LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082418\
Data File : BG036412.D
Acq On : 24 Aug 2018 13:45
Operator : JU/SJ
Sample : J4568-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 081718-DBRI-E-U-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	5.632	392	399	407	rBV	367585	568640	12.68%	3.019%
2	7.213	661	668	677	rBV	240584	403069	8.99%	2.140%
3	7.595	726	733	741	rBV	622816	1042229	23.23%	5.534%
4	8.065	804	813	820	rBV	185234	311525	6.94%	1.654%
5	8.388	861	868	876	rVB	807367	1379228	30.75%	7.323%
6	9.228	1002	1011	1019	rBV	681784	1218564	27.17%	6.470%
7	10.873	1282	1291	1299	rVB	250793	451823	10.07%	2.399%
8	13.318	1700	1707	1716	rVB	1916410	2921322	65.13%	15.511%
9	14.686	1933	1940	1950	rBV2	421351	699803	15.60%	3.716%
10	15.985	2156	2161	2167	rBV	104686	134913	3.01%	0.716%
11	16.173	2187	2193	2204	rBV	1055455	1555393	34.67%	8.258%
12	17.430	2401	2407	2416	rBV2	584776	881106	19.64%	4.678%
13	18.318	2554	2558	2564	rBV5	30241	44963	1.00%	0.239%
14	20.039	2845	2851	2862	rBV	3312241	4485684	100.00%	23.817%
15	21.355	3070	3075	3085	rBV2	51578	110987	2.47%	0.589%
16	21.696	3126	3133	3141	rVB	655959	1087018	24.23%	5.772%
17	23.053	3356	3364	3377	rBV	212810	506827	11.30%	2.691%
18	24.916	3671	3681	3692	rBV2	383514	1030975	22.98%	5.474%

Sum of corrected areas: 18834069

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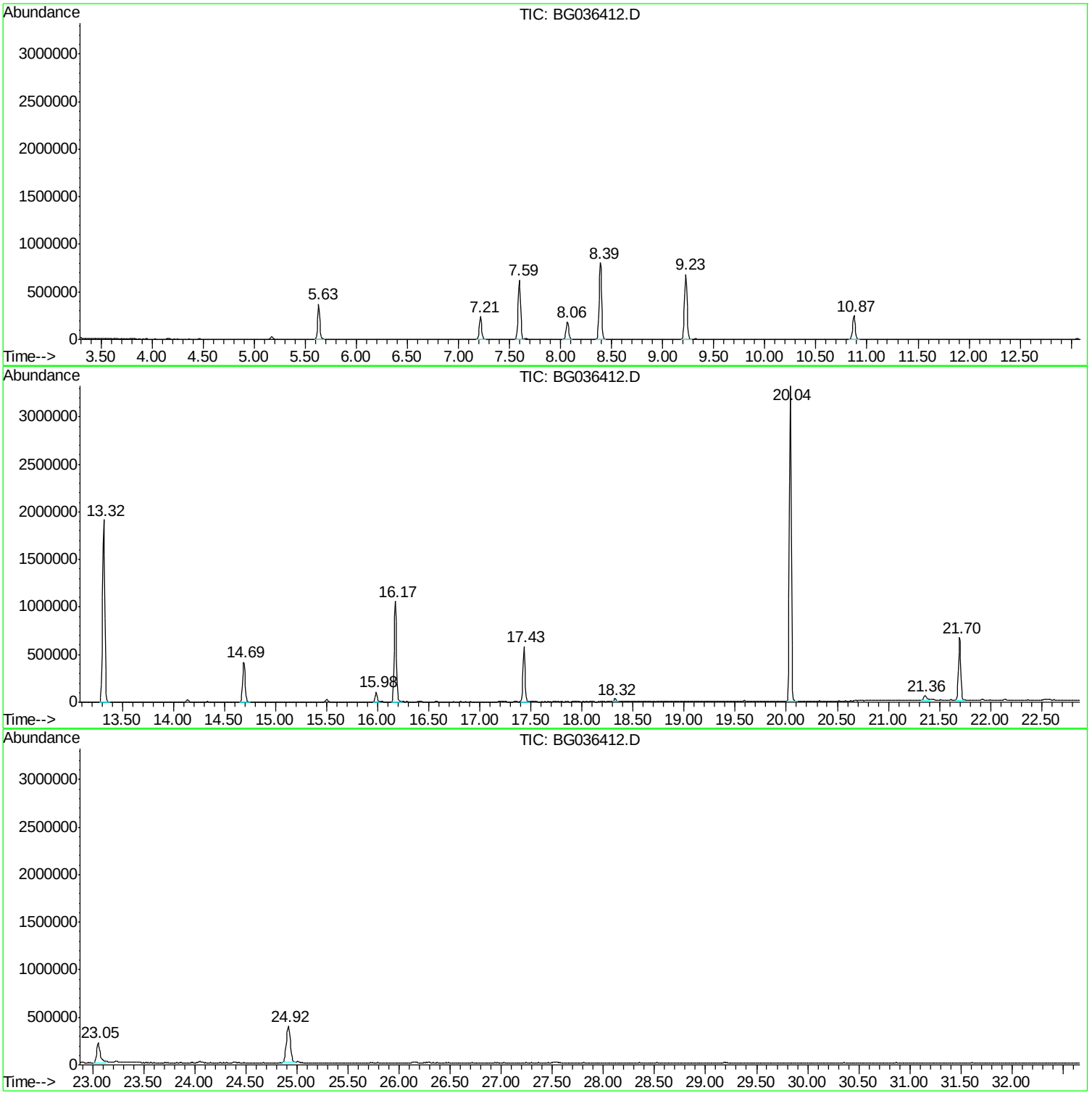
Instrument :
BNA_G
ClientSampleId :
081718-DBRI-E-U-S

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082418\
