

Supplementary Materials

Expanding the library of 1,2,4-oxadiazole derivatives: discovery of new Farnesoid X Receptor (FXR) antagonists/Pregnane X Receptor (PXR) agonists

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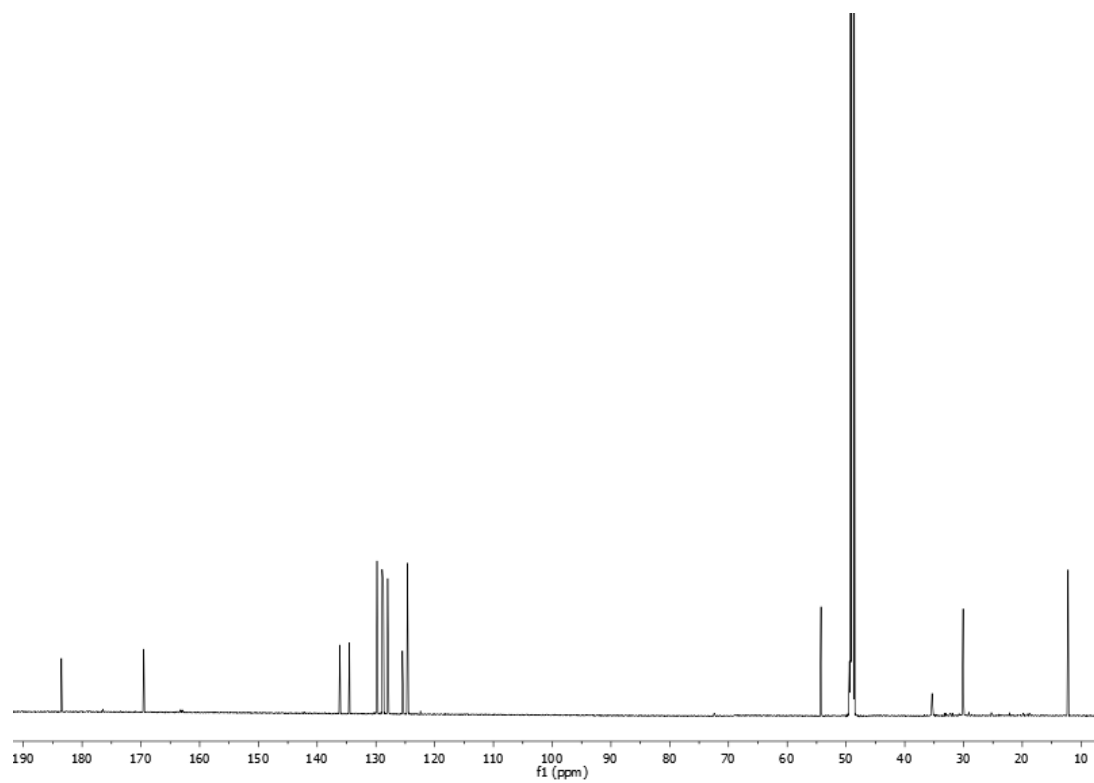
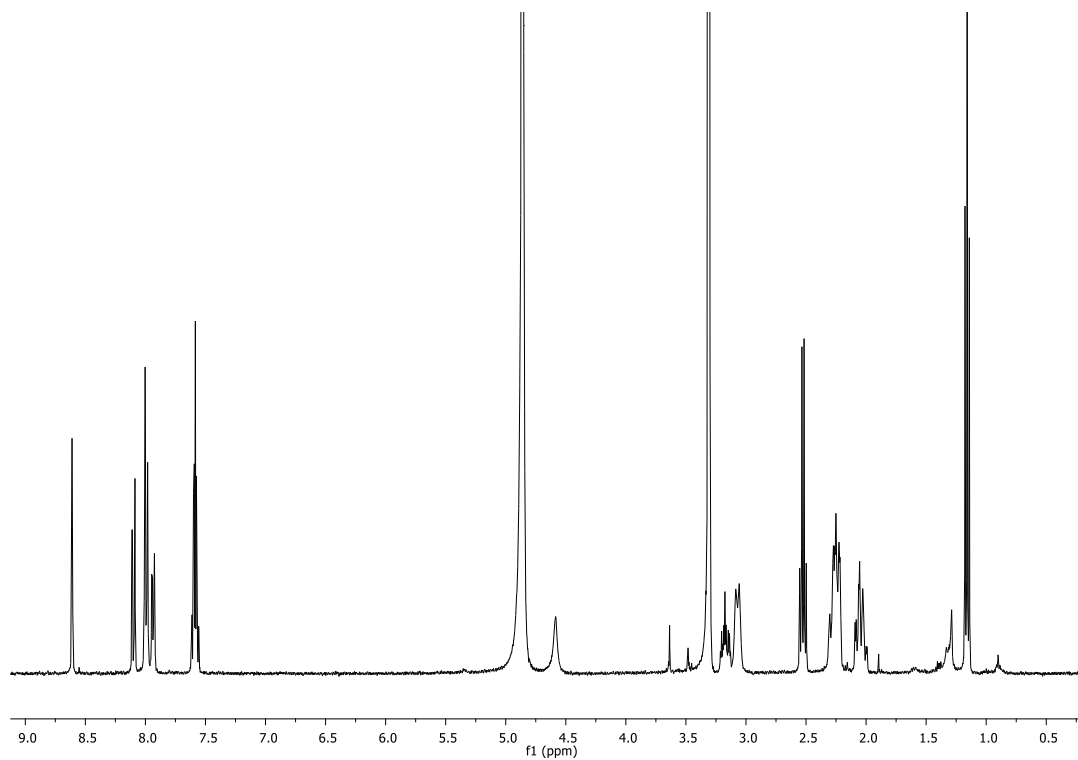
