

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
 Data File : BF097329.D
 Acq On : 3 Aug 2017 21:03
 Operator : SJ/JU
 Sample : I4559-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-GF-02-008-B

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	4.575	453	457	470	rBV	137152	234912	9.64%	1.109%
2	5.040	532	536	562	rBV	2041120	2436990	100.00%	11.504%
3	6.116	715	719	732	rBV	2092535	2333105	95.74%	11.014%
4	6.216	732	736	743	rVB	2272821	2191659	89.93%	10.346%
5	6.445	771	775	785	rBV	609276	592073	24.30%	2.795%
6	6.598	797	801	812	rBV	1772819	1611045	66.11%	7.605%
7	7.016	868	872	888	rBV	1542024	1509271	61.93%	7.125%
8	7.728	989	993	1002	rBV	849225	827528	33.96%	3.906%
9	8.798	1171	1175	1179	rBV	2392328	2316685	95.06%	10.936%
10	9.198	1240	1243	1248	rBV	366322	290099	11.90%	1.369%
11	9.463	1284	1288	1292	rBV	997860	849651	34.86%	4.011%
12	9.922	1363	1366	1369	rVB	54161	43101	1.77%	0.203%
13	10.139	1397	1403	1405	rBV	21454	29082	1.19%	0.137%
14	10.251	1418	1422	1432	rBV	1382995	1291371	52.99%	6.096%
15	10.386	1442	1445	1450	rBV	62724	71266	2.92%	0.336%
16	10.833	1517	1521	1524	rBV	39958	32481	1.33%	0.153%
17	10.933	1535	1538	1542	rBV	771628	738577	30.31%	3.487%
18	11.492	1630	1633	1640	rBV2	108957	114905	4.72%	0.542%
19	11.651	1657	1660	1667	rVB4	21041	34116	1.40%	0.161%
20	12.033	1719	1725	1727	rBV	31357	39572	1.62%	0.187%
21	12.051	1727	1728	1731	rVB	31778	25413	1.04%	0.120%
22	12.139	1740	1743	1747	rBV	61838	54735	2.25%	0.258%
23	12.363	1777	1781	1788	rVB	53581	57054	2.34%	0.269%
24	12.516	1803	1807	1811	rBV	1633354	1592128	65.33%	7.516%
25	12.769	1844	1850	1852	rBV6	21622	32023	1.31%	0.151%
26	13.439	1959	1964	1971	rBV2	106408	164930	6.77%	0.779%
27	13.557	1980	1984	1987	rBV	651401	594578	24.40%	2.807%
28	14.074	2066	2072	2077	rBV4	40766	74740	3.07%	0.353%
29	14.410	2125	2129	2133	rBV	93667	97643	4.01%	0.461%
30	14.551	2150	2153	2162	rVB2	40602	71747	2.94%	0.339%
31	14.633	2164	2167	2170	rBV2	32257	36241	1.49%	0.171%
32	14.845	2201	2203	2207	rVB	26455	25329	1.04%	0.120%
33	14.898	2208	2212	2216	rBV	436030	480841	19.73%	2.270%
34	15.098	2243	2246	2254	rVB7	22025	34293	1.41%	0.162%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

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	15.286	2274	2278	2282	rBV2	35816	57515	2.36%	0.272%
36	15.680	2341	2345	2352	rBV3	28612	46015	1.89%	0.217%
37	15.910	2381	2384	2391	rVB8	18441	25432	1.04%	0.120%
38	16.145	2421	2424	2429	rVB4	22344	34104	1.40%	0.161%
39	17.157	2590	2596	2604	rBV4	31330	91554	3.76%	0.432%

