LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061215\
Data File : BG017658.D
Acq On : 13 Jun 2015 4:54
Operator : TP/IZ
Sample : G2627-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-25

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-BG061215.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	5.110	408	412	419	rBV	202780	297421	9.34%	2.690%
2	6.732	682	688	697	rBV	133657	217169	6.82%	1.964%
3	7.066	738	745	756	rBV	402481	606376	19.04%	5.484%
4	7.525	818	823	831	rVB2	94680	147061	4.62%	1.330%
5	7.842	869	877	884	rBV	375919	563359	17.69%	5.095%
6	8.694	1013	1022	1033	rBV	260352	442303	13.89%	4.000%
7	10.322	1291	1299	1309	rBV	104287	190664	5.99%	1.724%
8	12.819	1717	1724	1735	rBV	839102	1199719	37.67%	10.850%
9	14.205	1954	1960	1968	rVB2	181980	275172	8.64%	2.489%
10	15.709	2209	2216	2229	rBV	914823	1264449	39.71%	11.436%
11	15.862	2236	2242	2248	rBV4	48080	73589	2.31%	0.666%
12	16.961	2423	2429	2436	rBV	289468	413316	12.98%	3.738%
13	17.871	2578	2584	2590	rBV7	36961	57330	1.80%	0.518%
14	17.942	2592	2596	2606	rVV3	127479	190604	5.99%	1.724%
15	19.164	2800	2804	2810	rBV7	26857	37357	1.17%	0.338%
16	19.605	2874	2879	2896	rBV	2280536	3184415	100.00%	28.800%
17	20.880	3092	3096	3104	rVB6	41643	59816	1.88%	0.541%
18	20.974	3106	3112	3119	rBV2	211885	288456	9.06%	2.609%
19	21.162	3135	3144	3150	rBV	513794	641374	20.14%	5.801%
20	22.172	3311	3316	3323	rBV	127622	228752	7.18%	2.069%
21	23.359	3512	3518	3525	rVB	321649	569472	17.88%	5.150%
22	23.665	3566	3570	3580	rBV8	41215	108853	3.42%	0.984%

Sum of corrected areas: 11057027

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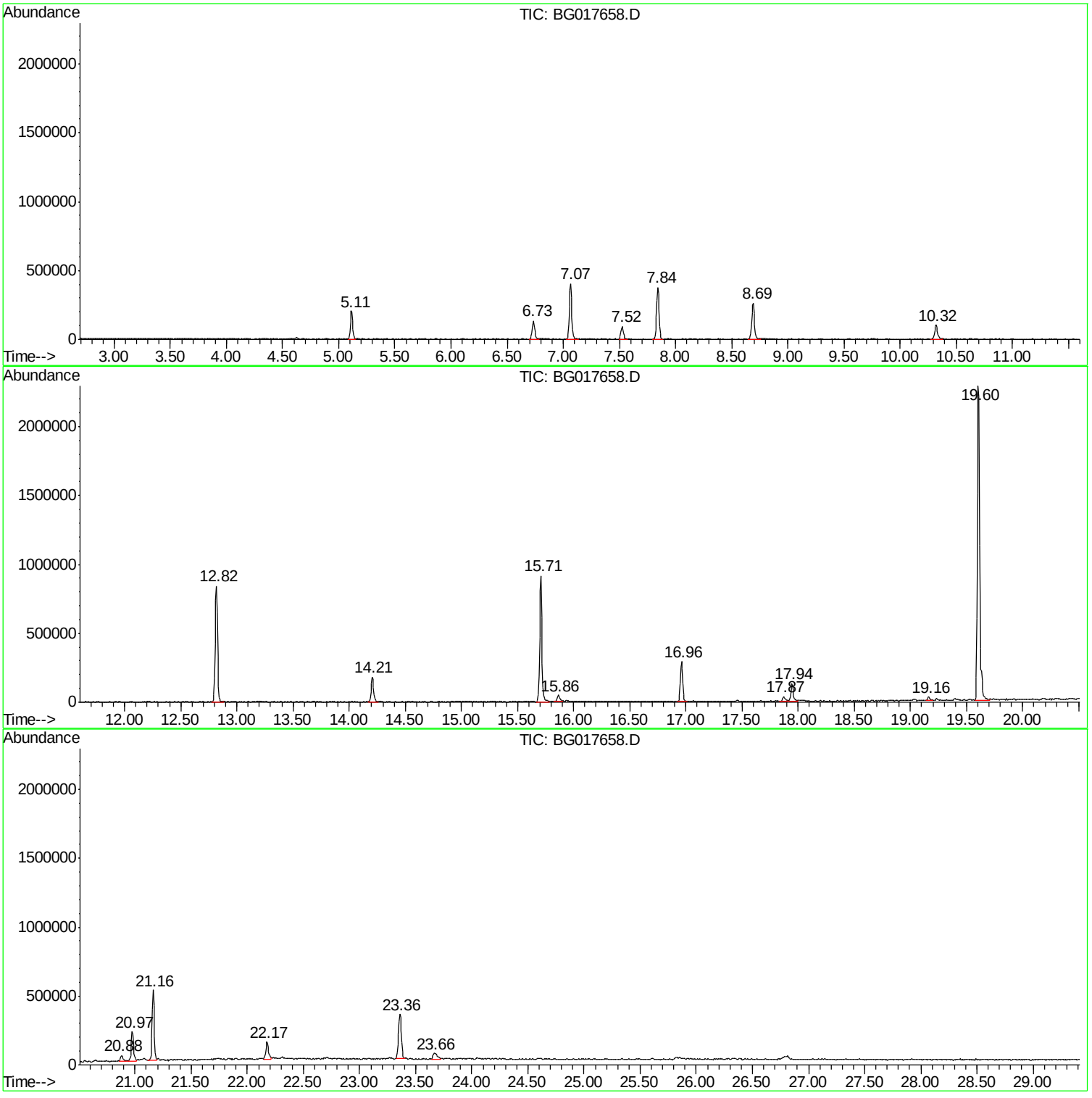
Instrument : BNA_G
ClientSampleId : MW-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG061215.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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Operator : TP/IZ