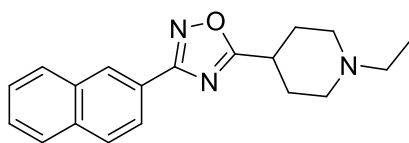
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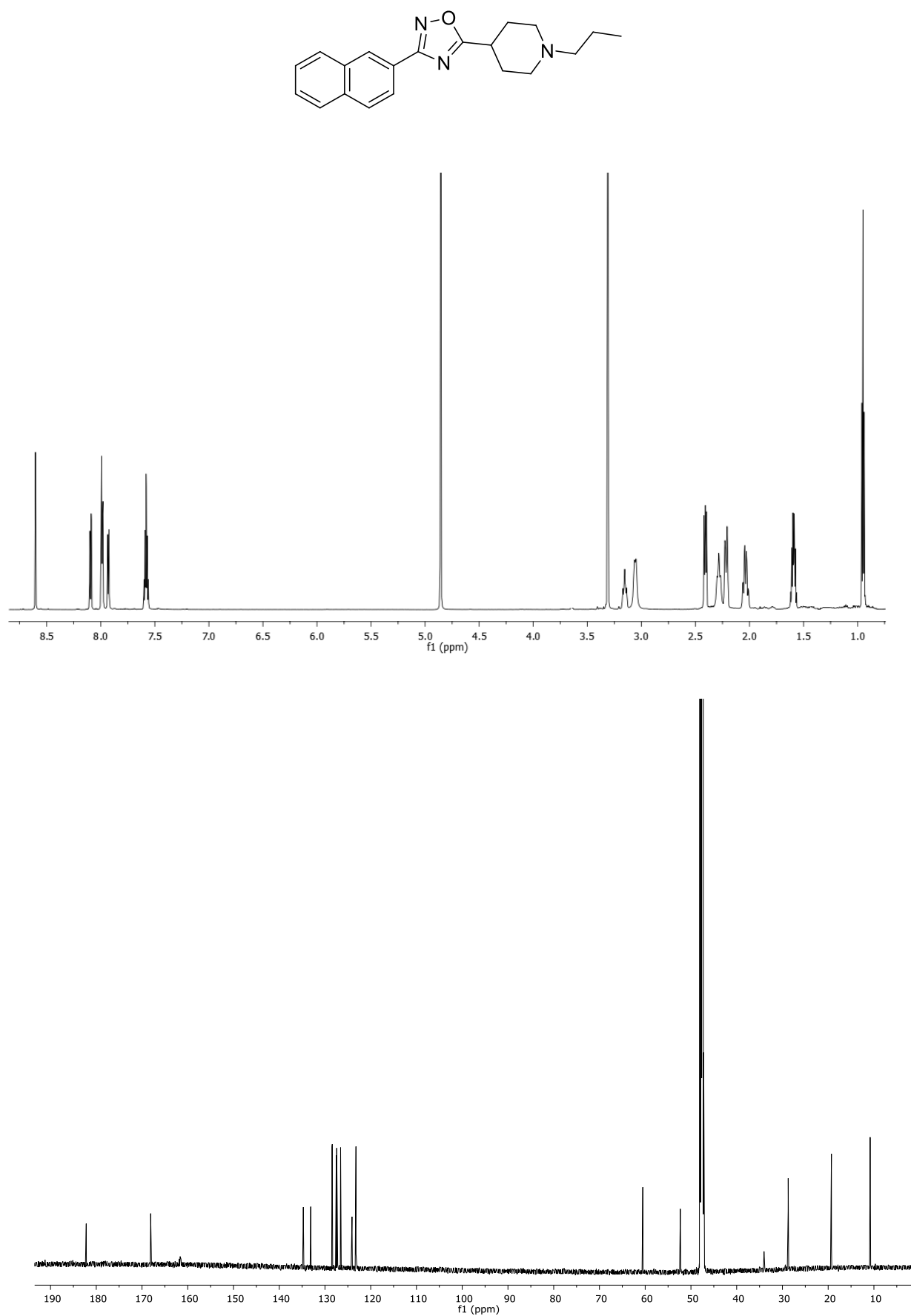
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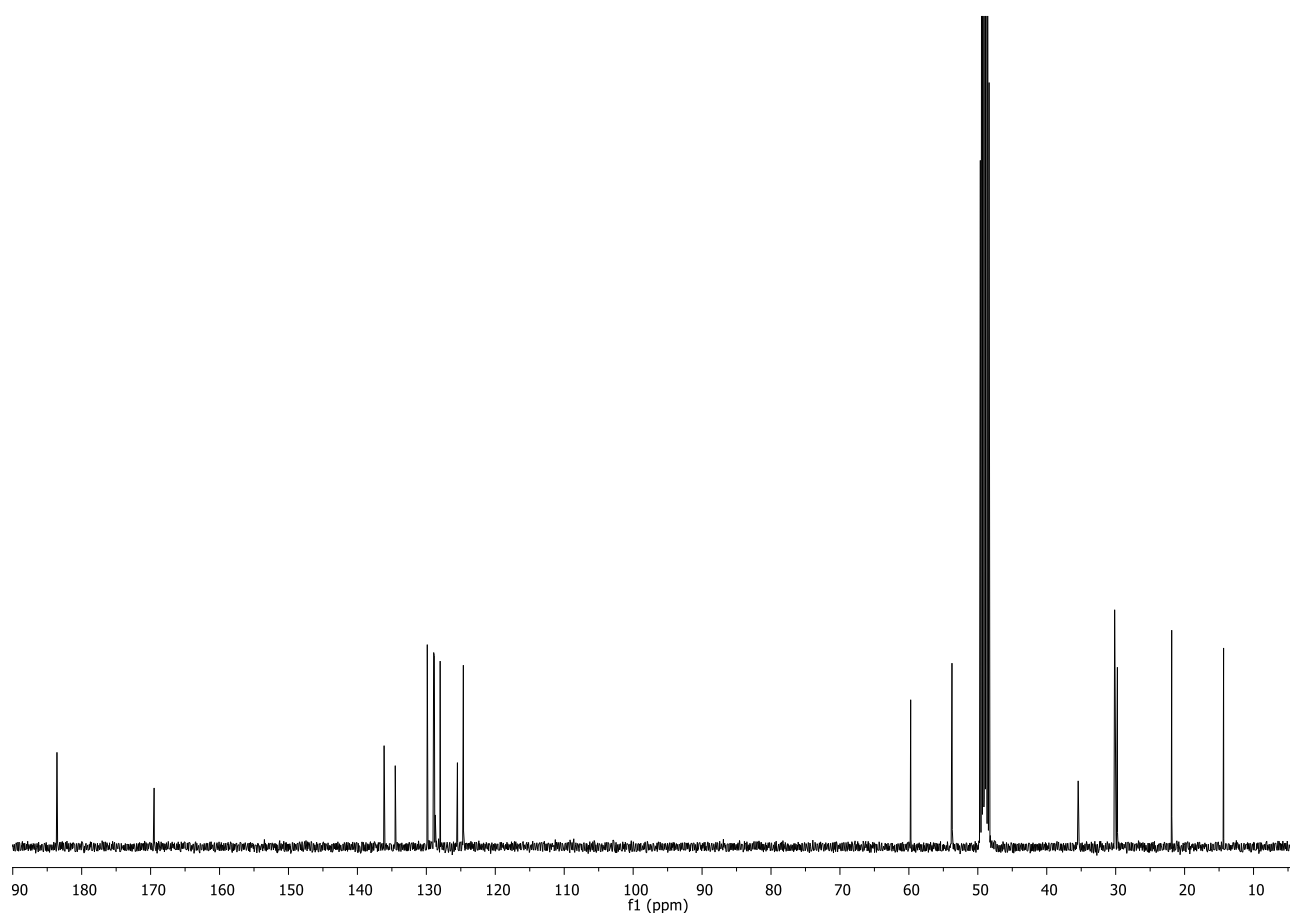
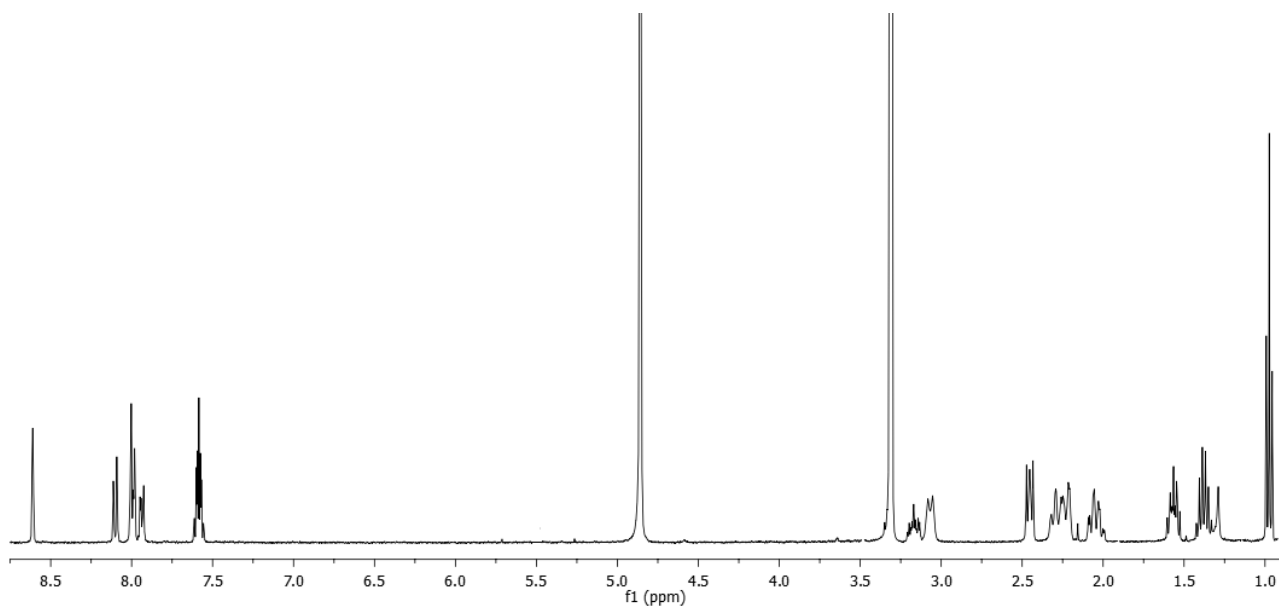
