LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033256.D
Acq On : 20 Mar 2018 1:22
Operator : SJ/JU
Sample : J1953-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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	30	36	46	rBV	159530	336280	9.13%	2.167%
2	3.588	46	51	61	rVB	103532	166149	4.51%	1.070%
3	6.314	508	515	531	rBV	135538	320327	8.70%	2.064%
4	6.848	600	606	615	rBV2	41220	92559	2.51%	0.596%
5	8.000	796	802	820	rBV2	78706	246536	6.69%	1.588%
6	8.400	863	870	892	rBV	308429	726247	19.72%	4.679%
7	8.893	948	954	967	rBV2	91556	209056	5.68%	1.347%
8	9.228	1003	1011	1022	rBV	501004	997871	27.09%	6.429%
9	10.092	1150	1158	1178	rBV	398598	939930	25.52%	6.056%
10	11.778	1437	1445	1458	rBV	139769	303943	8.25%	1.958%
11	14.134	1839	1846	1862	rBV	1289769	2284688	62.03%	14.720%
12	14.927	1973	1981	1986	rBV	34297	56272	1.53%	0.363%
13	15.339	2042	2051	2059	rBV	35461	55562	1.51%	0.358%
14	15.509	2074	2080	2090	rVB2	293737	495979	13.47%	3.195%
15	16.273	2206	2210	2216	rVB2	60235	79015	2.15%	0.509%
16	16.672	2269	2278	2282	rBV5	19619	43891	1.19%	0.283%
17	16.725	2282	2287	2292	rVB	46289	64131	1.74%	0.413%
18	16.984	2324	2331	2345	rBV	825725	1446110	39.26%	9.317%
19	17.131	2351	2356	2364	rVB	55129	93313	2.53%	0.601%
20	17.918	2485	2490	2494	rBV2	33230	47710	1.30%	0.307%
21	18.241	2538	2545	2557	rBV	431560	753079	20.45%	4.852%
22	19.034	2675	2680	2690	rBV	91197	159141	4.32%	1.025%
23	20.268	2886	2890	2897	rBV6	22034	36978	1.00%	0.238%
24	20.762	2968	2974	2987	rVB	2647772	3683235	100.00%	23.730%
25	22.107	3198	3203	3214	rBV2	110058	225065	6.11%	1.450%
26	22.595	3279	3286	3297	rVB2	428957	822905	22.34%	5.302%
27	24.487	3603	3608	3614	rVB4	23885	52079	1.41%	0.336%
28	26.390	3920	3932	3944	rBV2	229485	783202	21.26%	5.046%

Sum of corrected areas: 15521253

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
Data File : BG033256.D
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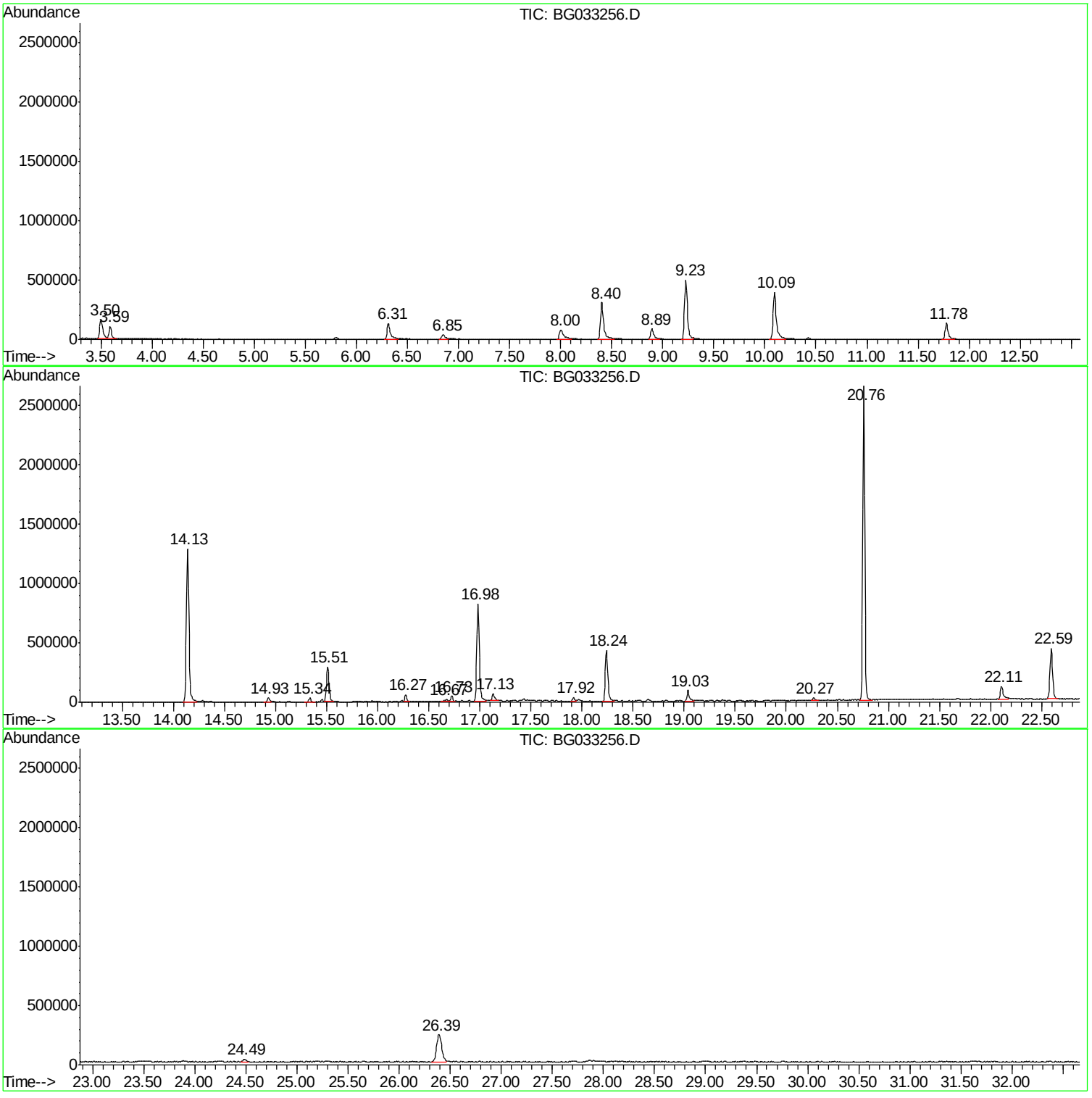
Operator : SJ/JU
Sample : J1953-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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



