

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
 Data File : BF096536.D
 Acq On : 6 Jul 2017 16:35
 Operator : SJ/MA
 Sample : I4036-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CIY-SB-101-0-50

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-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	4.904	474	479	492	rVB	263245	346236	16.44%	1.924%
2	5.328	546	551	554	rBV	2234425	2106691	100.00%	11.706%
3	6.351	720	725	736	rVB	2156553	2072892	98.40%	11.518%
4	6.481	743	747	751	rBV	2114021	2023058	96.03%	11.241%
5	6.710	783	786	790	rBV	782013	709829	33.69%	3.944%
6	6.869	809	813	817	rBV	1775217	1541848	73.19%	8.567%
7	7.275	876	882	885	rBV	1312719	1275527	60.55%	7.087%
8	7.375	894	899	908	rVB2	23262	27546	1.31%	0.153%
9	7.992	1000	1004	1008	rBV	1016563	917645	43.56%	5.099%
10	9.075	1183	1188	1191	rBV	1874515	1589140	75.43%	8.830%
11	9.469	1251	1255	1258	rBV	305718	276882	13.14%	1.538%
12	9.751	1298	1303	1306	rBV	932023	860850	40.86%	4.783%
13	10.192	1375	1378	1383	rVB	38958	32296	1.53%	0.179%
14	10.533	1432	1436	1445	rBV	938795	845185	40.12%	4.696%
15	10.669	1456	1459	1468	rBV	50527	64351	3.05%	0.358%
16	11.116	1530	1535	1537	rBV2	50555	46162	2.19%	0.256%
17	11.227	1550	1554	1557	rBV	807854	743936	35.31%	4.134%
18	11.251	1557	1558	1561	rVB	65167	41342	1.96%	0.230%
19	11.304	1561	1567	1570	rVB2	19682	22039	1.05%	0.122%
20	12.439	1757	1760	1764	rVB	69946	59965	2.85%	0.333%
21	12.486	1764	1768	1771	rBV	26821	23870	1.13%	0.133%
22	12.663	1793	1798	1801	rBV	65151	71134	3.38%	0.395%
23	12.815	1820	1824	1827	rBV	1011893	882709	41.90%	4.905%
24	12.951	1845	1847	1852	rBV	21022	29326	1.39%	0.163%
25	13.721	1974	1978	1983	rBV3	61338	82502	3.92%	0.458%
26	13.862	1998	2002	2005	rBV	727030	665066	31.57%	3.695%
27	14.621	2128	2131	2134	rBV	98846	96874	4.60%	0.538%
28	15.274	2237	2242	2247	rBV	454576	542226	25.74%	3.013%

