LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120117\
Data File : BG031343.D
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

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-BG111017.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	5.204	322	326	337	rVB	36849	65108	1.21%	0.264%
2	5.685	402	408	418	rBV	446254	804953	15.02%	3.269%
3	7.295	672	682	696	rBV	283442	585955	10.93%	2.379%
4	7.507	711	718	729	rBV	78493	134936	2.52%	0.548%
5	7.660	736	744	757	rBV	884763	1603471	29.91%	6.511%
6	8.130	817	824	838	rBV	208503	398019	7.43%	1.616%
7	8.453	865	879	893	rBV	855284	1550759	28.93%	6.297%
8	8.764	925	932	939	rBV3	40886	80409	1.50%	0.327%
9	9.234	1006	1012	1016	rBV	78170	131761	2.46%	0.535%
10	9.299	1016	1023	1044	rVB	630595	1328848	24.79%	5.396%
11	9.763	1094	1102	1107	rBV2	55473	99665	1.86%	0.405%
12	10.333	1193	1199	1207	rVB3	85261	160241	2.99%	0.651%
13	10.944	1290	1303	1309	rBV	291564	613560	11.45%	2.491%
14	12.812	1614	1621	1627	rVB	44424	80958	1.51%	0.329%
15	13.371	1708	1716	1729	rBV	2087774	3383454	63.12%	13.739%
16	14.751	1943	1951	1961	rBV2	496084	858028	16.01%	3.484%
17	16.238	2197	2204	2214	rBV	1590043	2596085	48.43%	10.542%
18	16.432	2231	2237	2250	rBV3	27689	62712	1.17%	0.255%
19	17.489	2410	2417	2426	rBV	727135	1151169	21.48%	4.674%
20	18.359	2560	2565	2573	rBV2	198785	328821	6.13%	1.335%
21	19.622	2775	2780	2790	rBV	246169	433820	8.09%	1.762%
22	20.080	2852	2858	2871	rBV	4015048	5360143	100.00%	21.765%
23	21.373	3075	3078	3088	rBV5	58889	120572	2.25%	0.490%
24	21.761	3138	3144	3154	rVB2	812062	1348234	25.15%	5.475%
25	25.057	3695	3705	3719	rVB2	443763	1345244	25.10%	5.462%

Sum of corrected areas: 24626925

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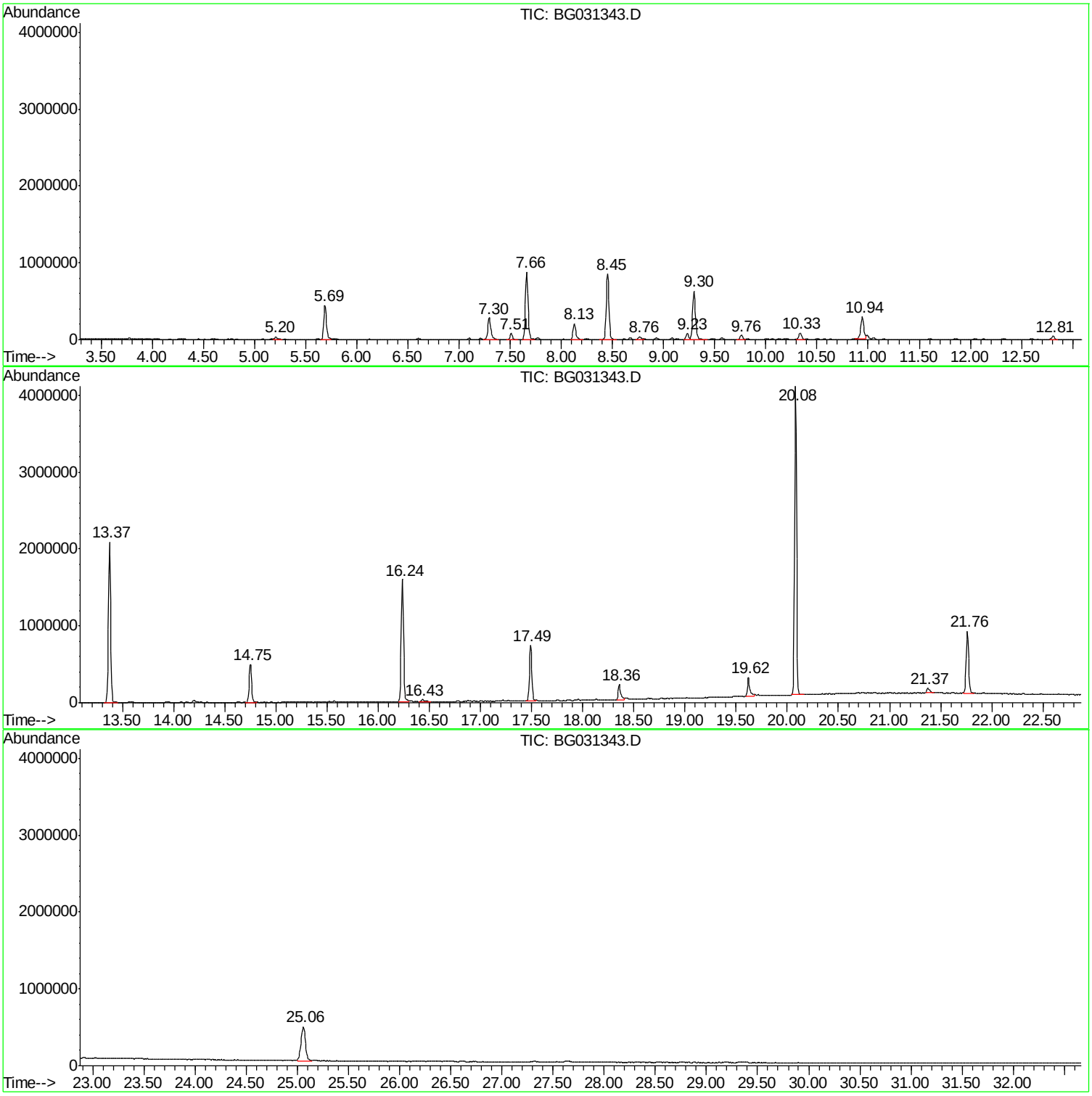
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120117\
Data File : BG031343.D
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

