LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM050517\
Data File : BM009923.D
Acq On : 06 May 2017 03:41
Operator : SJ/MA
Sample : I2893-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3070-PA1

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-BM050517.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	4.904	304	309	322	rVB	403377	576270	4.78%	1.151%
2	5.363	380	387	398	rBV	1324081	1994720	16.54%	3.986%
3	5.969	486	490	496	rVB	85426	122157	1.01%	0.244%
4	6.957	651	658	673	rBV	815228	1370220	11.36%	2.738%
5	7.310	711	718	733	rBV	2535347	4088813	33.90%	8.170%
6	7.775	791	797	804	rBV	487180	763249	6.33%	1.525%
7	8.092	841	851	861	rBV	2165172	3474358	28.81%	6.942%
8	8.951	988	997	1007	rBV	2253145	3649883	30.26%	7.293%
9	10.575	1264	1273	1280	rBV	603481	1037441	8.60%	2.073%
10	11.239	1380	1386	1397	rBV2	88722	166420	1.38%	0.333%
11	13.045	1685	1693	1703	rVB	5000447	6967241	57.76%	13.921%
12	14.433	1920	1929	1936	rBV2	896093	1385046	11.48%	2.767%
13	15.933	2177	2184	2195	rBV	4664690	6267695	51.97%	12.523%
14	16.151	2213	2221	2226	rBV5	136499	234252	1.94%	0.468%
15	17.186	2392	2397	2406	rVB2	1233179	1697020	14.07%	3.391%
16	18.068	2543	2547	2552	rBV2	161342	230758	1.91%	0.461%
17	19.351	2761	2765	2772	rBV3	173084	268861	2.23%	0.537%
18	19.815	2838	2844	2849	rVB	10333403	12061377	100.00%	24.099%
19	21.374	3105	3109	3116	rVB	1784017	2076513	17.22%	4.149%
20	23.680	3496	3501	3508	rVB	866957	1616862	13.41%	3.231%

Sum of corrected areas: 50049156

LSC Report - Integrated Chromatogram

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Operator : SJ/MA
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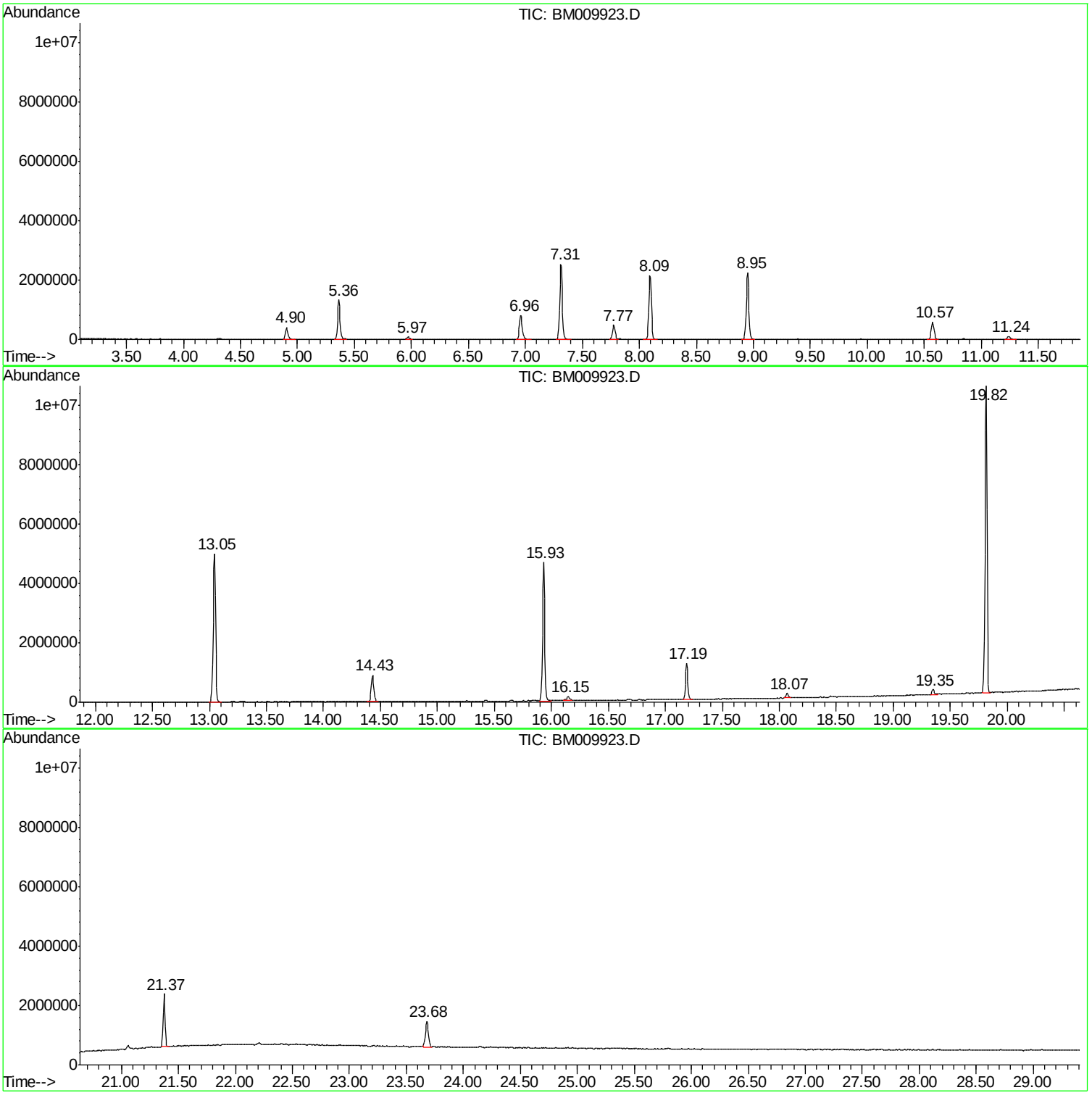
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
3070-PA1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

