LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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	3.475	26	32	43	rBV	155825	339084	10.37%	2.102%
2	3.569	43	48	59	rVB	132623	232021	7.10%	1.438%
3	5.767	417	422	429	rBV	21830	38020	1.16%	0.236%
4	6.284	503	510	522	rBV	226823	479100	14.65%	2.970%
5	7.970	789	797	816	rBV	136896	353828	10.82%	2.193%
6	8.369	857	865	884	rBV	501825	1059066	32.39%	6.565%
7	8.857	942	948	961	rBV	116135	267230	8.17%	1.657%
8	9.192	997	1005	1027	rBV	503782	1018884	31.16%	6.316%
9	10.056	1145	1152	1167	rBV	396353	872294	26.68%	5.408%
10	11.742	1430	1439	1451	rBV	181927	394849	12.08%	2.448%
11	14.104	1834	1841	1859	rBV	1272353	2158403	66.01%	13.380%
12	14.897	1970	1976	1984	rBV	57839	91856	2.81%	0.569%
13	15.297	2040	2044	2053	rVB2	43883	67051	2.05%	0.416%
14	15.473	2067	2074	2083	rBV2	354131	614331	18.79%	3.808%
15	16.237	2200	2204	2209	rVB	56612	76485	2.34%	0.474%
16	16.948	2317	2325	2340	rBV	1051865	1742033	53.28%	10.799%
17	17.095	2345	2350	2358	rVB	51245	85208	2.61%	0.528%
18	18.205	2532	2539	2547	rBV	461041	807781	24.70%	5.008%
19	19.004	2670	2675	2686	rBV2	99846	168216	5.14%	1.043%
20	20.232	2880	2884	2892	rBV5	39408	79001	2.42%	0.490%
21	20.726	2962	2968	2980	rBV	2462739	3269710	100.00%	20.270%
22	22.071	3192	3197	3205	rBV3	54180	107671	3.29%	0.667%
23	22.547	3271	3278	3289	rBV2	446588	904336	27.66%	5.606%
24	26.313	3904	3919	3934	rBV2	253193	904626	27.67%	5.608%

Sum of corrected areas: 16131084

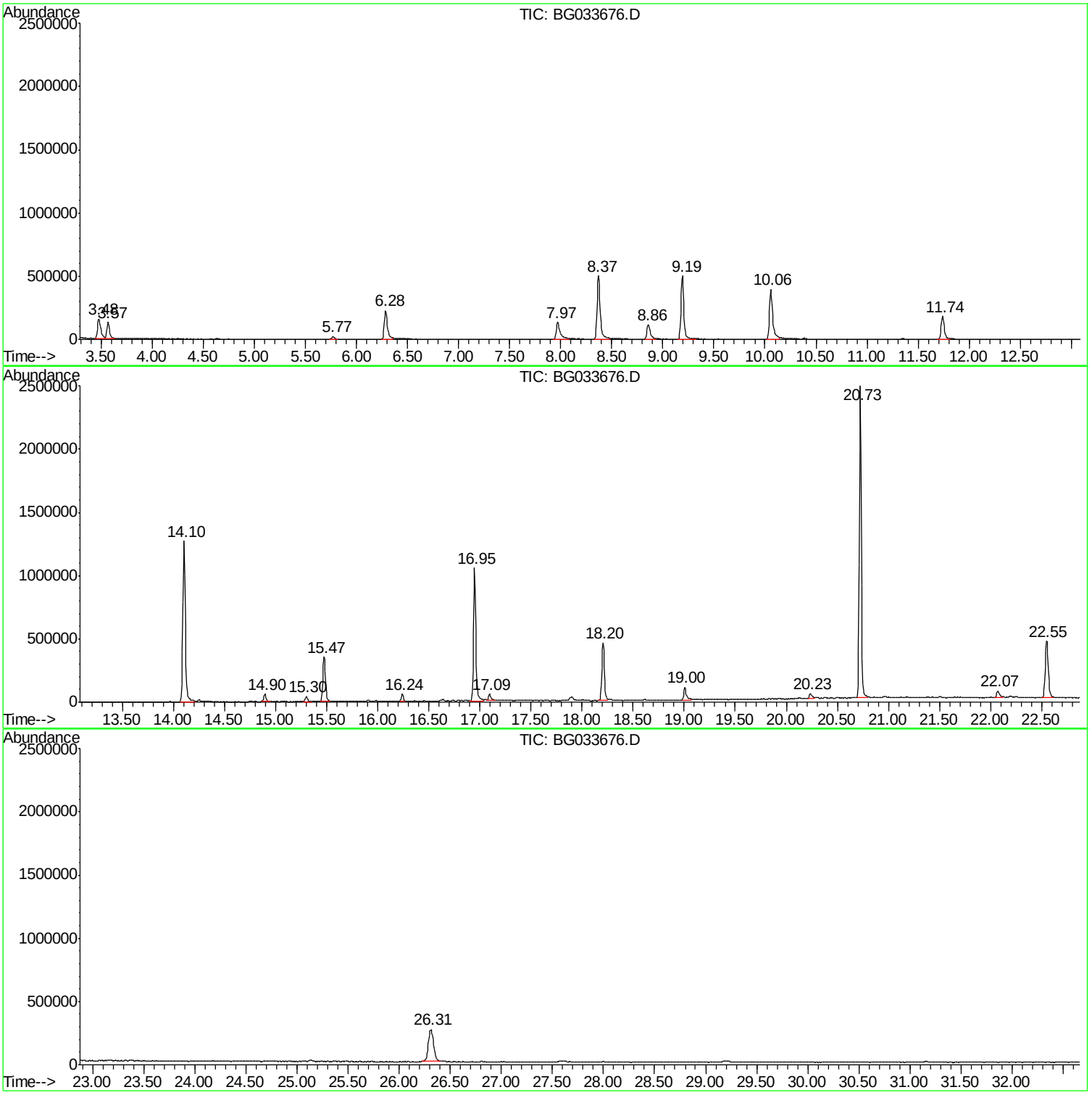
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

