LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033255.D
Acq On : 20 Mar 2018 00:44
Operator : SJ/JU
Sample : J1953-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-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_G\METHODS\8270-BG031918.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	3.499	29	36	47	rBV2	153516	320249	8.46%	2.007%
2	3.587	47	51	58	rVB	99322	148666	3.93%	0.932%
3	6.313	508	515	532	rBV2	144970	351178	9.28%	2.201%
4	6.848	601	606	620	rBV	37000	93149	2.46%	0.584%
5	8.000	793	802	819	rBV2	83556	279253	7.38%	1.750%
6	8.405	863	871	888	rBV	325715	750781	19.83%	4.705%
7	8.893	948	954	970	rBV2	98251	232416	6.14%	1.457%
8	9.228	1003	1011	1024	rBV	507130	1030993	27.24%	6.461%
9	10.091	1149	1158	1176	rBV	404857	945714	24.98%	5.927%
10	11.778	1438	1445	1457	rBV	145138	327925	8.66%	2.055%
11	14.139	1837	1847	1867	rBV	1390054	2402733	63.47%	15.058%
12	14.927	1975	1981	1993	rBV2	29853	55598	1.47%	0.348%
13	15.332	2045	2050	2057	rBV	35760	47878	1.26%	0.300%
14	15.508	2073	2080	2092	rBV2	294478	538037	14.21%	3.372%
15	16.272	2206	2210	2215	rVB3	59908	78767	2.08%	0.494%
16	16.719	2282	2286	2291	rVV2	54425	74758	1.97%	0.469%
17	16.977	2324	2330	2343	rBV	848804	1492102	39.42%	9.351%
18	17.124	2351	2355	2366	rVB2	50178	97518	2.58%	0.611%
19	18.241	2538	2545	2558	rBV	450900	794535	20.99%	4.979%
20	19.034	2676	2680	2687	rBV2	95199	142508	3.76%	0.893%
21	20.755	2967	2973	2984	rBV	2703106	3785441	100.00%	23.723%
22	22.101	3197	3202	3217	rBV3	100156	204237	5.40%	1.280%
23	22.594	3278	3286	3298	rVB	469380	910867	24.06%	5.708%
24	26.384	3920	3931	3945	rBV2	241148	851438	22.49%	5.336%

Sum of corrected areas: 15956741

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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Operator : SJ/JU
Sample : J1953-06
Misc :
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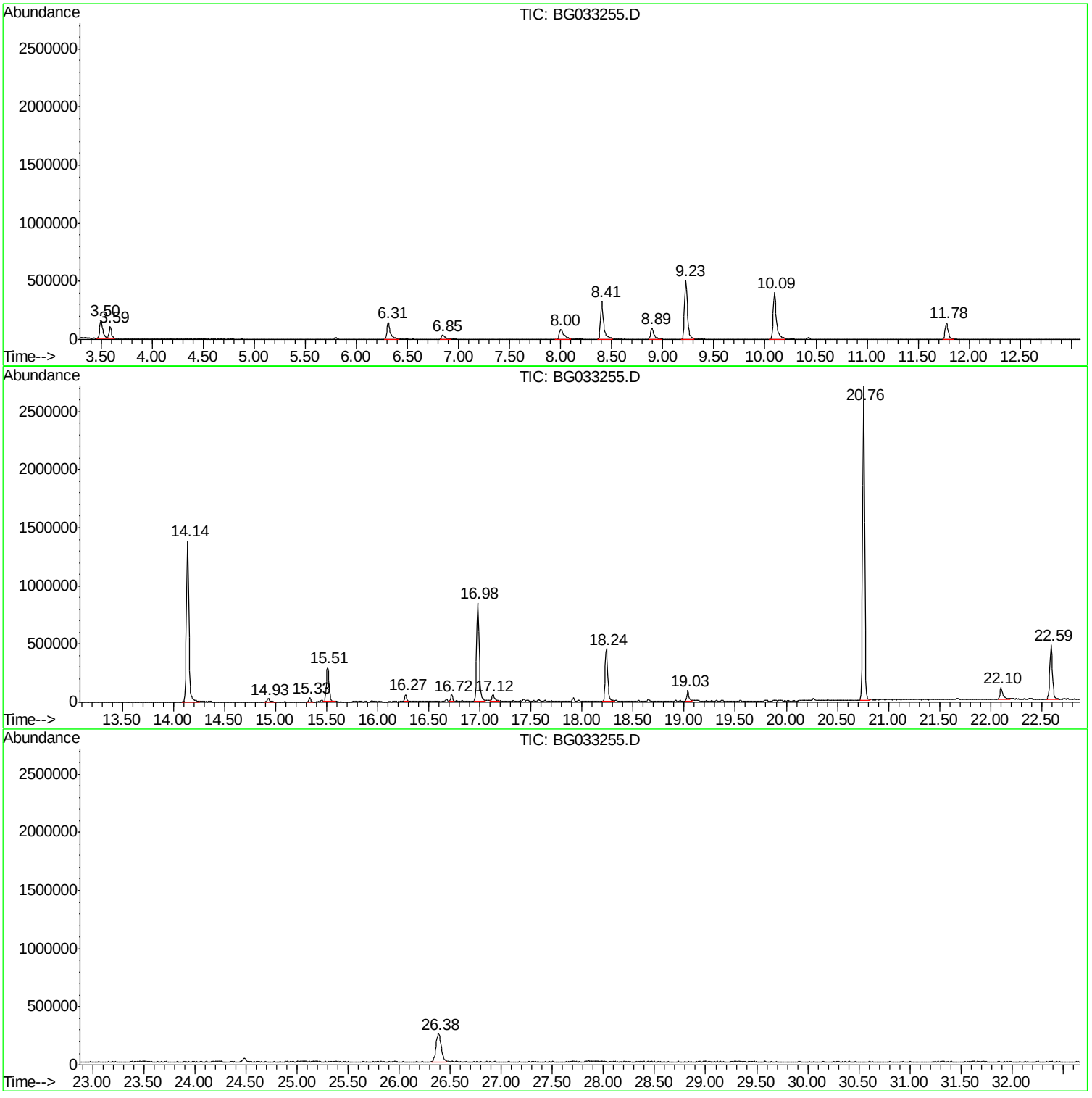
Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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\BG031918\
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Operator : SJ/JU
Sample : J1953-06
Misc :
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ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

