LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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	5.168	315	320	330	rVB	77802	122231	2.19%	0.442%
2	5.638	394	400	409	rBV	736245	1213892	21.79%	4.386%
3	7.225	663	670	683	rBV	541449	969781	17.41%	3.504%
4	7.595	725	733	740	rBV	1228244	2110388	37.89%	7.625%
5	8.059	804	812	817	rBV	193364	333781	5.99%	1.206%
6	8.382	859	867	875	rBV	999824	1699639	30.51%	6.141%
7	9.222	1002	1010	1023	rVB	883722	1586590	28.48%	5.733%
8	10.079	1149	1156	1165	rBV2	39912	93657	1.68%	0.338%
9	10.861	1281	1289	1294	rBV	265513	498498	8.95%	1.801%
10	11.507	1393	1399	1406	rBV3	105971	186758	3.35%	0.675%
11	13.305	1696	1705	1712	rBV	2402453	3809430	68.39%	13.765%
12	14.121	1838	1844	1854	rBV2	125767	208326	3.74%	0.753%
13	14.385	1884	1889	1894	rBV	59911	96649	1.74%	0.349%
14	14.479	1901	1905	1917	rVB	42919	79225	1.42%	0.286%
15	14.679	1930	1939	1945	rBV2	420147	714391	12.83%	2.581%
16	16.165	2185	2192	2201	rBV	1993814	3076134	55.22%	11.115%
17	16.353	2219	2224	2231	rVB3	58799	106554	1.91%	0.385%
18	16.718	2281	2286	2292	rBV3	40601	60586	1.09%	0.219%
19	16.958	2323	2327	2333	rVB	65438	99121	1.78%	0.358%
20	17.417	2400	2405	2412	rVB	572089	882232	15.84%	3.188%
21	17.693	2448	2452	2457	rVB	54115	70962	1.27%	0.256%
22	18.304	2552	2556	2565	rBV2	101490	155851	2.80%	0.563%
23	18.656	2609	2616	2625	rVV	726391	1239500	22.25%	4.479%
24	20.025	2843	2849	2858	rVB	4053816	5570189	100.00%	20.127%
25	21.329	3067	3071	3081	rVB3	89759	156227	2.80%	0.564%
26	21.687	3126	3132	3139	rVB	651373	1030467	18.50%	3.723%
27	22.545	3274	3278	3283	rVB3	44492	73251	1.32%	0.265%
28	22.950	3339	3347	3353	rBV6	84247	276370	4.96%	0.999%
29	24.912	3670	3681	3690	rVB2	356446	1036690	18.61%	3.746%
30	25.629	3796	3803	3807	rBV8	46175	118173	2.12%	0.427%

Sum of corrected areas: 27675543

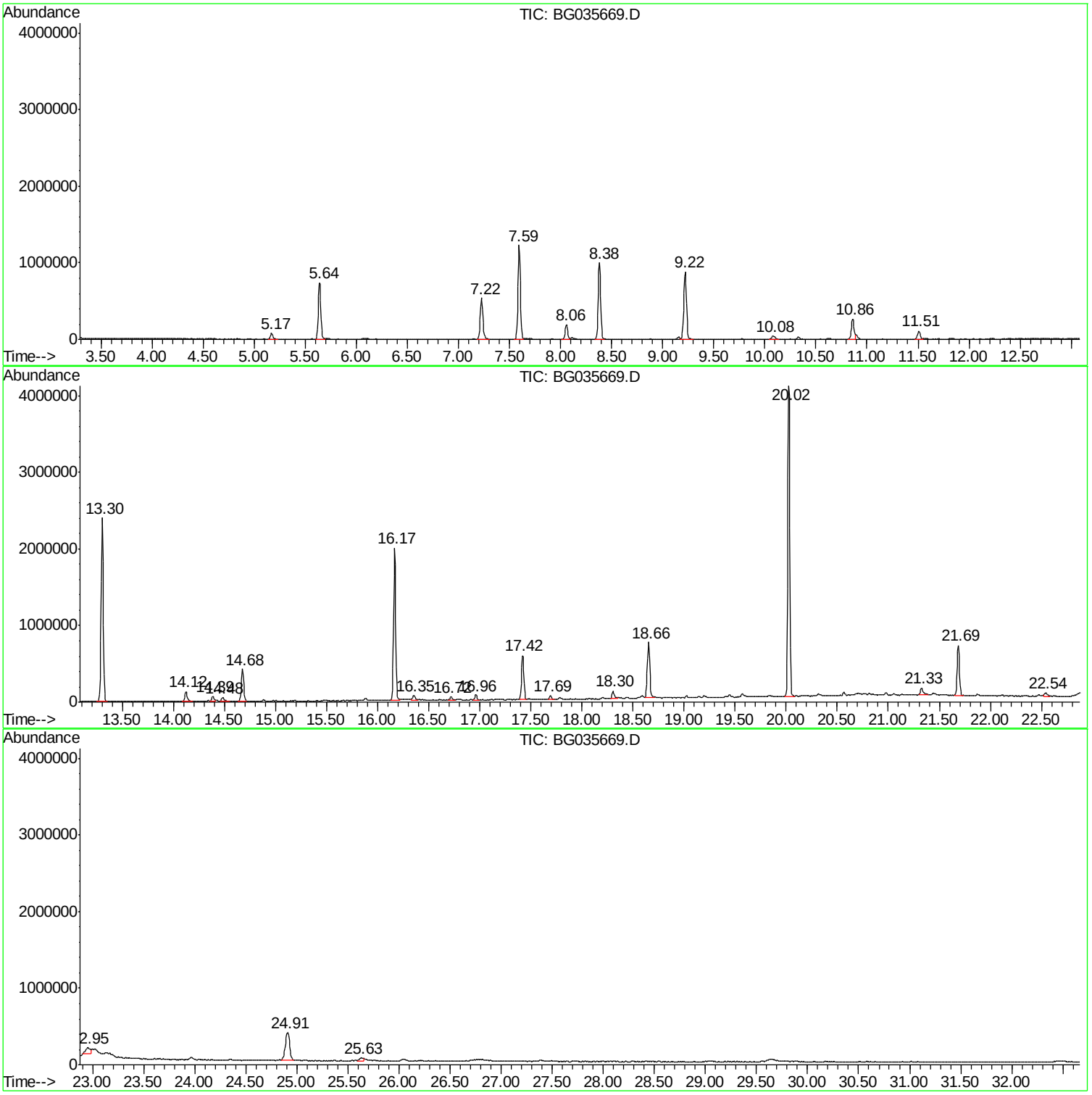
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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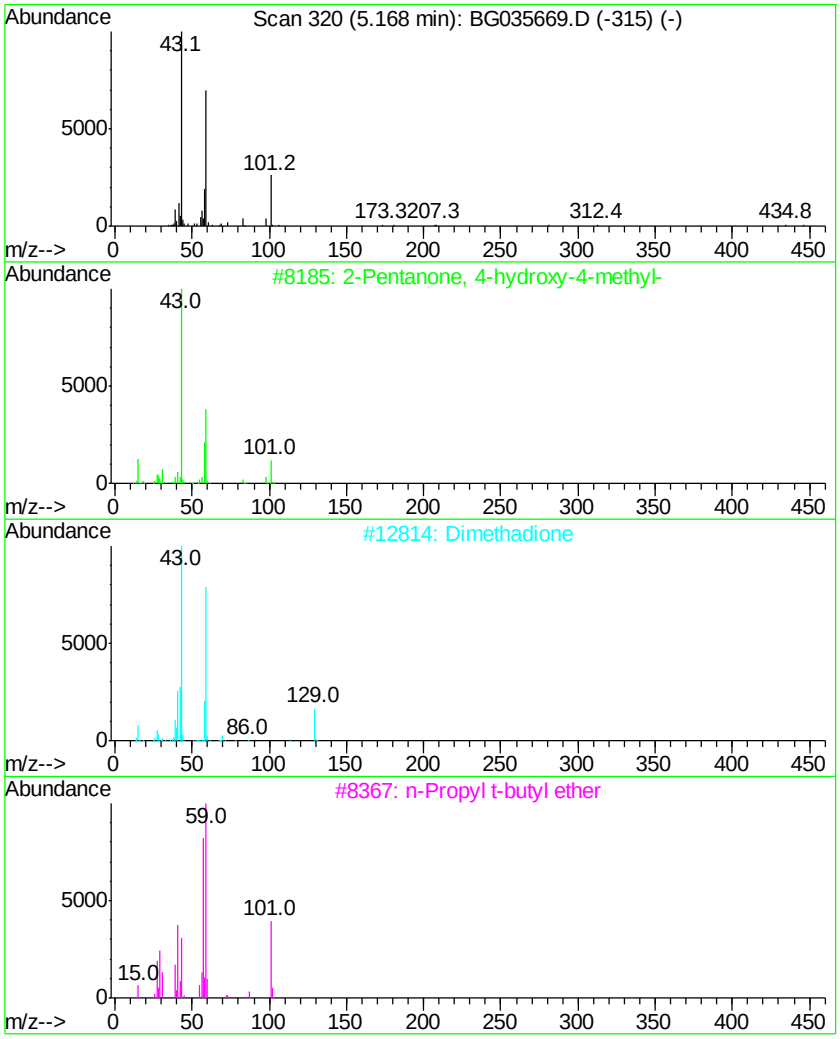
TIC Integration Parameters: LSCINT.P

