LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

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-BG060315.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	2.763	9	13	18	rBV	56138	72798	3.97%	0.785%
2	2.804	18	20	28	rVB	14729	21456	1.17%	0.231%
3	4.719	341	346	355	rVB	44100	65842	3.59%	0.710%
4	5.219	425	431	441	rBV	454356	652558	35.55%	7.037%
5	6.141	583	588	595	rBV2	15615	25721	1.40%	0.277%
6	6.834	698	706	718	rBV	463405	750466	40.89%	8.093%
7	7.163	754	762	772	rBV	473615	735940	40.10%	7.937%
8	7.622	831	840	845	rBV	71369	110708	6.03%	1.194%
9	7.939	885	894	903	rBV	332926	513636	27.98%	5.539%
10	8.785	1030	1038	1047	rBV	278971	461748	25.16%	4.980%
11	10.419	1309	1316	1325	rBV2	88685	153443	8.36%	1.655%
12	12.910	1733	1740	1748	rBV	705036	1039890	56.65%	11.215%
13	13.756	1877	1884	1894	rBV	91640	145468	7.93%	1.569%
14	14.290	1968	1975	1983	rBV3	153712	233001	12.69%	2.513%
15	15.795	2224	2231	2240	rBV	755855	1099079	59.88%	11.853%
16	17.046	2435	2444	2453	rBV	214309	312239	17.01%	3.367%
17	17.957	2594	2599	2604	rBV3	41289	62703	3.42%	0.676%
18	19.684	2887	2893	2899	rBV	1516204	1835479	100.00%	19.795%
19	20.953	3105	3109	3118	rBV	73447	104142	5.67%	1.123%
20	21.241	3153	3158	3168	rBV	282635	372868	20.31%	4.021%
21	22.410	3350	3357	3363	rBV	107287	139698	7.61%	1.507%
22	23.480	3532	3539	3547	rVB	186336	344840	18.79%	3.719%
23	25.771	3922	3929	3930	rBV7	10198	18869	1.03%	0.203%

Sum of corrected areas: 9272592

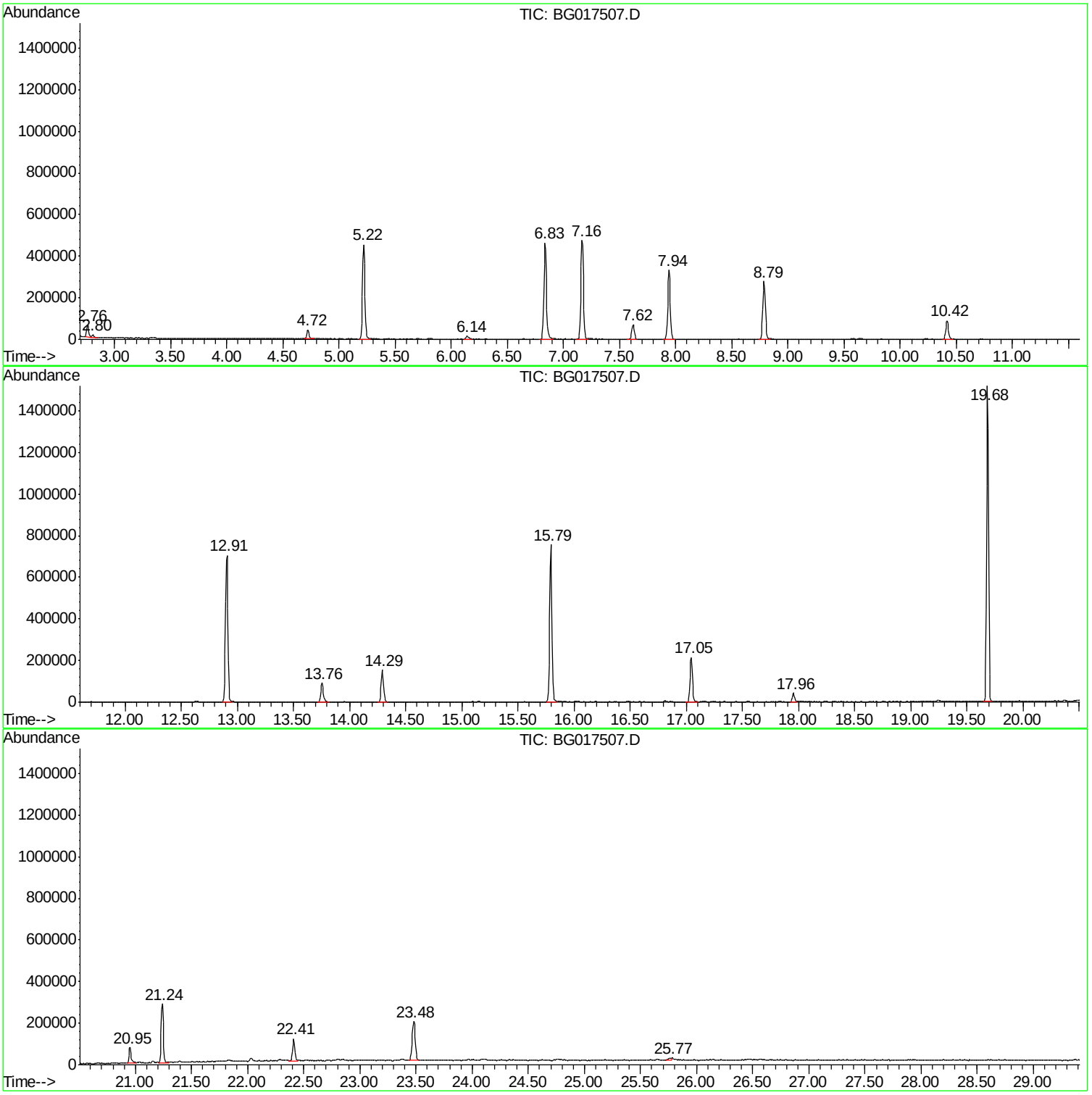
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.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\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