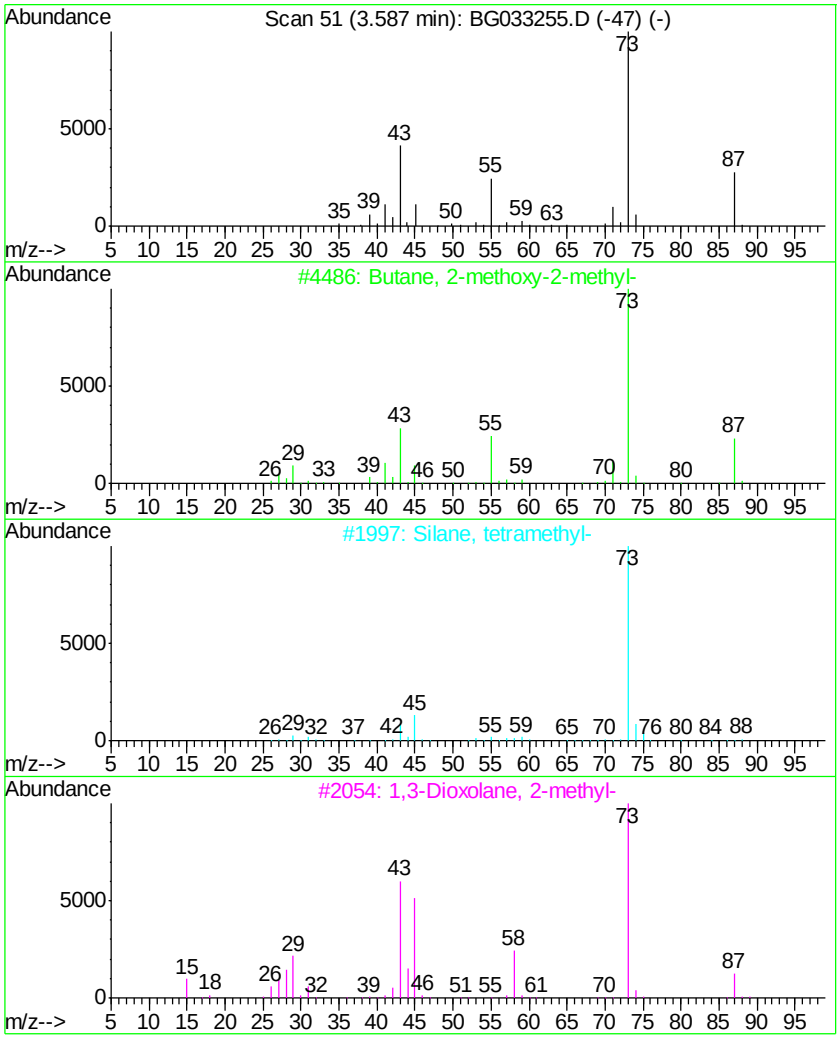
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

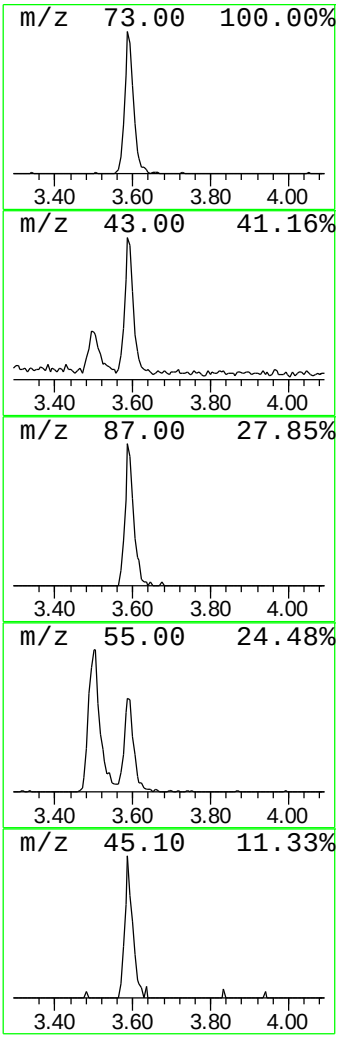
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	12.79 ng	148666	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG033255.D
Acq On : 20 Mar 2018 00:44
Operator : SJ/JU
Sample : J1953-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

