

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
 Data File : BF099050.D
 Acq On : 4 Oct 2017 00:30
 Operator : SJ/JU
 Sample : I5605-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-015

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-BF092317.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	2.157	9	12	31	rVB	170232	348131	11.96%	1.416%
2	5.098	508	512	524	rVB	462195	595852	20.47%	2.423%
3	5.492	574	579	583	rBV	2662784	2910275	100.00%	11.833%
4	6.504	745	751	754	rBV	2682225	2821603	96.95%	11.473%
5	6.645	770	775	778	rBV	3049877	2910348	100.00%	11.834%
6	6.875	810	814	817	rVB	818740	671700	23.08%	2.731%
7	7.034	833	841	844	rBV	2401098	2320722	79.74%	9.436%
8	7.439	904	910	913	rBV	1685049	1752370	60.21%	7.125%
9	8.157	1027	1032	1035	rBV	894837	815541	28.02%	3.316%
10	9.228	1209	1214	1217	rBV	3074424	2723669	93.59%	11.075%
11	9.616	1277	1280	1284	rBV	303513	243430	8.36%	0.990%
12	9.910	1326	1330	1333	rBV	783532	686644	23.59%	2.792%
13	10.698	1460	1464	1467	rBV	1261356	1120962	38.52%	4.558%
14	10.804	1479	1482	1487	rBV	37222	37908	1.30%	0.154%
15	11.392	1579	1582	1586	rBV	661919	563517	19.36%	2.291%
16	12.980	1847	1852	1855	rBV	2344168	2087782	71.74%	8.489%
17	13.863	1999	2002	2006	rBV	109819	115188	3.96%	0.468%
18	14.033	2027	2031	2034	rBV	774605	681309	23.41%	2.770%
19	14.486	2105	2108	2115	rBV5	18235	31269	1.07%	0.127%
20	15.133	2215	2218	2222	rBV2	43476	46459	1.60%	0.189%
21	15.509	2277	2282	2289	rBV	584430	735902	25.29%	2.992%
22	15.957	2354	2358	2363	rVB	52369	70941	2.44%	0.288%
23	16.462	2439	2444	2448	rBV2	40114	68346	2.35%	0.278%
24	17.062	2541	2546	2551	rVB	28971	54277	1.86%	0.221%
25	17.562	2626	2631	2642	rBV	37792	109406	3.76%	0.445%
26	18.603	2804	2808	2818	rVB9	30207	70030	2.41%	0.285%

