LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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-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	2.762	8	12	19	rBV	71724	99196	7.06%	1.036%
2	4.725	337	346	354	rBV	42872	66176	4.71%	0.691%
3	5.218	423	430	440	rBV	535687	807148	57.44%	8.429%
4	6.840	696	706	717	rBV	585977	929526	66.14%	9.707%
5	7.169	754	762	772	rBV	613710	952574	67.78%	9.948%
6	7.621	833	839	846	rBV	98348	153525	10.92%	1.603%
7	7.944	887	894	903	rVB	429200	669313	47.63%	6.990%
8	8.790	1027	1038	1047	rBV	375142	605766	43.11%	6.326%
9	10.418	1308	1315	1324	rBV	122443	211504	15.05%	2.209%
10	12.909	1732	1739	1745	rBV	776169	1093788	77.83%	11.422%
11	13.755	1877	1883	1891	rBV	41676	68520	4.88%	0.716%
12	14.290	1967	1974	1983	rBV2	164941	259732	18.48%	2.712%
13	15.794	2222	2230	2247	rBV	726769	1006710	71.64%	10.513%
14	17.045	2437	2443	2451	rBV2	198838	285942	20.35%	2.986%
15	17.950	2593	2597	2605	rBV3	45544	72236	5.14%	0.754%
16	19.243	2811	2817	2821	rBV5	11225	19164	1.36%	0.200%
17	19.683	2886	2892	2901	rBV	1174630	1405302	100.00%	14.675%
18	20.947	3104	3107	3113	rBV	70733	89608	6.38%	0.936%
19	21.158	3138	3143	3150	rVB	59170	78410	5.58%	0.819%
20	21.240	3152	3157	3162	rVV	263875	323644	23.03%	3.380%
21	21.499	3198	3201	3204	rVB5	19591	23929	1.70%	0.250%
22	22.786	3415	3420	3425	rBV7	19824	44804	3.19%	0.468%
23	23.479	3532	3538	3547	rVB	164877	309346	22.01%	3.230%

