LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100518\
Data File : BG037157.D
Acq On : 4 Oct 2018 16:13
Operator : JU/SJ
Sample : J5218-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 229-211-RBR250129

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-BG092018.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	5.139	311	315	322	rVB	66210	106870	2.99%	0.621%
2	5.609	388	395	412	rBV	632551	1140699	31.95%	6.627%
3	7.195	658	665	685	rBV	520639	1023450	28.67%	5.946%
4	7.565	720	728	748	rBV	705384	1348575	37.77%	7.835%
5	8.029	801	807	822	rBV	148172	301286	8.44%	1.750%
6	8.352	855	862	879	rBV	573758	1074992	30.11%	6.245%
7	9.193	998	1005	1018	rBV	433463	903378	25.30%	5.248%
8	10.838	1277	1285	1299	rBV	191568	397052	11.12%	2.307%
9	13.282	1692	1701	1719	rBV	1131656	1931506	54.10%	11.222%
10	14.657	1928	1935	1952	rVB2	317708	547272	15.33%	3.180%
11	16.143	2182	2188	2212	rBV	1024824	1752549	49.09%	10.182%
12	17.401	2396	2402	2416	rBV2	444313	767506	21.50%	4.459%
13	20.009	2840	2846	2860	rBV	2439322	3570189	100.00%	20.742%
14	21.320	3064	3069	3075	rBV4	16653	38335	1.07%	0.223%
15	21.396	3077	3082	3093	rBV	54572	111120	3.11%	0.646%
16	21.555	3105	3109	3115	rVB2	22229	36673	1.03%	0.213%
17	21.672	3121	3129	3144	rBV	521279	982489	27.52%	5.708%
18	21.854	3156	3160	3167	rVB2	28145	44431	1.24%	0.258%
19	22.459	3258	3263	3270	rBV	34450	55314	1.55%	0.321%
20	23.147	3374	3380	3386	rBV3	34883	65298	1.83%	0.379%
21	23.940	3510	3515	3524	rVB2	38103	82580	2.31%	0.480%
22	24.868	3663	3673	3693	rBV2	295762	930744	26.07%	5.407%

Sum of corrected areas: 17212308

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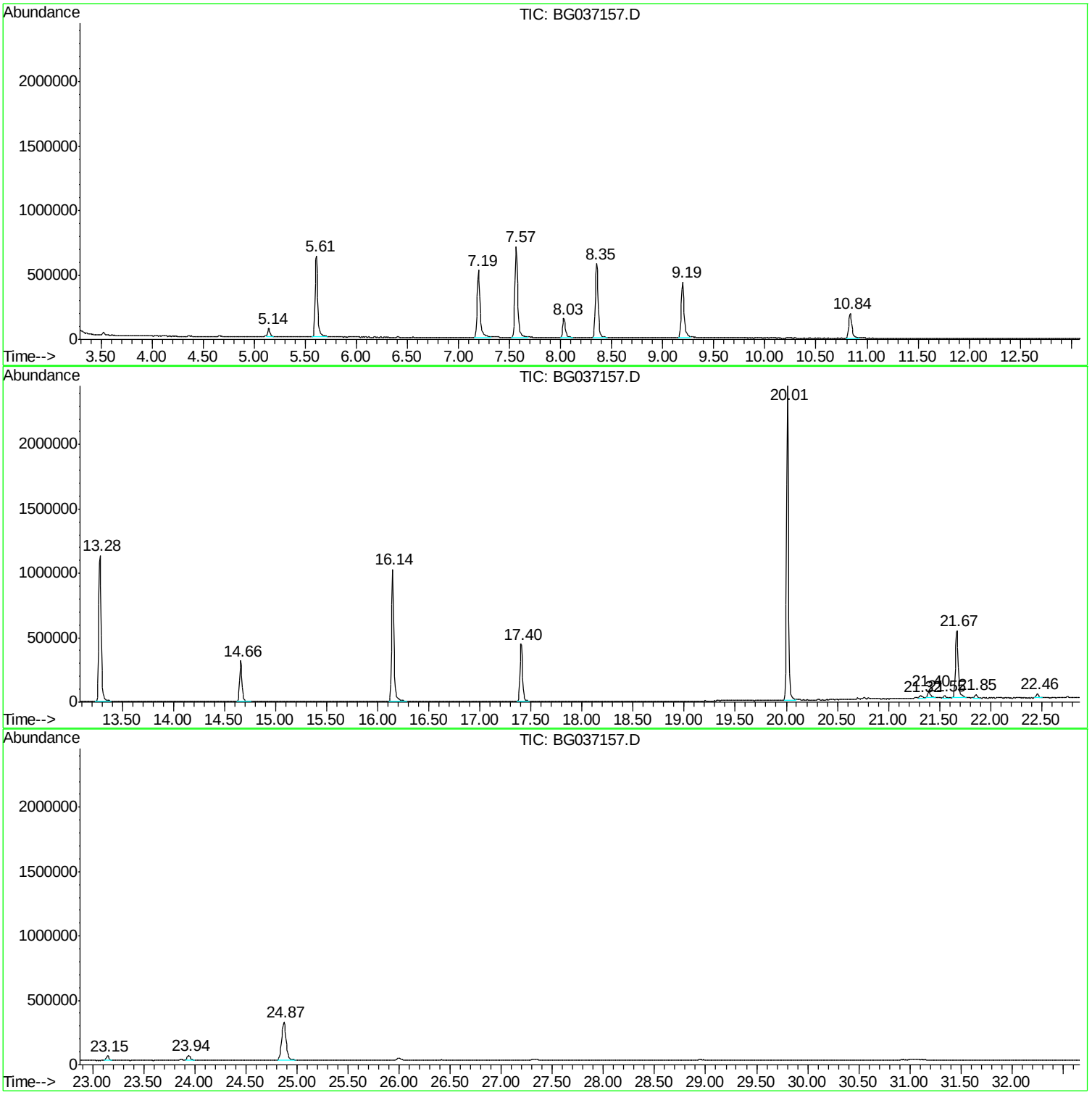
BNA_G
ClientSampleId :
229-211-RBR250129

