LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
Data File : BG057786.D
Acq On : 21 Jun 2023 15:55
Operator : CG/JU
Sample : PB153543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB153543BL

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-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057786.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.428	222	228	237	rBV	37280	52632	1.74%	0.399%
2	5.027	323	330	339	rVB	263584	381790	12.61%	2.893%
3	5.497	403	410	421	rBV	779952	1208473	39.90%	9.158%
4	7.084	672	680	688	rBV	769070	1276902	42.16%	9.676%
5	7.924	816	823	830	rBV	120563	198471	6.55%	1.504%
6	9.087	1012	1021	1030	rBV	420273	752629	24.85%	5.703%
7	10.727	1292	1300	1308	rVB	173246	301122	9.94%	2.282%
8	13.188	1712	1719	1728	rVB	1074088	1680713	55.49%	12.737%
9	14.557	1946	1952	1961	rVB	278174	431741	14.25%	3.272%
10	16.050	2199	2206	2213	rBV	932401	1456498	48.09%	11.037%
11	17.301	2413	2419	2426	rBV	409315	612942	20.24%	4.645%
12	19.922	2859	2865	2871	rBV	2314848	3028746	100.00%	22.952%
13	21.173	3072	3078	3082	rBV2	39434	77804	2.57%	0.590%
14	21.232	3083	3088	3093	rVB2	58761	99164	3.27%	0.751%
15	21.291	3094	3098	3103	rVV	118188	152481	5.03%	1.156%
16	21.555	3137	3143	3150	rVB2	422533	688058	22.72%	5.214%
