LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013118\
Data File : BG032464.D
Acq On : 31 Jan 2018 14:13
Operator : SJ/JU
Sample : J1364-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

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-BG012918.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	3.378	7	15	24	rBV4	28647	83452	3.12%	0.711%
2	3.466	24	30	40	rVB2	86370	167641	6.27%	1.428%
3	5.405	348	360	367	rBV2	17013	52131	1.95%	0.444%
4	6.157	481	488	498	rBV2	116928	238792	8.93%	2.034%
5	7.173	647	661	672	rBV3	20764	65564	2.45%	0.558%
6	7.831	767	773	788	rBV2	74507	184507	6.90%	1.571%
7	8.225	832	840	856	rBV	257380	530956	19.86%	4.522%
8	8.713	916	923	934	rBV	95528	184110	6.89%	1.568%
9	9.047	971	980	990	rBV	401486	766083	28.65%	6.525%
10	9.488	1049	1055	1067	rBV	39779	85514	3.20%	0.728%
11	9.911	1118	1127	1141	rBV	281812	557746	20.86%	4.750%
12	11.592	1406	1413	1425	rBV	133583	262966	9.83%	2.240%
13	12.103	1493	1500	1516	rBV	36361	100749	3.77%	0.858%
14	13.043	1653	1660	1672	rVB	38773	74819	2.80%	0.637%
15	13.313	1701	1706	1712	rBV3	21439	42720	1.60%	0.364%
16	13.971	1811	1818	1831	rBV	1111600	1798217	67.25%	15.315%
17	14.770	1947	1954	1960	rBV	50711	82275	3.08%	0.701%
18	15.346	2045	2052	2060	rBV2	248544	421602	15.77%	3.591%
19	16.821	2296	2303	2314	rBV	660535	1059316	39.62%	9.022%
20	18.078	2510	2517	2525	rBV2	329245	532485	19.91%	4.535%
21	18.901	2652	2657	2666	rVB2	91683	139803	5.23%	1.191%
22	20.140	2864	2868	2875	rBV	107249	160047	5.99%	1.363%
23	20.616	2943	2949	2956	rBV	2006836	2673994	100.00%	22.774%
24	21.950	3172	3176	3182	rVB9	32258	55126	2.06%	0.469%
25	22.408	3247	3254	3261	rBV2	384162	688955	25.77%	5.868%
26	26.092	3870	3881	3892	rVB	219729	731985	27.37%	6.234%

Sum of corrected areas: 11741555

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013118\
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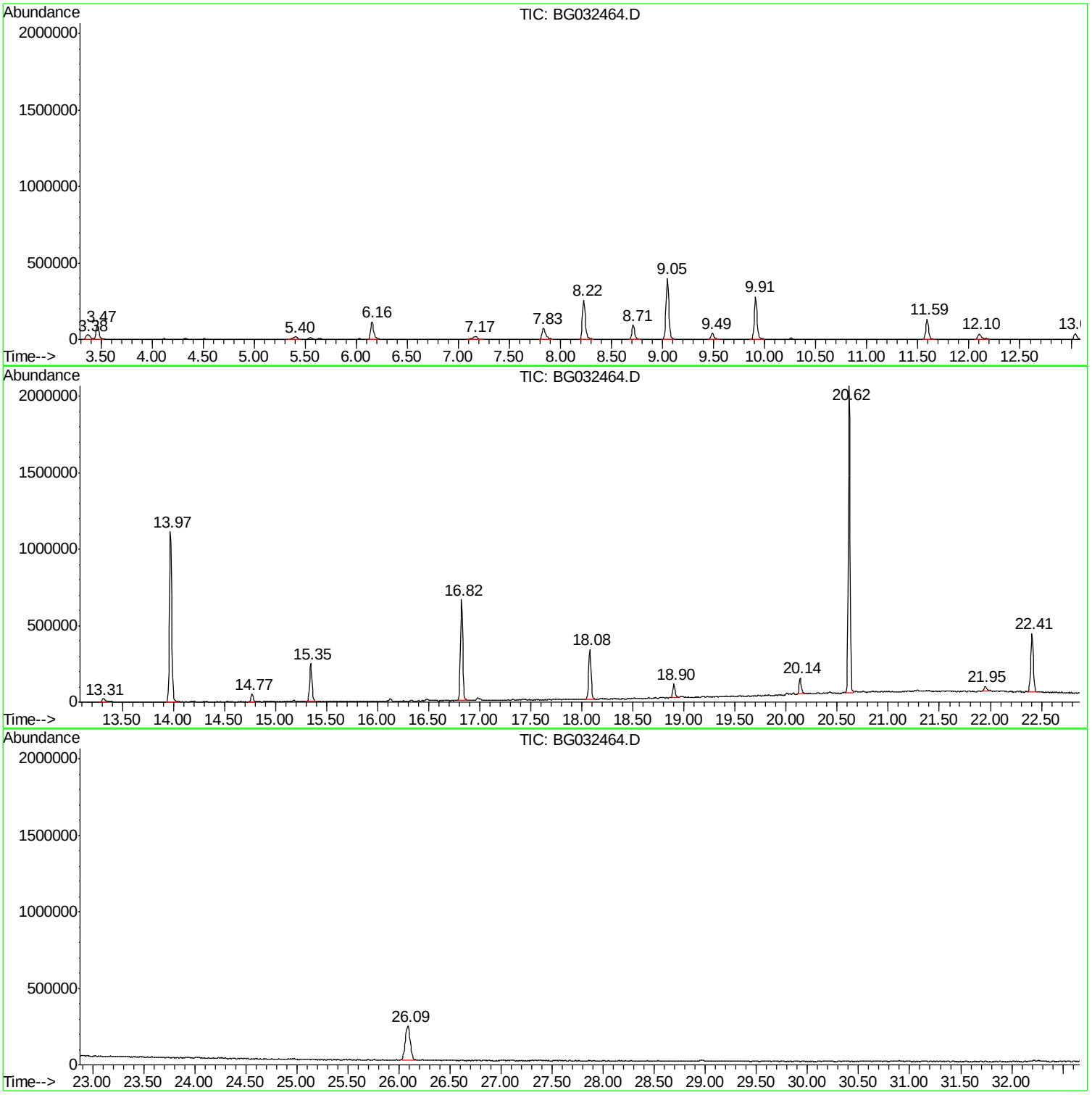
Acq On : 31 Jan 2018 14:13
Operator : SJ/JU
Sample : J1364-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Operator : SJ/JU
Sample : J1364-17
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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