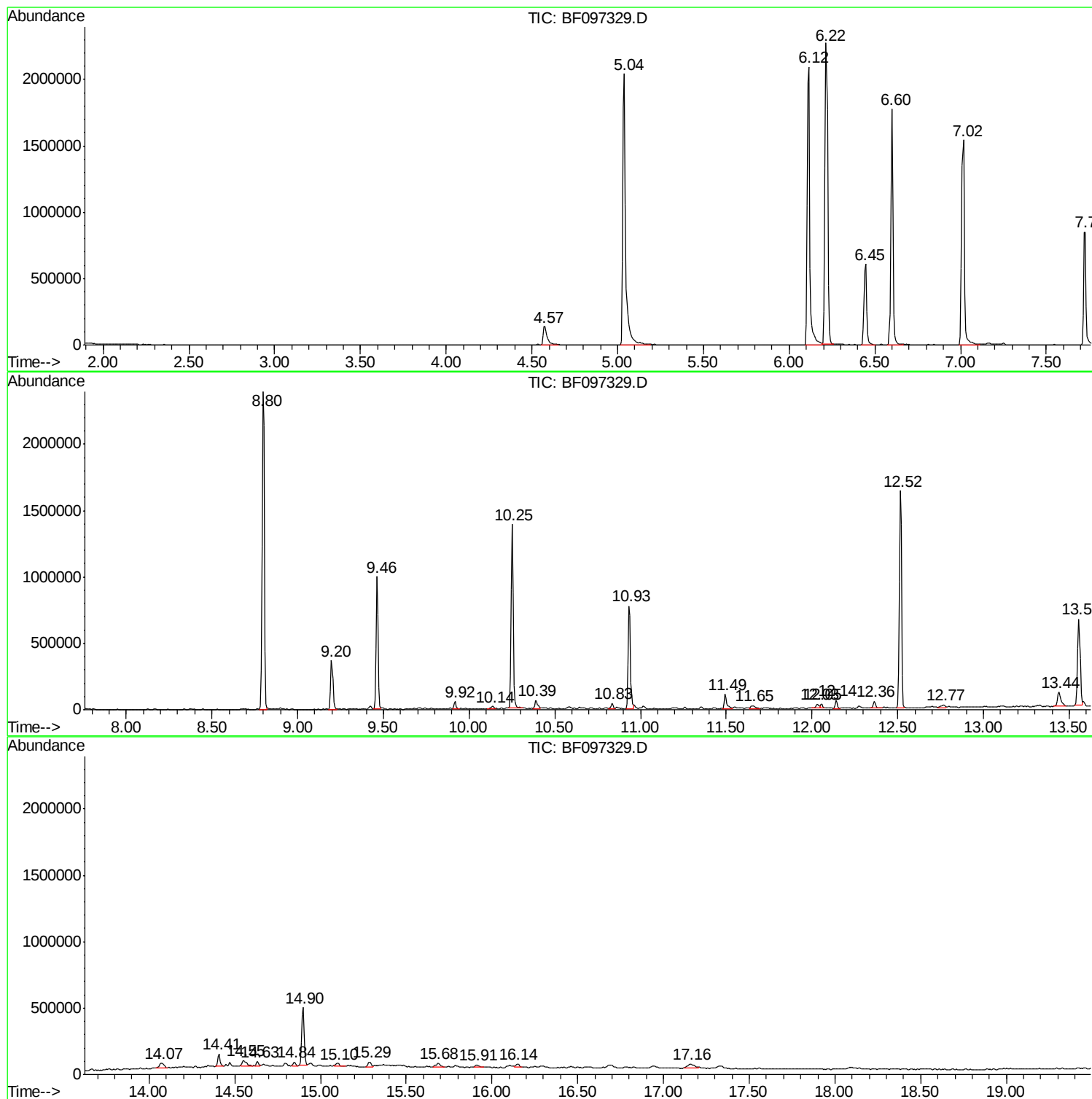
Sum of corrected areas: 21183804

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

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\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

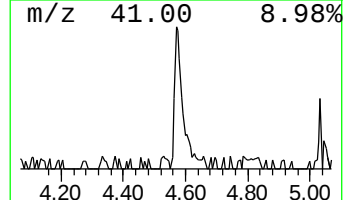
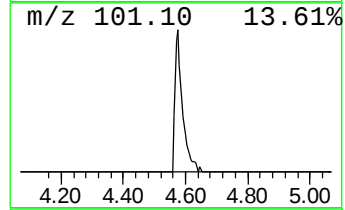
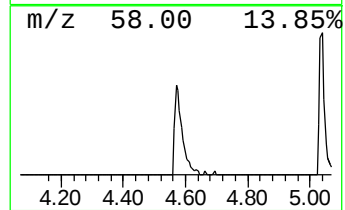
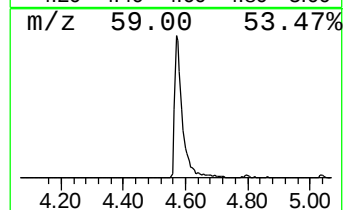
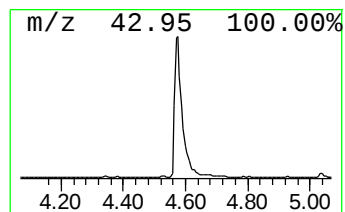
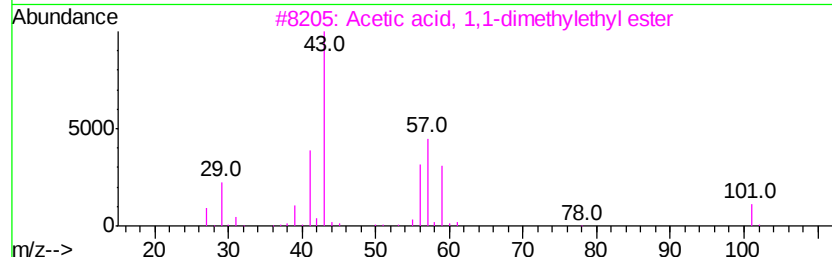
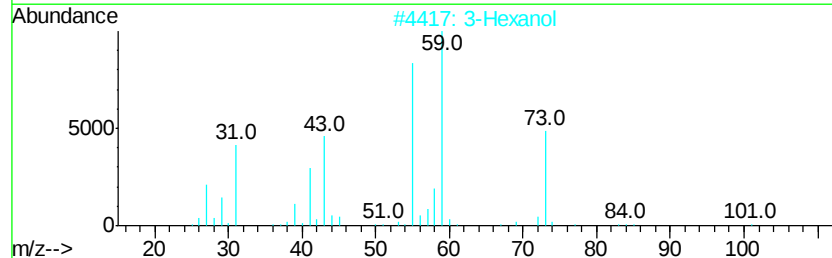
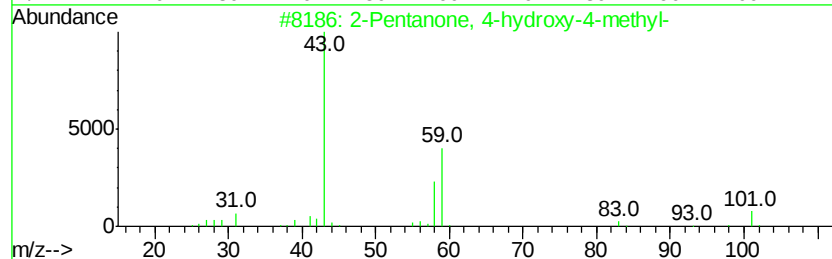
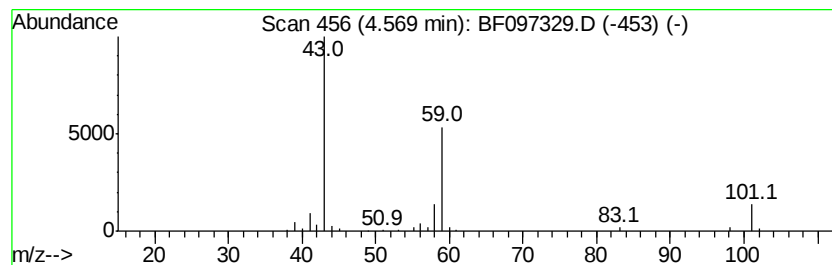
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	7.94 ng	234912	1,4-Dichlorobenzene-d4	6.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol	102	C6H14O	000623-37-0	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