17	24.710	3671	3680	3694	rVB2	270390	795756	26.27%	6.030%

Sum of corrected areas: 13195922

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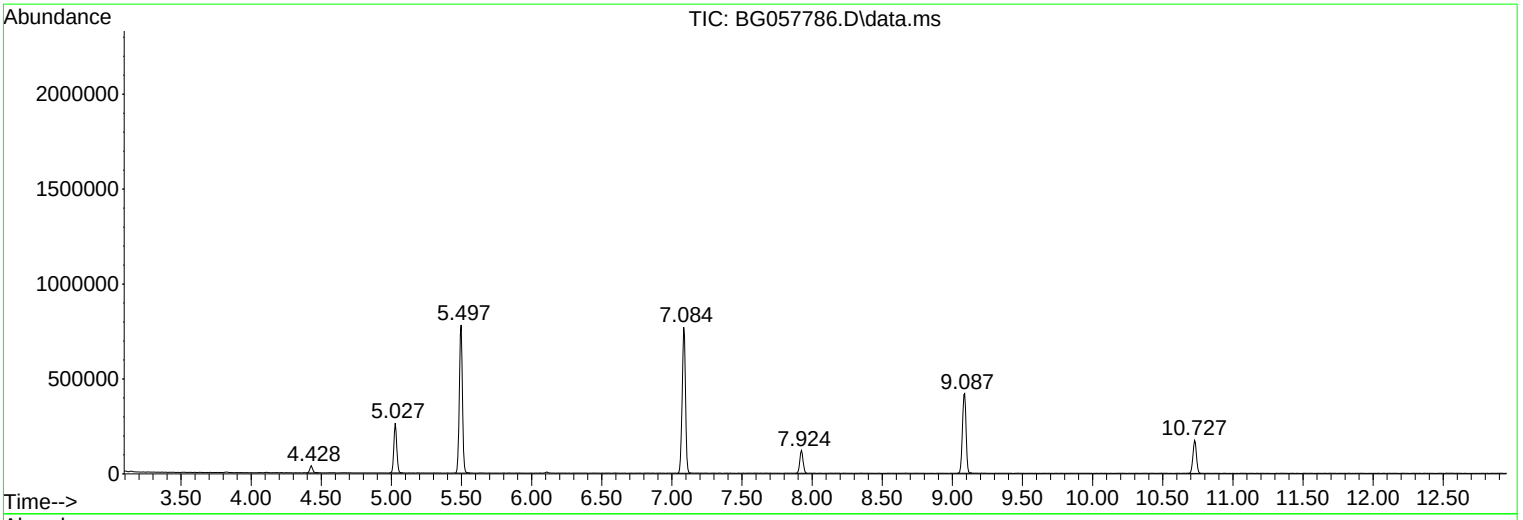
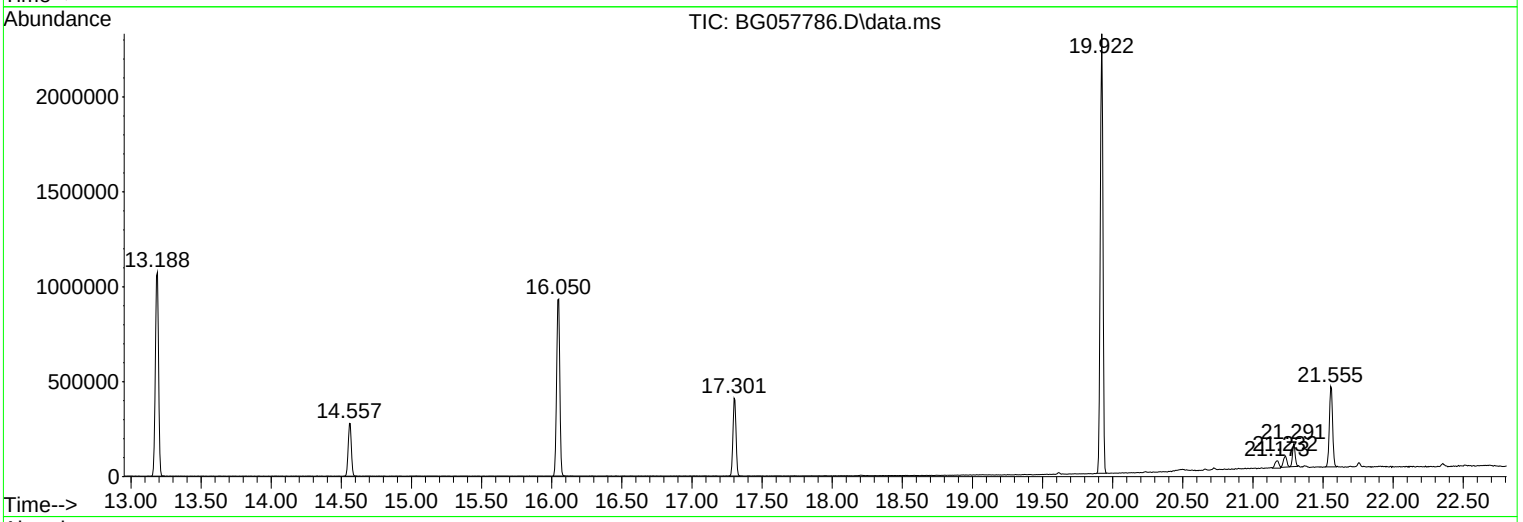
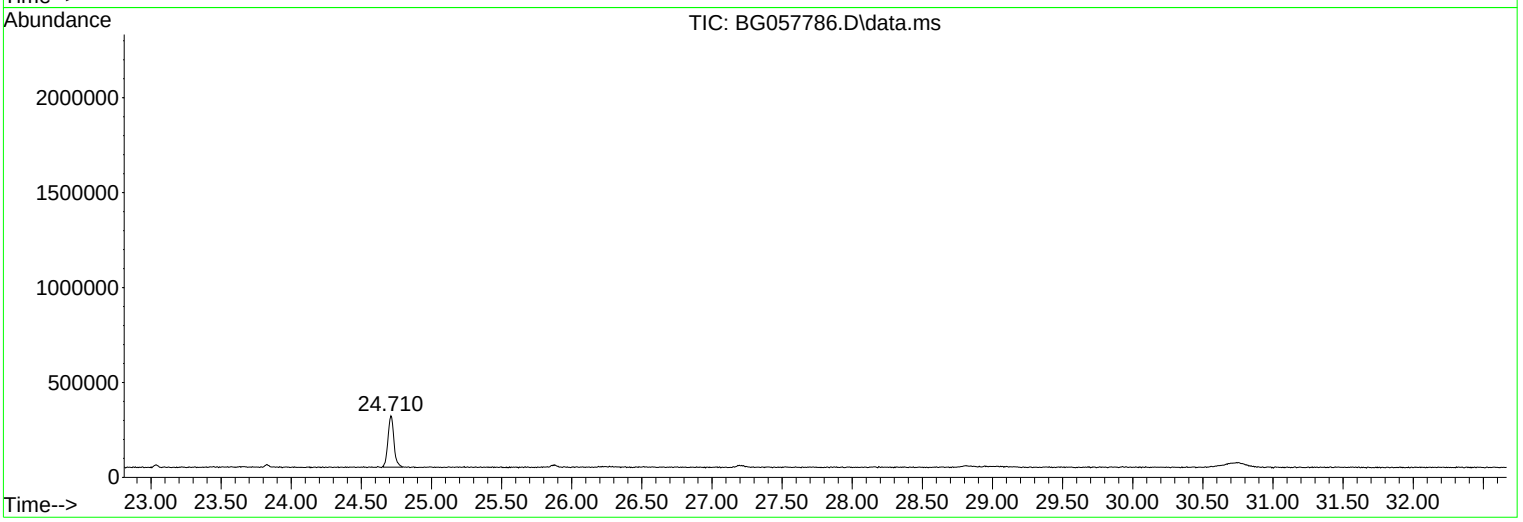
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

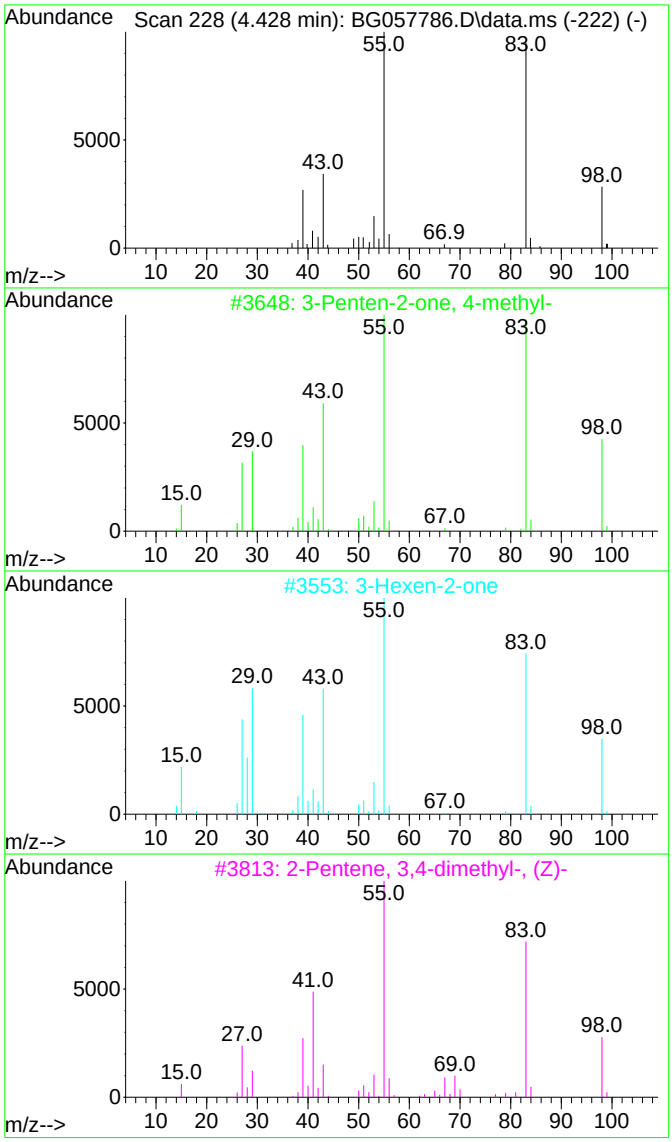
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

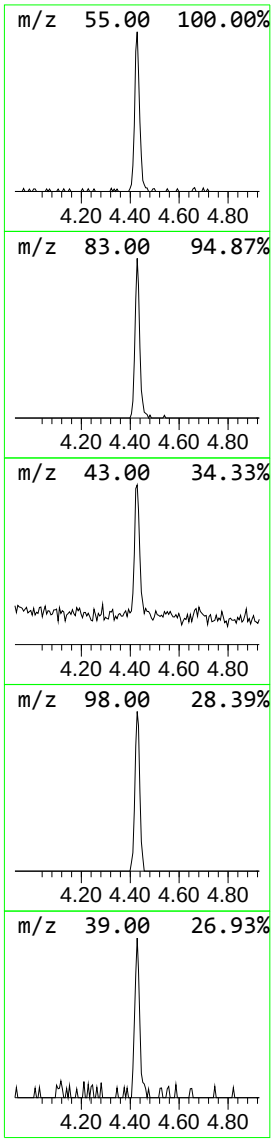
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.428	5.30 ng	52632	1,4-Dichlorobenzene-d4	7.924

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