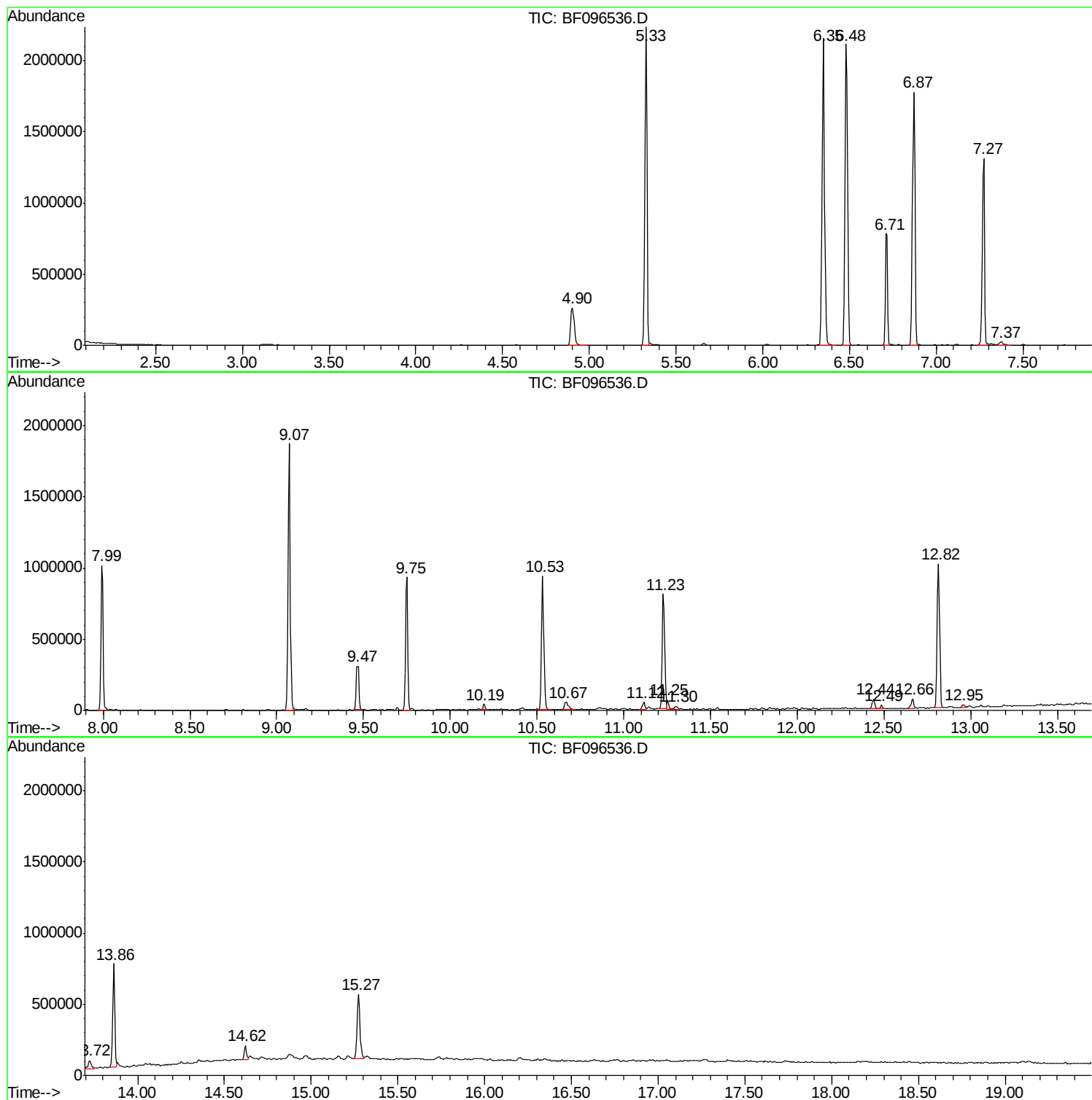
Sum of corrected areas: 17997127

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096536.D
Acq On : 6 Jul 2017 16:35
Operator : SJ/MA
Sample : I4036-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CIY-SB-101-0-50

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\BF070617\
Data File : BF096536.D
Acq On : 6 Jul 2017 16:35
Operator : SJ/MA
Sample : I4036-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CIY-SB-101-0-50

