LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

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_G\METHODS\8270-BG070816.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	5.700	480	487	496	rVB	1573624	2570682	23.01%	4.584%
2	7.005	704	709	716	rVB2	94776	173009	1.55%	0.308%
3	7.304	753	760	770	rVB	1193142	2064767	18.48%	3.681%
4	7.504	786	794	800	rBV5	87275	201620	1.80%	0.359%
5	7.680	816	824	834	rBV	2454150	4339777	38.84%	7.738%
6	8.156	896	905	910	rBV2	467079	943151	8.44%	1.682%
7	8.197	910	912	917	rVB3	89971	121181	1.08%	0.216%
8	8.479	953	960	966	rBV	1789171	3057244	27.36%	5.451%
9	9.326	1097	1104	1114	rBV	1785909	3208177	28.71%	5.720%
10	10.272	1258	1265	1269	rBV	61846	123604	1.11%	0.220%
11	10.982	1379	1386	1402	rVB	689158	1315535	11.77%	2.346%
12	11.635	1489	1497	1505	rBV6	55989	140972	1.26%	0.251%
13	11.870	1531	1537	1541	rBV3	77338	146051	1.31%	0.260%
14	13.056	1734	1739	1746	rBV6	93449	176919	1.58%	0.315%
15	13.209	1759	1765	1769	rBV4	110413	204378	1.83%	0.364%
16	13.421	1791	1801	1808	rVB	4631696	7475103	66.90%	13.328%
17	13.527	1815	1819	1825	rVB3	74928	112644	1.01%	0.201%
18	14.167	1924	1928	1933	rBV	75642	126068	1.13%	0.225%
19	14.796	2028	2035	2042	rVB2	1158605	1969728	17.63%	3.512%
20	14.954	2058	2062	2067	rBV8	62103	115364	1.03%	0.206%
21	15.571	2164	2167	2171	rBV2	92207	117799	1.05%	0.210%
22	16.294	2284	2290	2297	rVB	4823760	7307018	65.40%	13.028%
23	17.205	2441	2445	2449	rVB2	229703	296404	2.65%	0.528%
24	17.557	2499	2505	2514	rVB	1553081	2416004	21.62%	4.308%
25	18.421	2649	2652	2658	rBV3	262397	353514	3.16%	0.630%
26	19.690	2864	2868	2874	rVB2	262797	384849	3.44%	0.686%
27	20.154	2941	2947	2953	rVB	8056235	11173445	100.00%	19.922%
28	21.840	3229	3234	3243	rVB2	1612915	2761054	24.71%	4.923%
29	25.195	3798	3805	3817	rVB3	941503	2689010	24.07%	4.795%

Sum of corrected areas: 56085071

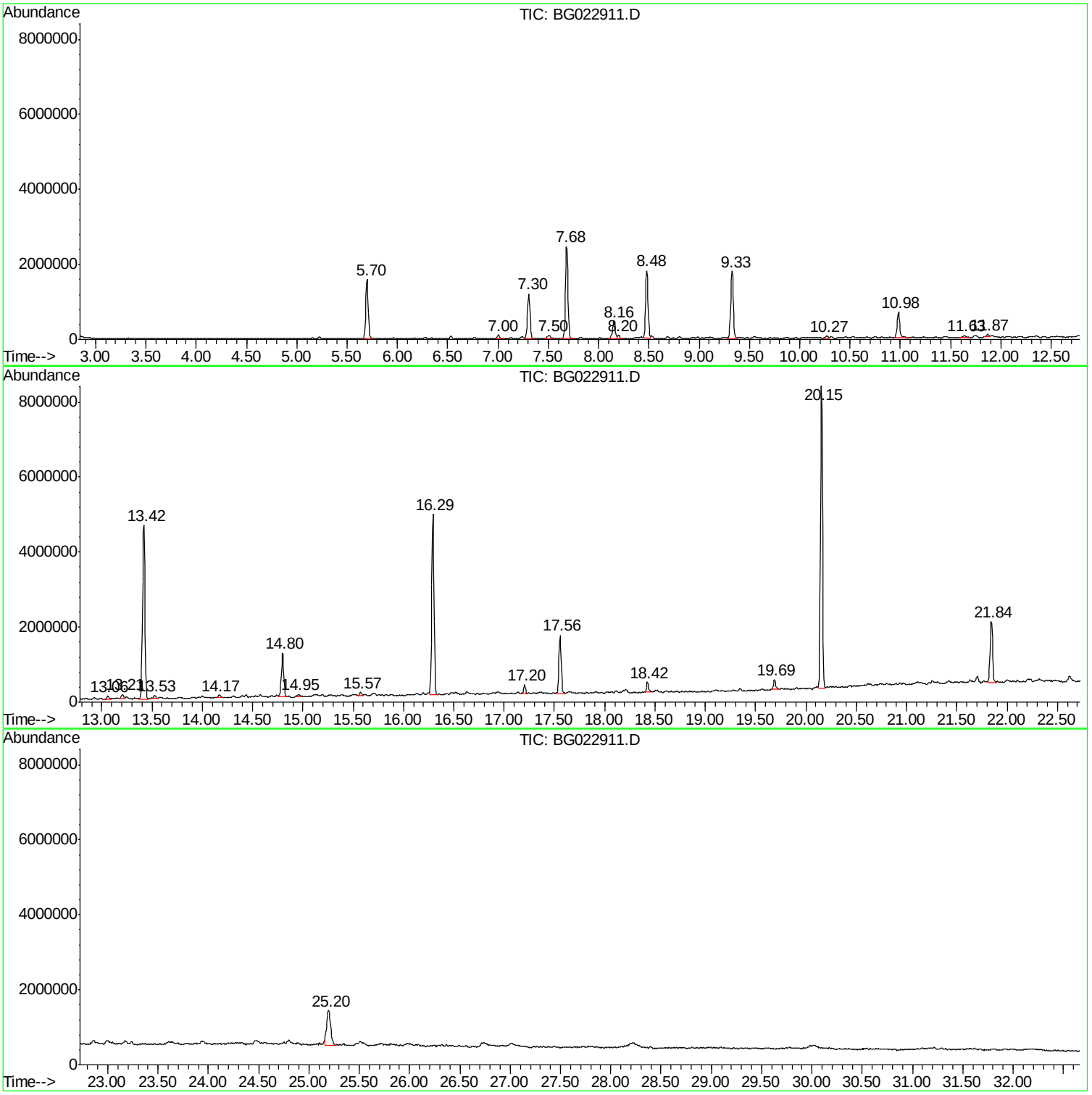
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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 G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

