LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062317\
Data File : BG027648.D
Acq On : 24 Jun 2017 2:29
Operator : SJ/JU
Sample : I3808-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DRUM-001-003-004-COMP

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-BG062117.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	5.643	293	299	306	rBV	20452	32599	1.93%	0.448%
2	6.090	368	375	387	rBV	145106	248302	14.69%	3.414%
3	7.641	632	639	652	rVB2	95483	178506	10.56%	2.454%
4	8.035	699	706	716	rBV	233246	427125	25.27%	5.873%
5	8.505	778	786	795	rBV	65521	121028	7.16%	1.664%
6	8.834	834	842	850	rBV	207534	389331	23.03%	5.353%
7	9.668	976	984	991	rBV	180656	336917	19.93%	4.633%
8	11.325	1258	1266	1273	rBV	89019	174290	10.31%	2.396%
9	11.965	1369	1375	1381	rBV2	11626	20522	1.21%	0.282%
10	13.710	1663	1672	1680	rBV	555619	863861	51.10%	11.878%
11	14.515	1803	1809	1819	rBV	53711	81813	4.84%	1.125%
12	15.085	1900	1906	1914	rBV2	158362	263731	15.60%	3.626%
13	15.796	2022	2027	2032	rBV	39950	58159	3.44%	0.800%
14	16.572	2152	2159	2169	rVB	498345	793095	46.91%	10.905%
15	16.742	2184	2188	2196	rBV4	15458	28873	1.71%	0.397%
16	17.835	2368	2374	2386	rVB	250386	400343	23.68%	5.505%
17	18.675	2511	2517	2527	rBV	80470	128612	7.61%	1.768%
18	19.868	2715	2720	2725	rVB	18800	23302	1.38%	0.320%
19	19.927	2726	2730	2738	rVV	39733	59022	3.49%	0.812%
20	20.414	2802	2813	2819	rBV	1223563	1690538	100.00%	23.245%
21	21.766	3038	3043	3049	rBV7	21577	48083	2.84%	0.661%
22	22.200	3110	3117	3129	rVB	246359	471004	27.86%	6.476%
23	25.837	3724	3736	3750	rBV3	129890	433689	25.65%	5.963%

Sum of corrected areas: 7272745

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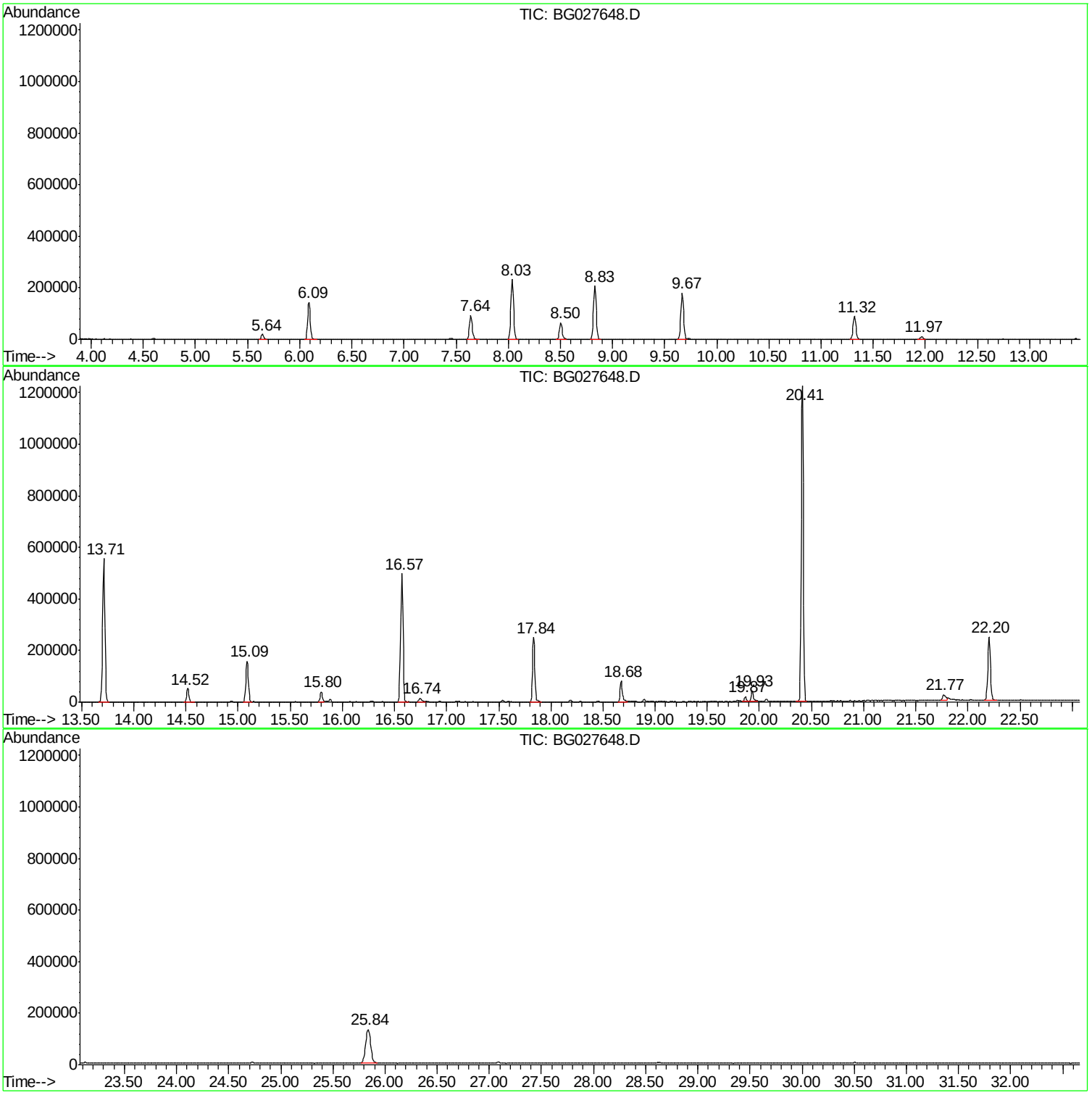
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DRUM-001-003-004-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.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

