LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093618.D
Acq On : 13 Mar 2017 20:12
Operator : SJ/MA
Sample : I2233-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

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-BF030717.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	2.435	45	48	60	rVB	86211	220345	3.94%	0.457%
2	4.161	196	199	201	rBV	84012	126317	2.26%	0.262%
3	4.207	201	203	217	rVV	76347	242653	4.33%	0.503%
4	4.401	217	220	228	rVB	71003	133115	2.38%	0.276%
5	4.870	259	261	278	rBV	1412044	2575612	46.00%	5.340%
6	5.316	298	300	320	rBV	4085259	5596224	99.95%	11.602%
7	5.716	333	335	346	rVB	67171	117034	2.09%	0.243%
8	6.367	390	392	400	rBV	3495202	5012682	89.52%	10.392%
9	6.481	400	402	405	rVB	4798703	4898539	87.49%	10.156%
10	6.710	419	422	429	rVB	980309	1038237	18.54%	2.152%
11	6.859	433	435	438	rBV	3783461	3996910	71.38%	8.286%
12	7.282	470	472	486	rBV	3046564	3605012	64.38%	7.474%
13	7.830	515	520	533	rBV6	14518	88516	1.58%	0.184%
14	8.002	533	535	547	rVB	1329127	1652719	29.52%	3.426%
15	8.722	596	598	605	rBV	57474	94910	1.70%	0.197%
16	8.825	605	607	613	rVB	63451	80373	1.44%	0.167%
17	9.076	627	629	632	rBV	4054121	5599199	100.00%	11.608%
18	9.762	686	689	690	rBV	1144786	1490367	26.62%	3.090%
19	9.796	690	692	698	rVB	119089	174267	3.11%	0.361%
20	10.322	733	738	741	rBV2	51380	95513	1.71%	0.198%
21	10.550	756	758	761	rBV2	2323825	2950602	52.70%	6.117%
22	11.248	817	819	825	rBV	1618189	1627535	29.07%	3.374%
23	12.836	955	958	961	rBV	4427645	4689155	83.75%	9.722%
24	13.899	1049	1051	1061	rVB	887837	1223373	21.85%	2.536%
25	15.305	1171	1174	1185	rVB	597449	905191	16.17%	1.877%

Sum of corrected areas: 48234400

LSC Report - Integrated Chromatogram

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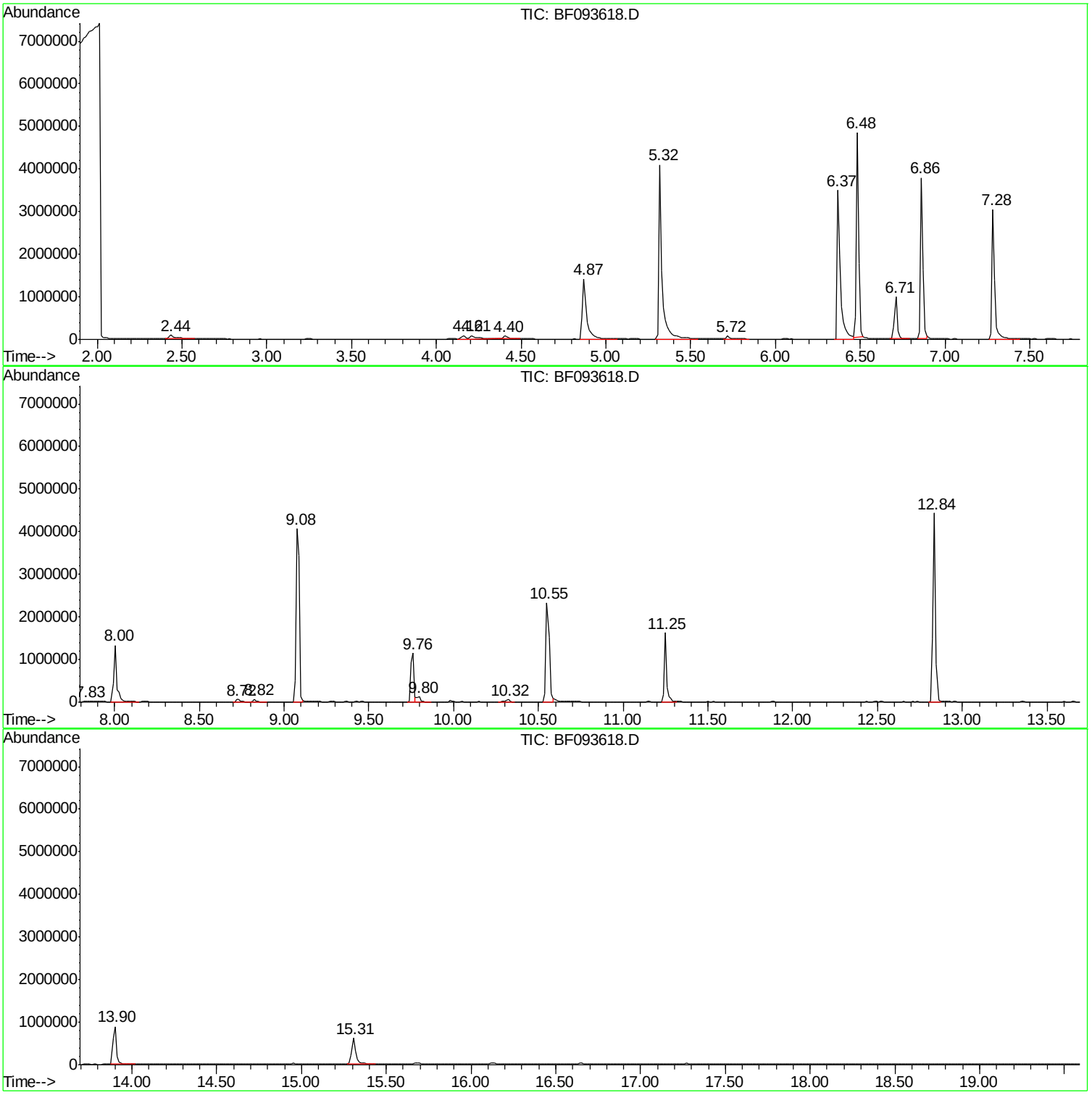
Operator : SJ/MA
Sample : I2233-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093618.D
Acq On : 13 Mar 2017 20:12
Operator : SJ/MA
Sample : I2233-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

