

Thiourea derivatives containing 4-arylthiazoles and D-glucose moiety: Design, synthesis, antimicrobial activity evaluation and molecular docking/dynamics simulations

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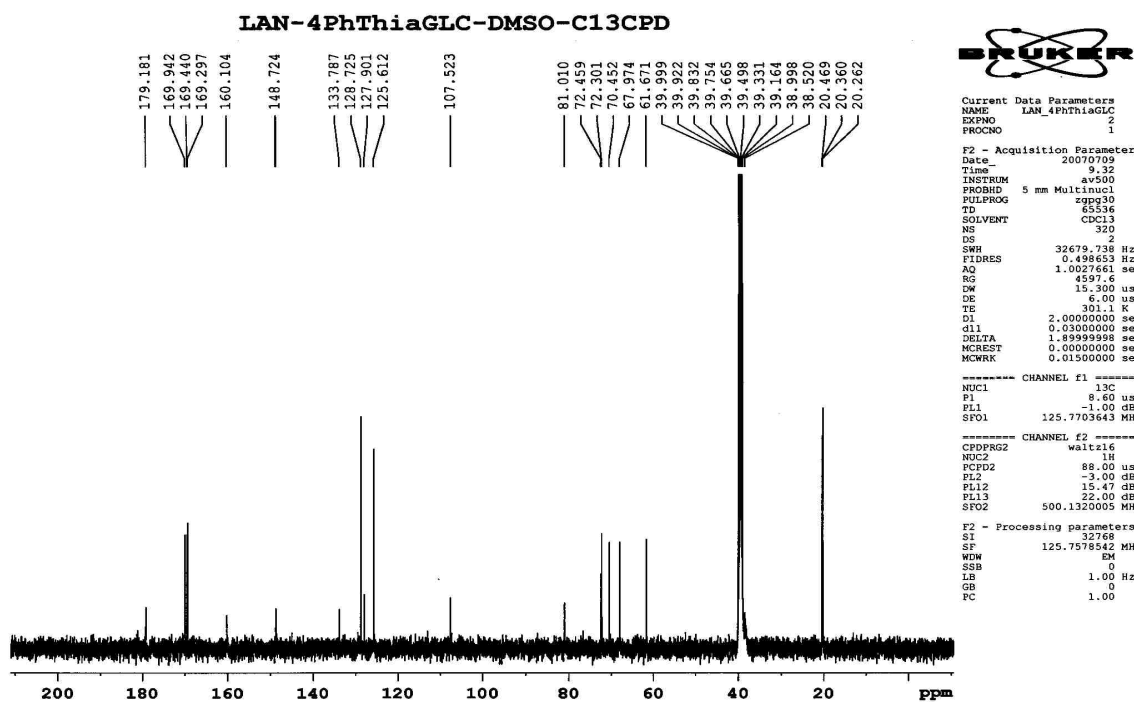
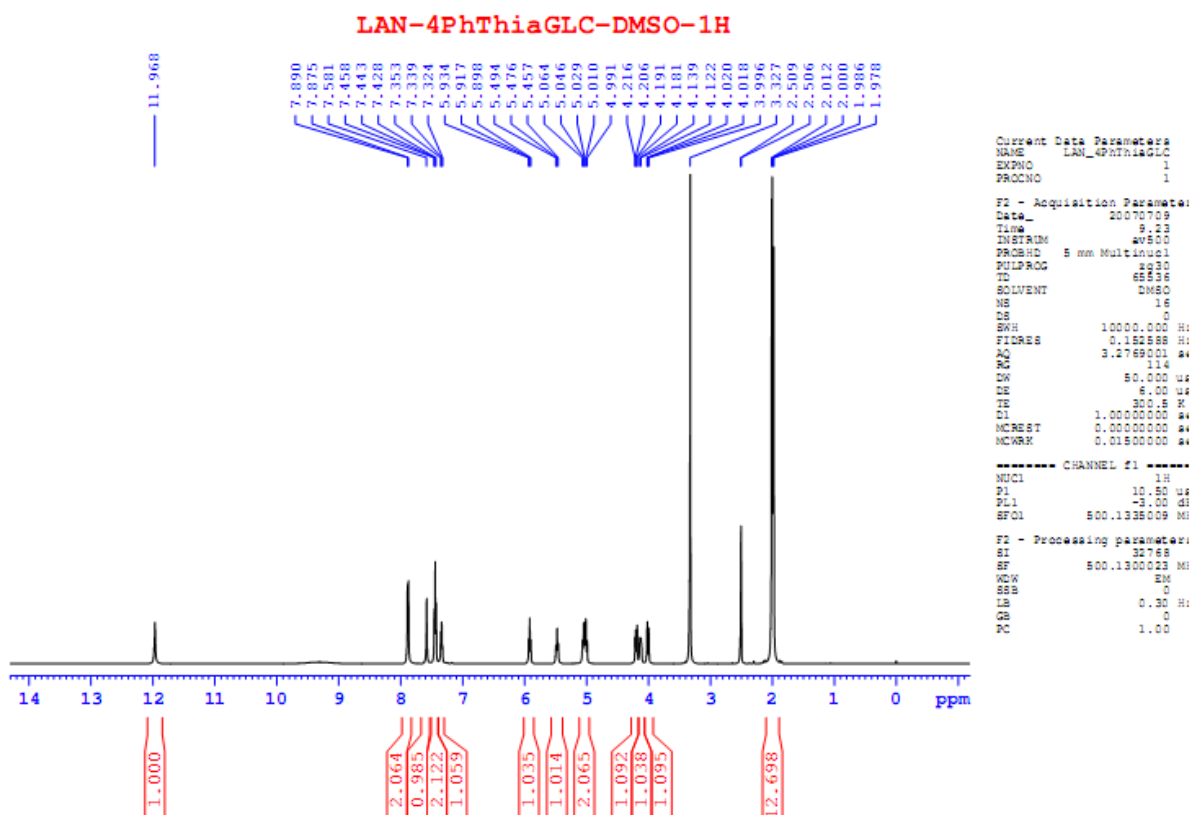
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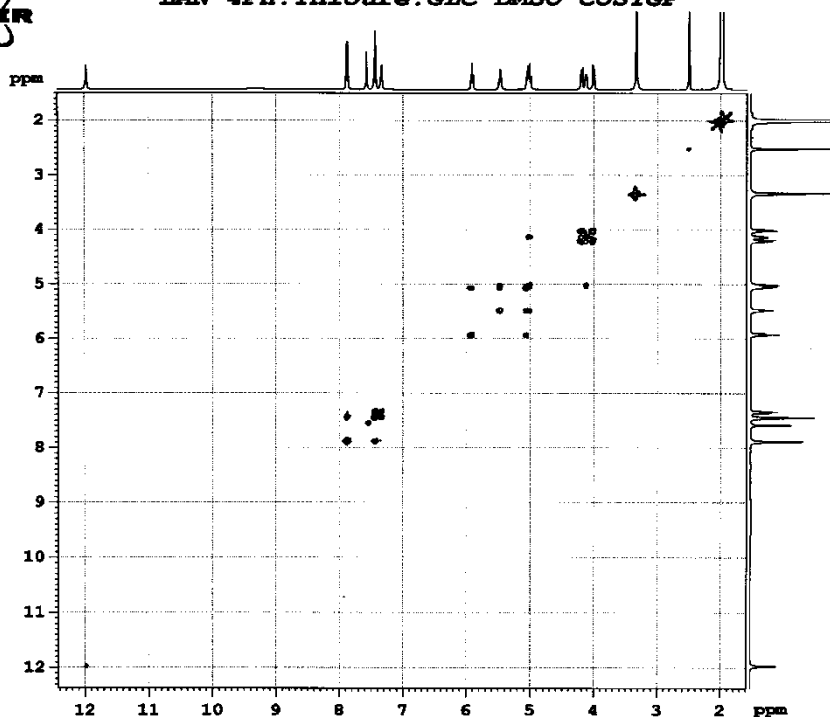
Selected NMR and mass spectra of compounds 4a-h

1-(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)-3-(4-phenylthiazole-2-yl)thiourea (**4a**)