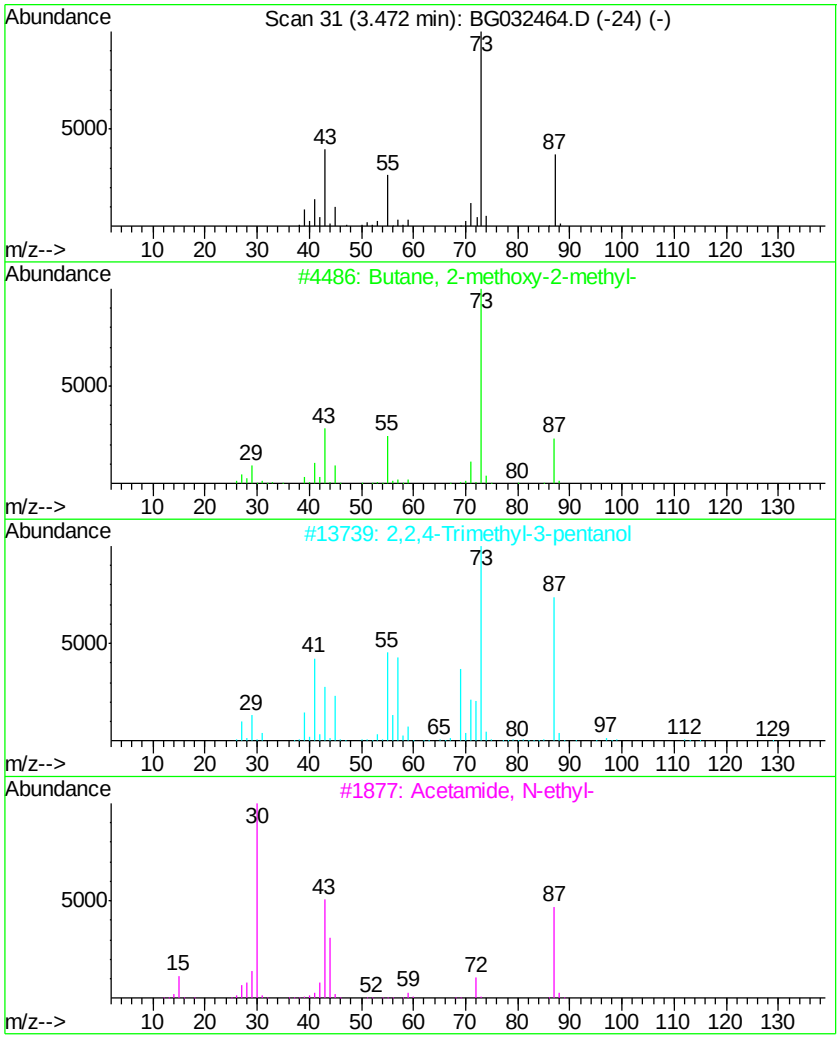
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

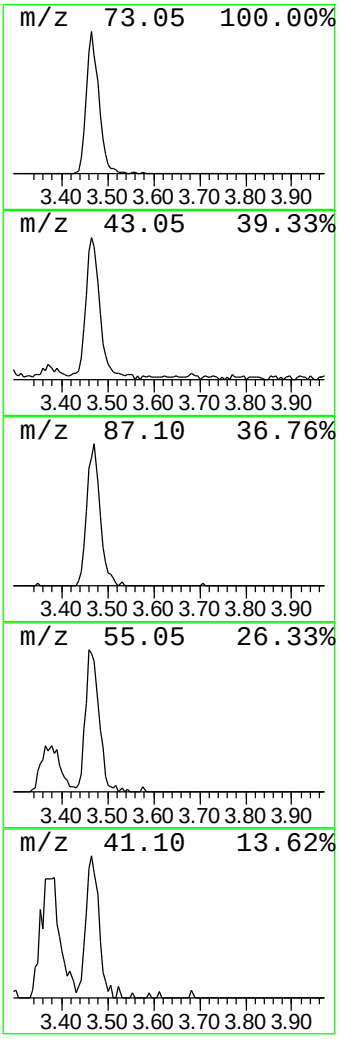
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.47	18.21 ng	167641	1,4-Dichlorobenzene-d4	8.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Data File : BG032464.D
Acq On : 31 Jan 2018 14:13
Operator : SJ/JU
Sample : J1364-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

