LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

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-BG050515.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	2.810	16	21	30	rBV	167858	267655	6.92%	1.573%
2	2.886	30	34	46	rVB	391354	538285	13.92%	3.164%
3	4.831	361	365	371	rVB2	26453	41670	1.08%	0.245%
4	5.313	441	447	455	rBV	417372	592775	15.33%	3.484%
5	6.917	713	720	728	rVB	275632	412467	10.67%	2.424%
6	7.258	771	778	787	rBV	768078	1188754	30.74%	6.987%
7	7.716	850	856	866	rBV	157494	255475	6.61%	1.502%
8	8.039	903	911	917	rBV	629166	989819	25.60%	5.818%
9	8.879	1047	1054	1062	rBV	554280	916714	23.71%	5.388%
10	10.513	1323	1332	1337	rBV	194994	331244	8.57%	1.947%
11	12.722	1702	1708	1713	rBV2	46768	70013	1.81%	0.412%
12	12.986	1745	1753	1760	rBV	1494436	2175004	56.24%	12.784%
13	14.367	1982	1988	1995	rBV2	309965	480744	12.43%	2.826%
14	15.090	2105	2111	2120	rVB2	38090	71193	1.84%	0.418%
15	15.859	2235	2242	2249	rBV	1638851	2285602	59.10%	13.434%
16	17.117	2449	2456	2461	rBV	461281	649786	16.80%	3.819%
17	18.016	2604	2609	2614	rBV2	86045	121331	3.14%	0.713%
18	19.297	2823	2827	2834	rBV4	96602	142412	3.68%	0.837%
19	19.749	2896	2904	2910	rBV	3091675	3867170	100.00%	22.730%
20	21.006	3115	3118	3123	rBV7	29974	46130	1.19%	0.271%
21	21.212	3147	3153	3156	rBV	46595	56318	1.46%	0.331%
22	21.294	3162	3167	3172	rVB	615801	715673	18.51%	4.206%
23	22.481	3365	3369	3374	rVB	81966	100846	2.61%	0.593%
24	23.562	3546	3553	3561	rVB	374606	696733	18.02%	4.095%

Sum of corrected areas: 17013813

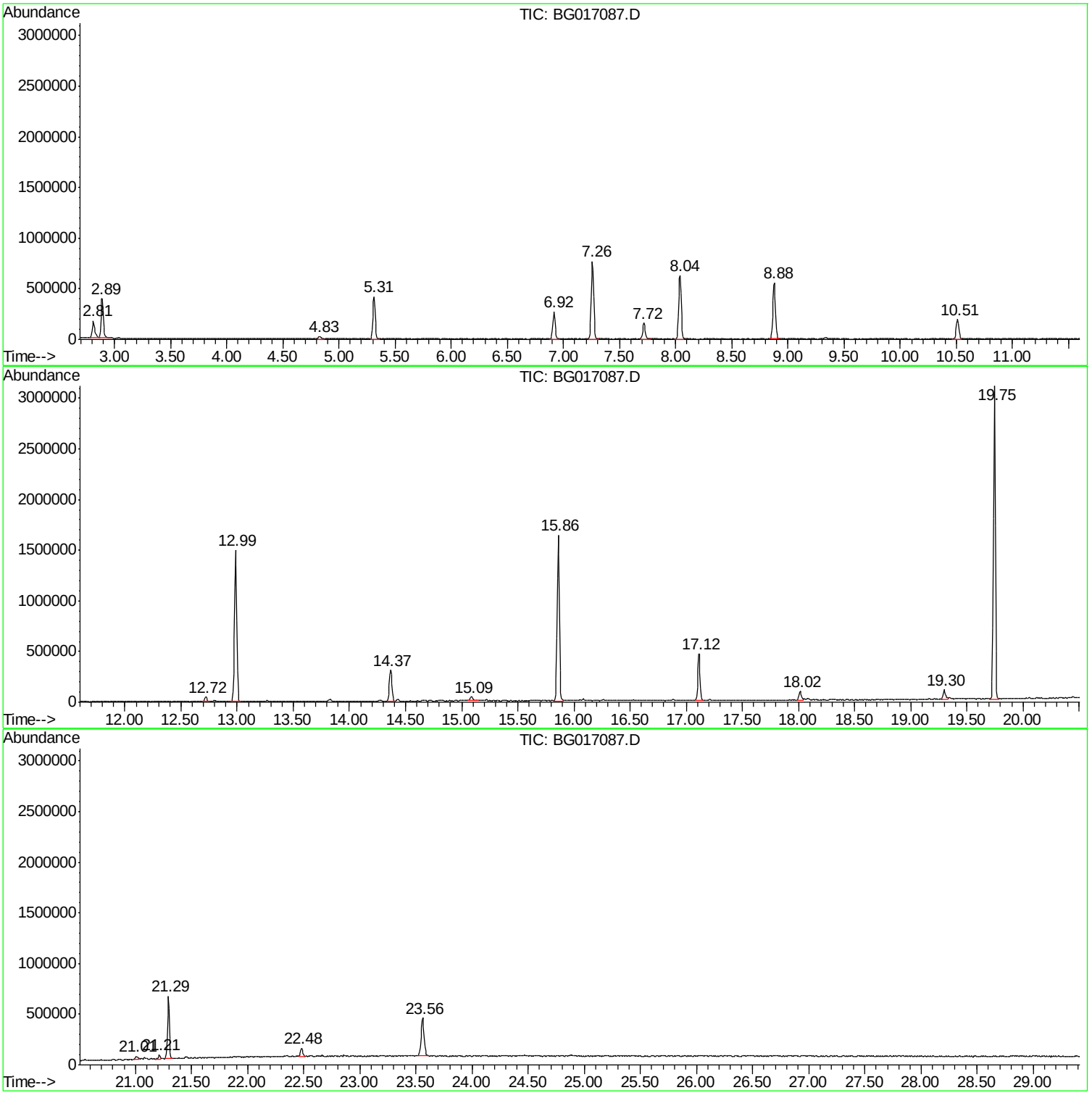
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