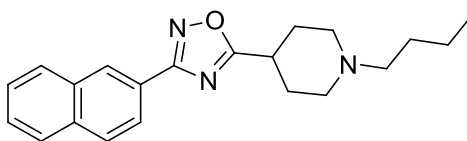
Figures S1-S2. ^1H (400 MHz) and ^{13}C NMR (100 MHz) in CD_3OD of compound **2**



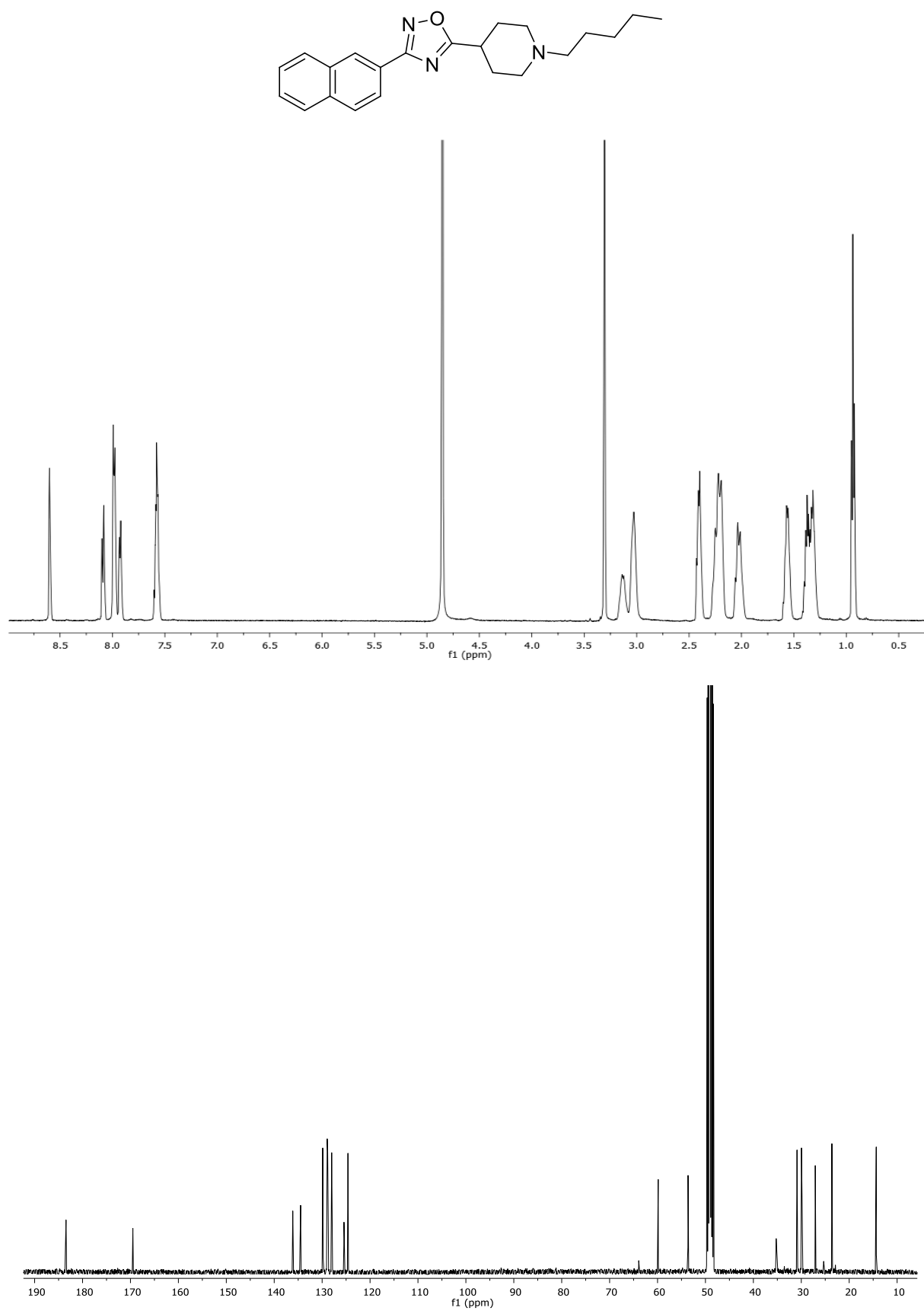
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Figures S7-S8. ^1H (400 MHz) and ^{13}C NMR (100 MHz) in CD_3OD of compound **5**