LAN-4PH.Thioure.GLC-DMSO-COSYGP



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PROCNO 1

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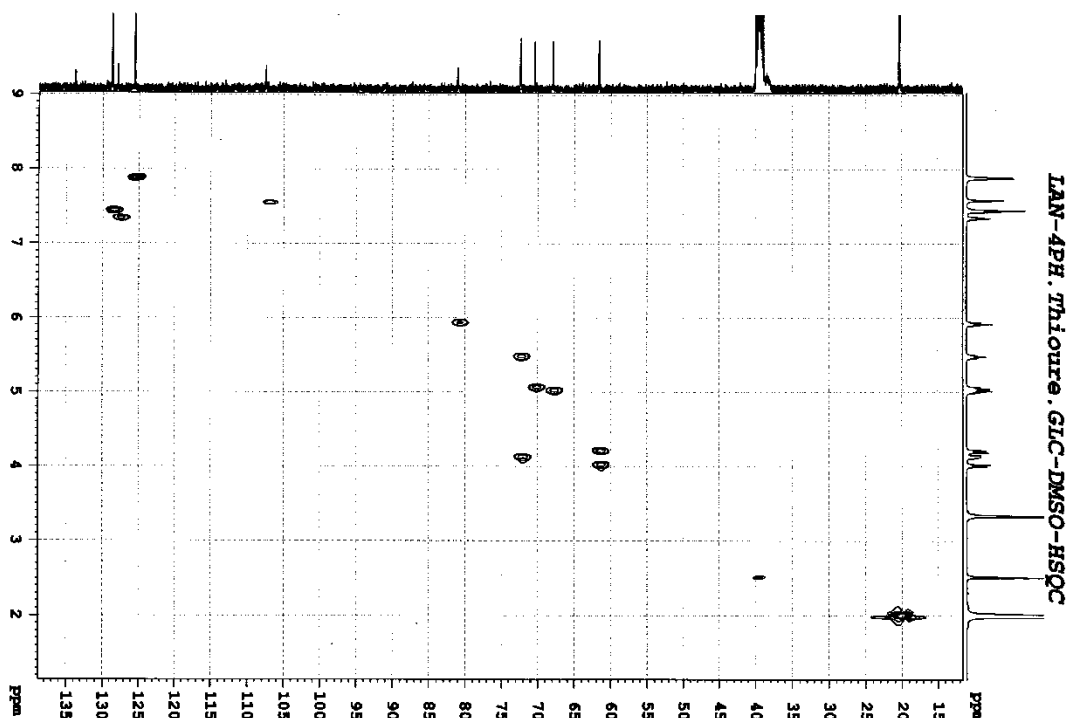
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GPX2 0.00 %
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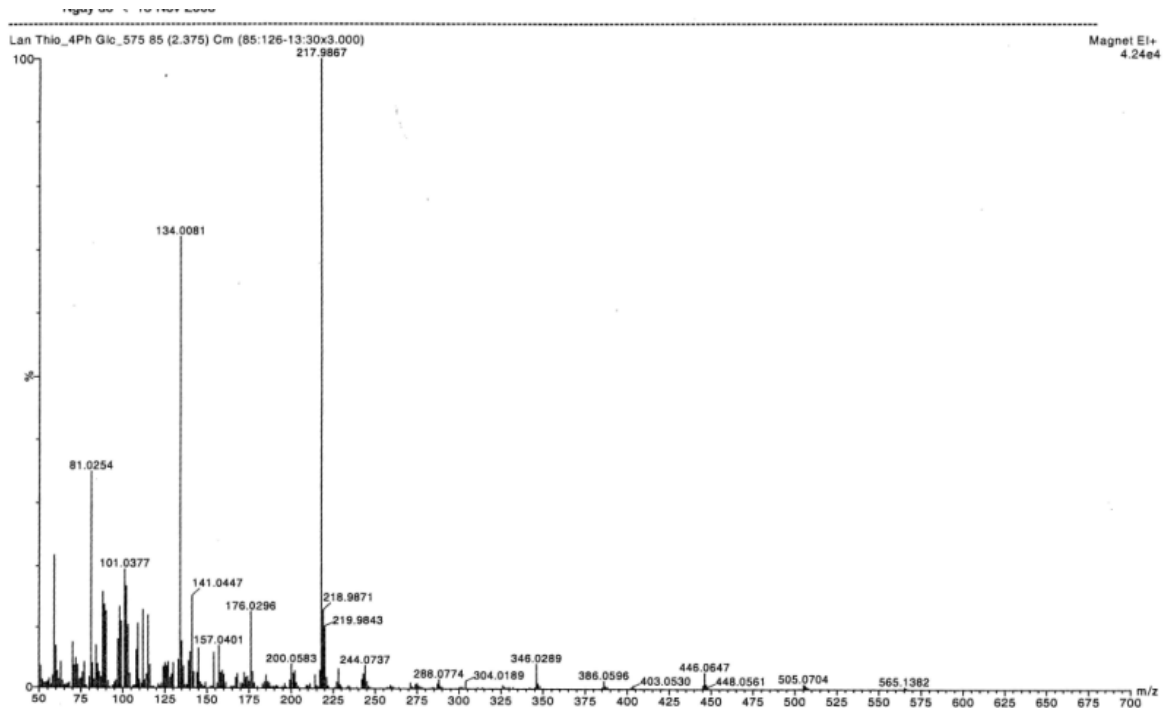
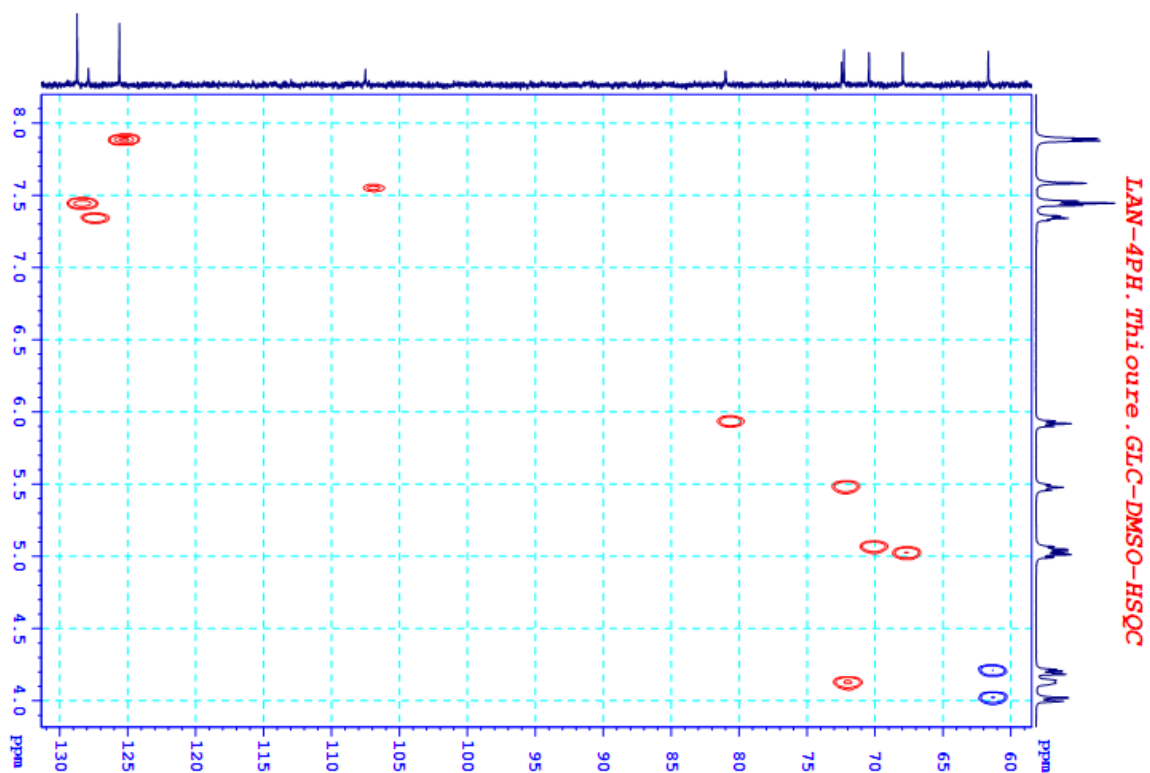
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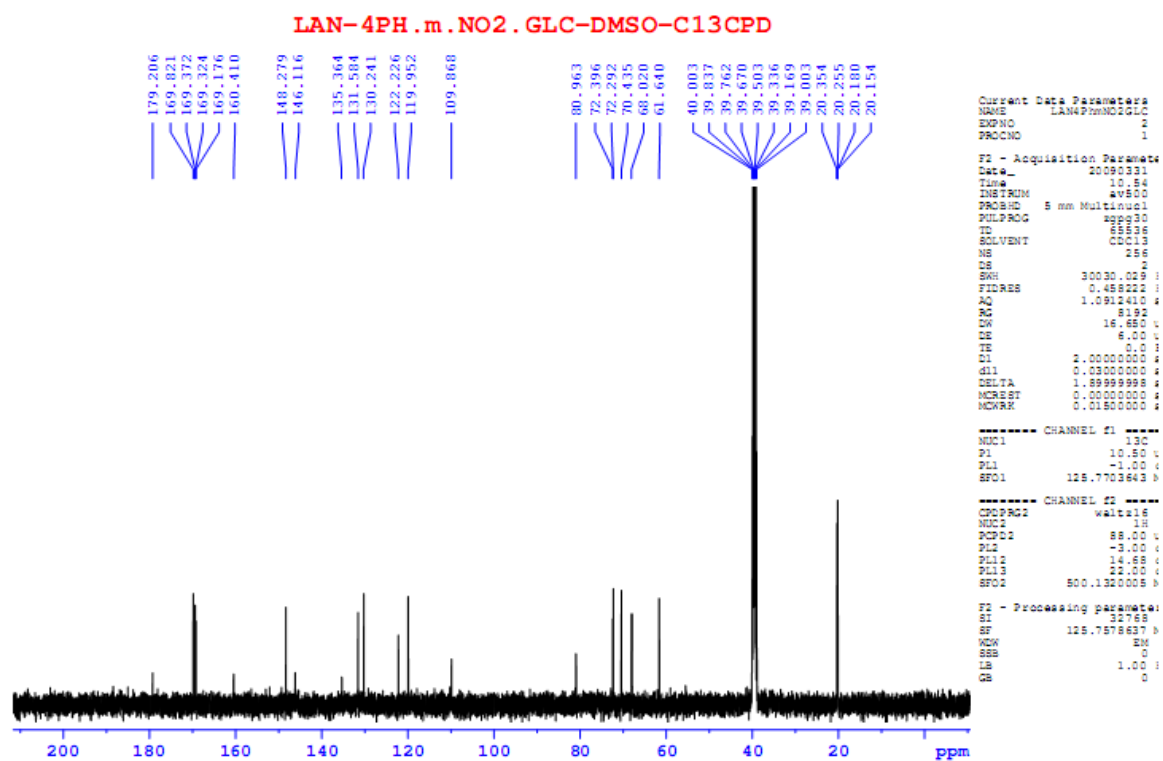
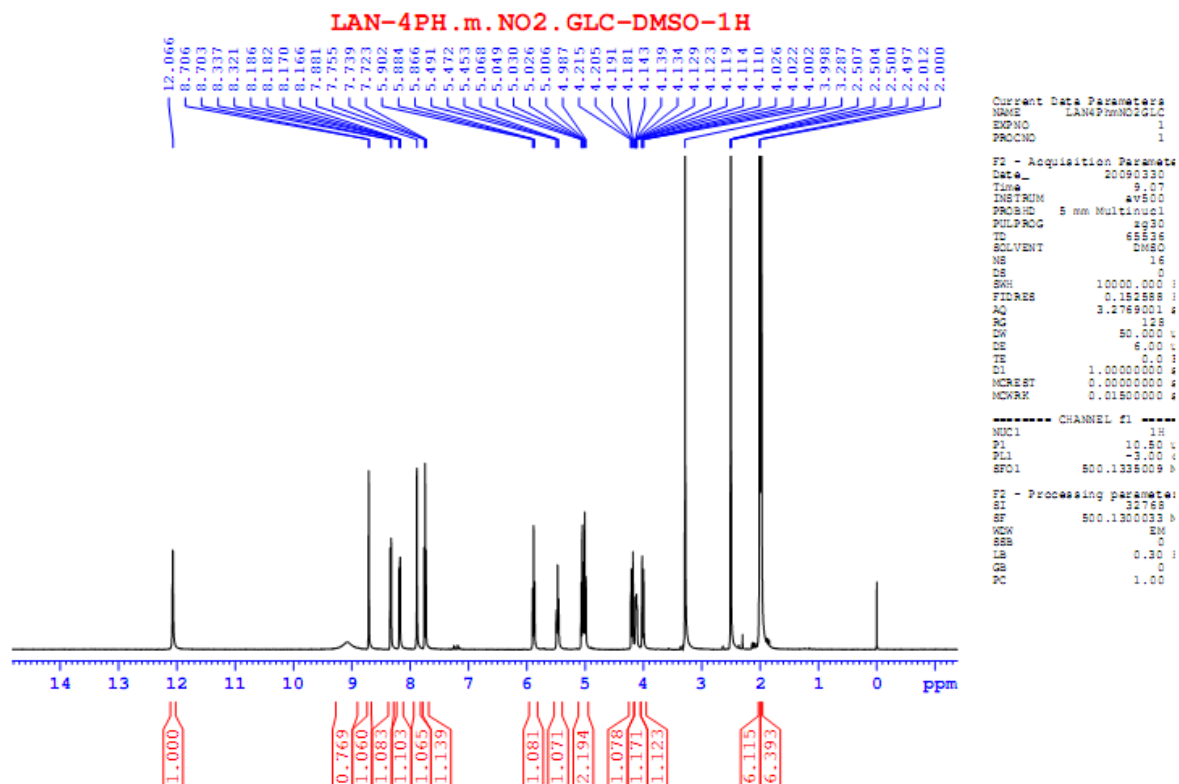
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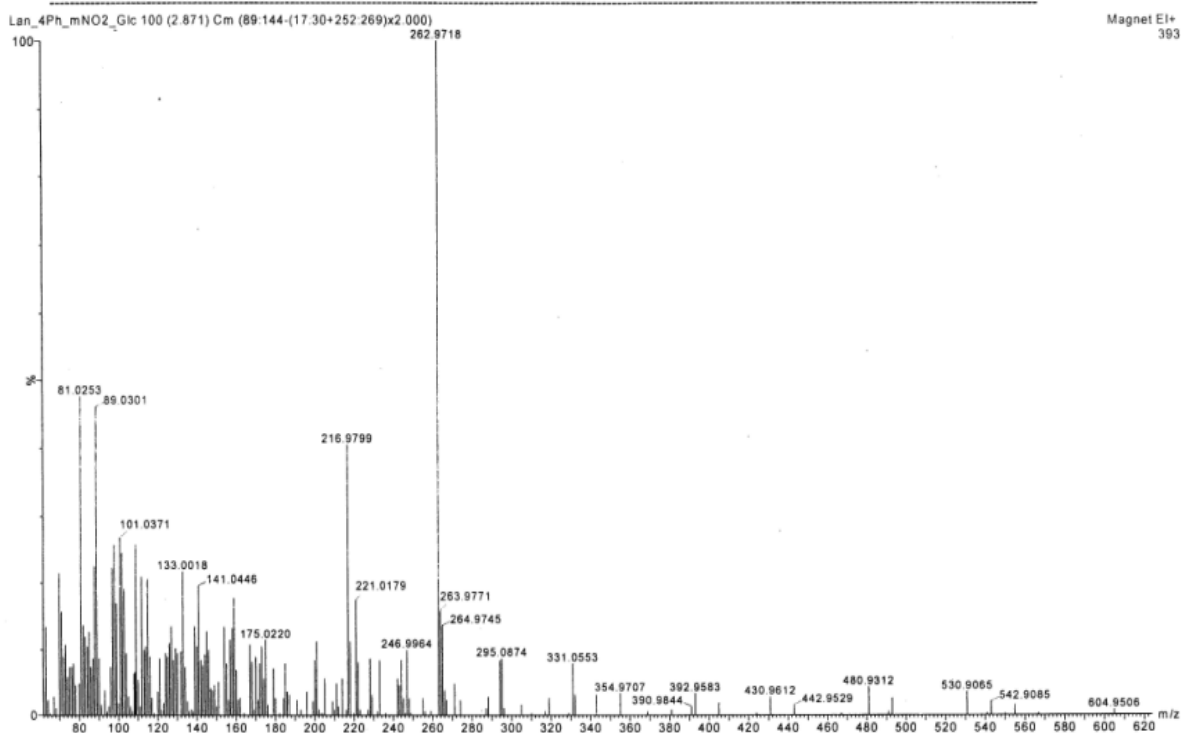