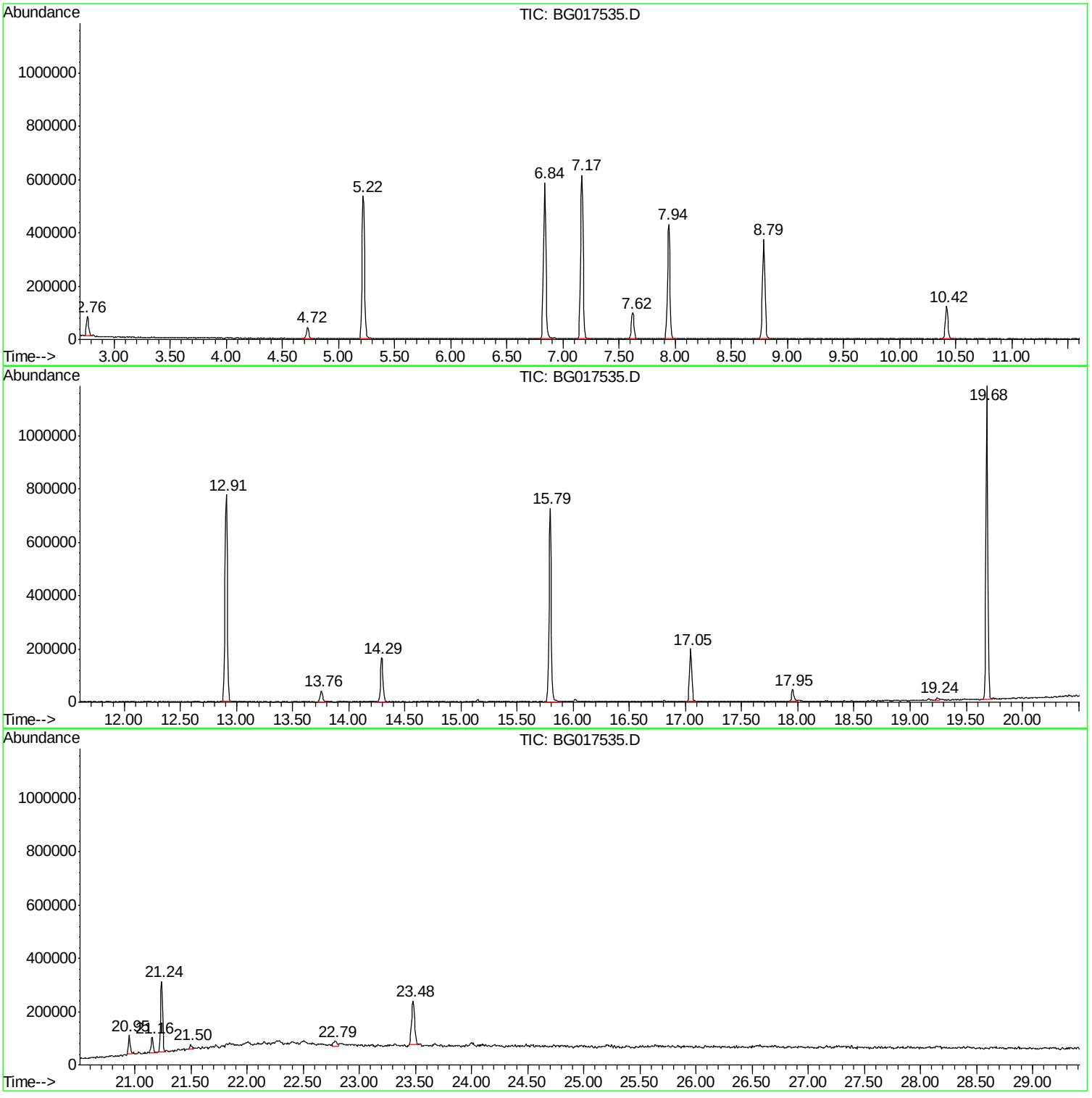
Sum of corrected areas: 9575863

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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 : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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

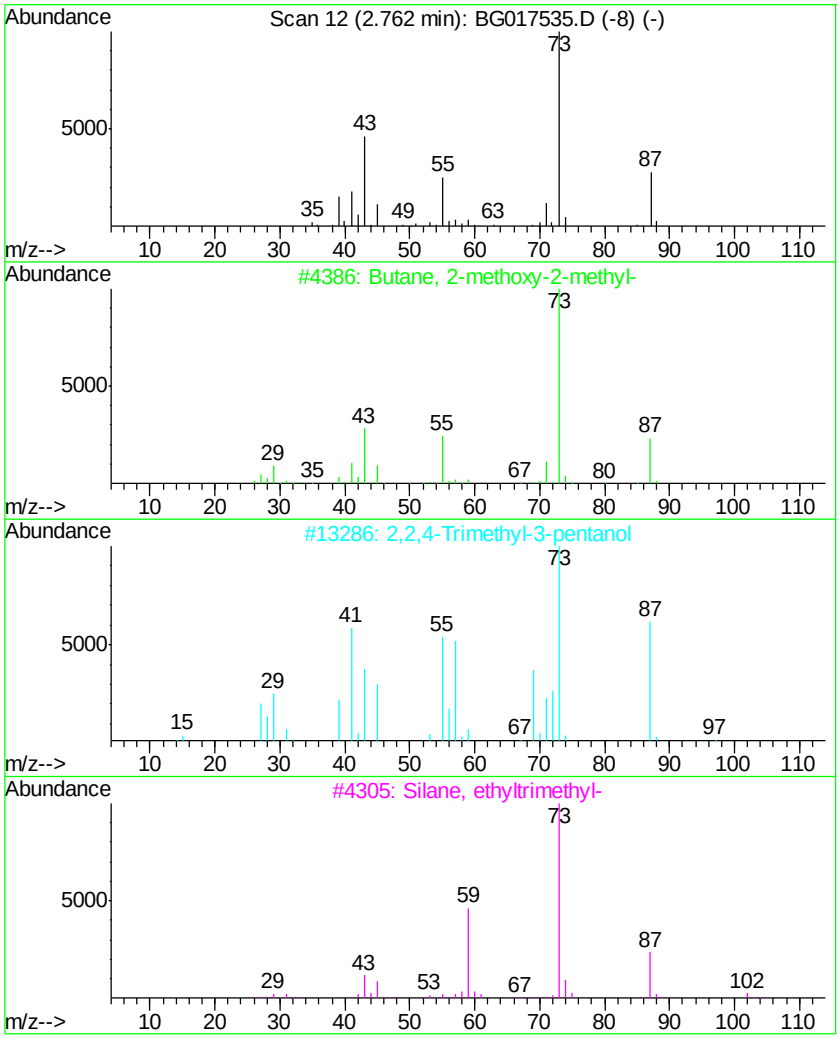
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

