LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035366.D
Acq On : 23 Jun 2018 13:32
Operator : JU/SJ
Sample : J3623-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-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-BG060718.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	5.169	315	320	328	rVB2	33719	56310	1.29%	0.307%
2	5.633	392	399	411	rBV	321272	524750	12.00%	2.862%
3	7.213	661	668	678	rBV	208644	388294	8.88%	2.118%
4	7.589	725	732	740	rBV	556844	979568	22.39%	5.343%
5	8.053	804	811	817	rBV	184274	310378	7.10%	1.693%
6	8.377	859	866	875	rVB	835787	1448923	33.12%	7.902%
7	9.217	1000	1009	1020	rBV	674569	1206643	27.58%	6.581%
8	10.855	1282	1288	1295	rBV	216786	391842	8.96%	2.137%
9	13.299	1697	1704	1713	rBV	1871116	2930859	67.00%	15.985%
10	14.122	1839	1844	1851	rBV	65922	98775	2.26%	0.539%
11	14.674	1931	1938	1948	rBV3	364191	624006	14.26%	3.403%
12	15.960	2153	2157	2162	rVB	109702	130370	2.98%	0.711%
13	16.160	2184	2191	2204	rBV	1011056	1487206	34.00%	8.111%
14	17.417	2398	2405	2412	rBV	508376	774843	17.71%	4.226%
15	18.298	2551	2555	2564	rBV2	58849	87069	1.99%	0.475%
16	19.567	2767	2771	2776	rBV4	35909	48150	1.10%	0.263%
17	20.025	2842	2849	2856	rBV	3362094	4374559	100.00%	23.859%
18	21.682	3124	3131	3139	rBV	543495	897408	20.51%	4.894%
19	23.027	3349	3360	3374	rBV	244822	658936	15.06%	3.594%
20	24.901	3669	3679	3692	rBV	300158	869733	19.88%	4.743%
21	26.053	3866	3875	3883	rBV10	15752	46643	1.07%	0.254%