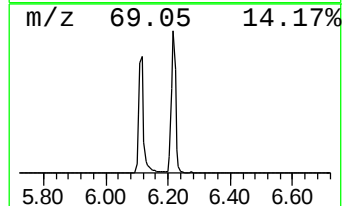
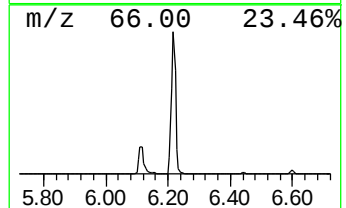
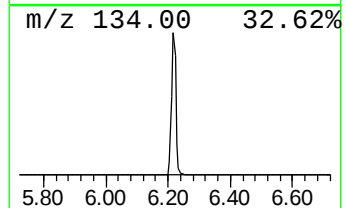
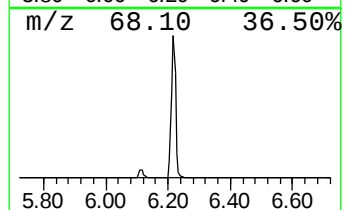
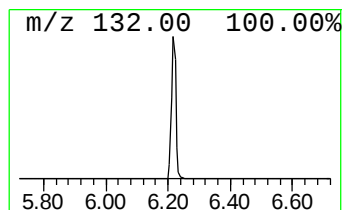
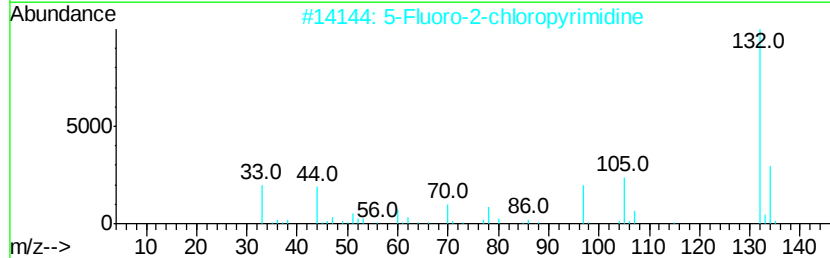
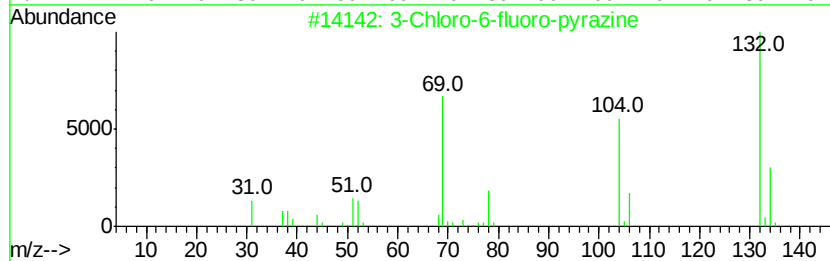
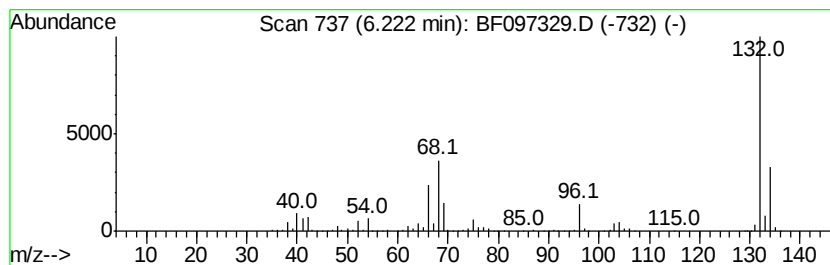
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	74.03 ng	2191660	1,4-Dichlorobenzene-d4	6.45