LAN-4PH.Thioure.GLC-DMSO-HSQC

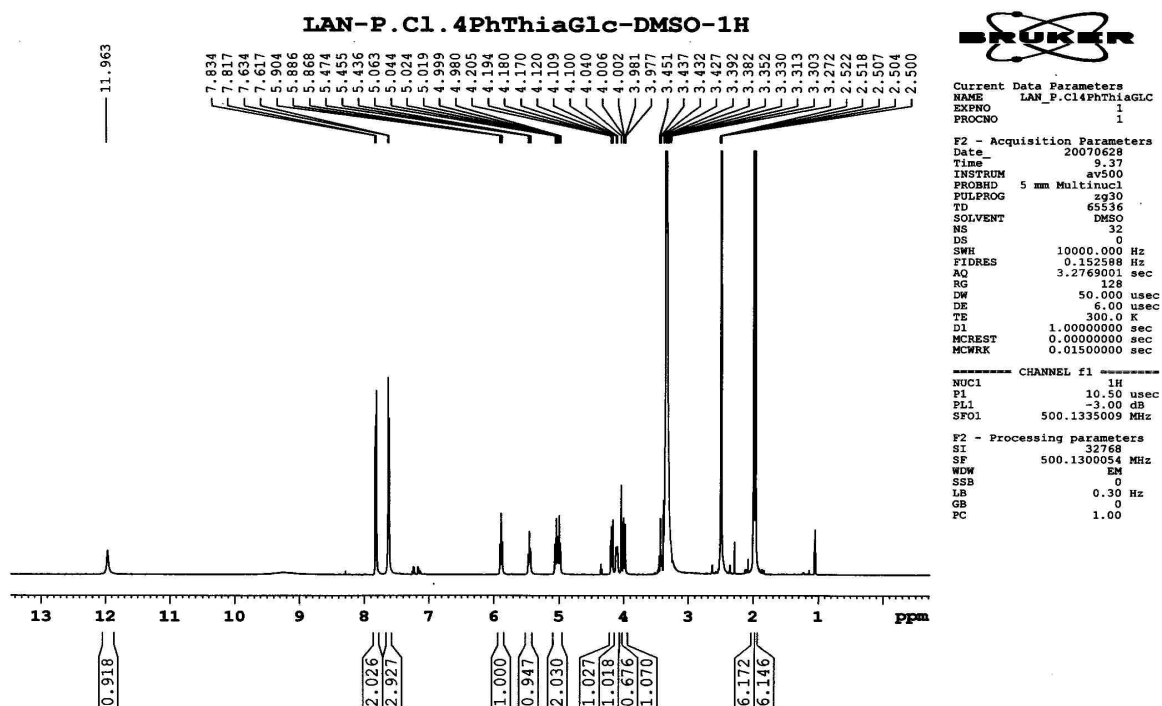


1-(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)-3-(4-(3-nitrophenyl)thiazole-2-yl)thiourea (4b)

