LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

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-BG040615.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	2.759	7	12	21	rBV	223917	359357	8.57%	1.531%
2	2.835	21	25	37	rVB	276894	363878	8.68%	1.550%
3	4.780	349	356	362	rBV	61785	87556	2.09%	0.373%
4	5.256	431	437	445	rBV	575659	812848	19.39%	3.464%
5	6.854	702	709	718	rBV	399070	617097	14.72%	2.629%
6	7.201	761	768	780	rBV	1031649	1614291	38.51%	6.878%
7	7.665	841	847	853	rBV	273036	421547	10.06%	1.796%
8	7.982	894	901	910	rBV	884081	1372099	32.73%	5.846%
9	8.822	1037	1044	1052	rBV	765010	1205492	28.76%	5.137%
10	10.450	1314	1321	1328	rBV	413793	675930	16.13%	2.880%
11	12.659	1691	1697	1705	rBV	29331	51469	1.23%	0.219%
12	12.929	1735	1743	1755	rVB	2131267	3132233	74.72%	13.346%
13	14.310	1971	1978	1987	rBV2	658810	971986	23.19%	4.142%
14	15.667	2205	2209	2215	rBV	46208	62915	1.50%	0.268%
15	15.802	2224	2232	2250	rBV	1548282	2257551	53.86%	9.619%
16	16.078	2273	2279	2287	rVB	68054	95428	2.28%	0.407%
17	17.048	2438	2444	2453	rBV2	836938	1199173	28.61%	5.110%
18	17.947	2593	2597	2606	rBV	174169	281003	6.70%	1.197%
19	18.041	2607	2613	2621	rVB2	153623	230860	5.51%	0.984%
20	19.087	2787	2791	2793	rBV3	31669	44431	1.06%	0.189%
21	19.234	2812	2816	2824	rBV	114389	164287	3.92%	0.700%
22	19.680	2886	2892	2897	rBV	3542749	4191782	100.00%	17.861%
23	20.479	3024	3028	3032	rBV3	49461	72061	1.72%	0.307%
24	20.908	3098	3101	3103	rBV	49786	51428	1.23%	0.219%
25	20.943	3103	3107	3117	rVB	268124	356551	8.51%	1.519%
26	21.143	3138	3141	3145	rBV	71583	81305	1.94%	0.346%
27	21.231	3151	3156	3161	rBV	936927	1177578	28.09%	5.018%
28	21.378	3178	3181	3184	rVB	74549	75060	1.79%	0.320%
29	21.760	3243	3246	3250	rVB3	60309	83380	1.99%	0.355%
30	21.807	3251	3254	3257	rBV2	56698	61411	1.47%	0.262%
31	22.265	3329	3332	3338	rVB3	61529	87794	2.09%	0.374%
32	22.771	3415	3418	3424	rVB	42397	60478	1.44%	0.258%
33	23.458	3529	3535	3545	rVB	612486	1148545	27.40%	4.894%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-PMW-11A

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-BG040615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