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

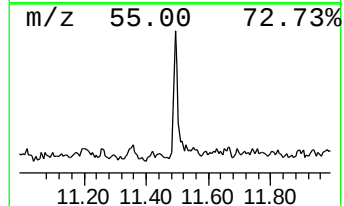
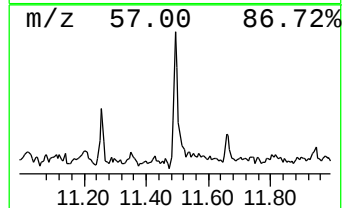
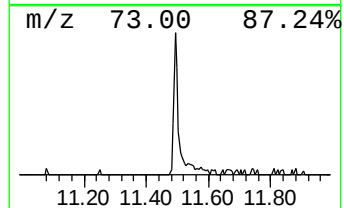
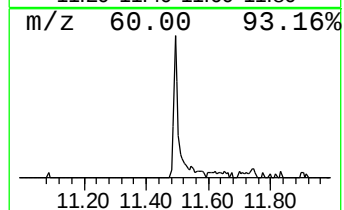
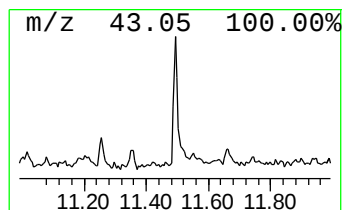
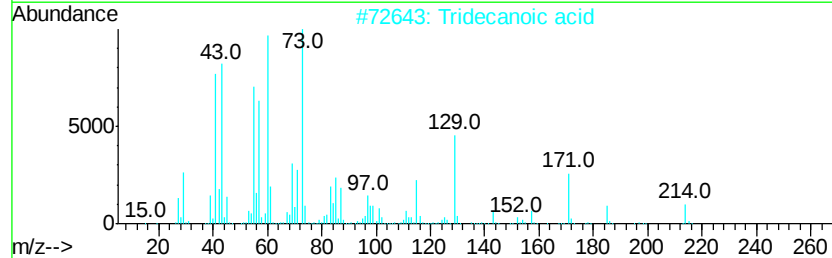
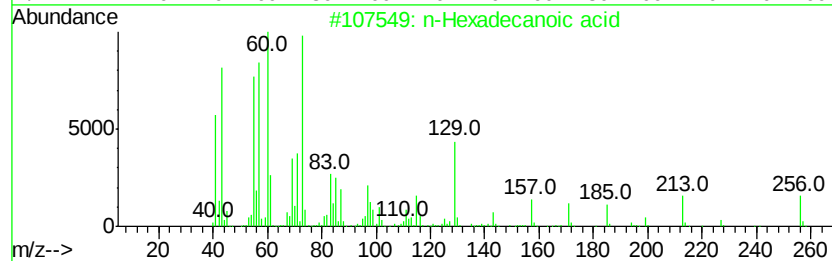
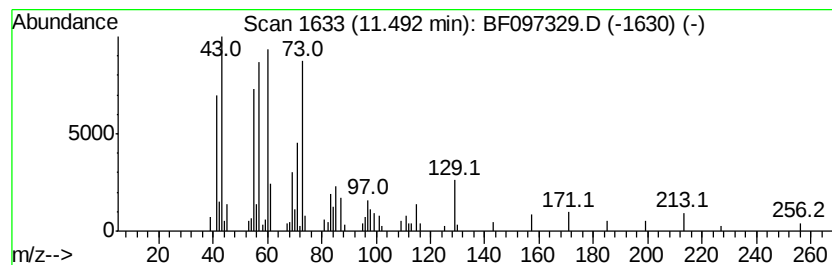
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	3.11 ng	114905	Phenanthrene-d10	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	Dodecane	170	C12H26	000112-40-3	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

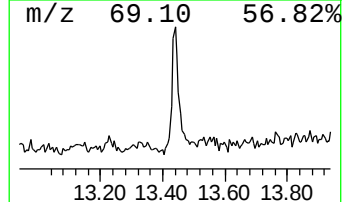
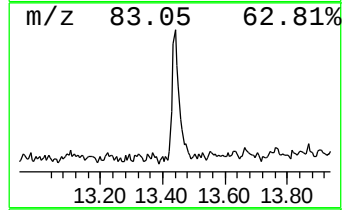
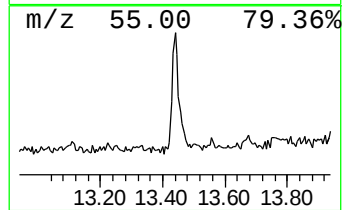
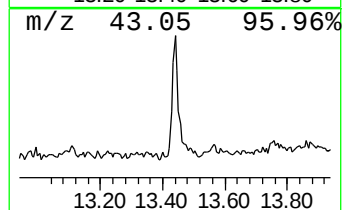
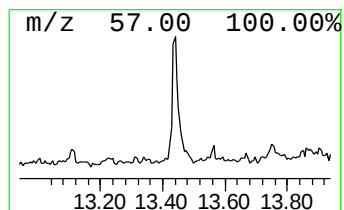
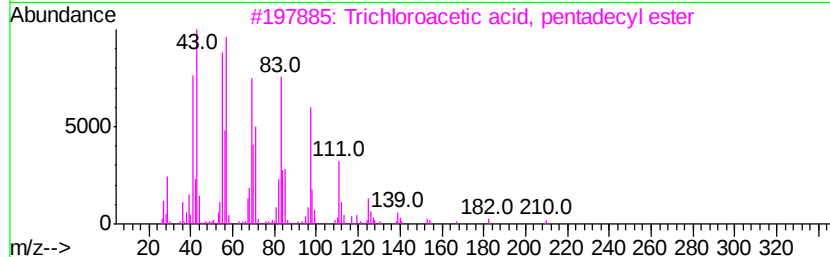
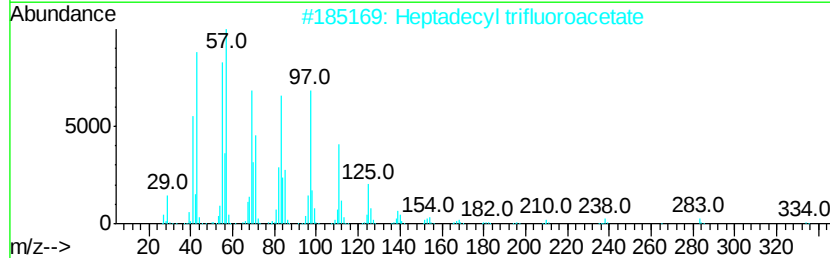
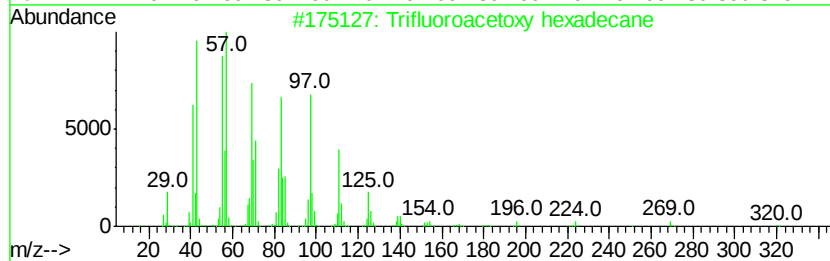
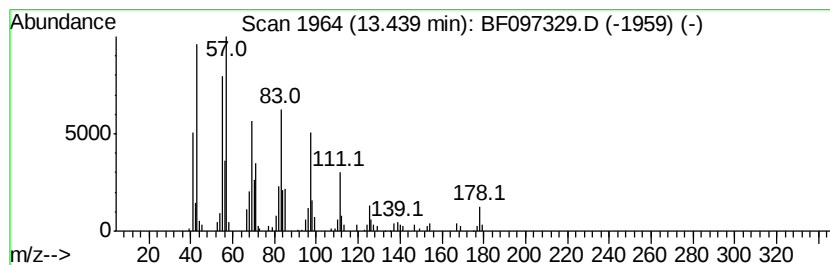
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	5.55 ng	164930	Chrysene-d12	13.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
4		1-Docosene	308	C22H44	001599-67-3	91
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