Data File : BG036412.D
Acq On : 24 Aug 2018 13:45
Operator : JU/SJ
Sample : J4568-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 081718-DBRI-E-U-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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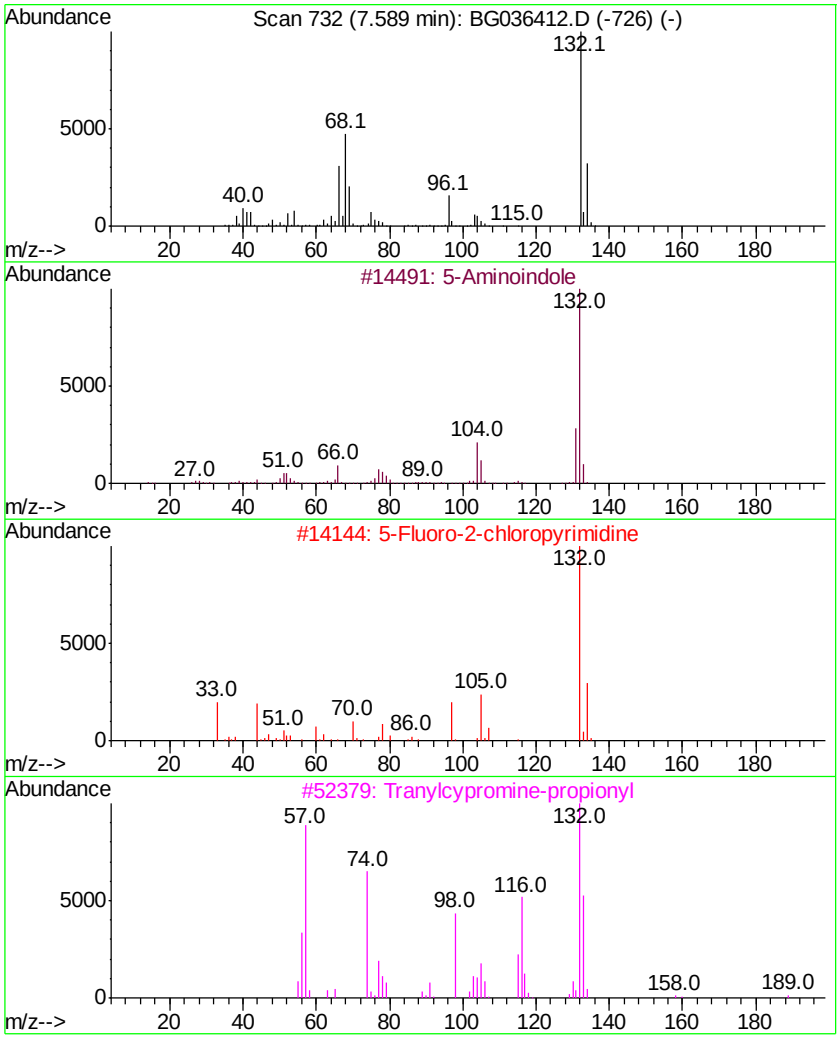
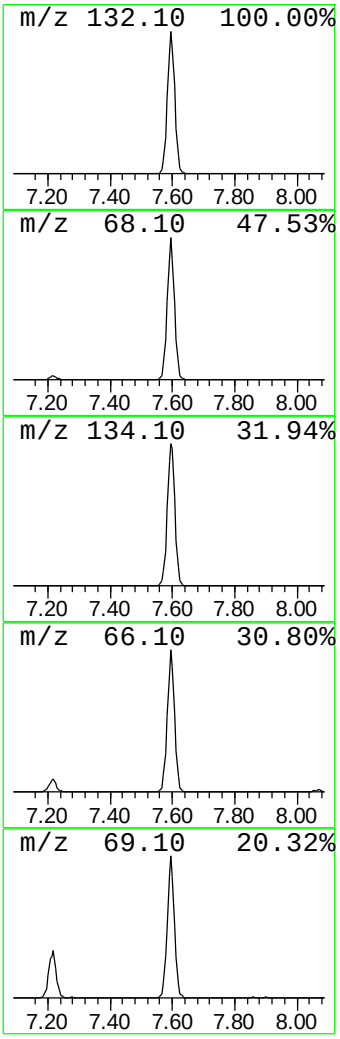
Peak Number 1 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	66.91 ng	1042230	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





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Misc :
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Instrument : BNA_G
ClientSampleId : 081718-DBRI-E-U-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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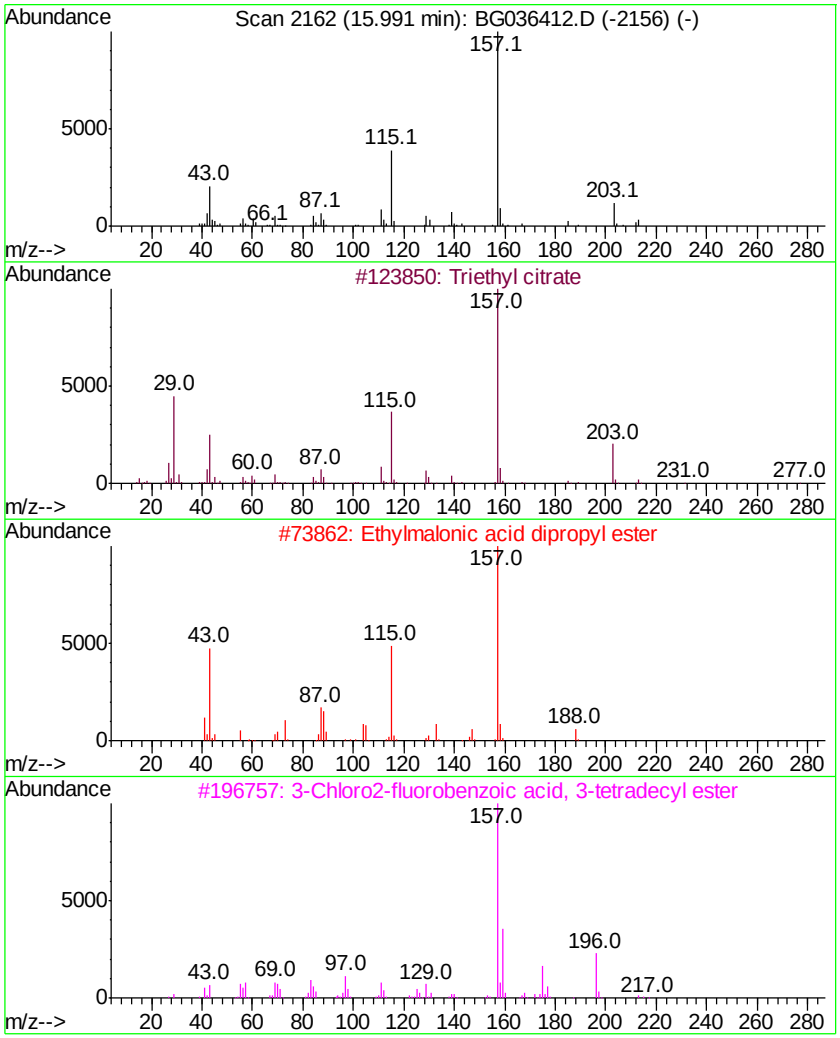