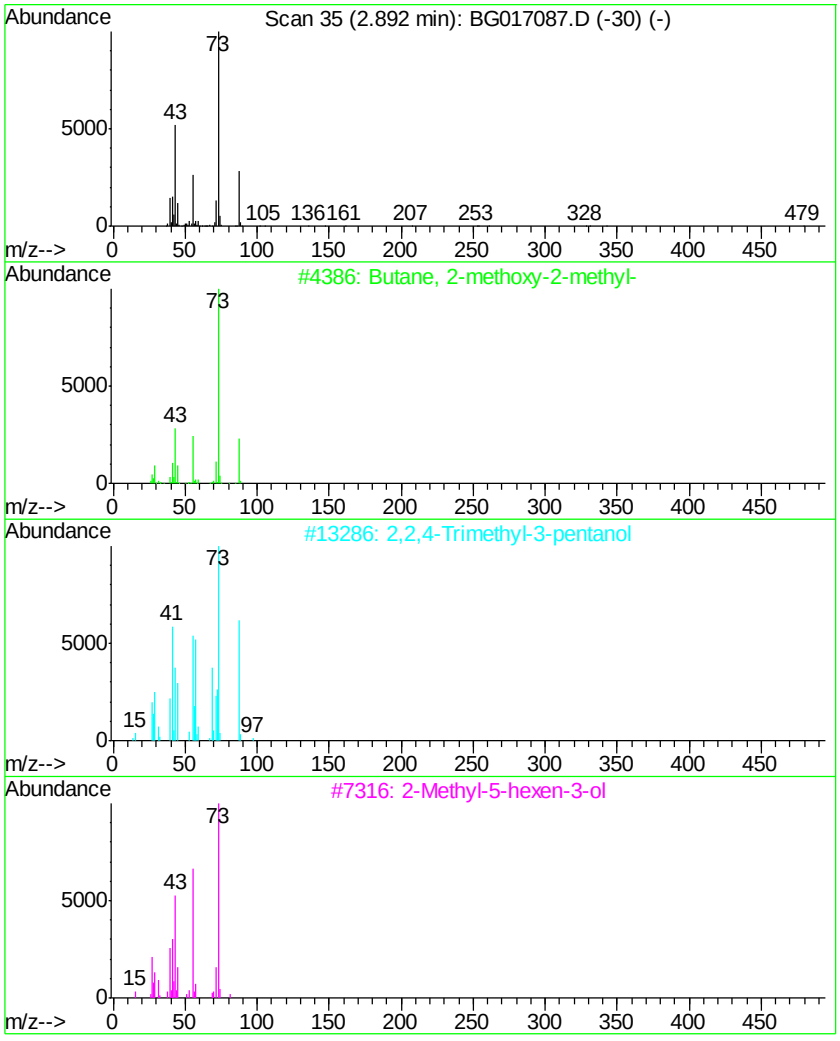
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

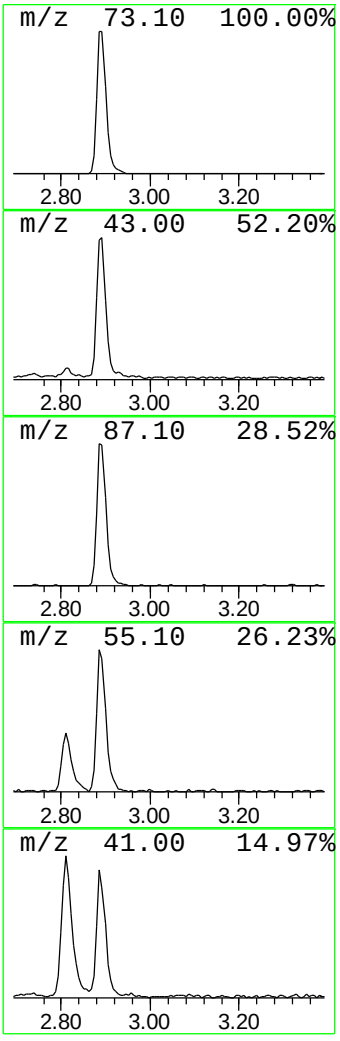
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	42.14 ng	538285	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

