

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
 Data File : BF099583.D
 Acq On : 17 Oct 2017 16:15
 Operator : SJ/JU
 Sample : I5776-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ENV-107-1(0-5)

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	5.057	501	505	519	rBV	308927	470818	15.51%	1.901%
2	5.457	568	573	592	rBV	2383075	2556467	84.22%	10.322%
3	6.469	739	745	757	rBV	2204040	2627665	86.57%	10.609%
4	6.598	763	767	770	rBV	2629543	2636136	86.85%	10.643%
5	6.822	802	805	813	rBV	558769	525509	17.31%	2.122%
6	6.981	828	832	836	rBV	2274053	2103743	69.31%	8.494%
7	7.392	897	902	905	rBV	1621525	1672403	55.10%	6.752%
8	8.104	1019	1023	1027	rBV	822558	730940	24.08%	2.951%
9	9.180	1200	1206	1209	rBV	3067062	3035405	100.00%	12.255%
10	9.574	1269	1273	1276	rBV	352838	279097	9.19%	1.127%
11	9.857	1317	1321	1325	rBV	894340	820798	27.04%	3.314%
12	10.651	1452	1456	1460	rBV	1645288	1691263	55.72%	6.828%
13	10.751	1470	1473	1481	rVB	38540	36687	1.21%	0.148%
14	11.345	1570	1574	1577	rBV	955321	841264	27.72%	3.397%
15	11.863	1658	1662	1667	rBV2	47096	55503	1.83%	0.224%
16	12.562	1777	1781	1785	rBV	87413	76829	2.53%	0.310%
17	12.739	1808	1811	1814	rVB2	65704	53712	1.77%	0.217%
18	12.792	1817	1820	1822	rVB	80704	61653	2.03%	0.249%
19	12.933	1839	1844	1847	rBV	2768841	2857058	94.12%	11.535%
20	13.439	1927	1930	1934	rBV	44231	36054	1.19%	0.146%
21	13.809	1988	1993	1997	rBV2	98443	117773	3.88%	0.476%
22	13.986	2019	2023	2026	rBV	859788	783542	25.81%	3.164%
23	14.809	2159	2163	2167	rVB	40677	43804	1.44%	0.177%
24	15.027	2196	2200	2203	rBV	24551	35948	1.18%	0.145%
25	15.056	2203	2205	2209	rVB2	26454	32379	1.07%	0.131%
26	15.451	2266	2272	2285	rVB	422419	546225	18.00%	2.205%
27	16.927	2518	2523	2531	rBV4	19375	39175	1.29%	0.158%

