

Supporting Information

Facile Preparation of N-Doped Graphitic Carbon Encapsulated Nickel Catalysts for Transfer hydrogenolysis of Lignin β -O-4 Model Compounds to Aromatics

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KEYWORDS: lignin β -O-4 model compounds; transfer hydrogenolysis; the encapsulated Ni; N-doped graphitic carbon shell; isopropanol

Table S1 The Ni content in various catalysts measured by ICP-OES

Catalysts	Ni content (wt%) by ICP-OES
Ni/NC-800	12.16
Ni@NC-600-H	2.67
Ni@NC-800-S	7.83
Ni/NC-800-S	10.33

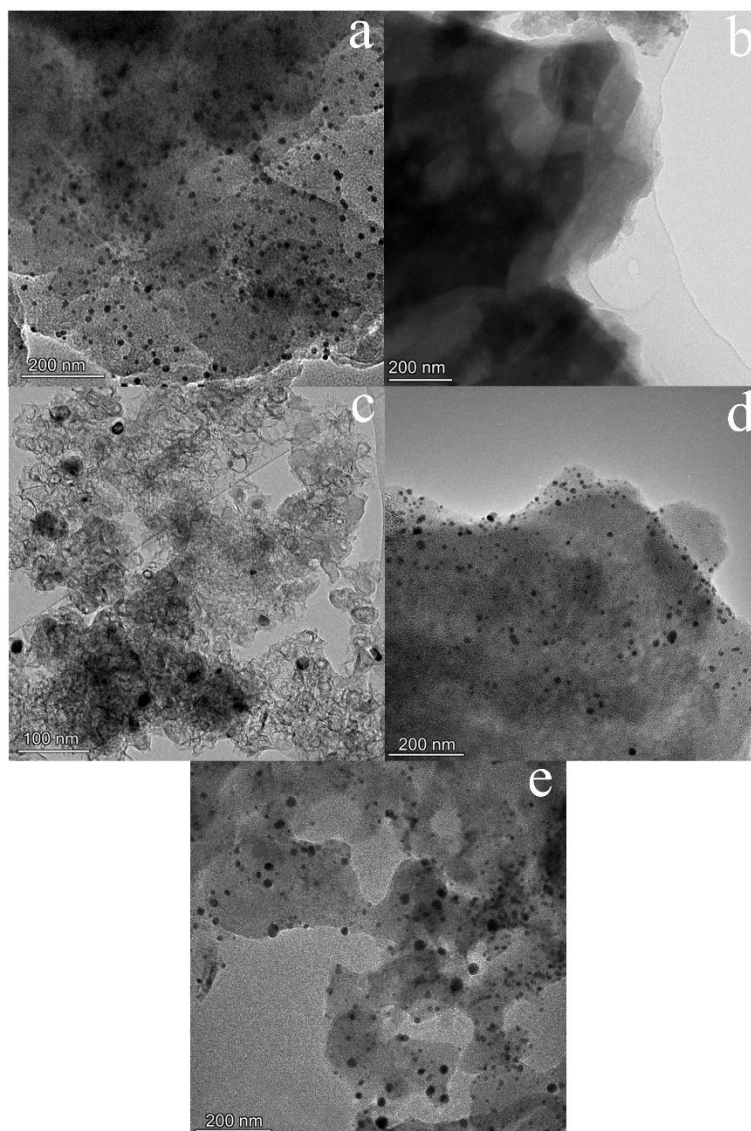


Figure S1 TEM images of Ni/NC-600 (a), Ni@NC-600-H (b), Ni@NC-800-S (c), Ni/NC-800 (d), and Ni/NC-800-S (e).