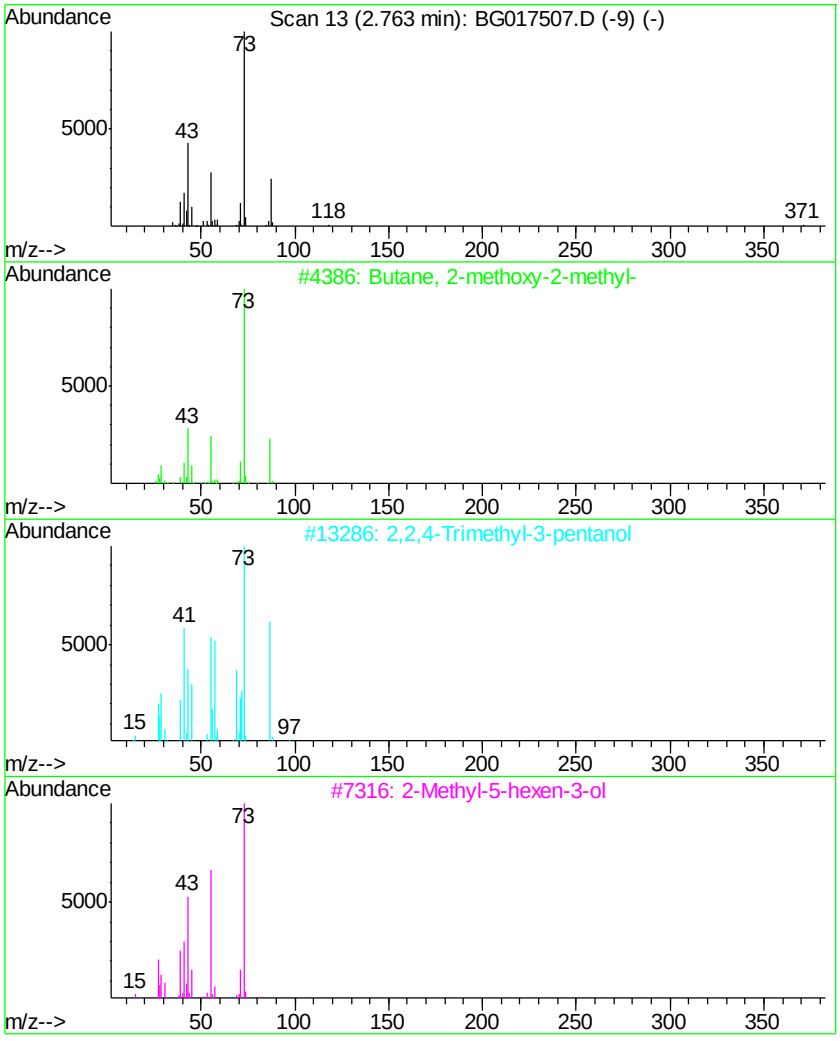
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