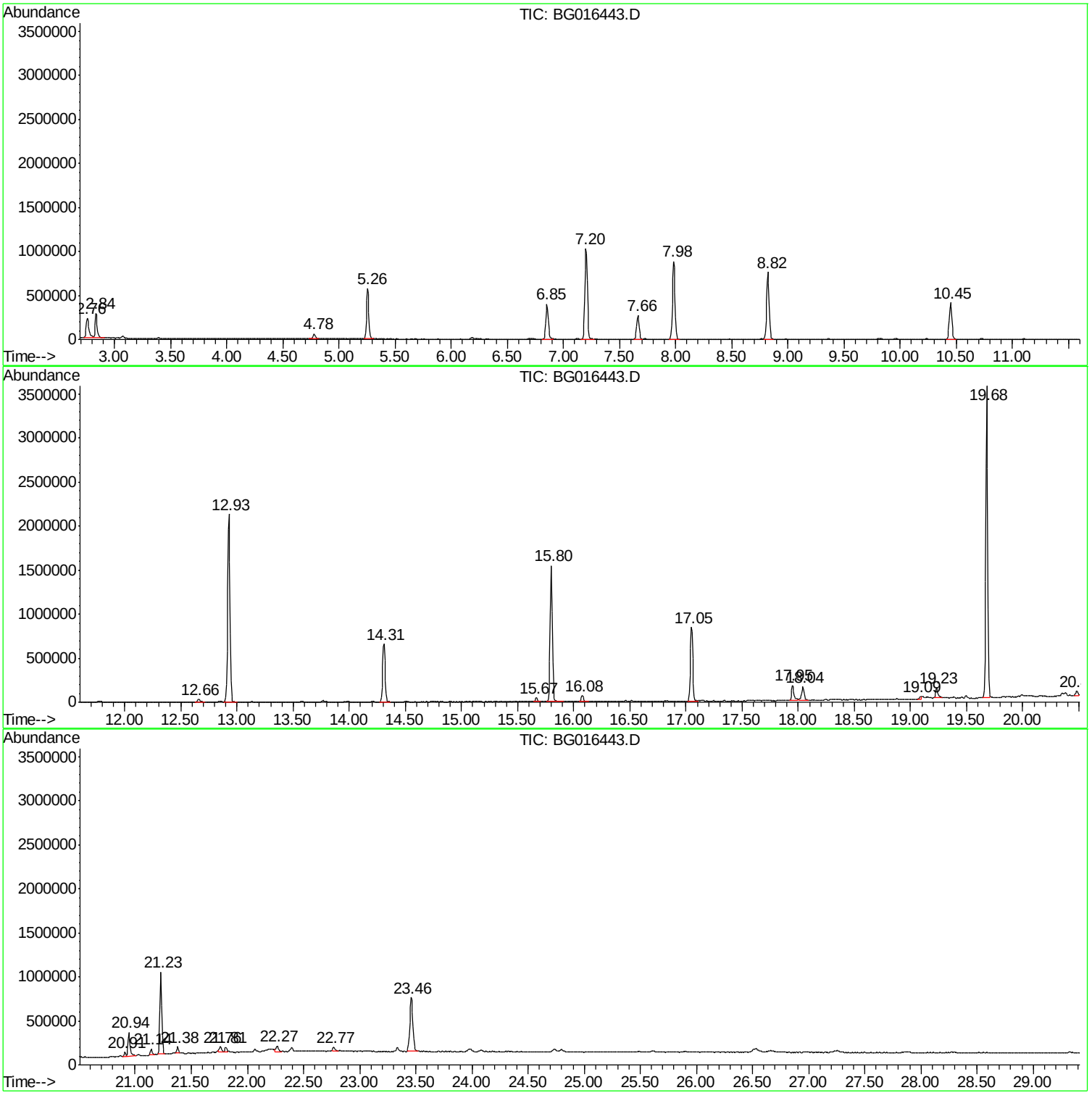
Sum of corrected areas: 23468804

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

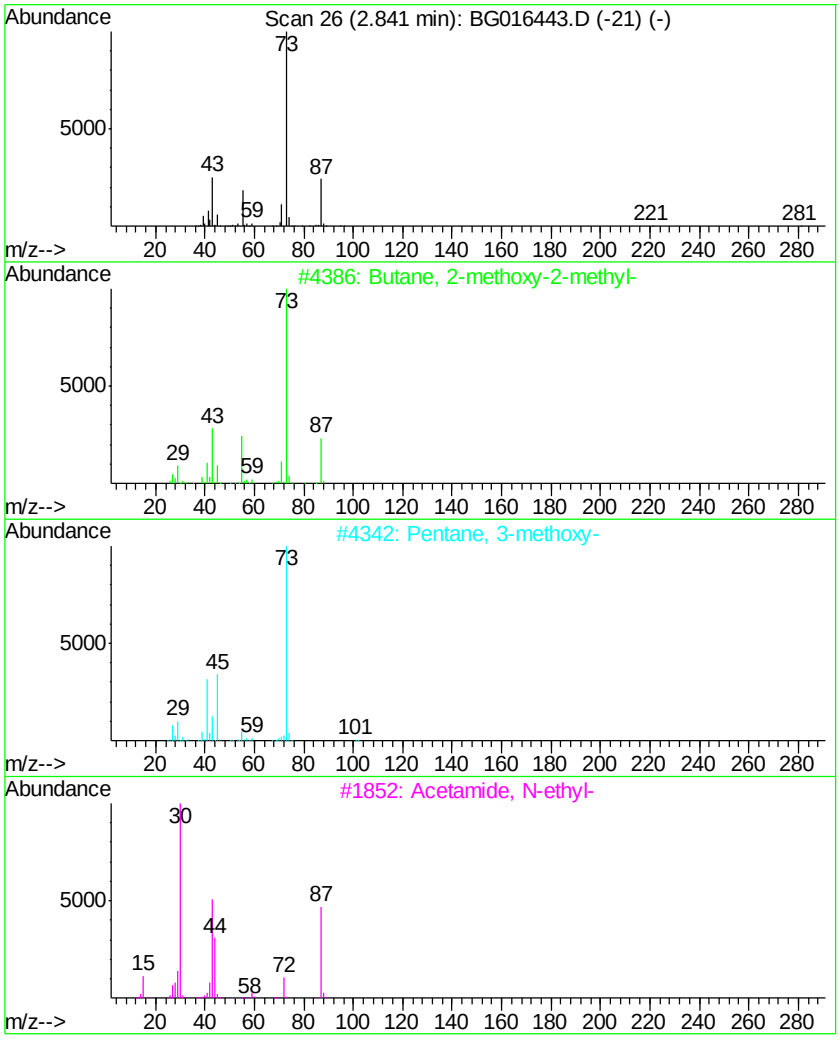
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