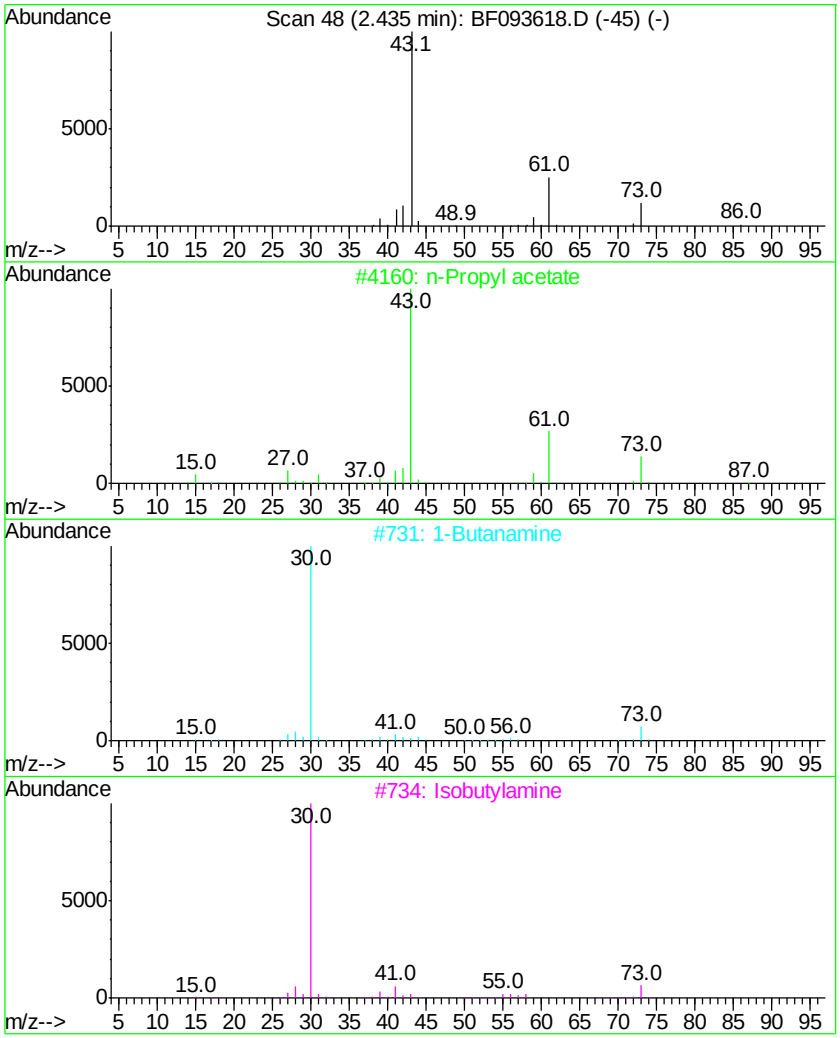
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

