LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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	5.120	409	414	424	rBV	174165	250699	9.14%	2.187%
2	6.137	580	587	593	rVB2	19090	28424	1.04%	0.248%
3	6.742	685	690	701	rVB3	92880	168902	6.16%	1.473%
4	7.071	737	746	756	rBV	396102	619525	22.59%	5.404%
5	7.529	818	824	830	rVB	119122	180497	6.58%	1.574%
6	7.846	870	878	887	rVB	427266	639842	23.33%	5.581%
7	8.692	1015	1022	1031	rBV	369648	597627	21.79%	5.213%
8	9.409	1138	1144	1150	rBV3	62827	112156	4.09%	0.978%
9	10.320	1294	1299	1305	rBV	146120	240122	8.75%	2.095%
10	12.318	1633	1639	1644	rVB9	17705	34808	1.27%	0.304%
11	12.776	1711	1717	1719	rBV2	42868	63349	2.31%	0.553%
12	12.817	1719	1724	1736	rVB	984679	1457334	53.13%	12.712%
13	13.669	1866	1869	1876	rVB2	21605	32542	1.19%	0.284%
14	14.204	1953	1960	1967	rBV2	253869	392460	14.31%	3.423%
15	14.662	2033	2038	2046	rBV4	45743	74479	2.72%	0.650%
16	15.708	2210	2216	2224	rBV	921196	1256009	45.79%	10.956%
17	16.959	2424	2429	2436	rBV	352625	493583	18.00%	4.305%
18	17.882	2580	2586	2591	rBV	249470	369338	13.47%	3.222%
19	19.016	2776	2779	2782	rBV5	17938	27640	1.01%	0.241%
20	19.168	2800	2805	2810	rBV	188216	276998	10.10%	2.416%
21	19.603	2873	2879	2884	rBV	2394536	2742857	100.00%	23.926%
22	20.878	3092	3096	3102	rVB2	96517	119616	4.36%	1.043%
23	21.078	3128	3130	3137	rVB8	20455	28060	1.02%	0.245%
24	21.160	3139	3144	3149	rBV	457918	581677	21.21%	5.074%
25	22.312	3336	3340	3343	rBV4	30154	41415	1.51%	0.361%
26	23.358	3511	3518	3525	rBV	282177	546996	19.94%	4.771%
27	24.597	3724	3729	3733	rBV8	44513	87191	3.18%	0.761%

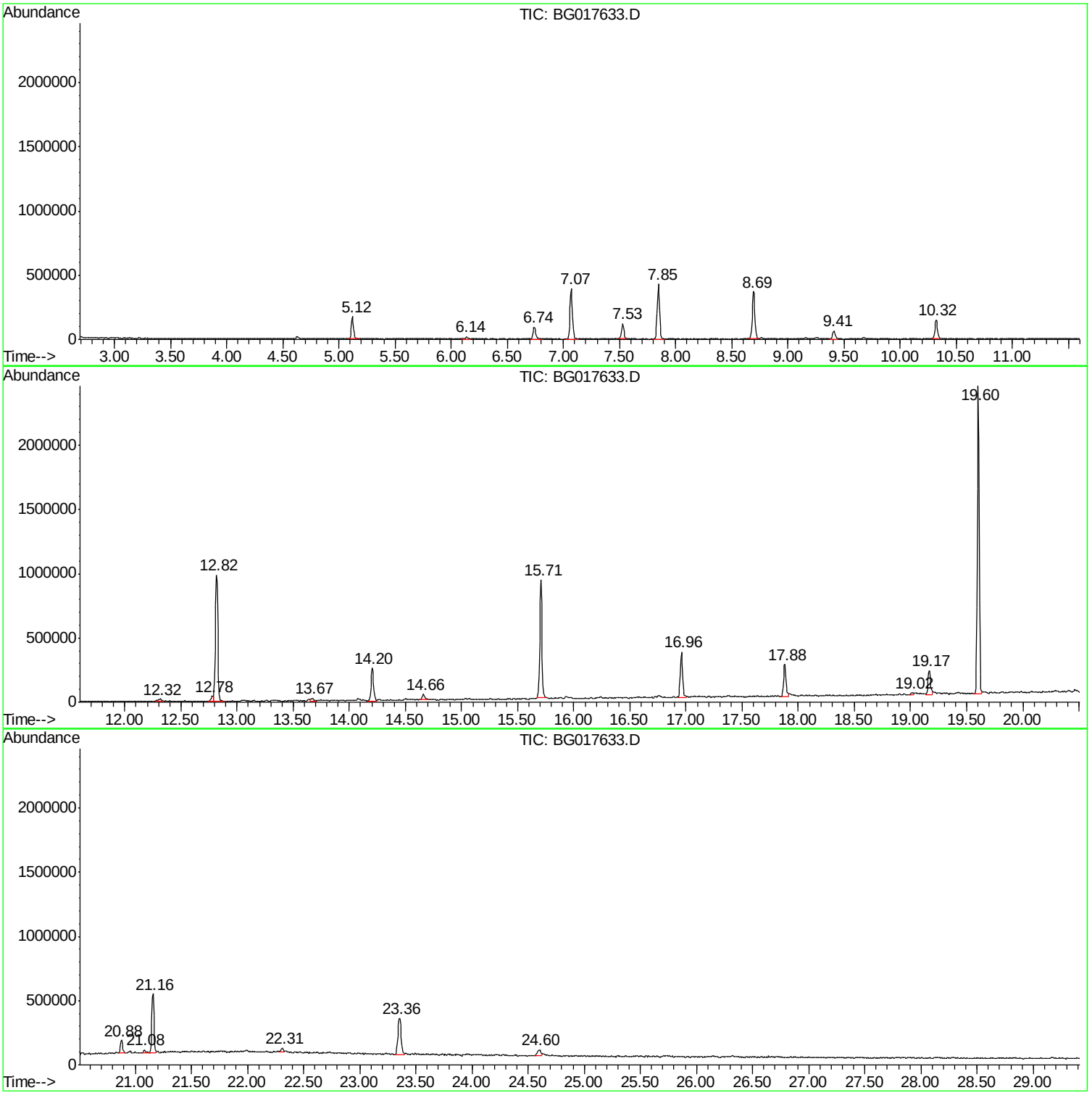
Sum of corrected areas: 11464146

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-5-6-3-15