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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TIC Integration Parameters: LSCINT.P

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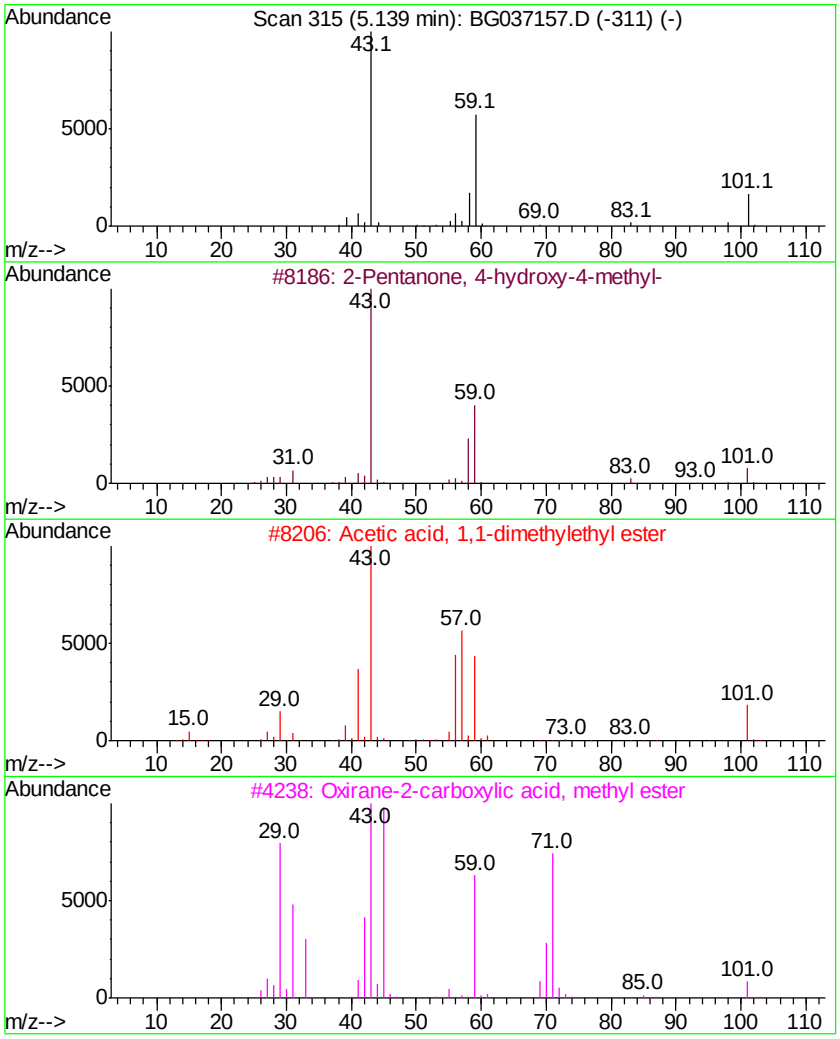
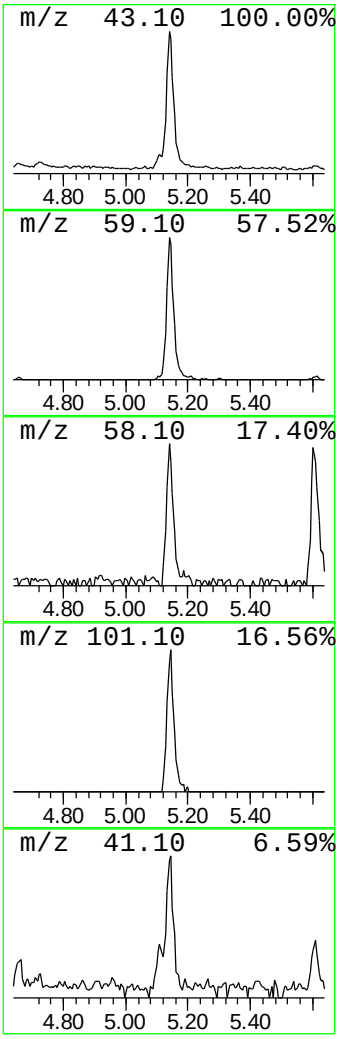
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	7.09 ng	106870	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : 229-211-RBR250129