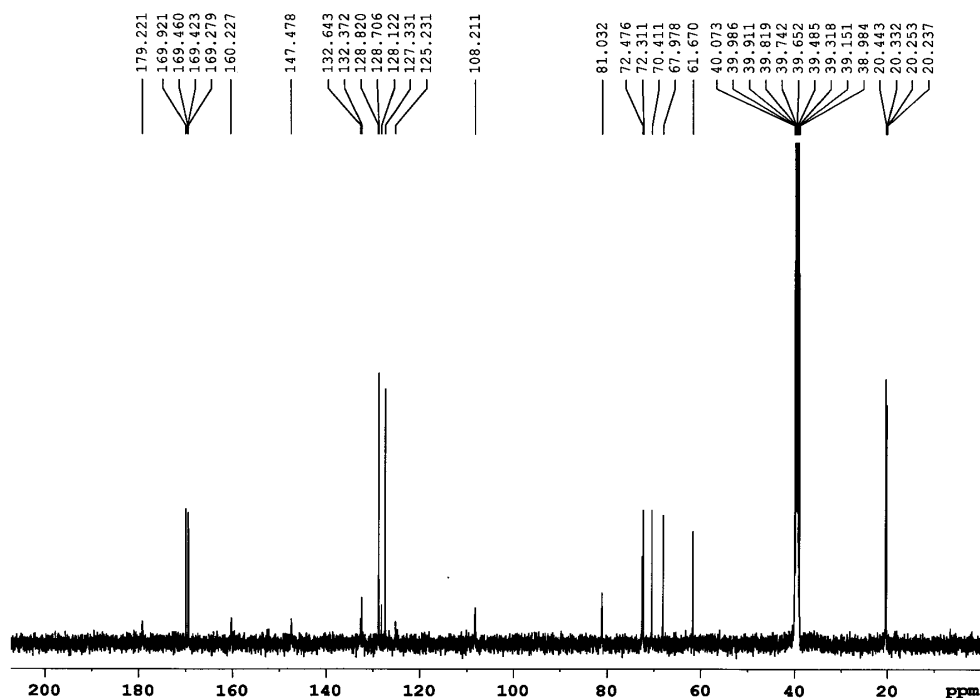




1-(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)-3-(4-(4-chlorophenyl)thiazole-2-yl)thiourea (4c)



