LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056278.D
Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056278.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.336	3	8	19	rVB	175478	252900	1.32%	0.535%
2	5.357	346	352	361	rBV	136946	205441	1.07%	0.435%
3	5.839	427	434	445	rBV	549901	879098	4.60%	1.860%
4	7.454	701	709	718	rBV	562000	949560	4.97%	2.009%
5	8.318	849	856	864	rBV	130847	221477	1.16%	0.469%
6	9.493	1048	1056	1067	rBV	323243	574186	3.00%	1.215%
7	11.150	1331	1338	1346	rVB	172767	309669	1.62%	0.655%
8	13.559	1739	1748	1755	rBV	1292933	1954246	10.22%	4.135%
9	14.928	1968	1981	1988	rBV	353554	586985	3.07%	1.242%
10	15.709	2099	2114	2122	rBV8	67119	314227	1.64%	0.665%
11	16.268	2204	2209	2214	rVB2	229886	329035	1.72%	0.696%
12	16.409	2227	2233	2242	rVB	927187	1388771	7.26%	2.939%
13	17.666	2442	2447	2453	rVB	468877	697081	3.65%	1.475%
14	19.570	2761	2771	2781	rBV	751650	2719155	14.22%	5.754%
15	19.669	2781	2788	2795	rVV	1304252	3385796	17.71%	7.165%
16	19.787	2795	2808	2820	rVV	6677437	19122234	100.00%	40.465%
17	19.881	2820	2824	2837	rVB	466250	1081853	5.66%	2.289%
18	20.239	2880	2885	2891	rVB	2622011	3419723	17.88%	7.237%
19	21.514	3095	3102	3108	rBV2	341491	895901	4.69%	1.896%
20	21.585	3109	3114	3119	rVV	577974	1195730	6.25%	2.530%
21	21.655	3119	3126	3133	rVV	3024855	4804623	25.13%	10.167%
22	21.732	3134	3139	3147	rVB	120288	198294	1.04%	0.420%
23	21.961	3172	3178	3187	rVB	485741	859019	4.49%	1.818%
24	25.404	3754	3764	3777	rVB2	289371	911550	4.77%	1.929%