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

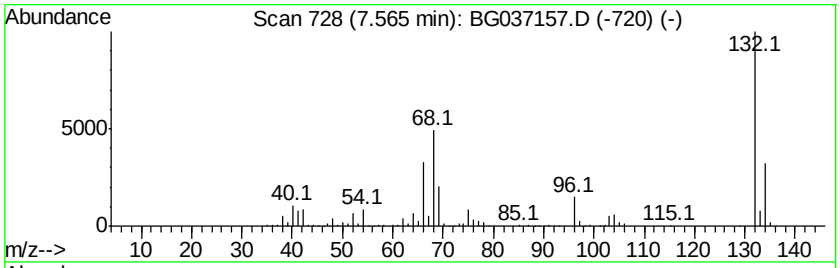
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

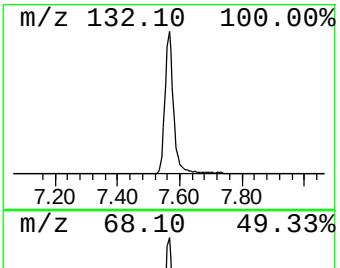
****

Peak Number 2 4-Chloro-6-fluoro-pyrimidine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	89.52 ng	1348580	1,4-Dichlorobenzene-d4	8.04

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	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Library Search Compound Report

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Operator : JU/SJ
Sample : J5218-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 229-211-RBR250129

