LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048399.D
Acq On : 17 Mar 2021 15:48
Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW-VAN-WINKLE-STREET

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-BG031621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.966	101	107	116	rVB	44593	70990	1.25%	0.240%
2	4.589	206	213	224	rBV	2562769	3790960	66.56%	12.816%
3	5.200	308	317	327	rBV	2090562	3318477	58.27%	11.219%
4	7.251	659	666	677	rBV	311697	539814	9.48%	1.825%
5	8.114	806	813	819	rBV	200004	349554	6.14%	1.182%
6	9.278	1000	1011	1018	rBV	534988	960633	16.87%	3.248%
7	10.935	1287	1293	1302	rVB	268645	484215	8.50%	1.637%
8	13.379	1701	1709	1715	rVB	1447424	2262688	39.73%	7.650%
9	14.196	1840	1848	1858	rBV	67307	107059	1.88%	0.362%
10	14.754	1936	1943	1950	rVB	465971	732139	12.86%	2.475%
11	17.503	2403	2411	2417	rBV	618459	937846	16.47%	3.171%
12	18.379	2557	2560	2568	rBV6	37923	69366	1.22%	0.235%
13	19.154	2687	2692	2698	rBV	85496	122291	2.15%	0.413%
14	19.654	2773	2777	2781	rBV7	35807	58986	1.04%	0.199%
15	20.112	2849	2855	2861	rVB	2960482	3689675	64.79%	12.474%
16	20.659	2944	2948	2952	rVB	67610	82736	1.45%	0.280%
17	21.387	3065	3072	3076	rBV2	797003	1627038	28.57%	5.501%
18	21.458	3076	3084	3088	rVV	1177414	2351010	41.28%	7.948%
19	21.516	3088	3094	3102	rVV	3629908	5695165	100.00%	19.254%
20	21.599	3104	3108	3113	rVB	241981	348284	6.12%	1.177%
21	21.793	3136	3141	3148	rVB	572412	944901	16.59%	3.195%
22	25.136	3701	3710	3718	rBV3	327881	1034969	18.17%	3.499%

Sum of corrected areas: 29578796

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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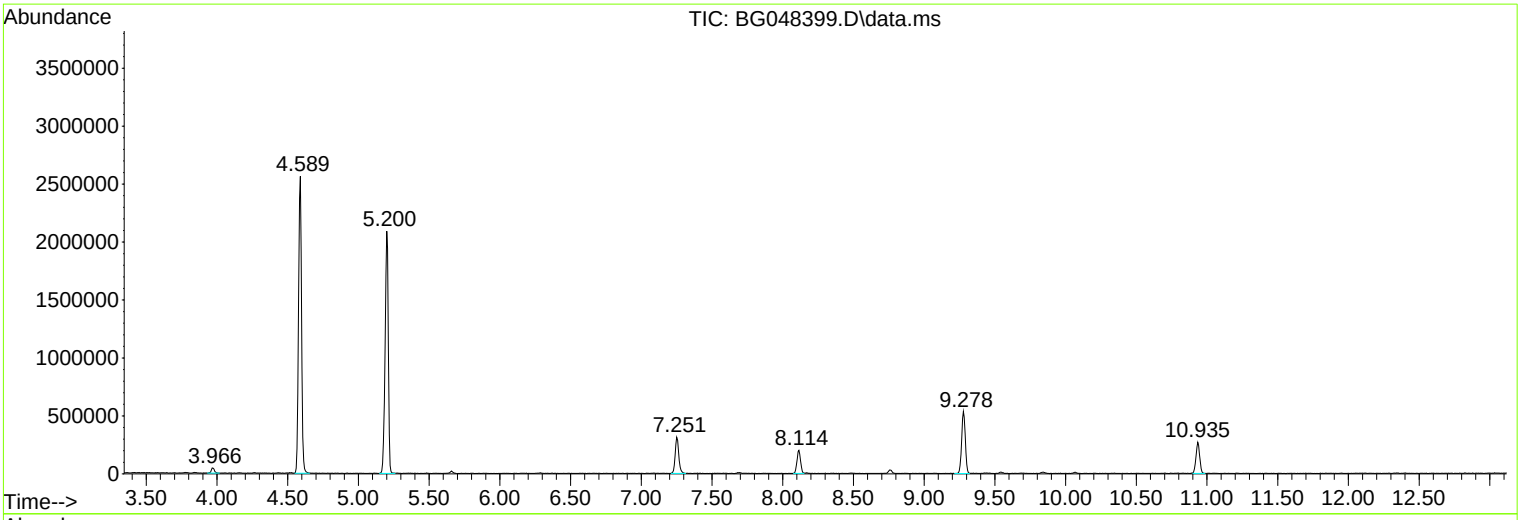
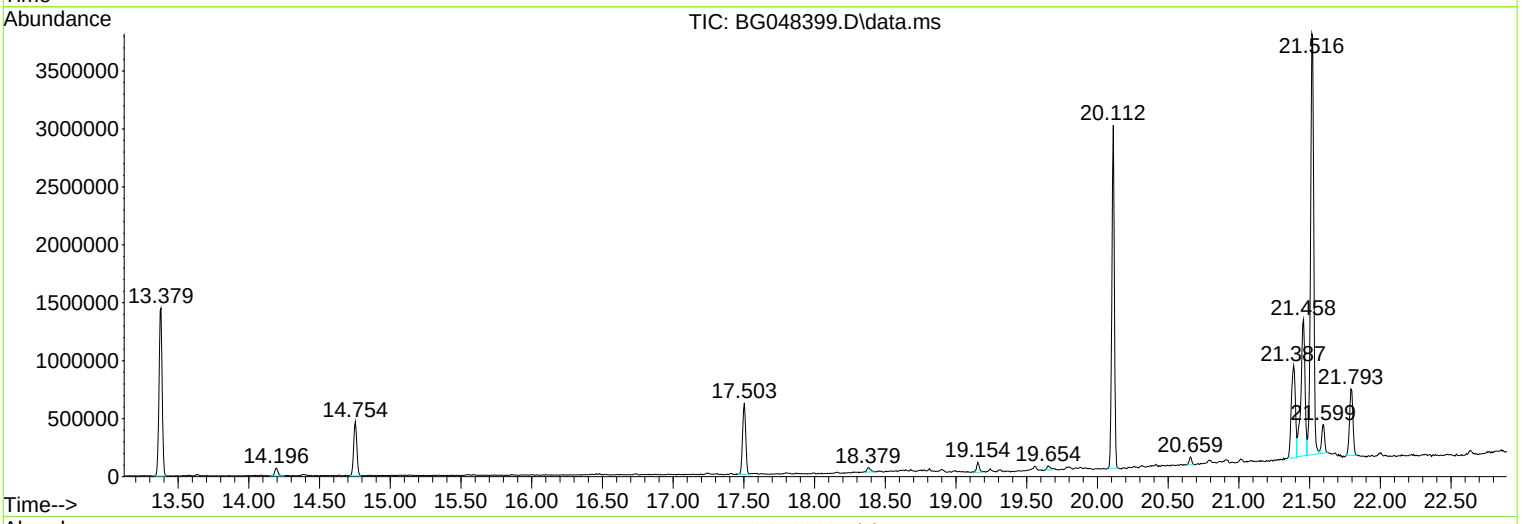
Acq On : 17 Mar 2021 15:48
Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

