

Data Path : Z:\HPCHEM1\BNA F\Data\BF041417\
 Data File : BF094433.D
 Acq On : 14 Apr 2017 17:29
 Operator : SJ/MA
 Sample : I2677-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 041117-DSDC-F-D-M

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-BF032217.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	2.963	178	183	189	rVB	136017	153220	3.16%	0.532%
2	3.898	338	342	349	rBV	177905	189234	3.90%	0.658%
3	4.316	410	413	426	rBV	1204703	1126107	23.19%	3.913%
4	5.393	592	596	608	rVB	786942	750492	15.46%	2.608%
5	5.522	613	618	621	rBV	2472041	2250889	46.36%	7.821%
6	5.769	656	660	664	rBV	969835	864067	17.80%	3.002%
7	5.951	686	691	694	rBV	3196710	3147090	64.81%	10.935%
8	6.422	765	771	775	rBV	2110511	2623131	54.02%	9.114%
9	7.269	910	915	919	rBV	1219727	1180564	24.31%	4.102%
10	8.598	1134	1141	1144	rBV	4199833	4855628	100.00%	16.872%
11	9.092	1221	1225	1228	rBV	66379	65583	1.35%	0.228%
12	9.404	1271	1278	1286	rVB2	1284147	1356125	27.93%	4.712%
13	10.004	1377	1380	1383	rVB	55777	50368	1.04%	0.175%
14	10.380	1439	1444	1448	rBV	1663423	1753253	36.11%	6.092%
15	10.586	1475	1479	1481	rBV	81572	85634	1.76%	0.298%
16	11.139	1570	1573	1577	rBV	69369	67964	1.40%	0.236%
17	11.227	1583	1588	1595	rVB	1357226	1370348	28.22%	4.761%
18	13.210	1918	1925	1929	rBV2	3521224	4576521	94.25%	15.902%
19	14.374	2118	2123	2134	rBV6	33401	69970	1.44%	0.243%
20	14.474	2134	2140	2144	rBV	1187729	1289370	26.55%	4.480%
21	16.092	2410	2415	2425	rVB	853042	954214	19.65%	3.316%