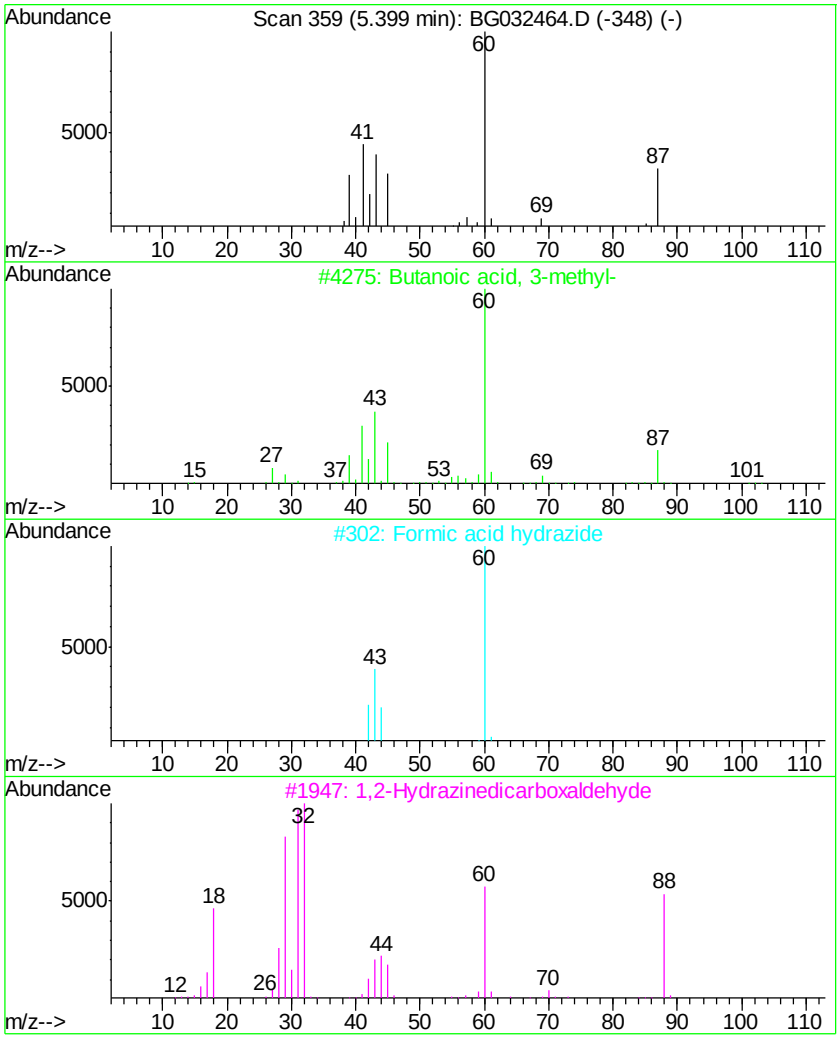
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

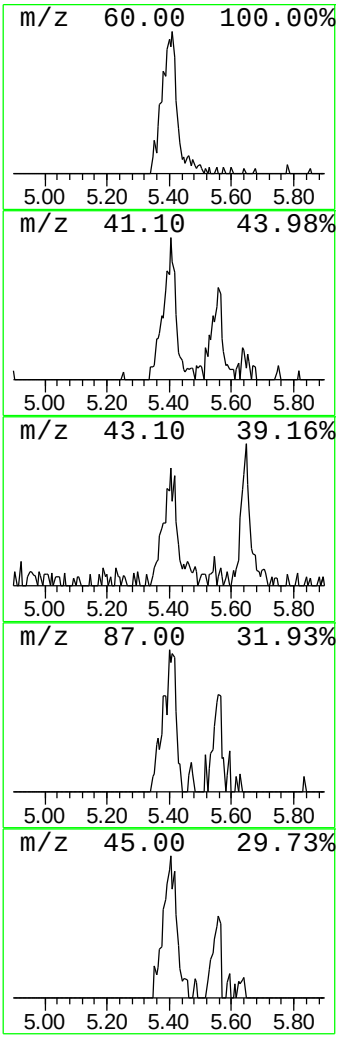
****

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.40	5.66 ng	52131	1,4-Dichlorobenzene-d4	8.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2	Formic acid hydrazide	60	CH4N2O	000624-84-0	50
3	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	38
4	(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	10
5	Butanoic acid	88	C4H8O2	000107-92-6	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG013118\
Data File : BG032464.D
Acq On : 31 Jan 2018 14:13
Operator : SJ/JU
Sample : J1364-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

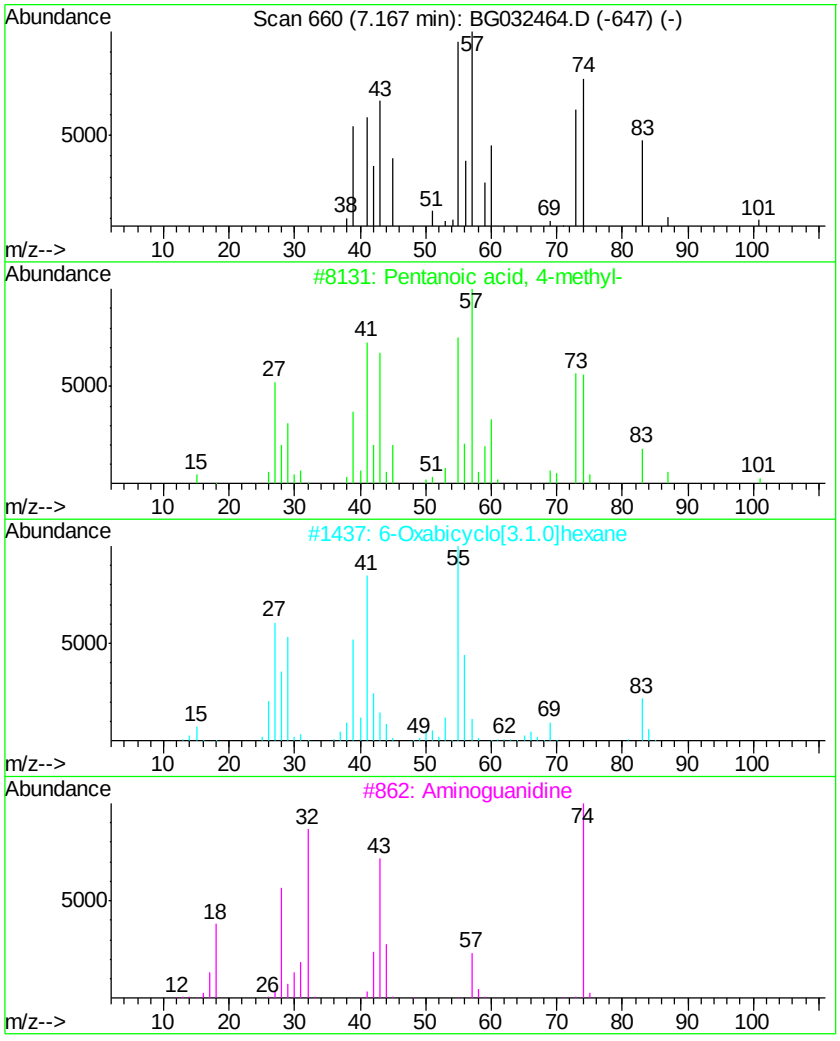
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