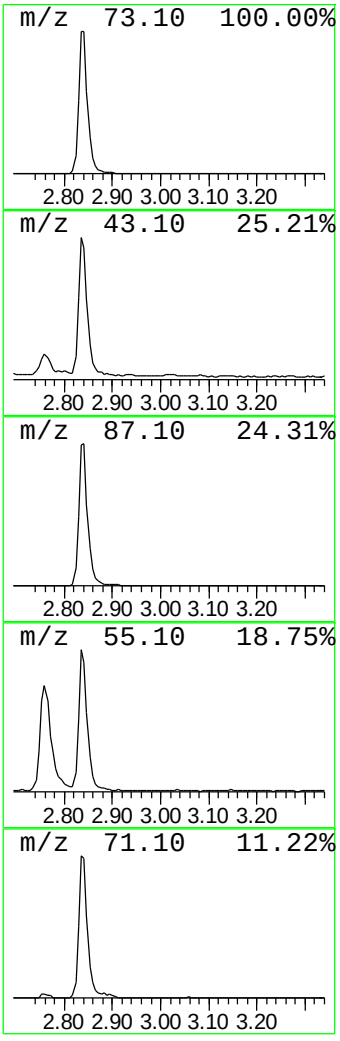
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	17.26 ng	363878	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

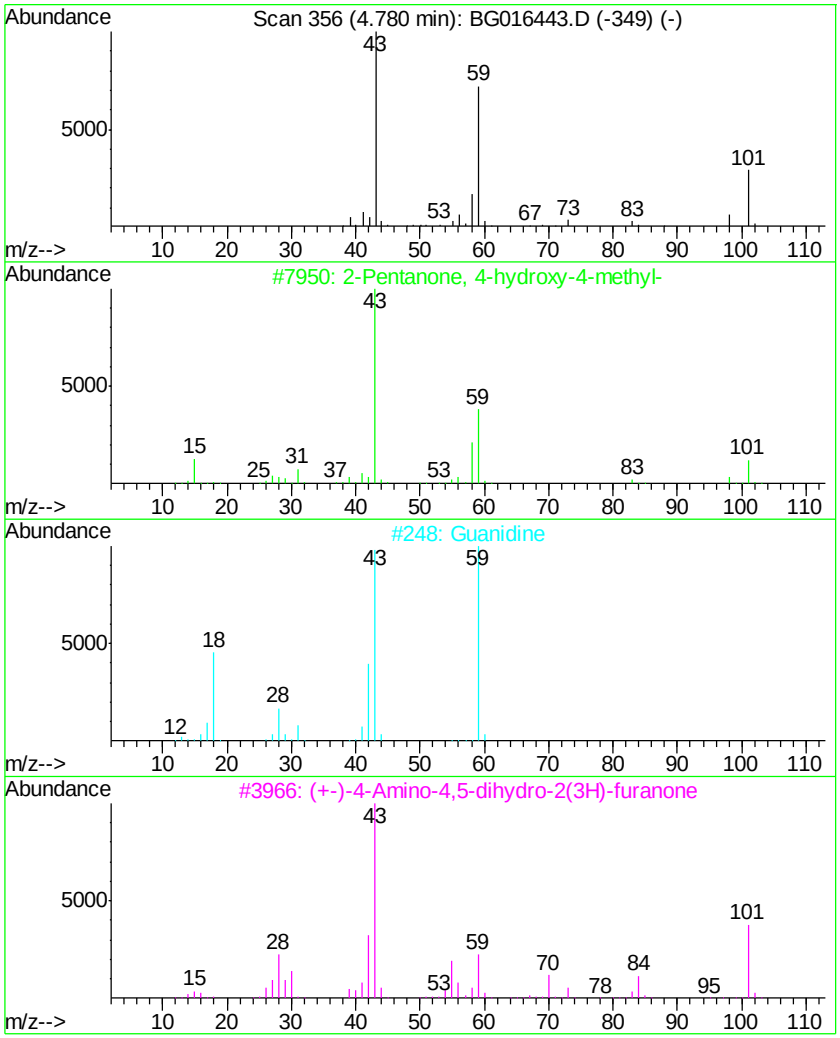
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

