LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009458.D
Acq On : 30 Mar 2017 19:33
Operator : SJ/MA
Sample : I2446-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-U-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_M\METHODS\8270-BM032217.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	4.375	215	219	227	rBV	102525	149419	1.66%	0.388%
2	4.969	315	320	332	rVB	651253	905252	10.06%	2.350%
3	5.422	391	397	408	rVB	880319	1242335	13.80%	3.225%
4	6.039	496	502	508	rBV	114101	167743	1.86%	0.435%
5	7.004	660	666	677	rBV	492042	768672	8.54%	1.996%
6	7.381	723	730	740	rBV	1450828	2352042	26.13%	6.106%
7	7.851	804	810	818	rVB	463086	750337	8.34%	1.948%
8	8.169	857	864	872	rBV	2163409	3399412	37.77%	8.826%
9	9.016	1000	1008	1018	rBV	1870538	3035320	33.72%	7.880%
10	10.645	1278	1285	1296	rBV	556564	942087	10.47%	2.446%
11	13.110	1696	1704	1711	rBV	4138434	6002704	66.69%	15.584%
12	13.945	1841	1846	1852	rBV2	62463	92367	1.03%	0.240%
13	14.492	1932	1939	1949	rBV2	743024	1160892	12.90%	3.014%
14	15.986	2187	2193	2201	rBV	1973992	2860473	31.78%	7.426%
15	17.239	2399	2406	2414	rBV2	984821	1431249	15.90%	3.716%
16	18.115	2548	2555	2560	rBV3	63527	94646	1.05%	0.246%
17	19.862	2846	2852	2857	rBV	7433256	9001409	100.00%	23.369%
18	21.103	3060	3063	3068	rBV5	111543	150705	1.67%	0.391%
19	21.415	3111	3116	3125	rBV	1608806	2033757	22.59%	5.280%
20	23.738	3505	3511	3522	rVB	1014354	1977157	21.96%	5.133%

Sum of corrected areas: 38517978