Sum of corrected areas: 18335265

LSC Report - Integrated Chromatogram

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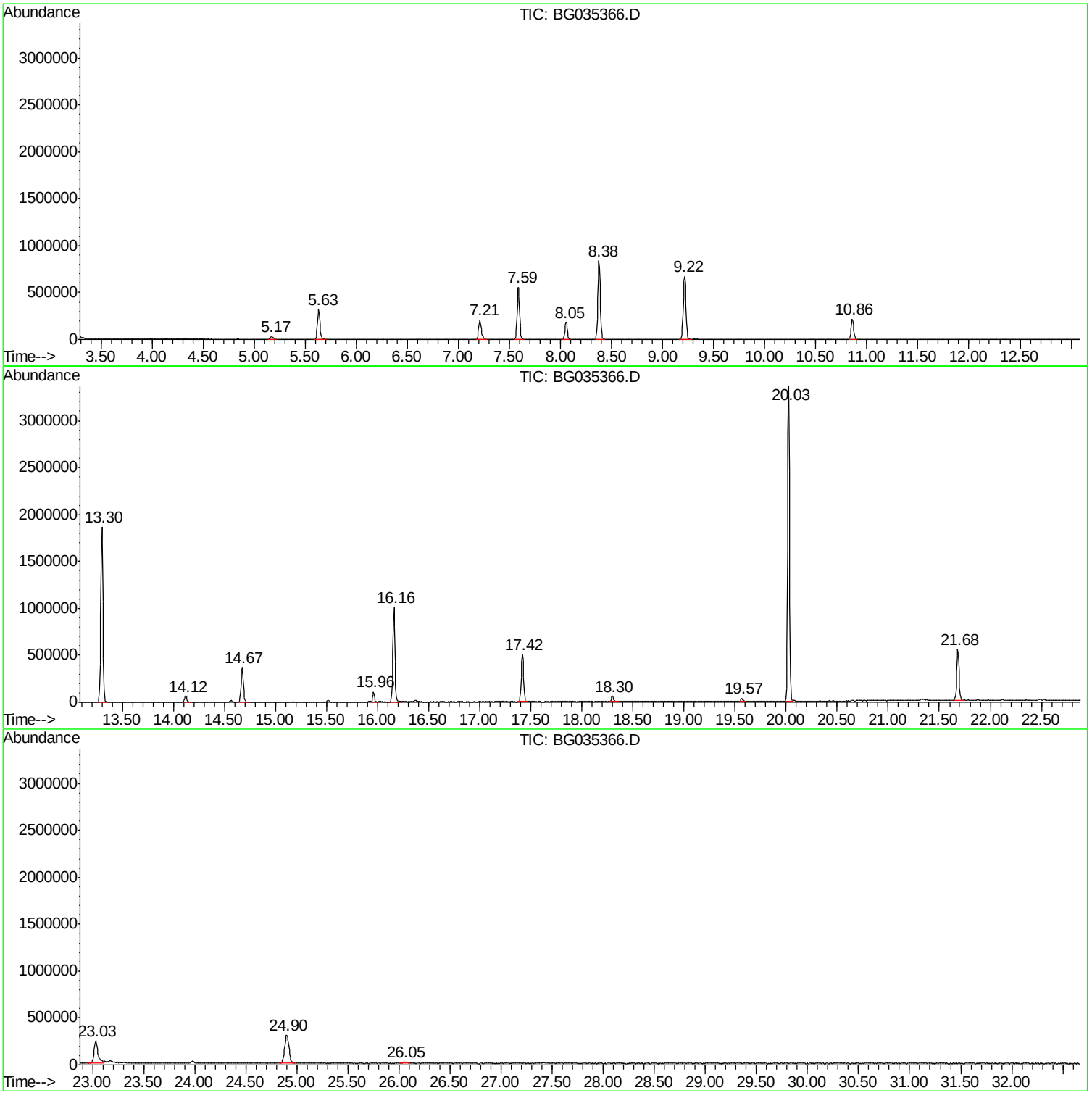
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
061918-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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Data File : BG035366.D
Acq On : 23 Jun 2018 13:32
Operator : JU/SJ
Sample : J3623-05
Misc :
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Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

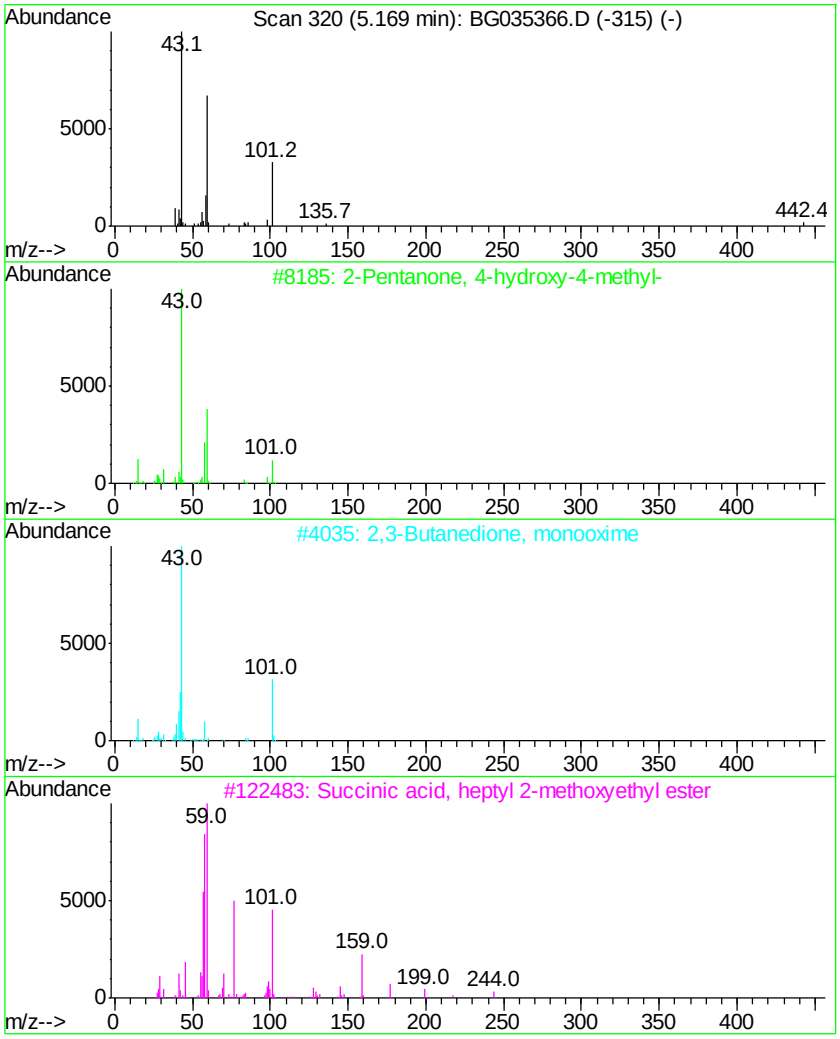
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

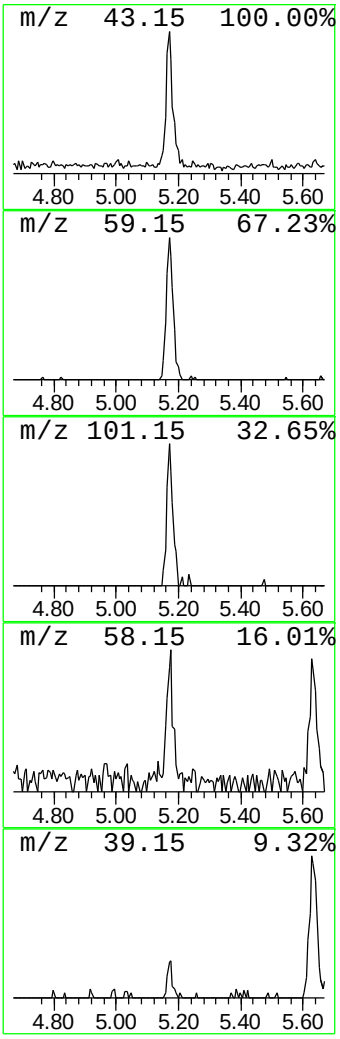