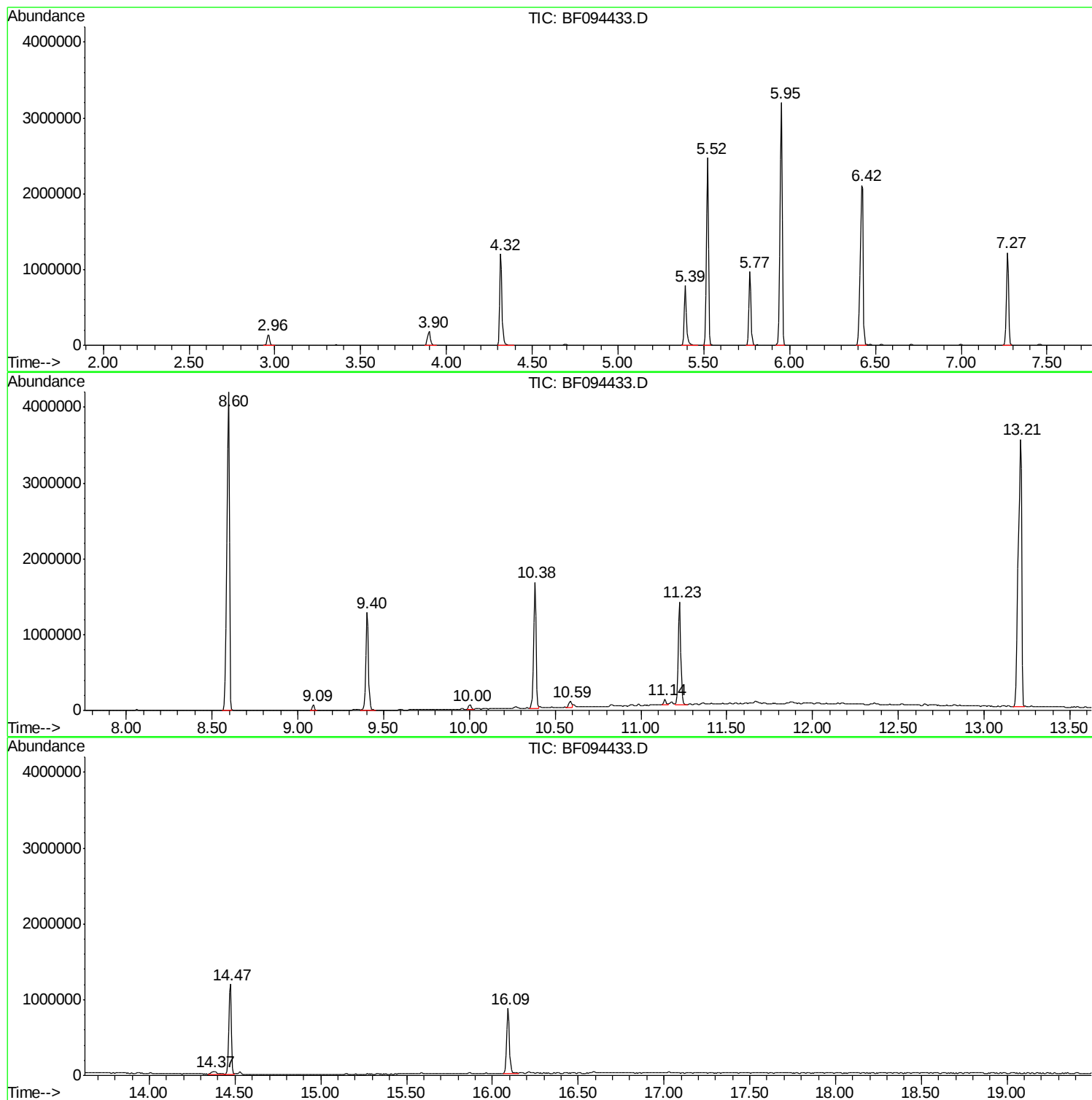
Sum of corrected areas: 28779772

Data Path : Z:\HPCHEM1\BNA F\Data\BF041417\
Data File : BF094433.D
Acq On : 14 Apr 2017 17:29
Operator : SJ/MA
Sample : I2677-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
041117-DSDC-F-D-M

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\Data\BF041417\
Data File : BF094433.D
Acq On : 14 Apr 2017 17:29
Operator : SJ/MA
Sample : I2677-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
041117-DSDC-F-D-M

