

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062017\
 Data File : BF096054.D
 Acq On : 20 Jun 2017 20:15
 Operator : SJ/MA
 Sample : I3676-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-5-6

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-BF060517.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	1.552	9	11	36	rVB	750296	1323135	73.99%	8.948%
2	4.469	503	507	523	rBV	45539	131209	7.34%	0.887%
3	5.181	624	628	656	rBV	689600	1505053	84.16%	10.179%
4	6.869	911	915	925	rBV	829270	1373702	76.81%	9.290%
5	6.951	925	929	953	rVB	1097984	1788335	100.00%	12.094%
6	7.292	982	987	999	rBV	265040	371110	20.75%	2.510%
7	7.528	1022	1027	1054	rBV	871610	1177156	65.82%	7.961%
8	8.210	1139	1143	1164	rBV	577936	876904	49.03%	5.930%
9	9.322	1328	1332	1346	rBV	362079	495955	27.73%	3.354%
10	11.104	1629	1635	1645	rBV	1285559	1556431	87.03%	10.526%
11	11.798	1749	1753	1760	rBV	145544	180952	10.12%	1.224%
12	12.145	1807	1812	1817	rBV2	372483	480358	26.86%	3.249%
13	12.186	1817	1819	1825	rVB2	16959	24011	1.34%	0.162%
14	13.004	1950	1958	1963	rBV	22519	30589	1.71%	0.207%
15	13.439	2028	2032	2048	rBV	512048	712736	39.85%	4.820%
16	13.768	2085	2088	2091	rBV2	24228	33286	1.86%	0.225%
17	14.539	2215	2219	2230	rVB	316453	439860	24.60%	2.975%
18	15.562	2389	2393	2400	rBV4	42564	54252	3.03%	0.367%
19	16.374	2527	2531	2534	rVB	20964	24804	1.39%	0.168%
20	16.674	2578	2582	2587	rBV2	41774	59664	3.34%	0.404%
21	16.921	2619	2624	2629	rVB	1038875	1183181	66.16%	8.002%
22	17.774	2766	2769	2772	rVB2	25575	24978	1.40%	0.169%
23	18.180	2834	2838	2845	rBV3	78363	147922	8.27%	1.000%
24	18.268	2849	2853	2859	rBV	333293	411516	23.01%	2.783%
25	18.597	2906	2909	2916	rVB	49730	63921	3.57%	0.432%
26	18.980	2971	2974	2978	rVB	33174	33092	1.85%	0.224%
27	19.944	3134	3138	3144	rVB	224587	282382	15.79%	1.910%

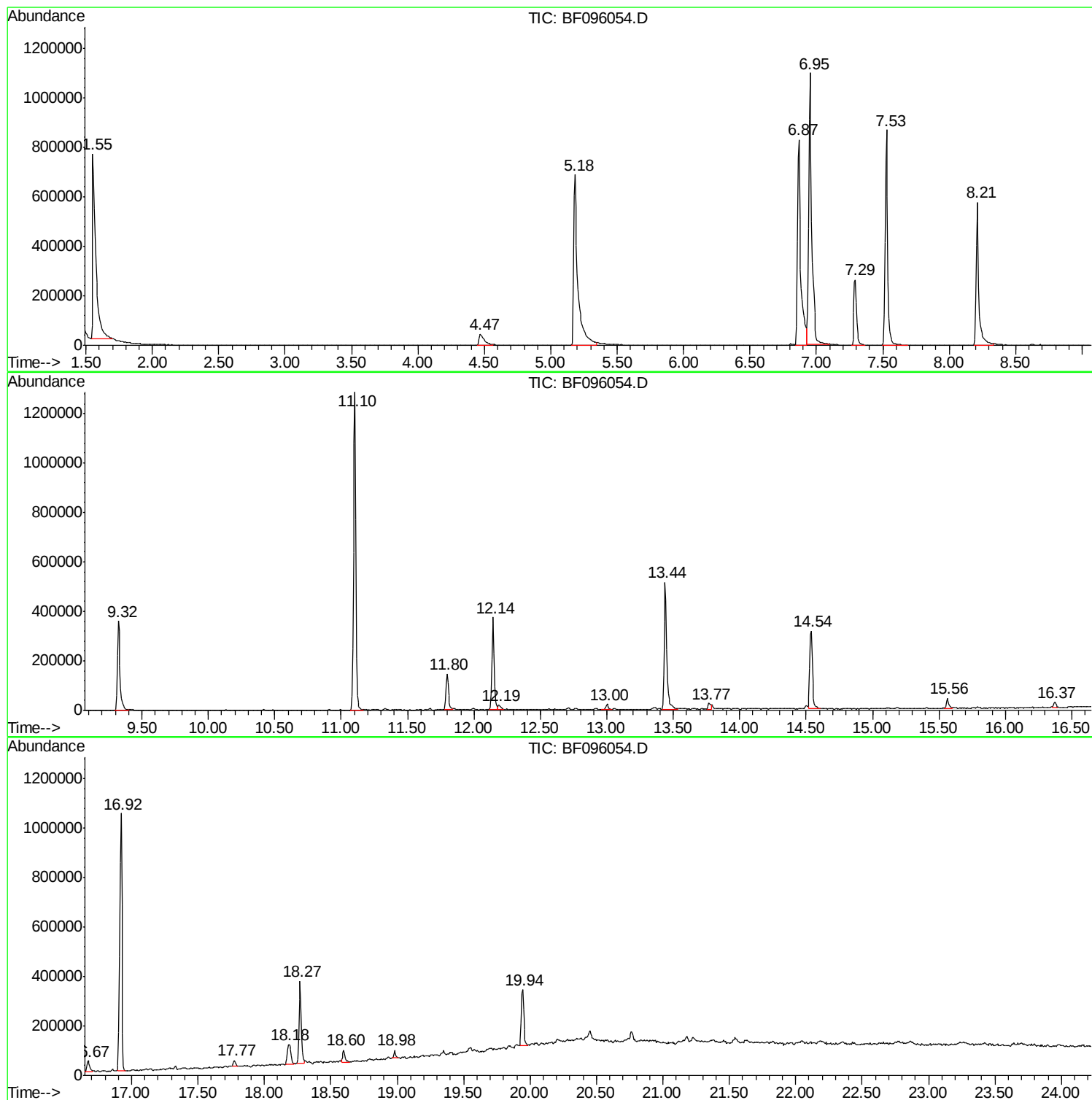
