

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
 Data File : BF099002.D
 Acq On : 2 Oct 2017 16:27
 Operator : SJ/JU
 Sample : I5534-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-114-1(10-16)

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-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	2.216	18	22	29	rVB	127666	171516	8.09%	0.868%
2	5.128	513	517	530	rVB	310107	355315	16.76%	1.798%
3	5.522	579	584	587	rBV	2262944	2021000	95.36%	10.227%
4	6.522	749	754	757	rBV	2083517	2007276	94.71%	10.158%
5	6.669	774	779	782	rBV	2393442	2119442	100.00%	10.725%
6	6.898	815	818	822	rBV	767384	656852	30.99%	3.324%
7	7.057	837	845	848	rBV	1805119	1739455	82.07%	8.802%
8	7.457	909	913	917	rBV	1240849	1267510	59.80%	6.414%
9	8.181	1032	1036	1040	rBV	1004771	880839	41.56%	4.457%
10	9.257	1213	1219	1222	rBV	2246357	1971133	93.00%	9.975%
11	9.645	1281	1285	1289	rBV	321755	274030	12.93%	1.387%
12	9.939	1330	1335	1339	rBV	1117023	935710	44.15%	4.735%
13	10.333	1398	1402	1405	rBV	461109	373519	17.62%	1.890%
14	10.727	1465	1469	1472	rBV	1361073	1213185	57.24%	6.139%
15	11.427	1584	1588	1591	rBV	1119755	908351	42.86%	4.597%
16	13.010	1853	1857	1860	rBV	1886167	1616504	76.27%	8.180%
17	13.892	2003	2007	2011	rBV	26664	31948	1.51%	0.162%
18	14.063	2033	2036	2040	rBV	696303	662938	31.28%	3.355%
19	15.551	2284	2289	2296	rBV	422079	528105	24.92%	2.672%
20	17.133	2551	2558	2563	rBV7	10628	26645	1.26%	0.135%