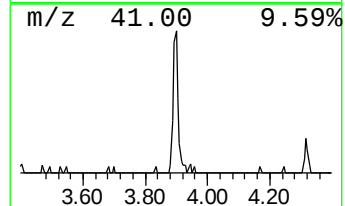
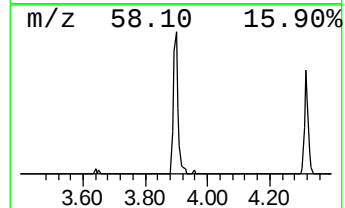
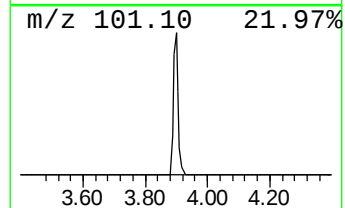
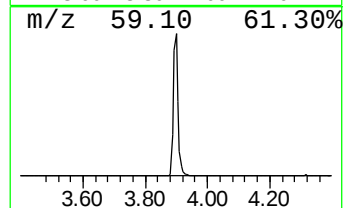
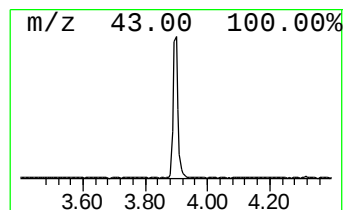
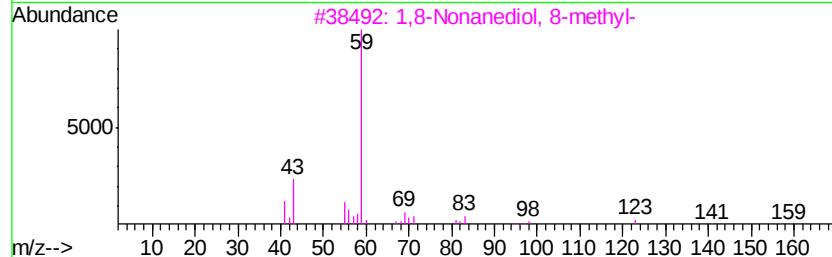
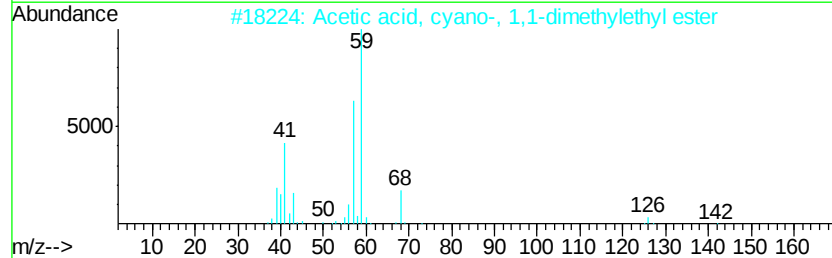
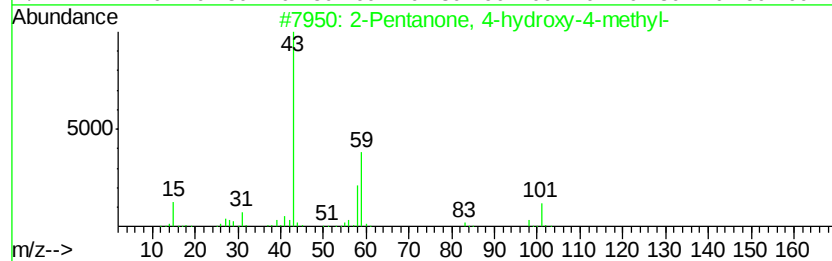
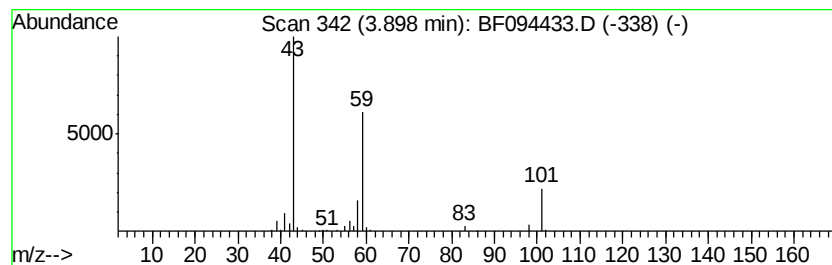
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
3.90	4.38 ng	189234	1,4-Dichlorobenzene-d4	5.77

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-dimethyl...	141	C7H11NO2	001116-98-9	25
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA F\Data\BF041417\
Data File : BF094433.D
Acq On : 14 Apr 2017 17:29
Operator : SJ/MA
Sample : I2677-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
041117-DSDC-F-D-M