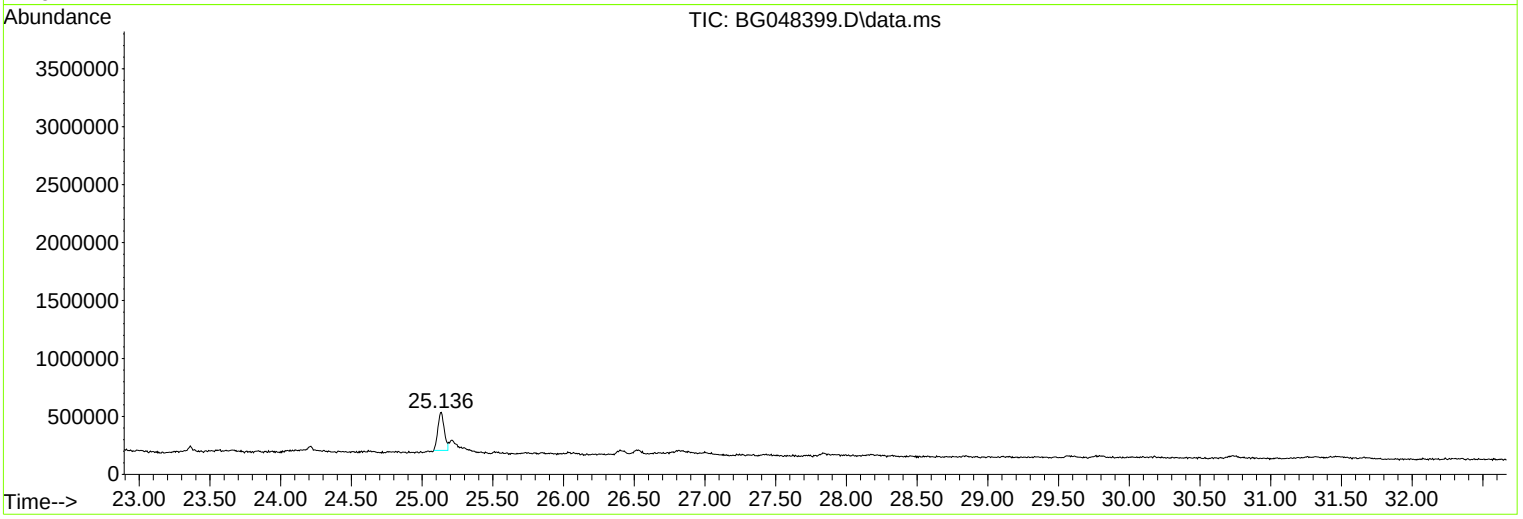
Instrument :
BNA_G
ClientSampleId :
SW-VAN-WINKLE-STREET

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.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 : BG048399.D
Acq On : 17 Mar 2021 15:48
Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