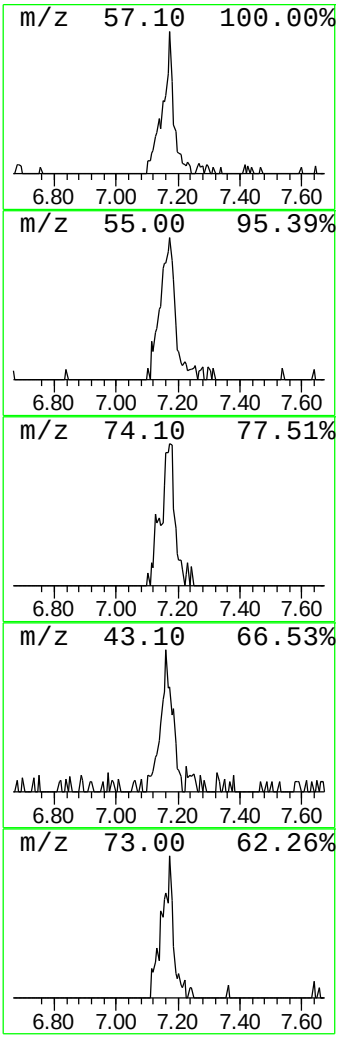
****

Peak Number 4 Pentanoic acid, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	7.12 ng	65564	1,4-Dichlorobenzene-d4	8.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	64
2	6-Oxabicyclo[3.1.0]hexane	84	C5H8O	000285-67-6	11
3	Aminoguanidine	74	CH6N4	000079-17-4	9
4	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	9
5	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013118\
Data File : BG032464.D
Acq On : 31 Jan 2018 14:13
Operator : SJ/JU
Sample : J1364-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

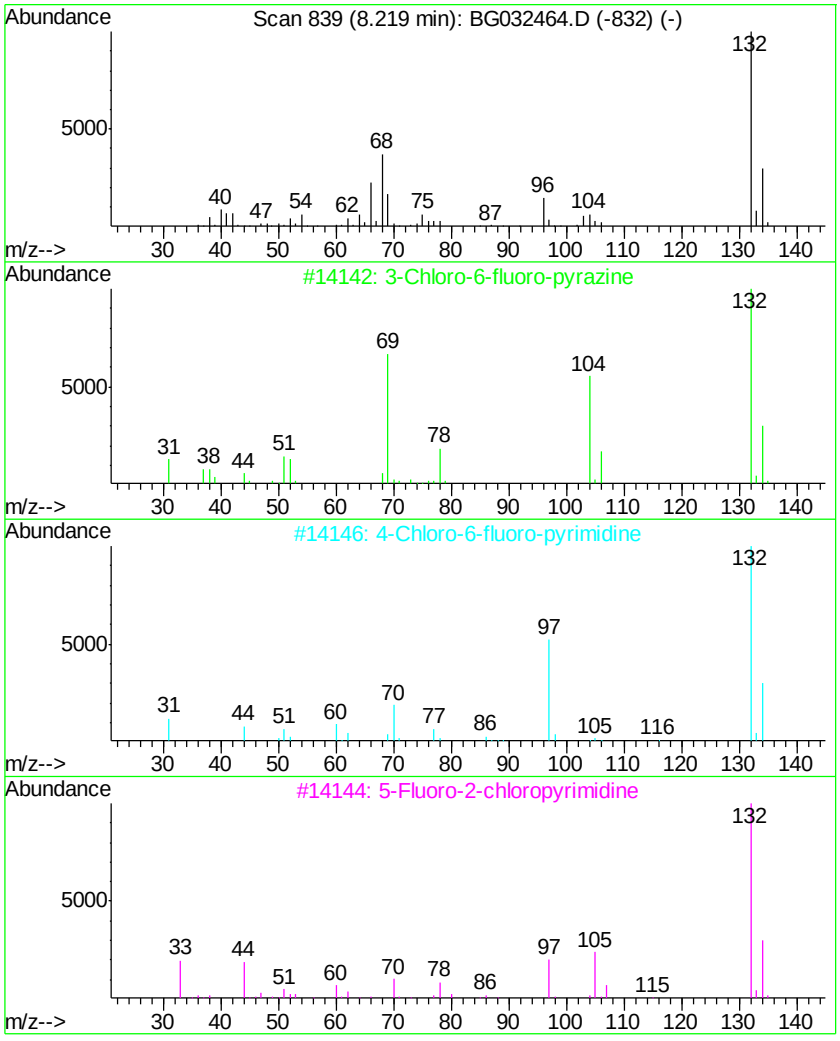
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

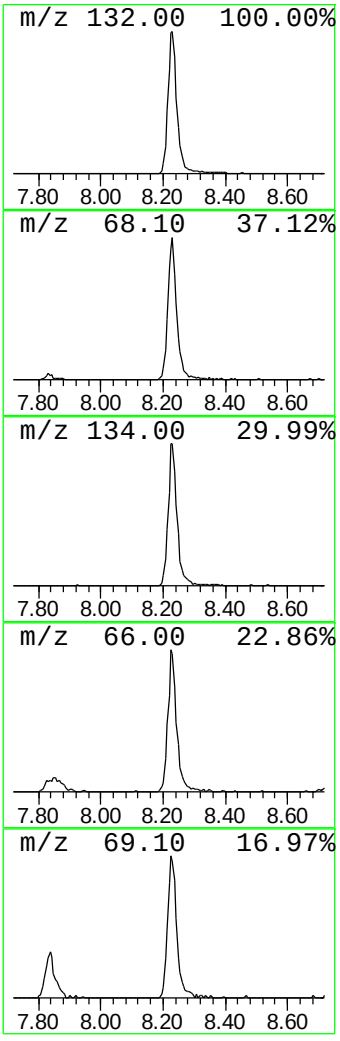
****

Peak Number 5 unknown8.22 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.22	57.68 ng	530956	1,4-Dichlorobenzene-d4	8.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG013118\
Data File : BG032464.D
Acq On : 31 Jan 2018 14:13
Operator : SJ/JU
Sample : J1364-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

