LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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	2.737	5	8	14	rVB	24829	36666	5.04%	0.721%
2	2.790	14	17	23	rVB4	6121	8389	1.15%	0.165%
3	4.706	338	343	350	rBV	17722	28734	3.95%	0.565%
4	5.199	422	427	438	rBB	186697	275168	37.85%	5.410%
5	6.821	696	703	714	rBV	191712	315078	43.34%	6.195%
6	7.150	753	759	769	rVB	200895	311949	42.91%	6.133%
7	7.608	831	837	844	rVB	80932	120776	16.61%	2.375%
8	7.925	885	891	899	rVB	145537	223464	30.74%	4.394%
9	8.771	1027	1035	1042	rBV	111377	194872	26.81%	3.831%
10	10.405	1306	1313	1325	rBV	99340	177465	24.41%	3.489%
11	12.896	1731	1737	1748	rVB	298195	428659	58.97%	8.428%
12	13.748	1876	1882	1891	rBV2	38806	61822	8.50%	1.216%
13	14.283	1967	1973	1982	rBV2	170329	249782	34.36%	4.911%
14	14.829	2062	2066	2072	rVB4	4837	7901	1.09%	0.155%
15	15.334	2148	2152	2159	rVB5	6358	9135	1.26%	0.180%
16	15.781	2220	2228	2236	rBV	275894	417770	57.47%	8.214%
17	17.038	2437	2442	2446	rBV2	217569	310580	42.72%	6.106%
18	17.073	2446	2448	2453	rVB	32032	42567	5.86%	0.837%
19	17.173	2461	2465	2469	rVB4	13937	20241	2.78%	0.398%
20	17.855	2577	2581	2583	rBV4	5029	7941	1.09%	0.156%
21	17.943	2593	2596	2605	rVV8	31498	61012	8.39%	1.200%
22	18.113	2621	2625	2629	rVB6	10705	16366	2.25%	0.322%
23	19.106	2789	2794	2798	rBV	55071	71417	9.82%	1.404%
24	19.236	2812	2816	2823	rVB9	16032	27383	3.77%	0.538%
25	19.435	2848	2850	2851	rBV2	8875	8172	1.12%	0.161%
26	19.465	2851	2855	2864	rVB	67092	108794	14.97%	2.139%