LAN-THIOURE.PCl.PH.ThiaGLC-DMSO-C13CPD



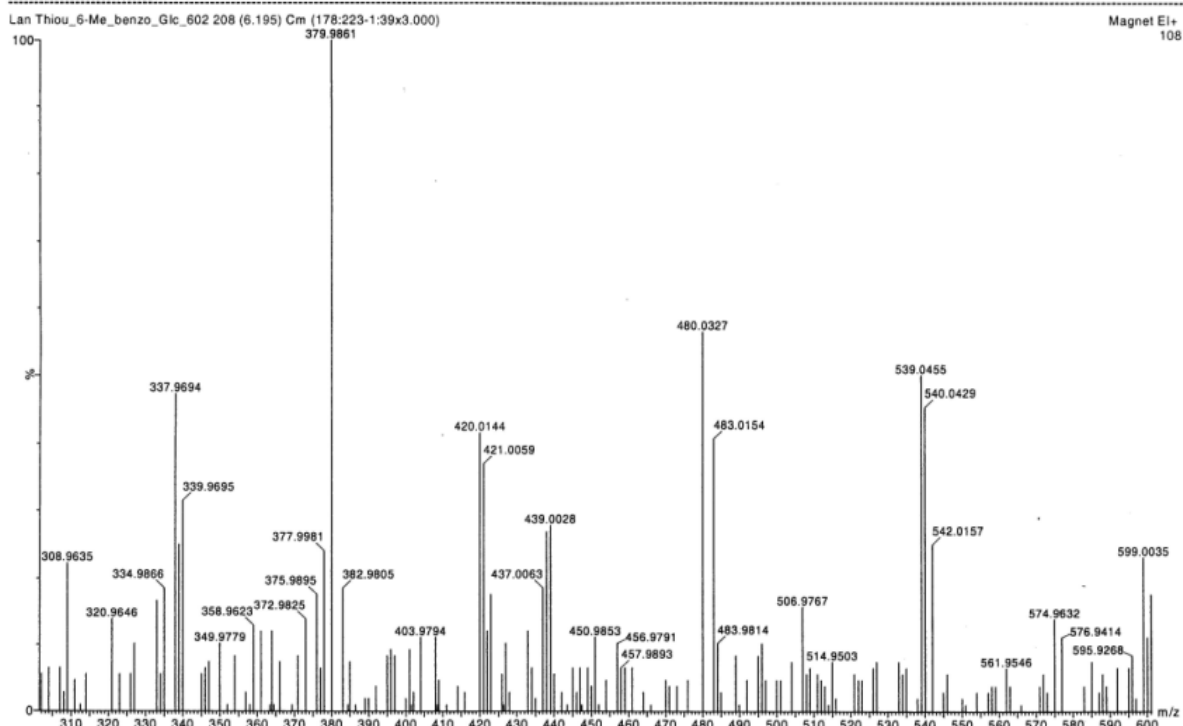
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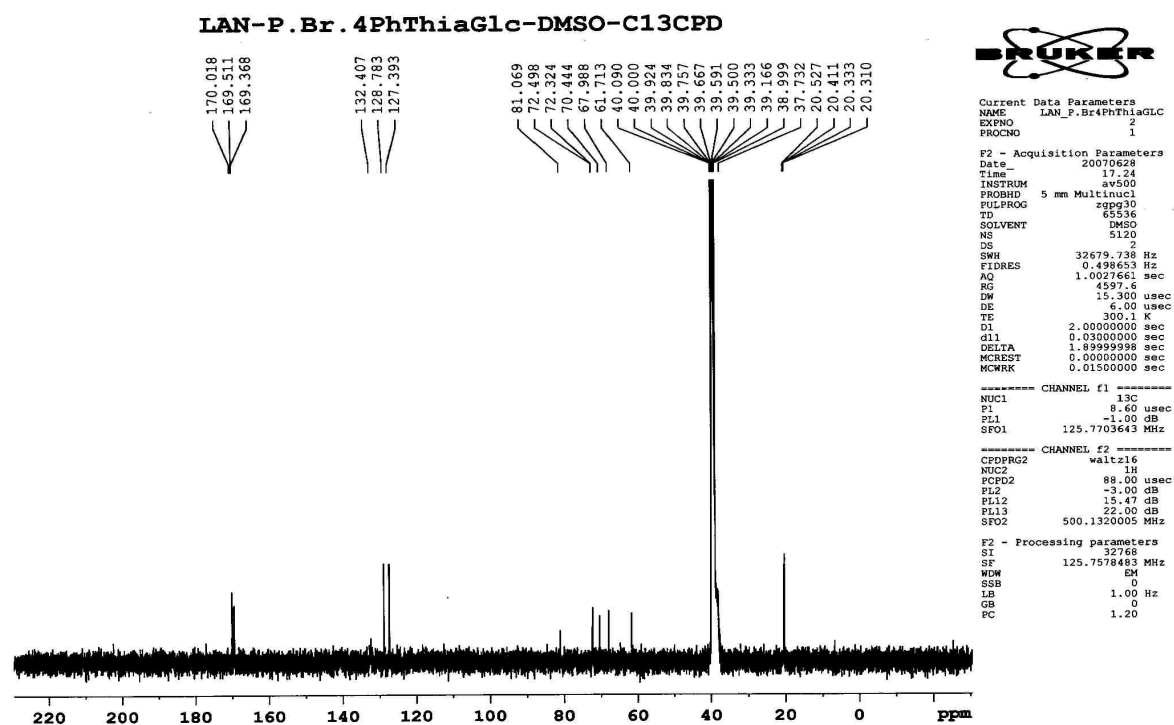
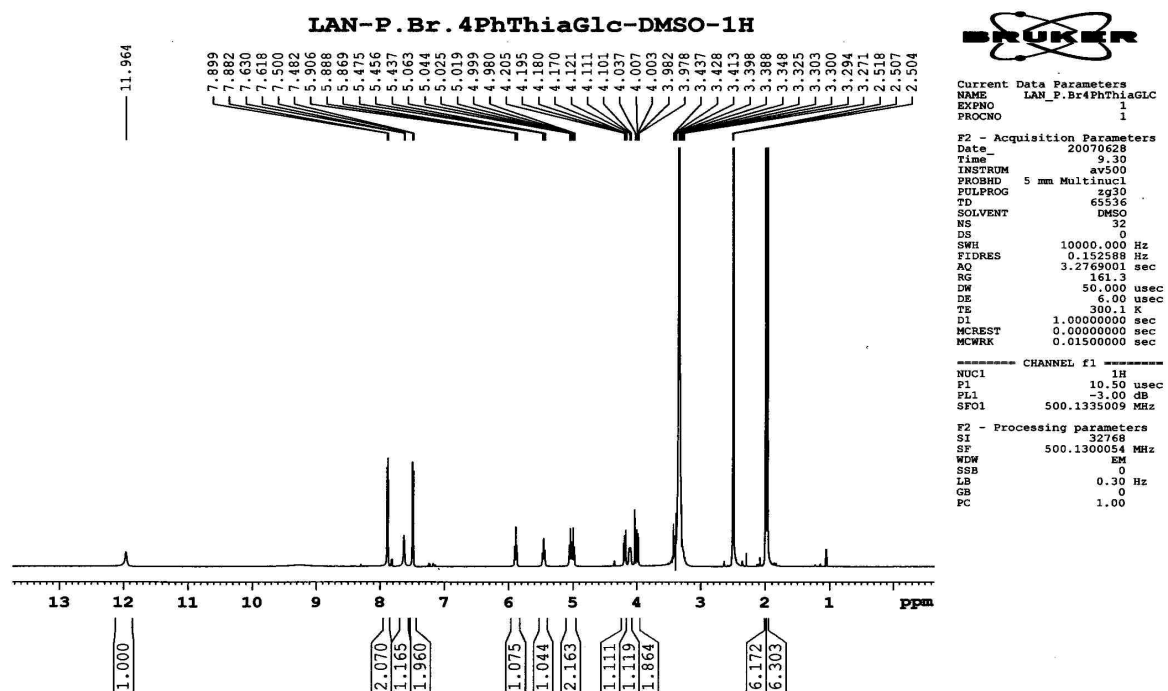
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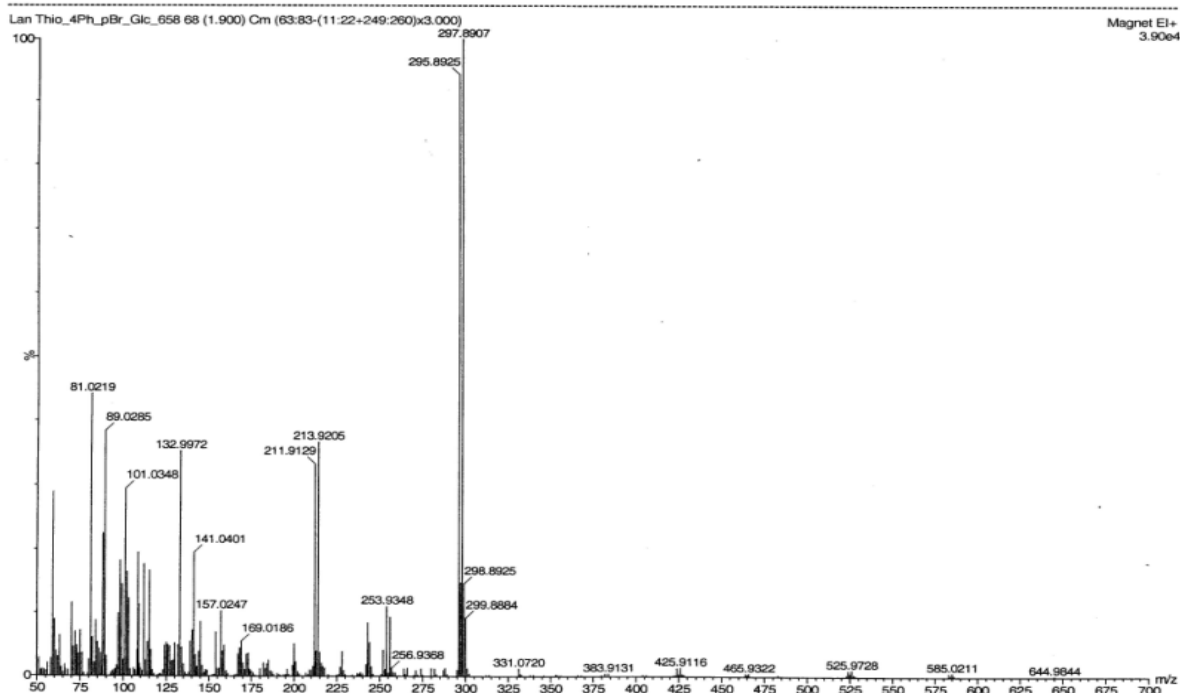
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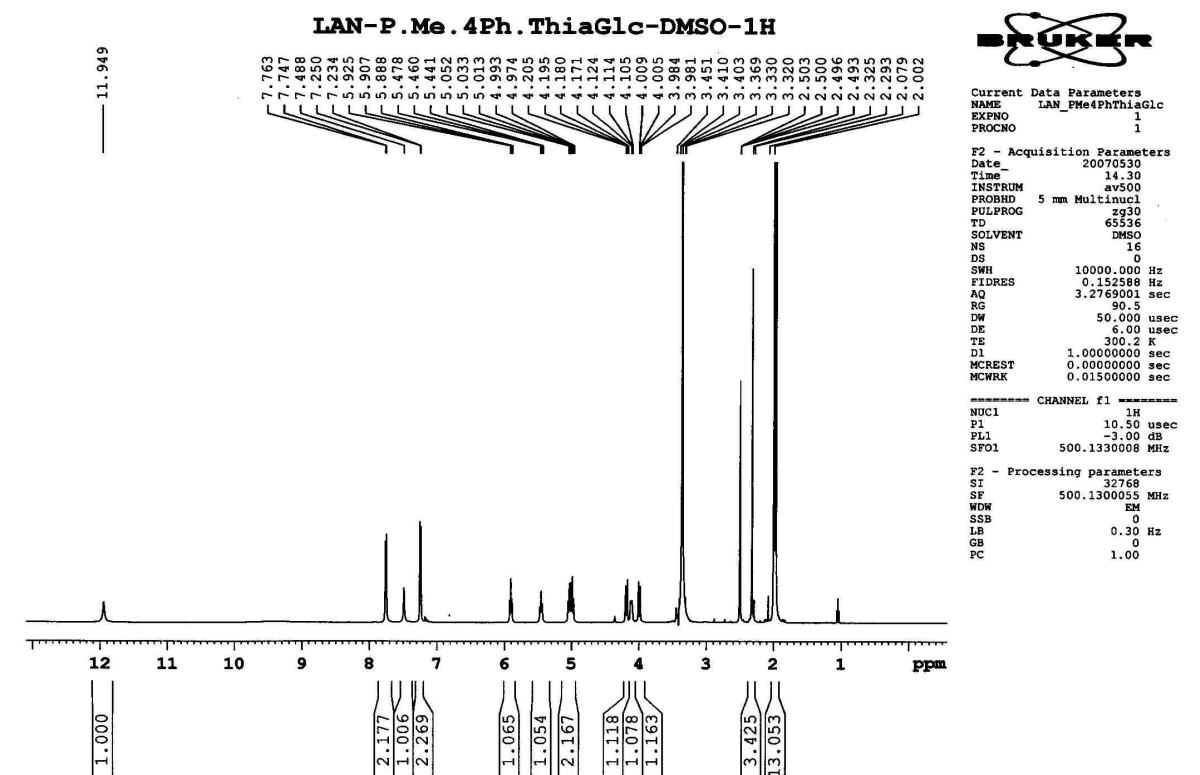


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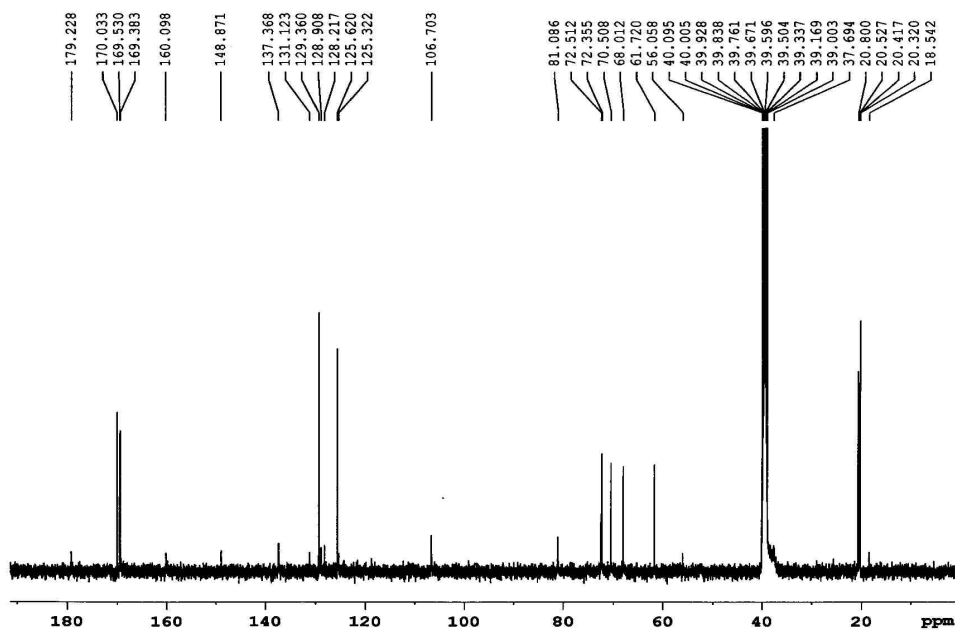




