LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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	2.761	7	12	21	rBV	372919	550138	11.64%	2.037%
2	2.837	21	25	36	rVB	424663	490569	10.38%	1.816%
3	3.072	61	65	77	rVB	222453	303216	6.42%	1.123%
4	4.782	350	356	363	rVB	57577	83736	1.77%	0.310%
5	5.258	431	437	447	rBV	631077	878663	18.59%	3.253%
6	5.346	447	452	459	rVB	37105	55976	1.18%	0.207%
7	6.856	699	709	721	rVB	413111	645944	13.67%	2.391%
8	7.203	761	768	777	rBV	1283021	1972485	41.74%	7.303%
9	7.667	840	847	854	rBV	287821	438644	9.28%	1.624%
10	7.984	894	901	911	rVB	1120935	1737868	36.77%	6.434%
11	8.824	1037	1044	1055	rBV	947008	1518257	32.13%	5.621%
12	10.452	1314	1321	1330	rBV	459192	744368	15.75%	2.756%
13	12.661	1691	1697	1709	rBV2	28778	53986	1.14%	0.200%
14	12.931	1735	1743	1755	rVB	2669512	3974570	84.10%	14.715%
15	14.306	1970	1977	1986	rVB2	722455	1115580	23.61%	4.130%
16	15.669	2204	2209	2215	rVB	54777	70538	1.49%	0.261%
17	15.798	2223	2231	2242	rBV	1629447	2472057	52.31%	9.152%
18	17.050	2438	2444	2453	rBV2	938540	1292962	27.36%	4.787%
19	17.949	2592	2597	2606	rBV	136581	215206	4.55%	0.797%
20	19.235	2811	2816	2823	rBV	84045	123627	2.62%	0.458%
21	19.494	2856	2860	2864	rVB	48236	51680	1.09%	0.191%
22	19.682	2886	2892	2900	rVB	3794801	4725991	100.00%	17.497%
23	20.481	3024	3028	3032	rBV3	57202	76266	1.61%	0.282%
24	20.945	3103	3107	3114	rBV	175125	225496	4.77%	0.835%
25	21.145	3137	3141	3145	rBV	126300	141414	2.99%	0.524%
26	21.227	3150	3155	3161	rBV	963946	1238945	26.22%	4.587%
27	21.380	3178	3181	3184	rVB	80298	81861	1.73%	0.303%
28	21.762	3242	3246	3251	rVB2	107761	174214	3.69%	0.645%
29	21.809	3251	3254	3257	rVB	70249	76400	1.62%	0.283%
30	22.067	3294	3298	3302	rBV	69915	94584	2.00%	0.350%
31	22.267	3329	3332	3340	rVB	74342	94210	1.99%	0.349%
32	22.391	3350	3353	3359	rVB	78753	102707	2.17%	0.380%
33	23.460	3529	3535	3547	rVB2	661364	1188523	25.15%	4.400%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-PMW-11M