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ClientSampleId :
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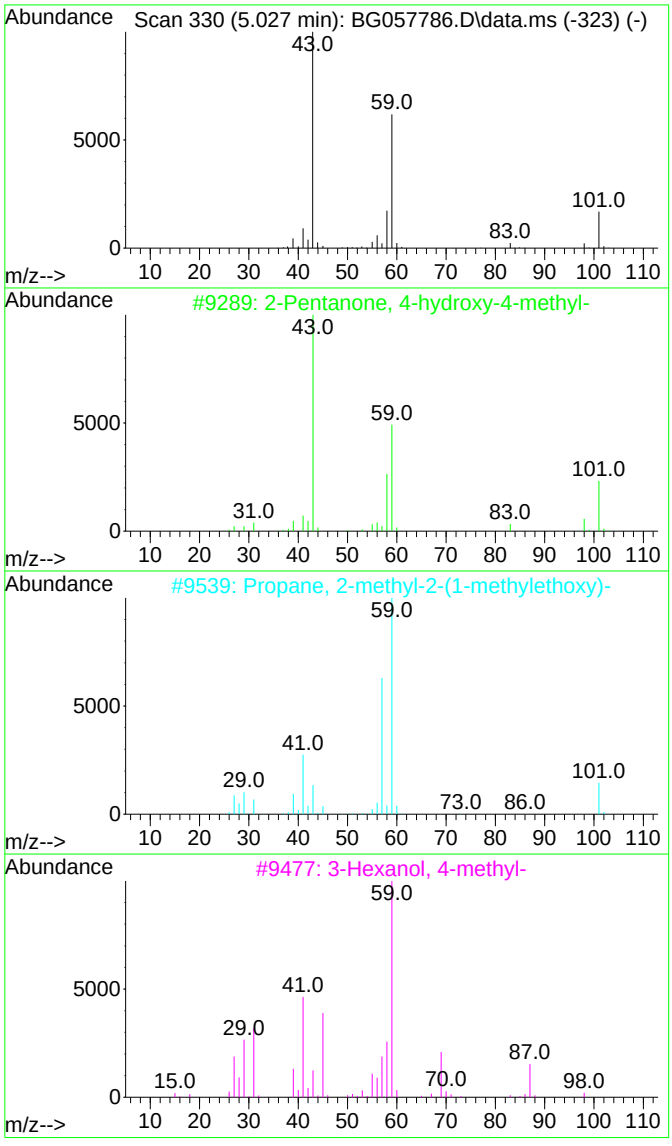
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

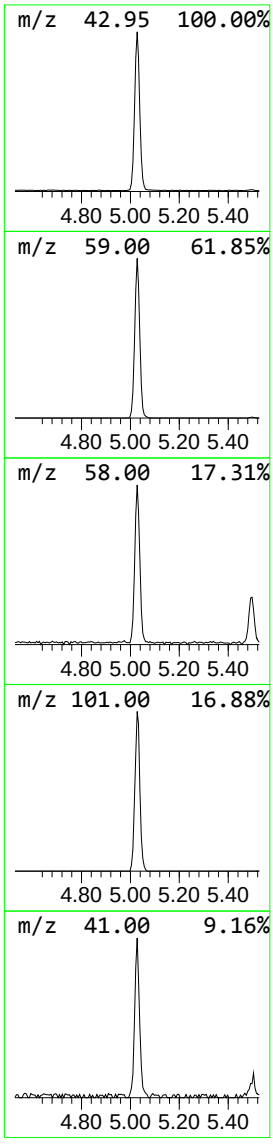
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	38.47 ng	381790	1,4-Dichlorobenzene-d4	7.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Operator : CG/JU
Sample : PB153543BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB153543BL

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TIC Library : C:\Database\NIST20.L
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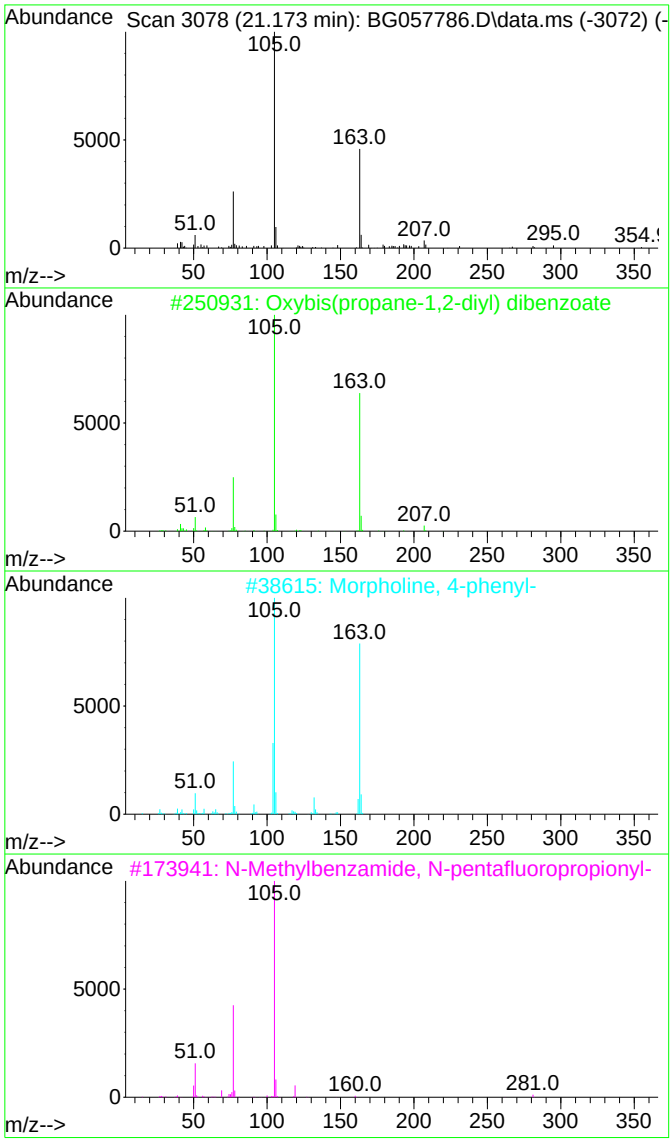