1-(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)-3-(4-(4-tolyl)thiazole-2-yl)thiourea (4e)



LAN-P.Me.4Ph.ThiaGlc-DMSO-C13CPD



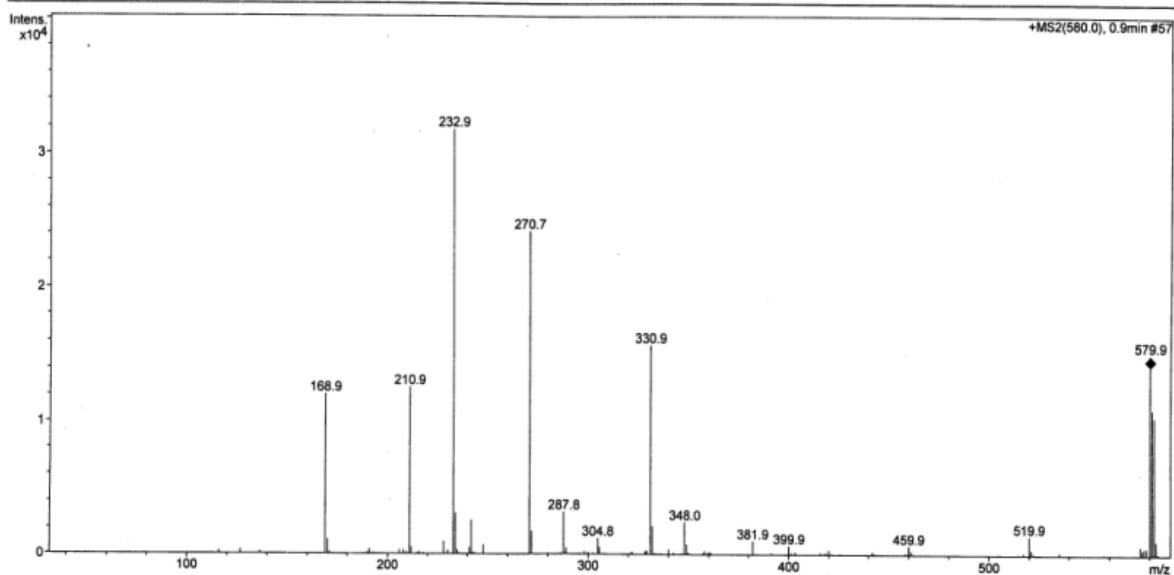
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RG 5160.6
DM 15.300 usec
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TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
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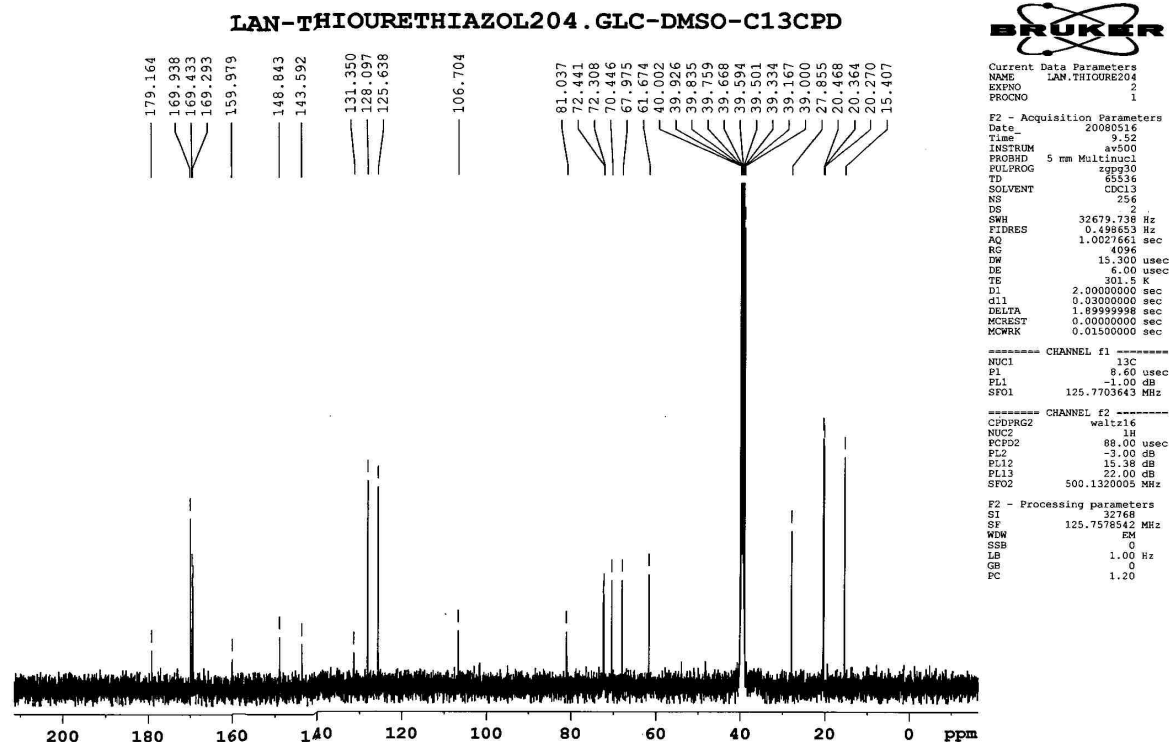
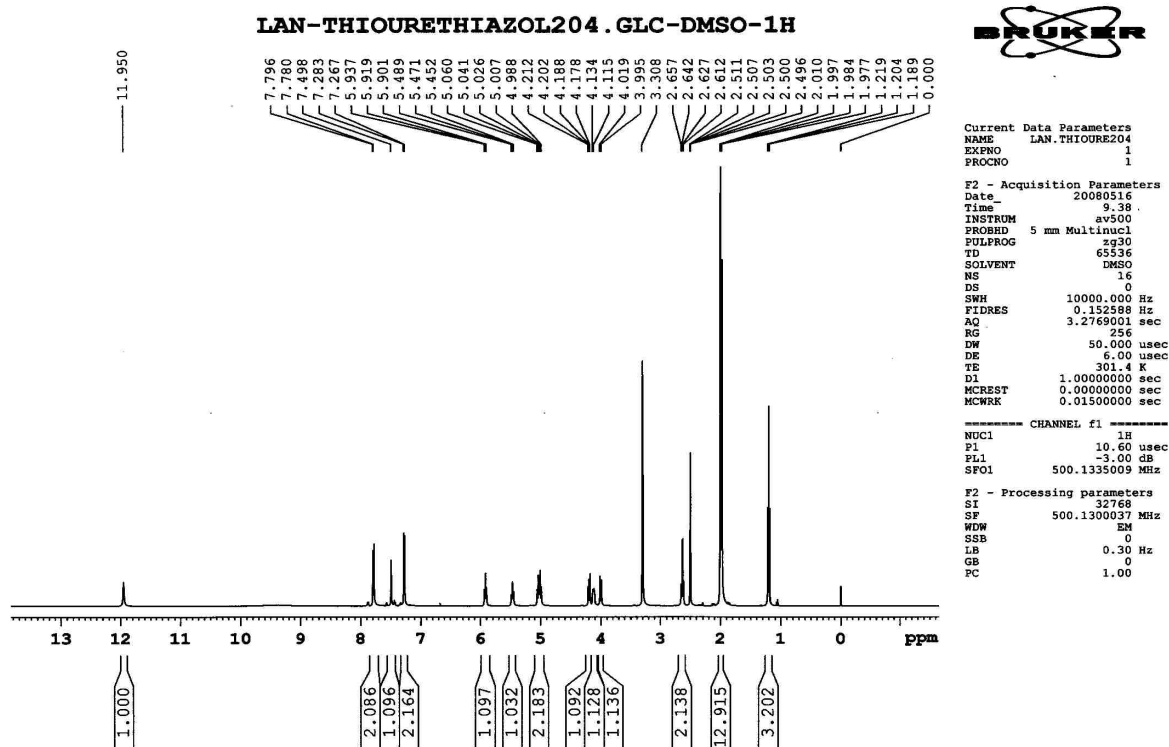
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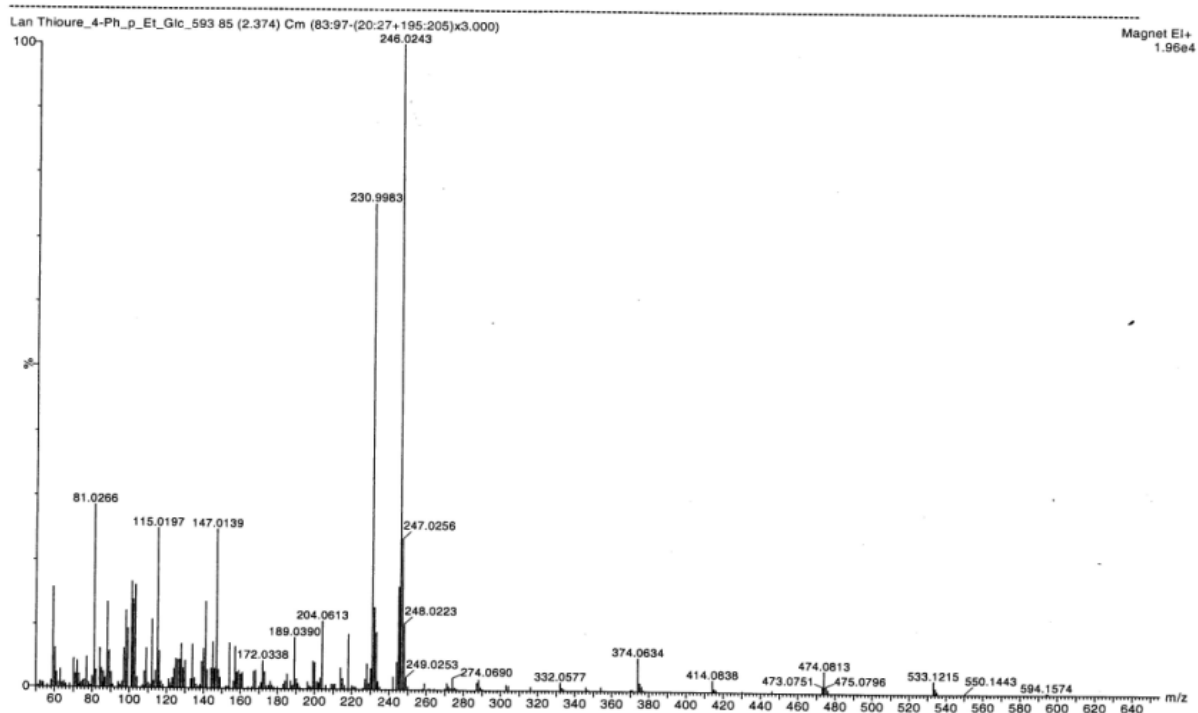
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PL13 22.00 dB
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F2 - Processing parameters
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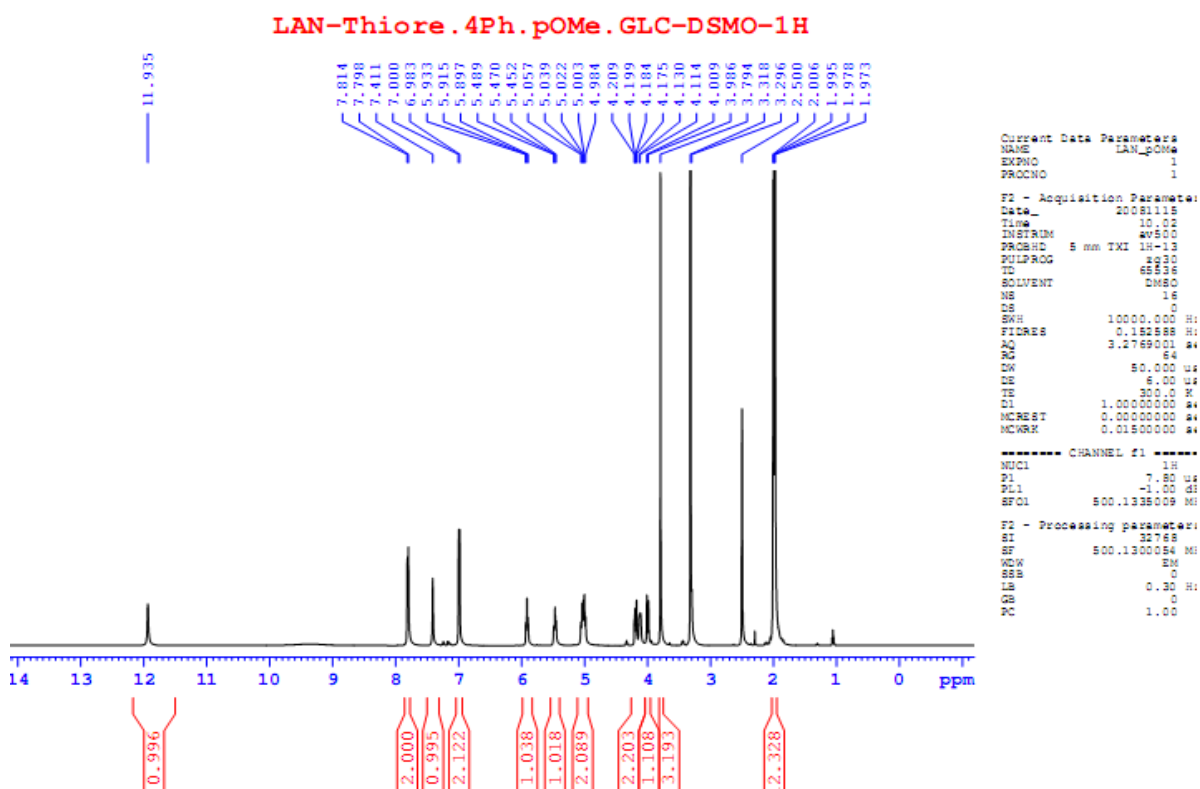