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: 27010681

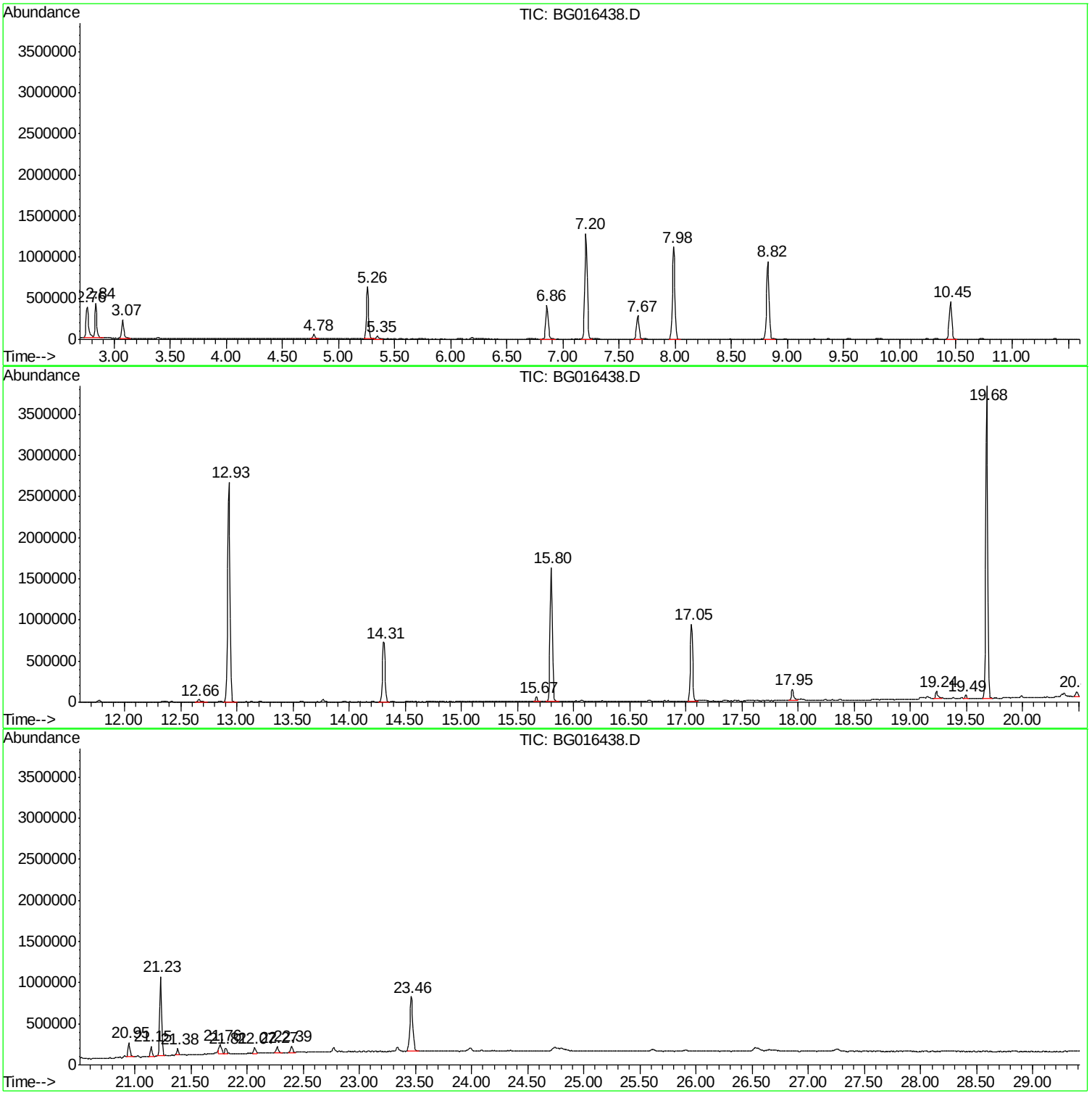
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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

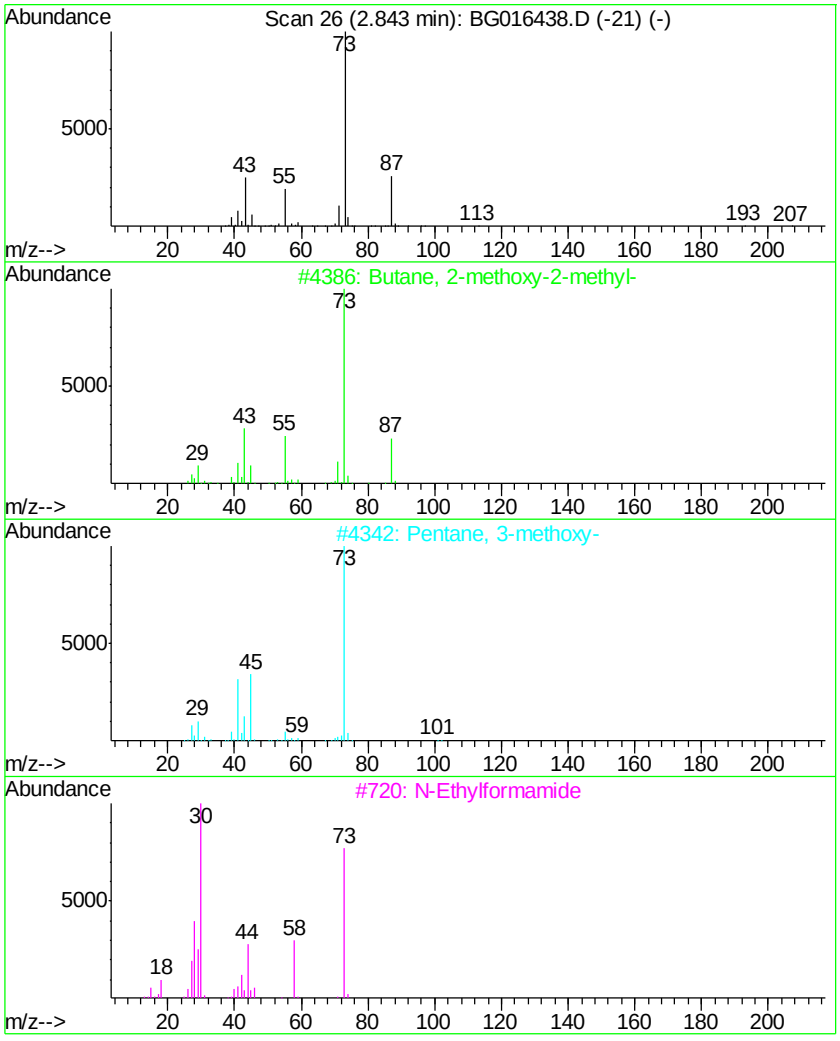
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