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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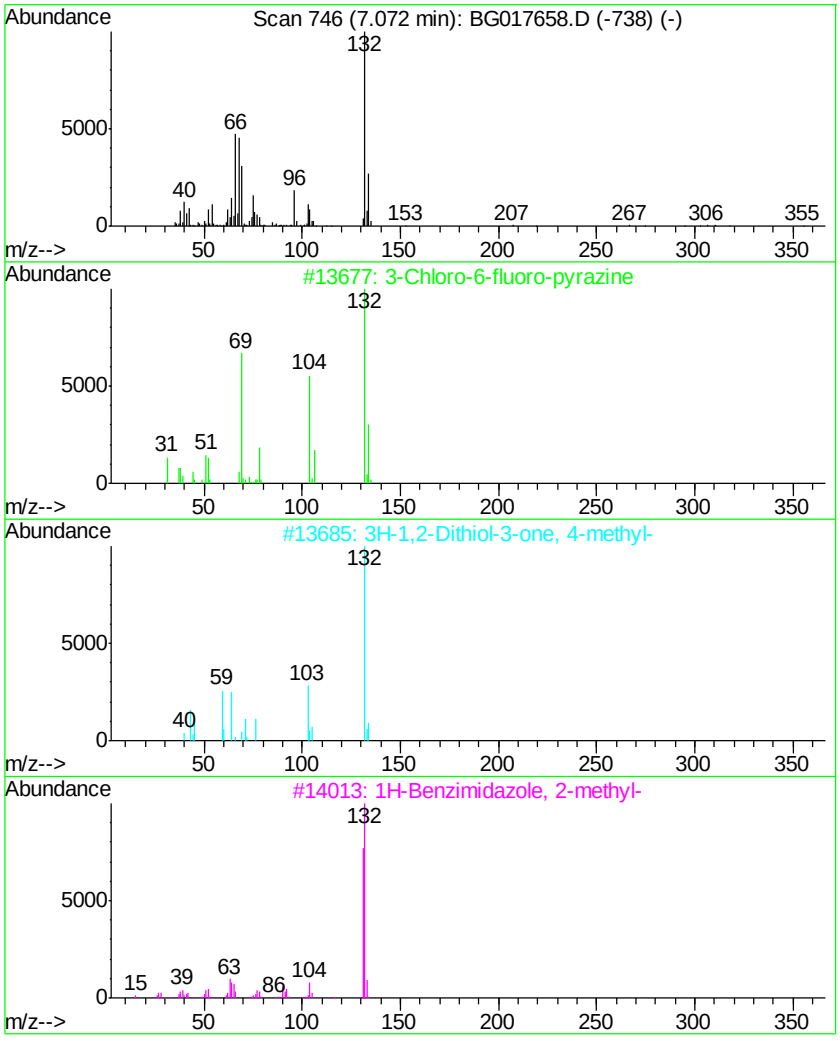
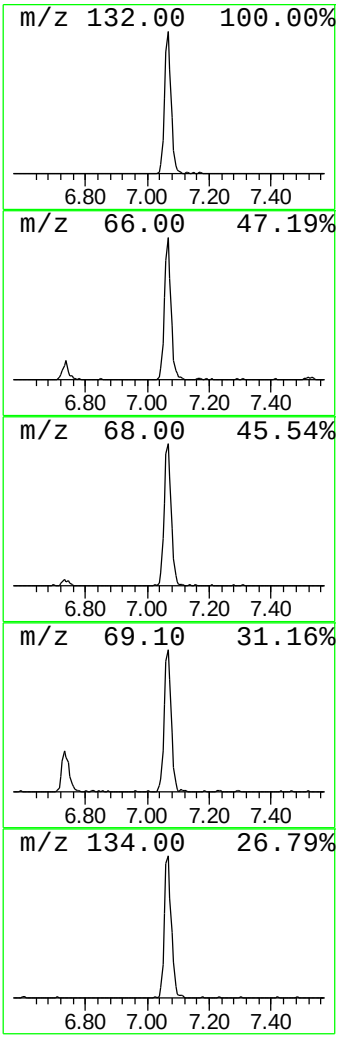
Peak Number 1 unknown7.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	82.47 ng	606376	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	3H-1,2-Dithiol-3-one, 4-methyl-	132	C4H4OS2	003620-10-8	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061215\
Data File : BG017658.D
Acq On : 13 Jun 2015 4:54
Operator : TP/IZ
Sample : G2627-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG061215.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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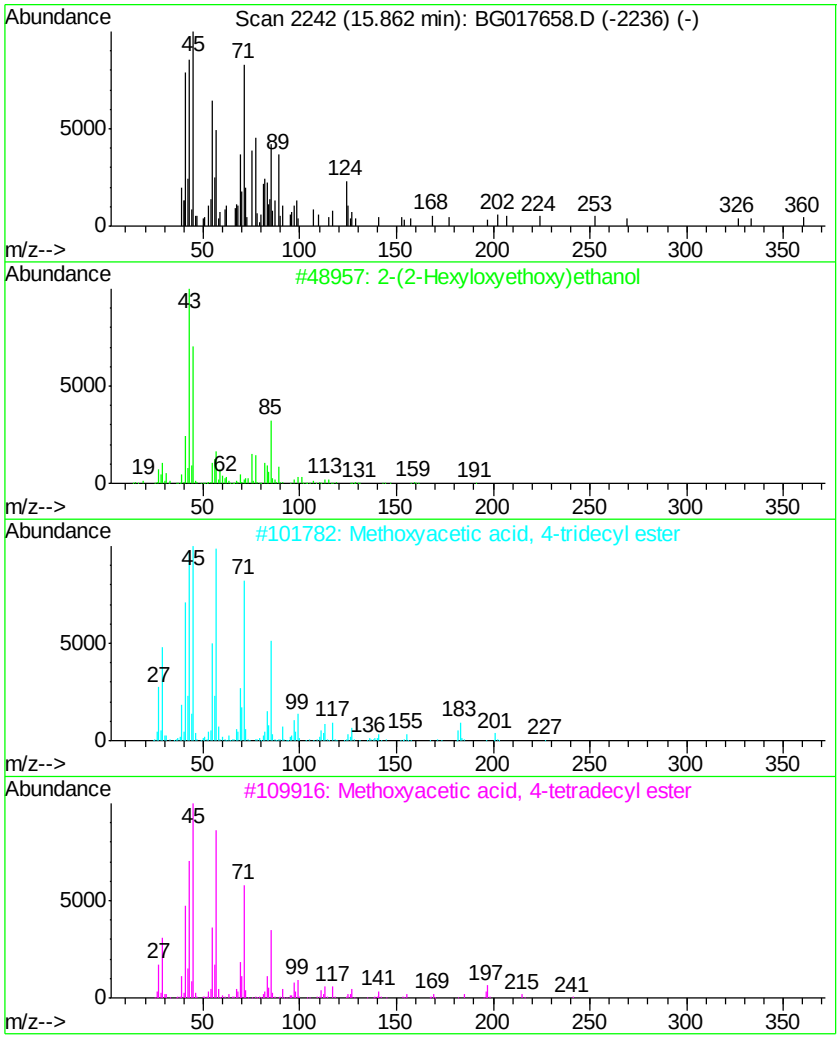
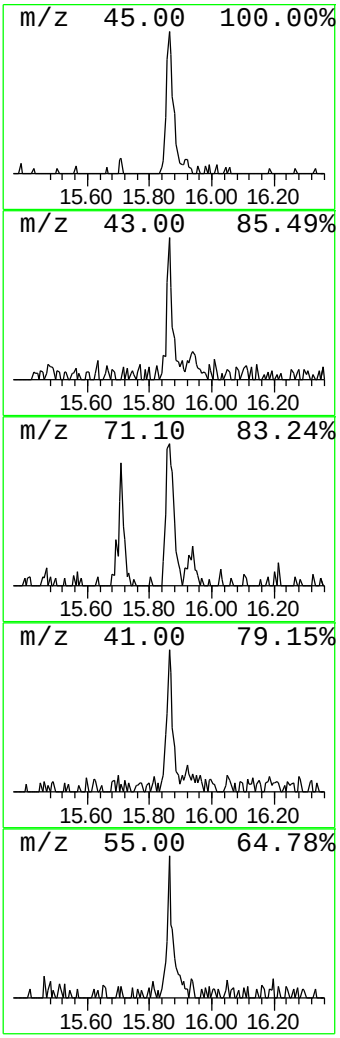
