LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020817\
Data File : BF092866.D
Acq On : 8 Feb 2017 21:13
Operator : SJ/MA
Sample : I1740-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 020317-PR-E-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-BF013017.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	4.407	201	203	210	rBV	170711	234232	5.00%	0.828%
2	5.058	257	260	263	rBV	1033675	1082981	23.09%	3.828%
3	5.493	295	298	300	rBV	1083502	1052903	22.45%	3.722%
4	5.893	331	333	336	rVB	201090	171784	3.66%	0.607%
5	6.521	386	388	392	rBV2	583384	719971	15.35%	2.545%
6	6.659	398	400	403	rBV	1892065	1816140	38.73%	6.420%
7	6.899	419	421	423	rBV	729030	786179	16.77%	2.779%
8	7.047	432	434	437	rBV	2351507	3087679	65.85%	10.915%
9	7.459	467	470	473	rBV	2057061	2553752	54.46%	9.028%
10	8.179	531	533	536	rBV	1241793	1060001	22.60%	3.747%
11	9.253	624	627	630	rBV	3759504	4431464	94.50%	15.665%
12	9.928	684	686	689	rBV	1096299	1156011	24.65%	4.087%
13	10.362	717	724	726	rBV	64650	69366	1.48%	0.245%
14	10.716	753	755	758	rBV2	1315455	1530481	32.64%	5.410%
15	10.830	763	765	770	rVB	78418	94997	2.03%	0.336%
16	11.276	802	804	810	rVB	38005	64743	1.38%	0.229%
17	11.413	814	816	819	rBV	1154884	1204617	25.69%	4.258%
18	13.002	952	955	958	rBV	3355390	4689278	100.00%	16.577%
19	13.905	1032	1034	1040	rBV3	23293	57846	1.23%	0.204%
20	14.054	1044	1047	1049	rBV	1430357	1277270	27.24%	4.515%
21	15.505	1170	1174	1180	rBV	756578	1146403	24.45%	4.053%