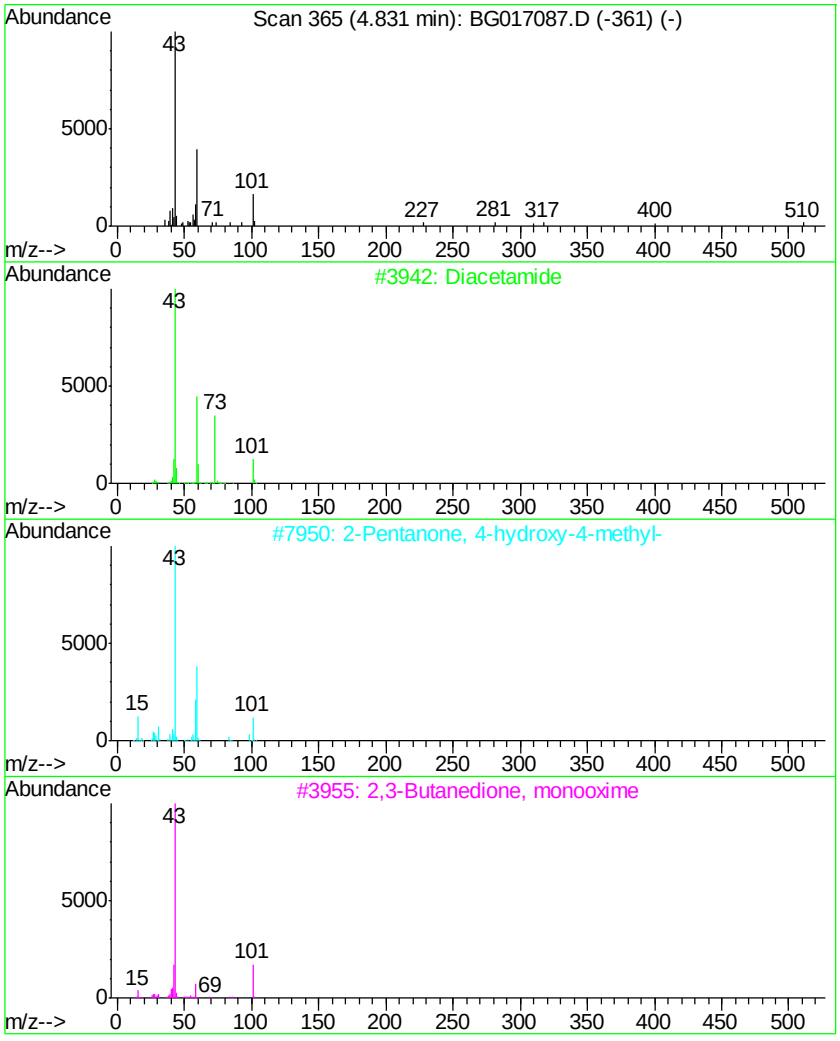
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

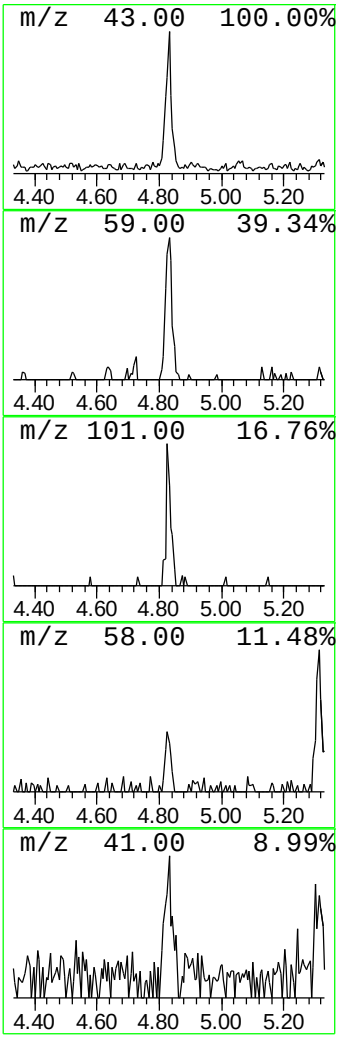
****

Peak Number 3 unknown4.83 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	3.26 ng	41670	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide	101	C4H7NO2	000625-77-4	38
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