Peak Number 3 unknown15.86 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.56 ng	73589	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Hexyloxyethoxy)ethanol	190	C10H22O3	000112-59-4	43
2	Methoxyacetic acid, 4-tridecyl e...	272	C16H32O3	1000282-04-7	38
3	Methoxyacetic acid, 4-tetradecyl...	286	C17H34O3	1000282-05-0	38
4	Methoxyacetic acid, 3-tetradecyl...	286	C17H34O3	1000282-04-9	38
5	Methoxyacetic acid, decyl ester	230	C13H26O3	259141-02-1	27





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061215\
Data File : BG017658.D
Acq On : 13 Jun 2015 4:54
Operator : TP/IZ
Sample : G2627-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG061215.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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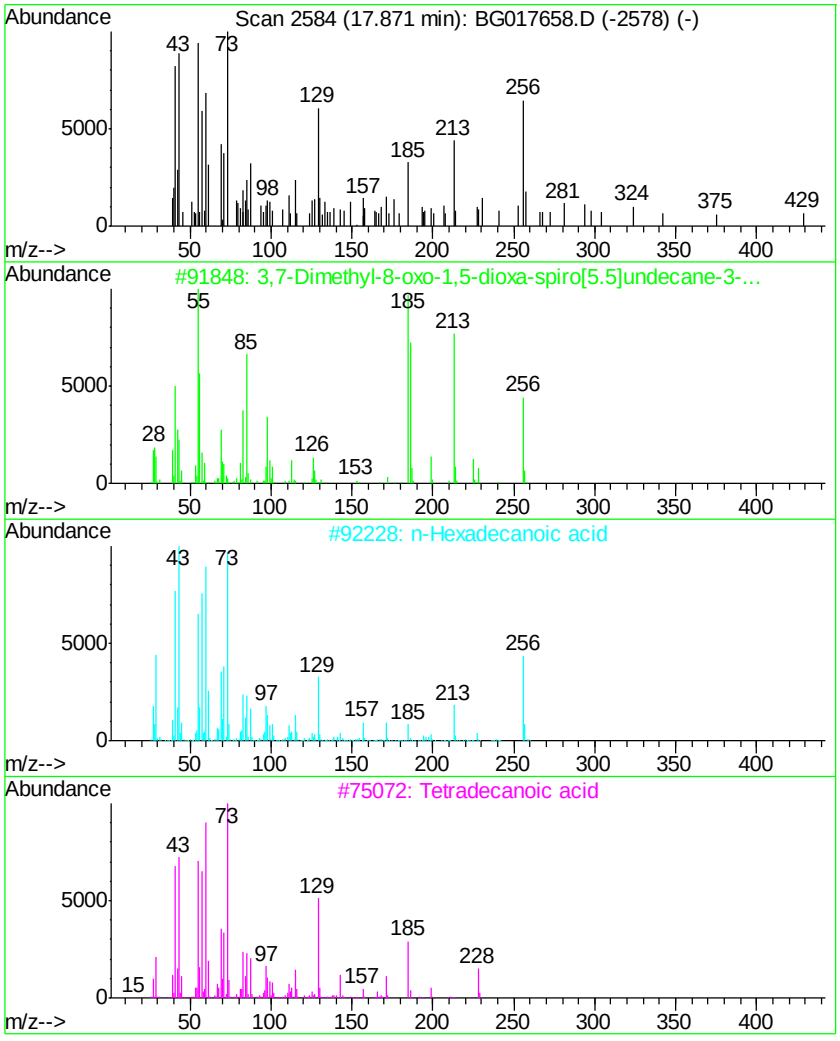
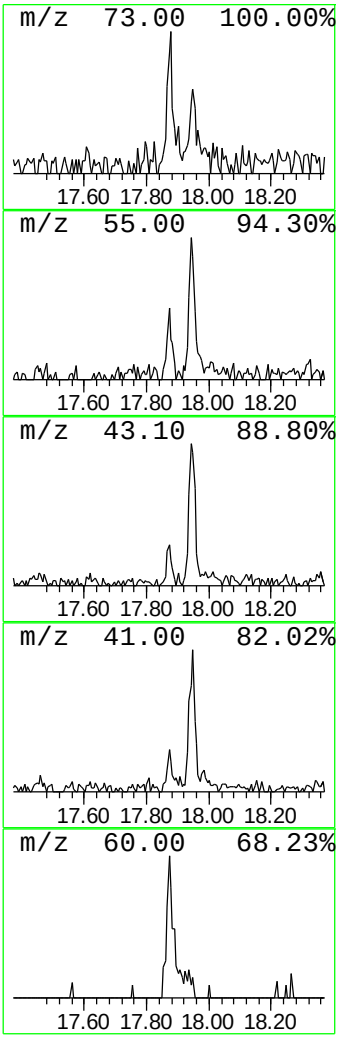
Peak Number 4 3,7-Dimethyl-8-oxo-1,5-diox... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	2.77 ng	57330	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Dimethyl-8-oxo-1,5-dioxa-spi...	256	C13H20O5	1000193-79-8	64