Library Search Compound Report

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Operator : SJ/JU
Sample : J1953-07
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ALS Vial : 12 Sample Multiplier: 1

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

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

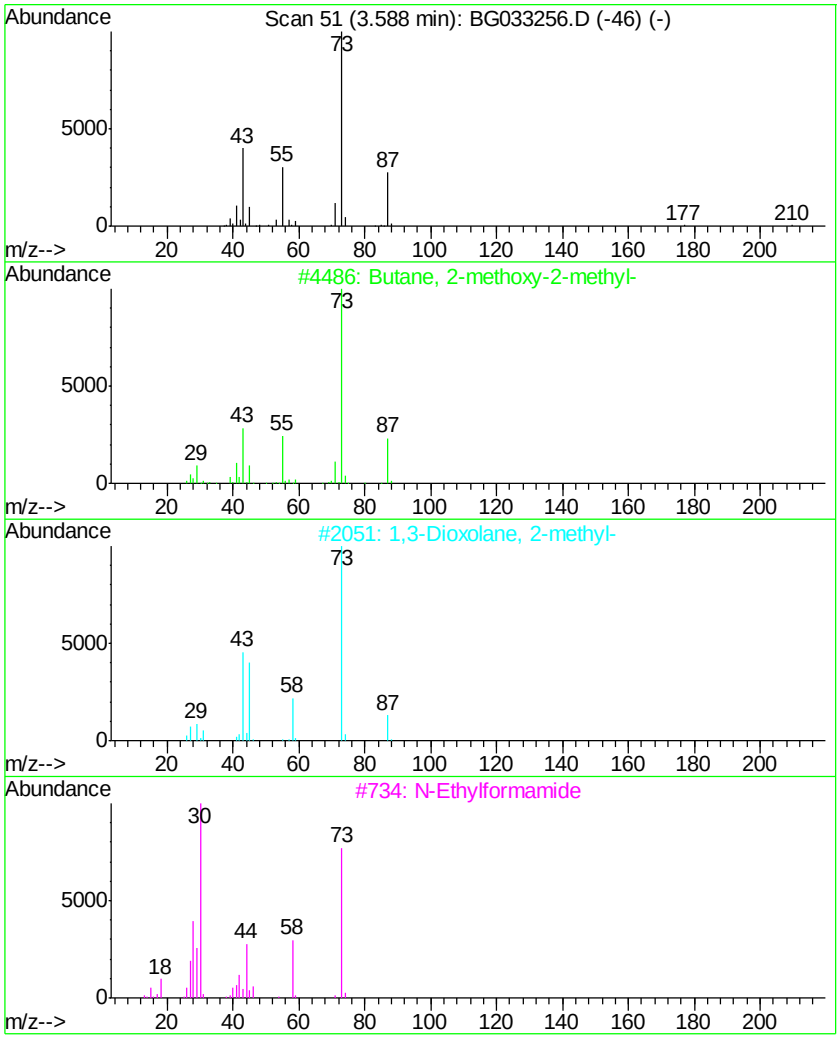
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

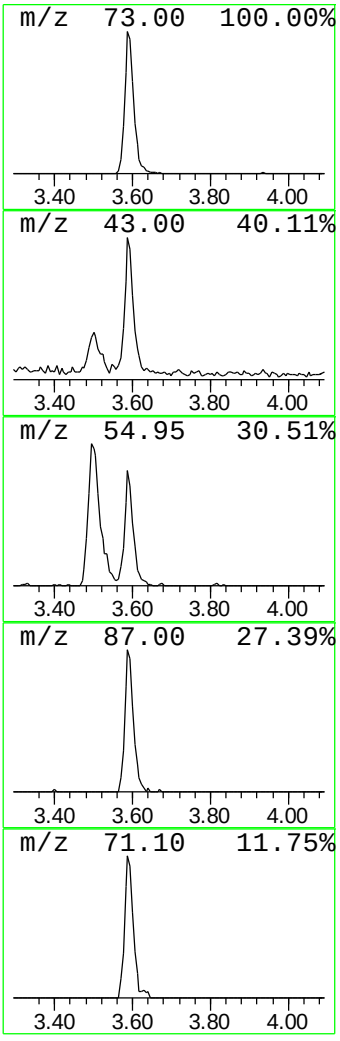
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	15.90 ng	166149	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	9
5	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9





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Acq On : 20 Mar 2018 1:22
Operator : SJ/JU
Sample : J1953-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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