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062317\
Data File : BG027648.D
Acq On : 24 Jun 2017 2:29
Operator : SJ/JU
Sample : I3808-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DRUM-001-003-004-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

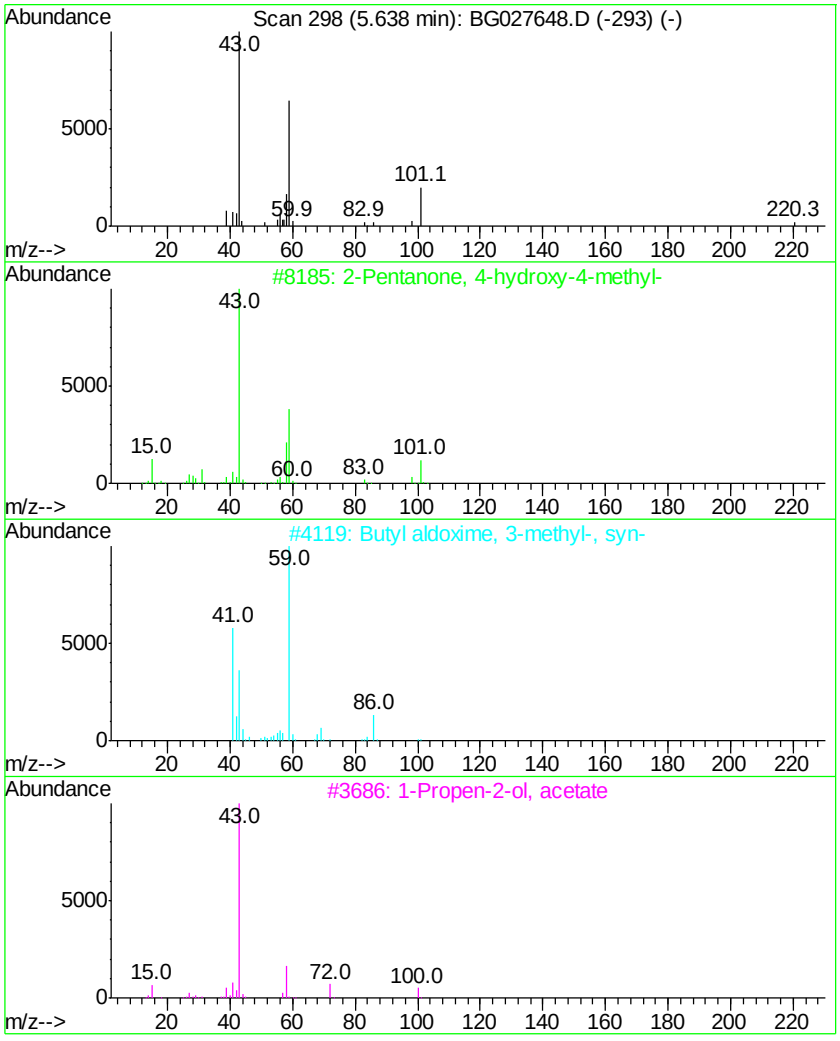
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