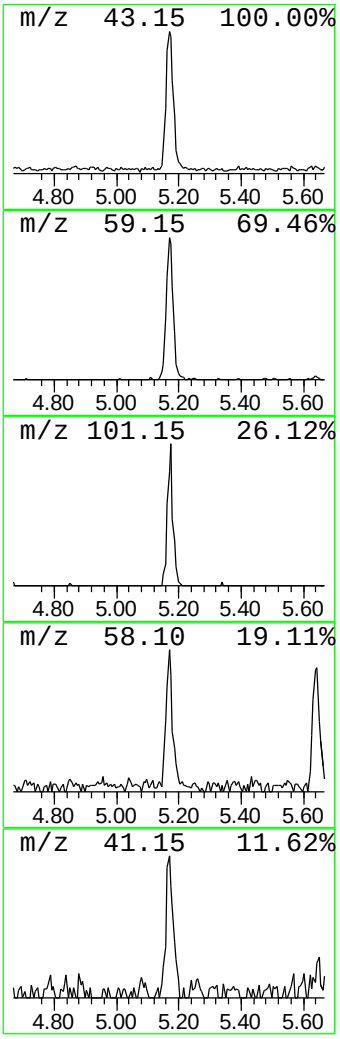
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	7.32 ng	122231	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Dimethadione	129	C5H7NO3	000695-53-4	33
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	25
4	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	25
5	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	25





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Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
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Misc :
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Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

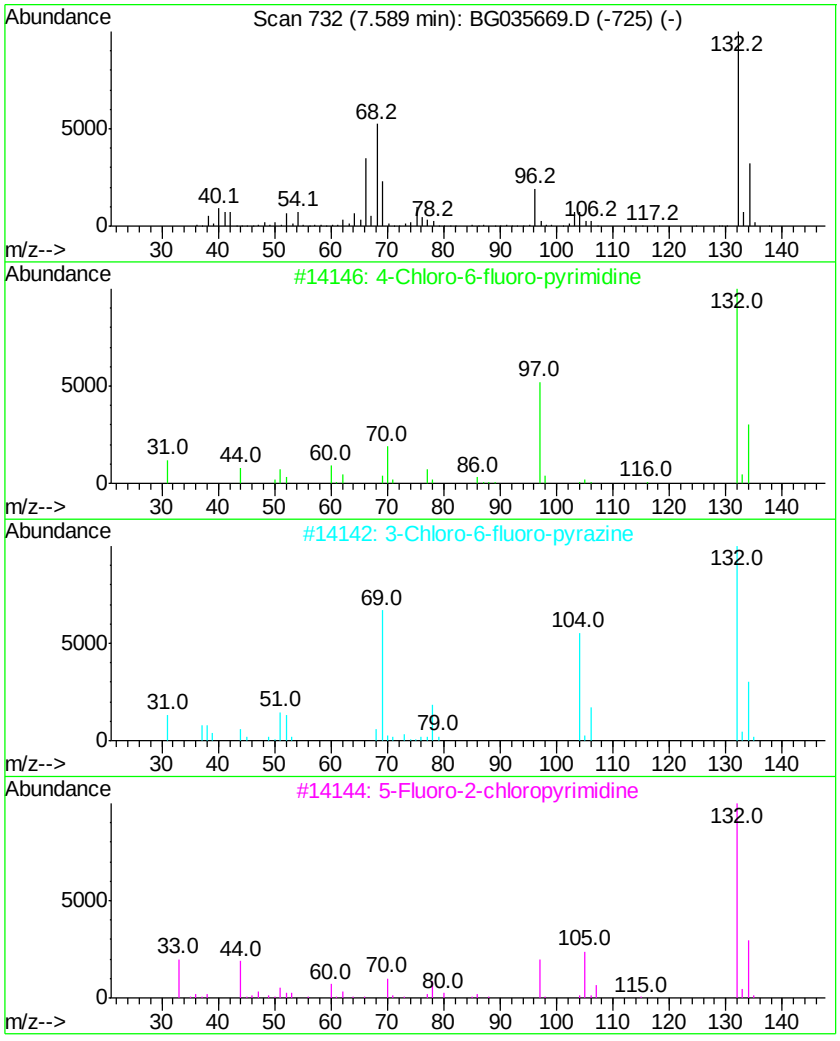
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

