LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094484.D
Acq On : 18 Apr 2017 13:57
Operator : SJ/MA
Sample : I2701-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S39-9004

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-BF041717.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	2.137	31	34	46	rBV	110105	166264	4.71%	0.523%
2	3.231	217	220	226	rBV	67665	84272	2.39%	0.265%
3	3.384	231	246	248	rBV5	35129	106981	3.03%	0.337%
4	3.607	282	284	286	rVB	117019	83141	2.36%	0.262%
5	3.942	337	341	348	rBV	374008	468898	13.28%	1.475%
6	4.331	402	407	410	rBV	3188306	3135438	88.83%	9.862%
7	5.401	584	589	605	rVB	2802405	3467586	98.24%	10.907%
8	5.525	605	610	614	rBV	3206007	3474039	98.43%	10.927%
9	5.772	648	652	656	rBV	874902	726176	20.57%	2.284%
10	5.948	678	682	686	rBV	2619235	2663072	75.45%	8.377%
11	6.425	757	763	766	rBV	1990850	2192206	62.11%	6.895%
12	6.589	787	791	797	rBV2	49237	60674	1.72%	0.191%
13	7.266	902	906	909	rBV	1102438	983576	27.87%	3.094%
14	8.589	1126	1131	1134	rBV	3680270	3529601	100.00%	11.102%
15	9.083	1211	1215	1219	rBV	845770	791641	22.43%	2.490%
16	9.395	1262	1268	1272	rBV2	977765	970034	27.48%	3.051%
17	9.995	1366	1370	1374	rVB	63640	55757	1.58%	0.175%
18	10.371	1429	1434	1438	rBV	1923394	2212431	62.68%	6.959%
19	10.577	1466	1469	1472	rBV	76545	80313	2.28%	0.253%
20	11.130	1559	1563	1567	rBV	46284	49075	1.39%	0.154%
21	11.218	1573	1578	1580	rBV	1077251	1101098	31.20%	3.463%
22	11.242	1580	1582	1586	rVB	172447	152013	4.31%	0.478%
23	11.307	1590	1593	1597	rVB	49433	43724	1.24%	0.138%