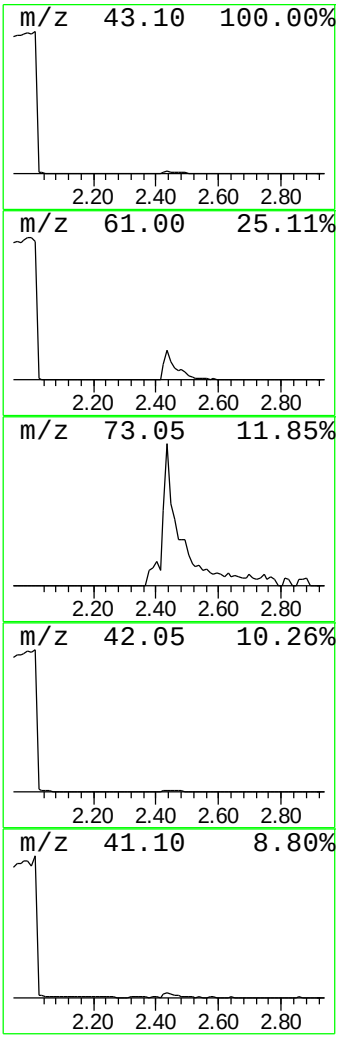
****

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	4.24 ng	220345	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	Acetohydroxamic Acid	75	C2H5NO2	000546-88-3	4
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4