Sum of corrected areas: 47256554

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ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
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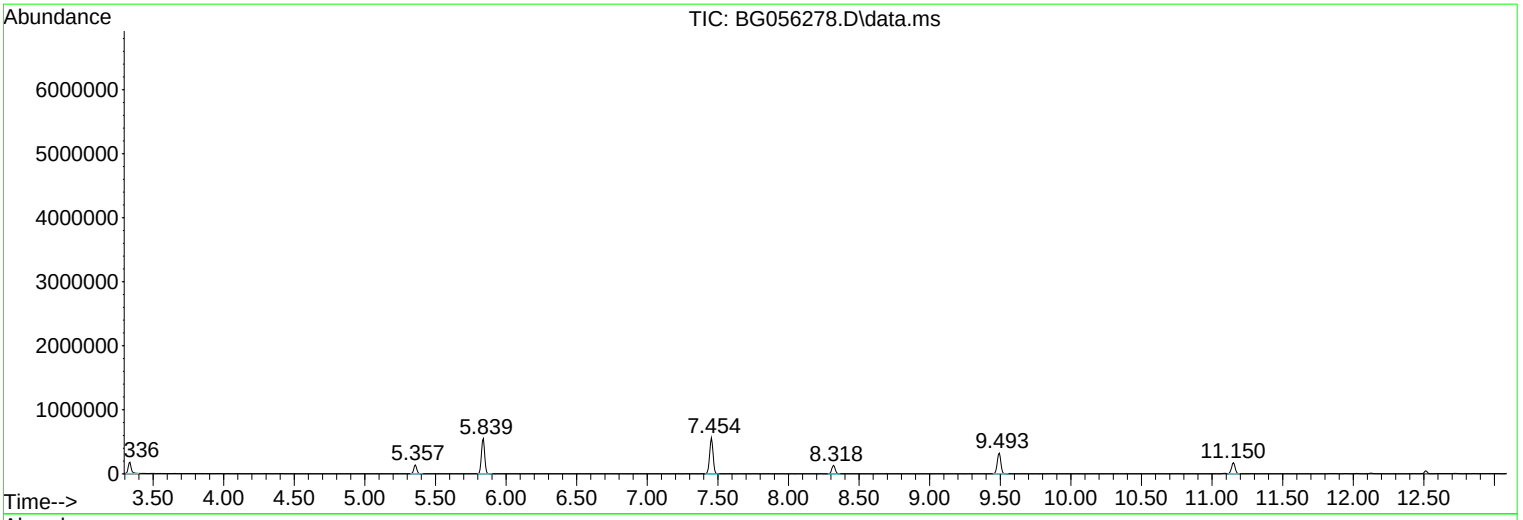
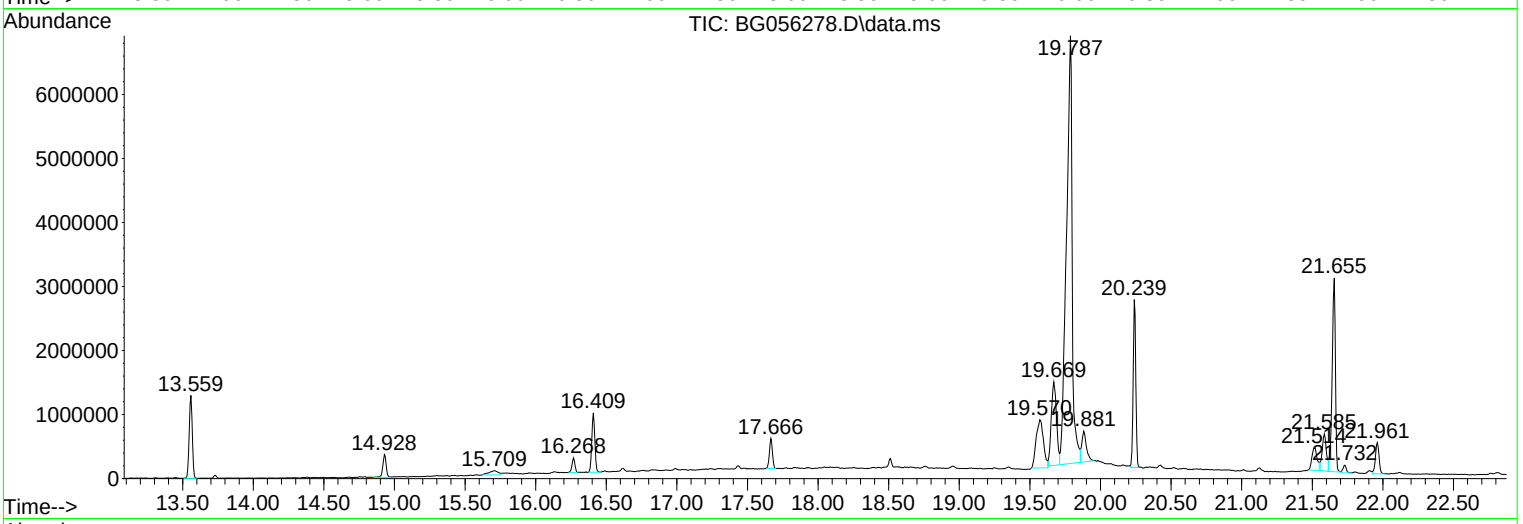
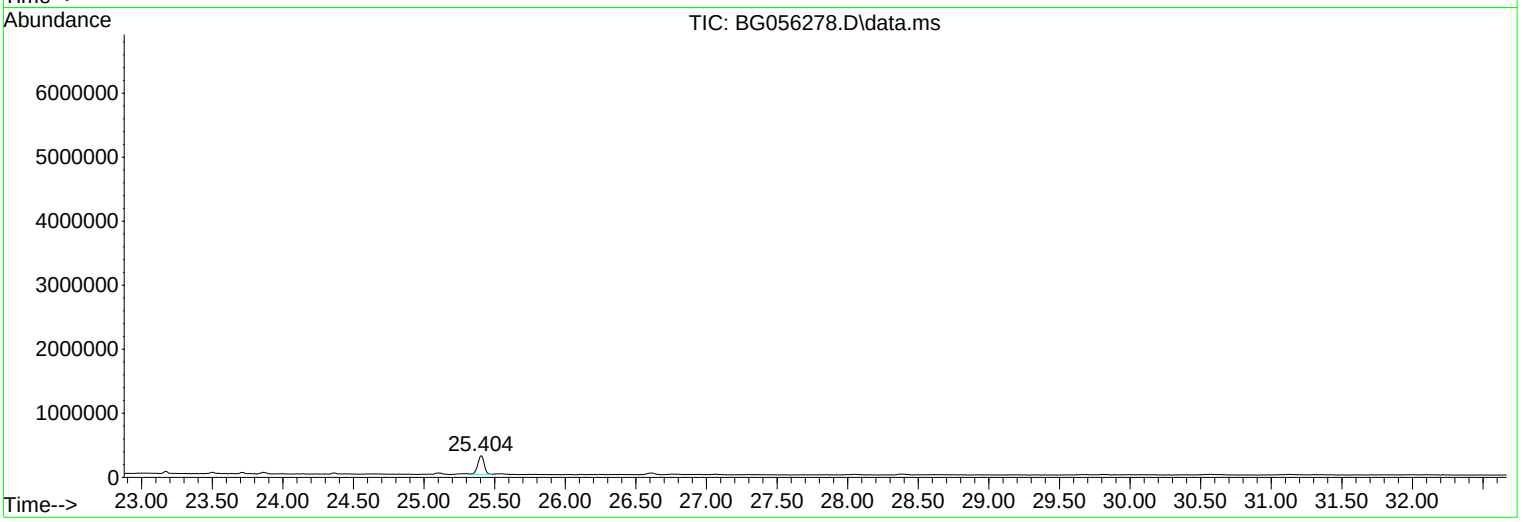
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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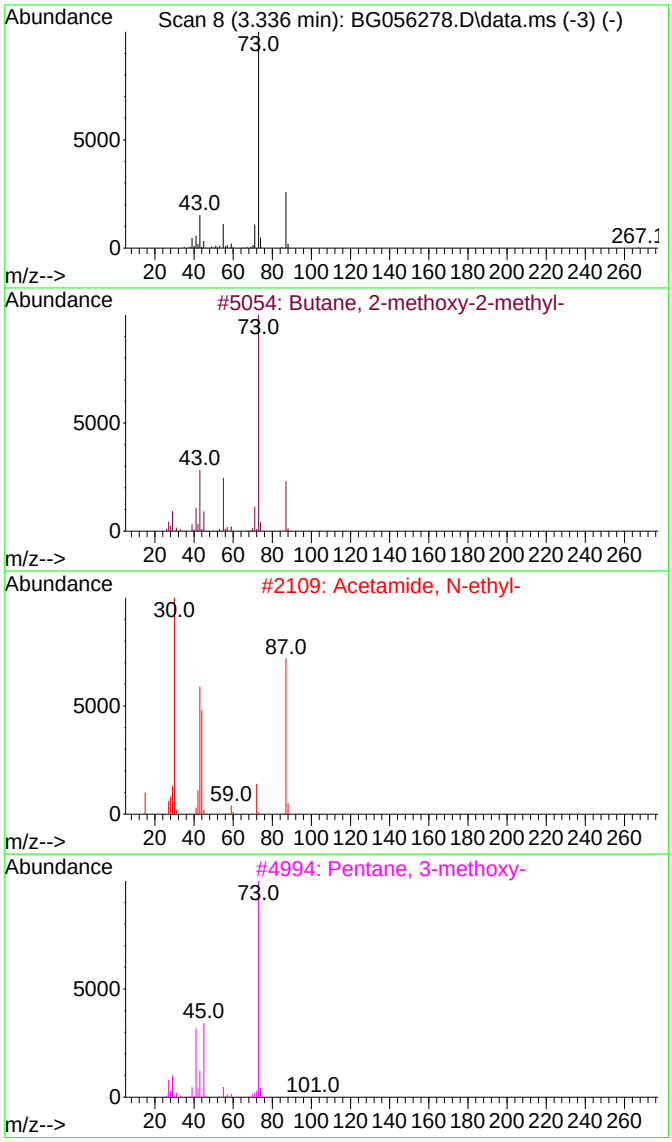
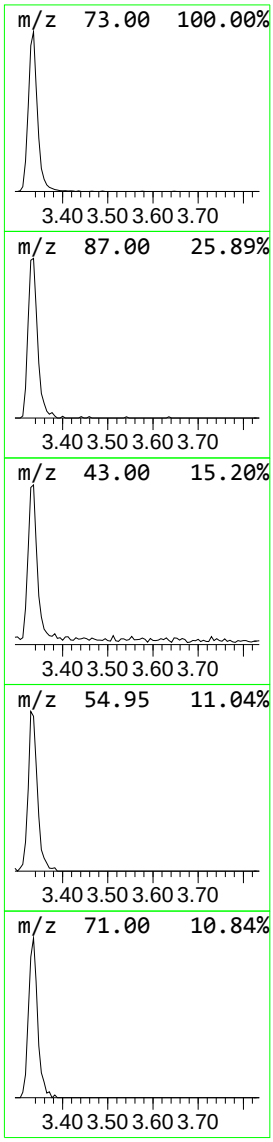
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.336	22.84 ng	252900	1,4-Dichlorobenzene-d4	8.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7