Sum of corrected areas: 14786494

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062017\
Data File : BF096054.D
Acq On : 20 Jun 2017 20:15
Operator : SJ/MA
Sample : I3676-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-5-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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\BF062017\
Data File : BF096054.D
Acq On : 20 Jun 2017 20:15
Operator : SJ/MA
Sample : I3676-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-5-6

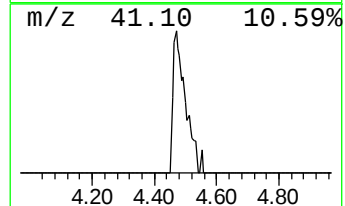
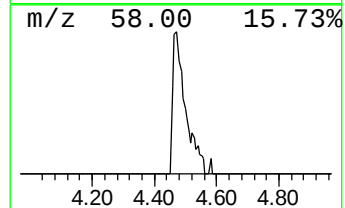
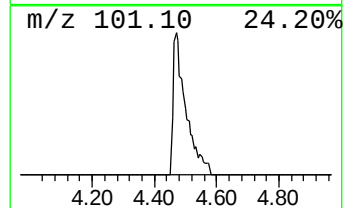
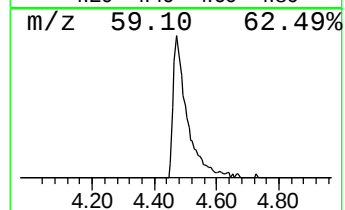
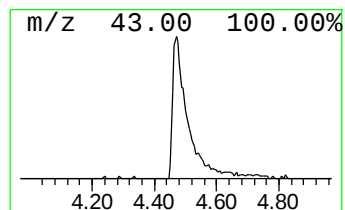
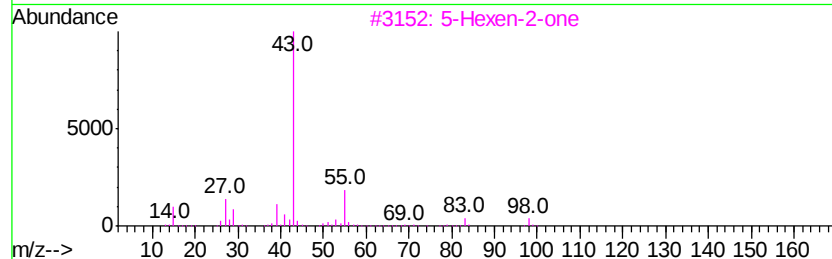
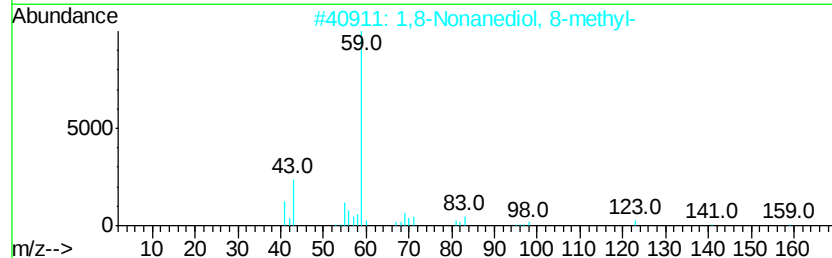
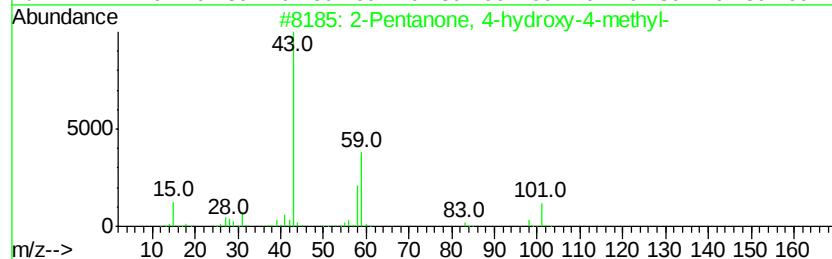
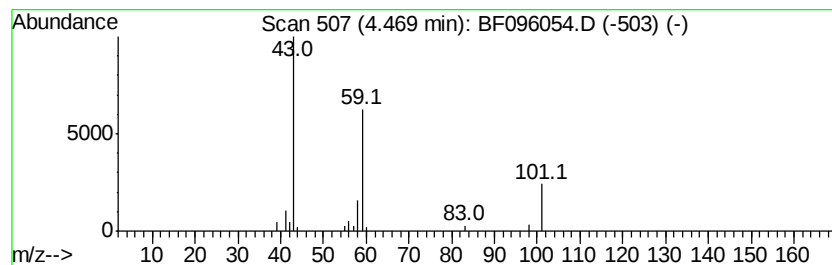