27	19.676	2886	2891	2895	rBV	616887	726963	100.00%	14.293%
28	19.717	2895	2898	2901	rVB5	6793	8161	1.12%	0.160%
29	19.964	2938	2940	2945	rVB6	13192	16153	2.22%	0.318%
30	20.481	3026	3028	3032	rVB5	12996	15316	2.11%	0.301%
31	20.945	3105	3107	3115	rVB7	29575	41522	5.71%	0.816%
32	21.151	3140	3142	3144	rVB3	26678	17035	2.34%	0.335%
33	21.233	3150	3156	3160	rBV	296700	403659	55.53%	7.936%
34	23.472	3531	3537	3542	rBV	181676	315225	43.36%	6.198%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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

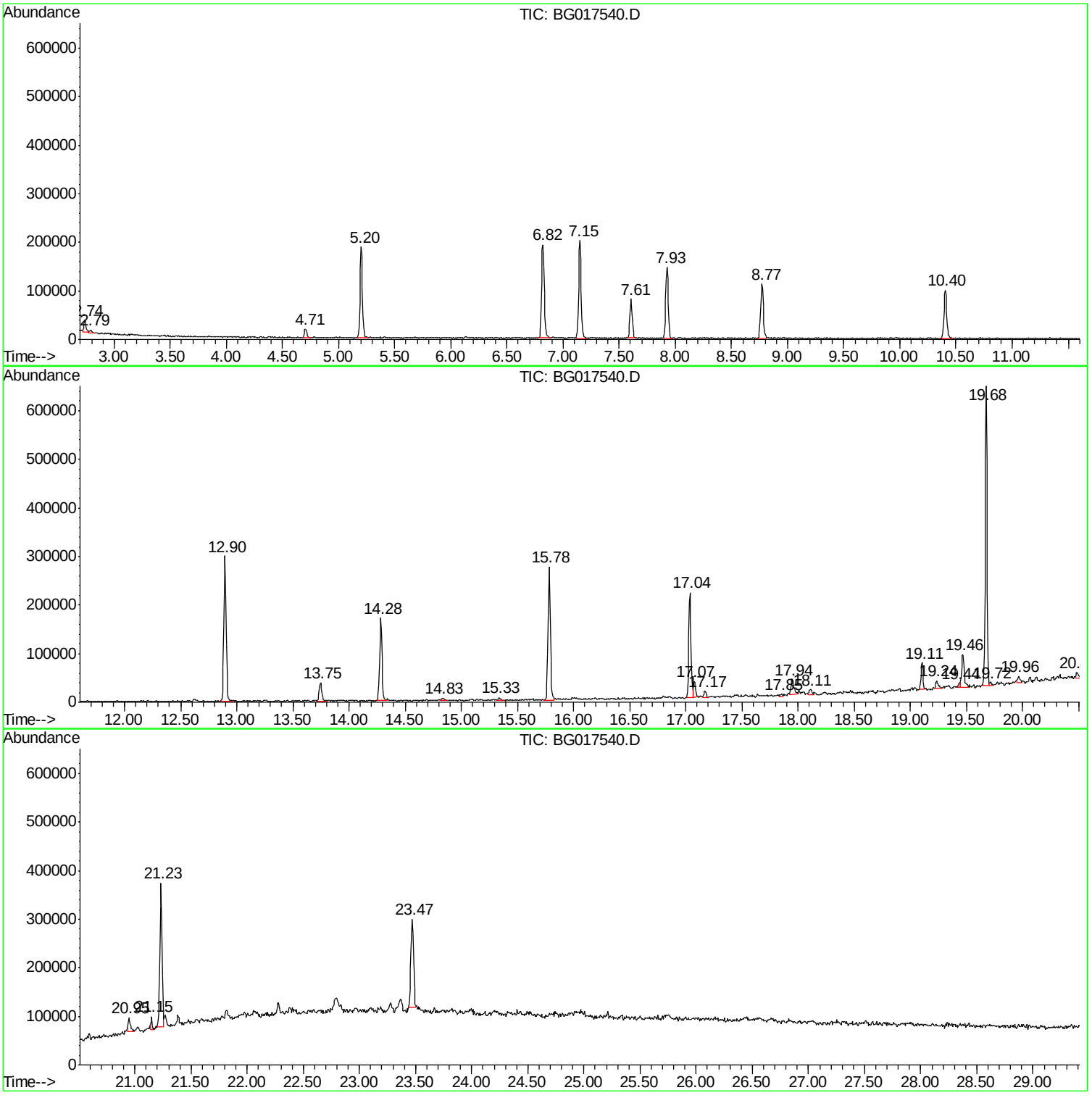
Sum of corrected areas: 5086137

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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