24	12.701	1826	1830	1835	rBV	134818	129089	3.66%	0.406%
25	12.977	1872	1877	1881	rVB	109798	118087	3.35%	0.371%
26	13.195	1909	1914	1918	rBV	2711654	3187236	90.30%	10.025%
27	14.371	2108	2114	2121	rVB4	24404	50403	1.43%	0.159%
28	14.459	2124	2129	2133	rBV	866885	972787	27.56%	3.060%
29	15.583	2315	2320	2324	rBV	30937	39774	1.13%	0.125%
30	16.083	2401	2405	2414	rVB	628449	696757	19.74%	2.192%

Sum of corrected areas: 31792143

LSC Report - Integrated Chromatogram

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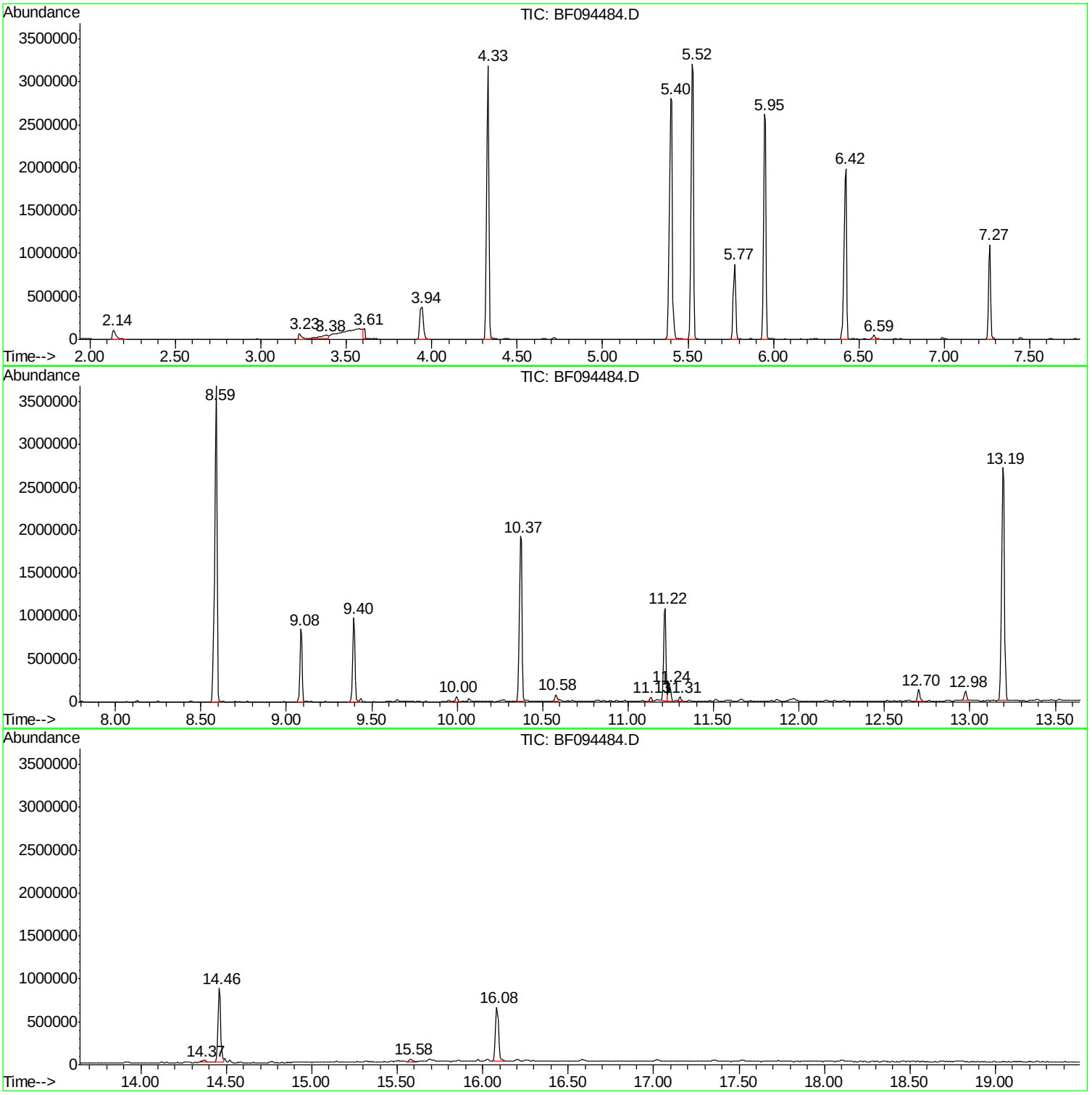
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S39-9004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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