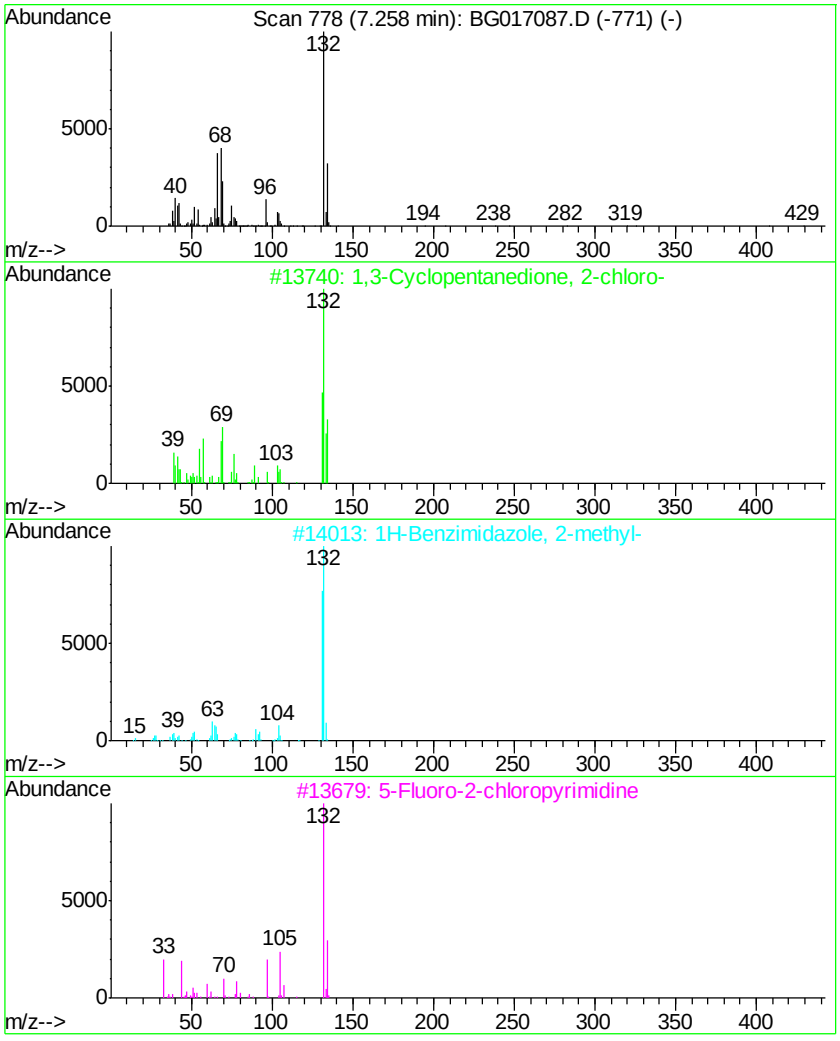
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

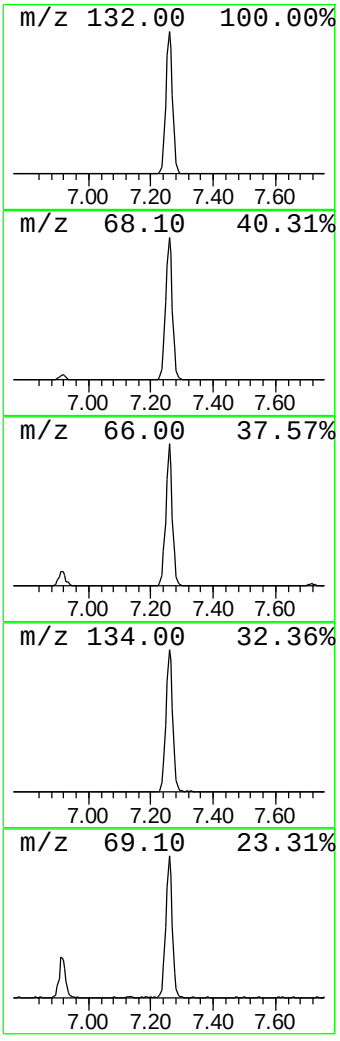
****

Peak Number 4 unknown7.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	93.06 ng	1188750	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

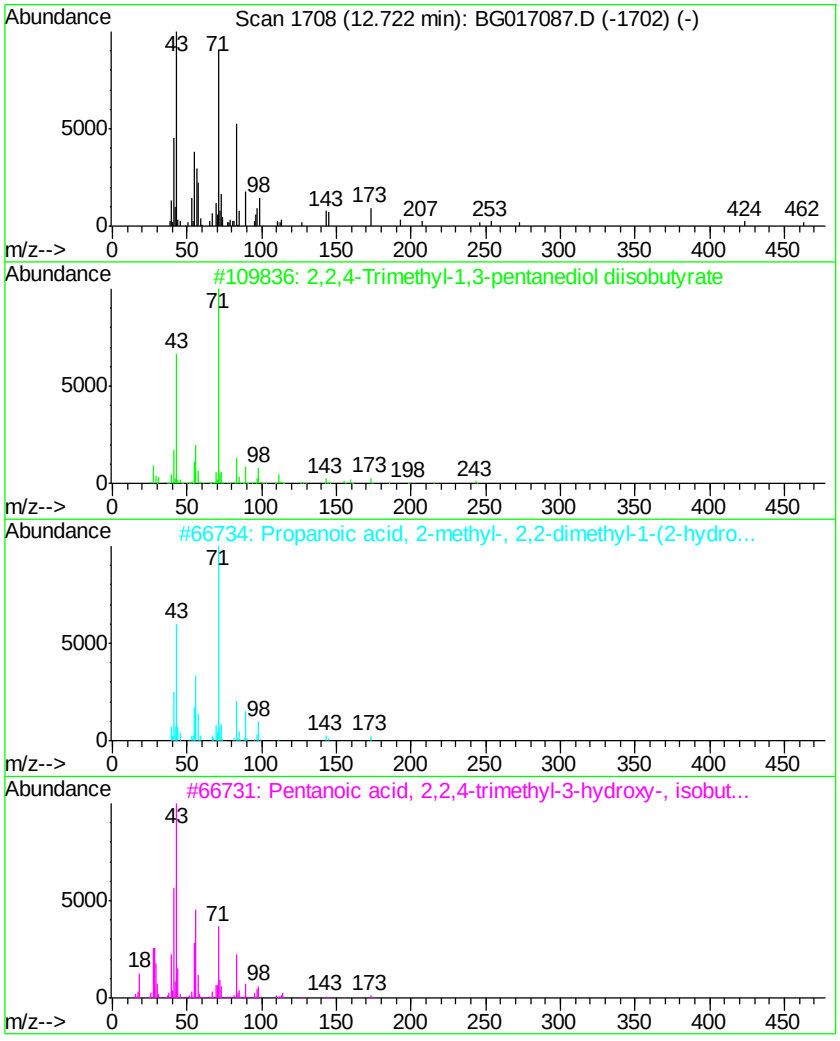
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