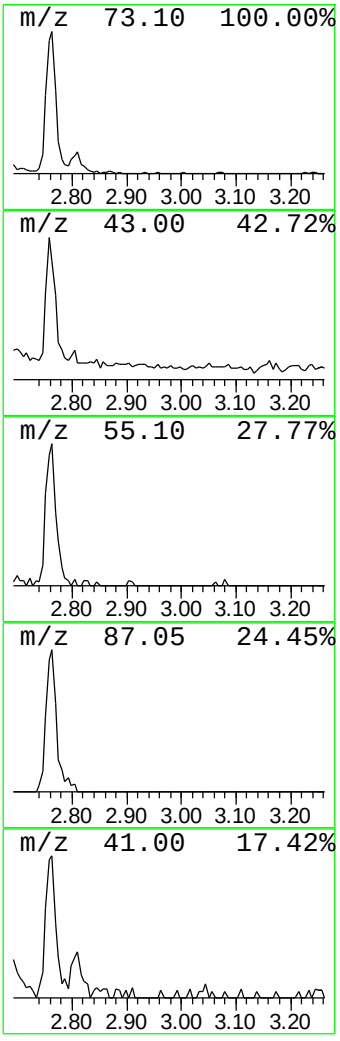
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.76	13.15 ng	72798	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

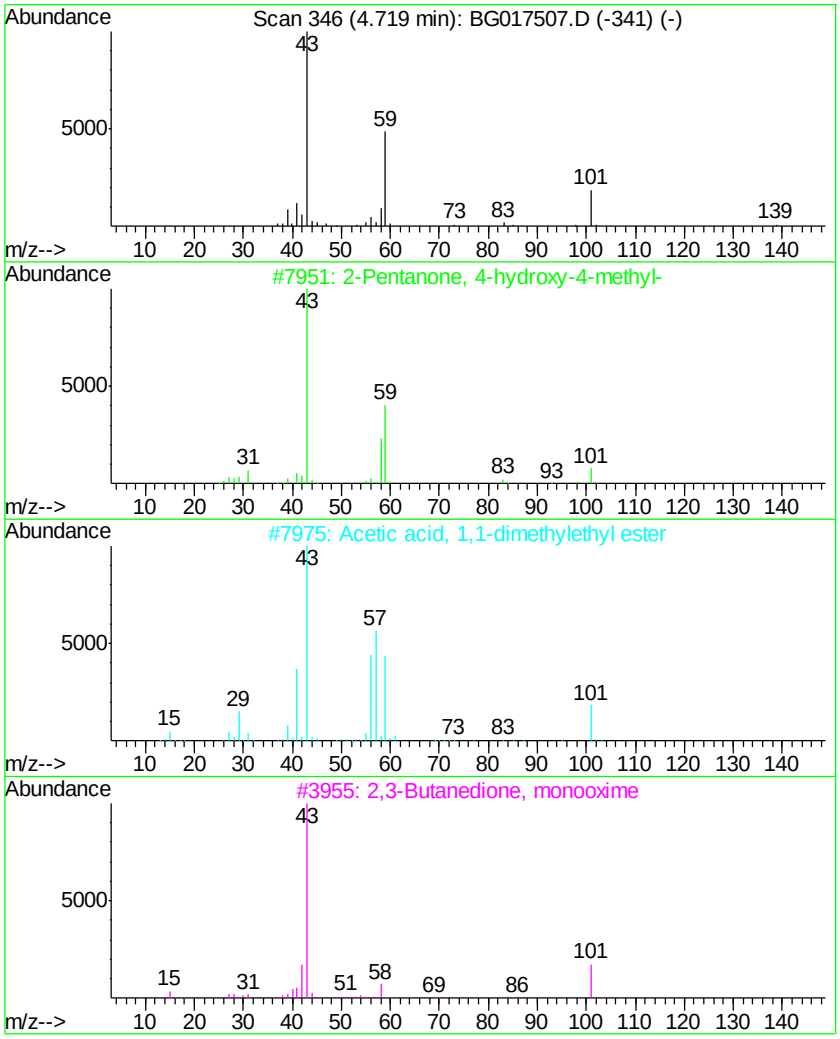
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

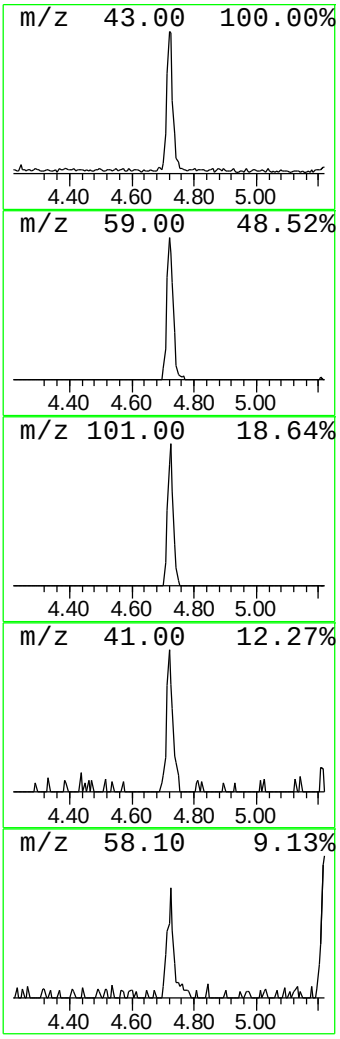
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	11.89 ng	65842	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Methanecarbothiolic acid	76	C2H4OS	000507-09-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