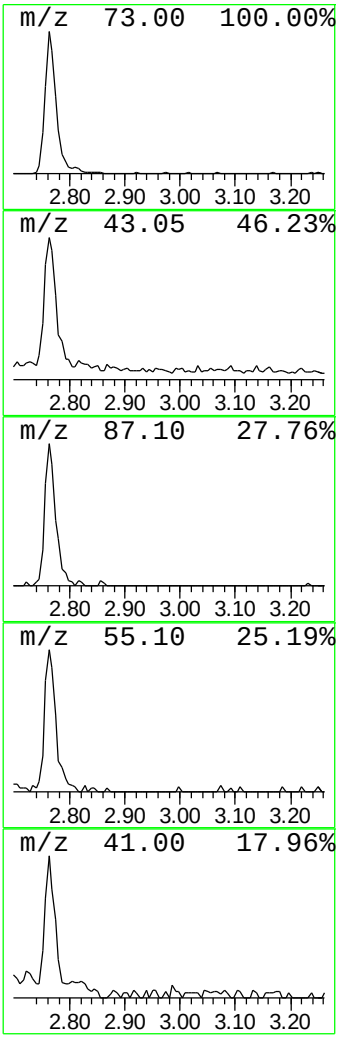
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.76	12.92 ng	99196	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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

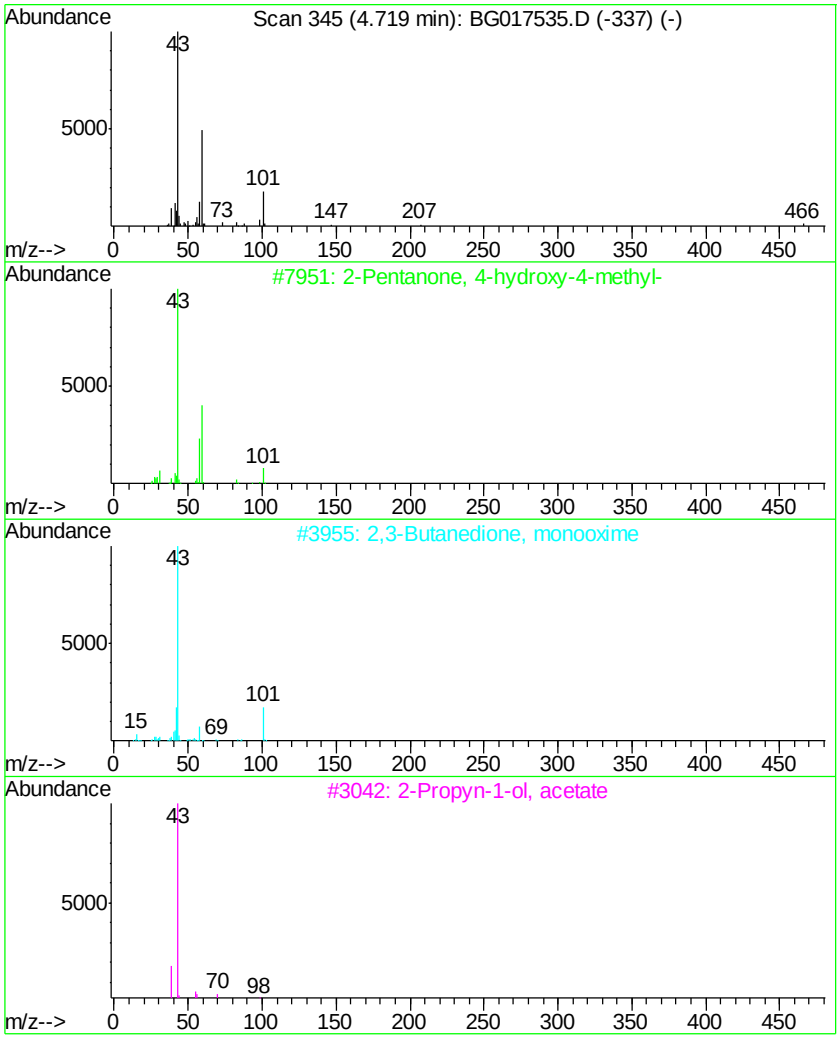
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

