

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
 Data File : BF098251.D
 Acq On : 2 Sep 2017 17:43
 Operator : SJ/JU
 Sample : I5073-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-2-COMP

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-BF081517.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	3.081	166	169	182	rBV	20969	55219	1.92%	0.242%
2	4.904	476	479	493	rVB	193198	267735	9.30%	1.172%
3	5.322	545	550	553	rBV	2533824	2705526	93.95%	11.847%
4	6.357	720	726	729	rBV	2621925	2879684	100.00%	12.610%
5	6.481	743	747	750	rBV	2707527	2698454	93.71%	11.816%
6	6.710	782	786	789	rBV	855651	681612	23.67%	2.985%
7	6.869	808	813	816	rBV	1900960	1792592	62.25%	7.850%
8	7.281	877	883	886	rBV	1649116	1699989	59.03%	7.444%
9	7.992	1000	1004	1013	rBV	1043657	859591	29.85%	3.764%
10	9.069	1182	1187	1190	rBV	2643534	2391101	83.03%	10.470%
11	9.463	1250	1254	1259	rBV	339428	297784	10.34%	1.304%
12	9.745	1298	1302	1306	rVB	939234	773004	26.84%	3.385%
13	10.180	1373	1376	1378	rVB	45450	30699	1.07%	0.134%
14	10.398	1409	1413	1417	rBV	43951	59446	2.06%	0.260%
15	10.533	1432	1436	1439	rBV	1384620	1227333	42.62%	5.374%
16	10.663	1453	1458	1465	rBV3	78673	136121	4.73%	0.596%
17	11.098	1530	1532	1534	rBV2	40951	34333	1.19%	0.150%
18	11.127	1534	1537	1544	rVB	68011	75230	2.61%	0.329%
19	11.227	1550	1554	1557	rBV	798537	662701	23.01%	2.902%
20	12.810	1819	1823	1827	rBV	1778016	1766472	61.34%	7.735%
21	13.710	1973	1976	1984	rBV	98975	124418	4.32%	0.545%
22	13.857	1997	2001	2005	rBV	702439	702079	24.38%	3.074%
23	14.345	2078	2084	2088	rBV3	47627	85765	2.98%	0.376%