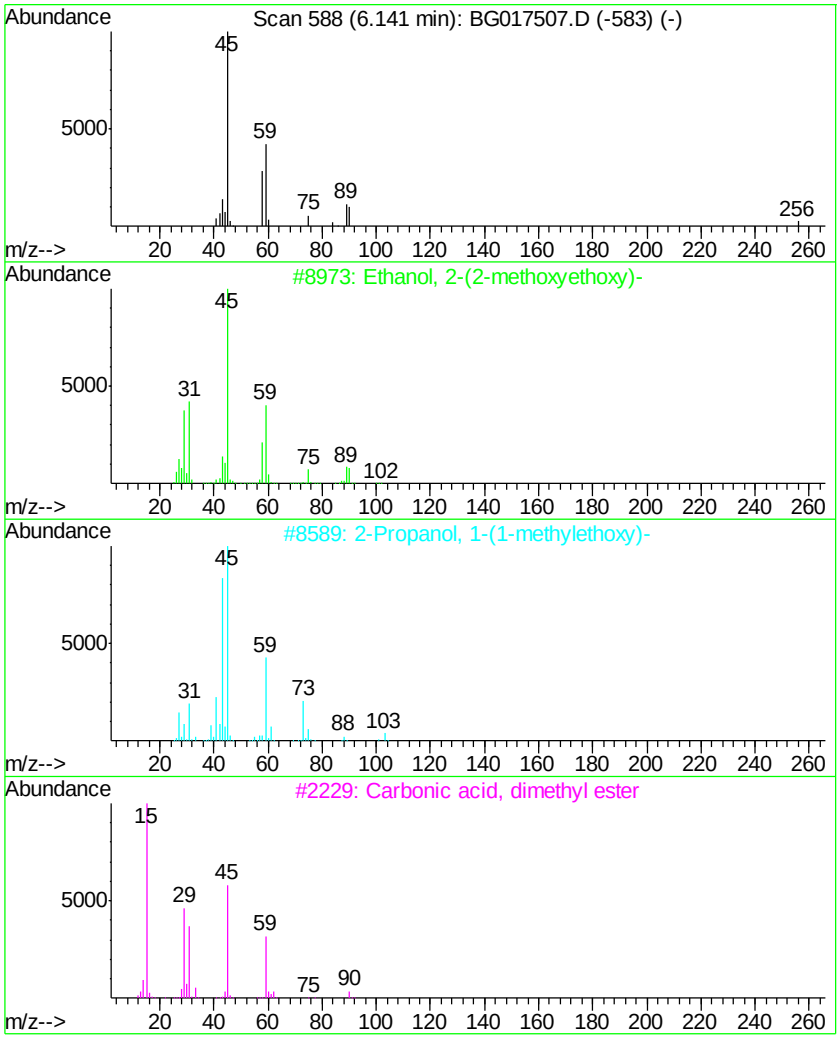
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

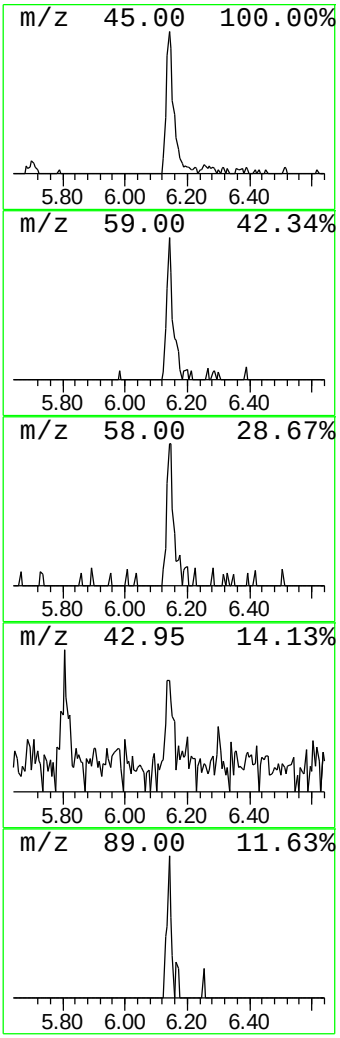
****

Peak Number 4 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	4.65 ng	25721	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	64
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	59
3	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38
4	Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	36
5	Ethanol, 2,2'-[oxybis(2,1-ethane...	194	C8H18O5	000112-60-7	28