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Acq On : 13 Mar 2017 20:12
Operator : SJ/MA
Sample : I2233-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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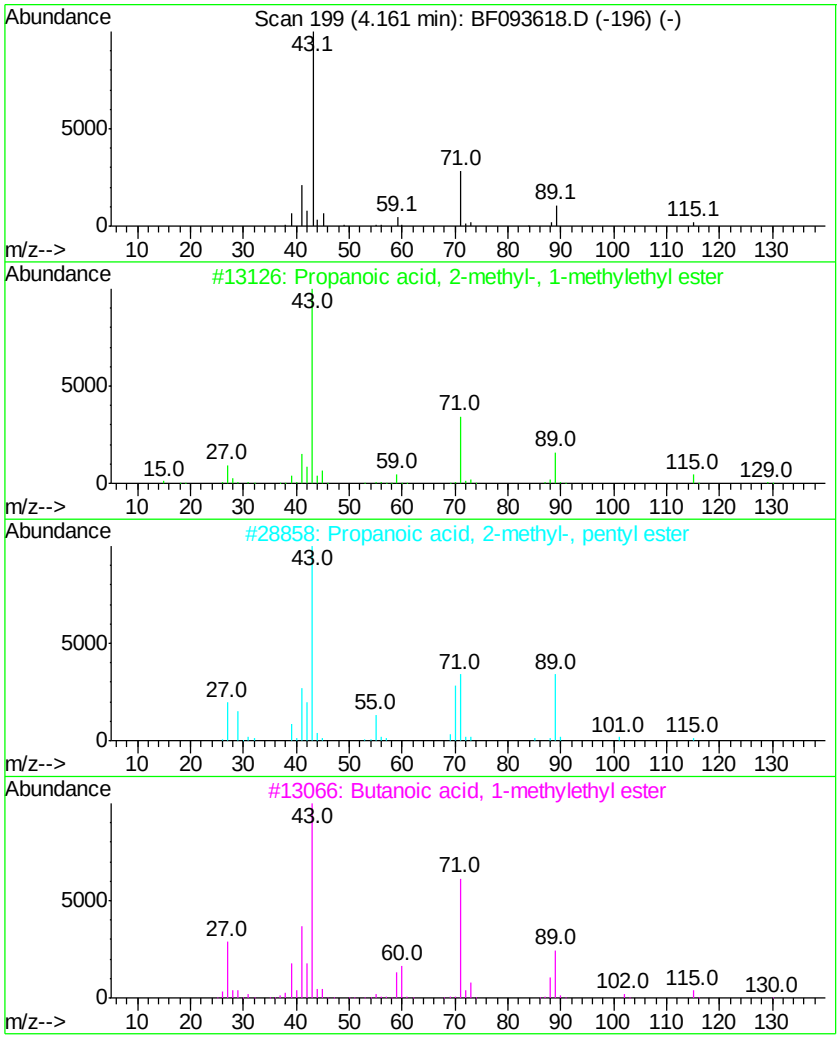
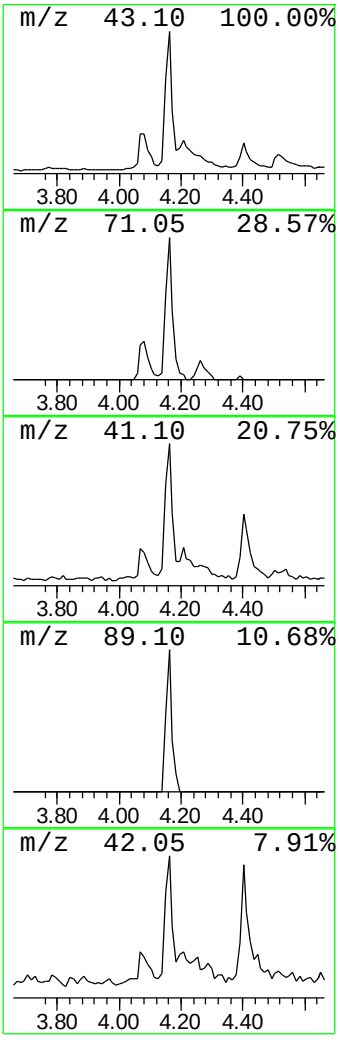
Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	2.43 ng	126317	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	36
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	33
4	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	27
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093618.D
Acq On : 13 Mar 2017 20:12
Operator : SJ/MA
Sample : I2233-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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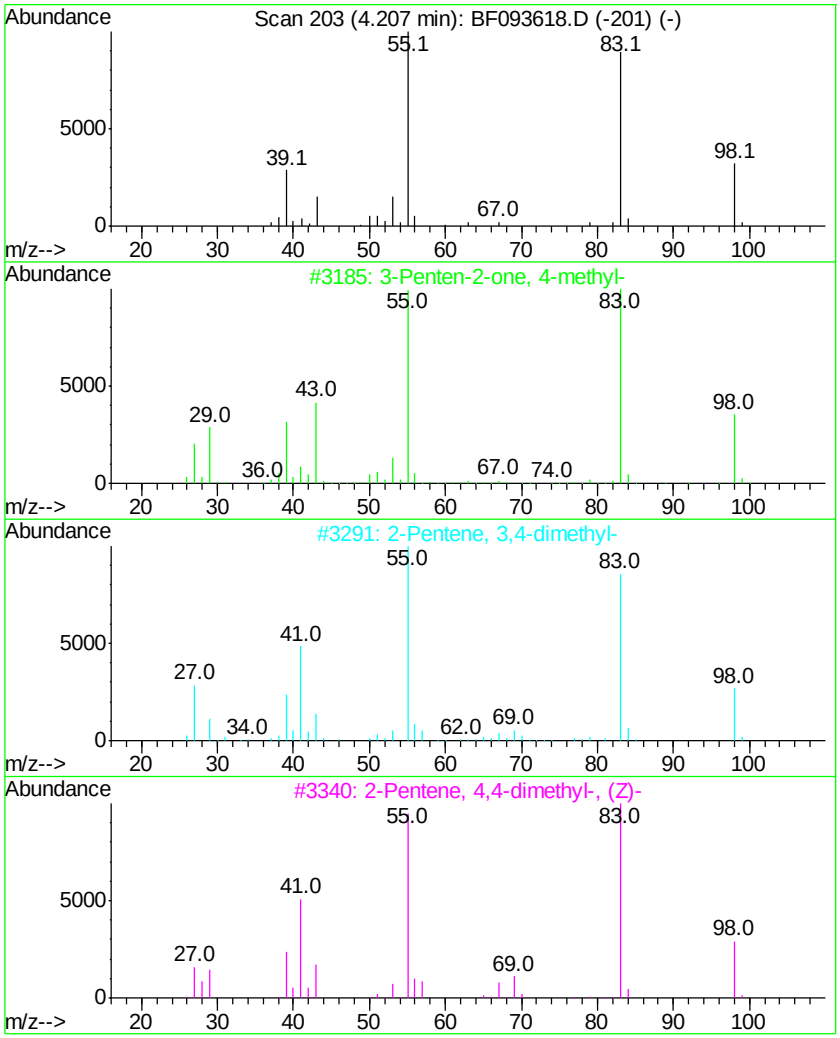
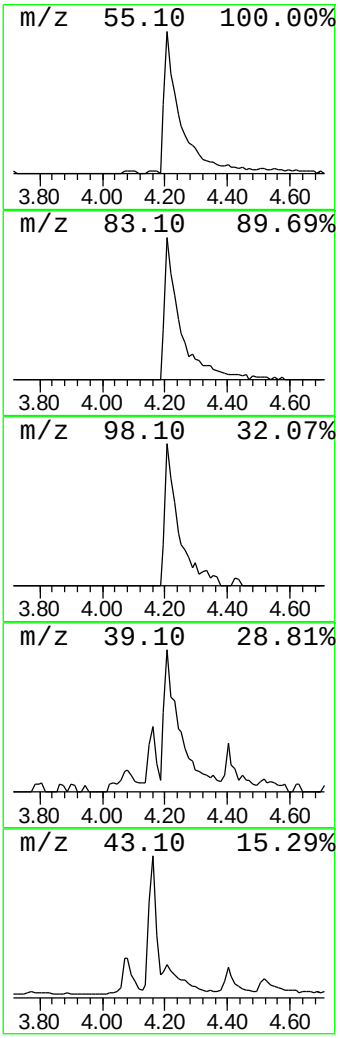
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.21	4.67 ng	242653	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80
3	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
4	3-Hexen-2-one	98	C6H10O	000763-93-9	72
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	64





