LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

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-BG120215.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	2.993	21	26	45	rBV	1562854	2086435	74.77%	12.388%
2	3.140	46	51	60	rVV4	36352	80818	2.90%	0.480%
3	3.216	60	64	77	rVB	79029	112896	4.05%	0.670%
4	5.191	395	400	410	rVB	122520	184054	6.60%	1.093%
5	5.661	471	480	490	rBV	563445	871840	31.24%	5.176%
6	7.265	743	753	763	rBV	618778	1054815	37.80%	6.263%
7	7.647	809	818	829	rBV	588657	986277	35.34%	5.856%
8	8.117	892	898	905	rBV	97291	159700	5.72%	0.948%
9	8.446	947	954	963	rVB	418662	710016	25.44%	4.216%
10	9.286	1089	1097	1105	rBV	390659	670957	24.04%	3.984%
11	10.937	1371	1378	1384	rBV	142783	247296	8.86%	1.468%
12	13.375	1785	1793	1801	rBV	1104263	1675107	60.03%	9.946%
13	14.192	1926	1932	1940	rVB	261962	379619	13.60%	2.254%
14	14.750	2018	2027	2035	rVB2	255104	404257	14.49%	2.400%
15	16.231	2272	2279	2290	rBV	1018599	1473171	52.79%	8.747%
16	17.488	2486	2493	2500	rBV	353709	530071	19.00%	3.147%
17	18.369	2638	2643	2654	rBV	93534	139776	5.01%	0.830%
18	19.633	2854	2858	2864	rBV2	37883	57362	2.06%	0.341%
19	20.097	2930	2937	2942	rBV	2105358	2790510	100.00%	16.568%
20	20.778	3045	3053	3059	rBV	30126	59274	2.12%	0.352%
21	20.996	3087	3090	3095	rBV5	19056	34785	1.25%	0.207%
22	21.043	3095	3098	3103	rVV2	33509	42426	1.52%	0.252%
23	21.401	3156	3159	3163	rVB3	37615	42580	1.53%	0.253%
24	21.554	3183	3185	3192	rVB2	27195	41322	1.48%	0.245%
25	21.765	3215	3221	3230	rVB	429052	681386	24.42%	4.046%
26	22.870	3404	3409	3414	rVB3	29204	50202	1.80%	0.298%
27	23.064	3434	3442	3443	rBV7	21655	44871	1.61%	0.266%
28	23.281	3473	3479	3492	rVB	134047	266794	9.56%	1.584%
29	23.510	3512	3518	3526	rVB	62144	129150	4.63%	0.767%
30	23.604	3532	3534	3541	rVB4	19965	34819	1.25%	0.207%
31	23.863	3571	3578	3585	rVB4	33010	90259	3.23%	0.536%
32	24.709	3720	3722	3734	rVB6	20638	47022	1.69%	0.279%
33	25.056	3771	3781	3791	rVB	223822	628862	22.54%	3.734%
34	25.772	3897	3903	3910	rVB3	13296	33899	1.21%	0.201%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

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-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

