LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043403.D
Acq On : 30 Oct 2019 16:41
Operator : JU
Sample : PB124406BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124406BL

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-BG102119.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	5.123	341	346	356	rBV	110894	174321	4.89%	1.121%
2	5.611	422	429	445	rBV	557127	963965	27.02%	6.198%
3	7.209	692	701	712	rBV	548297	1030478	28.89%	6.625%
4	7.561	754	761	770	rBV	599108	1060181	29.72%	6.816%
5	8.020	833	839	851	rBV	132684	224452	6.29%	1.443%
6	8.343	886	894	905	rBV	469944	842744	23.63%	5.418%
7	9.183	1030	1037	1058	rBV	295515	621851	17.43%	3.998%
8	10.828	1307	1317	1328	rBV	127604	277695	7.78%	1.785%
9	13.272	1725	1733	1748	rBV	979278	1683597	47.20%	10.824%
10	14.647	1959	1967	1980	rBV	266837	478234	13.41%	3.075%
11	16.139	2214	2221	2236	rBV	900143	1614722	45.27%	10.382%
12	17.397	2427	2435	2446	rBV2	342564	647774	18.16%	4.165%
13	20.006	2872	2879	2893	rBV	2516136	3567105	100.00%	22.934%
14	21.257	3086	3092	3097	rBV2	45380	91922	2.58%	0.591%
15	21.322	3097	3103	3108	rVV	65110	107474	3.01%	0.691%
16	21.380	3108	3113	3124	rVV	159070	301769	8.46%	1.940%
17	21.662	3153	3161	3177	rBV	457550	891768	25.00%	5.733%
18	23.930	3542	3547	3554	rVB7	20305	40421	1.13%	0.260%