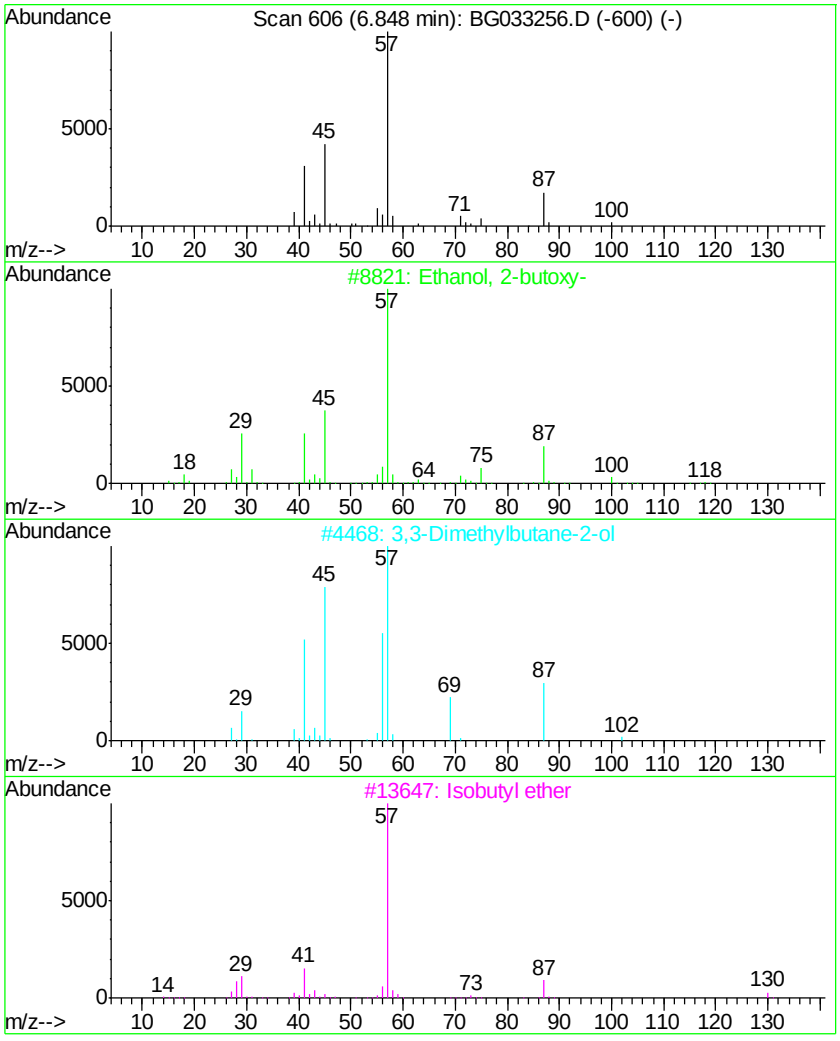
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

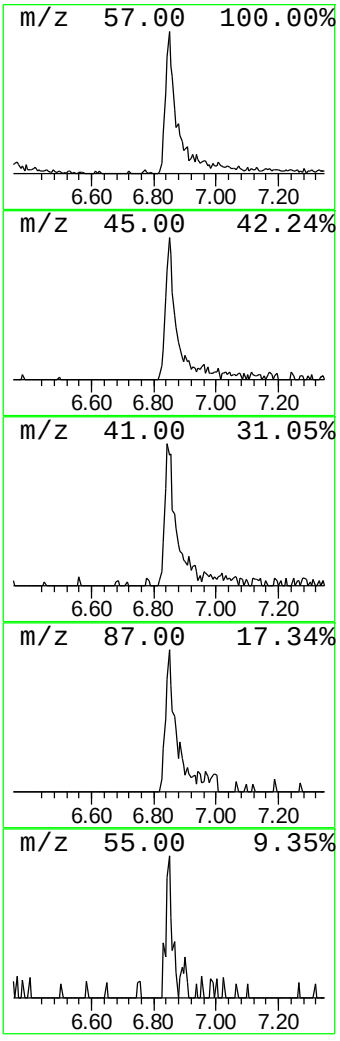
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	8.85 ng	92559	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	64
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	64
3	Isobutyl ether	130	C8H18O	000628-55-7	16
4	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	10
5	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	10





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Acq On : 20 Mar 2018 1:22
Operator : SJ/JU
Sample : J1953-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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

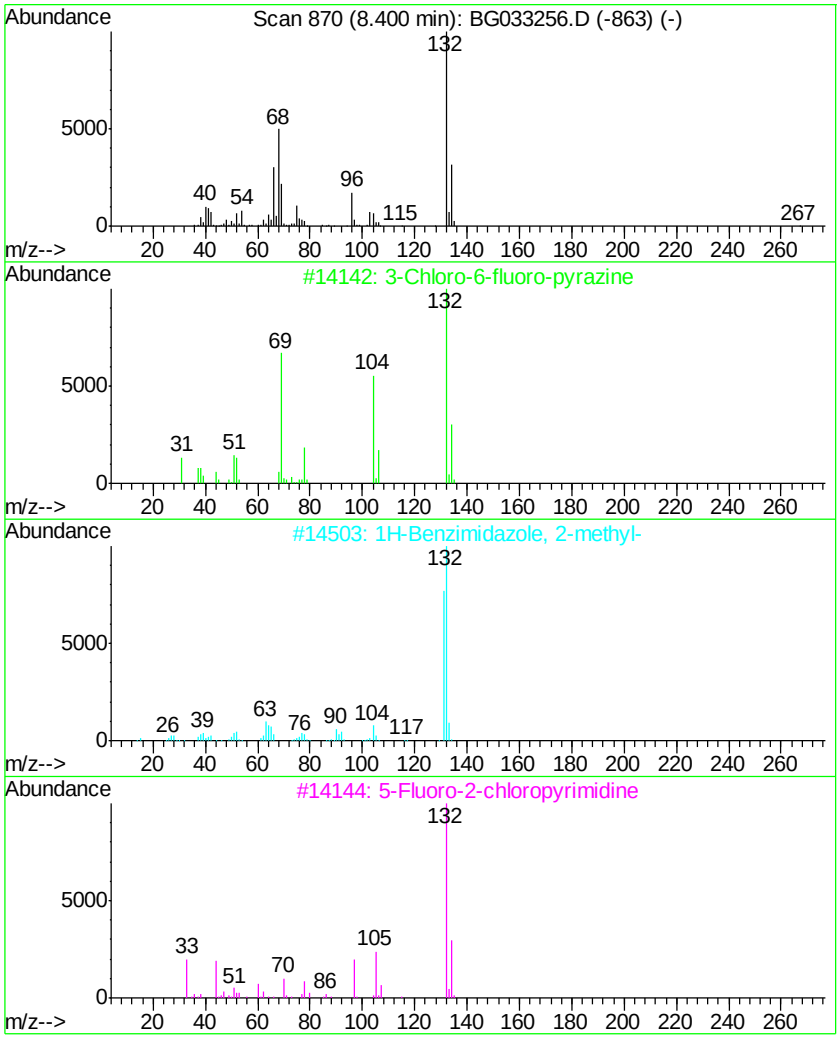
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