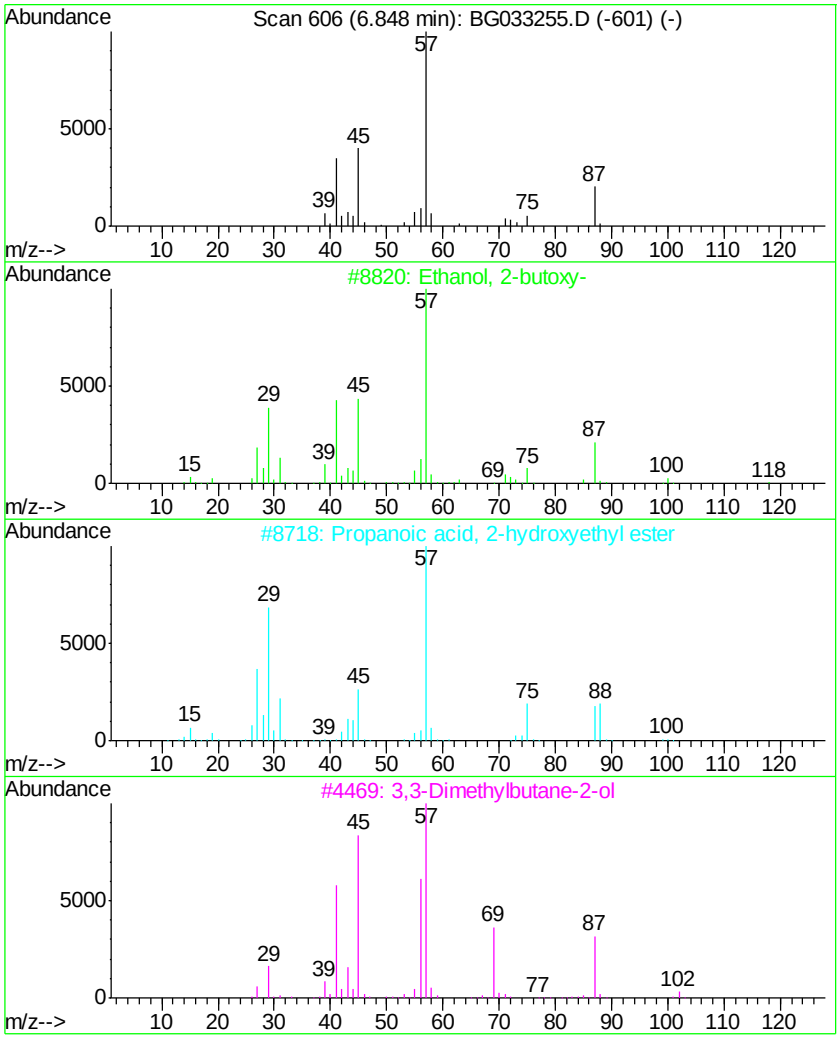
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