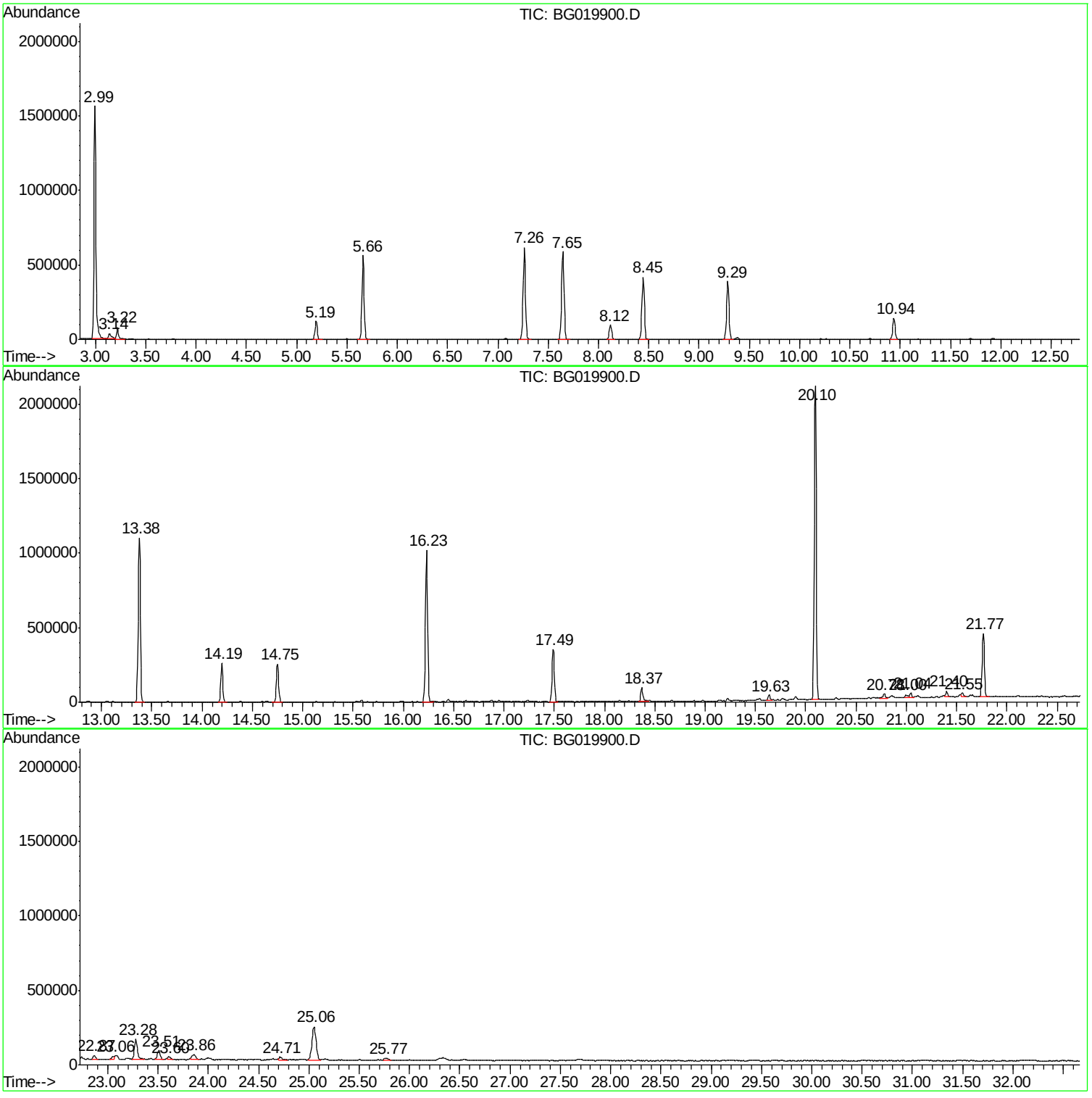
Sum of corrected areas: 16842628

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

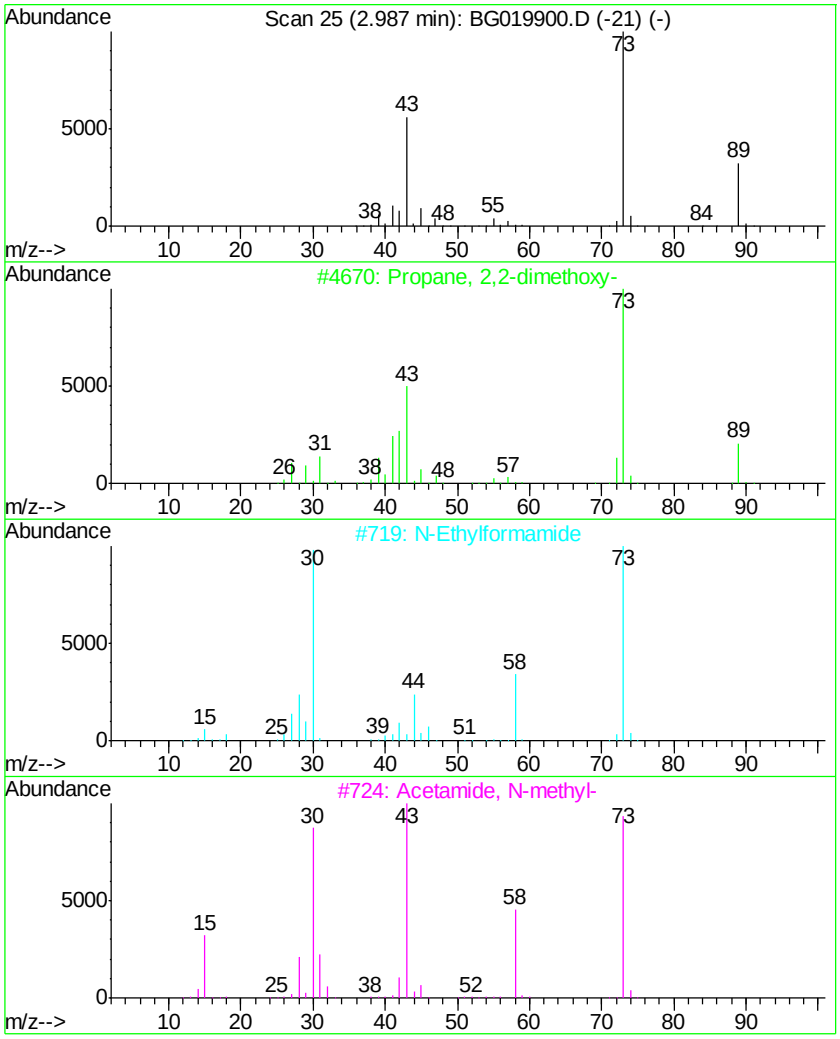
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