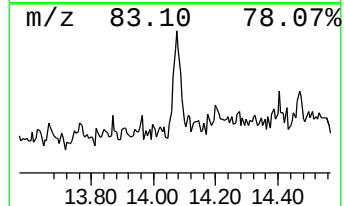
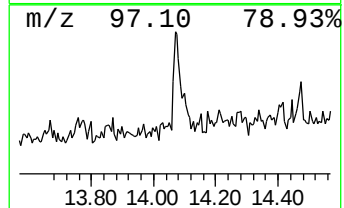
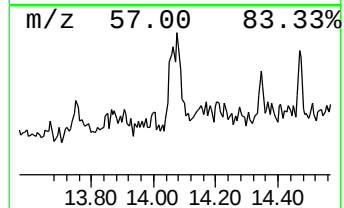
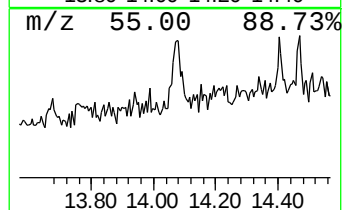
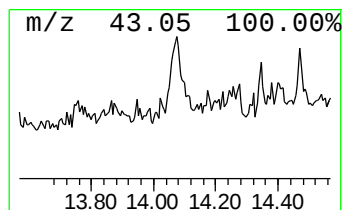
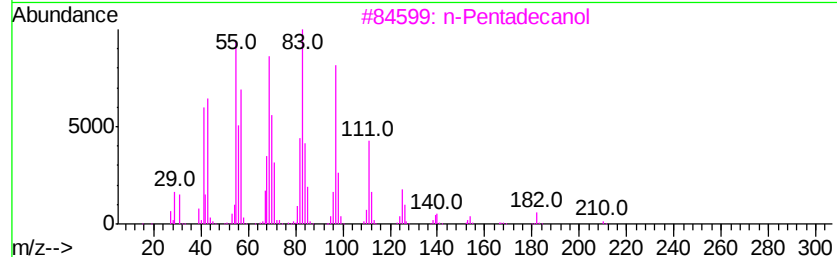
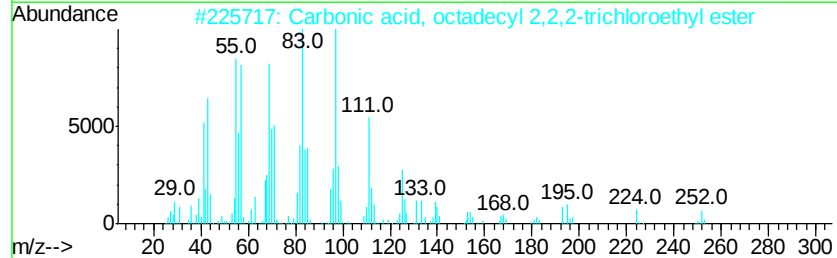
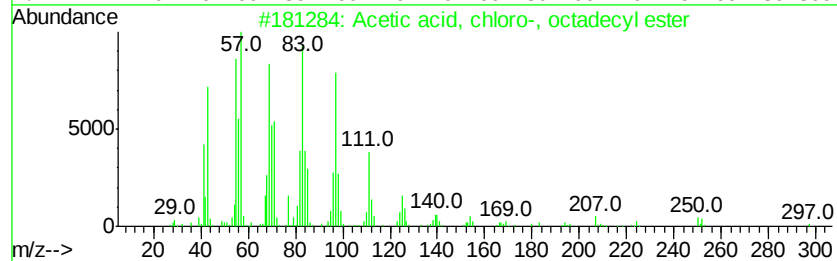
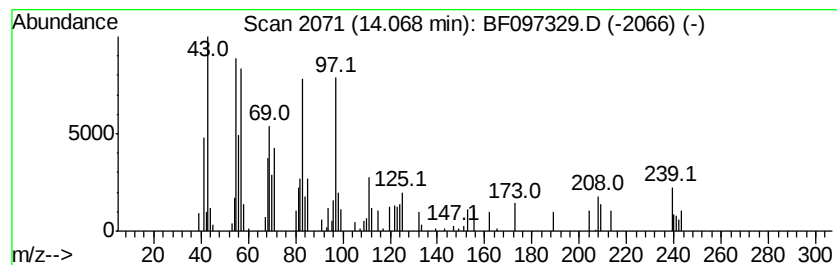
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Acetic acid, chloro-, octad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.51 ng	74740	Chrysene-d12	13.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	87
2		Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	83
3		n-Pentadecanol	228	C15H32O	000629-76-5	81
4		Cycloeicosane	280	C20H40	000296-56-0	74
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