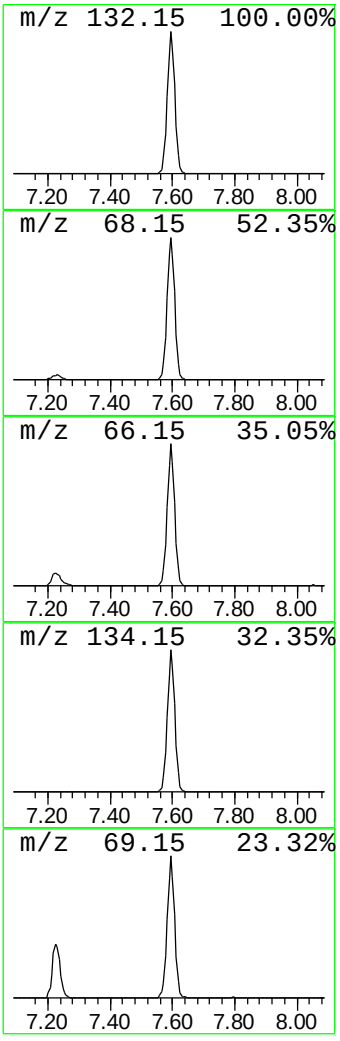
****

Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	126.45 ng	2110390	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
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TIC Library : C:\Database\NIST11.L
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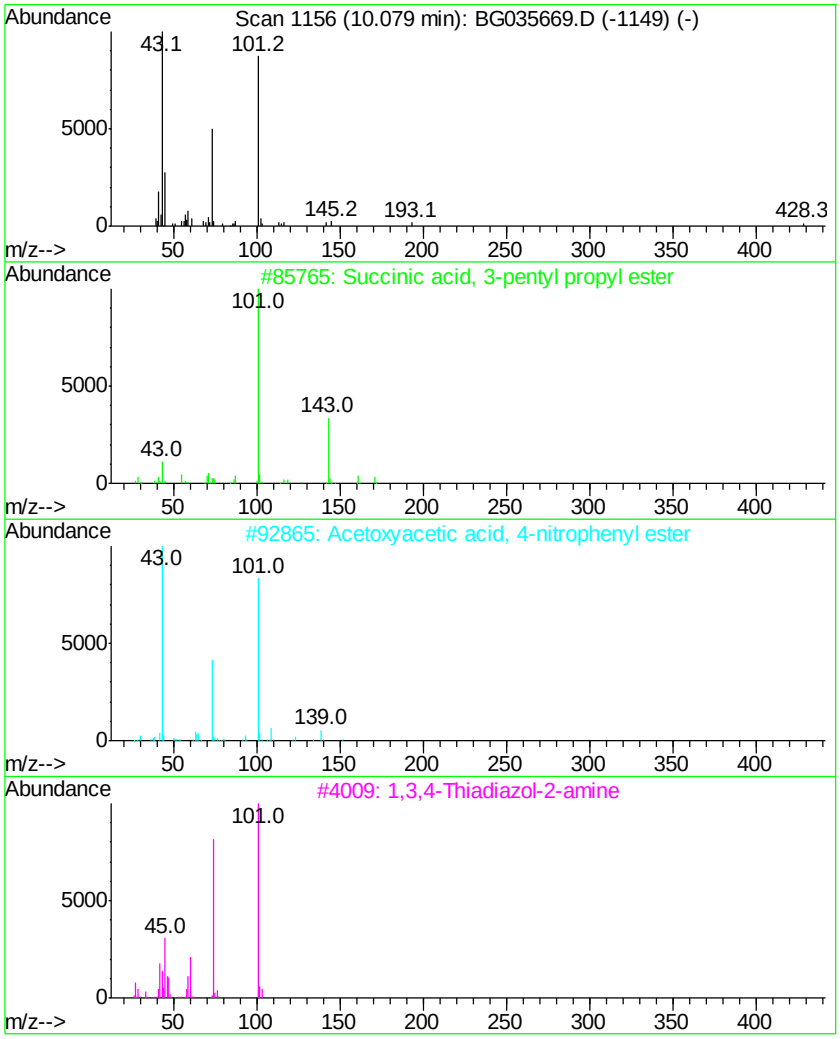
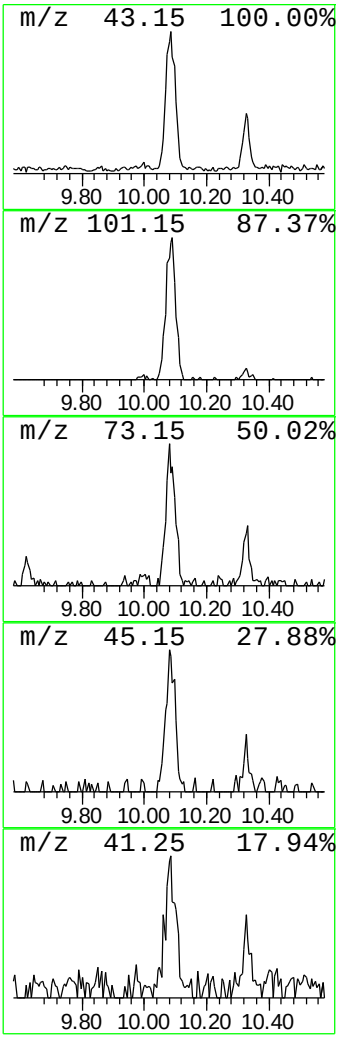
Peak Number 4 unknown10.08 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.08	3.76 ng	93657	Naphthalene-d8	10.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 3-pentyl propyl e...	230	C12H22O4	1000324-94-9	47
2	Acetoxyacetic acid, 4-nitrophenyl...	239	C10H9NO6	1000307-54-5	45
3	1,3,4-Thiadiazol-2-amine	101	C2H3N3S	004005-51-0	42
4	2,3,4-Trimethyl-d-xylose	192	C8H16O5	1000130-00-4	39
5	D-Xylose, 3,4,5-tri-O-methyl-	192	C8H16O5	069502-90-5	39





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

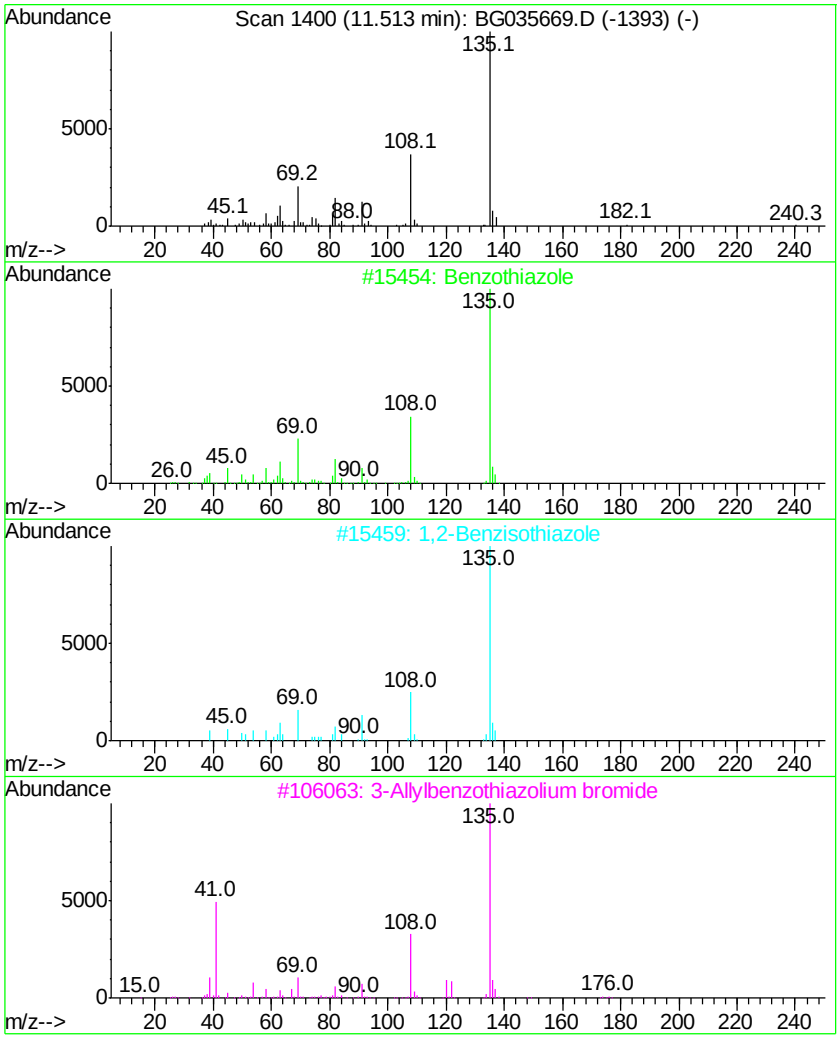
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

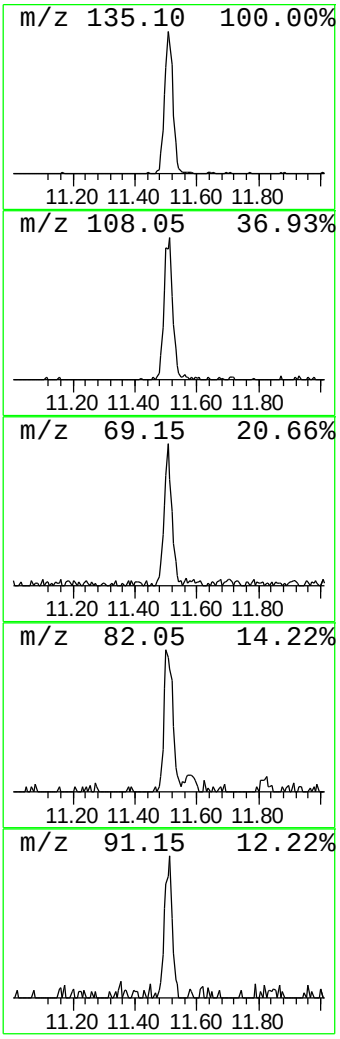
****

Peak Number 5 Benzothiazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.51	7.49 ng	186758	Naphthalene-d8	10.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	72
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	58
5	Adenine	135	C5H5N5	000073-24-5	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