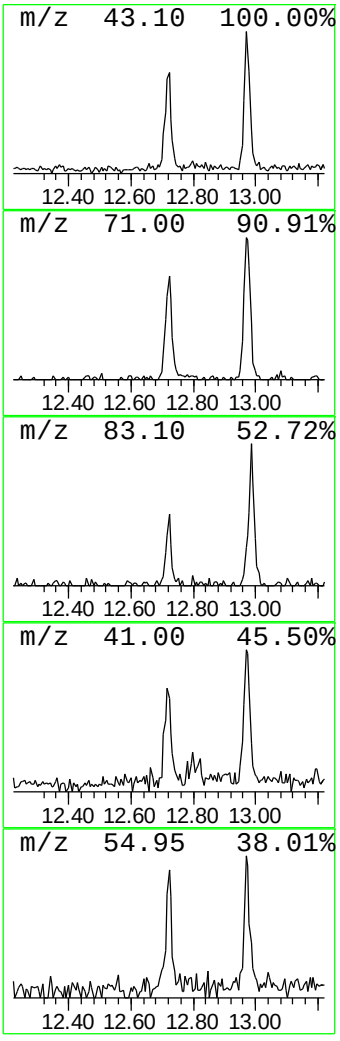
****

Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.91 ng	70013	Acenaphthene-d10	14.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	53
2	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	53
3	Pentanoic acid, 2,2,4-trimethyl-...	216	C12H24O3	244074-78-0	50
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	43
5	Butanoic acid, decyl ester	228	C14H28O2	005454-09-1	40





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

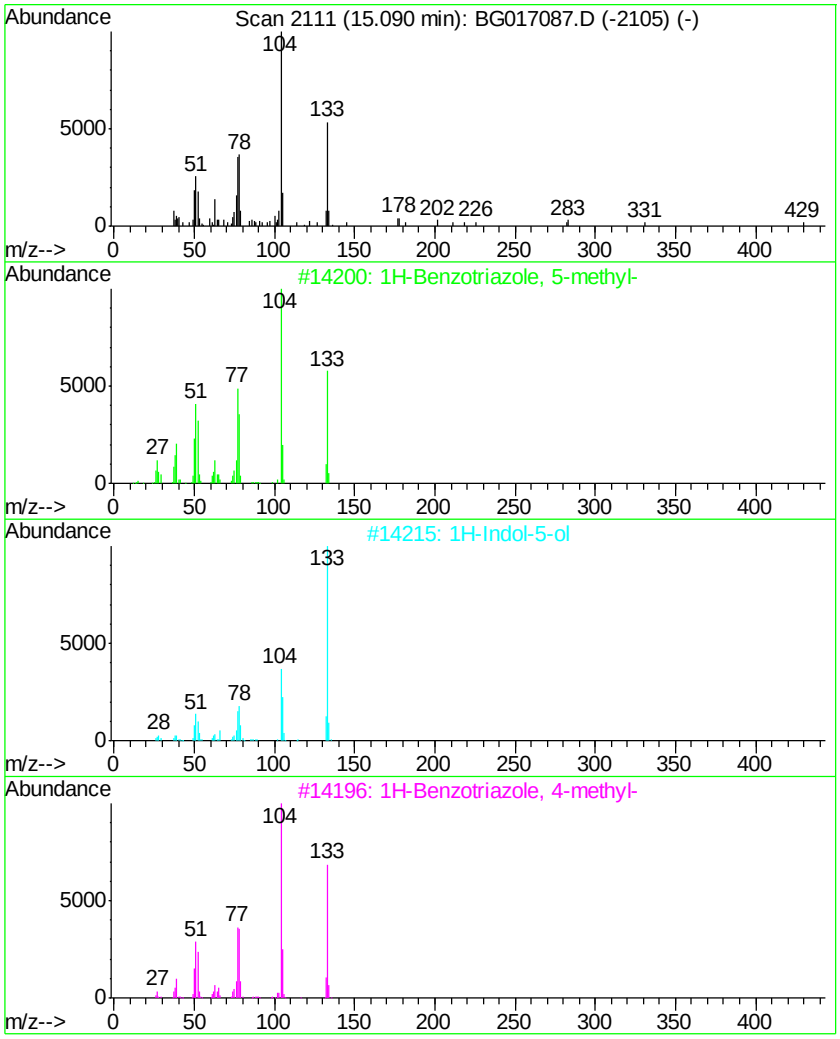
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