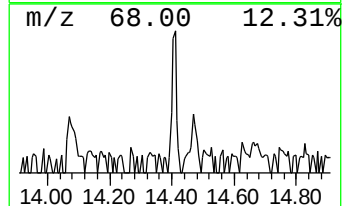
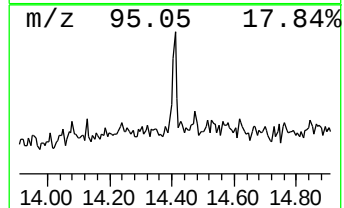
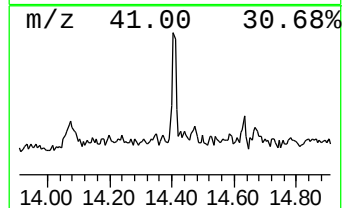
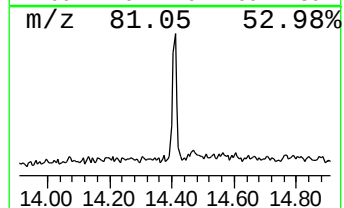
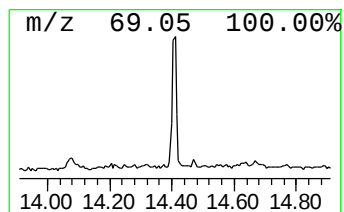
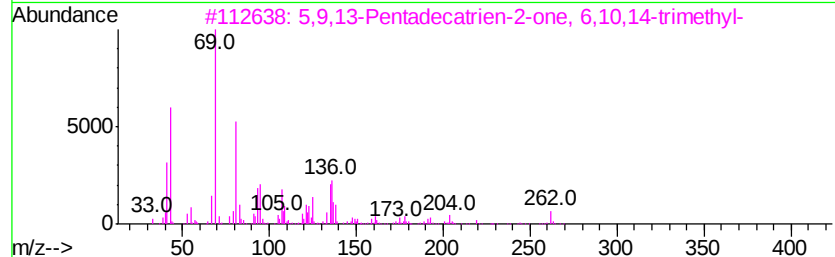
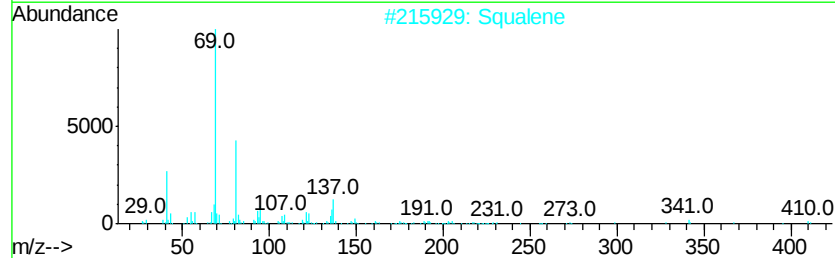
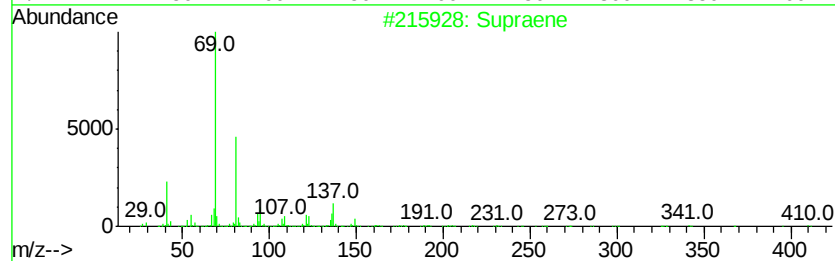
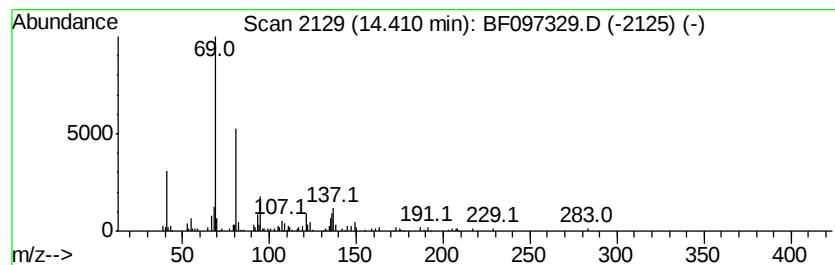
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	4.06 ng	97643	Perylene-d12	14.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	86
2		Squalene	410	C30H50	000111-02-4	86
3		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	000762-29-8	56
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	50
5		2,6-Dimethyl-2-trans-6-octadiene	138	C10H18	002609-23-6	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