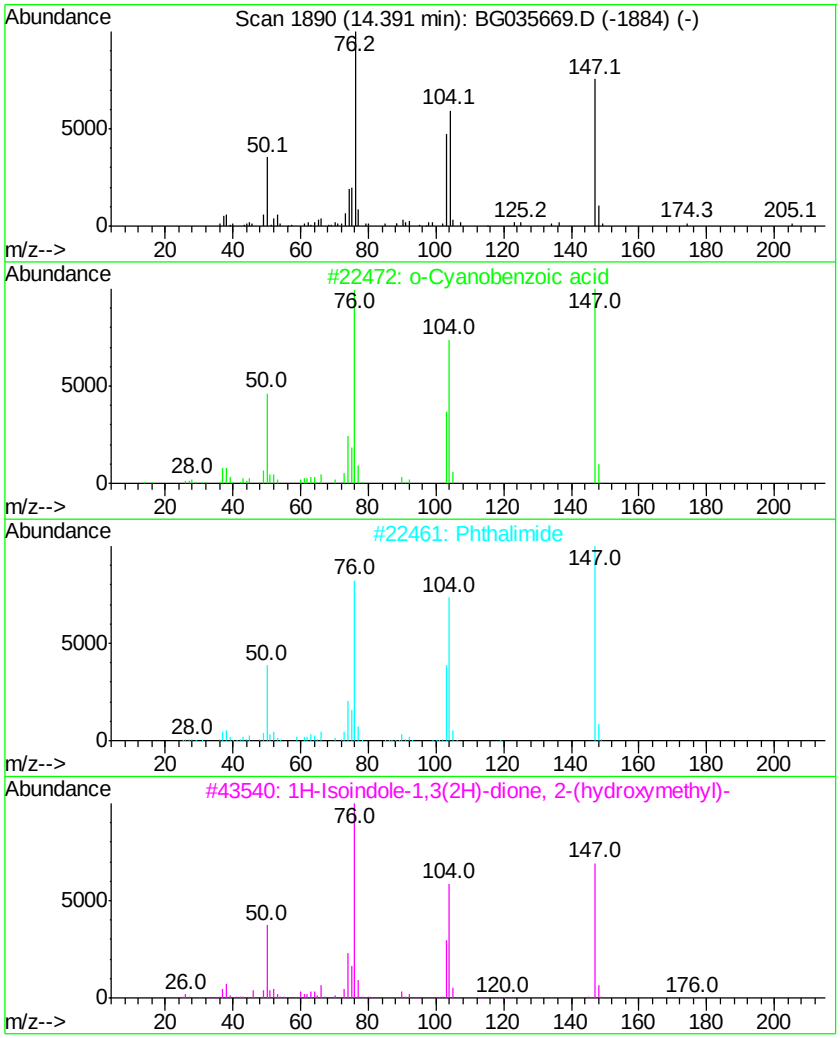
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

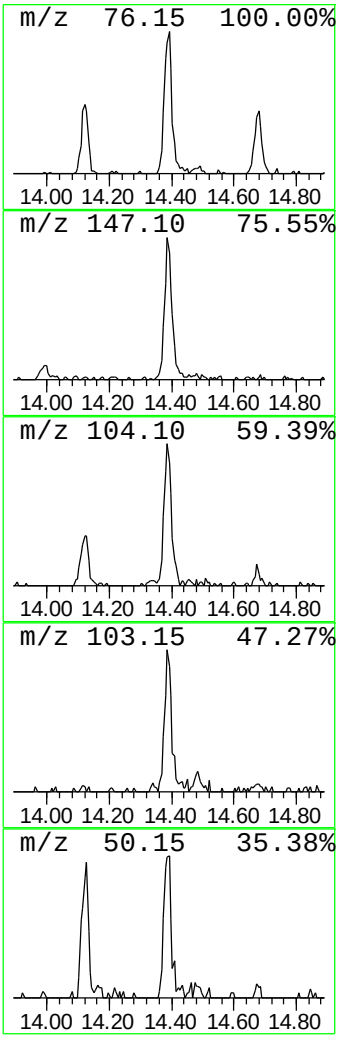
****

Peak Number 6 o-Cyanobenzoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	2.71 ng	96649	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cyanobenzoic acid	147	C8H5NO2	003839-22-3	91
2	Phthalimide	147	C8H5NO2	000085-41-6	90
3	1H-Isoindole-1,3(2H)-dione, 2-(h...	177	C9H7NO3	000118-29-6	83
4	Phthalimidomethyl 3-methoxybenzoate	311	C17H13NO5	1000224-82-4	83
5	N-[2-Acetamidoethylthio]phthalimide	264	C12H12N2O3S	025158-14-9	83





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Sample : J3964-01
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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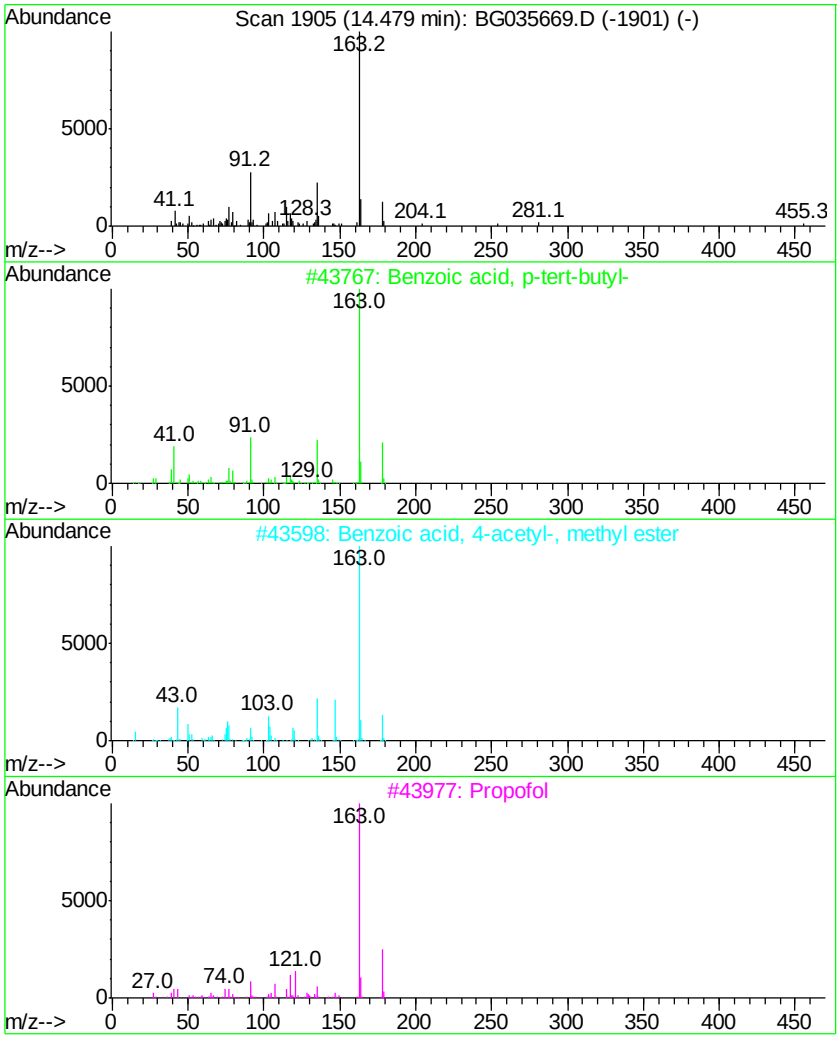
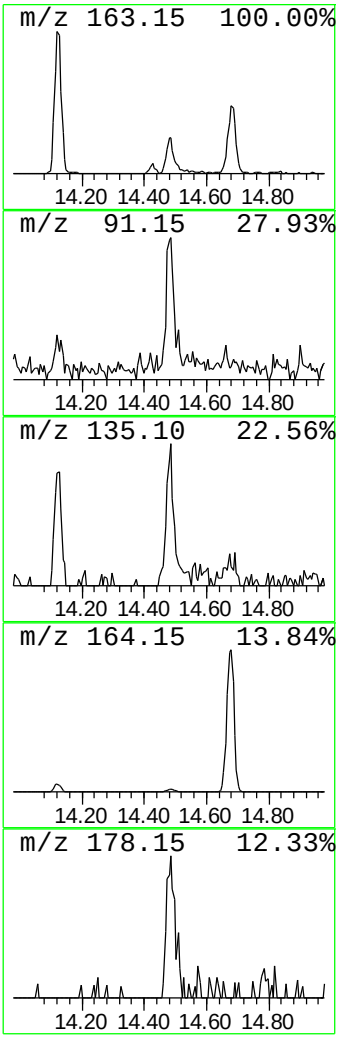
****