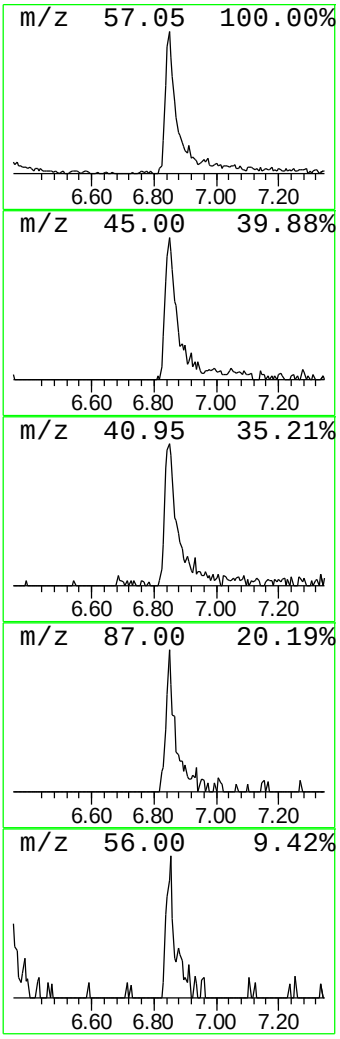
****

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	8.02 ng	93149	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Propanoic acid, 2-hydroxyethyl e...	118	C5H10O3	024567-27-9	32
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	27
4	3-Buten-2-ol	72	C4H8O	000598-32-3	25
5	n-Butyl ether	130	C8H18O	000142-96-1	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033255.D
Acq On : 20 Mar 2018 00:44
Operator : SJ/JU
Sample : J1953-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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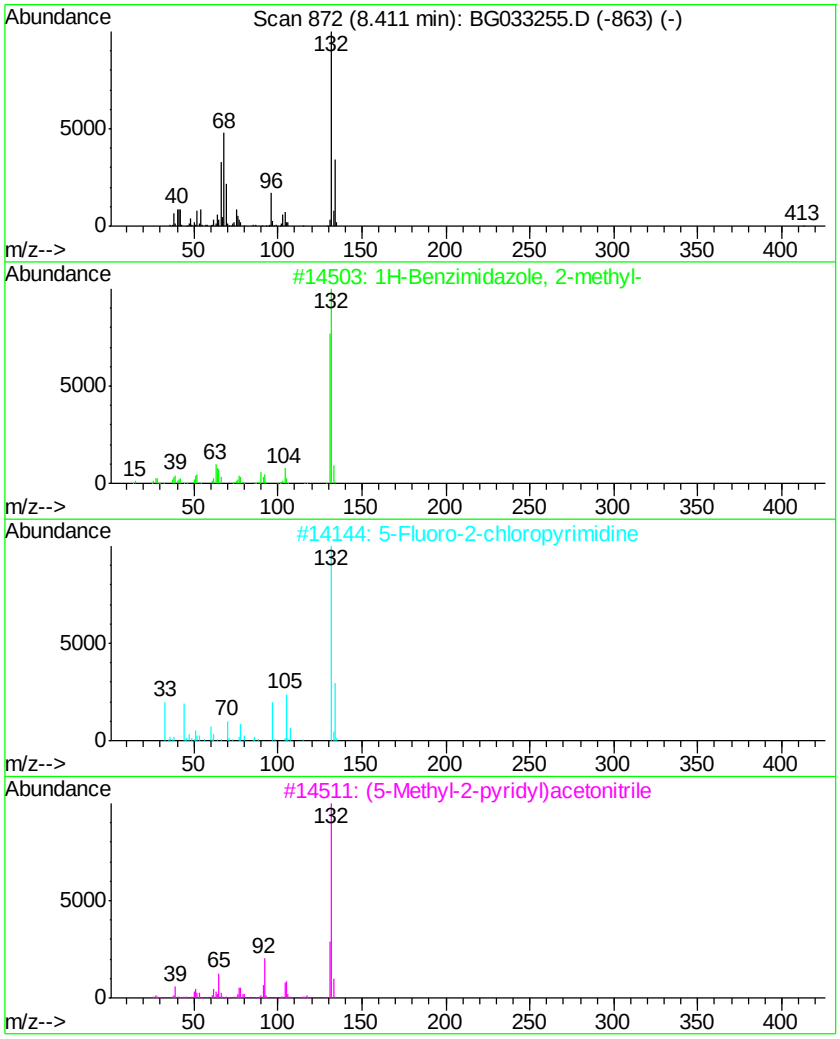
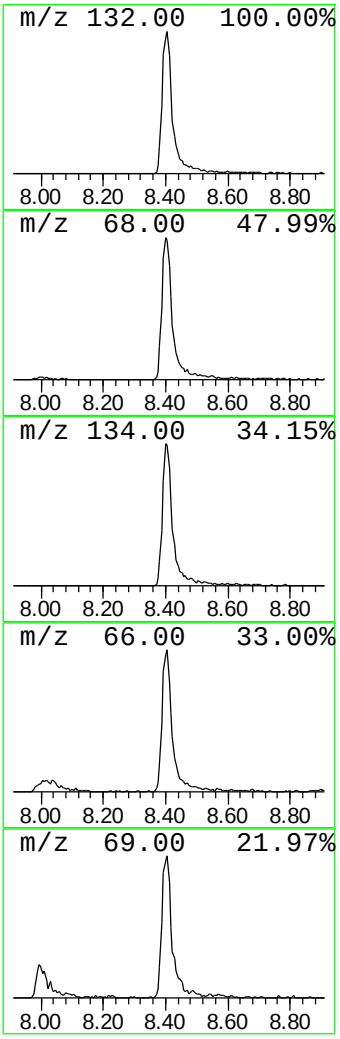
Peak Number 4 unknown8.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	64.61 ng	750781	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	30
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





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Operator : SJ/JU
Sample : J1953-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

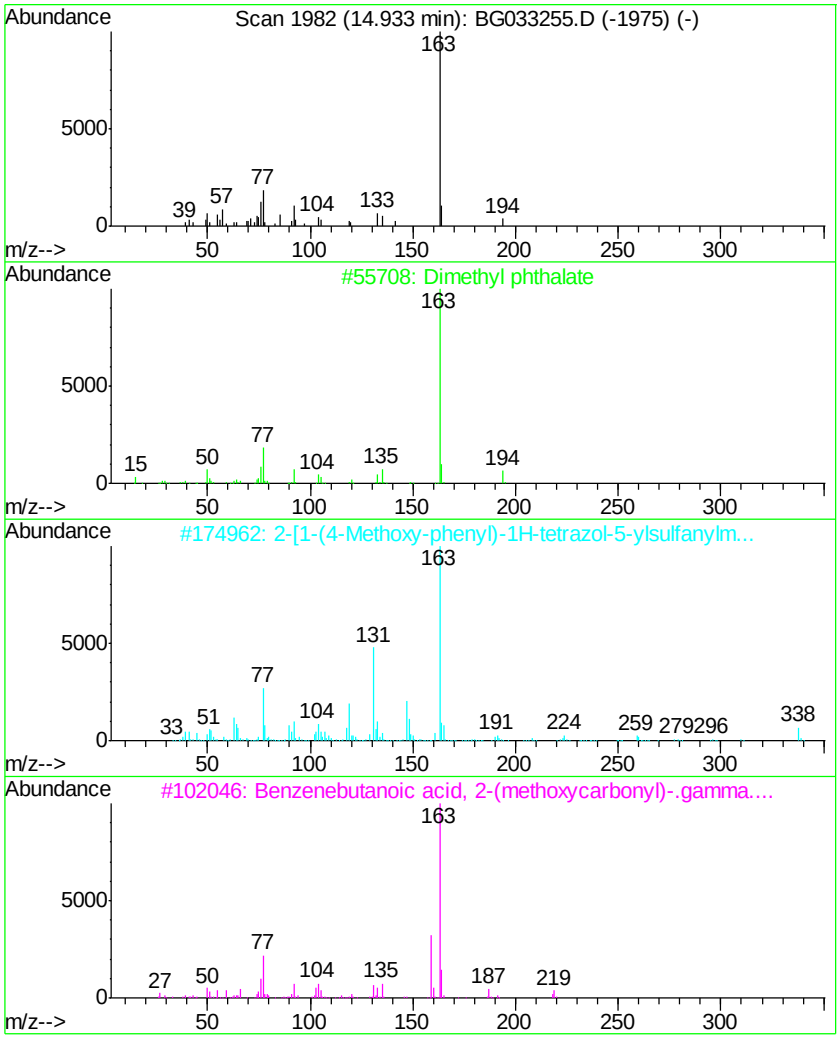
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

