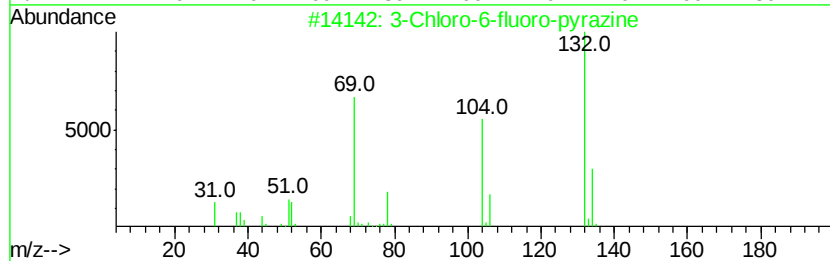
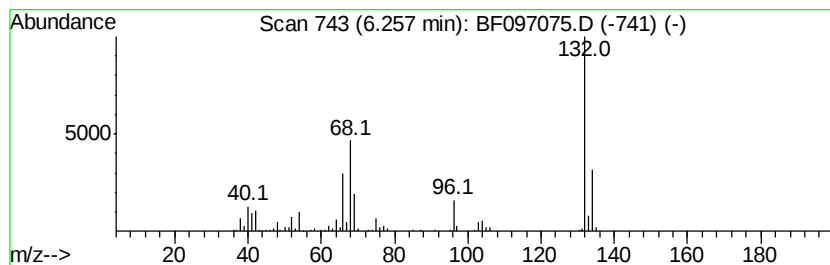
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	23.48 ng	820347	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

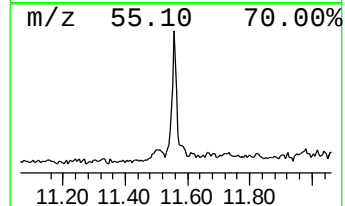
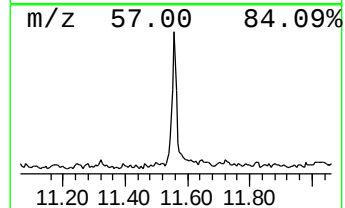
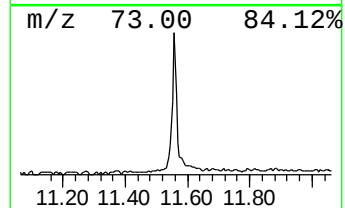
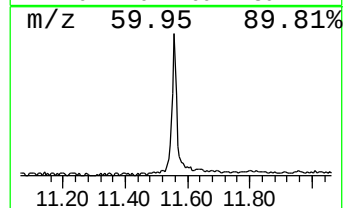
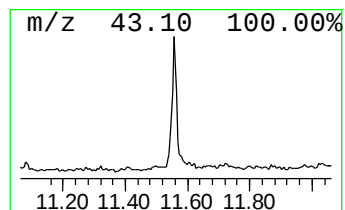
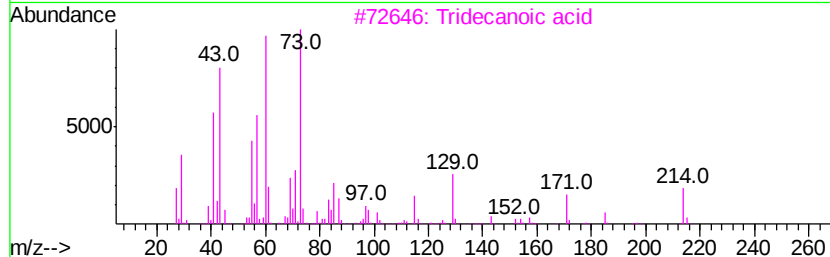
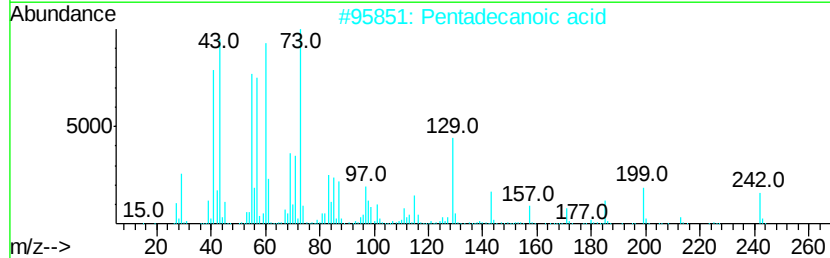
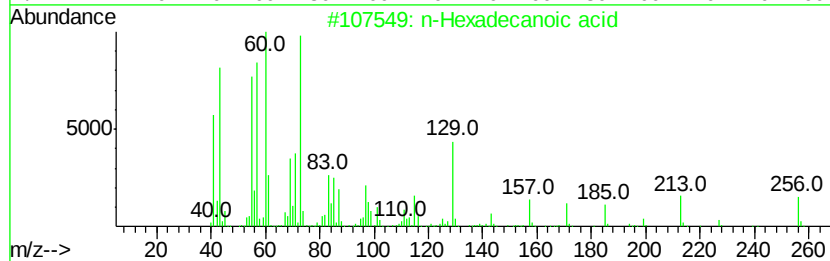
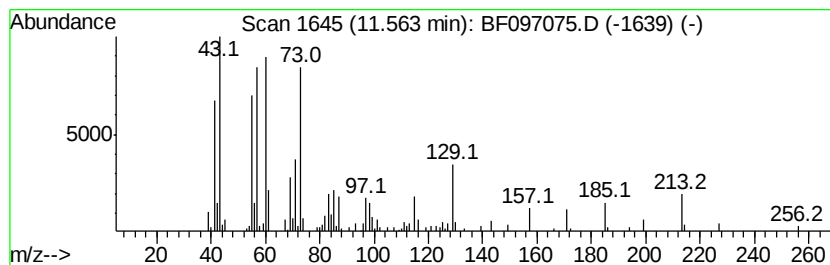
Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.56	5.22 ng	264060	Phenanthrene-d10	11.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

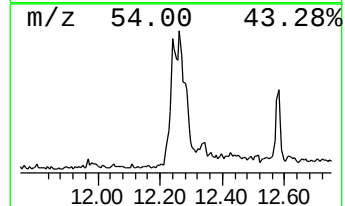
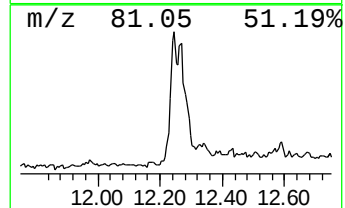
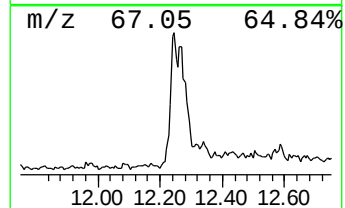
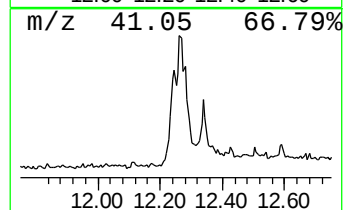
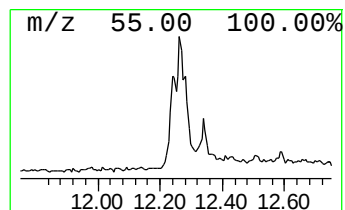
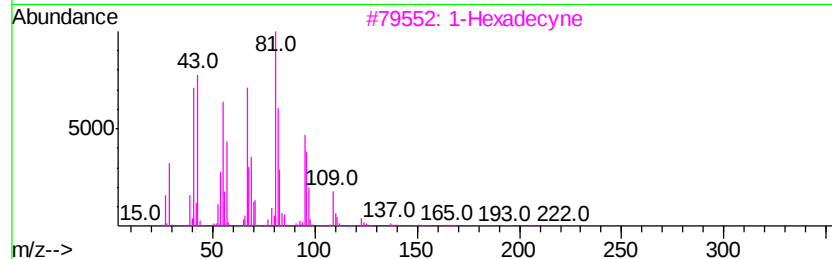
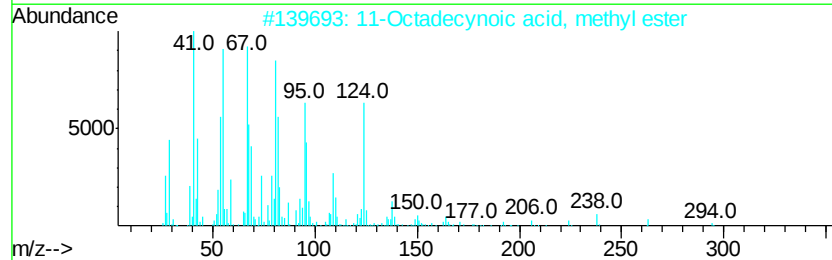
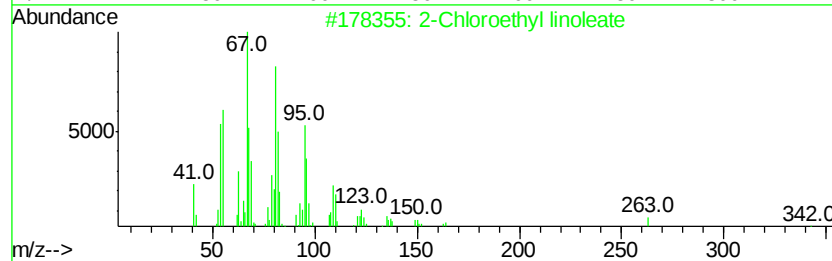
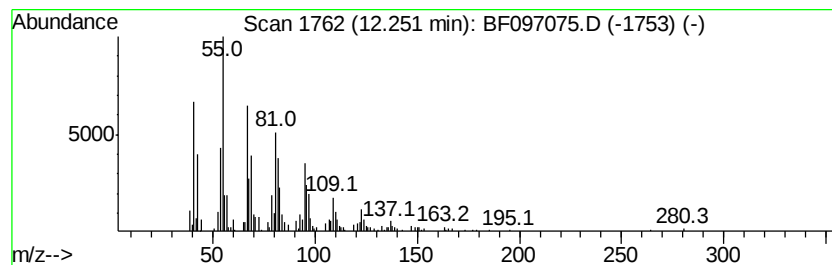
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Chloroethyl linoleate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	6.51 ng	328938	Phenanthrene-d10	11.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91
2		11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	91
3		1-Hexadecyne	222	C16H30	000629-74-3	91
4		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	90
5		11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