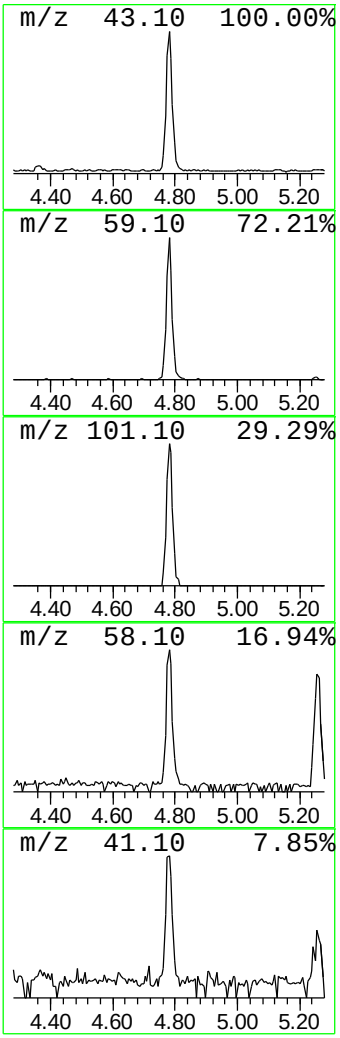
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	4.15 ng	87556	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Guanidine	59	CH5N3	000113-00-8	43
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

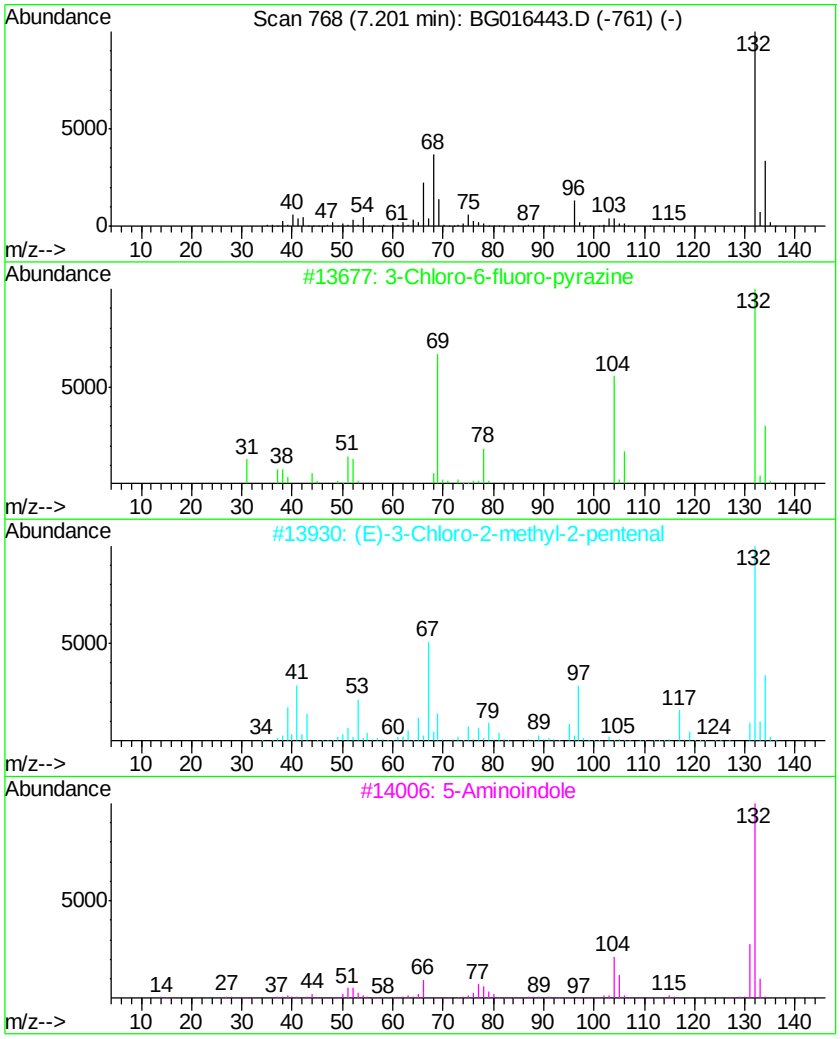
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