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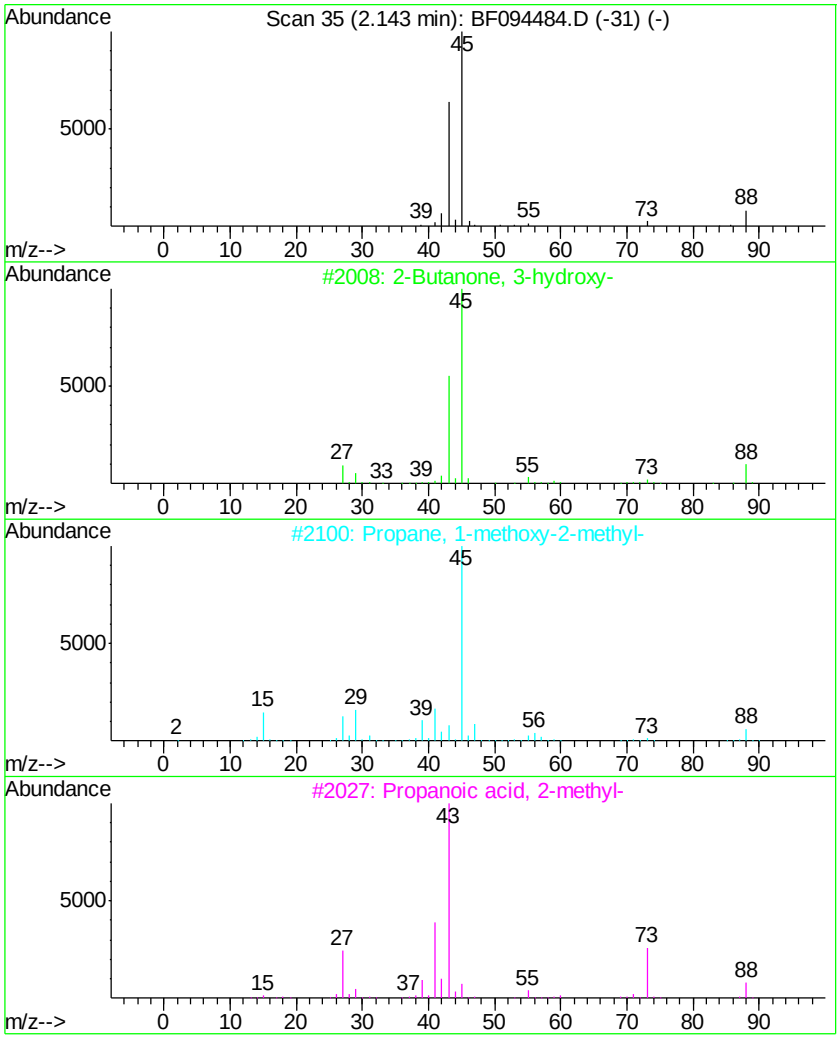
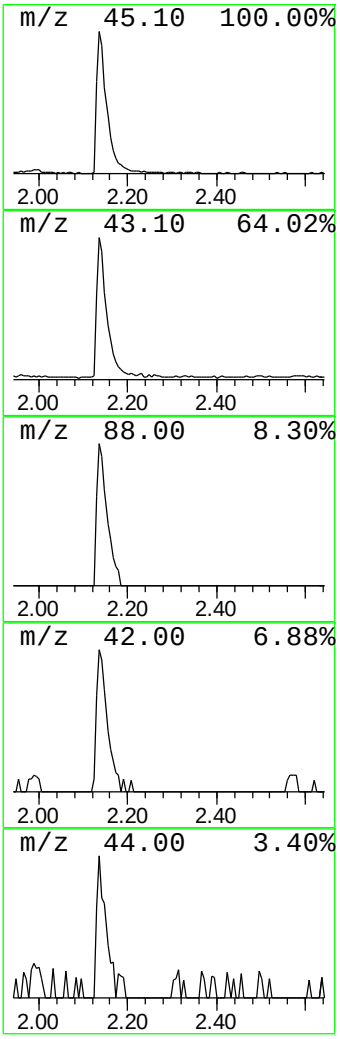
Peak Number 1 2-Butanone, 3-hydroxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	4.58 ng	166264	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-hydroxy-	88	C4H8O2	000513-86-0	78
2	Propane, 1-methoxy-2-methyl-	88	C5H12O	000625-44-5	56
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9
4	Ethanol, 2-(vinyloxy)-	88	C4H8O2	000764-48-7	9
5	2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9





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Operator : SJ/MA
Sample : I2701-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S39-9004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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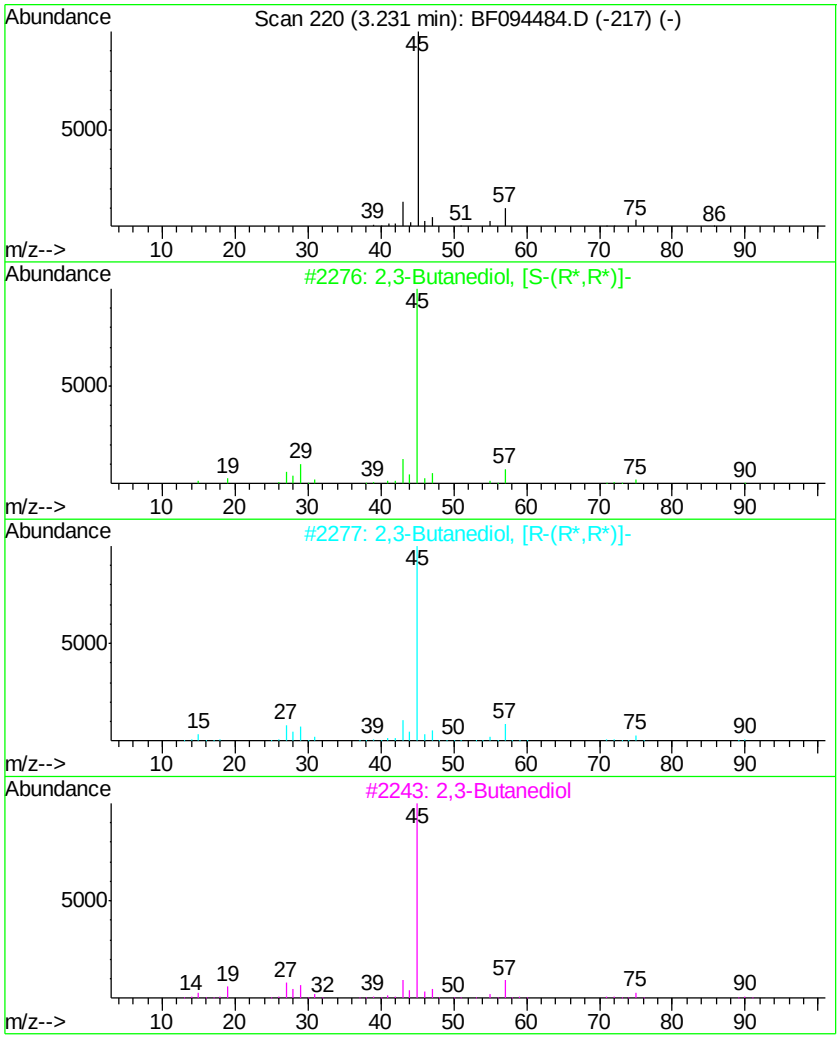