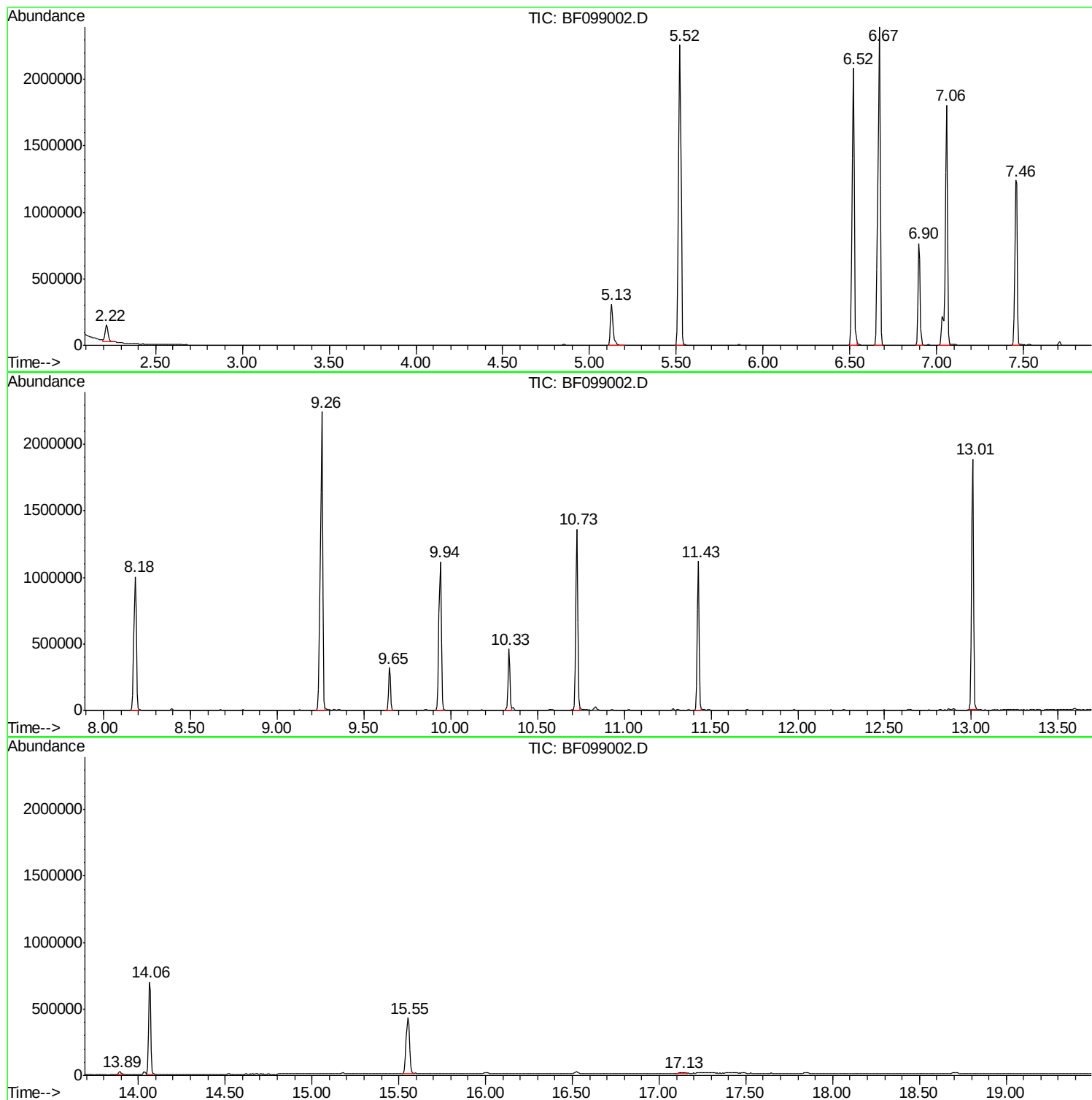
Sum of corrected areas: 19761273

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099002.D
Acq On : 2 Oct 2017 16:27
Operator : SJ/JU
Sample : I5534-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(10-16)

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\BF100217\
Data File : BF099002.D
Acq On : 2 Oct 2017 16:27
Operator : SJ/JU
Sample : I5534-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(10-16)

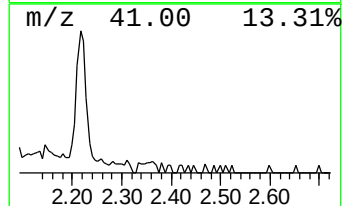
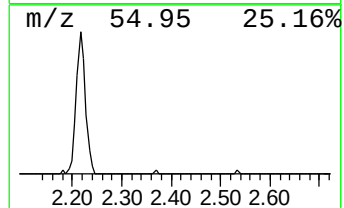