****

Peak Number 1 unknown5.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.63 ng	56310	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	38
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28
4	Pentanal, oxime	101	C5H11NO	000628-79-5	23
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23





Library Search Compound Report

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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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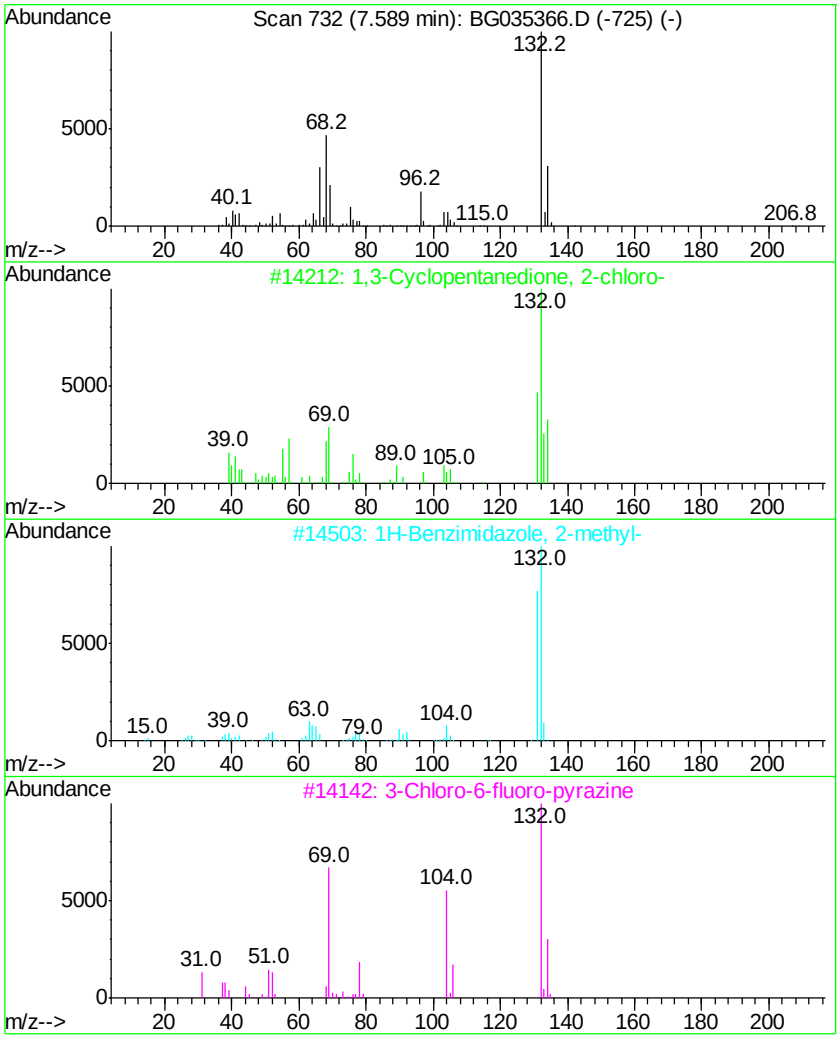
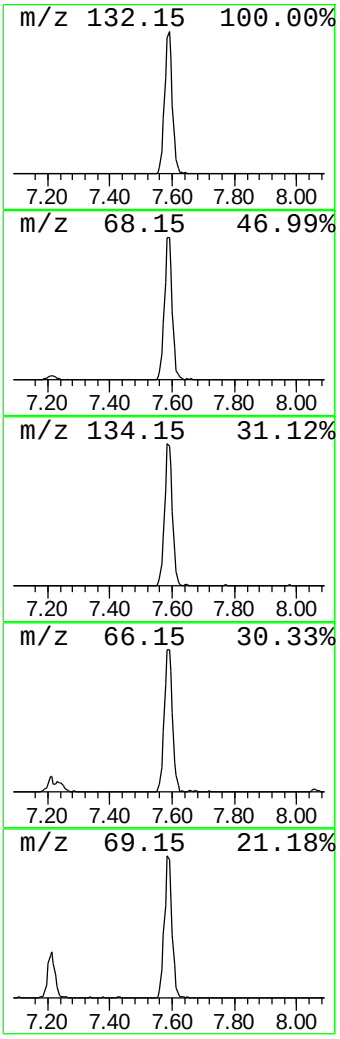
Peak Number 2 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	63.12 ng	979568	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035366.D
Acq On : 23 Jun 2018 13:32