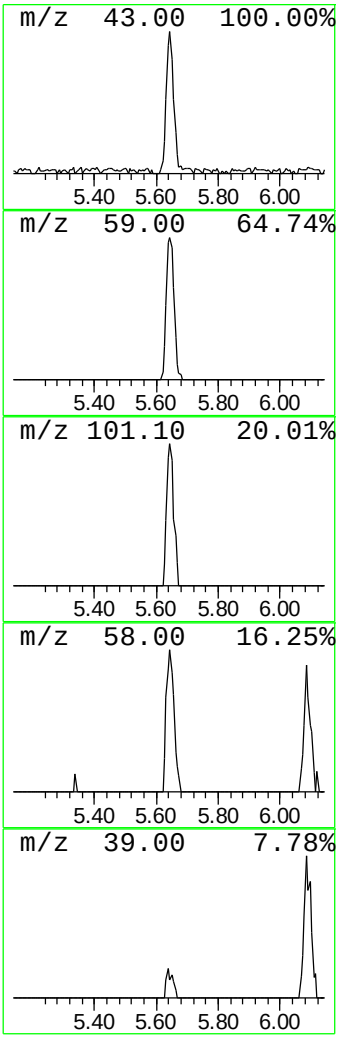
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	5.39 ng	32599	1,4-Dichlorobenzene-d4	8.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Operator : SJ/JU
Sample : I3808-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DRUM-001-003-004-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

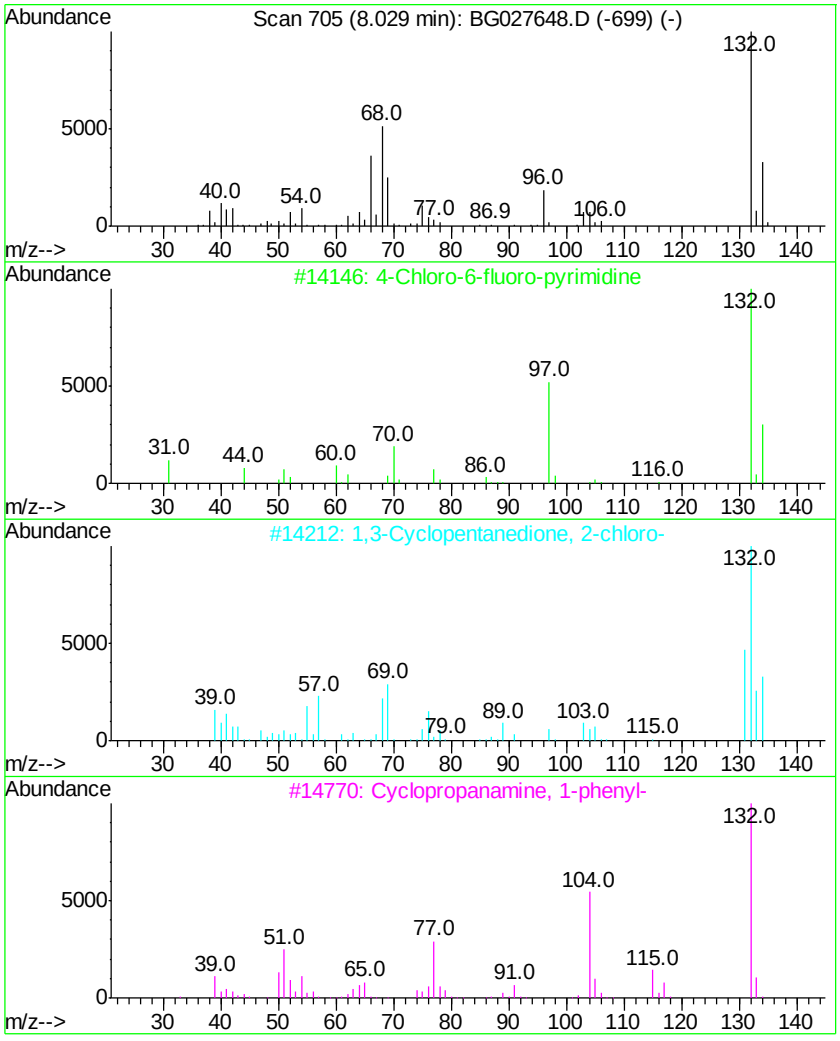
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