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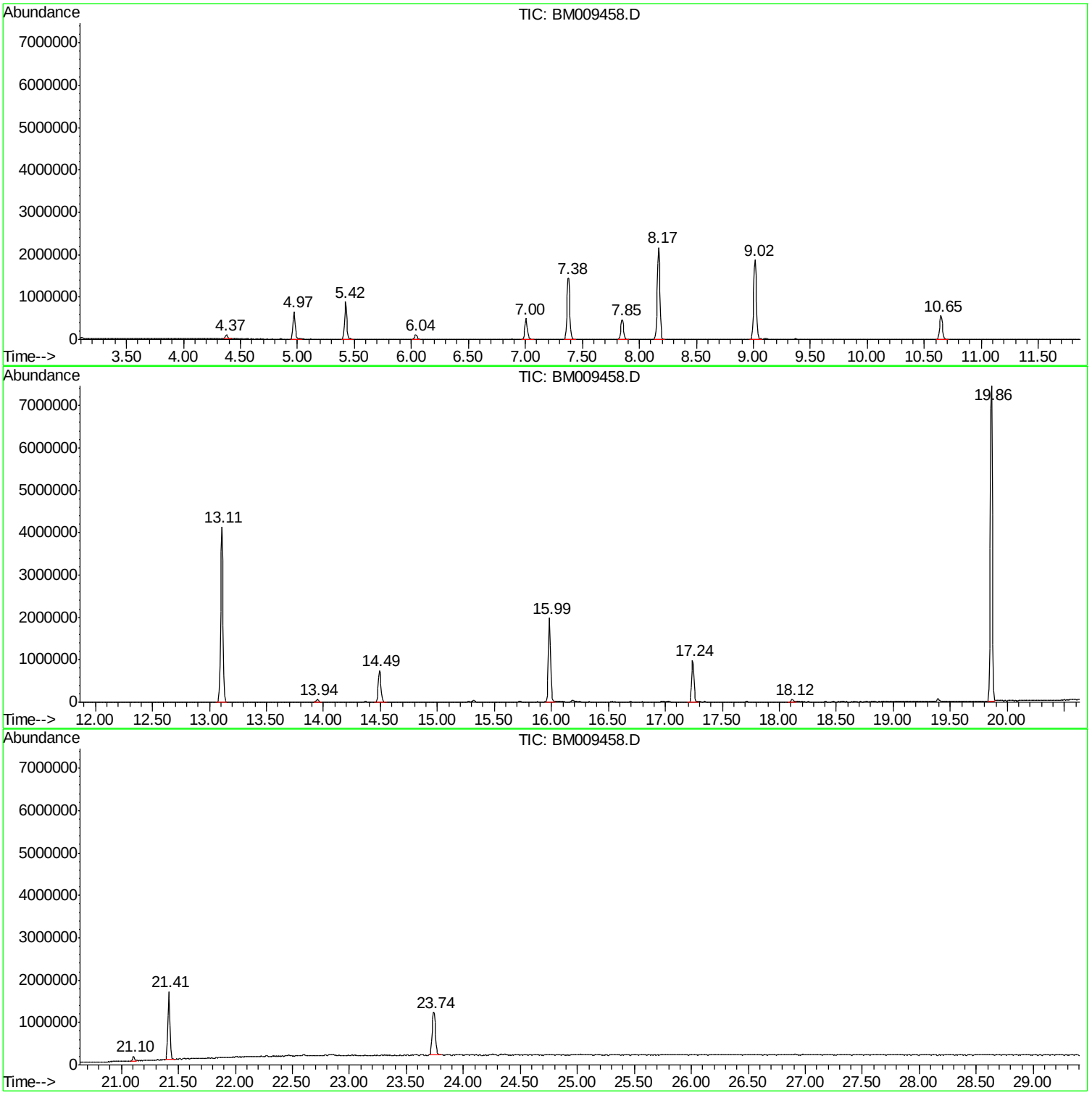
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
032817-PRRT-F-U-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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Data File : BM009458.D
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Operator : SJ/MA
Sample : I2446-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-U-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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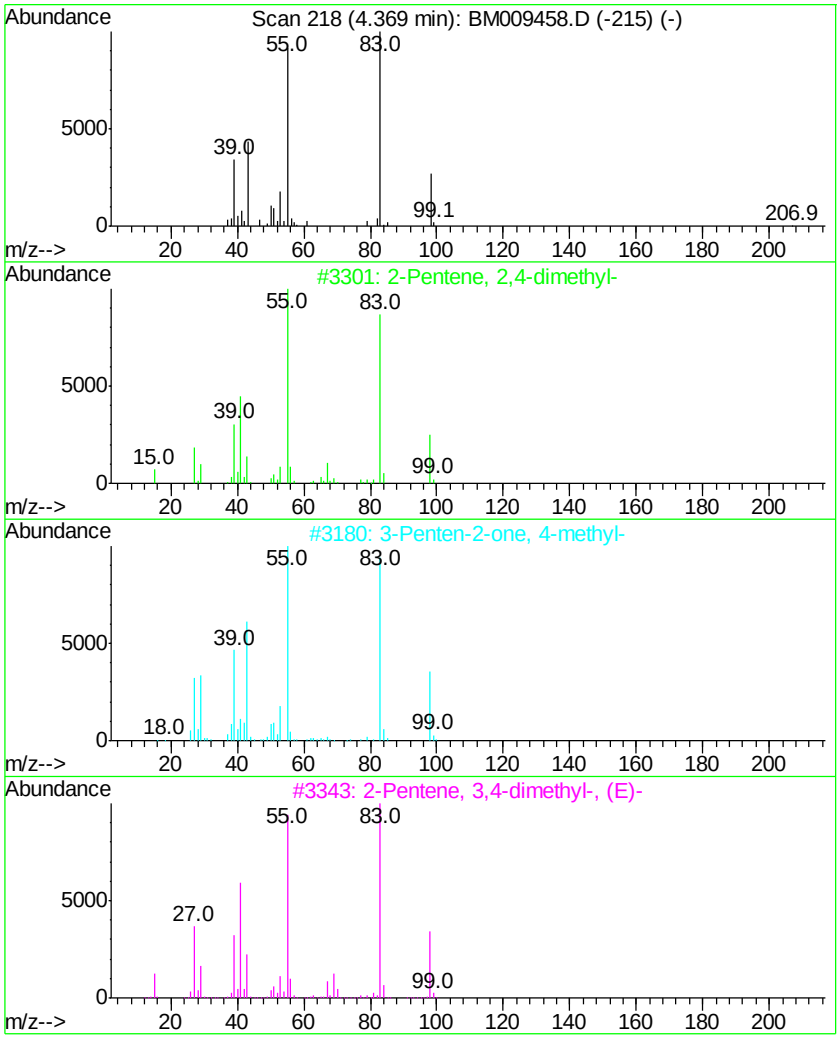
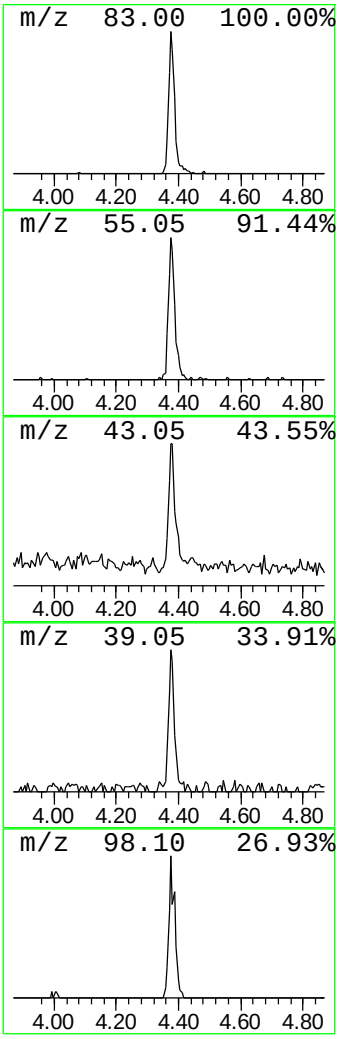