24	14.868	2171	2173	2179	rVB	23218	32398	1.13%	0.142%
25	14.945	2183	2186	2189	rBV	42624	49080	1.70%	0.215%
26	14.974	2189	2191	2196	rVB6	28793	35979	1.25%	0.158%
27	15.274	2237	2242	2246	rBV	567036	669680	23.26%	2.932%
28	15.710	2312	2316	2320	rVB3	31666	42795	1.49%	0.187%

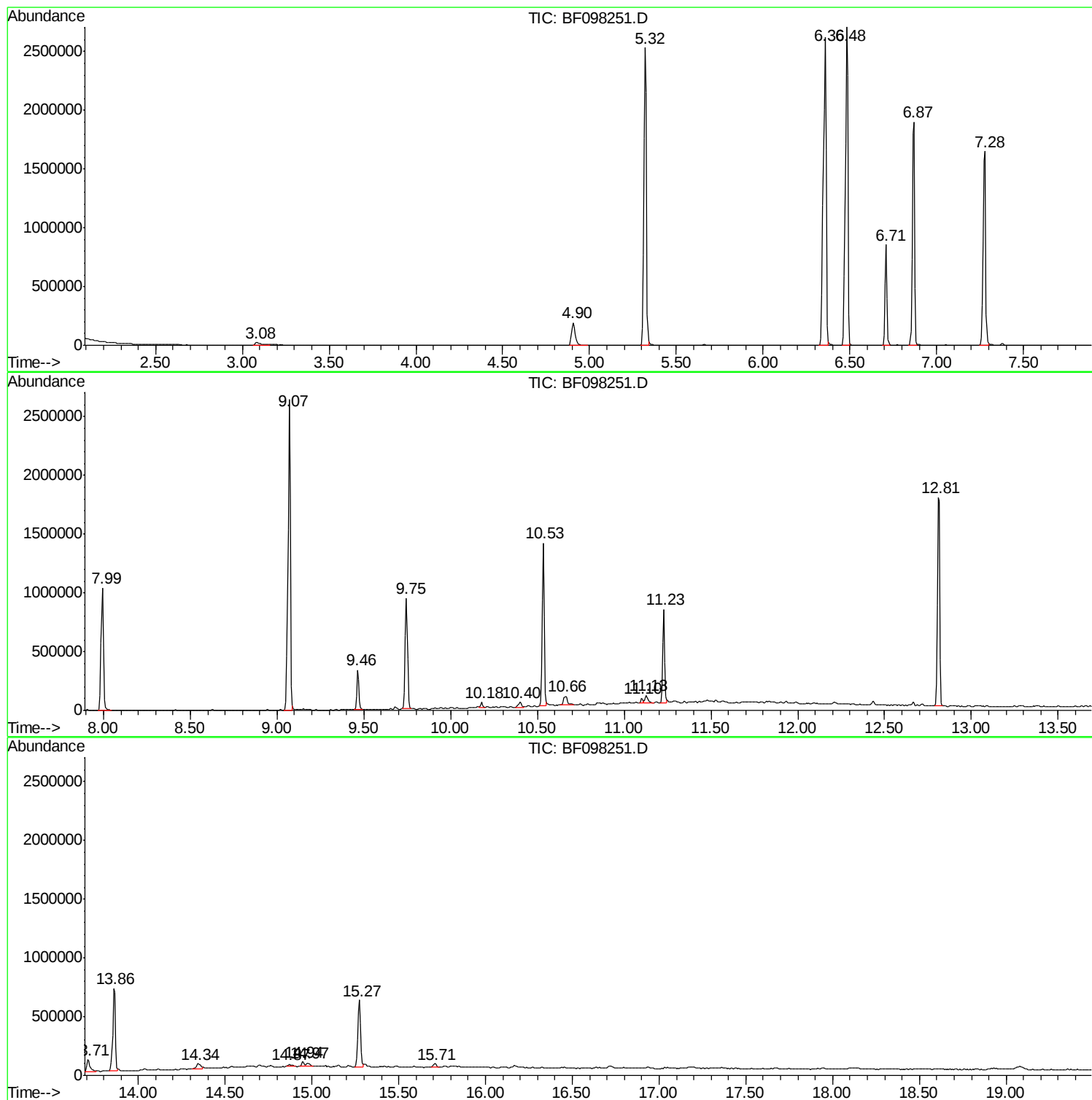
Sum of corrected areas: 22836820

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

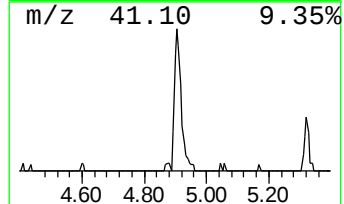
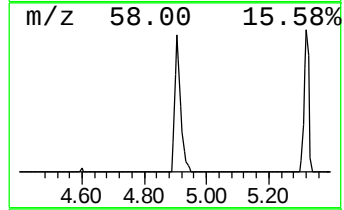
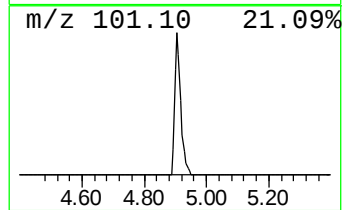
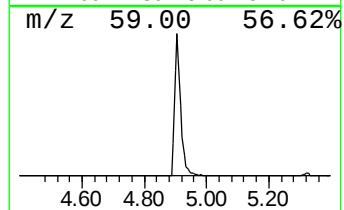
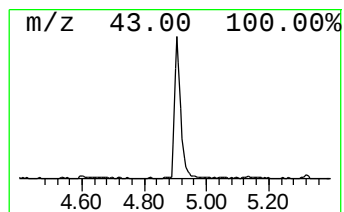
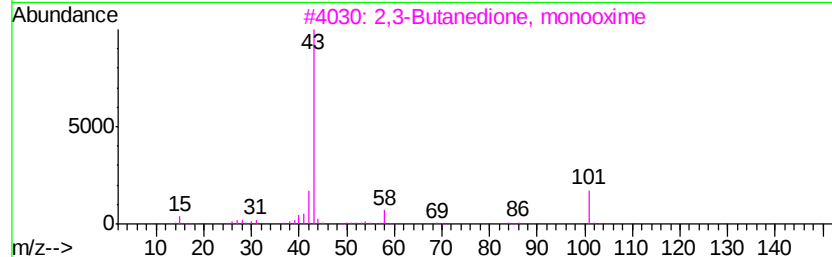
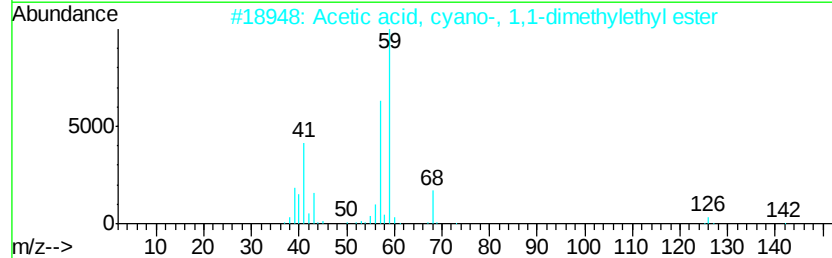
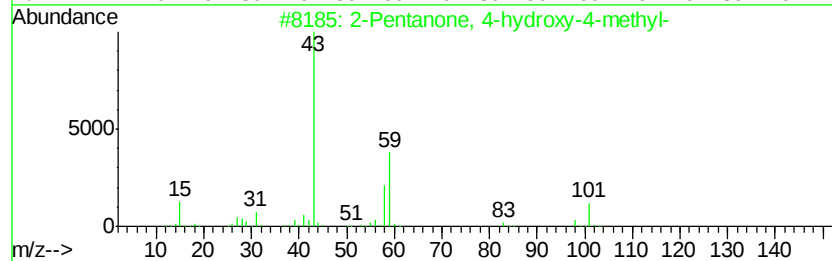
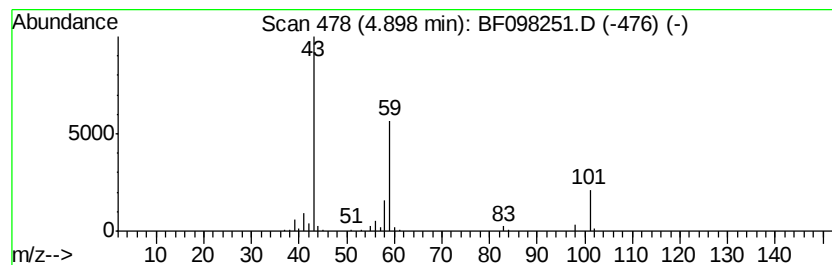
