Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093626.D
Acq On : 14 Mar 2017 00:12
Operator : SJ/MA
Sample : PB97546BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB97546BL

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	3.144	107	110	124	rBV	24761	101663	1.79%	0.204%
2	4.161	197	199	218	rBV	887204	1592509	28.01%	3.194%
3	4.859	258	260	285	rBV	2206109	3982783	70.05%	7.989%
4	5.316	298	300	323	rBV	2964107	5685545	100.00%	11.404%
5	5.704	332	334	345	rVB	132750	198610	3.49%	0.398%
6	6.367	390	392	400	rBV	4404091	5139435	90.39%	10.309%
7	6.482	400	402	405	rVB	4594815	5052816	88.87%	10.135%
8	6.710	420	422	431	rVB	896528	1131625	19.90%	2.270%
9	6.859	433	435	438	rBV	3862819	3778768	66.46%	7.580%
10	7.282	470	472	487	rBV	2939937	3361416	59.12%	6.743%
11	8.002	532	535	547	rBV	1361646	1493988	26.28%	2.997%
12	9.076	626	629	632	rBV	3618163	5418978	95.31%	10.870%
13	9.762	686	689	691	rBV	1223900	1572928	27.67%	3.155%
14	10.551	756	758	761	rBV2	2190993	2748604	48.34%	5.513%
15	11.248	817	819	825	rBV	1663425	1620695	28.51%	3.251%
16	12.836	955	958	961	rBV	4347248	4538269	79.82%	9.103%
17	13.899	1049	1051	1062	rBV	1012561	1404204	24.70%	2.817%
18	15.305	1171	1174	1187	rBV	665976	1030839	18.13%	2.068%

