

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
 Data File : BG048027.D
 Acq On : 27 Jan 2021 11:44
 Operator : CG/JU
 Sample : PB134351BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB134351BL

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-BG012521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048027.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.682	391	399	409	rBV	956133	1479909	33.65%	8.783%
2	7.274	662	670	677	rBV	928222	1558484	35.43%	9.249%
3	8.126	808	815	822	rBV2	160270	269351	6.12%	1.598%
4	9.290	1004	1013	1020	rBV	550164	971038	22.08%	5.763%
5	10.941	1286	1294	1302	rBV	208490	362456	8.24%	2.151%
6	13.373	1701	1708	1717	rVB	1415667	2176159	49.47%	12.915%
7	14.748	1936	1942	1949	rBV2	339562	520942	11.84%	3.092%
8	16.229	2187	2194	2206	rBV	1262177	1884269	42.84%	11.182%
9	17.492	2403	2409	2416	rVB	456189	696063	15.82%	4.131%
10	18.367	2553	2558	2564	rBV5	26597	47618	1.08%	0.283%
11	20.089	2845	2851	2857	rBV	3347824	4398507	100.00%	26.103%
12	21.358	3061	3067	3072	rBV2	63191	131895	3.00%	0.783%
13	21.423	3073	3078	3083	rVV	96182	159172	3.62%	0.945%
14	21.481	3083	3088	3095	rVB	236914	345622	7.86%	2.051%
15	21.763	3129	3136	3142	rBV	579553	979174	22.26%	5.811%
16	25.048	3686	3695	3703	rBV2	322722	869726	19.77%	5.161%

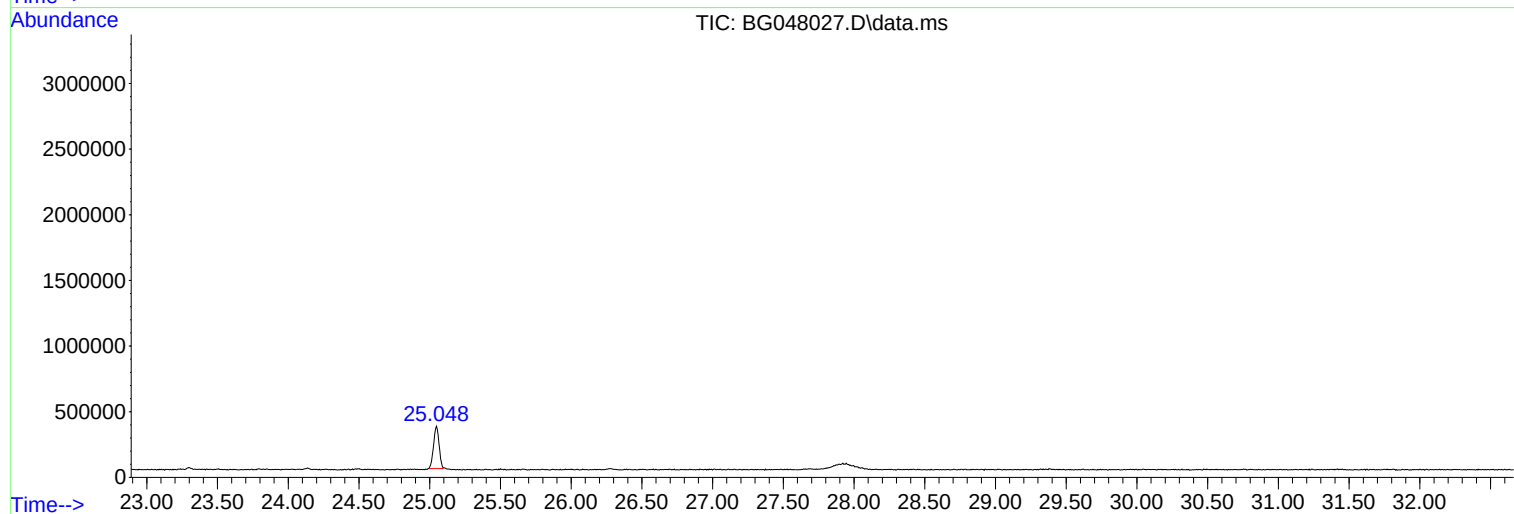
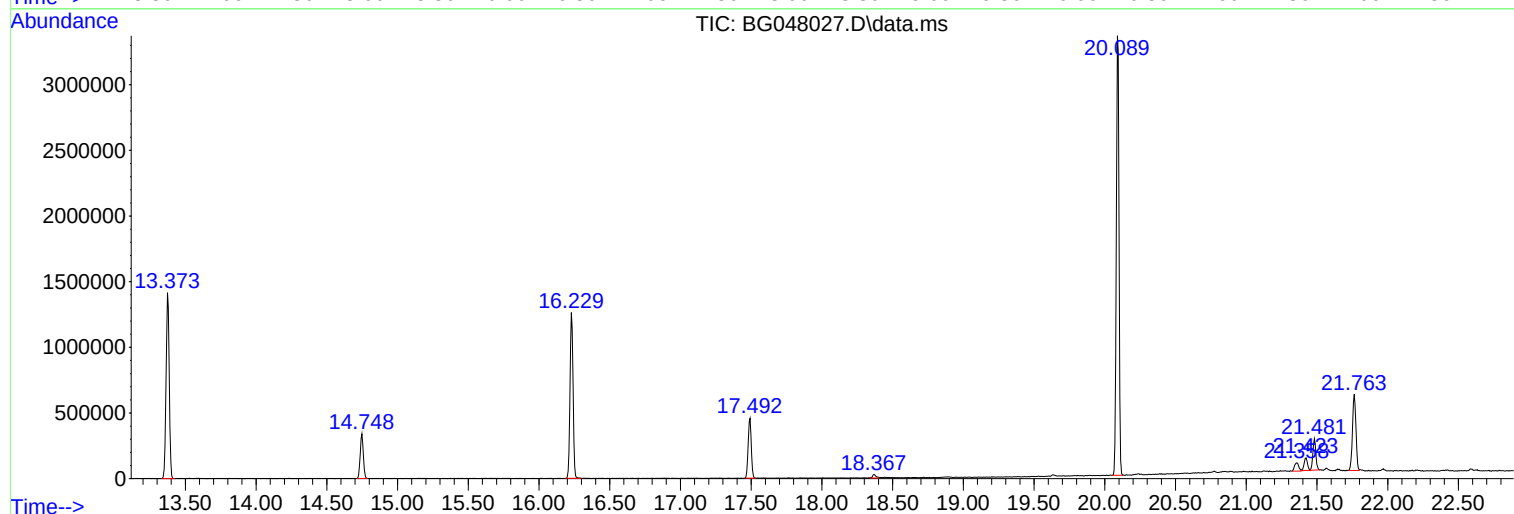
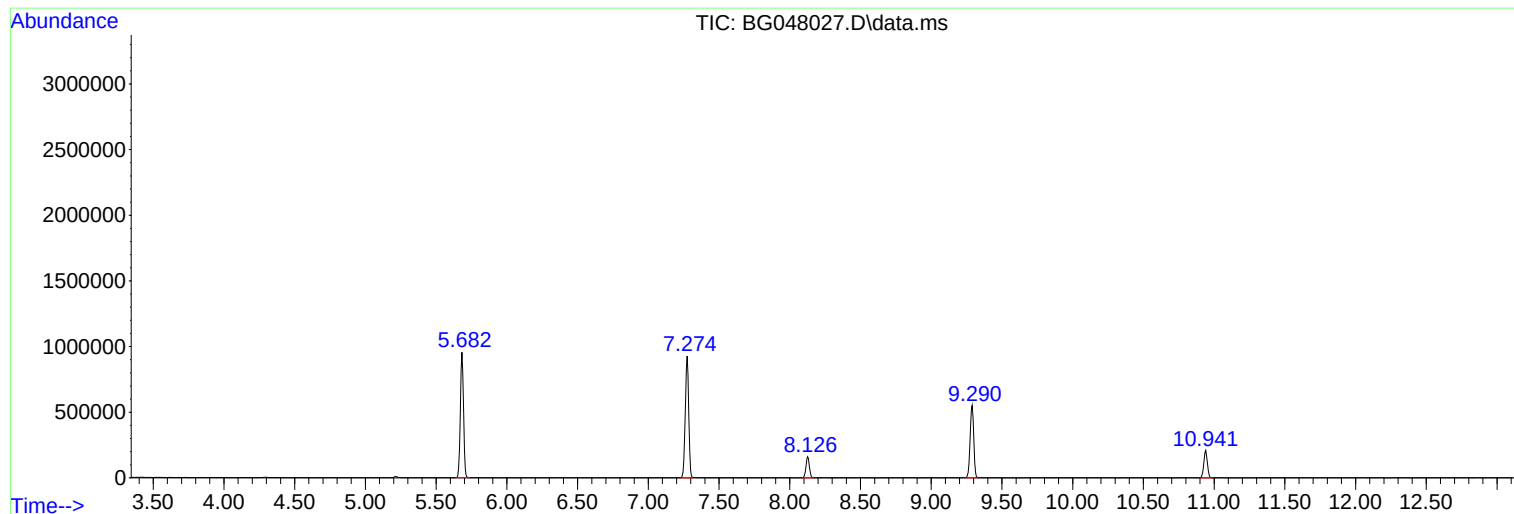
Sum of corrected areas: 16850385

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048027.D
Acq On : 27 Jan 2021 11:44
Operator : CG/JU
Sample : PB134351BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB134351BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048027.D
Acq On : 27 Jan 2021 11:44
Operator : CG/JU
Sample : PB134351BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB134351BL

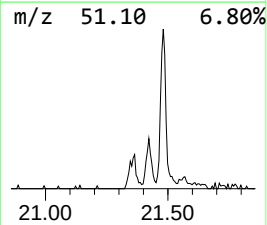
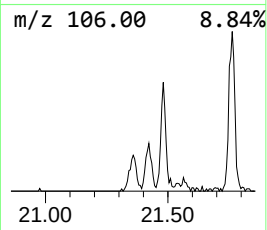
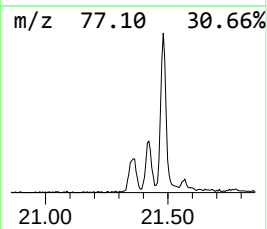