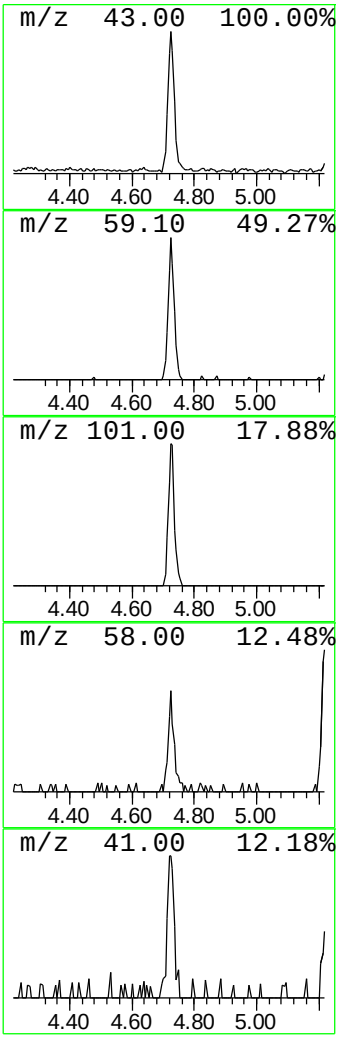
****

Peak Number 2 unknown4.72 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	8.62 ng	66176	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	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Butanamide	87	C4H9NO	000541-35-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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

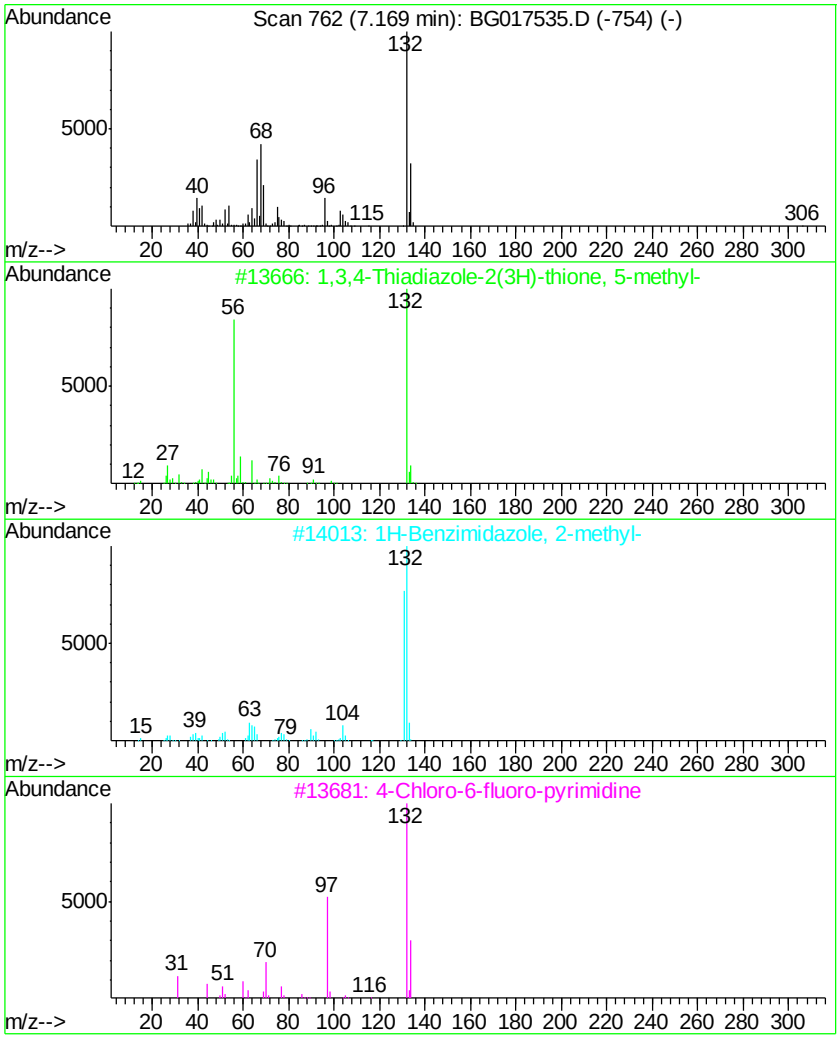
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