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4	Lumiflavine	256	C13H12N4O2	001088-56-8	30
5	Isopropyl Palmitate	298	C19H38O2	000142-91-6	30





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061215\
Data File : BG017658.D
Acq On : 13 Jun 2015 4:54
Operator : TP/IZ
Sample : G2627-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG061215.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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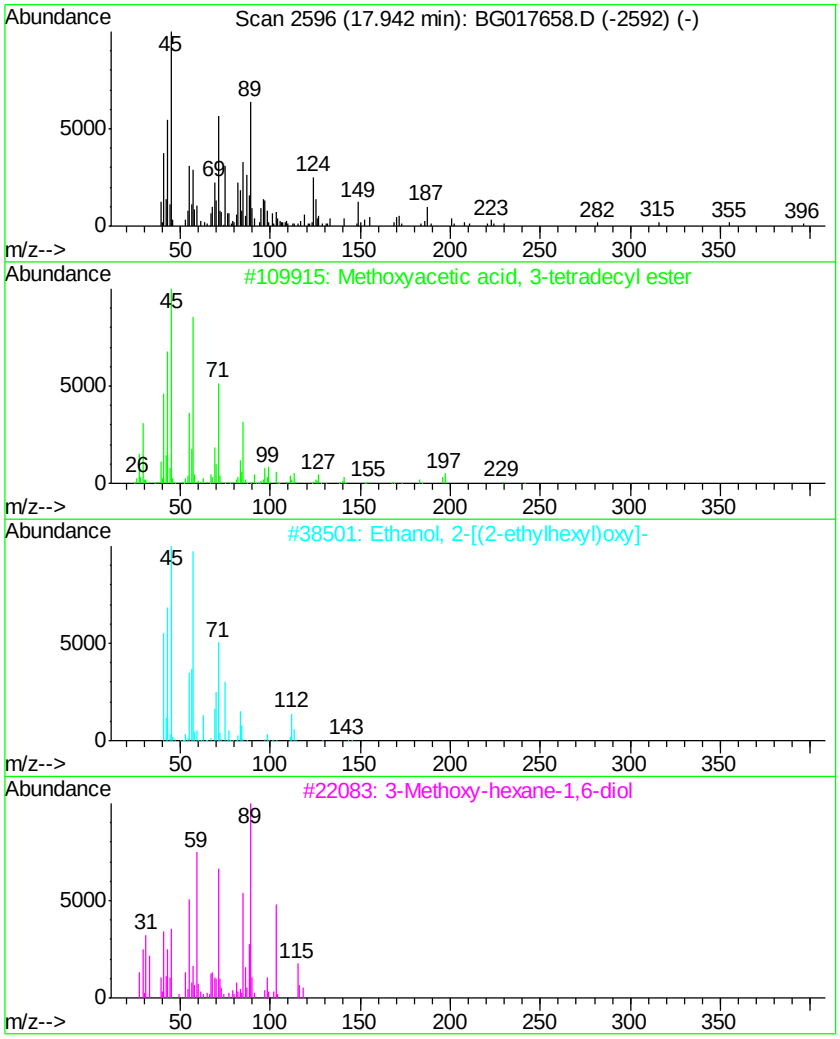
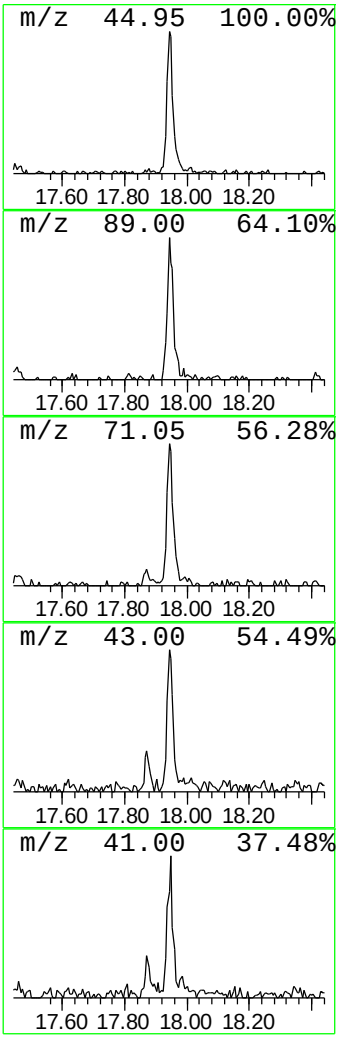
Peak Number 5 unknown17.94 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.94	9.22 ng	190604	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 3-tetradecyl...	286	C17H34O3	1000282-04-9	43
2	Ethanol, 2-[(2-ethylhexyl)oxy]-	174	C10H22O2	001559-35-9	35
