LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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	2.760	7	12	21	rBV	341785	569065	13.52%	2.207%
2	2.837	21	25	39	rVB	370554	470183	11.17%	1.824%
3	4.781	349	356	364	rBV	70931	102692	2.44%	0.398%
4	5.257	429	437	444	rBV	550251	771595	18.33%	2.993%
5	6.855	702	709	719	rBV	389572	612929	14.56%	2.377%
6	7.202	761	768	778	rBV	1122070	1703373	40.46%	6.607%
7	7.666	840	847	853	rVB	303440	447869	10.64%	1.737%
8	7.983	893	901	909	rVB	1016075	1574639	37.40%	6.107%
9	8.824	1036	1044	1053	rBV	849925	1338402	31.79%	5.191%
10	10.234	1278	1284	1297	rBV	153008	258619	6.14%	1.003%
11	10.451	1314	1321	1329	rBV	441311	708255	16.82%	2.747%
12	11.755	1535	1543	1554	rBV3	63173	139310	3.31%	0.540%
13	12.931	1736	1743	1750	rBV	2268341	3313216	78.70%	12.851%
14	13.765	1879	1885	1894	rBV	71153	102739	2.44%	0.398%
15	14.305	1967	1977	1987	rBV2	653146	1032877	24.54%	4.006%
16	15.669	2201	2209	2214	rBV	125436	175391	4.17%	0.680%
17	15.798	2225	2231	2243	rBV	1452830	2098370	49.85%	8.139%
18	16.074	2274	2278	2285	rVB	35892	53857	1.28%	0.209%
19	17.049	2438	2444	2450	rBV2	870772	1235172	29.34%	4.791%
20	17.819	2571	2575	2581	rBV7	29910	58286	1.38%	0.226%
21	17.948	2592	2597	2606	rBV	301004	445179	10.57%	1.727%
22	18.042	2609	2613	2621	rVB	91934	138411	3.29%	0.537%
23	19.088	2787	2791	2793	rBV2	57227	81300	1.93%	0.315%
24	19.112	2793	2795	2800	rVB5	42589	58865	1.40%	0.228%
25	19.229	2812	2815	2826	rVB	106309	155622	3.70%	0.604%
26	19.493	2857	2860	2865	rVB4	40371	47170	1.12%	0.183%
27	19.681	2886	2892	2898	rBV	3223685	4209766	100.00%	16.328%
28	20.481	3024	3028	3032	rVB2	58488	80373	1.91%	0.312%
29	20.945	3102	3107	3115	rBV	438194	635473	15.10%	2.465%
30	21.144	3138	3141	3147	rVB	92248	107135	2.54%	0.416%
31	21.227	3150	3155	3160	rBV	1014727	1260772	29.95%	4.890%
32	21.379	3177	3181	3193	rBV	85014	125500	2.98%	0.487%
33	21.808	3251	3254	3260	rBV3	67792	82475	1.96%	0.320%
34	22.390	3349	3353	3359	rVB	216963	307204	7.30%	1.192%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

35	22.766	3415	3417	3423	rVB2	53556	69226	1.64%	0.268%
36	23.459	3528	3535	3544	rBV2	631371	1211440	28.78%	4.699%

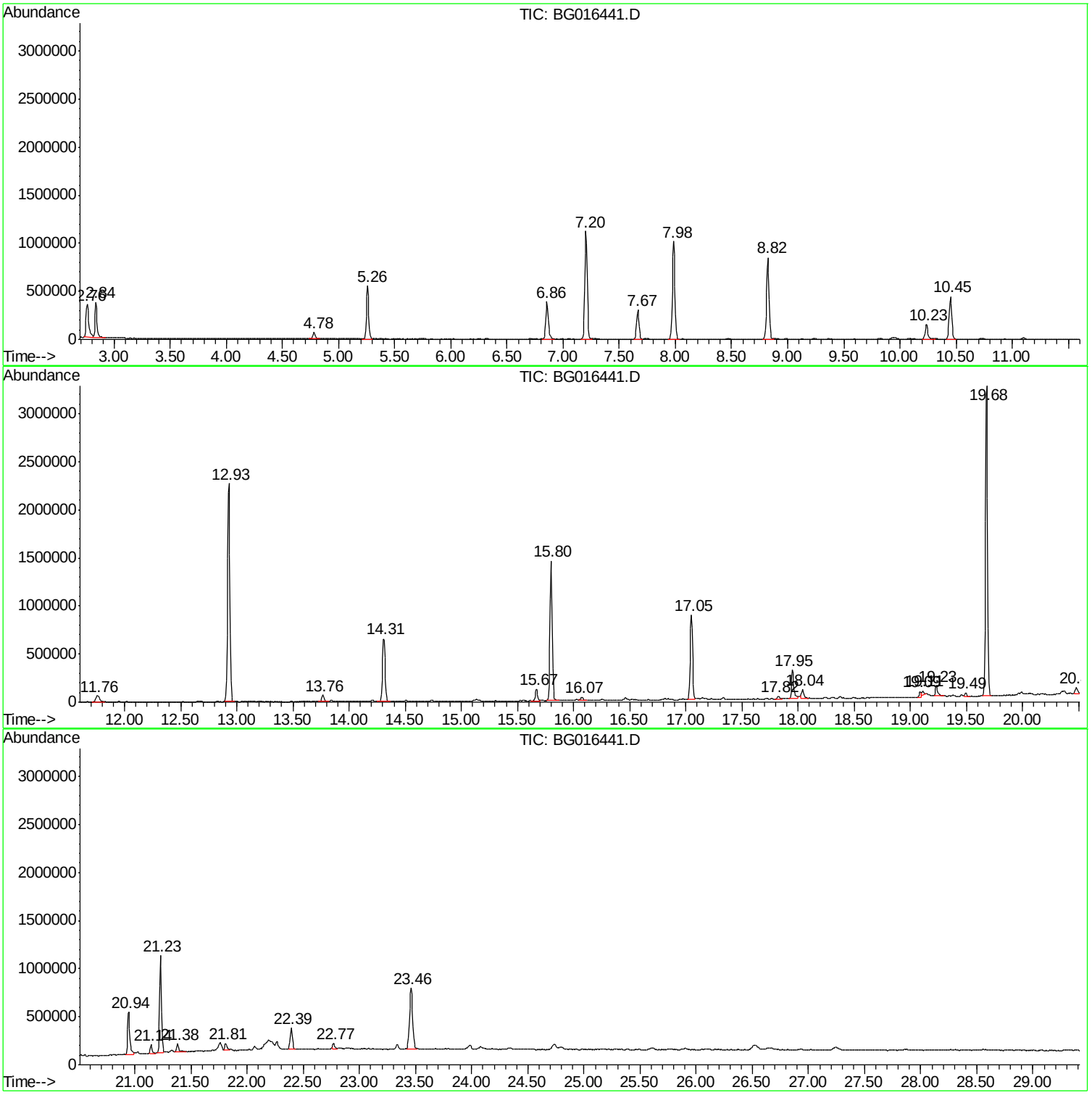
Sum of corrected areas: 25782750

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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 : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