Peak Number 7 Benzoic acid, p-tert-butyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	2.22 ng	79225	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	90
2	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	80
3	Propofol	178	C12H18O	002078-54-8	64
4	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	59
5	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	59





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Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

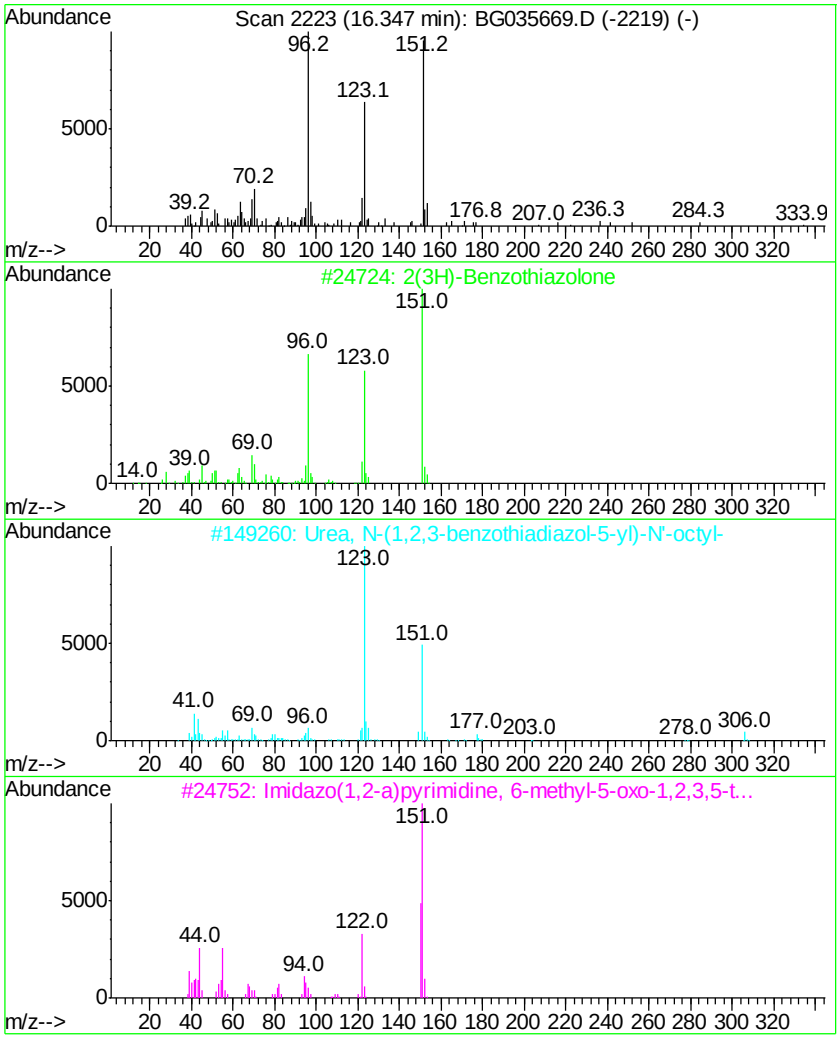
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

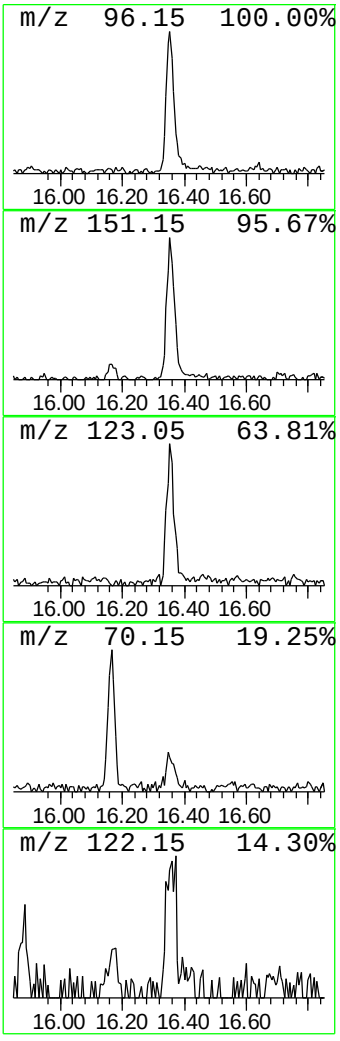
****

Peak Number 8 2(3H)-Benzothiazolone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	2.42 ng	106554	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2	Urea, N-(1,2,3-benzothiadiazol-5...	306	C15H22N4OS	1000318-87-5	38
3	Imidazo(1,2-a)pyrimidine, 6-meth...	151	C7H9N3O	026955-11-3	38
4	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	35
5	Benzene, fluoro-	96	C6H5F	000462-06-6	27





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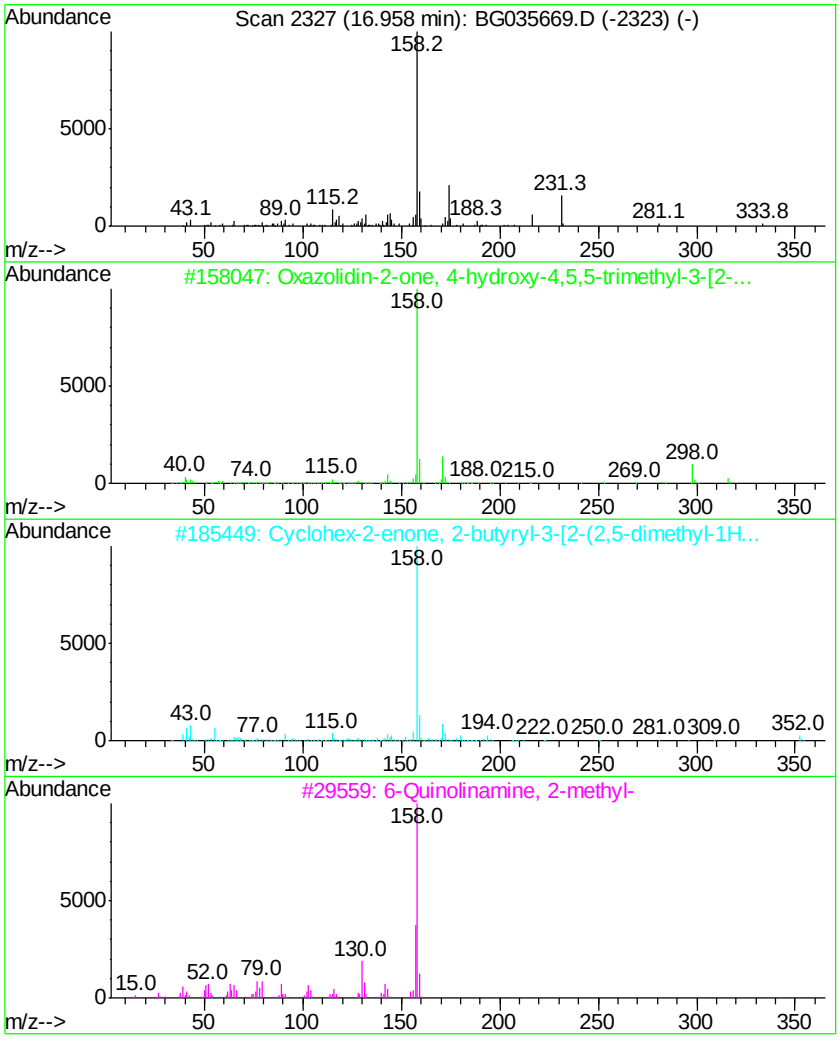
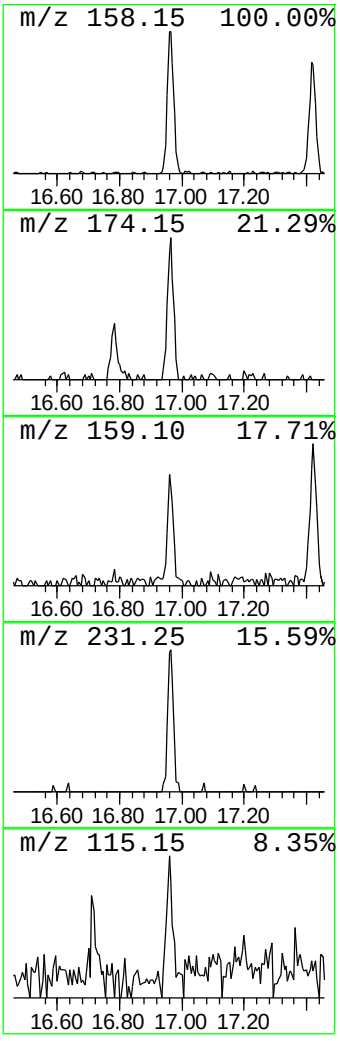
****