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

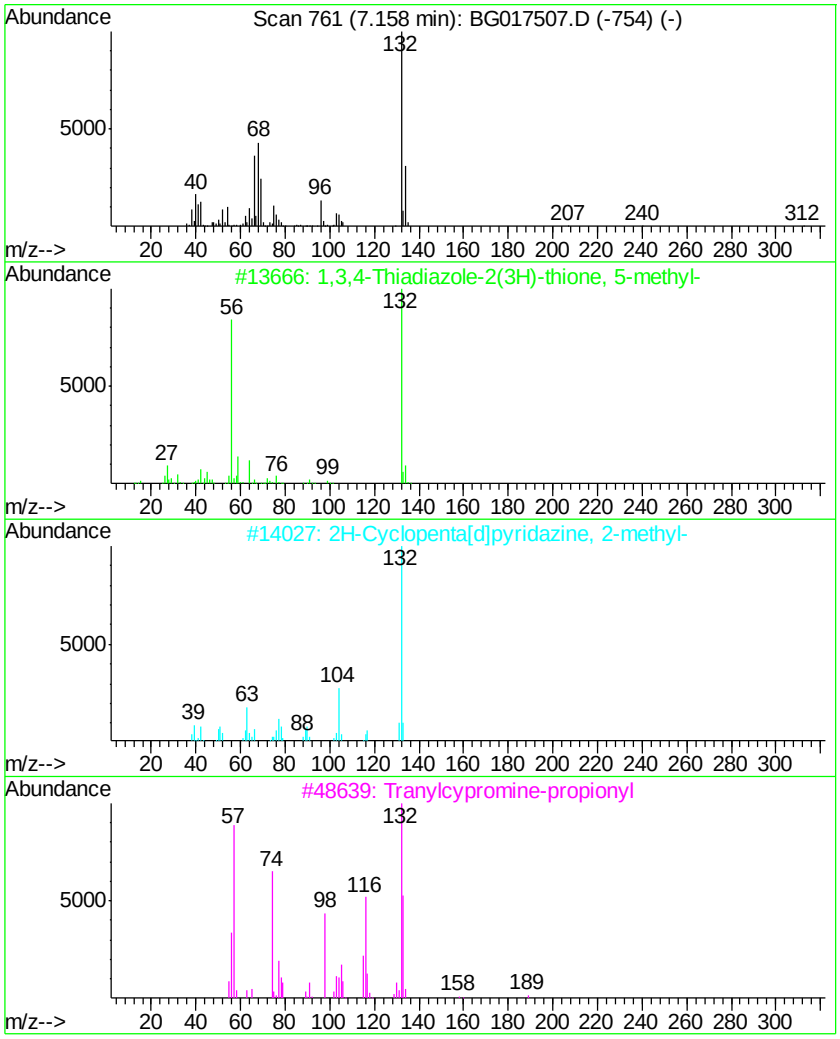
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

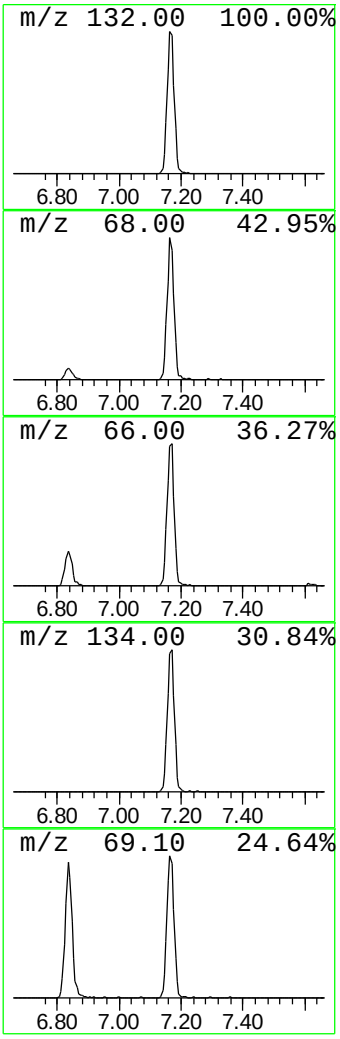
****

Peak Number 5 unknown7.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	132.95 ng	735940	1,4-Dichlorobenzene-d4	7.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