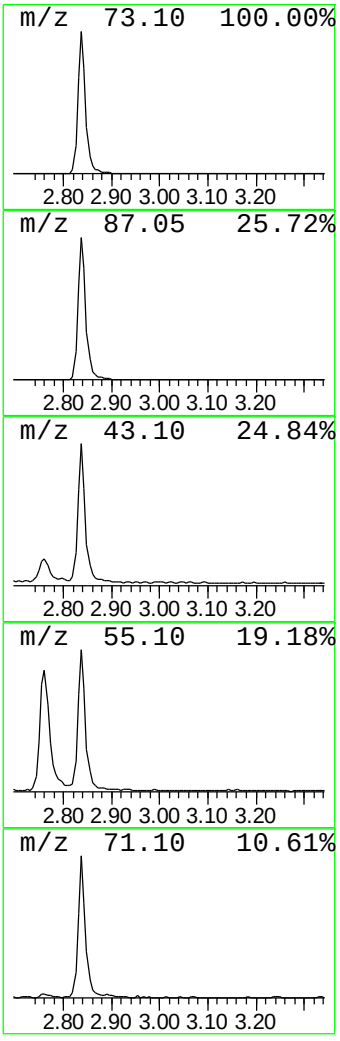
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	22.37 ng	490569	1,4-Dichlorobenzene-d4	7.67

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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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

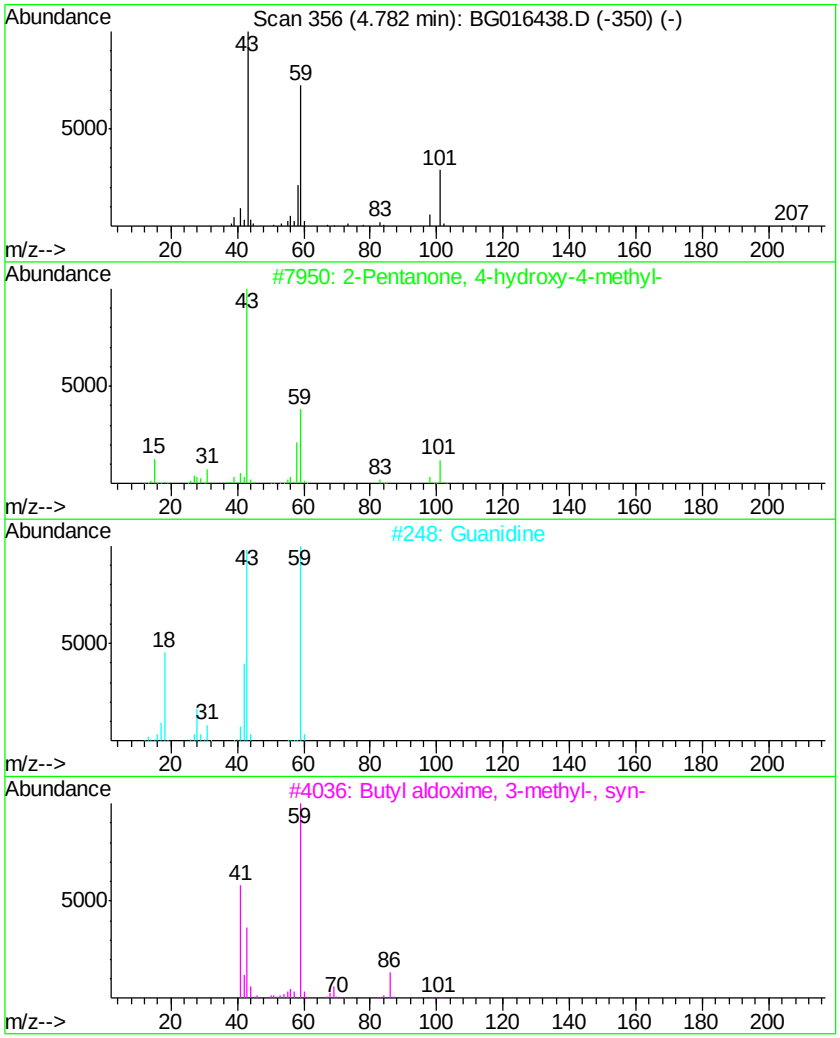
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

