

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
 Data File : BF096648.D
 Acq On : 11 Jul 2017 17:01
 Operator : SJ/JU
 Sample : PB100554BL
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB100554BL

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-BF070117.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	4.881	469	475	487	rVB	369634	540981	19.39%	2.386%
2	5.304	542	547	550	rBV	2480465	2457462	88.07%	10.838%
3	6.328	715	721	724	rBV	2350966	2419947	86.73%	10.673%
4	6.457	738	743	746	rBV	2444110	2443486	87.57%	10.777%
5	6.681	778	781	785	rBV	681602	584948	20.96%	2.580%
6	6.839	804	808	812	rBV	2085509	1895427	67.93%	8.360%
7	7.245	872	877	880	rBV	1643409	1561477	55.96%	6.887%
8	7.963	995	999	1003	rBV	983404	889402	31.87%	3.923%
9	9.045	1177	1183	1186	rBV	2649713	2790364	100.00%	12.307%
10	9.716	1292	1297	1301	rBV	1018428	910575	32.63%	4.016%
11	10.498	1425	1430	1445	rBV	1445517	1548418	55.49%	6.829%
12	11.192	1544	1548	1552	rBV	1004563	837146	30.00%	3.692%
13	12.780	1813	1818	1821	rBV	2338704	2252792	80.73%	9.936%
14	13.821	1991	1995	1999	rBV	697633	628969	22.54%	2.774%
15	14.921	2178	2182	2186	rBV	26632	28996	1.04%	0.128%
16	15.215	2227	2232	2238	rBV	425722	519723	18.63%	2.292%
17	15.268	2238	2241	2245	rVB2	41725	50028	1.79%	0.221%
18	15.668	2304	2309	2314	rBV2	47861	68317	2.45%	0.301%
19	16.127	2381	2387	2393	rBV2	40368	70477	2.53%	0.311%
20	16.662	2472	2478	2484	rBV4	30708	67897	2.43%	0.299%
21	17.298	2579	2586	2594	rBV3	25260	60512	2.17%	0.267%
22	18.056	2708	2715	2724	rVB5	17916	46483	1.67%	0.205%

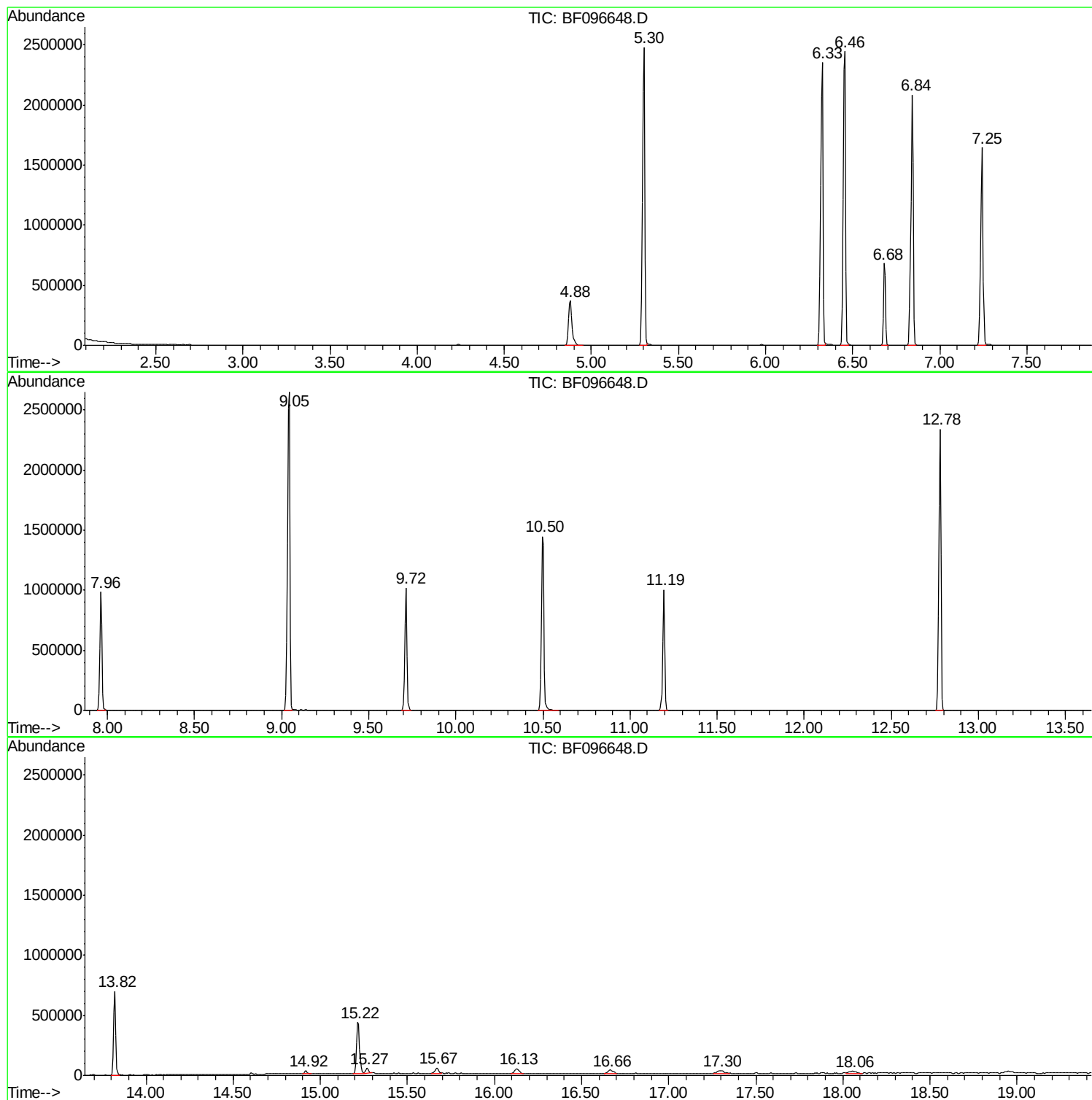