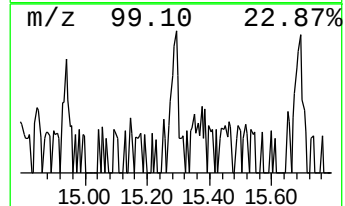
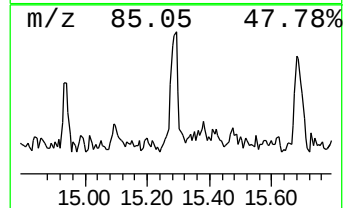
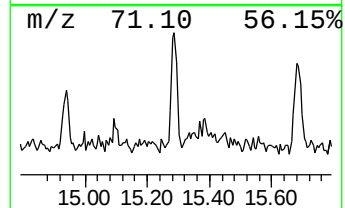
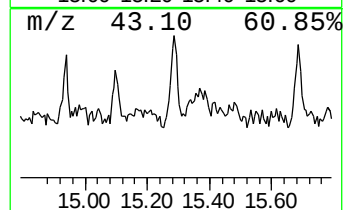
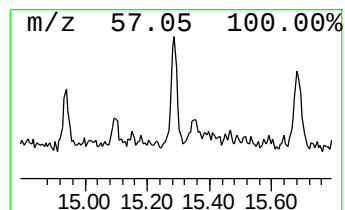
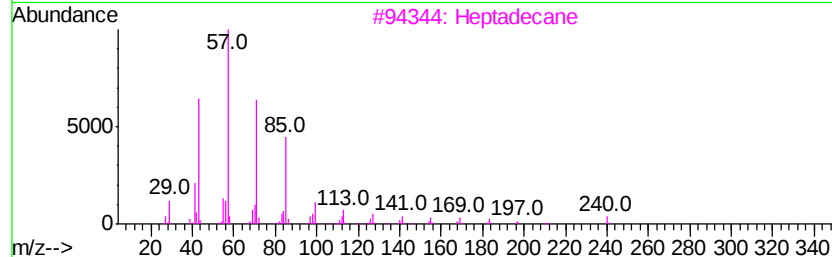
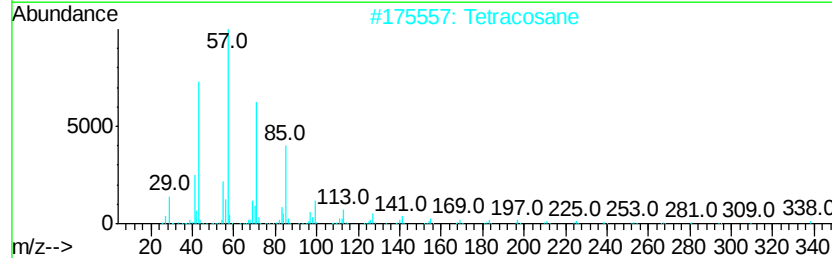
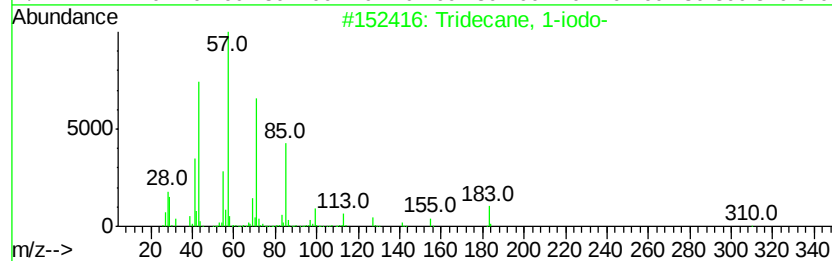
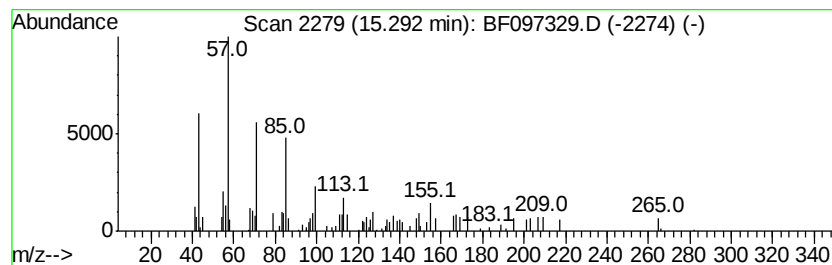
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.39 ng	57515	Perylene-d12	14.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
2		Tetracosane	338	C24H50	000646-31-1	64
3		Heptadecane	240	C17H36	000629-78-7	64
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59
5		Eicosane	282	C20H42	000112-95-8	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