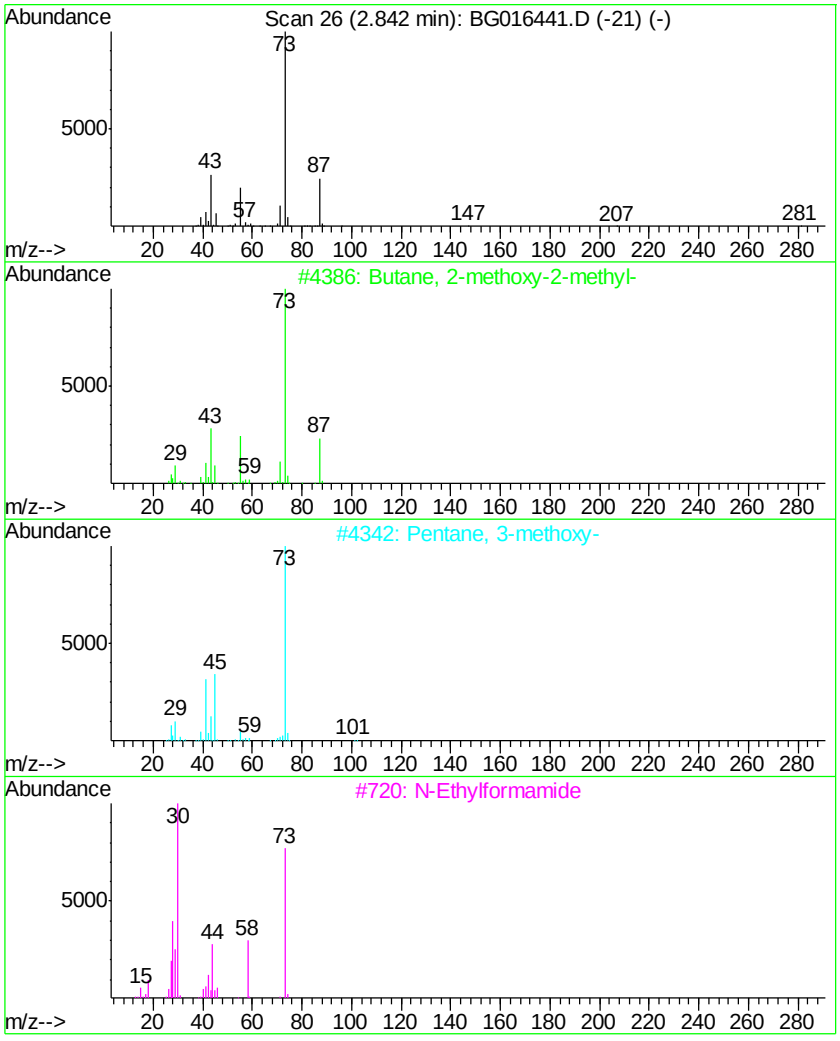
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

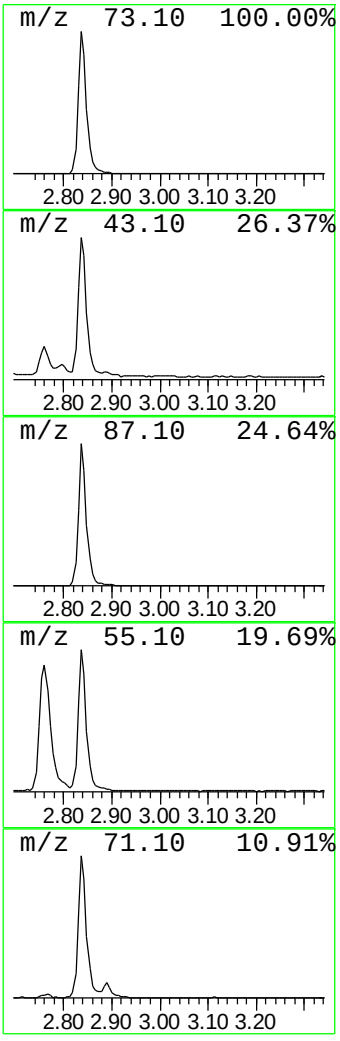
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	21.00 ng	470183	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	7
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

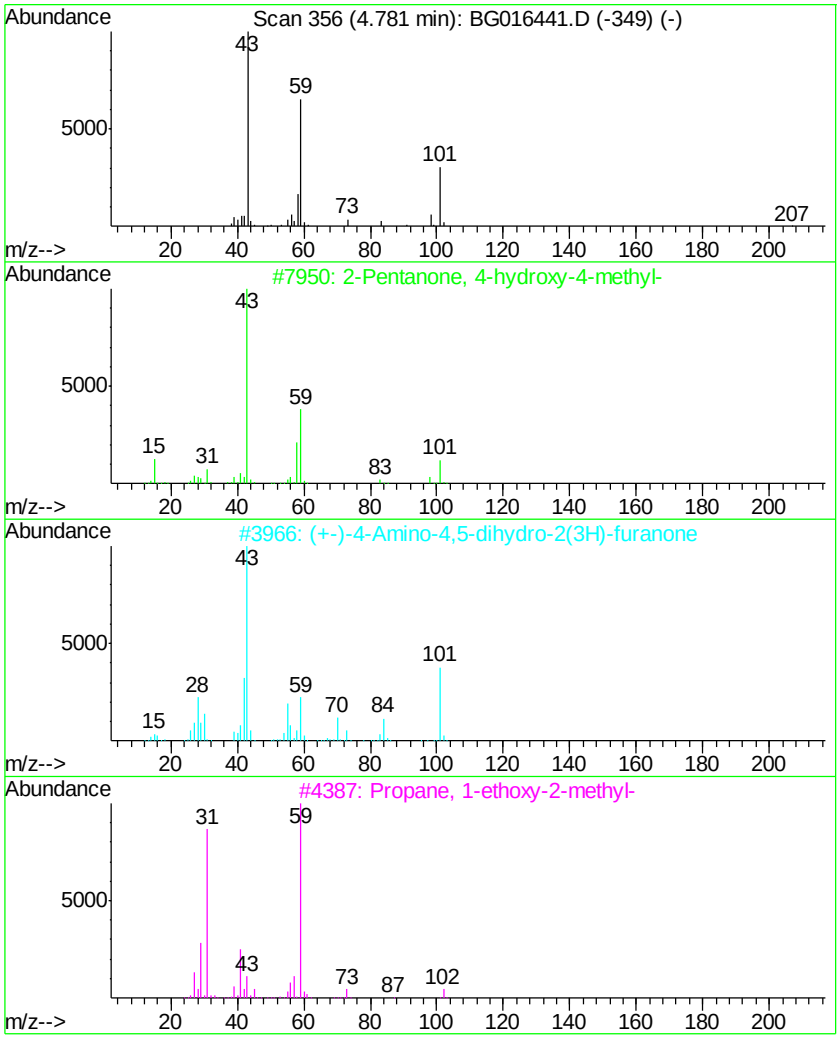
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