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Data File : BG056278.D
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Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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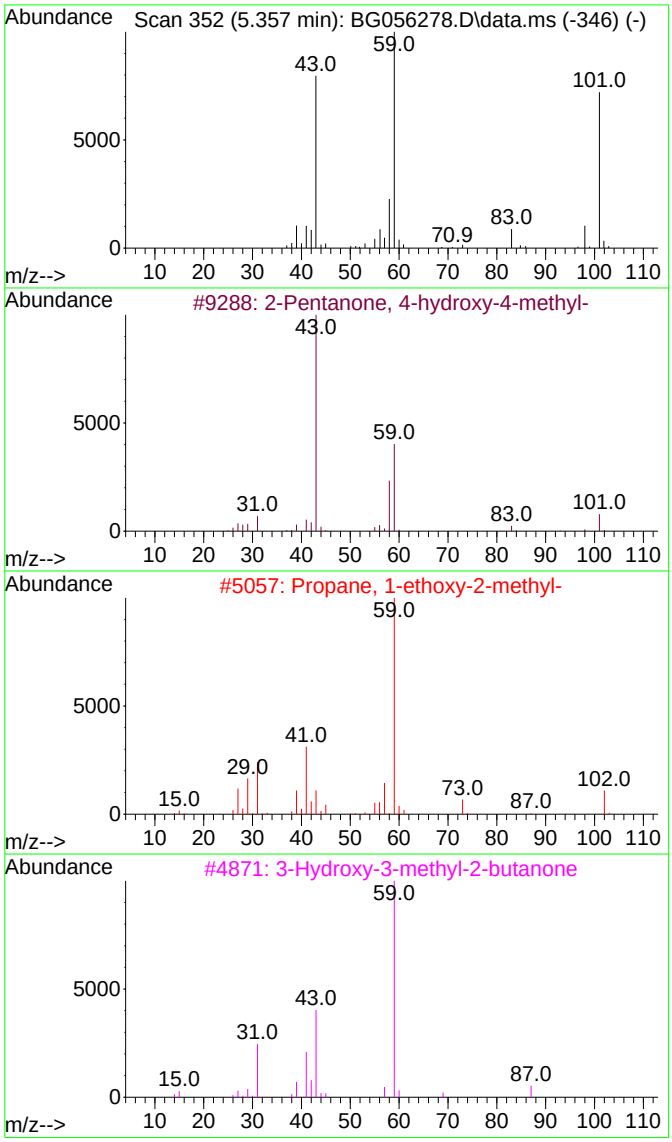
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

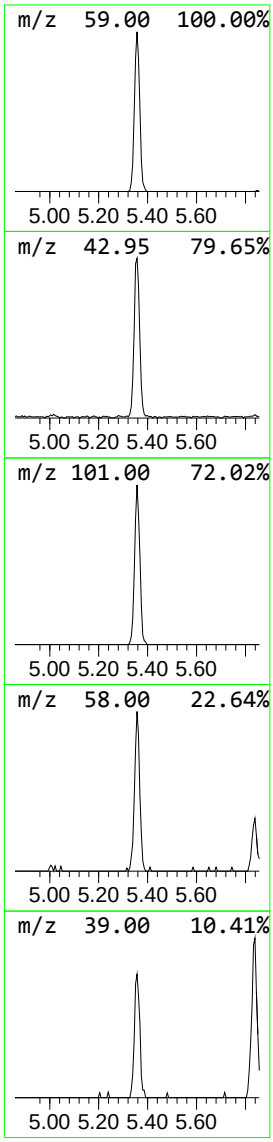
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.357	18.55 ng	205441	1,4-Dichlorobenzene-d4	8.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	2,4-Dimethyl-2,4-pentanediol	132	C7H16O2	024892-49-7	25
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25





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Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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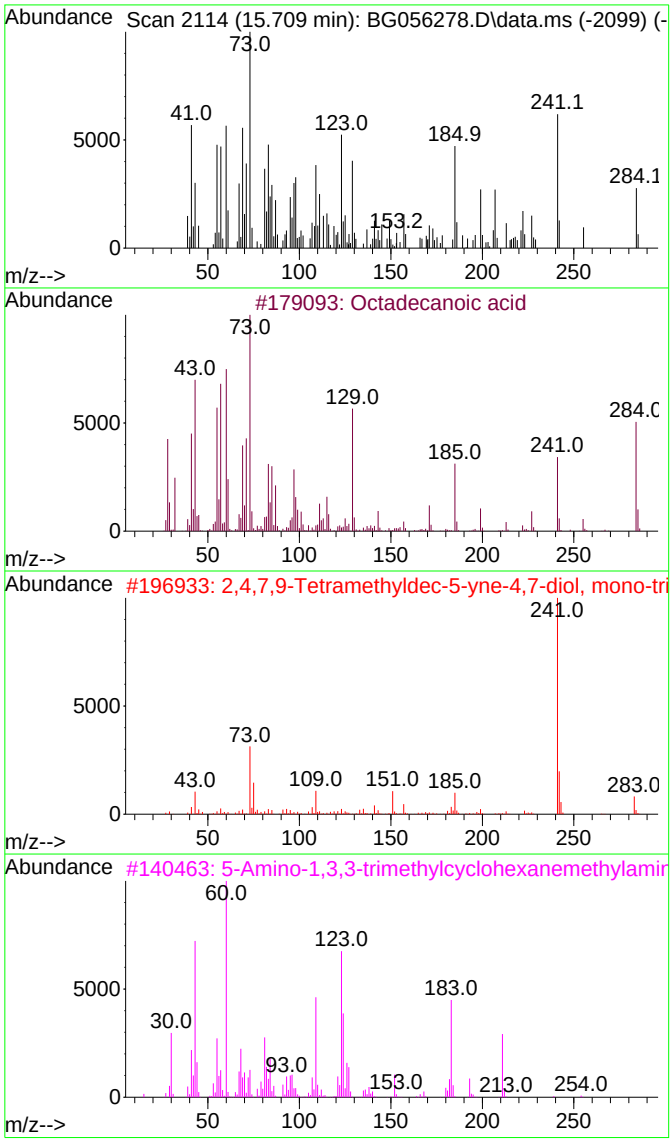
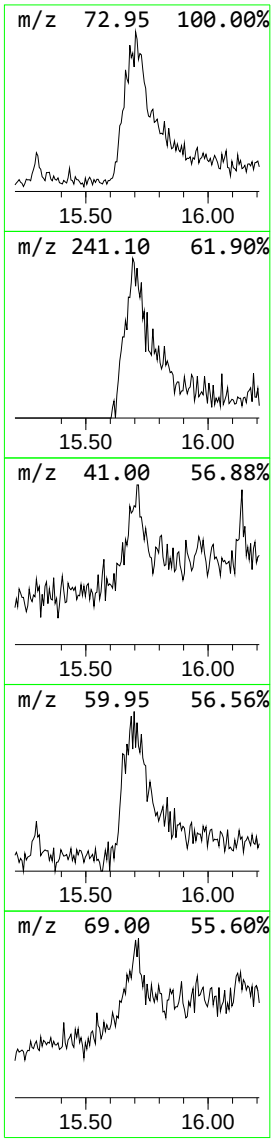
****

Peak Number 3 unknown15.709 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.709	10.71 ng	314227	Acenaphthene-d10	14.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	20
2	2,4,7,9-Tetramethyldec-5-yne-4,7...	298	C17H34O2Si	1010473-18-6	14
3	5-Amino-1,3,3-trimethylcyclohexa...	254	C14H26N2O2	1000454-06-5	12
4	7-Butylbenz[a]anthracene	284	C22H20	018868-65-0	11
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	11





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Data File : BG056278.D
Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