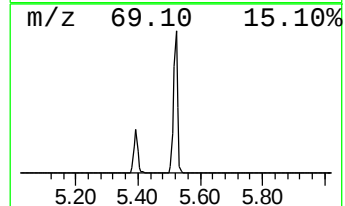
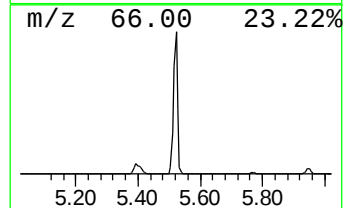
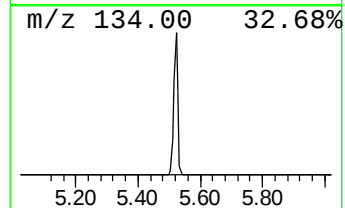
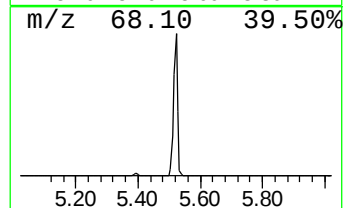
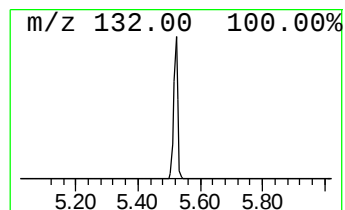
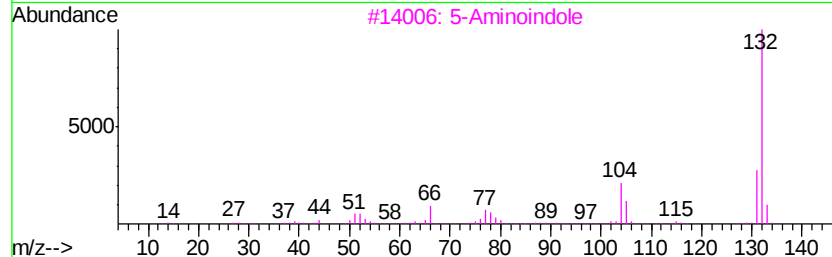
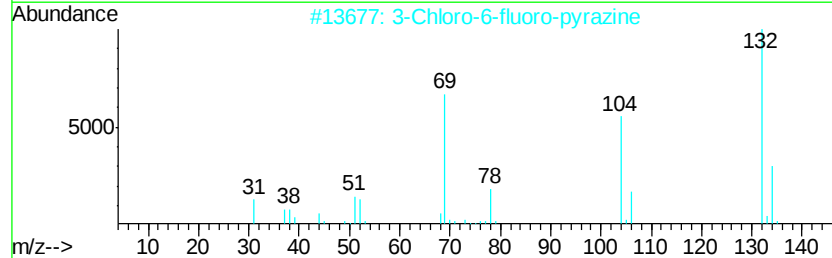
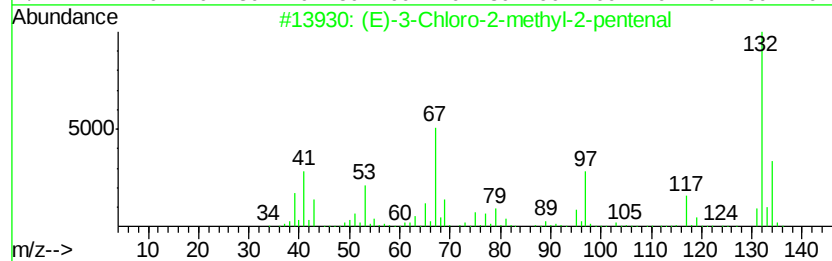
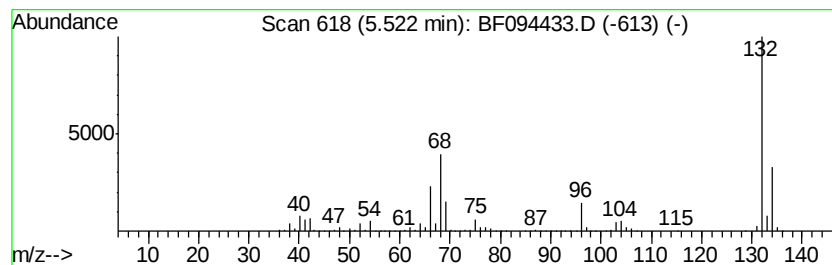
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.52 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	52.10 ng	2250890	1,4-Dichlorobenzene-d4	5.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\HPCHEM1\BNA_F\Data\BF041417\
Data File : BF094433.D
Acq On : 14 Apr 2017 17:29
Operator : SJ/MA
Sample : I2677-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
041117-DSDC-F-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.90	4.4	ng	189234	1	5.77	864067	20.0
unknown5.52	5.52	52.1	ng	2250890	1	5.77	864067	20.0