Peak Number 1 2-Pentene, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	3.98 ng	149419	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	3-Hexen-2-one	98	C6H10O	000763-93-9	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





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Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-U-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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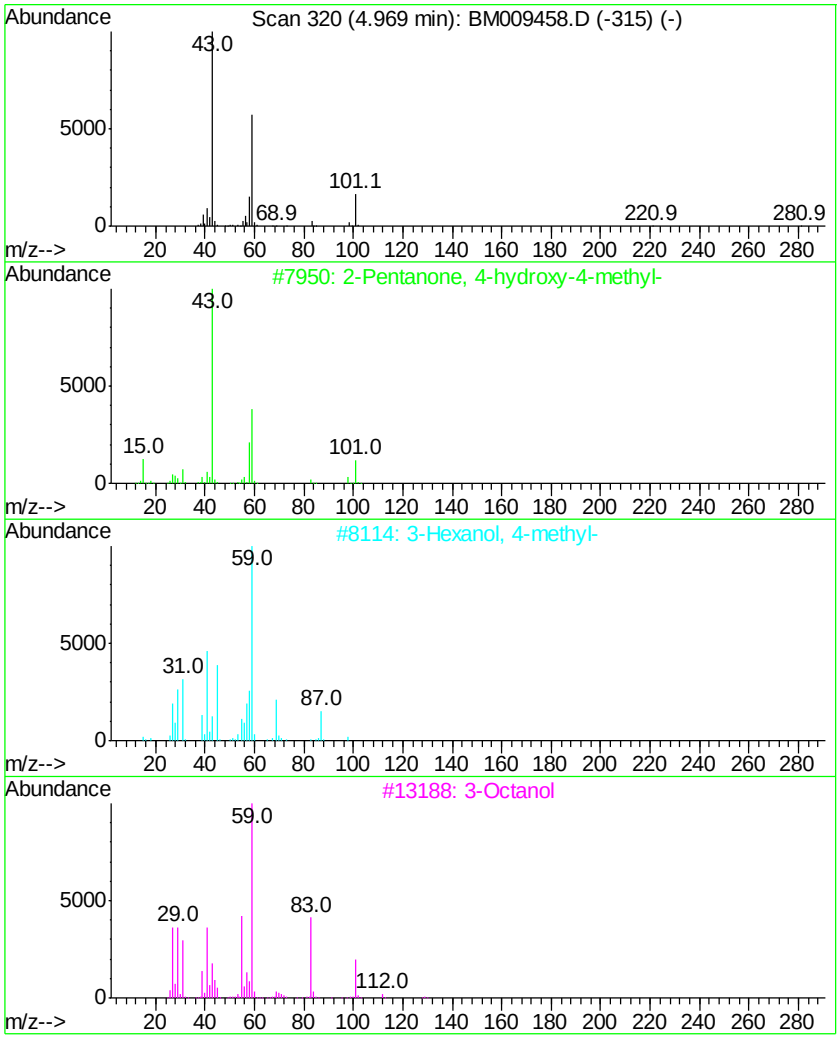
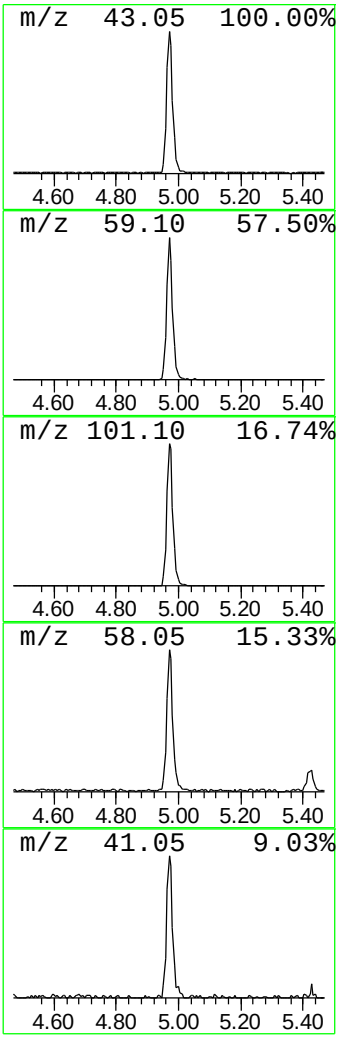
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	24.13 ng	905252	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	3-Octanol	130	C8H18O	000589-98-0	33
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25





Library Search Compound Report