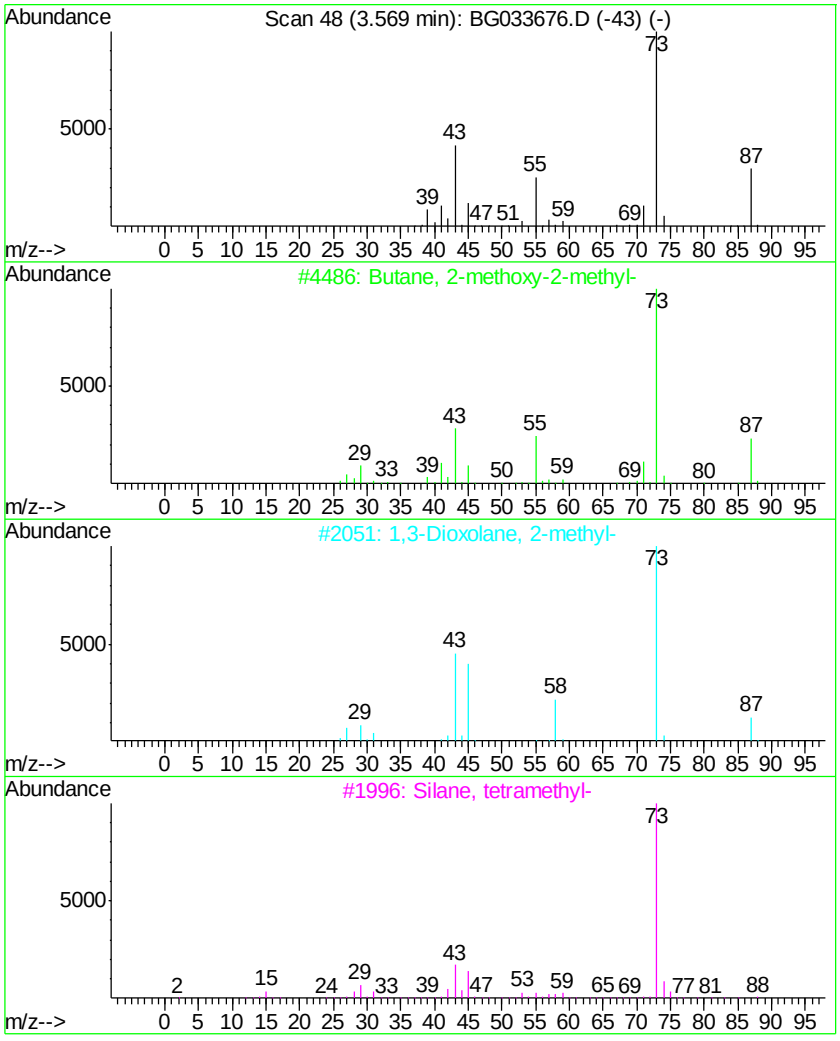
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

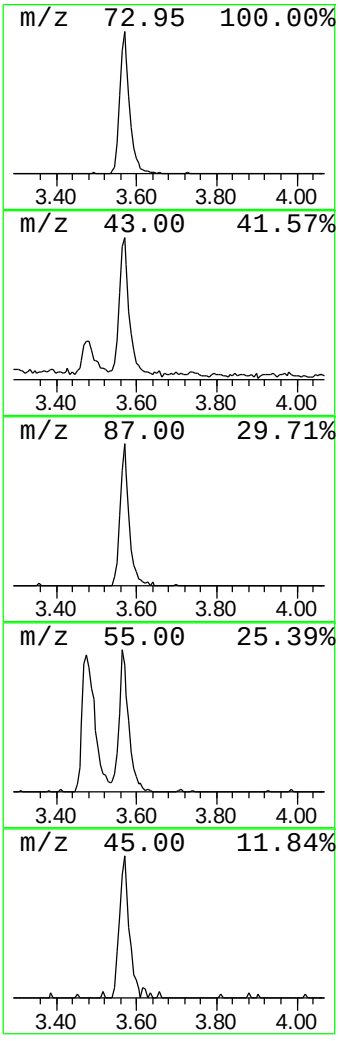
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	17.36 ng	232021	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