19	24.859	3694	3705	3719	rBV2	305309	933248	26.16%	6.000%

Sum of corrected areas: 15553721

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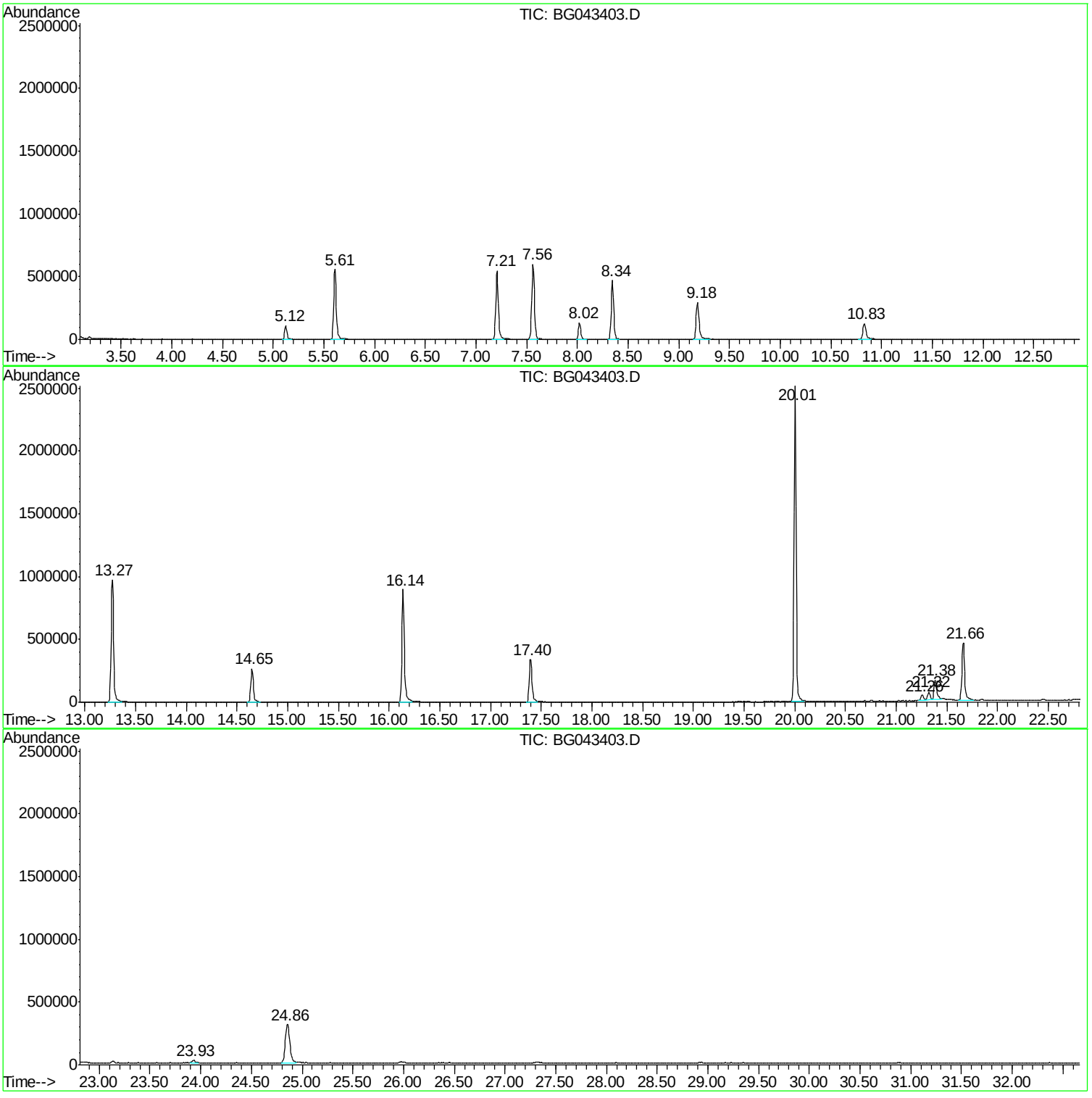
Instrument :
BNA_G
ClientSampleId :
PB124406BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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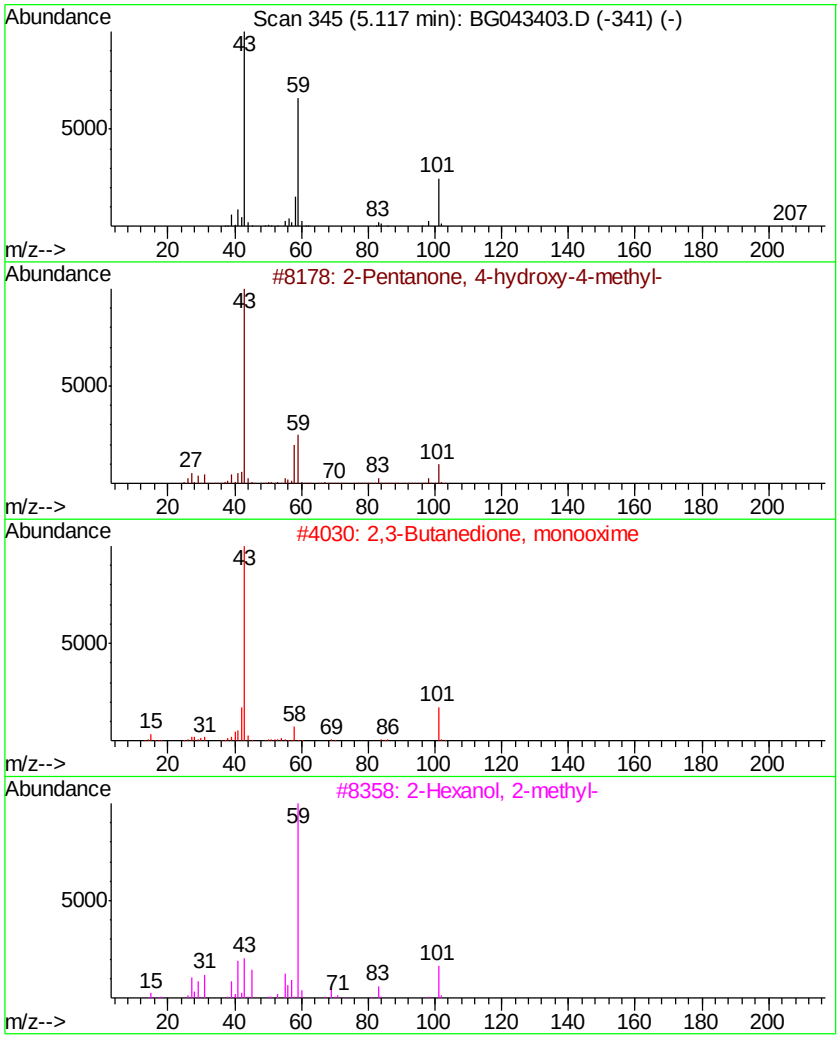
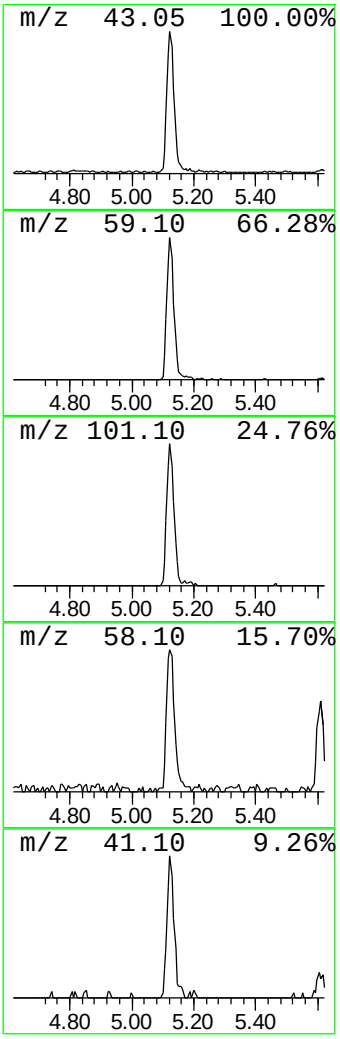
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	15.53 ng	174321	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Library Search Compound Report

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Data File : BG043403.D