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Data File : BM009458.D
Acq On : 30 Mar 2017 19:33
Operator : SJ/MA
Sample : I2446-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-U-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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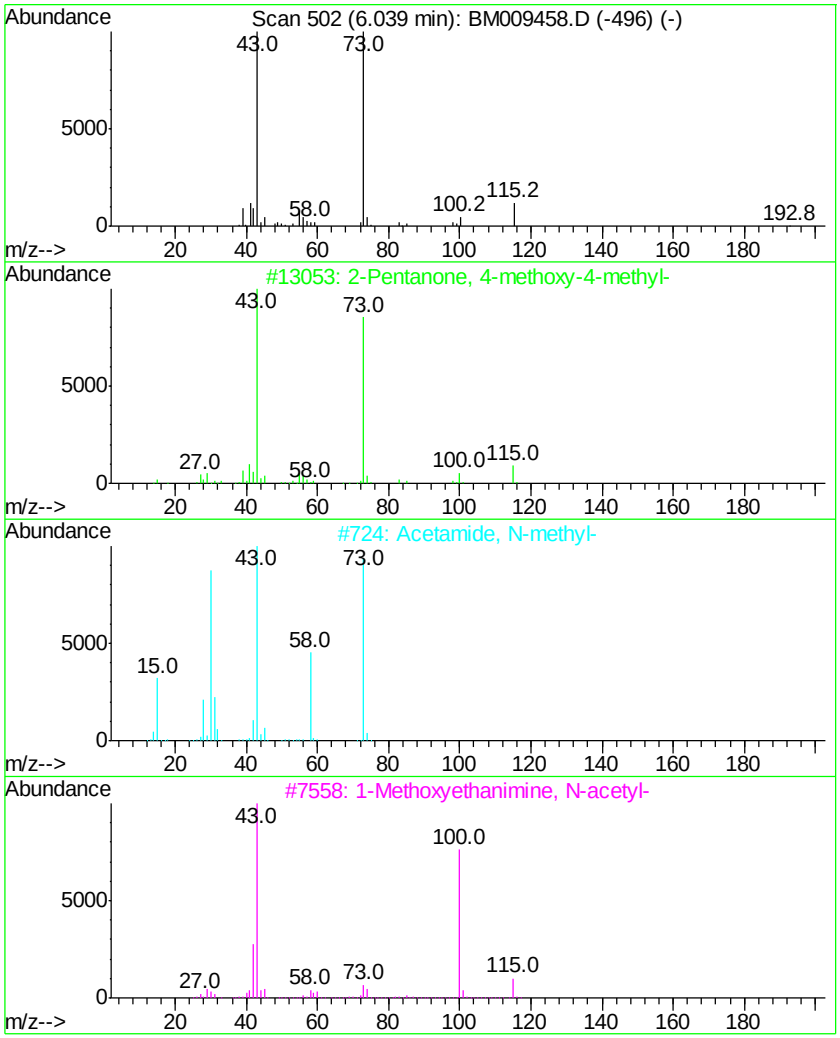
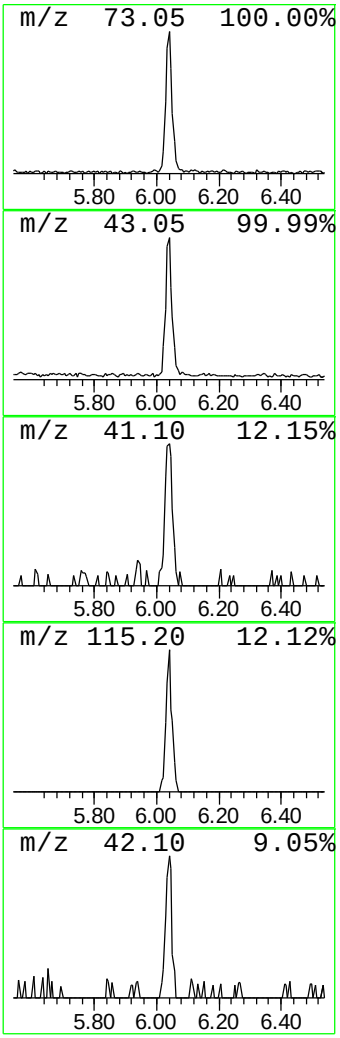
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.04	4.47 ng	167743	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	17
4	Heptane	100	C7H16	000142-82-5	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Sample : I2446-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032817-PRRT-F-U-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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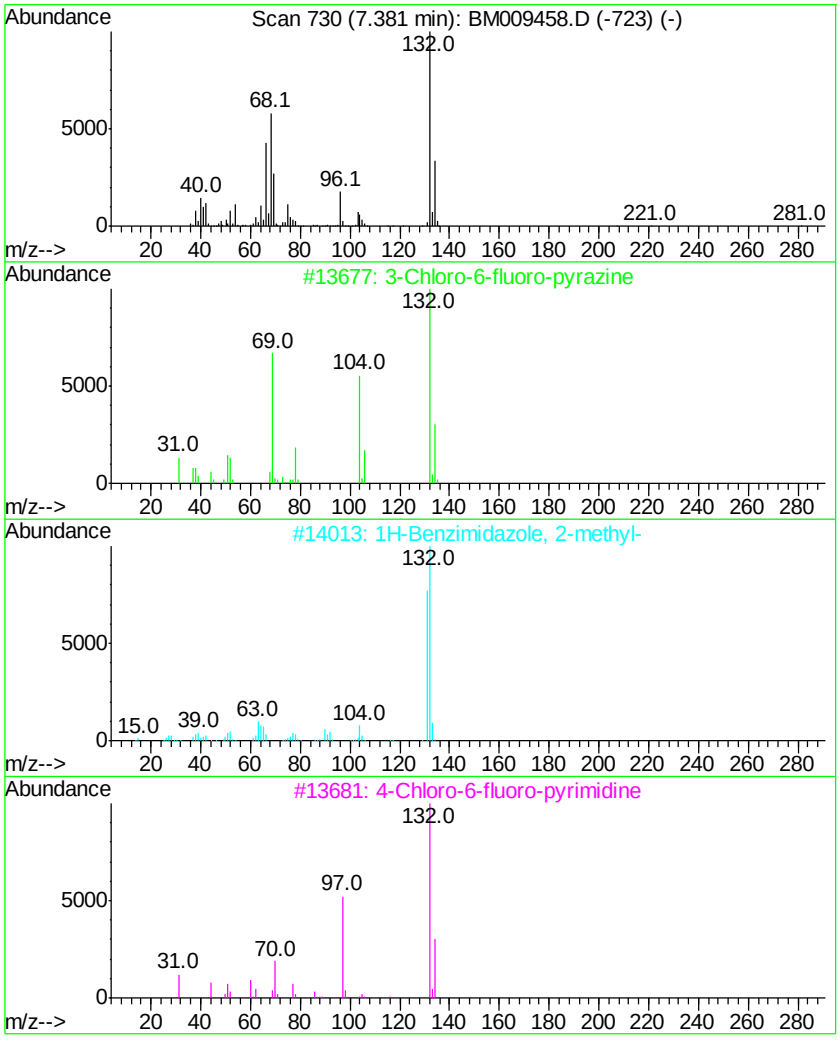