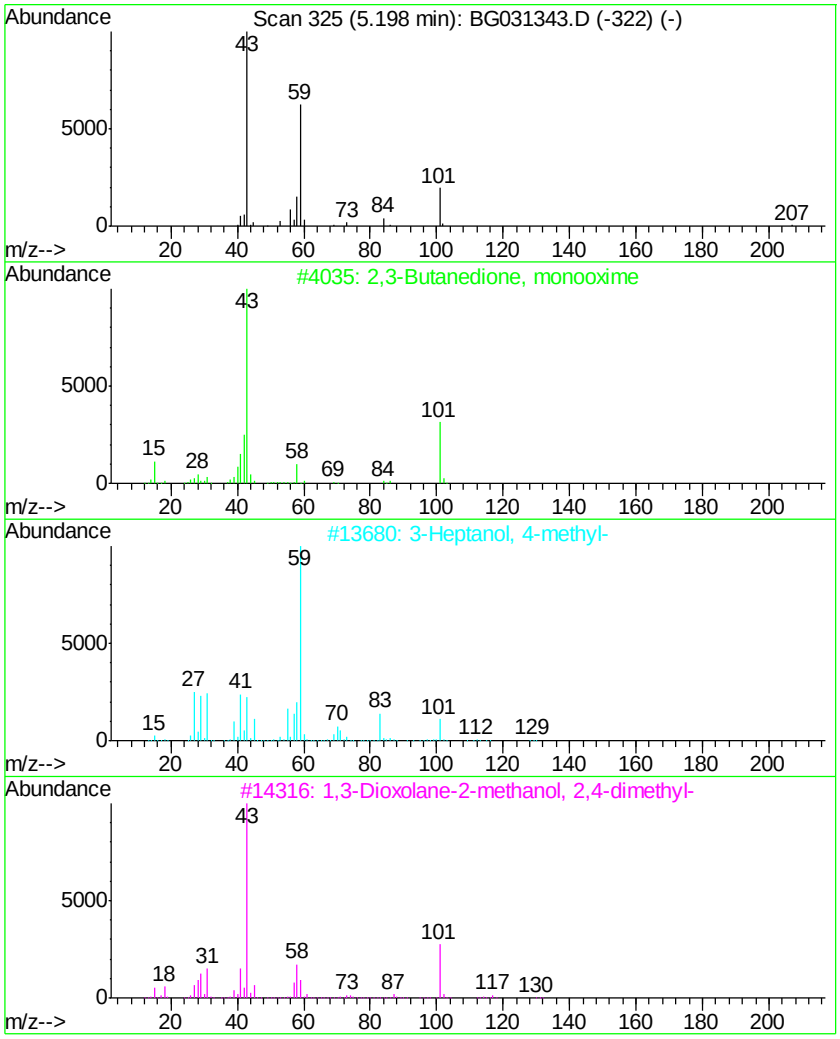
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

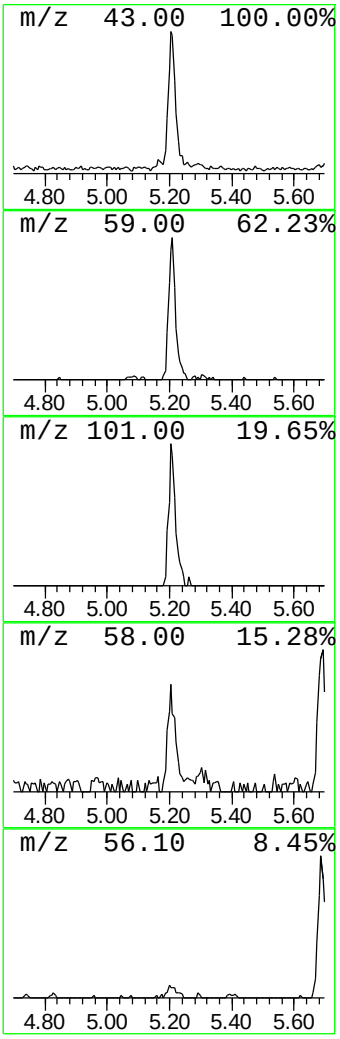
****

Peak Number 1 unknown5.20 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.27 ng	65108	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	37
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Data File : BG031343.D
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