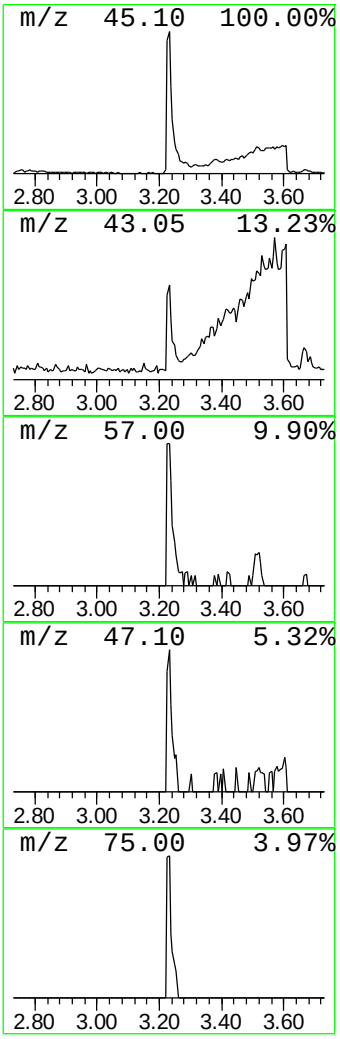
Peak Number 2 2,3-Butanediol, [S-(R*,R*)]- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	2.32 ng	84272	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanediol, [S-(R*,R*)]-	90	C4H10O2	019132-06-0	83
2	2,3-Butanediol, [R-(R*,R*)]-	90	C4H10O2	024347-58-8	64
3	2,3-Butanediol	90	C4H10O2	000513-85-9	64
4	(S)-2-Hydroxypropanoic acid	90	C3H6O3	000079-33-4	9
5	Thiirane	60	C2H4S	000420-12-2	9





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Data File : BF094484.D
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Operator : SJ/MA
Sample : I2701-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S39-9004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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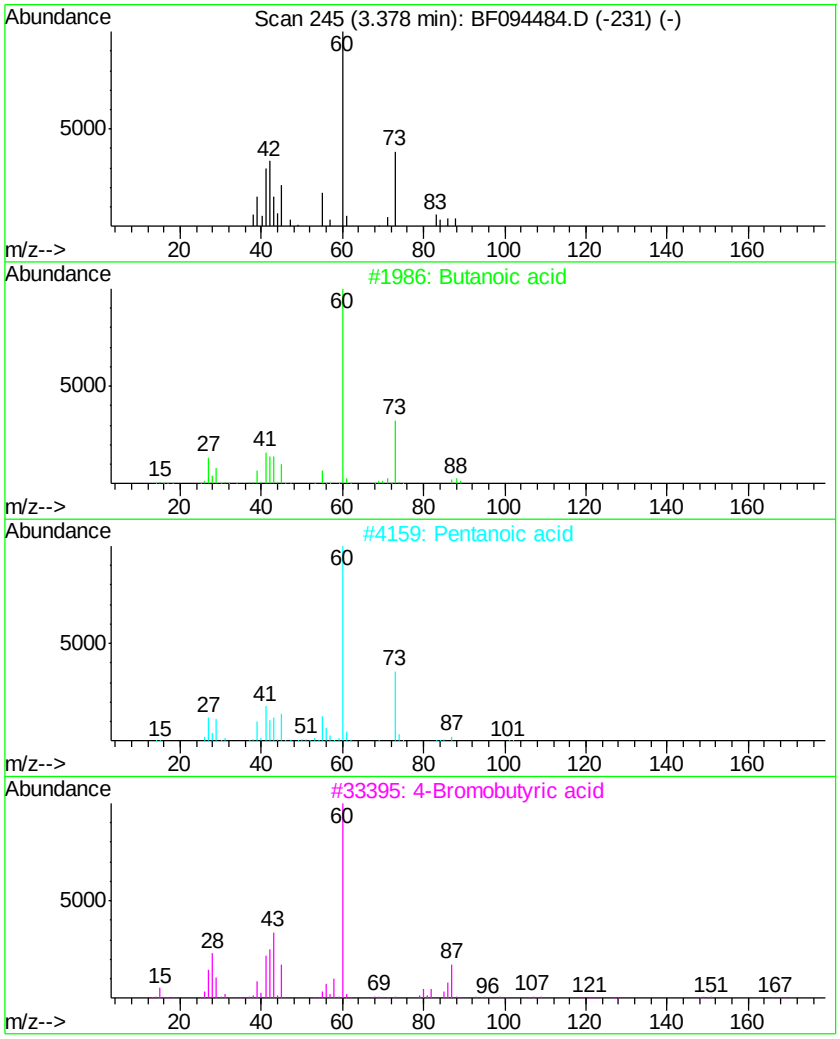