Sum of corrected areas: 28288098

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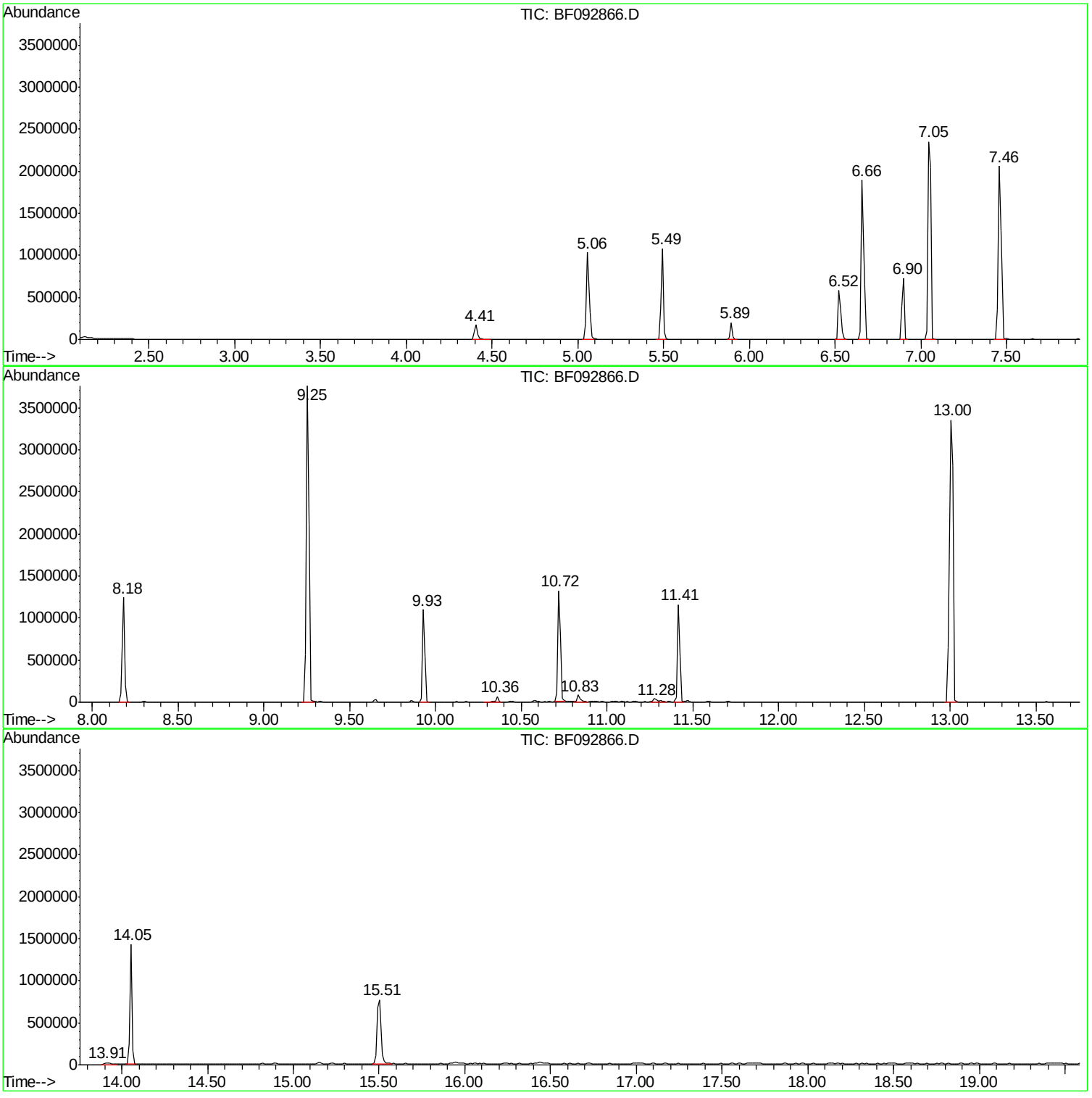
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
020317-PR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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\BF020817\
Data File : BF092866.D
Acq On : 8 Feb 2017 21:13
Operator : SJ/MA
Sample : I1740-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 020317-PR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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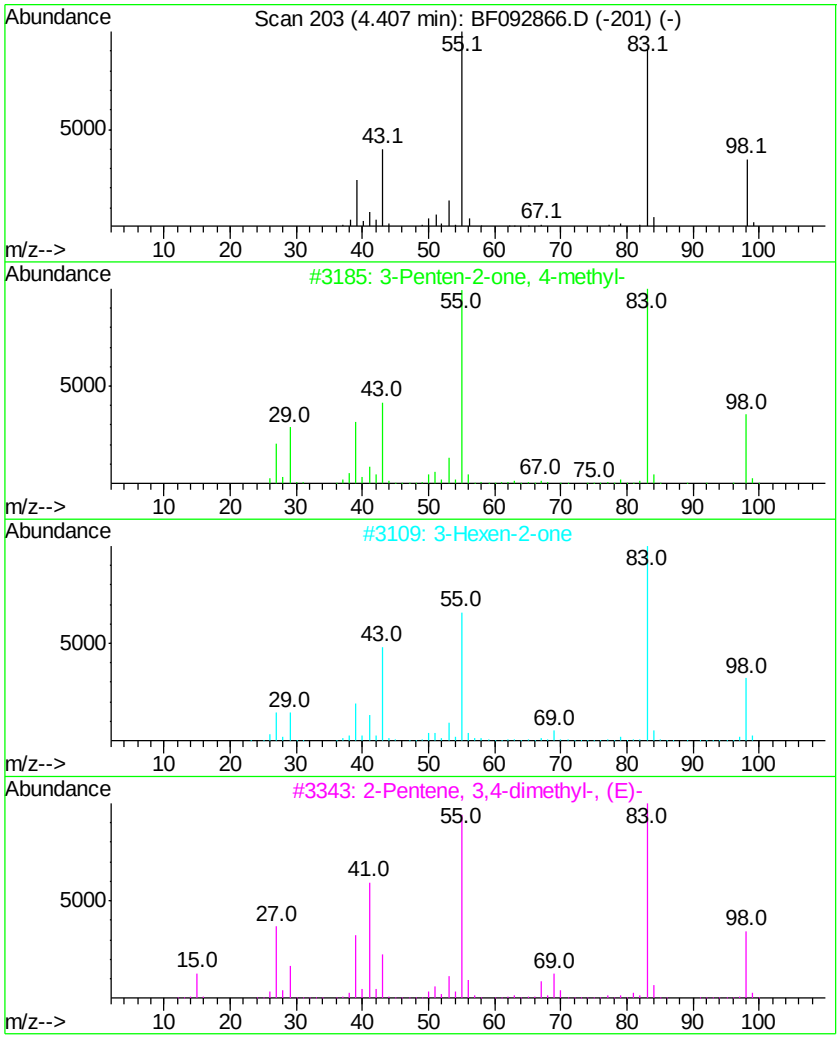
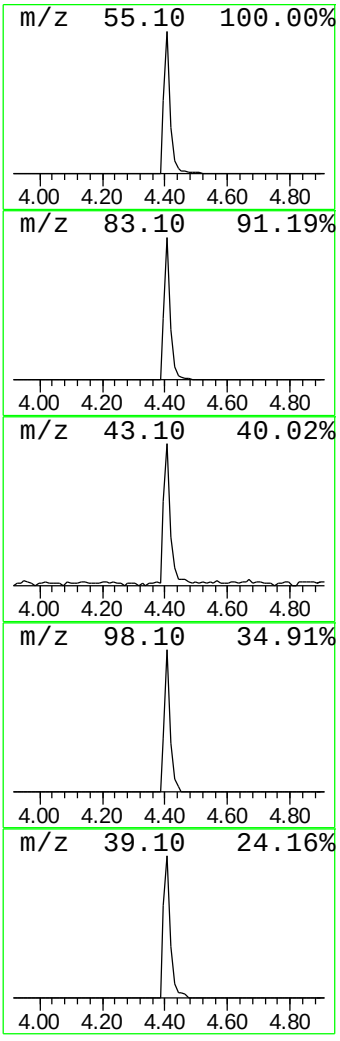
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	5.96 ng	234232	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020817\