3	3-Methoxy-hexane-1,6-diol	148	C7H16O3	1000193-45-4	35
4	2-Tetradecanol	214	C14H30O	004706-81-4	27
5	12-Crown-4	176	C8H16O4	000294-93-9	27





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Sample : G2627-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG061215.M
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TIC Library : C:\DATABASE\NIST02.L
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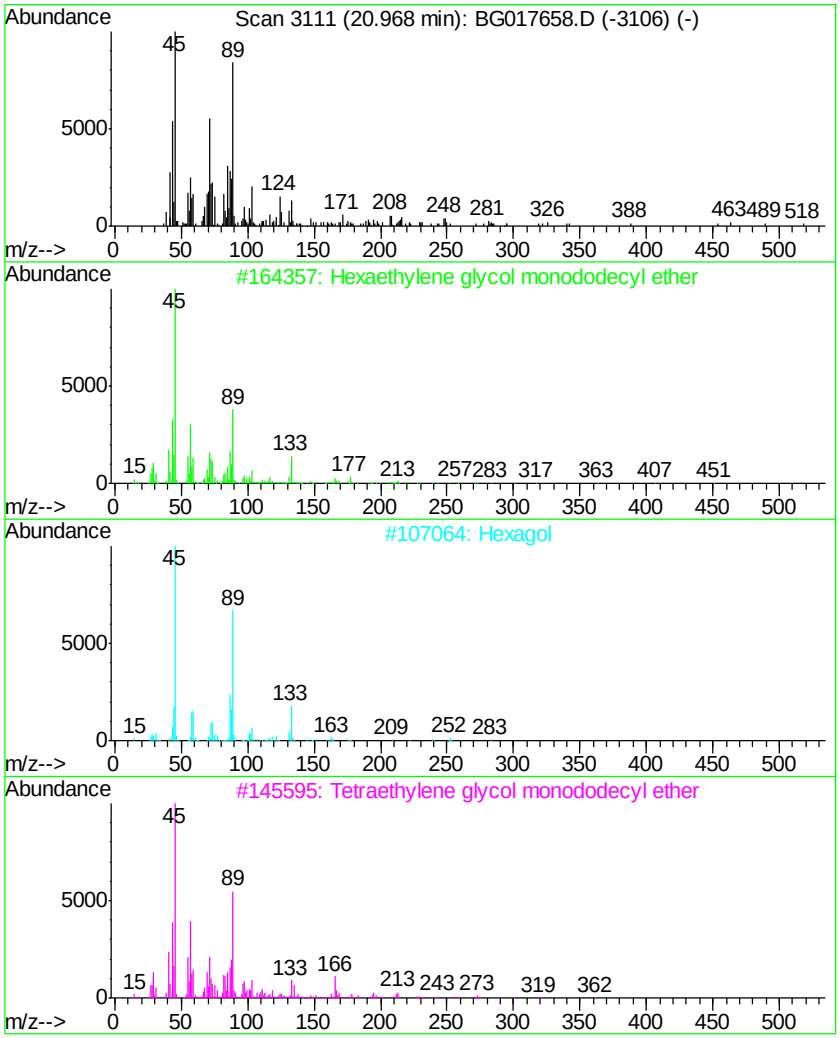
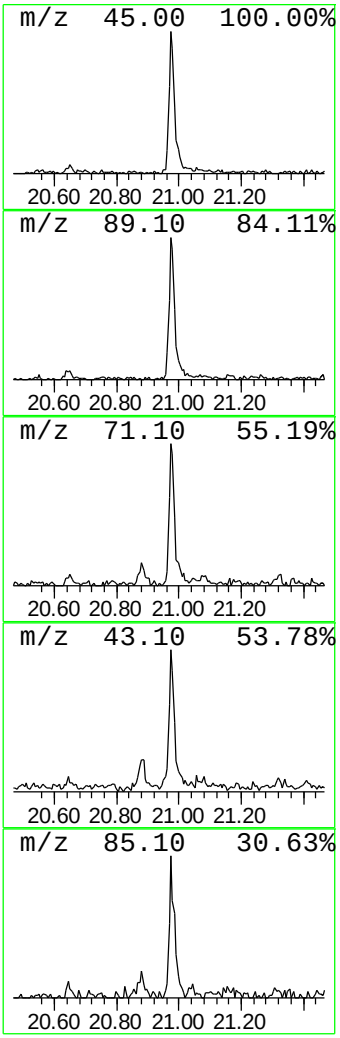
Peak Number 6 Hexaethylene glycol monodod... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	8.99 ng	288456	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	78
2	Hexagol	282	C12H26O7	002615-15-8	58
3	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	56
4	3-Methylseleno-2-benzo[b]thiophe...	256	C10H8OSSe	039857-04-0	47
5	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	47





