LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

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-BG070816.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	2.891	6	9	23	rVB6	54492	137737	1.46%	0.207%
2	3.037	29	34	53	rVB	4726304	7147997	76.01%	10.757%
3	5.223	400	406	415	rVB	411244	652768	6.94%	0.982%
4	5.699	479	487	497	rBV	2299751	3769852	40.09%	5.673%
5	7.309	753	761	771	rBV	2658587	4703906	50.02%	7.079%
6	7.679	815	824	839	rBV	2485838	4430990	47.12%	6.668%
7	8.149	897	904	911	rBV	477482	817990	8.70%	1.231%
8	8.478	949	960	968	rBV	1795680	3201557	34.05%	4.818%
9	9.324	1096	1104	1112	rBV	1696647	3070890	32.66%	4.621%
10	9.430	1115	1122	1127	rBV2	73178	128419	1.37%	0.193%
11	10.981	1378	1386	1395	rBV	712147	1295482	13.78%	1.950%
12	13.419	1791	1801	1811	rBV	4430532	7179891	76.35%	10.805%
13	14.242	1933	1941	1949	rBV	1731886	2680692	28.51%	4.034%
14	14.800	2029	2036	2043	rBV2	1171265	1896466	20.17%	2.854%
15	15.617	2171	2175	2180	rVB	80969	111523	1.19%	0.168%
16	16.292	2283	2290	2302	rBV	3852146	5979761	63.59%	8.999%
17	16.480	2317	2322	2334	rBV2	112743	226926	2.41%	0.342%
18	17.274	2452	2457	2461	rBV	133997	185789	1.98%	0.280%
19	17.550	2498	2504	2510	rBV2	1403656	2254143	23.97%	3.392%
20	18.014	2580	2583	2589	rVB	114076	148678	1.58%	0.224%
21	18.419	2647	2652	2658	rBV	493355	754934	8.03%	1.136%
22	19.600	2848	2853	2857	rVB	267121	374267	3.98%	0.563%
23	19.683	2863	2867	2874	rBV2	223090	345707	3.68%	0.520%
24	19.824	2888	2891	2898	rVB3	134886	184544	1.96%	0.278%
25	19.959	2911	2914	2919	rVB	238289	339612	3.61%	0.511%
26	20.153	2941	2947	2954	rBV	6997961	9403494	100.00%	14.151%
27	21.463	3166	3170	3175	rBV6	140873	242502	2.58%	0.365%
28	21.857	3230	3237	3243	rBV2	1449206	2617874	27.84%	3.940%
29	25.229	3803	3811	3823	rVB	748527	2164696	23.02%	3.258%

Sum of corrected areas: 66449087

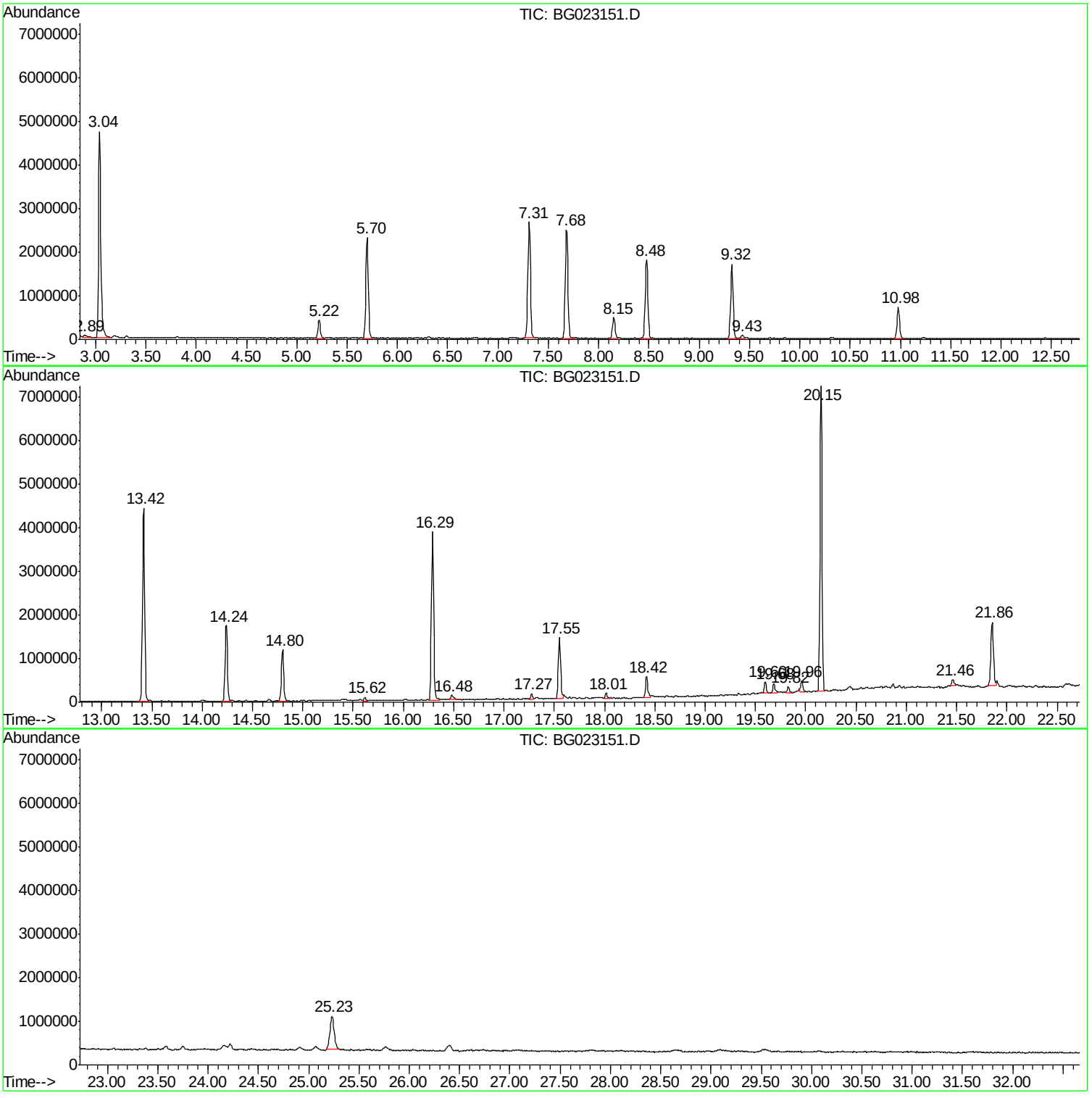
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