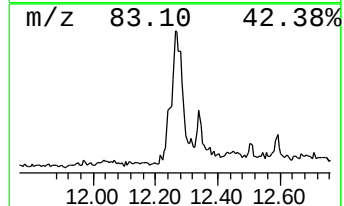
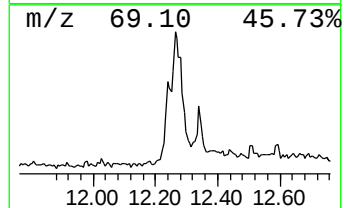
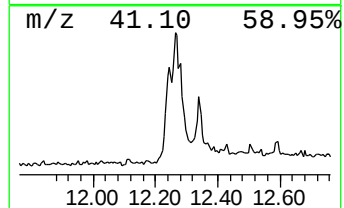
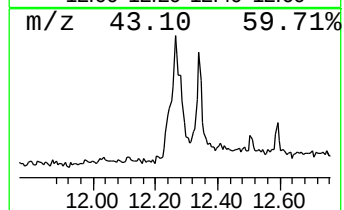
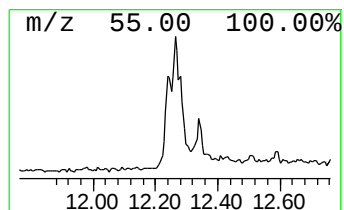
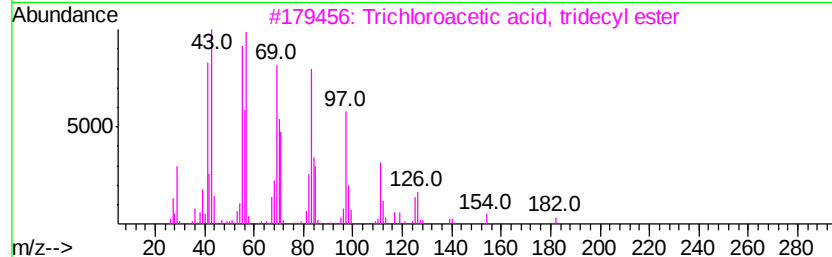
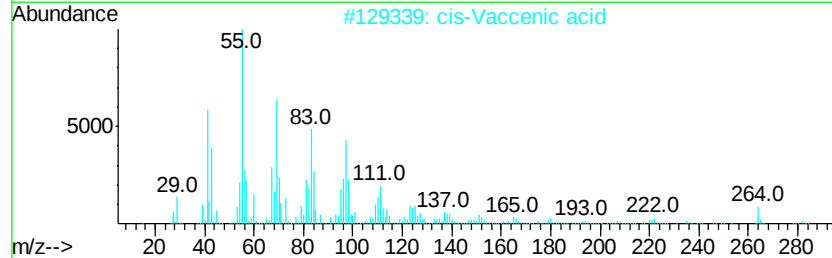
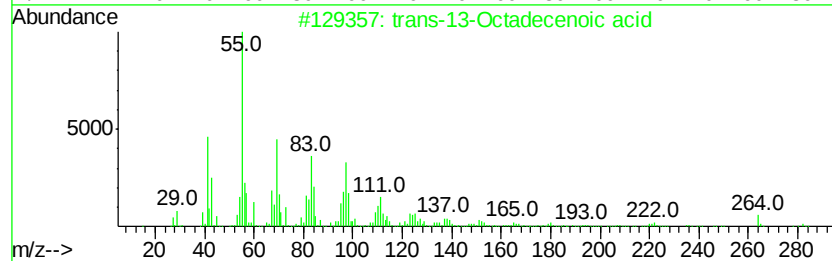
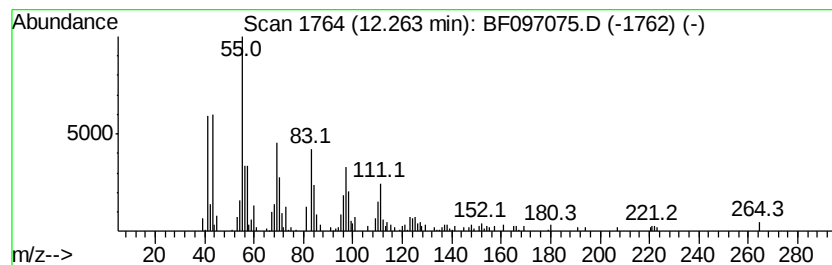
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 trans-13-Octadecenoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	12.92 ng	652905	Phenanthrene-d10	11.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	86
2		cis-Vaccenic acid	282	C18H34O2	000506-17-2	86
3		Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	52
4		1-Tridecene	182	C13H26	002437-56-1	50
5		Decyl trifluoroacetate	254	C12H21F3O2	000333-88-0	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

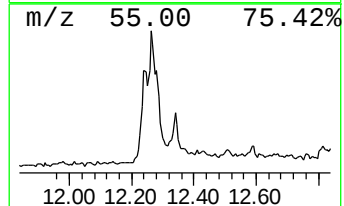
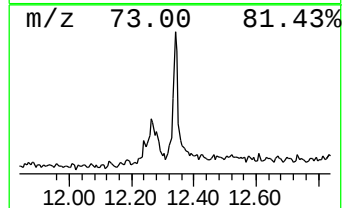
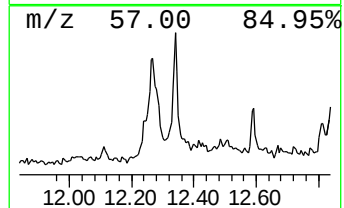
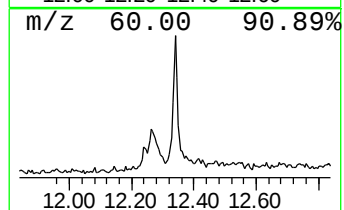
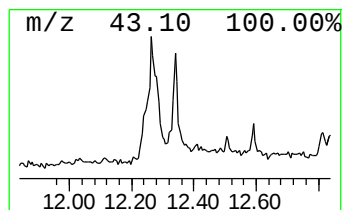
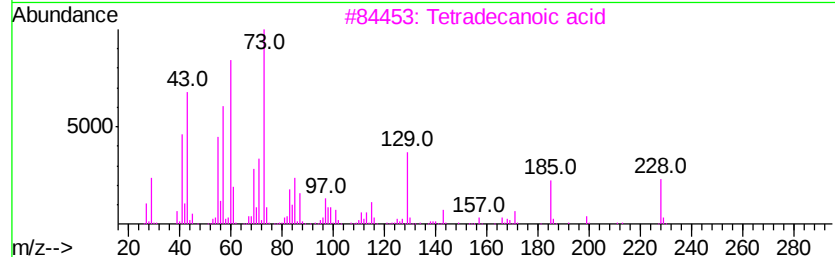
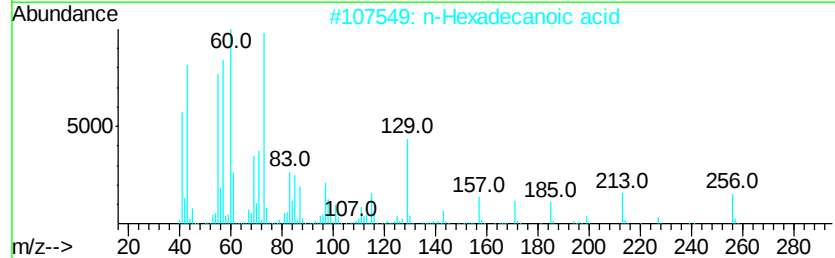
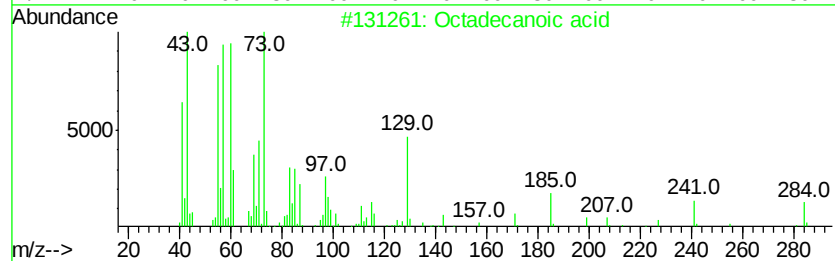
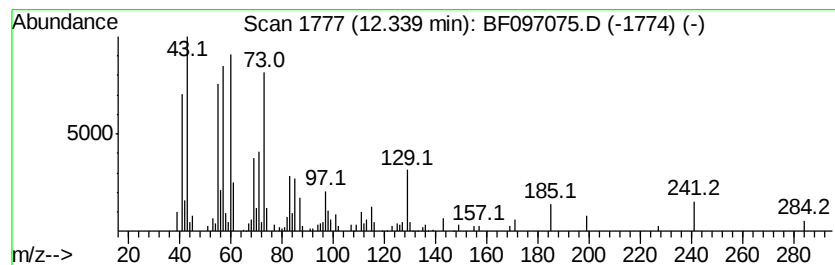
Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.34	7.09 ng	207609	Chrysene-d12		13.62	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	91
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