Peak Number 9 Oxazolidin-2-one, 4-hydroxy... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	2.25 ng	99121	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one, 4-hydroxy-4,5,...	316	C18H24N2O3	1000276-64-3	53
2	Cyclohex-2-enone, 2-butyryl-3-[2...	352	C22H28N2O2	1000302-14-2	53
3	6-Quinolinamine, 2-methyl-	158	C10H10N2	065079-19-8	50
4	4-Aminoquinaldine	158	C10H10N2	006628-04-2	47
5	Spiro[2H-1-benzopyran-2,2'-[2H]i...	495	C31H33N3O3	077031-67-5	42





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Sample : J3964-01
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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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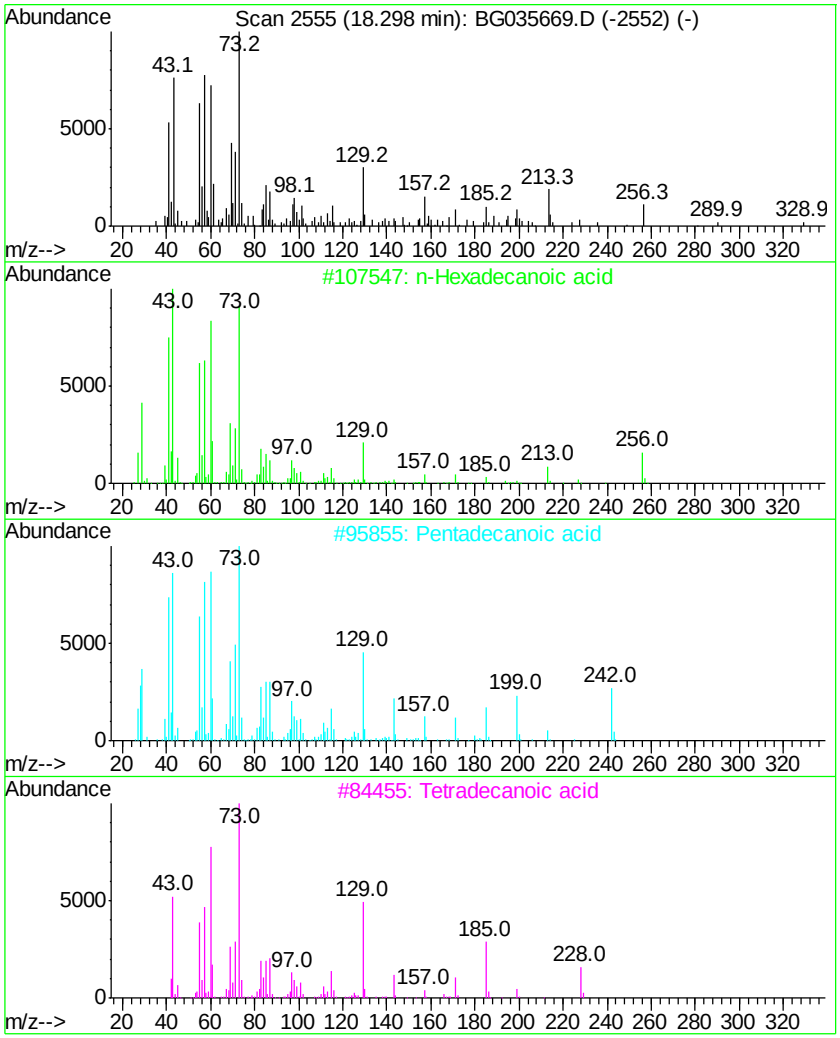
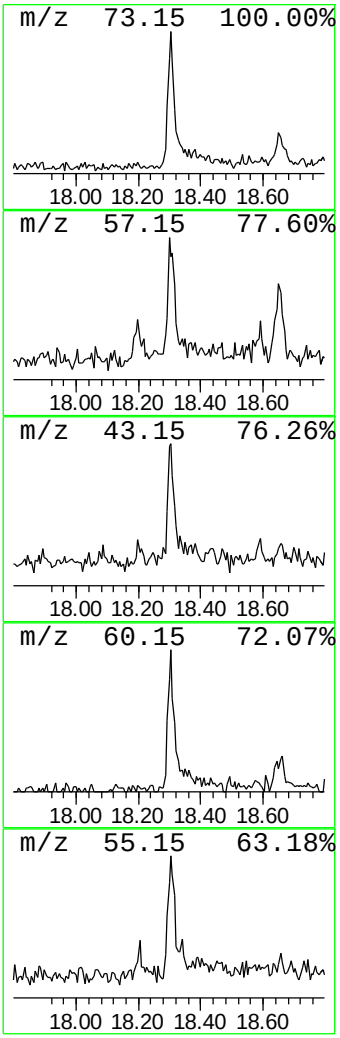
Peak Number 10 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.53 ng	155851	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Octadecanoic acid	284	C18H36O2	000057-11-4	58





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Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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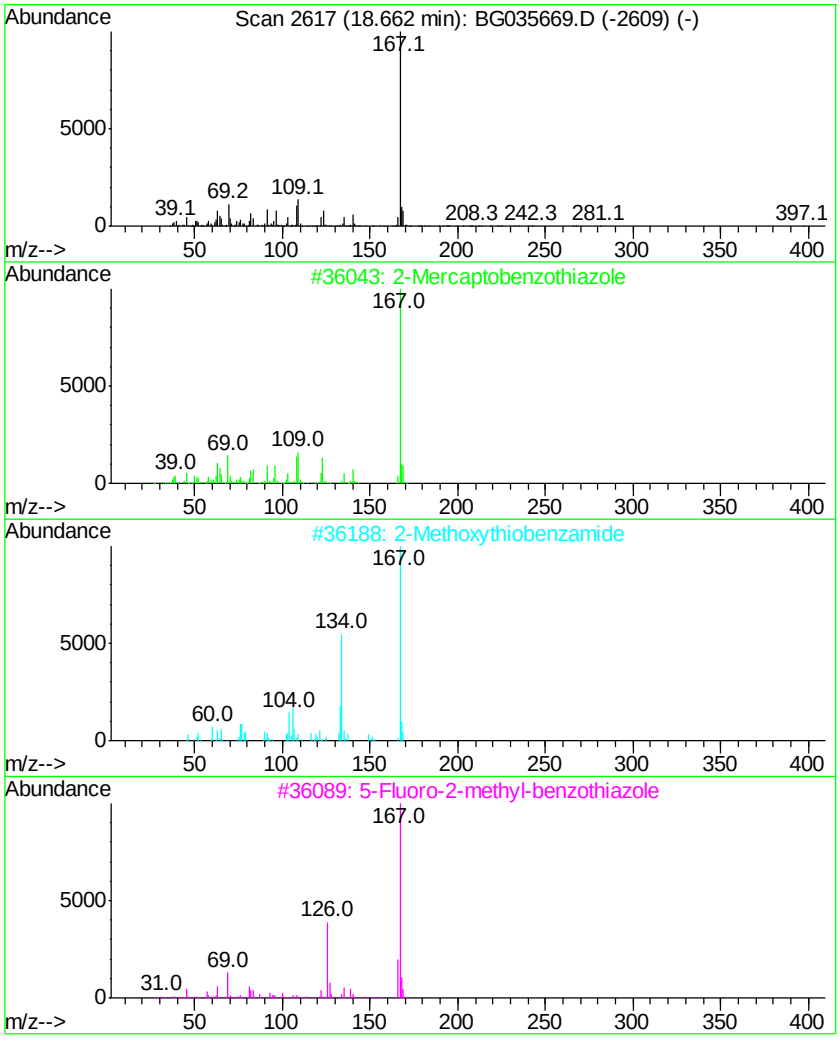
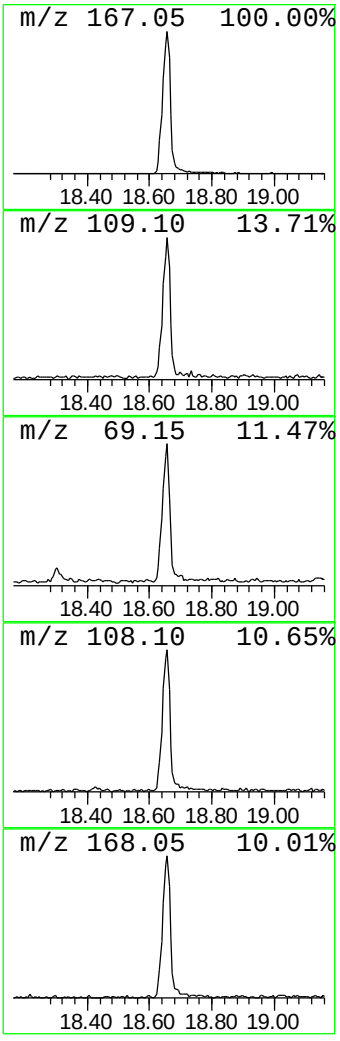
Peak Number 11 2-Mercaptobenzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.66	28.10 ng	1239500	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2	2-Methoxythiobenzamide	167	C8H9NOS	042590-97-6	53
3	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	52
4	Thioguanine	167	C5H5N5S	000154-42-7	50
5	1,3-Benzodioxole, 5-nitro-	167	C7H5NO4	002620-44-2	47





