LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091118\
Data File : BG036660.D
Acq On : 11 Sep 2018 17:32
Operator : JU/SJ
Sample : J4841-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

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-BG082318.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	5.158	313	318	324	rBV	38964	58582	1.28%	0.294%
2	5.622	389	397	410	rBV	364915	589042	12.87%	2.954%
3	7.203	659	666	676	rBV	231676	424907	9.28%	2.131%
4	7.585	723	731	738	rBV	633419	1074846	23.49%	5.389%
5	8.055	804	811	817	rBV	197994	341213	7.46%	1.711%
6	8.378	858	866	874	rBV	828821	1437481	31.41%	7.208%
7	9.212	1000	1008	1017	rBV	713855	1264283	27.63%	6.339%
8	10.857	1281	1288	1295	rBV	284453	496209	10.84%	2.488%
9	13.301	1696	1704	1714	rBV	1944177	2989181	65.32%	14.988%
10	13.566	1743	1749	1757	rBV	431776	673855	14.72%	3.379%
11	14.124	1838	1844	1850	rBV	216523	313653	6.85%	1.573%
12	14.676	1931	1938	1946	rBV2	447722	716806	15.66%	3.594%
13	15.787	2122	2127	2141	rBV	96126	188561	4.12%	0.945%
14	16.163	2183	2191	2204	rBV	954155	1516351	33.13%	7.603%
15	17.420	2399	2405	2414	rBV2	626718	938433	20.51%	4.705%
16	18.301	2550	2555	2563	rBV2	62346	99902	2.18%	0.501%
17	19.477	2750	2755	2759	rVB2	44358	56458	1.23%	0.283%
18	20.029	2841	2849	2858	rBV	3410474	4576337	100.00%	22.946%
19	21.363	3068	3076	3089	rBV5	40894	182210	3.98%	0.914%
20	21.686	3124	3131	3143	rBV2	578862	1048375	22.91%	5.257%
21	24.894	3665	3677	3690	rBV	290638	957130	20.91%	4.799%

Sum of corrected areas: 19943815

LSC Report - Integrated Chromatogram

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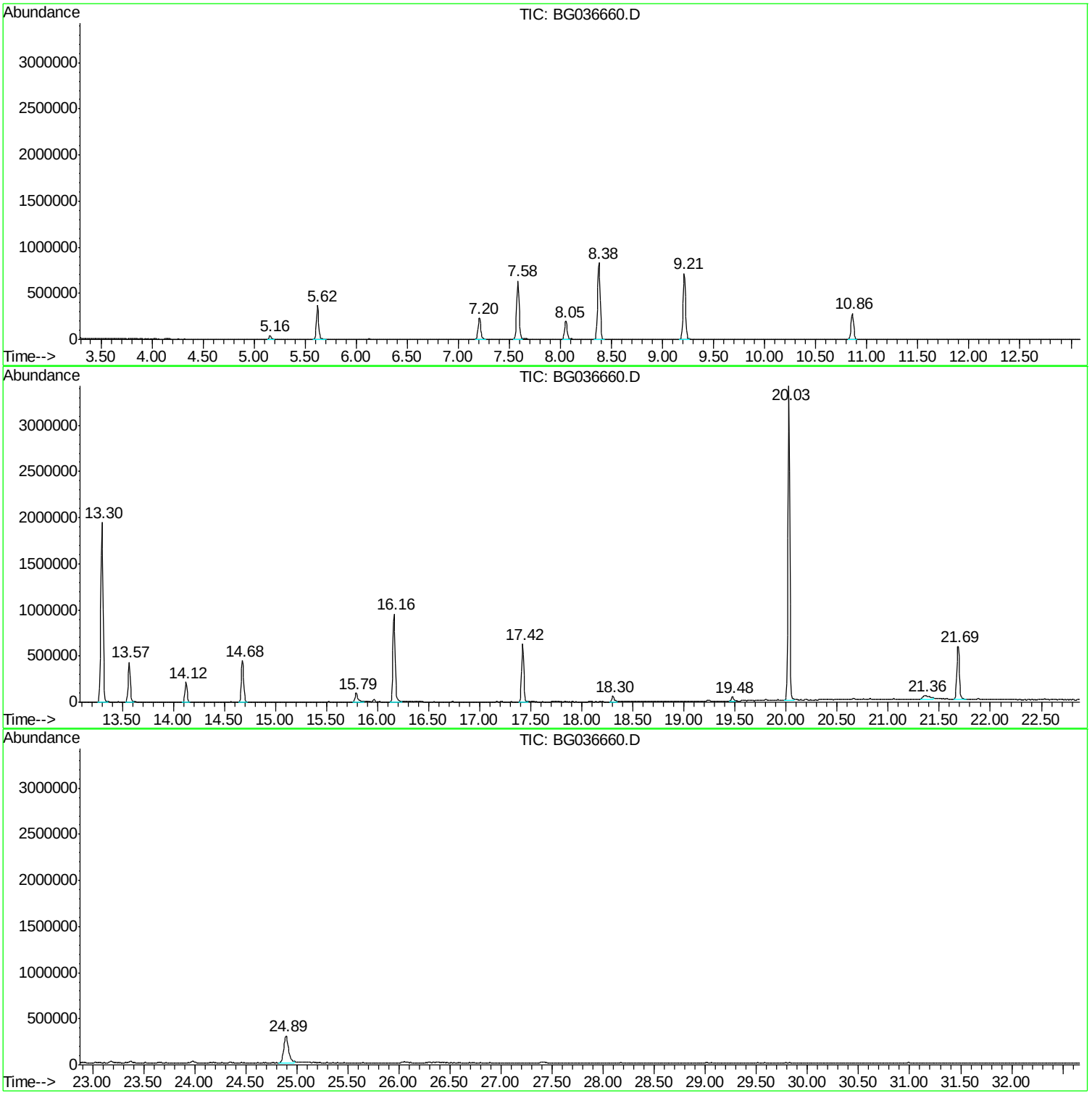
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091118\
Data File : BG036660.D
Acq On : 11 Sep 2018 17:32
Operator : JU/SJ
Sample : J4841-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