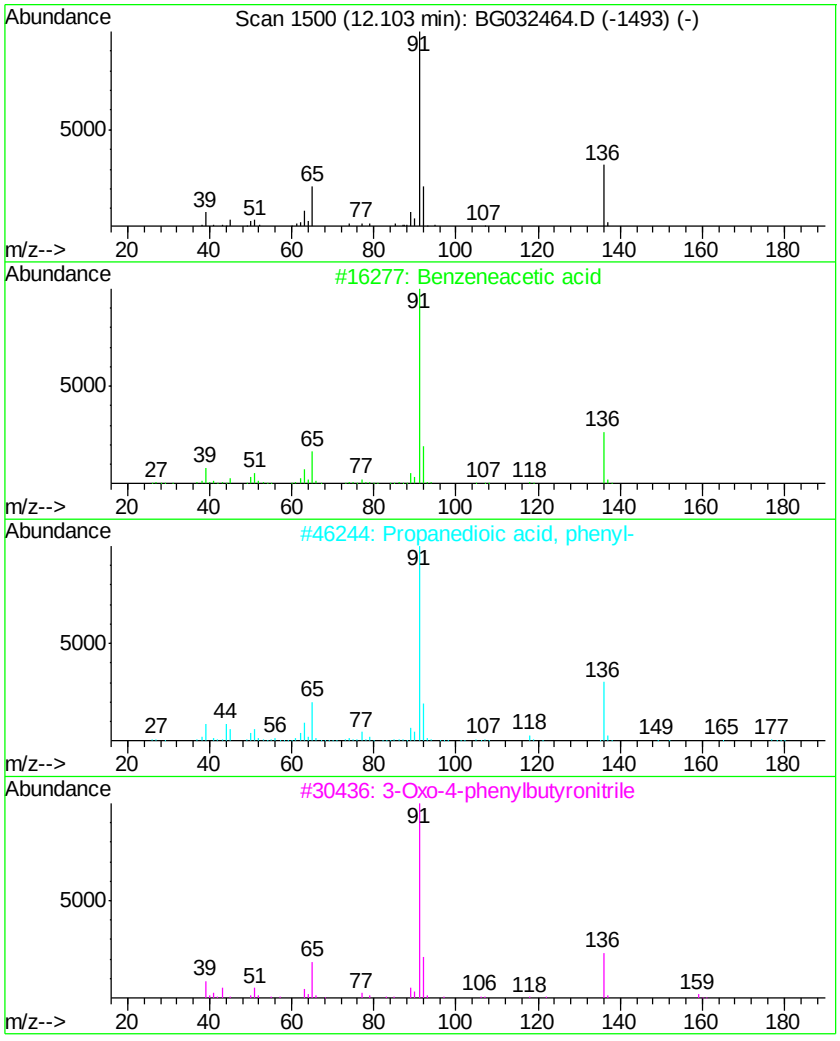
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

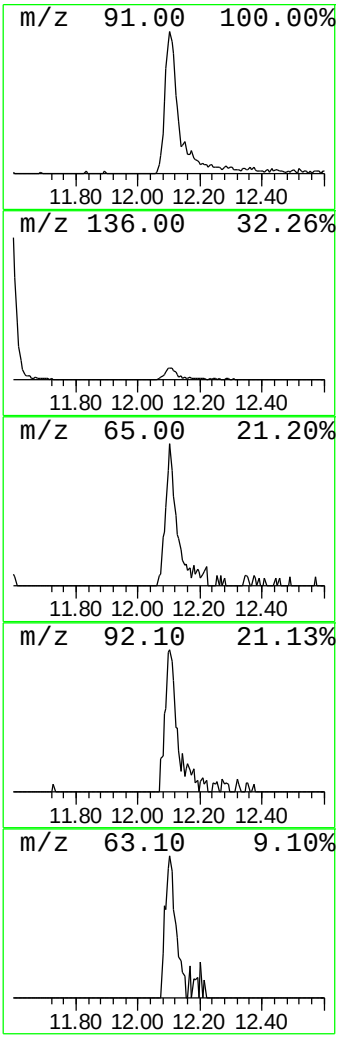
****

Peak Number 7 Benzeneacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	7.66 ng	100749	Naphthalene-d8	11.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	91
2	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	74
3	3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	59
4	Benzeneacetaldehyde	120	C8H8O	000122-78-1	53
5	Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	47





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Operator : SJ/JU
Sample : J1364-17
Misc :
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Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