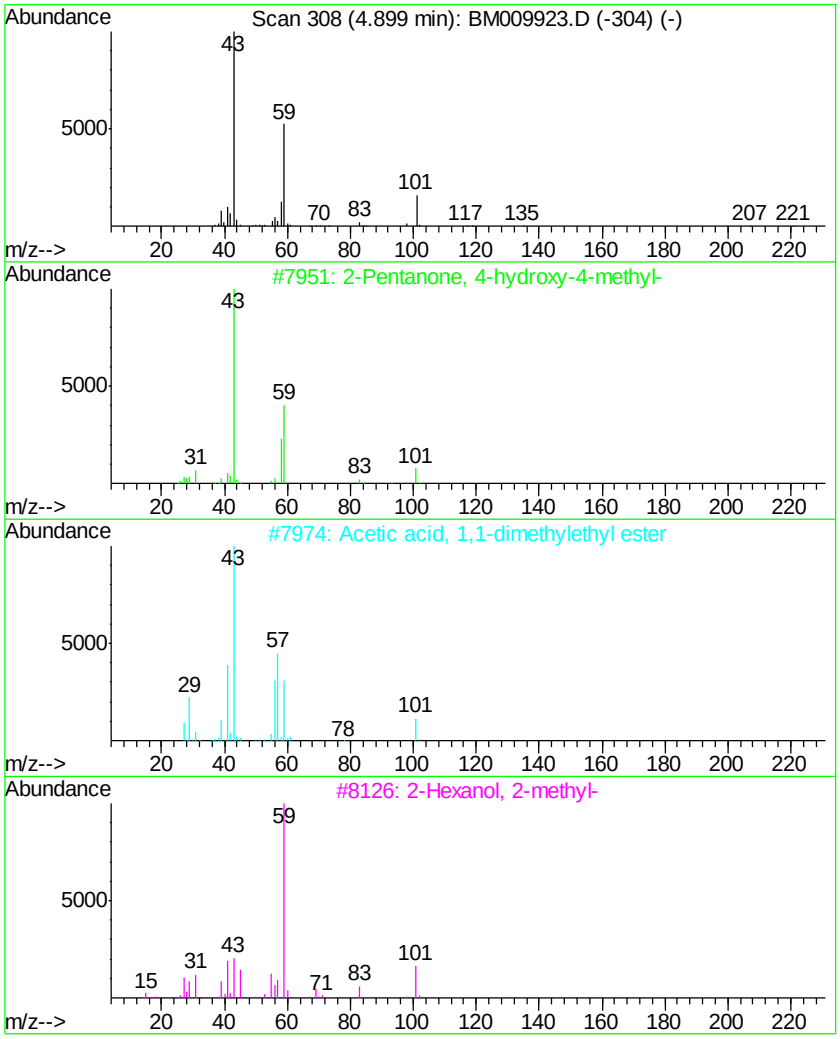
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