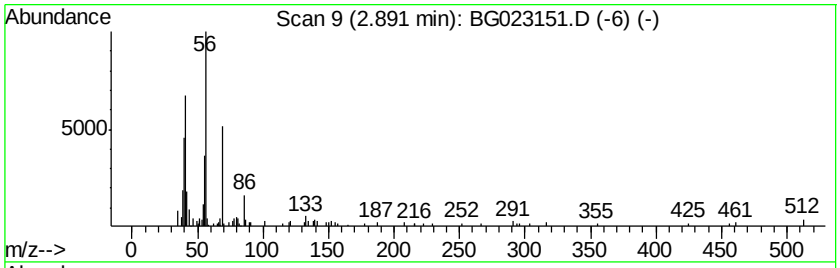
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

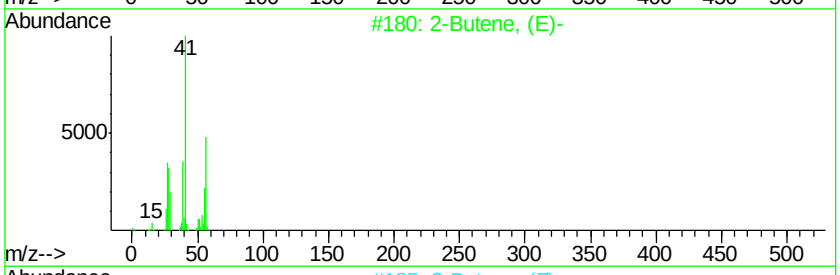
****

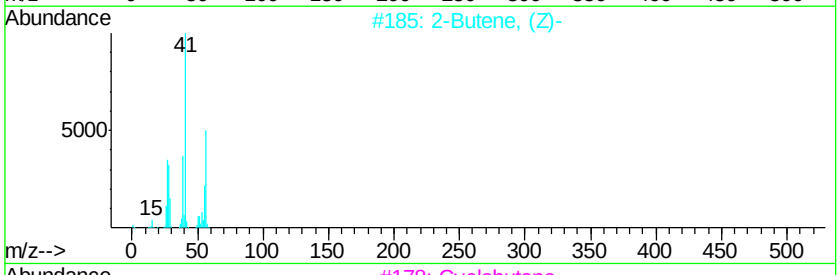
Peak Number 1 2-Butene, (E)- Concentration Rank 6

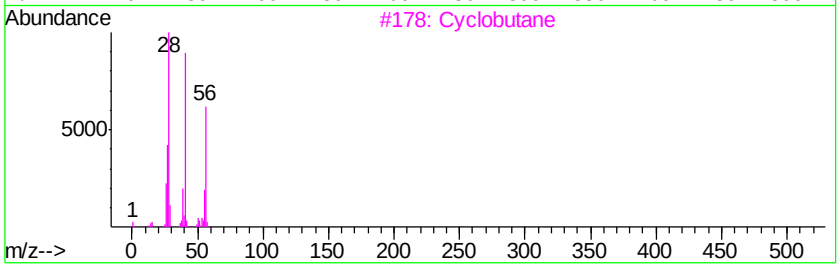
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	3.37 ng	137737	1,4-Dichlorobenzene-d4	8.15

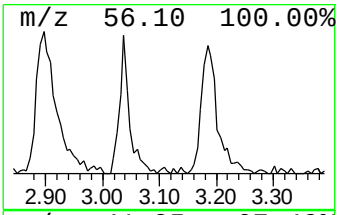
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, (E)-	56	C4H8	000624-64-6	52
2	2-Butene, (Z)-	56	C4H8	000590-18-1	50
3	Cyclobutane	56	C4H8	000287-23-0	50
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	40
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	40