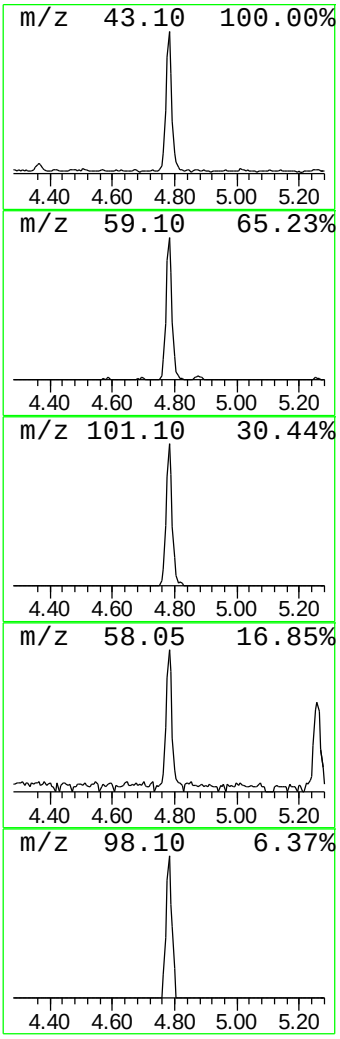
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	4.59 ng	102692	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	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
4	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	17
5	Hexanamide	115	C6H13NO	000628-02-4	17





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

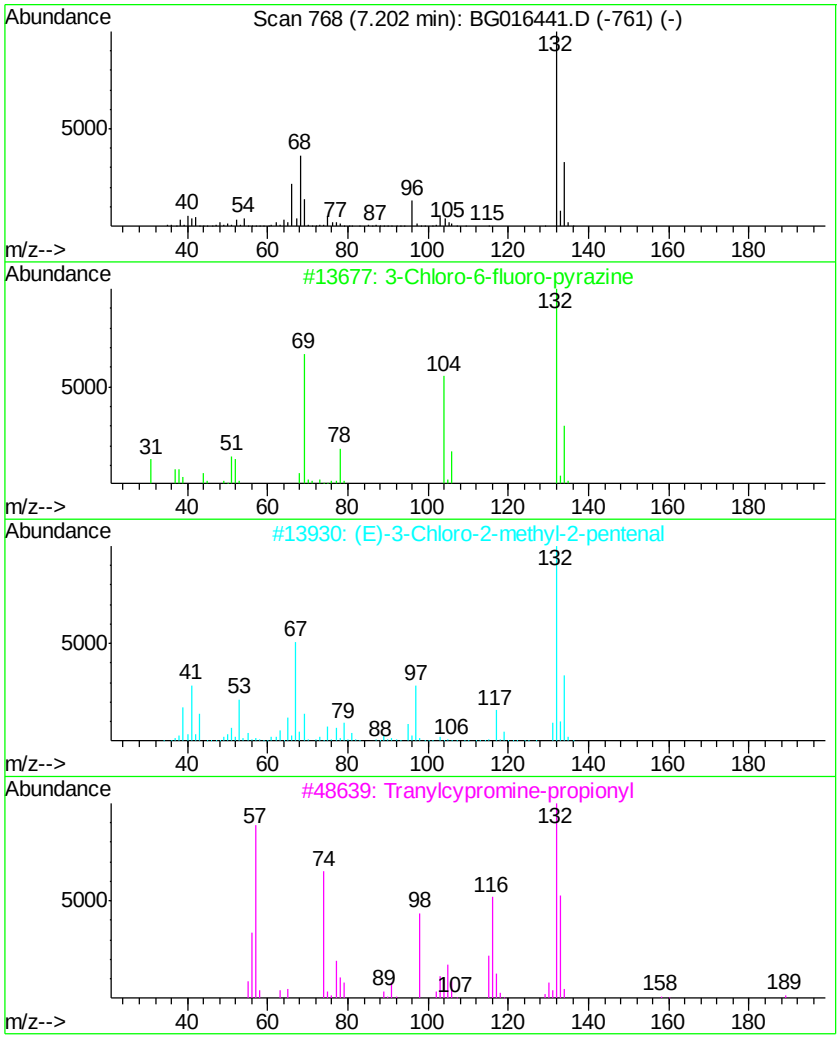
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

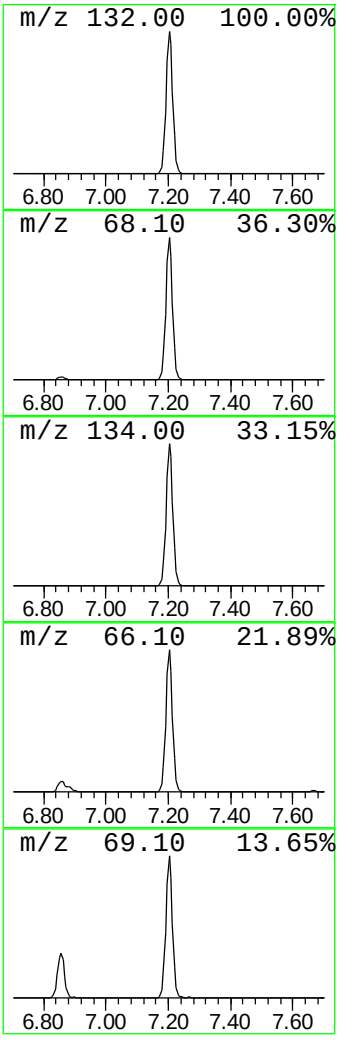
****

Peak Number 4 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	76.07 ng	1703370	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