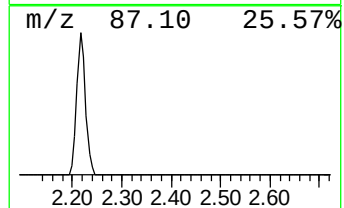
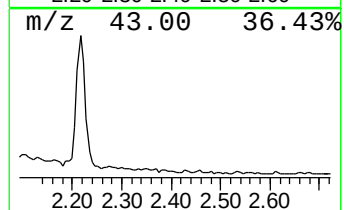
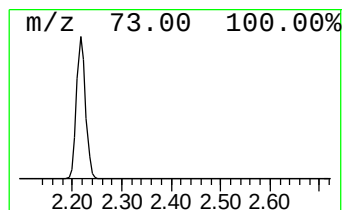
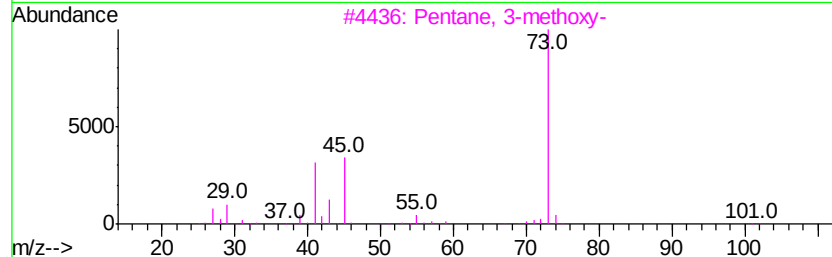
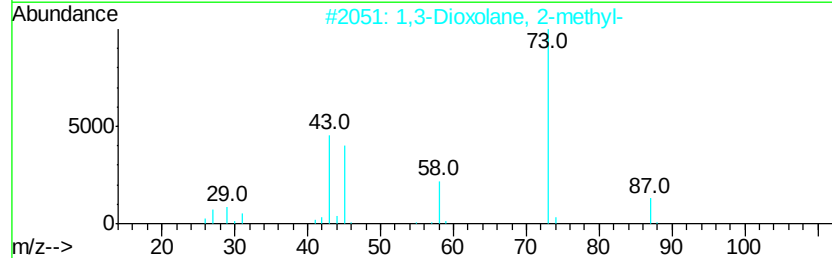
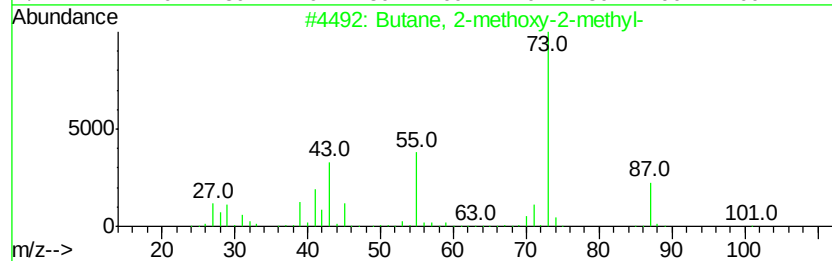
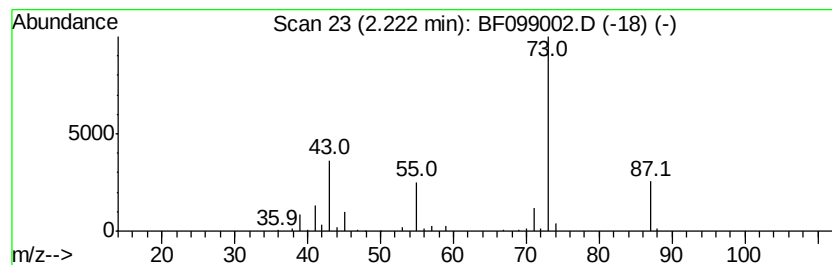
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.22	5.22 ng	171516	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
Data File : BF099002.D
Acq On : 2 Oct 2017 16:27
Operator : SJ/JU
Sample : I5534-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(10-16)