Figures S9-S10. ^1H (400 MHz) and ^{13}C NMR (100 MHz) in CD_3OD of compound **6**

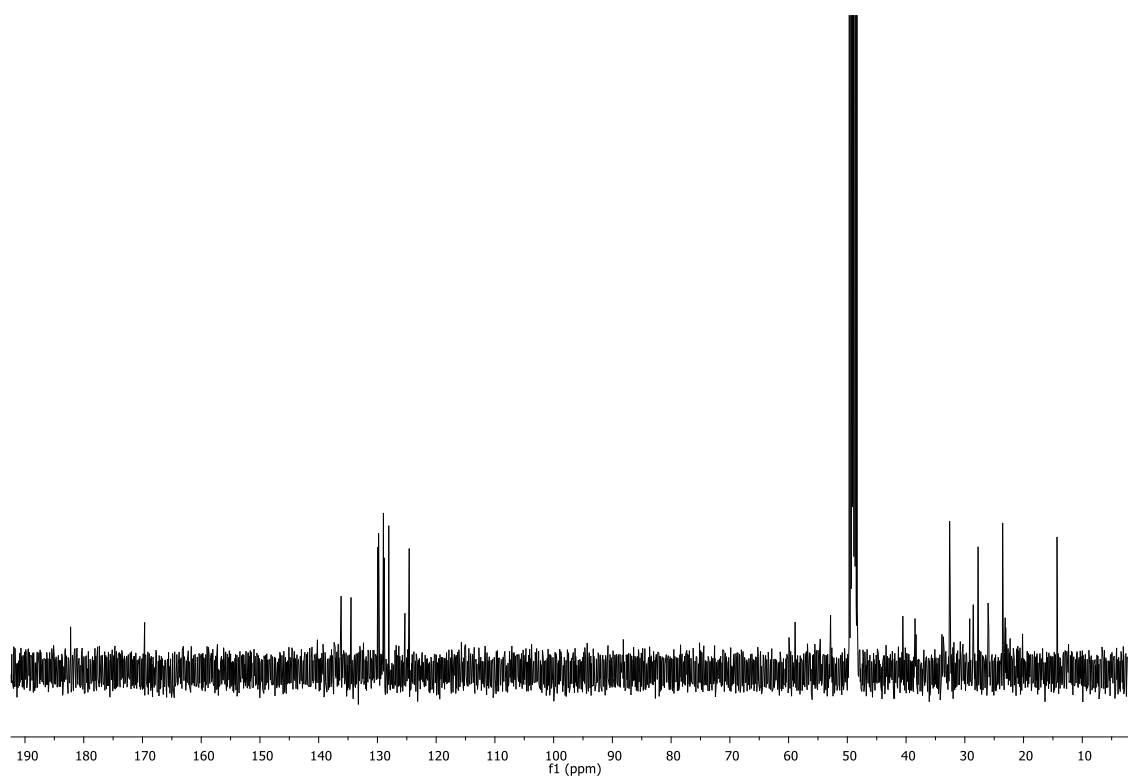
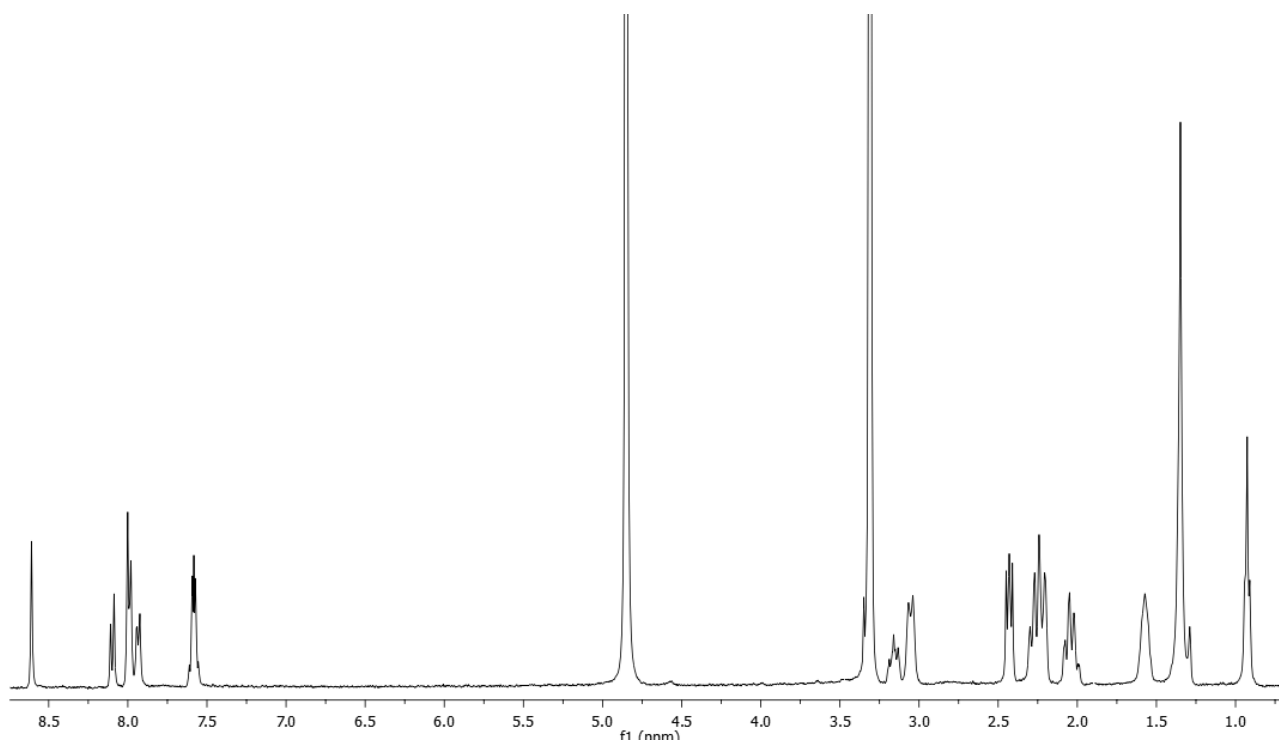
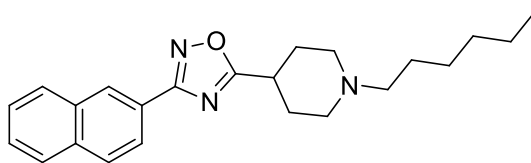
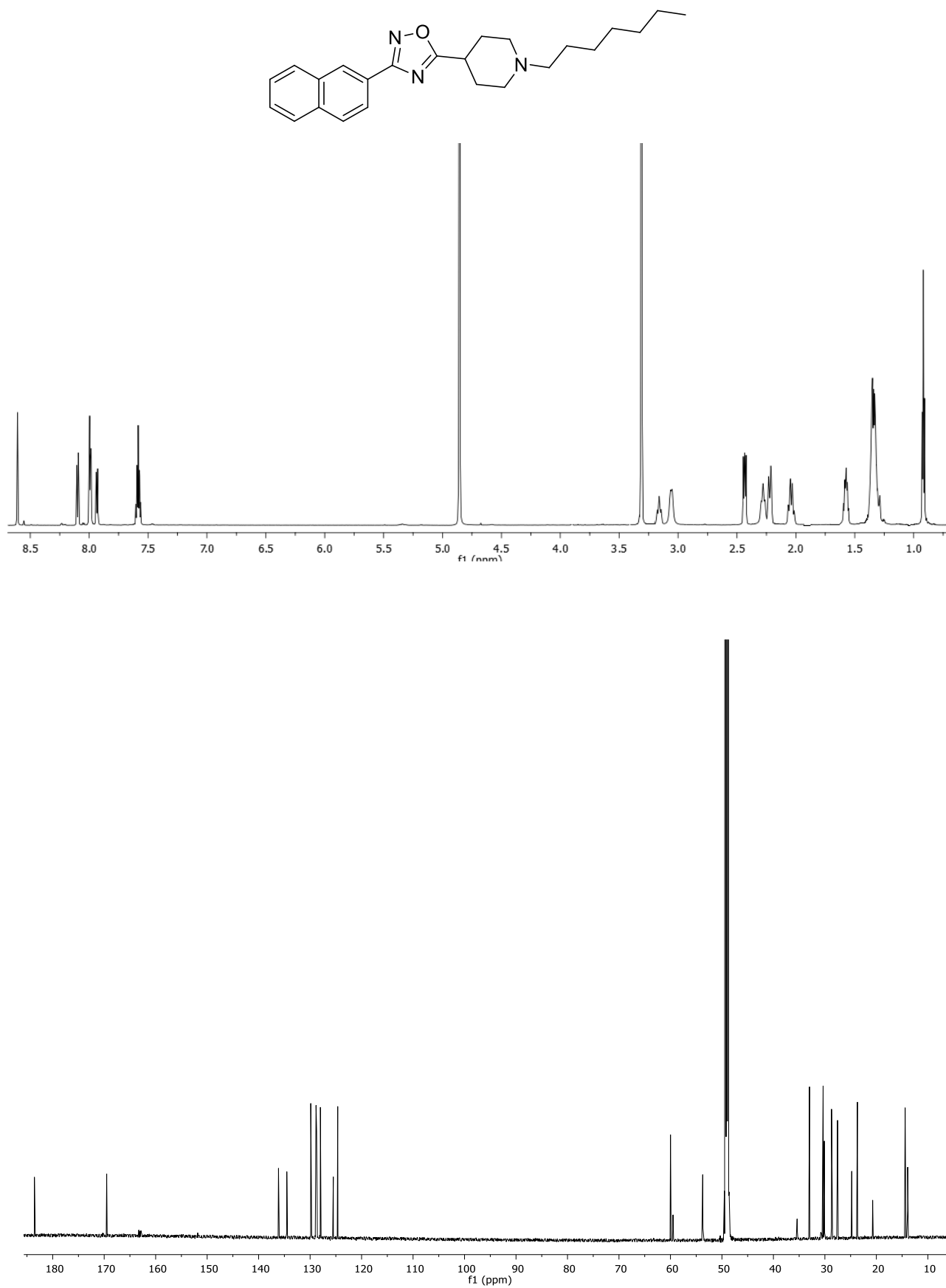
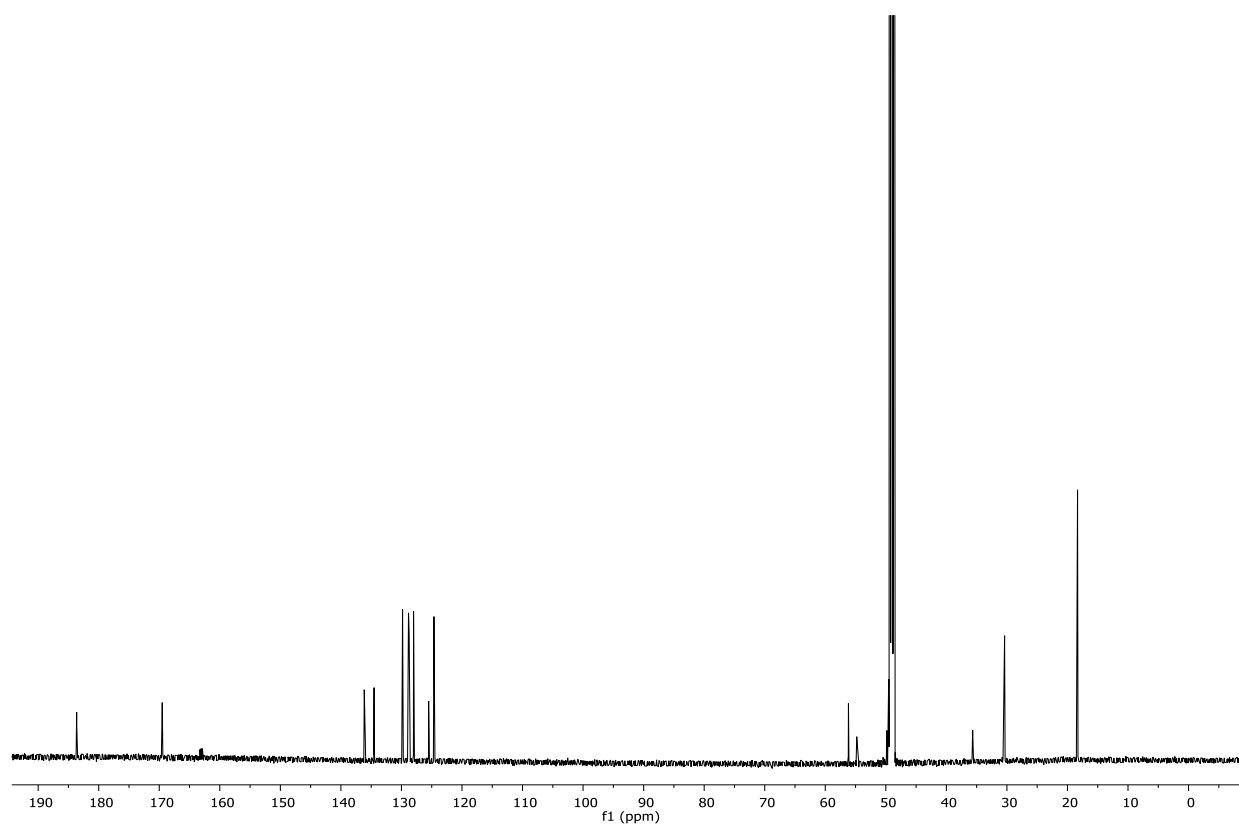