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	7.86 ng	267735	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

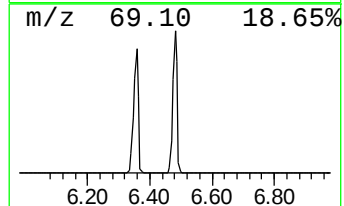
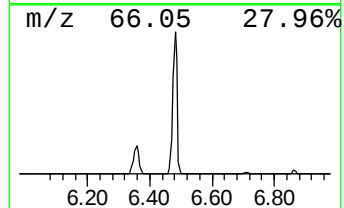
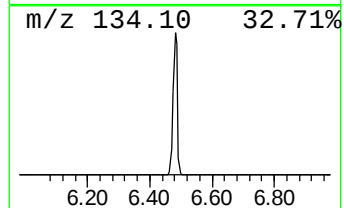
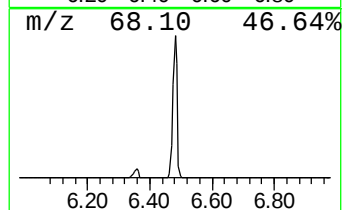
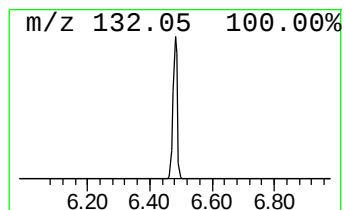
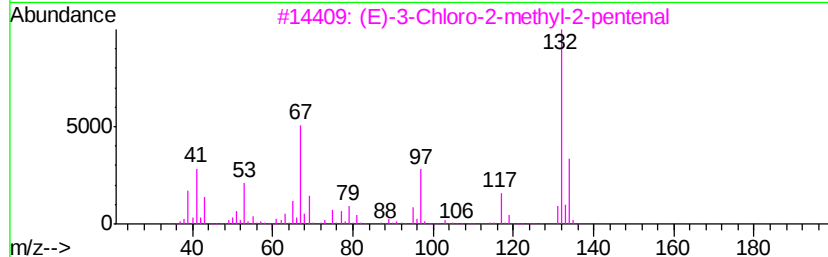
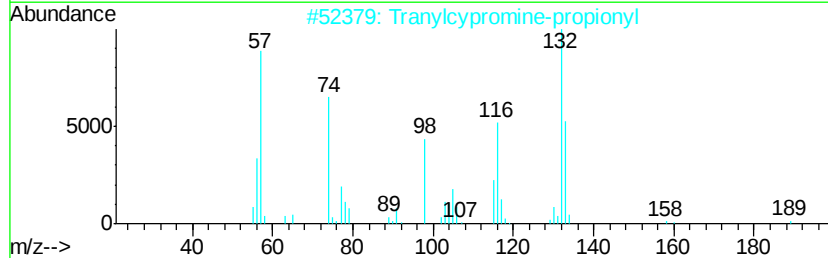
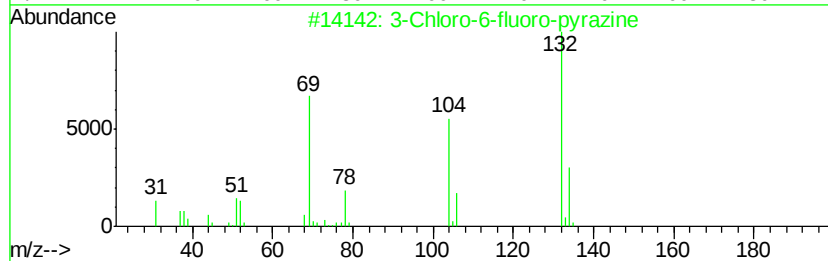
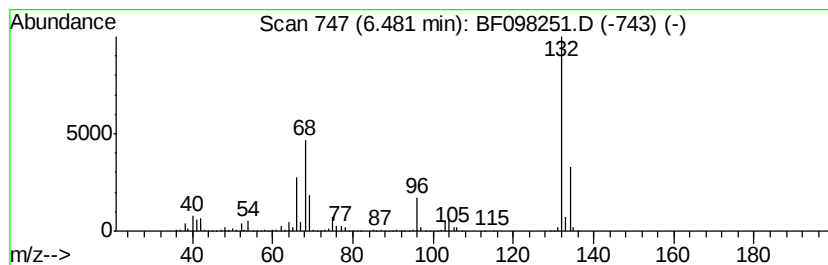
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	79.18 ng	2698450	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

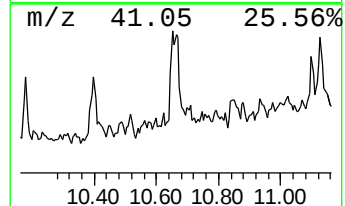
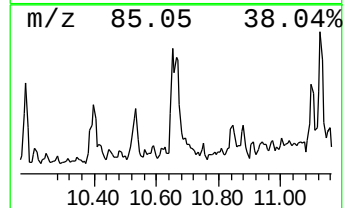
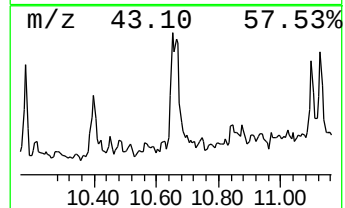
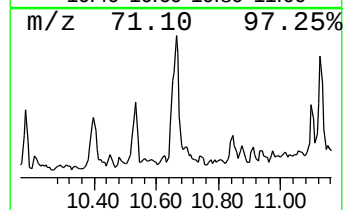