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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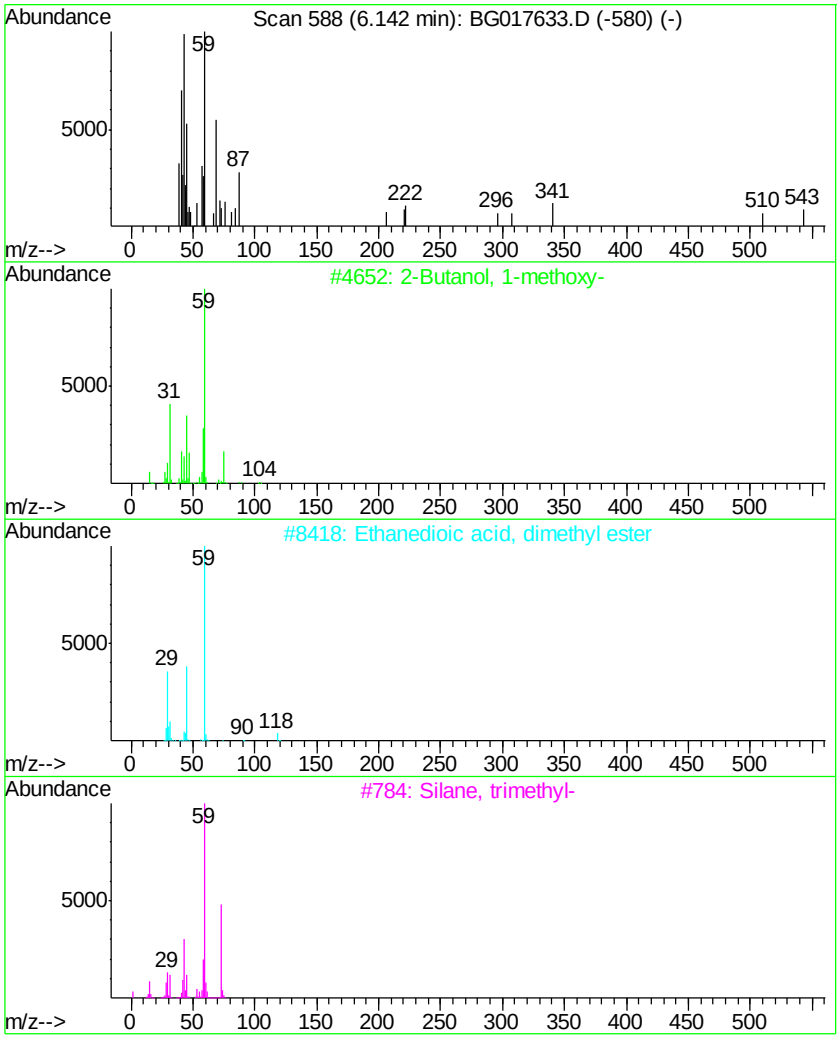
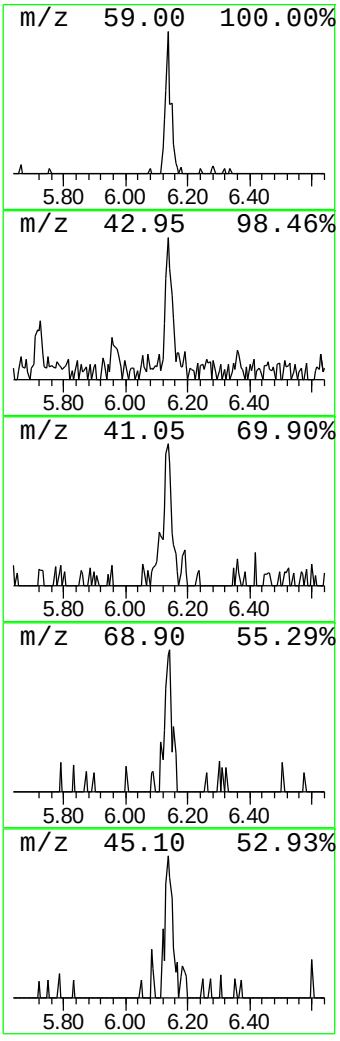
Peak Number 1 unknown6.14 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	3.15 ng	28424	1,4-Dichlorobenzene-d4	7.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	33
2	Ethanedioic acid, dimethyl ester	118	C4H6O4	000553-90-2	32
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	28
4	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	9
5	2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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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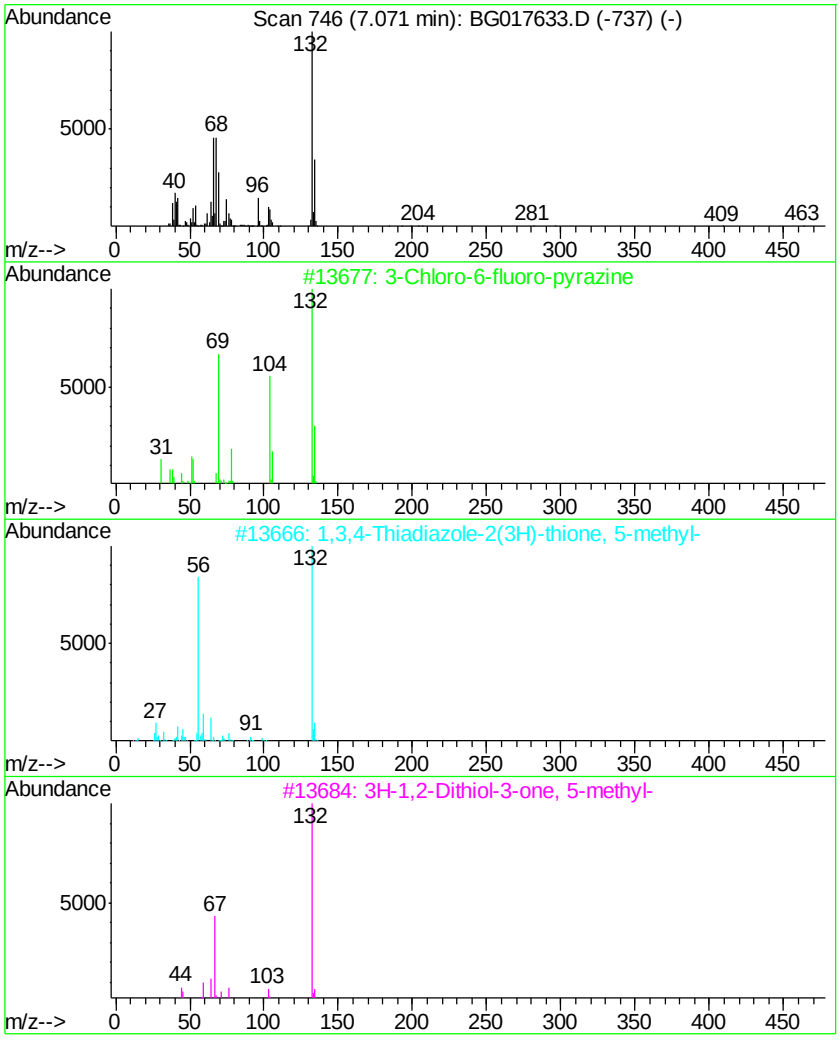
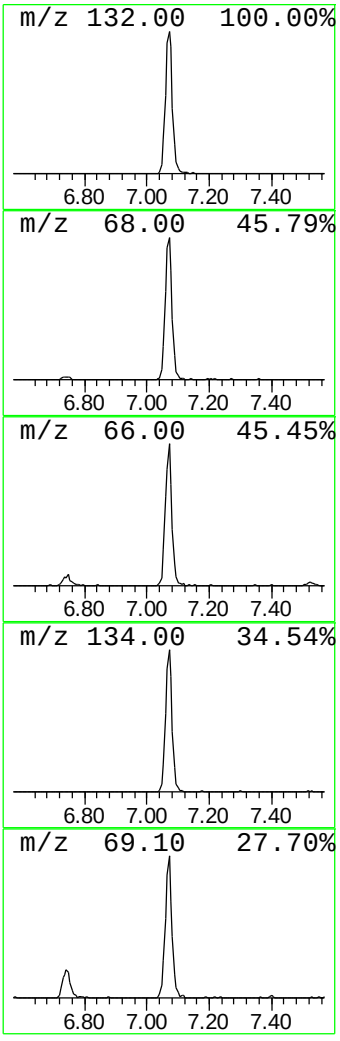