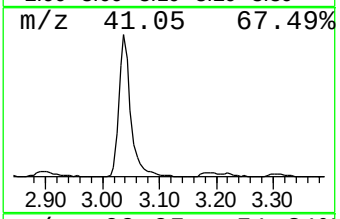


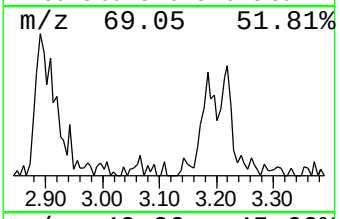


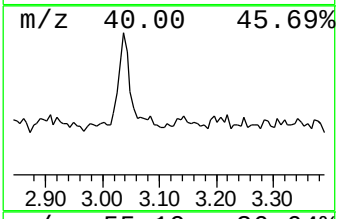


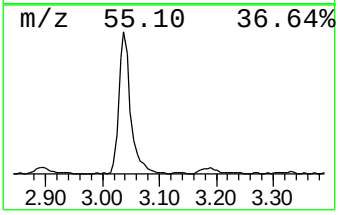












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

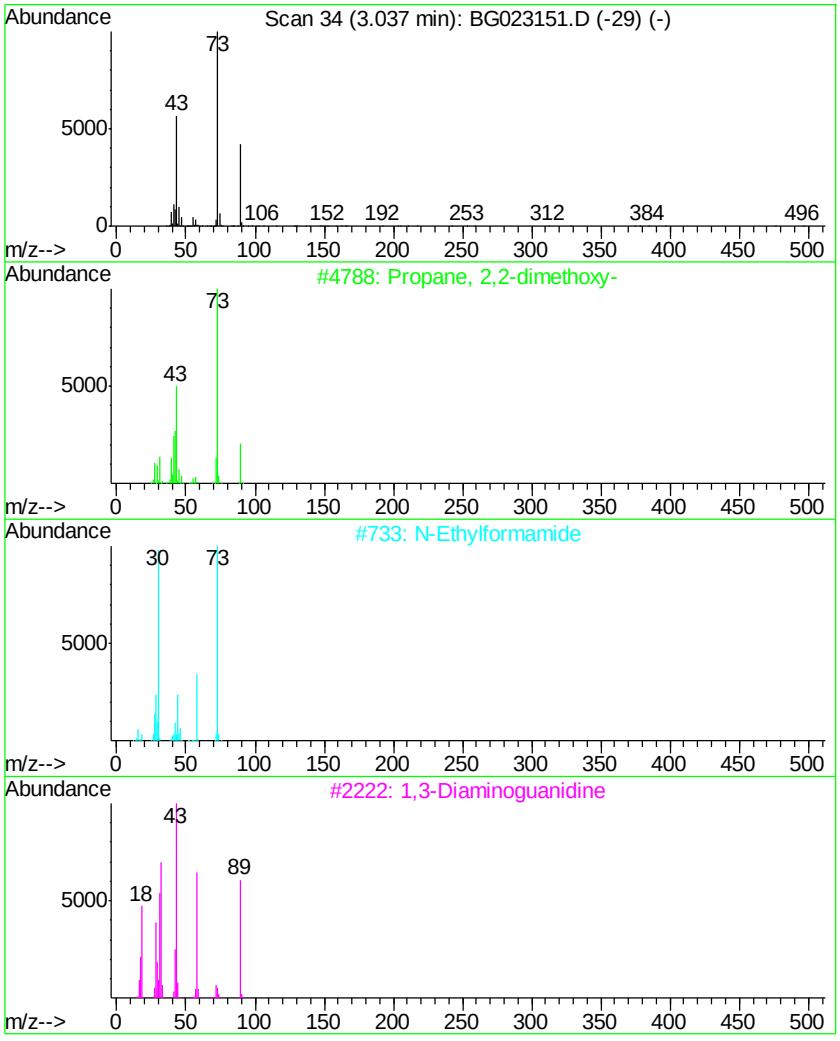
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

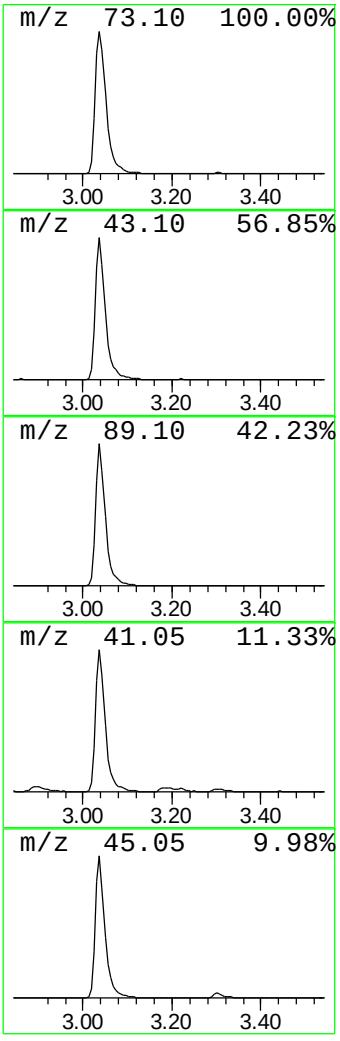
****

Peak Number 2 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	174.77 ng	7148000	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