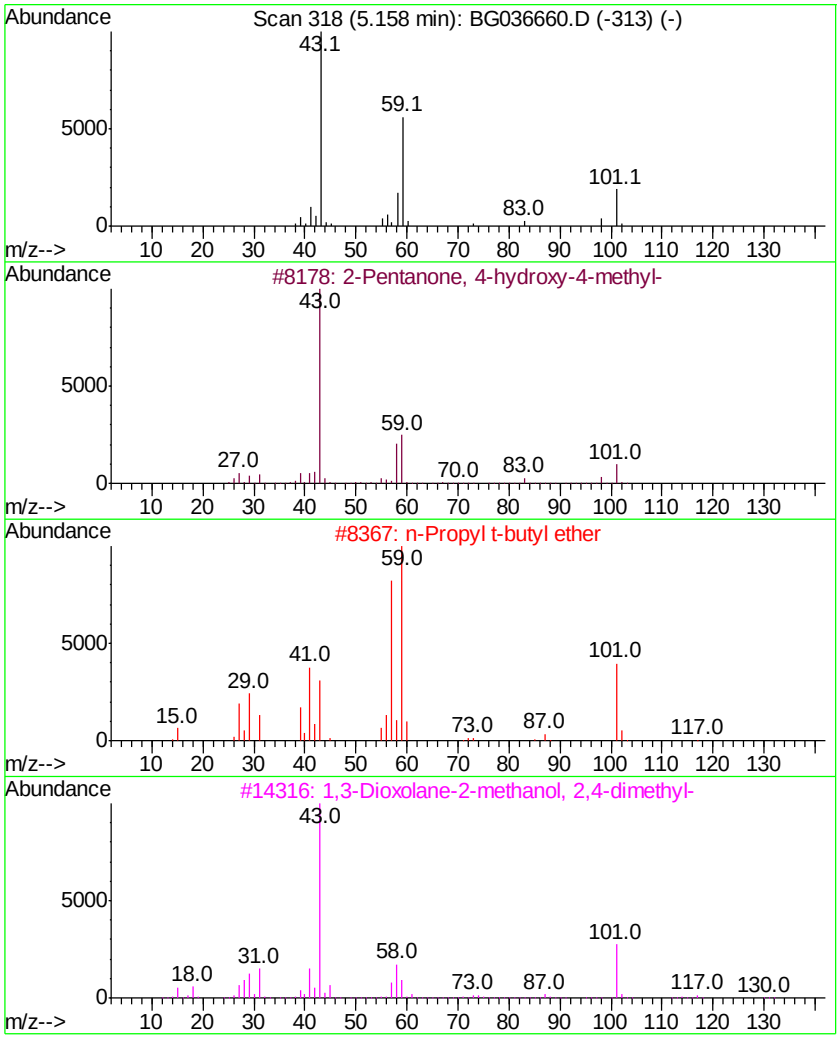
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