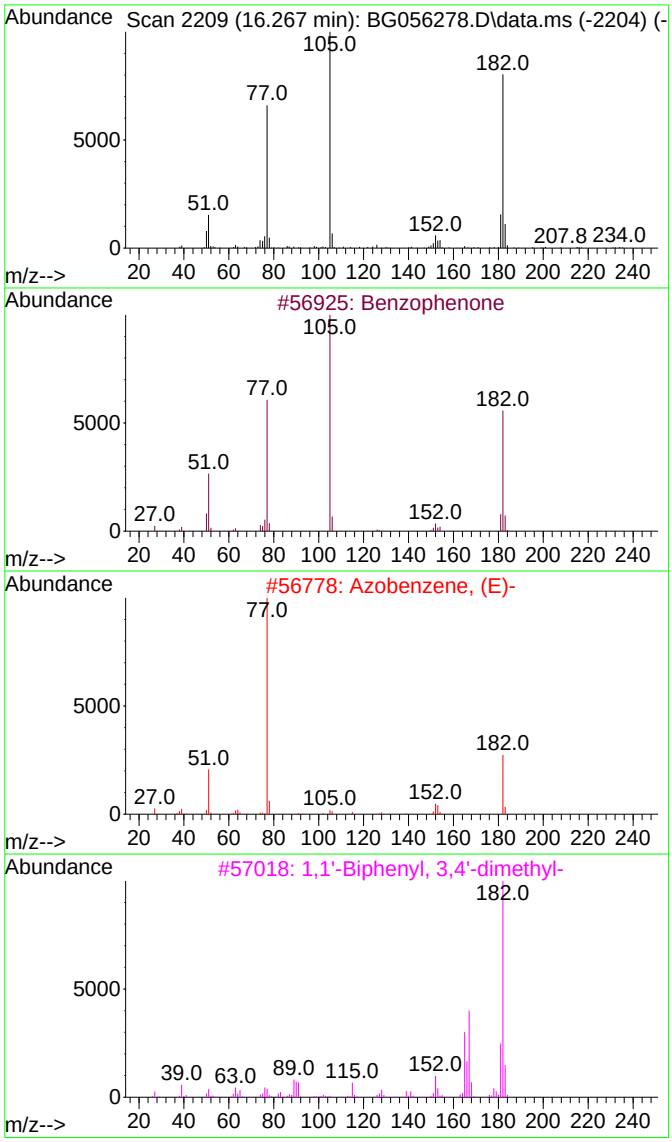
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

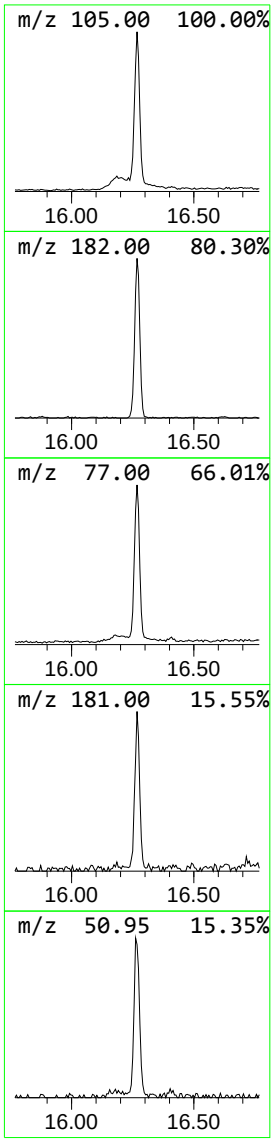
****

Peak Number 4 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.267	11.21 ng	329035	Acenaphthene-d10	14.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	94
2	Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	49
4	2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	47
5	9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	46





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Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

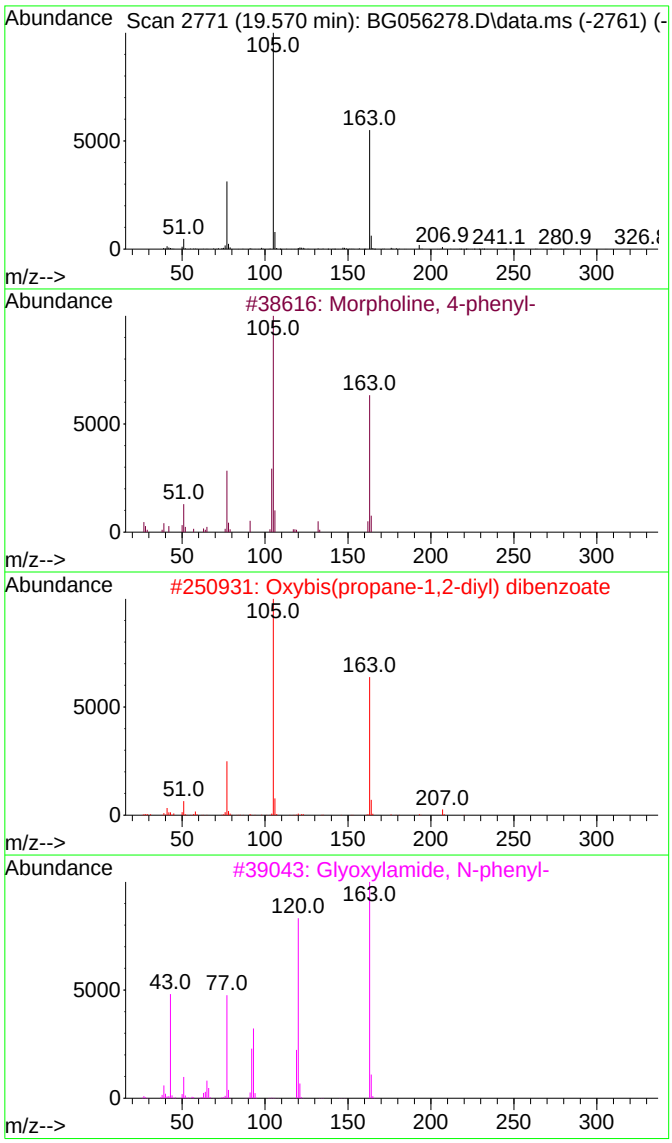
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

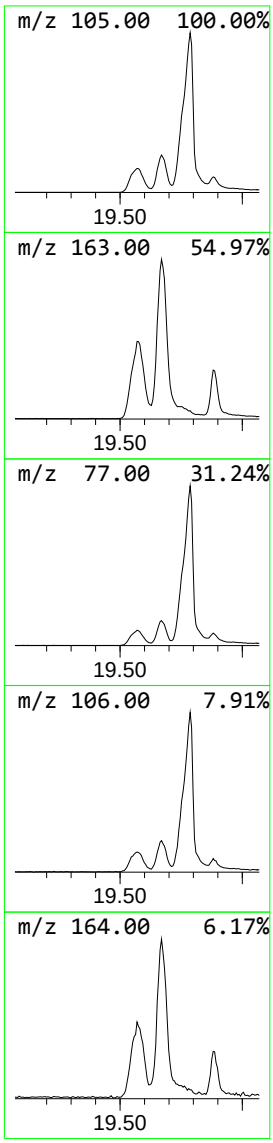
****

Peak Number 5 Morpholine, 4-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.570	78.02 ng	2719160	Phenanthrene-d10	17.666