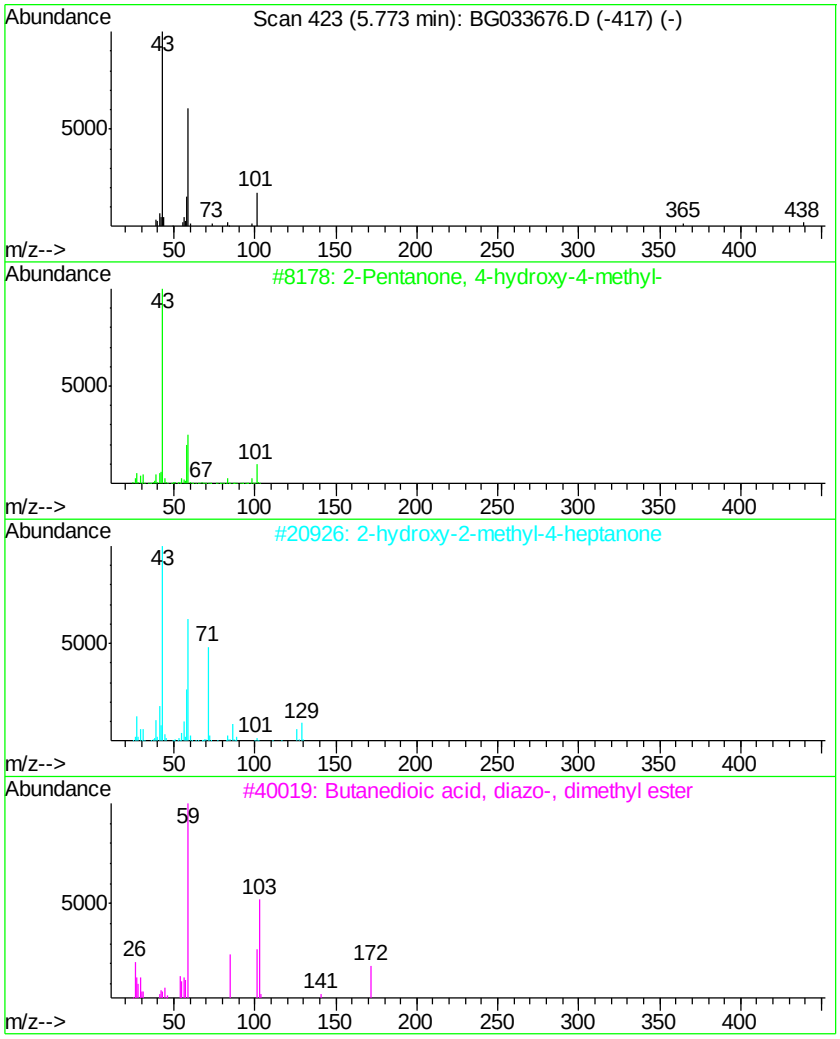
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

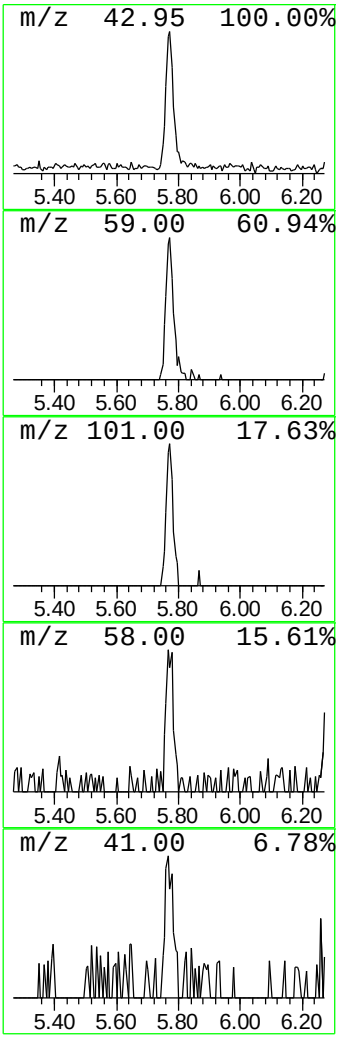
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	2.85 ng	38020	1,4-Dichlorobenzene-d4	8.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2-hydroxy-2-methyl-4-heptanone	144	C8H16O2	054862-91-8	38
3	Butanedioic acid, diazo-, dimeth...	172	C6H8N2O4	055514-36-8	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