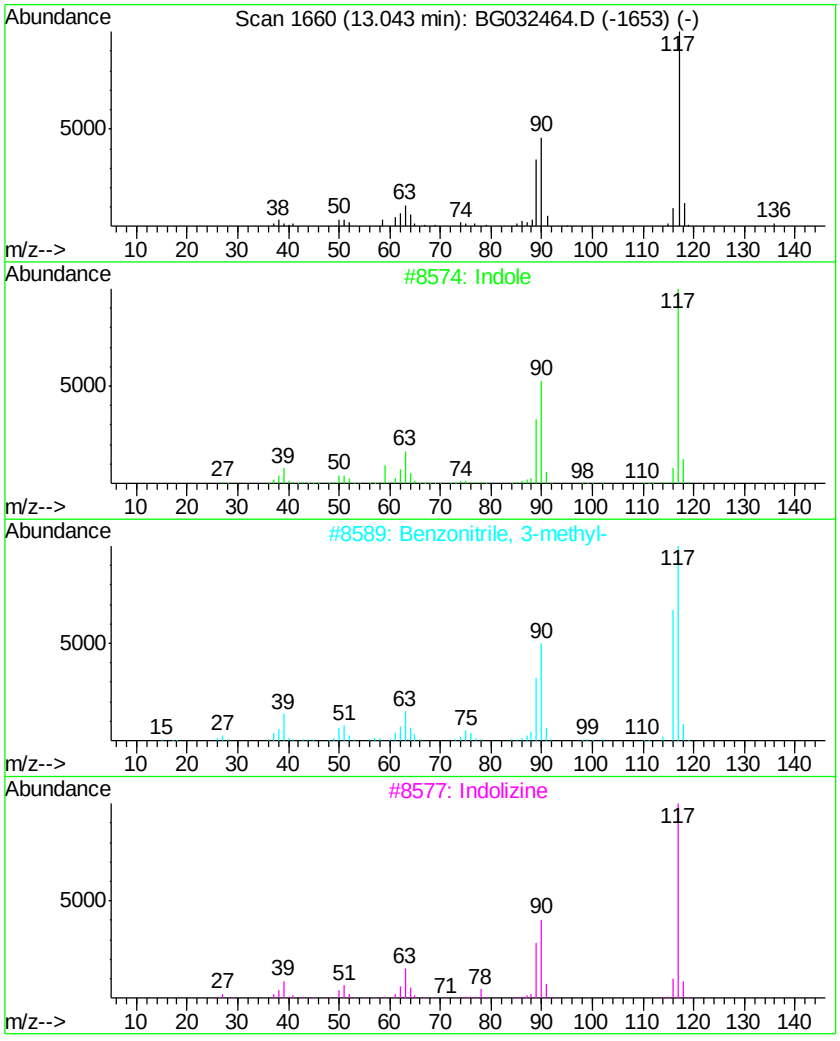
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

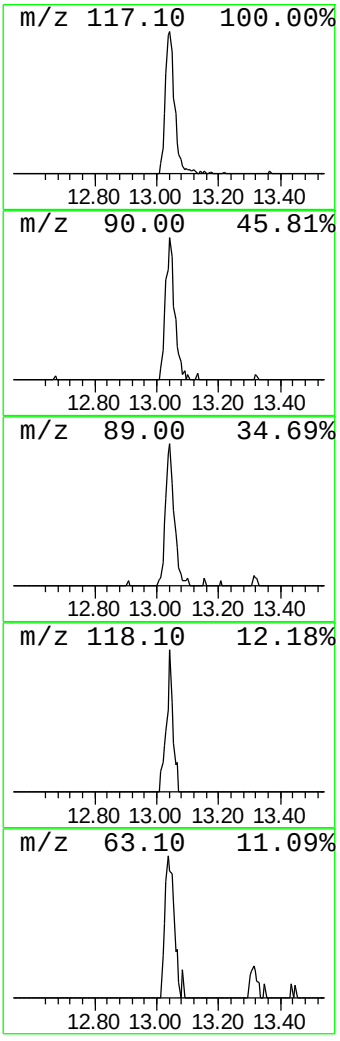
****

Peak Number 8 Indole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.04	5.69 ng	74819	Naphthalene-d8	11.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	94
2	Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	91
3	Indolizine	117	C8H7N	000274-40-8	91
4	Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	91
5	Benzyl nitrile	117	C8H7N	000140-29-4	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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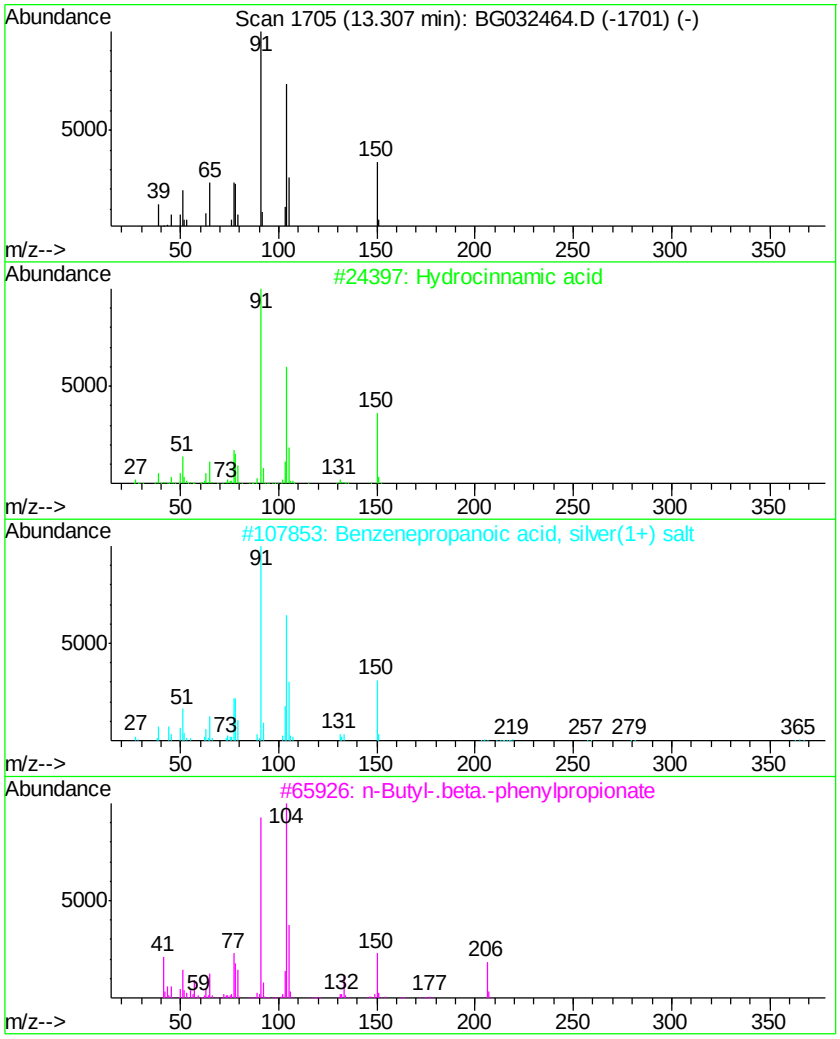
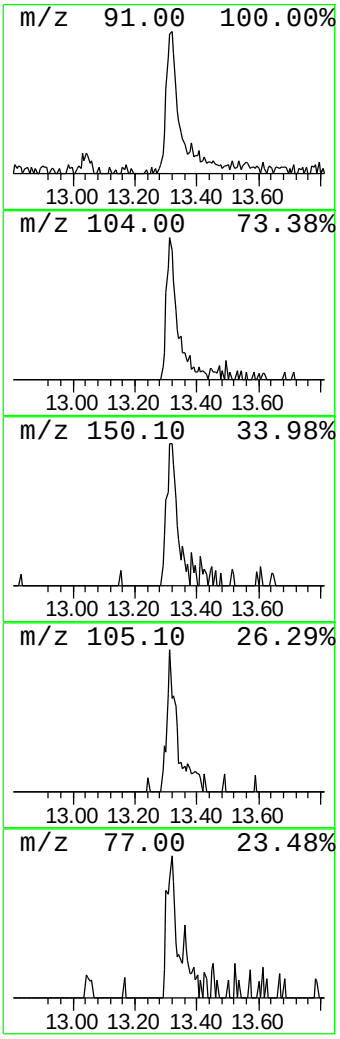
****