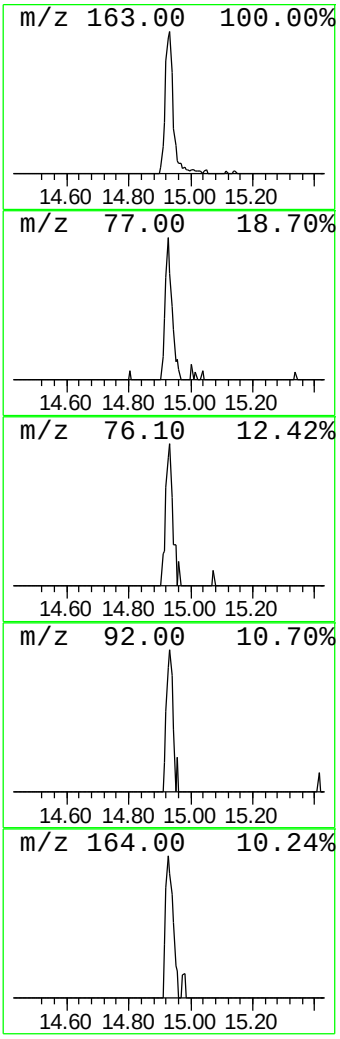
****

Peak Number 6 Dimethyl phthalate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.07 ng	55598	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl phthalate	194	C10H10O4	000131-11-3	94
2	2-[1-(4-Methoxy-phenyl)-1H-tetra...	338	C16H14N6OS	1000301-37-5	72
3	Benzenebutanoic acid, 2-(methoxy...	250	C13H14O5	054103-08-1	64
4	Benzoic acid, 2-(1-oxopropyl)-, ...	192	C11H12O3	032025-37-9	64
5	Methyl 4-methylpentan-2-yl phtha...	264	C15H20O4	1000373-82-3	59





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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Acq On : 20 Mar 2018 00:44
Operator : SJ/JU
Sample : J1953-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

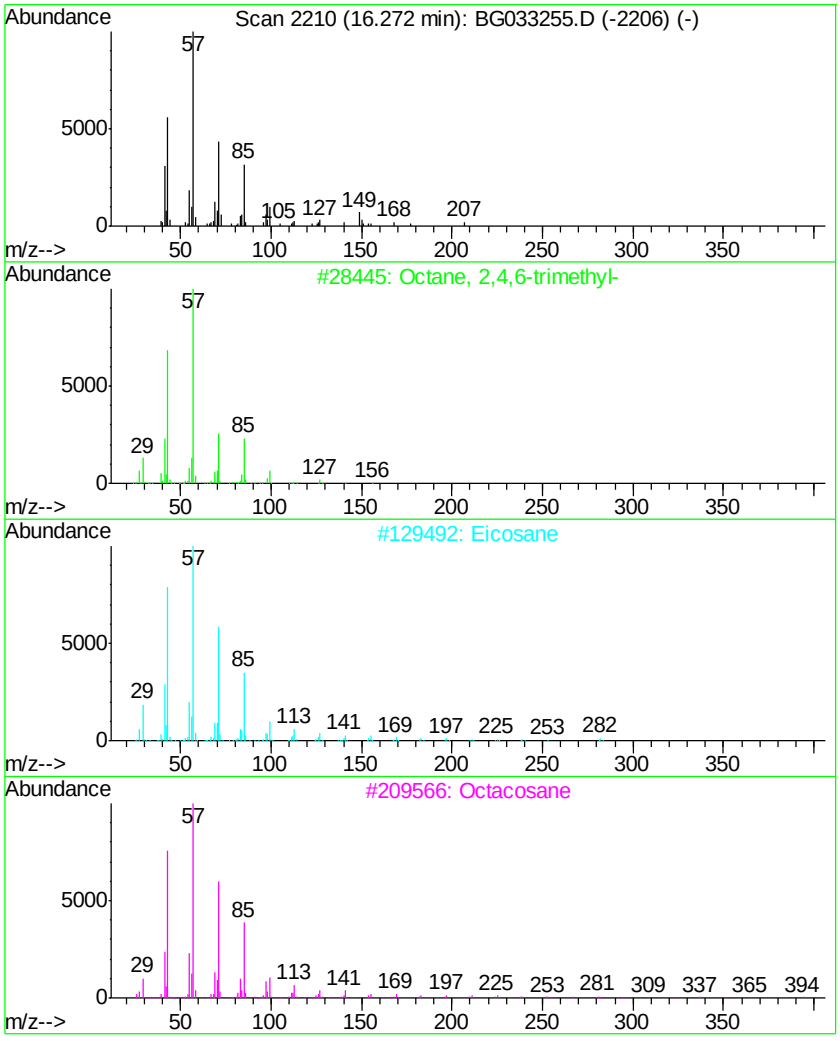
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