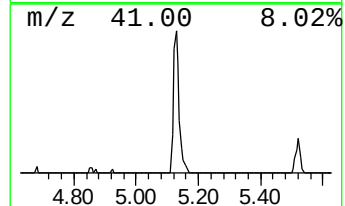
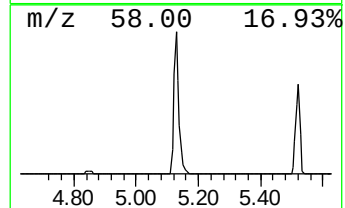
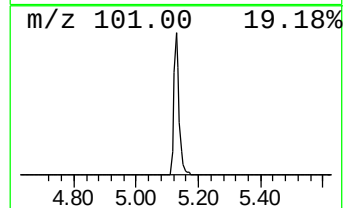
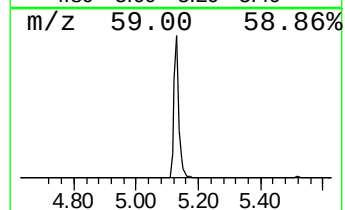
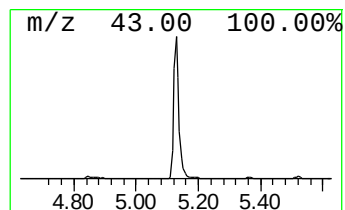
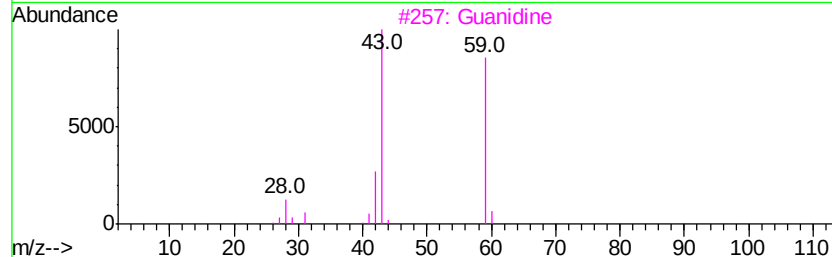
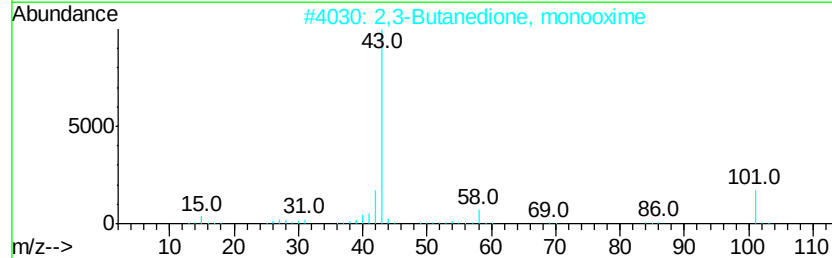
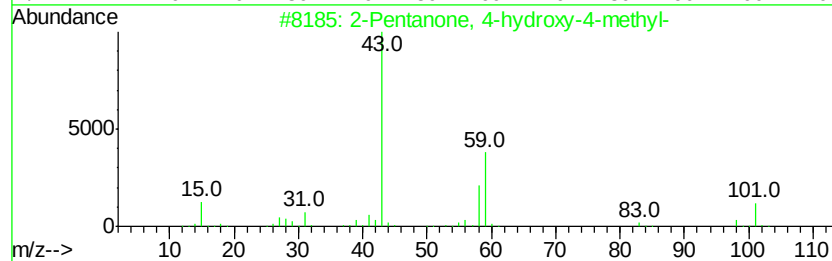
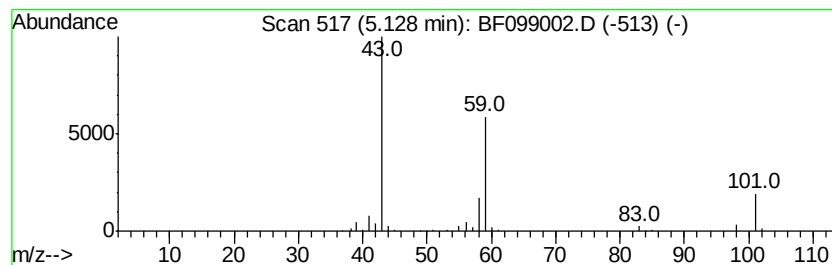
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	10.82 ng	355315	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Guanidine	59	CH5N3	000113-00-8	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
Data File : BF099002.D
Acq On : 2 Oct 2017 16:27
Operator : SJ/JU
Sample : I5534-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(10-16)