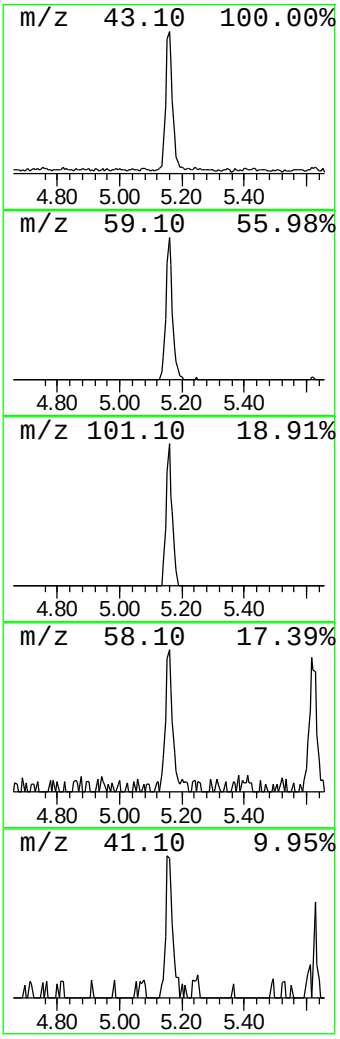
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	3.43 ng	58582	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	17
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
5	Acetone	58	C3H6O	000067-64-1	9