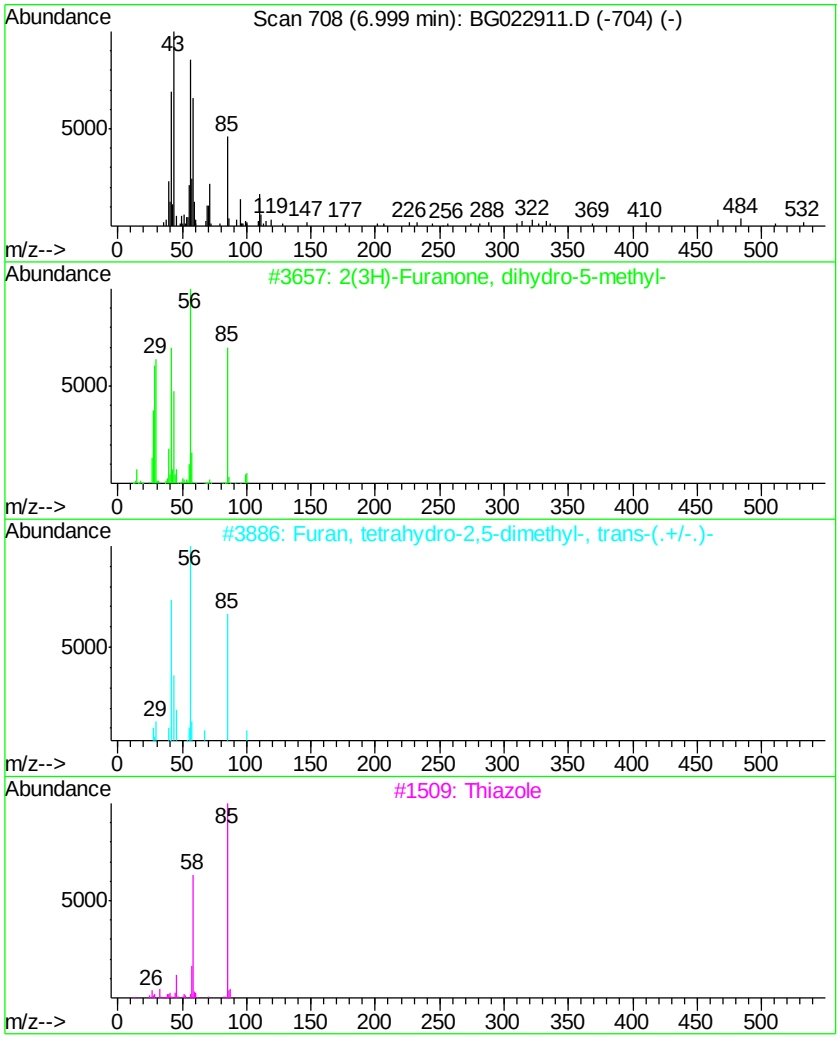
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

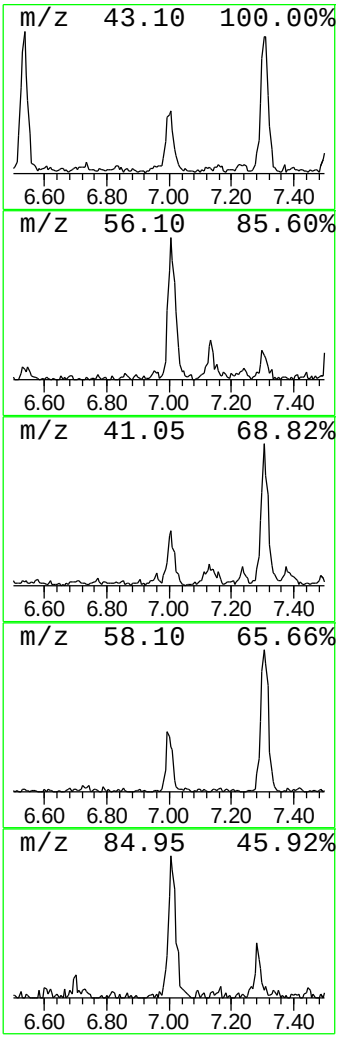
****

Peak Number 1 2(3H)-Furanone, dihydro-5-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	3.67 ng	173009	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5-methyl-	100	C5H8O2	000108-29-2	52
2	Furan, tetrahydro-2,5-dimethyl-,...	100	C6H12O	038484-59-2	50
3	Thiazole	85	C3H3NS	000288-47-1	38
4	Oxirane, (2-methylbutyl)-	114	C7H14O	053229-42-8	37
5	Furan, tetrahydro-2,4-dimethyl-,...	100	C6H12O	039168-01-9	35





Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

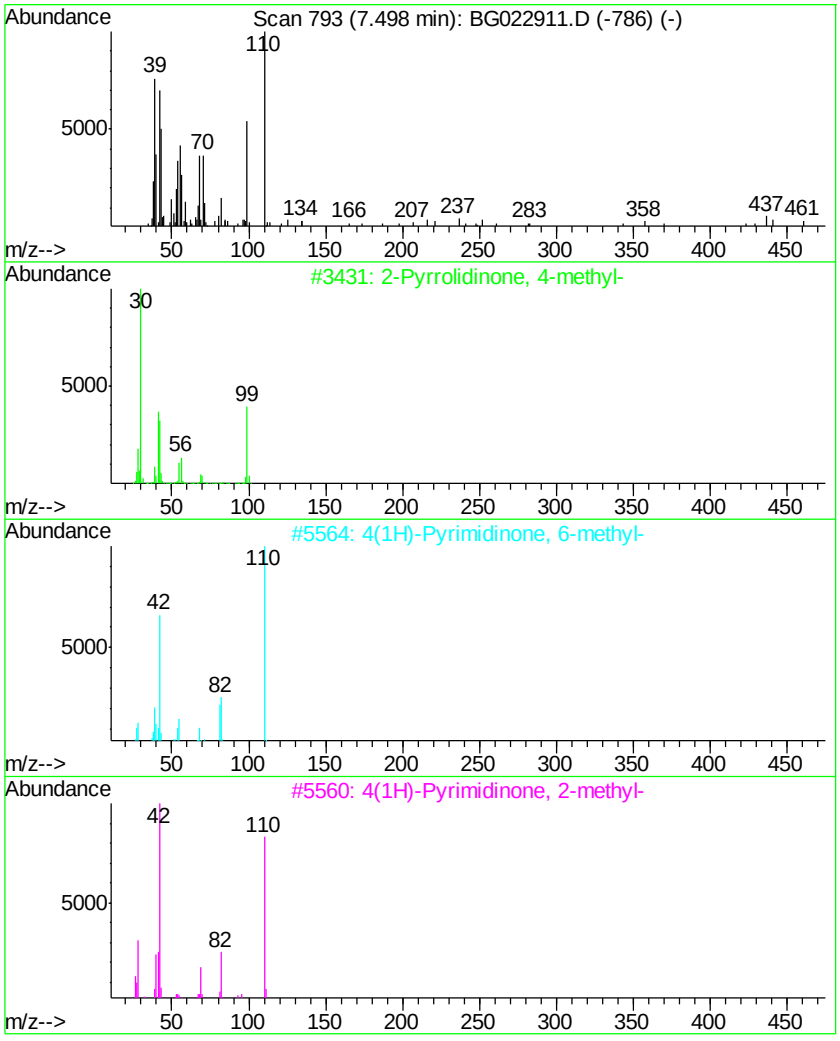
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

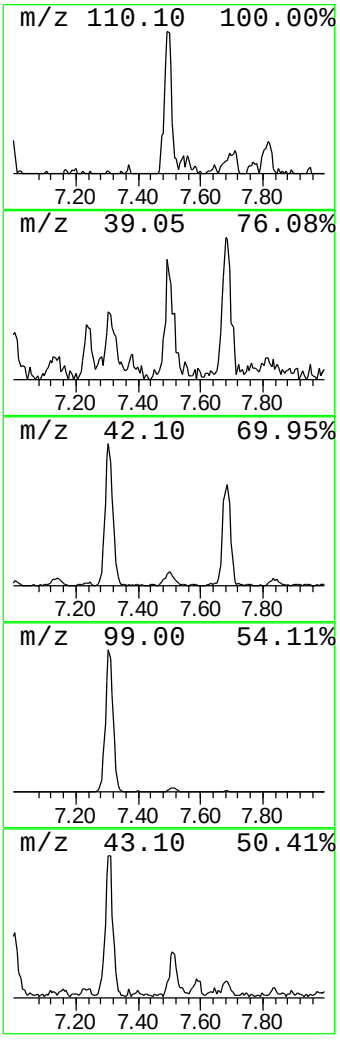
****

Peak Number 2 unknown7.50 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	4.28 ng	201620	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 4-methyl-	99	C5H9NO	1000197-00-3	38
2	4(1H)-Pyrimidinone, 6-methyl-	110	C5H6N2O	003524-87-6	27
3	4(1H)-Pyrimidinone, 2-methyl-	110	C5H6N2O	019875-04-8	27
4	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	22
5	Cholestan-3-one, cyclic 1,2-etha...	430	C29H50O2	025328-53-4	22





Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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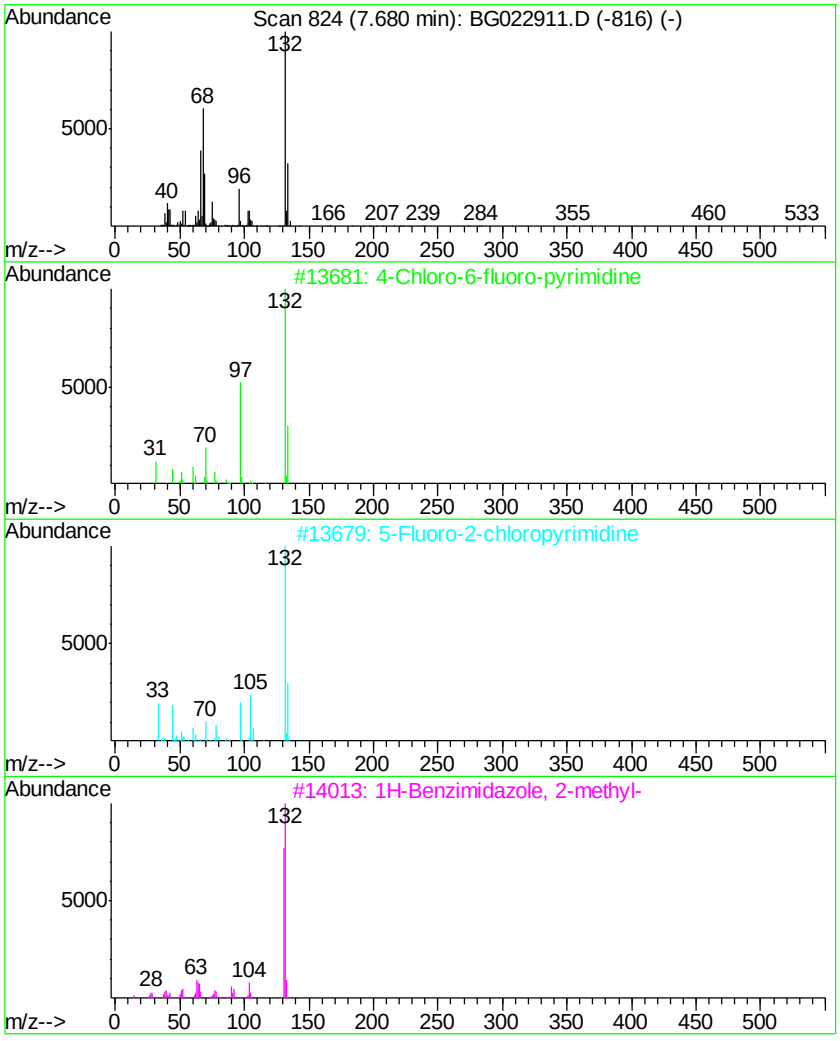
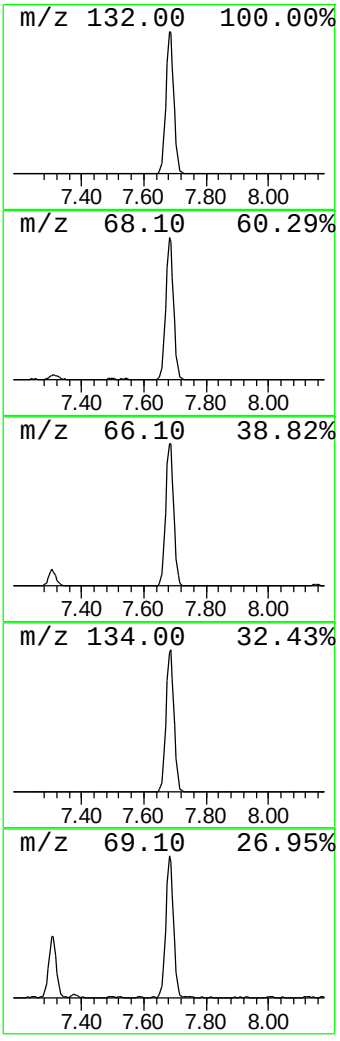
Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	92.03 ng	4339780	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

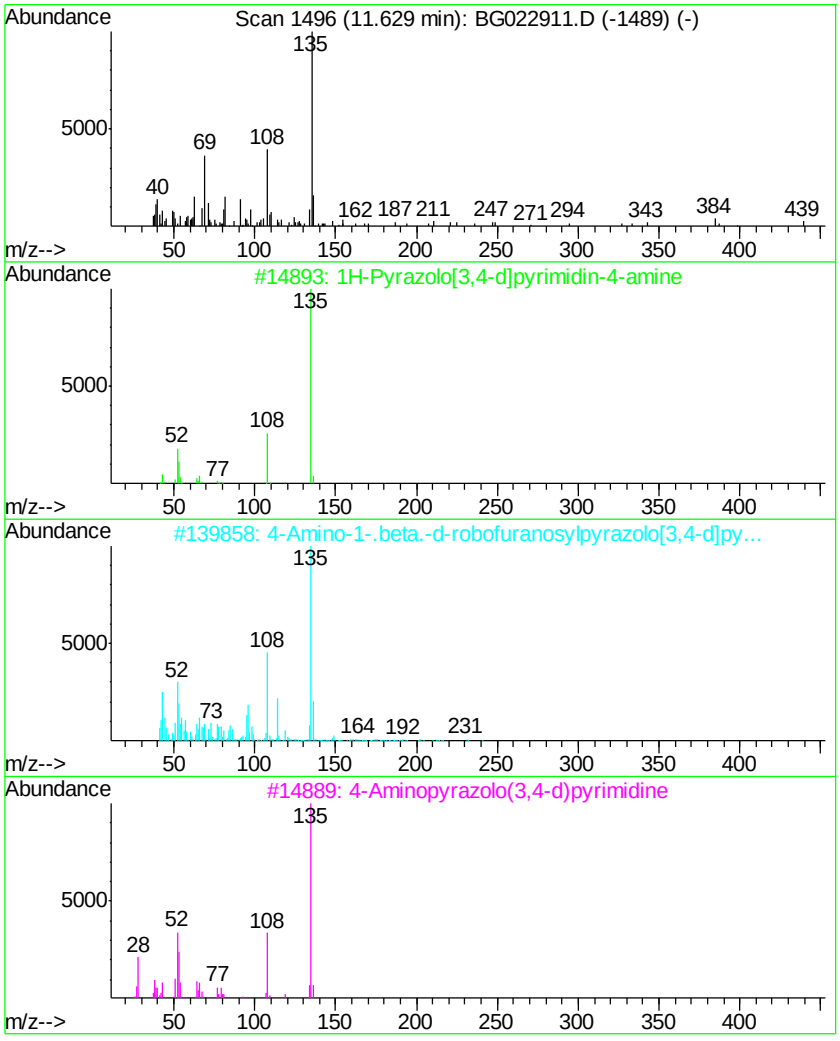
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

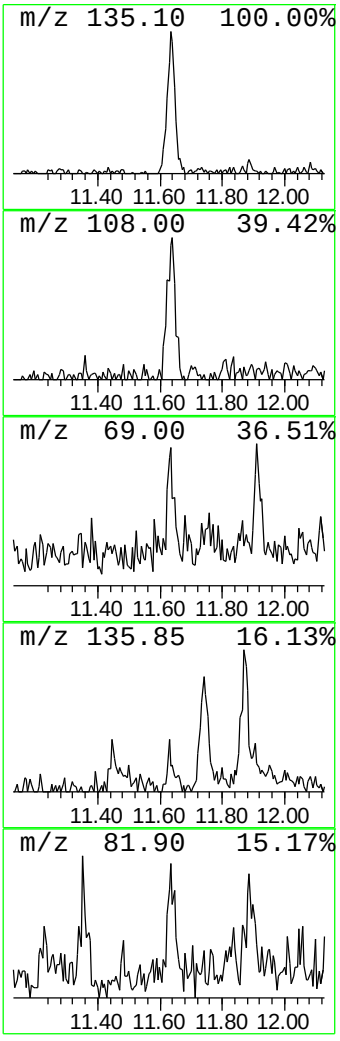
****

Peak Number 5 1H-Pyrazolo[3,4-d]pyrimidin... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	2.14 ng	140972	Naphthalene-d8	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	72
2	4-Amino-1-.beta.-d-robofuranosyl...	347	C10H14N5O7P	028072-48-2	56
3	4-Aminopyrazolo(3,4-d)pyrimidine	135	C5H5N5	020289-44-5	50
4	Adenine	135	C5H5N5	000073-24-5	50
5	Benzothiazole	135	C7H5NS	000095-16-9	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