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Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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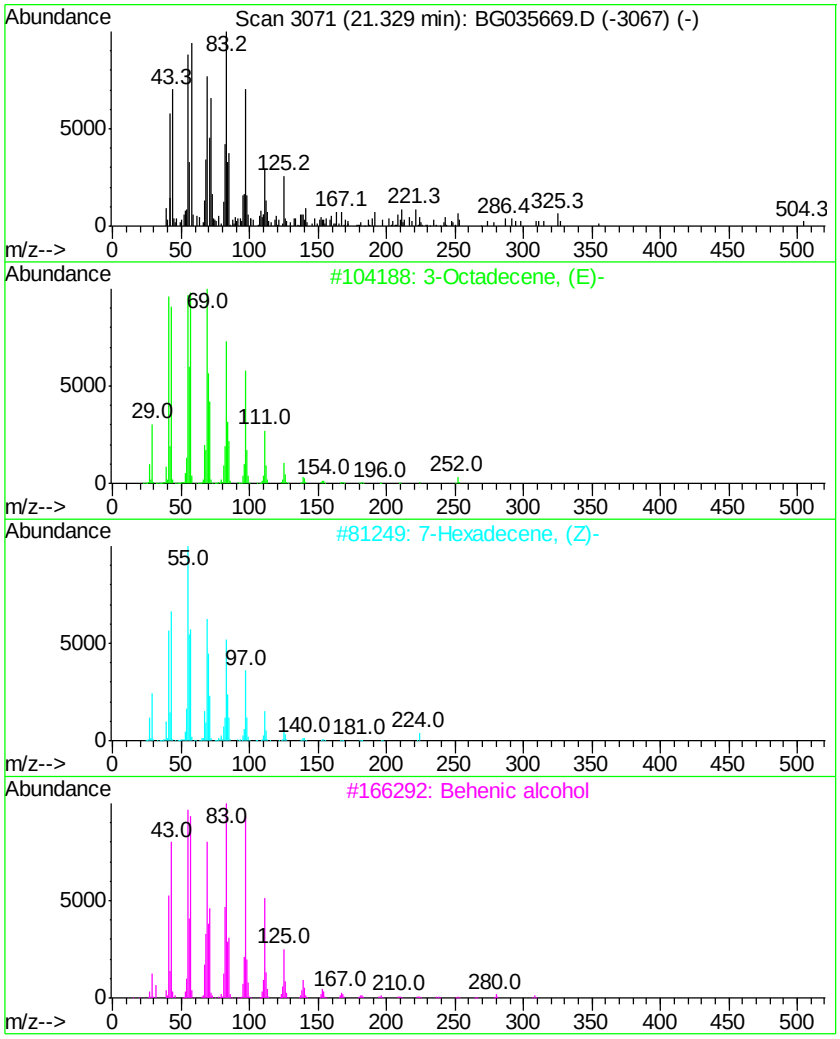
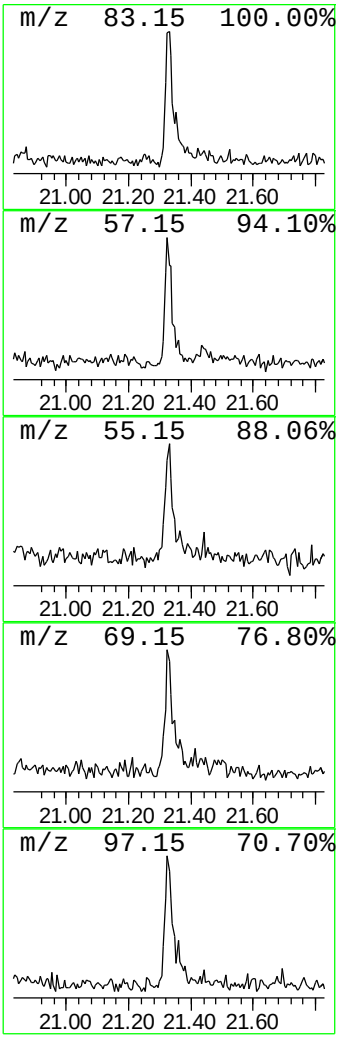
Peak Number 12 3-Octadecene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	3.03 ng	156227	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	92
2	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	91
3	Behenic alcohol	326	C22H46O	000661-19-8	87
4	1-Heneicosanol	312	C21H44O	015594-90-8	87
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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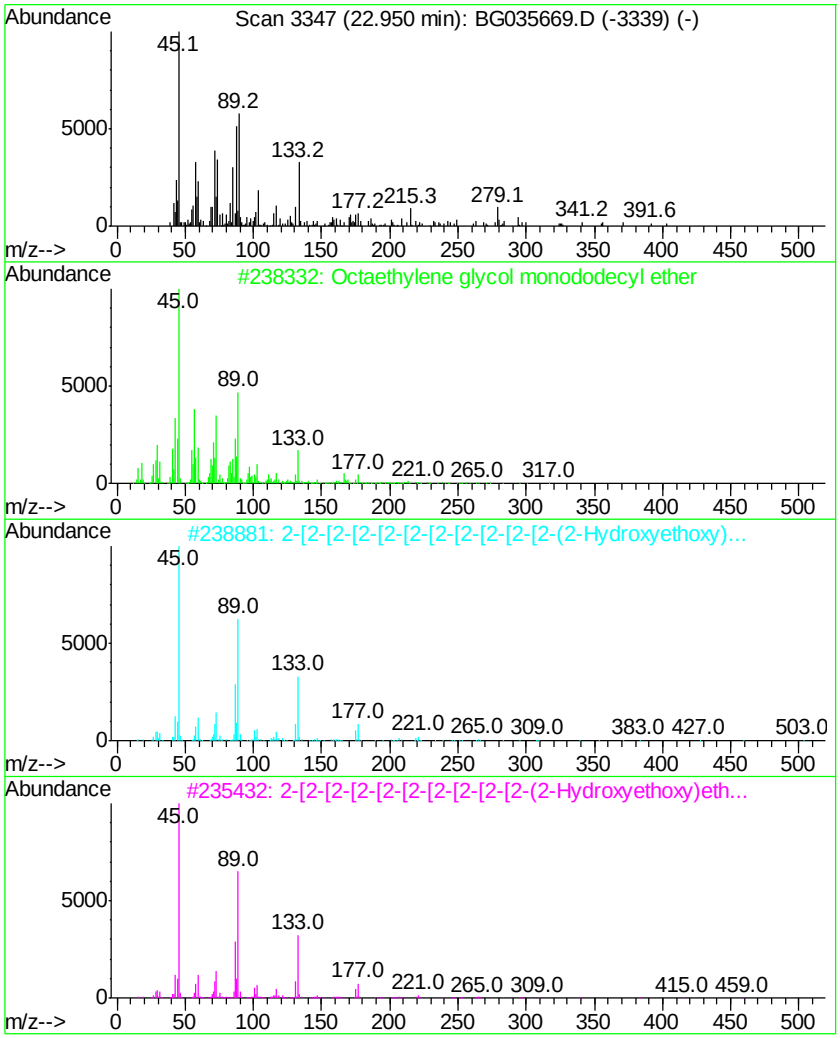
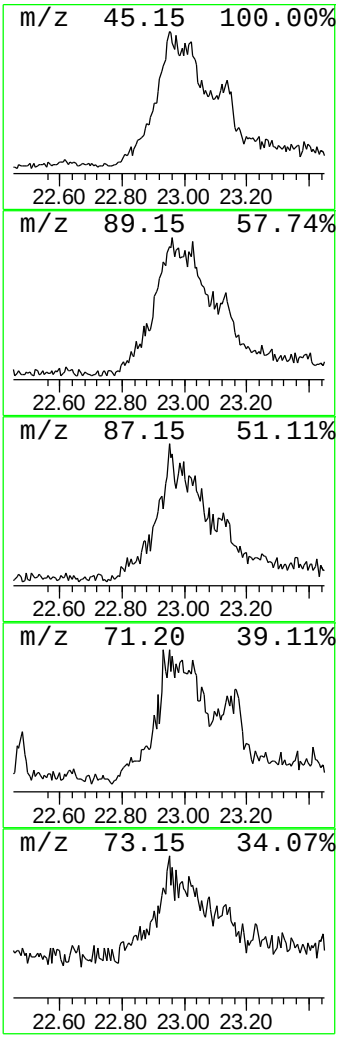
Peak Number 13 Octaethylene glycol monodod... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.95	5.36 ng	276370	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octaethylene glycol monododecyl ...	538	C28H58O9	003055-98-9	59
2	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	49
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	49
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	43
5	1-Chloro-3-methoxy-propan-2-ol, ...	238	C10H23ClO2Si	1000373-19-3	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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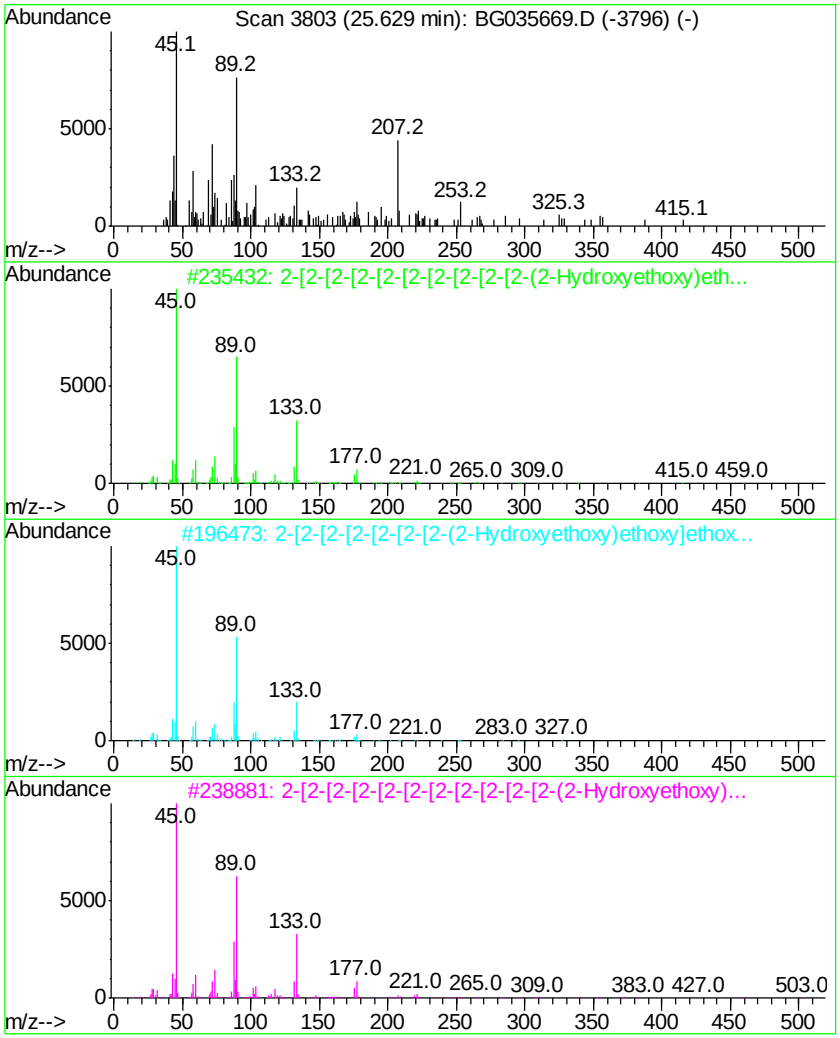
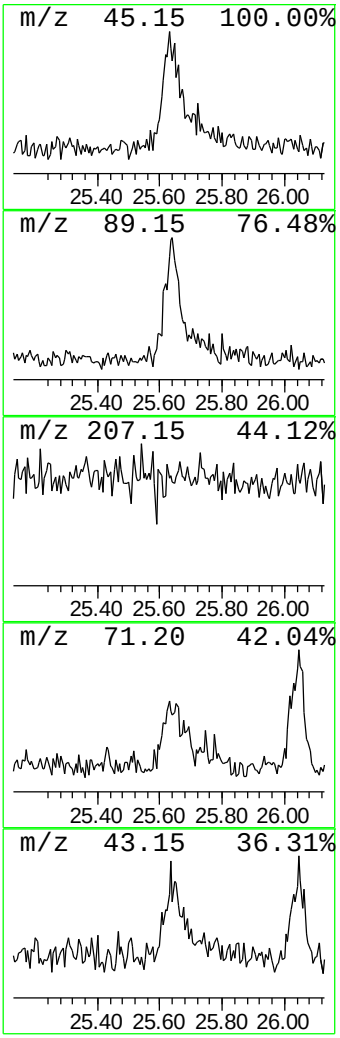