Data File : BF092866.D
Acq On : 8 Feb 2017 21:13
Operator : SJ/MA
Sample : I1740-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 020317-PR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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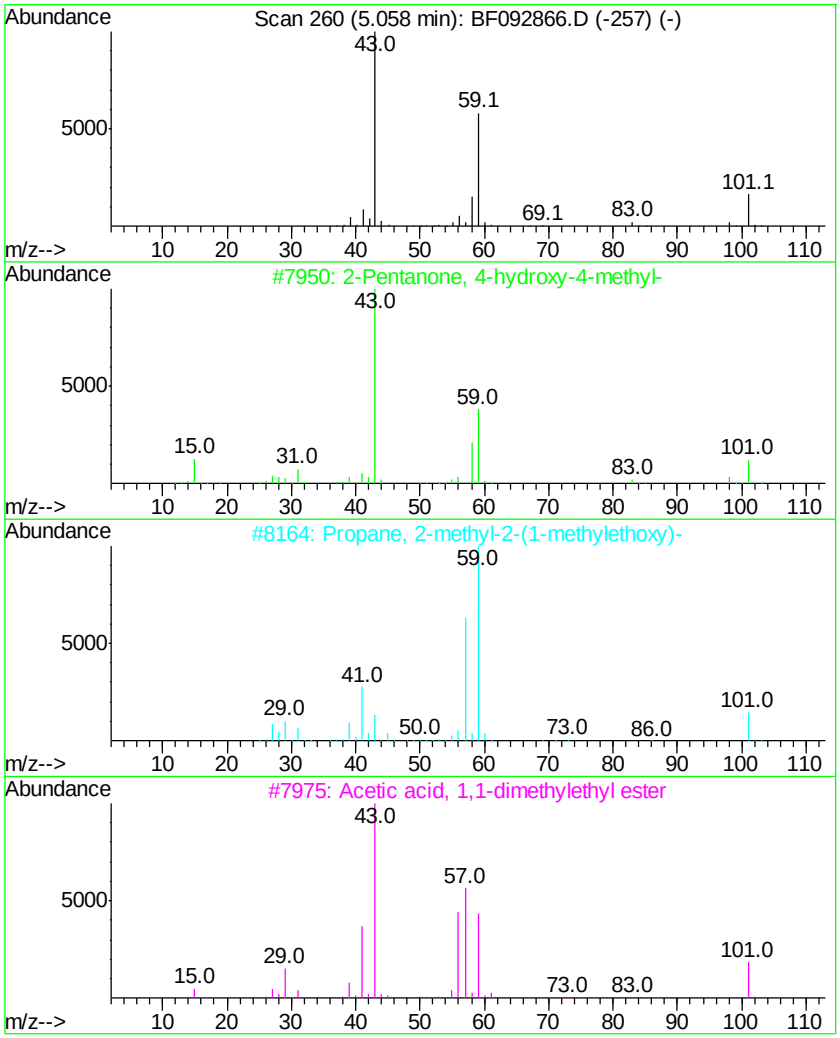
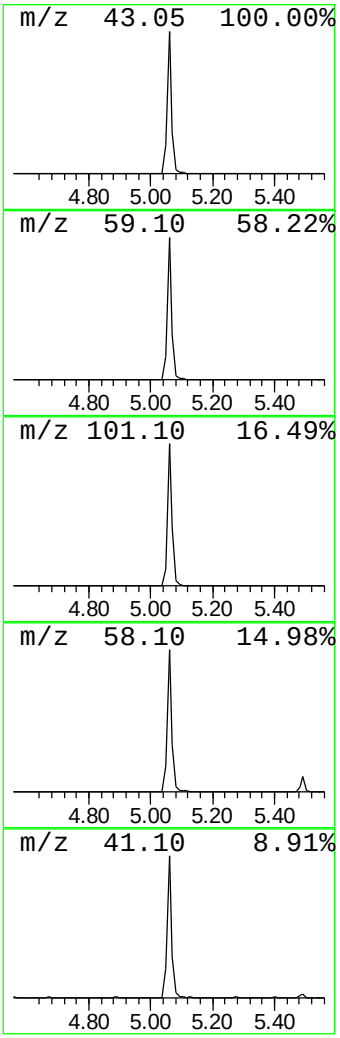
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	27.55 ng	1082980	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





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Acq On : 8 Feb 2017 21:13
Operator : SJ/MA
Sample : I1740-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 