Sum of corrected areas: 22673827

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB100554BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB100554BL

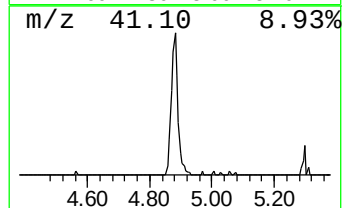
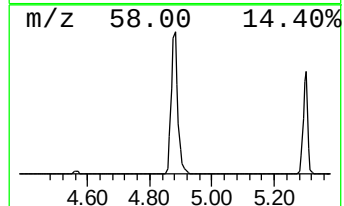
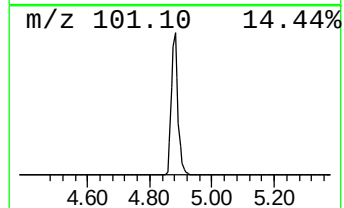
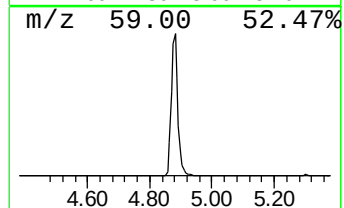
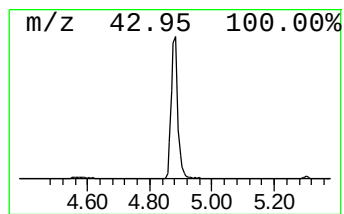
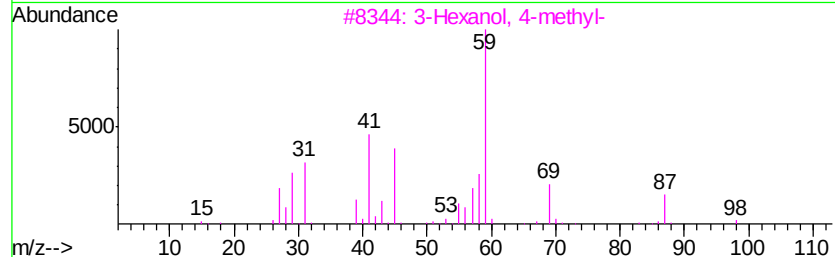
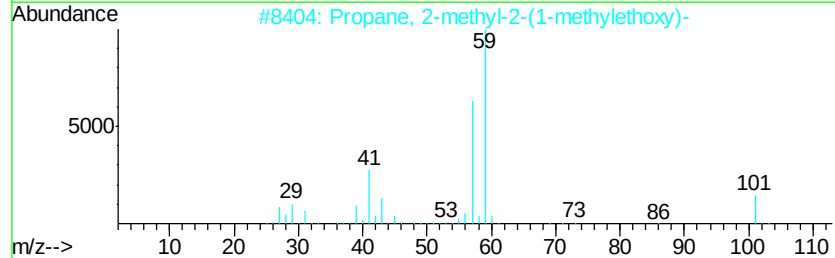
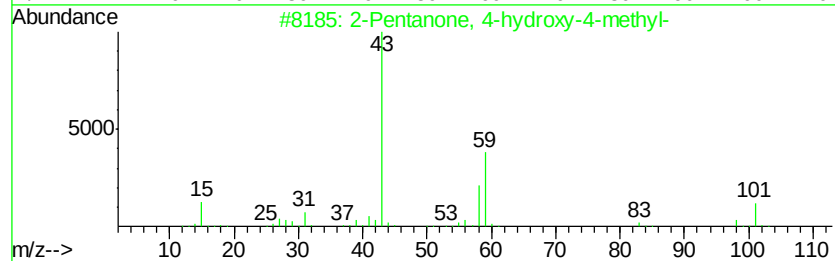
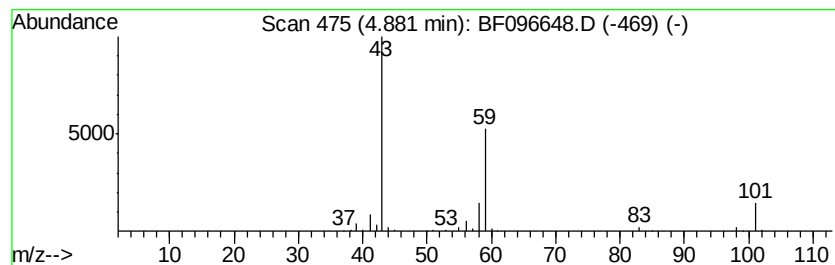
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.88	18.50 ng	540981	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB100554BL

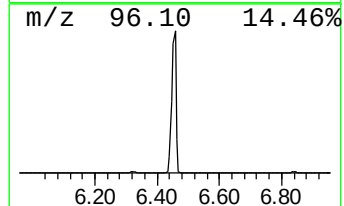
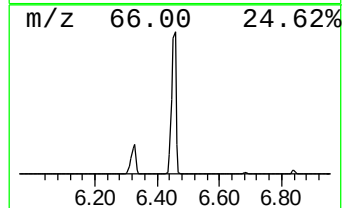
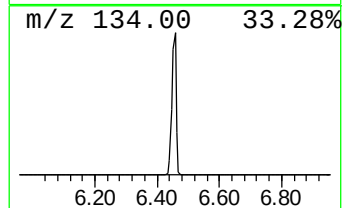