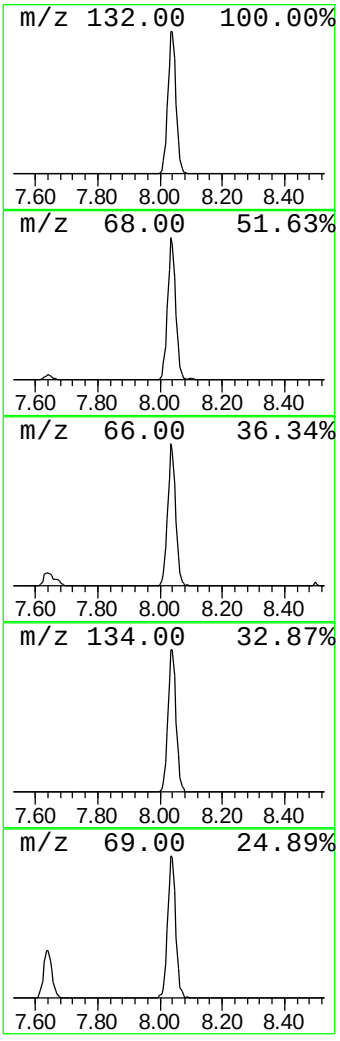
****

Peak Number 2 unknown8.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.03	70.58 ng	427125	1,4-Dichlorobenzene-d4	8.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16





Data Path : Z:\HPCHEM1\BNA G\DATA\BG062317\
Data File : BG027648.D
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Operator : SJ/JU
Sample : I3808-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DRUM-001-003-004-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

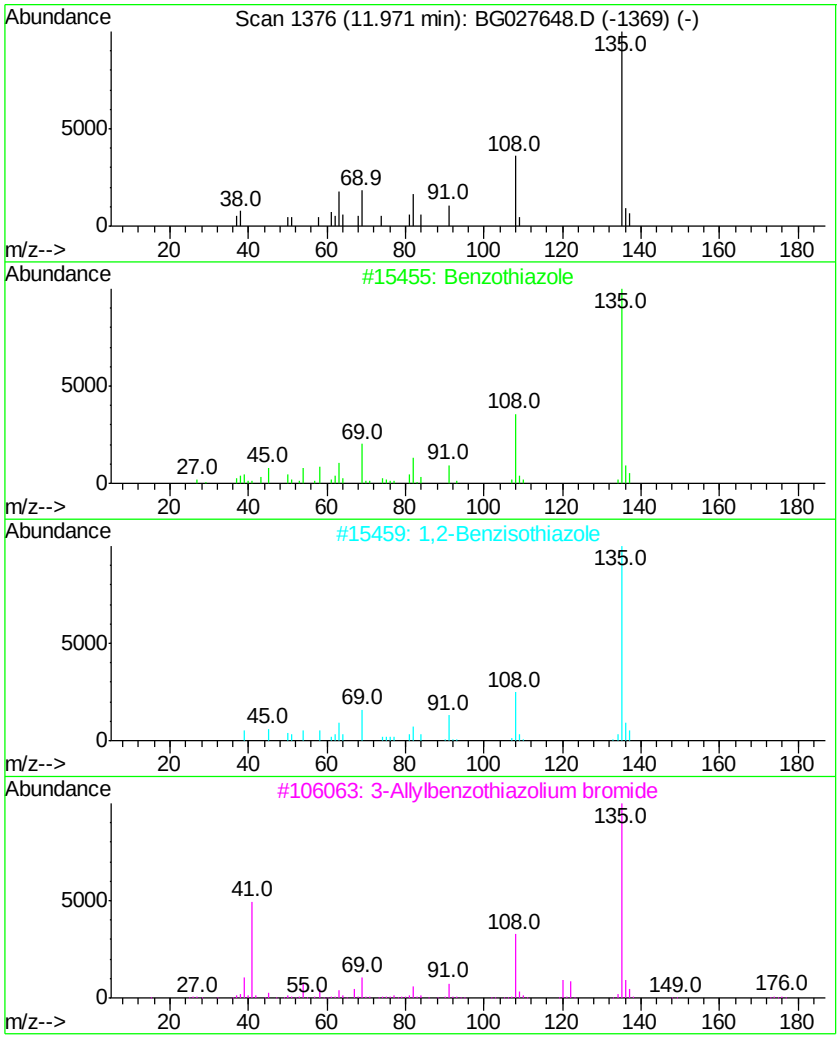
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

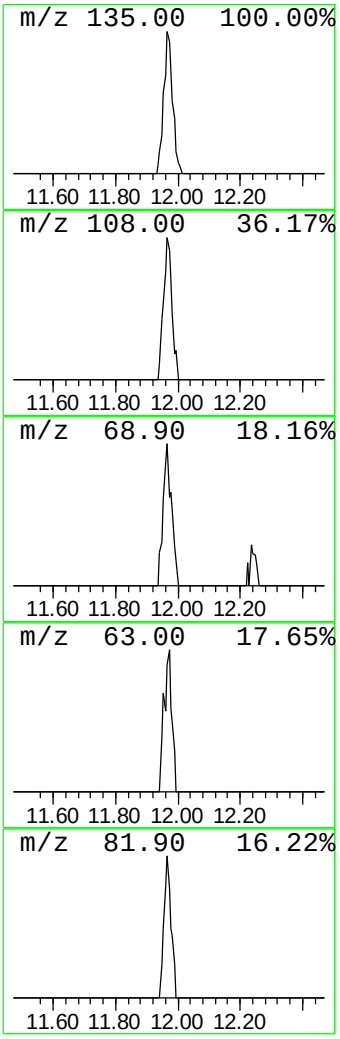
****

Peak Number 4 Benzothiazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.35 ng	20522	Naphthalene-d8	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	91
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	64
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	59
4	Adenine	135	C5H5N5	000073-24-5	52
5	Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	000459-22-3	52