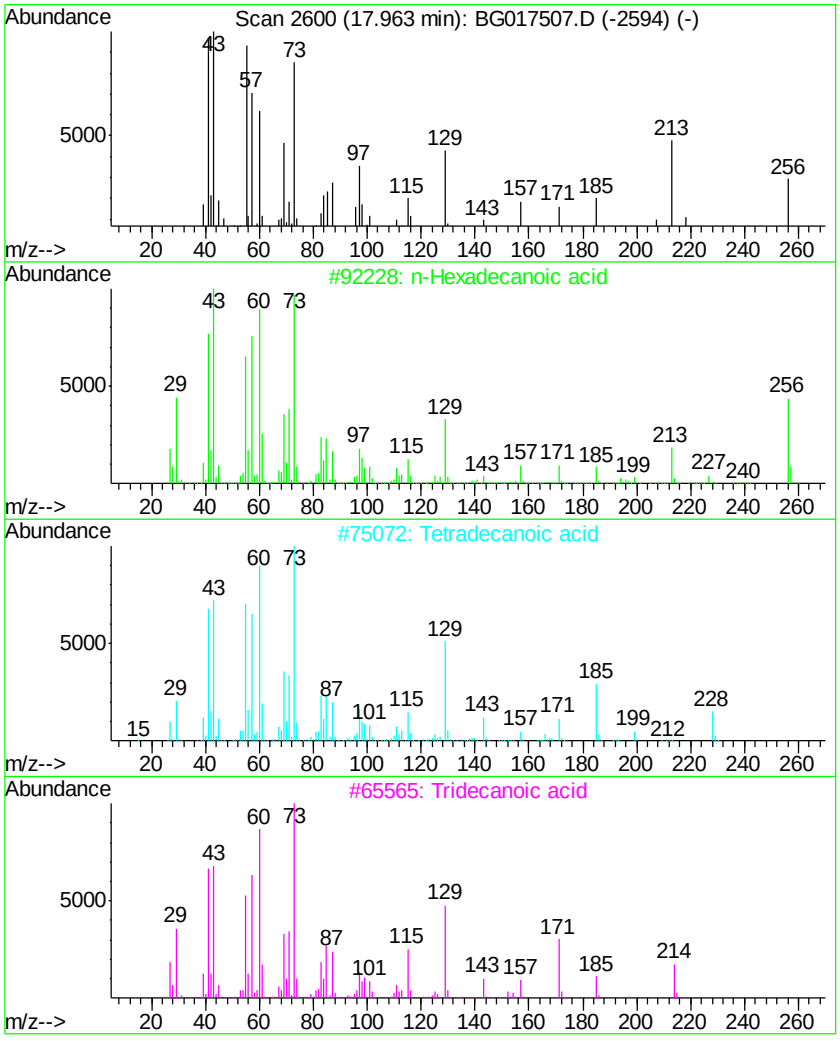
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

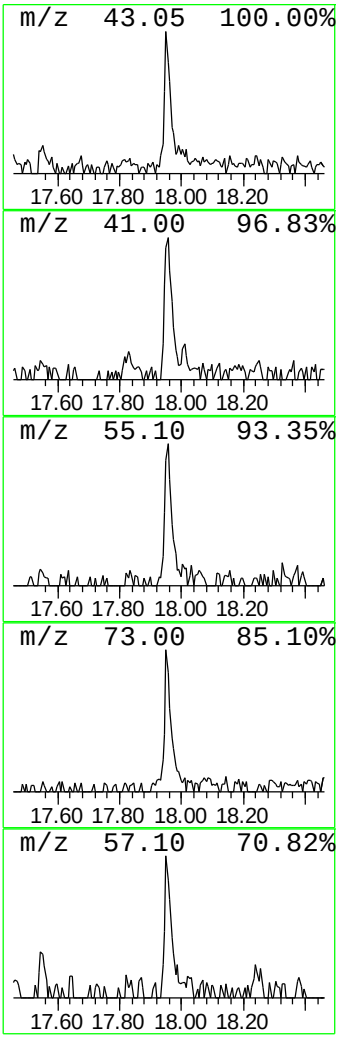
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	4.02 ng	62703	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
3	Tridecanoic acid	214	C13H26O2	000638-53-9	47
4	.alpha.-D-Galactopyranoside, met...	334	C17H34O6	1000157-55-9	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