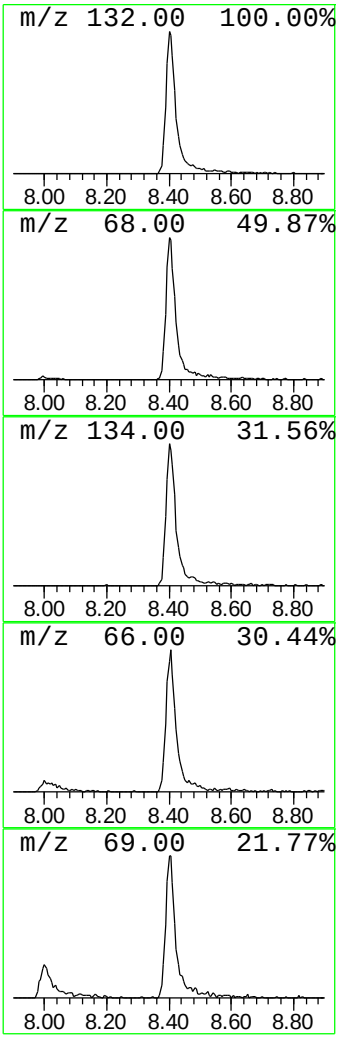
****

Peak Number 4 unknown8.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	69.48 ng	726247	1,4-Dichlorobenzene-d4	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-S

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

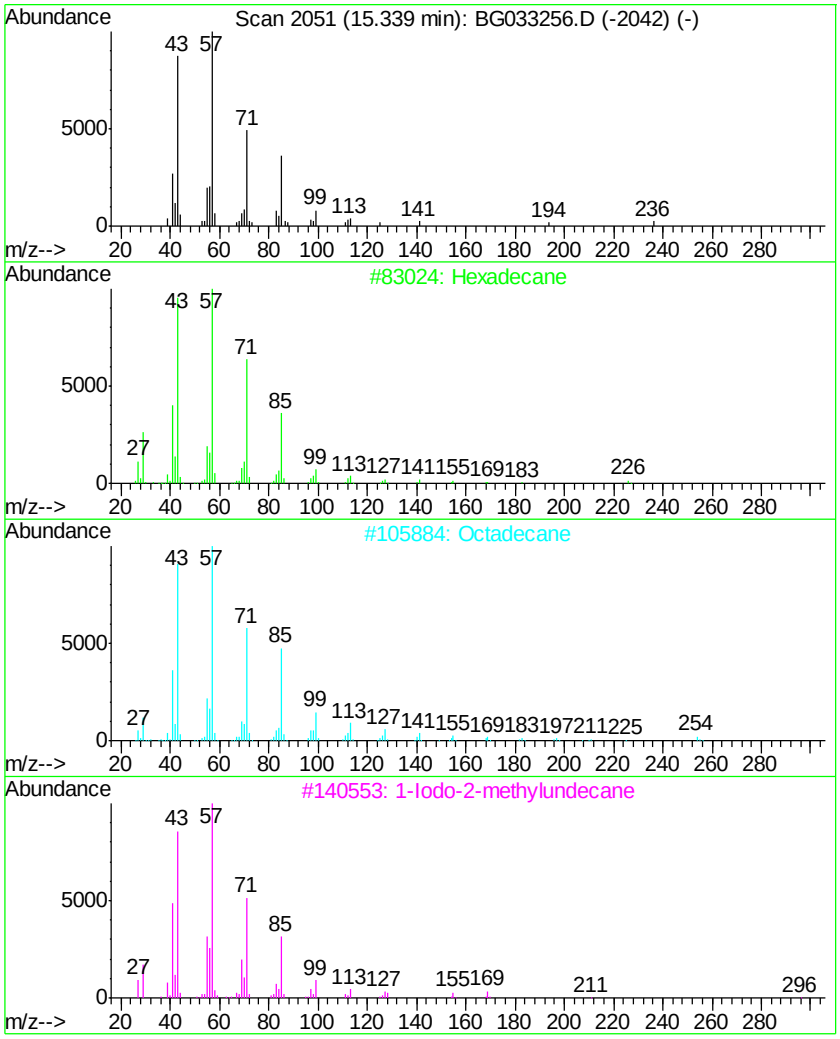
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

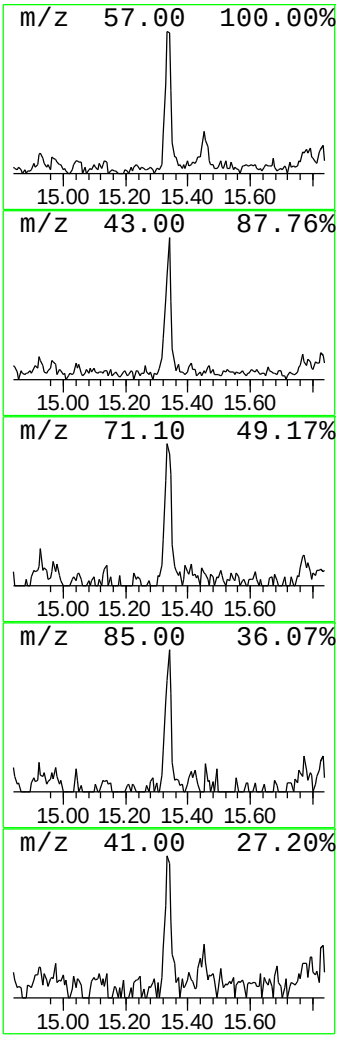
****

Peak Number 6 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.24 ng	55562	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Octadecane	254	C18H38	000593-45-3	86
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
4	Tridecane	184	C13H28	000629-50-5	78
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	78