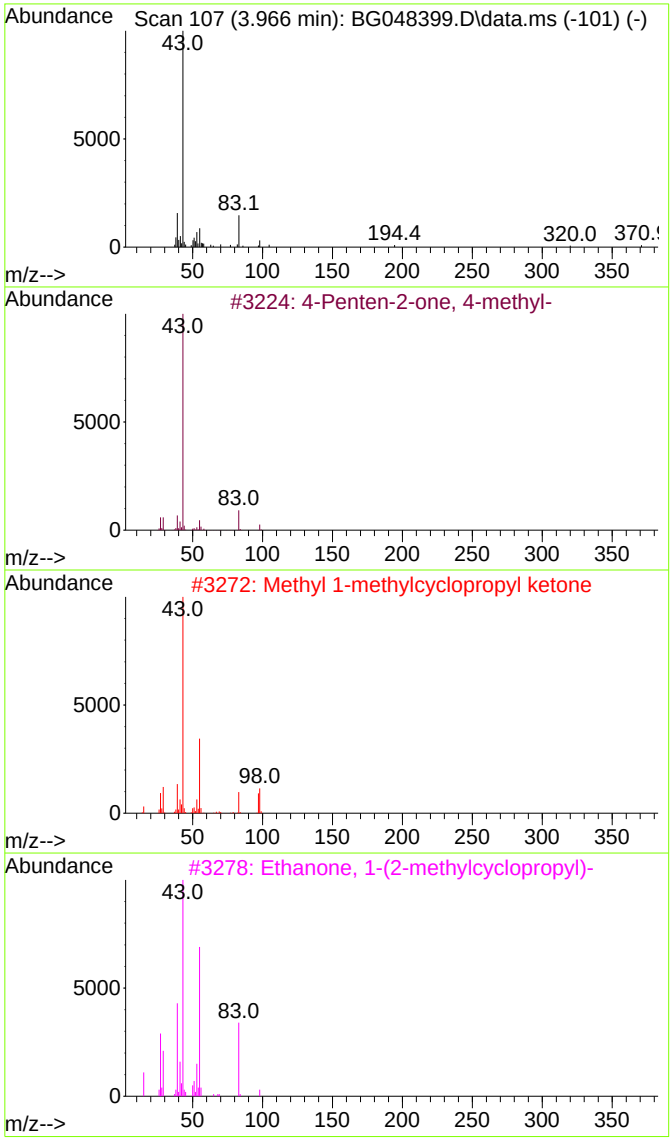
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

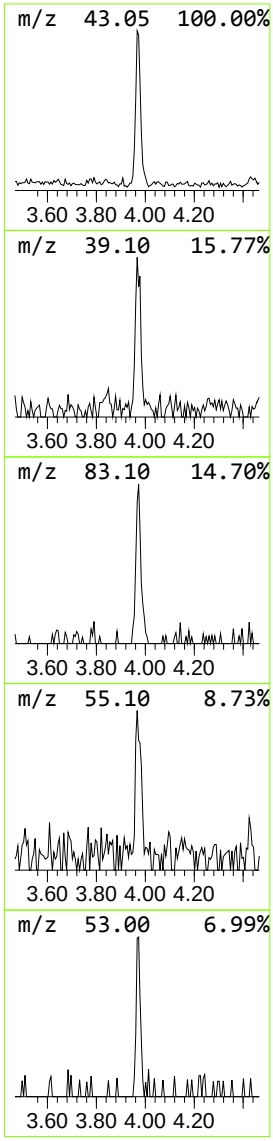
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.966	4.06 ng	70990	1,4-Dichlorobenzene-d4	8.109

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	53
2	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	42
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	12
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9





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Data File : BG048399.D
Acq On : 17 Mar 2021 15:48
Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-VAN-WINKLE-STREET

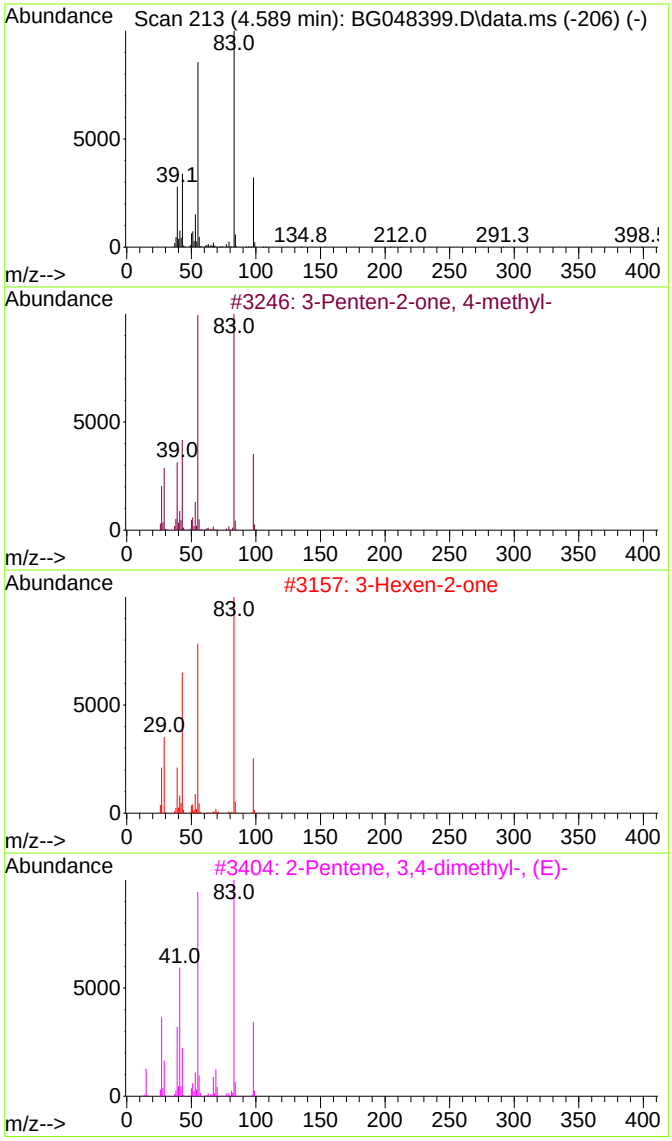
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

