

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030321\
 Data File : BG048317.D
 Acq On : 3 Mar 2021 17:38
 Operator : CG/JU
 Sample : M1544-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TT-040-IDWSO-20210301

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-BG021021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.688	393	400	410	rBV	538305	902825	37.65%	8.011%
2	7.309	668	676	689	rBV	545684	1022172	42.63%	9.069%
3	8.102	804	811	820	rBV	131813	229602	9.57%	2.037%
4	9.283	1003	1012	1025	rBV	313731	638547	26.63%	5.666%
5	10.923	1281	1291	1303	rBV	151792	305673	12.75%	2.712%
6	13.361	1698	1706	1717	rBV	732304	1278251	53.30%	11.342%
7	14.736	1934	1940	1952	rVB2	263219	448511	18.70%	3.980%
8	16.234	2188	2195	2209	rBV	758033	1235151	51.51%	10.959%
9	17.485	2401	2408	2417	rBV	390808	614396	25.62%	5.451%
10	19.107	2678	2684	2689	rBV	47414	74172	3.09%	0.658%
11	19.512	2749	2753	2758	rBV8	15505	30070	1.25%	0.267%
12	20.082	2844	2850	2858	rBV	1876885	2398026	100.00%	21.277%
13	21.346	3058	3065	3068	rBV	54079	116883	4.87%	1.037%
14	21.404	3072	3075	3081	rVV	80282	150519	6.28%	1.336%
15	21.475	3081	3087	3095	rVB	200931	313811	13.09%	2.784%
16	21.763	3130	3136	3143	rBV	453602	762895	31.81%	6.769%
17	25.059	3687	3697	3708	rVB2	251138	748977	31.23%	6.645%

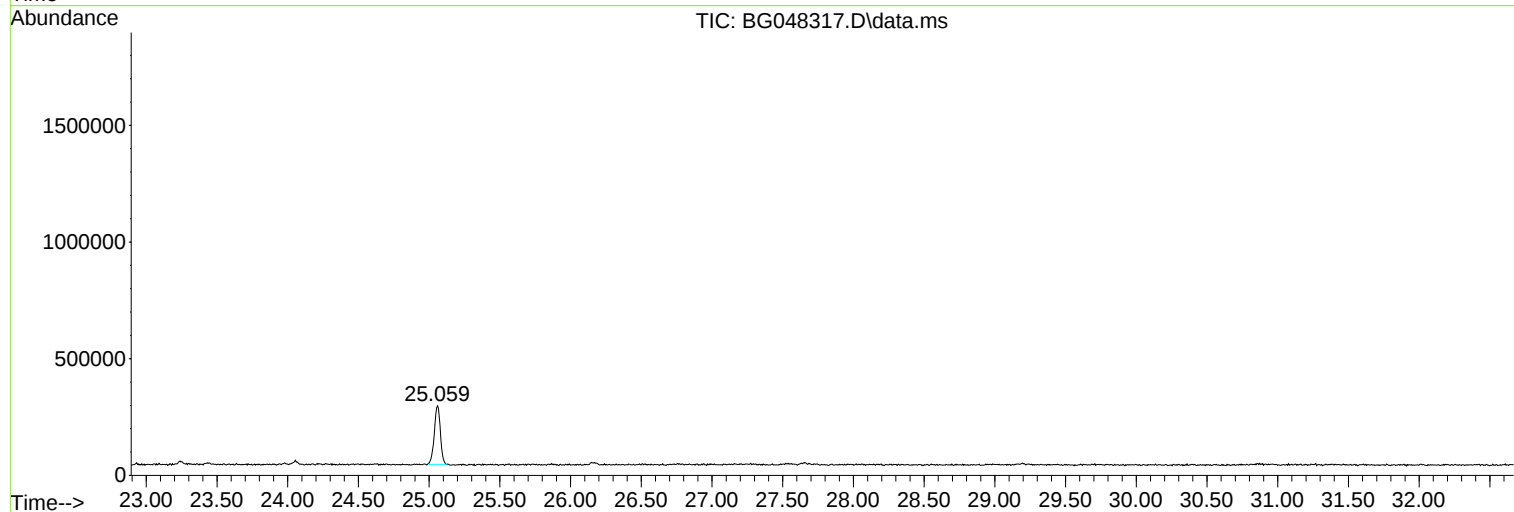
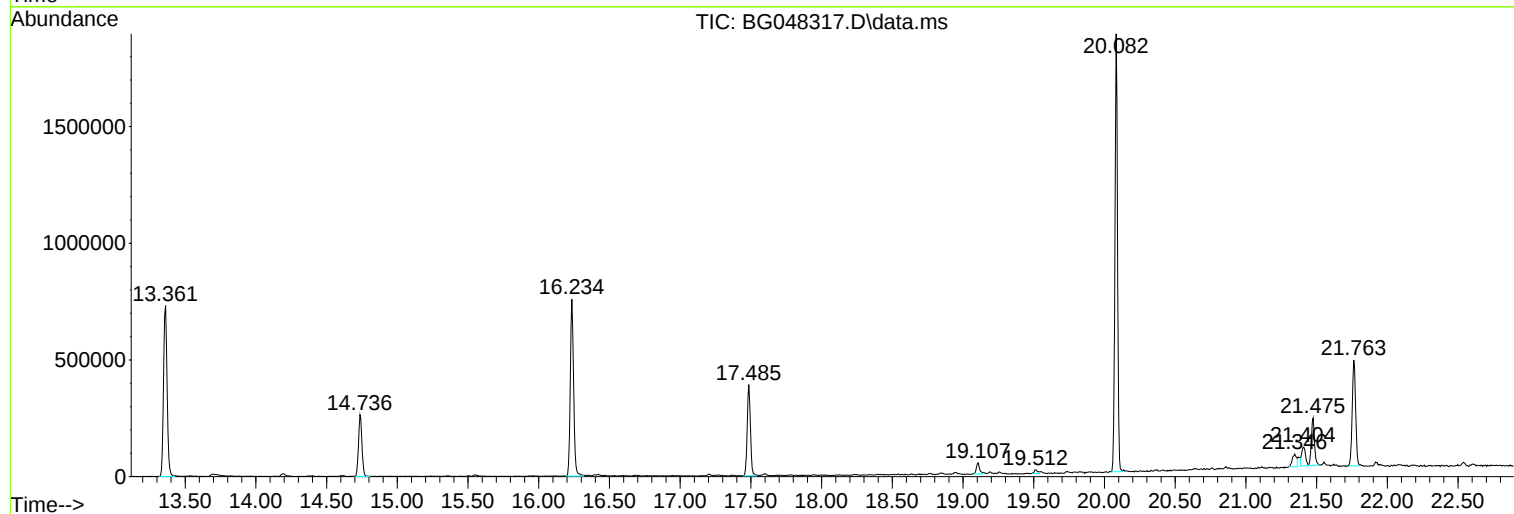
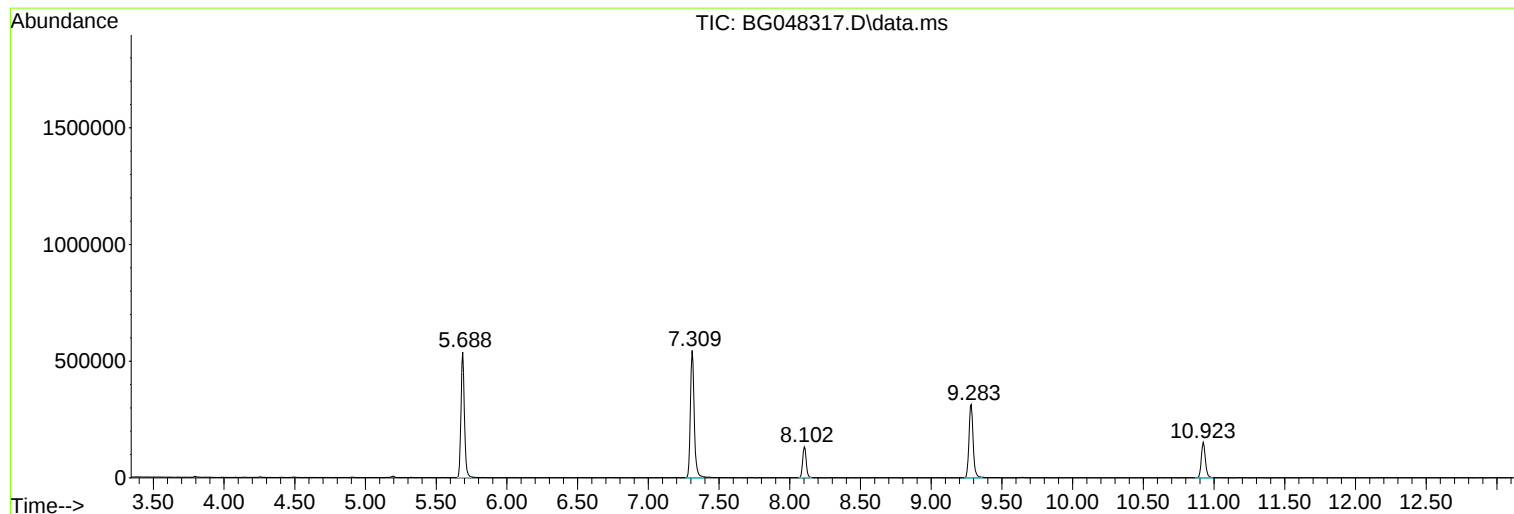
Sum of corrected areas: 11270481

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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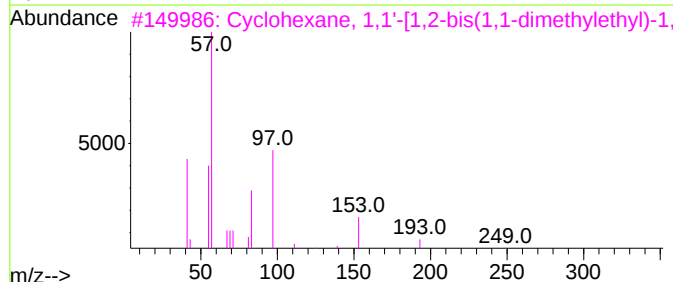
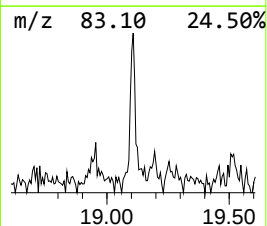
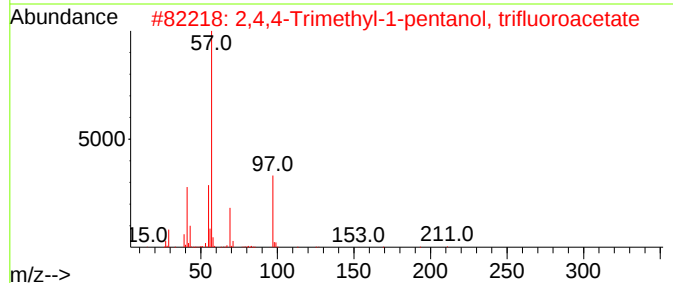