Data Path : Z:\HPCHEM1\BNA G\DATA\BG031918\
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Acq On : 20 Mar 2018 1:22
Operator : SJ/JU
Sample : J1953-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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

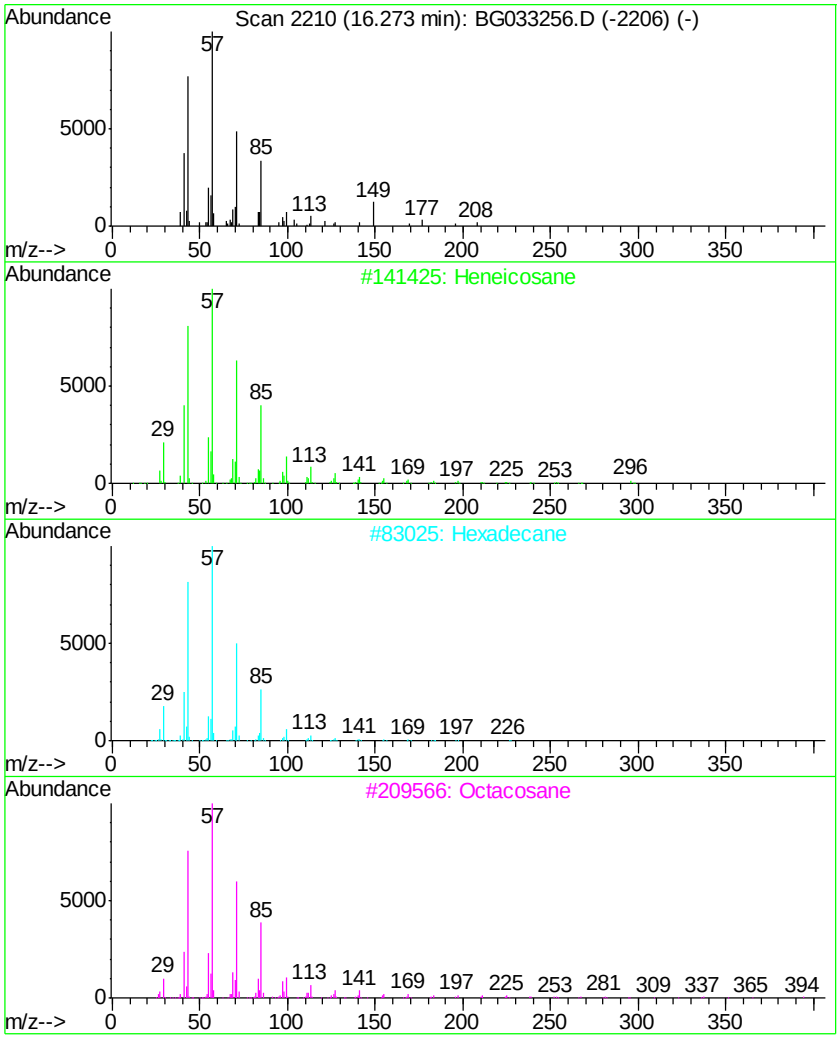
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

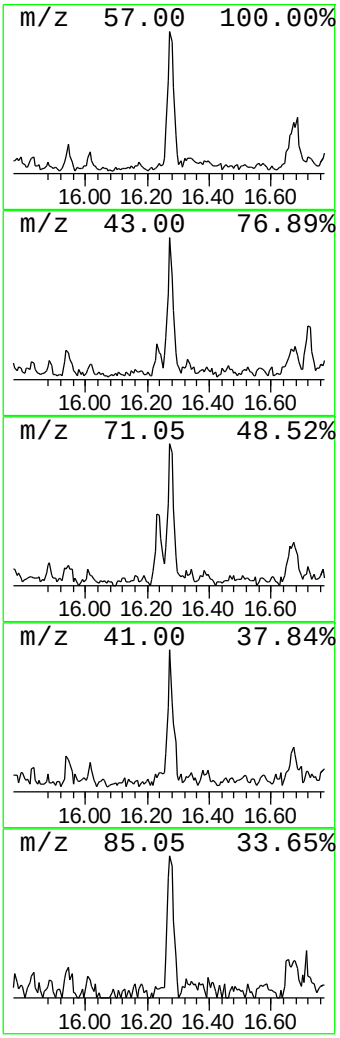
****

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	3.19 ng	79015	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	80
2	Hexadecane	226	C16H34	000544-76-3	80
3	Octacosane	394	C28H58	000630-02-4	80
4	Eicosane	282	C20H42	000112-95-8	80
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	72





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Operator : SJ/JU
Sample : J1953-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