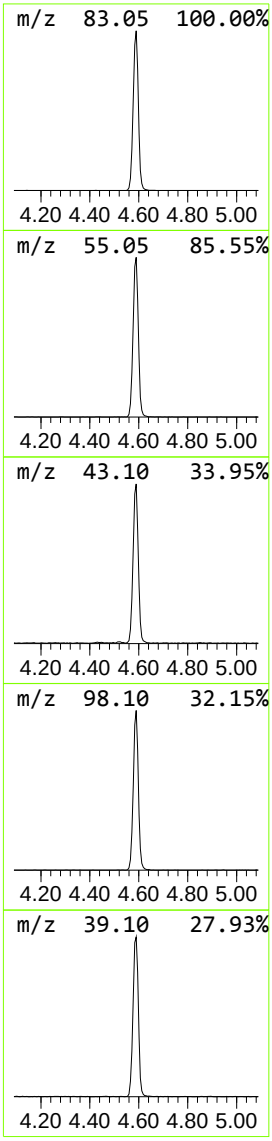
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.589	216.90 ng	3790960	1,4-Dichlorobenzene-d4	8.109

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048399.D
Acq On : 17 Mar 2021 15:48
Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-VAN-WINKLE-STREET

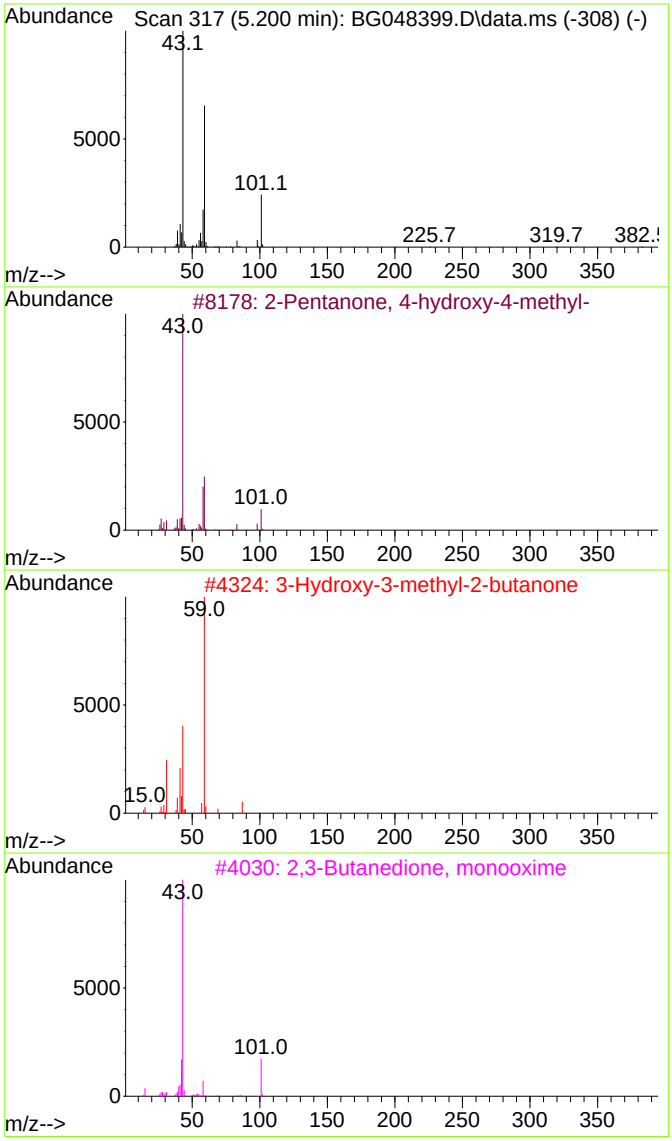
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