1-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)-3-(4-(4-ethylphenyl)thiazole-2-yl)thiourea (4f)

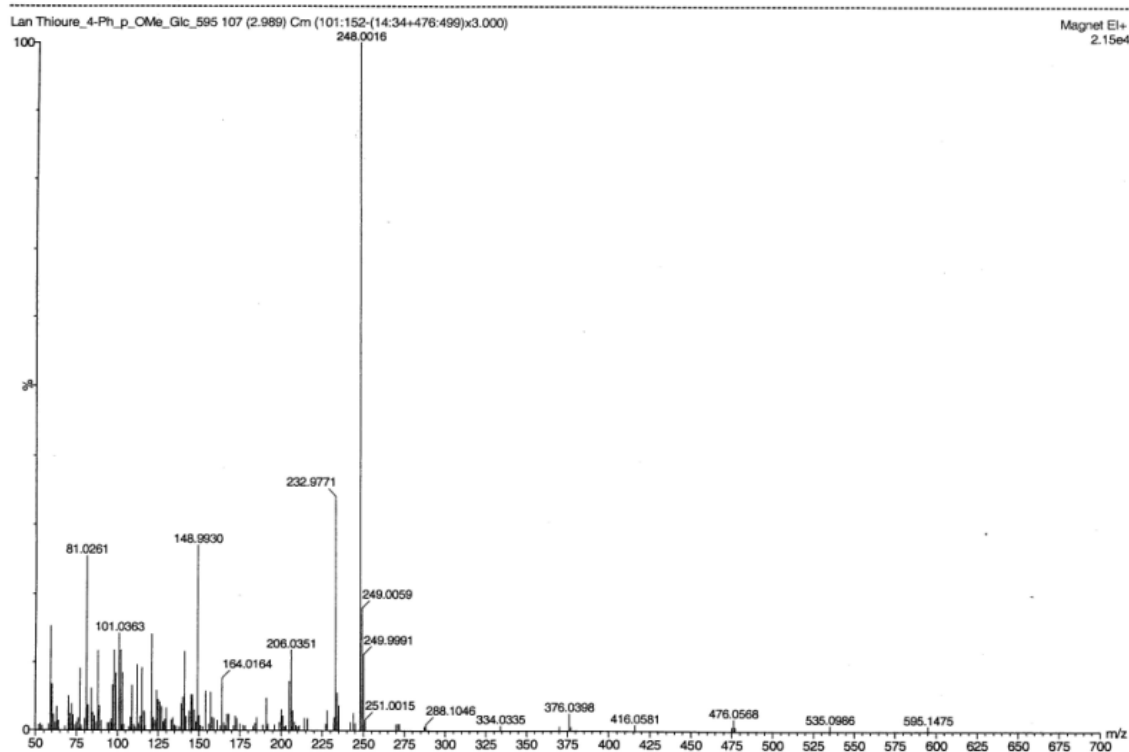
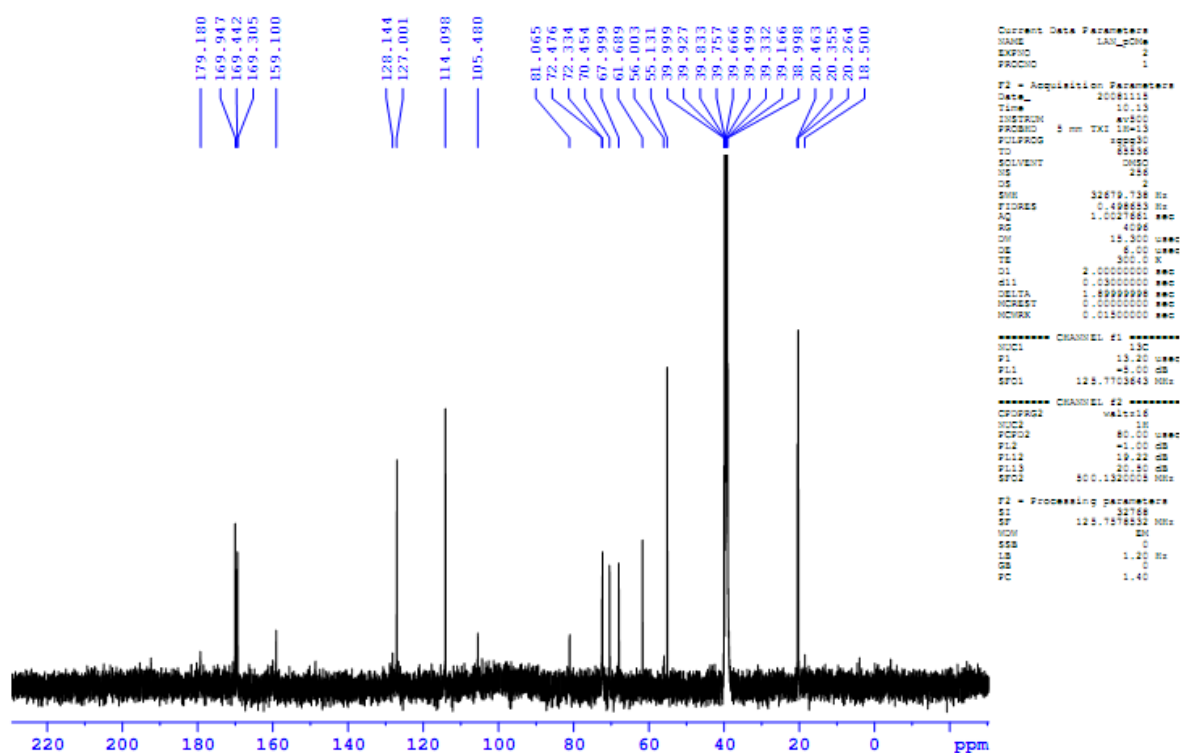