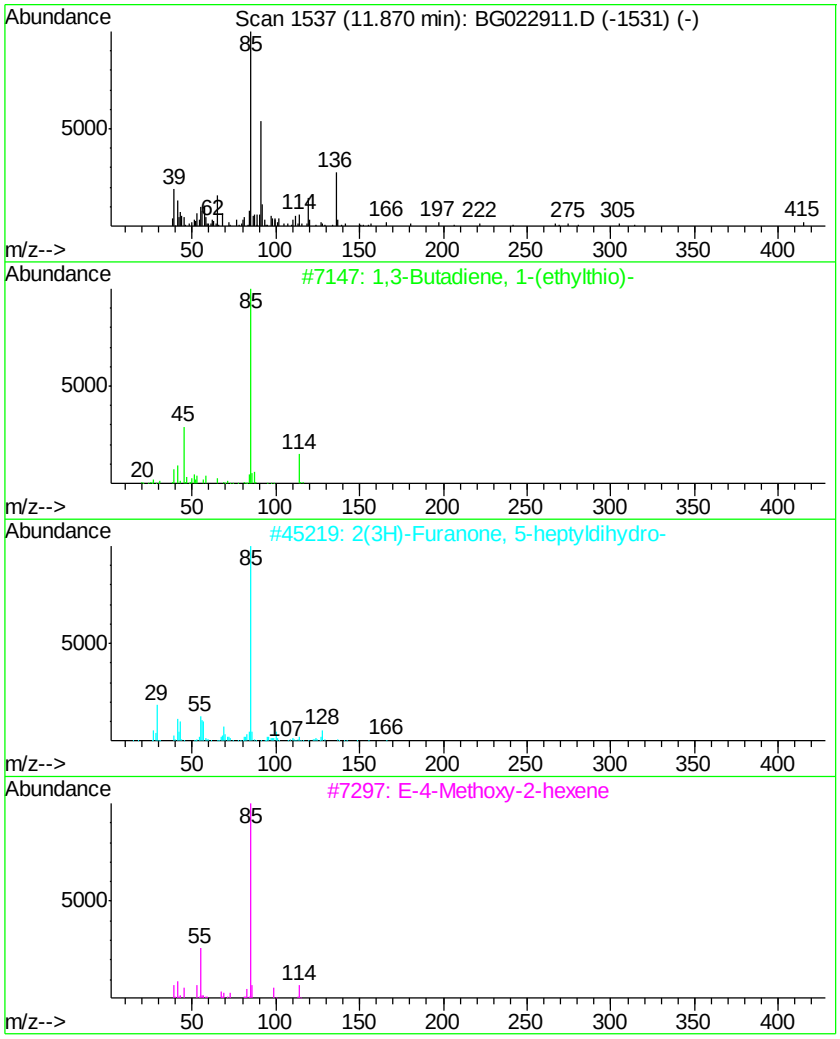
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

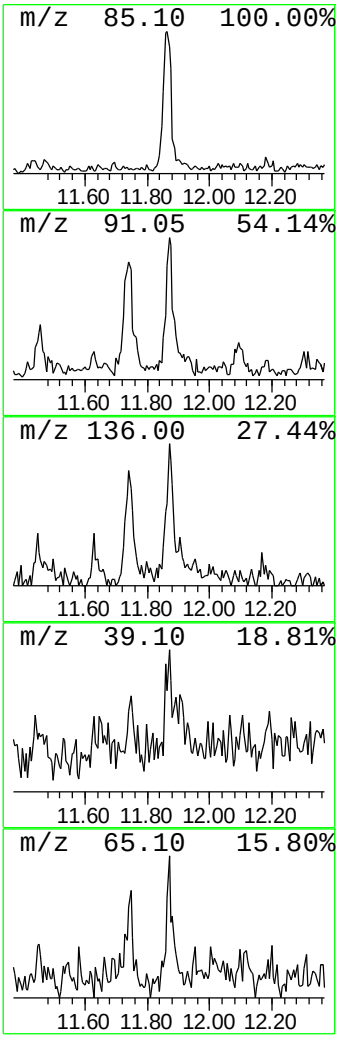
****

Peak Number 6 unknown11.87 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.22 ng	146051	Naphthalene-d8	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1-(ethylthio)-	114	C6H10S	010574-85-3	49
2	2(3H)-Furanone, 5-heptyldihydro-	184	C11H20O2	000104-67-6	47
3	E-4-Methoxy-2-hexene	114	C7H14O	1000279-61-2	47
4	.gamma. Dodecalactone	198	C12H22O2	002305-05-7	47
5	2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2	000706-14-9	43





Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
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Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