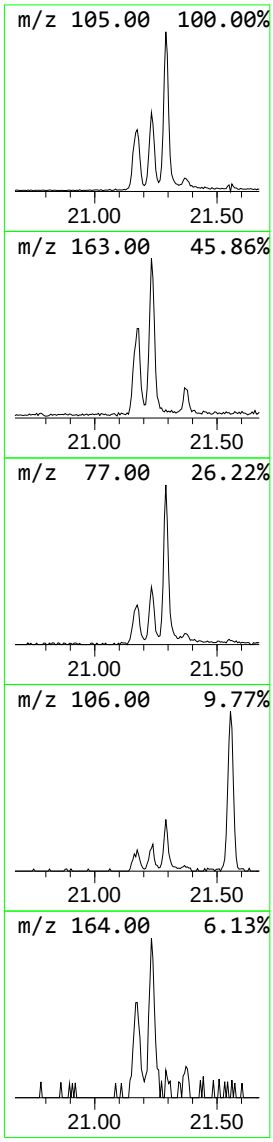
****
Peak Number 3 Oxybis(propane-1,2-diyl) di... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.173	2.26 ng	77804	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	78
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	35
4	Phenylglyoxylic acid, 2-methylbu...	220	C13H16O3	1010453-46-2	35
5	3-Buten-1-one, 2,2-dimethyl-1-ph...	174	C12H14O	062894-04-6	35





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Instrument :
BNA_G
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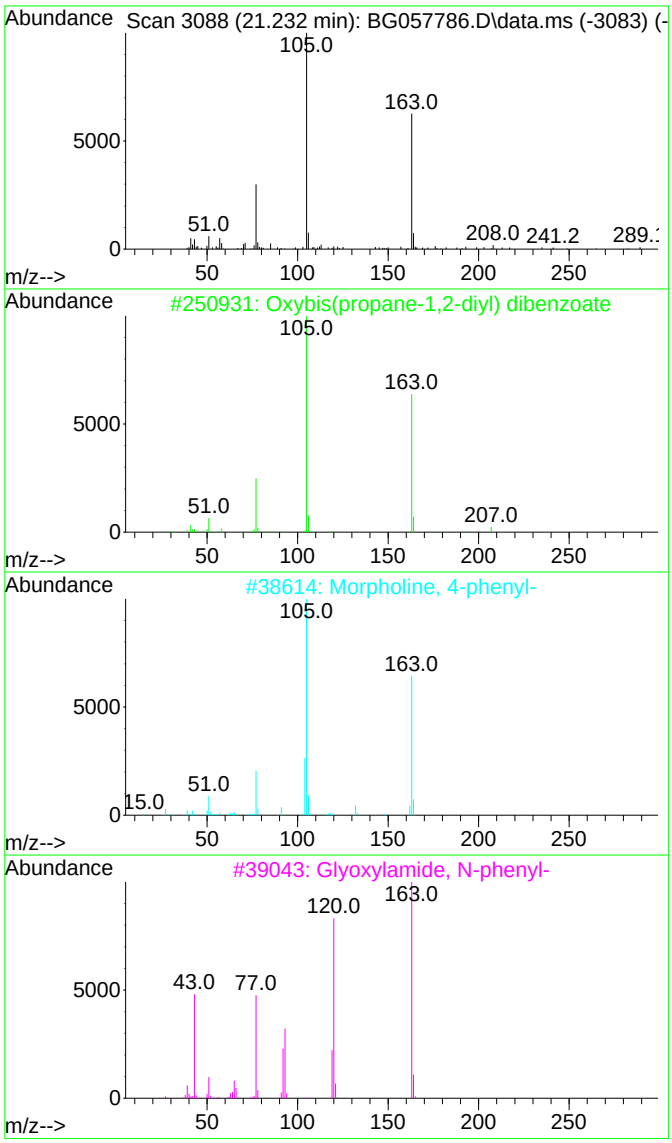