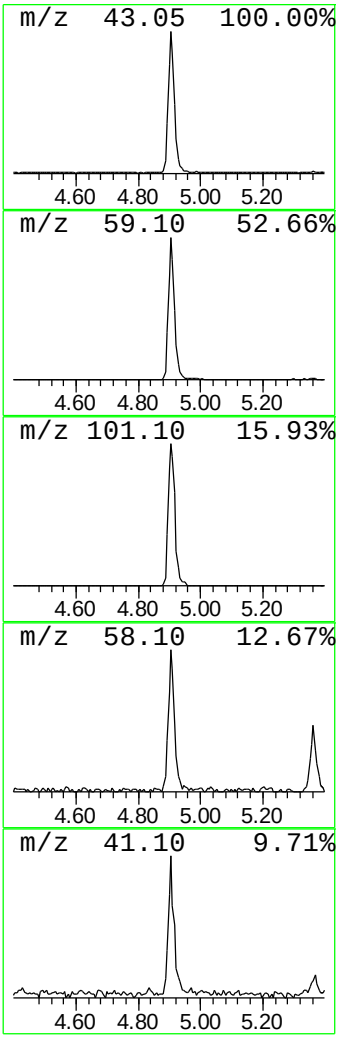
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	15.10 ng	576270	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Library Search Compound Report

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Data File : BM009923.D
Acq On : 06 May 2017 03:41
Operator : SJ/MA
Sample : I2893-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3070-PA1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

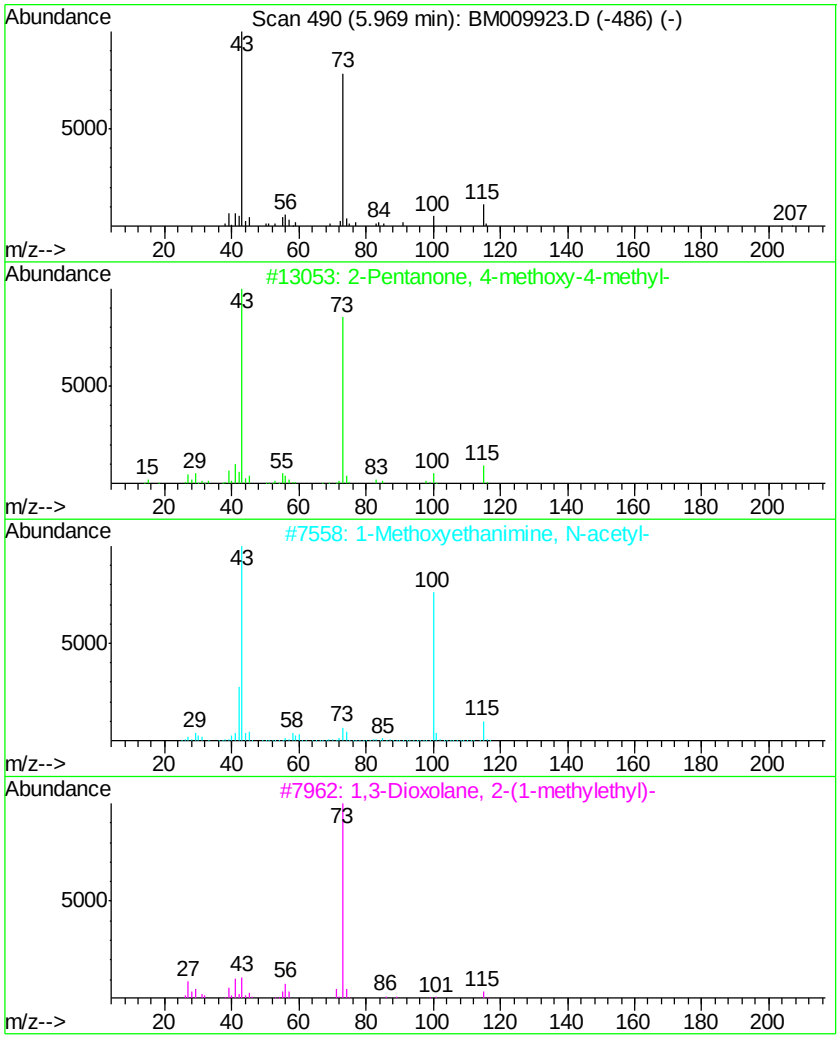
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