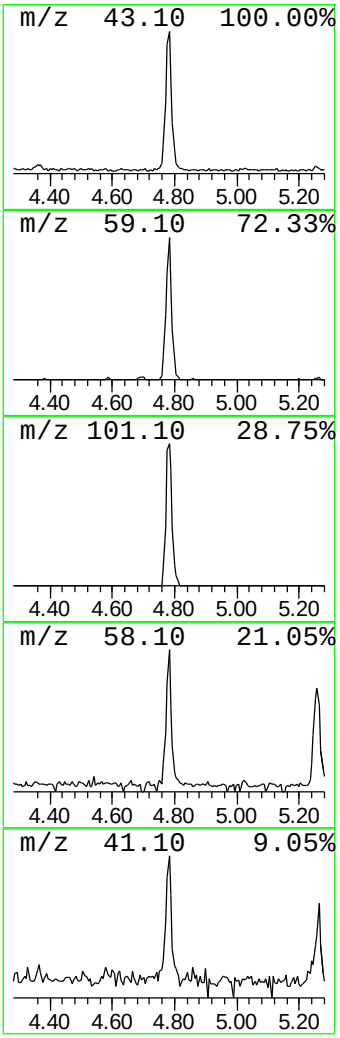
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	3.82 ng	83736	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Guanidine	59	CH5N3	000113-00-8	38
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	27
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	16





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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

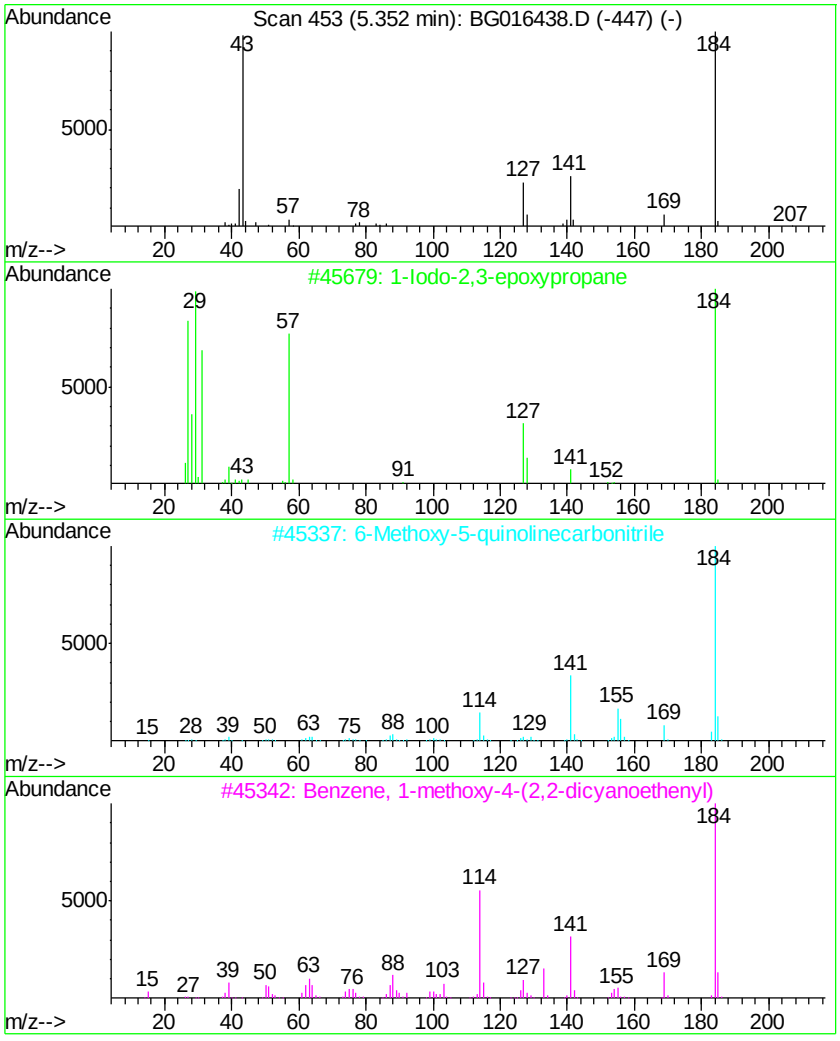
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