Operator : JU/SJ
Sample : J3623-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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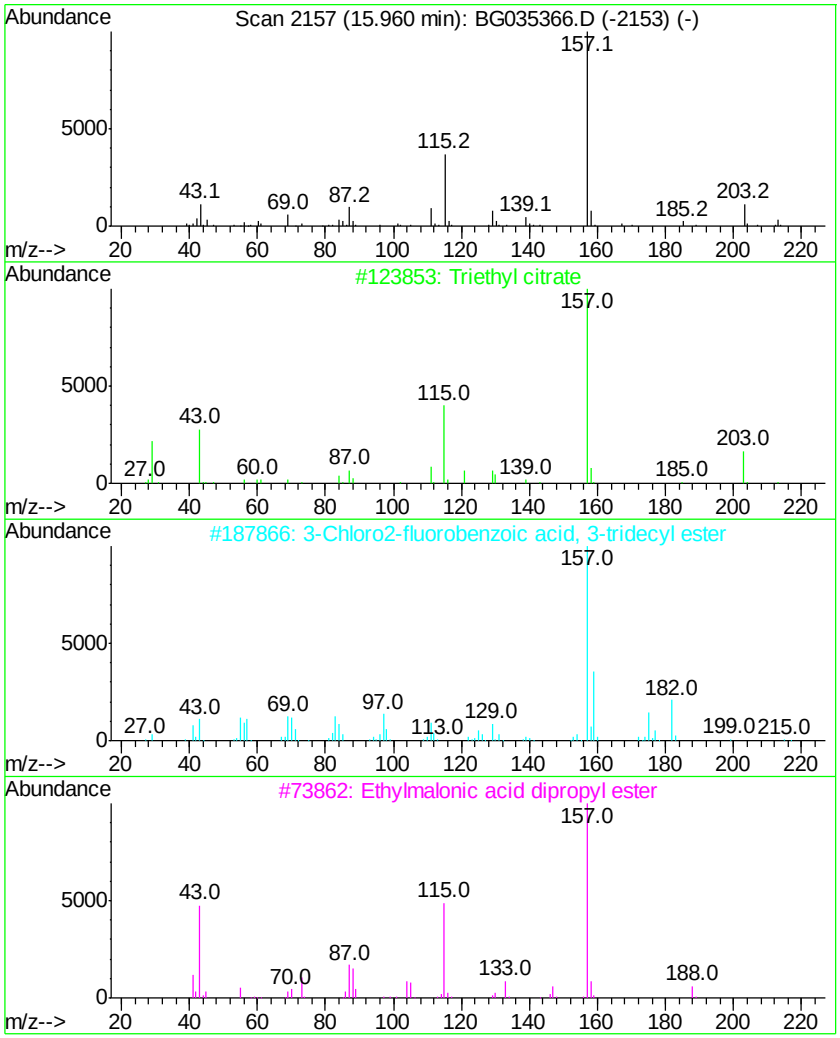
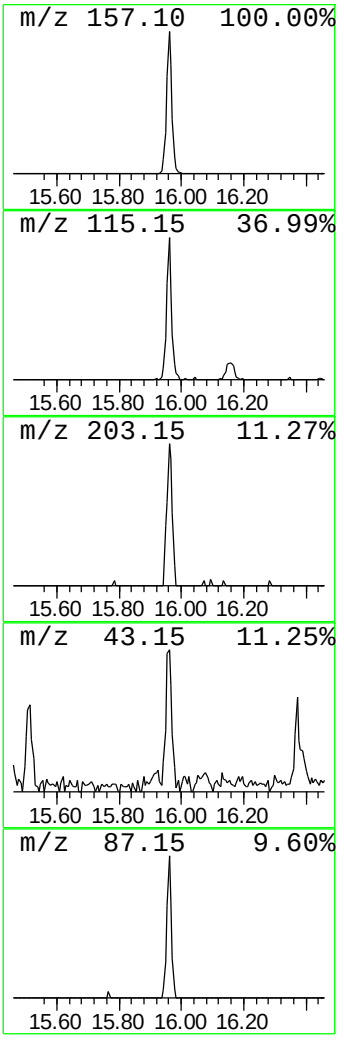
Peak Number 4 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	4.18 ng	130370	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	3-Chloro2-fluorobenzoic acid, 3-...	356	C20H30ClFO2	1000338-64-3	40
3	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	38
4	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	38
5	3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClFO2	1000338-64-4	36





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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061918-DBRI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