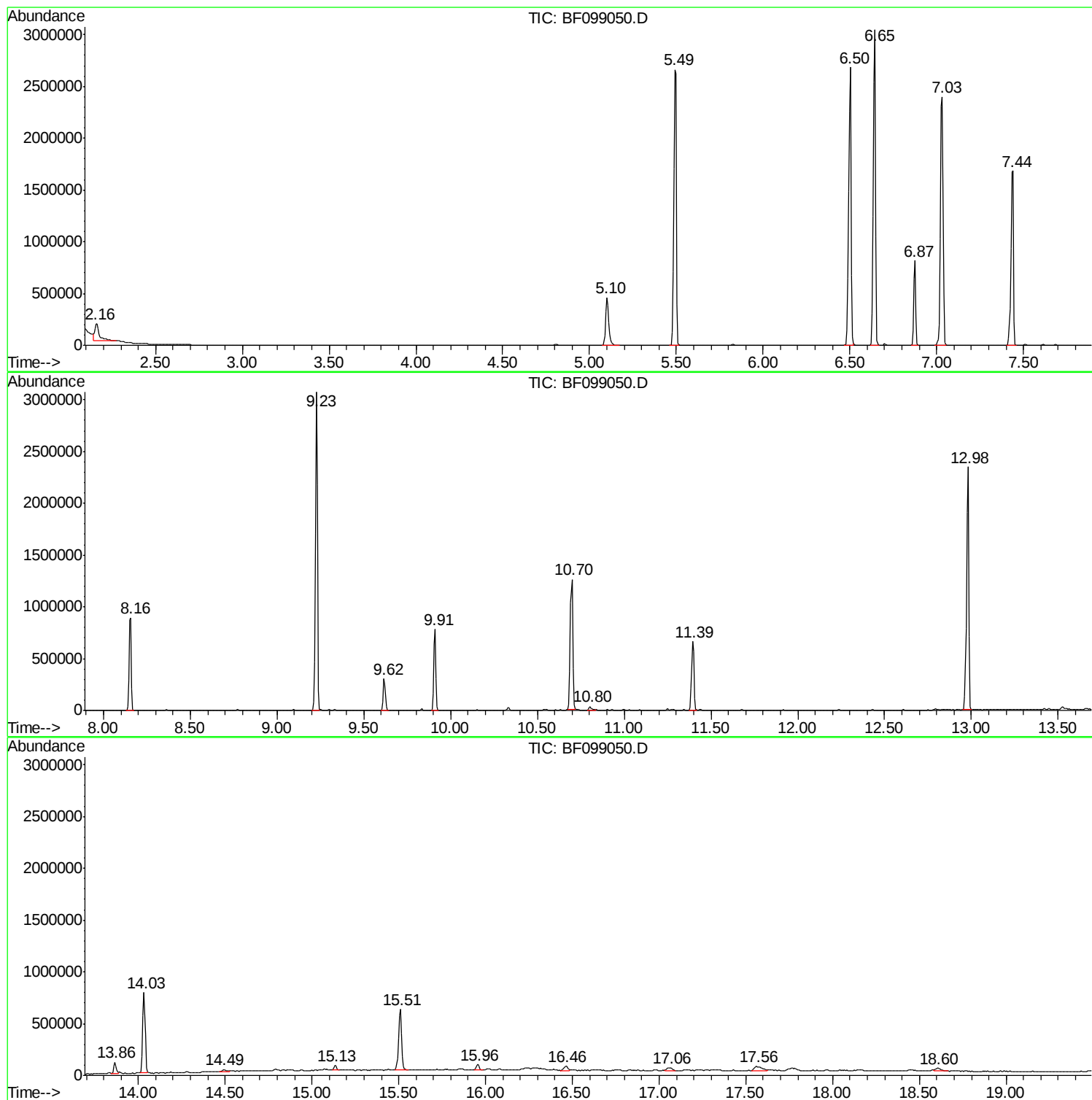
Sum of corrected areas: 24593581

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099050.D
Acq On : 4 Oct 2017 00:30
Operator : SJ/JU
Sample : I5605-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF100317\
Data File : BF099050.D
Acq On : 4 Oct 2017 00:30
Operator : SJ/JU
Sample : I5605-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-015

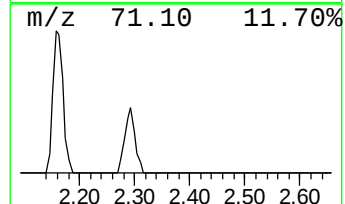
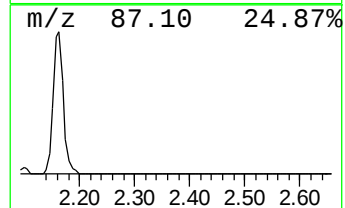
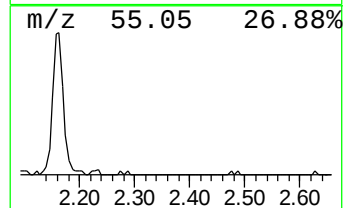
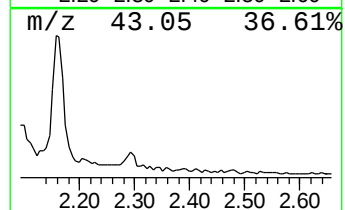
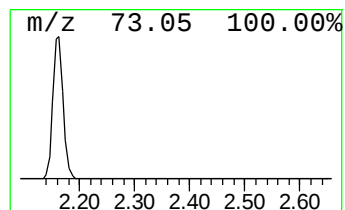
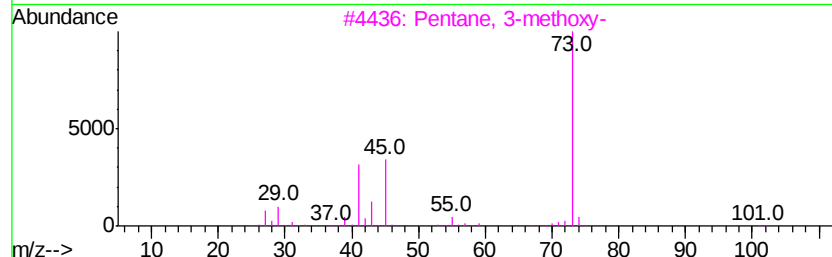
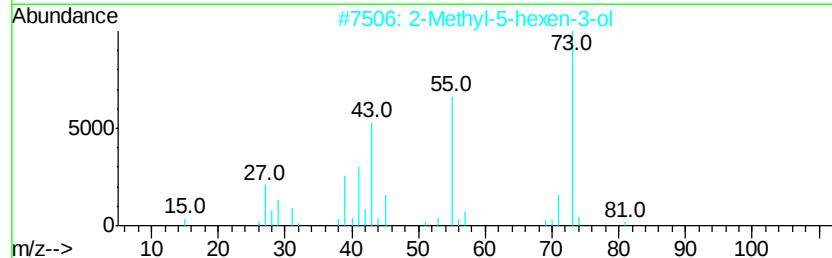
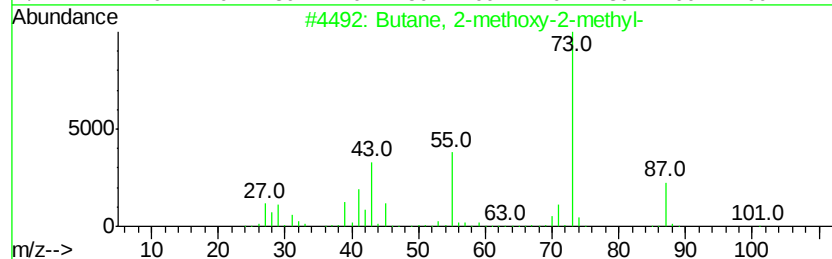
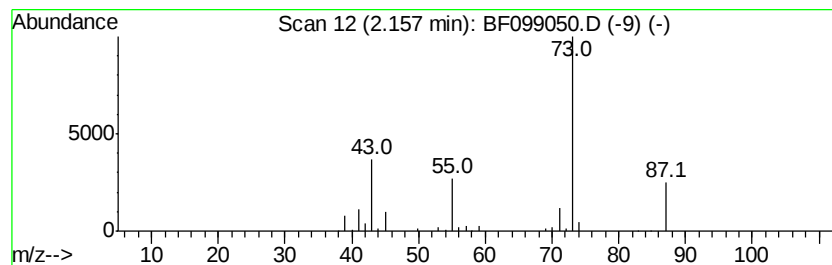
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	10.37 ng	348131	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099050.D