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Data File : BF093618.D
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Operator : SJ/MA
Sample : I2233-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

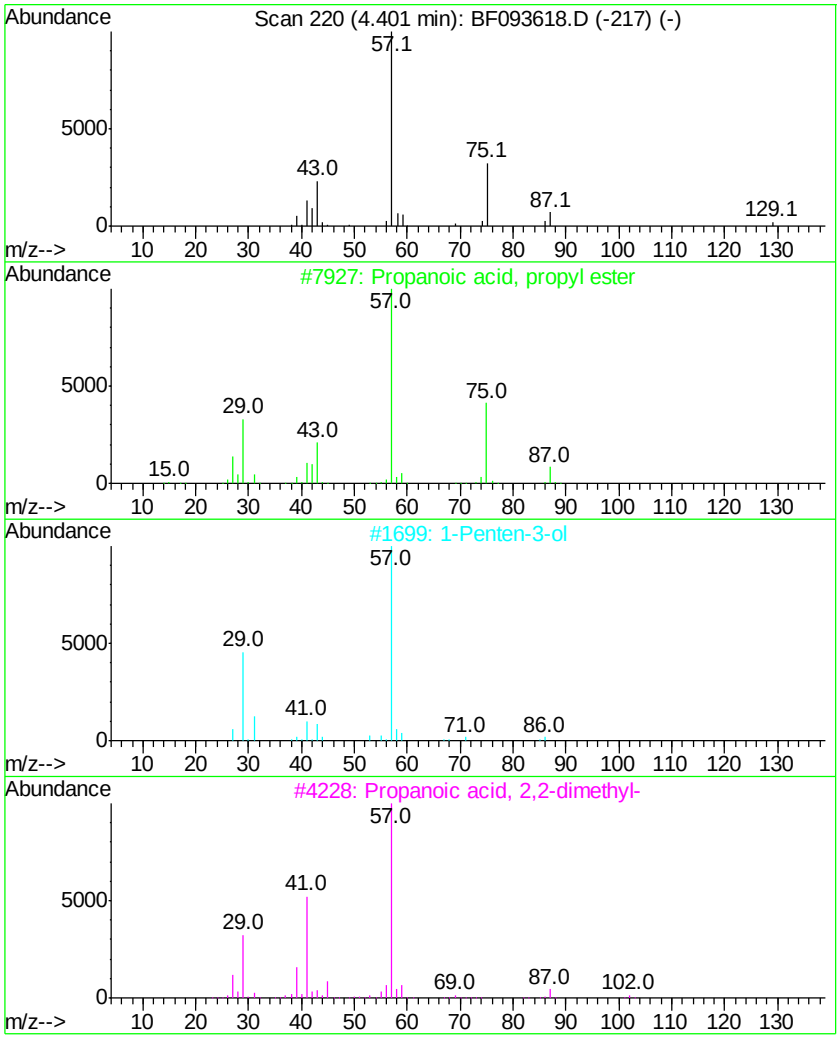
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

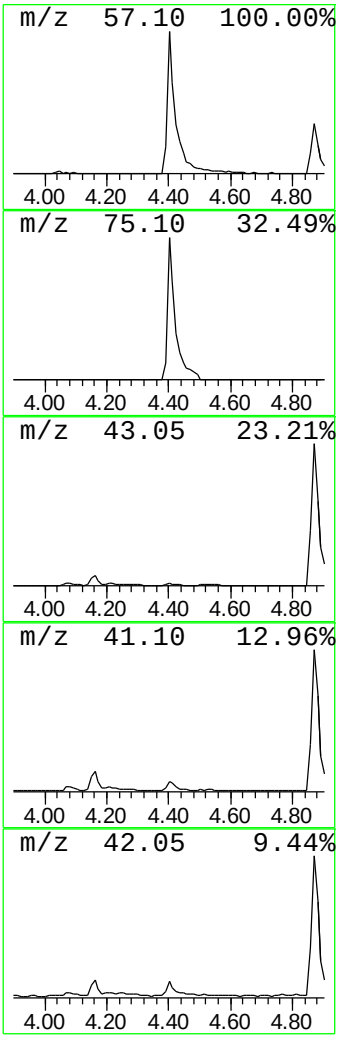
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	2.56 ng	133115	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
2	1-Penten-3-ol	86	C5H10O	000616-25-1	16
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
4	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	9
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9