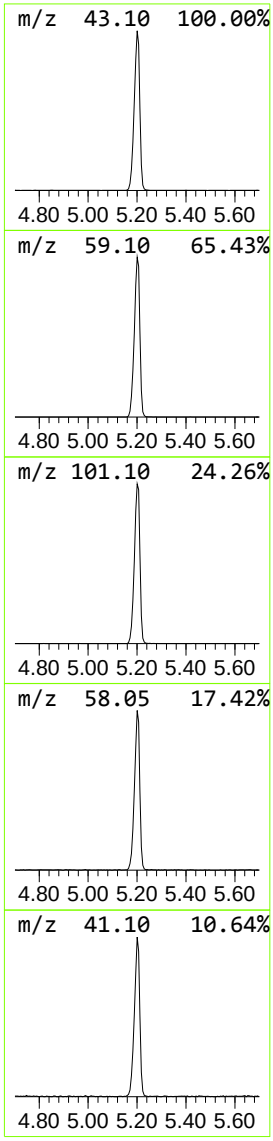
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.200	189.87 ng	3318480	1,4-Dichlorobenzene-d4	8.109

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Acetone	58	C3H6O	000067-64-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Acq On : 17 Mar 2021 15:48
Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-VAN-WINKLE-STREET

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

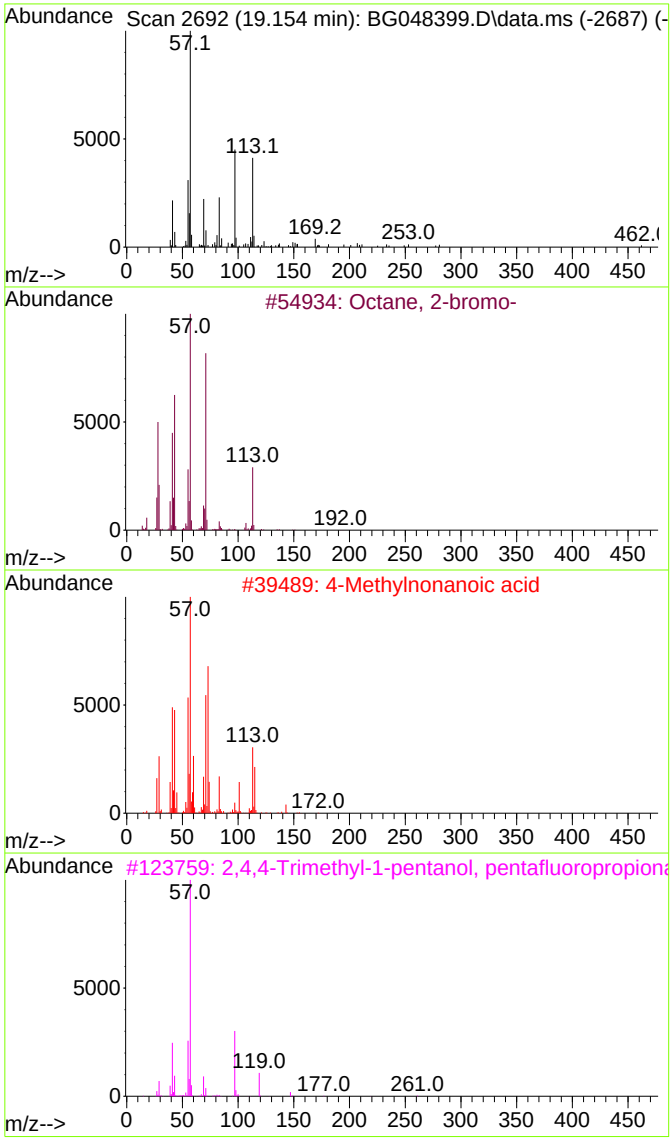
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

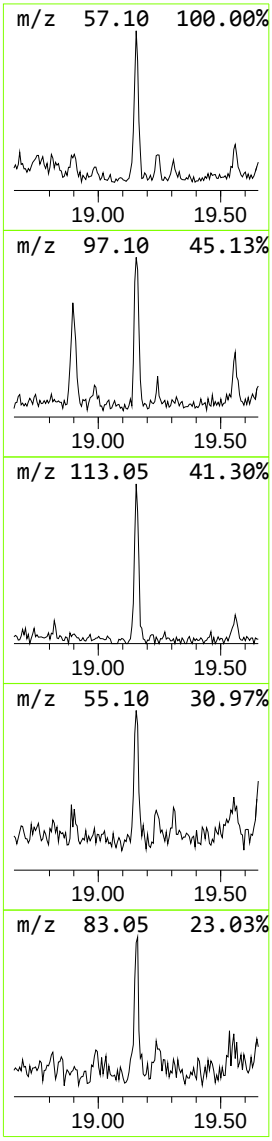
****

Peak Number 4 unknown19.15 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.154	2.61 ng	122291	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
2	4-Methylnonanoic acid	172	C10H20O2	045019-28-1	33
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	27
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	25
5	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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Instrument :
BNA_G
ClientSampleId :
SW-VAN-WINKLE-STREET