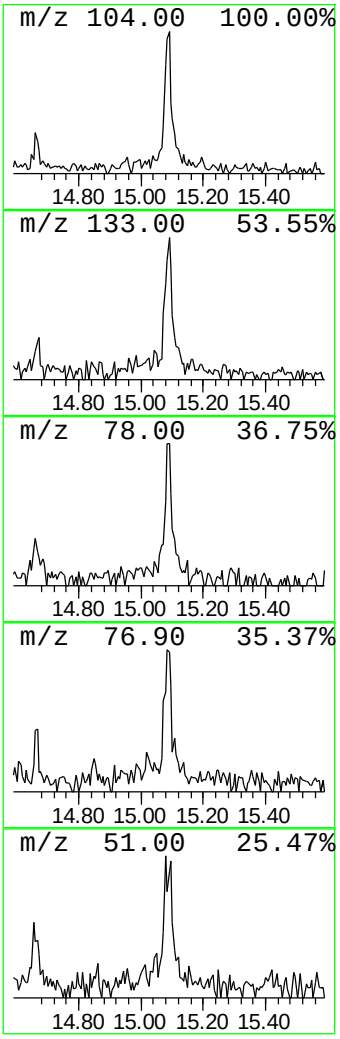
****

Peak Number 7 1H-Benzotriazole, 5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.96 ng	71193	Acenaphthene-d10	14.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	94
2	1H-Indol-5-ol	133	C8H7NO	001953-54-4	91
3	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	90
4	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	80
5	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

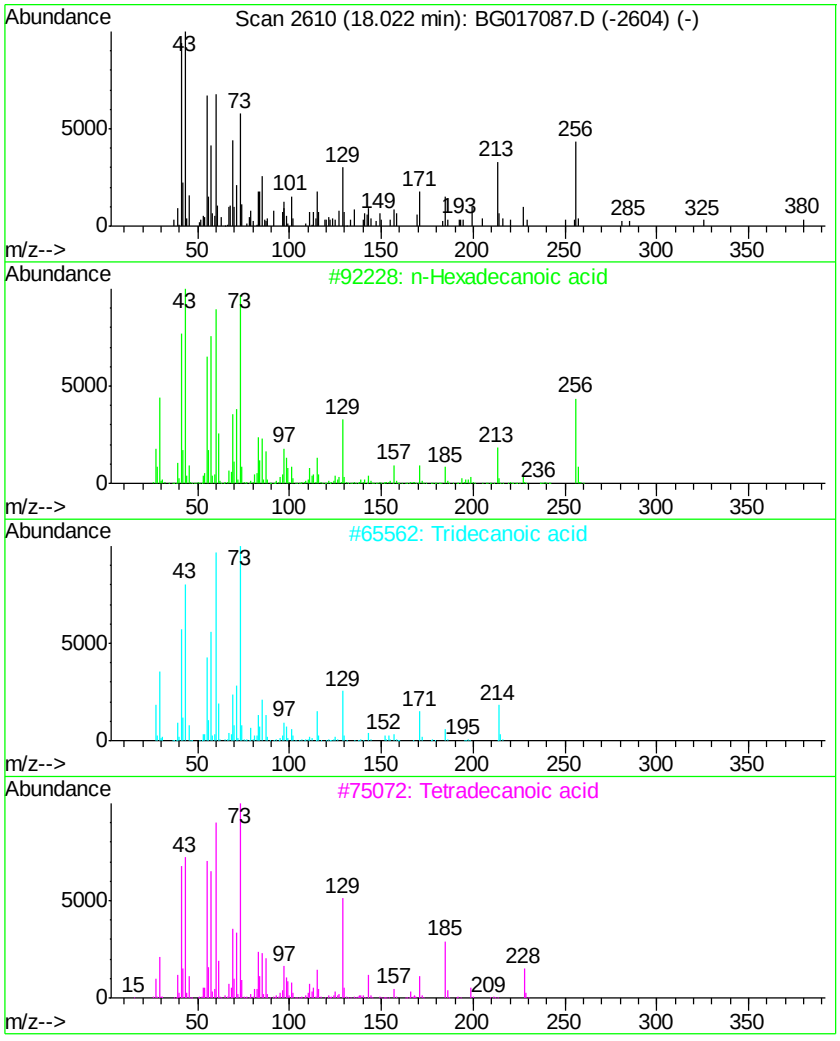
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

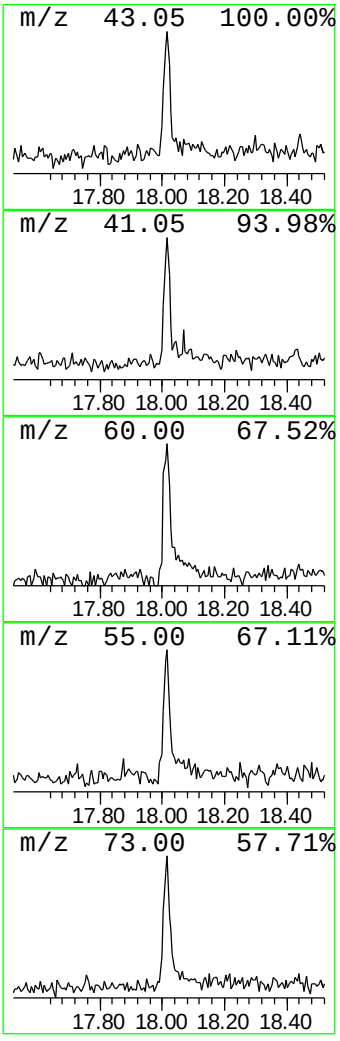
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.02	3.73 ng	121331	Phenanthrene-d10	17.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2	Tridecanoic acid	214	C13H26O2	000638-53-9	47
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