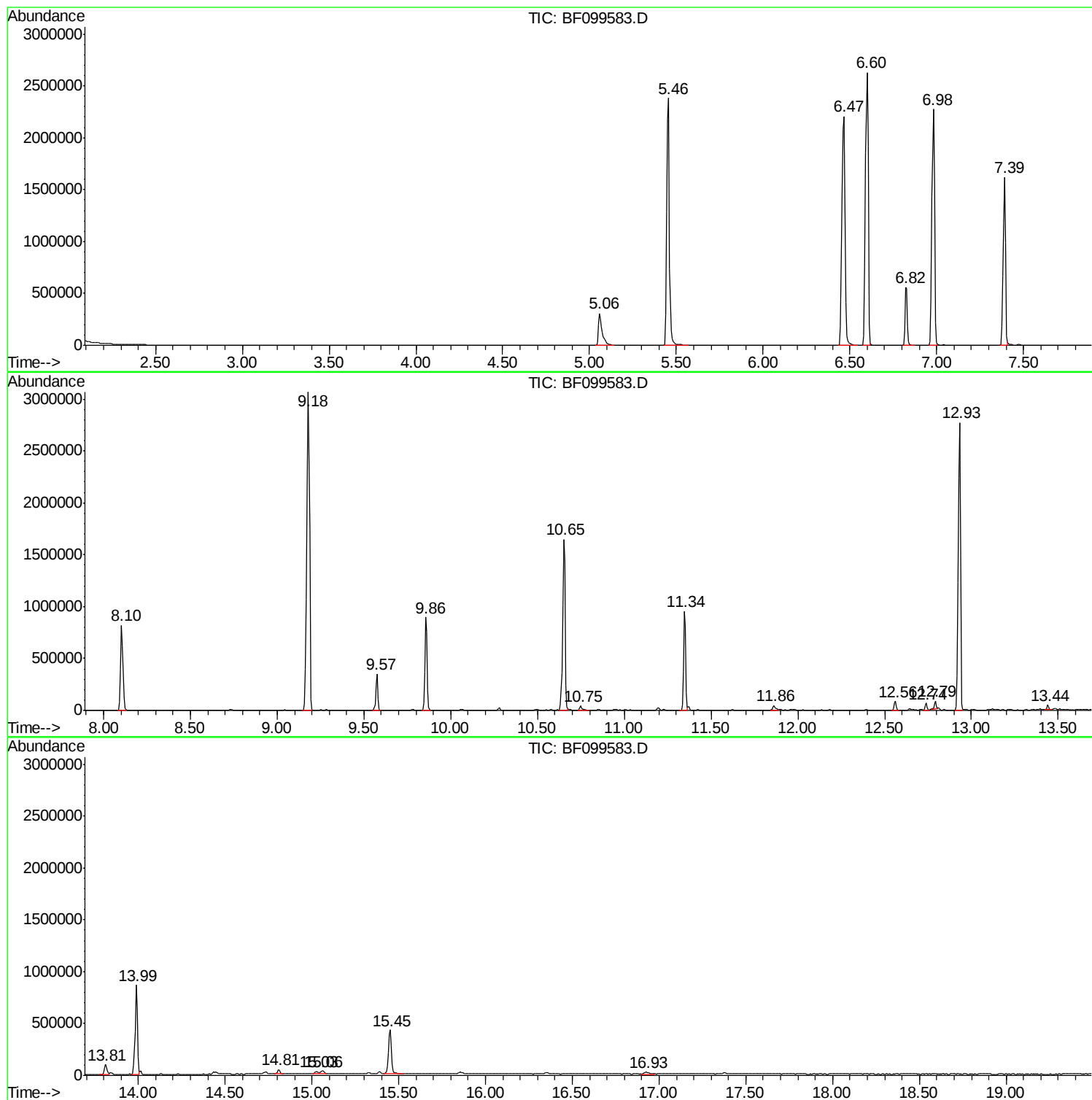
Sum of corrected areas: 24767850

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099583.D
Acq On : 17 Oct 2017 16:15
Operator : SJ/JU
Sample : I5776-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-107-1(0-5)

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\BF101717\
Data File : BF099583.D
Acq On : 17 Oct 2017 16:15
Operator : SJ/JU
Sample : I5776-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-107-1(0-5)