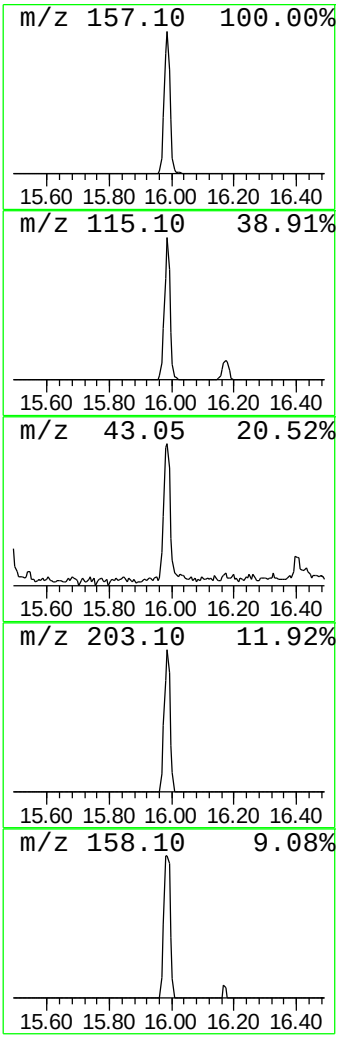
Peak Number 3 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	3.86 ng	134913	Acenaphthene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	87
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClFO2	1000338-64-6	50
4	3-Chloro2-fluorobenzoic acid, 3-...	342	C19H28ClFO2	1000338-63-8	42
5	3-Chloro2-fluorobenzoic acid, 6-...	384	C22H34ClFO2	1000338-65-3	40





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Data File : BG036412.D
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Sample : J4568-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 081718-DBRI-E-U-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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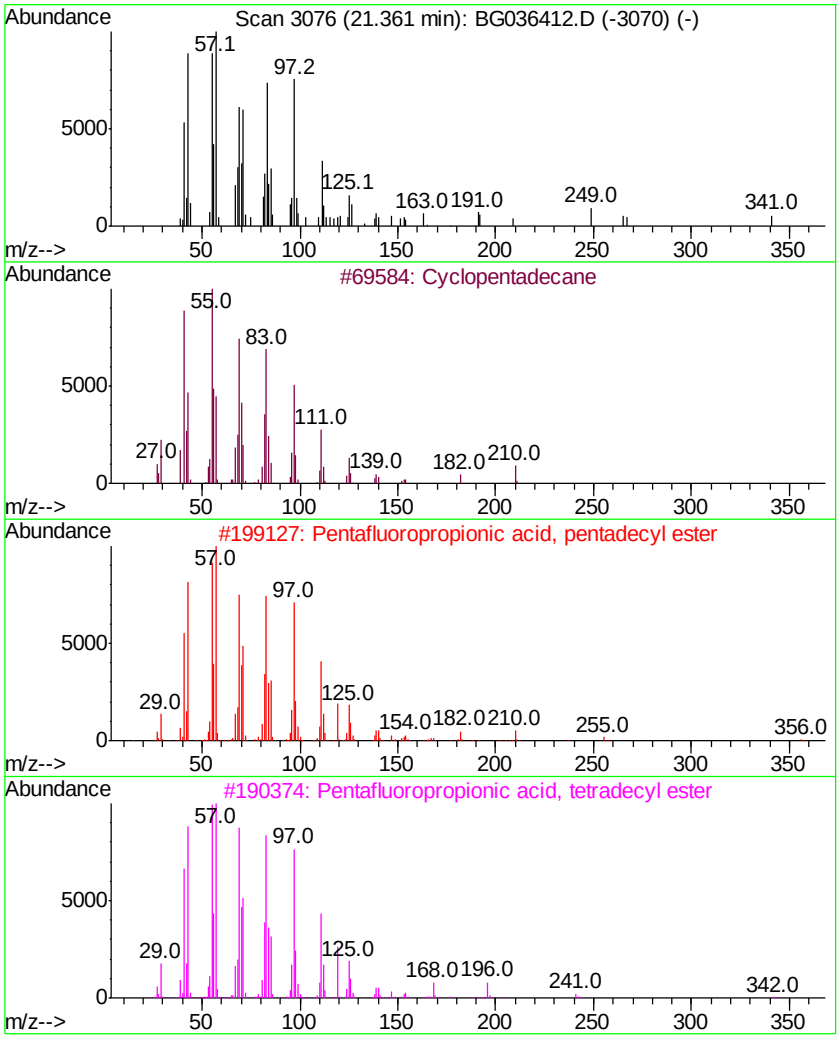