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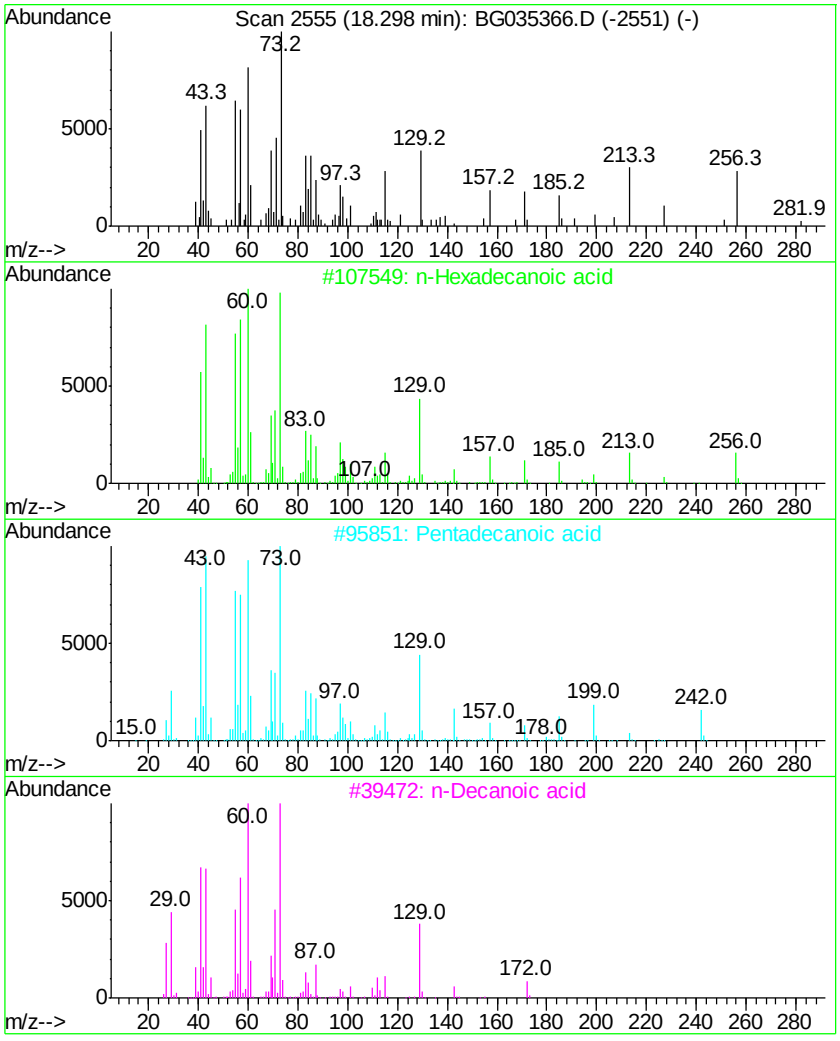
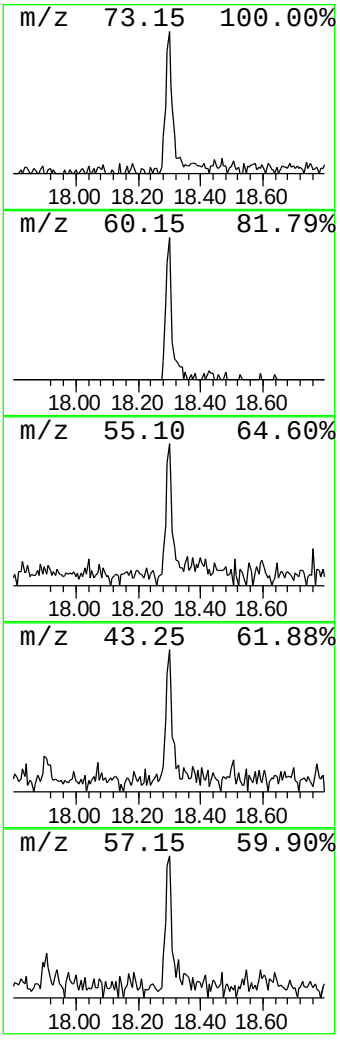
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.25 ng	87069	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	58
4	Dodecanoic acid	200	C12H24O2	000143-07-7	43
5	Eicosane	282	C20H42	000112-95-8	15





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Misc :
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Instrument : BNA_G
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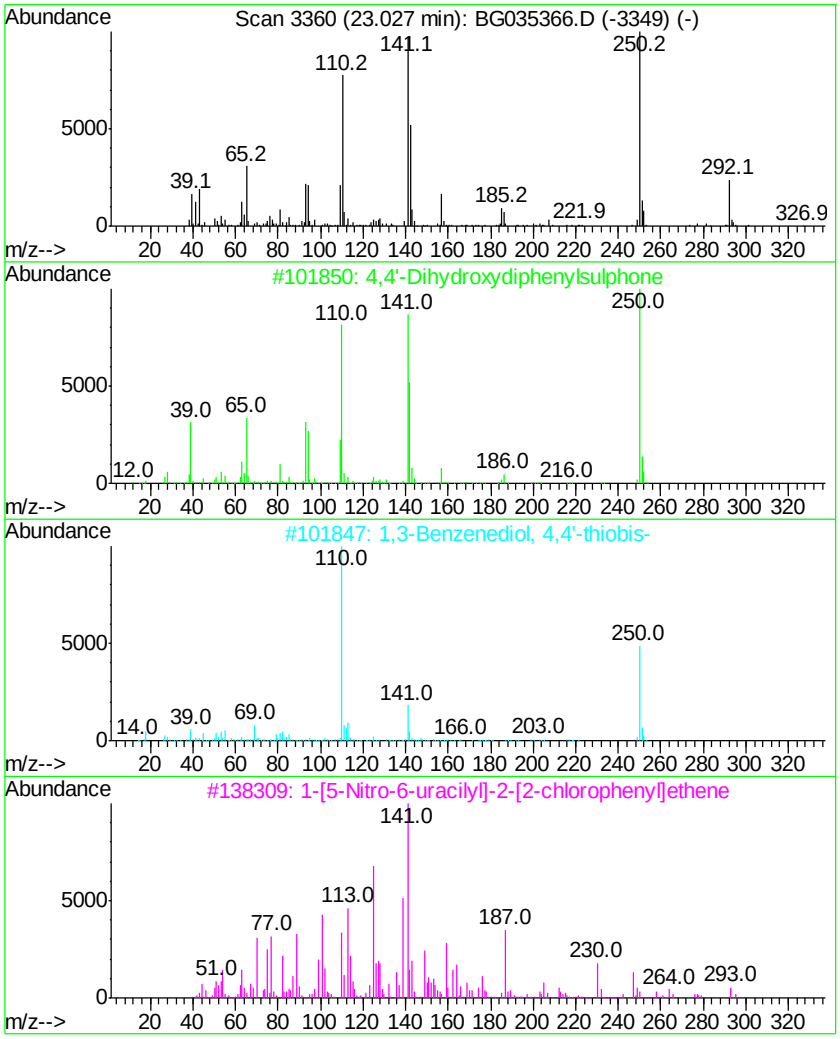
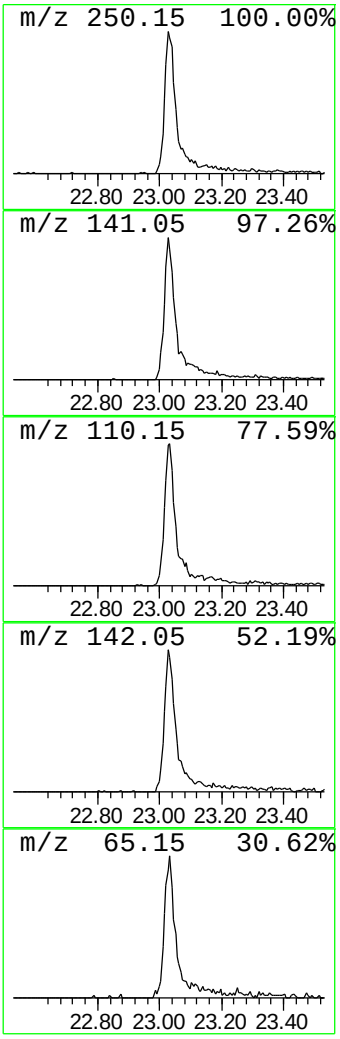
****

Peak Number 6 4,4'-Dihydroxydiphenylsulphone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.03	14.69 ng	658936	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	99
2	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	64
3	1-[5-Nitro-6-uracilyl]-2-[2-chlo...	293	C12H8ClN3O4	296798-53-3	18
4	Bis(5-methyl-2-pyrimidinyl) disu...	250	C10H10N4S2	1000326-74-2	18
5	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	14





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.17	5.17	3.6	ng	56310	1	8.05	310378	20.0
unknown7.59	7.59	63.1	ng	979568	1	8.05	310378	20.0
Triethyl citrate	15.96	4.2	ng	130370	3	14.67	624006	20.0
n-Hexadecanoic acid	18.30	2.3	ng	87069	4	17.42	774843	20.0
4,4'-Dihydroxydip...	23.03	14.7	ng	658936	5	21.68	897408	20.0