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Operator : SJ/MA
Sample : I2233-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

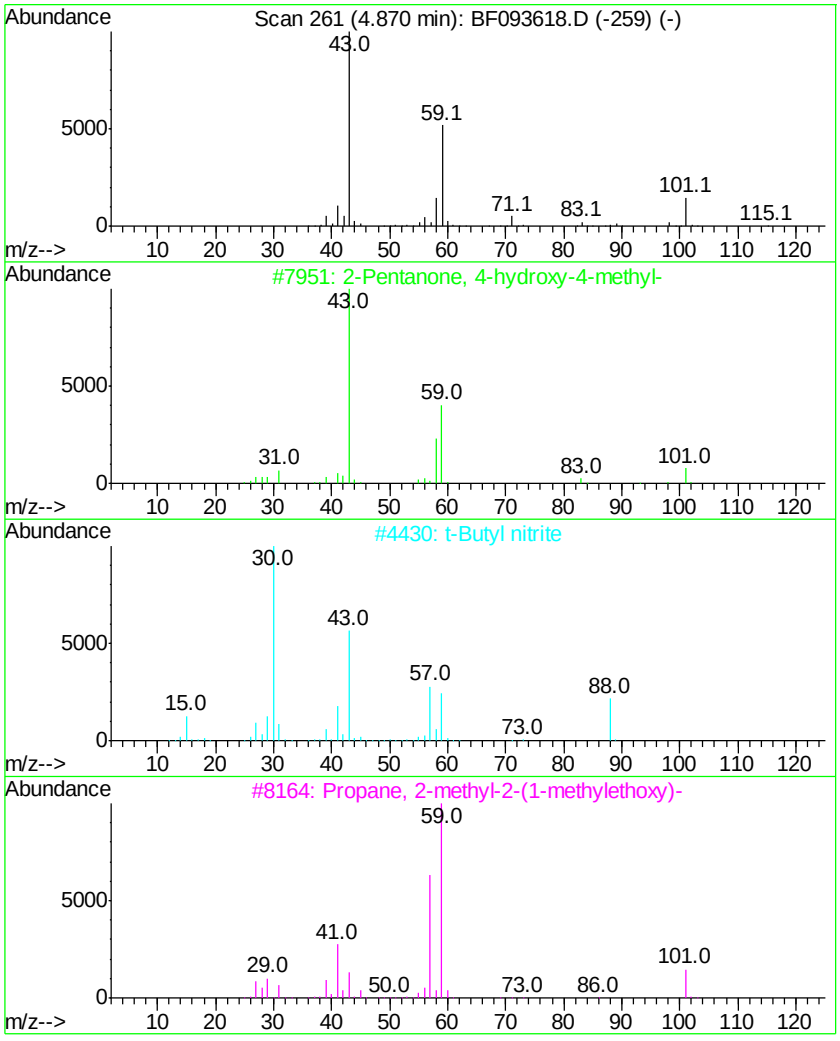
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

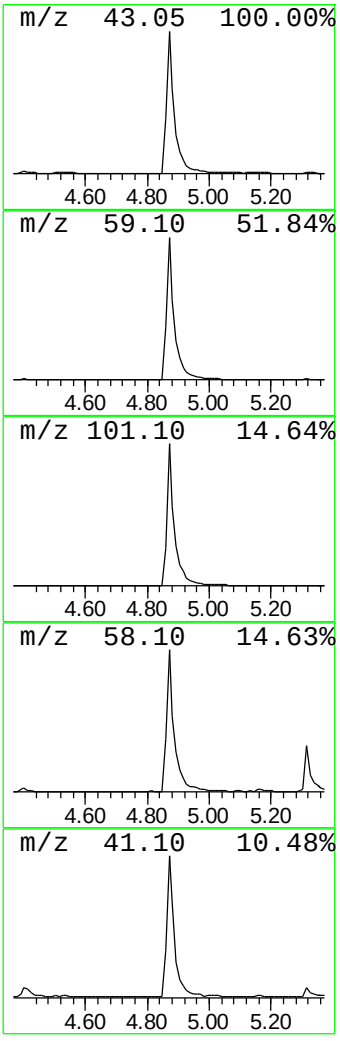
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	49.62 ng	2575610	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	45
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	25
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : FRAC-TANK-BOTTOM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