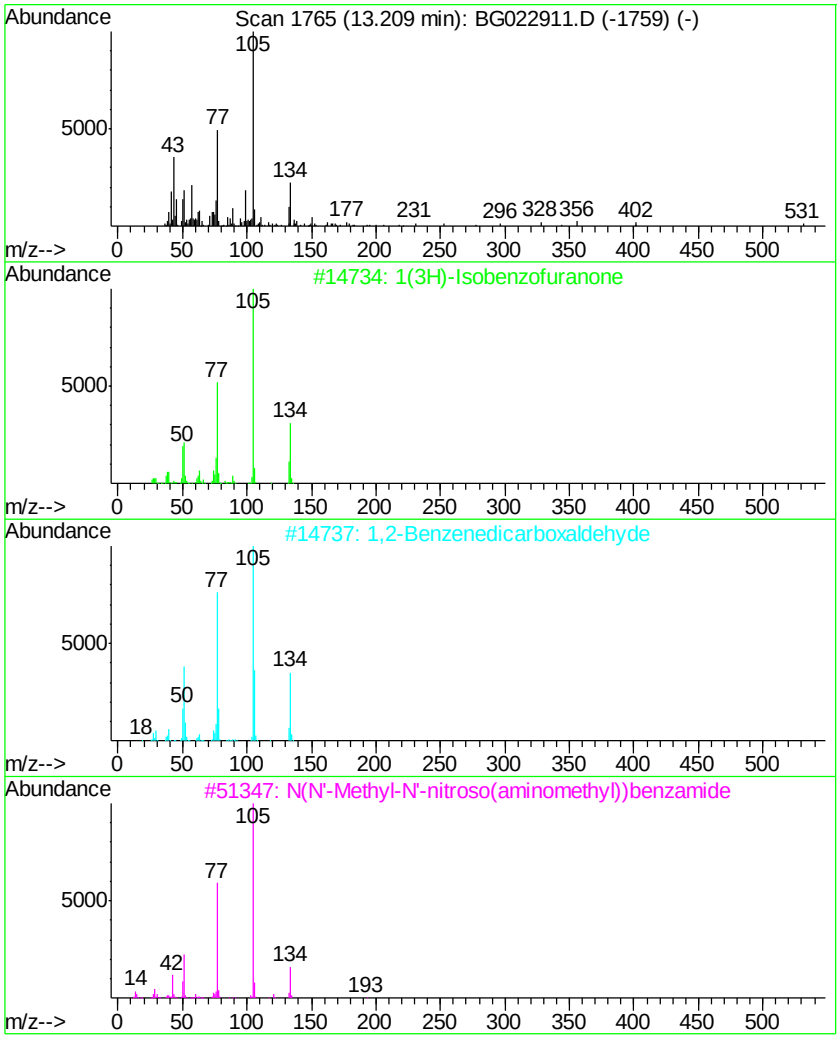
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

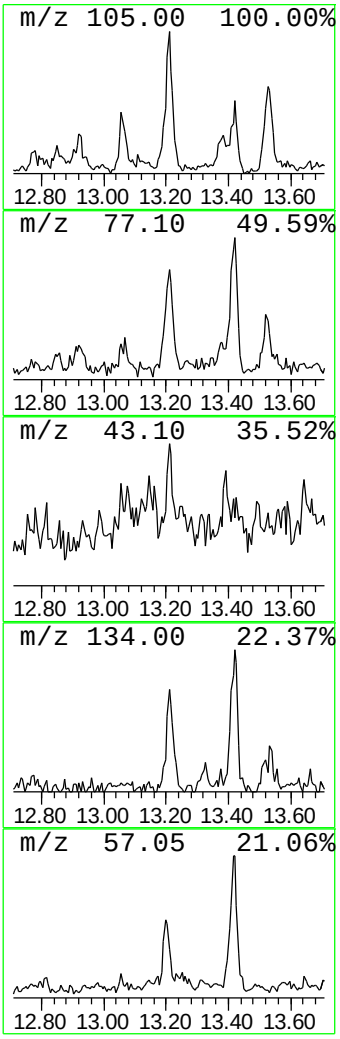
****

Peak Number 7 1(3H)-Isobenzofuranone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.08 ng	204378	Acenaphthene-d10	14.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(3H)-Isobenzofuranone	134	C8H6O2	000087-41-2	81
2	1,2-Benzenedicarboxaldehyde	134	C8H6O2	000643-79-8	64
3	N(N'-Methyl-N'-nitroso(aminometh...	193	C9H11N3O2	059665-02-0	50
4	1-Propanone, 1-phenyl-	134	C9H10O	000093-55-0	47
5	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	43





Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

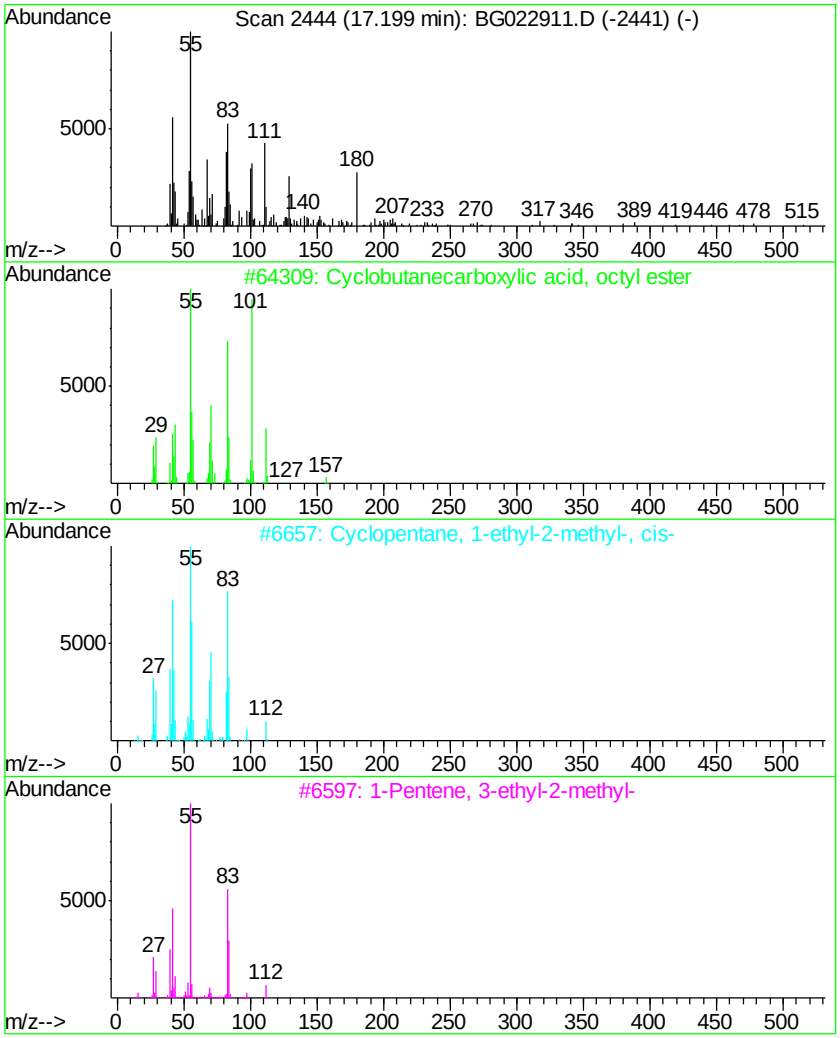
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