Peak Number 9 Hydrocinnamic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.31	3.25 ng	42720	Naphthalene-d8	11.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	83
2	Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	80
3	n-Butyl-.beta.-phenylpropionate	206	C13H18O2	020627-49-0	59
4	Acetic acid, trifluoro-, 2-phenyl...	218	C10H9F3O2	055419-66-4	47
5	3H-2-Benzopyran-3-imine, 1,4-dih...	147	C9H9NO	038866-67-0	43





Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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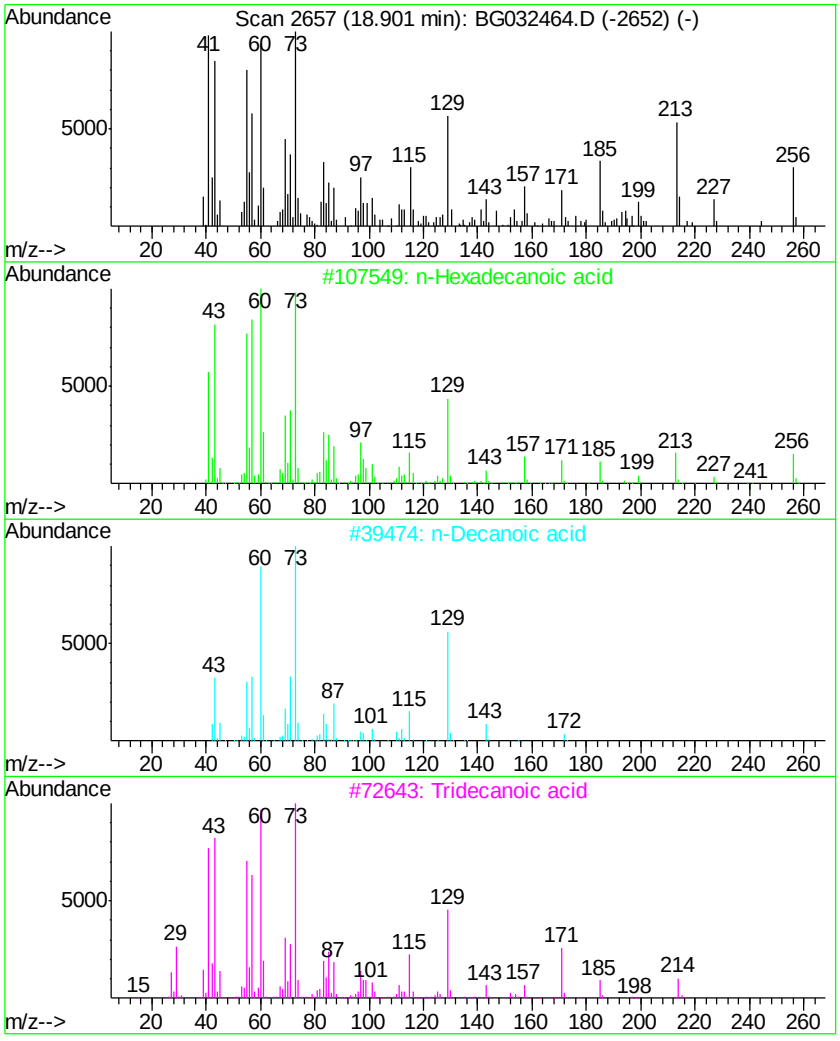
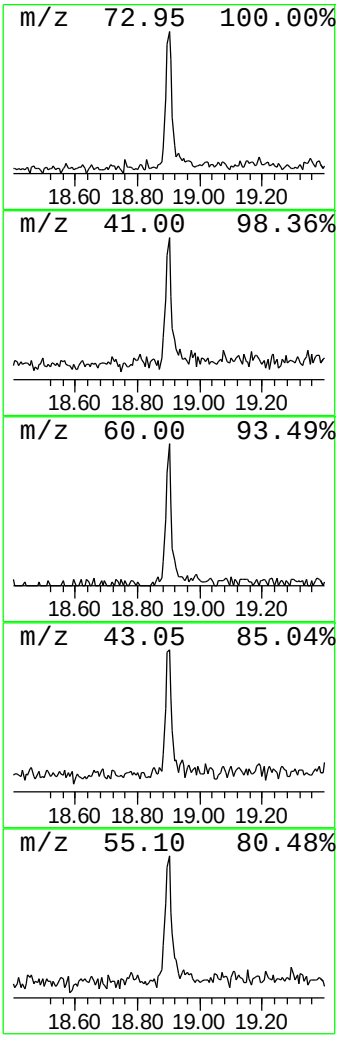
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.90	5.25 ng	139803	Phenanthrene-d10	18.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