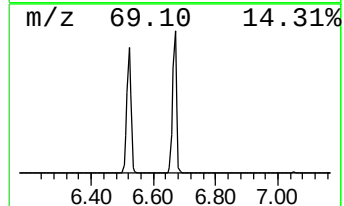
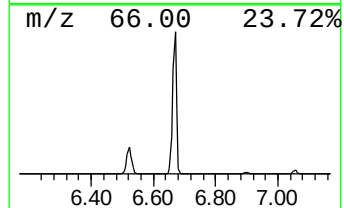
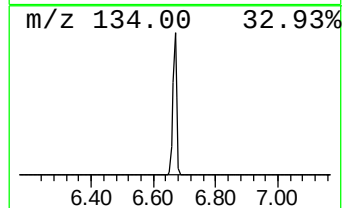
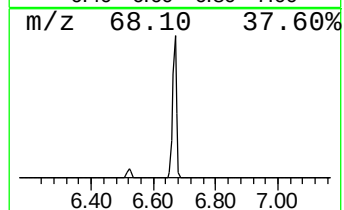
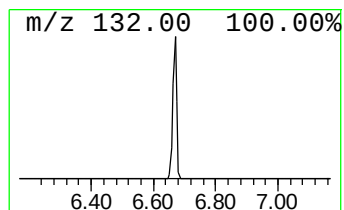
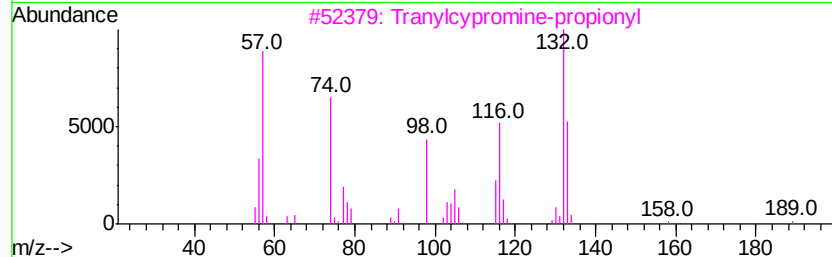
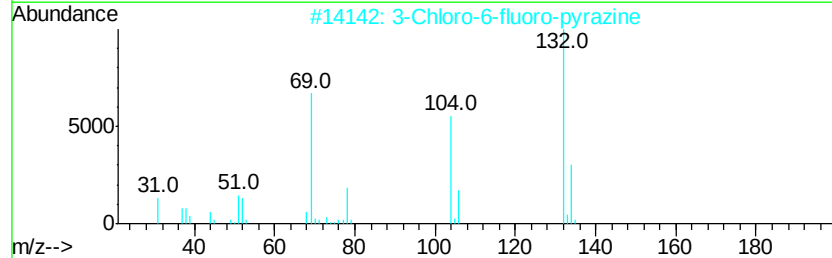
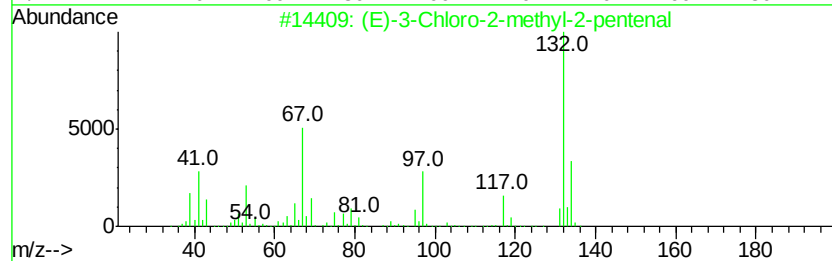
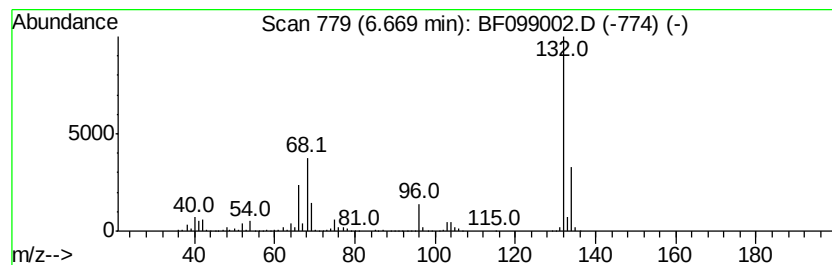
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	64.53 ng	2119440	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		Tranvlcypromine-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\BF100217\
Data File : BF099002.D
Acq On : 2 Oct 2017 16:27
Operator : SJ/JU
Sample : I5534-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