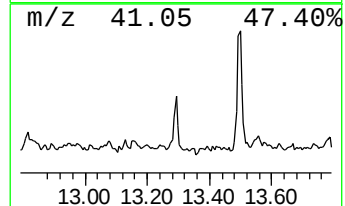
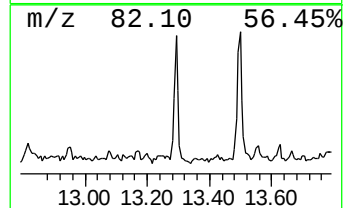
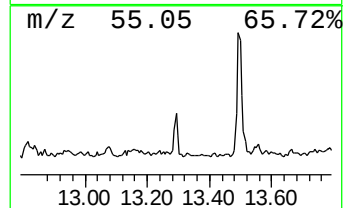
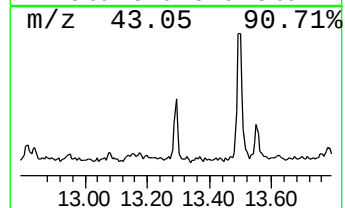
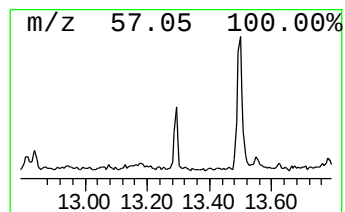
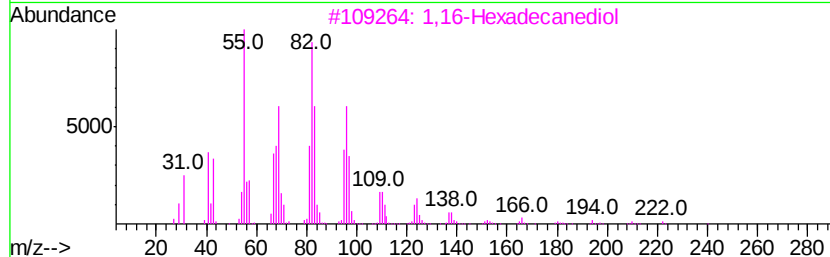
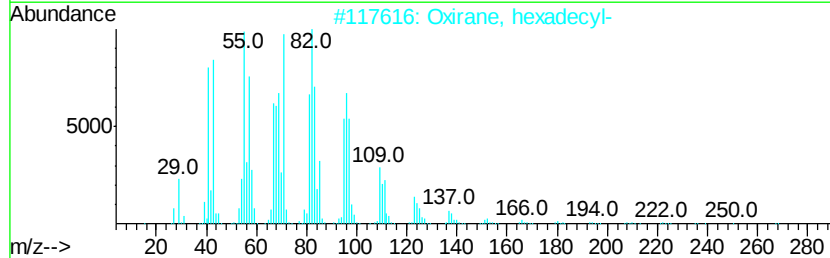
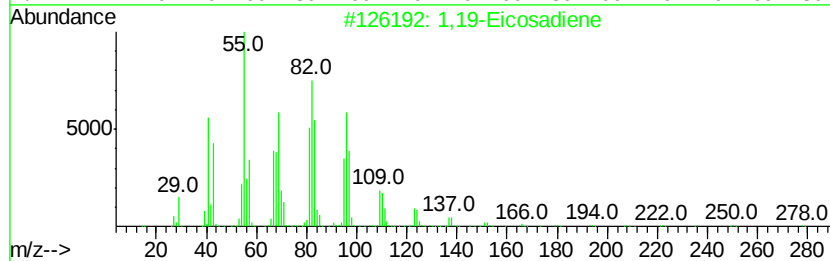
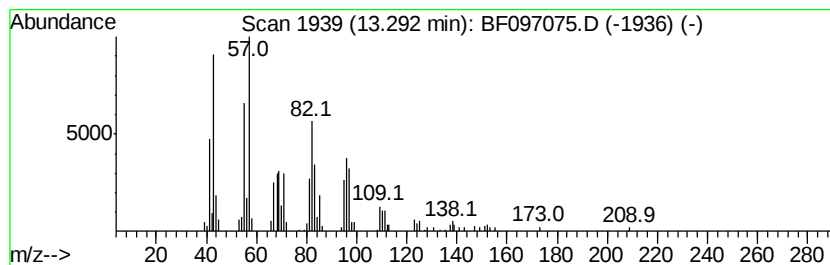
Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,19-Eicosadiene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.29	3.99 ng	116777	Chrysene-d12	13.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	87
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
3	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	81
4	Hexadecanal	240	C16H32O	000629-80-1	80
5	Pentadecanal-	226	C15H30O	002765-11-9	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

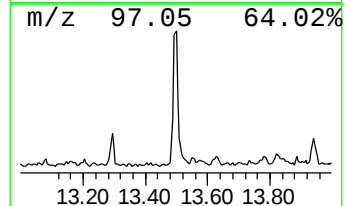
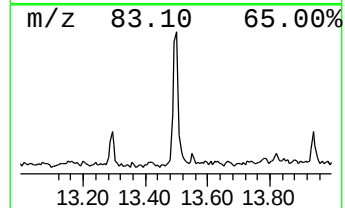
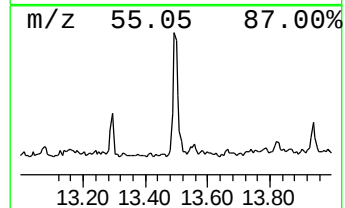
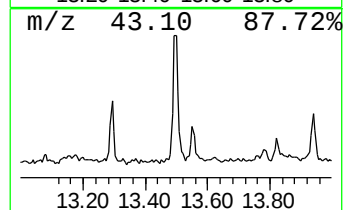
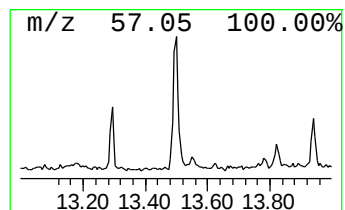
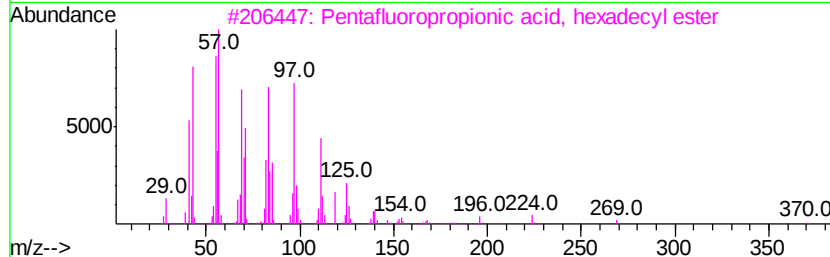
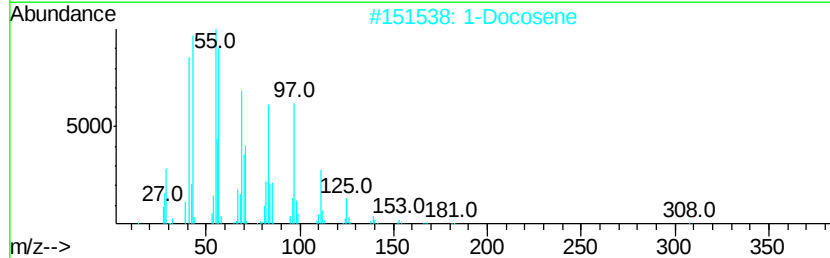
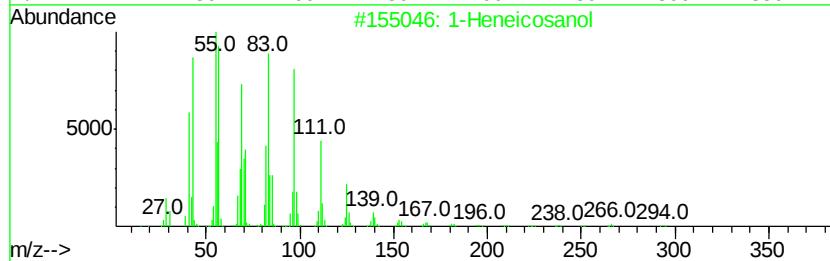
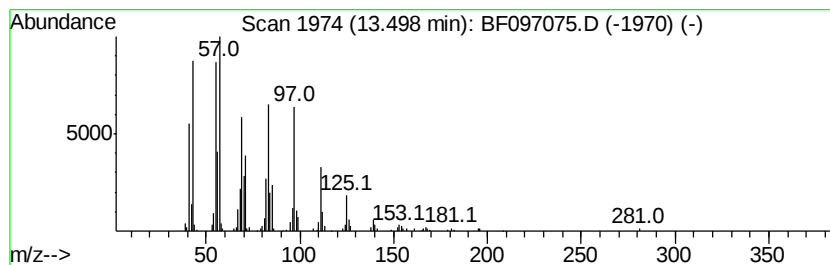
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	11.35 ng	332188	Chrysene-d12	13.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	93
2	1-Docosene		308	C22H44	001599-67-3	91
3	Pentafluoropropionic acid, hexad...		388	C19H33F5O2	006222-07-7	91
4	Trifluoroacetoxv hexadecane		338	C18H33F3O2	006222-03-3	91
5	Pentafluoropropionic acid, hepta...		402	C20H35F5O2	959218-78-1	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