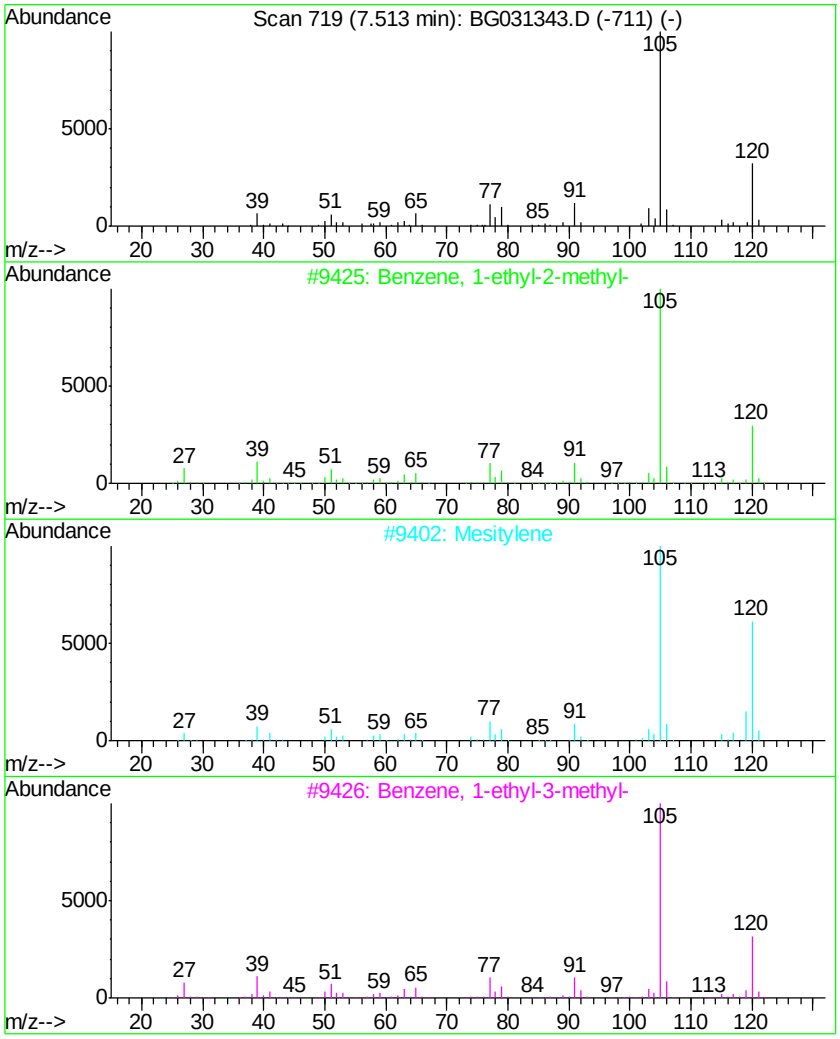
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

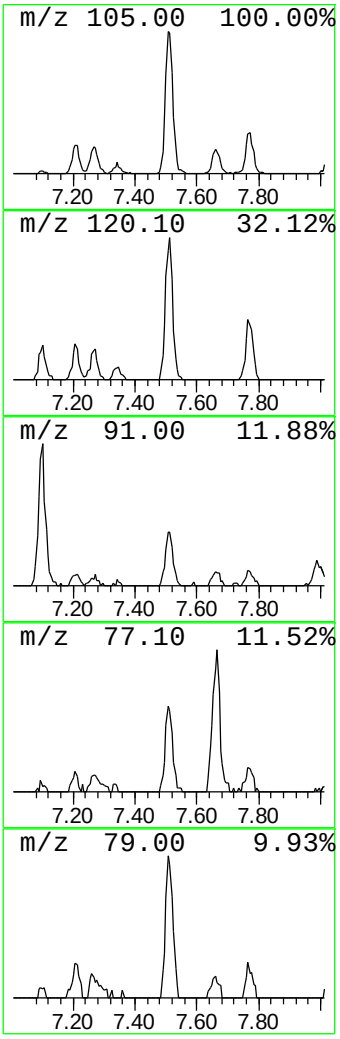
****

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.51	6.78 ng	134936	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120117\
Data File : BG031343.D
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

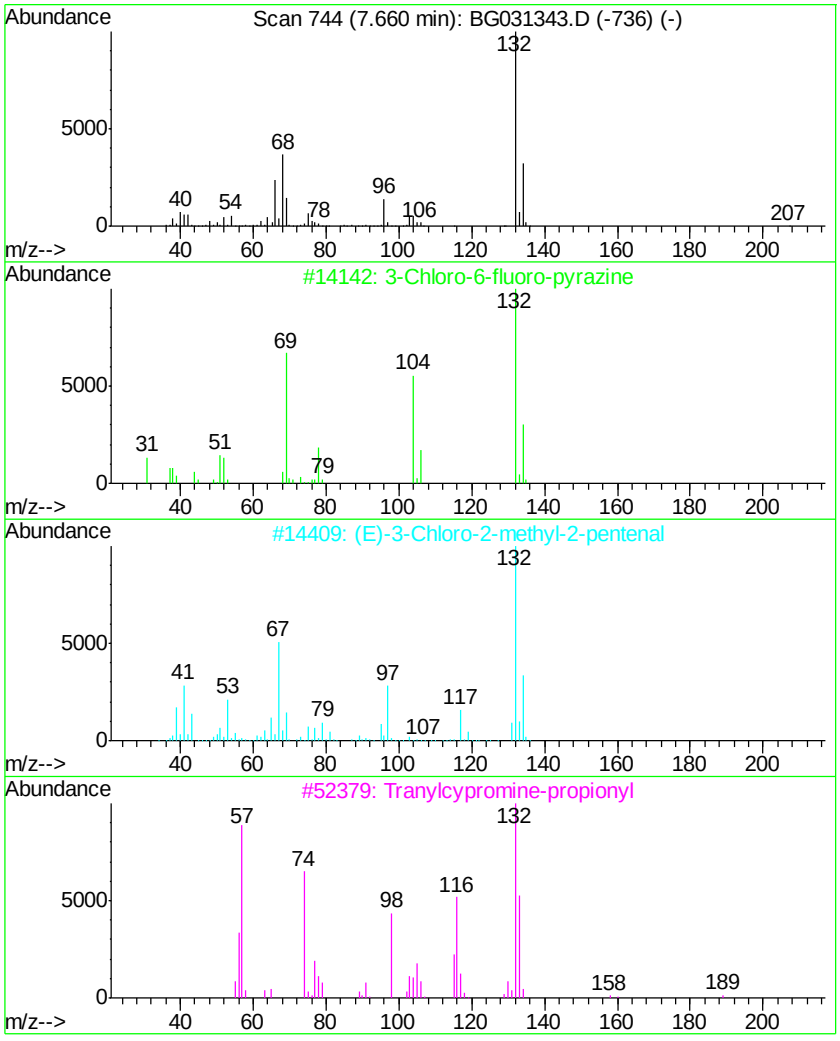
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