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

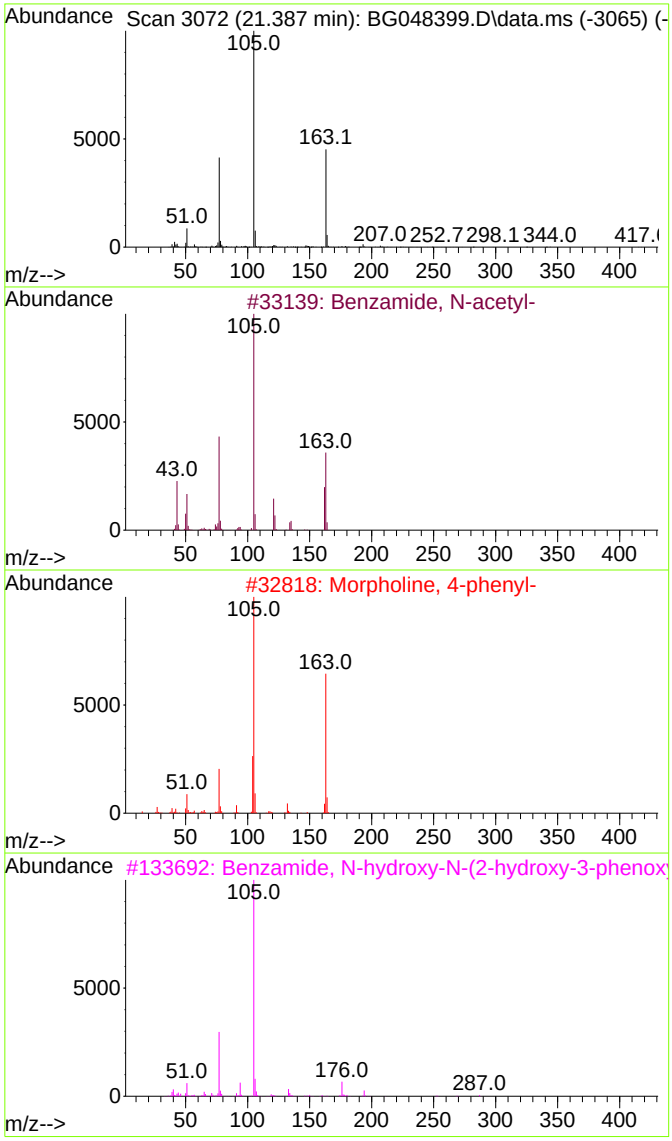
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

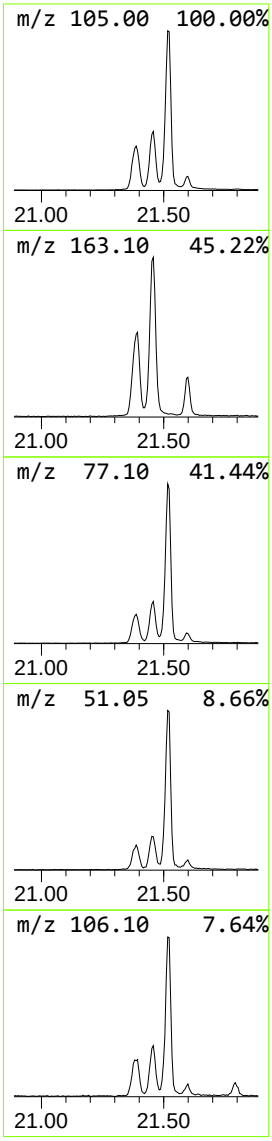
****

Peak Number 5 Benzamide, N-acetyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.387	34.44 ng	1627040	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	56
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	50
3	Benzamide, N-hydroxy-N-(2-hydrox...	287	C16H17NO4	309921-11-7	43
4	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	43
5	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
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Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-VAN-WINKLE-STREET

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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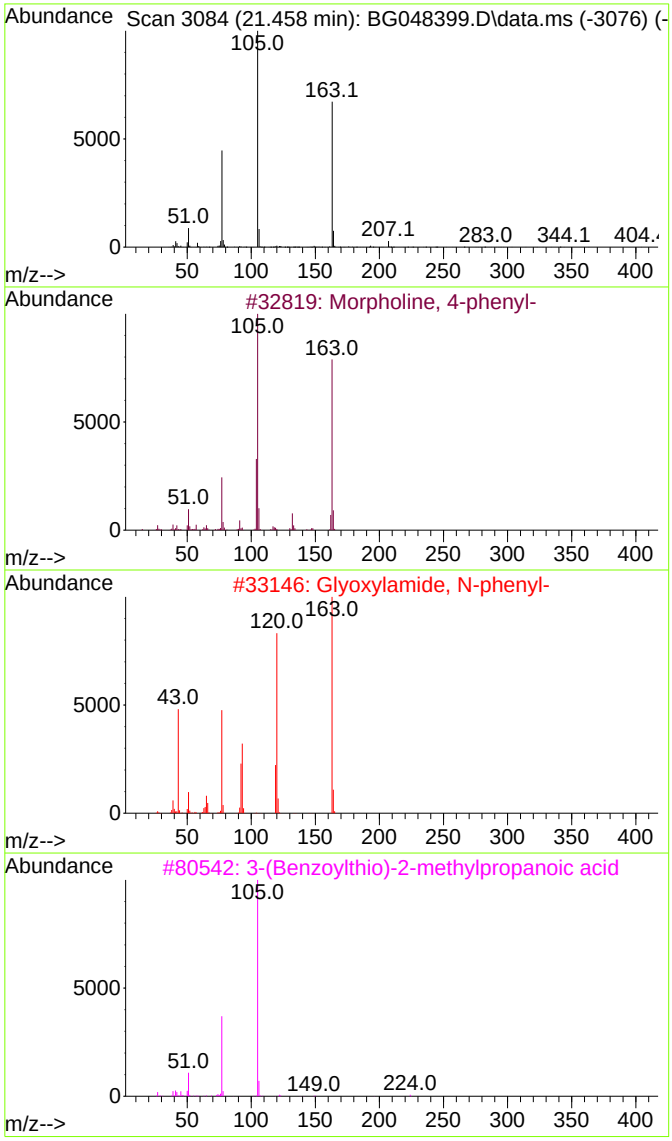
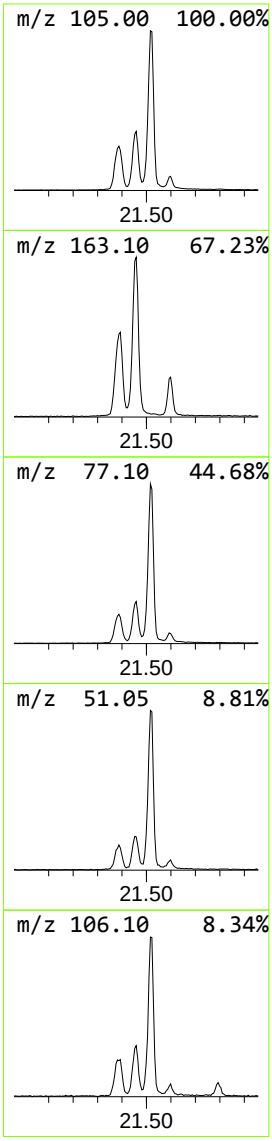
****