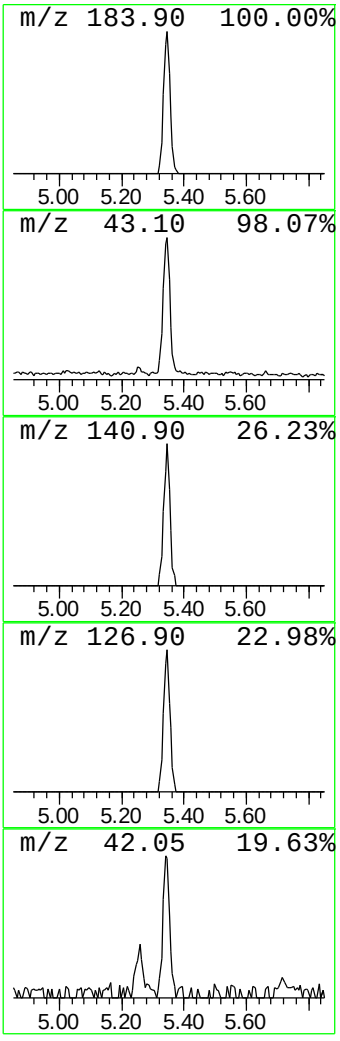
****

Peak Number 5 unknown5.35 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.35	2.55 ng	55976	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2,3-epoxypropane	184	C3H5IO	000624-57-7	28
2	6-Methoxy-5-quinolinecarbonitrile	184	C11H8N2O	087299-97-6	28
3	Benzene, 1-methoxy-4-(2,2-dicyan...	184	C11H8N2O	002826-26-8	9
4	1,1'-Biphenyl, 2-methoxy-	184	C13H12O	000086-26-0	9
5	Benzene, 1-methoxy-3-(2,2-dicyan...	184	C11H8N2O	002972-72-7	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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

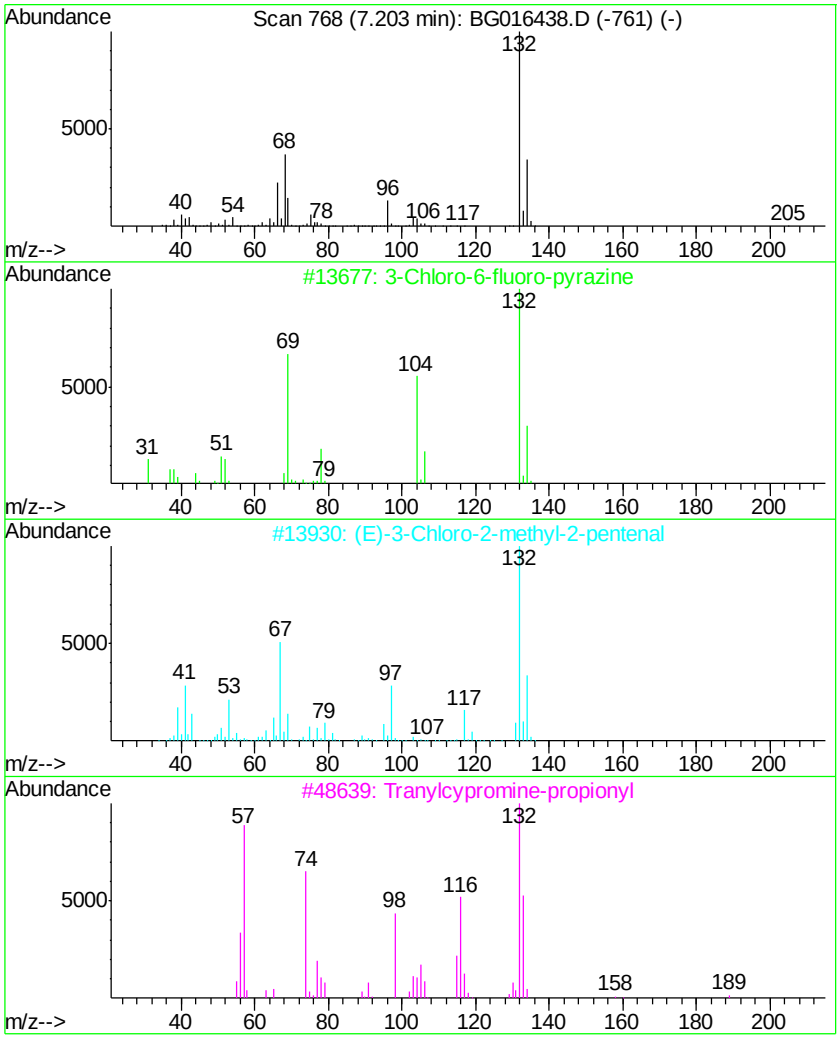
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

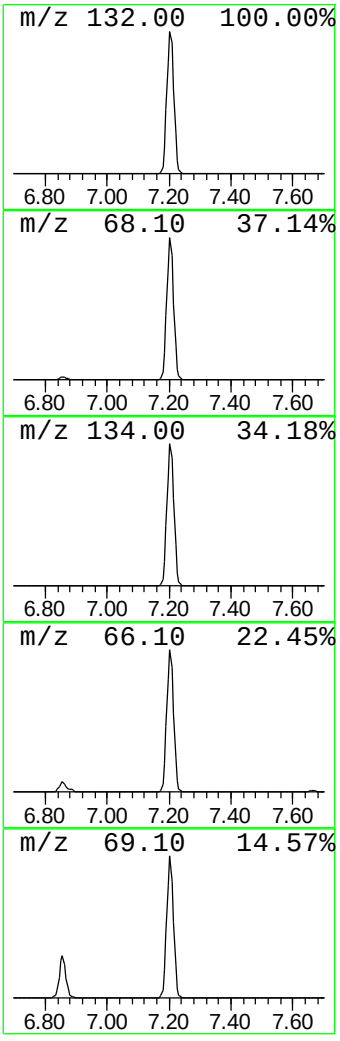
****

Peak Number 6 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	89.94 ng	1972490	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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