Acq On : 4 Oct 2017 00:30
Operator : SJ/JU
Sample : I5605-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-015

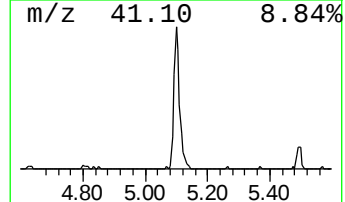
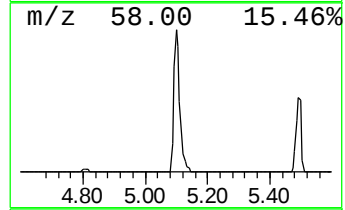
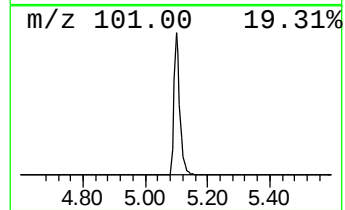
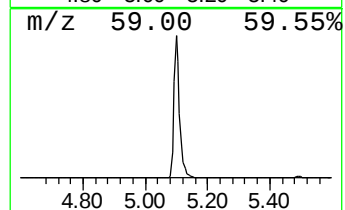
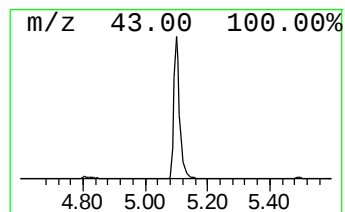
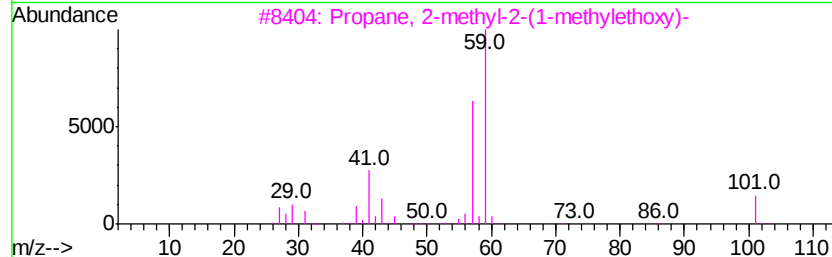
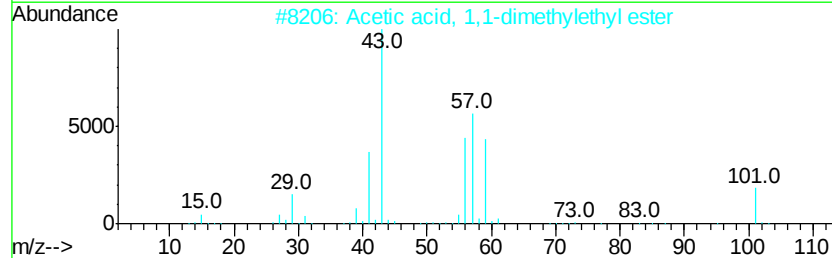
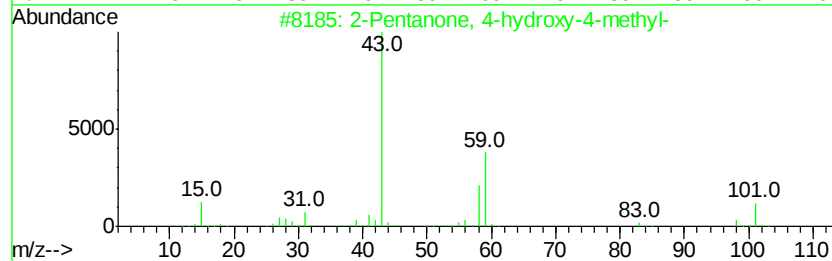
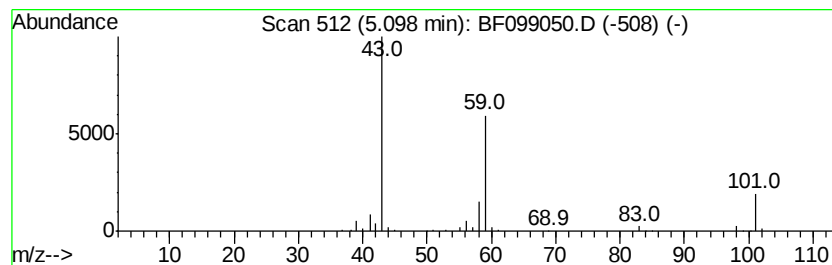
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	17.74 ng	595852	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099050.D
Acq On : 4 Oct 2017 00:30
Operator : SJ/JU
Sample : I5605-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-015

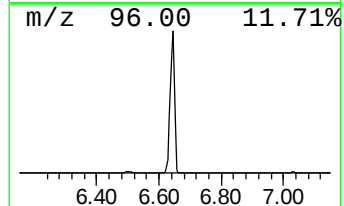
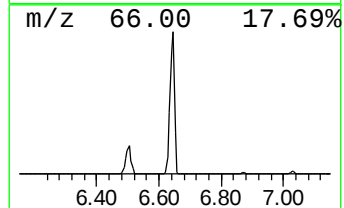
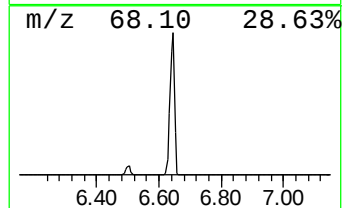