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

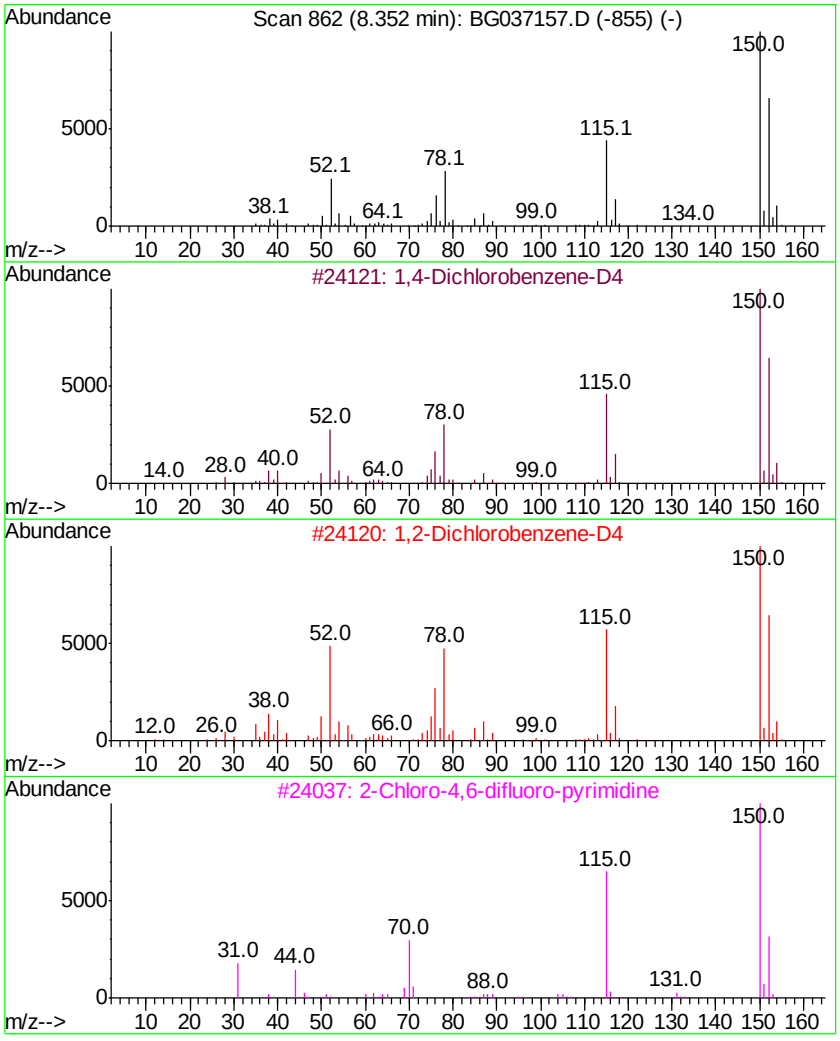
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

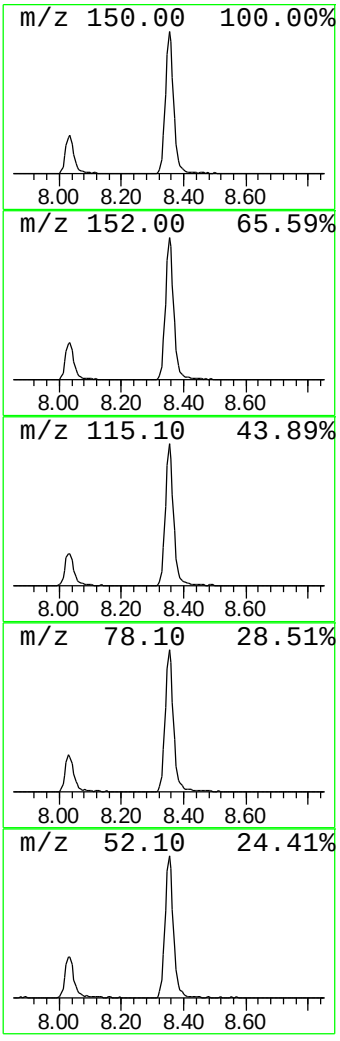
****

Peak Number 3 1,4-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.35	71.36 ng	1074990	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	95
2	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
3	2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	35
4	2-Bromo-3'-nitroacetophenone	243	C8H6BrNO3	002227-64-7	14
5	2-Bromo-2'-nitroacetophenone	243	C8H6BrNO3	006851-99-6	14





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Sample : J5218-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 229-211-RBR250129