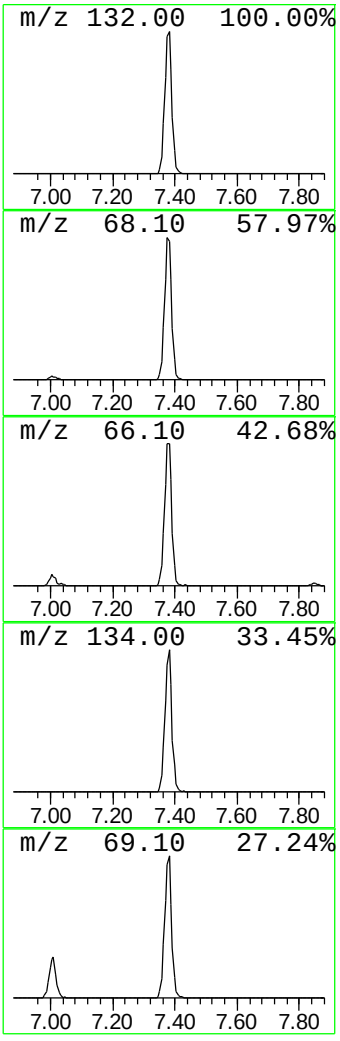
Peak Number 4 unknown7.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	62.69 ng	2352040	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9





Tentatively Identified Compound (LSC) summary

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Sample : I2446-02
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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
2-Pentene, 2,4-di...	4.37	4.0	ng	149419	1	7.85	750337	20.0
2-Pentanone, 4-hy...	4.97	24.1	ng	905252	1	7.85	750337	20.0
2-Pentanone, 4-me...	6.04	4.5	ng	167743	1	7.85	750337	20.0
unknown7.38	7.38	62.7	ng	2352040	1	7.85	750337	20.0