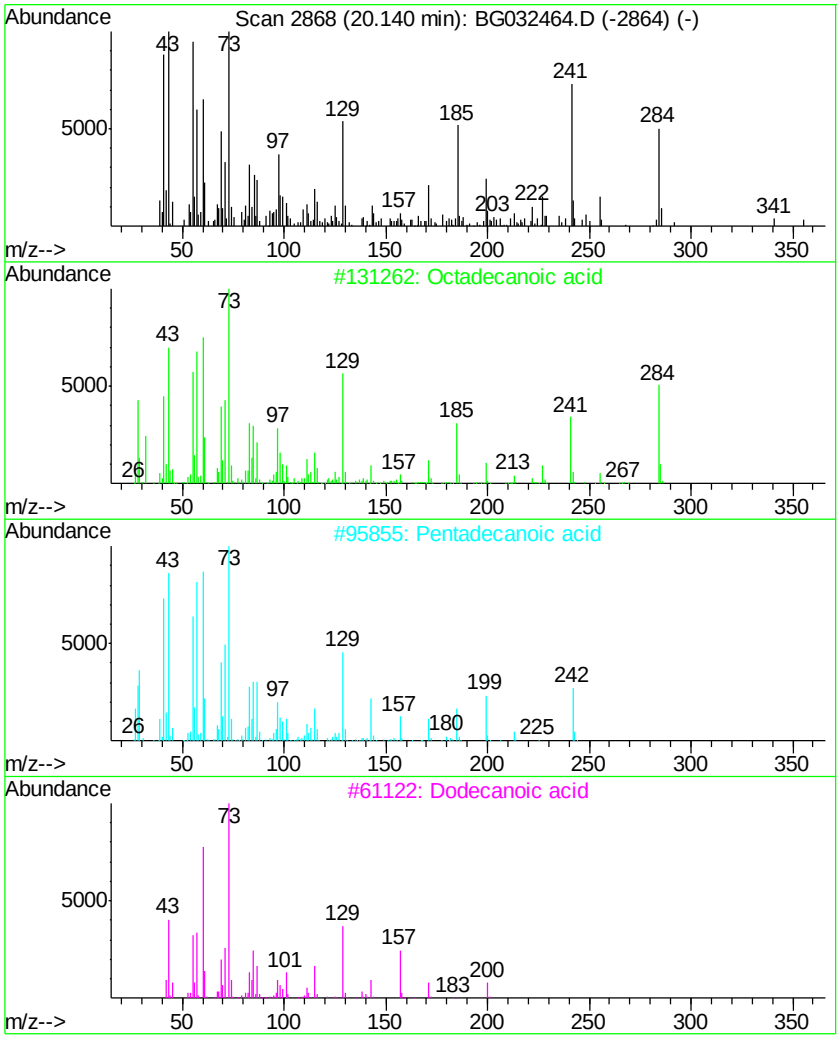
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

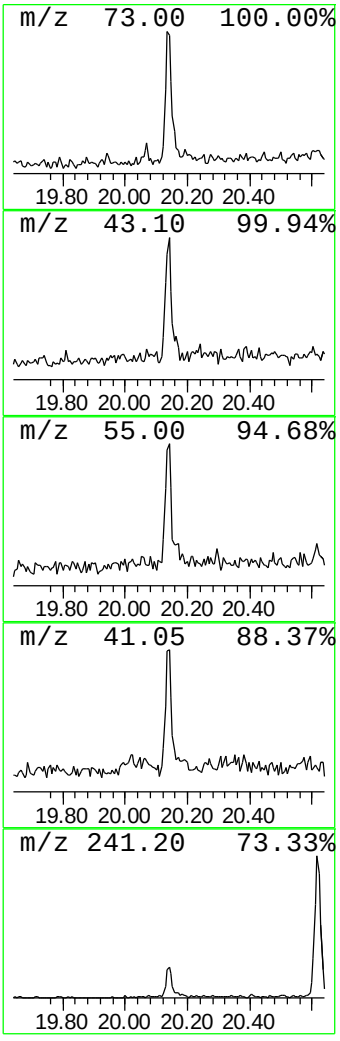
****

Peak Number 11 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.14	6.01 ng	160047	Phenanthrene-d10	18.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	41
3	Dodecanoic acid	200	C12H24O2	000143-07-7	41
4	Tridecanoic acid	214	C13H26O2	000638-53-9	30
5	1-Methyl-1-n-decyloxy-1-silacycl...	256	C15H32OSi	1000216-91-2	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG013118\
Data File : BG032464.D
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Operator : SJ/JU
Sample : J1364-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-07

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.47	18.2	ng	167641	1	8.71	184110	20.0
Butanoic acid, 3-...	5.40	5.7	ng	52131	1	8.71	184110	20.0
Pentanoic acid, 4...	7.17	7.1	ng	65564	1	8.71	184110	20.0
unknown8.22	8.22	57.7	ng	530956	1	8.71	184110	20.0
Benzeneacetic acid	12.10	7.7	ng	100749	2	11.59	262966	20.0
Indole	13.04	5.7	ng	74819	2	11.59	262966	20.0
Hydrocinnamic acid	13.31	3.3	ng	42720	2	11.59	262966	20.0
n-Hexadecanoic acid	18.90	5.3	ng	139803	4	18.08	532485	20.0
Octadecanoic acid	20.14	6.0	ng	160047	4	18.08	532485	20.0