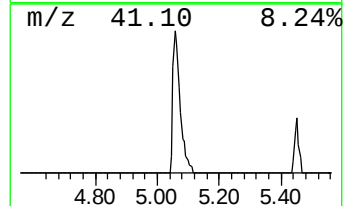
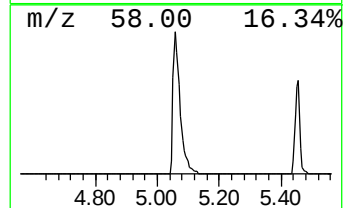
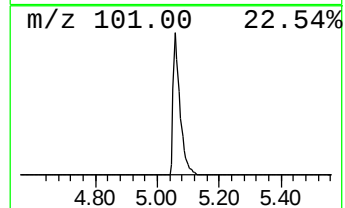
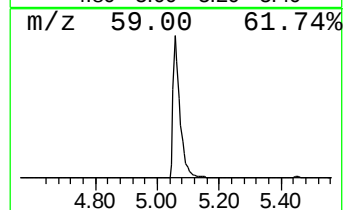
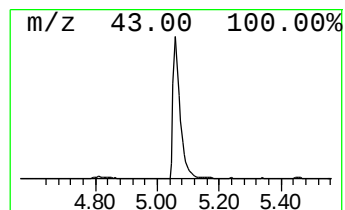
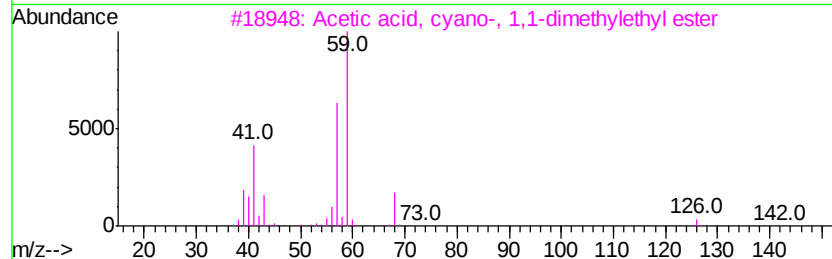
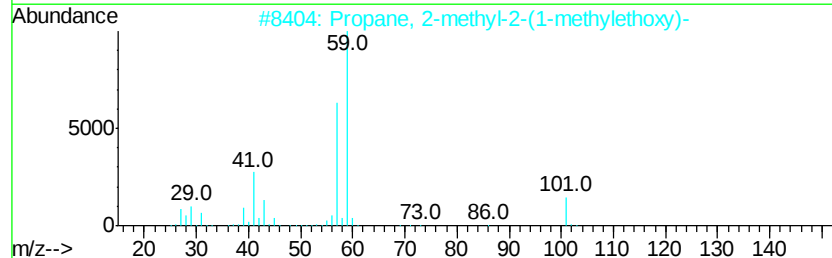
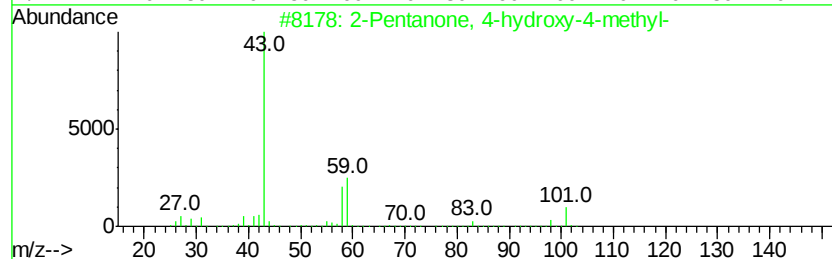
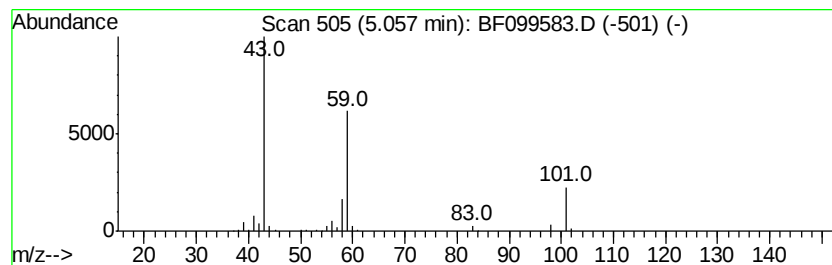
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	17.92 ng	470818	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099583.D
Acq On : 17 Oct 2017 16:15
Operator : SJ/JU
Sample : I5776-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-107-1(0-5)