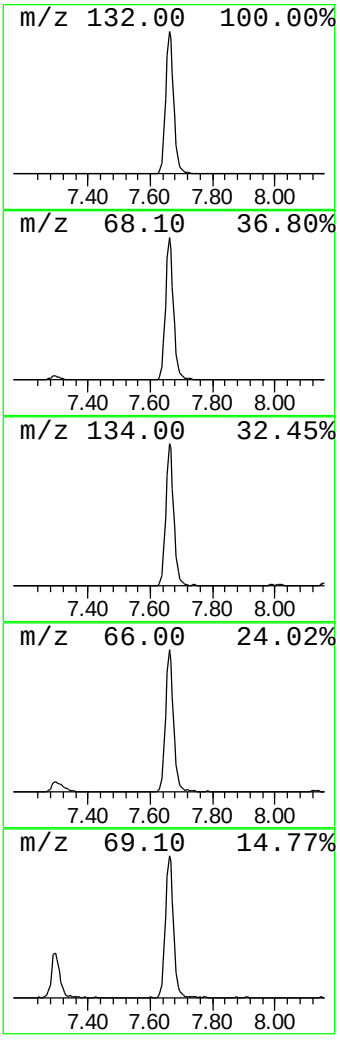
****

Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	80.57 ng	1603470	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120117\
Data File : BG031343.D
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

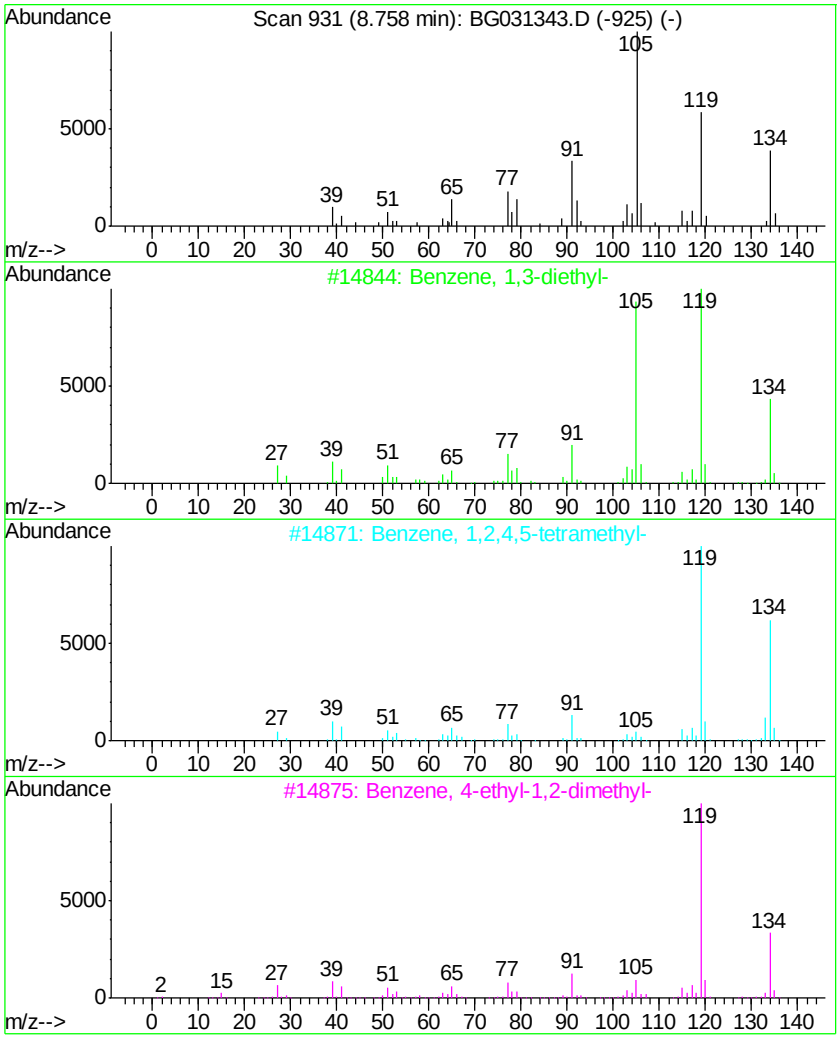
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

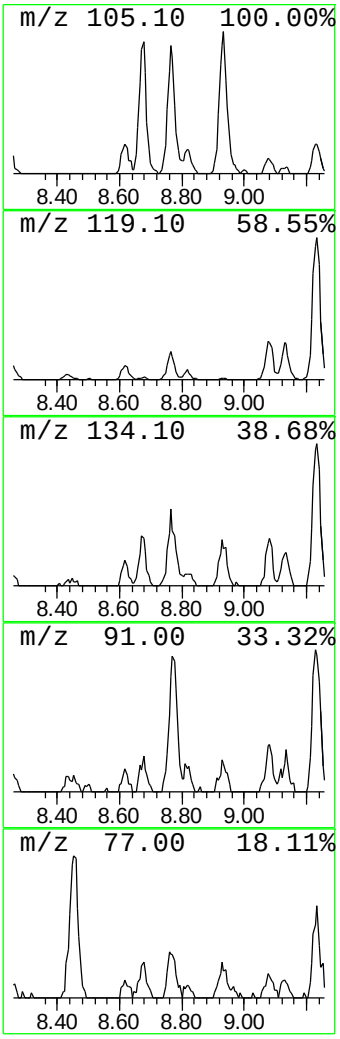
****

Peak Number 5 Benzene, 1,3-diethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	4.04 ng	80409	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	78
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	74
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	68
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	68
5	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	68