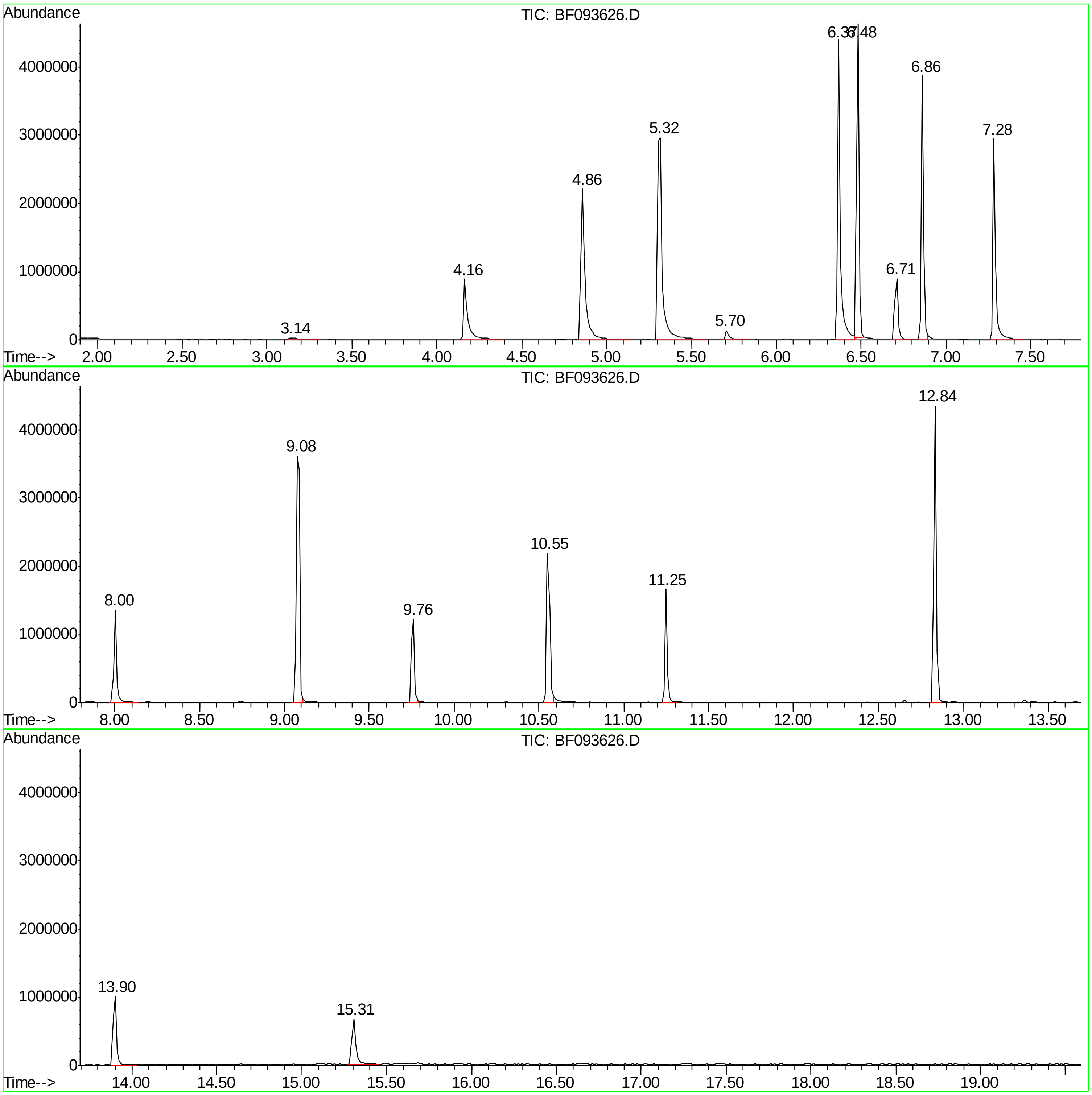
Sum of corrected areas: 49853675

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093626.D
Acq On : 14 Mar 2017 00:12
Operator : SJ/MA
Sample : PB97546BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB97546BL

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093626.D
Acq On : 14 Mar 2017 00:12
Operator : SJ/MA
Sample : PB97546BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB97546BL

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

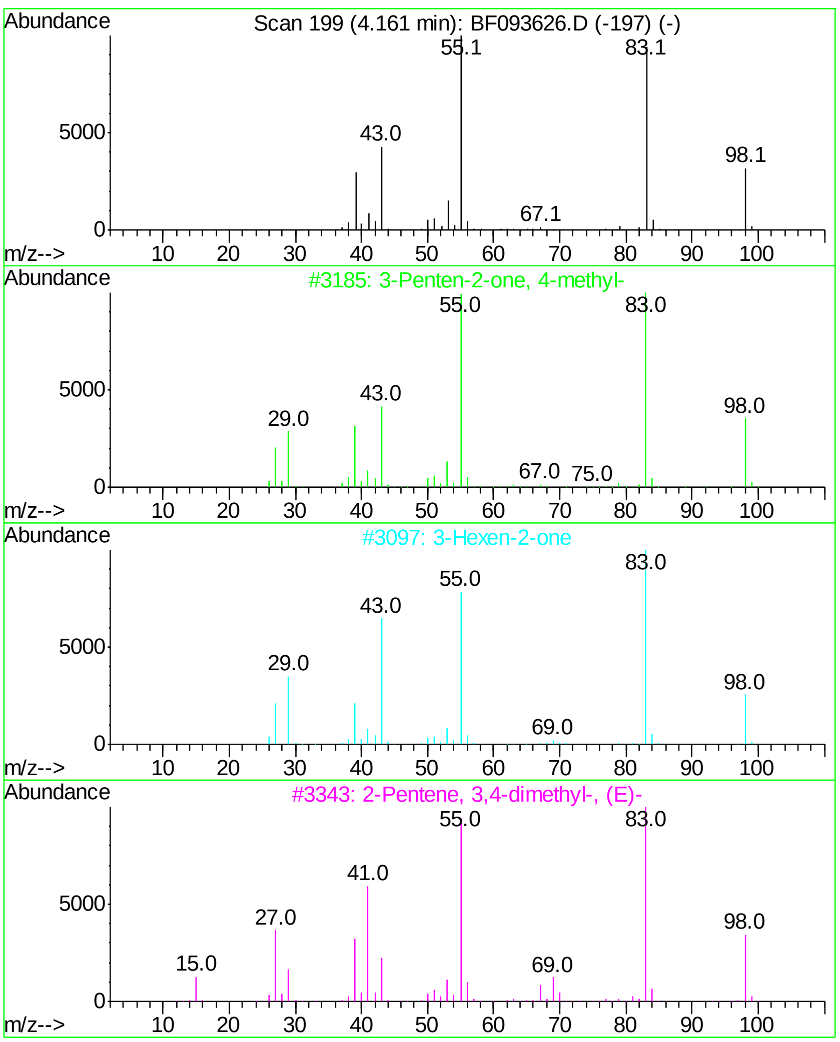
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