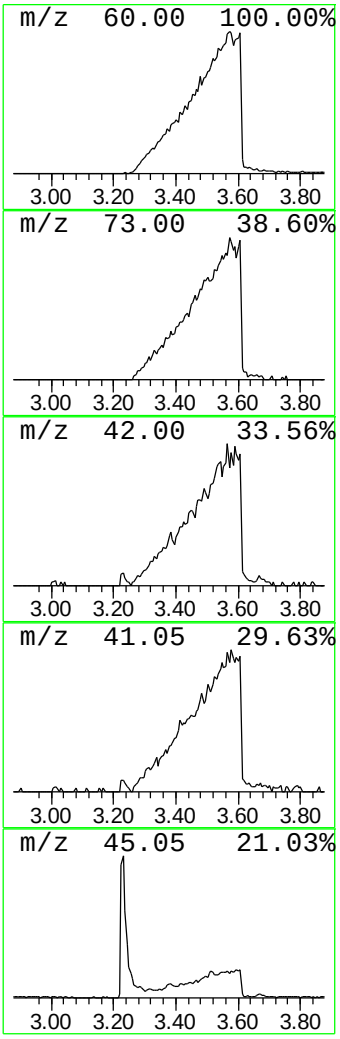
Peak Number 3 Butanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	2.95 ng	106981	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	72
2	Pentanoic acid	102	C5H10O2	000109-52-4	38
3	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
4	Propanoic acid, 3-hydroxy-	90	C3H6O3	000503-66-2	9
5	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	9





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ClientSampleId : S39-9004

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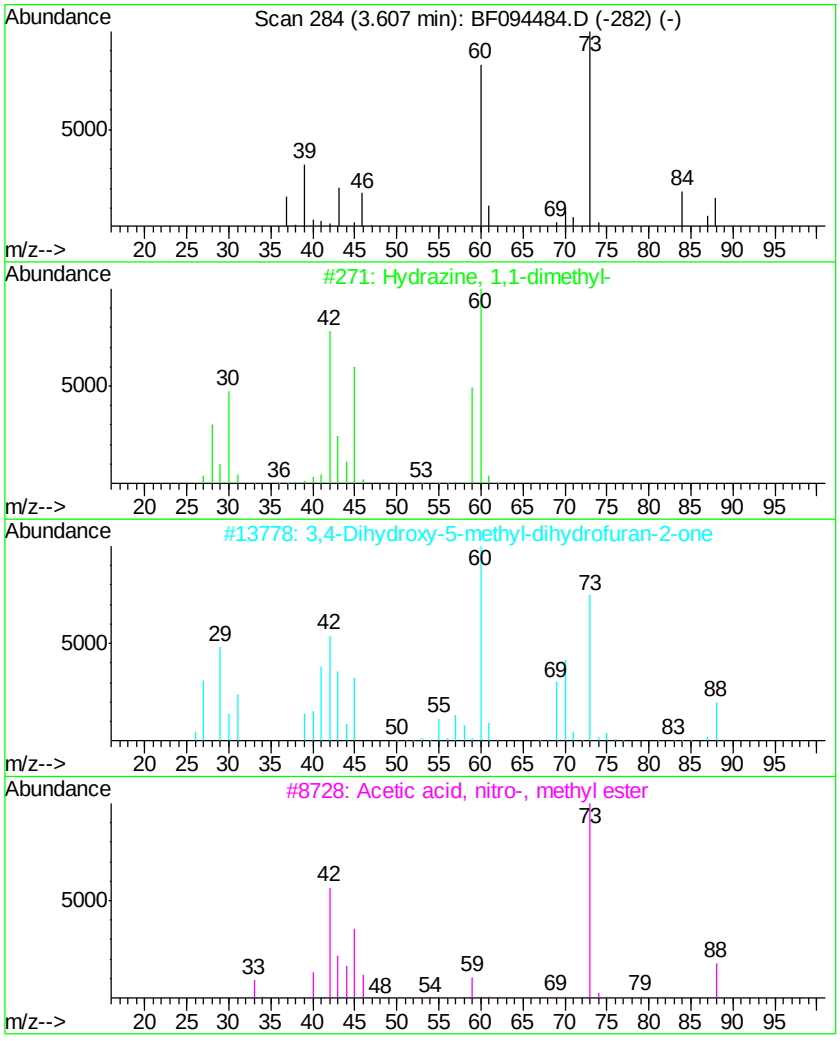
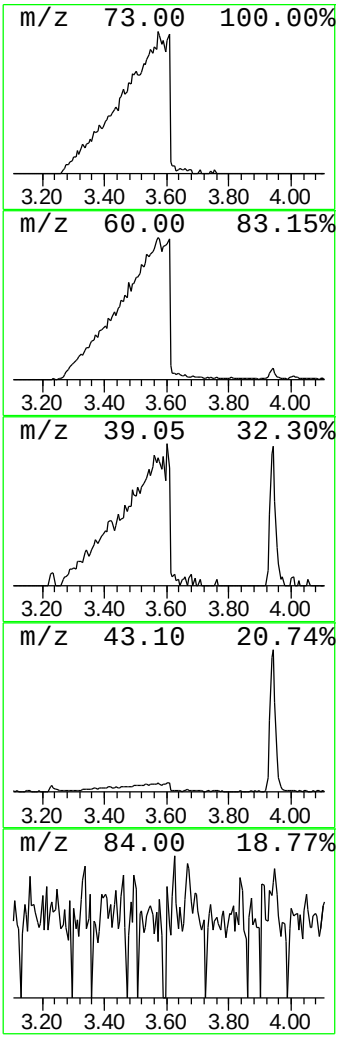