020317-PR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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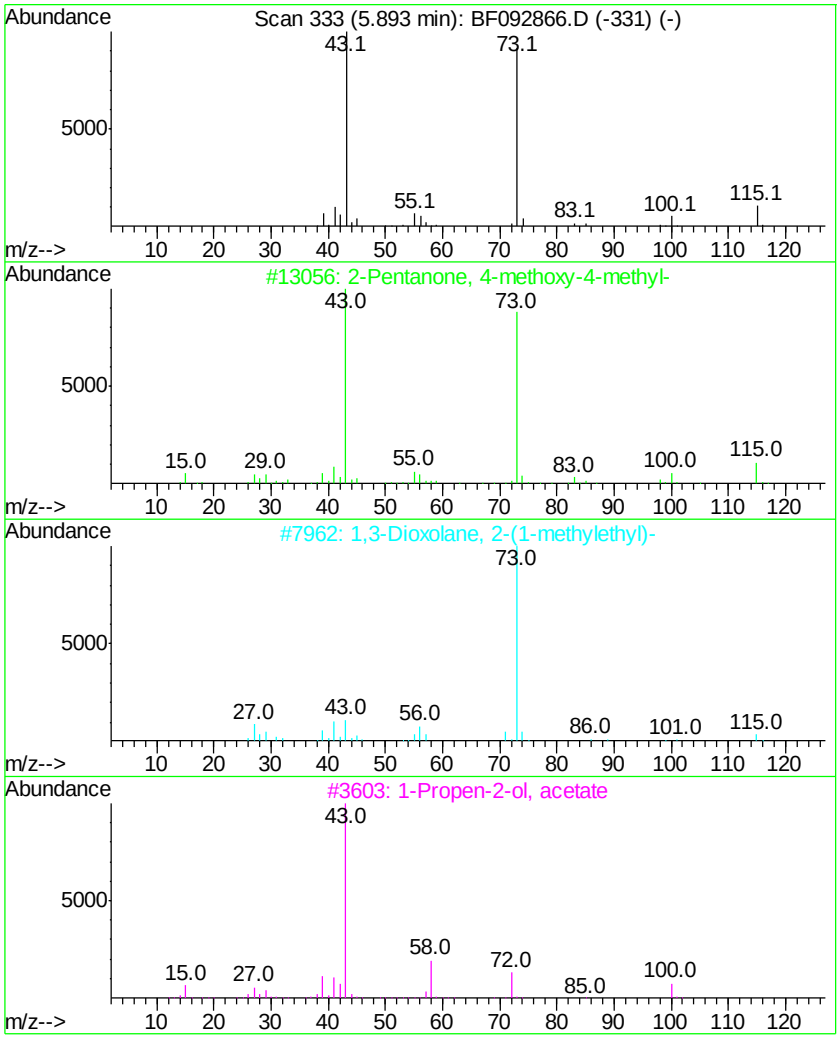
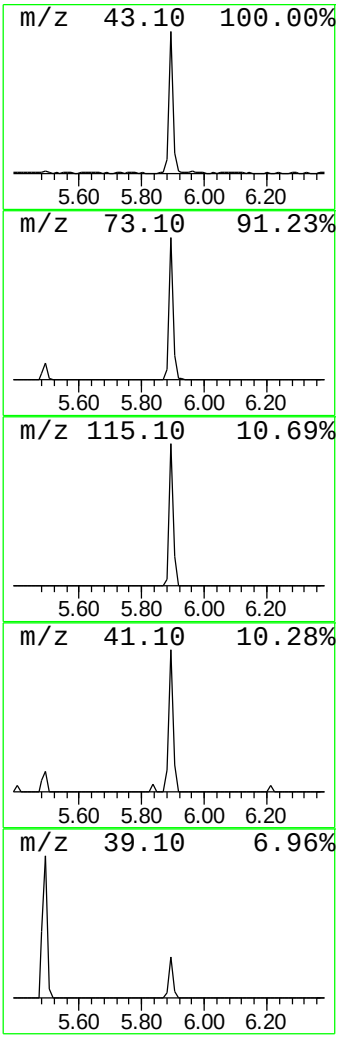
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.37 ng	171784	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Heptane	100	C7H16	000142-82-5	9





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Acq On : 8 Feb 2017 21:13
Operator : SJ/MA
Sample : I1740-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 020317-PR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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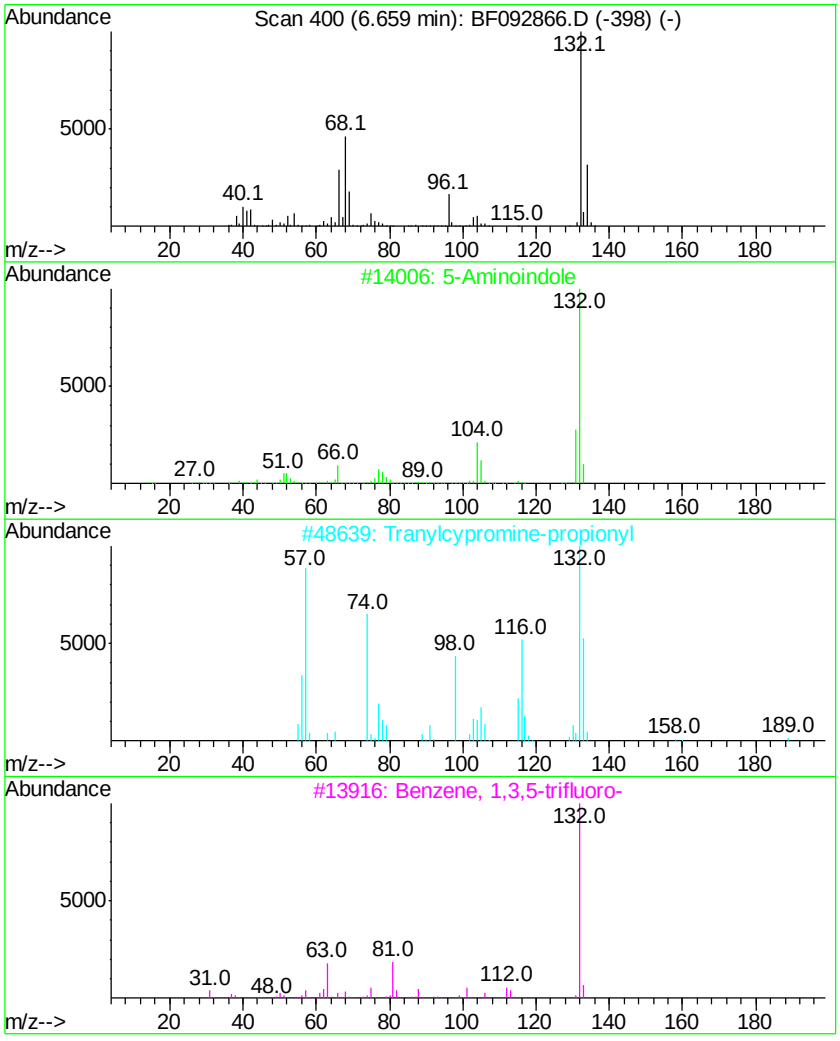
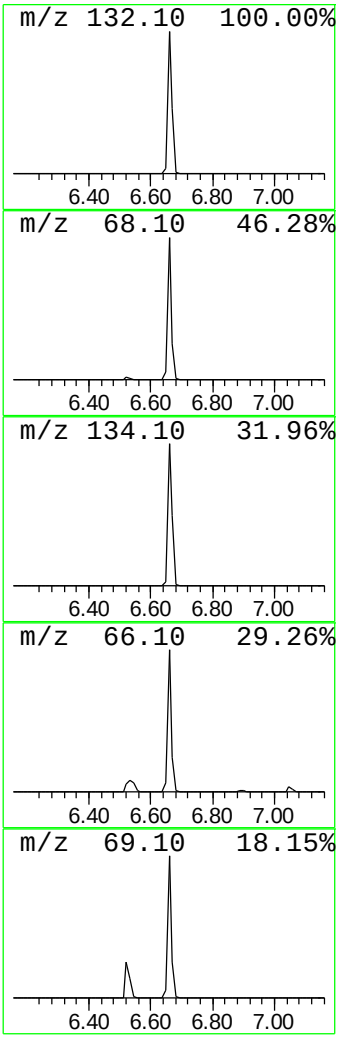
Peak Number 4 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	46.20 ng	1816140	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Tentatively Identified Compound (LSC) summary

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Acq On : 8 Feb 2017 21:13
Operator : SJ/MA
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Misc :
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Instrument : BNA_F
ClientSampleId : 020317-PR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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
3-Penten-2-one, 4...	4.41	6.0	ng	234232	1	6.90	786179	20.0
2-Pentanone, 4-hy...	5.06	27.6	ng	1082980	1	6.90	786179	20.0
2-Pentanone, 4-me...	5.89	4.4	ng	171784	1	6.90	786179	20.0
unknown6.66	6.66	46.2	ng	1816140	1	6.90	786179	20.0