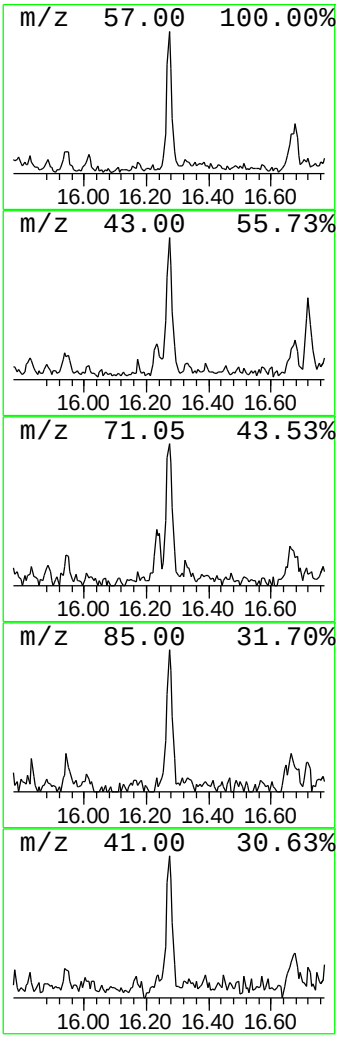
****

Peak Number 7 Octane, 2,4,6-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	2.93 ng	78767	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	86
2	Eicosane	282	C20H42	000112-95-8	86
3	Octacosane	394	C28H58	000630-02-4	83
4	Nonadecane	268	C19H40	000629-92-5	80
5	Heneicosane	296	C21H44	000629-94-7	72





Library Search Compound Report

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Operator : SJ/JU
Sample : J1953-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

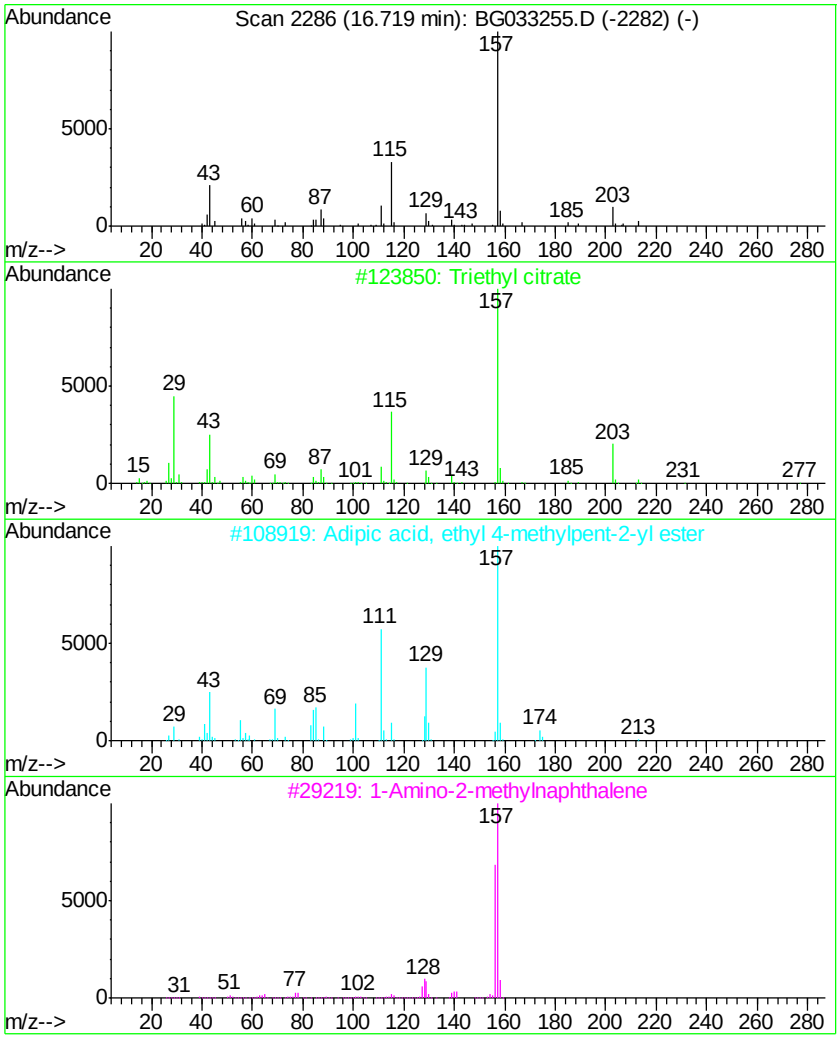
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

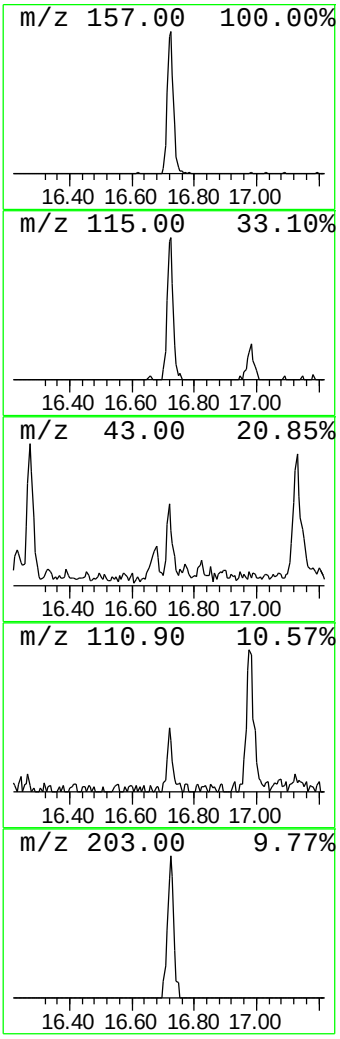
****

Peak Number 8 Triethyl citrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.78 ng	74758	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	87
2	Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	42
3	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	38
4	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	38
5	N-Methoxy-2,2-dicarbomethoxyazir...	189	C7H11NO5	053084-34-7	37