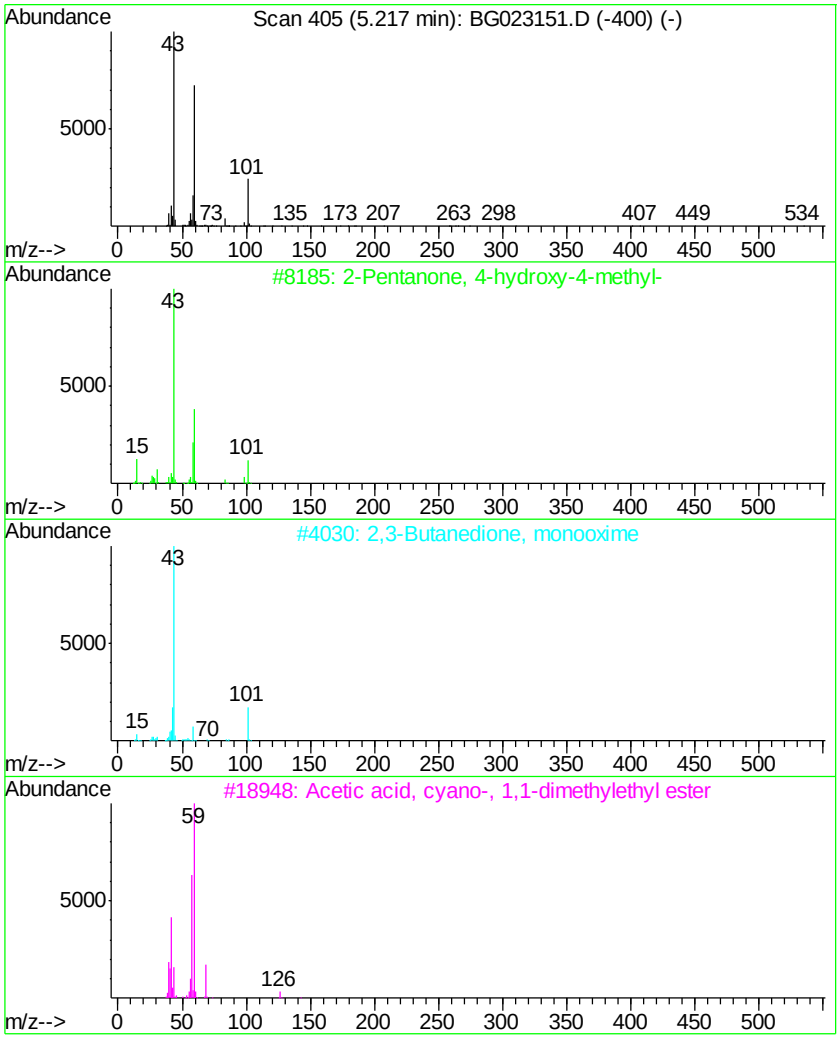
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

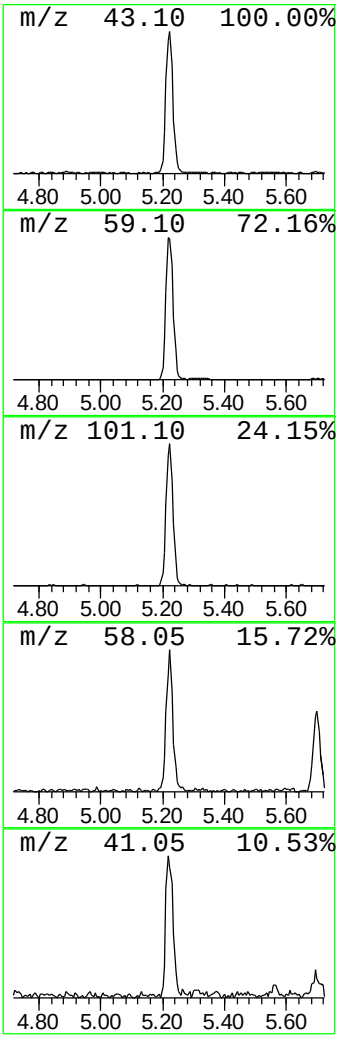
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	15.96 ng	652768	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