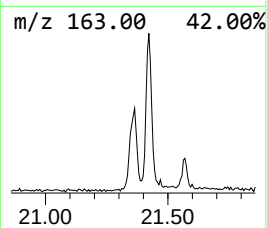
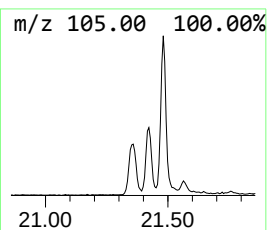
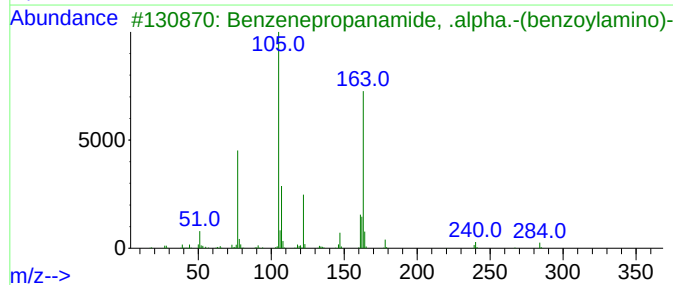
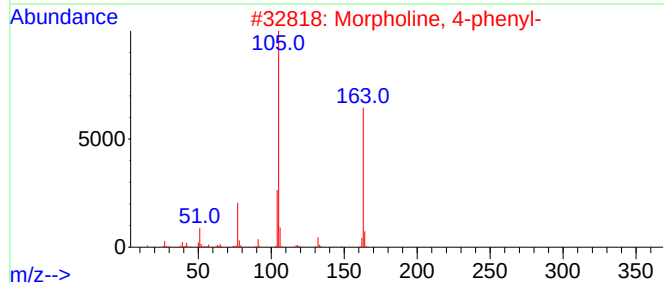
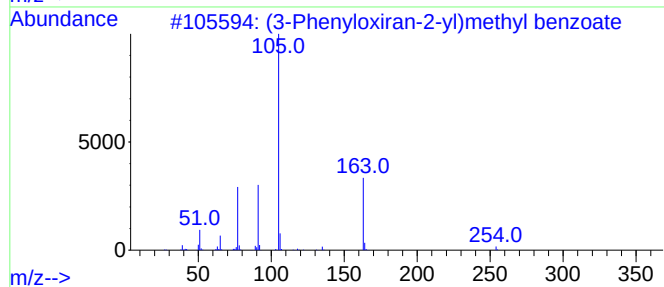
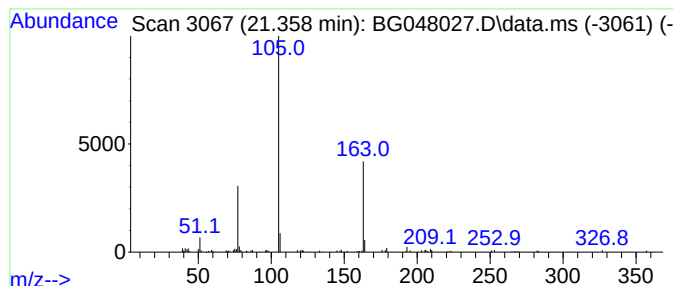
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (3-Phenyloxiran-2-yl)methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.358	2.69 ng	131895	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	72
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
3			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	45
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	27
5			Crotonic acid, 2-benzamido-, met...	219	C12H13NO3	105909-91-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048027.D
Acq On : 27 Jan 2021 11:44
Operator : CG/JU
Sample : PB134351BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB134351BL

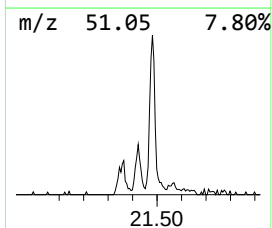
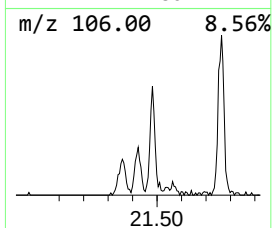