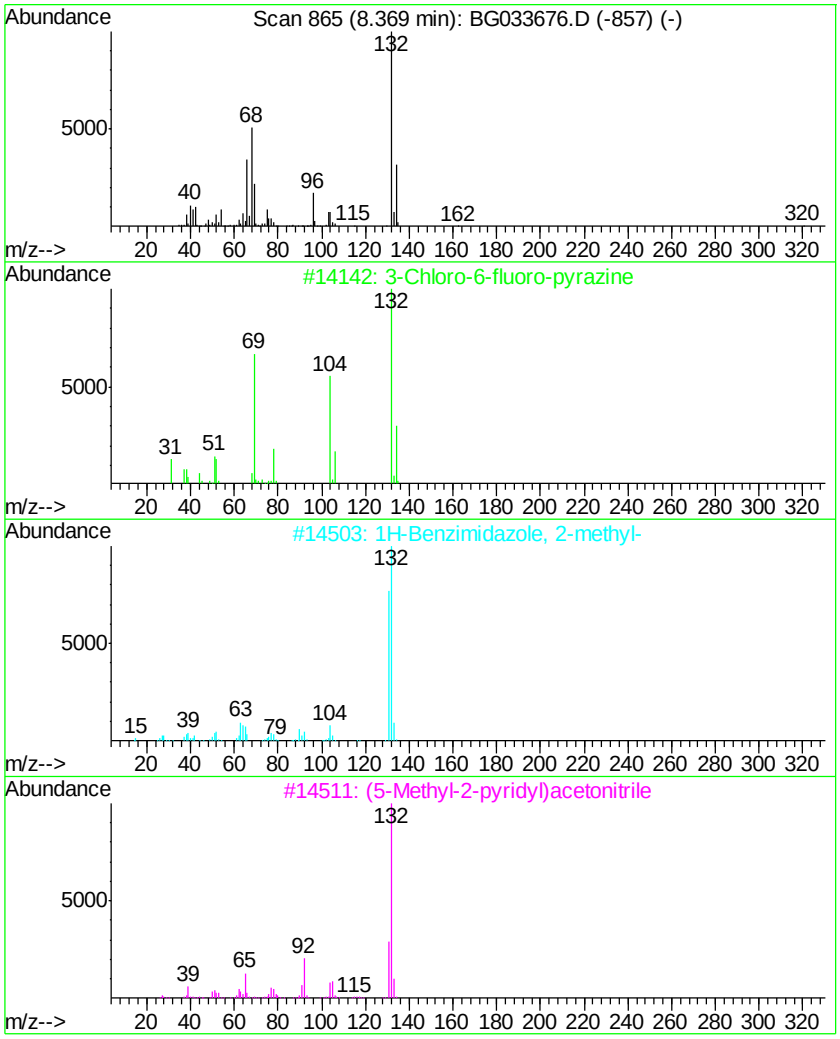
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

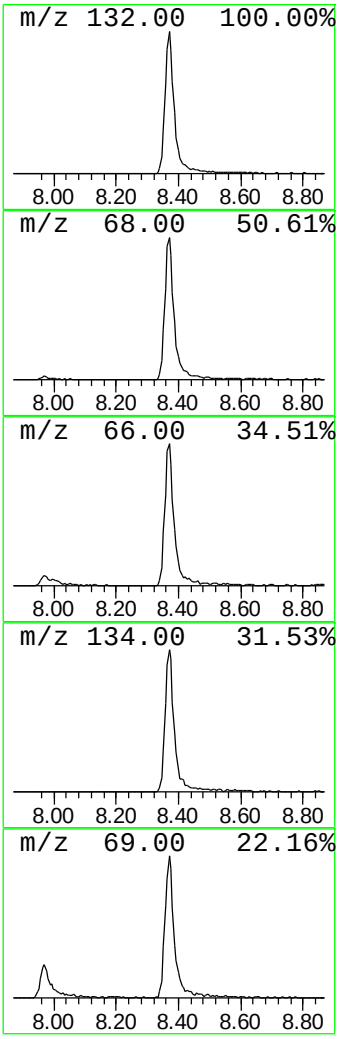
****

Peak Number 4 unknown8.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	79.26 ng	1059070	1,4-Dichlorobenzene-d4	8.86

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-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

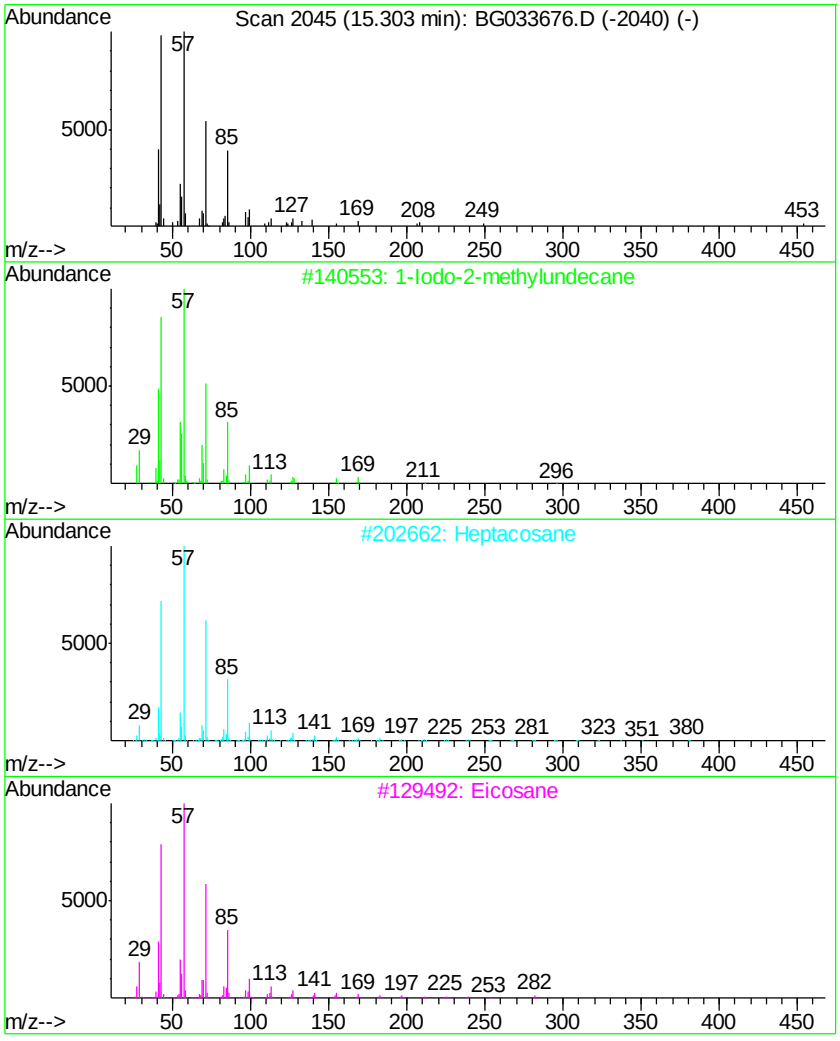
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