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Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

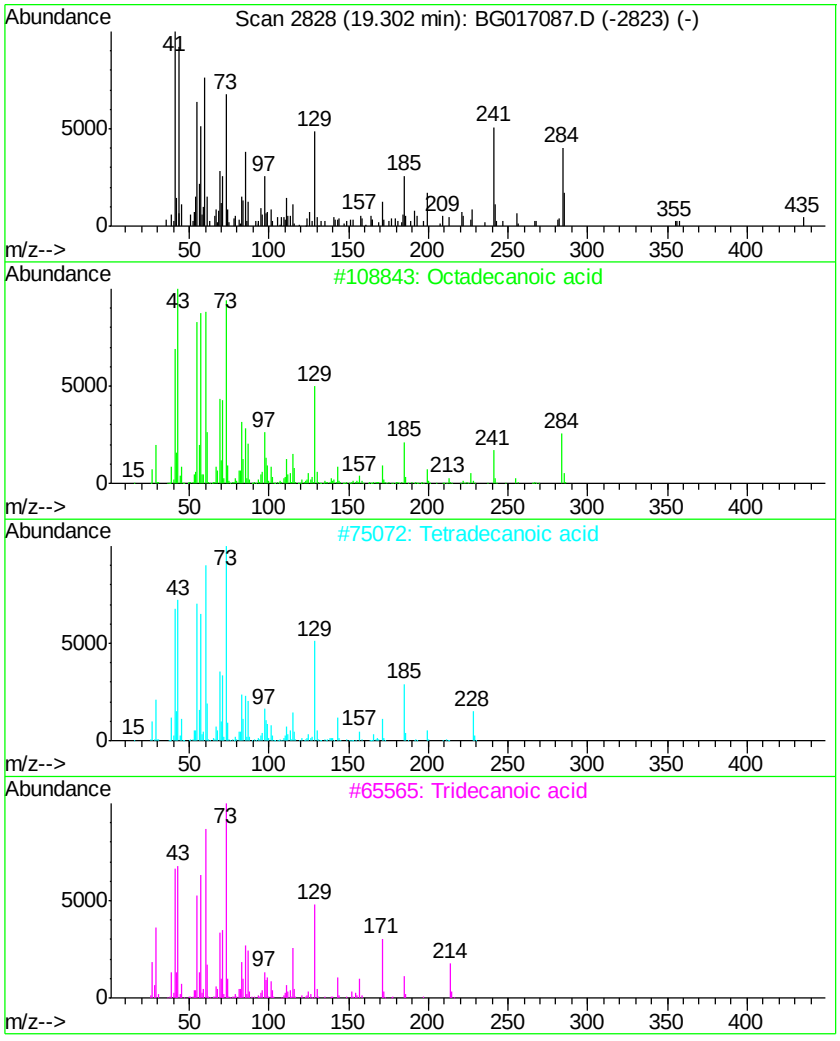
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

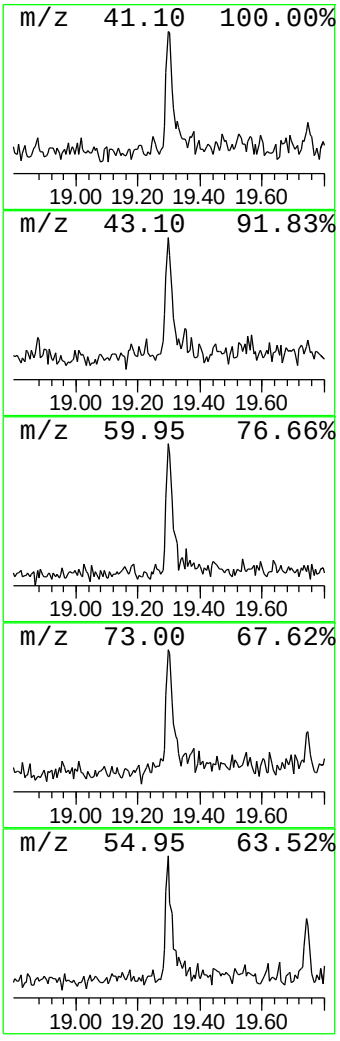
****

Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.30	3.98 ng	142412	Chrysene-d12	21.29

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	47
3	Tridecanoic acid	214	C13H26O2	000638-53-9	43
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





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Sample : G2194-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