Peak Number 2 unknown7.07 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	68.65 ng	619525	1,4-Dichlorobenzene-d4	7.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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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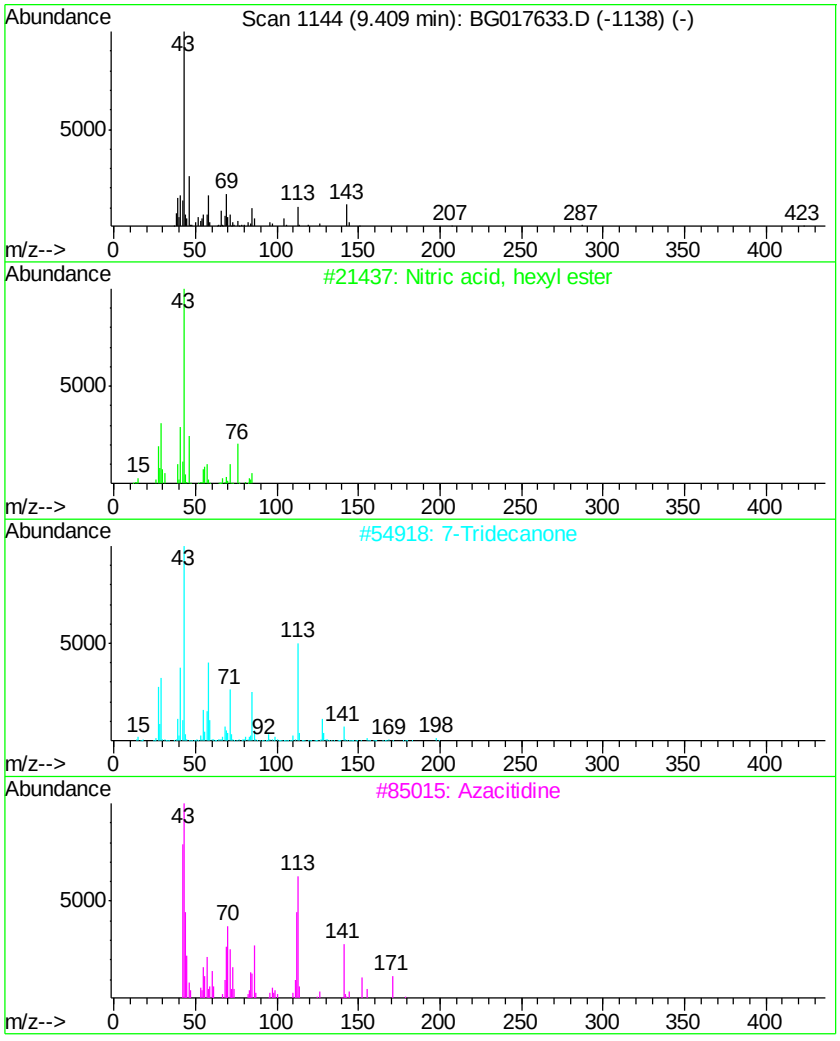
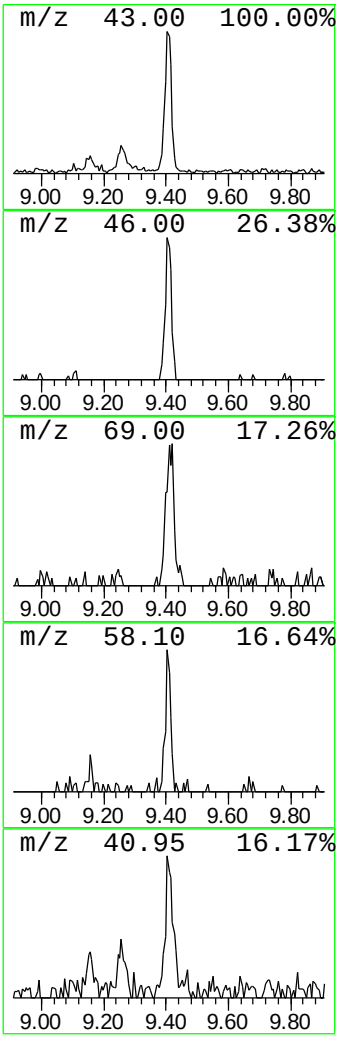
Peak Number 4 unknown9.41 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	9.34 ng	112156	Naphthalene-d8	10.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nitric acid, hexyl ester	147	C6H13NO3	020633-11-8	12
2	7-Tridecanone	198	C13H26O	000462-18-0	10
3	Azacitidine	244	C8H12N4O5	000320-67-2	10
4	2-Hexane isothiocyanate	143	C7H13NS	005334-87-2	9
5	2-(Dimethylamino)-3-methyl-1-butene	113	C7H15N	007694-48-6	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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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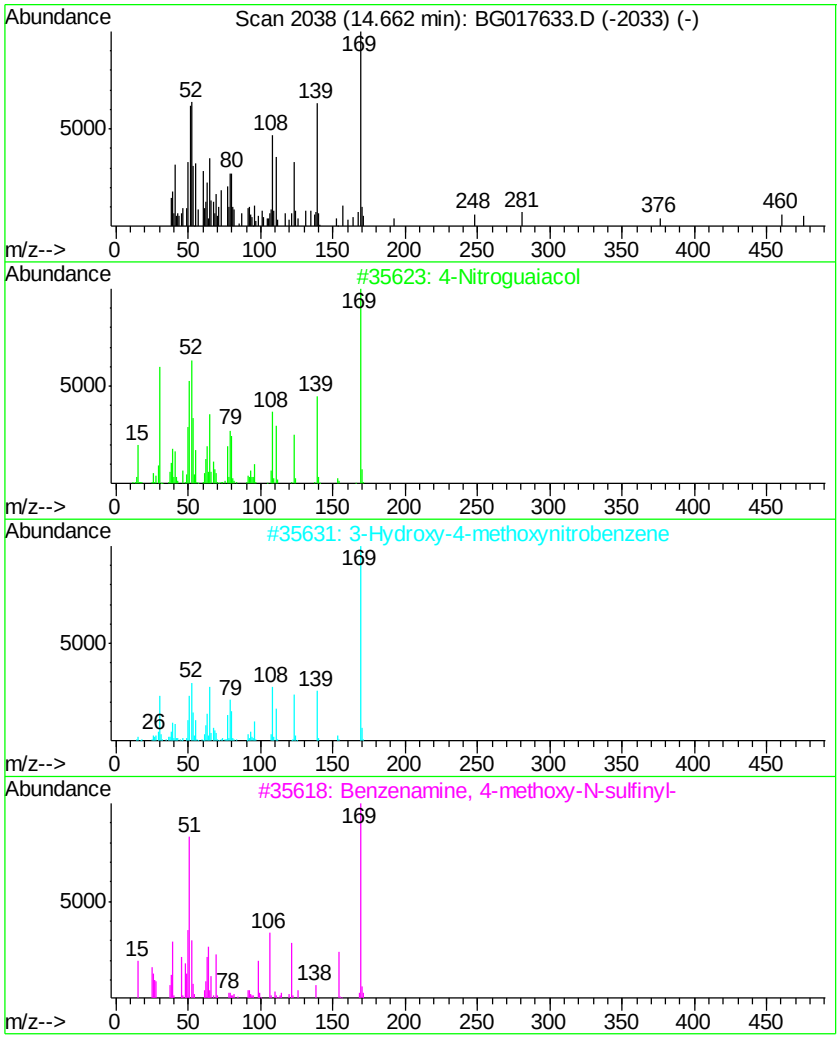