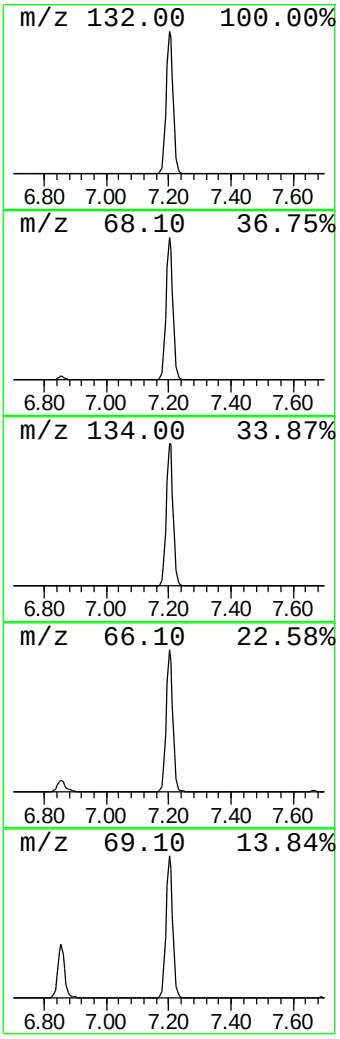
****

Peak Number 4 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	76.59 ng	1614290	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

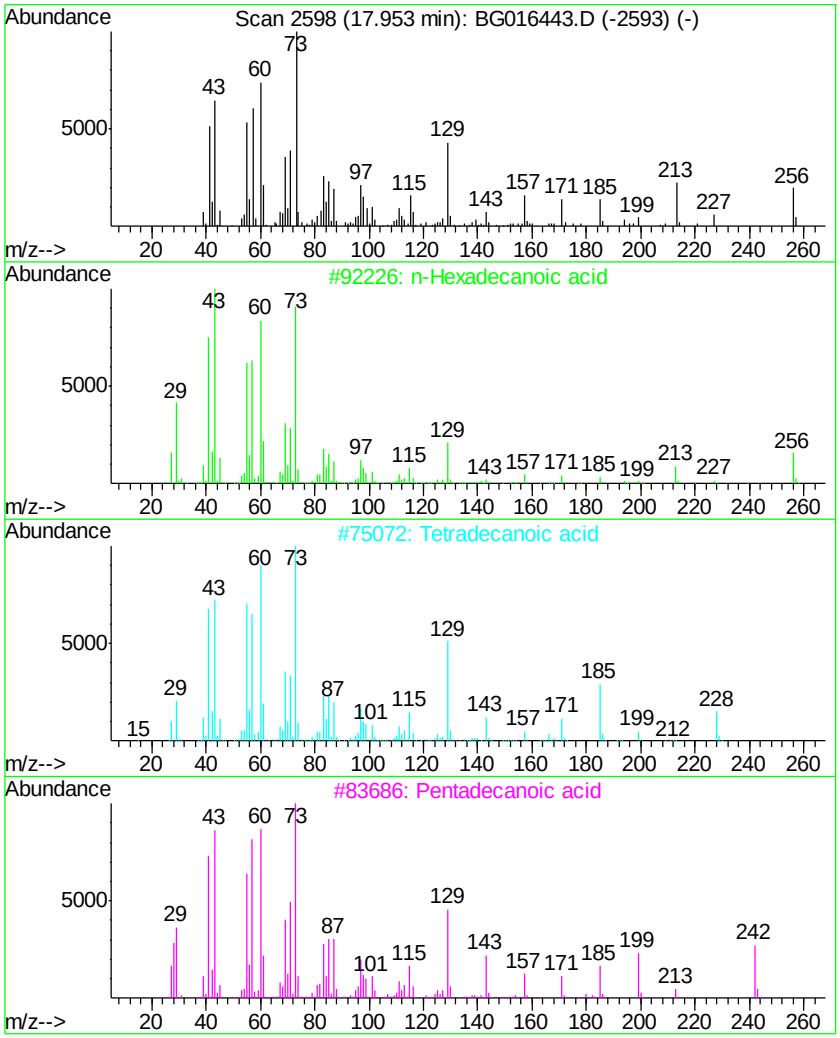
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

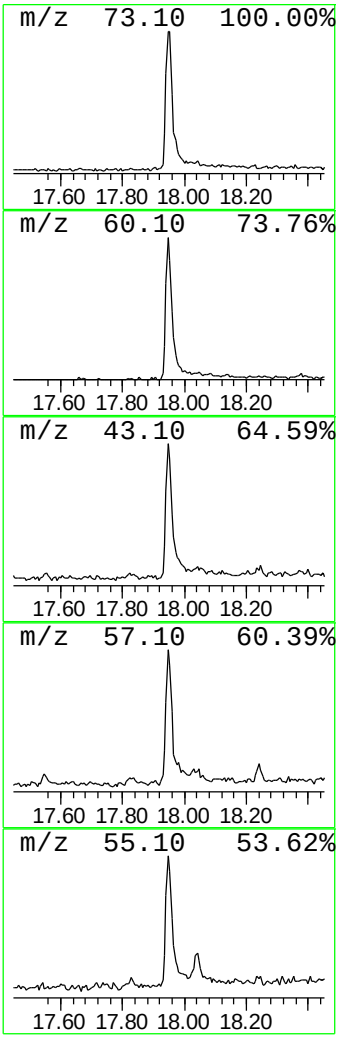
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	4.69 ng	281003	Phenanthrene-d10	17.05