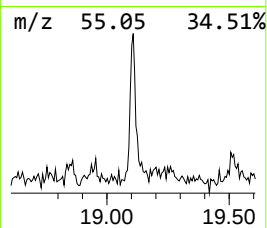
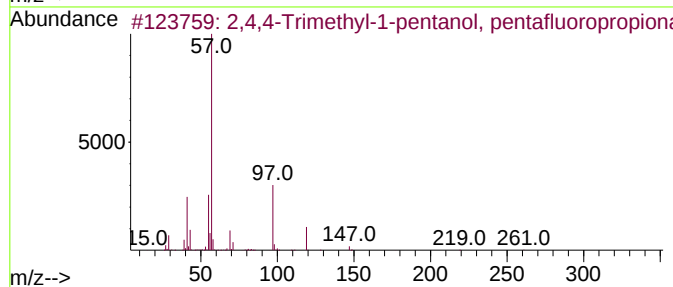
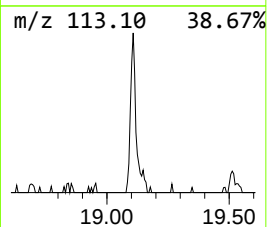
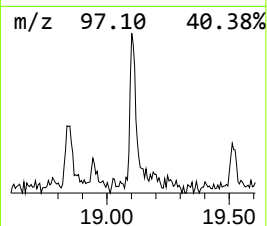
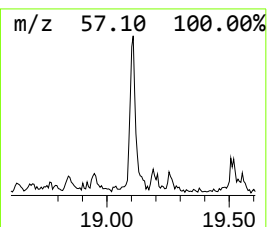
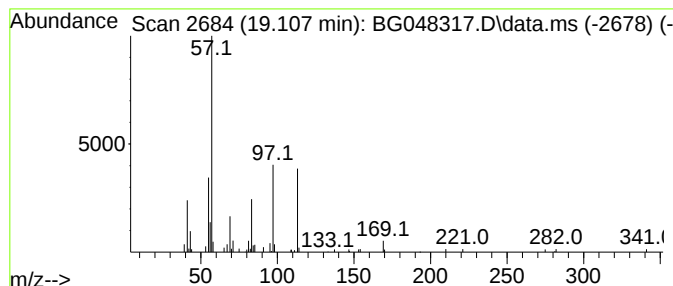
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown19.107 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.107	2.41 ng	74172	Phenanthrene-d10	17.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F502	1000365-51-0	27		
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F302	1000365-19-5	27		
3	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	23		
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	17		
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	16		



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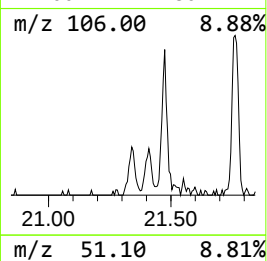
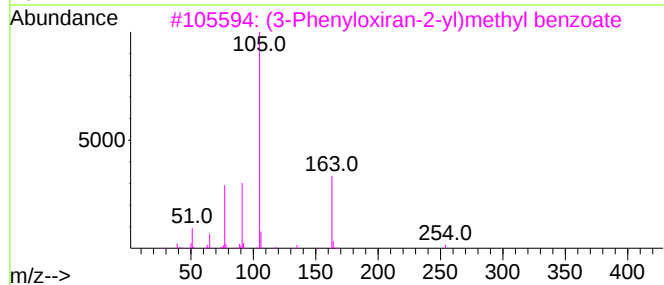