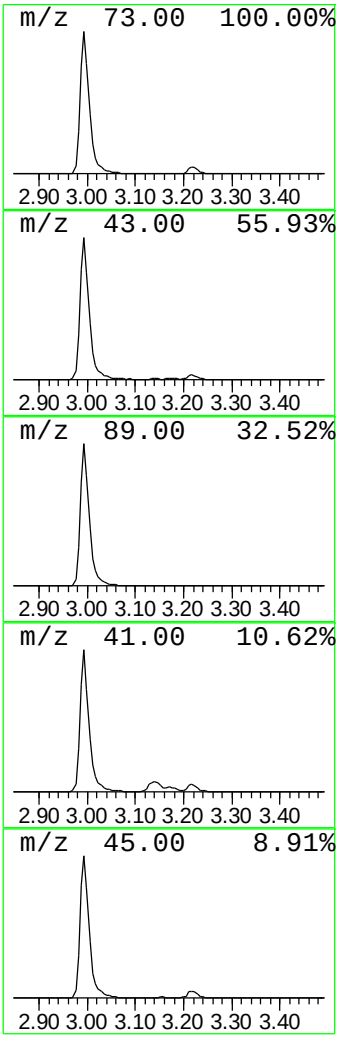
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	261.29 ng	2086440	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

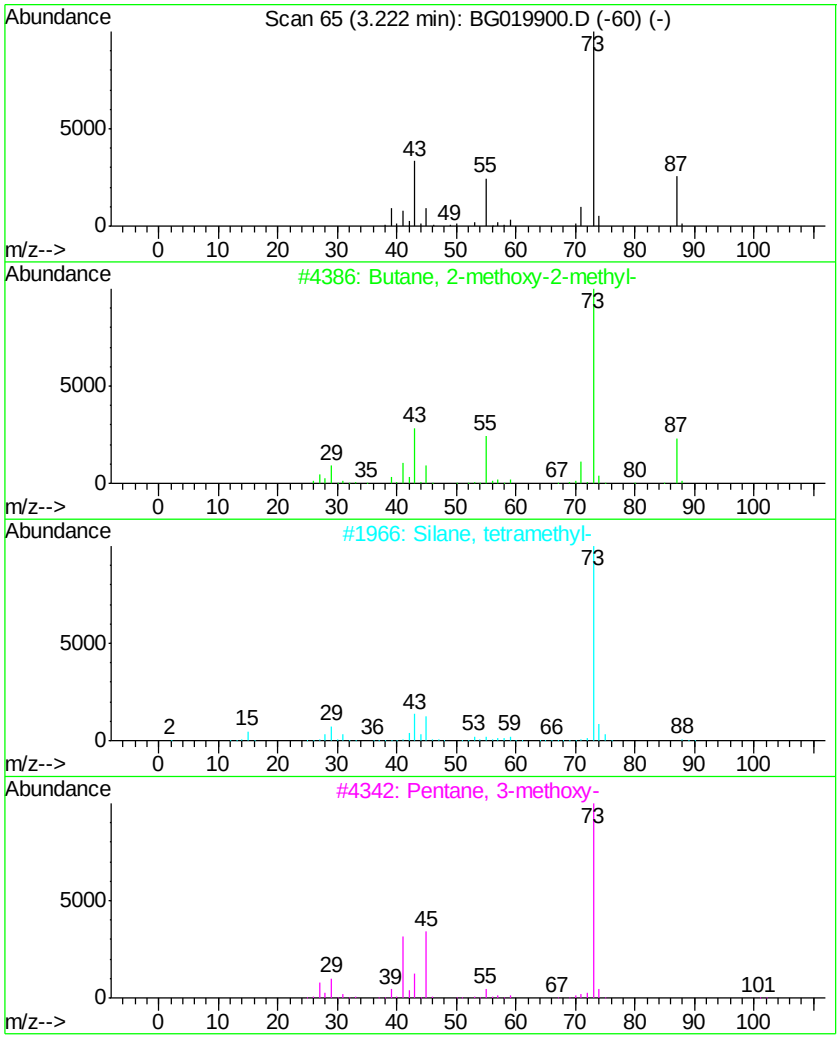
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

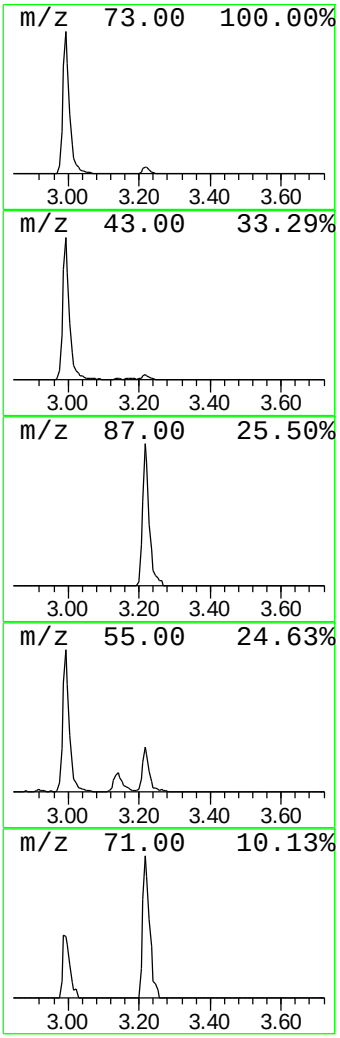
****

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	14.14 ng	112896	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	22
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