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	7.07 ng	131209	1,4-Dichlorobenzene-d4	7.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062017\
Data File : BF096054.D
Acq On : 20 Jun 2017 20:15
Operator : SJ/MA
Sample : I3676-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-5-6

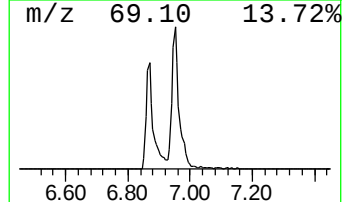
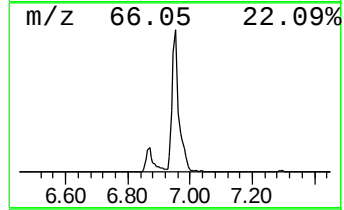
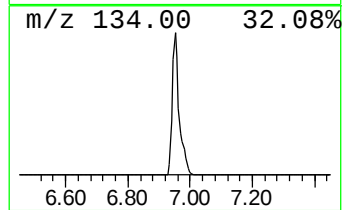
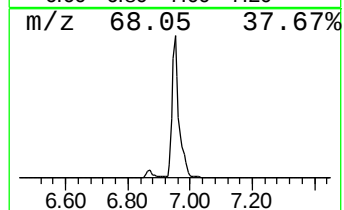
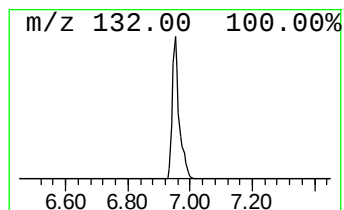
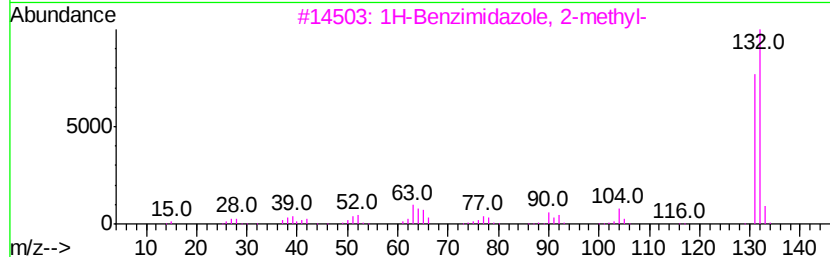
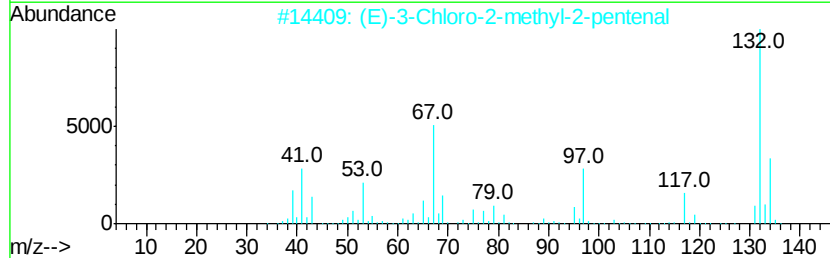
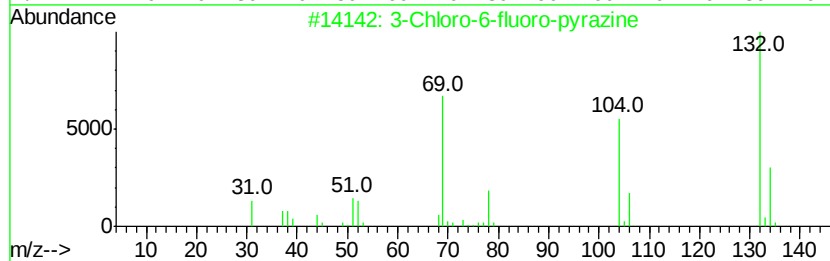
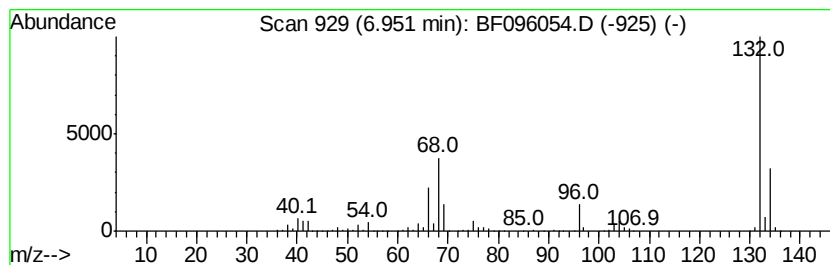
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.95 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	96.38 ng	1788340	1,4-Dichlorobenzene-d4	7.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062017\
Data File : BF096054.D
Acq On : 20 Jun 2017 20:15
Operator : SJ/MA
Sample : I3676-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-5-6