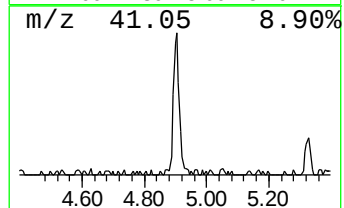
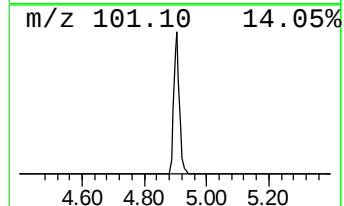
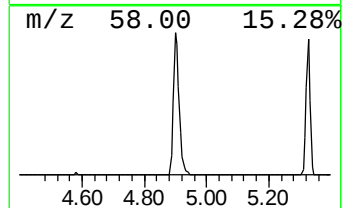
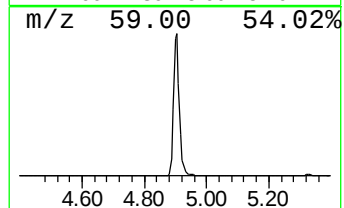
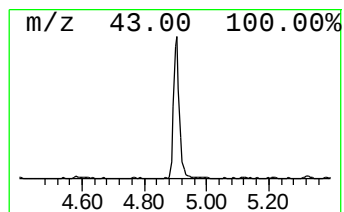
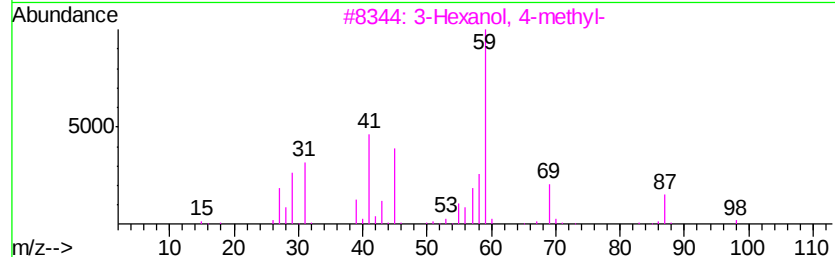
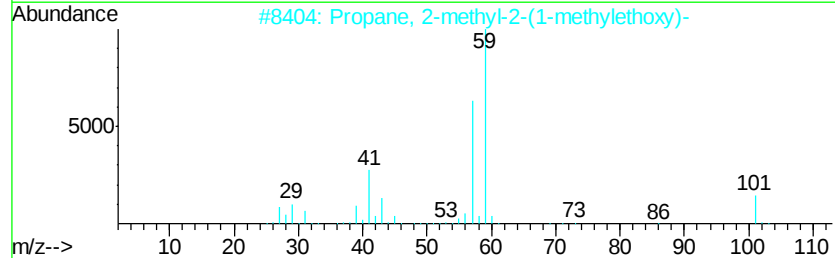
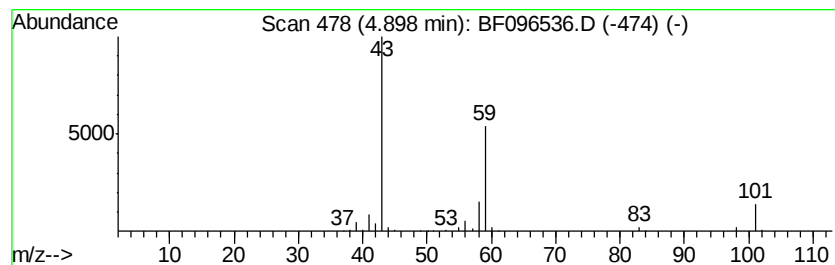
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	9.76 ng	346236	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096536.D
Acq On : 6 Jul 2017 16:35
Operator : SJ/MA
Sample : I4036-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CIY-SB-101-0-50