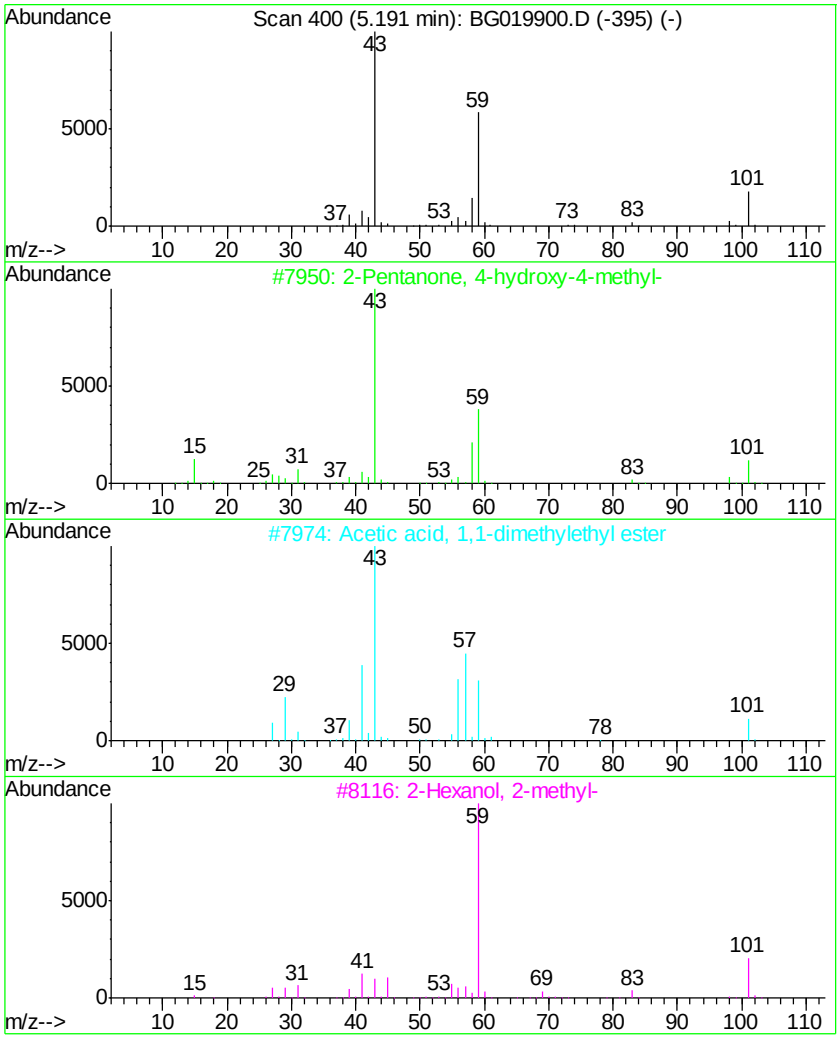
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

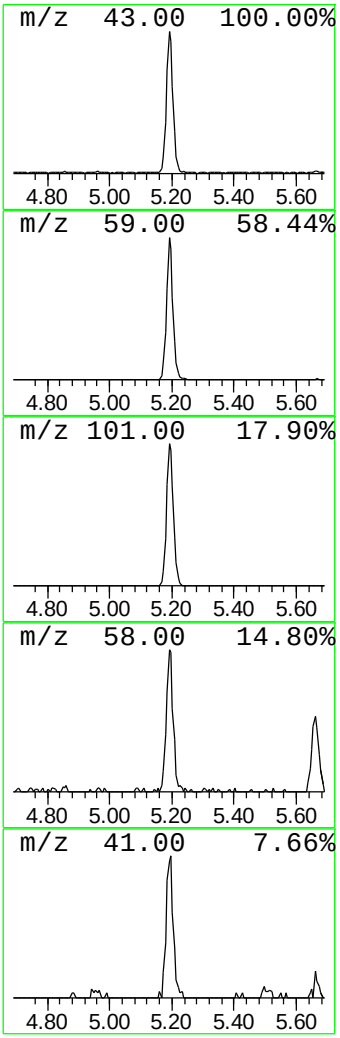
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	23.05 ng	184054	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

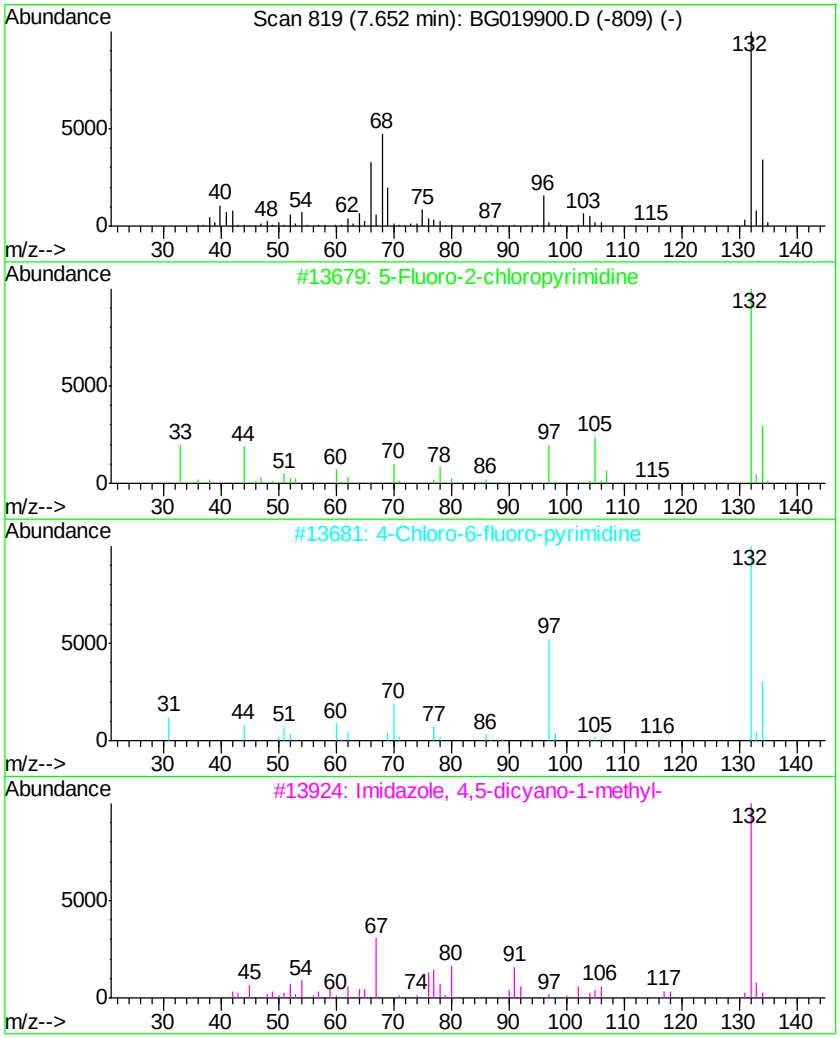
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