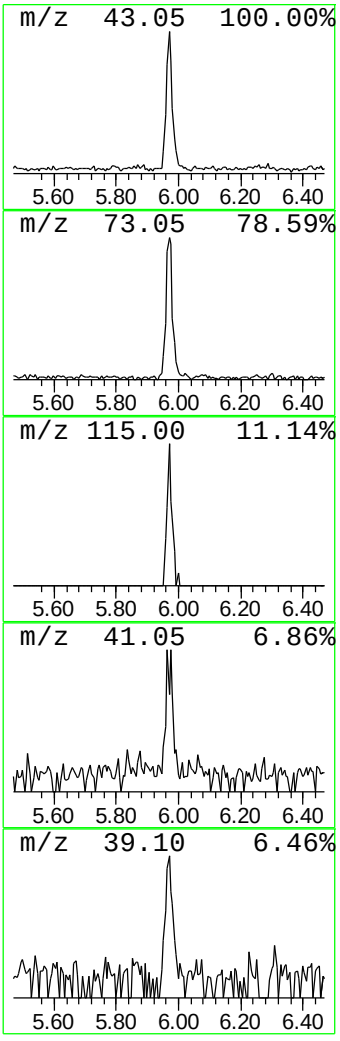
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	3.20 ng	122157	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	47
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	32
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	25





Library Search Compound Report

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Acq On : 06 May 2017 03:41
Operator : SJ/MA
Sample : I2893-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3070-PA1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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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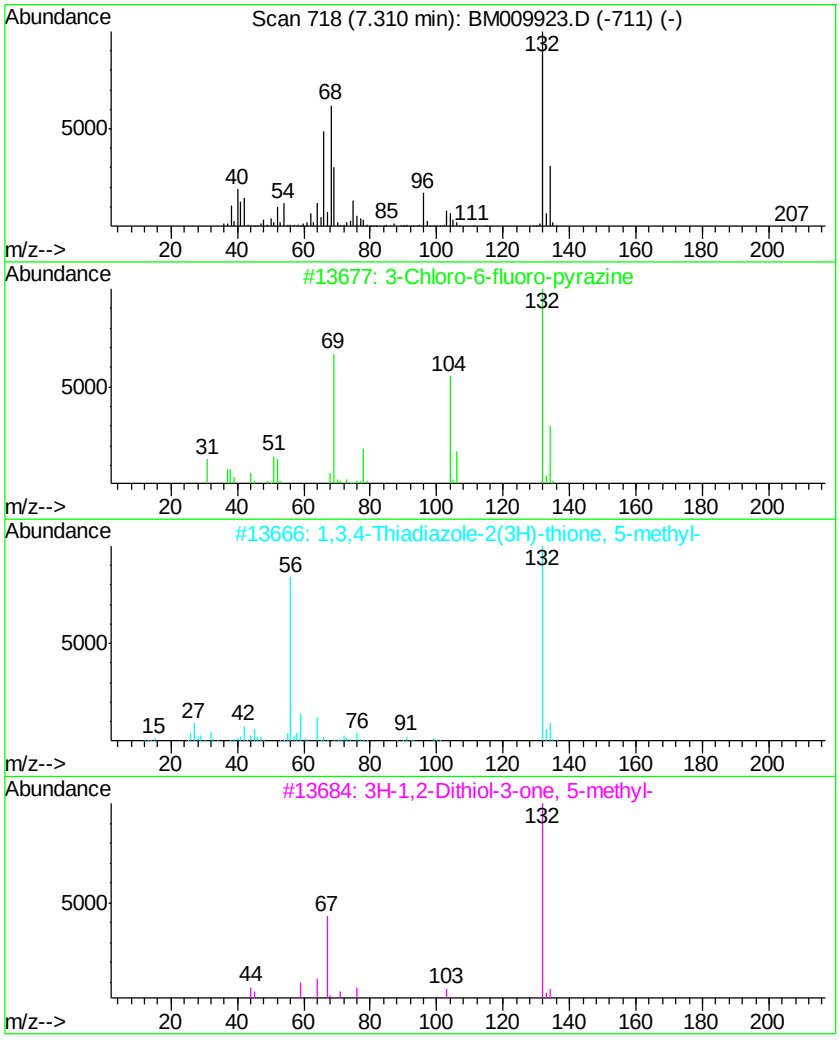
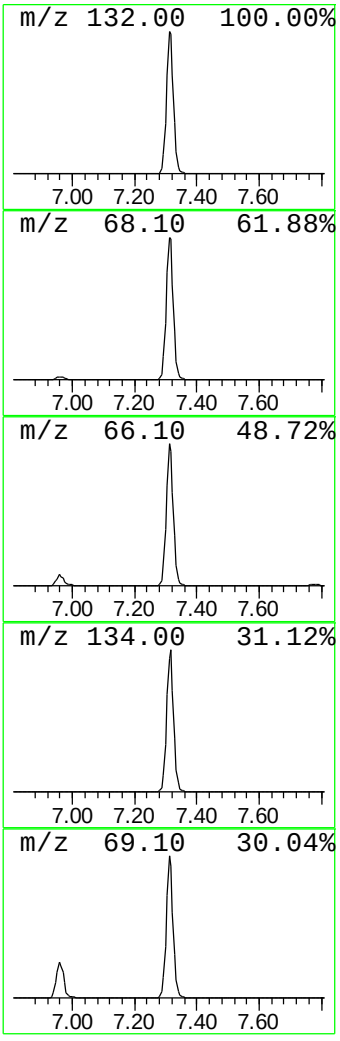
Peak Number 3 unknown7.31 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	107.14 ng	4088810	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