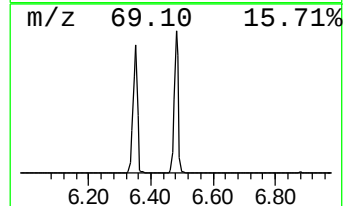
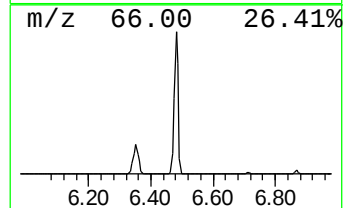
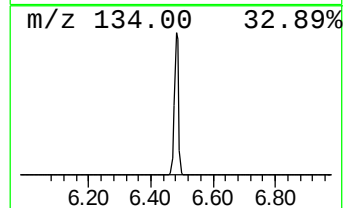
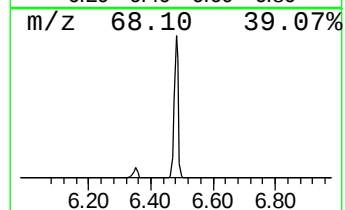
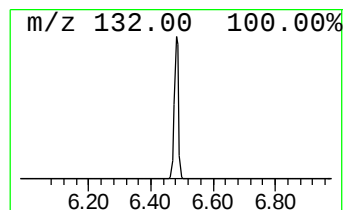
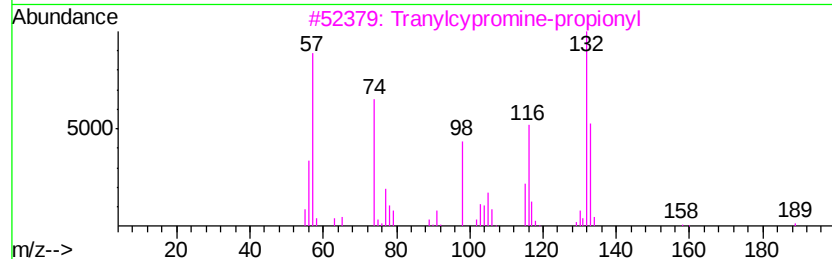
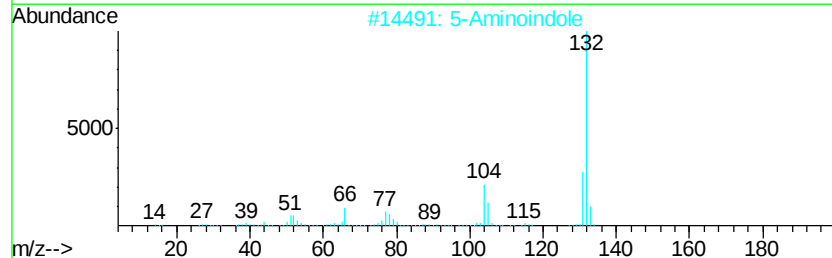
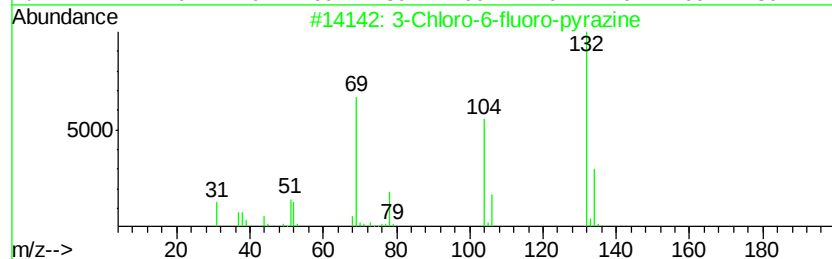
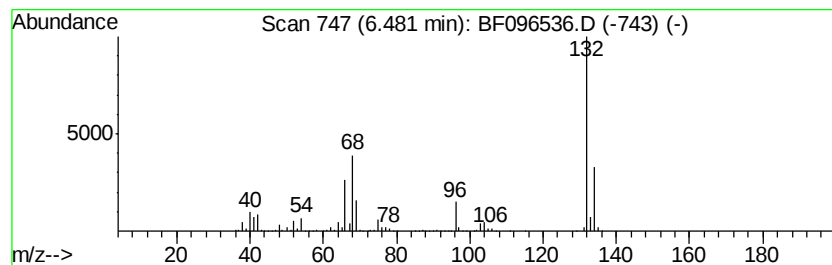
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	57.00 ng	2023060	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096536.D
Acq On : 6 Jul 2017 16:35
Operator : SJ/MA
Sample : I4036-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