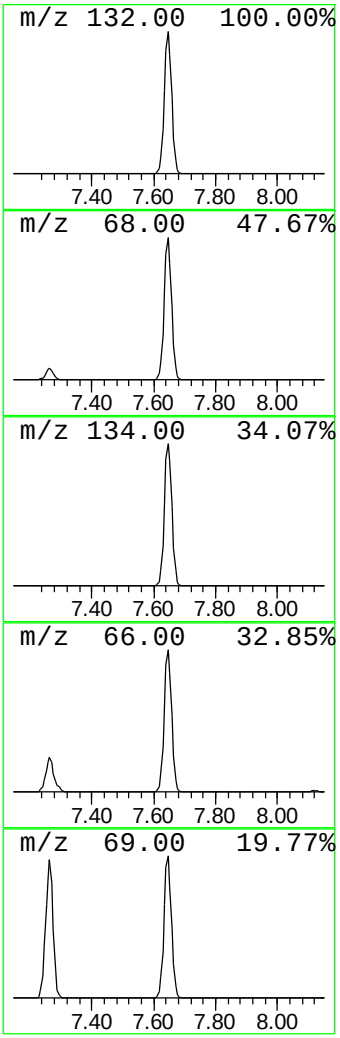
****

Peak Number 5 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	123.52 ng	986277	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

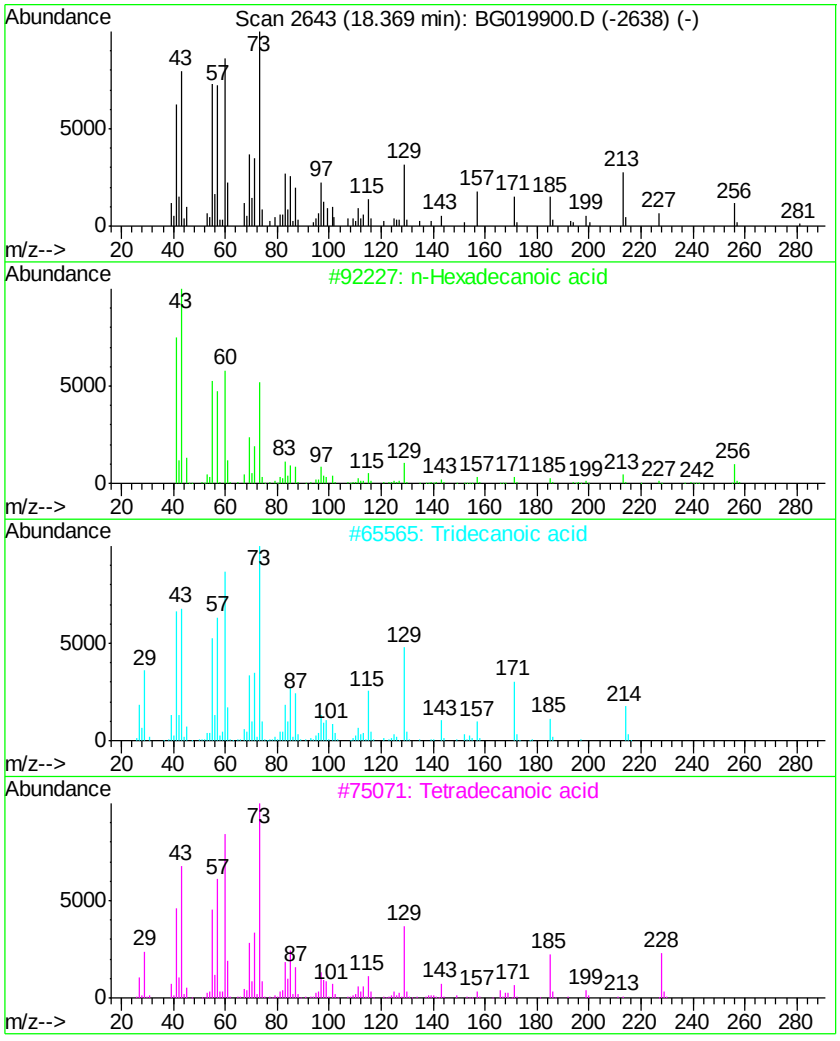
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