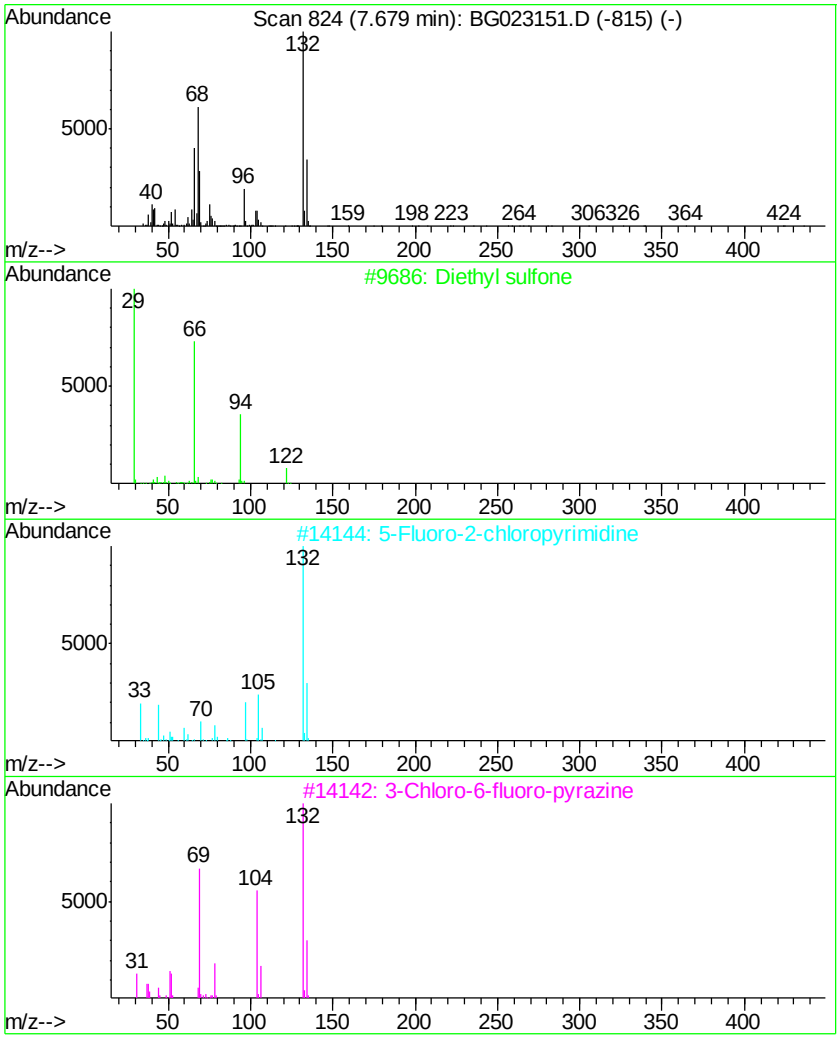
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

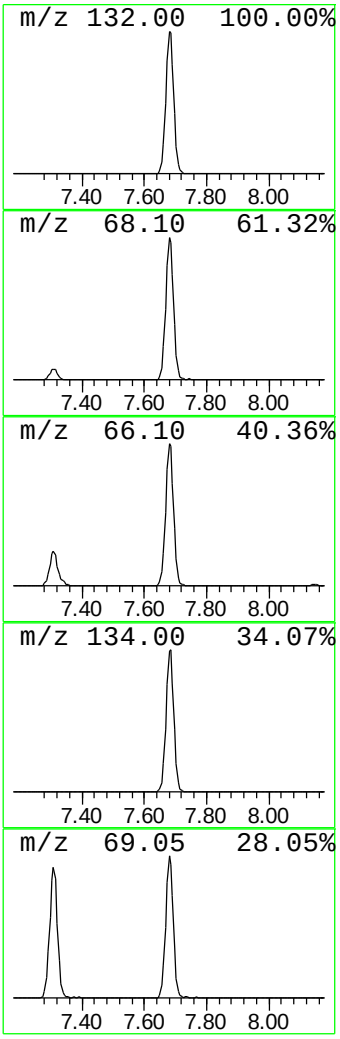
****

Peak Number 4 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	108.34 ng	4430990	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl sulfone	122	C4H10O2S	000597-35-3	17
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

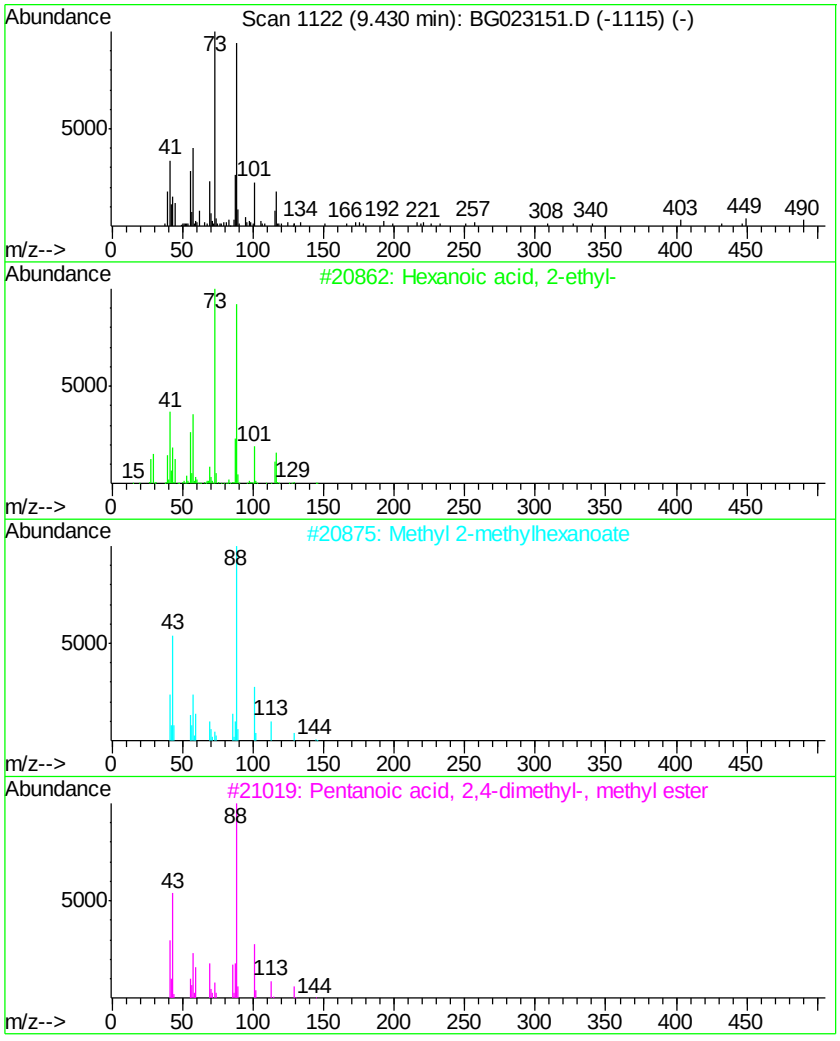
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