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	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	11





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

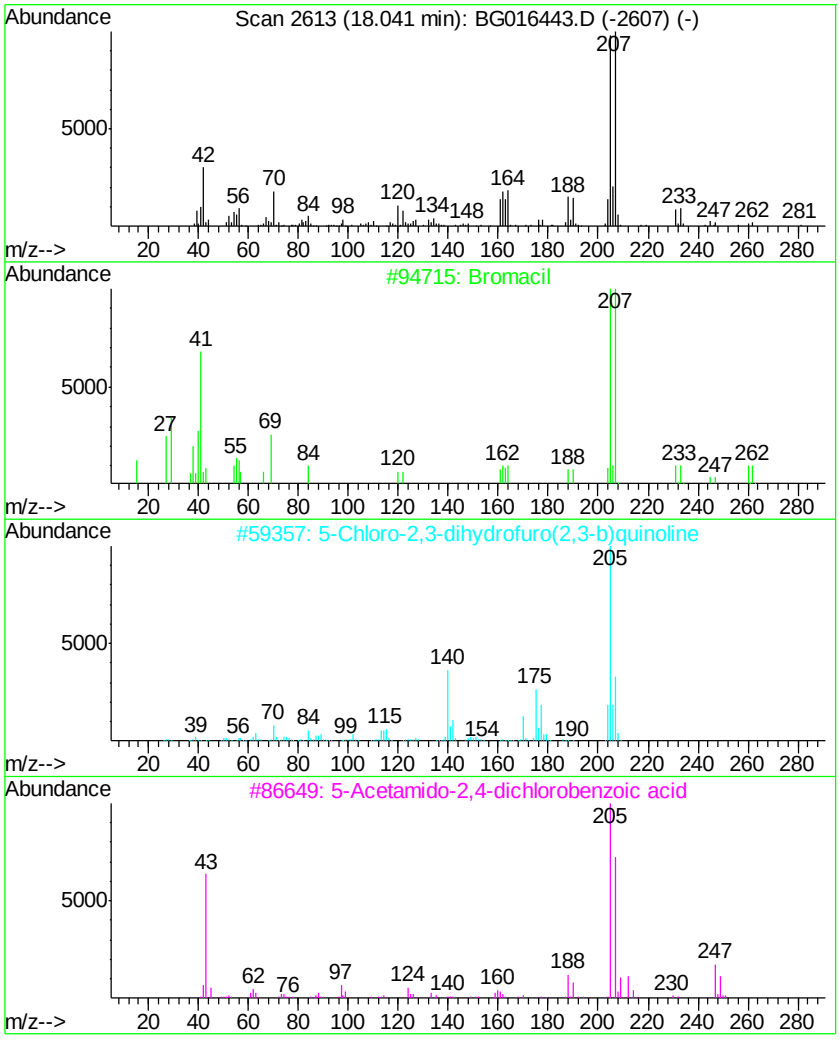
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

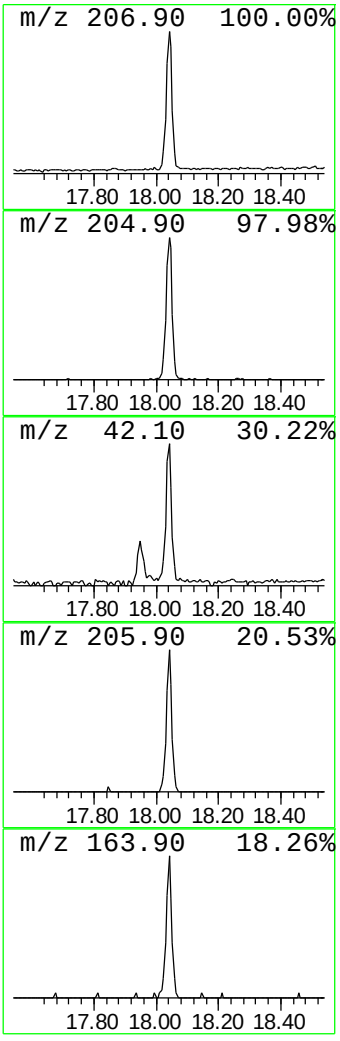
****

Peak Number 7 Bromacil Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	3.85 ng	230860	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromacil	260	C9H13BrN2O2	000314-40-9	93
2	5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	38
3	5-Acetamido-2,4-dichlorobenzoic ...	247	C9H7Cl2NO3	050602-49-8	38
4	7-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-91-0	37
5	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	36