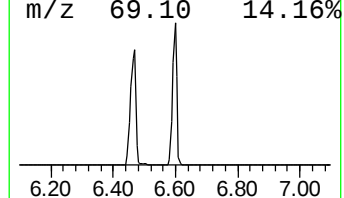
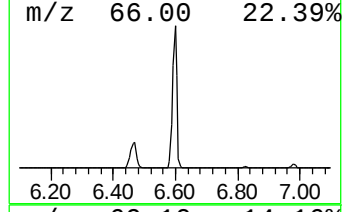
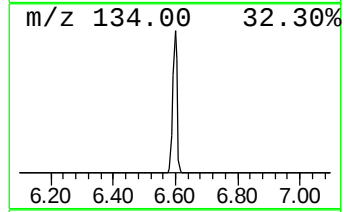
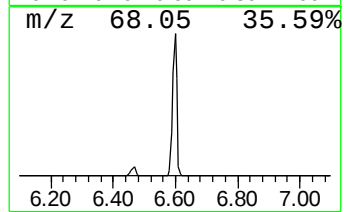
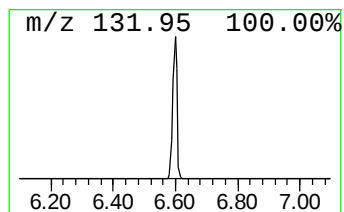
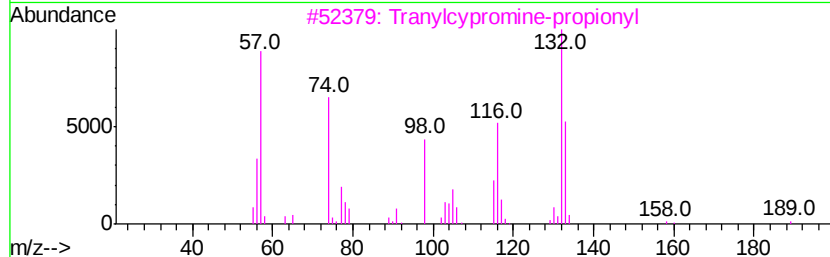
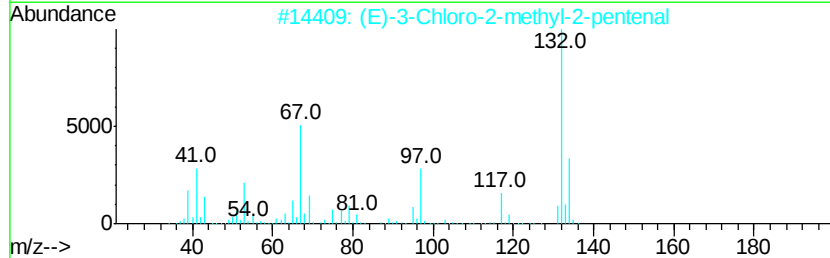
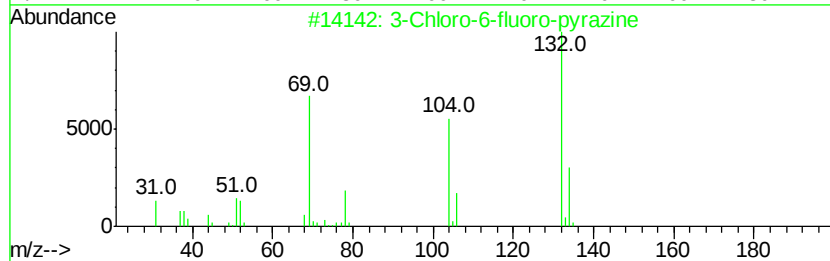
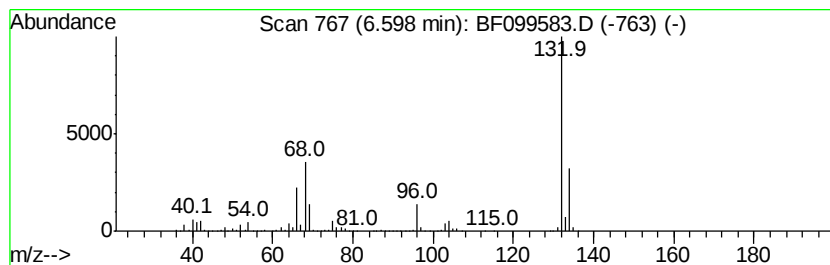
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	100.33 ng	2636140	1,4-Dichlorobenzene-d4	6.83

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099583.D
Acq On : 17 Oct 2017 16:15
Operator : SJ/JU
Sample : I5776-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-107-1(0-5)