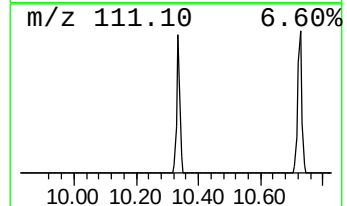
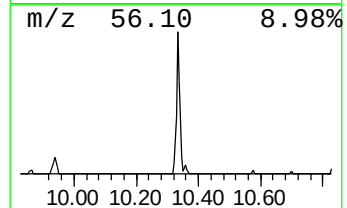
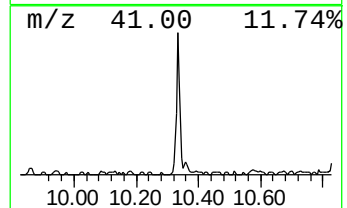
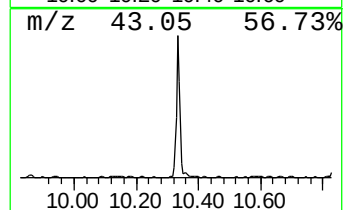
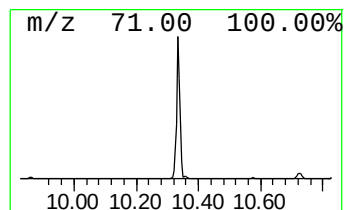
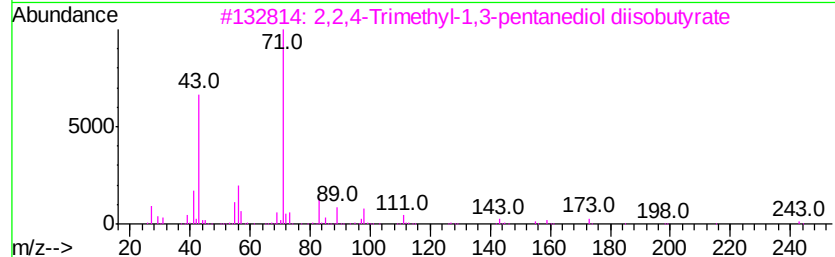
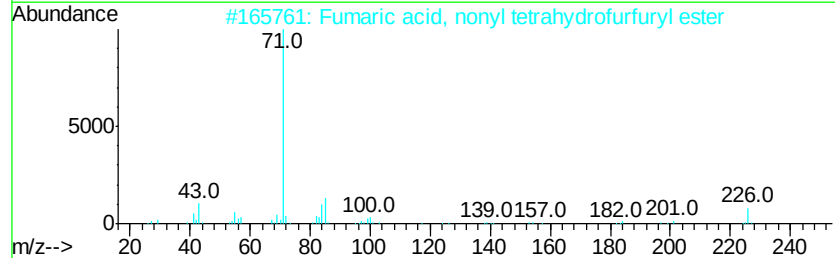
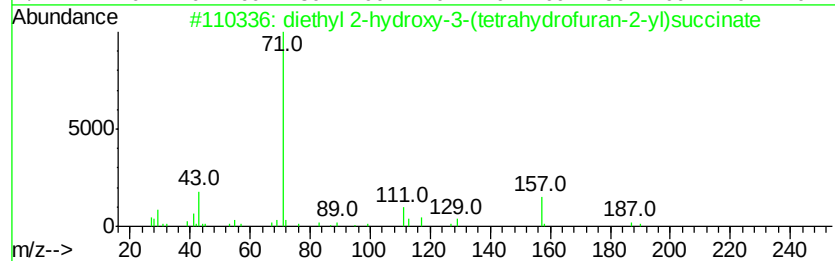
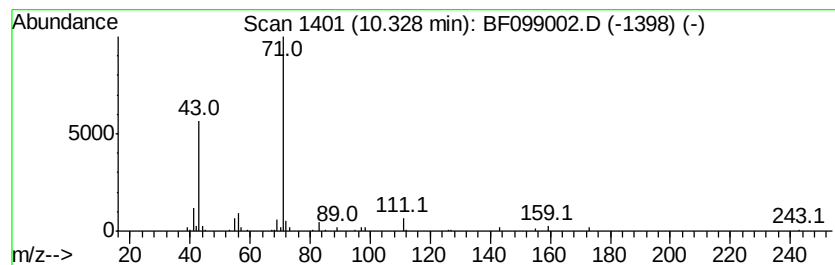
Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(10-16)

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 diethyl 2-hydroxy-3-(tetrahydrofuran-2-yl)succinate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	7.98 ng	373519	Acenaphthene-d10	9.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	diethyl 2-hydroxy-3-(tetrahydrofuran-2-yl)succinate	260 C12H20O6	1000365-67-1	64
2	Fumaric acid, nonyl tetrahydrofuran-2-yl ester	326 C18H30O5	1000330-58-3	64
3	2,2,4-Trimethyl-1,3-pentanediol	286 C16H30O4	006846-50-0	56
4	4-Hexen-3-ol, 2-methyl-	114 C7H14O	004798-60-1	50
5	2-Furanmethanol, tetrahydro-, ac-	144 C7H12O3	000637-64-9	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
Data File : BF099002.D
Acq On : 2 Oct 2017 16:27
Operator : SJ/JU
Sample : I5534-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-114-1(10-16)

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...	2.22	5.2	ng	171516	1	6.90	656852	20.0
2-Pentanone, 4-hy...	5.13	10.8	ng	355315	1	6.90	656852	20.0
unknown6.67	6.67	64.5	ng	2119440	1	6.90	656852	20.0
diethyl 2-hydroxy...	10.33	8.0	ng	373519	3	9.94	935710	20.0