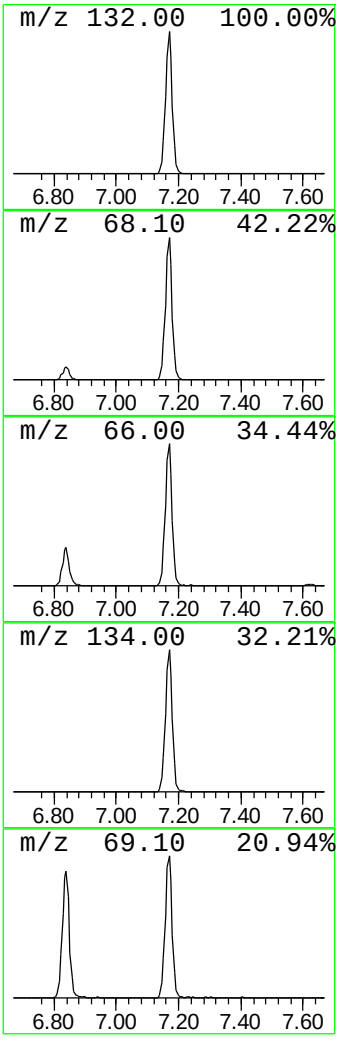
****

Peak Number 3 unknown7.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	124.09 ng	952574	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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

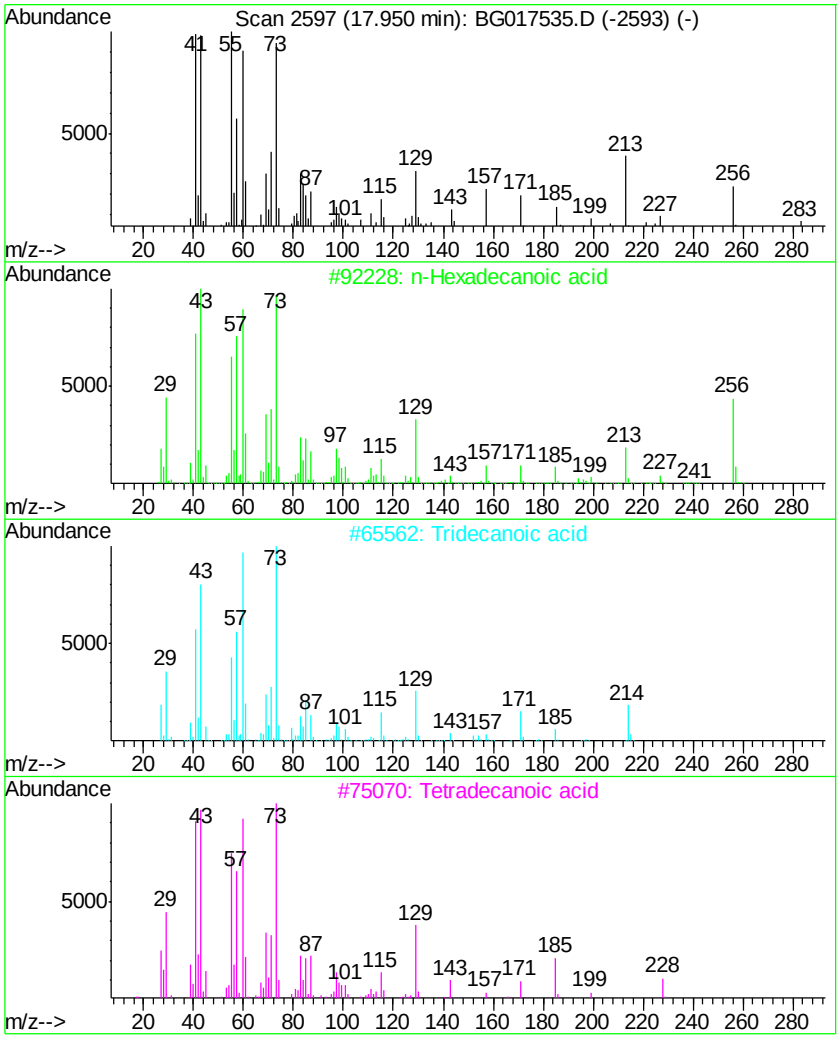
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