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124406BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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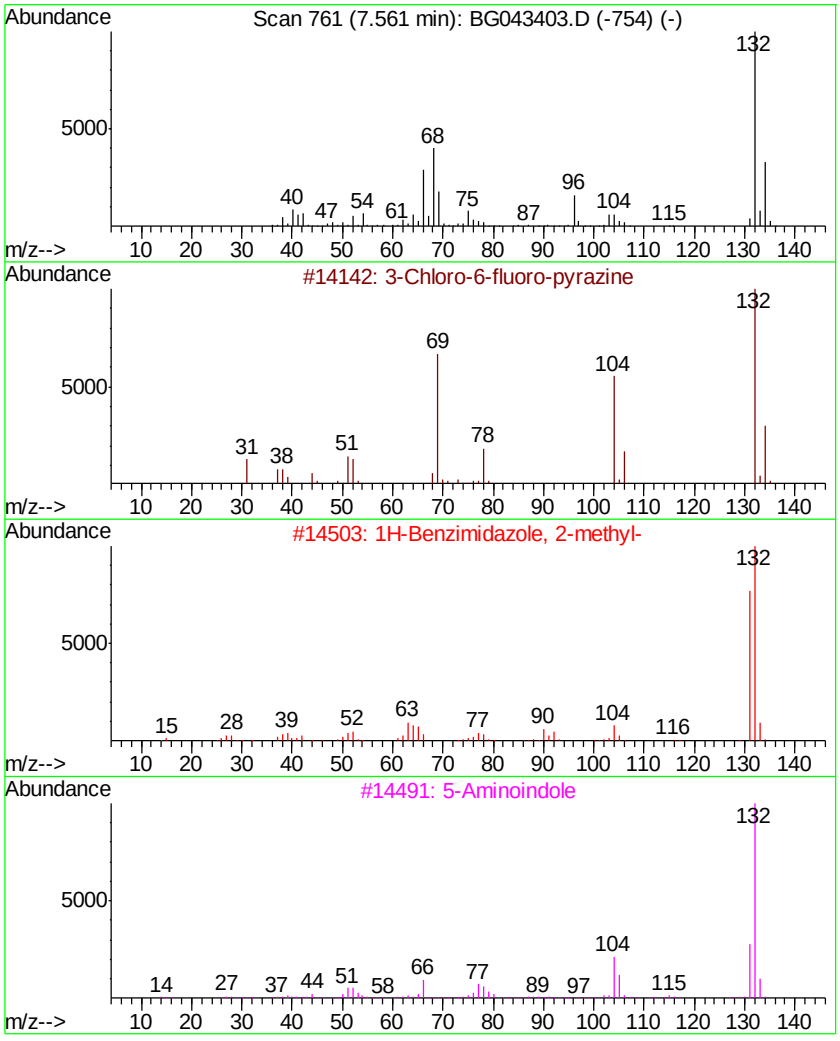
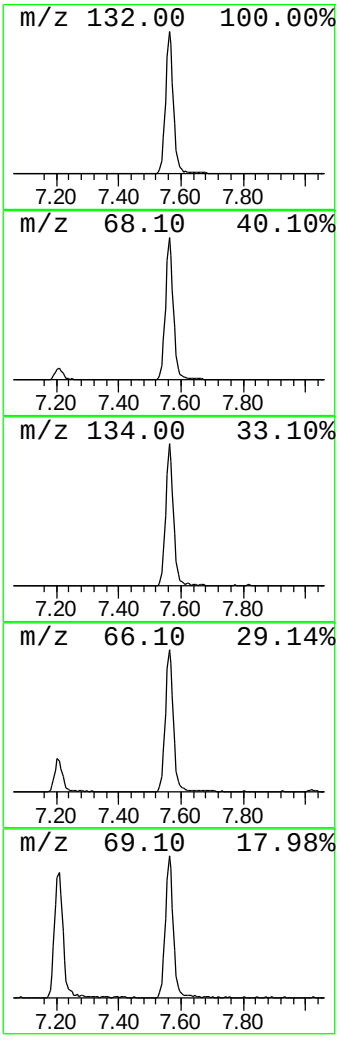
Peak Number 2 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	94.47 ng	1060180	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Instrument : BNA_G
ClientSampleId : PB124406BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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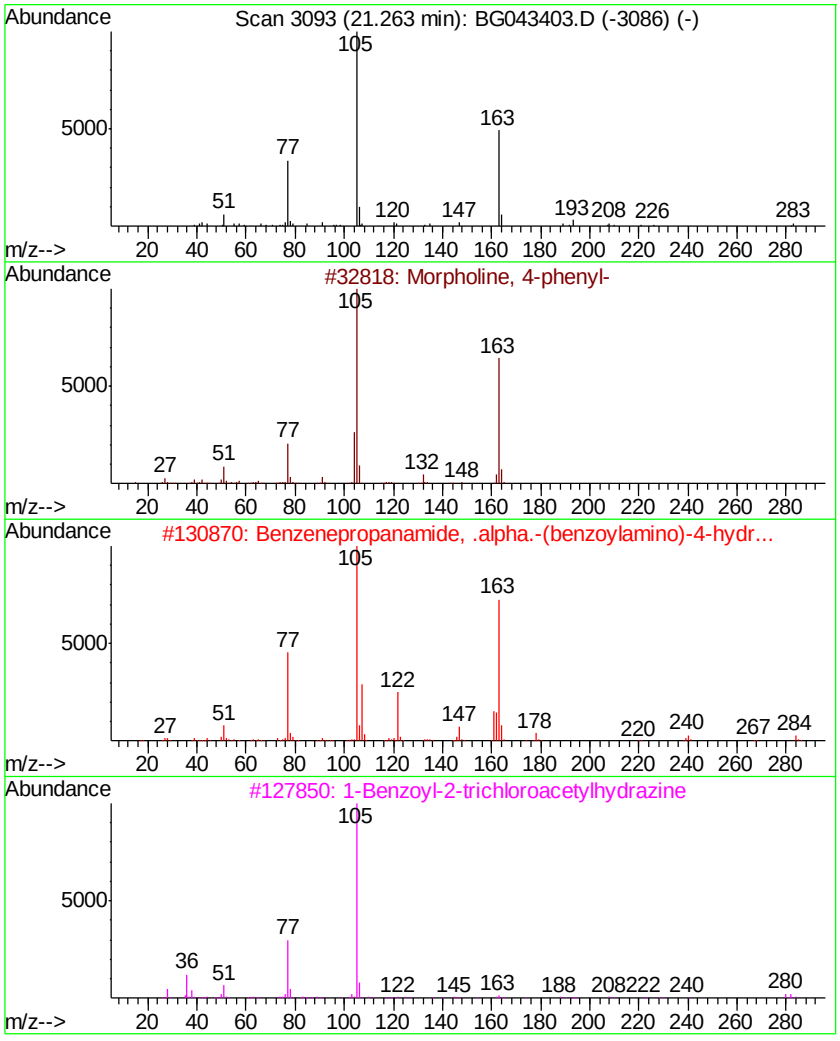
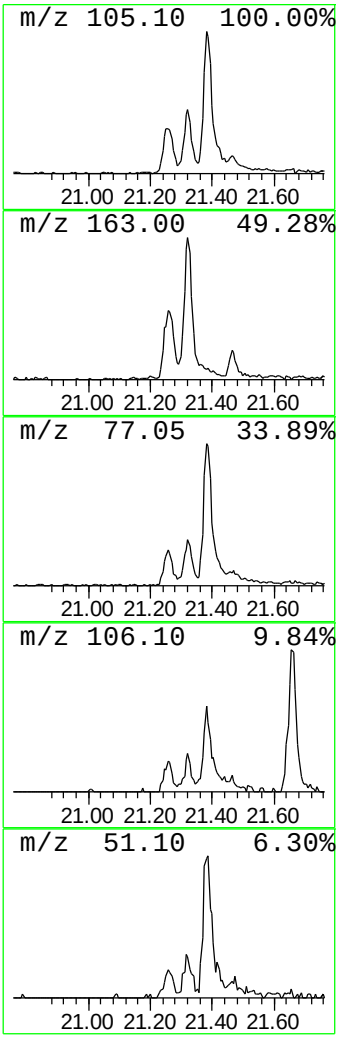