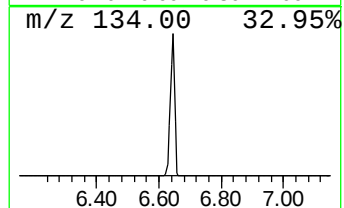
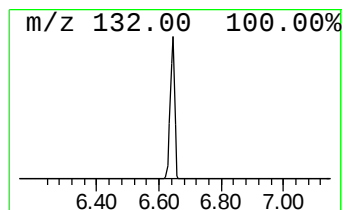
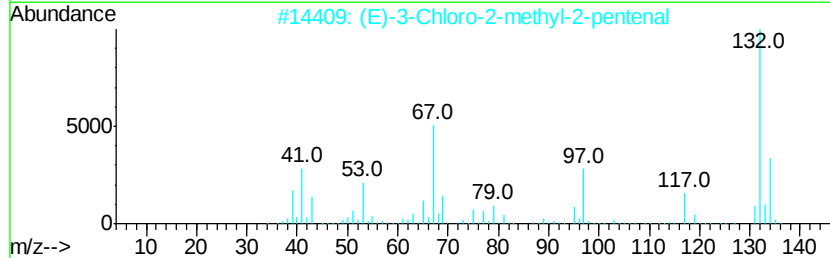
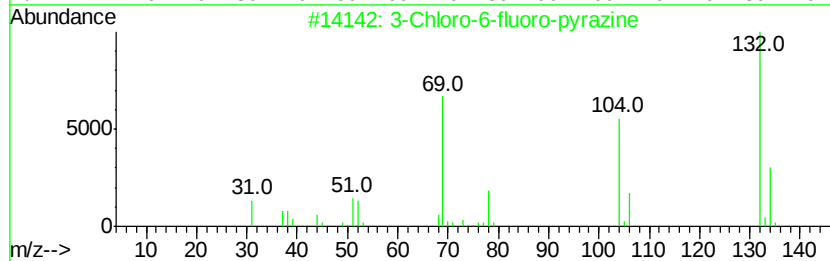
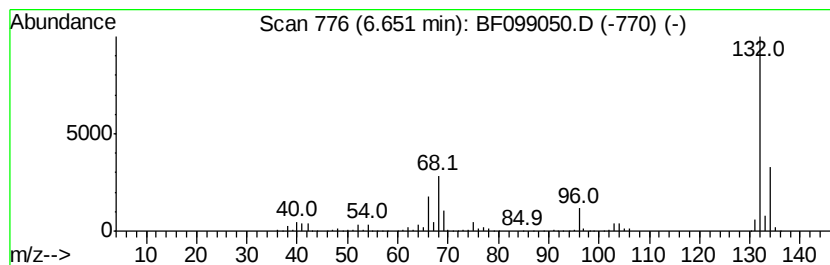
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	86.66 ng	2910350	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
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	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099050.D
Acq On : 4 Oct 2017 00:30
Operator : SJ/JU
Sample : I5605-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-015

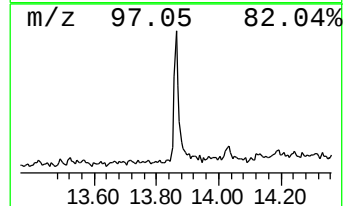
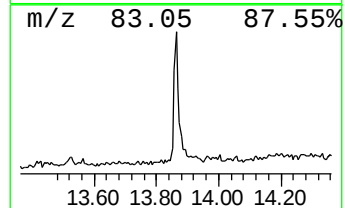
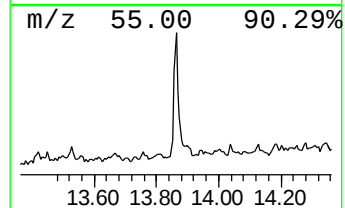
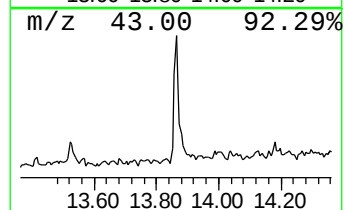
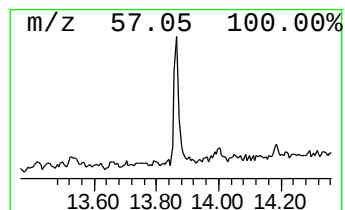
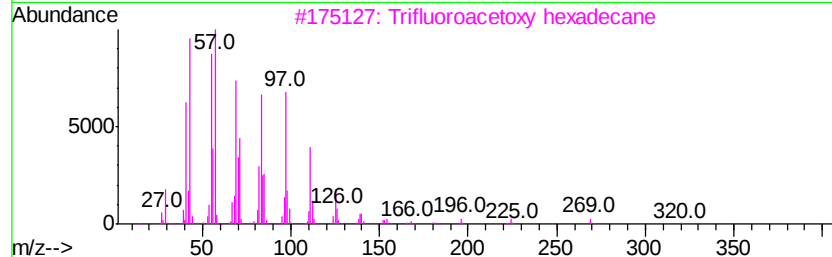
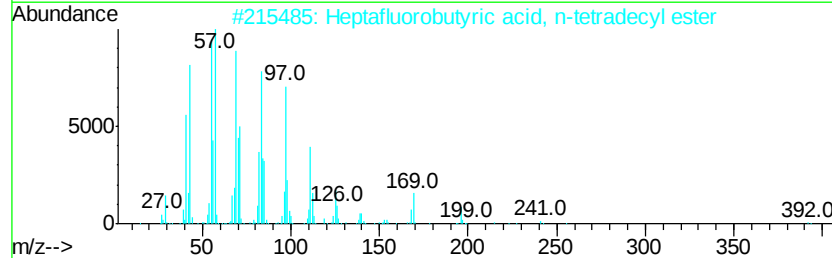