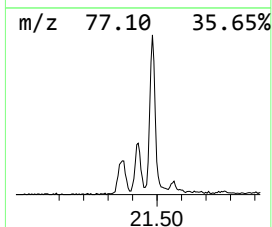
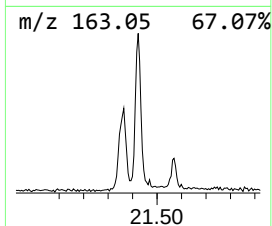
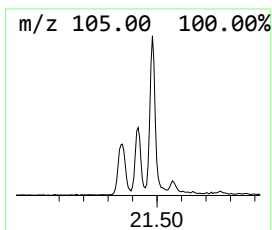
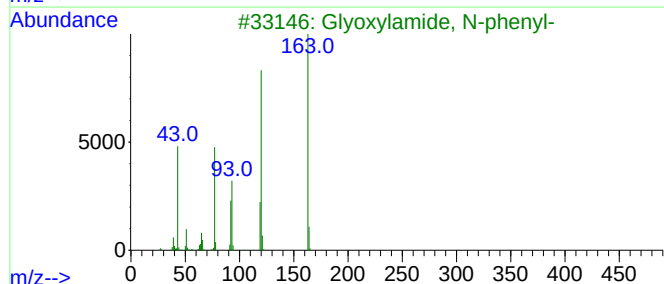
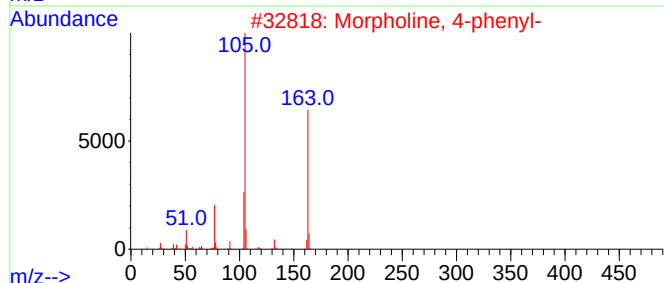
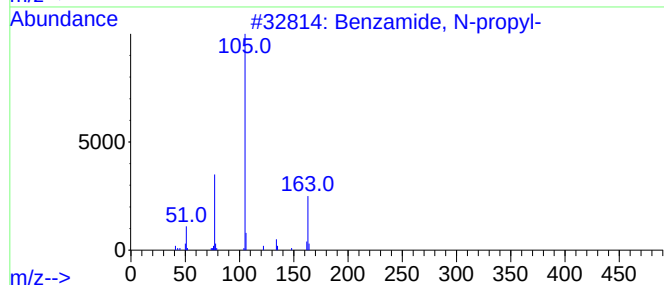
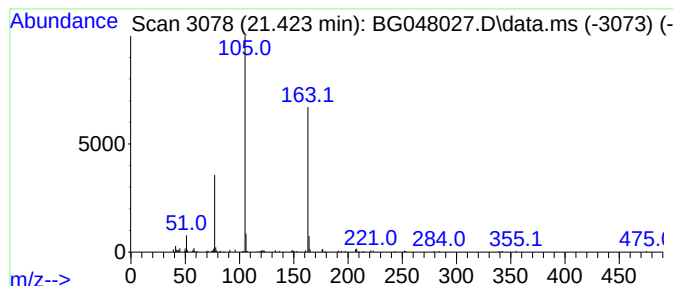
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzamide, N-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.423	3.25 ng	159172	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
4			1,1'-(p-Phenylene)bis(2-phenylet...	342	C22H14O4	003363-97-1	35
5			1-Deoxy-2,3,4,5-tetrabenzyl-d-ly...	552	C33H28O8	1000124-89-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048027.D
Acq On : 27 Jan 2021 11:44
Operator : CG/JU
Sample : PB134351BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

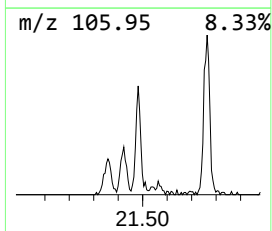
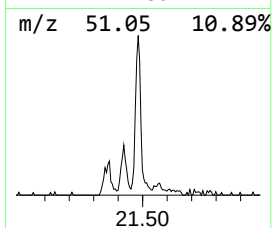
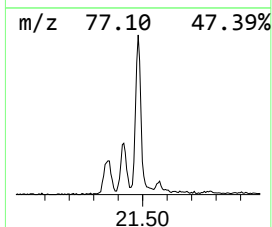
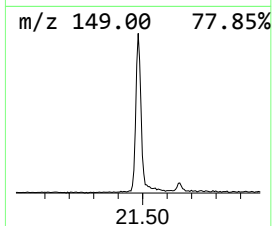
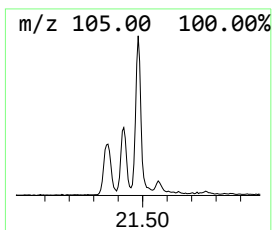