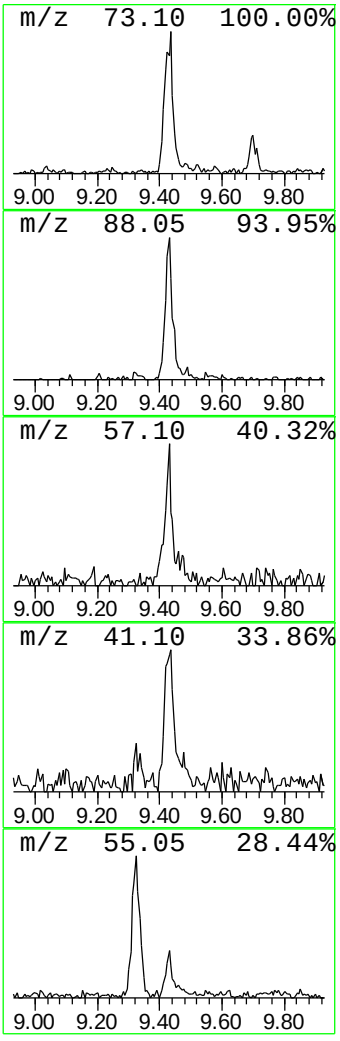
****

Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.43	3.14 ng	128419	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2	Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	42
3	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	42
4	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	40
5	Octanoic acid, ethyl ester	172	C10H20O2	000106-32-1	40





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Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
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Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

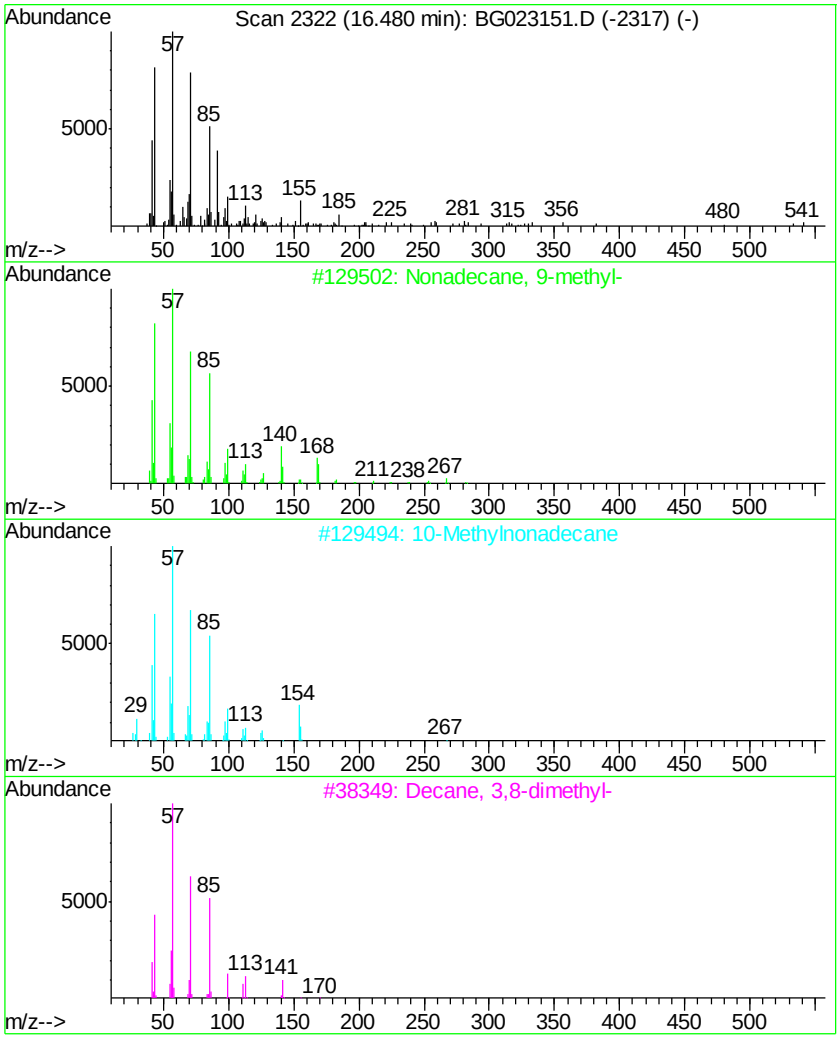
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