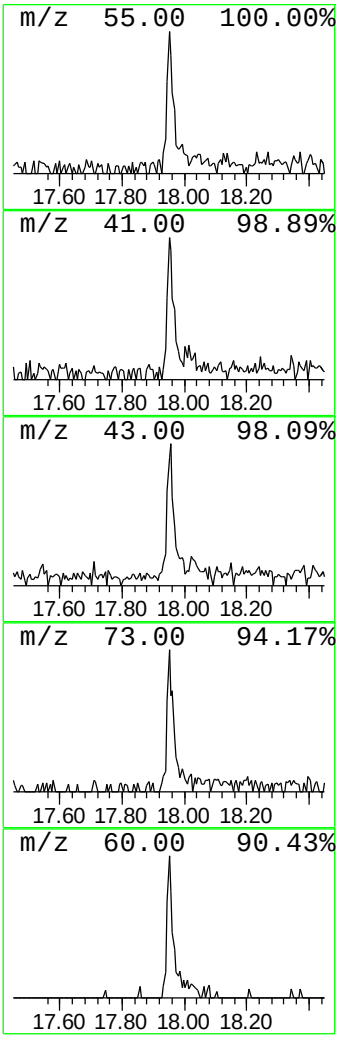
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	5.05 ng	72236	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	49
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	n-Decanoic acid	172	C10H20O2	000334-48-5	45





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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