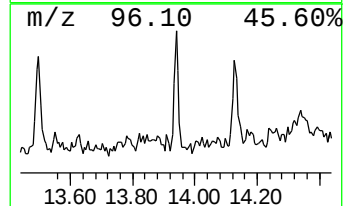
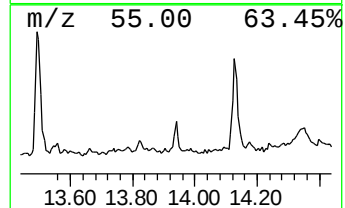
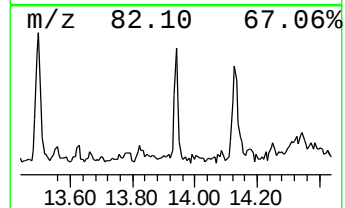
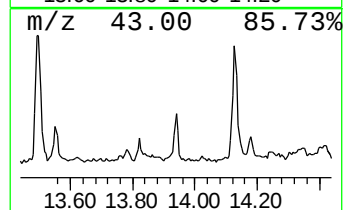
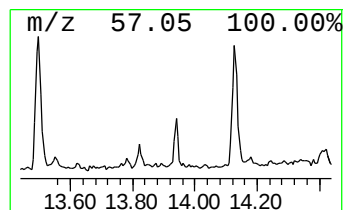
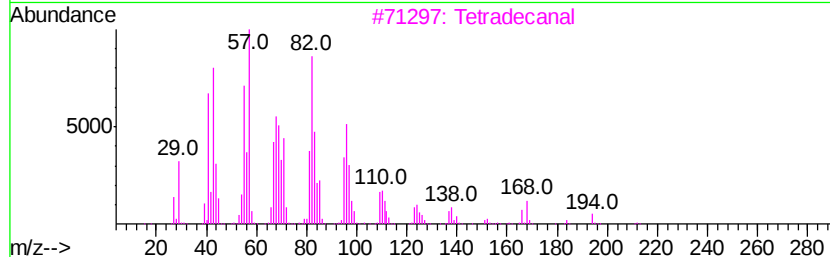
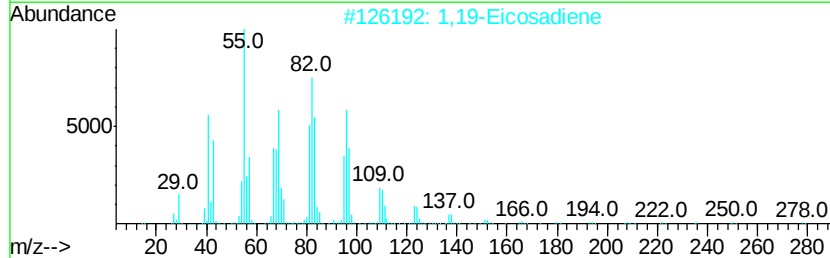
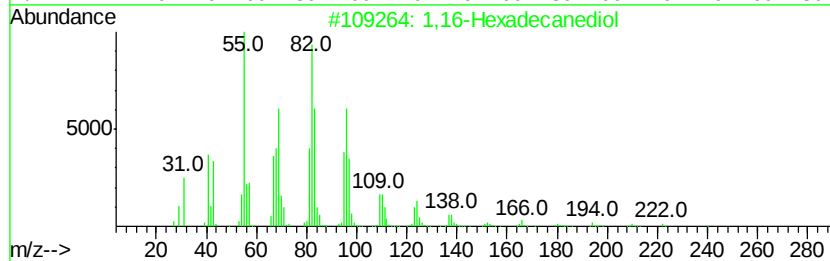
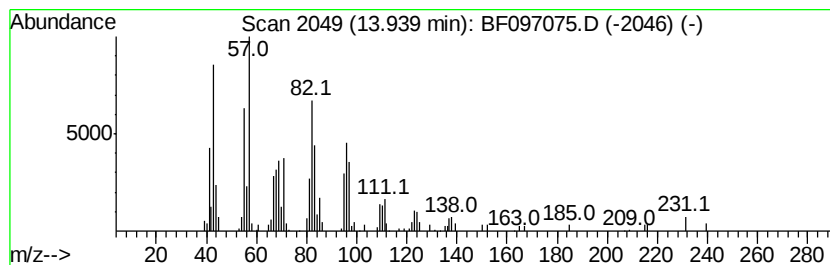
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,16-Hexadecanediol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.24 ng	94768	Chrysene-d12	13.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	91
2		1,19-Eicosadiene	278	C20H38	014811-95-1	91
3		Tetradecanal	212	C14H28O	000124-25-4	90
4		17-Octadecenal	266	C18H34O	056554-86-0	90
5		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

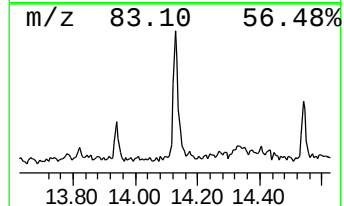
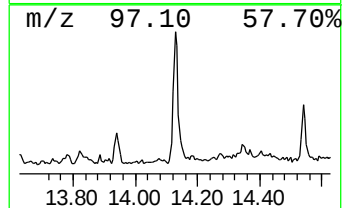
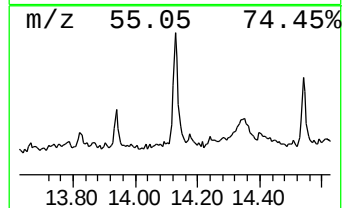
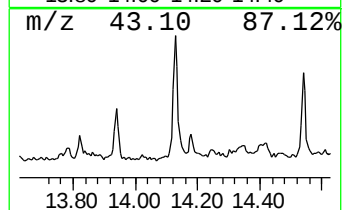
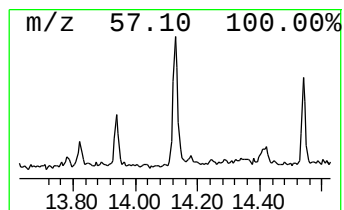
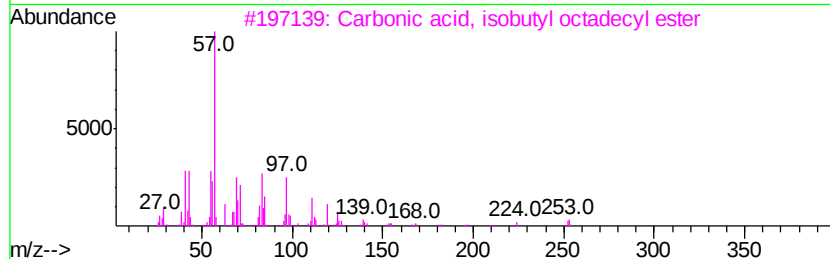
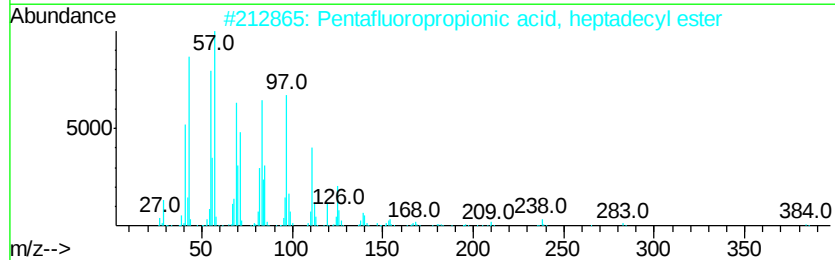
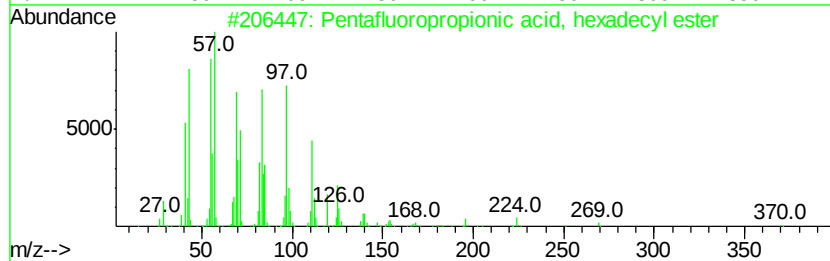
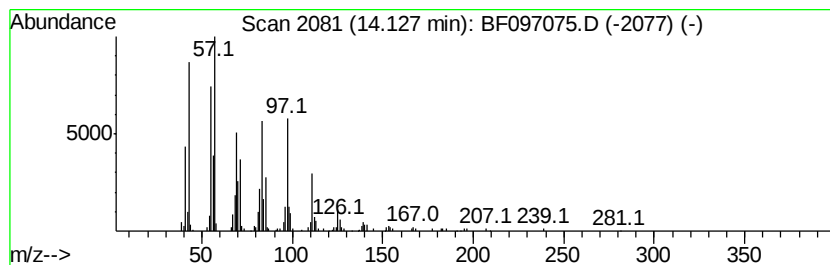
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	9.96 ng	291436	Chrysene-d12	13.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	94
2		Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	91
3		Carbonic acid, isobutyl octadecyl ester	370	C23H46O3	1000314-61-5	91
4		1-Docosene	308	C22H44	001599-67-3	90
5		1-Octadecanol	270	C18H38O	000112-92-5	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

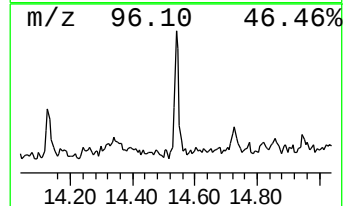
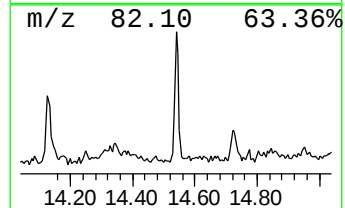
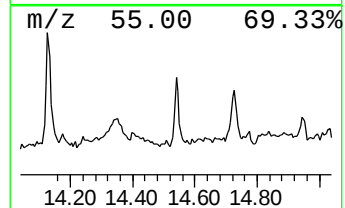
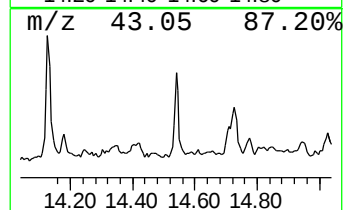
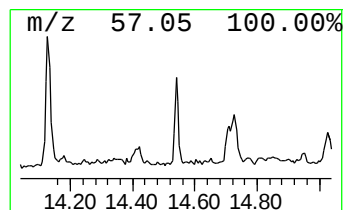
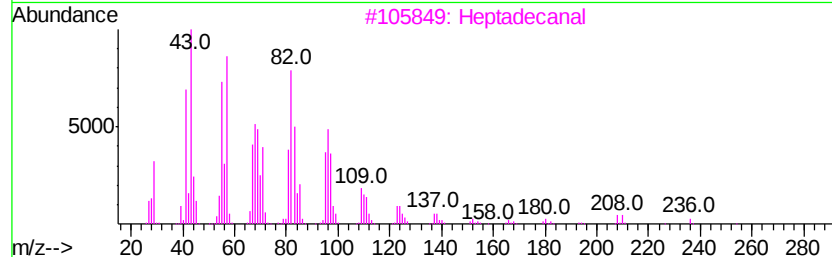
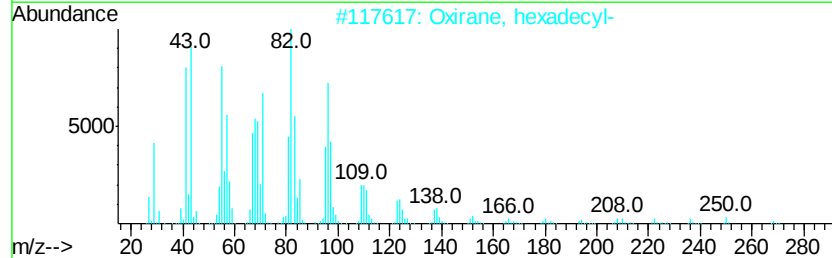
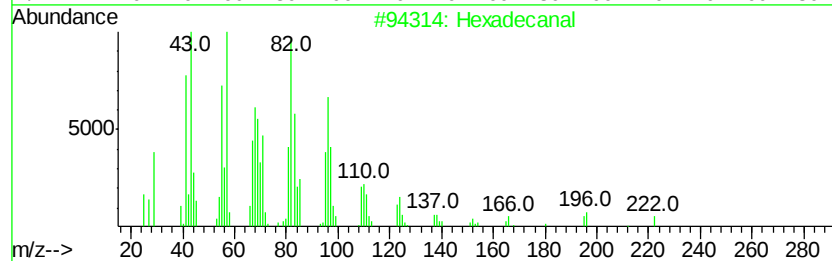
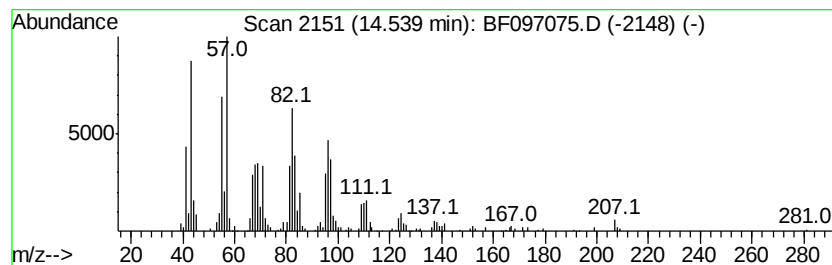
Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.54	6.26 ng	185150	Perylene-d12		14.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Heptadecanal	254	C17H34O	1000376-70-0	91
4	Octadecanal	268	C18H36O	000638-66-4	91
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

