

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061623\
 Data File : BG057736.D
 Acq On : 16 Jun 2023 15:54
 Operator : CG/JU
 Sample : PB153486BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB153486BL

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-BG061323.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057736.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.039	326	332	340	rVB	158377	233105	8.60%	2.081%
2	5.503	404	411	423	rVB	654823	1001013	36.95%	8.938%
3	7.089	673	681	692	rBV	653811	1071055	39.53%	9.564%
4	7.930	816	824	831	rBV	99162	161575	5.96%	1.443%
5	9.093	1014	1022	1033	rBV	341499	590935	21.81%	5.276%
6	10.732	1294	1301	1310	rVB	139251	249121	9.20%	2.224%
7	13.188	1711	1719	1726	rBV	930438	1438735	53.11%	12.847%
8	14.563	1946	1953	1961	rVB	232265	363756	13.43%	3.248%
9	16.049	2199	2206	2218	rVB	814206	1203748	44.43%	10.748%
10	17.307	2412	2420	2428	rBV	365347	521368	19.24%	4.655%
11	19.927	2859	2866	2871	rBV	2053424	2709193	100.00%	24.191%
12	21.179	3073	3079	3084	rBV	31678	60924	2.25%	0.544%
13	21.232	3084	3088	3094	rVV2	63922	107118	3.95%	0.956%
14	21.296	3094	3099	3109	rVB	135135	195900	7.23%	1.749%
15	21.561	3138	3144	3151	rBV2	386650	589618	21.76%	5.265%
16	21.766	3175	3179	3185	rVB	29767	39438	1.46%	0.352%
17	22.366	3277	3281	3287	rVB	21881	33909	1.25%	0.303%
18	24.716	3671	3681	3692	rBV2	226396	628892	23.21%	5.615%

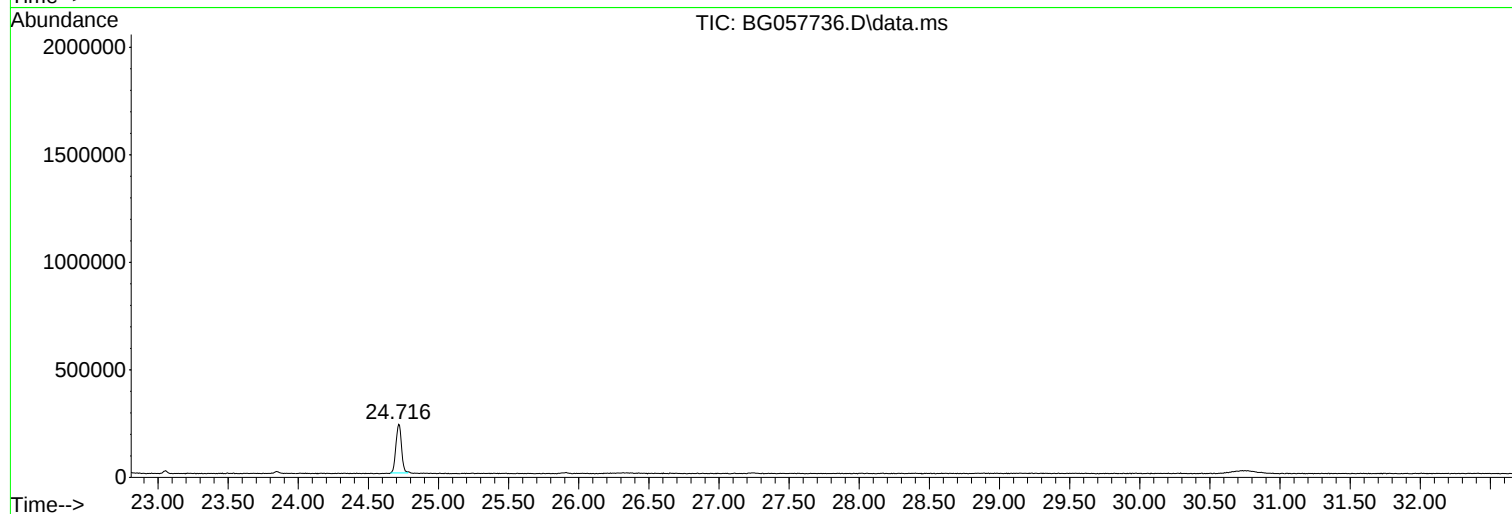
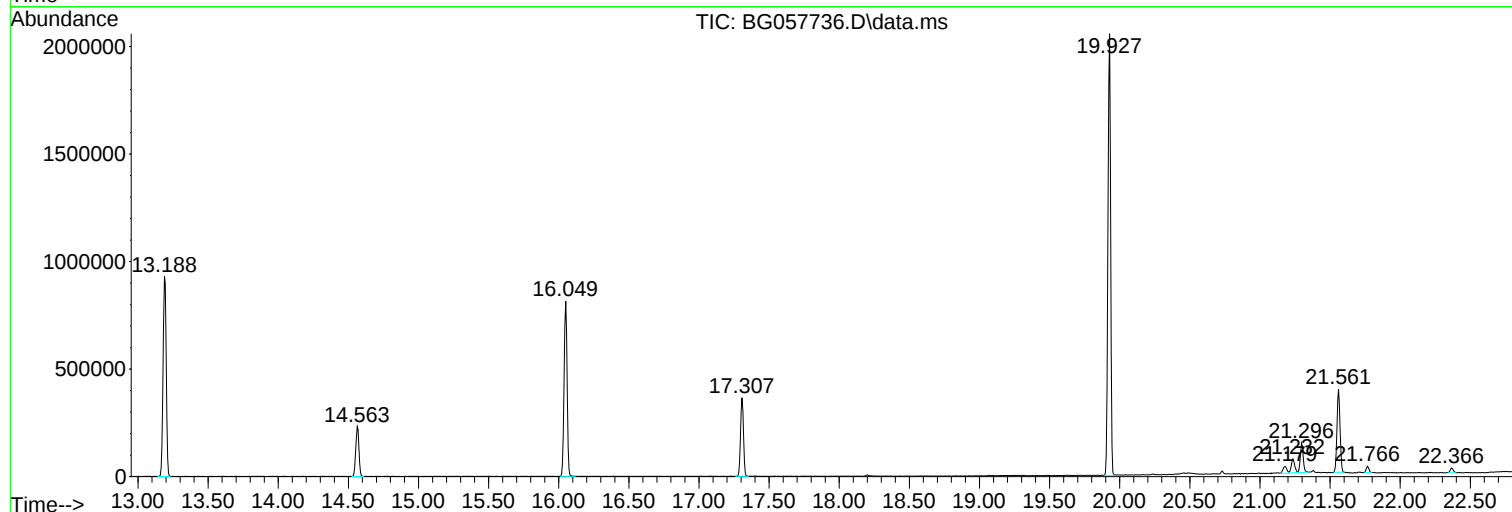
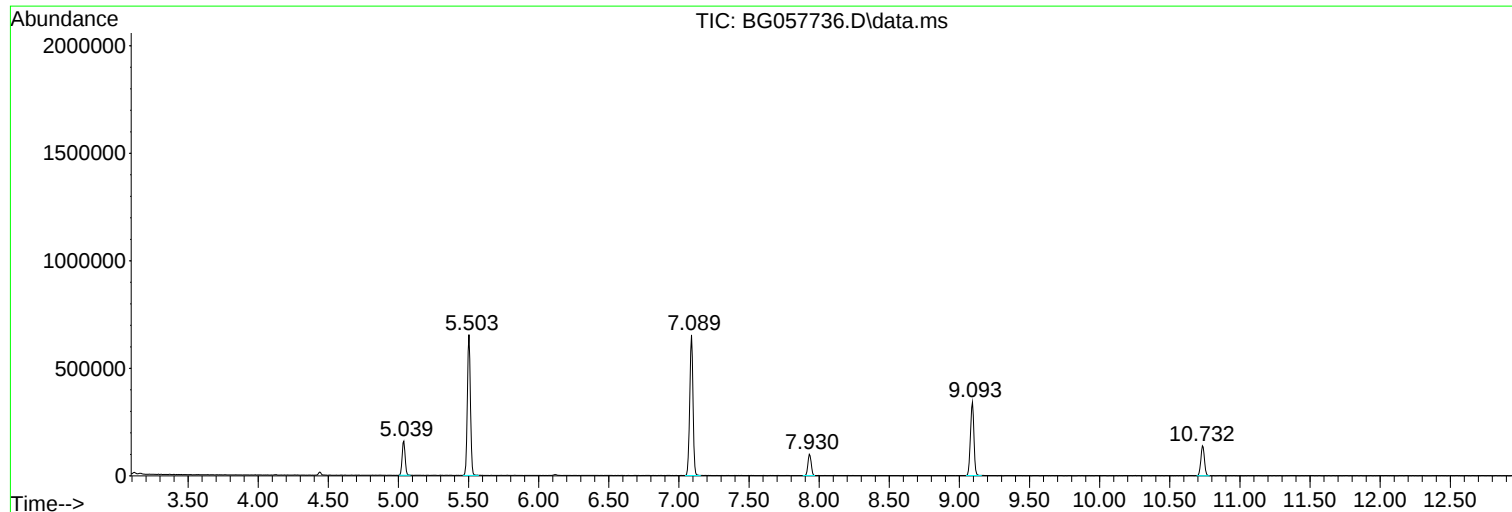
Sum of corrected areas: 11199403

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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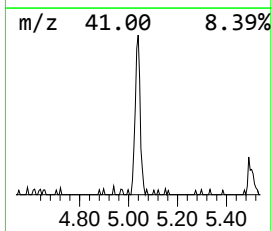