Peak Number 14 2-[2-[2-[2-[2-[2-[2-[2-[2-[... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.63	2.28 ng	118173	Perylene-d12	24.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	59
2	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	59
3	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	59
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	59
5	1,4,7,10,13,16-Hexaoxanonadecane...	320	C16H32O6	1000163-65-3	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071618\
Data File : BG035669.D
Acq On : 16 Jul 2018 14:41
Operator : JU/SJ
Sample : J3964-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : N48967

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	7.3	ng	122231	1	8.06	333781	20.0
unknown7.59	7.59	126.5	ng	2110390	1	8.06	333781	20.0
unknown10.08	10.08	3.8	ng	93657	2	10.86	498498	20.0
Benzothiazole	11.51	7.5	ng	186758	2	10.86	498498	20.0
o-Cyanobenzoic acid	14.39	2.7	ng	96649	3	14.68	714391	20.0
Benzoic acid, p-t...	14.48	2.2	ng	79225	3	14.68	714391	20.0
2(3H)-Benzothiazo...	16.35	2.4	ng	106554	4	17.42	882232	20.0
Oxazolidin-2-one,...	16.96	2.3	ng	99121	4	17.42	882232	20.0
n-Hexadecanoic acid	18.30	3.5	ng	155851	4	17.42	882232	20.0
2-Mercaptobenzoth...	18.66	28.1	ng	1239500	4	17.42	882232	20.0
3-Octadecene, (E)-	21.33	3.0	ng	156227	5	21.69	1030470	20.0
Octaethylene glyc...	22.95	5.4	ng	276370	5	21.69	1030470	20.0
2-[2-[2-[2-[2-[2-...	25.63	2.3	ng	118173	6	24.90	1036690	20.0