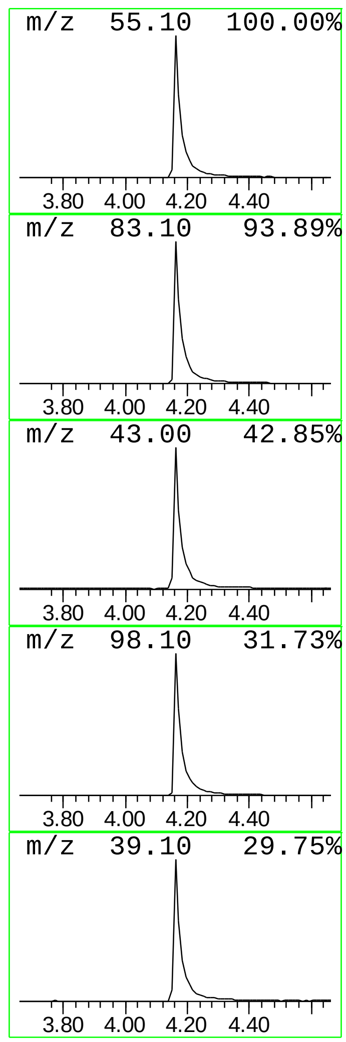
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	28.15 ng	1592510	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	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Library Search Compound Report

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Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093626.D
Acq On    : 14 Mar 2017  00:12
Operator  : SJ/MA
Sample    : PB97546BL
Misc      :
ALS Vial  : 26   Sample Multiplier: 1