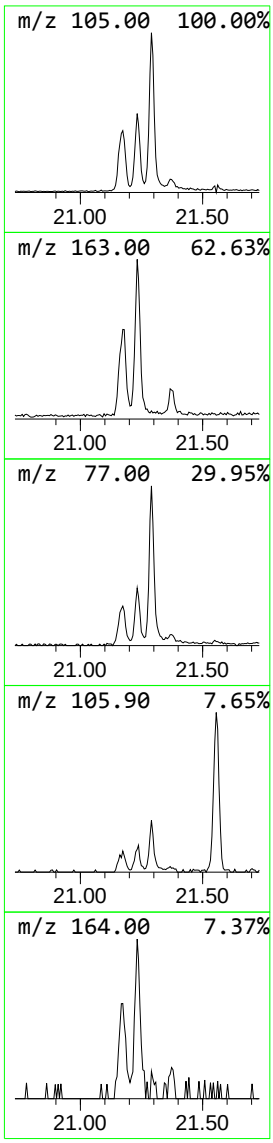
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.232	2.88 ng	99164	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	80
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
4	Benzoic acid, (3-isopropyl-6-met...	283	C17H17NO3	039870-46-7	35
5	3-Benzoylaminochromone	265	C16H11NO3	1000243-49-5	35





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ALS Vial : 3 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
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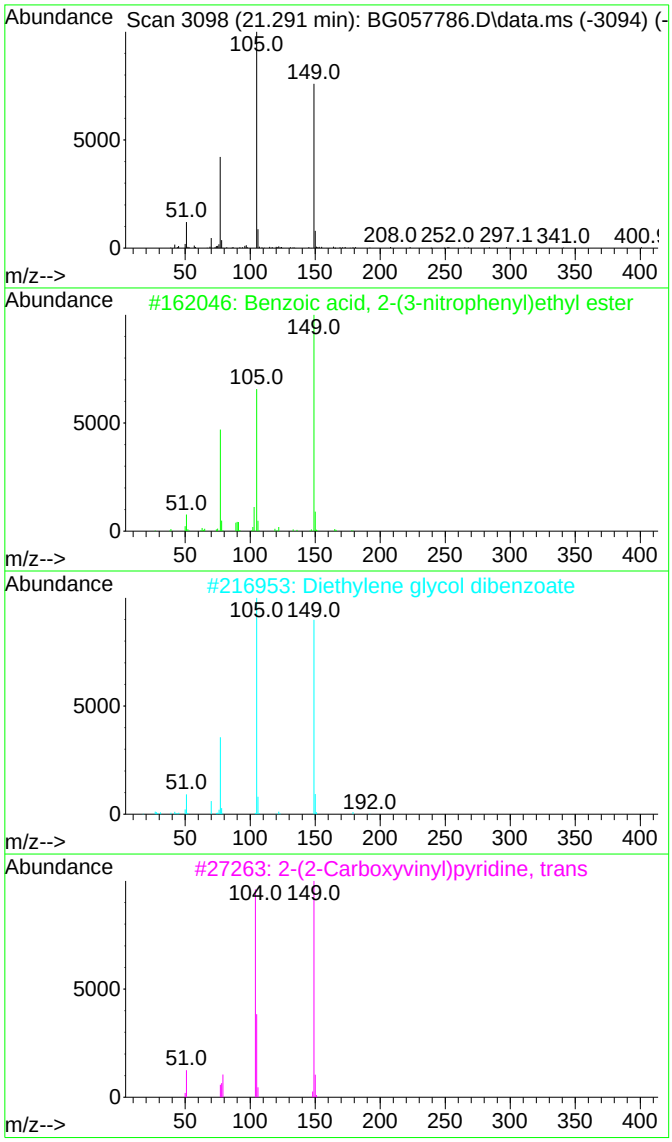
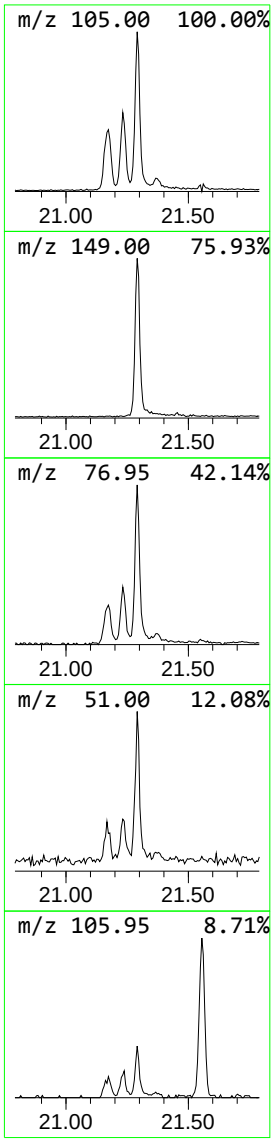
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzoic acid, 2-(3-nitrophe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.291	4.43 ng	152481	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	53
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	38
5	Phthalic acid, hexyl 2-methylbut...	320	C19H28O4	1000322-81-4	38





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.428	5.3	ng	52632	1	7.924	198471	20.0
2-Pentanone, 4-...	5.027	38.5	ng	381790	1	7.924	198471	20.0
Oxybis(propane-...	21.173	2.3	ng	77804	5	21.555	688058	20.0
Morpholine, 4-p...	21.232	2.9	ng	99164	5	21.555	688058	20.0
Benzoic acid, 2...	21.291	4.4	ng	152481	5	21.555	688058	20.0