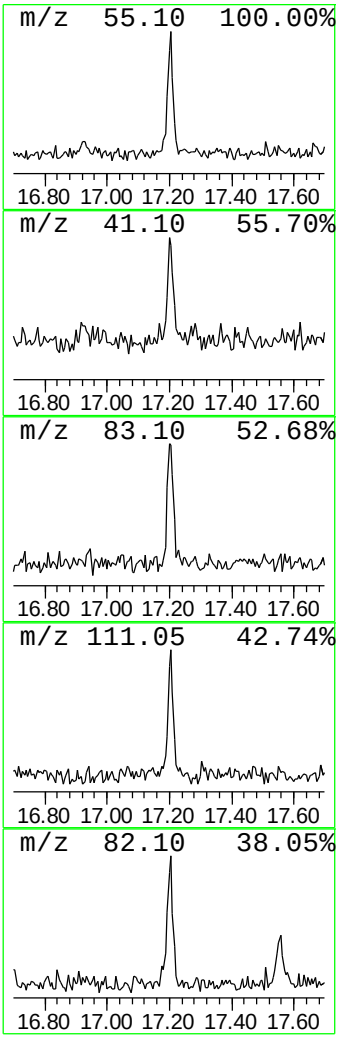
****

Peak Number 8 unknown17.20 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	2.45 ng	296404	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanecarboxylic acid, octy...	212	C13H24O2	1000280-40-5	38
2	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	18
3	1-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-66-6	14
4	Cyclohexane, 1,1'-[methylenebis(...	212	C13H24O2	001453-21-0	12
5	3-Ethyl-2-hexene	112	C8H16	000620-00-8	11





Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
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Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

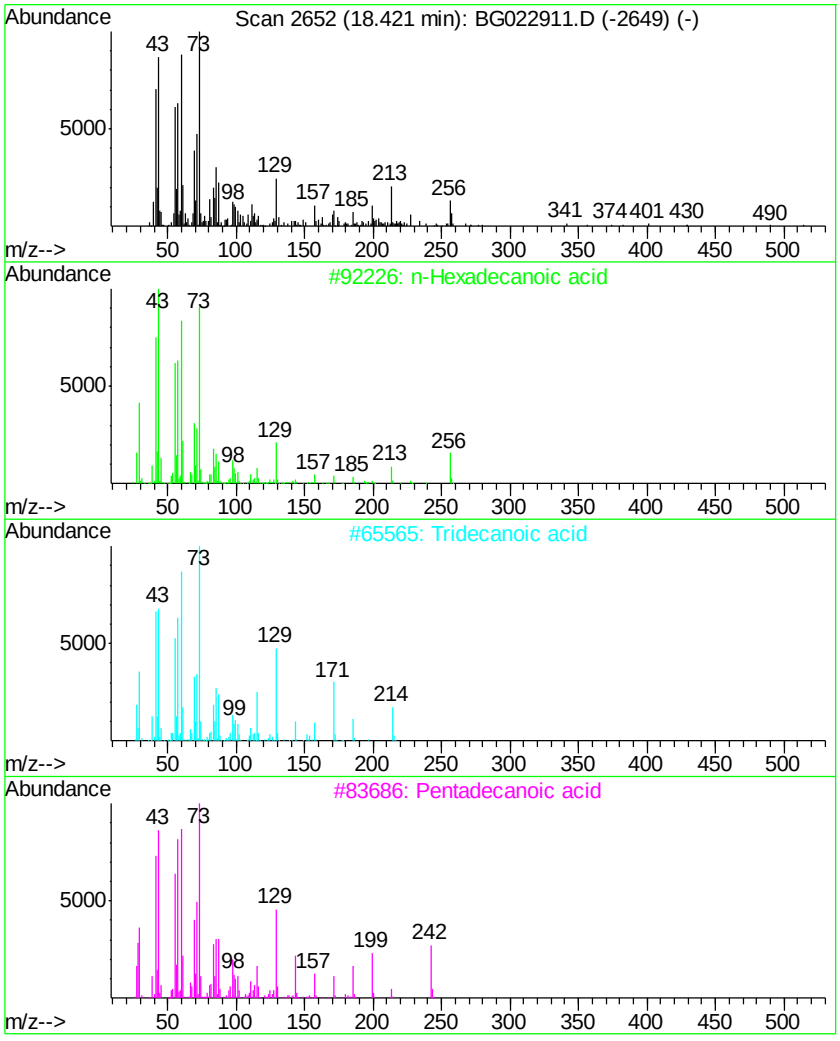
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