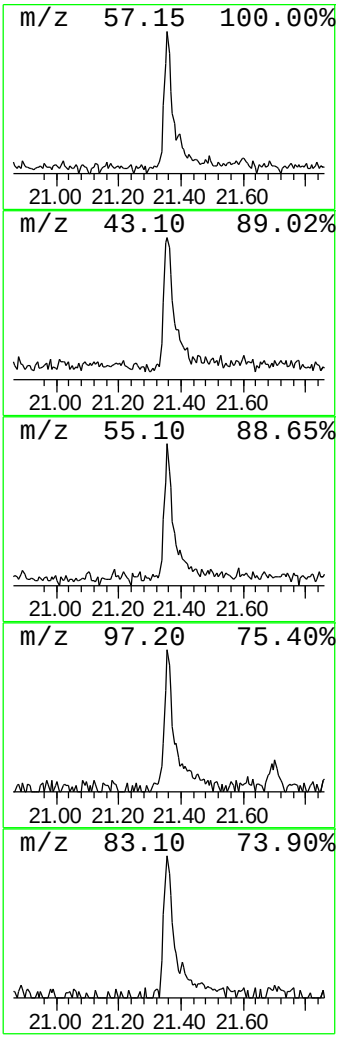
Peak Number 4 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.36	2.04 ng	110987	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93





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Operator : JU/SJ
Sample : J4568-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 081718-DBRI-E-U-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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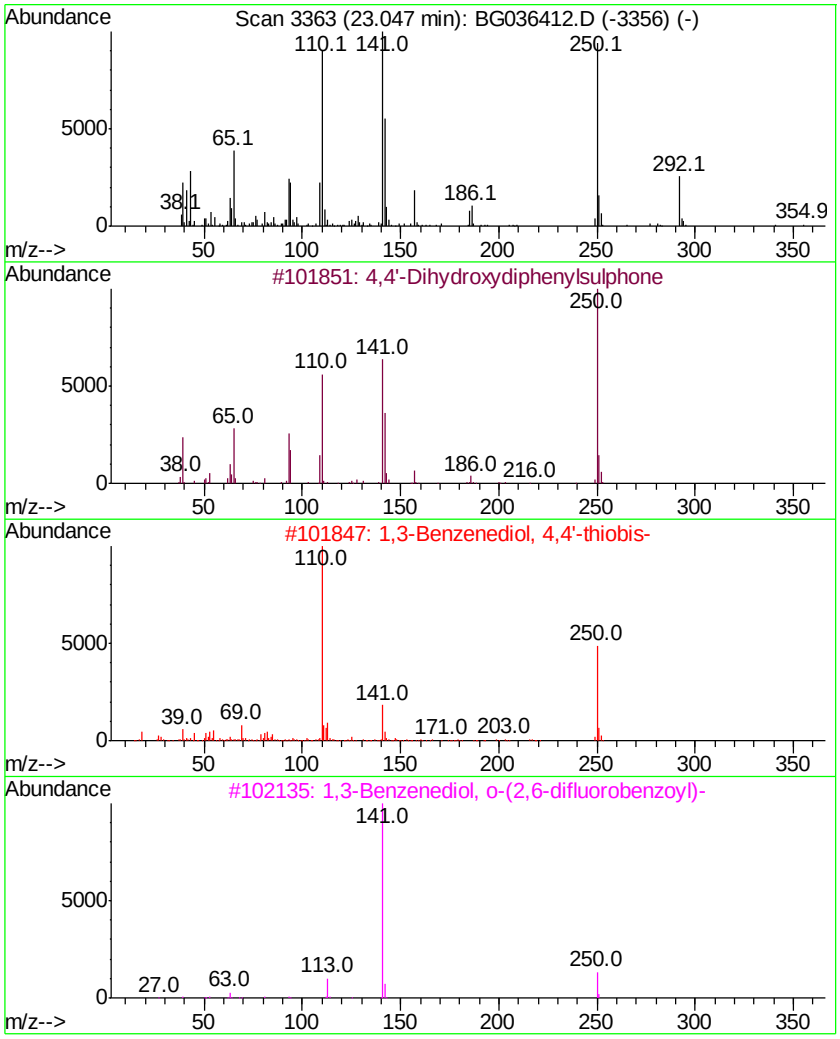
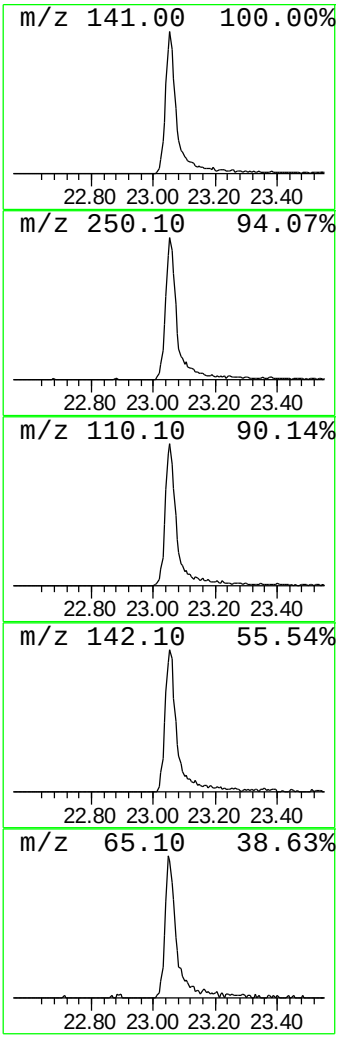
Peak Number 5 4,4'-Dihydroxydiphenylsulphone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.05	9.33 ng	506827	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	93
2	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	53
3	1,3-Benzenediol, o-(2,6-difluoro...	250	C13H8F2O3	1000330-83-2	25
4	4,4'-Thiodibenzenethiol	250	C12H10S3	019362-77-7	25
5	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	25





Tentatively Identified Compound (LSC) summary

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Data File : BG036412.D
Acq On : 24 Aug 2018 13:45
Operator : JU/SJ
Sample : J4568-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 081718-DBRI-E-U-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.59	7.59	66.9	ng	1042230	1	8.06	311525	20.0
Triethyl citrate	15.99	3.9	ng	134913	3	14.69	699803	20.0
Cyclopentadecane	21.36	2.0	ng	110987	5	21.70	1087020	20.0
4,4'-Dihydroxydip...	23.05	9.3	ng	506827	5	21.70	1087020	20.0