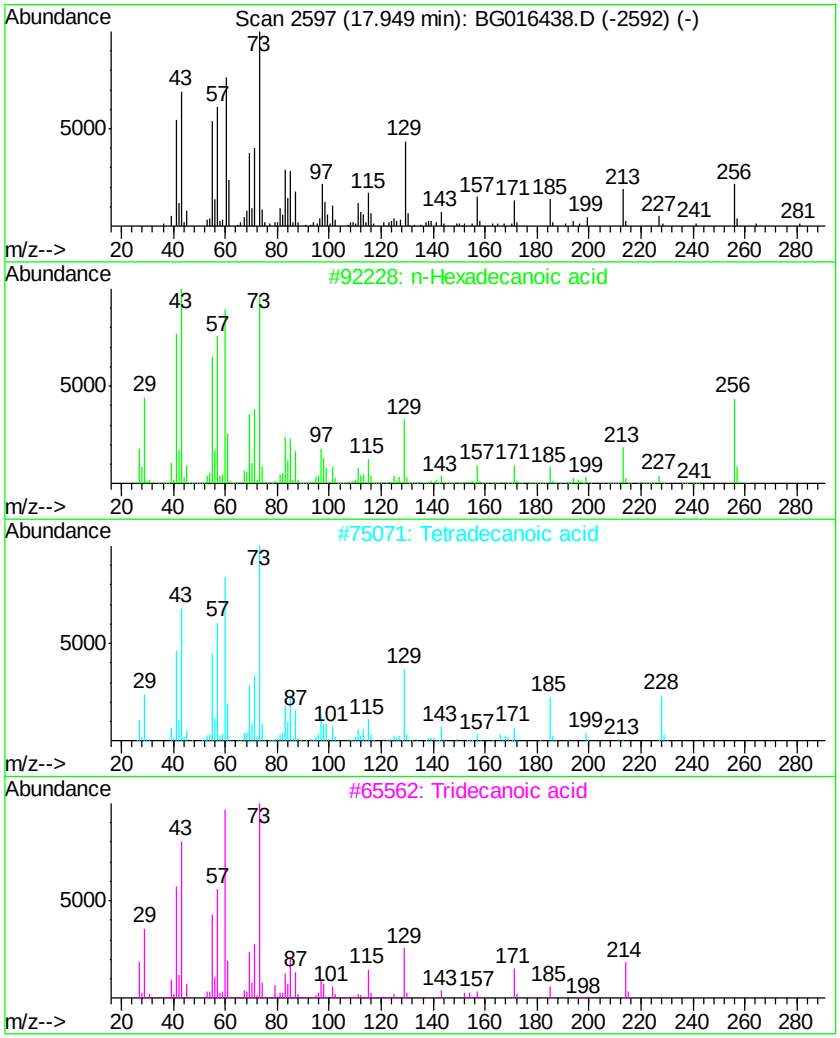
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

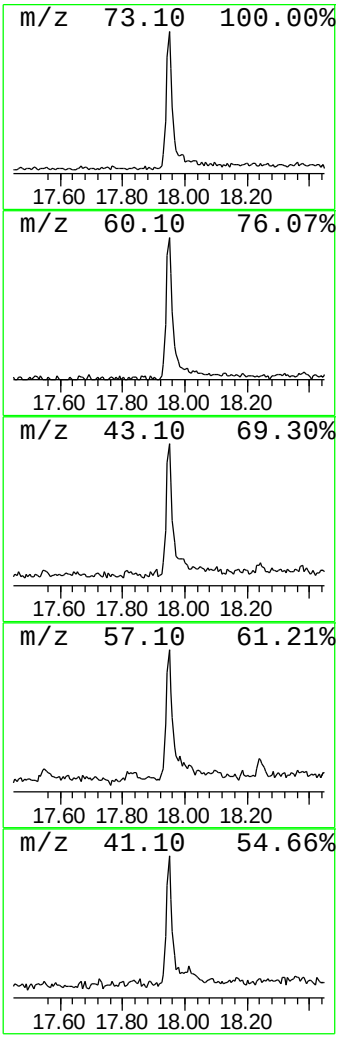
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	3.33 ng	215206	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	41