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

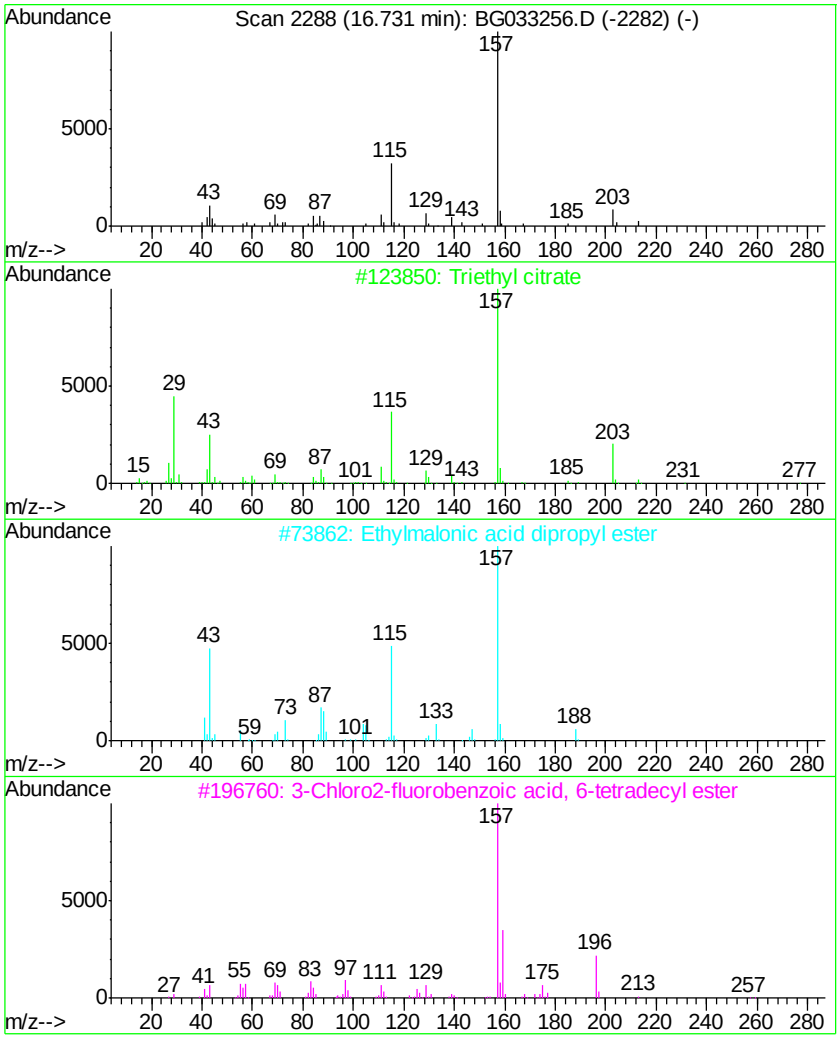
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

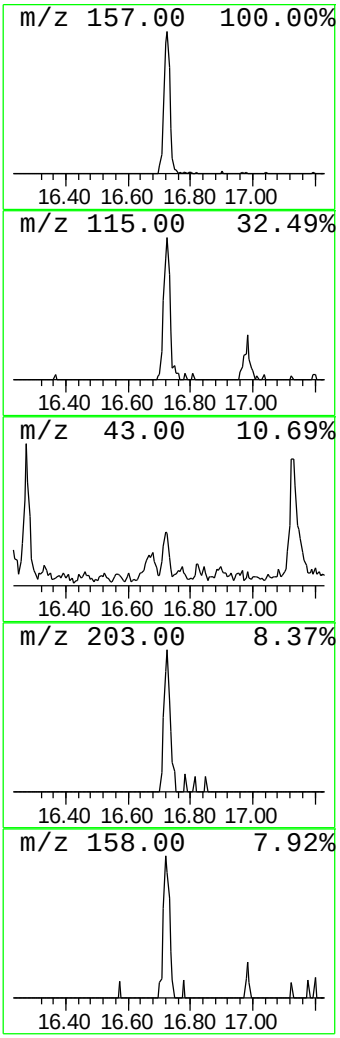
****

Peak Number 8 Triethyl citrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	2.59 ng	64131	Acenaphthene-d10	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	86
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
3	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClFO2	1000338-64-9	36
4	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	36
5	3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClFO2	1000338-64-6	36





Library Search Compound Report

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

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

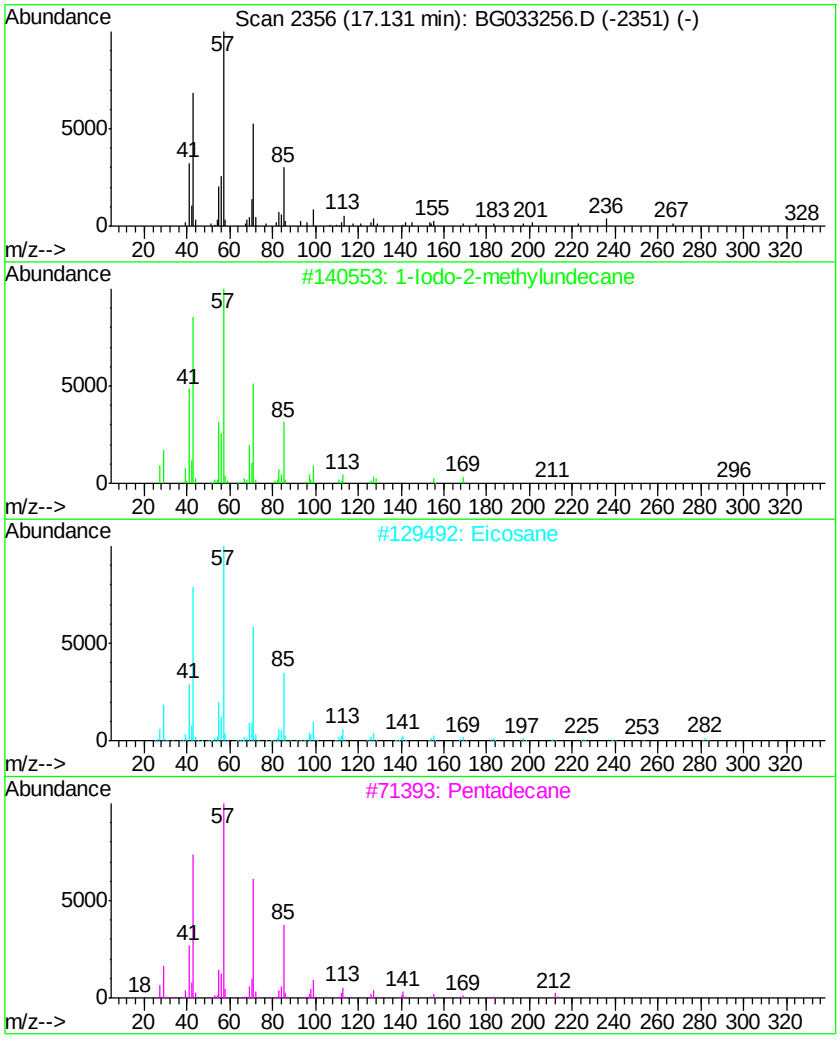
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