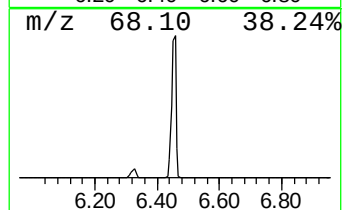
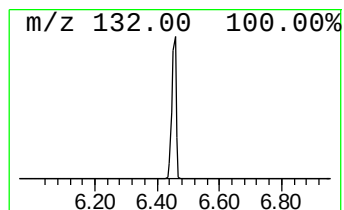
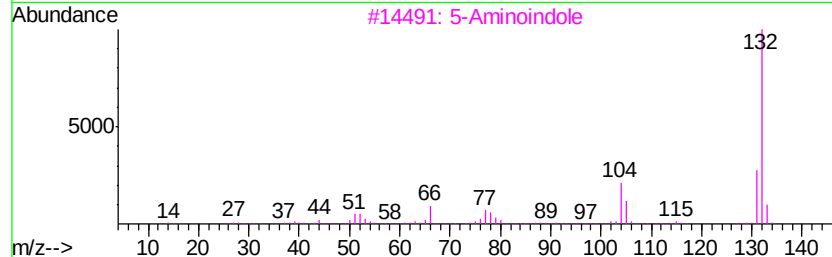
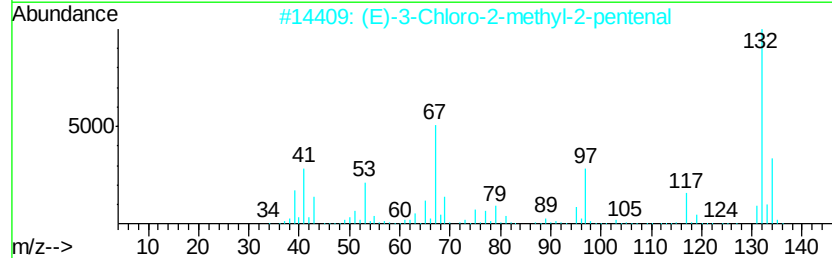
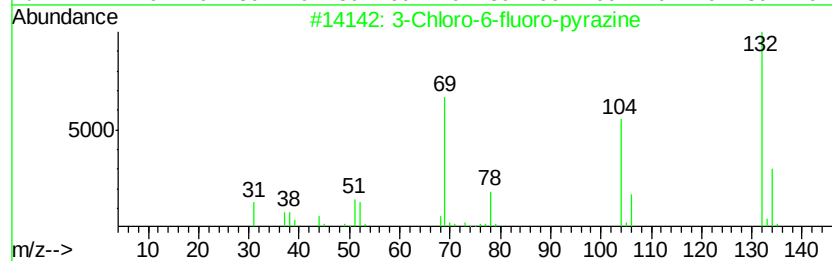
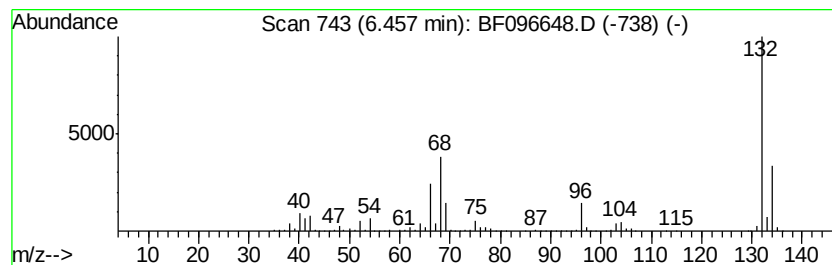
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	83.55 ng	2443490	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

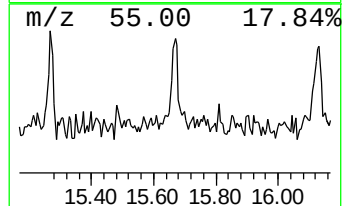
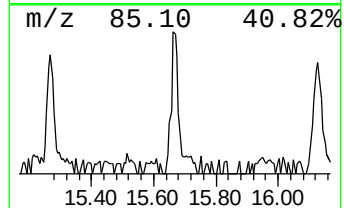
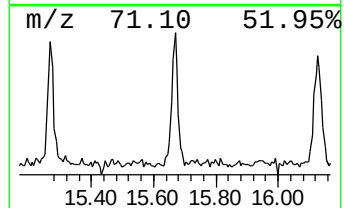
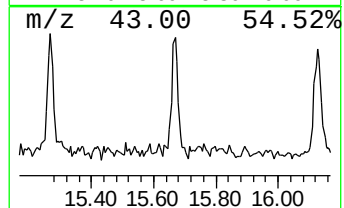
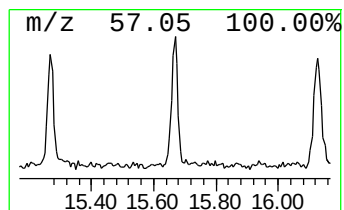
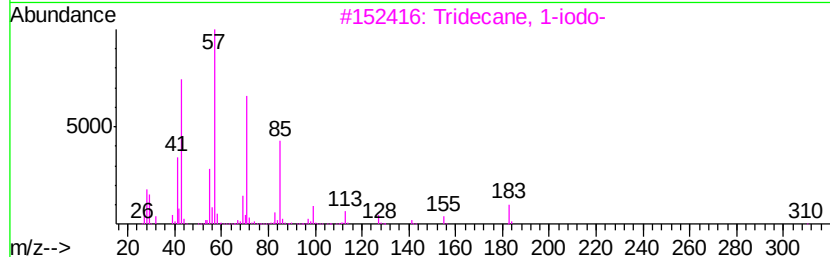
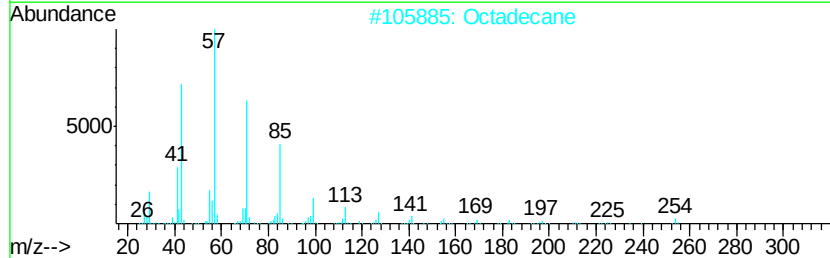
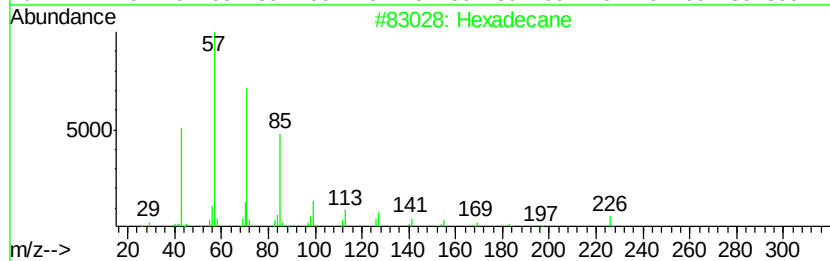
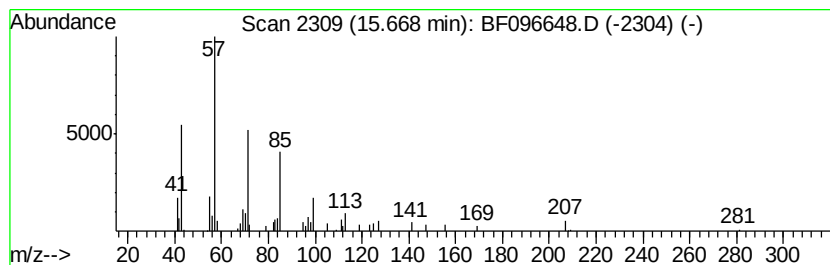
Instrument :
BNA_F
ClientSampleId :