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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

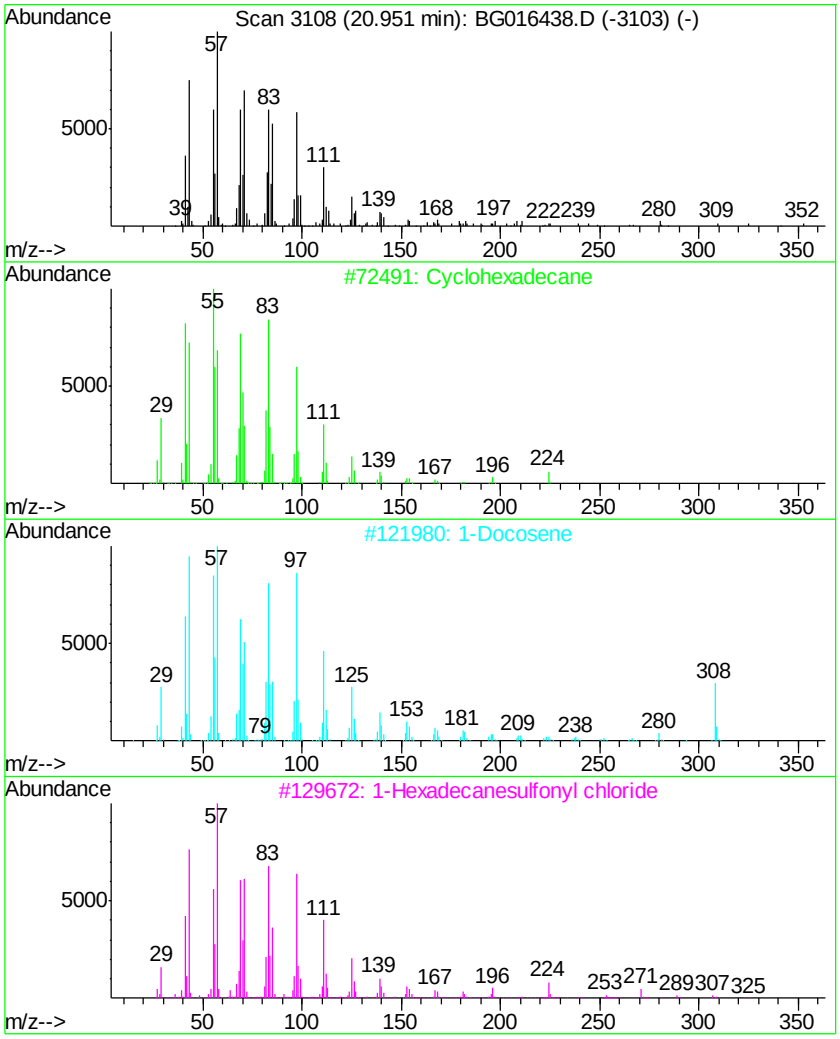
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

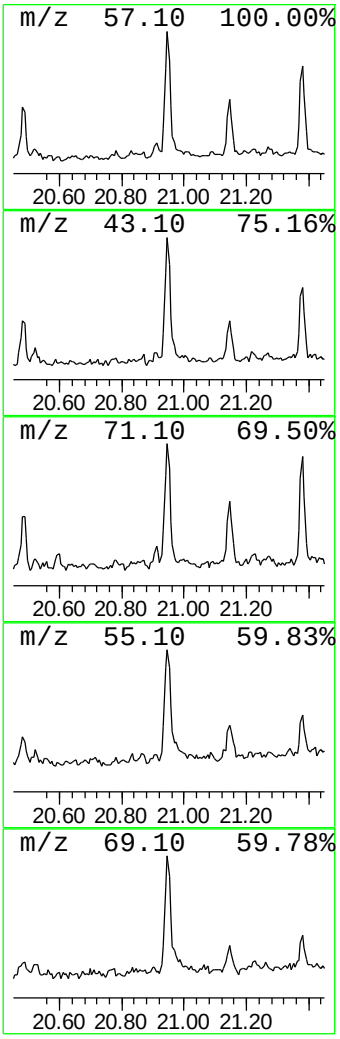
****

Peak Number 9 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	3.64 ng	225496	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	1-Docosene	308	C22H44	001599-67-3	93
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	86
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81





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Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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