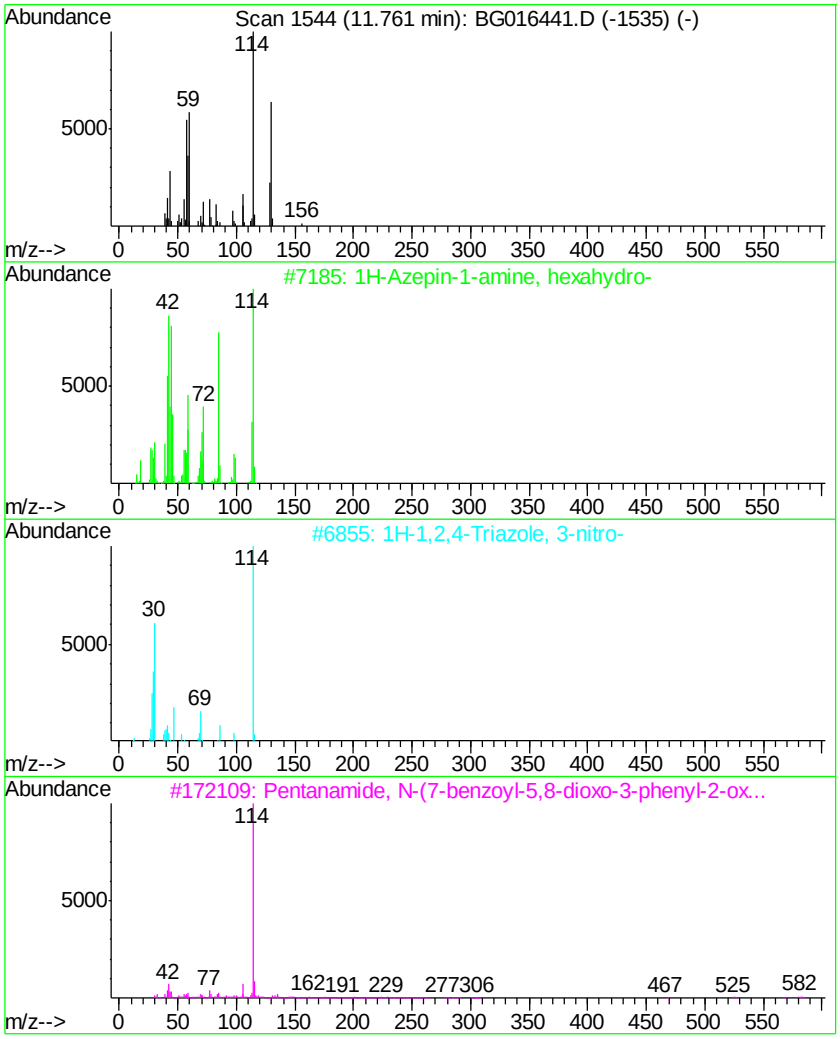
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

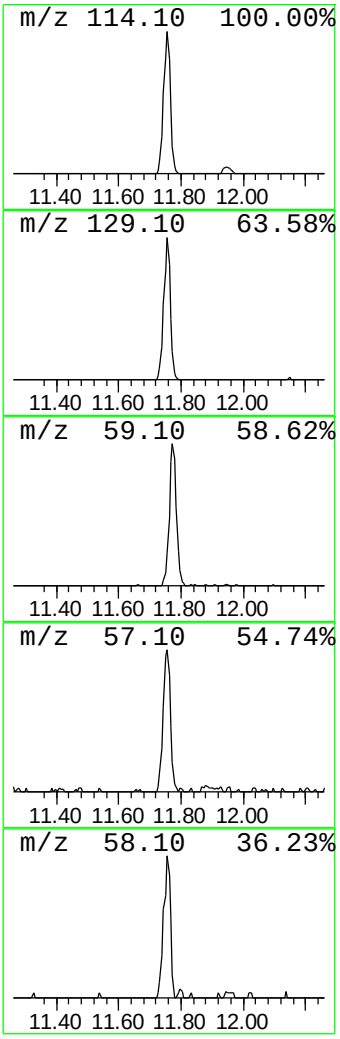
****

Peak Number 7 unknown11.76 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	3.93 ng	139310	Naphthalene-d8	10.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Azepin-1-amine, hexahydro-	114	C6H14N2	005906-35-4	27
2	1H-1,2,4-Triazole, 3-nitro-	114	C2H2N4O2	024807-55-4	27
3	Pentanamide, N-(7-benzoyl-5,8-di...	582	C34H38N4O5	021761-48-8	17
4	1-[3,4-Dichlorophenyl]-3-[4-[[2-...	437	C20H29Cl2N7	051386-82-4	12
5	2,4(1H,3H)-Pyrimidinedione, dihy...	114	C4H6N2O2	000504-07-4	12