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Operator : SJ/MA
Sample : I2893-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 3070-PA1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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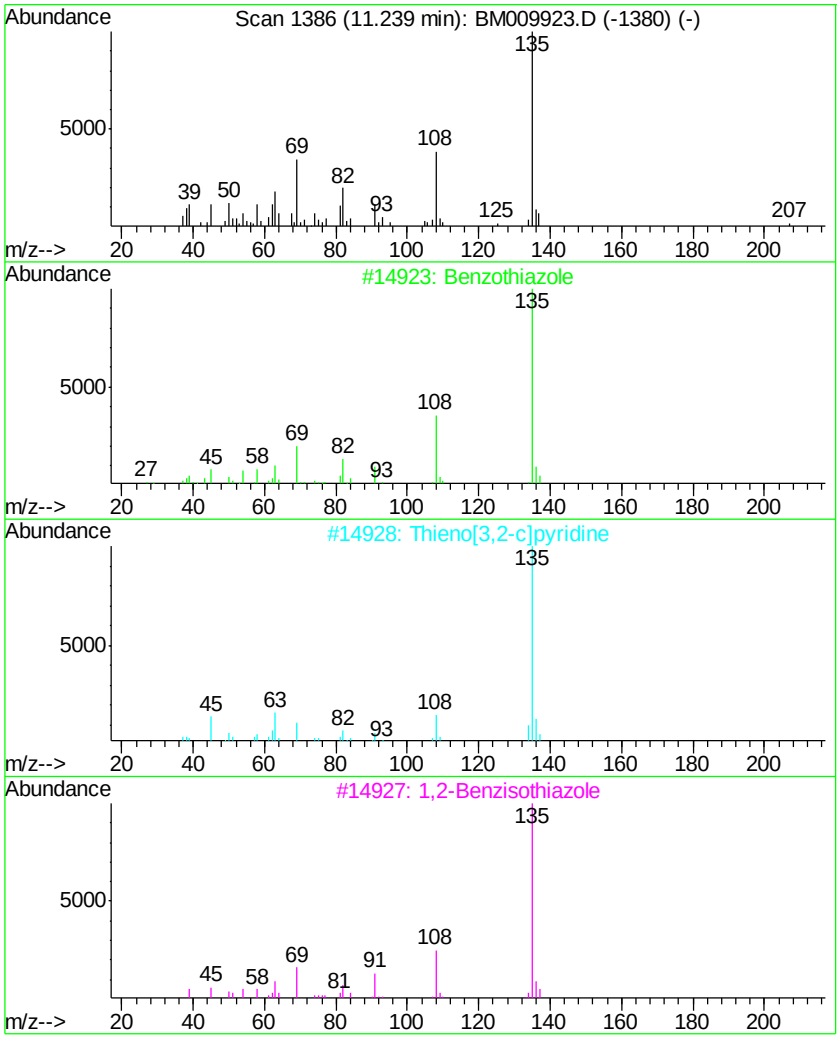
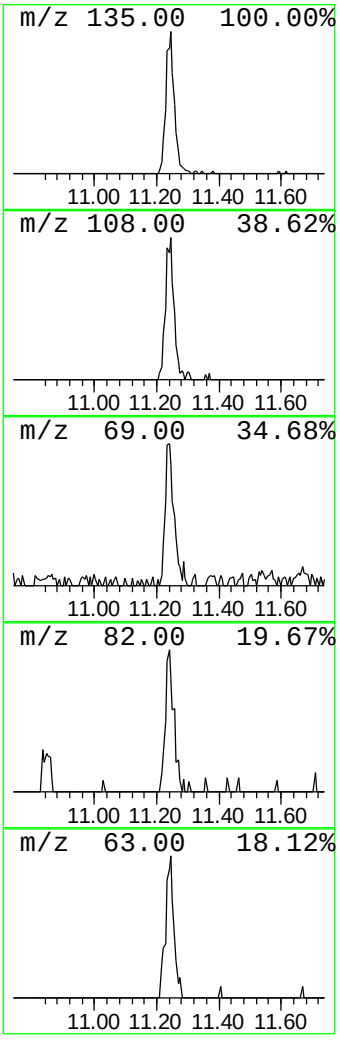
Peak Number 5 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	3.21 ng	166420	Naphthalene-d8	10.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	62
3	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	58
4	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	53
5	Adenine	135	C5H5N5	000073-24-5	52