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120117\
Data File : BG031343.D
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

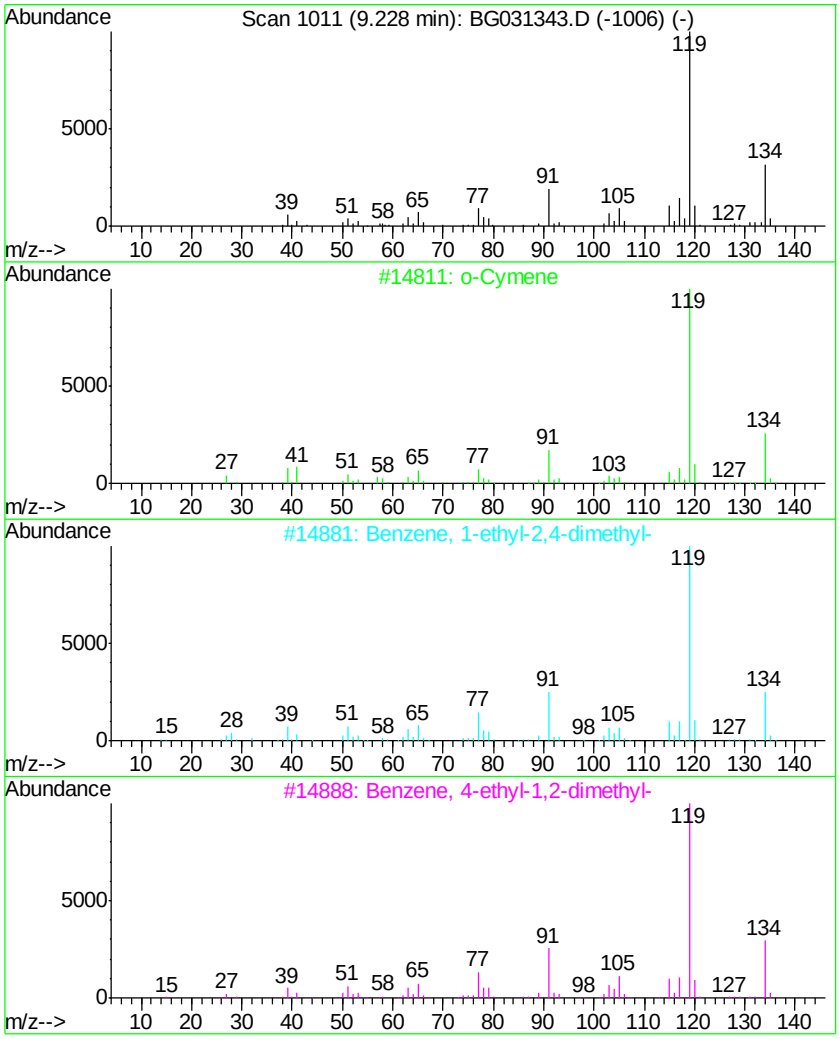
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

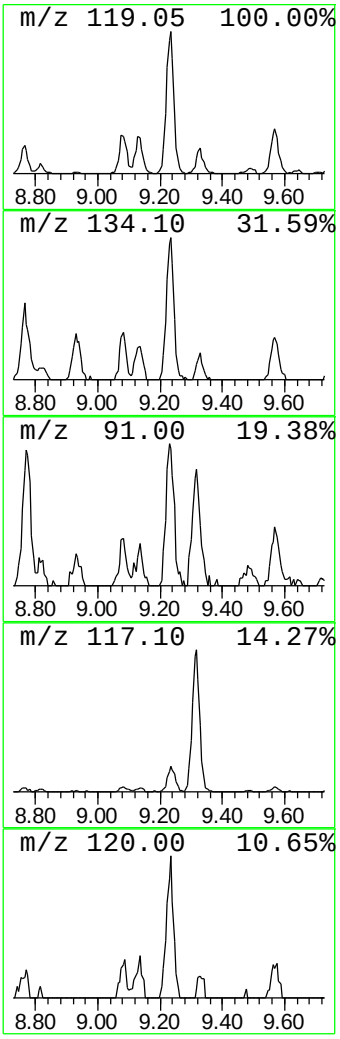
****

Peak Number 6 o-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.23	6.62 ng	131761	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
4	p-Cymene	134	C10H14	000099-87-6	93
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93





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Data File : BG031343.D
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Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