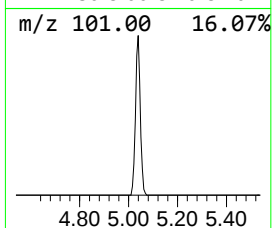
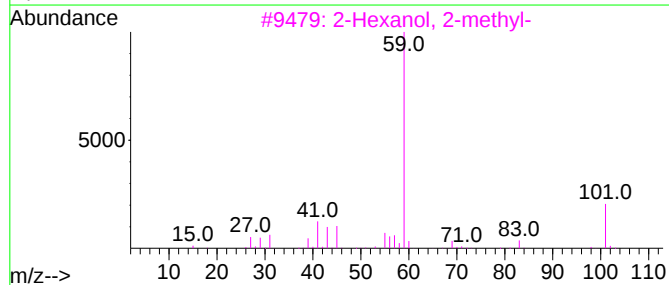
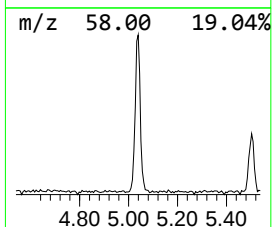
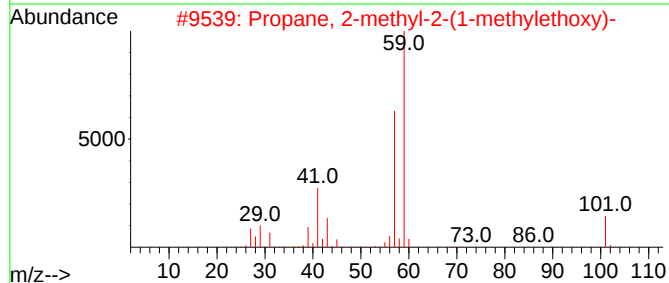
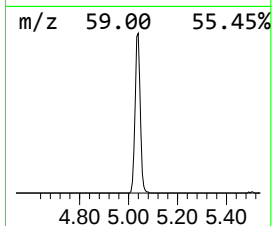
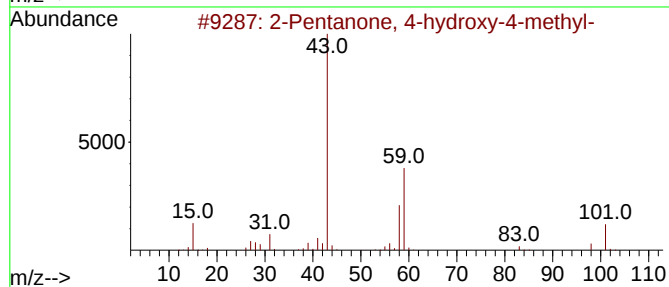
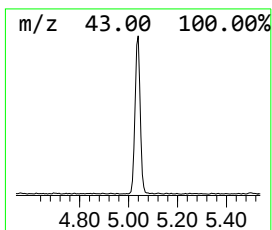
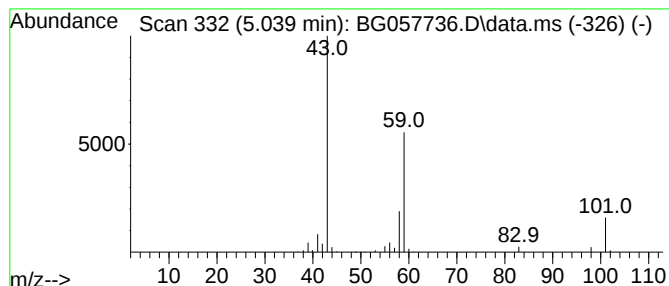
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.039	28.85 ng	233105	1,4-Dichlorobenzene-d4	7.935

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	28		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		



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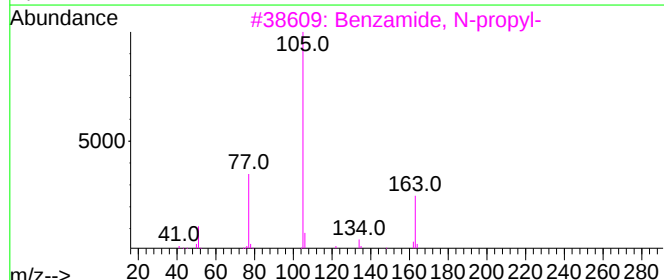
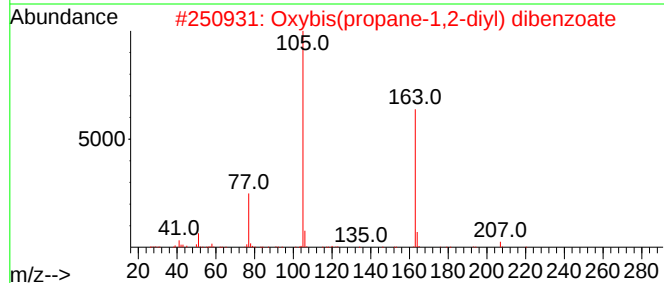
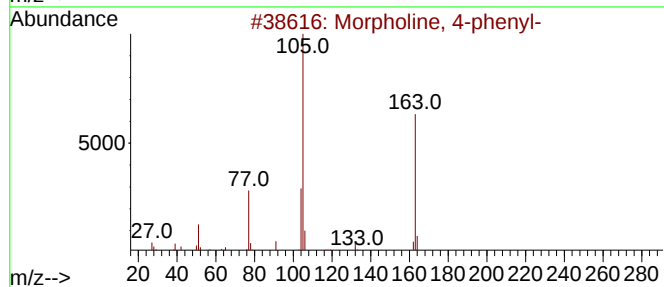
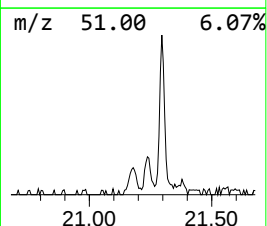
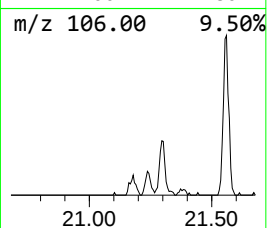
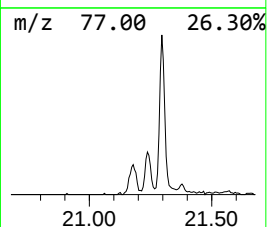