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

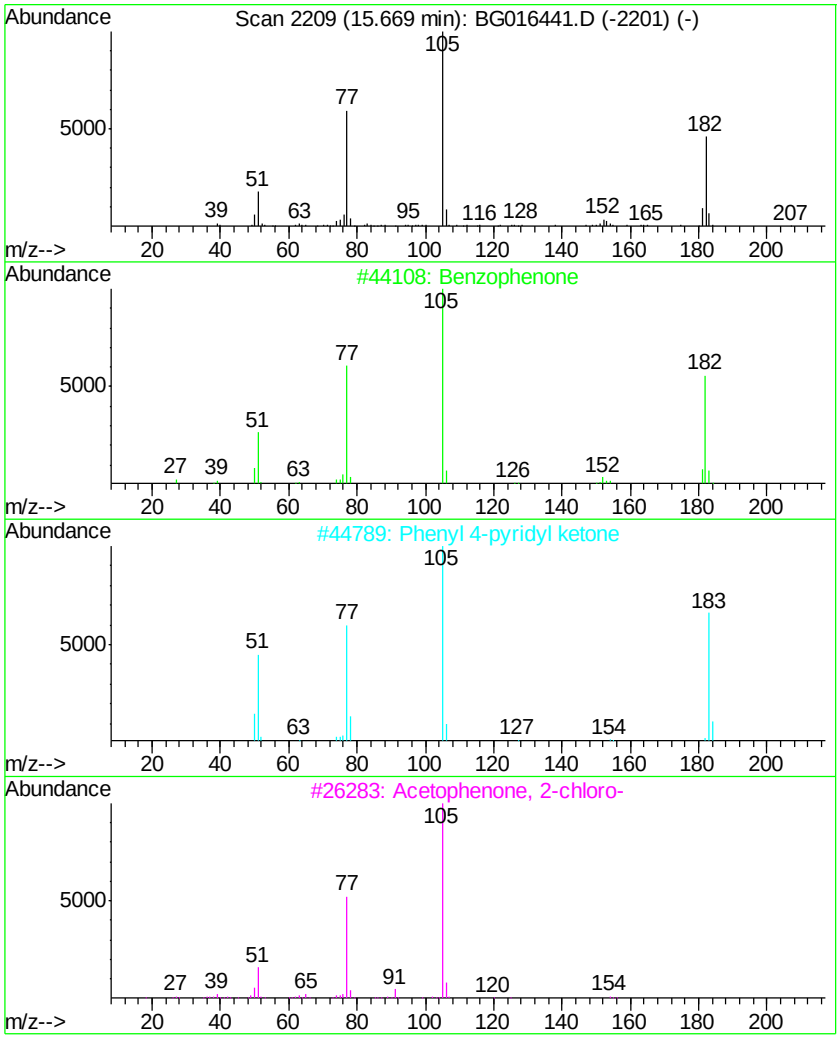
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

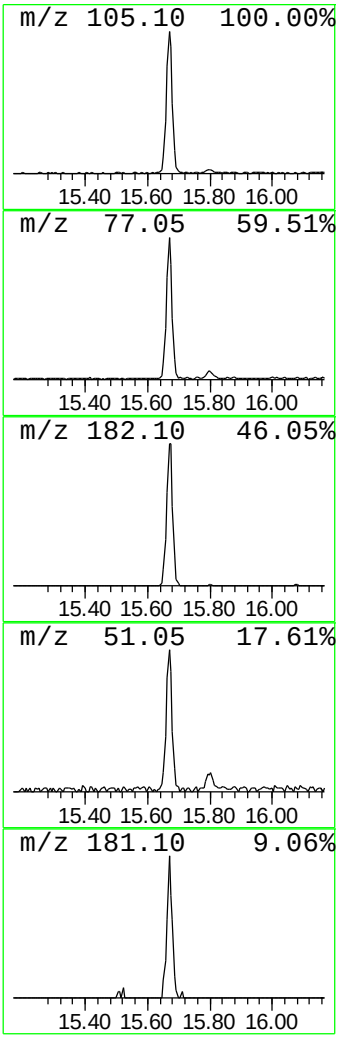
****

Peak Number 8 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	3.40 ng	175391	Acenaphthene-d10	14.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	47
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4	2-Pyrazoline-5-carbonitrile, 2-b...	199	C11H9N3O	067872-68-8	43
5	Vinyl benzoate	148	C9H8O2	000769-78-8	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

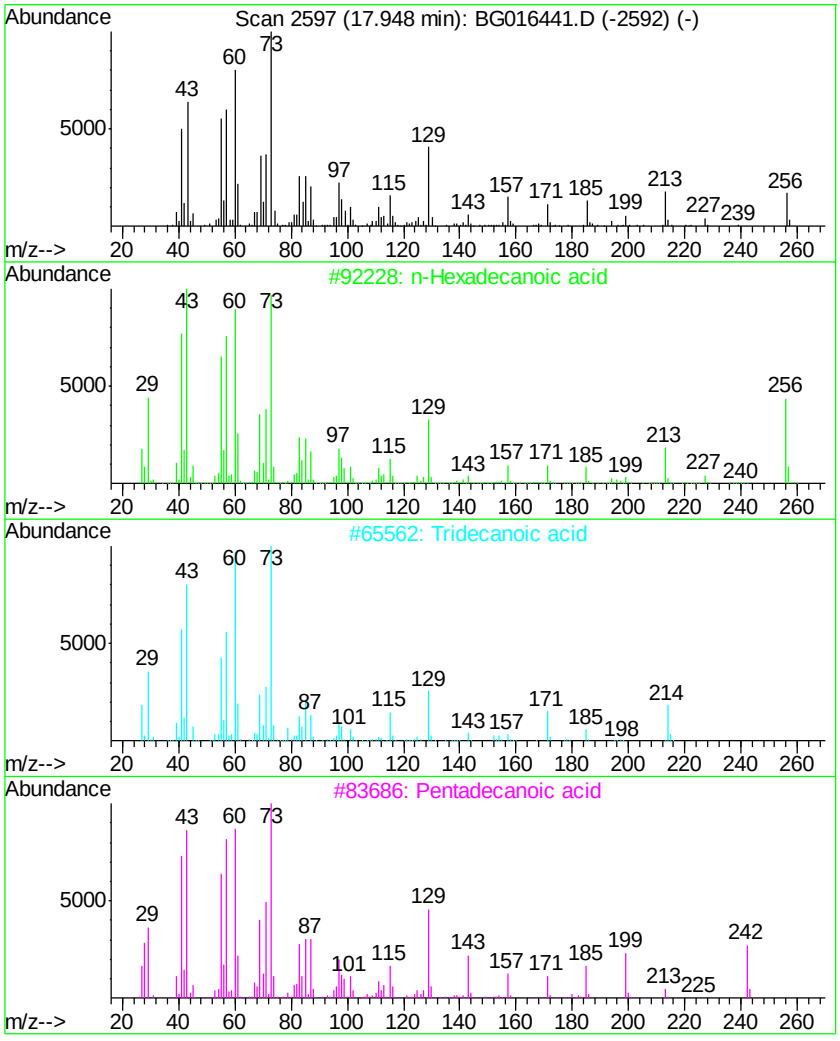
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