PB100554BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.67	2.63 ng	68317	Perylene-d12	15.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Octadecane	254	C18H38	000593-45-3	90
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4	Heneicosane	296	C21H44	000629-94-7	86
5	Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB100554BL

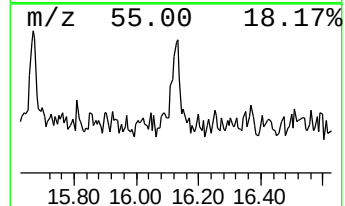
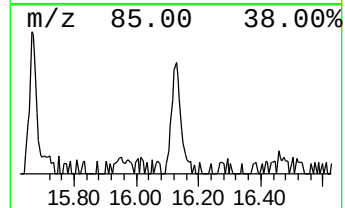
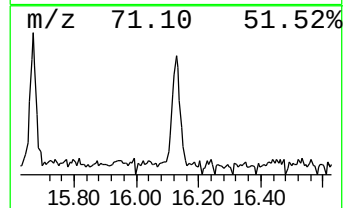
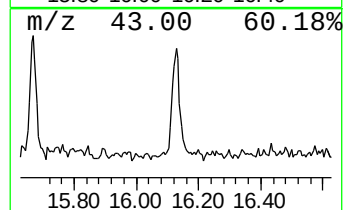
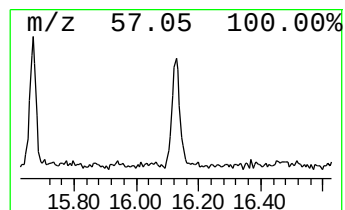
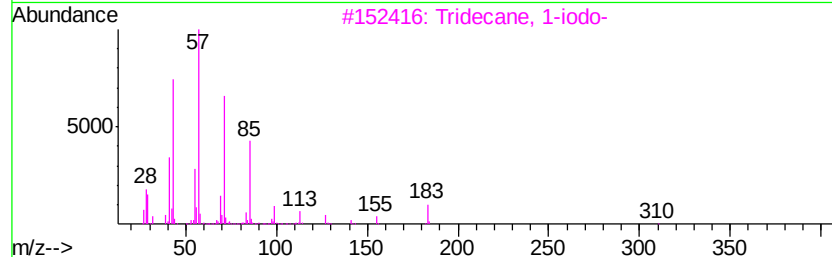
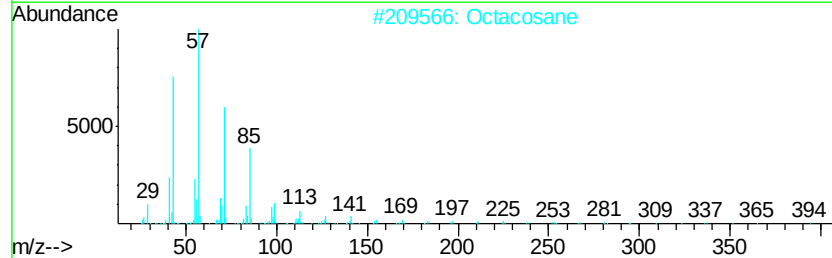
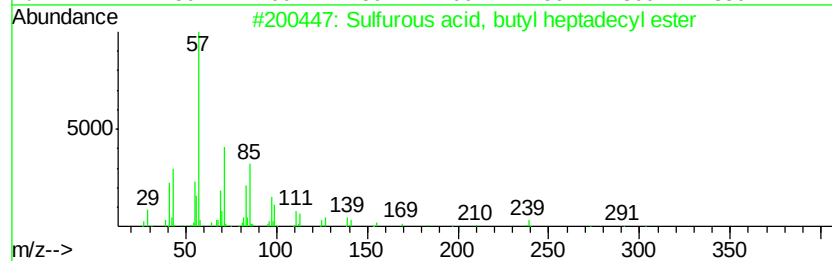
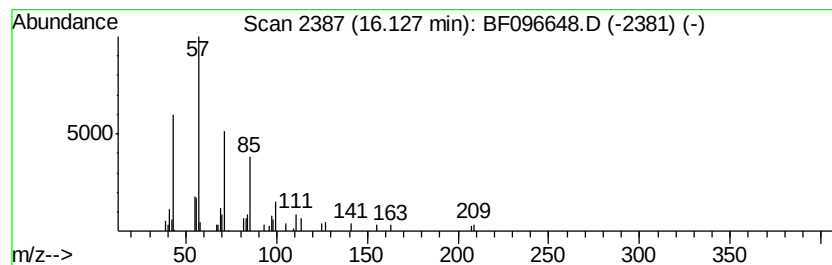