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Instrument : BNA_M
ClientSampleId : 3070-PA1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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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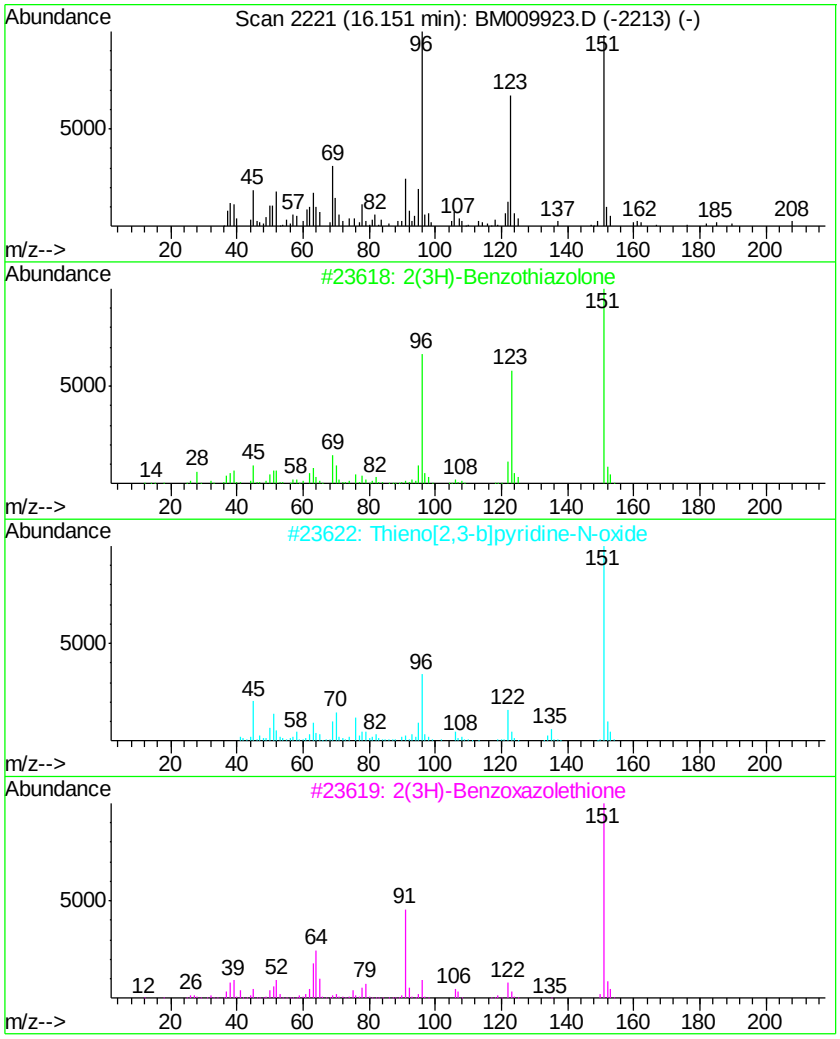
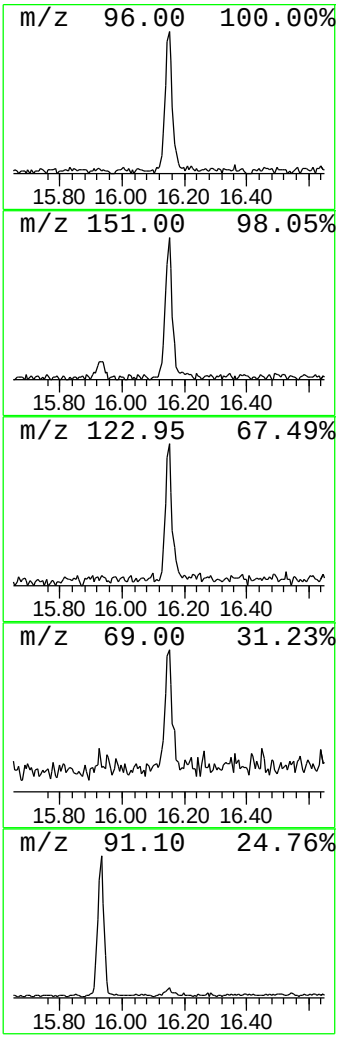
Peak Number 6 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	2.76 ng	234252	Phenanthrene-d10	17.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	46
3	2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	43
4	N-Methylsalicylamide	151	C8H9NO2	001862-88-0	35
5	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	35