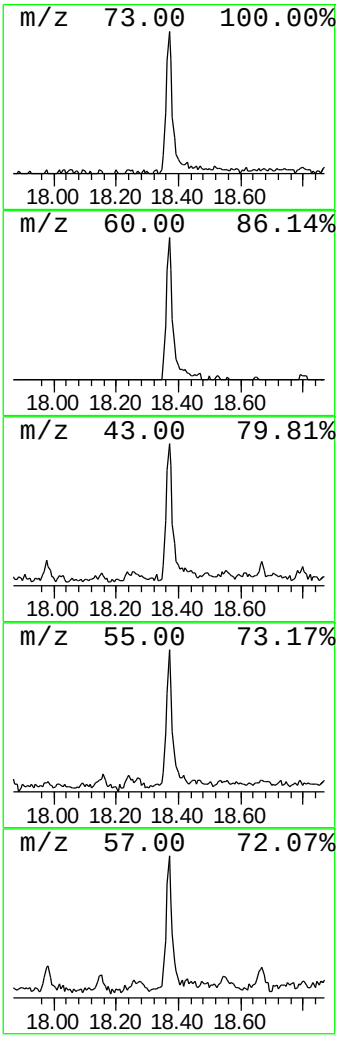
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	5.27 ng	139776	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	49





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

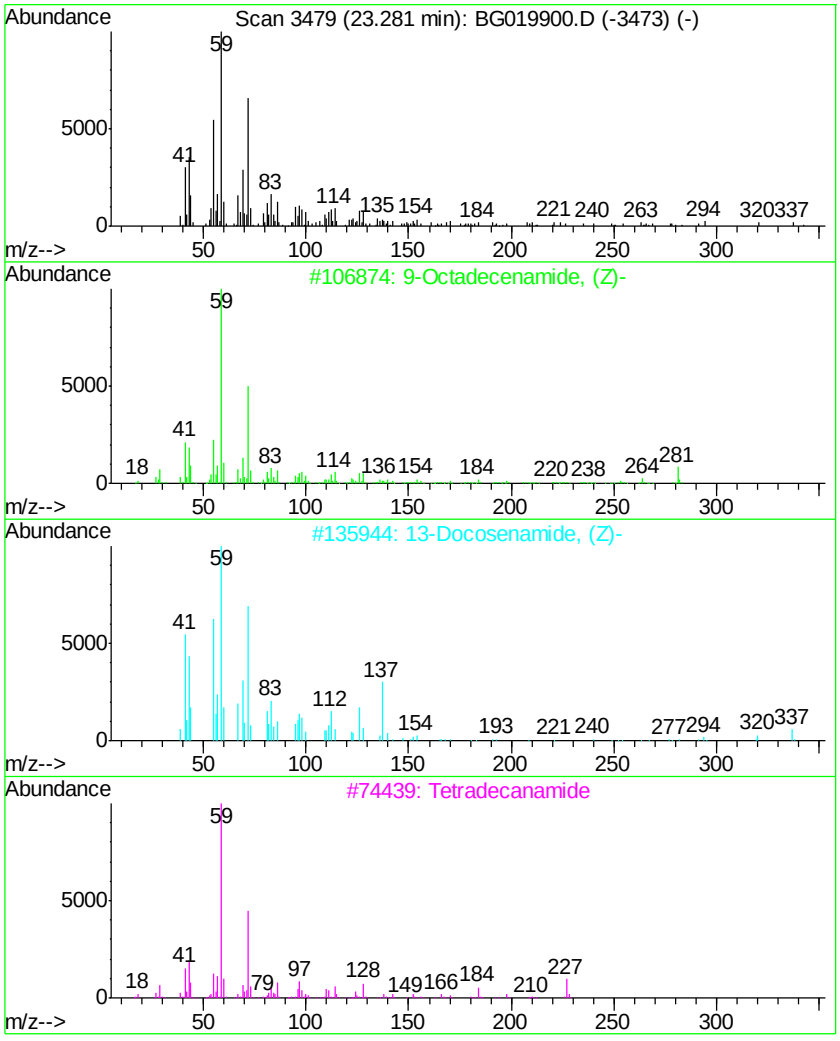
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