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Data File : BG036660.D
Acq On : 11 Sep 2018 17:32
Operator : JU/SJ
Sample : J4841-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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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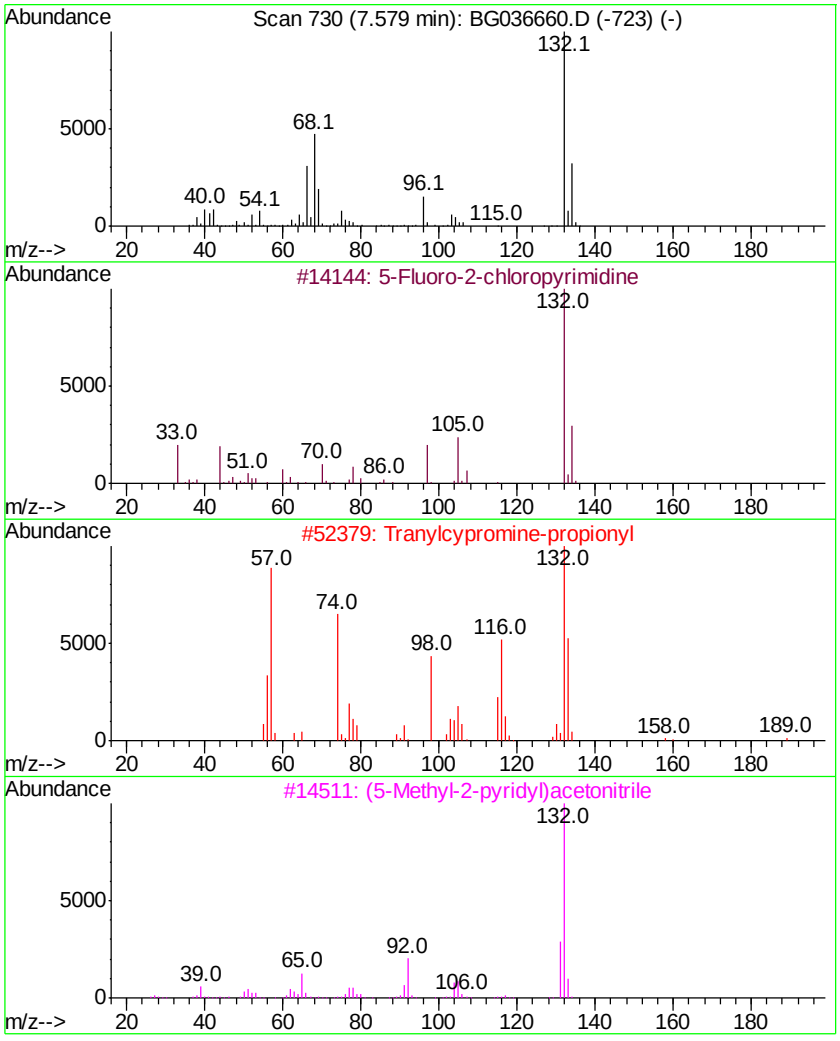
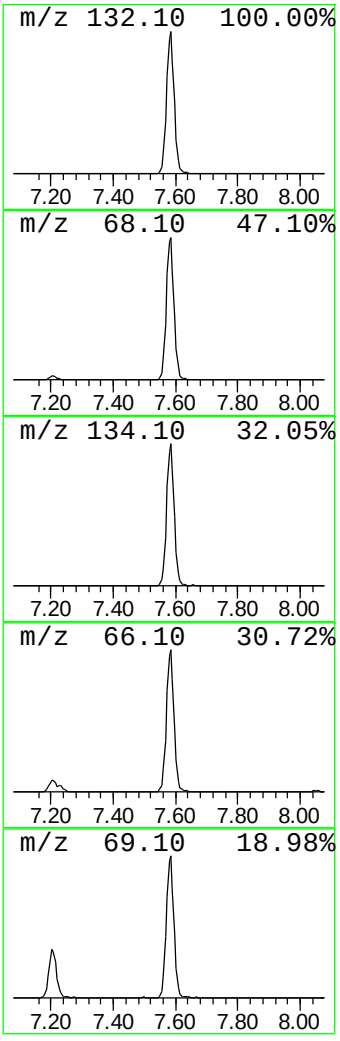
Peak Number 2 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	63.00 ng	1074850	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091118\
Data File : BG036660.D
Acq On : 11 Sep 2018 17:32
Operator : JU/SJ
Sample : J4841-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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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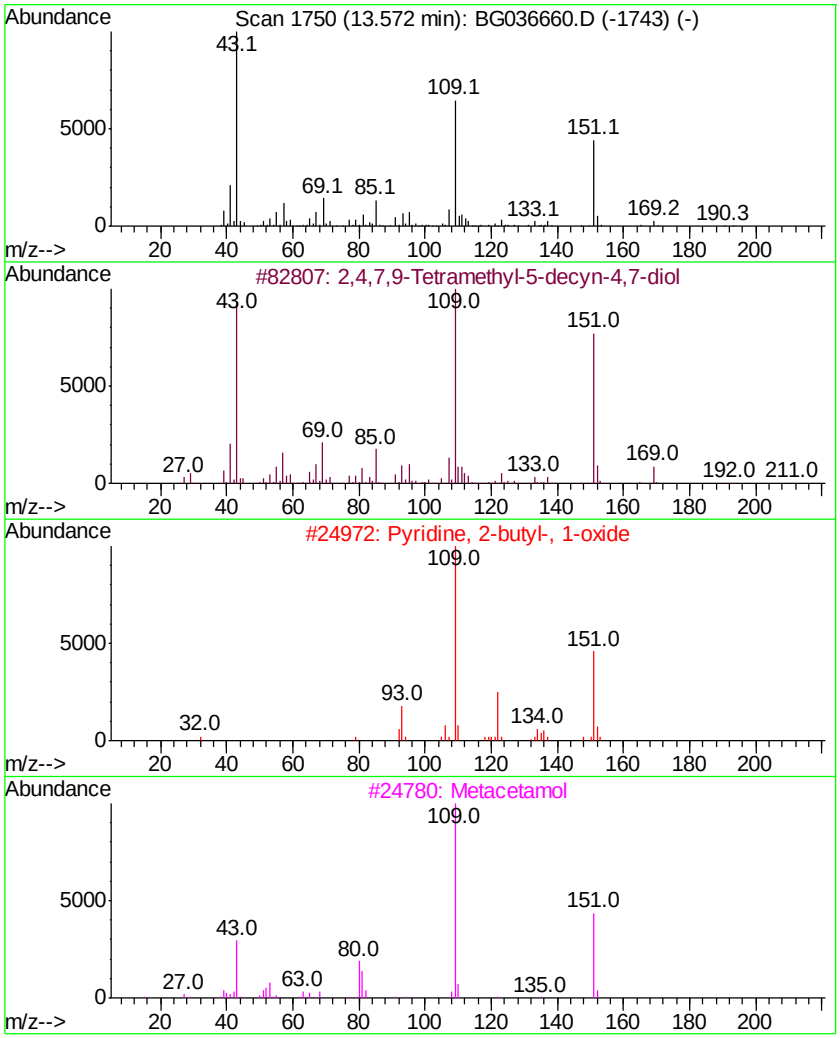
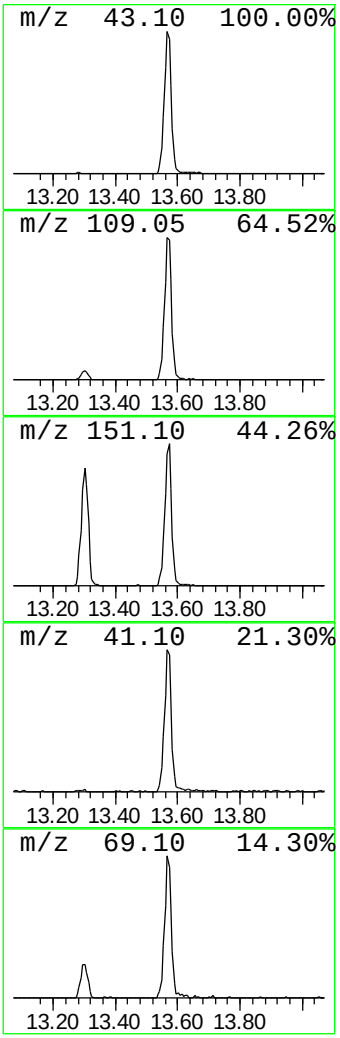
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	18.80 ng	673855	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Metacetamol	151	C8H9NO2	000621-42-1	53
4	Acetaminophen	151	C8H9NO2	000103-90-2	53
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53