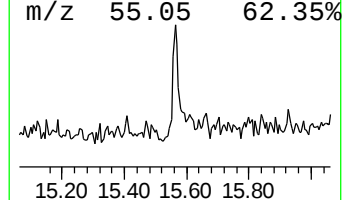
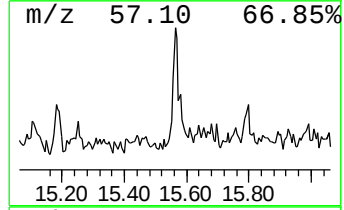
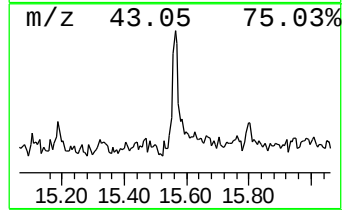
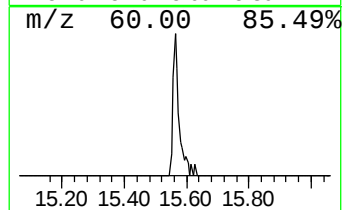
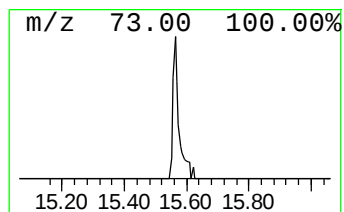
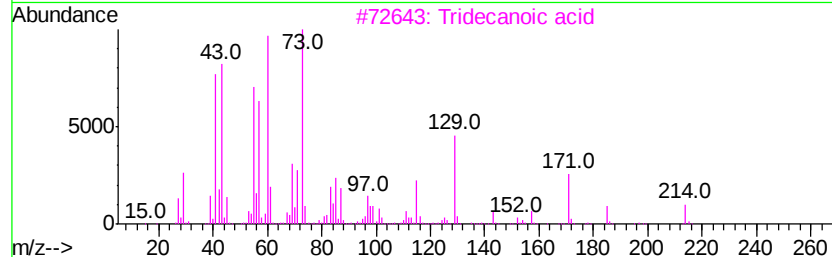
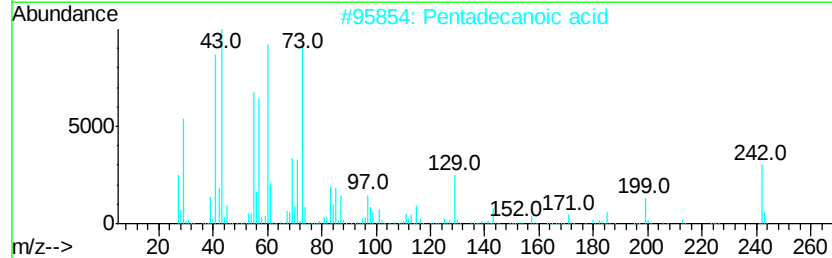
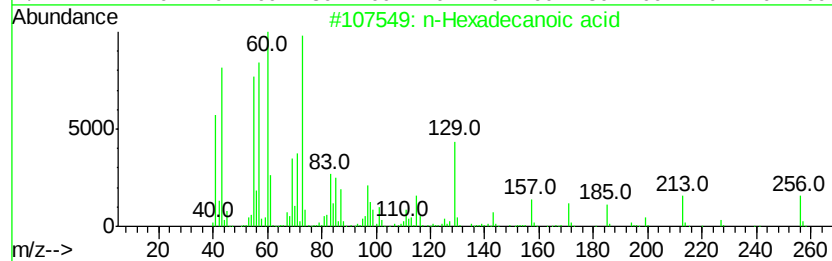
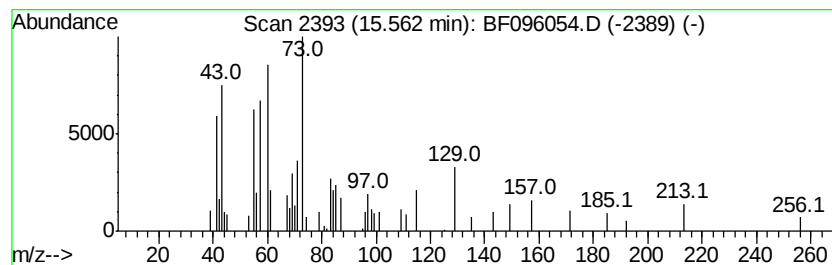
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	2.47 ng	54252	Phenanthrene-d10	14.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062017\
Data File : BF096054.D
Acq On : 20 Jun 2017 20:15
Operator : SJ/MA
Sample : I3676-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-5-6

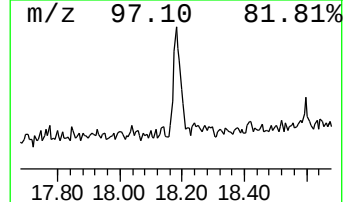
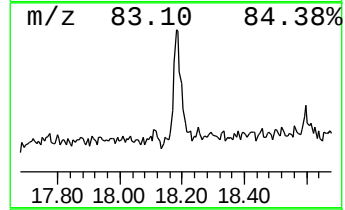
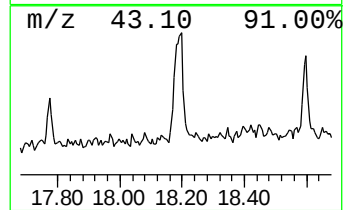
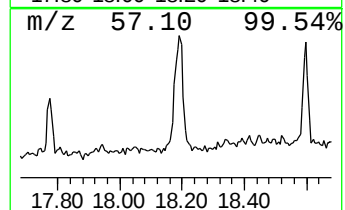
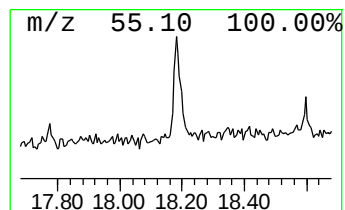
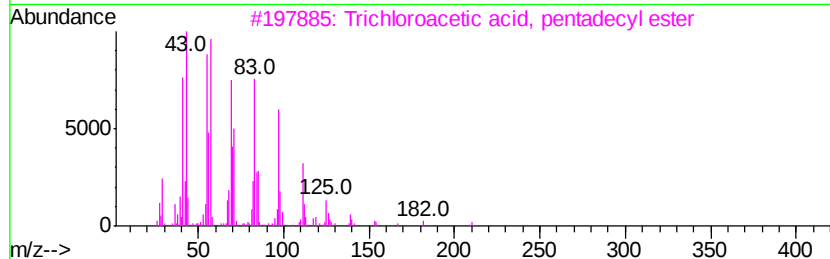