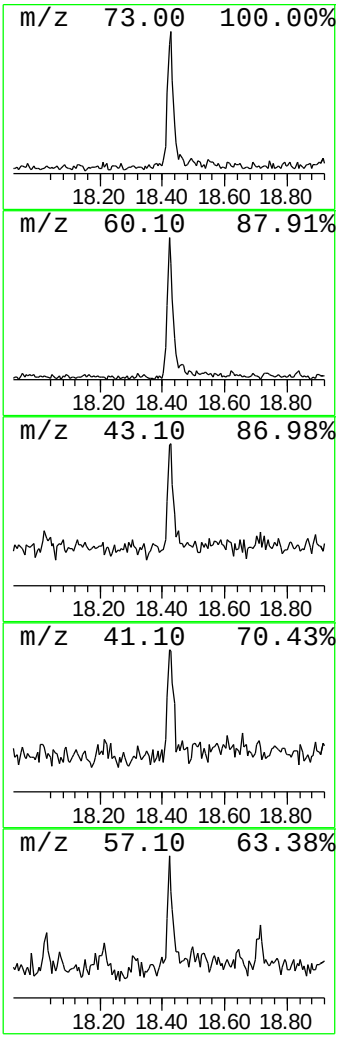
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.93 ng	353514	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

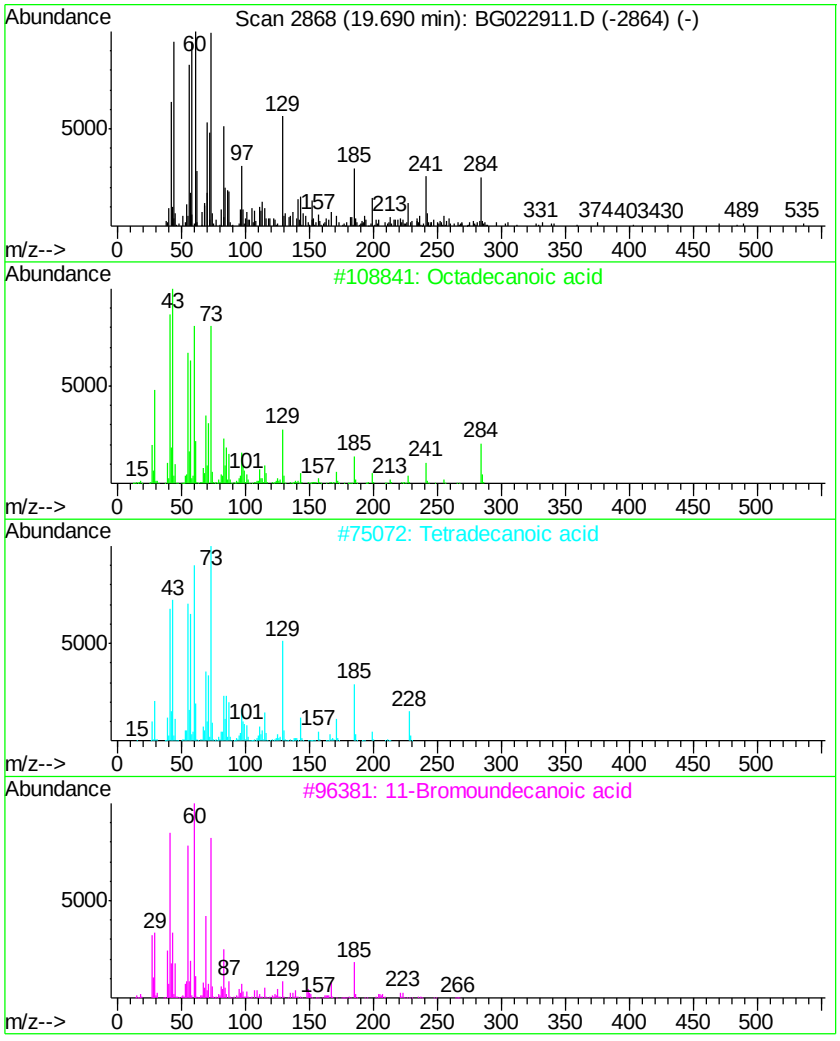
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

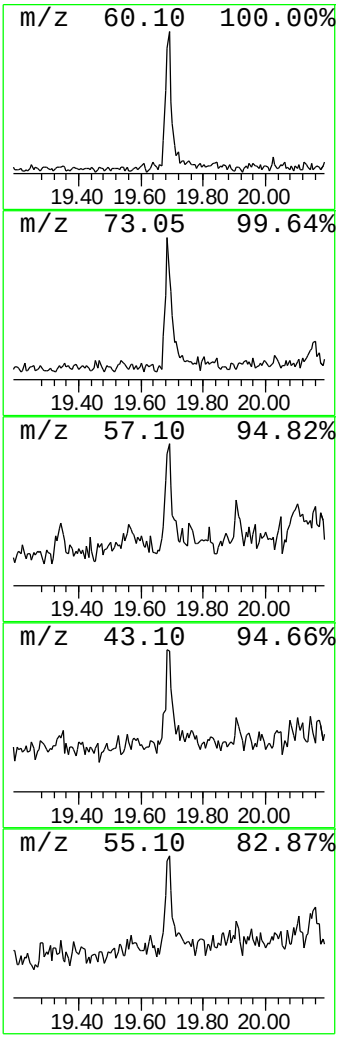
****

Peak Number 10 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.19 ng	384849	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Undecanoic acid	186	C11H22O2	000112-37-8	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG070816\
Data File : BG022911.D
Acq On : 8 Jul 2016 1:23
Operator : UM/SJ
Sample : H3834-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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(3H)-Furanone, d...	7.00	3.7	ng	173009	1	8.16	943151	20.0
unknown7.50	7.50	4.3	ng	201620	1	8.16	943151	20.0
unknown7.68	7.68	92.0	ng	4339780	1	8.16	943151	20.0
1H-Pyrazolo[3,4-d...	11.63	2.1	ng	140972	2	10.98	1315540	20.0
unknown11.87	11.87	2.2	ng	146051	2	10.98	1315540	20.0
1(3H)-Isobenzofur...	13.21	2.1	ng	204378	3	14.80	1969730	20.0
unknown17.20	17.20	2.5	ng	296404	4	17.56	2416000	20.0
n-Hexadecanoic acid	18.42	2.9	ng	353514	4	17.56	2416000	20.0
Octadecanoic acid	19.69	3.2	ng	384849	4	17.56	2416000	20.0