Library Search Compound Report

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Data File : BG036660.D
Acq On : 11 Sep 2018 17:32
Operator : JU/SJ
Sample : J4841-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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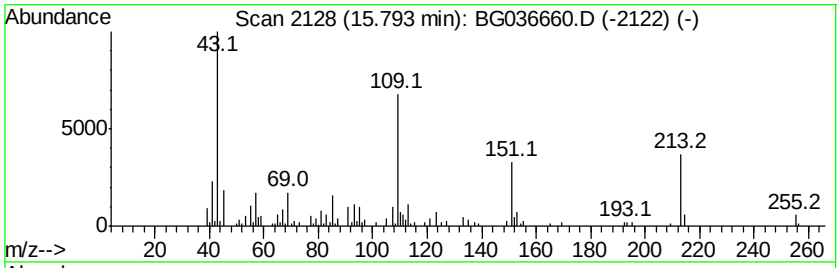
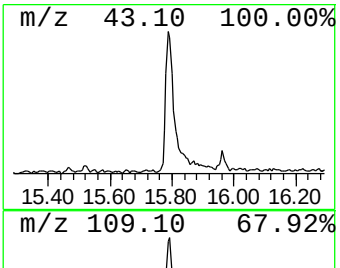
****

Peak Number 5 Camphorsulfonic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	5.26 ng	188561	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	53
2	Camphorsulfonic acid	232	C10H16O4S	003144-16-9	43
3	Metacetamol	151	C8H9NO2	000621-42-1	38
4	Acetaminophen	151	C8H9NO2	000103-90-2	38
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091118\
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Acq On : 11 Sep 2018 17:32
Operator : JU/SJ
Sample : J4841-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