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ClientSampleId : 3070-PA1

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

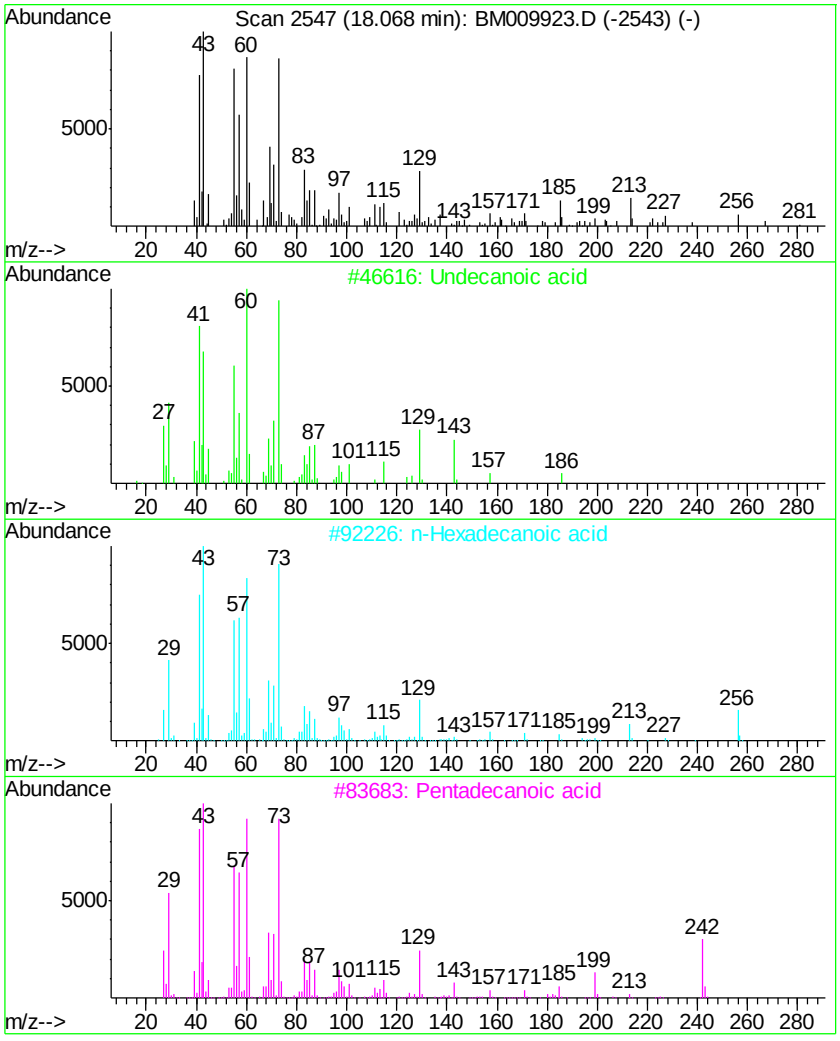
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