Peak Number 6 Morpholine, 4-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.458	49.76 ng	2351010	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	53
3	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	43
4	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	43
5	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	43





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Data File : BG048399.D
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Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-VAN-WINKLE-STREET

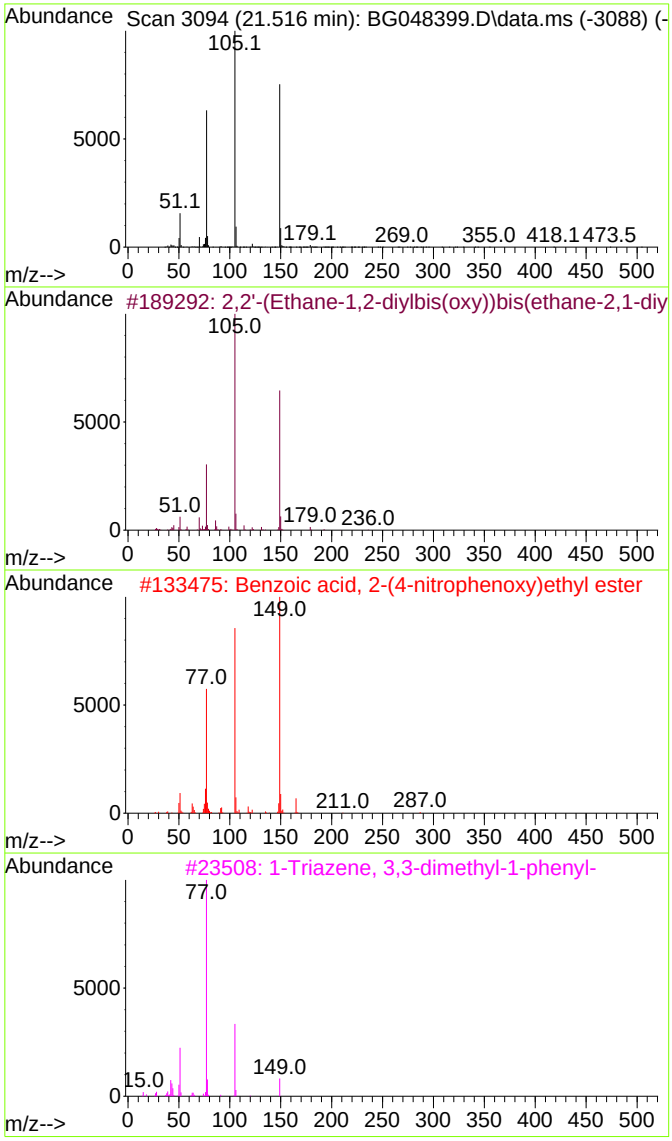
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

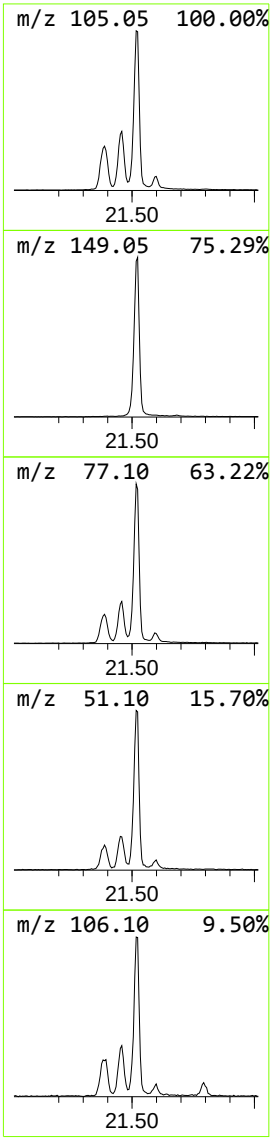
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.516	120.55 ng	5695170	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	74
3	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	72
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