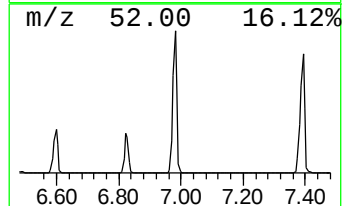
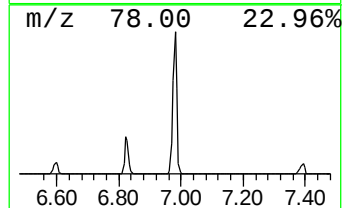
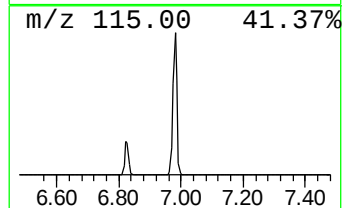
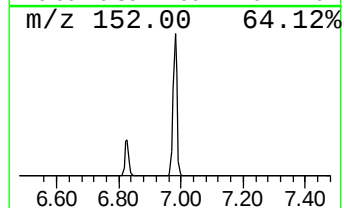
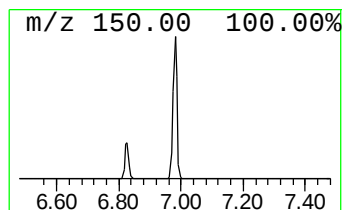
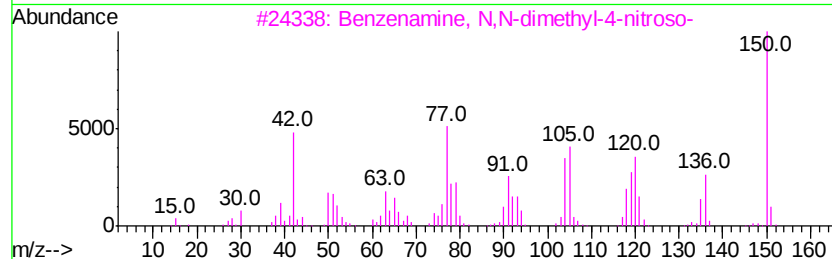
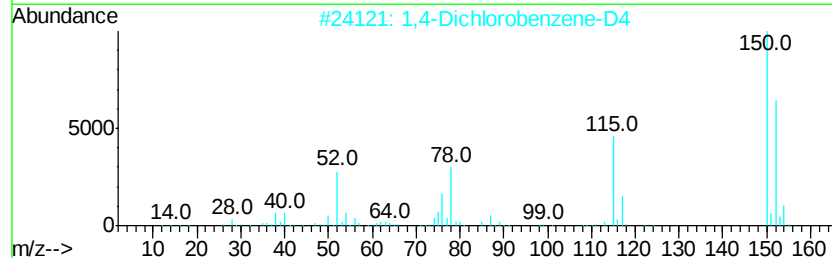
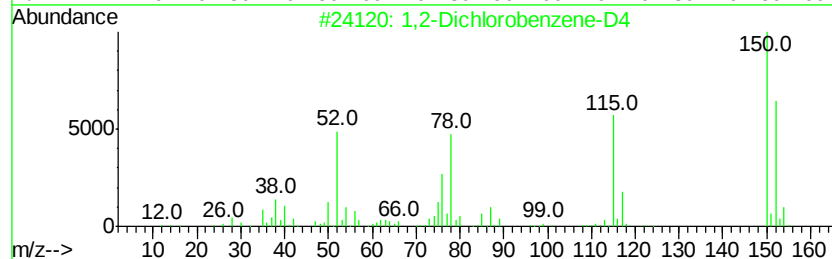
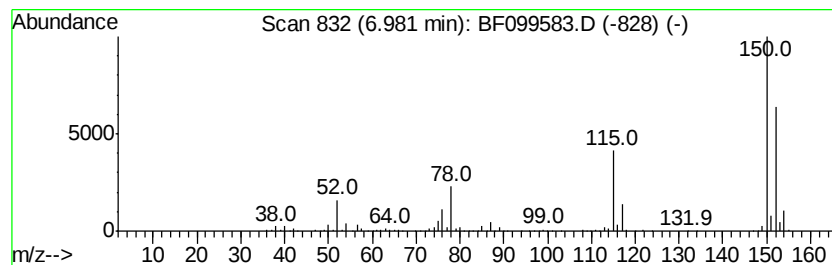
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,2-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	80.06 ng	2103740	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
2		1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
3		Benzenamine, N,N-dimethyl-4-nitr...	150	C8H10N2O	000138-89-6	32
4		2,6-Diaminopurine	150	C5H6N6	001904-98-9	12
5		But-2-yne-1,4-diol, 0,0'-bis(3-n...	384	C18H12N2O8	055709-58-5	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099583.D
Acq On : 17 Oct 2017 16:15
Operator : SJ/JU
Sample : I5776-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-107-1(0-5)