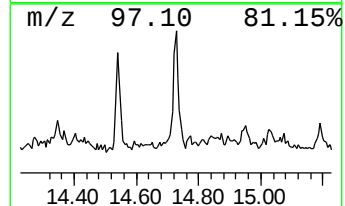
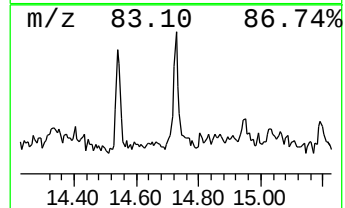
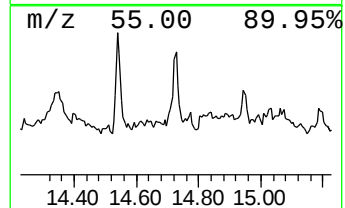
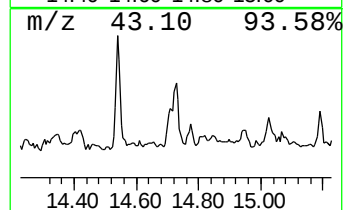
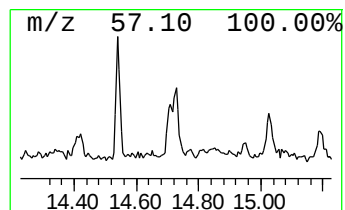
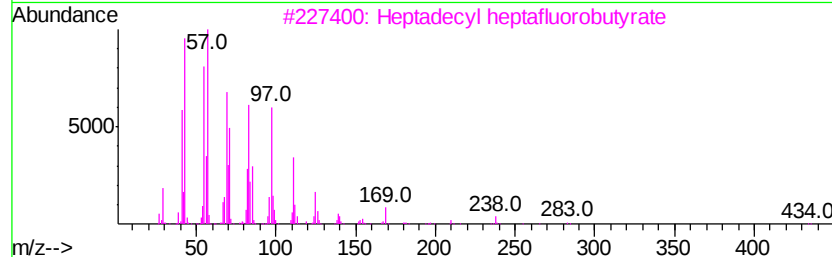
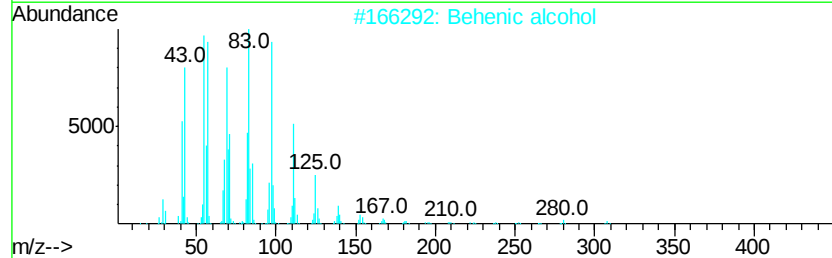
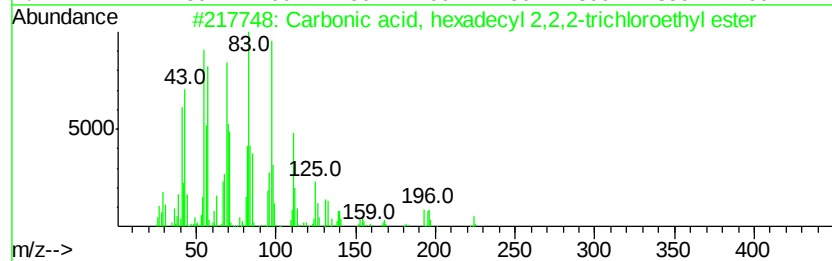
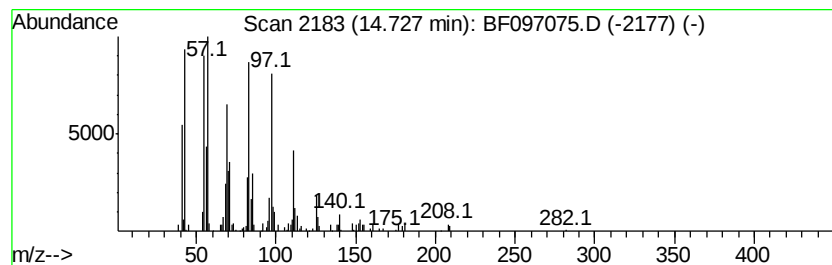
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Carbonic acid, hexadecyl 2,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	4.65 ng	137498	Perylene-d12	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	90
2			Behenic alcohol	326	C22H46O	000661-19-8	87
3			Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	87
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
5			Heptacosyl acetate	438	C29H58O2	1000351-78-2	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

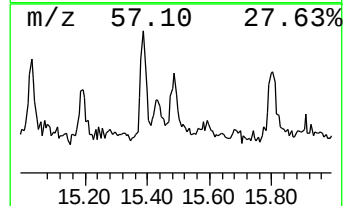
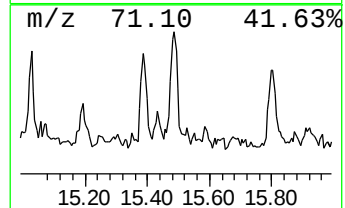
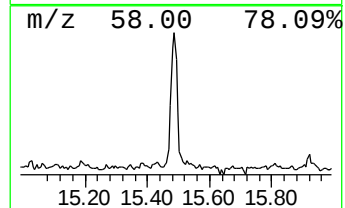
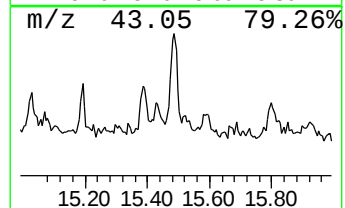
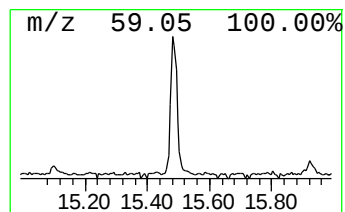
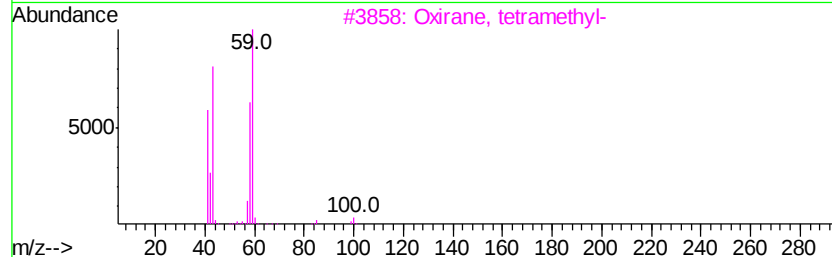
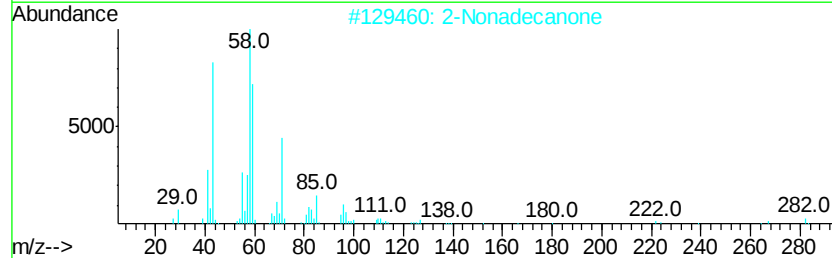
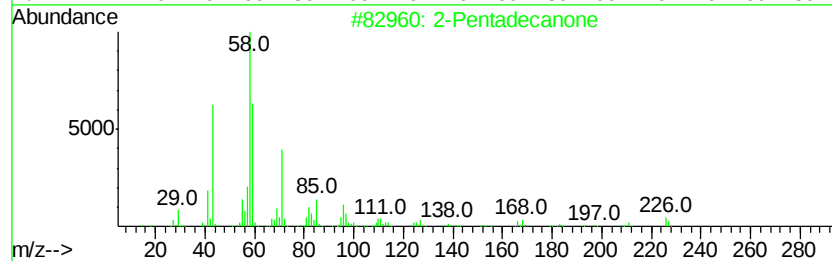
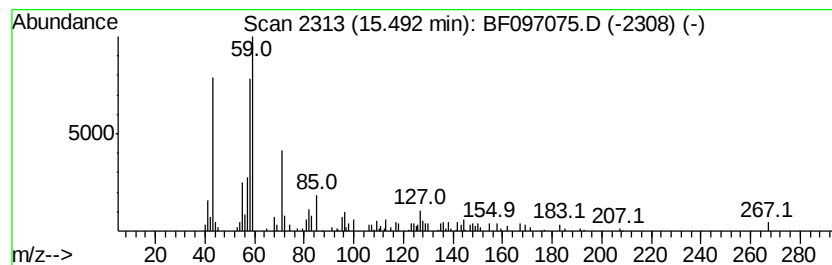
Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2-Pentadecanone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.49	3.60 ng	106329	Perylene-d12	14.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentadecanone	226	C15H30O	002345-28-0	53
2	2-Nonadecanone	282	C19H38O	000629-66-3	53
3	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	50
4	2-Tridecanone	198	C13H26O	000593-08-8	50
5	2-Dodecanone	184	C12H24O	006175-49-1	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