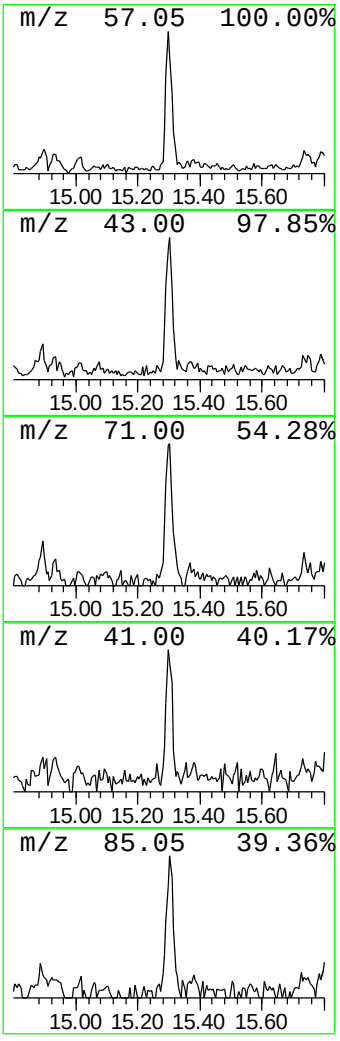
****

Peak Number 6 1-Iodo-2-methylundecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	2.18 ng	67051	Acenaphthene-d10	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
2	Heptacosane	380	C27H56	000593-49-7	72
3	Eicosane	282	C20H42	000112-95-8	72
4	Tridecane	184	C13H28	000629-50-5	72
5	Hexadecane	226	C16H34	000544-76-3	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

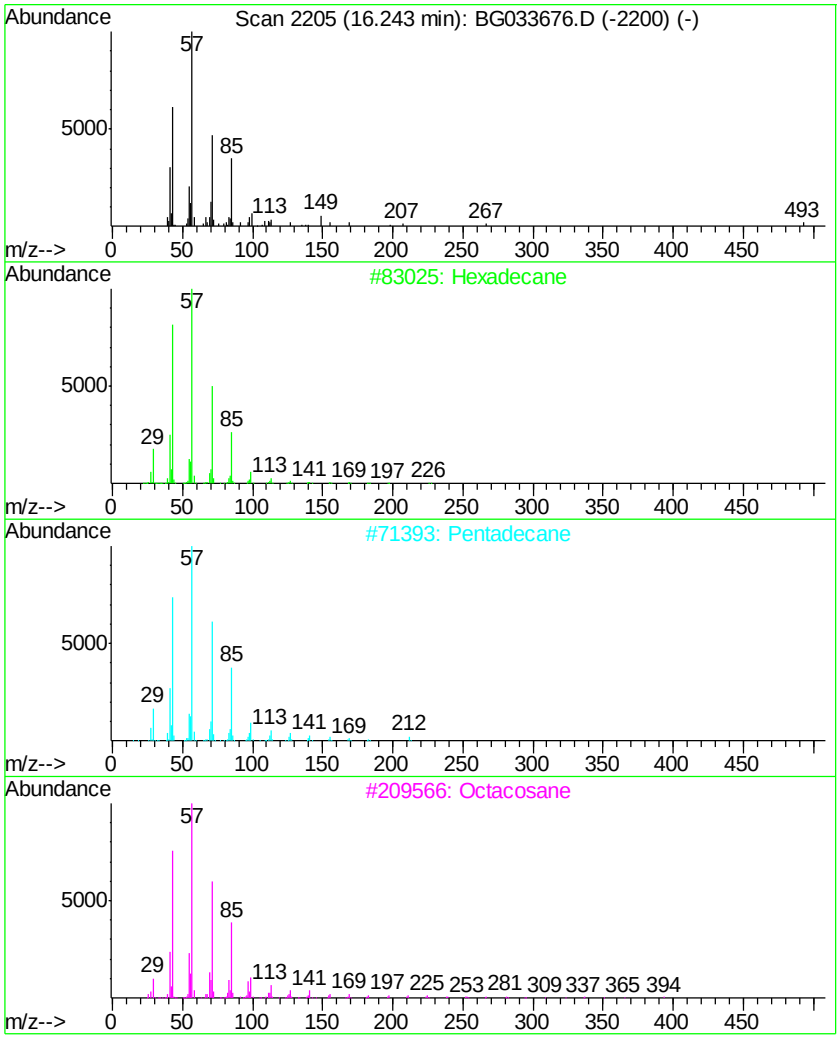
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