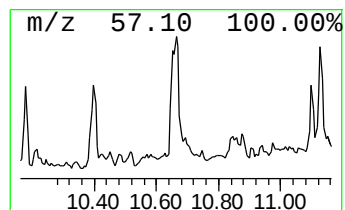
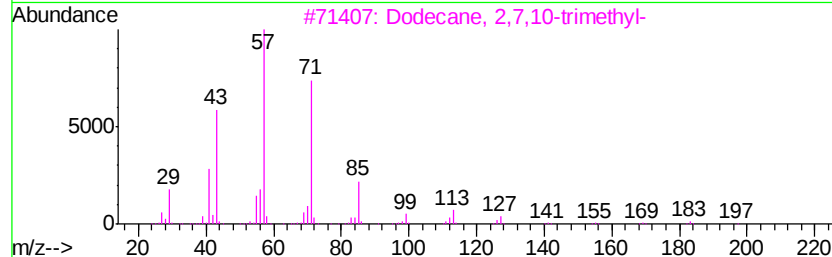
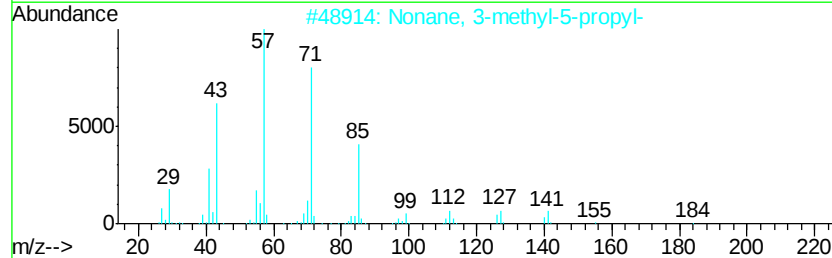
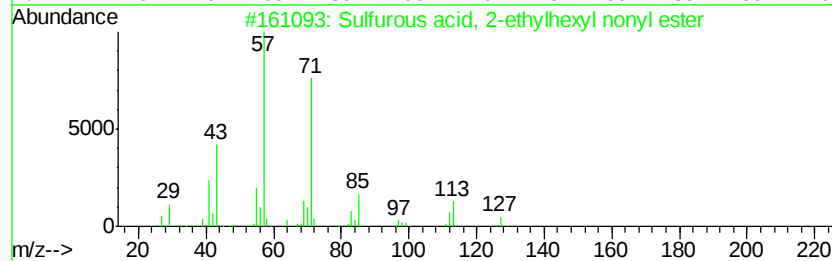
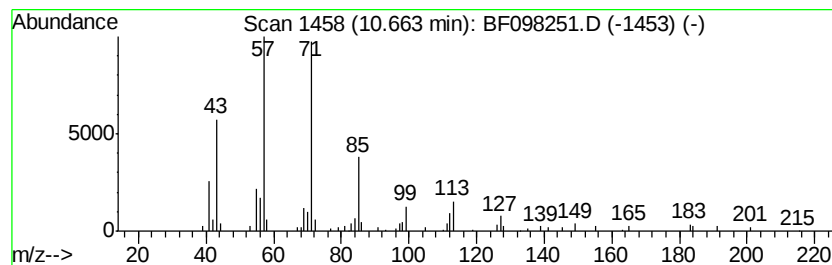
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Sulfurous acid, 2-ethylhexy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	4.11 ng	136121	Phenanthrene-d10	11.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	72
2			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	72
3			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
4			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
5			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

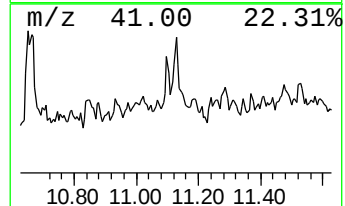
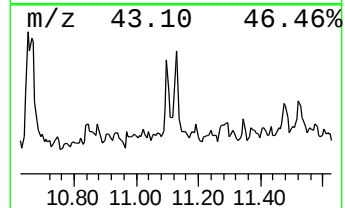
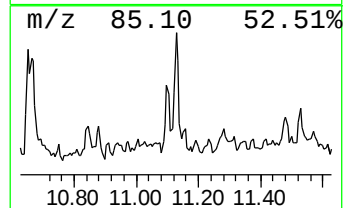