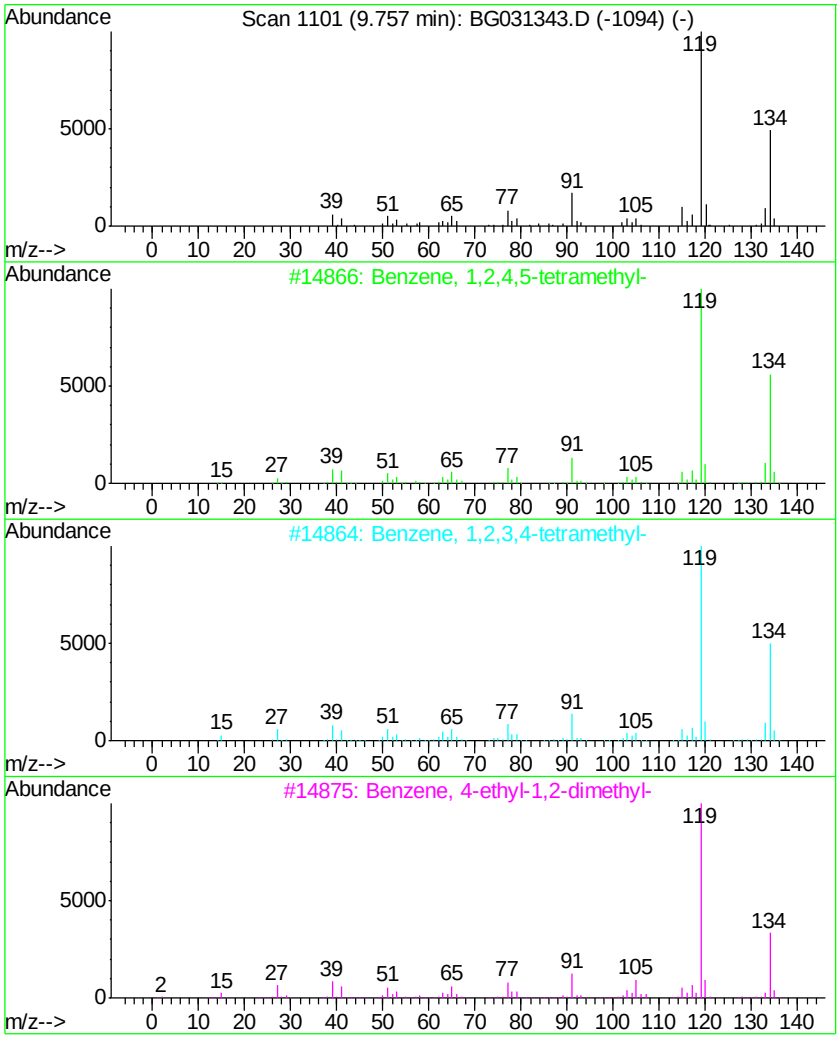
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

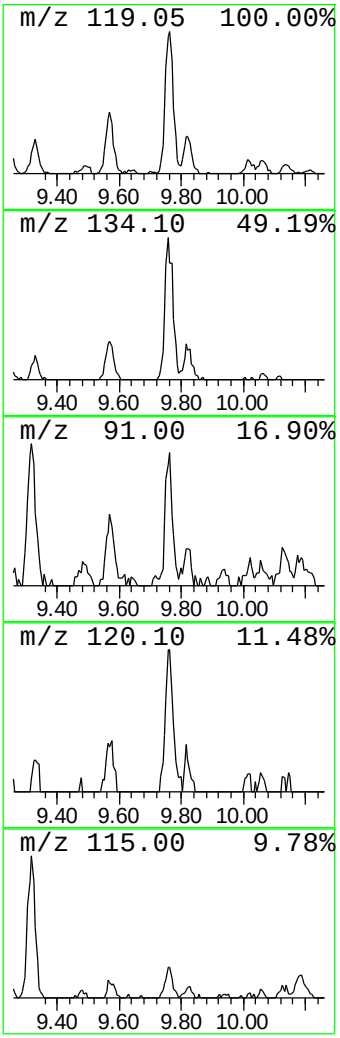
****

Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.25 ng	99665	Naphthalene-d8	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91





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Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

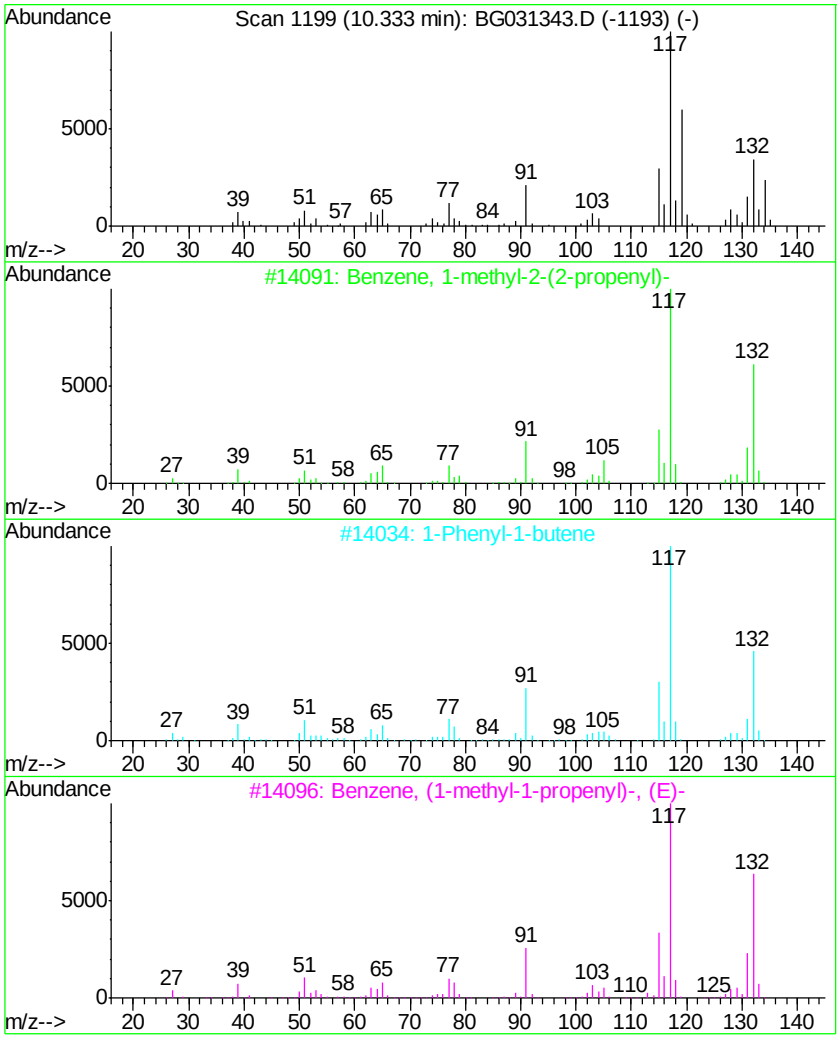
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