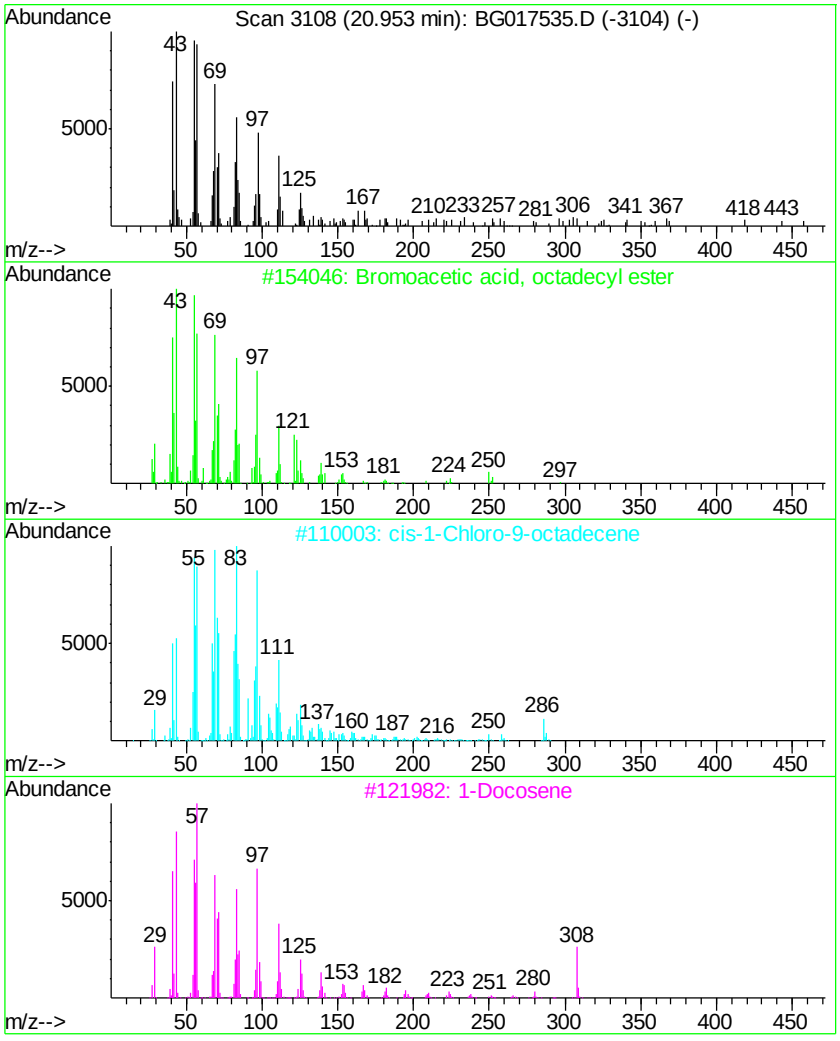
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

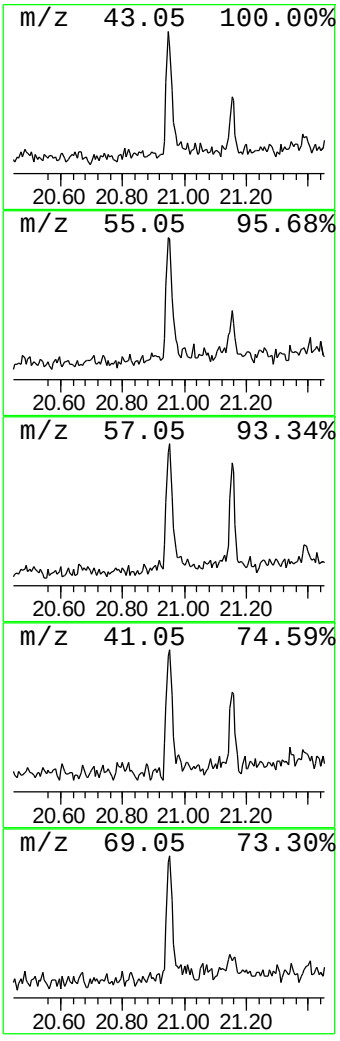
****

Peak Number 6 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	5.54 ng	89608	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
2	cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	89
3	1-Docosene	308	C22H44	001599-67-3	83
4	1-Eicosanol	298	C20H42O	000629-96-9	81
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	81





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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