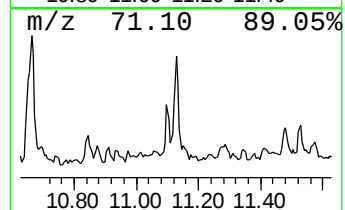
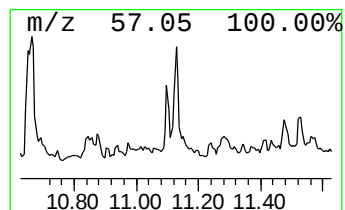
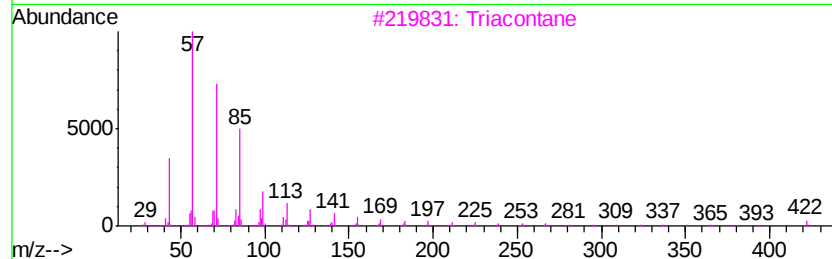
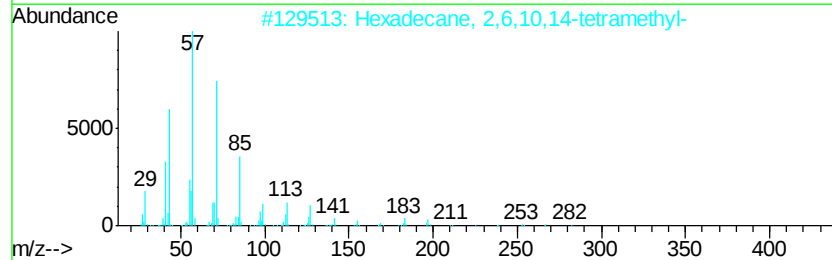
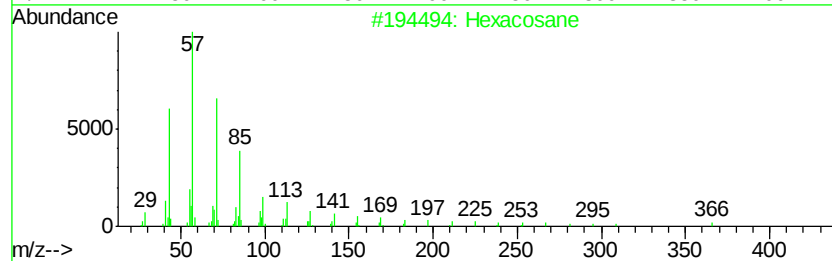
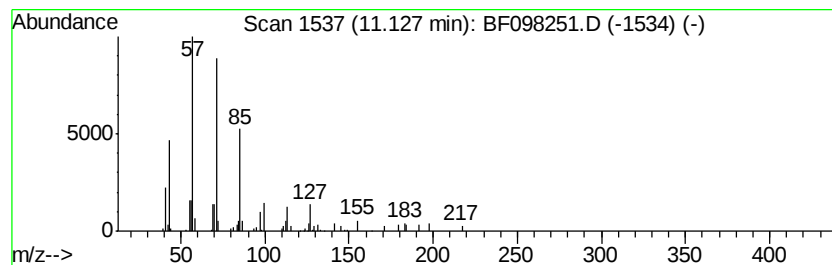
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.13	2.27 ng	75230	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
3		Triacontane	422	C30H62	000638-68-6	83
4		Heptadecane	240	C17H36	000629-78-7	80
5		Heneicosane	296	C21H44	000629-94-7	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

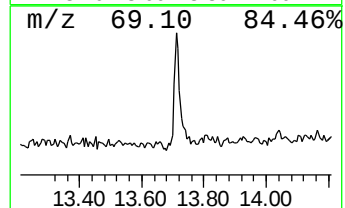
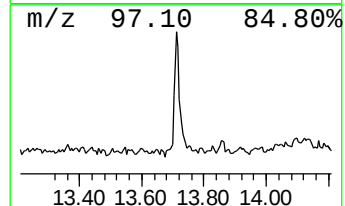
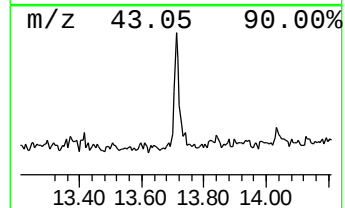
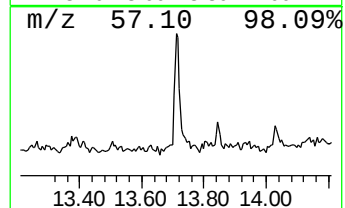
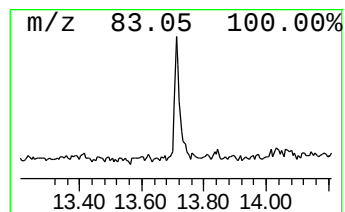
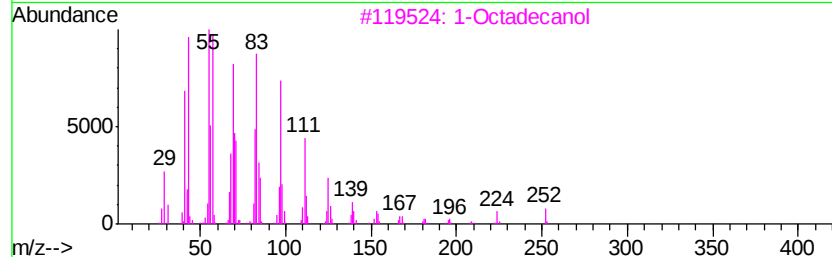