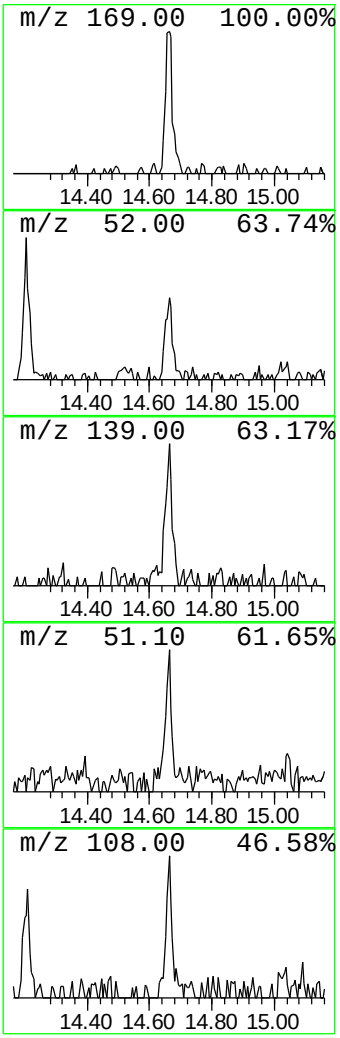
Peak Number 5 4-Nitroguaiacol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.80 ng	74479	Acenaphthene-d10	14.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nitroguaiacol	169	C7H7NO4	003251-56-7	99
2	3-Hydroxy-4-methoxynitrobenzene	169	C7H7NO4	000636-93-1	46
3	Benzenamine, 4-methoxy-N-sulfinyl-	169	C7H7NO2S	013165-69-0	45
4	2-Methoxy-3,5-dinitropyridine	199	C6H5N3O5	018617-40-8	43
5	Benzothiazole, 2-chloro-	169	C7H4ClNS	000615-20-3	30





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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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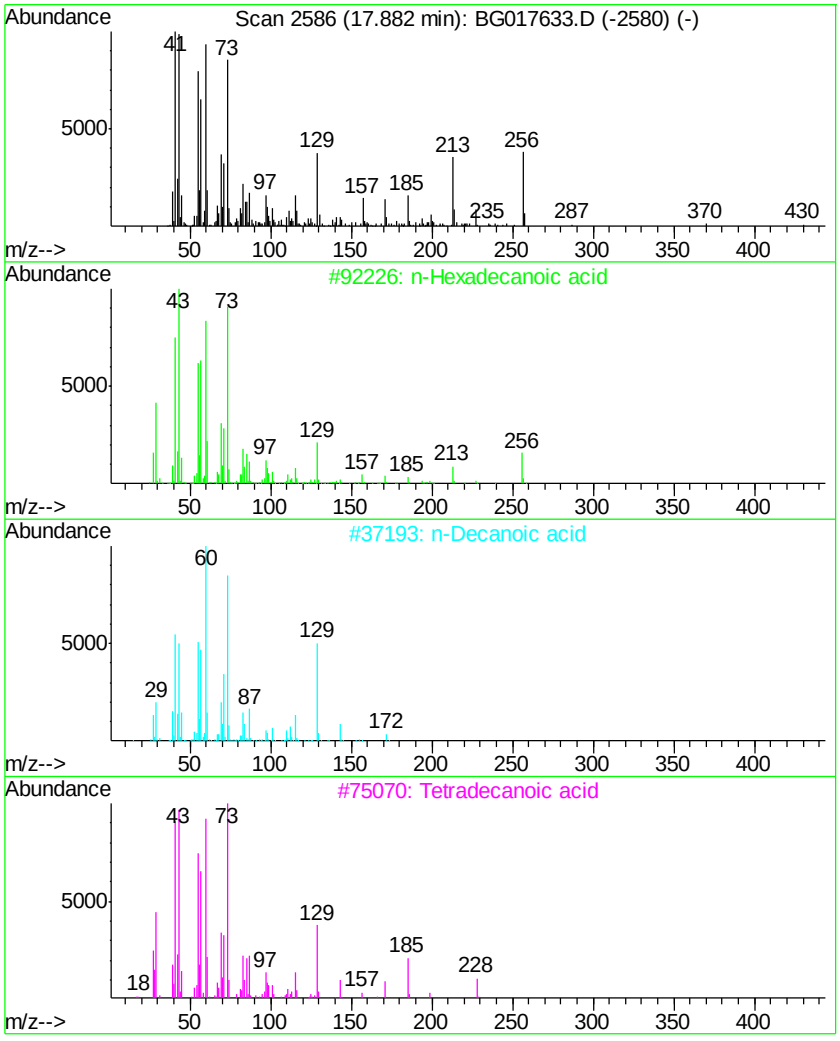
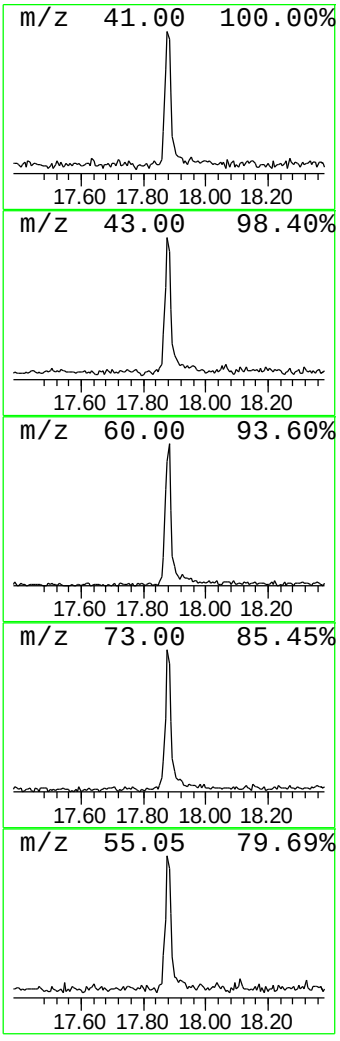
Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	14.97 ng	369338	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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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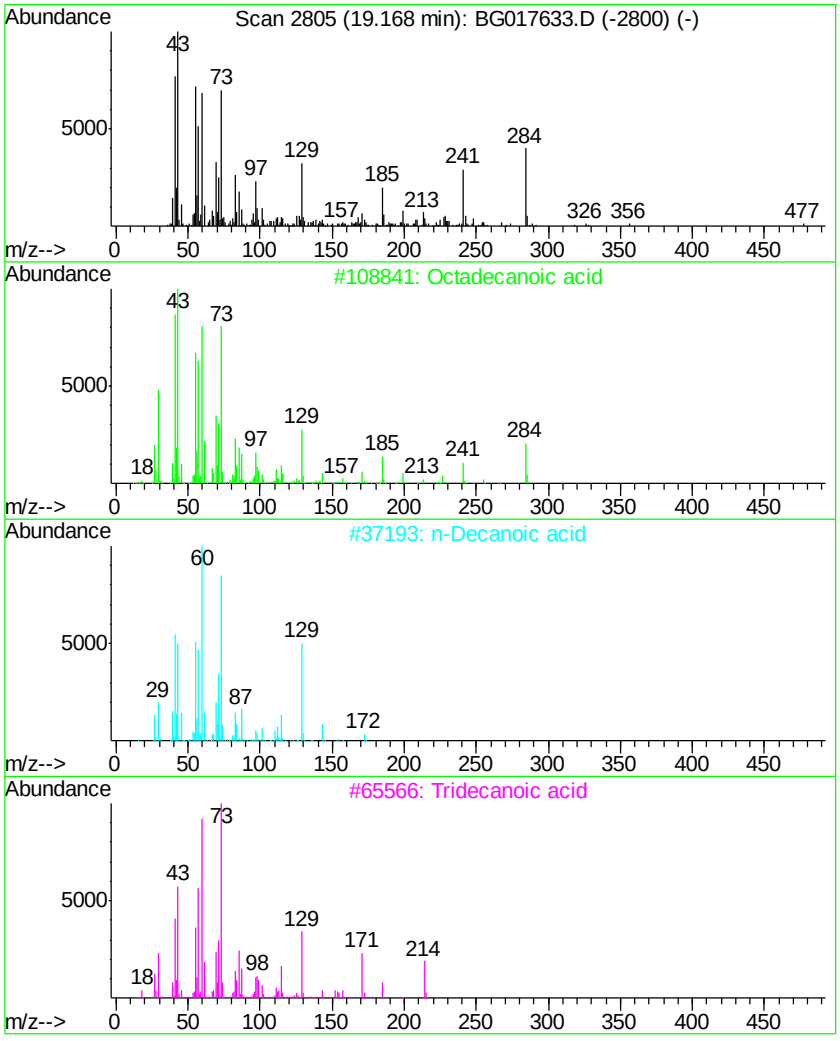
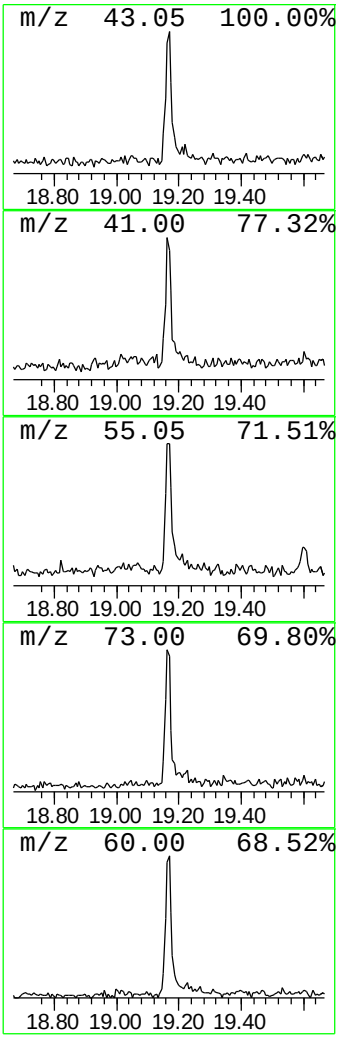
Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.17	9.52 ng	276998	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	76
2	n-Decanoic acid	172	C10H20O2	000334-48-5	38
3	Tridecanoic acid	214	C13H26O2	000638-53-9	30
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	27
5	Undecanoic acid	186	C11H22O2	000112-37-8	22





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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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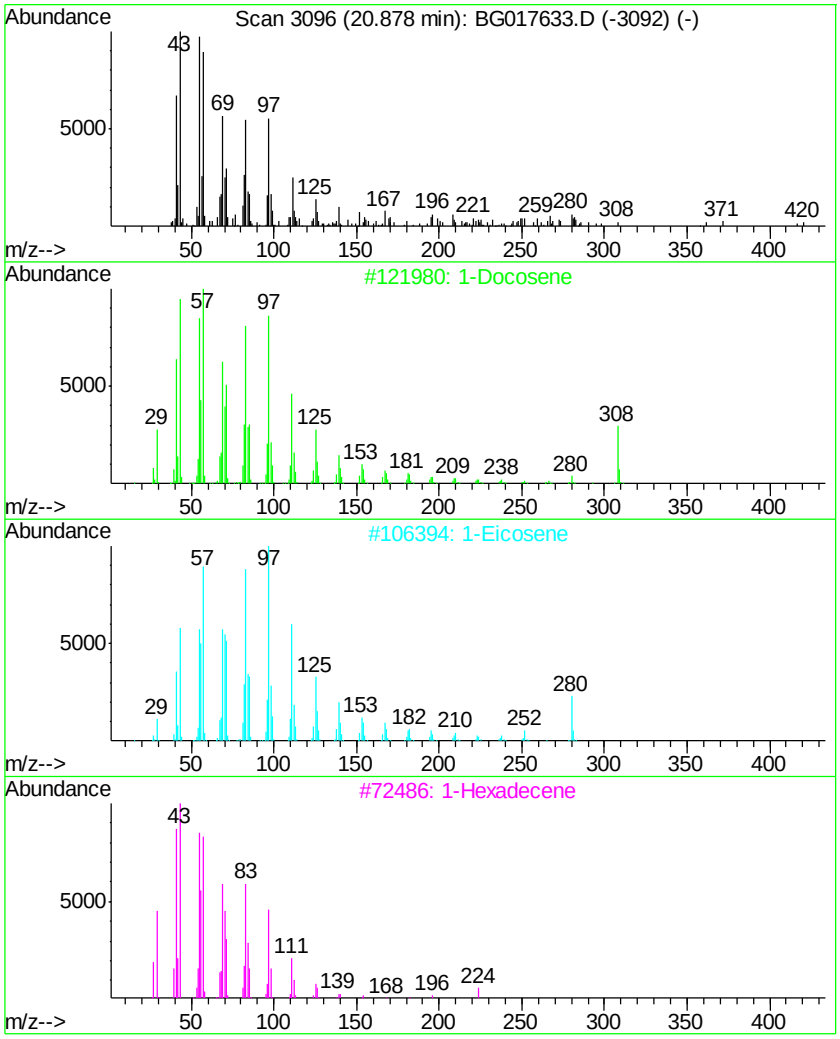
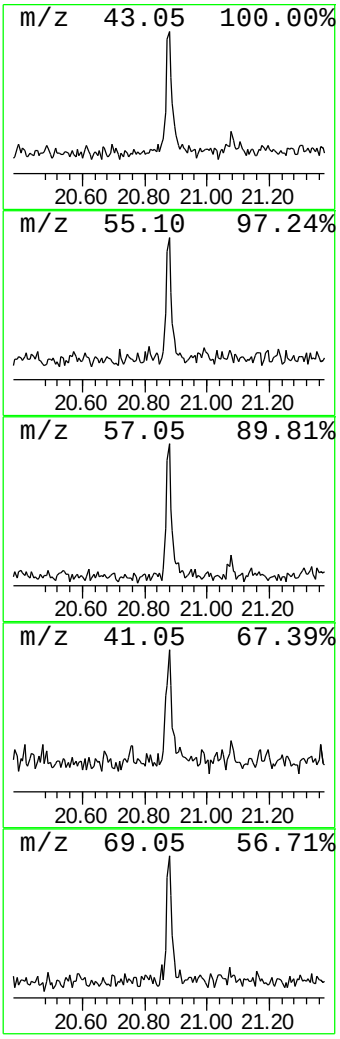