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Data File : BG027648.D
Acq On : 24 Jun 2017 2:29
Operator : SJ/JU
Sample : I3808-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DRUM-001-003-004-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.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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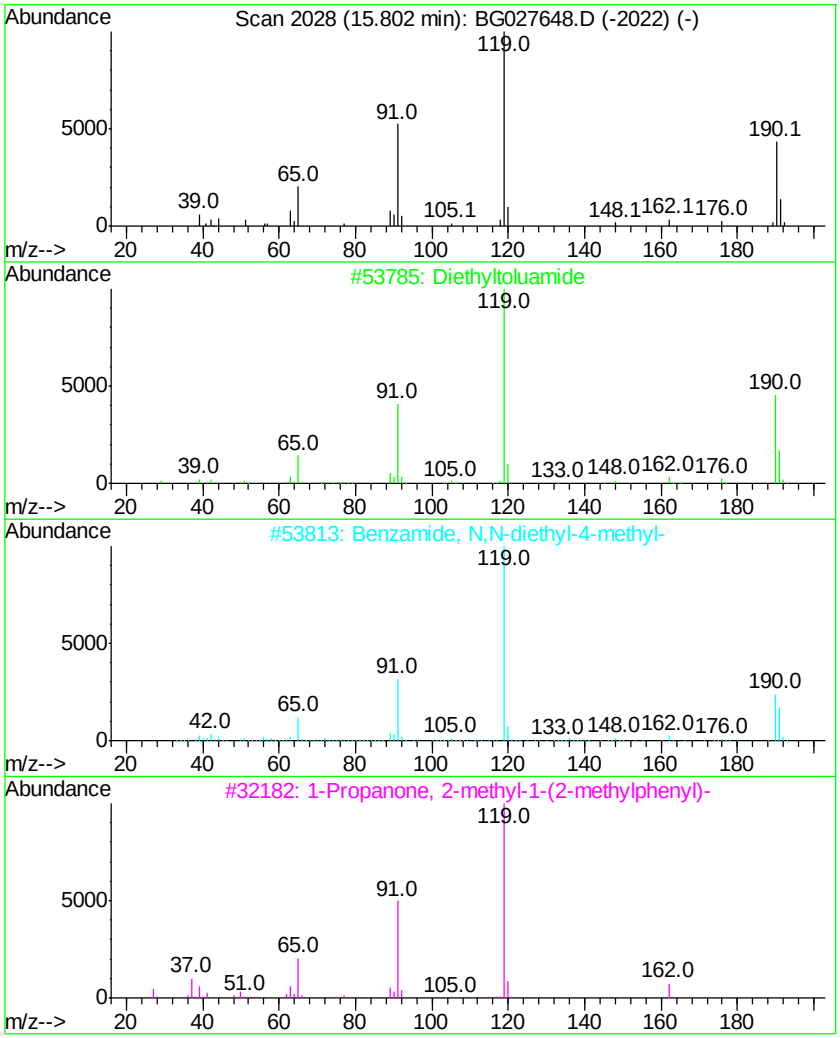
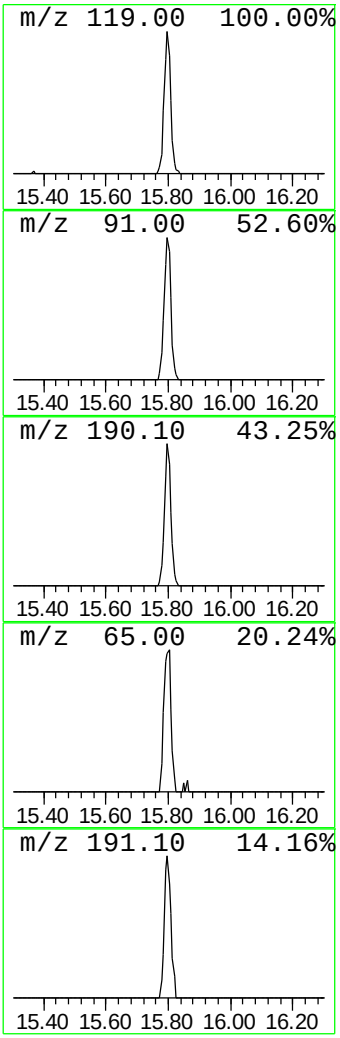
Peak Number 5 Diethyltoluamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	4.41 ng	58159	Acenaphthene-d10	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	76
3	1-Propanone, 2-methyl-1-(2-methy...	162	C11H14O	002040-21-3	52
4	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	000140-76-1	52
5	4-Methylbenzoic acid, pentafluor...	302	C14H7F5O2	1000354-15-1	50