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Sulfurous acid, butyl hepta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.71 ng	70477	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	90
2		Octacosane	394	C28H58	000630-02-4	86
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4		Pentadecane	212	C15H32	000629-62-9	86
5		Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB100554BL

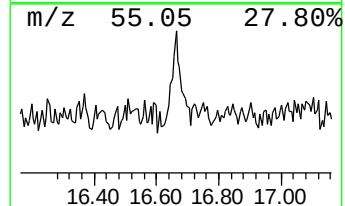
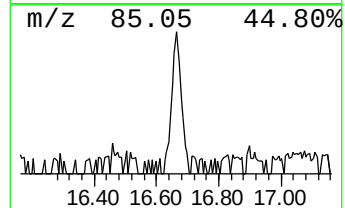
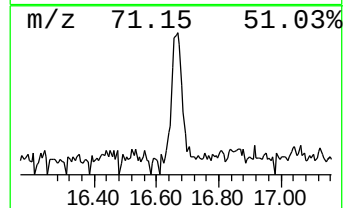
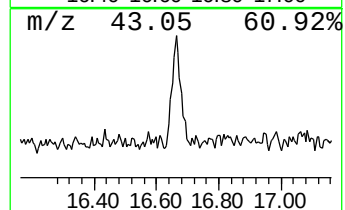
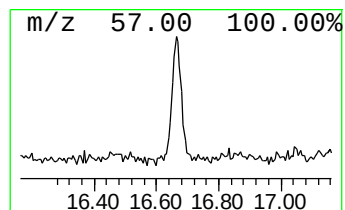
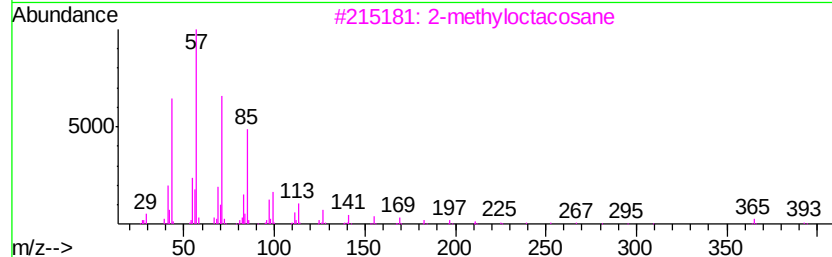
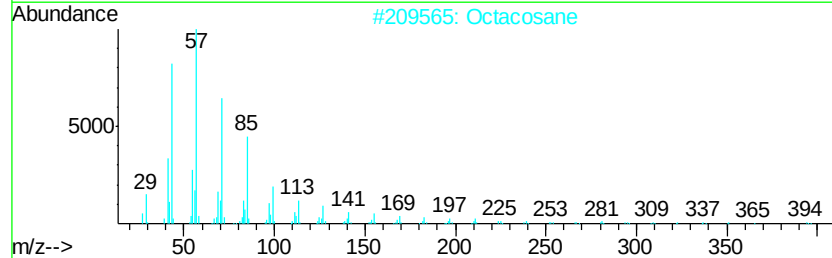
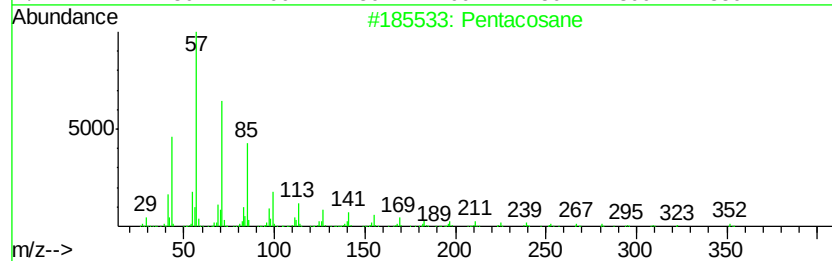
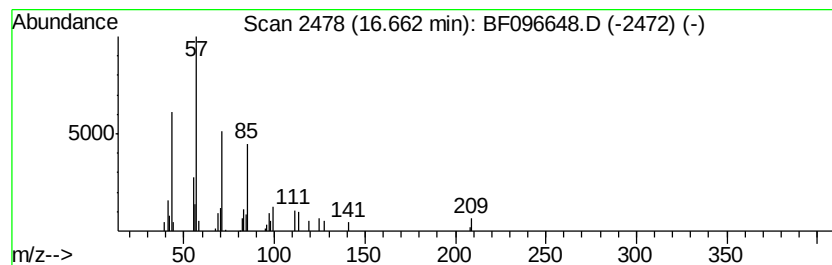
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	2.61 ng	67897	Perylene-d12	15.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	86