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

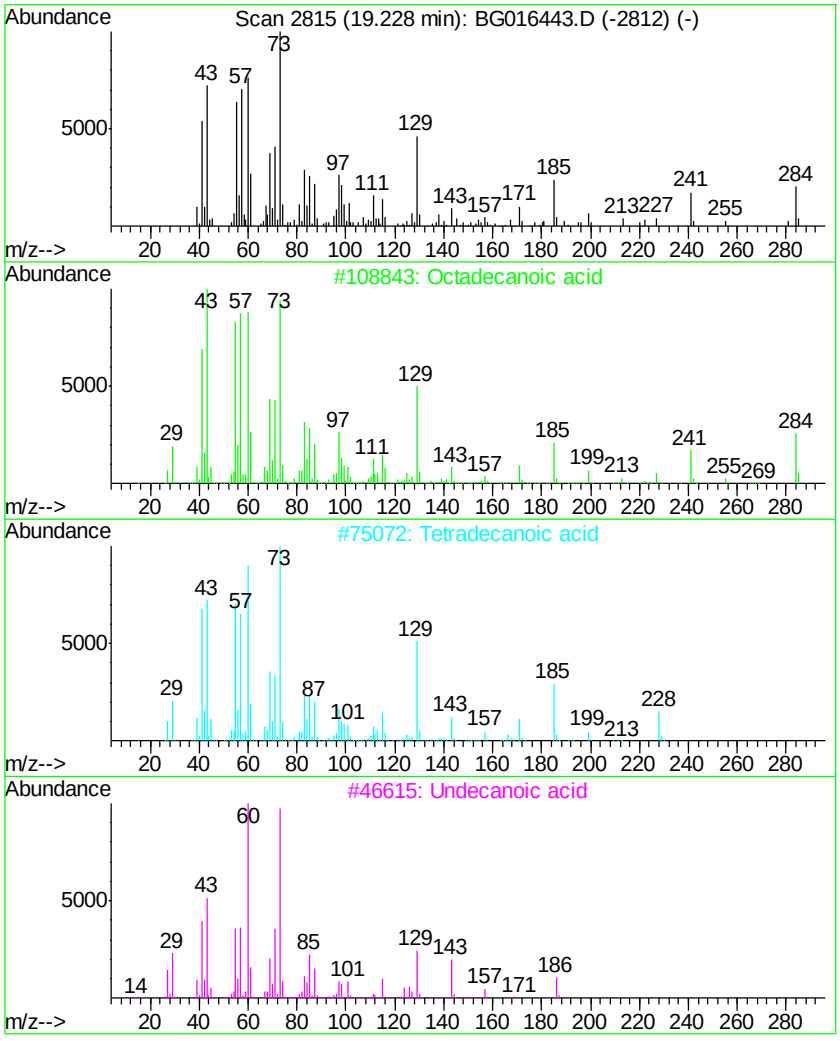
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

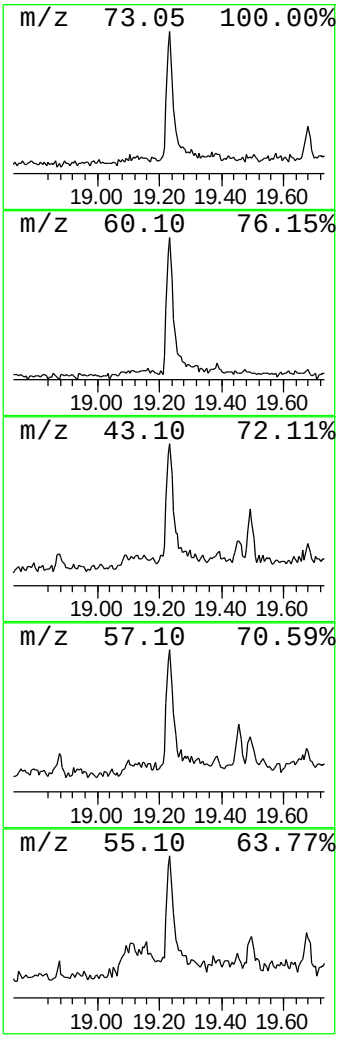
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	2.79 ng	164287	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