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	40
4	1,3-Benzenediol, monobenzoate	214	C13H10O3	000136-36-7	38
5	Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38





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Data File : BG056278.D
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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TIC Library : C:\Database\NIST20.L
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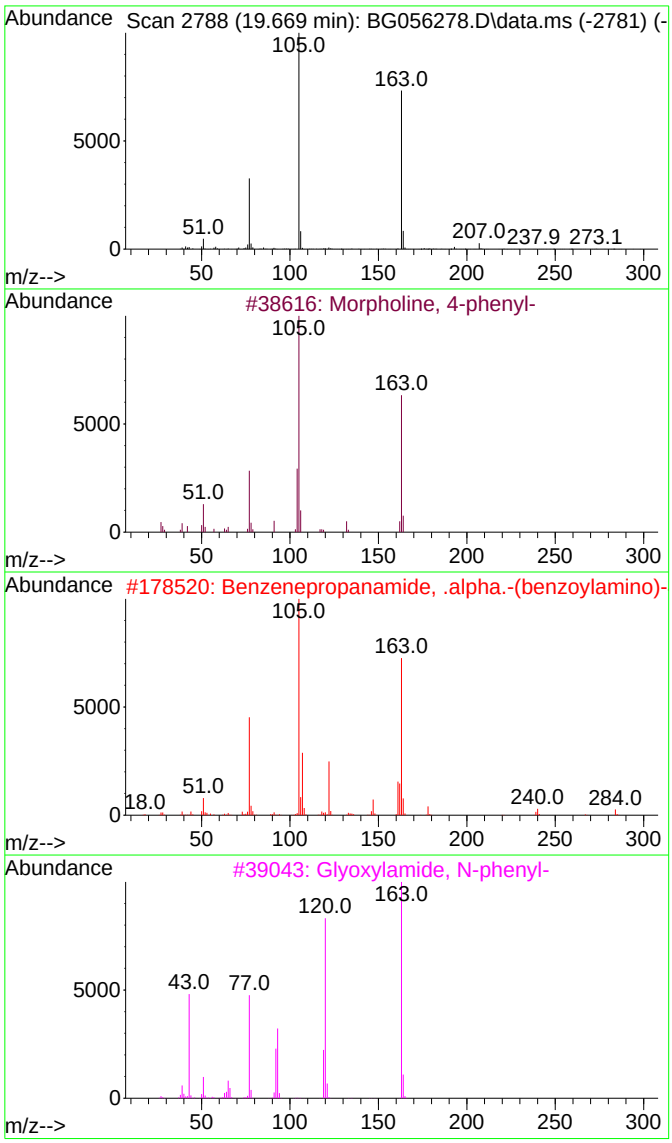
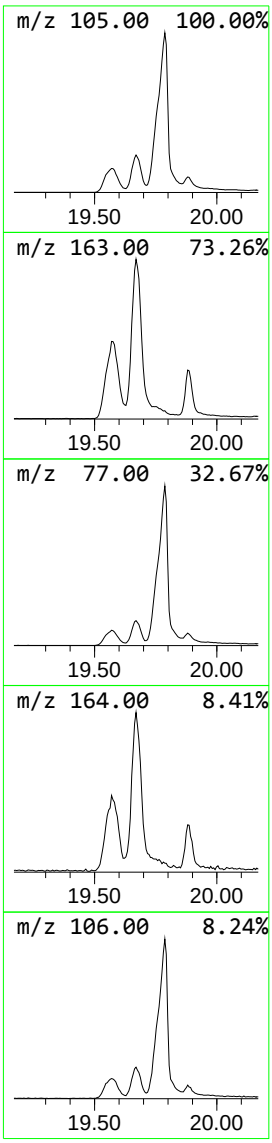
****

Peak Number 6 unknown19.669 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.669	97.14 ng	3385800	Phenanthrene-d10	17.666

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	78
2	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	43
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	42
4	Phenylglyoxylic acid, pentyl ester	220	C13H16O3	1000453-46-0	22
5	1,3-Benzenediol, monobenzoate	214	C13H10O3	000136-36-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056278.D
Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

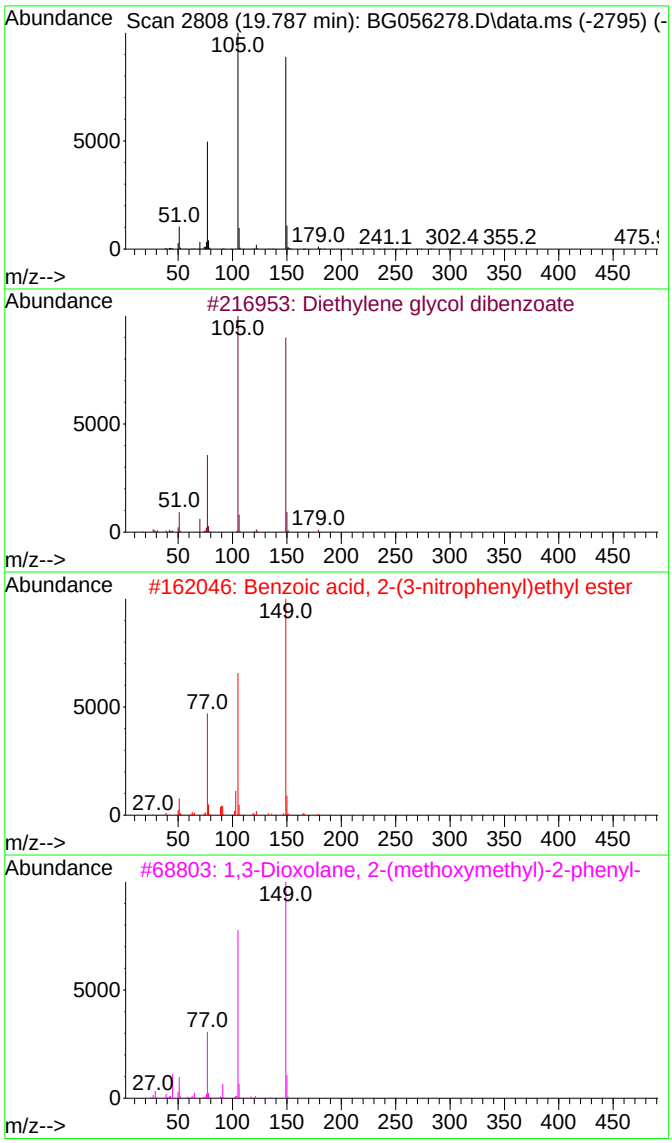
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