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Instrument : BNA_G
ClientSampleId : MW-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG061215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

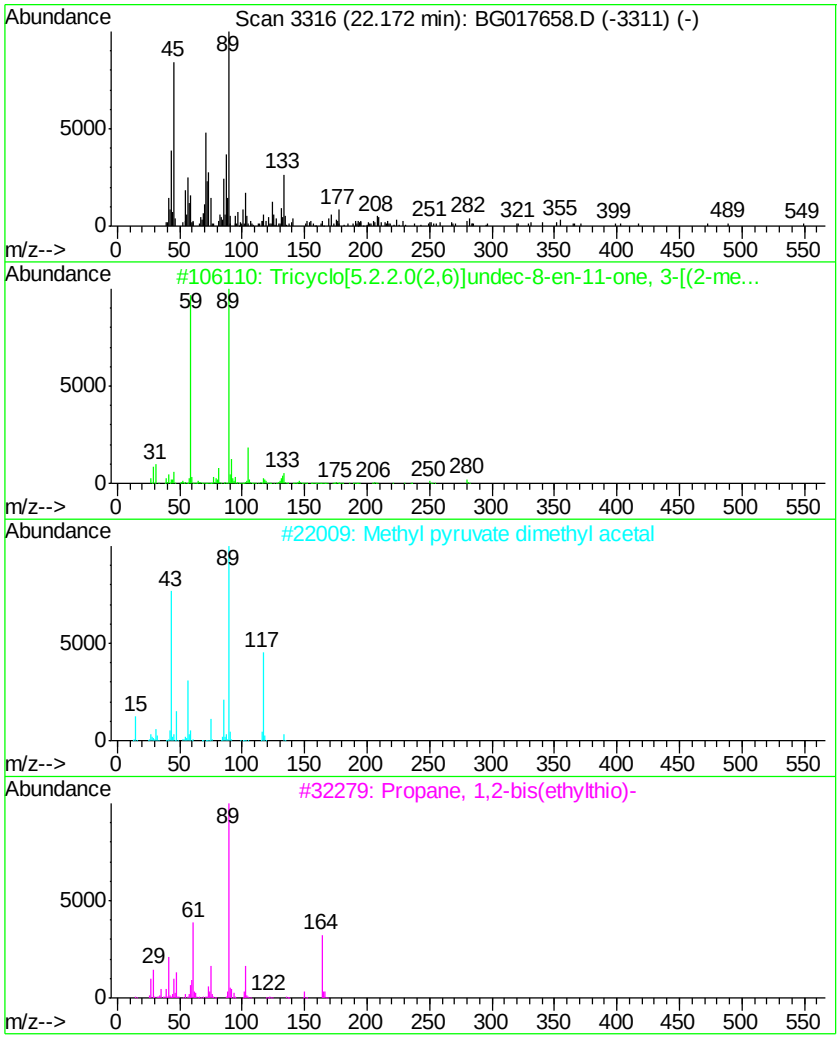
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

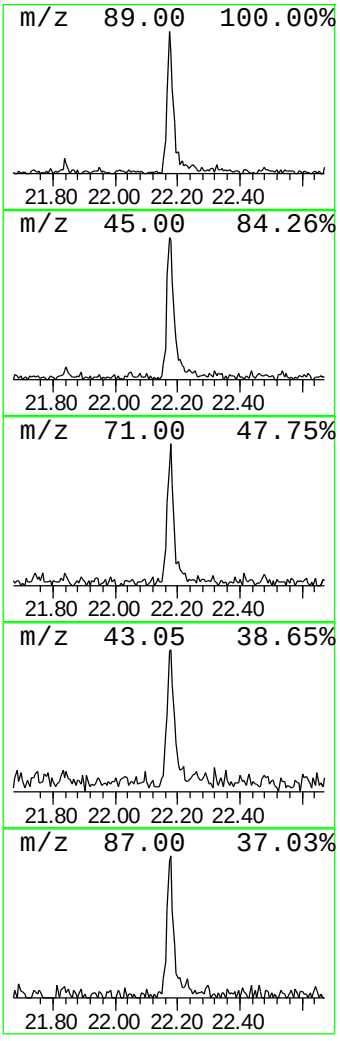
****

Peak Number 7 unknown22.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.17	7.13 ng	228752	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[5.2.2.0(2,6)]undec-8-en...	280	C16H24O4	1000154-01-3	49
2	Methyl pyruvate dimethyl acetal	148	C6H12O4	010076-48-9	47
3	Propane, 1,2-bis(ethylthio)-	164	C7H16S2	054410-62-7	47
4	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	45
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	45





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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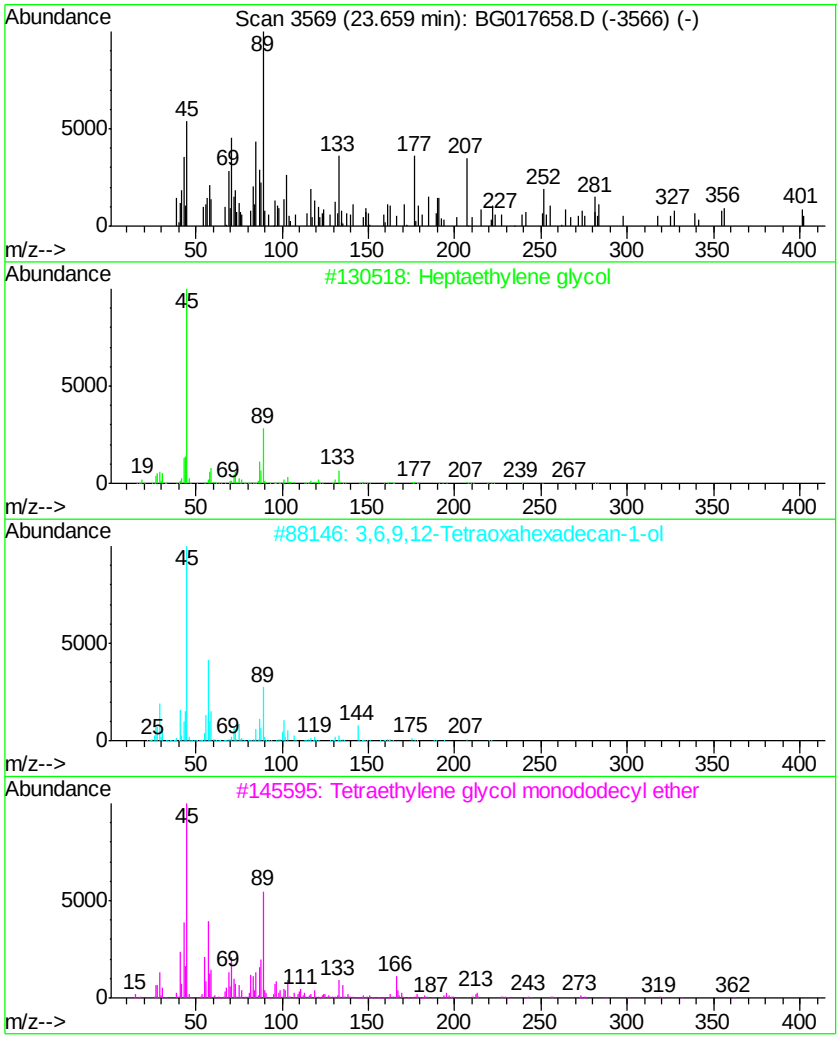