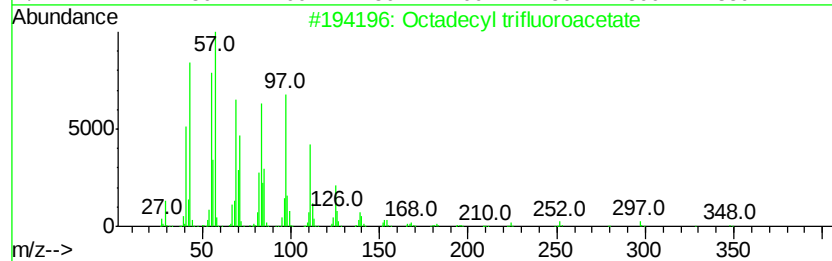
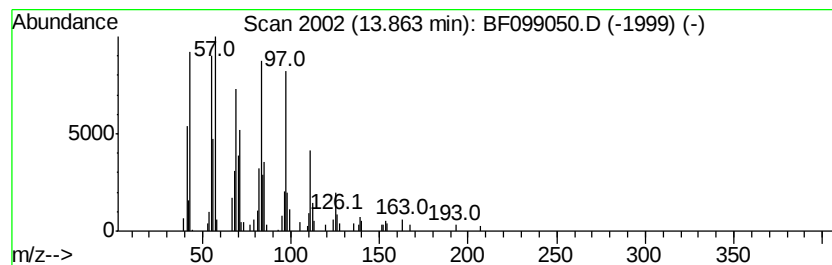
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.38 ng	115188	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
5		1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099050.D
Acq On : 4 Oct 2017 00:30
Operator : SJ/JU
Sample : I5605-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

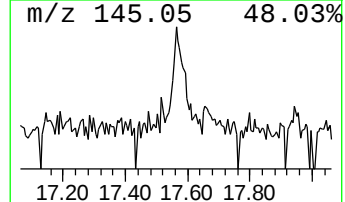
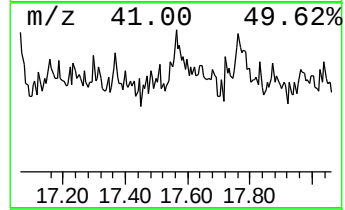
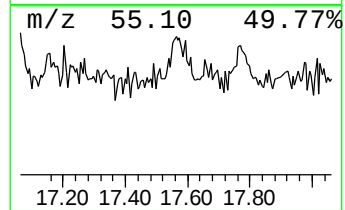
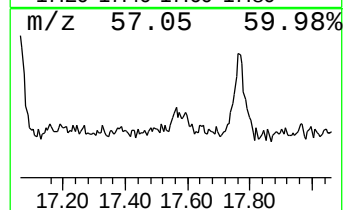
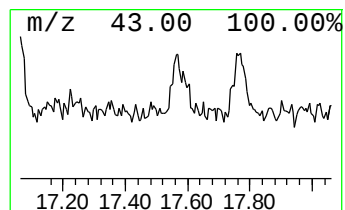
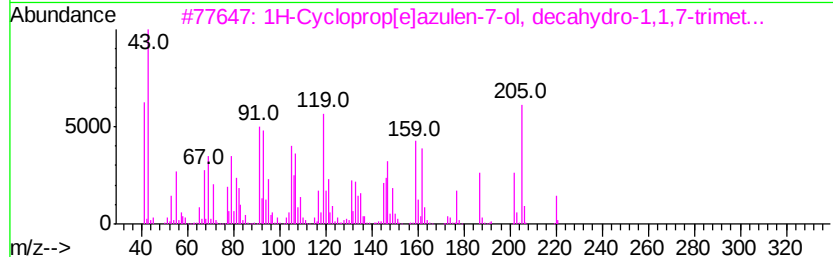
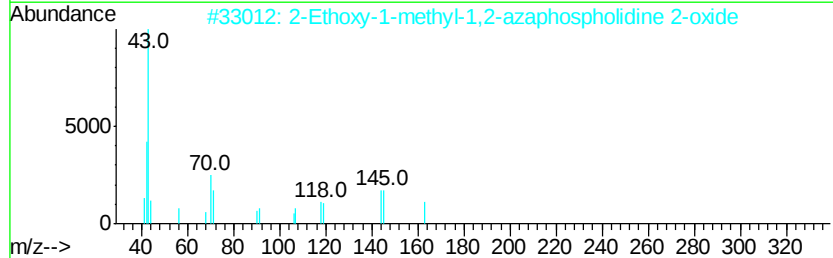
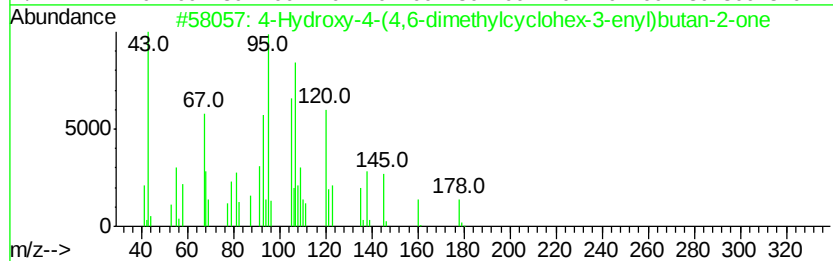
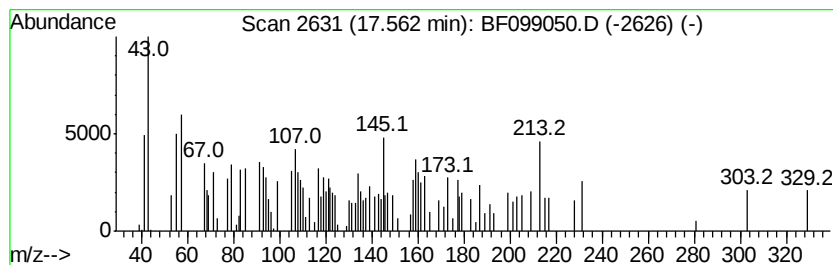
Instrument :
BNA_F
ClientSampleId :
FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown17.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.56	2.97 ng	109406	Perylene-d12	15.51		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	10	
2	2-Ethoxy-1-methyl-1,2-azaphospho...	163	C6H14N02P	054008-32-1	9	
3	1H-Cycloprop[elazulen-7-ol, deca...	220	C15H24O	006750-60-3	9	
4	Androst-5-ene,1-acetoxy-16,17-di...	386	C25H38O3	294866-91-4	9	
5	Azuleno[5,6-c]furan-3(1H)-one, 8...	310	C17H26O5	071305-64-1	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099050.D
Acq On : 4 Oct 2017 00:30
Operator : SJ/JU
Sample : I5605-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-015

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.16	10.4	ng	348131	1	6.87	671700	20.0
2-Pentanone, 4-hy...	5.10	17.7	ng	595852	1	6.87	671700	20.0
unknown6.65	6.65	86.7	ng	2910350	1	6.87	671700	20.0
Octadecyl trifluo...	13.86	3.4	ng	115188	5	14.03	681309	20.0
unknown17.56	17.56	3.0	ng	109406	6	15.51	735902	20.0