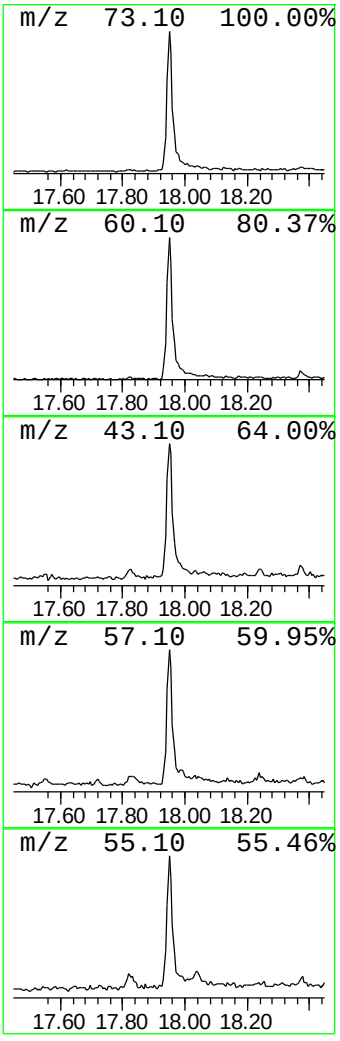
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	7.21 ng	445179	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

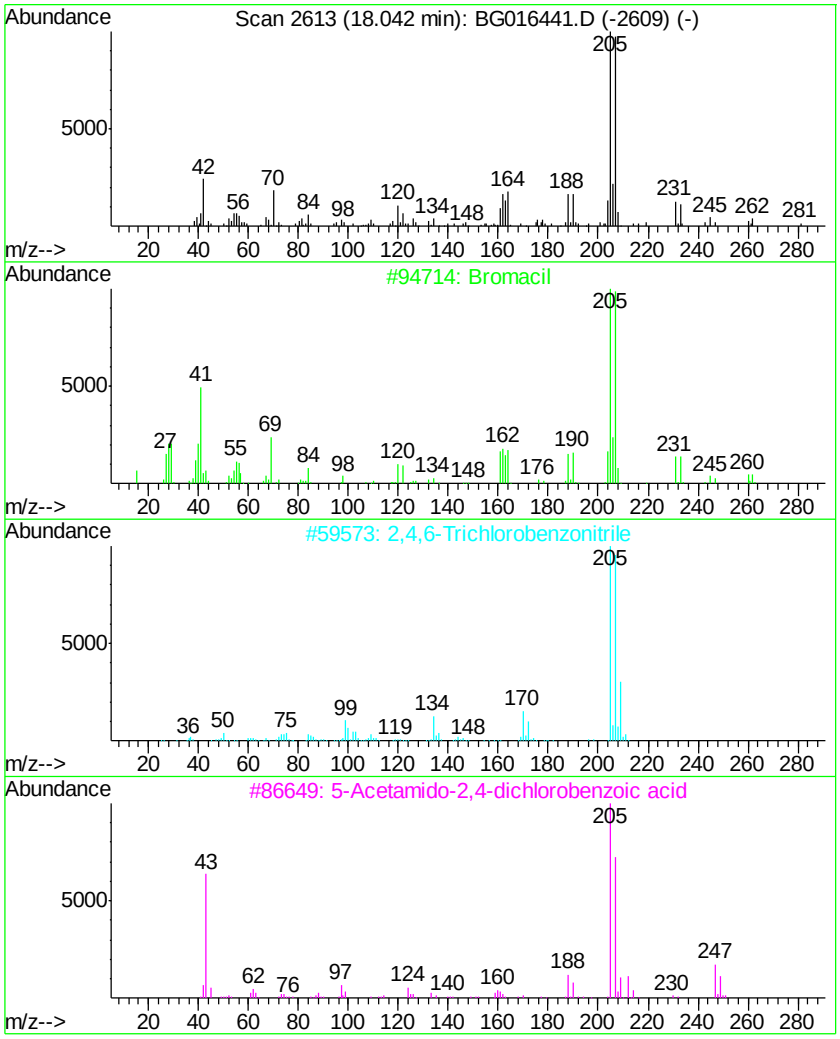
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

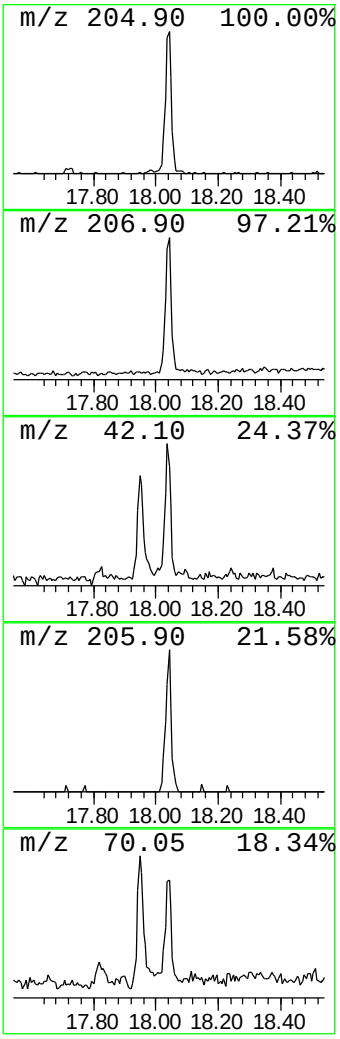
****

Peak Number 10 Bromacil Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	2.24 ng	138411	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromacil	260	C9H13BrN2O2	000314-40-9	92
2	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	58
3	5-Acetamido-2,4-dichlorobenzoic ...	247	C9H7Cl2NO3	050602-49-8	53
4	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	45
5	Indolizine, 2-(4-methylphenyl)-	207	C15H13N	007496-81-3	35