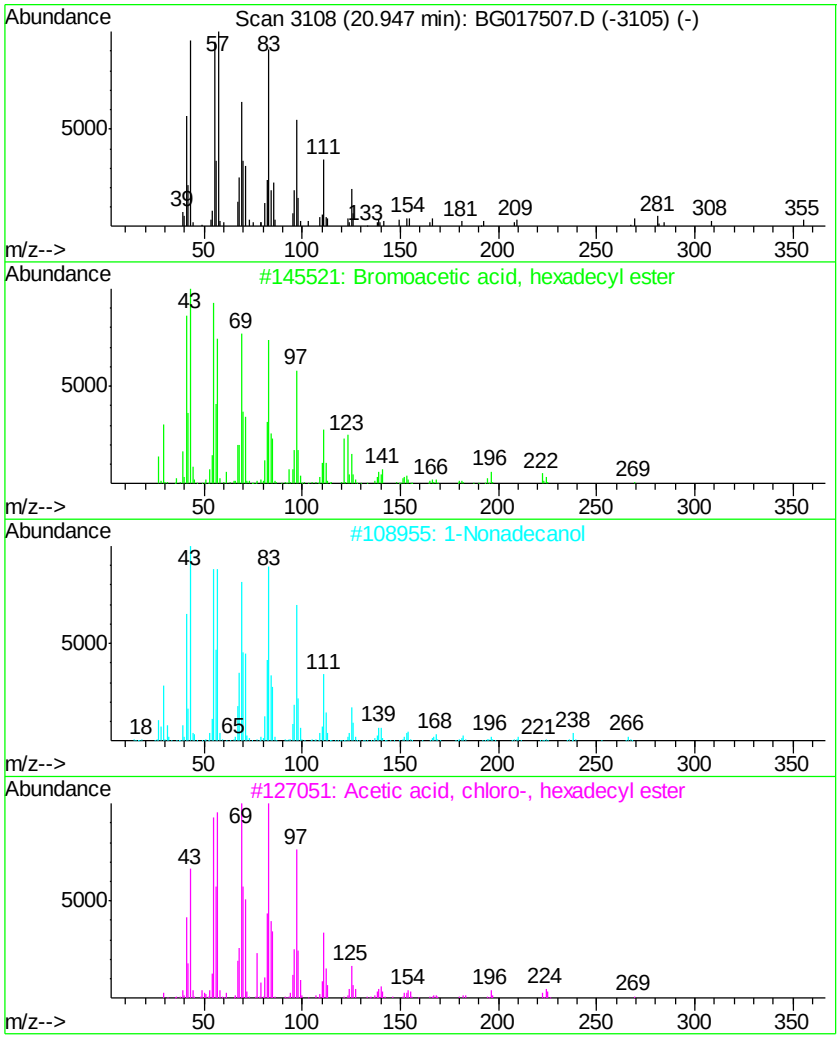
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

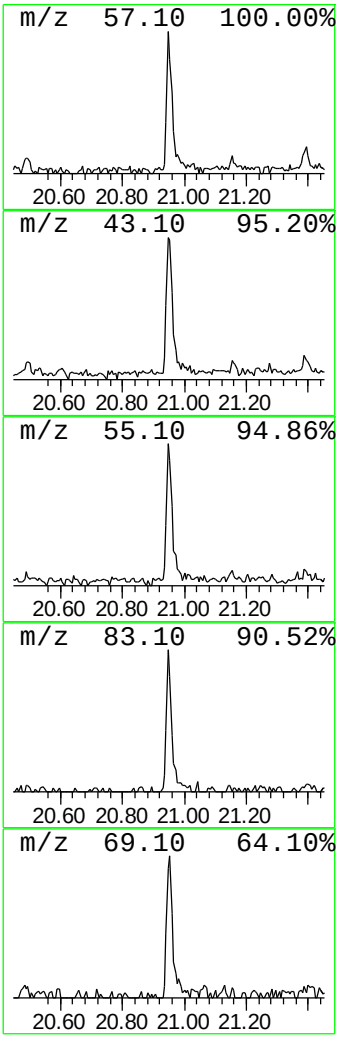
****

Peak Number 8 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	5.59 ng	104142	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2	1-Nonadecanol	284	C19H40O	001454-84-8	94
3	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	94
4	1-Eicosene	280	C20H40	003452-07-1	93
5	1-Eicosanol	298	C20H42O	000629-96-9	92