2	Octacosane		394	C28H58	000630-02-4	86
3	2-methyloctacosane		408	C29H60	1000376-72-8	86
4	Heptacosane		380	C27H56	000593-49-7	86
5	Hexatriacontane		507	C36H74	000630-06-8	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB100554BL

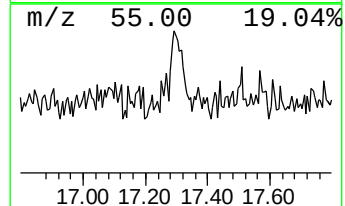
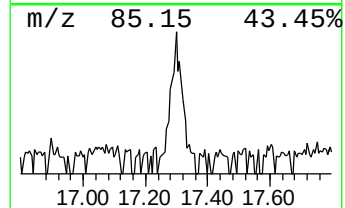
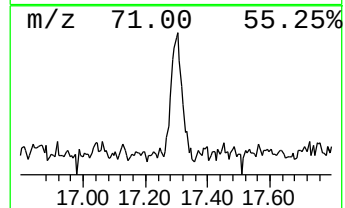
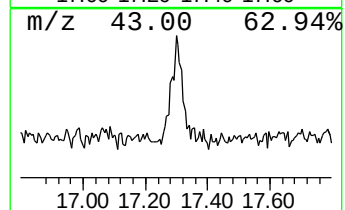
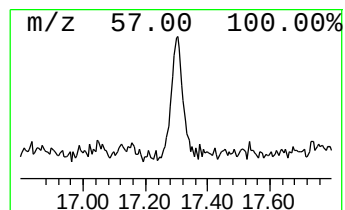
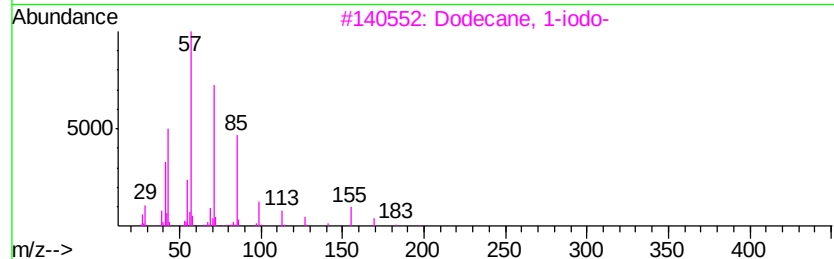
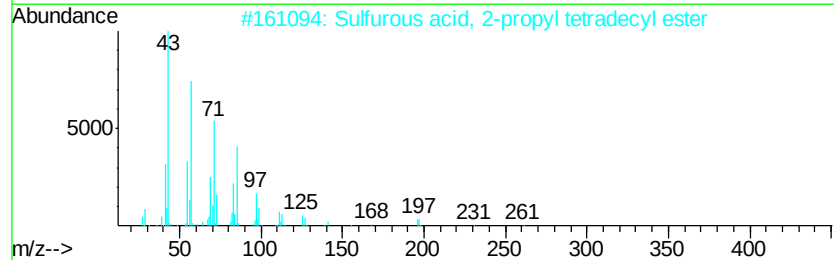
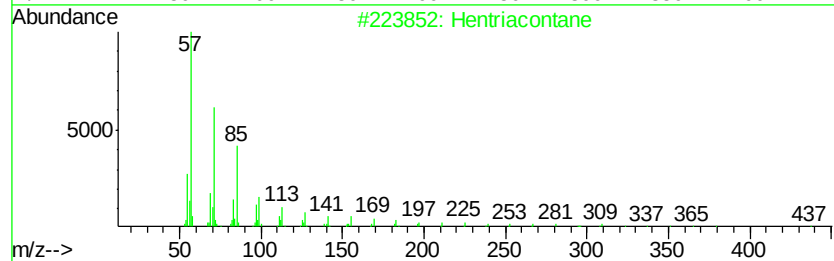
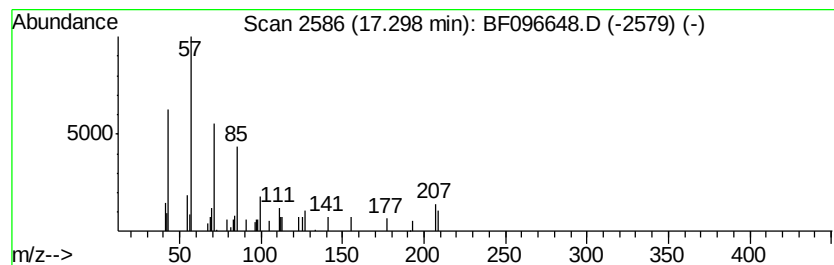
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	2.33 ng	60512	Perylene-d12	15.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	59
2	Sulfurous acid, 2-propyl tetradec...		320	C17H36O3S	1000309-12-5	59
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	53
4	Heptadecane		240	C17H36	000629-78-7	53
5	Heneicosane		296	C21H44	000629-94-7	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071117\
Data File : BF096648.D
Acq On : 11 Jul 2017 17:01
Operator : SJ/JU
Sample : PB100554BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB100554BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.88	18.5	ng	540981	1	6.68	584948	20.0
unknown6.46	6.46	83.5	ng	2443490	1	6.68	584948	20.0
Hexadecane	15.67	2.6	ng	68317	6	15.22	519723	20.0
Sulfurous acid, b...	16.13	2.7	ng	70477	6	15.22	519723	20.0
Pentacosane	16.66	2.6	ng	67897	6	15.22	519723	20.0
Hentriacontane	17.30	2.3	ng	60512	6	15.22	519723	20.0