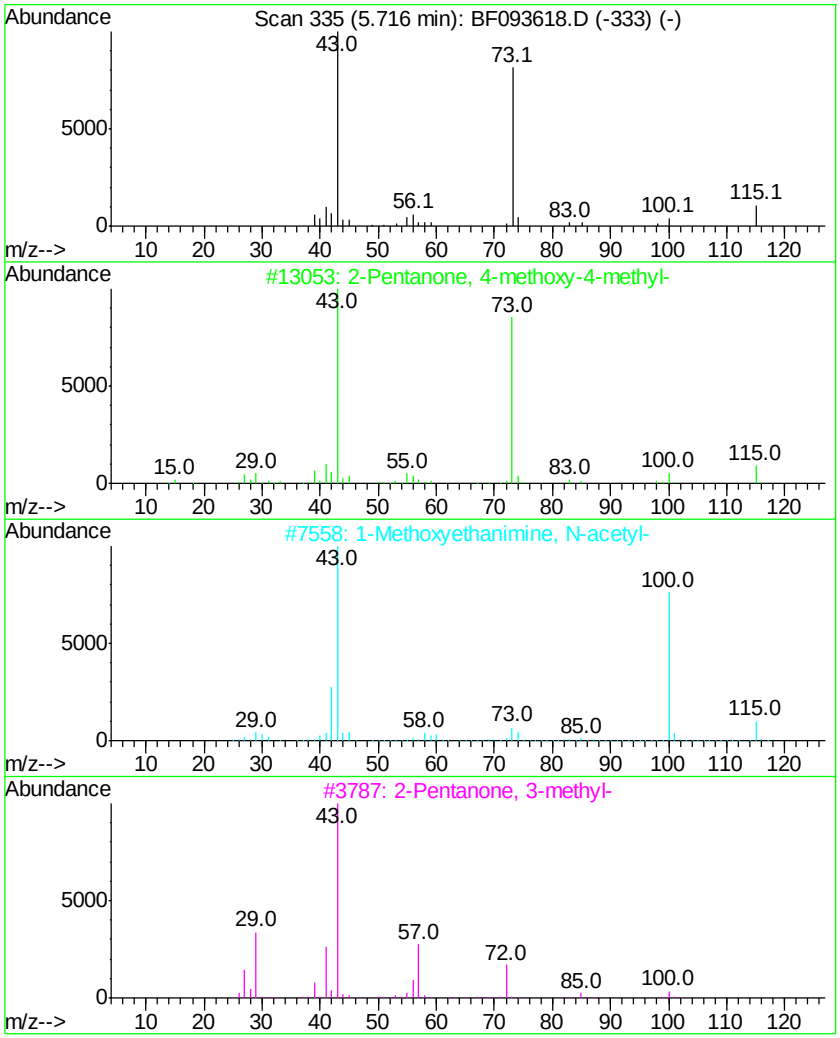
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