Peak Number 4 unknown3.61 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	2.29 ng	83141	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7
2	3,4-Dihydroxy-5-methyl-dihydrofu...	132	C5H8O4	1000193-83-1	4
3	Acetic acid, nitro-, methyl ester	119	C3H5NO4	002483-57-0	4
4	Pentanoic acid	102	C5H10O2	000109-52-4	4
5	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	3





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Data File : BF094484.D
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Operator : SJ/MA
Sample : I2701-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S39-9004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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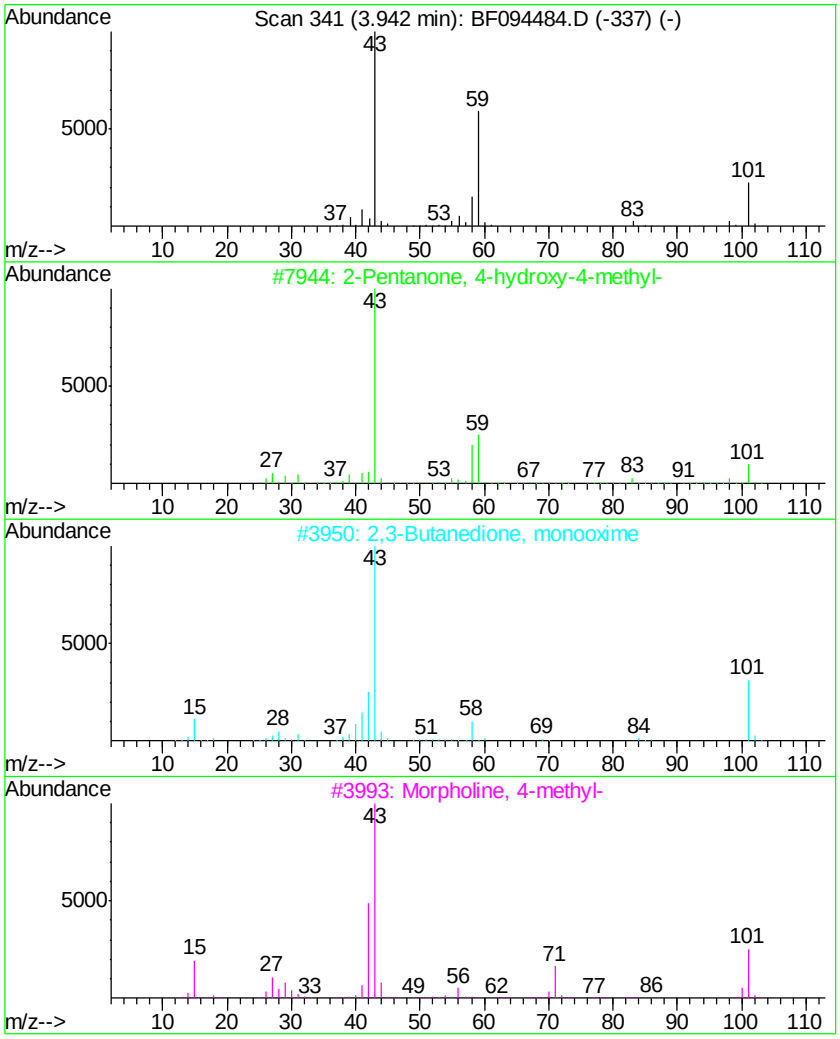
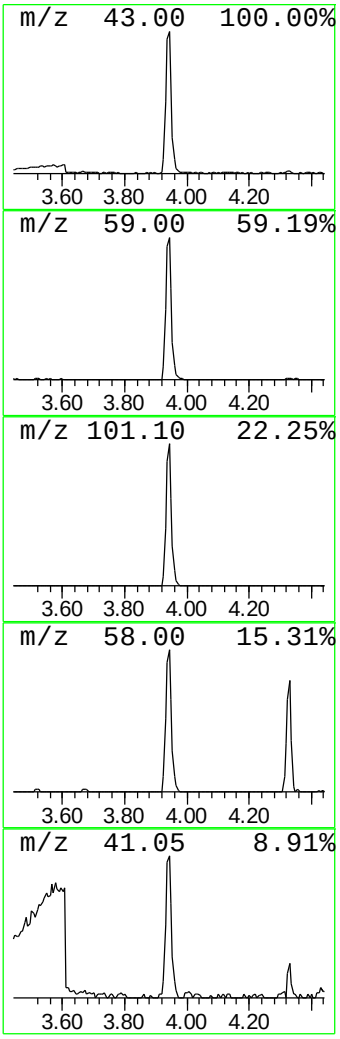