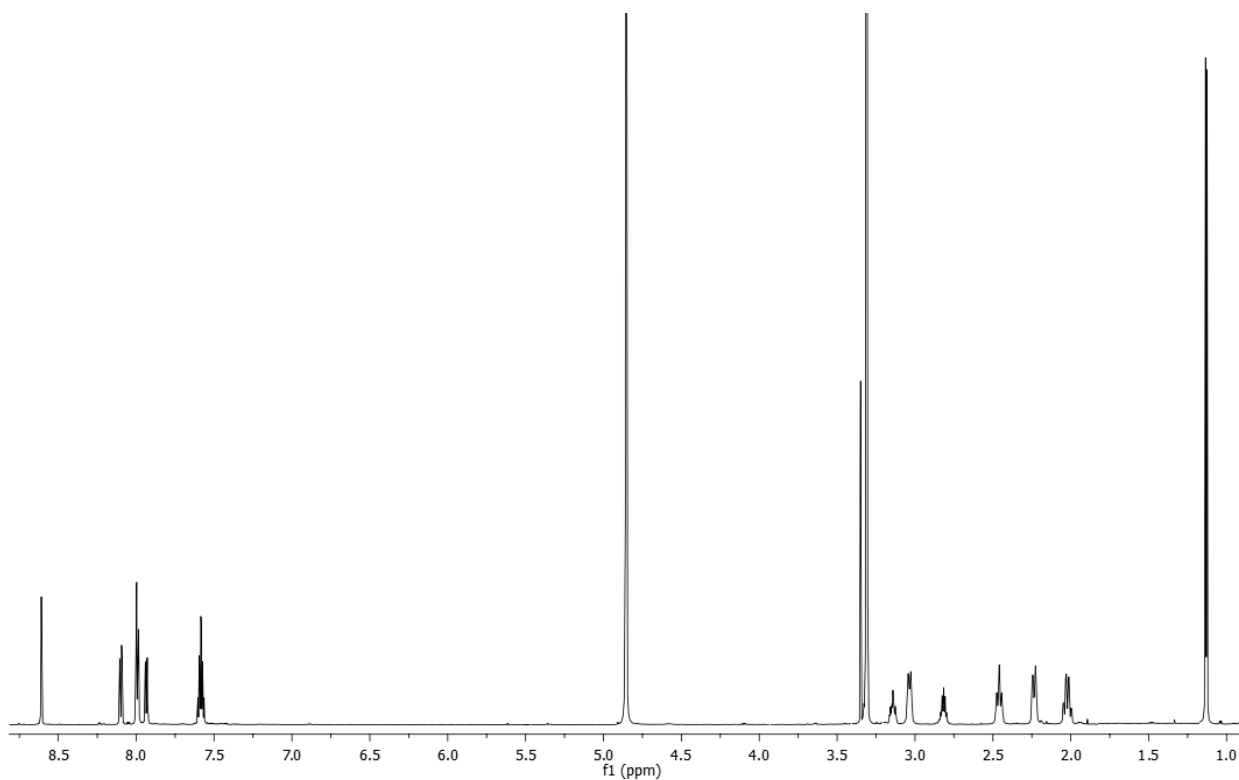
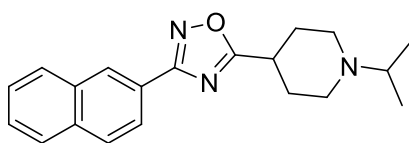


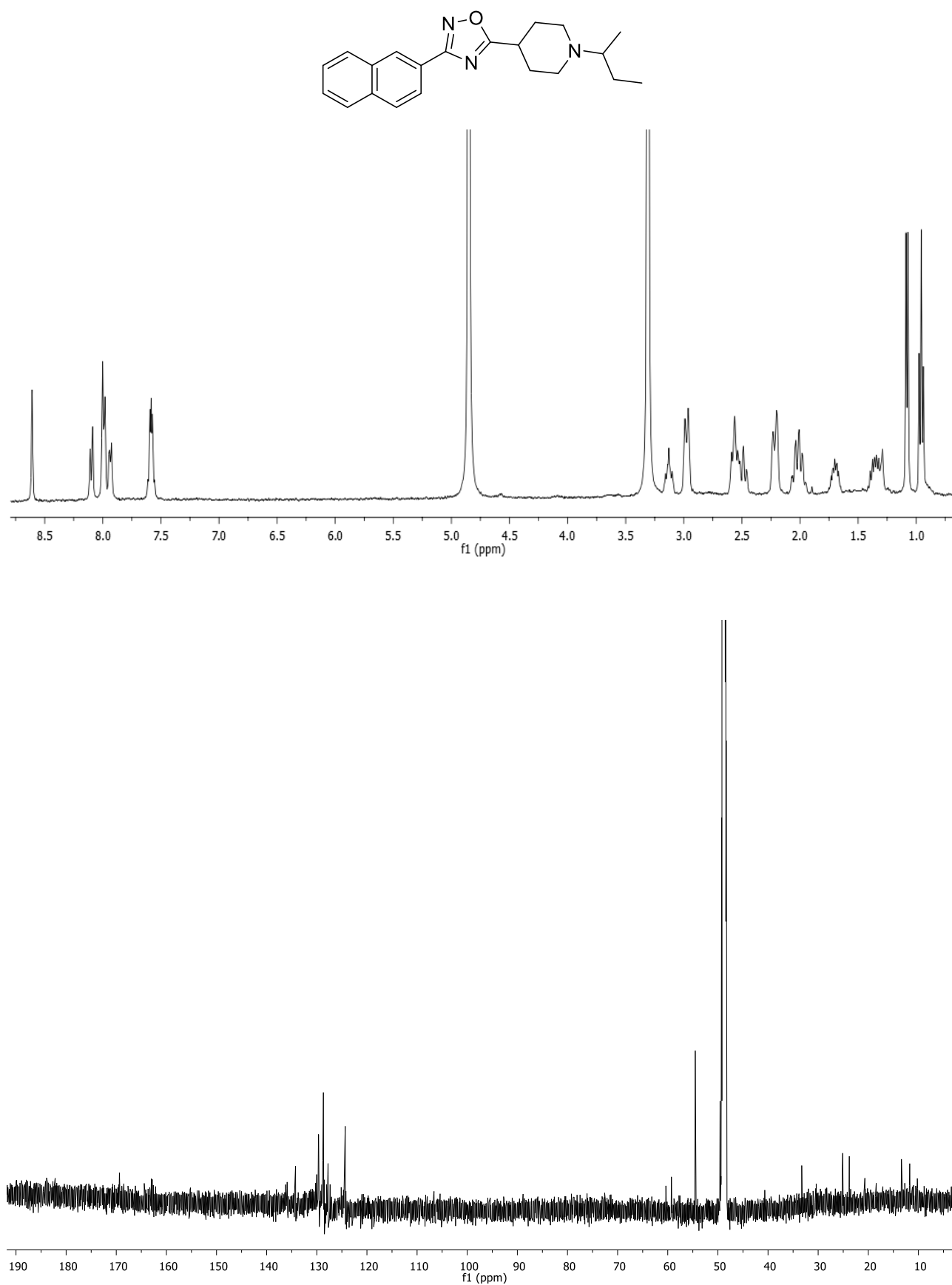
Figure S11-S12. ^1H (700 MHz) and ^{13}C NMR (175 MHz) in CD_3OD of compound **7**



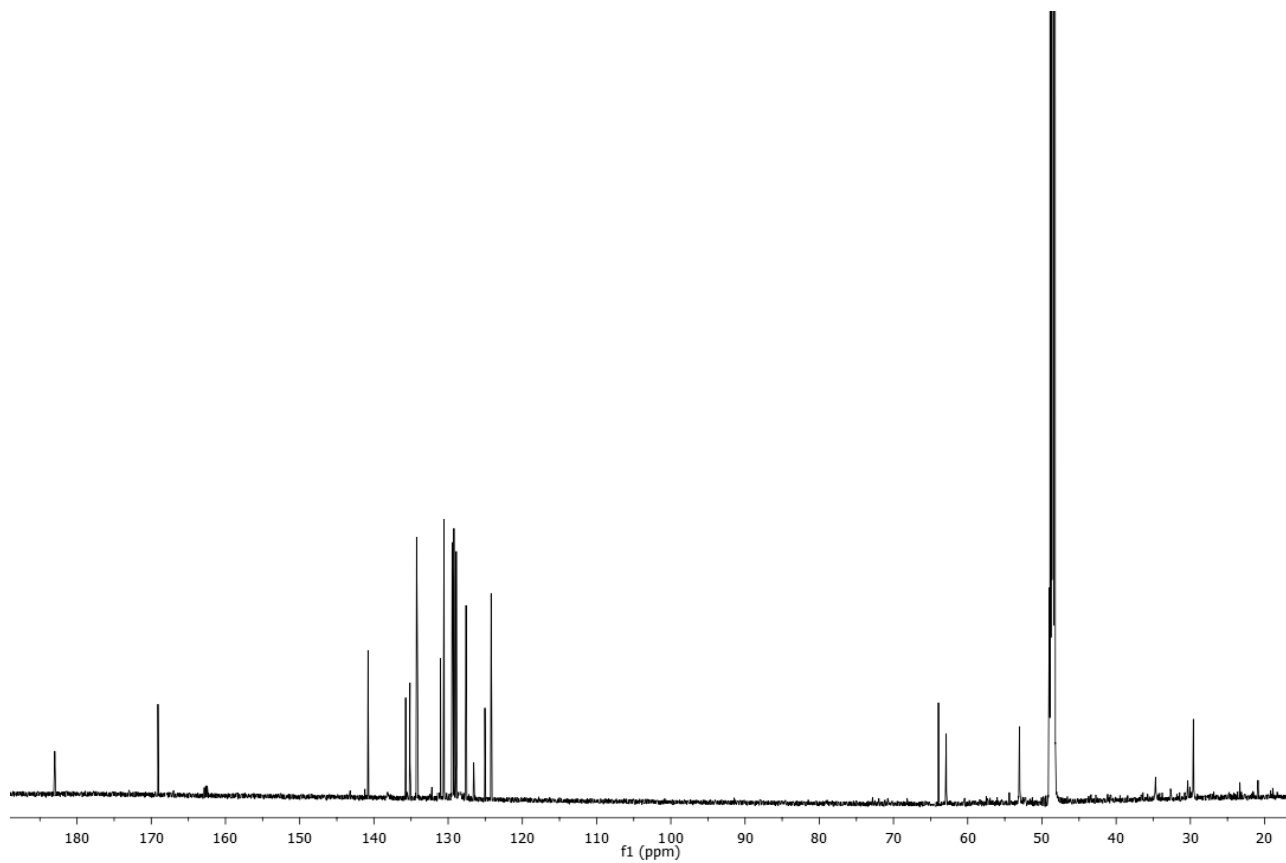
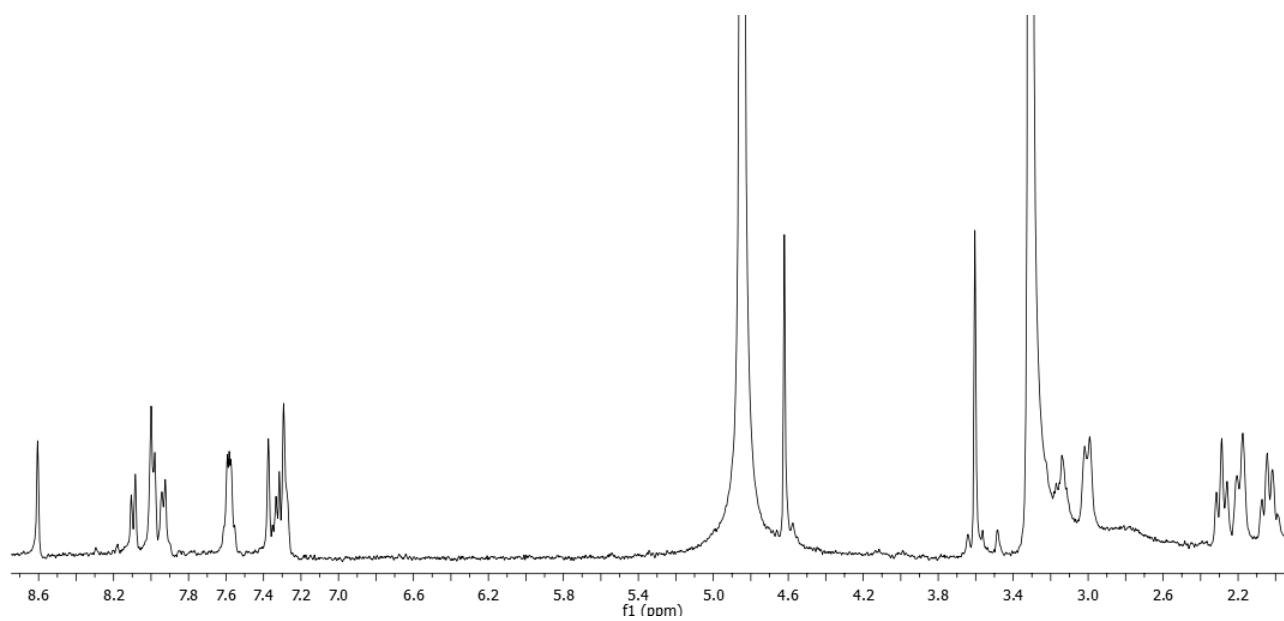