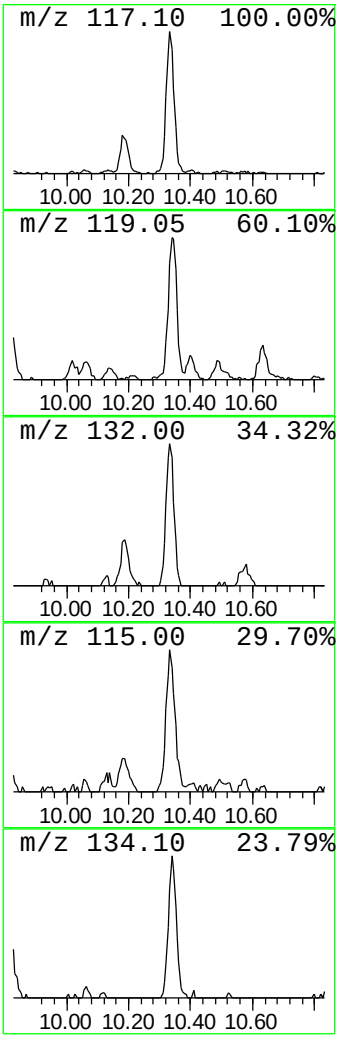
****

Peak Number 8 Benzene, 1-methyl-2-(2-prop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	5.22 ng	160241	Naphthalene-d8	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	70
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	62
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	62





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Sample : I6653-02
Misc :
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Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
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TIC Library : C:\Database\NIST11.L
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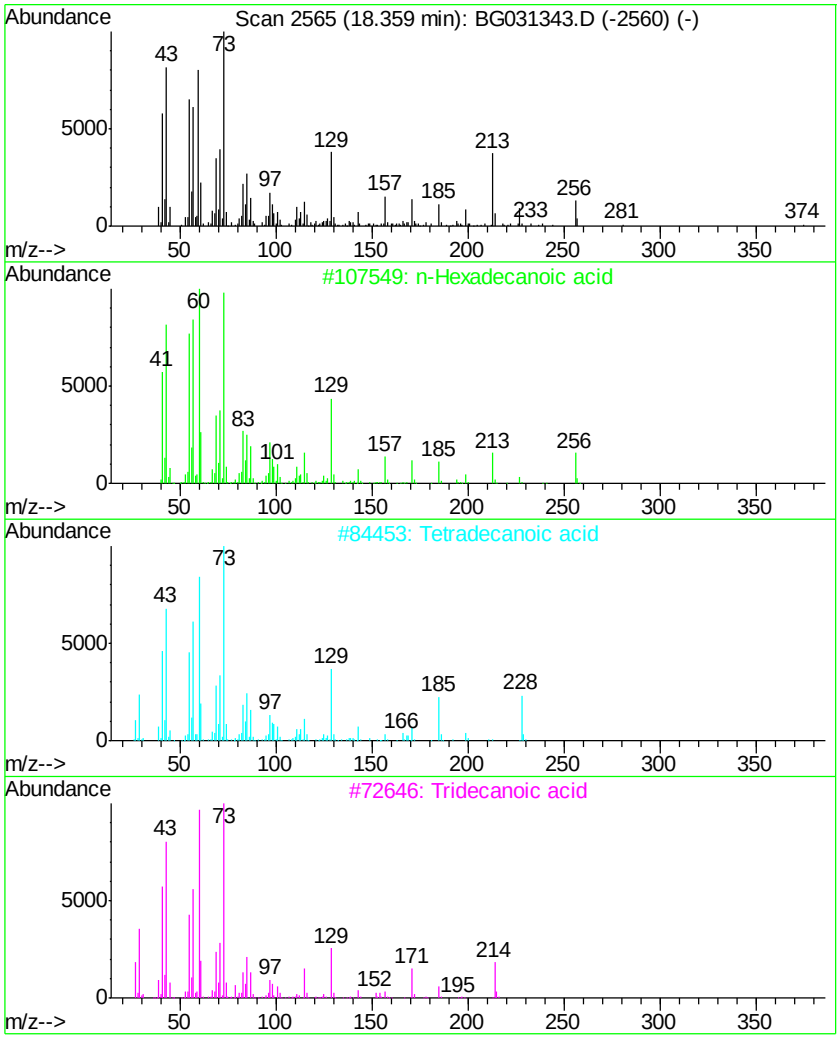
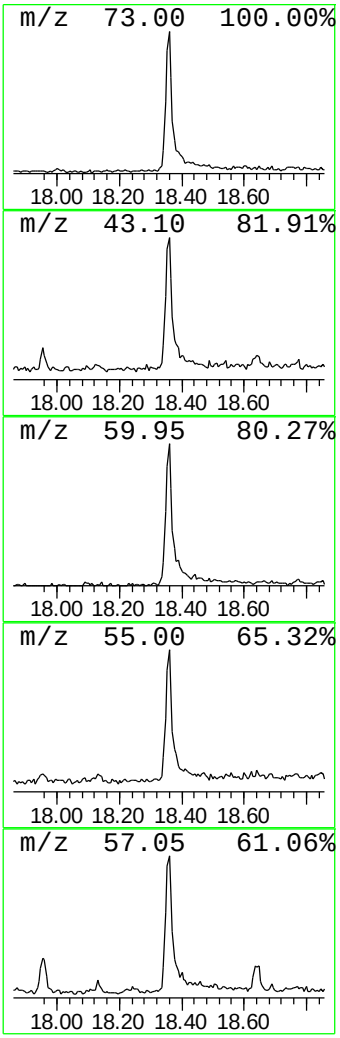
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	5.71 ng	328821	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Octadecanoic acid	284	C18H36O2	000057-11-4	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