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Operator : SJ/JU
Sample : I3808-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DRUM-001-003-004-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.M
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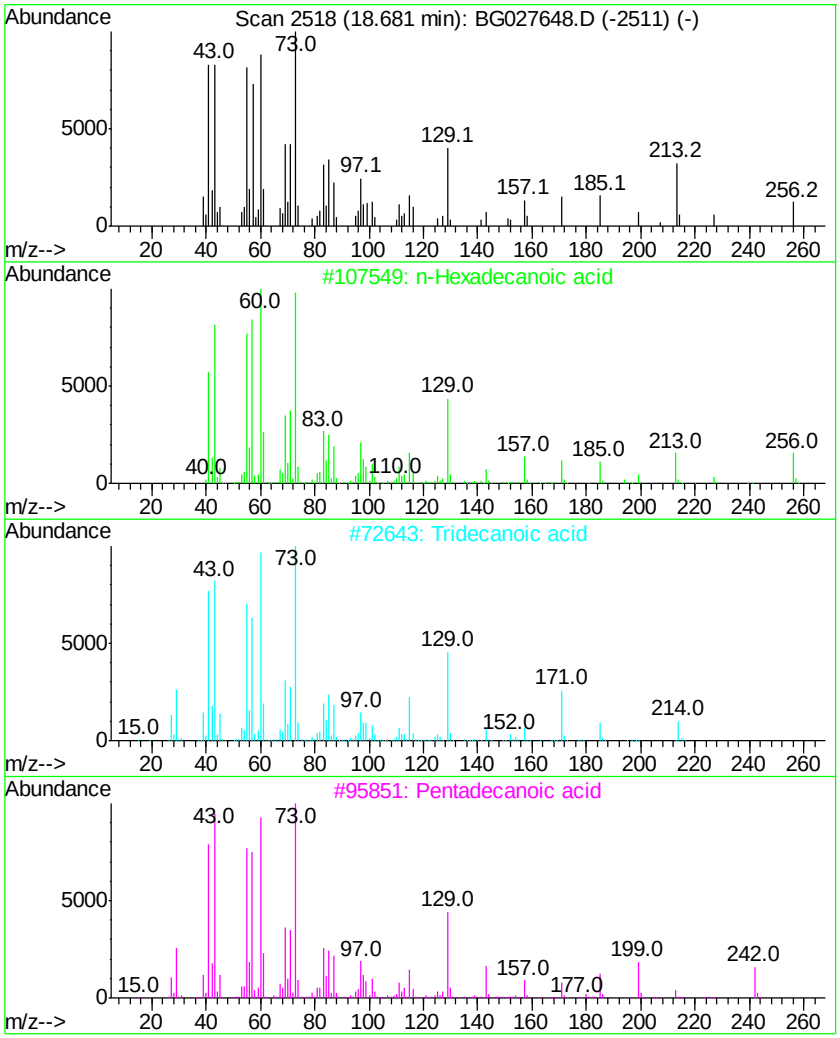
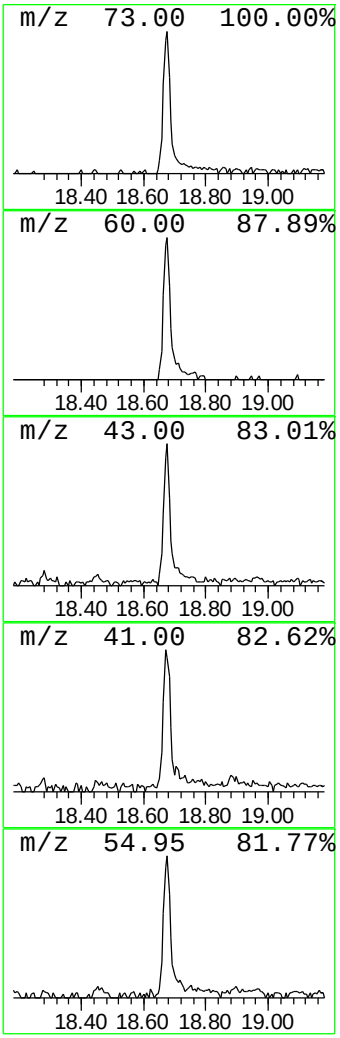
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.68	6.43 ng	128612	Phenanthrene-d10	17.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20