Peak Number 8 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.88	4.11 ng	119616	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	1-Eicosene	280	C20H40	003452-07-1	91
3	1-Hexadecene	224	C16H32	000629-73-2	89
4	Cyclotetradecane	196	C14H28	000295-17-0	83
5	1-Octadecanethiol	286	C18H38S	002885-00-9	83





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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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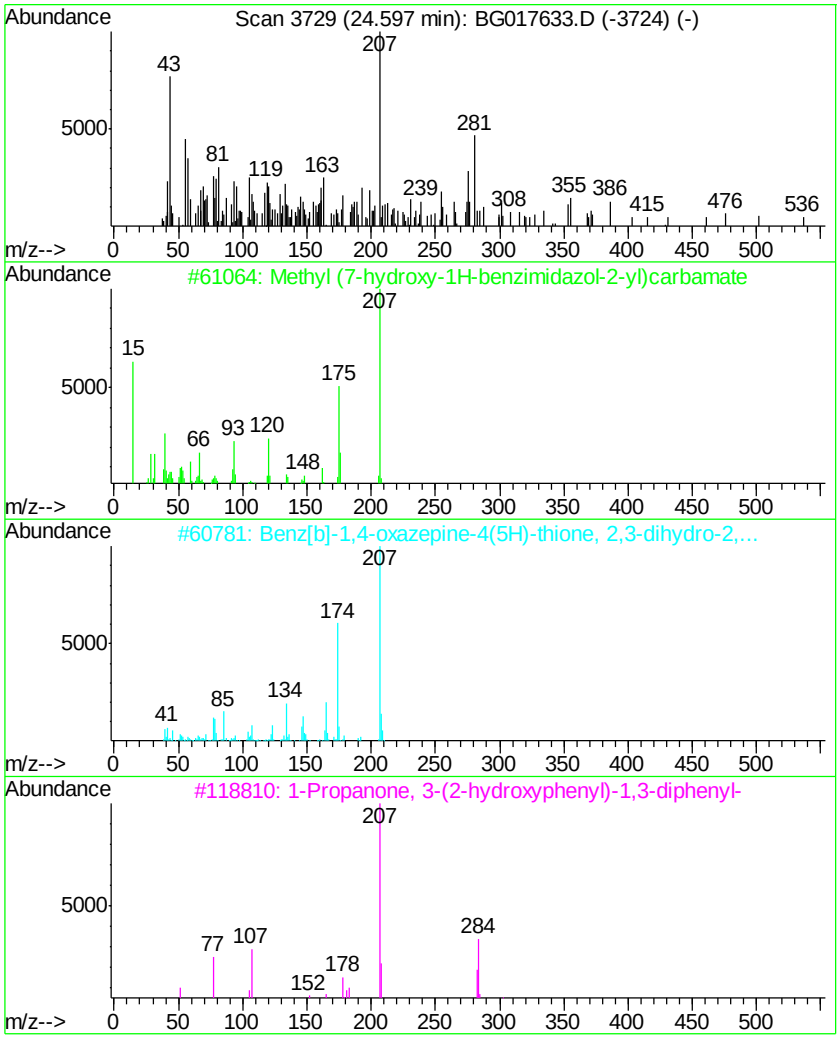
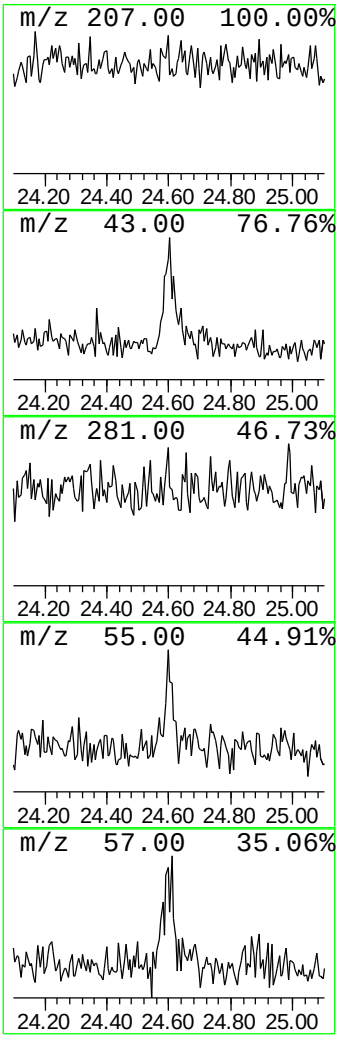
Peak Number 9 unknown24.60 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.60	3.19 ng	87191	Perylene-d12	23.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl (7-hydroxy-1H-benzimidazo...	207	C9H9N3O3	041261-35-2	41
2	Benz[b]-1,4-oxazepine-4(5H)-thio...	207	C11H13NOS	1000258-63-4	38
3	1-Propanone, 3-(2-hydroxyphenyl)...	302	C21H18O2	004376-83-4	35
4	N-Methyl-1-adamantaneacetamide	207	C13H21NO	031897-93-5	35
5	Benzothiazoline, 3-methyl-2-[(tr...	276	C10H7F3N2S2	118215-08-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017633.D
Acq On : 12 Jun 2015 7:33
Operator : TP/IZ
Sample : G2523-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-5-6-3-15

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
unknown6.14	6.14	3.1	ng	28424	1	7.53	180497	20.0
unknown7.07	7.07	68.7	ng	619525	1	7.53	180497	20.0
unknown9.41	9.41	9.3	ng	112156	2	10.32	240122	20.0
4-Nitroguaiacol	14.66	3.8	ng	74479	3	14.20	392460	20.0
n-Hexadecanoic acid	17.88	15.0	ng	369338	4	16.96	493583	20.0
Octadecanoic acid	19.17	9.5	ng	276998	5	21.16	581677	20.0
1-Docosene	20.88	4.1	ng	119616	5	21.16	581677	20.0
unknown24.60	24.60	3.2	ng	87191	6	23.36	546996	20.0