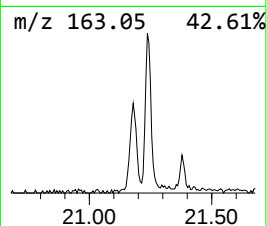
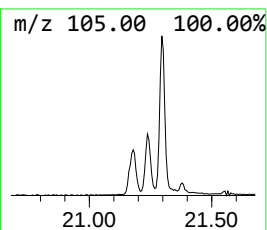
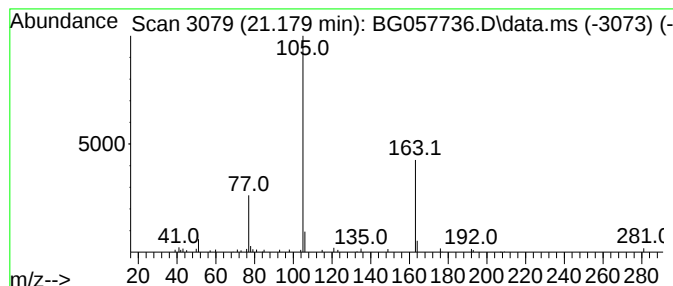
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Peak Number 2 Morpholine, 4-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.179	2.07 ng	60924	Chrysene-d12	21.561

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	64
3			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	43
4			(5-tert-Butyl-2-hydroxyphenyl)(p...	254	C17H18O2	1000468-68-2	35
5			benzamide, N-[4-[7-(benzoyloxy)-...	461	C29H19NO5	1010399-44-9	35



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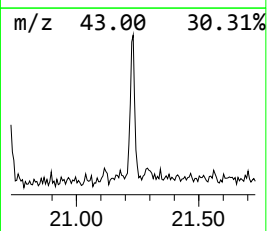
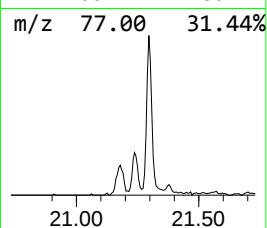
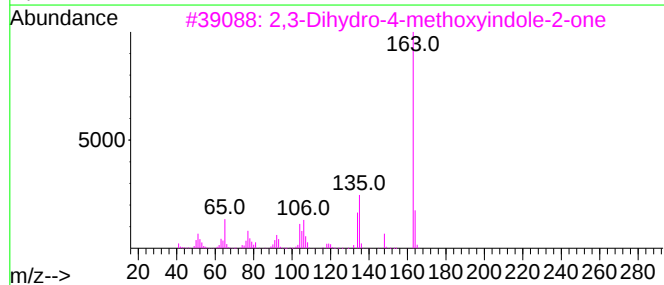
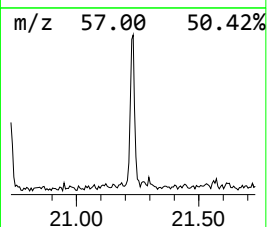
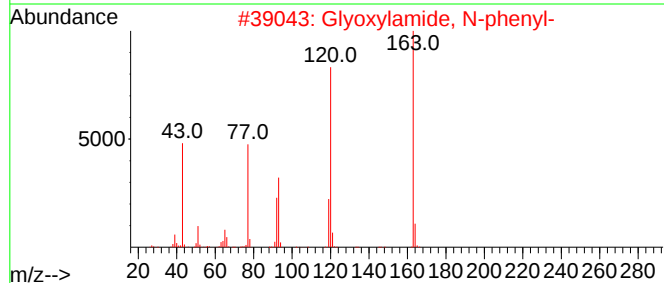
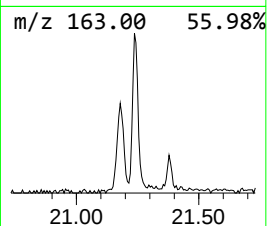