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Misc :
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Instrument : BNA_G
ClientSampleId : DRUM-001-003-004-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.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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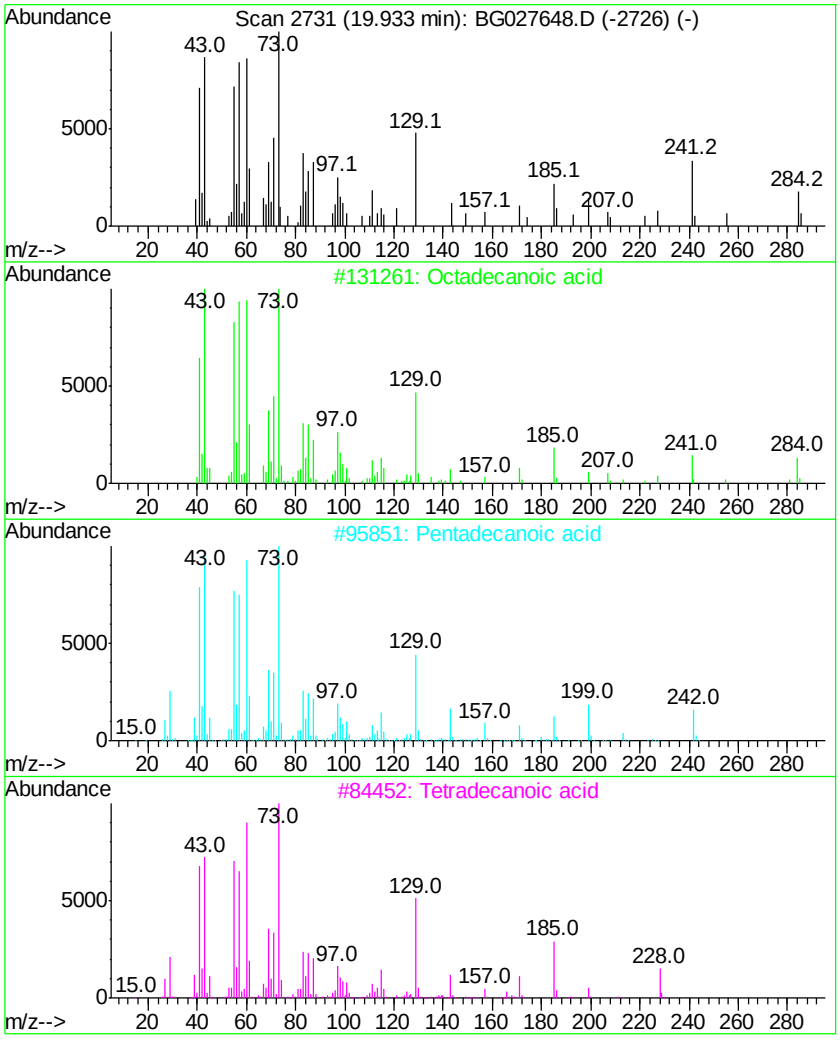
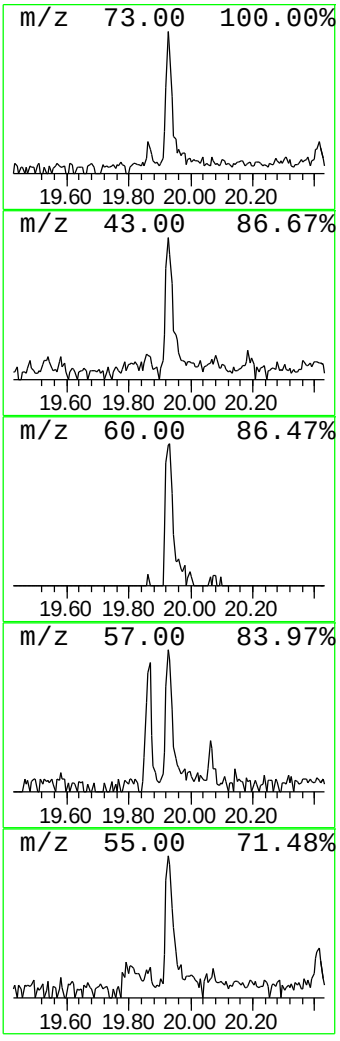
Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.93	2.95 ng	59022	Phenanthrene-d10	17.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