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

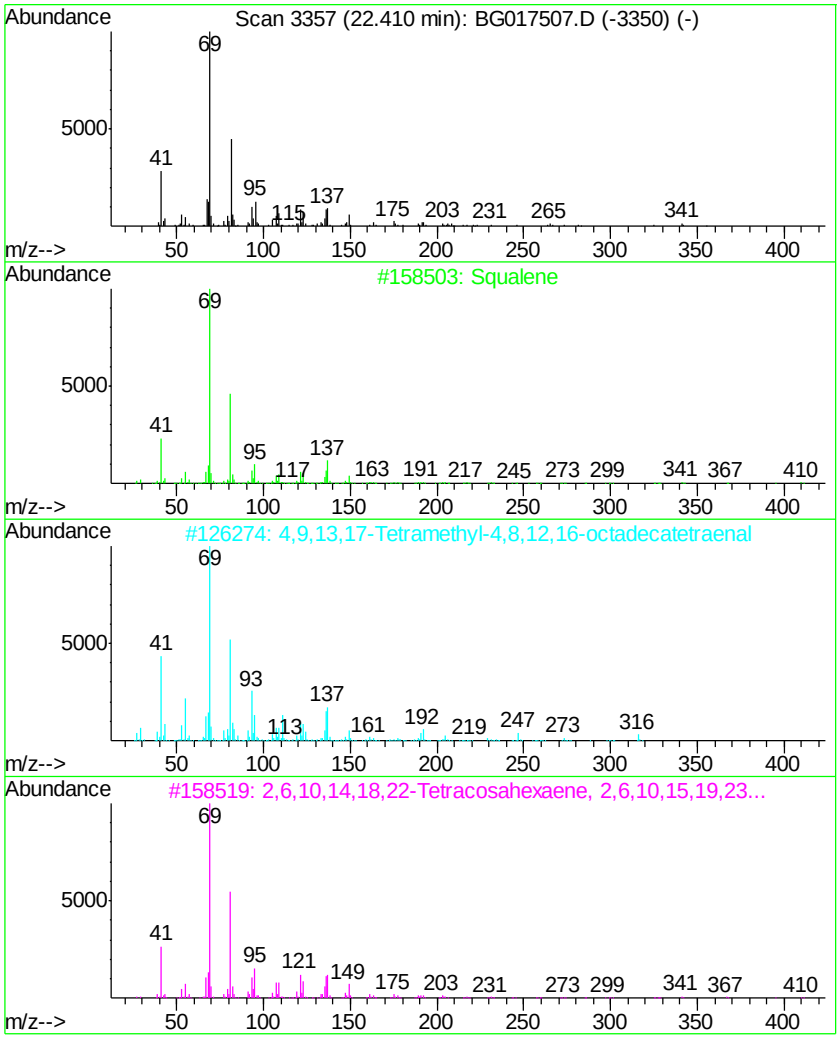
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

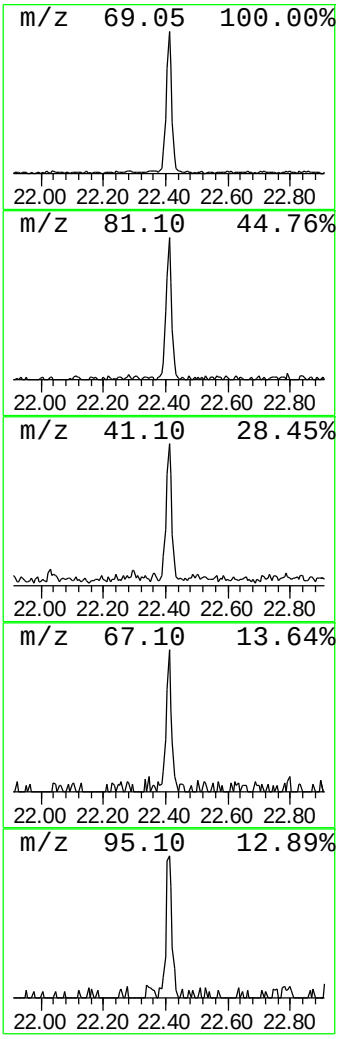
****

Peak Number 9 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	8.10 ng	139698	Perylene-d12	23.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
3	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	78
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017507.D
Acq On : 6 Jun 2015 21:14
Operator : TP/IZ
Sample : G2550-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-040

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.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...	2.76	13.2	ng	72798	1	7.62	110708	20.0
2-Pentanone, 4-hy...	4.72	11.9	ng	65842	1	7.62	110708	20.0
Ethanol, 2-(2-met...	6.14	4.7	ng	25721	1	7.62	110708	20.0
unknown7.16	7.16	132.9	ng	735940	1	7.62	110708	20.0
n-Hexadecanoic acid	17.96	4.0	ng	62703	4	17.05	312239	20.0
Bromoacetic acid,...	20.95	5.6	ng	104142	5	21.24	372868	20.0
Squalene	22.41	8.1	ng	139698	6	23.48	344840	20.0