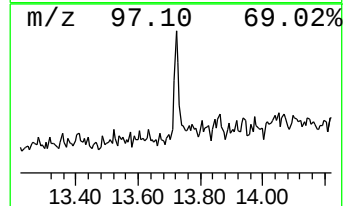
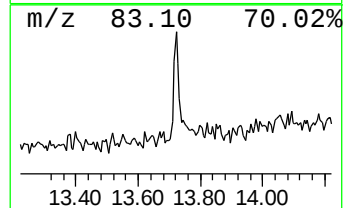
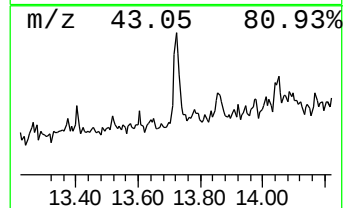
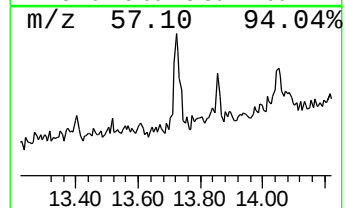
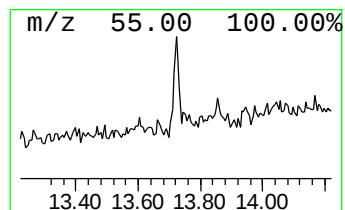
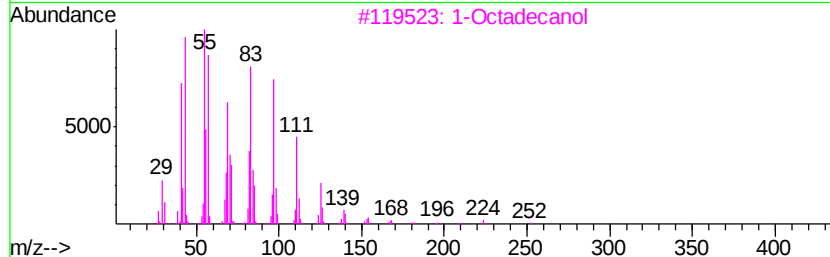
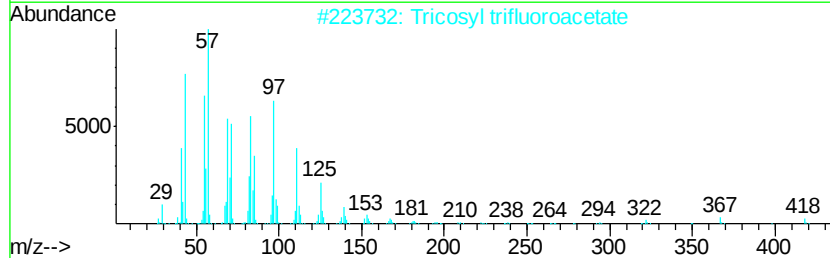
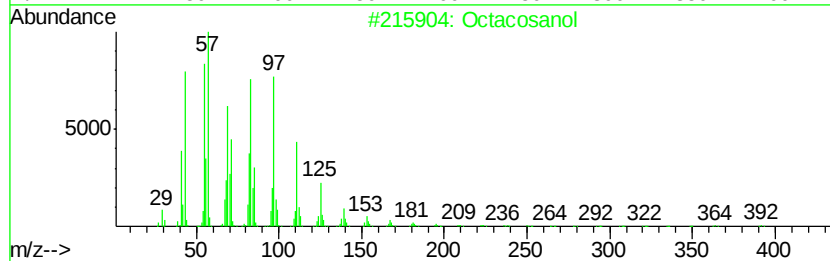
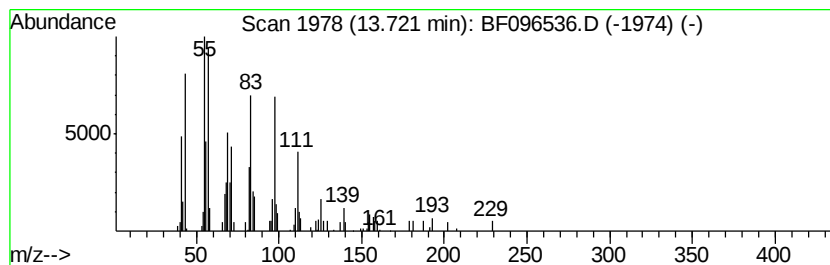
Instrument :
BNA_F
ClientSampleId :
CIY-SB-101-0-50

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 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	2.48 ng	82502	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
3	1-Octadecanol	270	C18H38O	000112-92-5	87
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096536.D
Acq On : 6 Jul 2017 16:35
Operator : SJ/MA
Sample : I4036-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CIY-SB-101-0-50