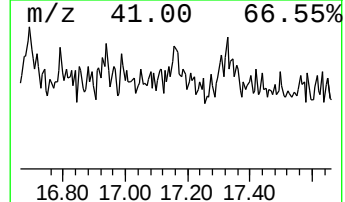
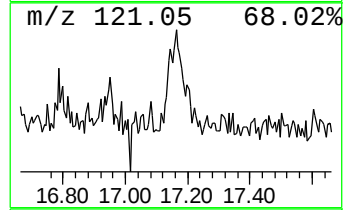
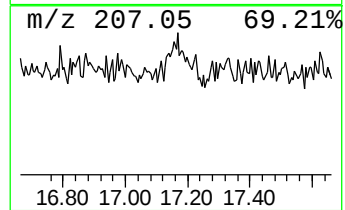
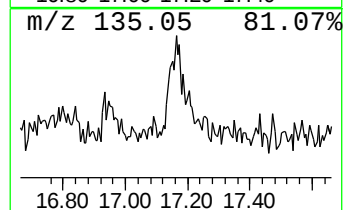
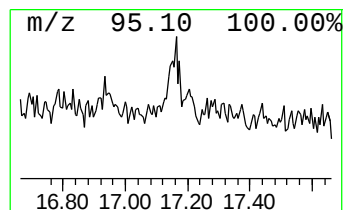
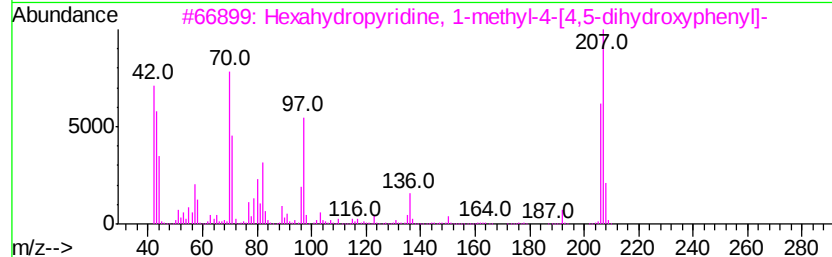
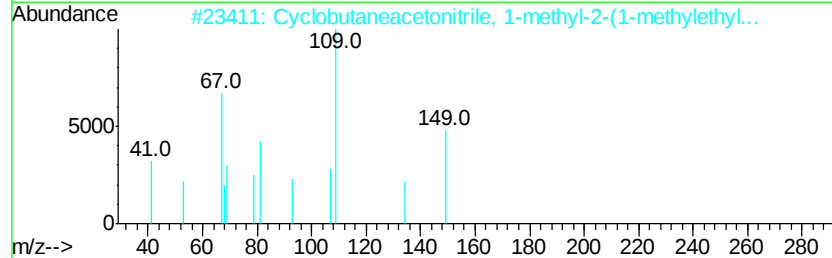
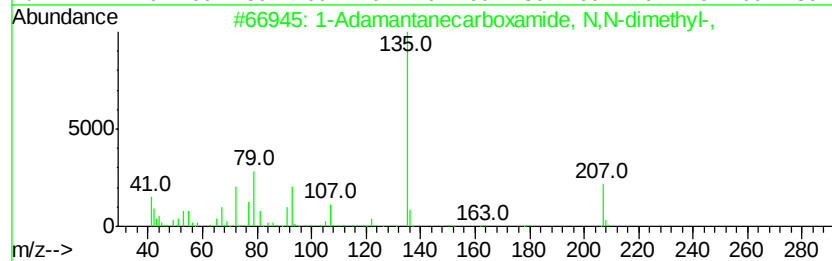
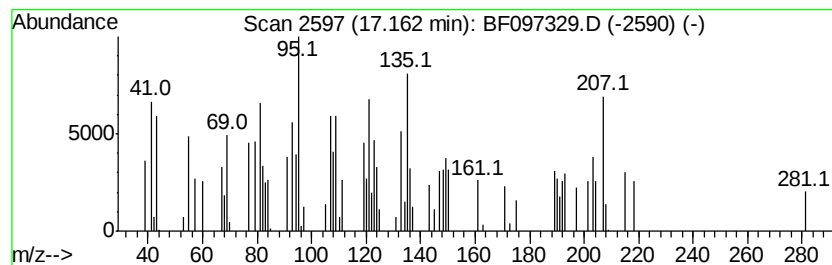
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.16 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	3.81 ng	91554	Perylene-d12	14.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Adamantanecarboxamide, N,N-dim...	207	C13H21NO	001502-00-7	11
2			Cyclobutaneacetonitrile, 1-methv...	149	C10H15N	055760-14-0	11
3			Hexahydrodropyridine, 1-methyl-4-[4...	207	C12H17N02	094427-47-1	11
4			2-Bromothiophenol	188	C6H5BrS	006320-02-1	10
5			8-Chloro-5-quinolinecarboxylic acid	207	C10H6ClN02	121490-68-4	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097329.D
Acq On : 3 Aug 2017 21:03
Operator : SJ/JU
Sample : I4559-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-008-B

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
2-Pentanone, 4-hy...	4.57	7.9	ng	234912	1	6.45	592073	20.0
unknown6.22	6.22	74.0	ng	2191660	1	6.45	592073	20.0
n-Hexadecanoic acid	11.49	3.1	ng	114905	4	10.93	738577	20.0
Trifluoroacetoxy ...	13.44	5.5	ng	164930	5	13.56	594578	20.0
Acetic acid, chlo...	14.07	2.5	ng	74740	5	13.56	594578	20.0
Supraene	14.41	4.1	ng	97643	6	14.90	480841	20.0
Tridecane, 1-iodo-	15.29	2.4	ng	57515	6	14.90	480841	20.0
unknown17.16	17.16	3.8	ng	91554	6	14.90	480841	20.0