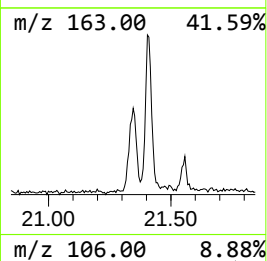
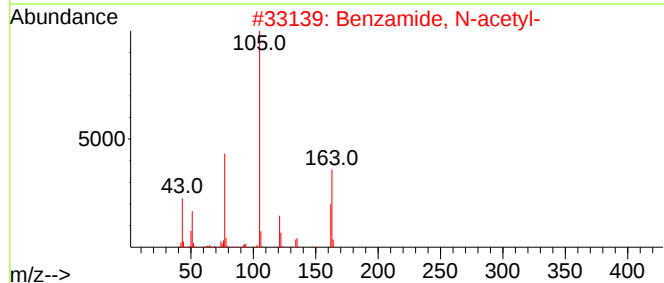
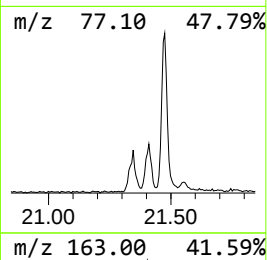
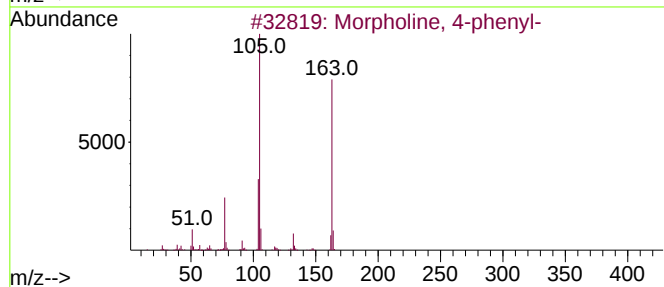
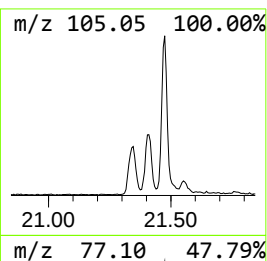
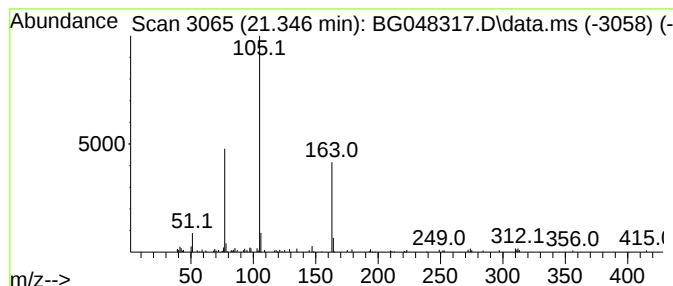
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Peak Number 2 Morpholine, 4-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.346	3.06 ng	116883	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	56
3			(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	50
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	38
5			Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	38



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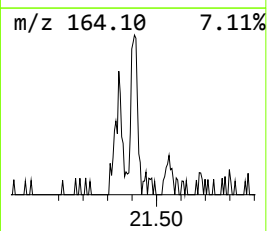
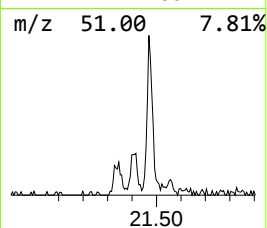
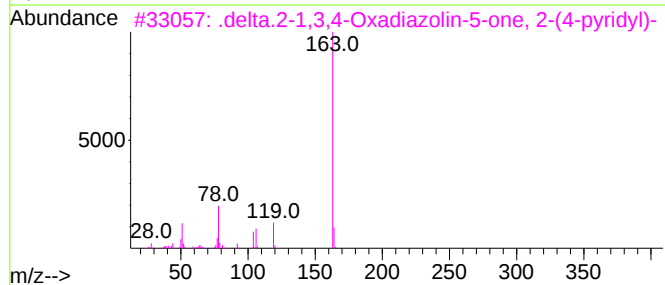