Peak Number 4 Morpholine, 4-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	2.06 ng	91922	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	56
3	1-Benzoyl-2-trichloroacetylhydra...	280	C9H7Cl3N2O2	090273-66-8	38
4	Isovaleric acid, 2-benzamido-, e...	249	C14H19NO3	061131-42-8	35
5	Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	35





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Instrument : BNA_G
ClientSampleId : PB124406BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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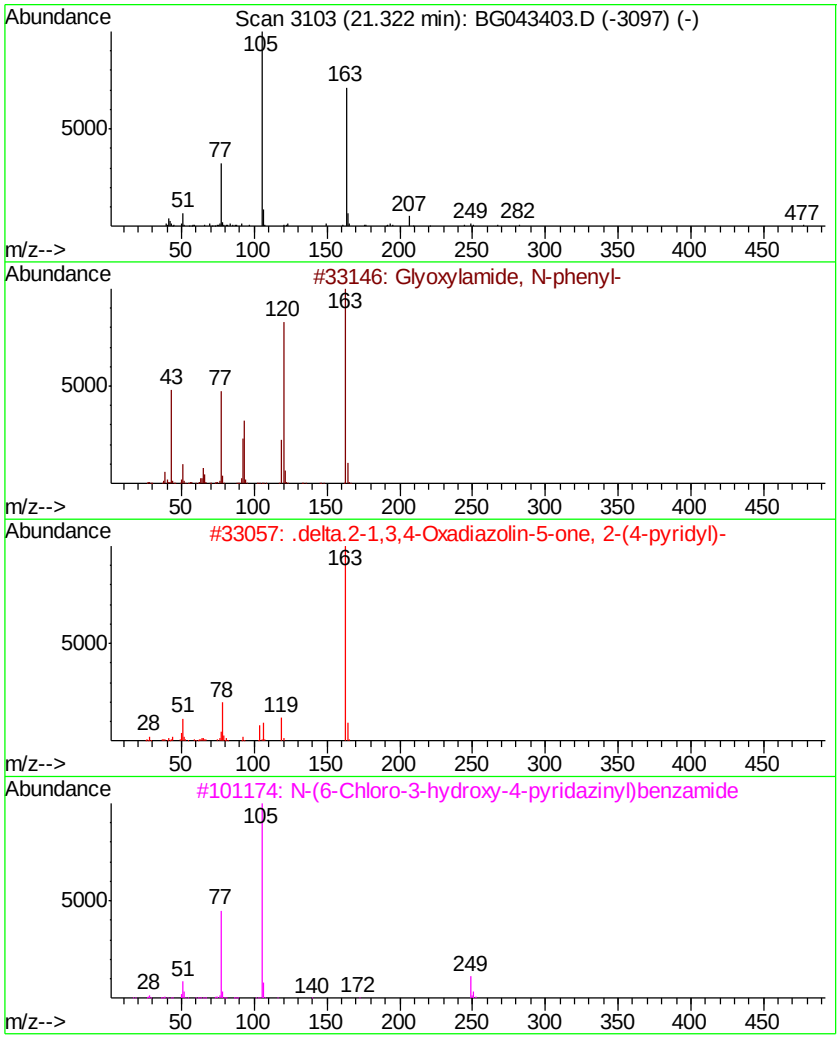
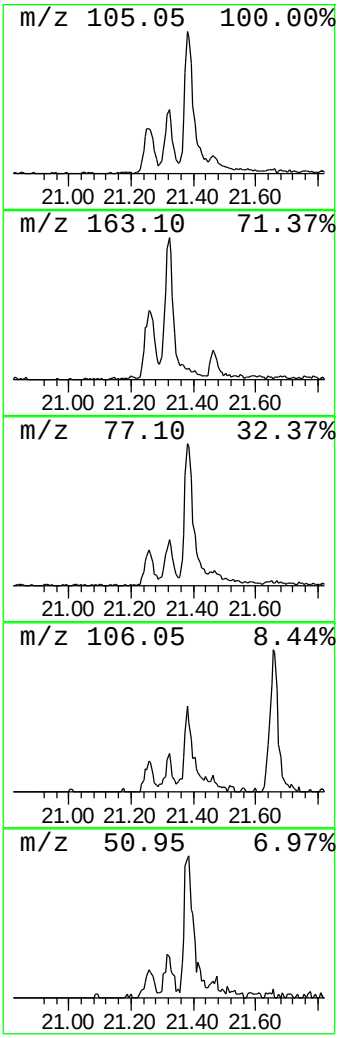