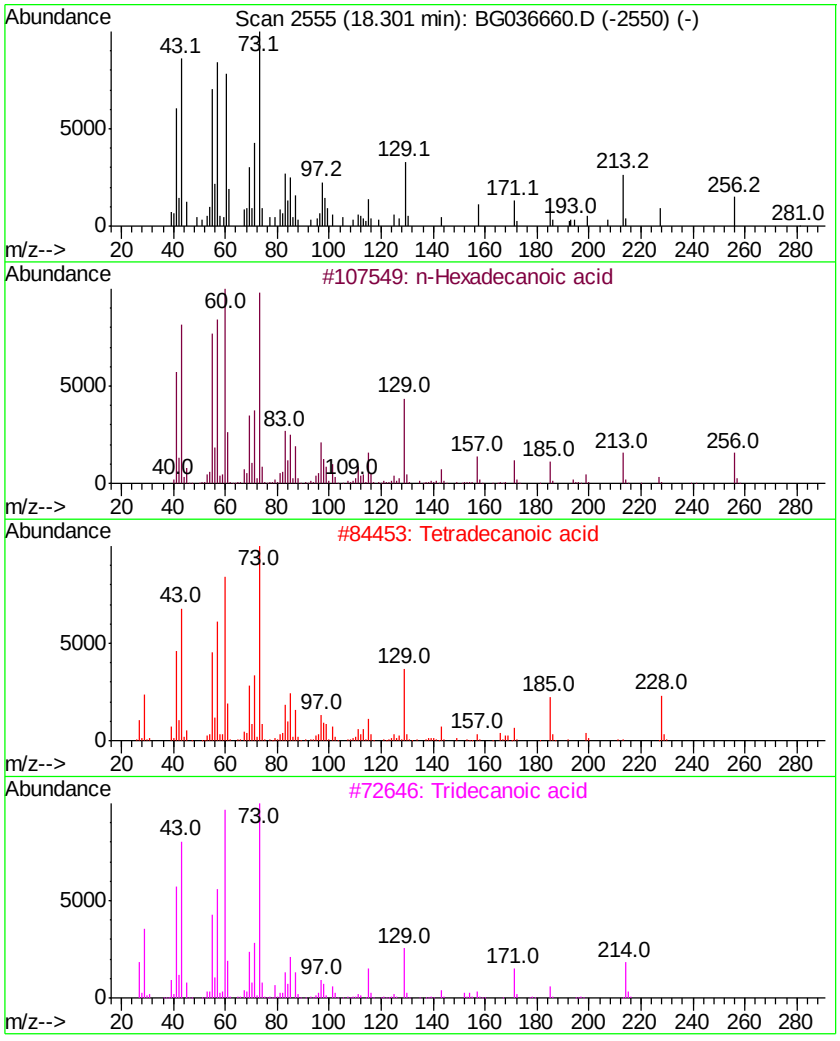
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

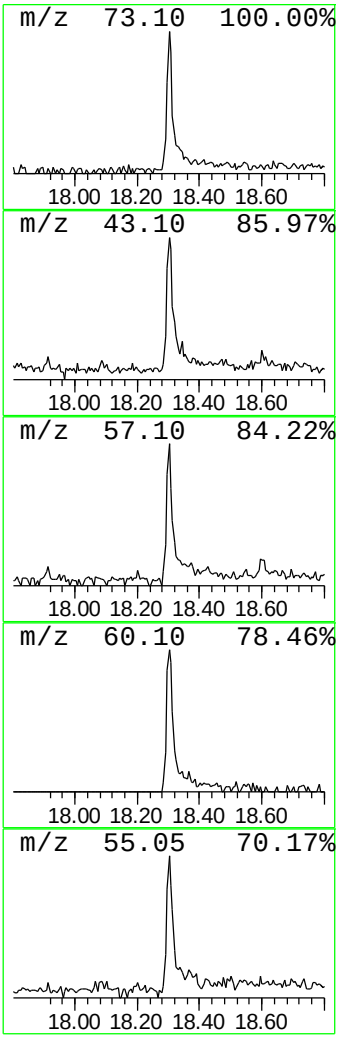
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.13 ng	99902	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50





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Misc :
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Instrument : BNA_G
ClientSampleId : 090718-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