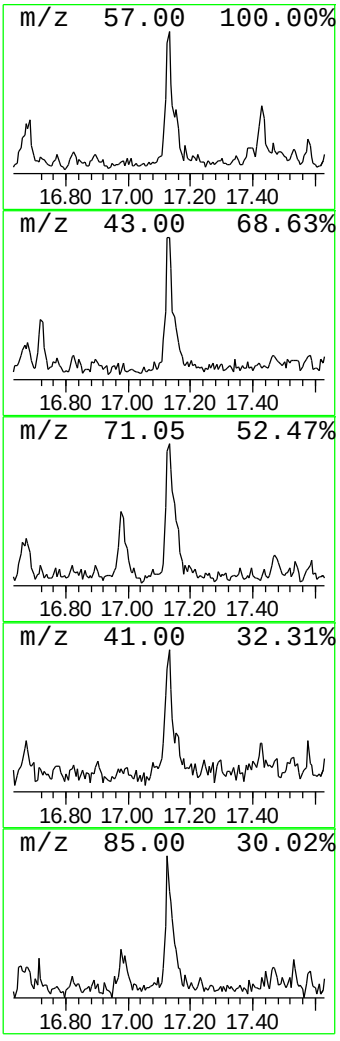
****

Peak Number 9 1-Iodo-2-methylundecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	2.48 ng	93313	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	86
2	Eicosane	282	C20H42	000112-95-8	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Dodecane	170	C12H26	000112-40-3	72





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Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-S

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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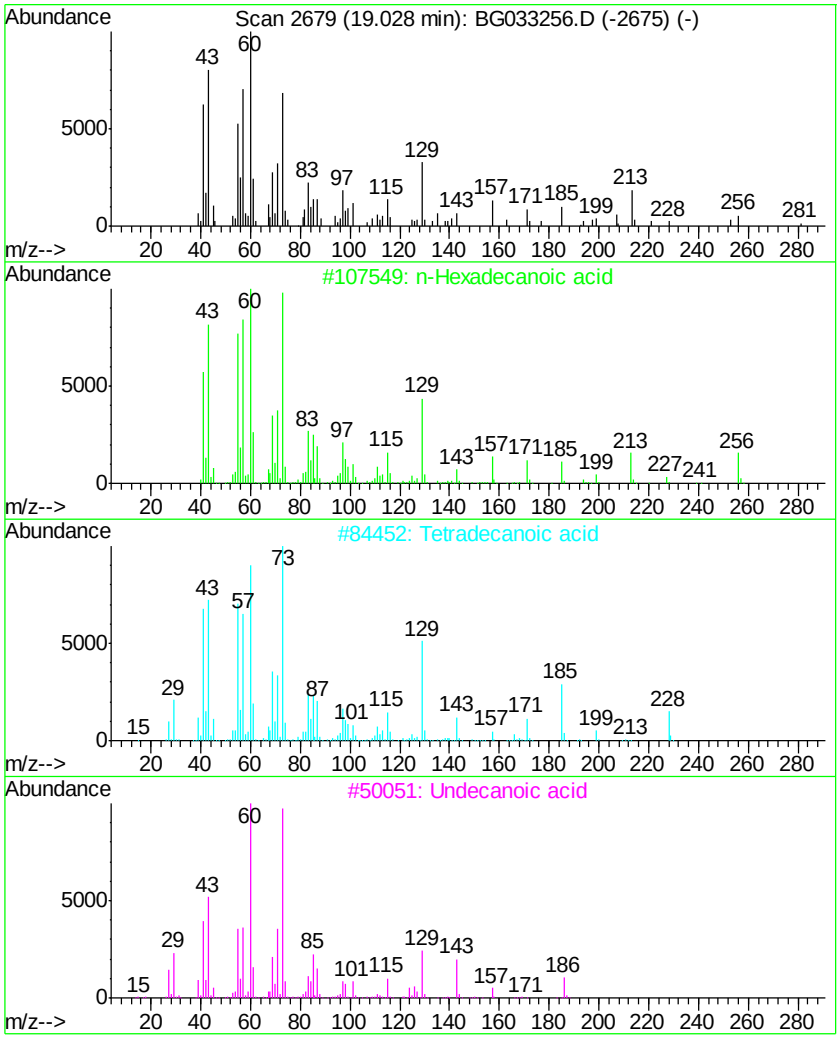
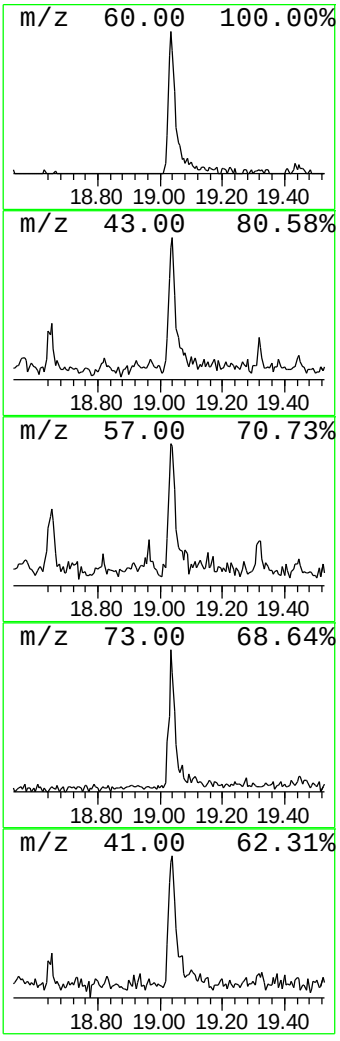
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	4.23 ng	159141	Phenanthrene-d10	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Misc :
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-S