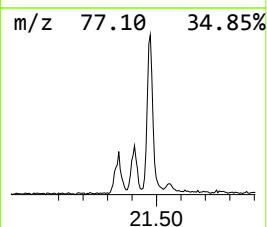
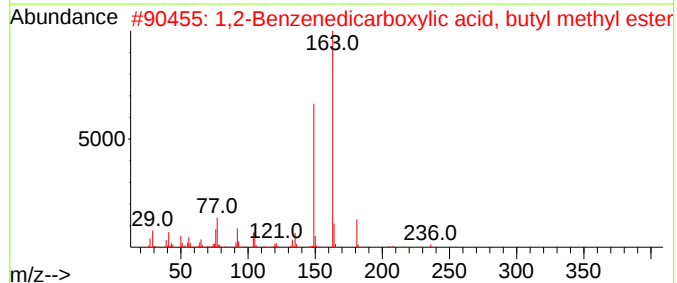
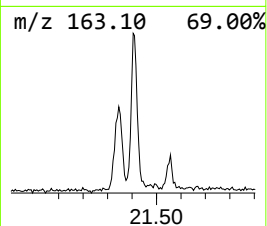
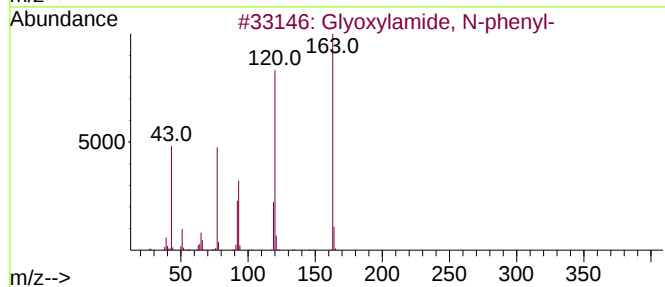
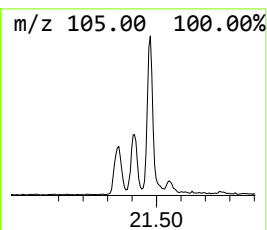
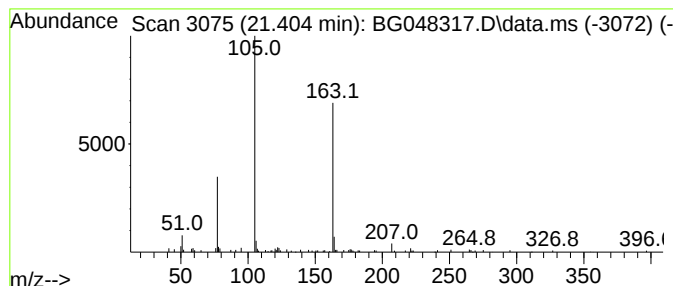
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Peak Number 3 unknown21.404 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.404	3.95 ng	150519	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
2			1,2-Benzenedicarboxylic acid, bu...	236	C13H16O4	034006-76-3	40
3			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	38
4			2-Benzoyloxyacetophenone	240	C15H12O3	004010-33-7	27
5			Benzohydrazide, N2-(5-hydroxyimi...	285	C13H11N5O3	1000268-99-0	27



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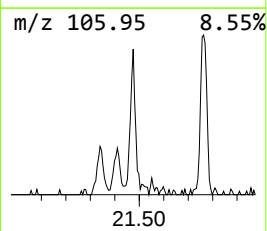
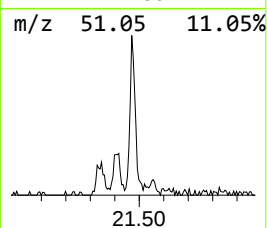