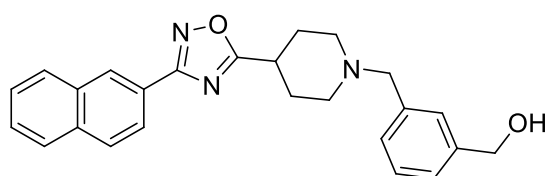
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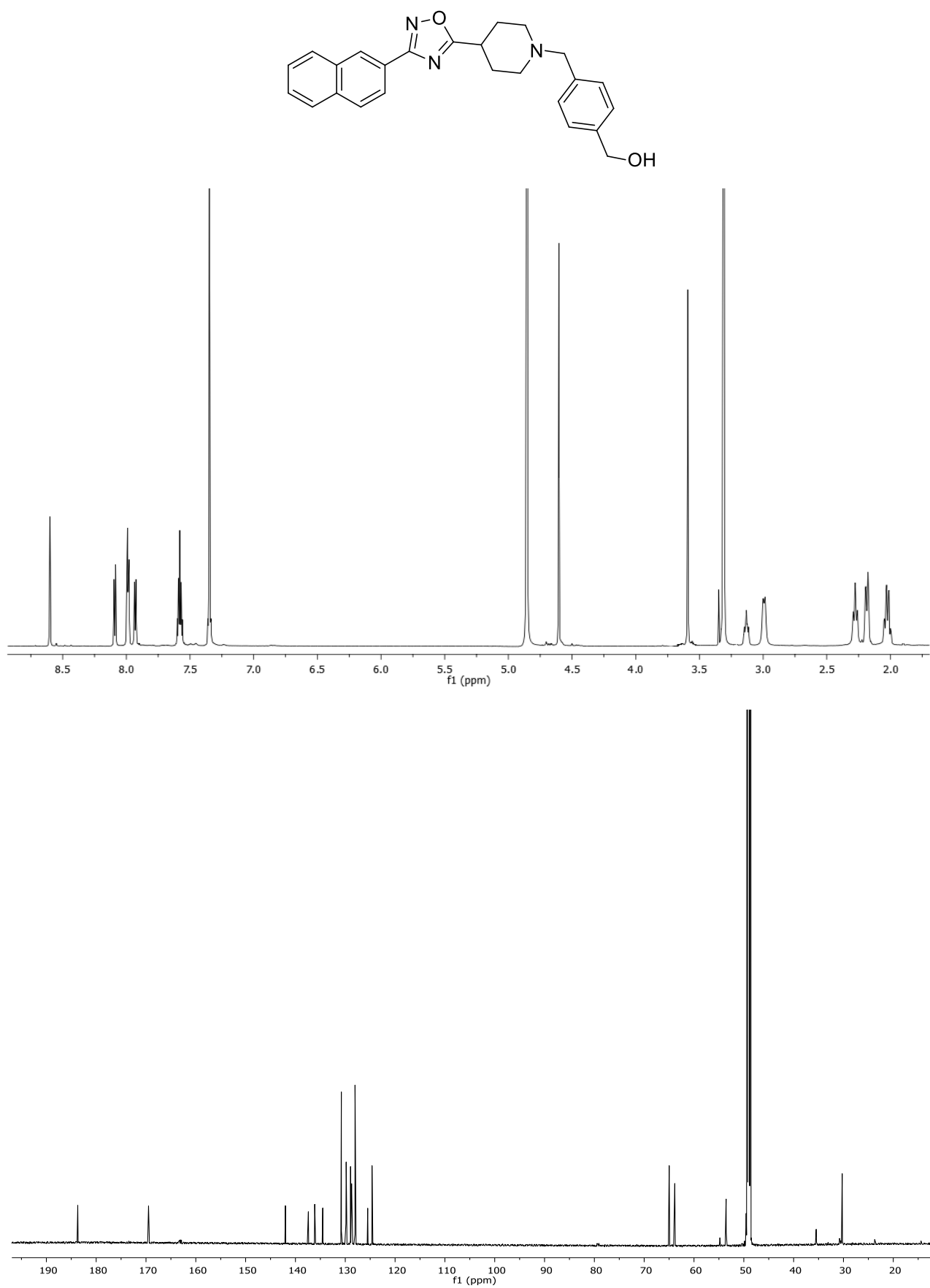
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Figures S17-18. ^1H (400 MHz) and ^{13}C NMR (100 MHz) in CD_3OD of compound **10**