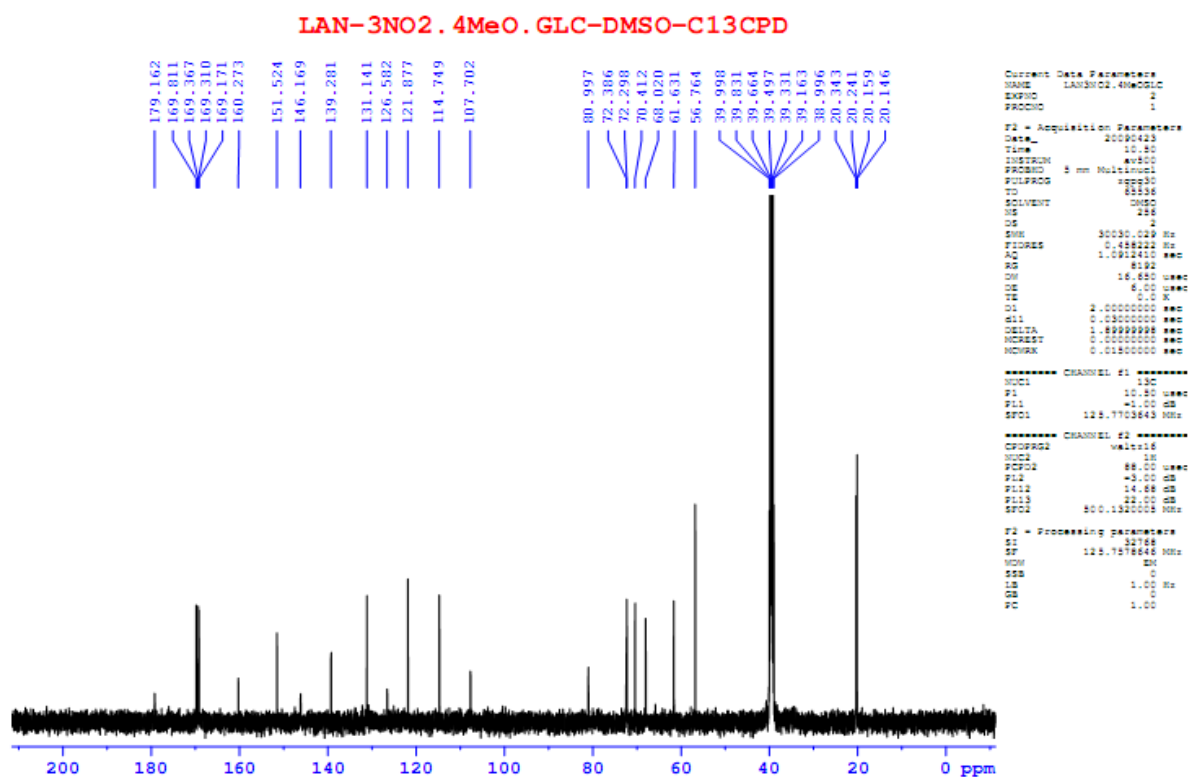
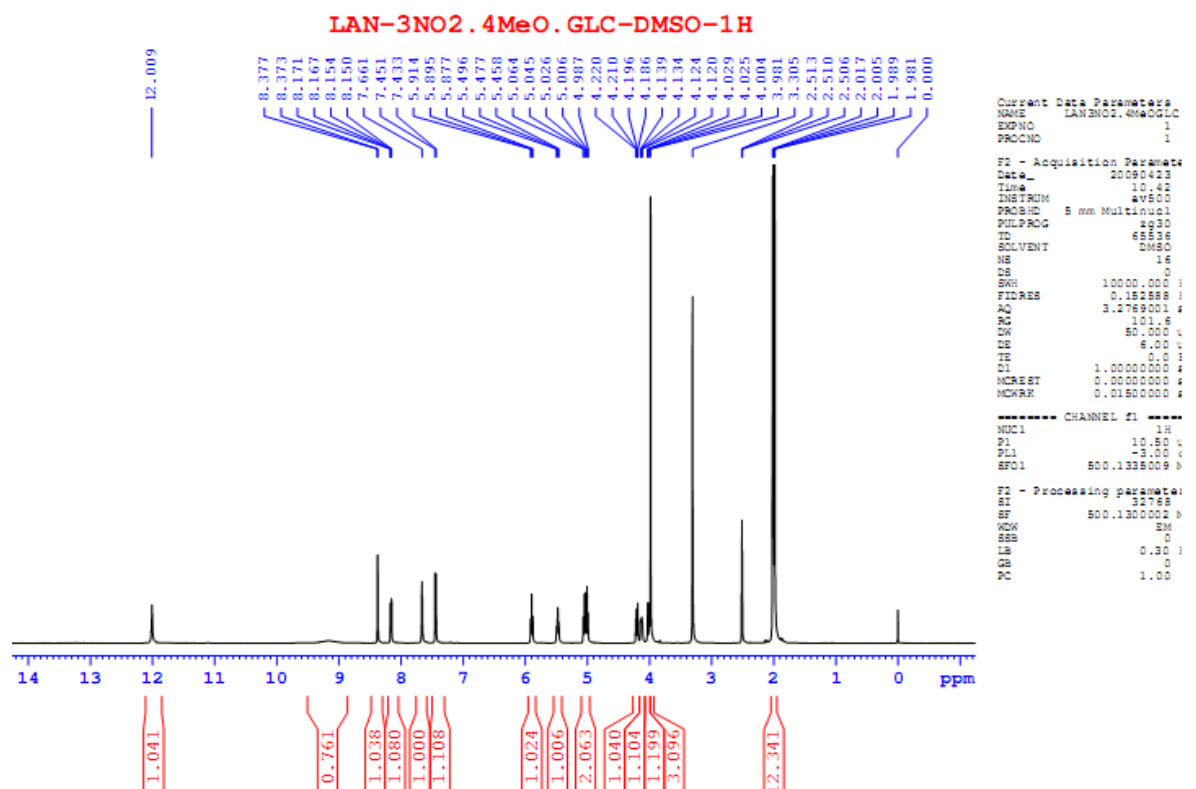
1-(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)-3-(4-(4-methoxyphenyl)thiazole-2-yl)thiourea
(4g)



LAN-Thiore.4Ph.pOMe.GLC-DSMO-C13CPD



1-(2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl)-3-(4-(4-methoxy-3-nitrophenyl)thiazole-2-yl)thiourea (**4h**)



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