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
```

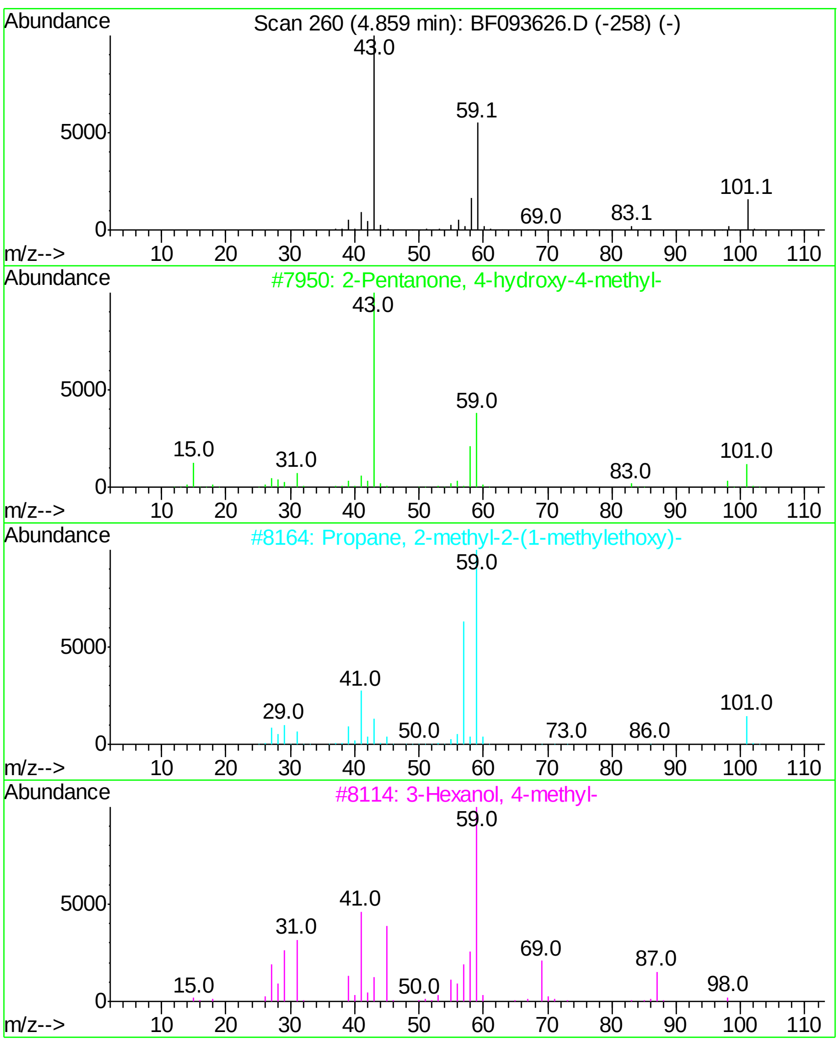
Instrument : BNA_F
ClientSampleId : PB97546BL

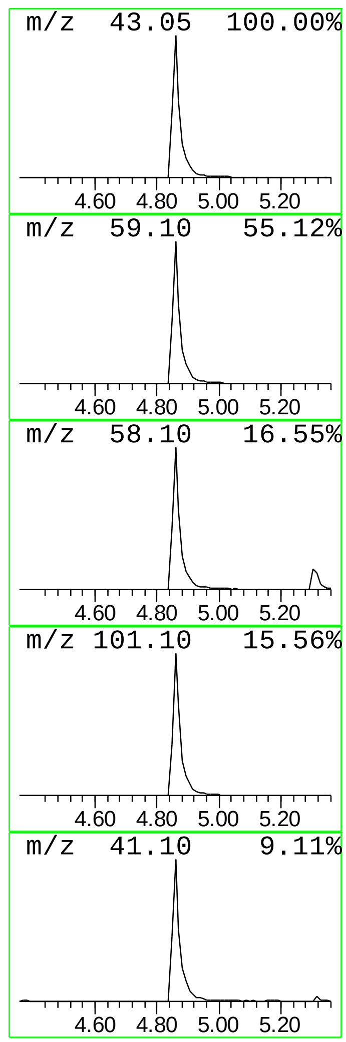
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	70.39 ng	3982780	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Library Search Compound Report