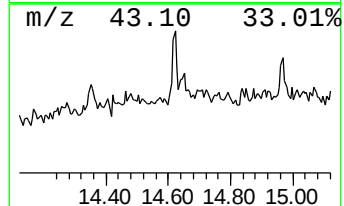
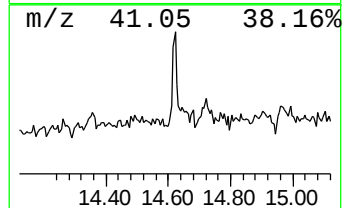
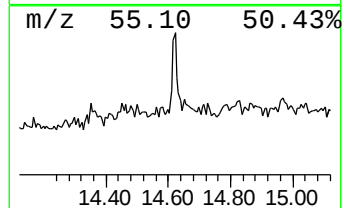
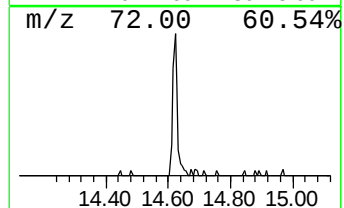
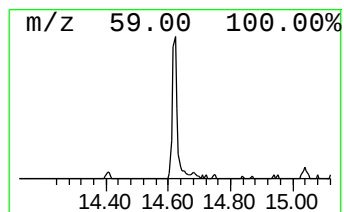
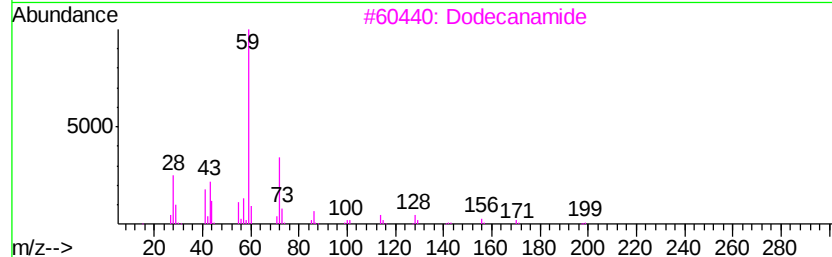
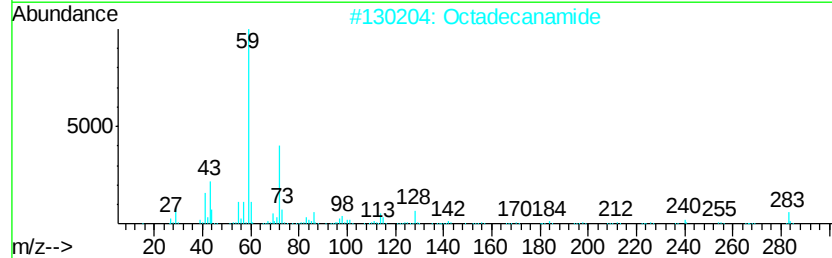
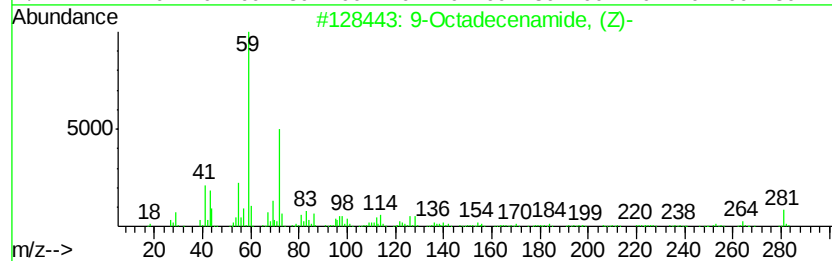
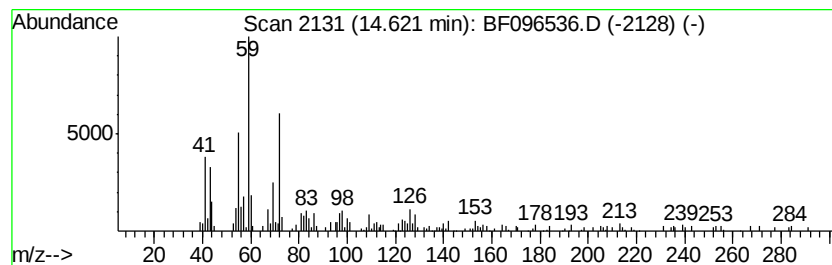
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.57 ng	96874	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90	
2	Octadecanamide	283	C18H37NO	000124-26-5	64	
3	Dodecanamide	199	C12H25NO	001120-16-7	50	
4	Octanamide	143	C8H17NO	000629-01-6	50	
5	Hexanamide	115	C6H13NO	000628-02-4	47	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096536.D
Acq On : 6 Jul 2017 16:35
Operator : SJ/MA
Sample : I4036-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CIY-SB-101-0-50

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...	4.90	9.8	ng	346236	1	6.72	709829	20.0
unknown6.48	6.48	57.0	ng	2023060	1	6.72	709829	20.0
Octacosanol	13.72	2.5	ng	82502	5	13.86	665066	20.0
9-Octadecenamide,...	14.62	3.6	ng	96874	6	15.27	542226	20.0