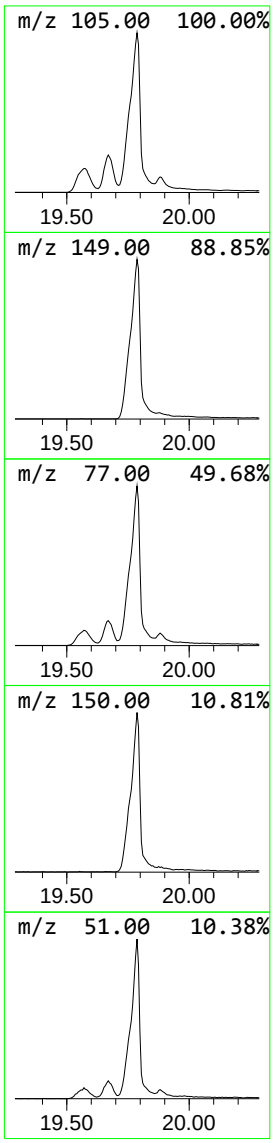
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.787	548.64 ng	19122200	Phenanthrene-d10	17.666

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	59





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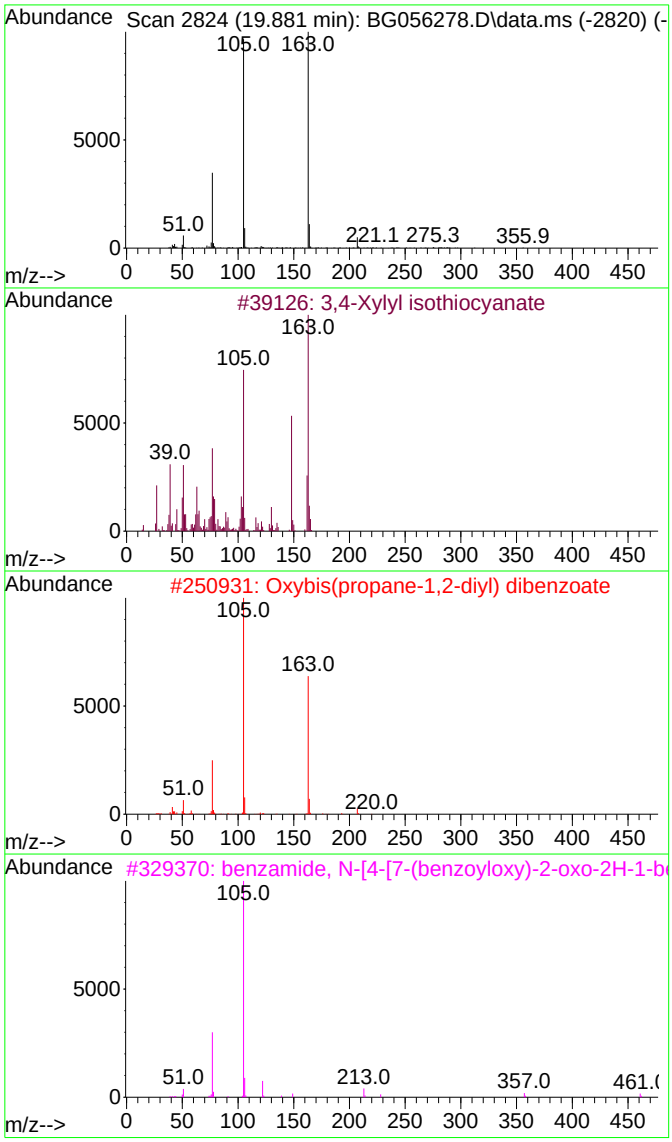
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

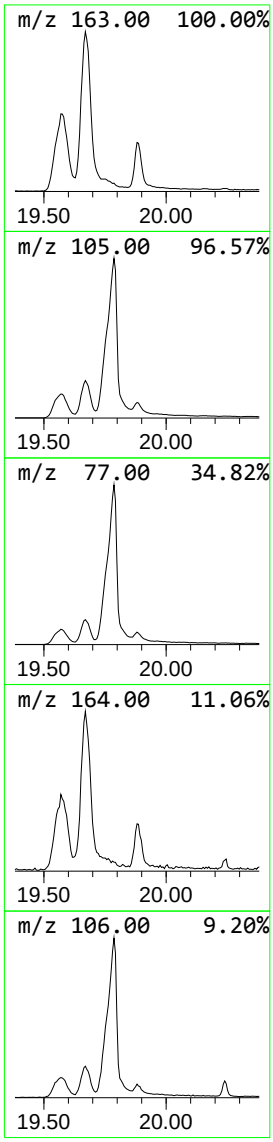
****

Peak Number 8 3,4-Xylyl isothiocyanate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.881	25.19 ng	1081850	Chrysene-d12	21.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Xylyl isothiocyanate	163	C9H9NS	019241-17-9	64
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	50
3	benzamide, N-[4-[7-(benzoyloxy)-...	461	C29H19NO5	1010399-44-9	14
4	Benzamide, N-benzoyl-N-(2-triflu...	369	C21H14F3NO2	1000262-58-9	14
5	4-Nitrophenyl benzoate	243	C13H9NO4	000959-22-8	14





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ALS Vial : 5 Sample Multiplier: 1

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BNA_G
ClientSampleId :
VNJ-207

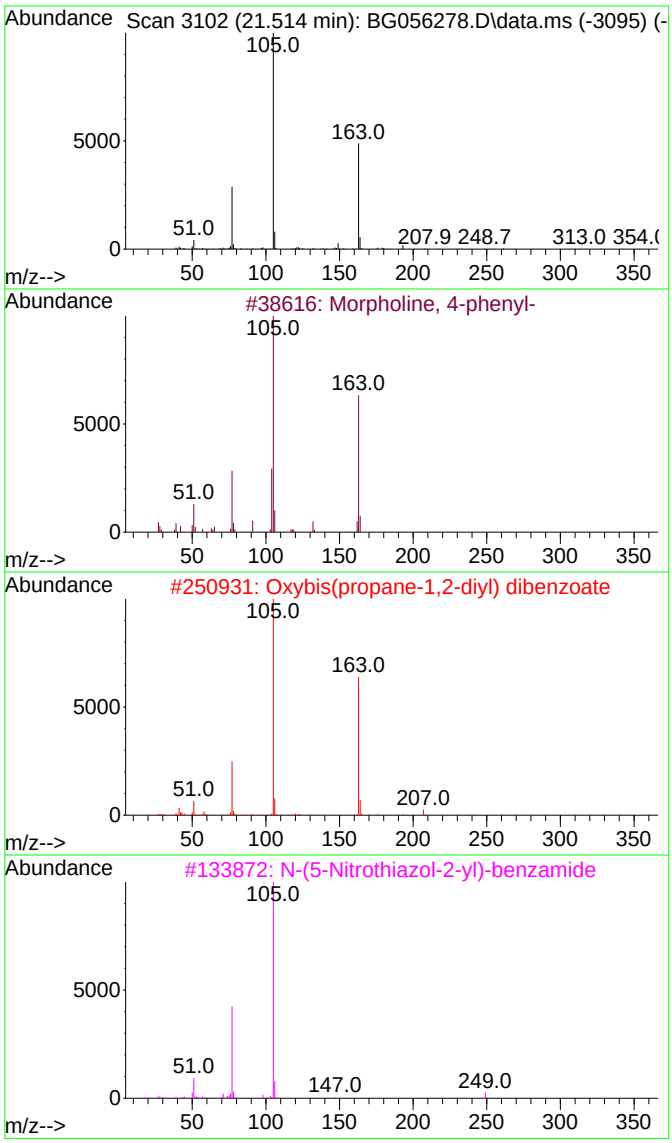
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