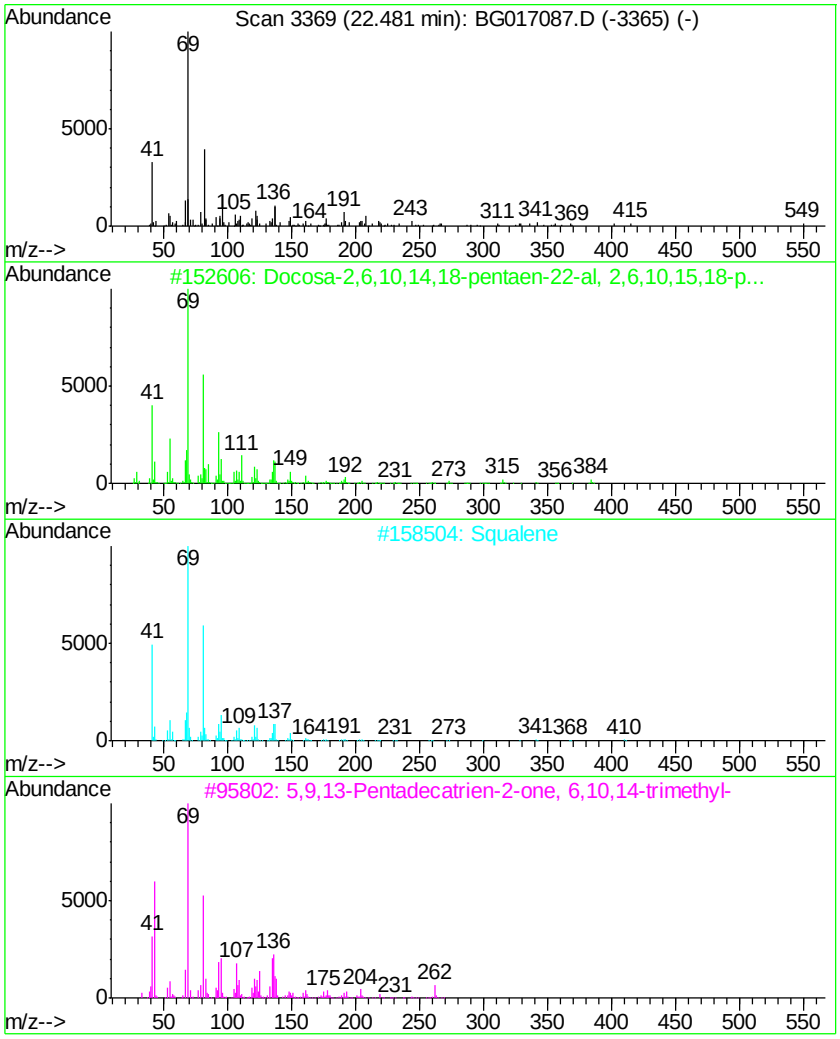
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

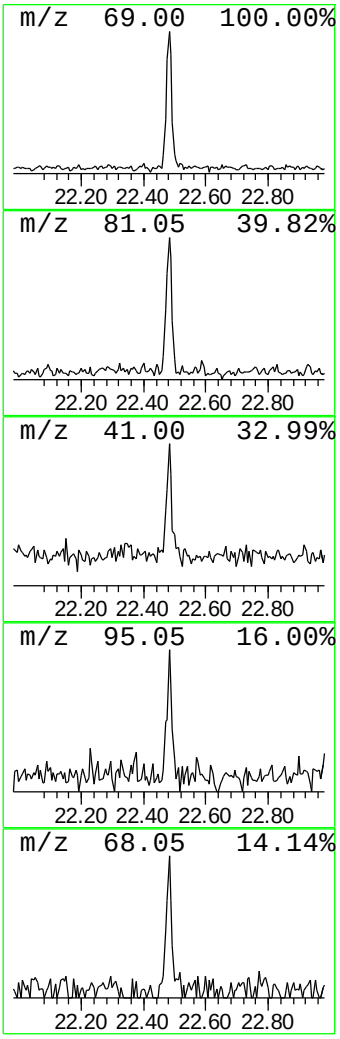
****

Peak Number 10 Docosa-2,6,10,14,18-pentaen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	2.89 ng	100846	Perylene-d12	23.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
2	Squalene	410	C30H50	007683-64-9	72
3	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	000762-29-8	64
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64
5	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051215\
Data File : BG017087.D
Acq On : 12 May 2015 17:42
Operator : TP/IZ
Sample : G2194-14
Misc :
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Instrument : BNA_G
ClientSampleId : TU021-TW-02

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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...	2.89	42.1	ng	538285	1	7.72	255475	20.0
unknown4.83	4.83	3.3	ng	41670	1	7.72	255475	20.0
unknown7.26	7.26	93.1	ng	1188750	1	7.72	255475	20.0
2,2,4-Trimethyl-1...	12.72	2.9	ng	70013	3	14.37	480744	20.0
1H-Benzotriazole,...	15.09	3.0	ng	71193	3	14.37	480744	20.0
n-Hexadecanoic acid	18.02	3.7	ng	121331	4	17.12	649786	20.0
Octadecanoic acid	19.30	4.0	ng	142412	5	21.29	715673	20.0
Docosa-2,6,10,14,...	22.48	2.9	ng	100846	6	23.56	696733	20.0