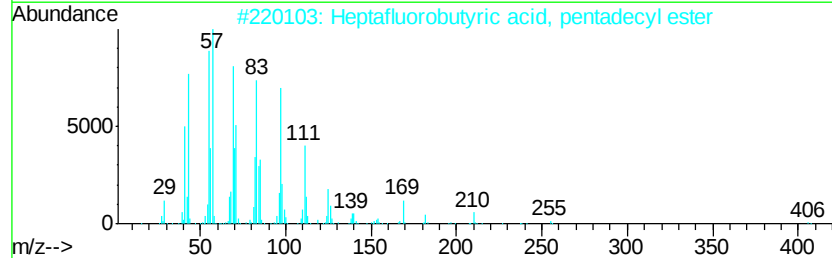
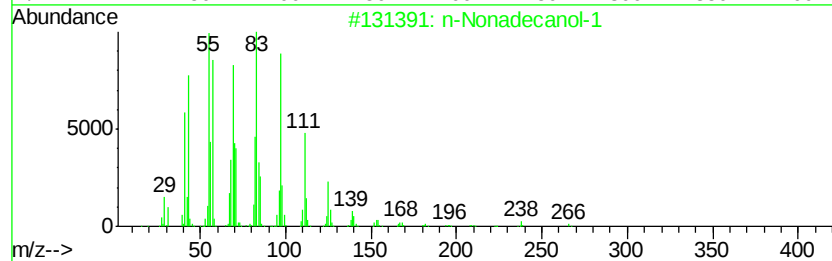
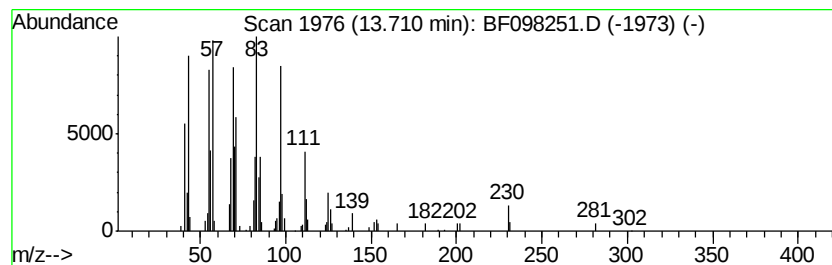
Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.71	3.54 ng	124418	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	1-Octadecanol	270	C18H38O	000112-92-5	93
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	92
5	Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

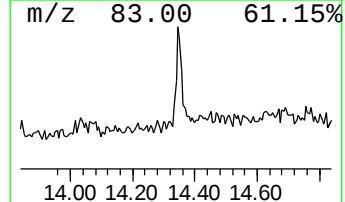
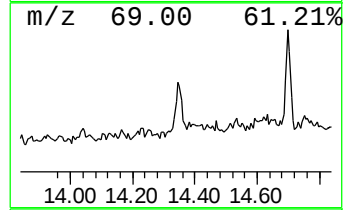
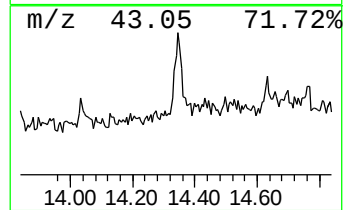
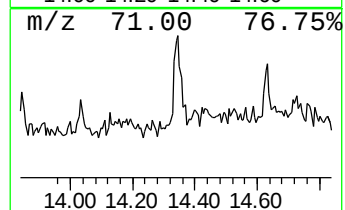
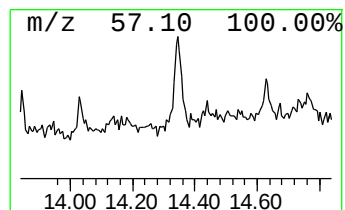
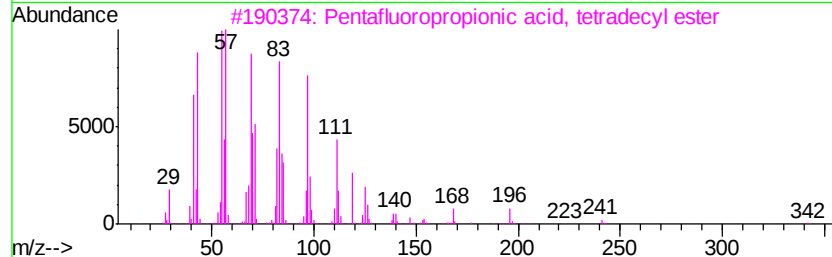
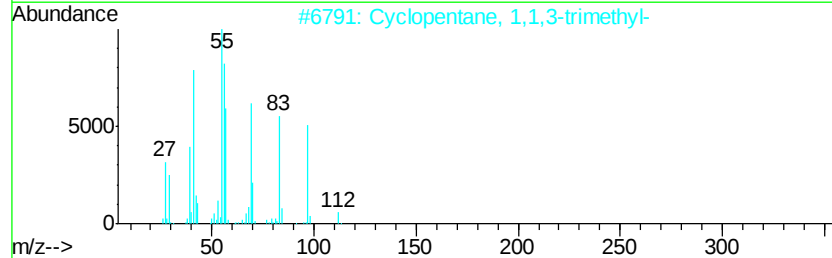
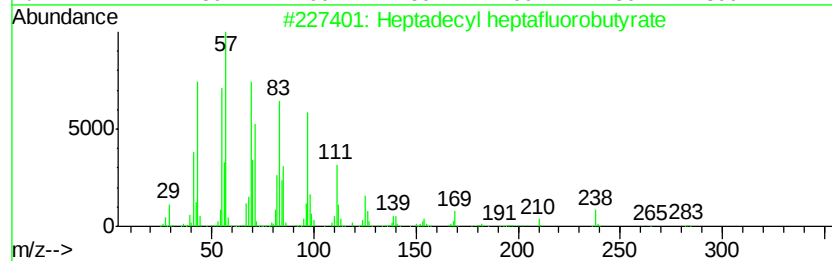
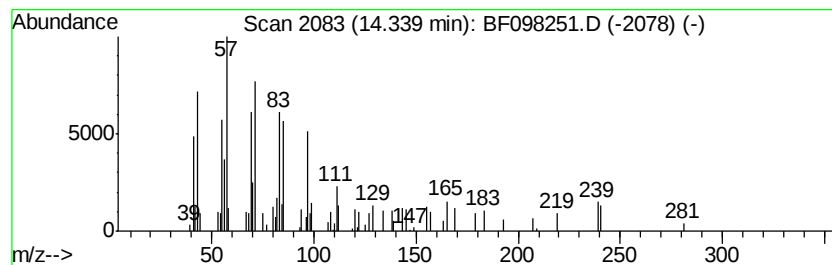
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.44 ng	85765	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
2		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	58
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	53
4		1-Docosene	308	C22H44	001599-67-3	52
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
Data File : BF098251.D
Acq On : 2 Sep 2017 17:43
Operator : SJ/JU
Sample : I5073-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	7.9	ng	267735	1	6.71	681612	20.0
unknown6.48	6.48	79.2	ng	2698450	1	6.71	681612	20.0
Sulfurous acid, 2...	10.66	4.1	ng	136121	4	11.23	662701	20.0
Hexacosane	11.13	2.3	ng	75230	4	11.23	662701	20.0
n-Nonadecanol-1	13.71	3.5	ng	124418	5	13.86	702079	20.0
Heptadecyl heptaf...	14.34	2.4	ng	85765	5	13.86	702079	20.0