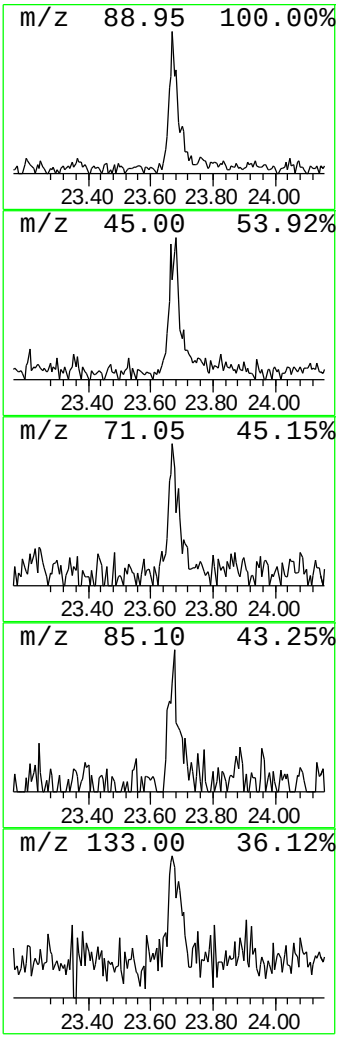
Peak Number 8 Heptaethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.66	3.82 ng	108853	Perylene-d12	23.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	72
2	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	72
3	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	64
4	1,3,4-Trimethoxy-butan-2-ol	164	C7H16O4	033469-04-4	56
5	3-(2,5,8,11,14-Pentaoxacyclohexa...	510	C24H46O11	1000110-99-4	50





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.07	7.07	82.5	ng	606376	1	7.52	147061	20.0
unknown15.86	15.86	3.6	ng	73589	4	16.96	413316	20.0
3,7-Dimethyl-8-ox...	17.87	2.8	ng	57330	4	16.96	413316	20.0
unknown17.94	17.94	9.2	ng	190604	4	16.96	413316	20.0
Hexaethylene glyc...	20.97	9.0	ng	288456	5	21.16	641374	20.0
unknown22.17	22.17	7.1	ng	228752	5	21.16	641374	20.0
Heptaethylene glycol	23.66	3.8	ng	108853	6	23.36	569472	20.0