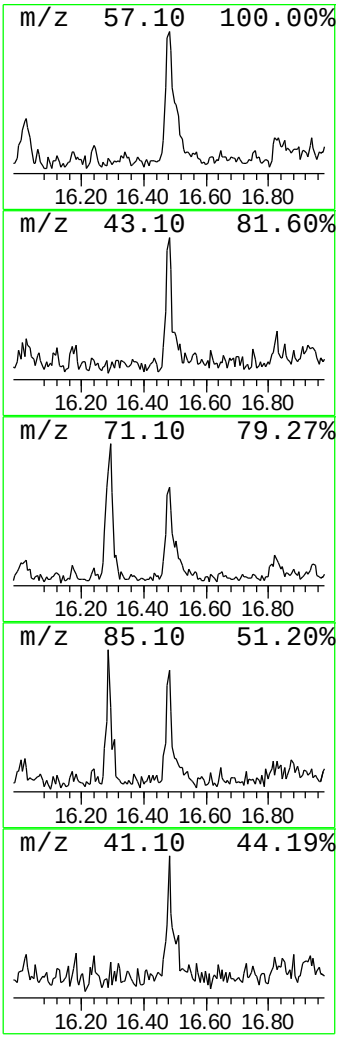
****

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	2.01 ng	226926	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	10-Methylnonadecane	282	C20H42	056862-62-5	90
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86





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Sample : H3951-03
Misc :
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Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

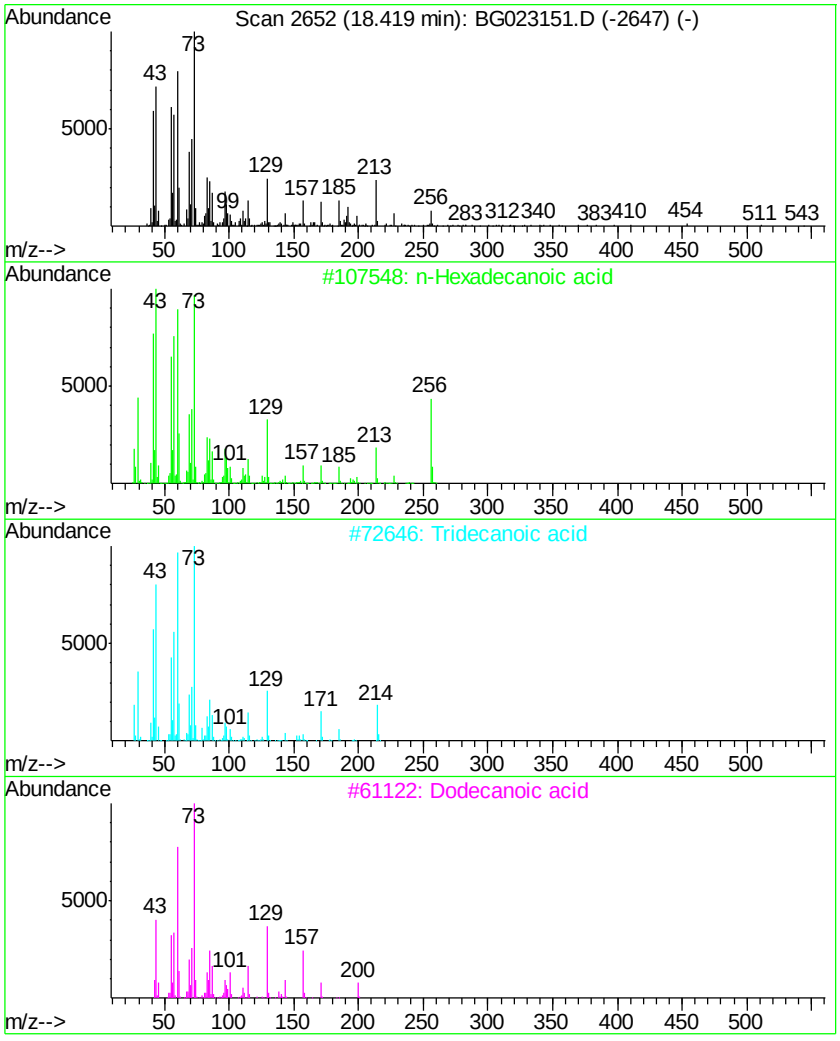
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

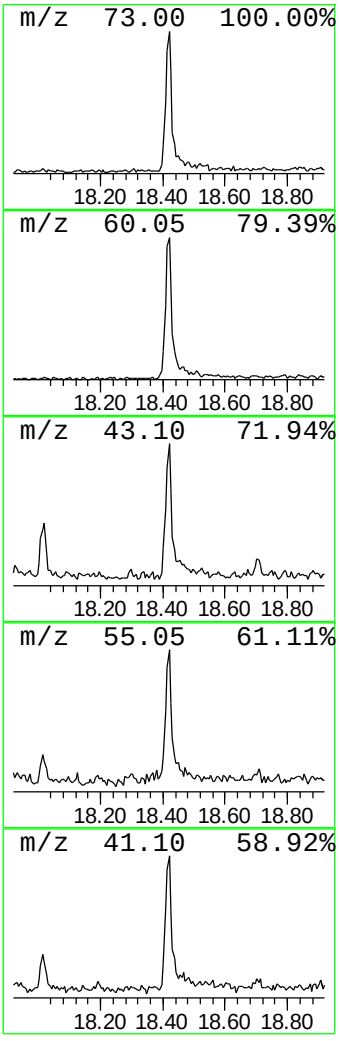
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	6.70 ng	754934	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Dodecanoic acid	200	C12H24O2	000143-07-7	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	43