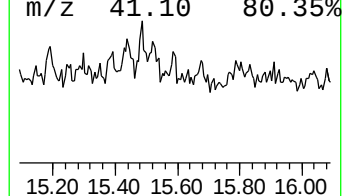
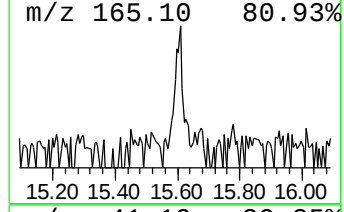
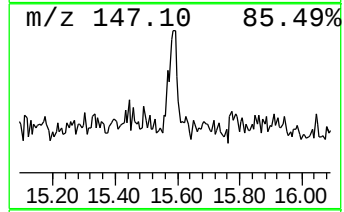
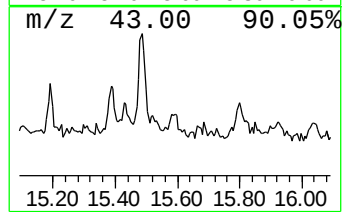
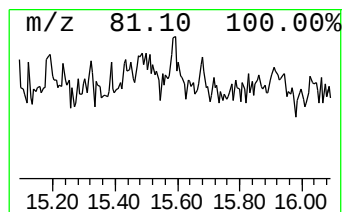
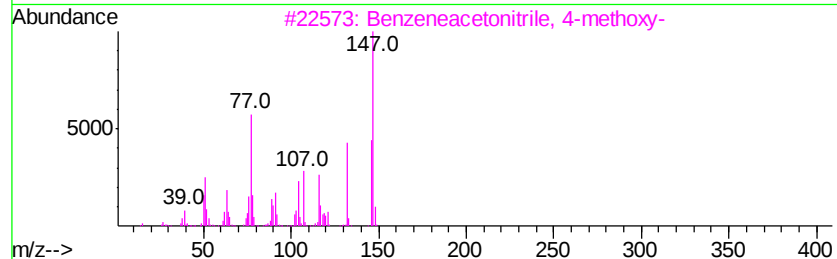
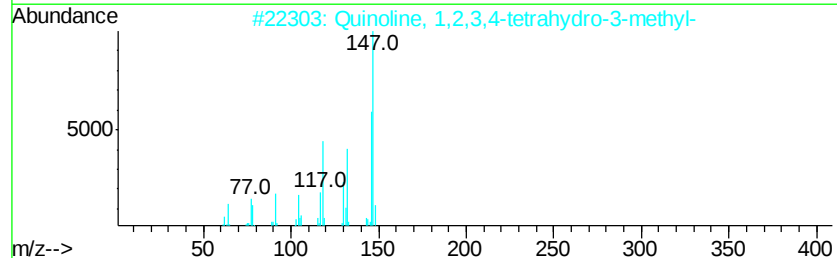
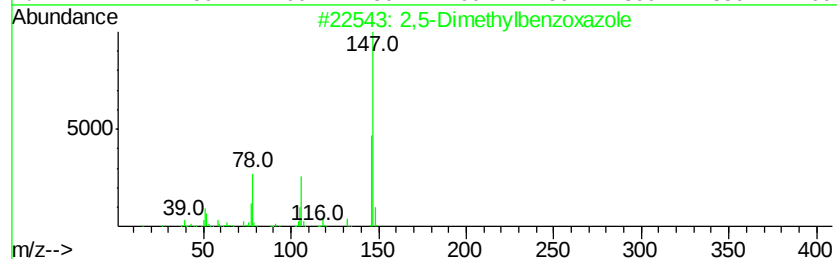
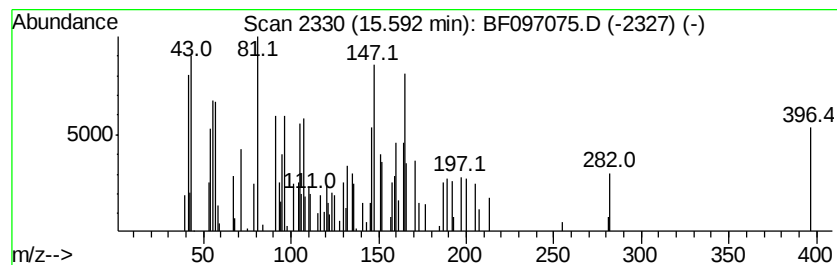
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown15.59 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	2.73 ng	80762	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Dimethylbenzoxazole	147	C9H9NO	005676-58-4	30
2		Quinoline, 1,2,3,4-tetrahydro-3-...	147	C10H13N	020668-20-6	30
3		Benzeneacetonitrile, 4-methoxy-	147	C9H9NO	000104-47-2	30
4		Carbazochrome	236	C10H12N4O3	000069-81-8	27
5		Benzonitrile, 2-methoxy-6-methyl-	147	C9H9NO	053005-44-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

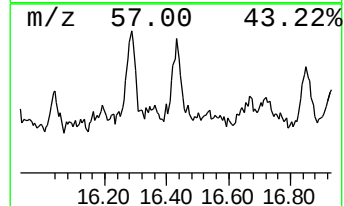
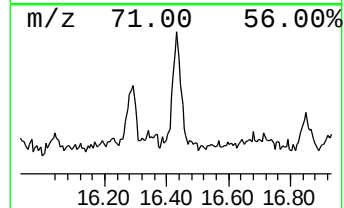
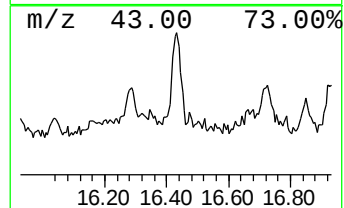
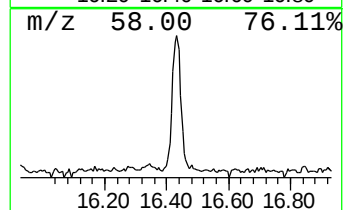
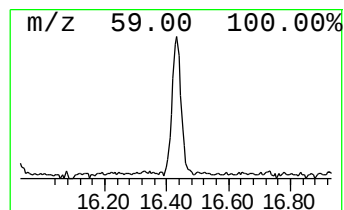
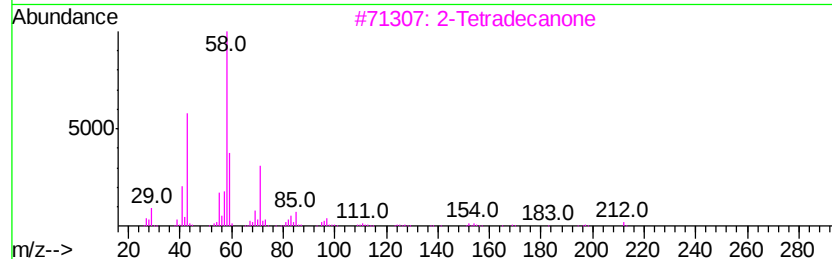
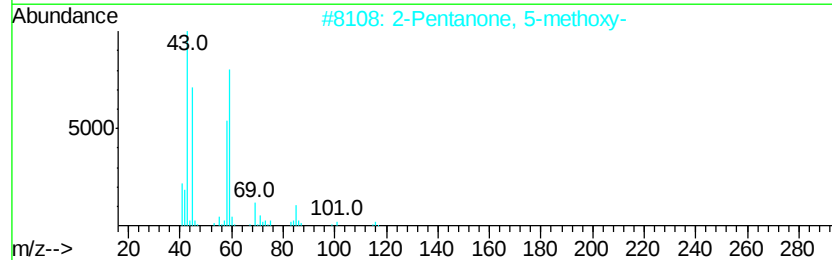
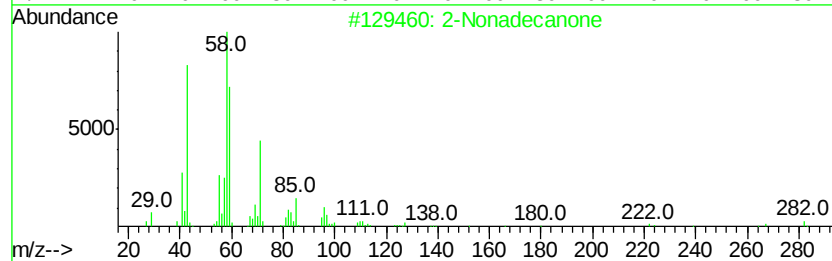
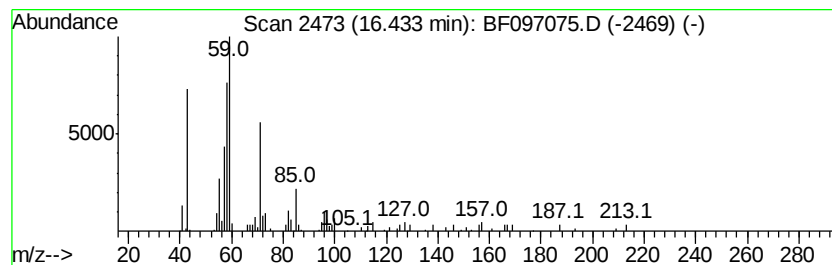
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 2-Nonadecanone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	4.05 ng	119641	Perylene-d12	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonadecanone	282	C19H38O	000629-66-3	68
2			2-Pentanone, 5-methoxy-	116	C6H12O2	017429-04-8	53
3			2-Tetradecanone	212	C14H28O	002345-27-9	50
4			2-Tridecanone	198	C13H26O	000593-08-8	50
5			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