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Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093626.D
Acq On    : 14 Mar 2017  00:12
Operator  : SJ/MA
Sample    : PB97546BL
Misc      :
ALS Vial  : 26   Sample Multiplier: 1

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
```
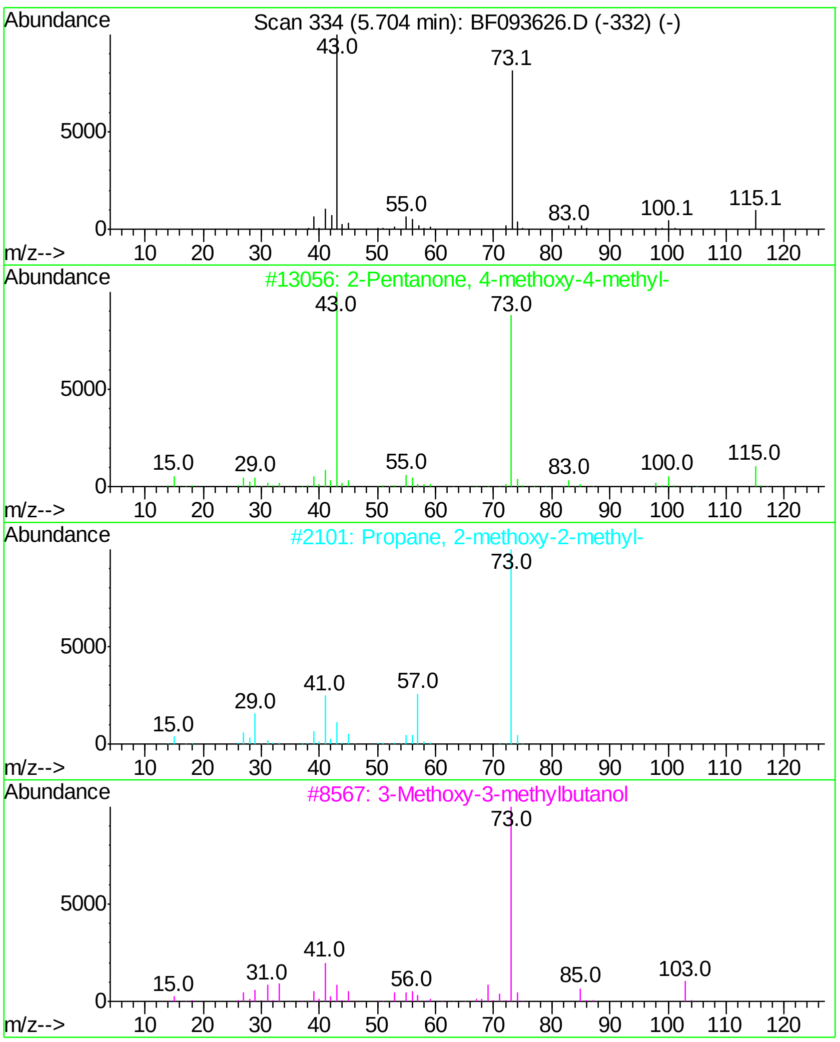
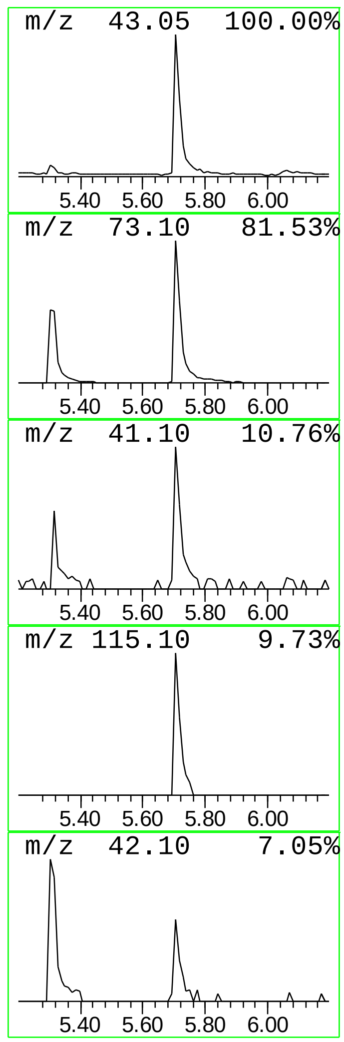