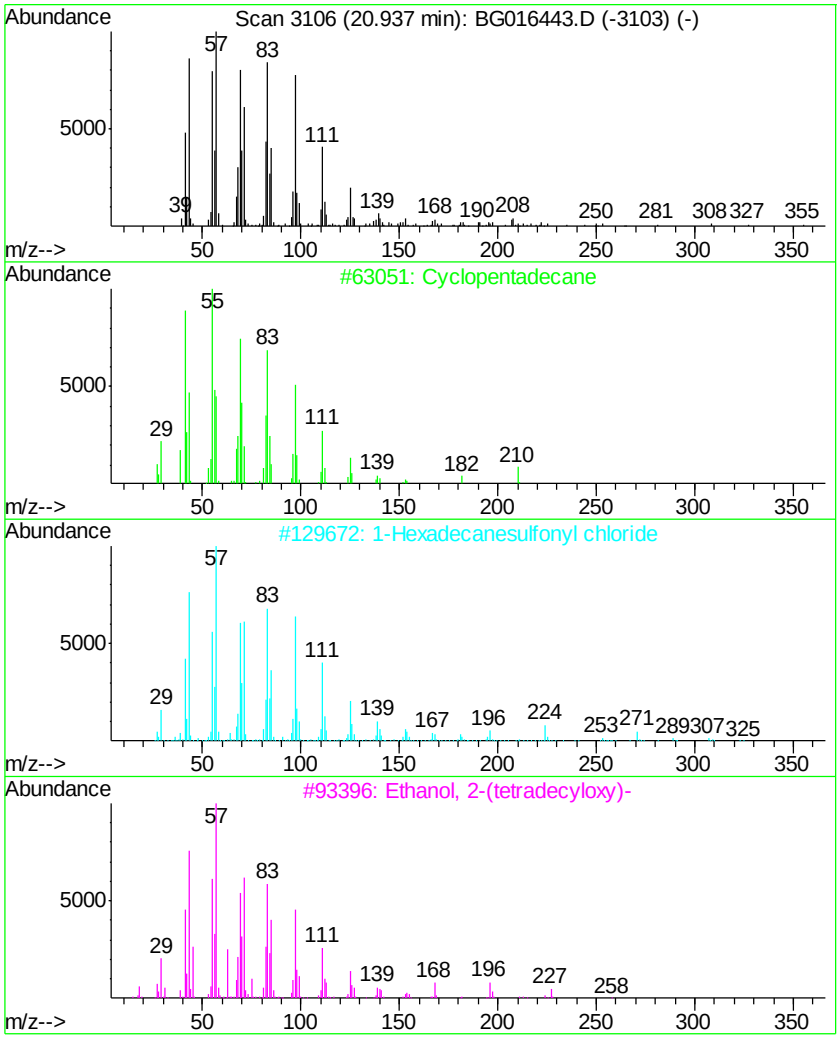
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

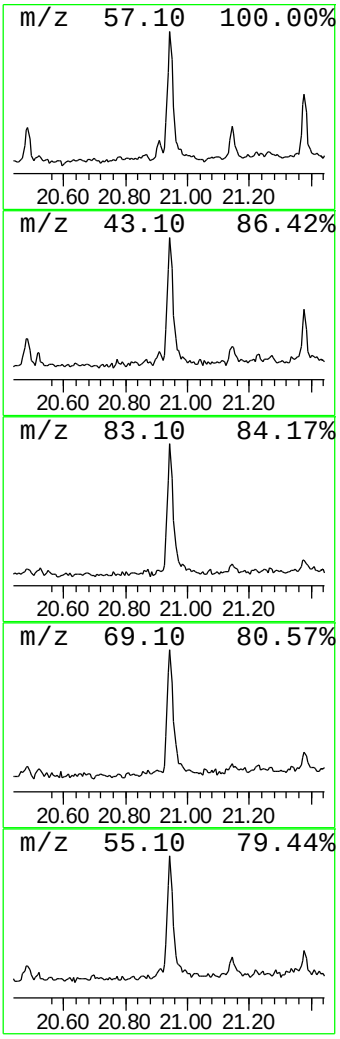
****

Peak Number 9 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	6.06 ng	356551	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	1-Docosene	308	C22H44	001599-67-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016443.D
Acq On : 16 Apr 2015 4:52
Operator : TP/IZ
Sample : G1829-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.84	17.3	ng	363878	1	7.66	421547	20.0
2-Pentanone, 4-hy...	4.78	4.2	ng	87556	1	7.66	421547	20.0
unknown7.20	7.20	76.6	ng	1614290	1	7.66	421547	20.0
n-Hexadecanoic acid	17.95	4.7	ng	281003	4	17.05	1199170	20.0
Bromacil	18.04	3.9	ng	230860	4	17.05	1199170	20.0
Octadecanoic acid	19.23	2.8	ng	164287	5	21.23	1177580	20.0
Cyclopentadecane	20.94	6.1	ng	356551	5	21.23	1177580	20.0