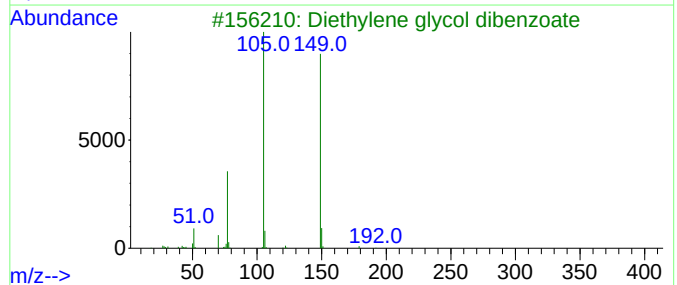
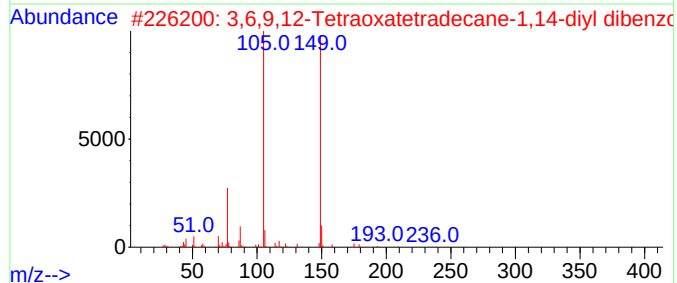
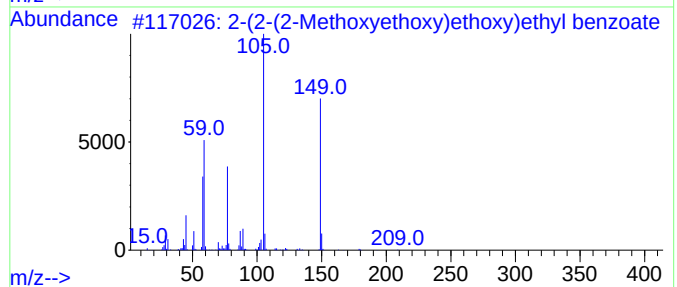
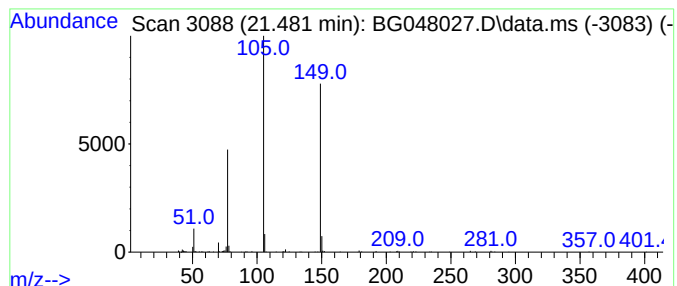
Instrument :
BNA_G
ClientSampleId :
PB134351BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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-(2-(2-Methoxyethoxy)ethox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.481	7.06 ng	345622	Chrysene-d12	21.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	74
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
4	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048027.D
Acq On : 27 Jan 2021 11:44
Operator : CG/JU
Sample : PB134351BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB134351BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(3-Phenyloxiran...	21.358	2.7	ng	131895	5	21.763	979174	20.0
Benzamide, N-pr...	21.423	3.3	ng	159172	5	21.763	979174	20.0
2-(2-(2-Methoxy...	21.481	7.1	ng	345622	5	21.763	979174	20.0