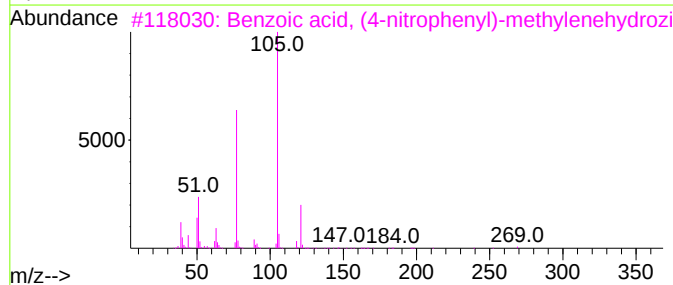
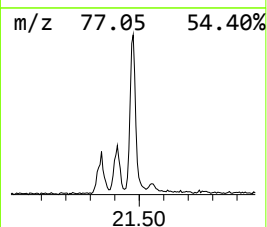
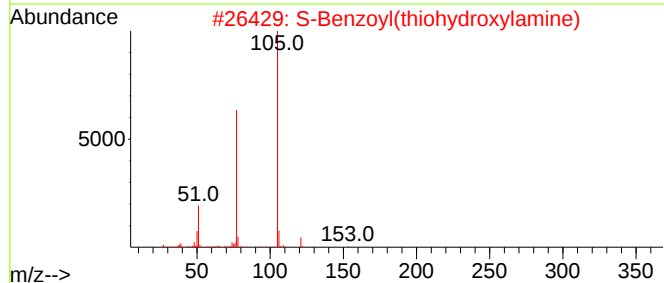
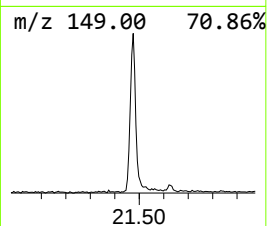
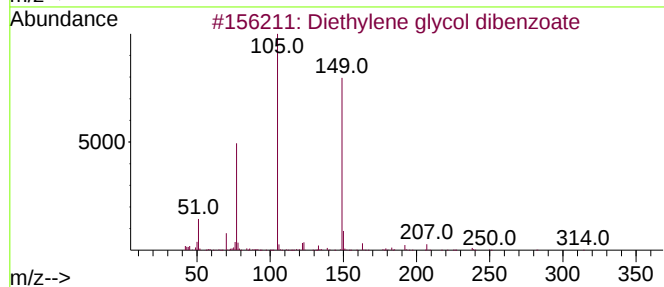
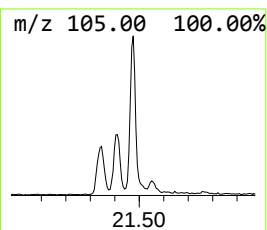
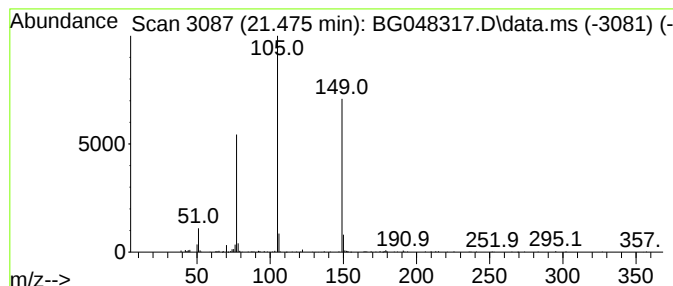
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.475	8.23 ng	313811	Chrysene-d12	21.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2			S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
3			Benzoic acid, (4-nitrophenyl)-me...	269	C14H11N3O3	028123-77-5	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown19.107	19.107	2.4	ng	74172	4	17.485	614396	20.0
Morpholine, 4-p...	21.346	3.1	ng	116883	5	21.763	762895	20.0
unknown21.404	21.404	4.0	ng	150519	5	21.763	762895	20.0
Diethylene glyc...	21.475	8.2	ng	313811	5	21.763	762895	20.0