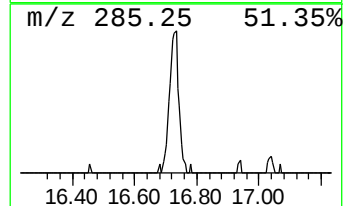
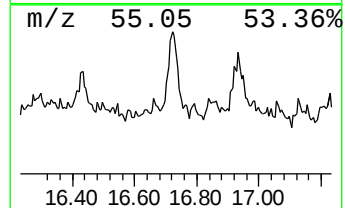
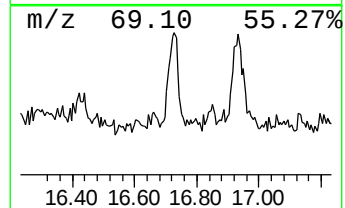
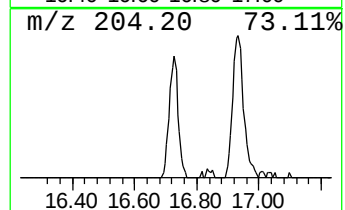
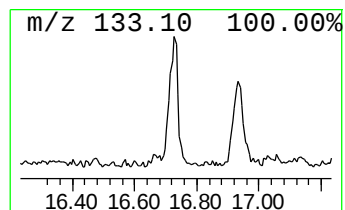
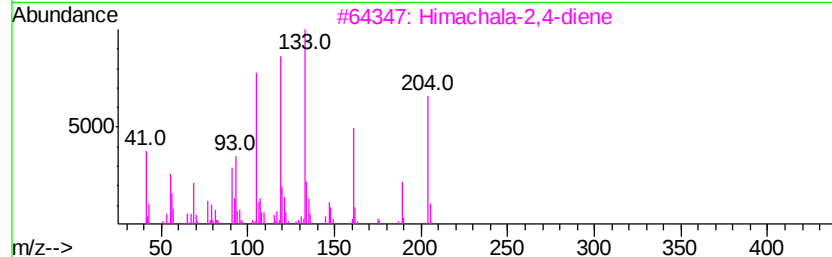
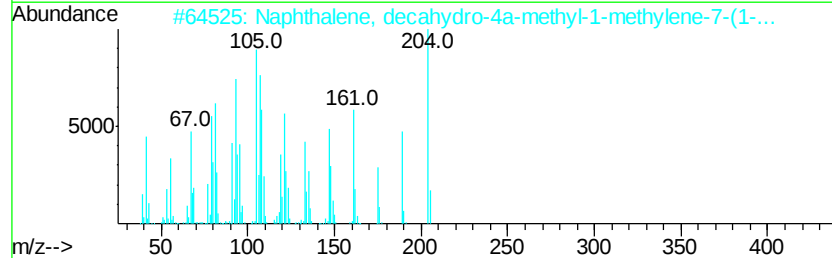
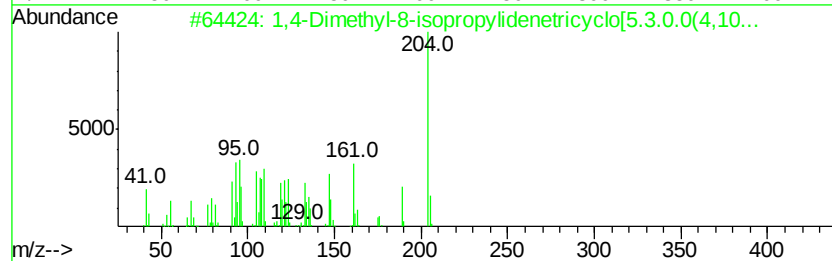
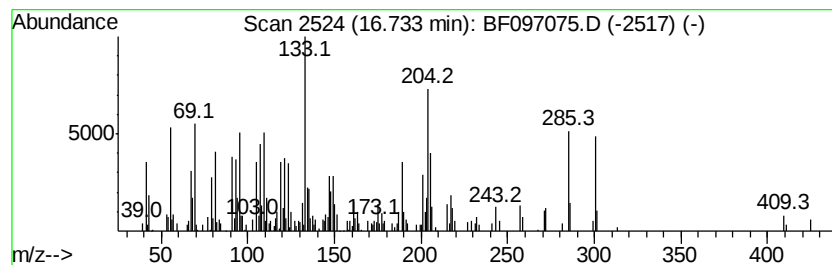
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown16.73 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	15.21 ng	449731	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	46
2		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	30
3		Himachala-2,4-diene	204	C15H24	060909-27-5	30
4		1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	27
5		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

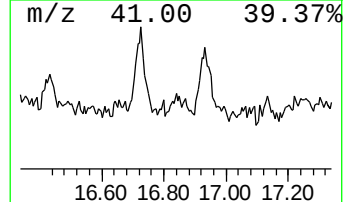
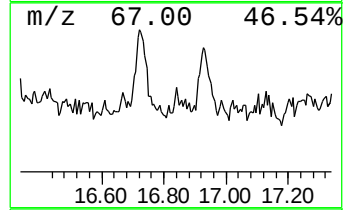
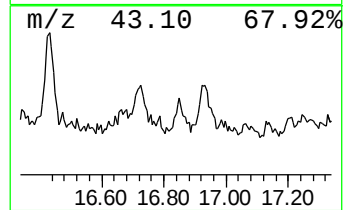
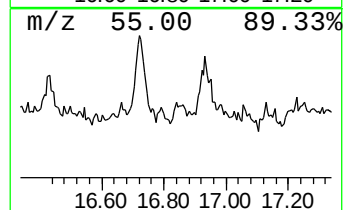
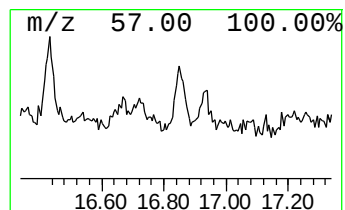
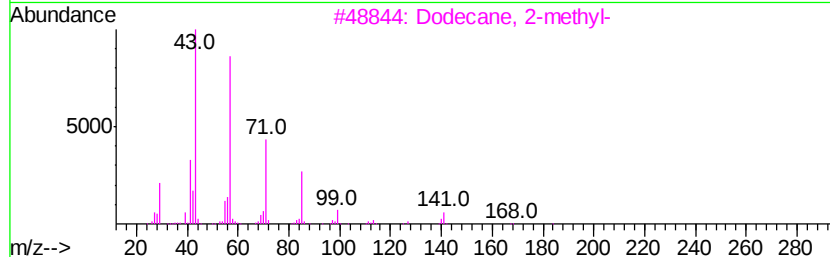
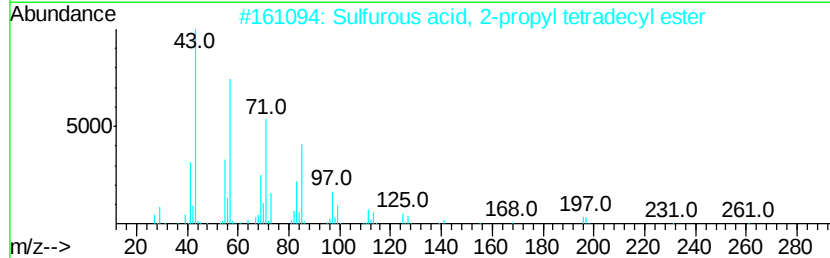
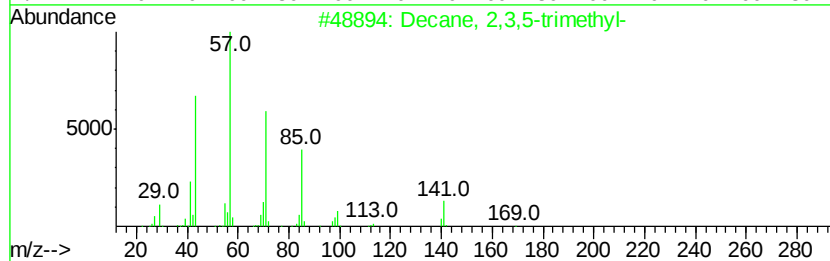
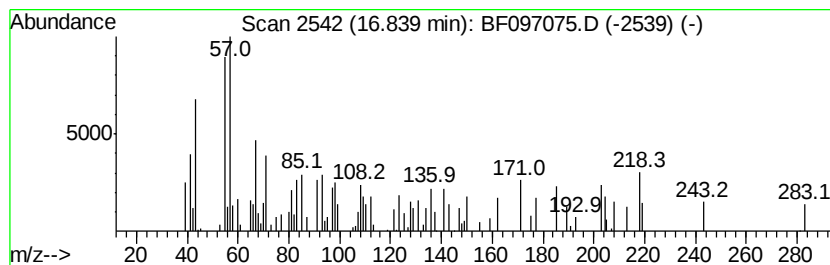
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown16.84 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	2.42 ng	71533	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	27
2		Sulfurous acid, 2-propyl tetradecyl	320	C17H36O3S	1000309-12-5	27
3		Dodecane, 2-methyl-	184	C13H28	001560-97-0	22
4		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	22
5		Hexatriacontane	507	C36H74	000630-06-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