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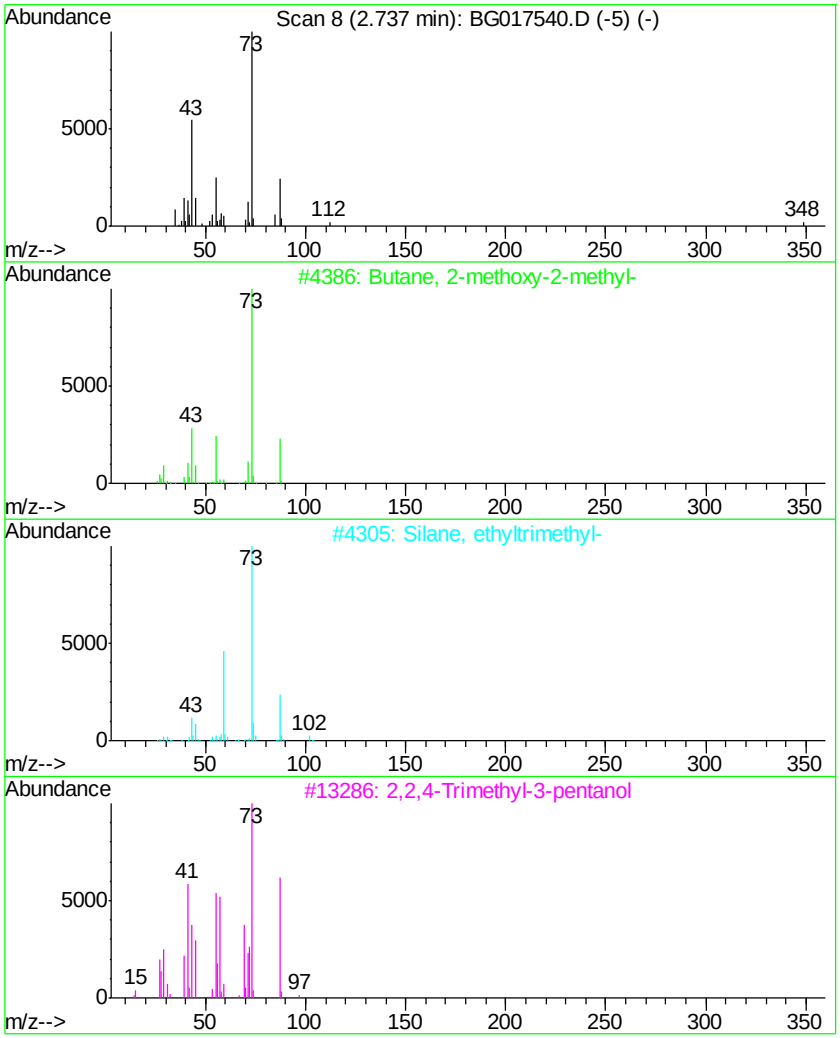
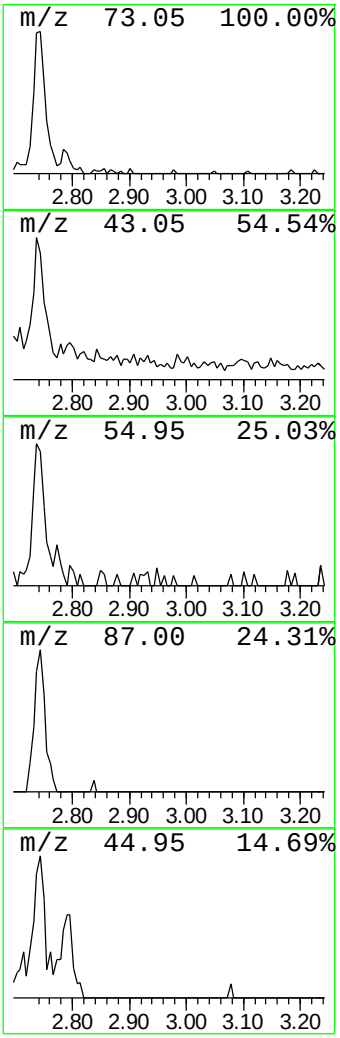
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.74	6.07 ng	36666	1,4-Dichlorobenzene-d4	7.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
4	Methyl 2-acetamidoacrylate	143	C6H9NO3	035356-70-8	23
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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

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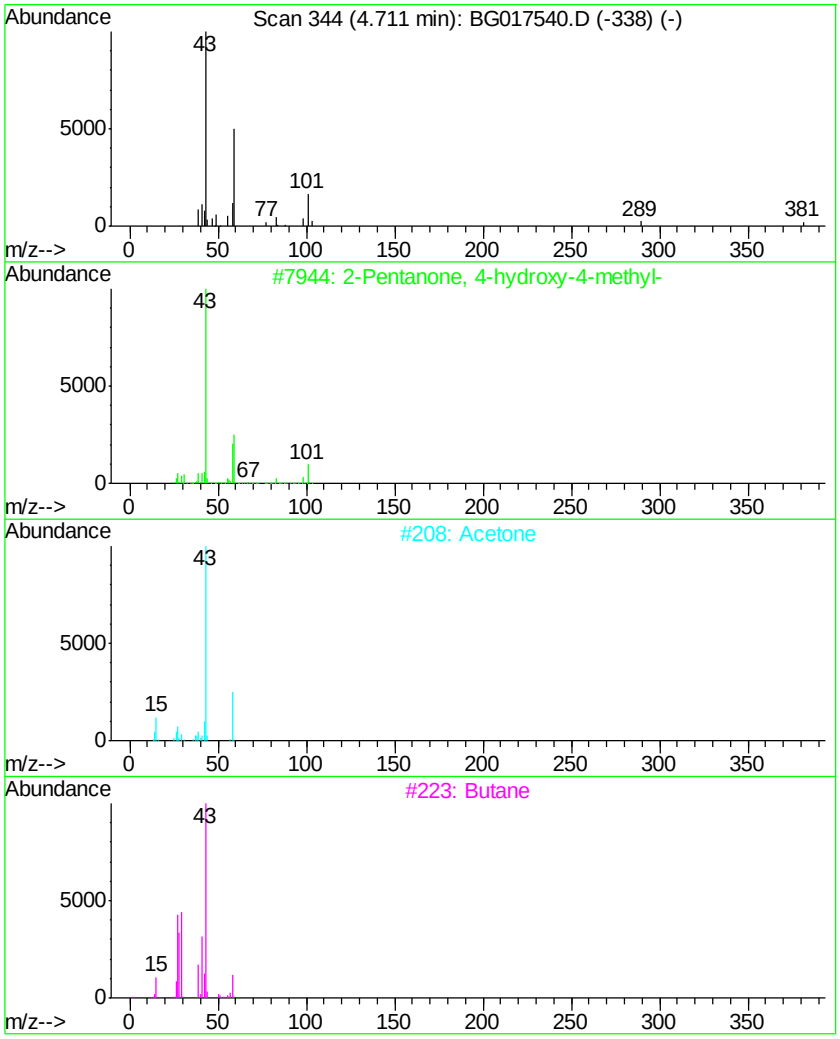
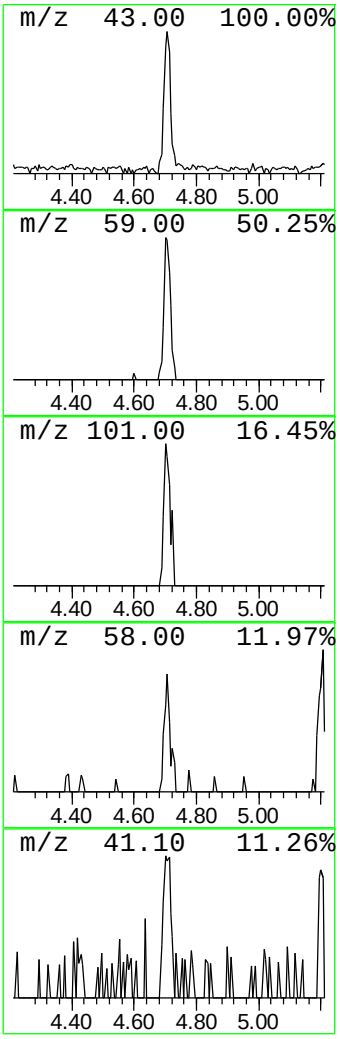
Peak Number 2 unknown4.71 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	4.76 ng	28734	1,4-Dichlorobenzene-d4	7.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetone	58	C3H6O	000067-64-1	12