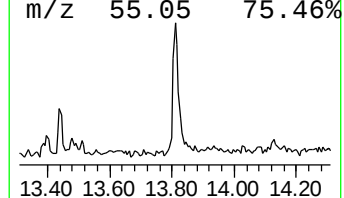
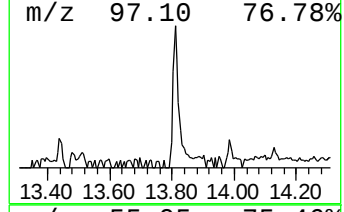
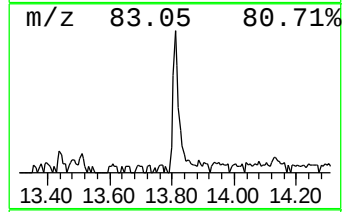
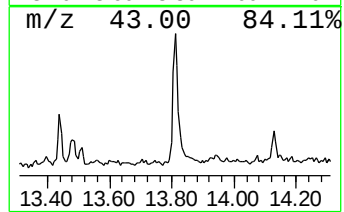
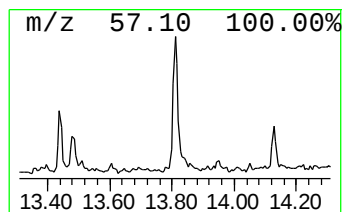
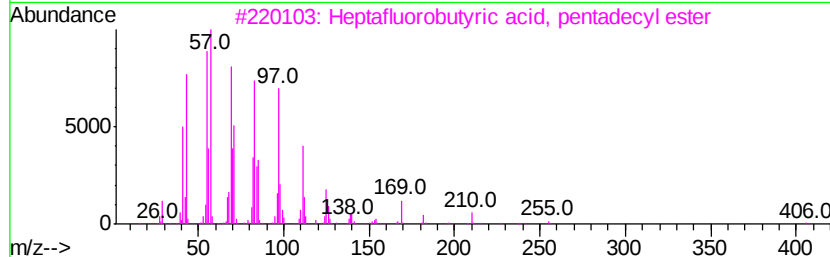
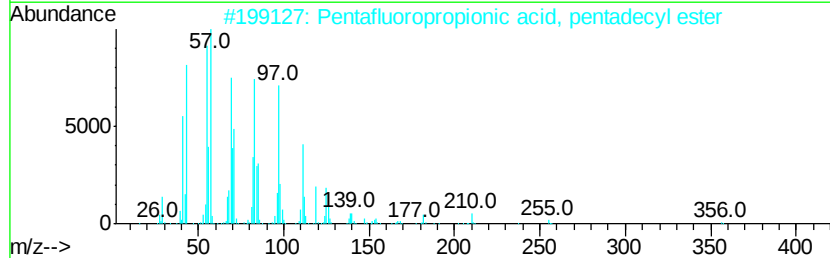
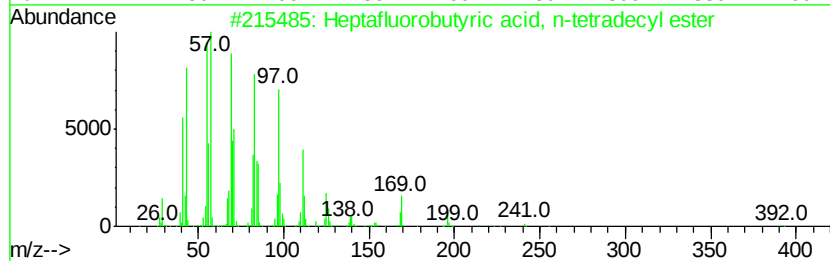
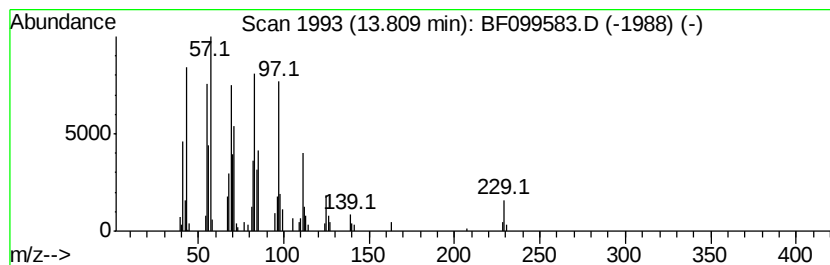
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.01 ng	117773	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
4		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
5		1-Heptacosanol	396	C27H56O	002004-39-9	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099583.D
Acq On : 17 Oct 2017 16:15
Operator : SJ/JU
Sample : I5776-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-107-1(0-5)

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
2-Pentanone, 4-hy...	5.06	17.9	ng	470818	1	6.83	525509	20.0
3-Chloro-6-fluoro...	6.60	100.3	ng	2636140	1	6.83	525509	20.0
1,2-Dichlorobenze...	6.98	80.1	ng	2103740	1	6.83	525509	20.0
Heptafluorobutyri...	13.81	3.0	ng	117773	5	13.99	783542	20.0