Figures S19-S20. ^1H (700 MHz) and ^{13}C NMR (175 MHz) in CD_3OD of compound **11**



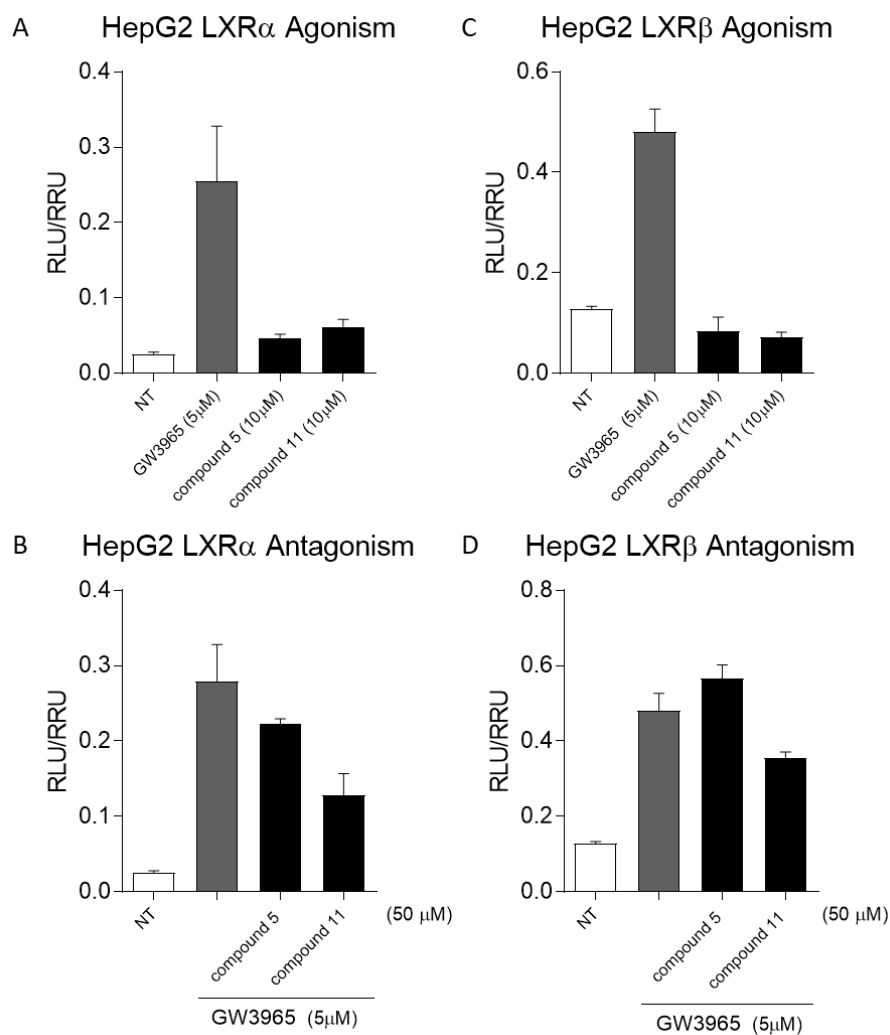


Figure S21. Activity towards LXR α and LXR β in transactivation assay in agonism and antagonism. **A** and **C**) HepG2 cells were stimulated with **GW3965** (GW, 5 μ M) as positive control and compounds **5** and **11** (10 μ M); **B** and **D**) HepG2 cells were stimulated with 50 μ M of compounds **5** and **11** in combination with the relative positive control. Results are expressed as mean $\pm$ SEM. * p < 0.05 versus not treated cells (NT).