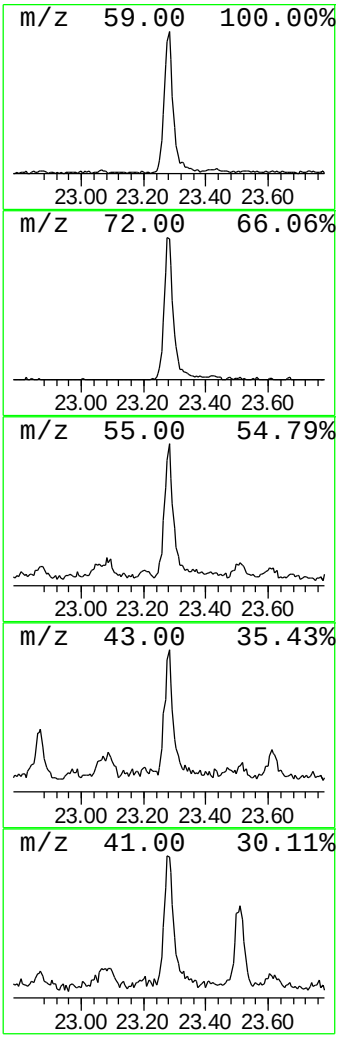
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	7.83 ng	266794	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Octadecanamide	283	C18H37NO	000124-26-5	72
5	Dodecanamide	199	C12H25NO	001120-16-7	59





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

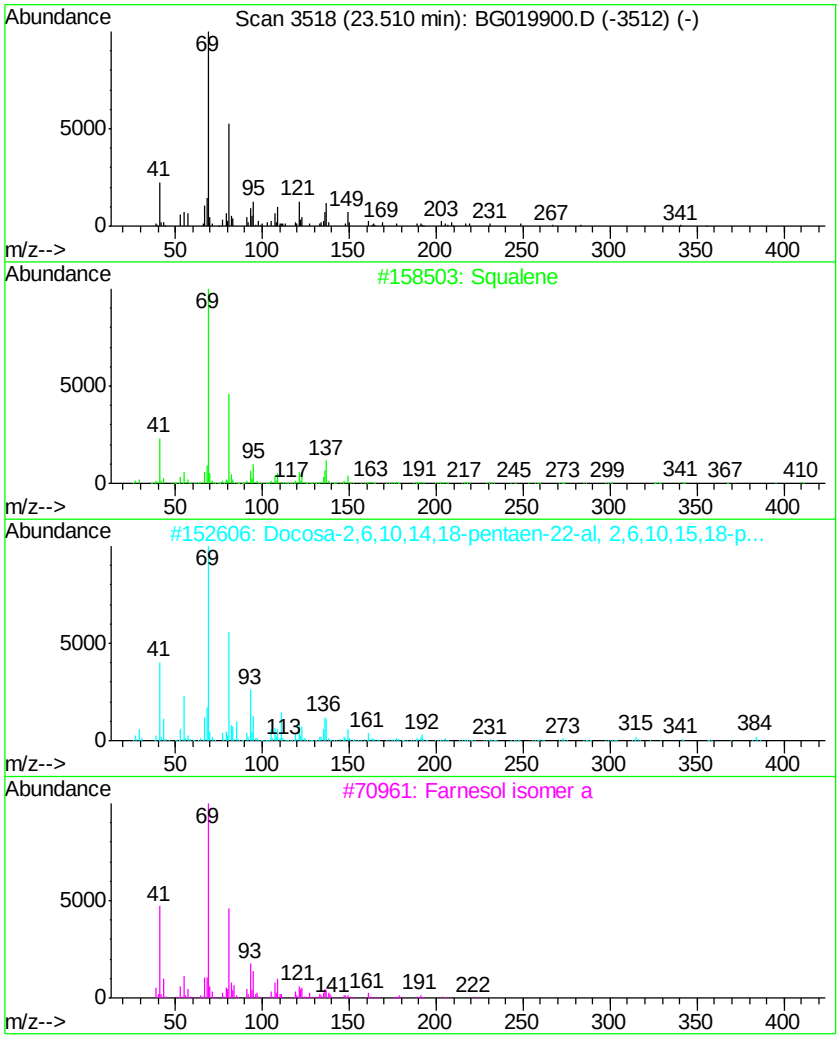
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

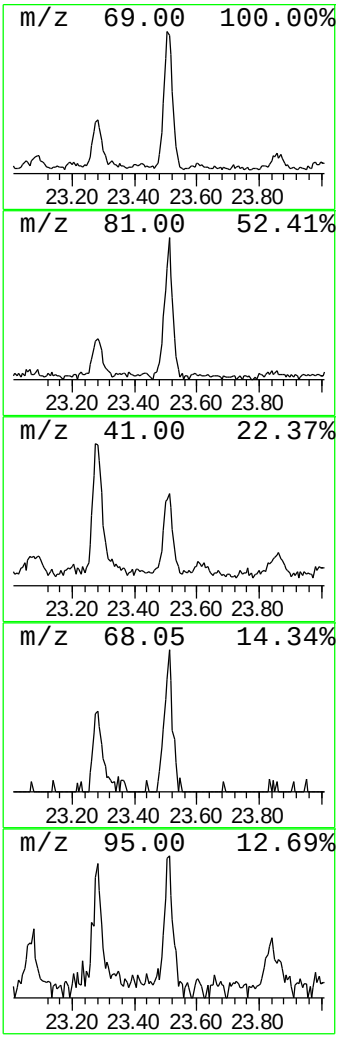
****

Peak Number 9 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	4.11 ng	129150	Perylene-d12	25.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