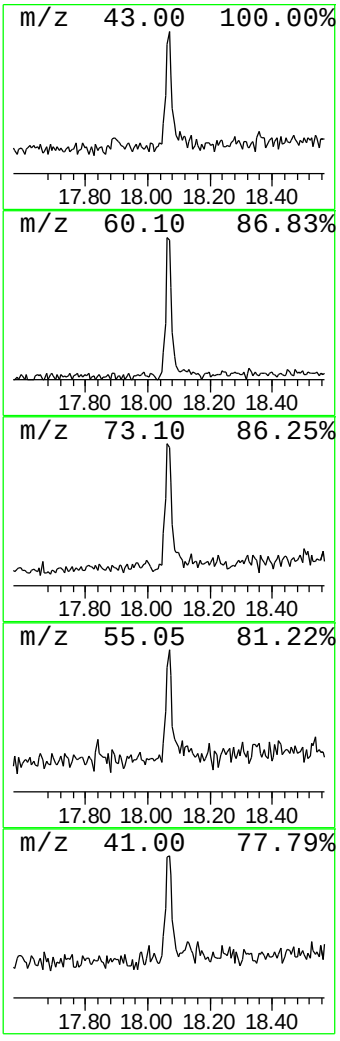
****

Peak Number 7 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	2.72 ng	230758	Phenanthrene-d10	17.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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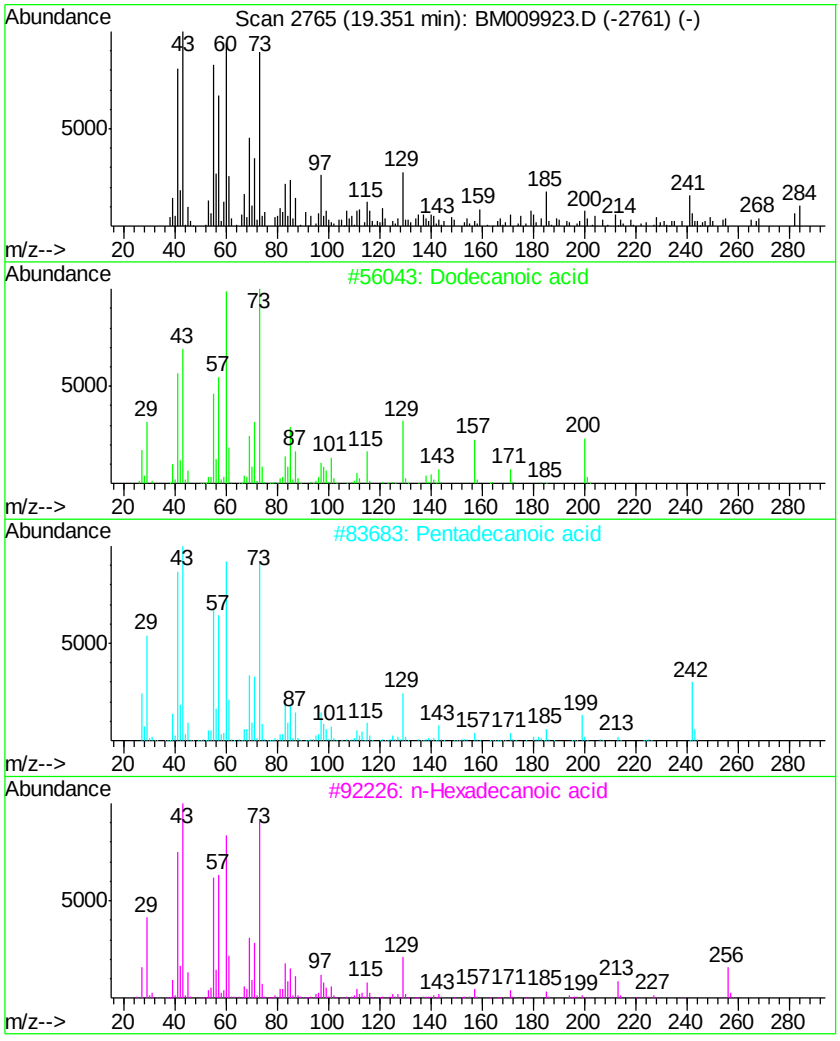
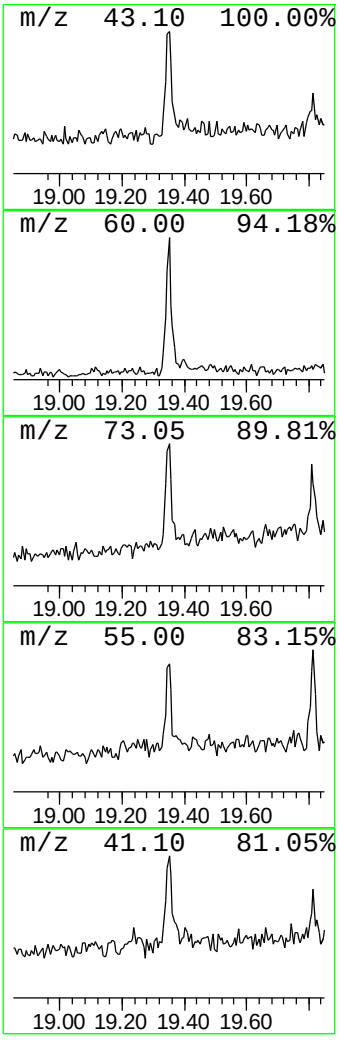
****

Peak Number 8 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	2.59 ng	268861	Chrysene-d12	21.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	76
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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-Pentanone, 4-hy...	4.90	15.1	ng	576270	1	7.77	763249	20.0
2-Pentanone, 4-me...	5.97	3.2	ng	122157	1	7.77	763249	20.0
unknown7.31	7.31	107.1	ng	4088810	1	7.77	763249	20.0
Benzothiazole	11.24	3.2	ng	166420	2	10.57	1037440	20.0
2(3H)-Benzothiazo...	16.15	2.8	ng	234252	4	17.19	1697020	20.0
Undecanoic acid	18.07	2.7	ng	230758	4	17.19	1697020	20.0
Dodecanoic acid	19.35	2.6	ng	268861	5	21.37	2076510	20.0