3	Butane	58	C4H10	000106-97-8	9
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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

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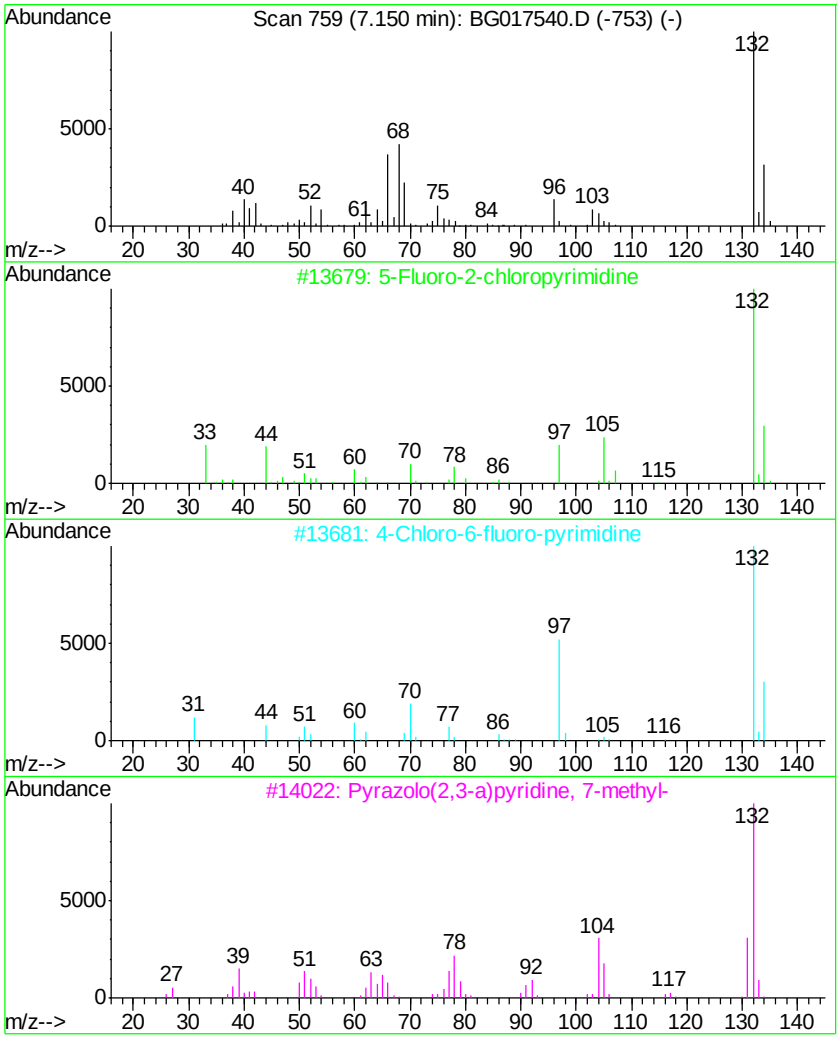
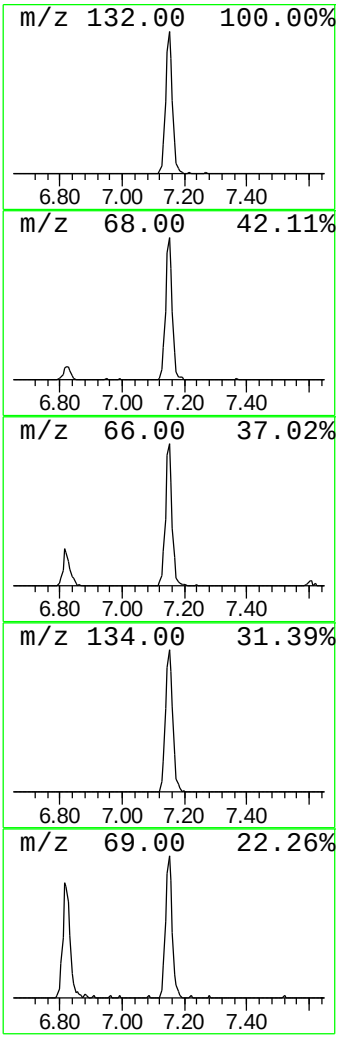
Peak Number 3 unknown7.15 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.15	51.66 ng	311949	1,4-Dichlorobenzene-d4	7.61

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	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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

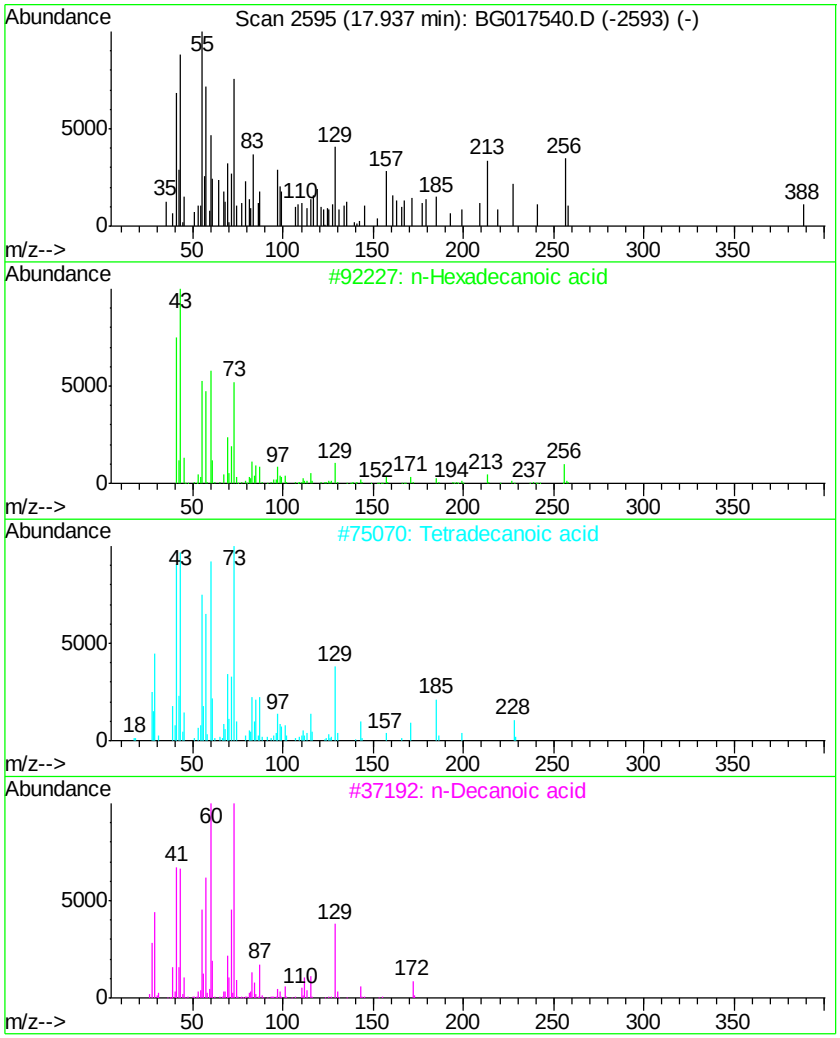
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