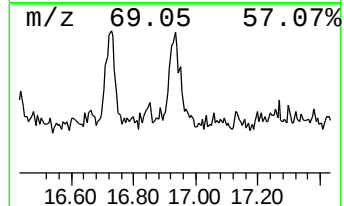
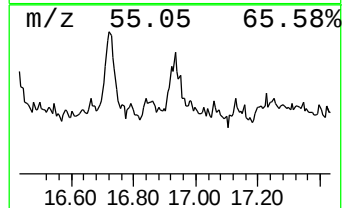
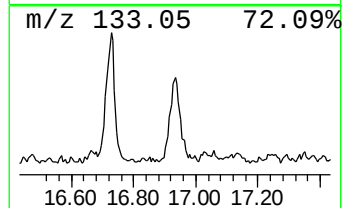
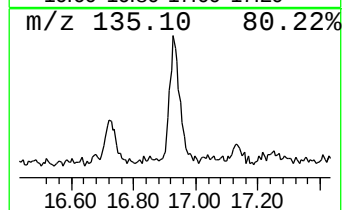
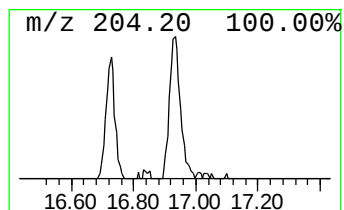
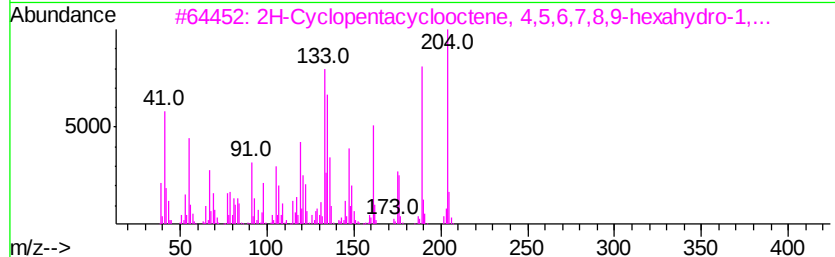
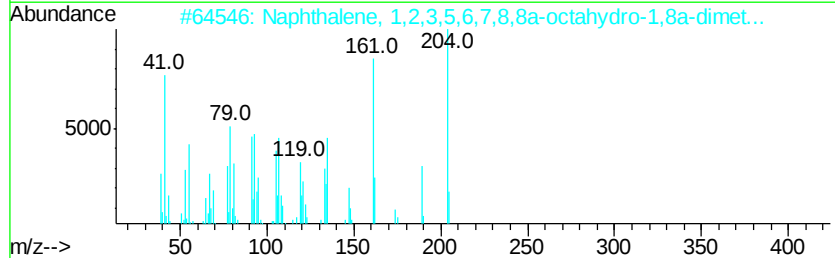
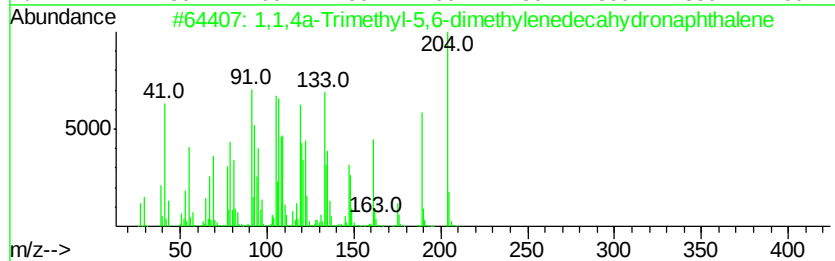
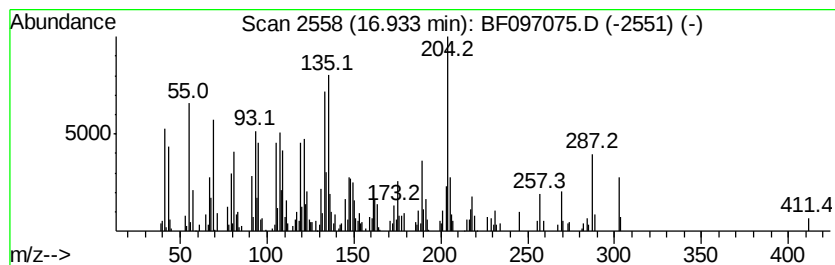
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	15.51 ng	458628	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	58
2		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	49
3		2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	46
4		cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	43
5		Guaia-3,9-diene	204	C15H24	000489-83-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097075.D
Acq On : 26 Jul 2017 15:07
Operator : SJ/JU
Sample : I4443-06 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-M7-BASE

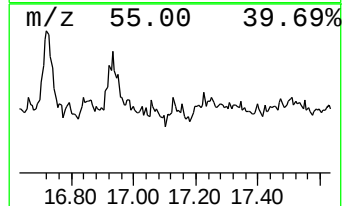
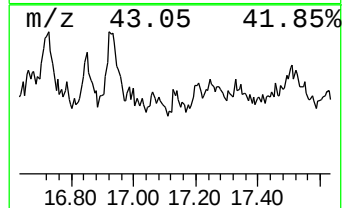
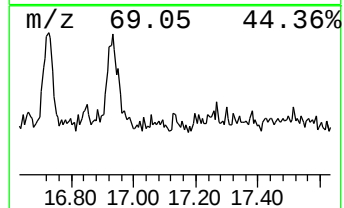
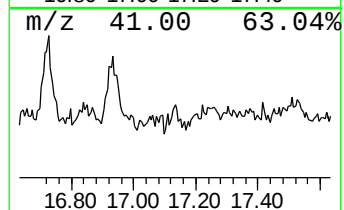
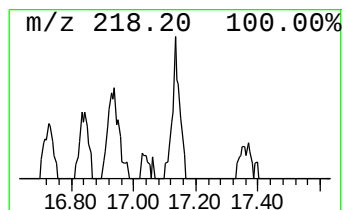
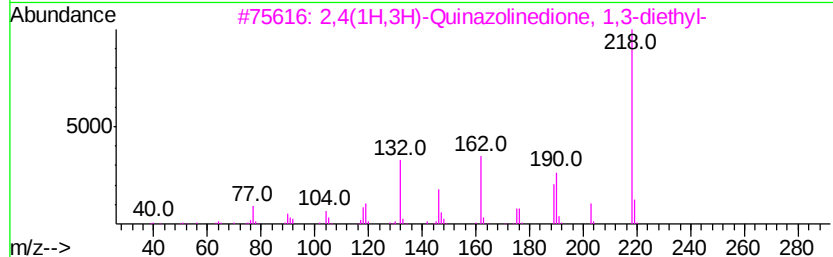
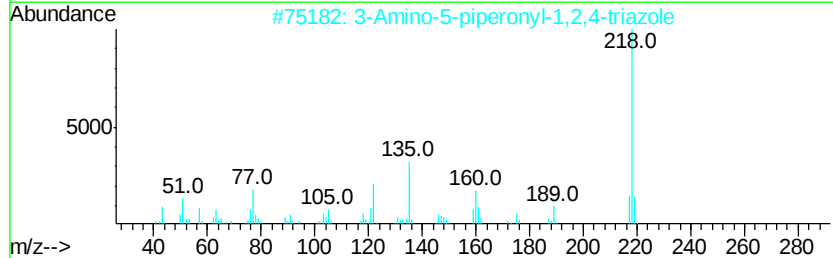
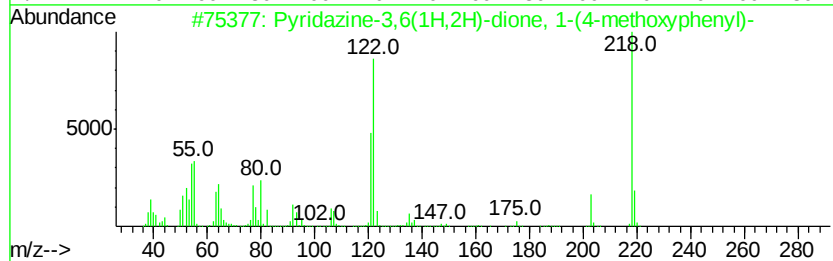
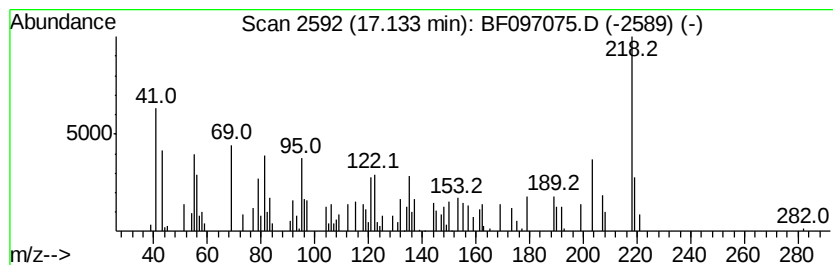
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown17.13 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.52 ng	74675	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyridazine-3,6(1H,2H)-dione, 1-(...	218	C11H10N2O3	060399-10-2	43
2		3-Amino-5-piperonyl-1,2,4-triazole	218	C10H10N4O2	014730-92-8	43
3		2,4(1H,3H)-Quinazolinodione, 1,3...	218	C12H14N2O2	002049-84-5	38
4		1,4-Naphthoquinone, 6-ethyl-2,5-...	218	C12H10O4	013378-87-5	38
5		.beta.-Amyrin trimethylsilyl ether	498	C33H58OSi	001721-67-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
 Data File : BF097075.D
 Acq On : 26 Jul 2017 15:07
 Operator : SJ/JU
 Sample : I4443-06 5X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-M7-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
unknown6.26	6.26	23.5	ng	820347	1	6.49	698736	20.0
n-Hexadecanoic acid	11.56	5.2	ng	264060	4	11.00	1010900	20.0
2-Chloroethyl lin...	12.25	6.5	ng	328938	4	11.00	1010900	20.0
trans-13-Octadece...	12.26	12.9	ng	652905	4	11.00	1010900	20.0
Octadecanoic acid	12.34	7.1	ng	207609	5	13.62	585253	20.0
1,19-Eicosadiene	13.29	4.0	ng	116777	5	13.62	585253	20.0
1-Heneicosanol	13.50	11.4	ng	332188	5	13.62	585253	20.0
1,16-Hexadecanediol	13.94	3.2	ng	94768	5	13.62	585253	20.0
Pentafluoropropio...	14.13	10.0	ng	291436	5	13.62	585253	20.0
Hexadecanal	14.54	6.3	ng	185150	6	14.97	591538	20.0
Carbonic acid, he...	14.73	4.7	ng	137498	6	14.97	591538	20.0
2-Pentadecanone	15.49	3.6	ng	106329	6	14.97	591538	20.0
unknown15.59	15.59	2.7	ng	80762	6	14.97	591538	20.0
2-Nonadecanone	16.43	4.0	ng	119641	6	14.97	591538	20.0
unknown16.73	16.73	15.2	ng	449731	6	14.97	591538	20.0
unknown16.84	16.84	2.4	ng	71533	6	14.97	591538	20.0
1,1,4a-Trimethyl-...	16.93	15.5	ng	458628	6	14.97	591538	20.0
unknown17.13	17.13	2.5	ng	74675	6	14.97	591538	20.0