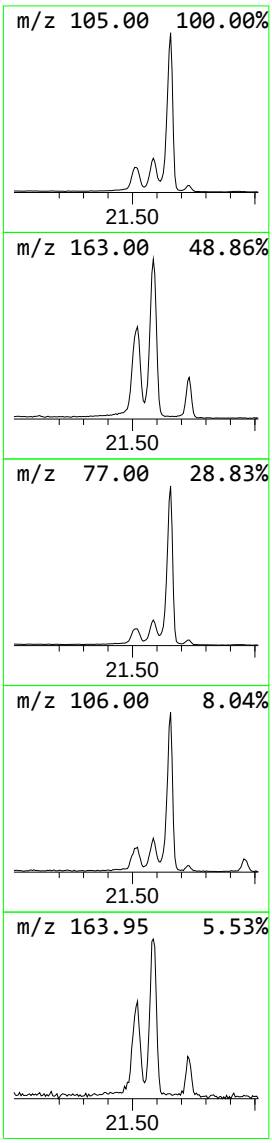
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Oxybis(propane-1,2-diyl) di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	20.86 ng	895901	Chrysene-d12	21.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	80
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
3	N-(5-Nitrothiazol-2-yl)-benzamide	249	C10H7N3O3S	064398-84-1	38
4	Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38
5	Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056278.D
Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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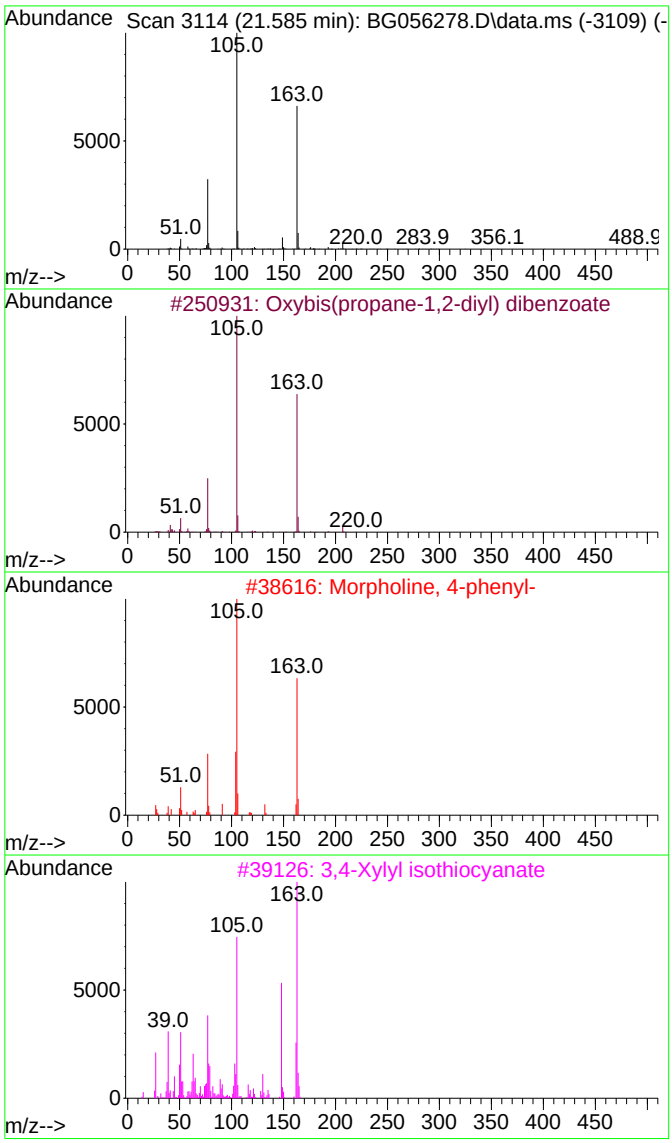
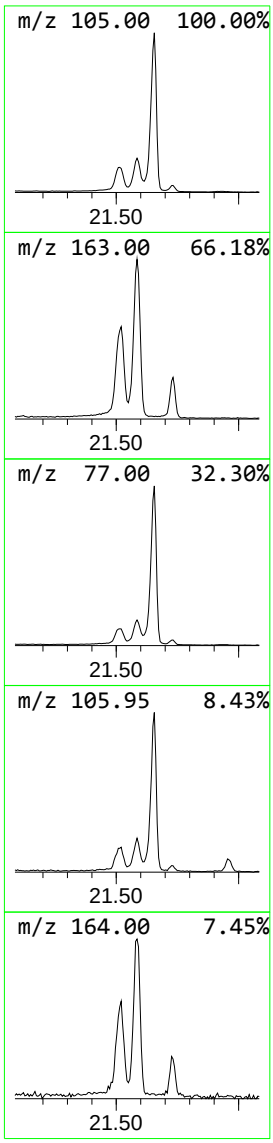
Peak Number 10 unknown21.585 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.585	27.84 ng	1195730	Chrysene-d12	21.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3	3,4-Xylyl isothiocyanate	163	C9H9NS	019241-17-9	64
4	Methyl octyl phthalate	292	C17H24O4	091485-83-5	38
5	Phenylglyoxylic acid, pentyl ester	220	C13H16O3	1000453-46-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056278.D
Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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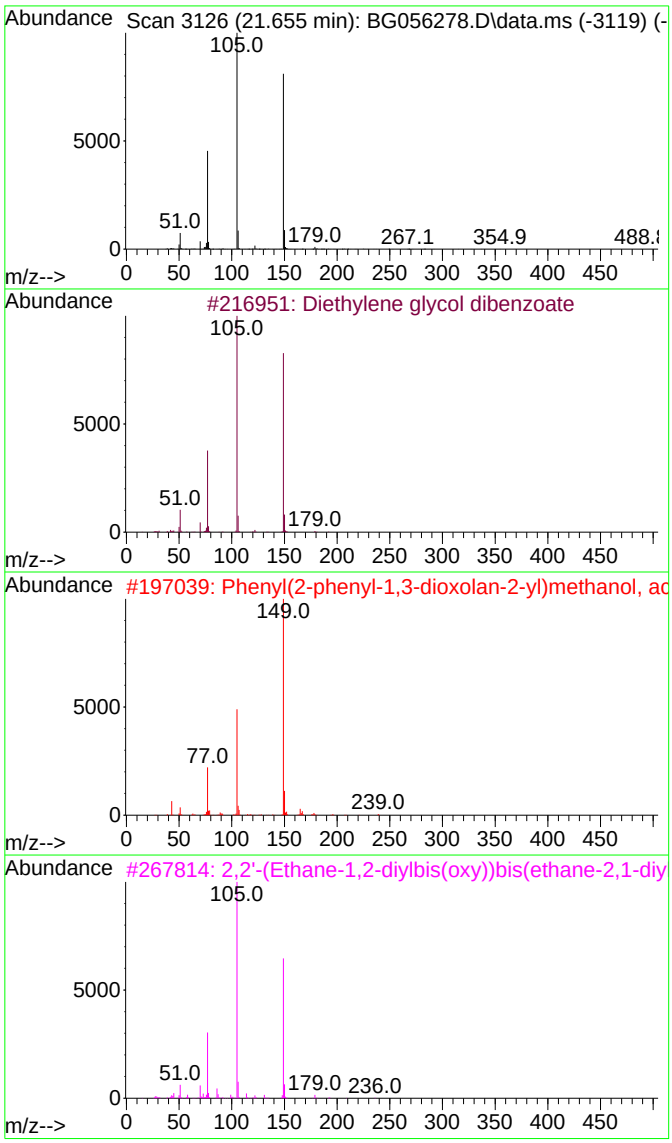
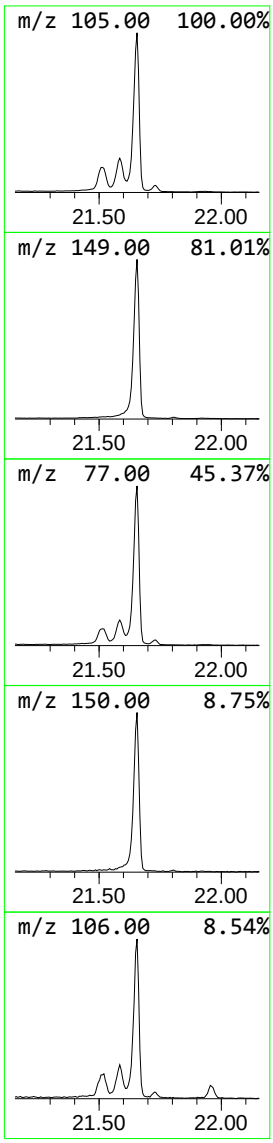
Peak Number 11 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.655	111.86 ng	4804620	Chrysene-d12	21.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	83
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	83
5	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056278.D
Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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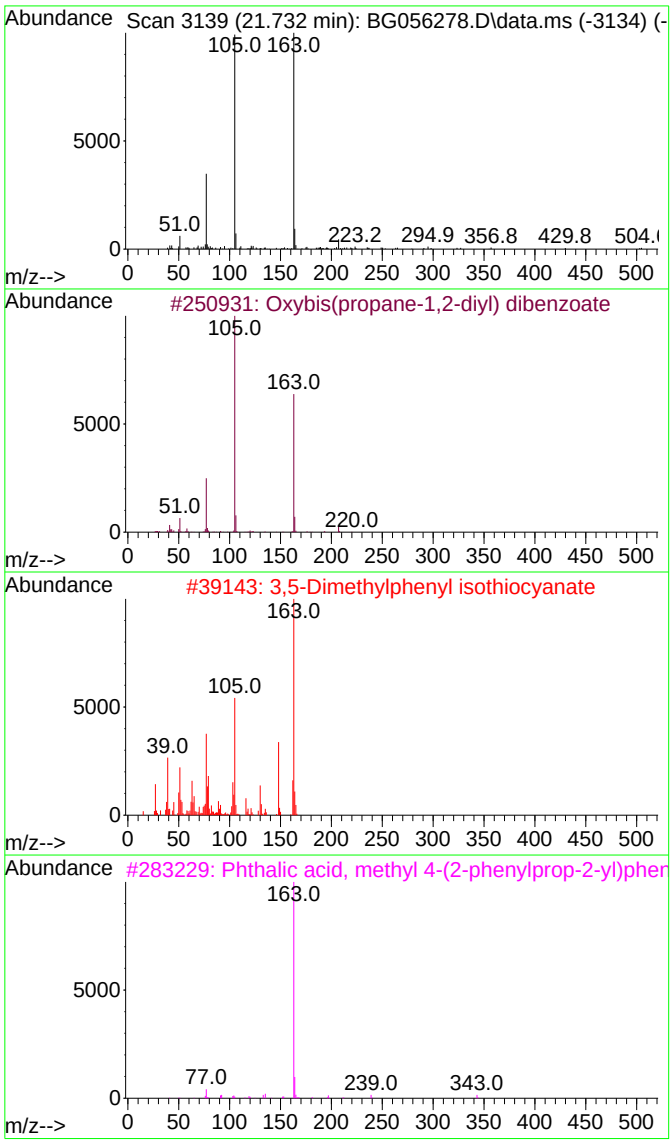
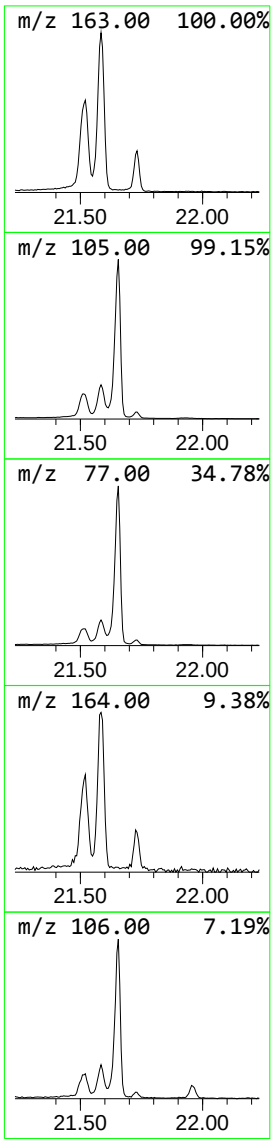
Peak Number 12 unknown21.732 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.732	4.62 ng	198294	Chrysene-d12	21.961