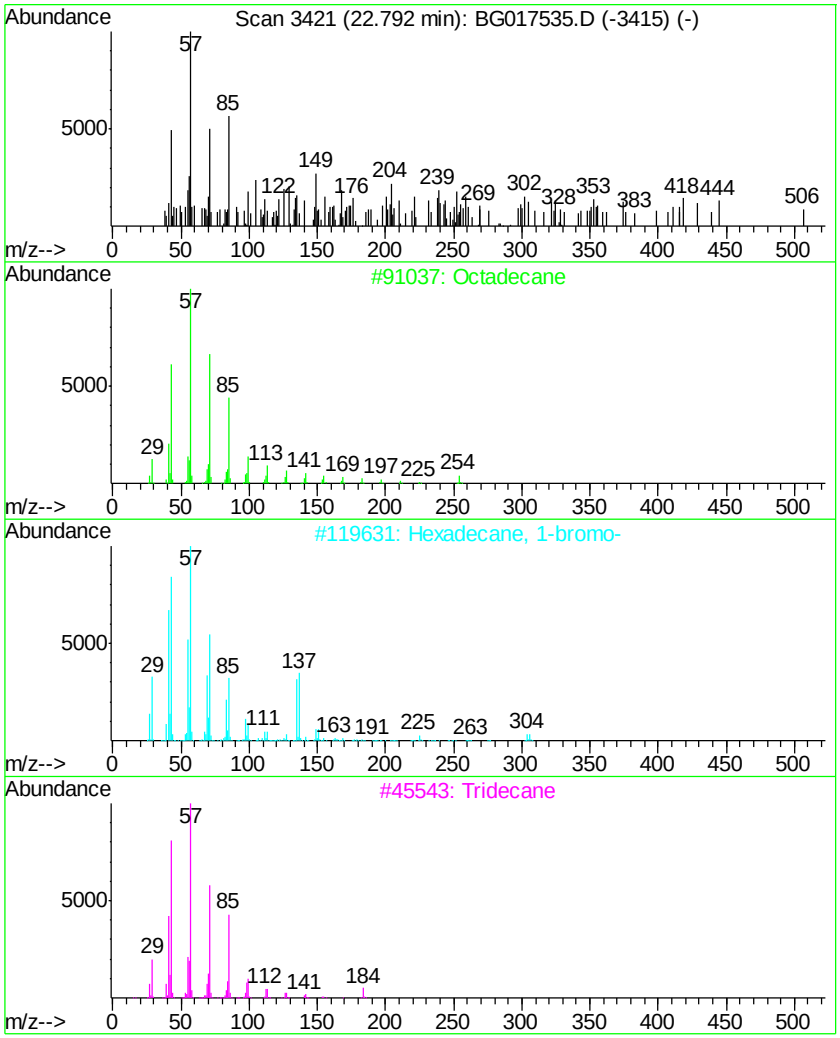
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

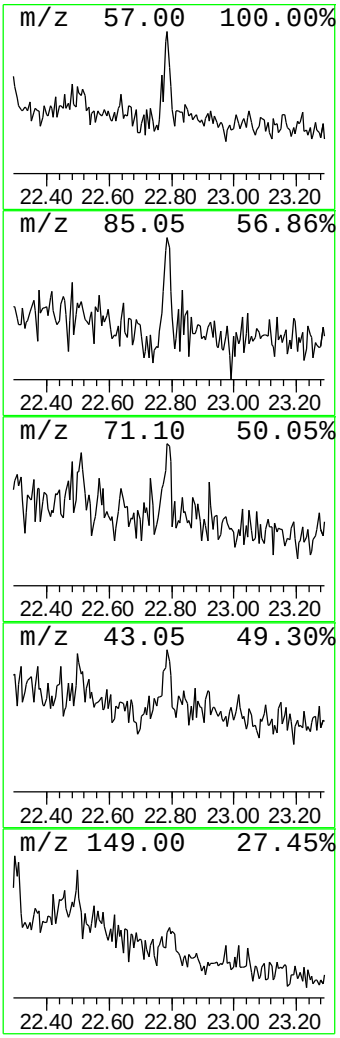
****

Peak Number 7 unknown22.79 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.79	2.90 ng	44804	Perylene-d12	23.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	41
2	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	41
3	Tridecane	184	C13H28	000629-50-5	38
4	Propanoic acid, 2,2-dimethyl-, c...	150	C6H11ClO2	018997-19-8	38
5	Pentadecane	212	C15H32	000629-62-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060615\
Data File : BG017535.D
Acq On : 7 Jun 2015 15:09
Operator : TP/IZ
Sample : G2507-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PIER2-1(0-2)

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	12.9	ng	99196	1	7.62	153525	20.0
unknown4.72	4.72	8.6	ng	66176	1	7.62	153525	20.0
unknown7.17	7.17	124.1	ng	952574	1	7.62	153525	20.0
n-Hexadecanoic acid	17.95	5.0	ng	72236	4	17.05	285942	20.0
Bromoacetic acid,...	20.95	5.5	ng	89608	5	21.24	323644	20.0
unknown22.79	22.79	2.9	ng	44804	6	23.48	309346	20.0