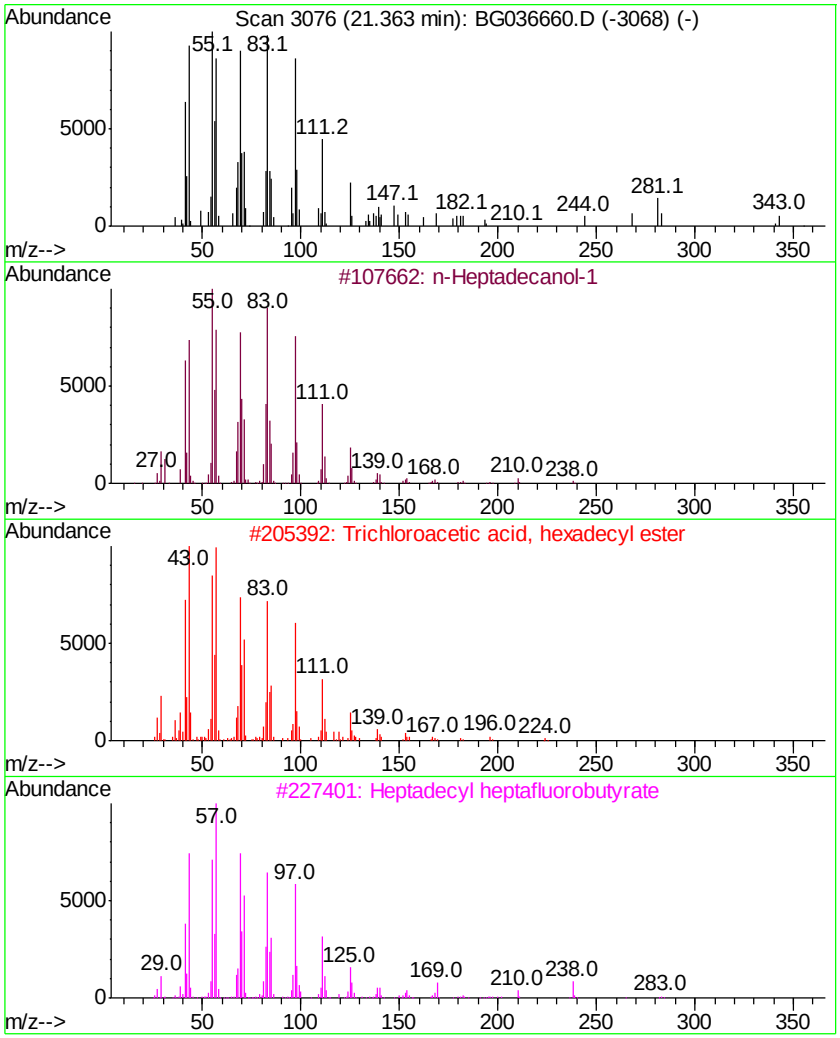
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

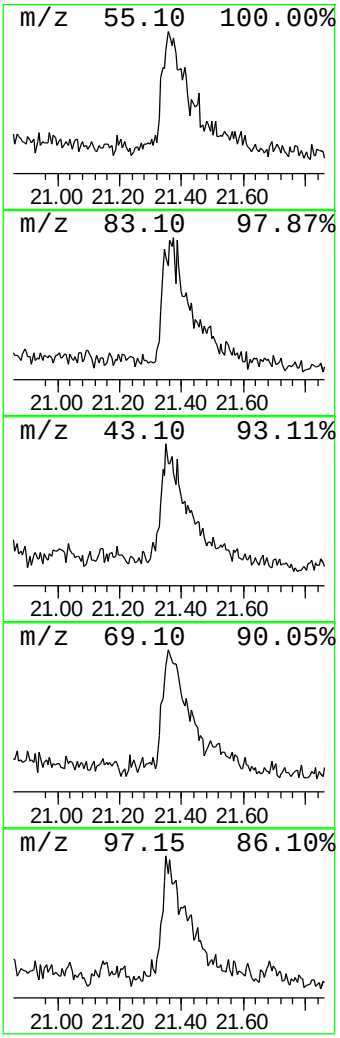
****

Peak Number 7 n-Heptadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.36	3.48 ng	182210	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	80
4	Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	70
5	10-Heneicosene (c,t)	294	C21H42	095008-11-0	70





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	3.4	ng	58582	1	8.05	341213	20.0
unknown7.58	7.58	63.0	ng	1074850	1	8.05	341213	20.0
2,4,7,9-Tetrameth...	13.57	18.8	ng	673855	3	14.68	716806	20.0
Camphorsulfonic acid	15.79	5.3	ng	188561	3	14.68	716806	20.0
n-Hexadecanoic acid	18.30	2.1	ng	99902	4	17.42	938433	20.0
n-Heptadecanol-1	21.36	3.5	ng	182210	5	21.68	1048380	20.0