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

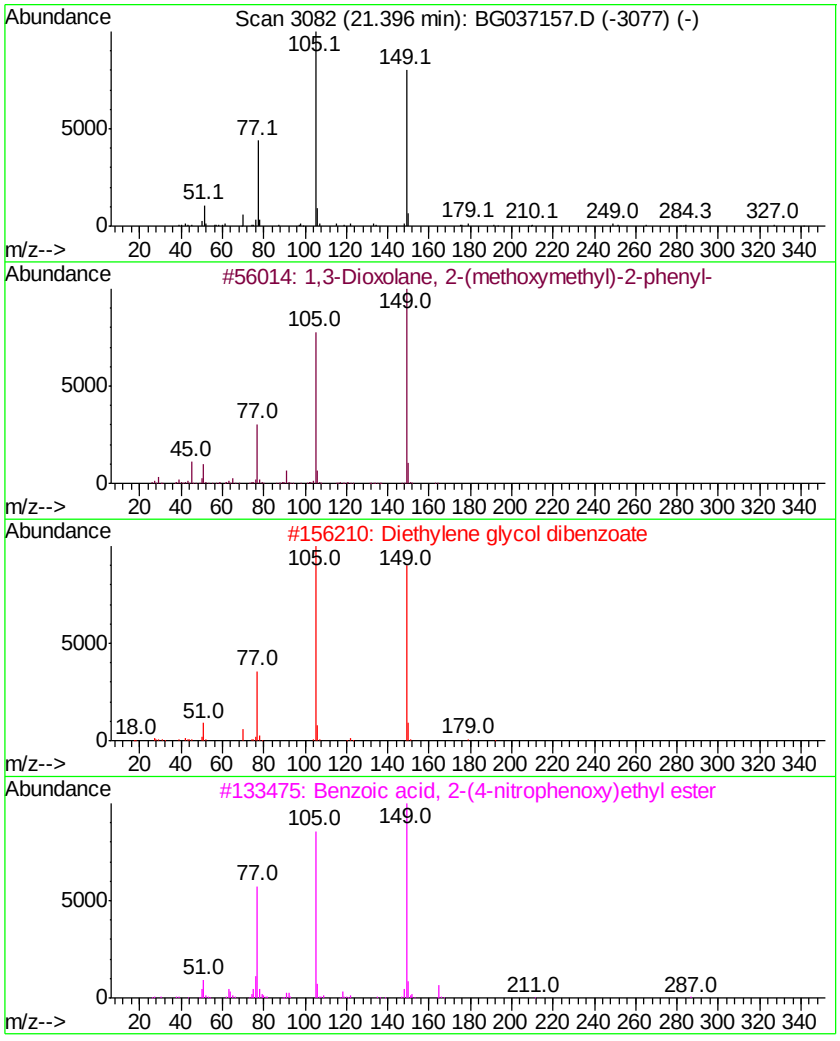
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

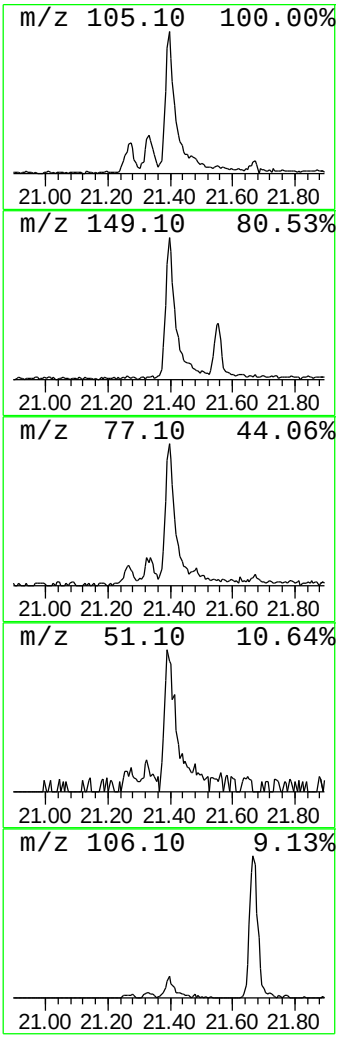
****

Peak Number 4 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.26 ng	111120	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	56
4	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	43
5	Hippuric-benzaldehyde azalactone	249	C16H11NO2	000842-74-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100518\
Data File : BG037157.D
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 229-211-RBR250129

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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...	5.14	7.1	ng	106870	1	8.04	301286	20.0
4-Chloro-6-fluoro...	7.57	89.5	ng	1348580	1	8.04	301286	20.0
1,4-Dichlorobenze...	8.35	71.4	ng	1074990	1	8.04	301286	20.0
1,3-Dioxolane, 2-...	21.40	2.3	ng	111120	5	21.67	982489	20.0