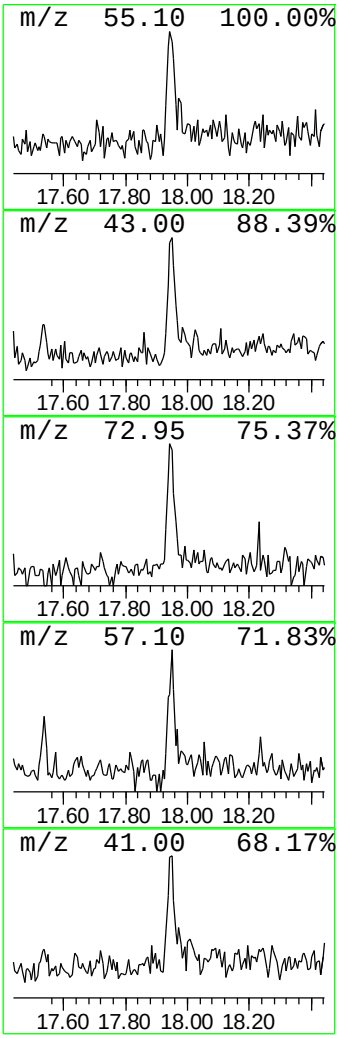
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	3.93 ng	61012	Phenanthrene-d10	17.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	n-Decanoic acid	172	C10H20O2	000334-48-5	43
4	Tridecanoic acid	214	C13H26O2	000638-53-9	27
5	Nonanoic acid	158	C9H18O2	000112-05-0	27





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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

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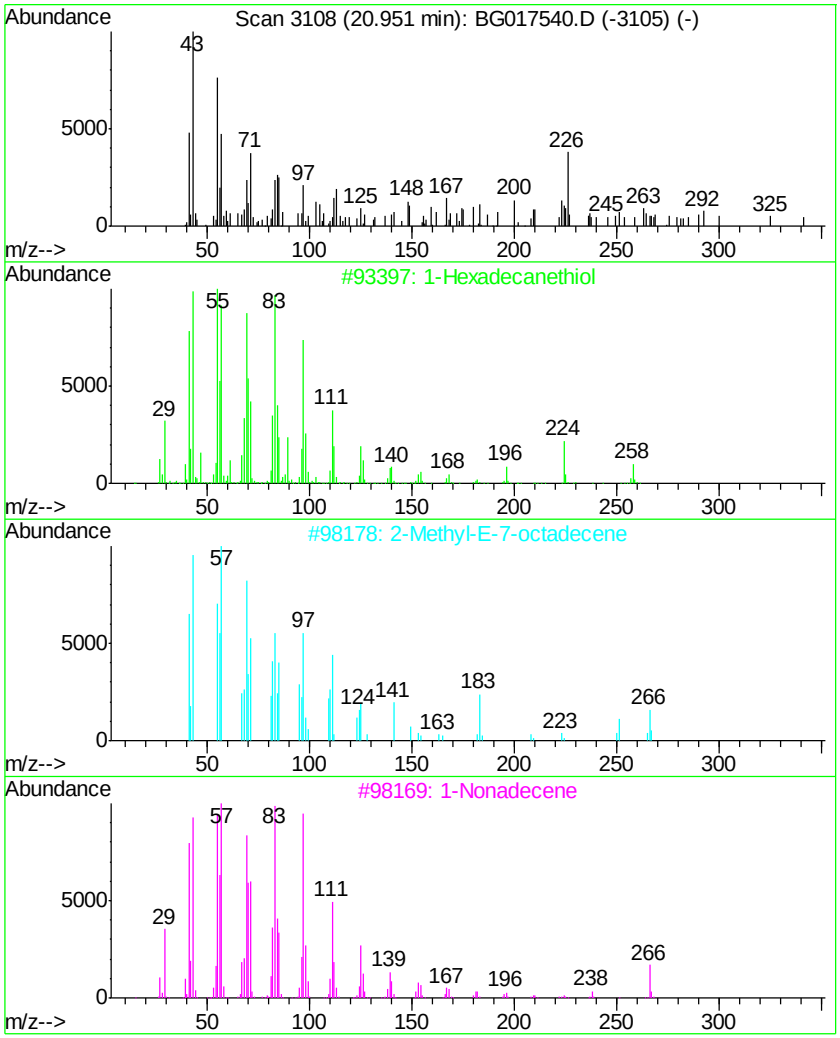
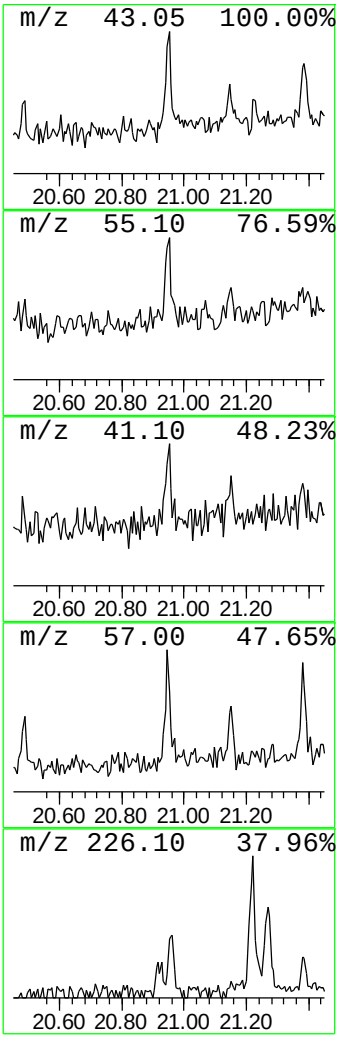
Peak Number 6 1-Hexadecanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	2.06 ng	41522	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanethiol	258	C16H34S	002917-26-2	52
2	2-Methyl-E-7-octadecene	266	C19H38	1000130-92-3	40
3	1-Nonadecene	266	C19H38	018435-45-5	38
4	Cyclopentane, 1-(2-decyldodecyl)...	406	C29H58	055429-26-0	37
5	Heneicosane, 11-cyclopentyl-	364	C26H52	006703-81-7	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060815\
Data File : BG017540.D
Acq On : 8 Jun 2015 13:24
Operator : TP/IZ
Sample : G2464-05 2X
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11D

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...	2.74	6.1	ng	36666	1	7.61	120776	20.0
unknown4.71	4.71	4.8	ng	28734	1	7.61	120776	20.0
unknown7.15	7.15	51.7	ng	311949	1	7.61	120776	20.0
n-Hexadecanoic acid	17.94	3.9	ng	61012	4	17.04	310580	20.0
1-Hexadecanethiol	20.95	2.1	ng	41522	5	21.23	403659	20.0