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

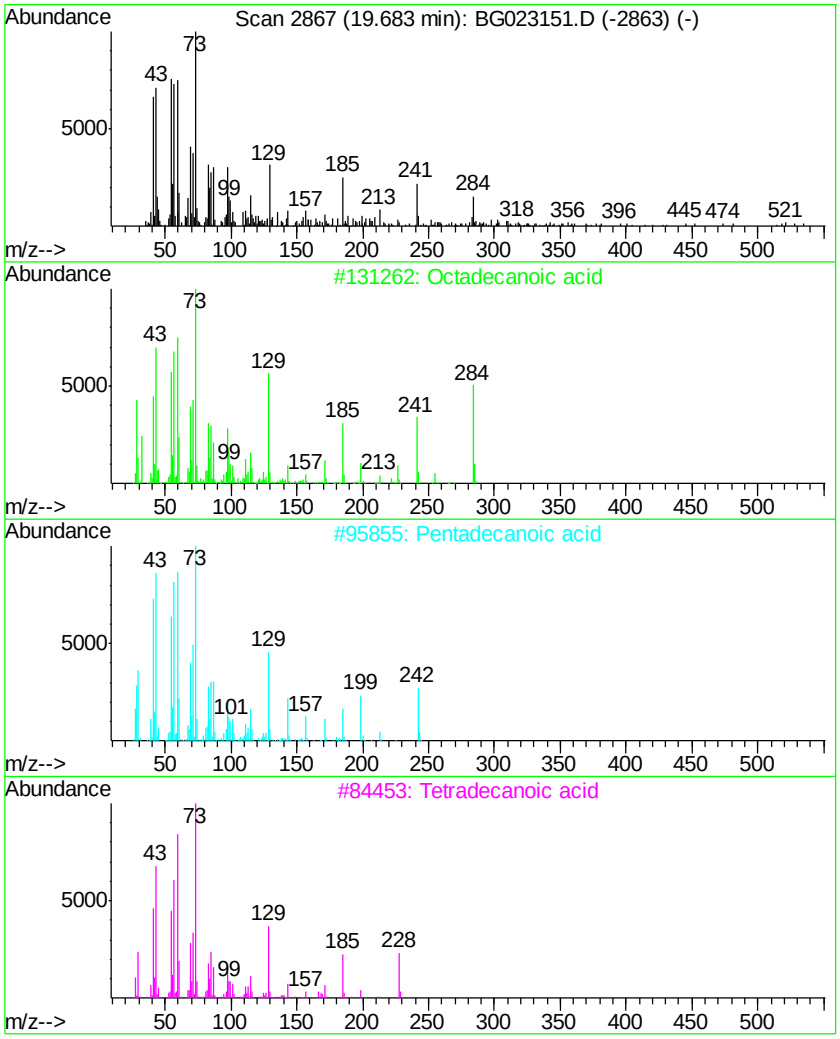
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

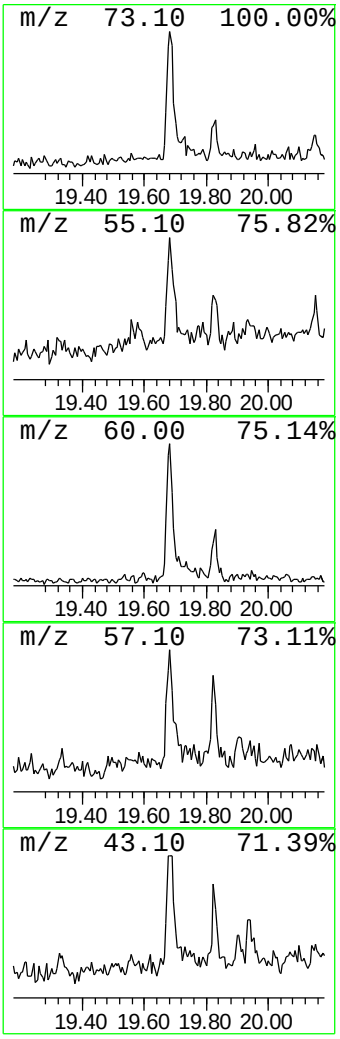
****

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	3.07 ng	345707	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	89
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071616\
Data File : BG023151.D
Acq On : 16 Jul 2016 17:43
Operator : UM/SJ
Sample : H3951-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LSS-SB-SB01(7-9ft)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
2-Butene, (E)-	2.89	3.4	ng	137737	1	8.15	817990	20.0
unknown3.04	3.04	174.8	ng	7148000	1	8.15	817990	20.0
2-Pentanone, 4-hy...	5.22	16.0	ng	652768	1	8.15	817990	20.0
unknown7.68	7.68	108.3	ng	4430990	1	8.15	817990	20.0
Hexanoic acid, 2-...	9.43	3.1	ng	128419	1	8.15	817990	20.0
Nonadecane, 9-met...	16.48	2.0	ng	226926	4	17.55	2254140	20.0
n-Hexadecanoic acid	18.42	6.7	ng	754934	4	17.55	2254140	20.0
Octadecanoic acid	19.68	3.1	ng	345707	4	17.55	2254140	20.0