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

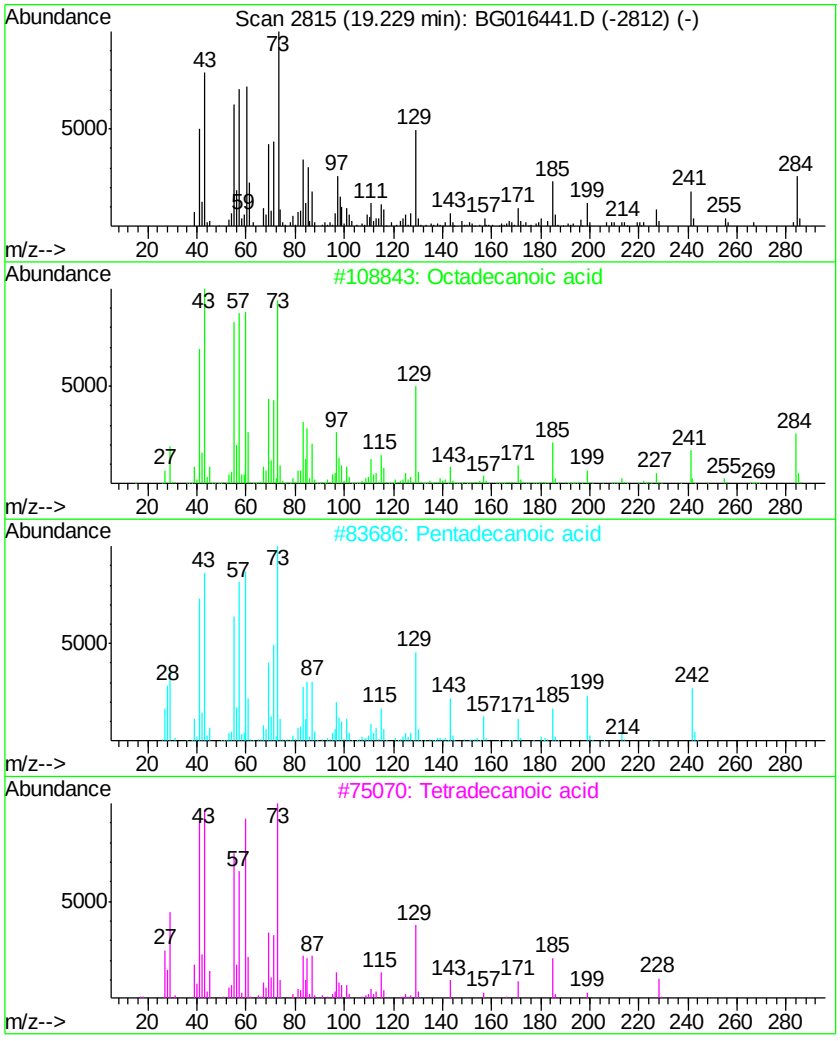
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

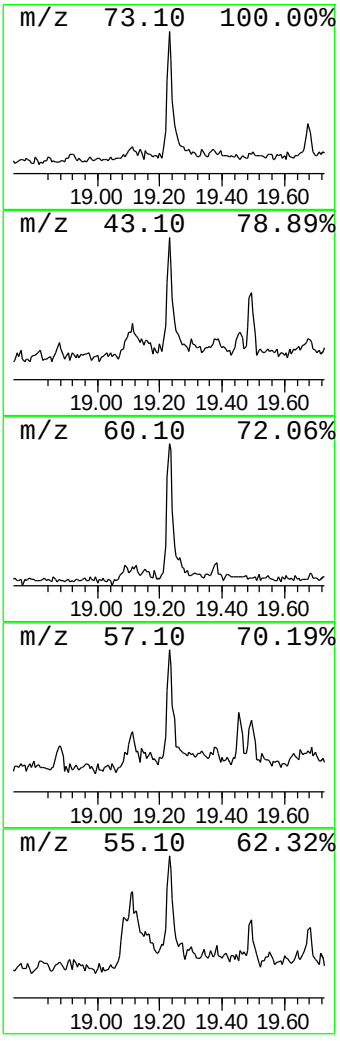
****

Peak Number 11 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	2.47 ng	155622	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

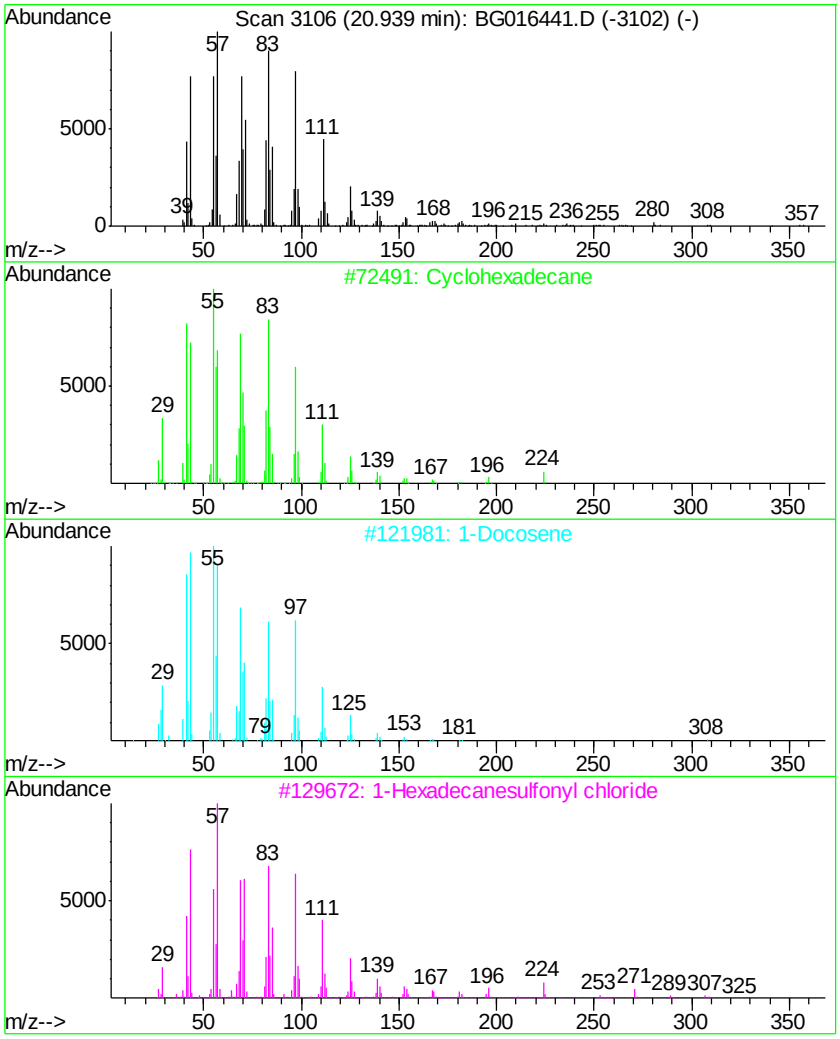
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