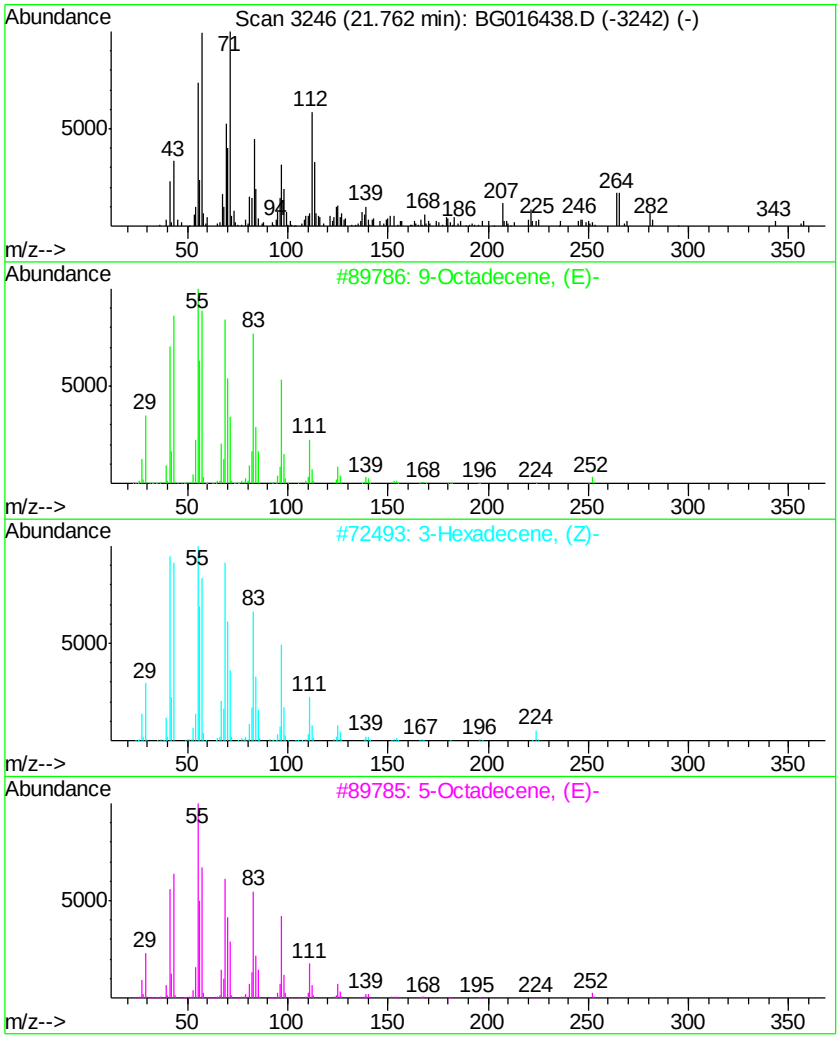
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

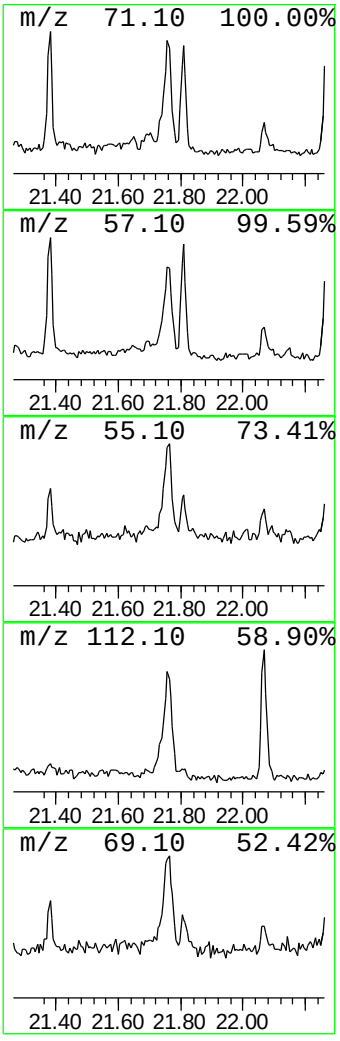
****

Peak Number 10 9-Octadecene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.76	2.81 ng	174214	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-	252	C18H36	007206-25-9	64
2	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	45
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	45
4	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	38
5	Cyclododecane	168	C12H24	000294-62-2	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016438.D
Acq On : 16 Apr 2015 1:59
Operator : TP/IZ
Sample : G1829-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11M

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	22.4	ng	490569	1	7.67	438644	20.0
2-Pentanone, 4-hy...	4.78	3.8	ng	83736	1	7.67	438644	20.0
unknown5.35	5.35	2.5	ng	55976	1	7.67	438644	20.0
unknown7.20	7.20	89.9	ng	1972490	1	7.67	438644	20.0
n-Hexadecanoic acid	17.95	3.3	ng	215206	4	17.05	1292960	20.0
Cyclohexadecane	20.95	3.6	ng	225496	5	21.23	1238950	20.0
9-Octadecene, (E)-	21.76	2.8	ng	174214	5	21.23	1238950	20.0