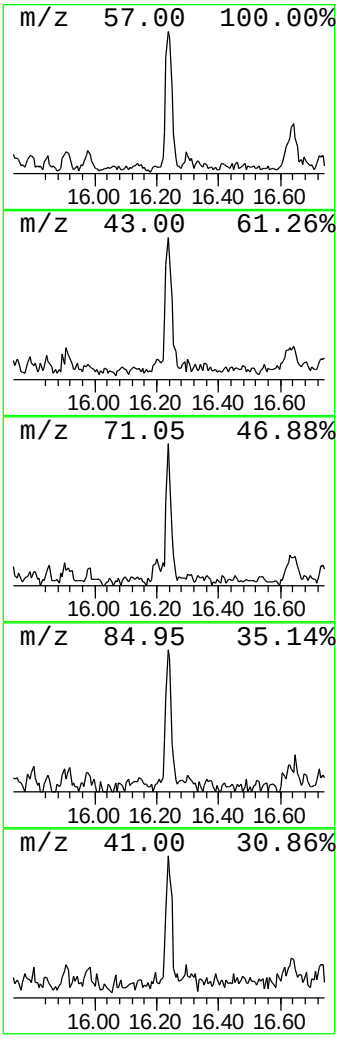
****

Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	2.49 ng	76485	Acenaphthene-d10	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Pentadecane	212	C15H32	000629-62-9	80
3	Octacosane	394	C28H58	000630-02-4	80
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72
5	Tetratetracontane	619	C44H90	007098-22-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

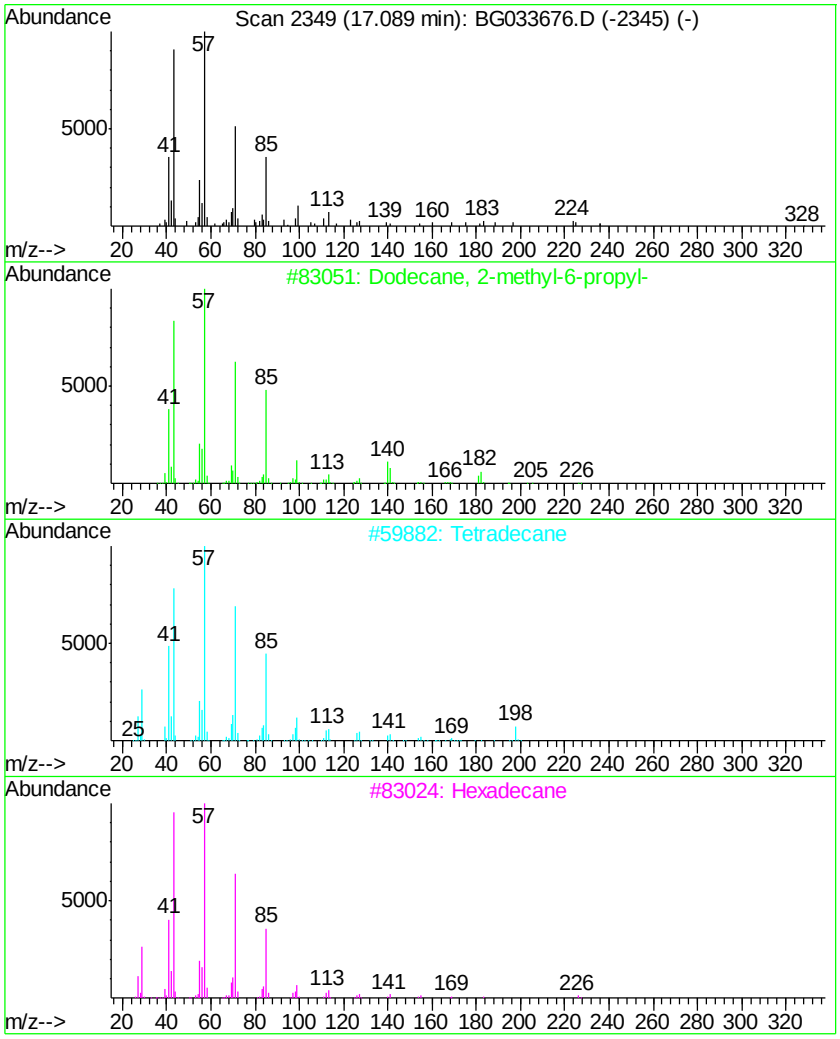
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