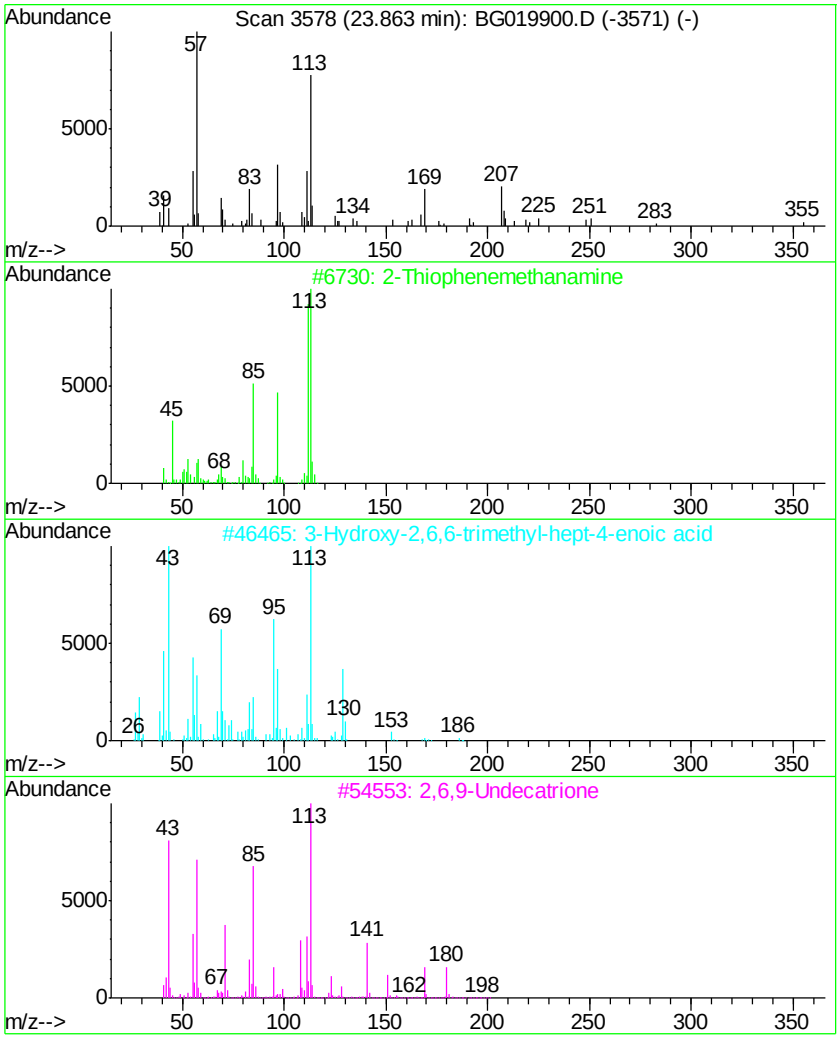
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

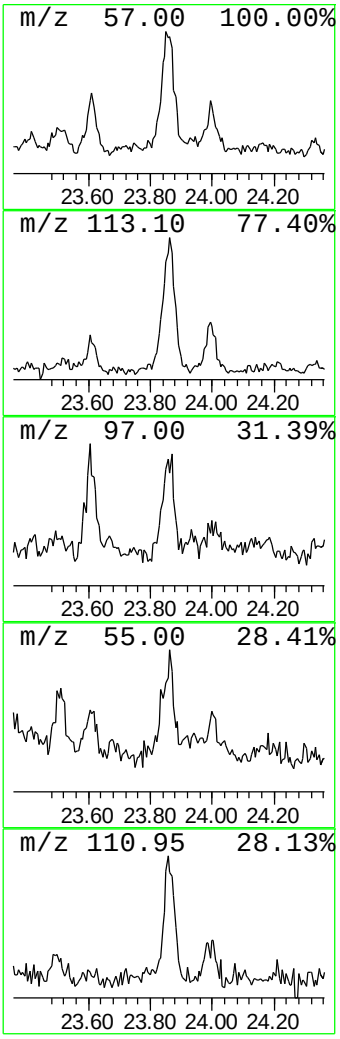
****

Peak Number 10 unknown23.86 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.86	2.87 ng	90259	Perylene-d12	25.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenemethanamine	113	C5H7NS	027757-85-3	49
2	3-Hydroxy-2,6,6-trimethyl-hept-4...	186	C10H18O3	1000185-34-0	38
3	2,6,9-Undecatrione	198	C11H18O3	078975-91-4	38
4	5-Hydroxy-6-methyl-12,13-dioxa-t...	270	C14H22O5	1000193-88-4	38
5	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120315\
Data File : BG019900.D
Acq On : 4 Dec 2015 10:15
Operator : UM/NP
Sample : G4609-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CF-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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
Propane, 2,2-dime...	2.99	261.3	ng	2086440	1	8.12	159700	20.0
Butane, 2-methoxy...	3.22	14.1	ng	112896	1	8.12	159700	20.0
2-Pentanone, 4-hy...	5.19	23.1	ng	184054	1	8.12	159700	20.0
unknown7.65	7.65	123.5	ng	986277	1	8.12	159700	20.0
n-Hexadecanoic acid	18.37	5.3	ng	139776	4	17.49	530071	20.0
9-Octadecenamide,...	23.28	7.8	ng	266794	5	21.77	681386	20.0
Squalene	23.51	4.1	ng	129150	6	25.05	628862	20.0
unknown23.86	23.86	2.9	ng	90259	6	25.05	628862	20.0