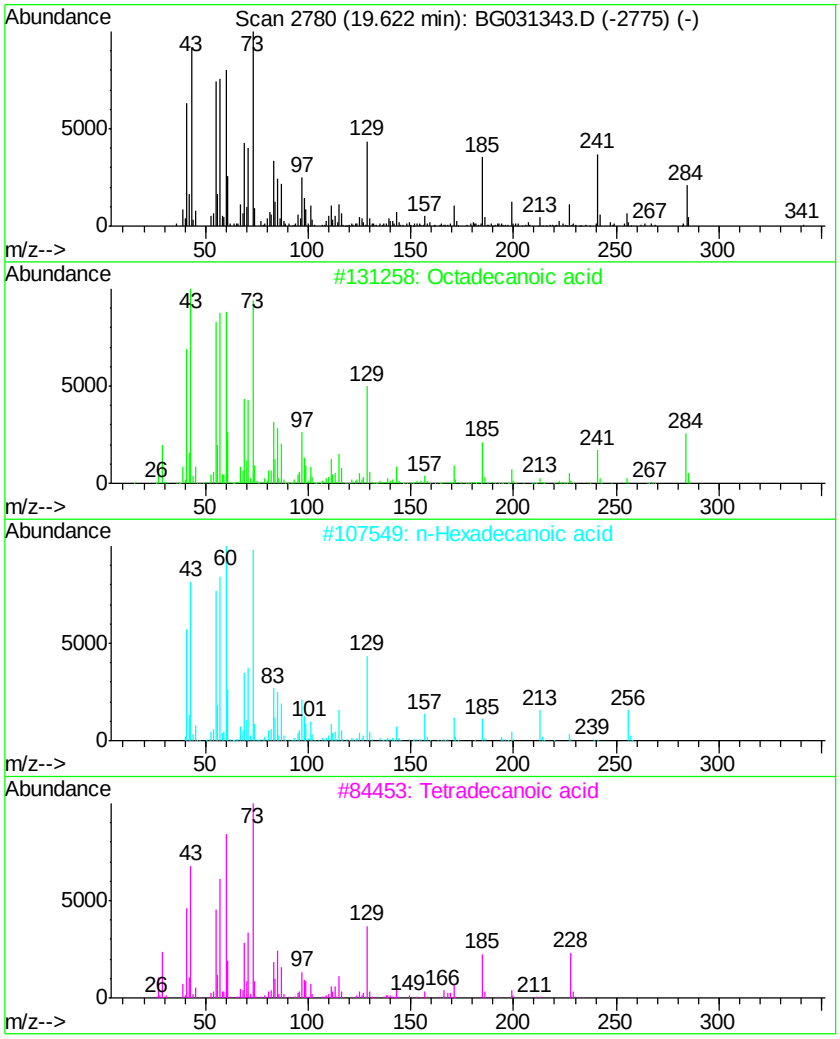
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

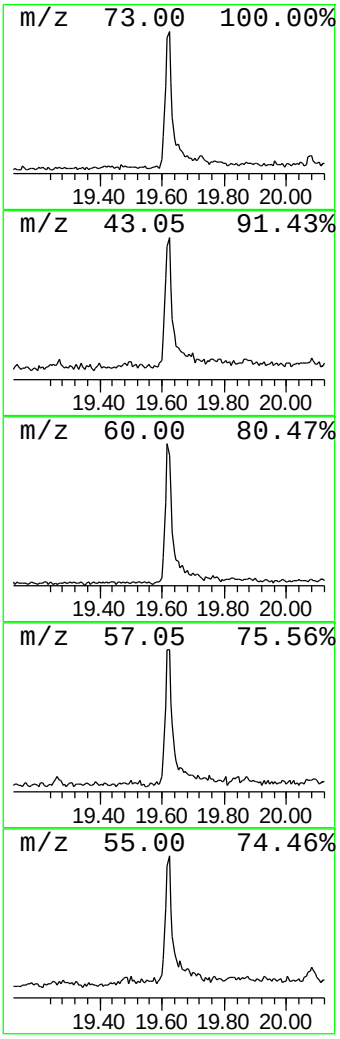
****

Peak Number 10 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	7.54 ng	433820	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120117\
Data File : BG031343.D
Acq On : 2 Dec 2017 7:37
Operator : SJ/JU
Sample : I6653-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG111017.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
unknown5.20	5.20	3.3	ng	65108	1	8.13	398019	20.0
Benzene, 1-ethyl-...	7.51	6.8	ng	134936	1	8.13	398019	20.0
unknown7.66	7.66	80.6	ng	1603470	1	8.13	398019	20.0
Benzene, 1,3-diet...	8.76	4.0	ng	80409	1	8.13	398019	20.0
o-Cymene	9.23	6.6	ng	131761	1	8.13	398019	20.0
Benzene, 1,2,4,5-...	9.76	3.3	ng	99665	2	10.94	613560	20.0
Benzene, 1-methyl...	10.33	5.2	ng	160241	2	10.94	613560	20.0
n-Hexadecanoic acid	18.36	5.7	ng	328821	4	17.49	1151170	20.0
Octadecanoic acid	19.62	7.5	ng	433820	4	17.49	1151170	20.0