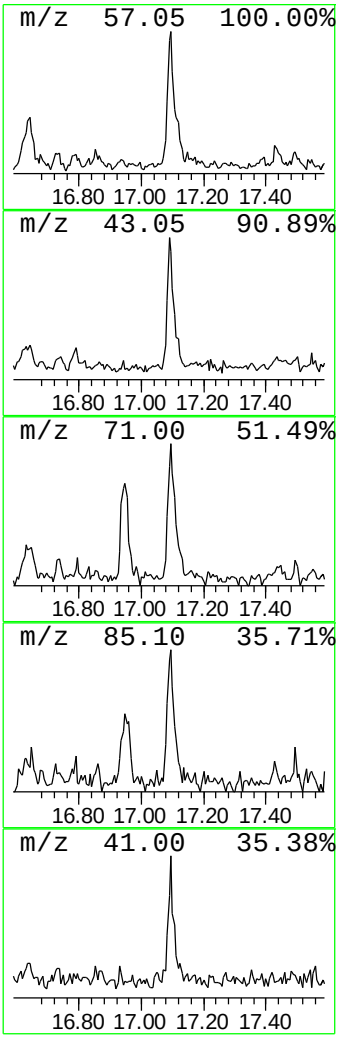
****

Peak Number 8 Dodecane, 2-methyl-6-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	2.11 ng	85208	Phenanthrene-d10	18.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
2	Tetradecane	198	C14H30	000629-59-4	80
3	Hexadecane	226	C16H34	000544-76-3	72
4	Tridecane	184	C13H28	000629-50-5	72
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	70





Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

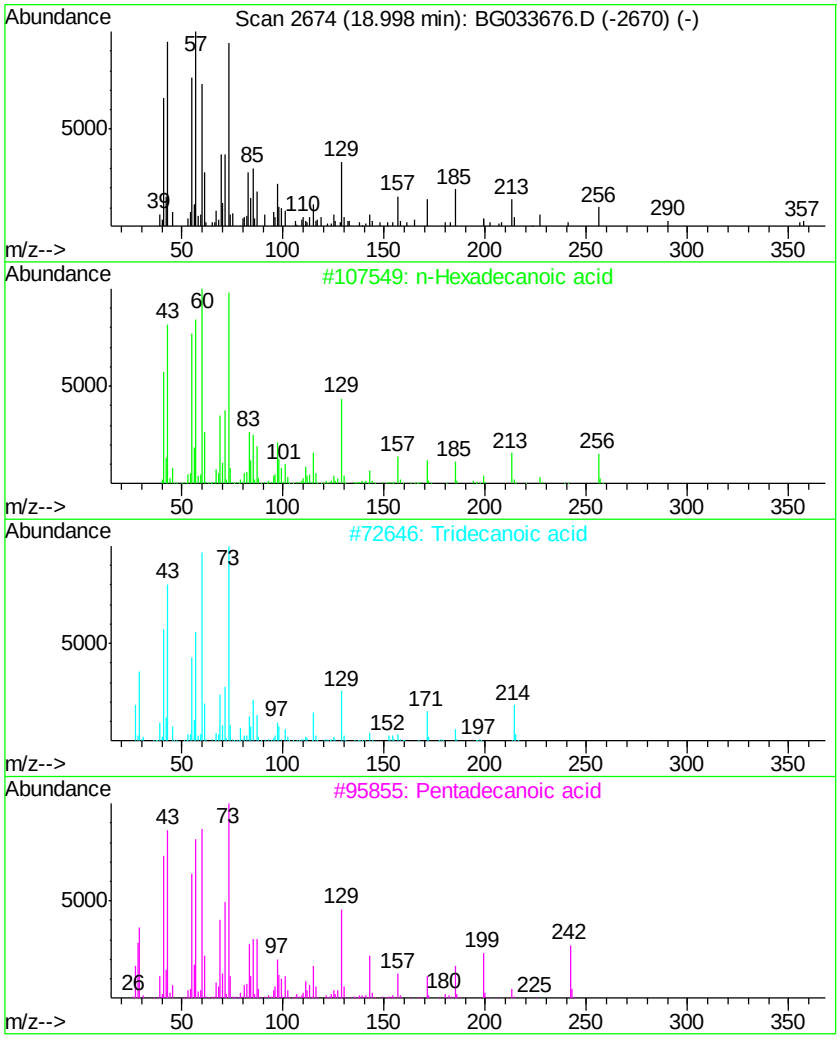
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

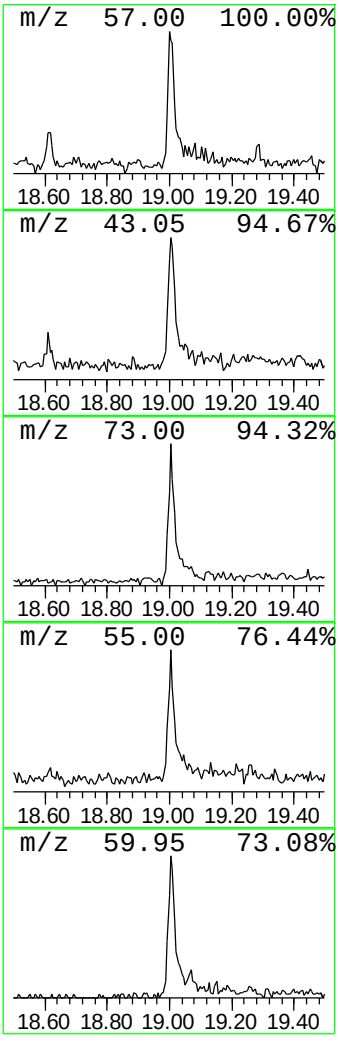
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.00	4.16 ng	168216	Phenanthrene-d10	18.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	42





Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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

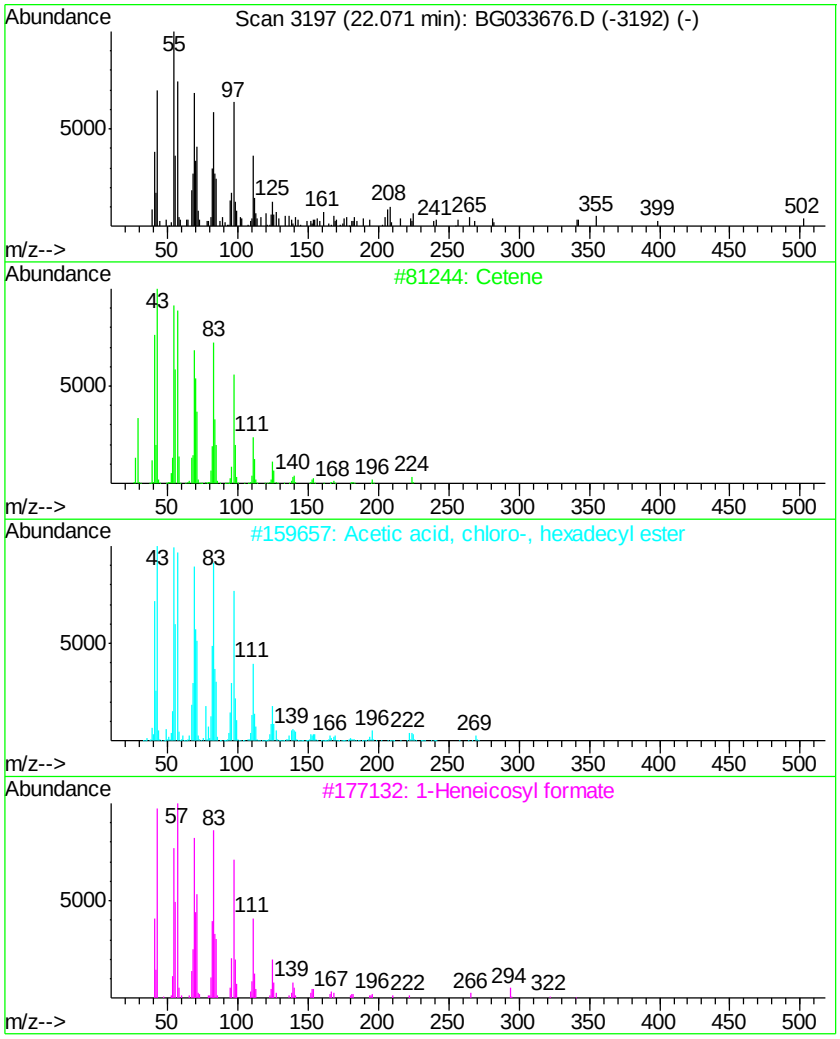
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

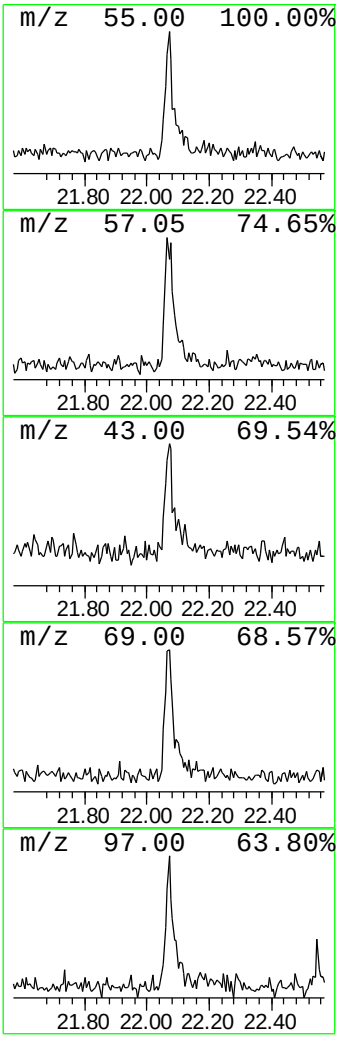
****

Peak Number 10 Cetene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.38 ng	107671	Chrysene-d12	22.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	90
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040918\
Data File : BG033676.D
Acq On : 9 Apr 2018 12:15
Operator : SJ/JU
Sample : J2236-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101

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...	3.57	17.4	ng	232021	1	8.86	267230	20.0
2-Pentanone, 4-hy...	5.77	2.9	ng	38020	1	8.86	267230	20.0
unknown8.37	8.37	79.3	ng	1059070	1	8.86	267230	20.0
1-Iodo-2-methylun...	15.30	2.2	ng	67051	3	15.47	614331	20.0
Hexadecane	16.24	2.5	ng	76485	3	15.47	614331	20.0
Dodecane, 2-methy...	17.09	2.1	ng	85208	4	18.20	807781	20.0
n-Hexadecanoic acid	19.00	4.2	ng	168216	4	18.20	807781	20.0
Cetene	22.07	2.4	ng	107671	5	22.55	904336	20.0