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

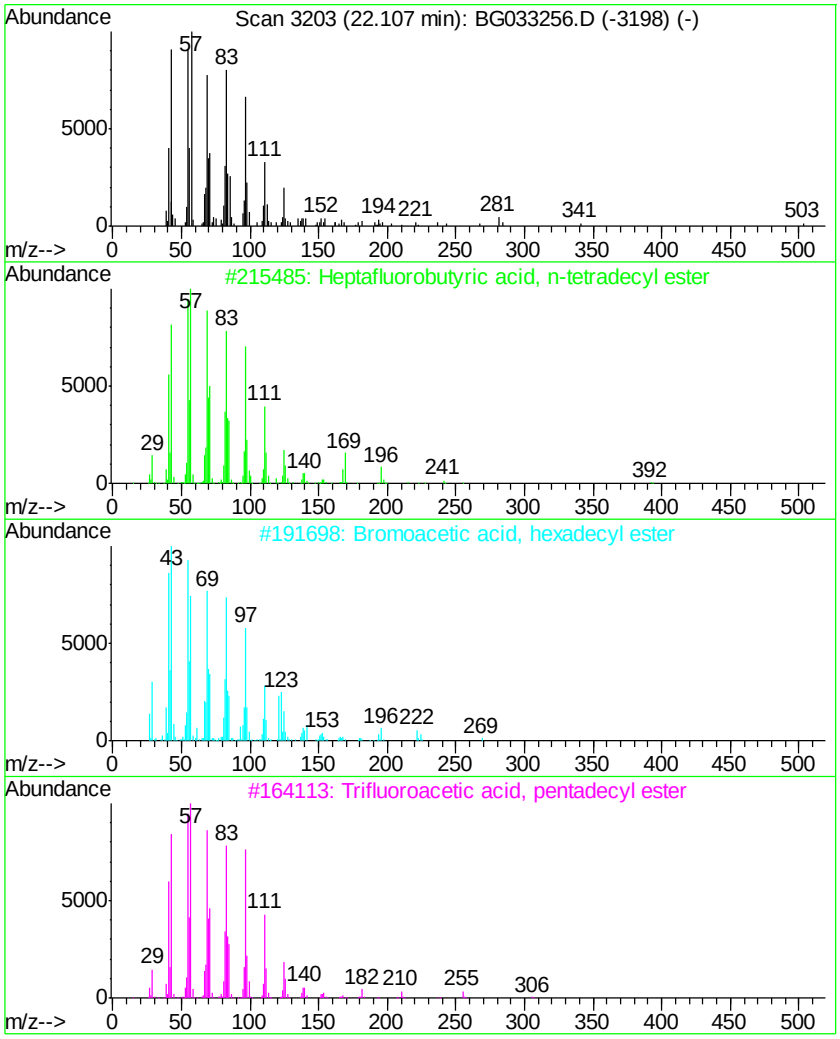
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

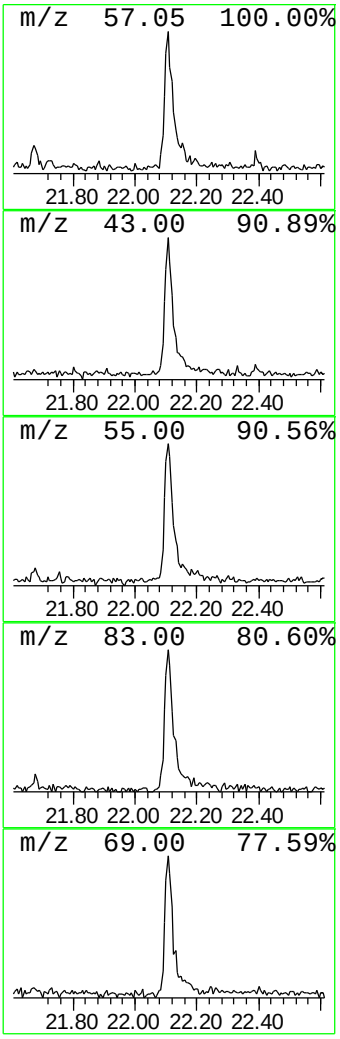
****

Peak Number 11 Heptafluorobutyric acid, n-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.11	5.47 ng	225065	Chrysene-d12	22.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG031918\
Data File : BG033256.D
Acq On : 20 Mar 2018 1:22
Operator : SJ/JU
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Instrument : BNA_G
ClientSampleId : 031418-JETT-E-D-S

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.59	15.9	ng	166149	1	8.89	209056	20.0
Ethanol, 2-butoxy-	6.85	8.8	ng	92559	1	8.89	209056	20.0
unknown8.40	8.40	69.5	ng	726247	1	8.89	209056	20.0
Hexadecane	15.34	2.2	ng	55562	3	15.51	495979	20.0
Heneicosane	16.27	3.2	ng	79015	3	15.51	495979	20.0
Triethyl citrate	16.73	2.6	ng	64131	3	15.51	495979	20.0
1-Iodo-2-methylun...	17.13	2.5	ng	93313	4	18.24	753079	20.0
n-Hexadecanoic acid	19.03	4.2	ng	159141	4	18.24	753079	20.0
Heptafluorobutyri...	22.11	5.5	ng	225065	5	22.59	822905	20.0