Peak Number 5 unknown21.32 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	2.41 ng	107474	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
2	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	38
3	N-(6-Chloro-3-hydroxy-4-pyridazi...	249	C11H8ClN3O2	117892-39-4	35
4	2-Benzoylamino-3-phenyl-N,N-dime...	294	C18H18N2O2	1000287-00-0	35
5	Hippuric-benzaldehyde azalactone	249	C16H11NO2	000842-74-0	35





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB124406BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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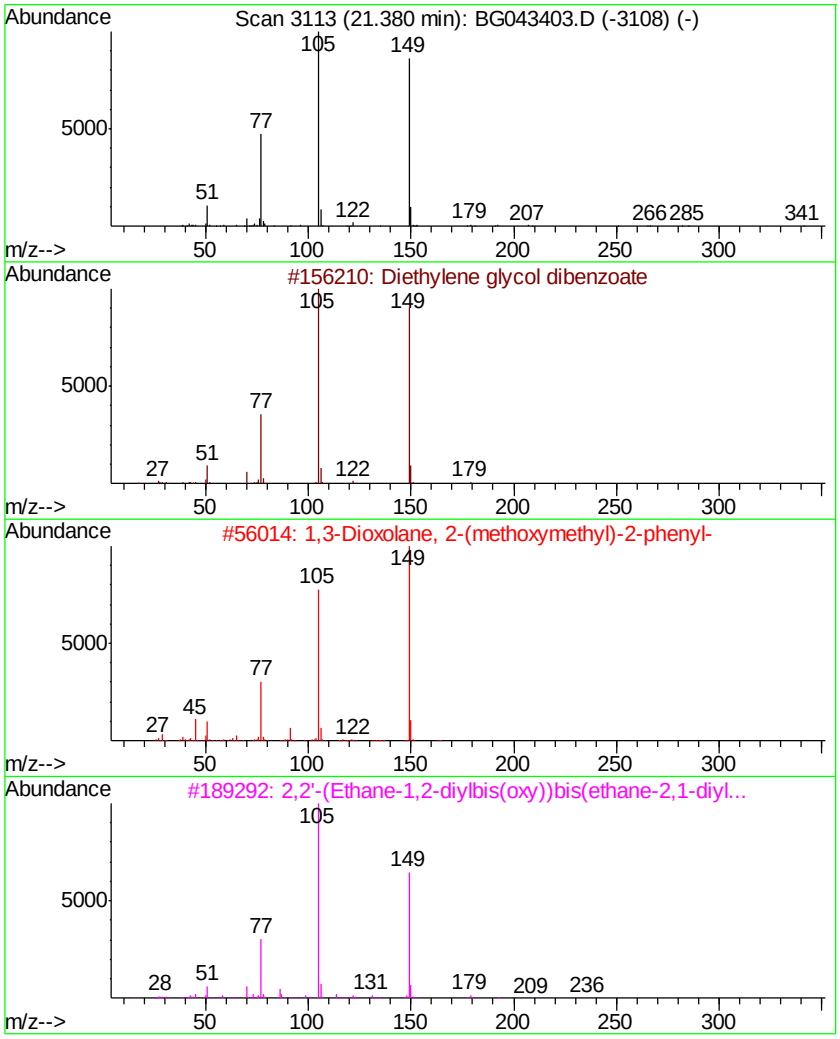