Instrument : BNA_F
ClientSampleId : PB97546BL

```
**********************************************************************
Peak Number  3  2-Pentanone, 4-methoxy-4-me...  Concentration Rank  5
```

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	3.51 ng	198610	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	$C_7H_{14}O_2$	000107-70-0	83
2	Propane, 2-methoxy-2-methyl-	88	$C_5H_{12}O$	001634-04-4	17
3	3-Methoxy-3-methylbutanol	118	$C_6H_{14}O_2$	056539-66-3	17
4	Ethanone, 1-(3-ethyloxiranyl)-	114	$C_6H_{10}O_2$	017257-81-7	10
5	2-Pentanone, 3-methyl-	100	$C_6H_{12}O$	000565-61-7	10





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Data File : BF093626.D
Acq On : 14 Mar 2017 00:12
Operator : SJ/MA
Sample : PB97546BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB97546BL

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

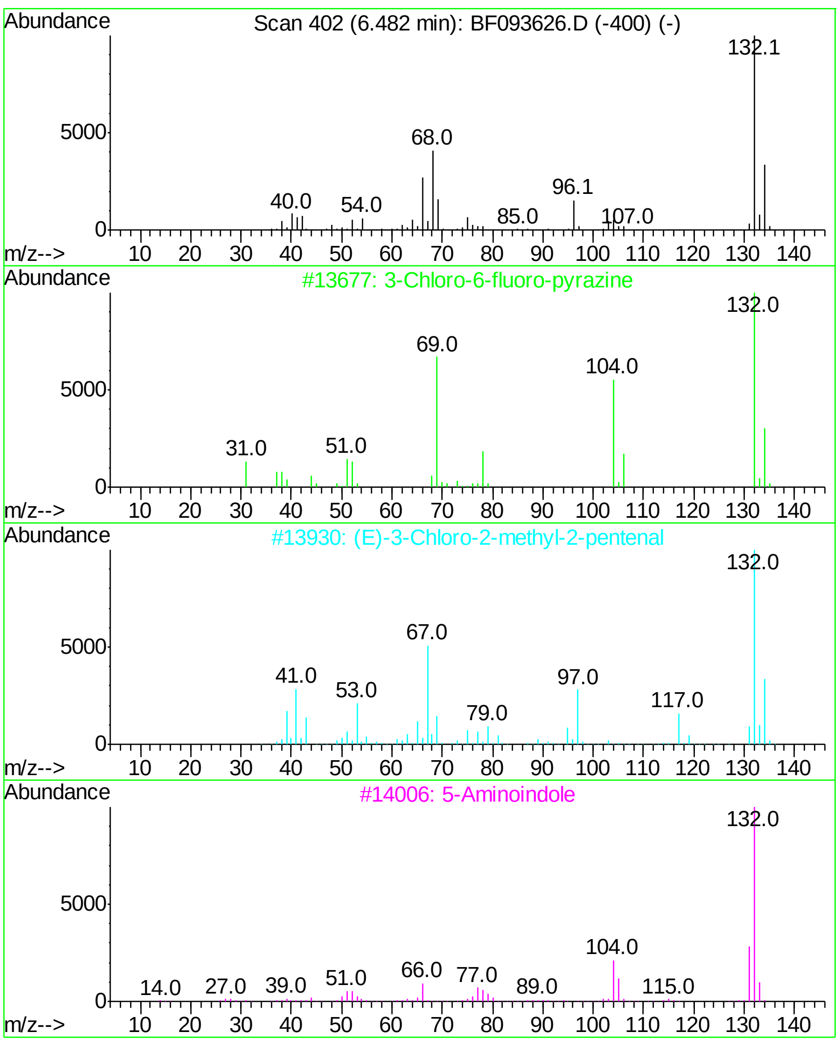
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

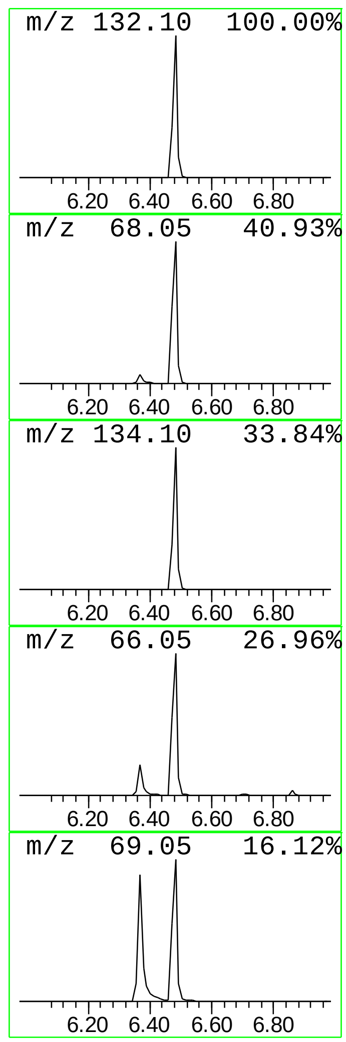
****

Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	89.30 ng	5052820	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093626.D
Acq On : 14 Mar 2017 00:12
Operator : SJ/MA
Sample : PB97546BL
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB97546BL

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.16	28.1	ng	1592510	1	6.71	1131630	20.0
2-Pentanone, 4-hy...	4.86	70.4	ng	3982780	1	6.71	1131630	20.0
2-Pentanone, 4-me...	5.70	3.5	ng	198610	1	6.71	1131630	20.0
unknown6.48	6.48	89.3	ng	5052820	1	6.71	1131630	20.0