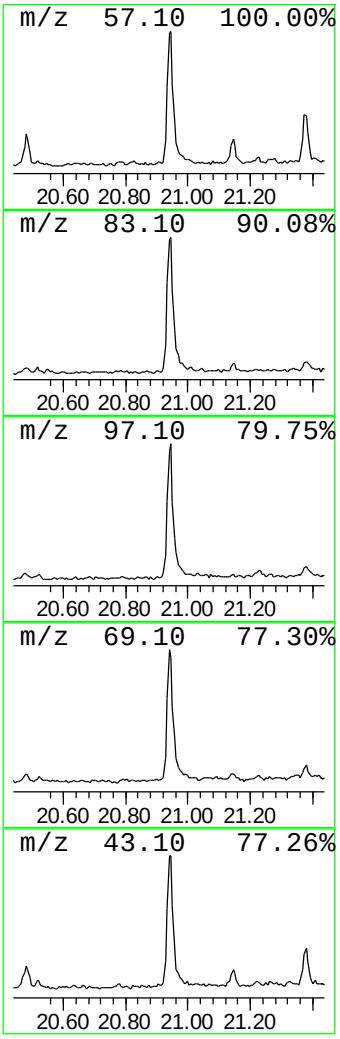
****

Peak Number 12 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	10.08 ng	635473	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Cyclotetracosane	336	C24H48	000297-03-0	90





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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

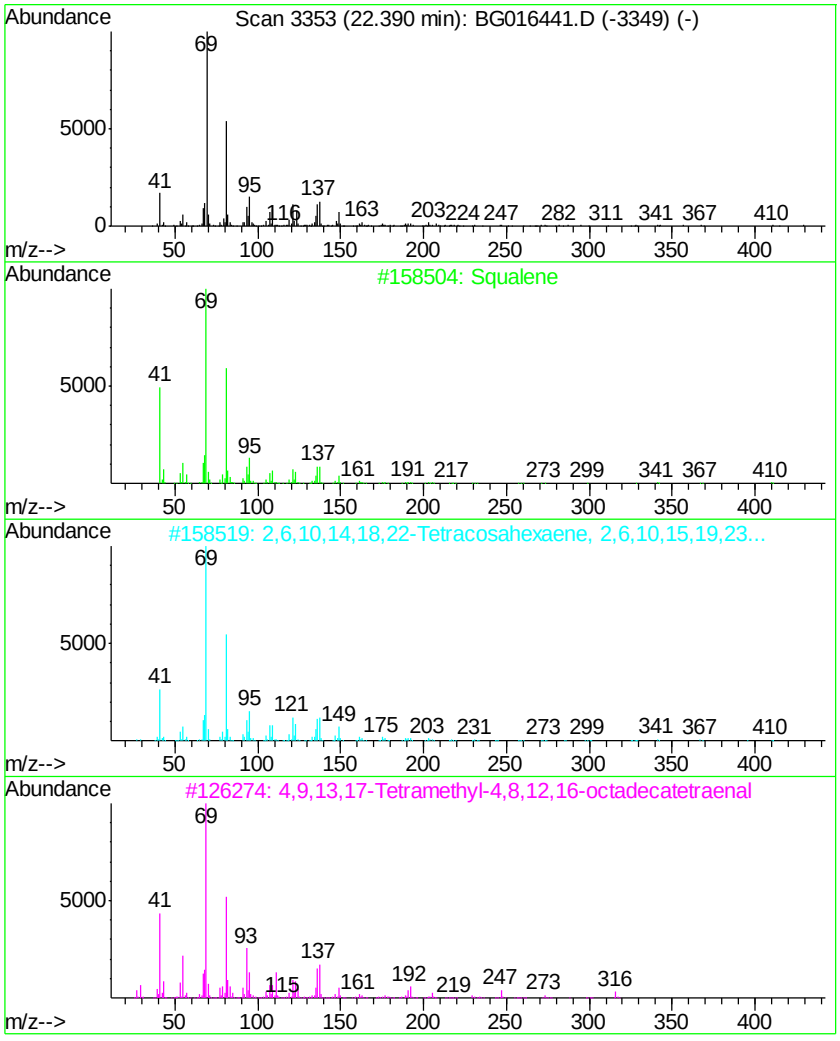
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

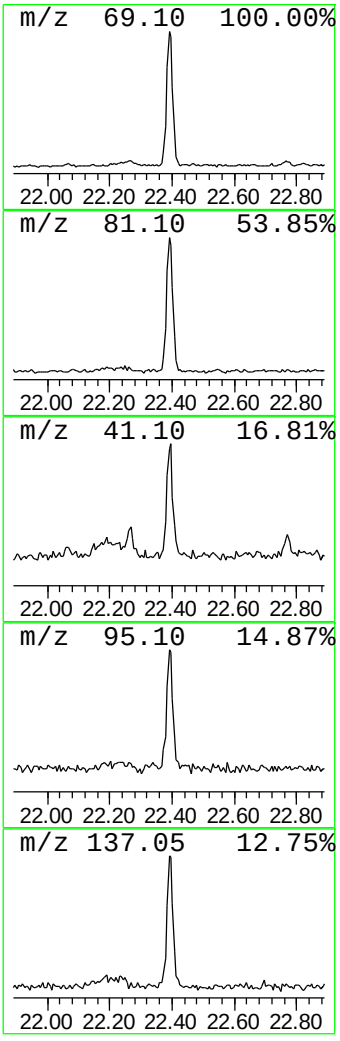
****

Peak Number 13 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	5.07 ng	307204	Perylene-d12	23.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	99
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	98
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016441.D
Acq On : 16 Apr 2015 3:43
Operator : TP/IZ
Sample : G1829-18
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PO-010

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	21.0	ng	470183	1	7.67	447869	20.0
2-Pentanone, 4-hy...	4.78	4.6	ng	102692	1	7.67	447869	20.0
unknown7.20	7.20	76.1	ng	1703370	1	7.67	447869	20.0
unknown11.76	11.76	3.9	ng	139310	2	10.45	708255	20.0
Benzophenone	15.67	3.4	ng	175391	3	14.31	1032880	20.0
n-Hexadecanoic acid	17.95	7.2	ng	445179	4	17.05	1235170	20.0
Bromacil	18.04	2.2	ng	138411	4	17.05	1235170	20.0
Octadecanoic acid	19.23	2.5	ng	155622	5	21.23	1260770	20.0
Cyclohexadecane	20.94	10.1	ng	635473	5	21.23	1260770	20.0
Squalene	22.39	5.1	ng	307204	6	23.46	1211440	20.0