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	12.91 ng	468898	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	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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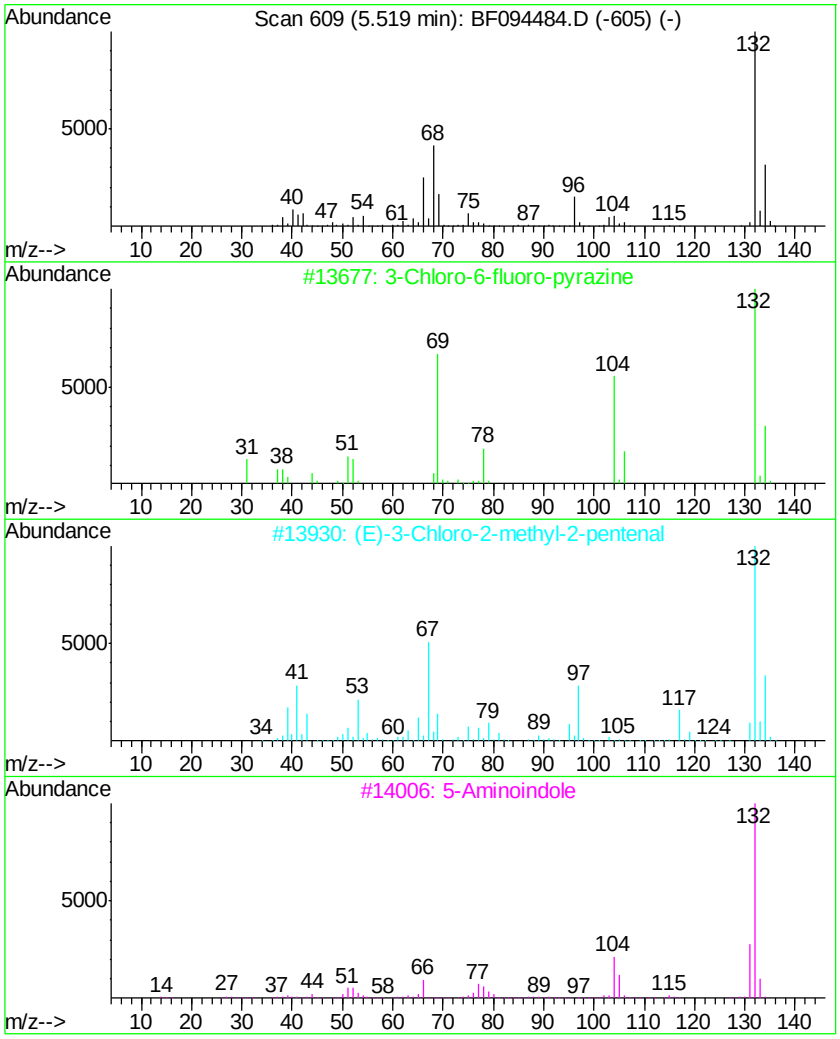
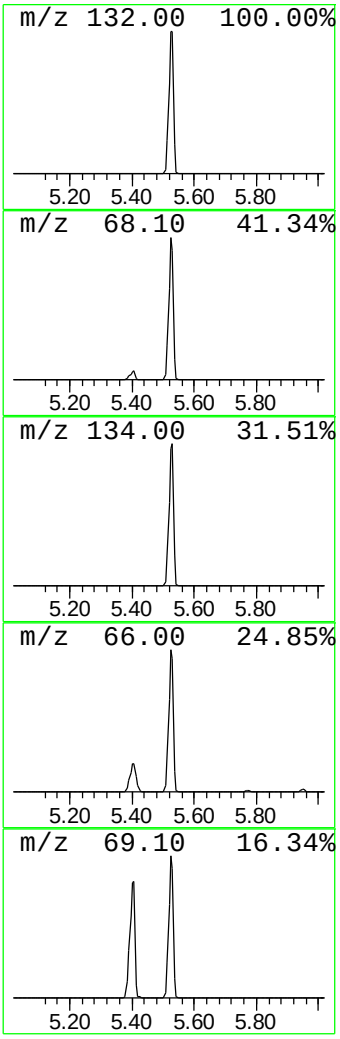
Peak Number 6 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	95.68 ng	3474040	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Butanone, 3-hyd...	2.14	4.6	ng	166264	1	5.77	726176	20.0
2,3-Butanediol, [...	3.23	2.3	ng	84272	1	5.77	726176	20.0
Butanoic acid	3.38	3.0	ng	106981	1	5.77	726176	20.0
unknown3.61	3.61	2.3	ng	83141	1	5.77	726176	20.0
2-Pentanone, 4-hy...	3.94	12.9	ng	468898	1	5.77	726176	20.0
unknown5.52	5.52	95.7	ng	3474040	1	5.77	726176	20.0