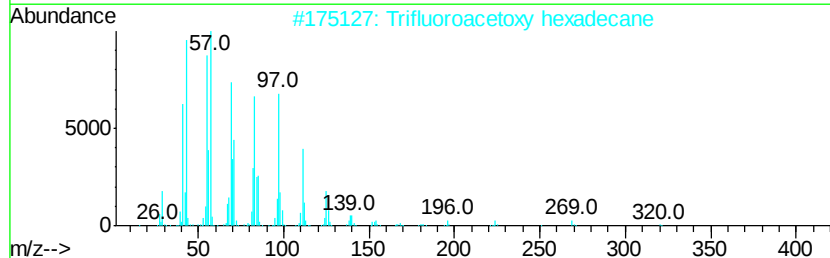
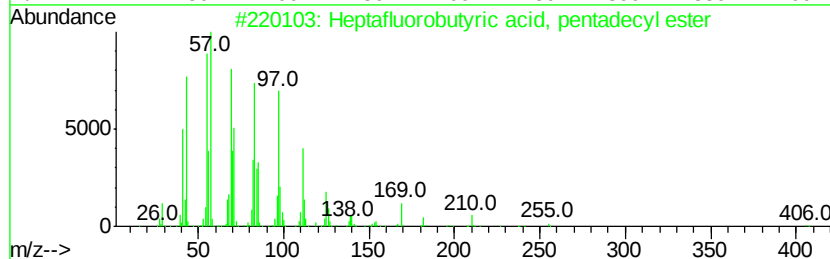
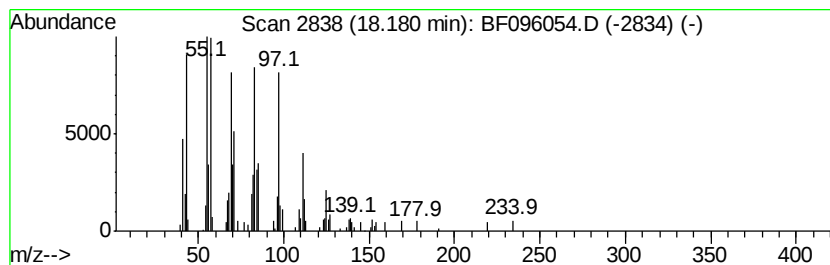
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.18	7.19 ng	147922	Chrysene-d12	18.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	89
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	89



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062017\
Data File : BF096054.D
Acq On : 20 Jun 2017 20:15
Operator : SJ/MA
Sample : I3676-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-5-6

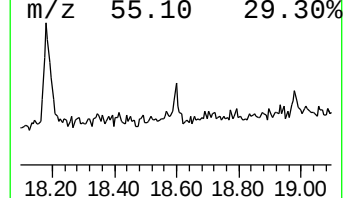
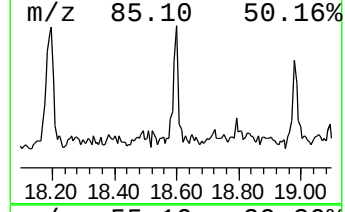
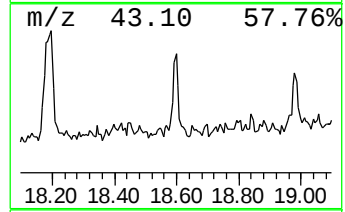
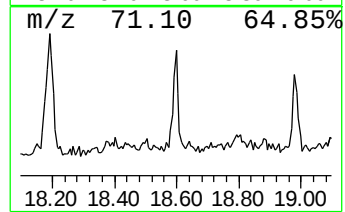
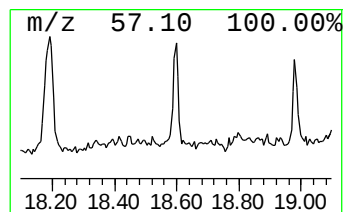
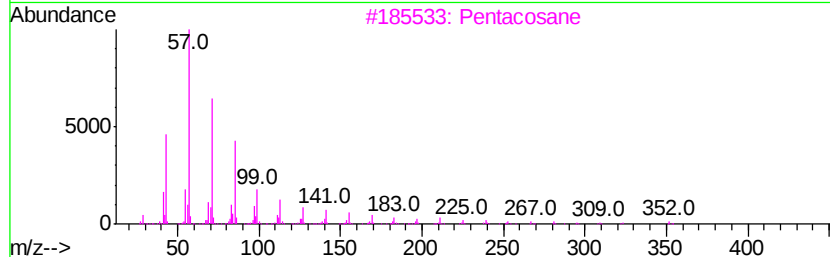
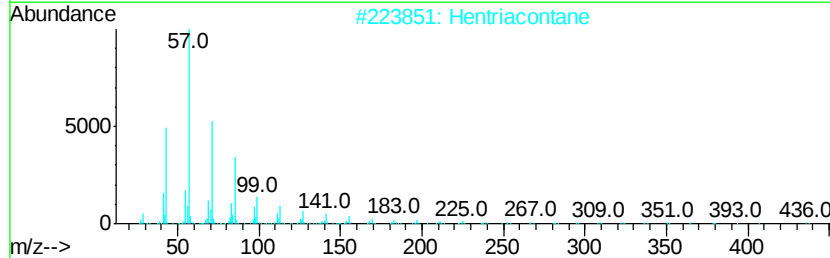
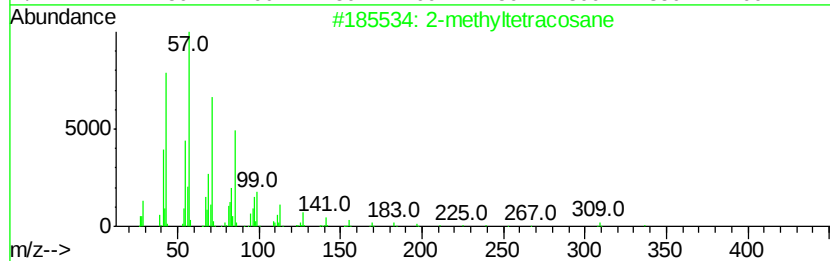
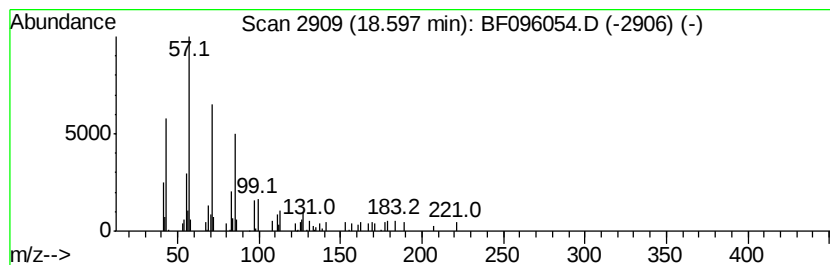
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyltetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.60	3.11 ng	63921	Chrysene-d12	18.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyltetracosane		352	C25H52	1000376-72-6	90
2	Hentriacontane		437	C31H64	000630-04-6	80
3	Pentacosane		352	C25H52	000629-99-2	72
4	Tetratetracontane		619	C44H90	007098-22-8	72
5	Sulfurous acid, dodecyl 2-propyl...		292	C15H32O3S	1000309-12-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062017\
Data File : BF096054.D
Acq On : 20 Jun 2017 20:15
Operator : SJ/MA
Sample : I3676-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-5-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.47	7.1	ng	131209	1	7.29	371110	20.0
unknown6.95	6.95	96.4	ng	1788340	1	7.29	371110	20.0
n-Hexadecanoic acid	15.56	2.5	ng	54252	4	14.54	439860	20.0
Heptafluorobutyri...	18.18	7.2	ng	147922	5	18.27	411516	20.0
2-methyltetracosane	18.60	3.1	ng	63921	5	18.27	411516	20.0