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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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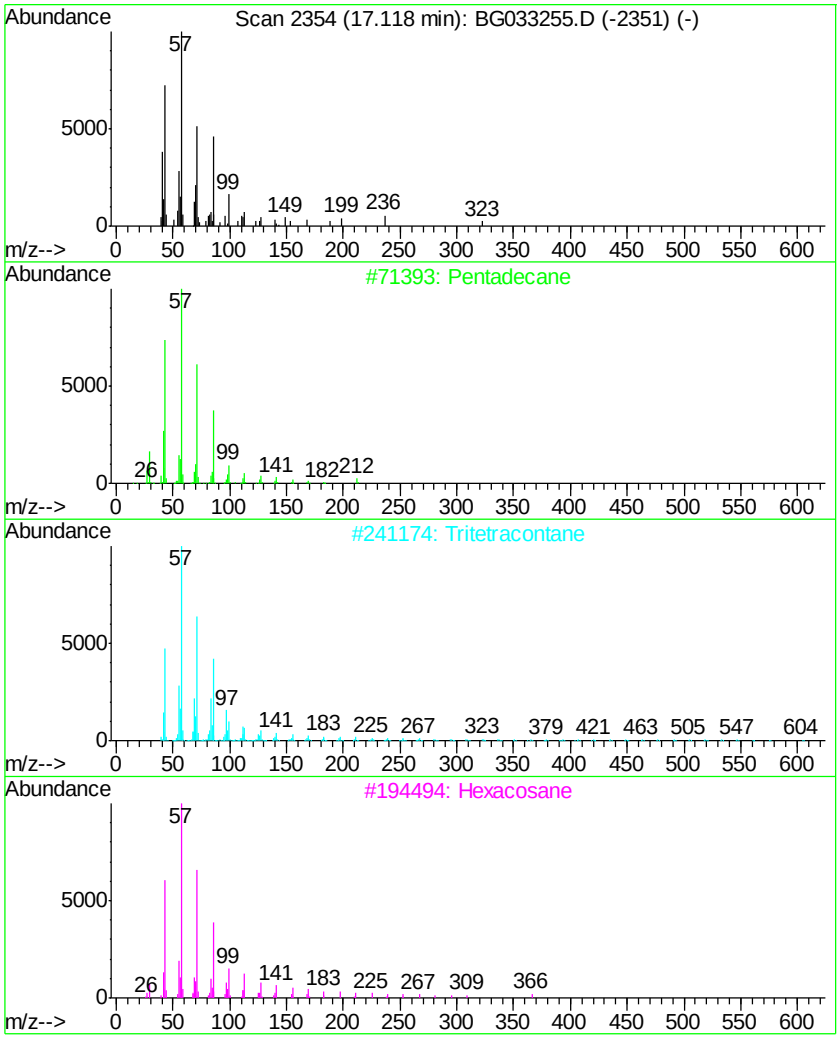
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

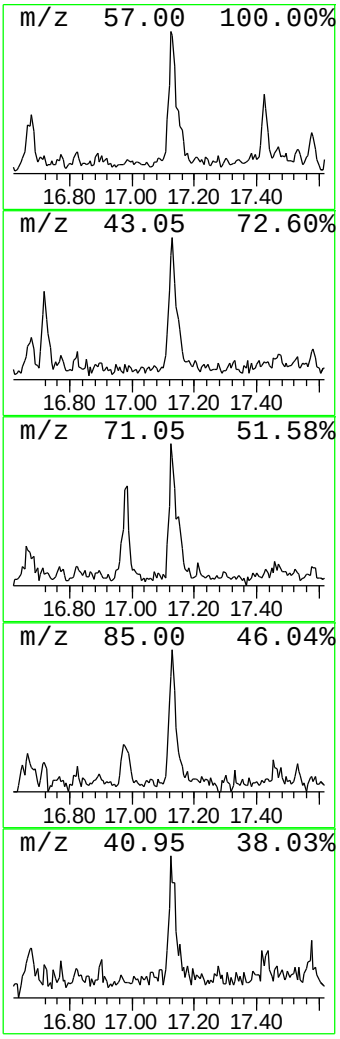
****

Peak Number 9 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	2.45 ng	97518	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Tritetracontane	605	C43H88	007098-21-7	80
3	Hexacosane	366	C26H54	000630-01-3	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Octacosane	394	C28H58	000630-02-4	72





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Sample : J1953-06
Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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TIC Library : C:\Database\NIST11.L
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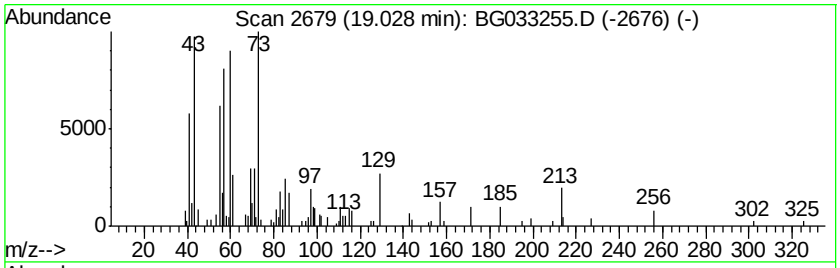
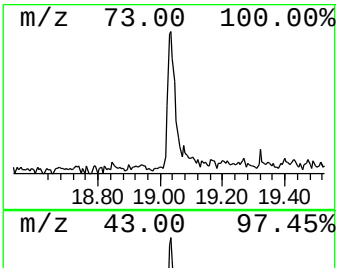
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	3.59 ng	142508	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Octadecanoic acid	284	C18H36O2	000057-11-4	49
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	35