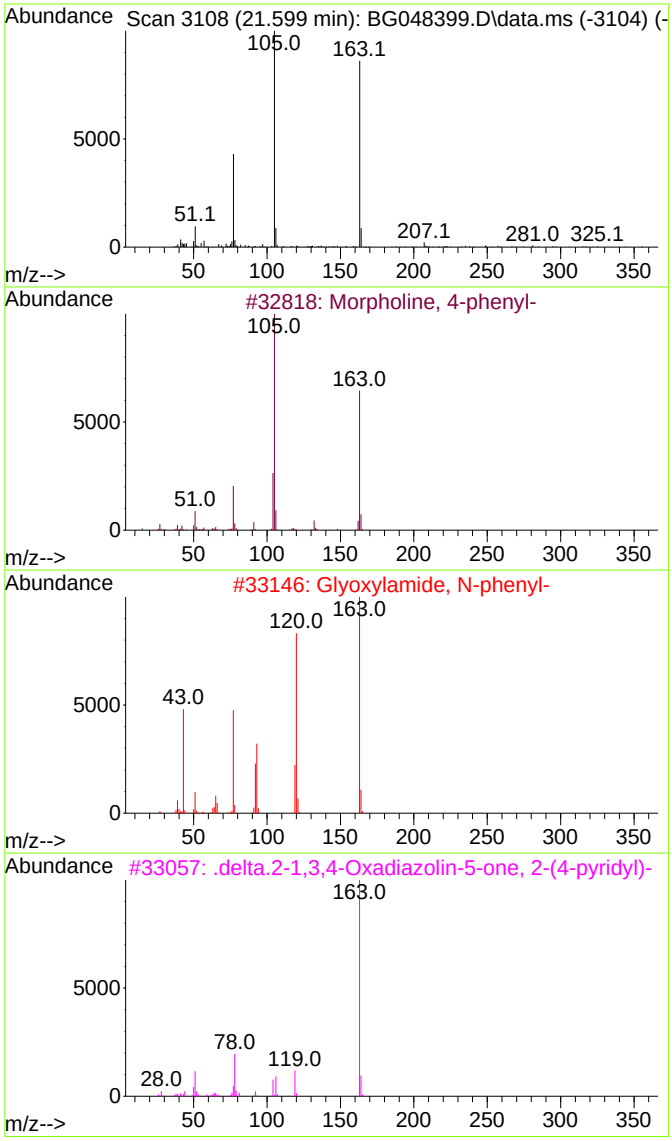
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

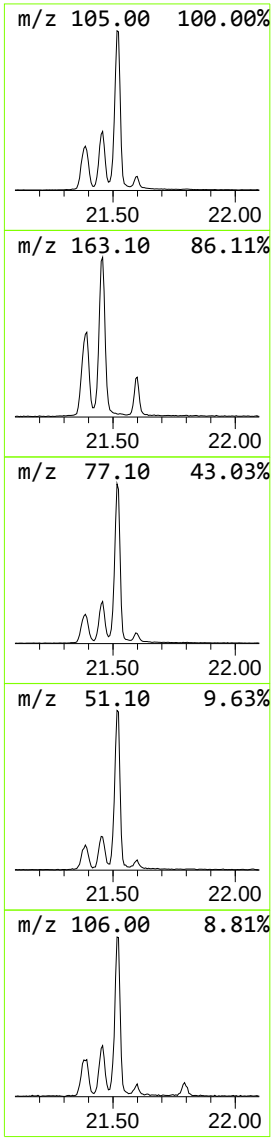
****

Peak Number 8 Glyoxylamide, N-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.599	7.37 ng	348284	Chrysene-d12	21.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	64
3	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	47
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	35
5	Thiobenzoic acid, S-n-butyl ester	194	C11H14OS	007269-35-4	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG031721\
Data File : BG048399.D
Acq On : 17 Mar 2021 15:48
Operator : CG/JU
Sample : M1686-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW-VAN-WINKLE-STREET

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031621.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
4-Penten-2-one,...	3.966	4.1	ng	70990	1	8.109	349554	20.0
3-Penten-2-one,...	4.589	216.9	ng	3790960	1	8.109	349554	20.0
2-Pentanone, 4-...	5.200	189.9	ng	3318480	1	8.109	349554	20.0
unknown19.15	19.154	2.6	ng	122291	4	17.503	937846	20.0
Benzamide, N-ac...	21.387	34.4	ng	1627040	5	21.793	944901	20.0
Morpholine, 4-p...	21.458	49.8	ng	2351010	5	21.793	944901	20.0
2,2'-(Ethane-1,...	21.516	120.6	ng	5695170	5	21.793	944901	20.0
Glyoxylamide, N...	21.599	7.4	ng	348284	5	21.793	944901	20.0