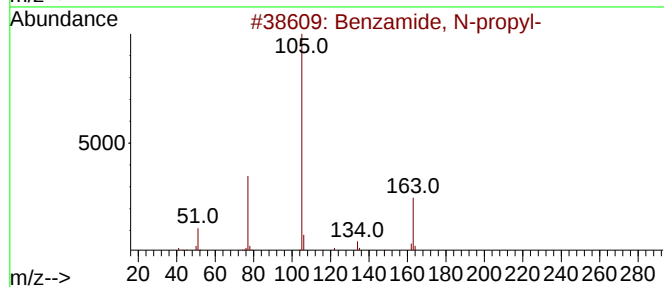
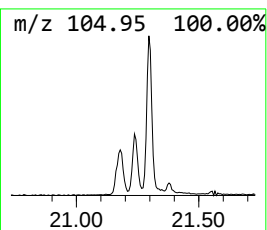
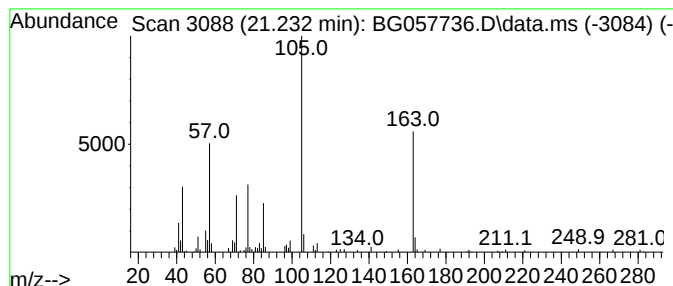
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Peak Number 3 unknown21.232 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.232	3.63 ng	107118	Chrysene-d12	21.561	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	47
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	35
3	2,3-Dihydro-4-methoxyindole-2-one	163	C9H9NO2	007699-17-4	14
4	Heneicosane	296	C21H44	000629-94-7	14
5	Hippuric-benzaldehyde azalactone	249	C16H11NO2	000842-74-0	14



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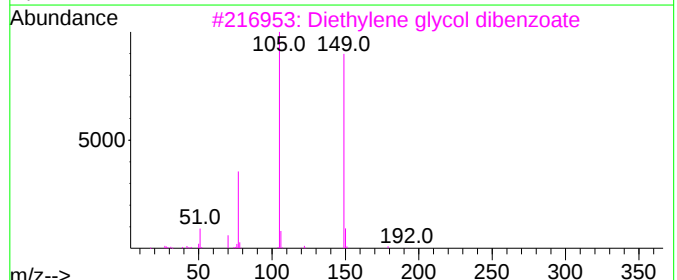
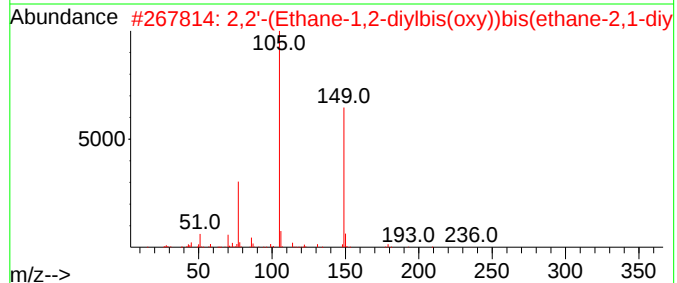
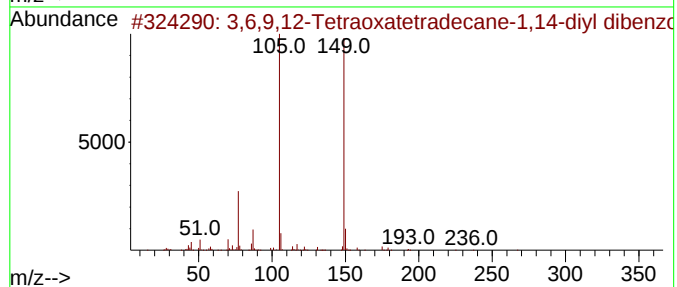
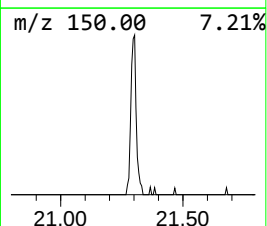
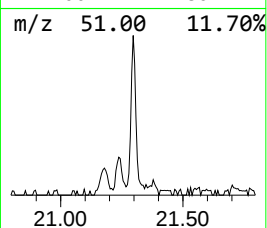