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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

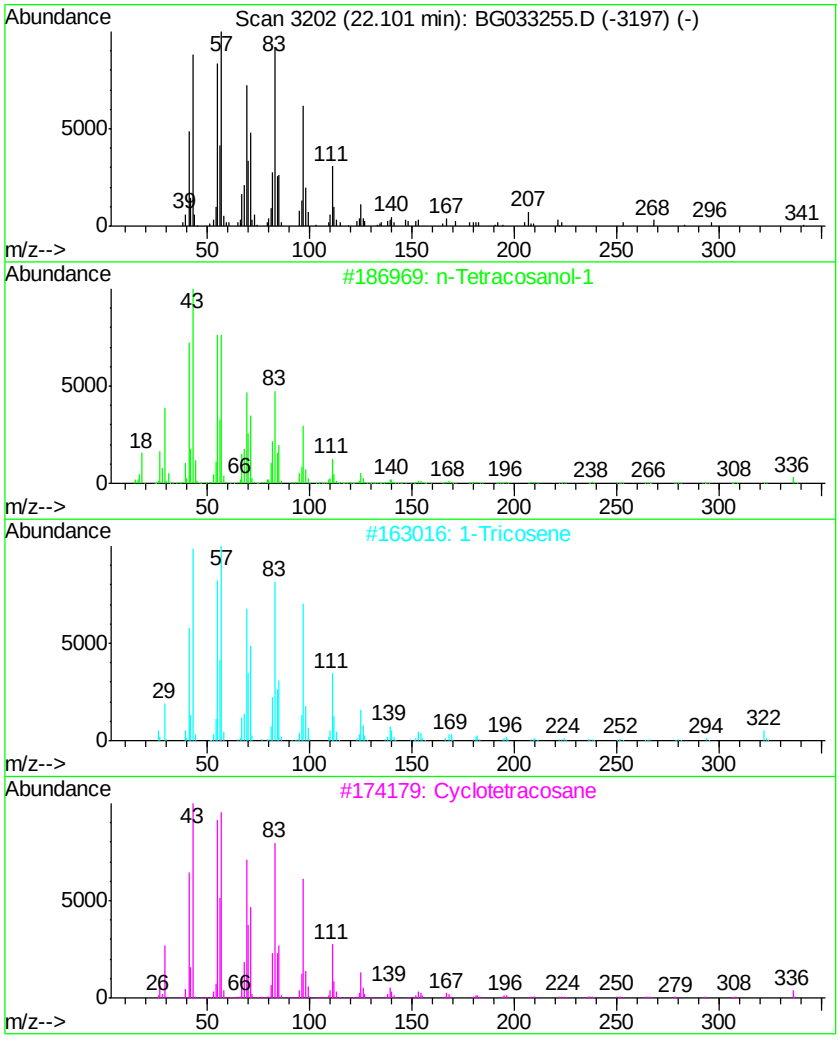
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

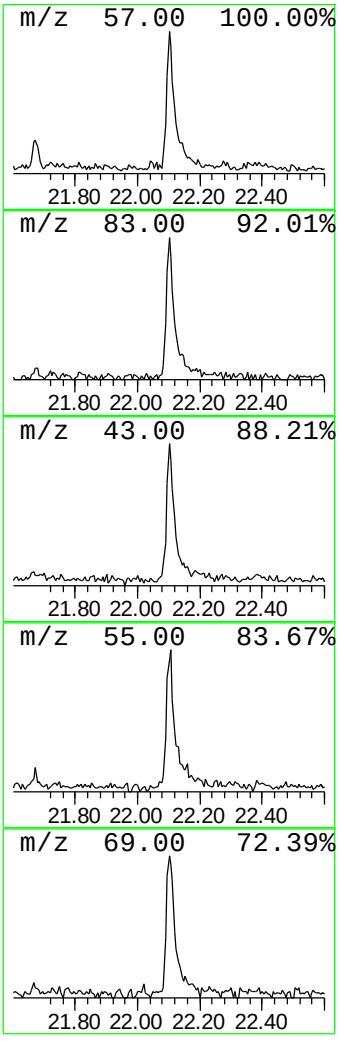
****

Peak Number 11 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.10	4.48 ng	204237	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Tricosene	322	C23H46	018835-32-0	91
3	Cyclotetracosane	336	C24H48	000297-03-0	91
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87





Tentatively Identified Compound (LSC) summary

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Data File : BG033255.D
Acq On : 20 Mar 2018 00:44
Operator : SJ/JU
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Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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...	3.59	12.8	ng	148666	1	8.89	232416	20.0
Ethanol, 2-butoxy-	6.85	8.0	ng	93149	1	8.89	232416	20.0
unknown8.41	8.41	64.6	ng	750781	1	8.89	232416	20.0
Dimethyl phthalate	14.93	2.1	ng	55598	3	15.51	538037	20.0
Octane, 2,4,6-tri...	16.27	2.9	ng	78767	3	15.51	538037	20.0
Triethyl citrate	16.72	2.8	ng	74758	3	15.51	538037	20.0
Pentadecane	17.12	2.5	ng	97518	4	18.24	794535	20.0
n-Hexadecanoic acid	19.03	3.6	ng	142508	4	18.24	794535	20.0
n-Tetracosanol-1	22.10	4.5	ng	204237	5	22.59	910867	20.0