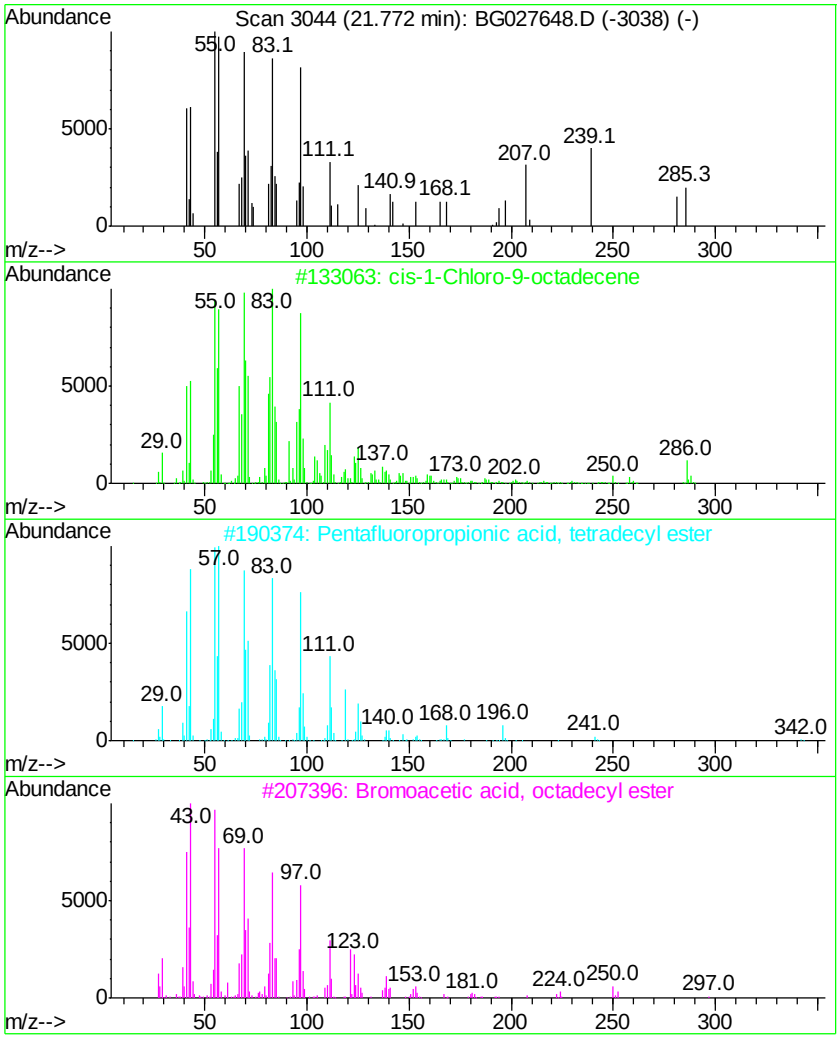
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

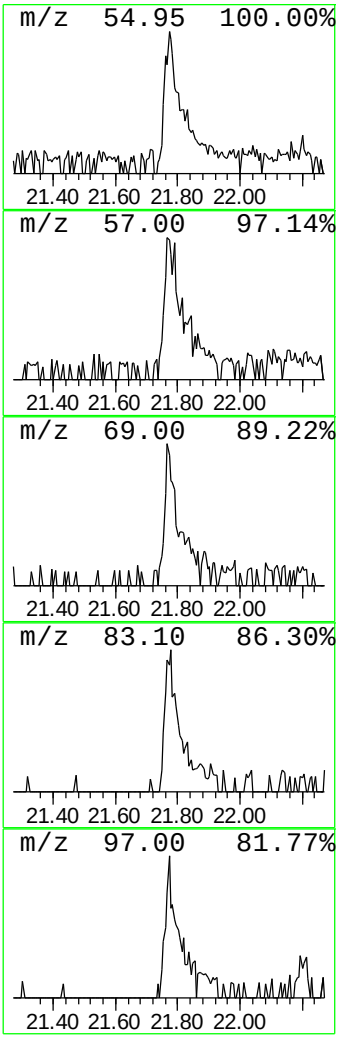
****

Peak Number 8 cis-1-Chloro-9-octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.77	2.04 ng	48083	Chrysene-d12	22.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	64
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	60
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	60
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	50
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	50





Tentatively Identified Compound (LSC) summary

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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...	5.64	5.4	ng	32599	1	8.50	121028	20.0
unknown8.03	8.03	70.6	ng	427125	1	8.50	121028	20.0
Benzothiazole	11.97	2.4	ng	20522	2	11.32	174290	20.0
Diethyltoluamide	15.80	4.4	ng	58159	3	15.09	263731	20.0
n-Hexadecanoic acid	18.68	6.4	ng	128612	4	17.84	400343	20.0
Octadecanoic acid	19.93	3.0	ng	59022	4	17.84	400343	20.0
cis-1-Chloro-9-oc...	21.77	2.0	ng	48083	5	22.20	471004	20.0