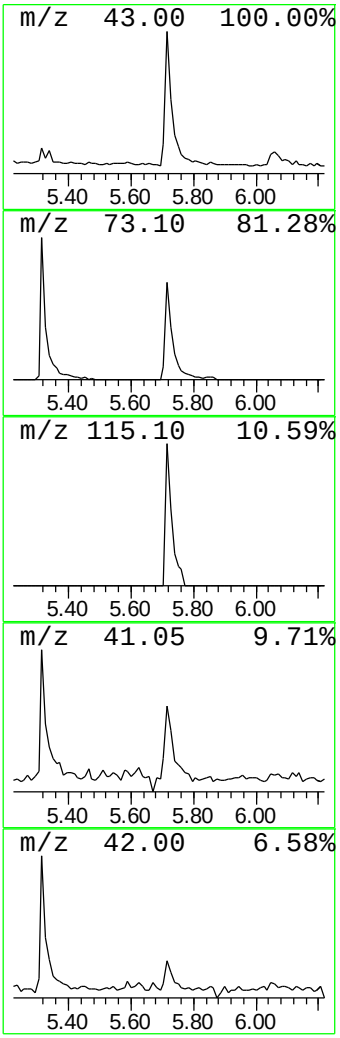
****

Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.25 ng	117034	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	47
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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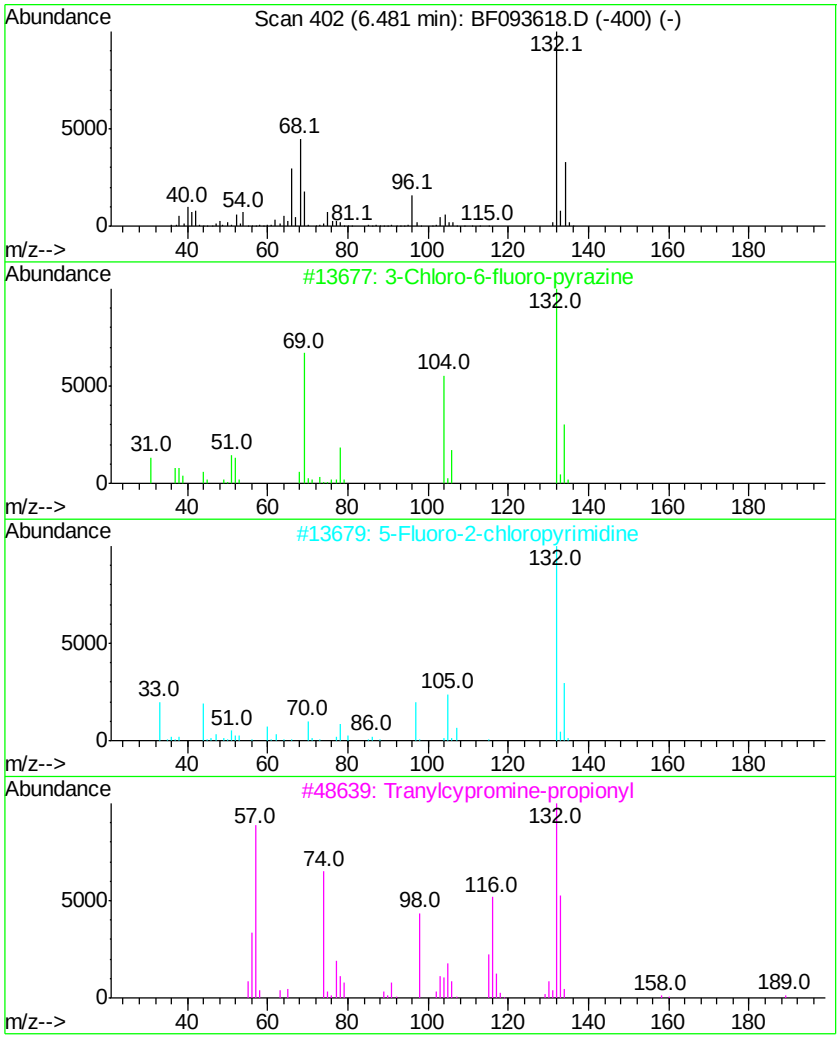
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

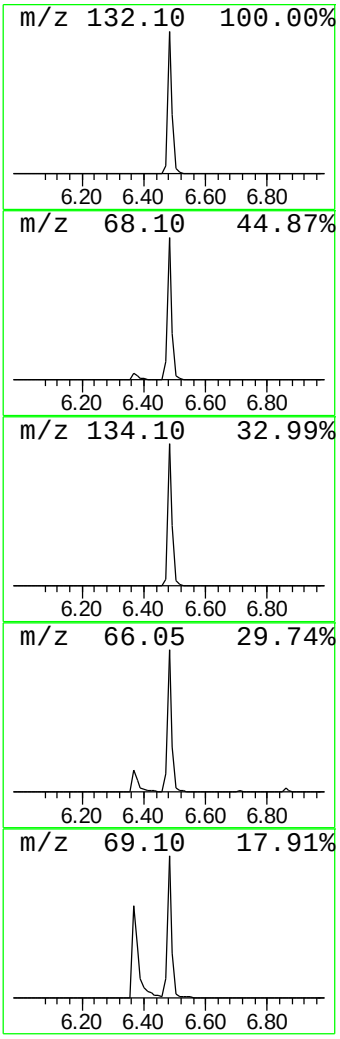
****

Peak Number 7 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	94.36 ng	4898540	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.44	4.2	ng	220345	1	6.71	1038240	20.0
Propanoic acid, 2...	4.16	2.4	ng	126317	1	6.71	1038240	20.0
3-Penten-2-one, 4...	4.21	4.7	ng	242653	1	6.71	1038240	20.0
Propanoic acid, p...	4.40	2.6	ng	133115	1	6.71	1038240	20.0
2-Pentanone, 4-hy...	4.87	49.6	ng	2575610	1	6.71	1038240	20.0
2-Pentanone, 4-me...	5.72	2.3	ng	117034	1	6.71	1038240	20.0
unknown6.48	6.48	94.4	ng	4898540	1	6.71	1038240	20.0