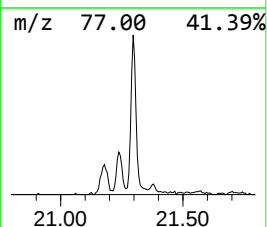
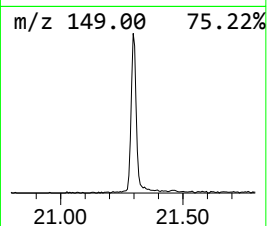
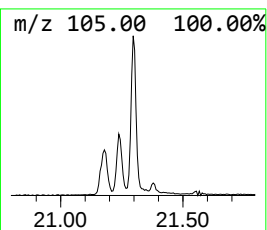
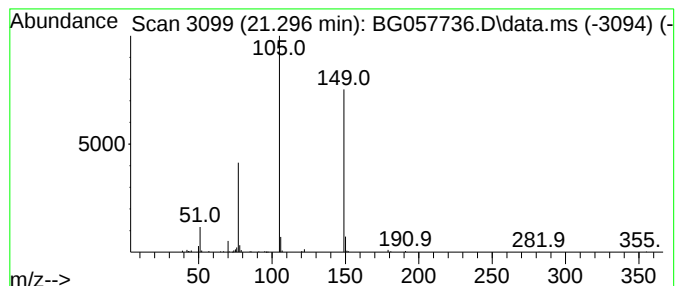
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Peak Number 4 3,6,9,12-Tetraoxatetradecan... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.296	6.64 ng	195900	Chrysene-d12	21.561	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	83
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
4	N-(5-Nitrothiazol-2-yl)-benzamide	249	C10H7N3O3S	064398-84-1	35
5	N-(4-Methylthiazol-2-yl)benzamide	218	C11H10N2OS	037529-67-2	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.039	28.9	ng	233105	1	7.935	161575	20.0
Morpholine, 4-p...	21.179	2.1	ng	60924	5	21.561	589618	20.0
unknown21.232	21.232	3.6	ng	107118	5	21.561	589618	20.0
3,6,9,12-Tetrao...	21.296	6.6	ng	195900	5	21.561	589618	20.0