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	50
2	3,5-Dimethylphenyl isothiocyanate	163	C9H9NS	040046-30-8	39
3	Phthalic acid, methyl 4-(2-pheny...	374	C24H22O4	1000315-62-1	28
4	Phthalic acid, 2,6-dimethoxyphen...	316	C17H16O6	1010315-74-1	28
5	Phthalic acid, 4-isopropylphenyl...	298	C18H18O4	1000315-65-7	28





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011323\
Data File : BG056278.D
Acq On : 13 Jan 2023 15:11
Operator : CG/JU
Sample : 01129-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.336	22.8	ng	252900	1	8.318	221477	20.0
2-Pentanone, 4-...	5.357	18.6	ng	205441	1	8.318	221477	20.0
unknown15.709	15.709	10.7	ng	314227	3	14.928	586985	20.0
Benzophenone	16.267	11.2	ng	329035	3	14.928	586985	20.0
Morpholine, 4-p...	19.570	78.0	ng	2719160	4	17.666	697081	20.0
unknown19.669	19.669	97.1	ng	3385800	4	17.666	697081	20.0
Diethylene glyc...	19.787	548.6	ng	19122200	4	17.666	697081	20.0
3,4-Xylyl isoth...	19.881	25.2	ng	1081850	5	21.961	859019	20.0
Oxybis(propane-...	21.514	20.9	ng	895901	5	21.961	859019	20.0
unknown21.585	21.585	27.8	ng	1195730	5	21.961	859019	20.0
Phenyl(2-phenyl...	21.655	111.9	ng	4804620	5	21.961	859019	20.0
unknown21.732	21.732	4.6	ng	198294	5	21.961	859019	20.0