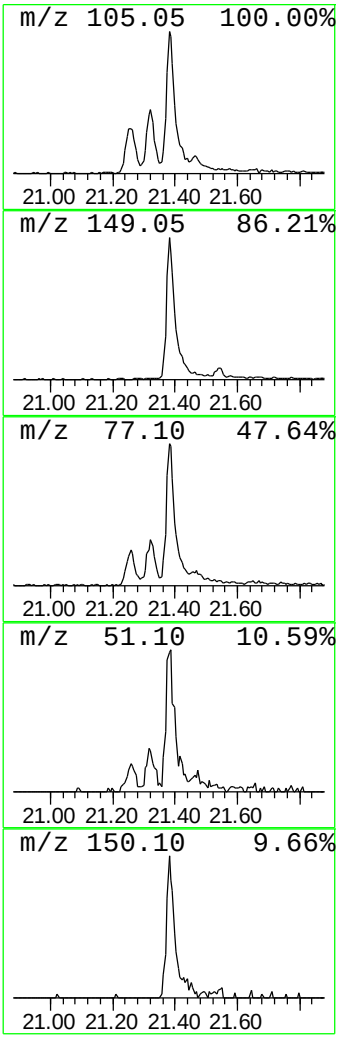
Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	6.77 ng	301769	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	78
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	74





Tentatively Identified Compound (LSC) summary

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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...	5.12	15.5	ng	174321	1	8.02	224452	20.0
unknown7.56	7.56	94.5	ng	1060180	1	8.02	224452	20.0
Morpholine, 4-phe...	21.26	2.1	ng	91922	5	21.66	891768	20.0
unknown21.32	21.32	2.4	ng	107474	5	21.66	891768	20.0
Diethylene glycol...	21.38	6.8	ng	301769	5	21.66	891768	20.0