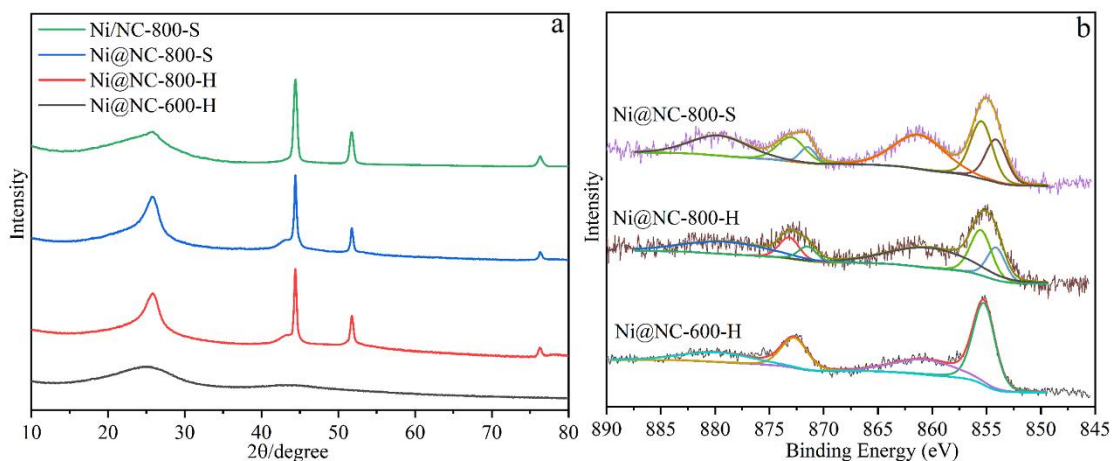


Figure S2 (a) XRD patterns of Ni@NC-600-H, Ni@NC-800-H, Ni@NC-800-S, and Ni/NC-800-S. (b) XPS Ni 2p spectra of Ni@NC-600-H, Ni@NC-800-H, and Ni@NC-800-S.

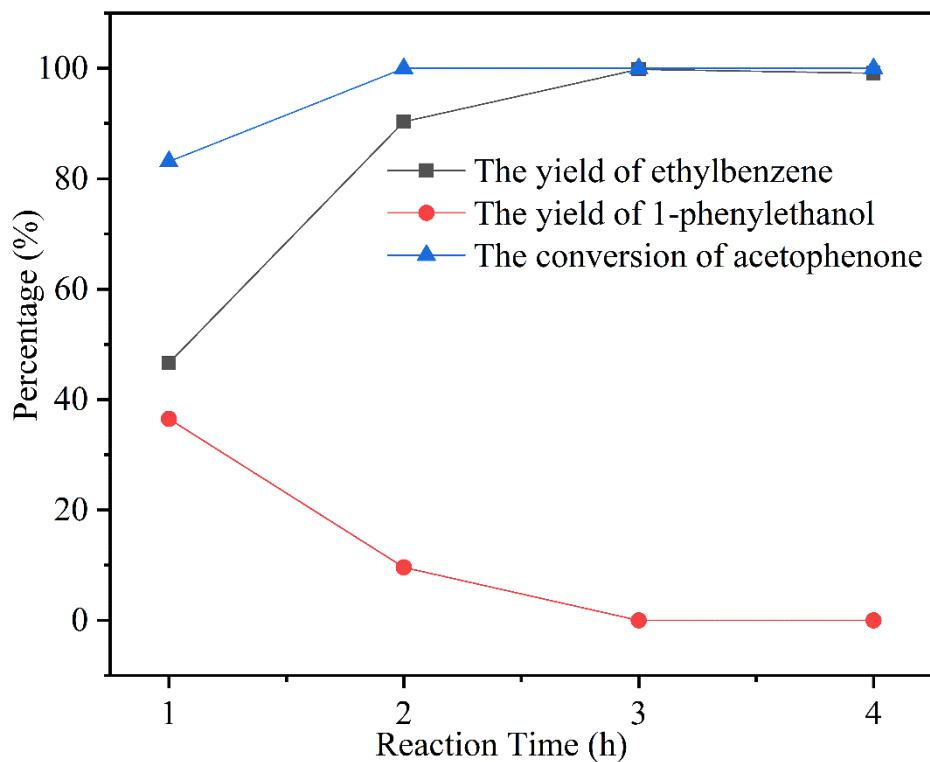


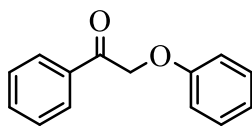
Figure S3 The effect of reaction time for the conversion of acetophenone over Ni@NC-800-H at 180 °C.

Synthesis of the β -O-4 lignin alcohol and ketone model compounds and detailed NMR characterizations

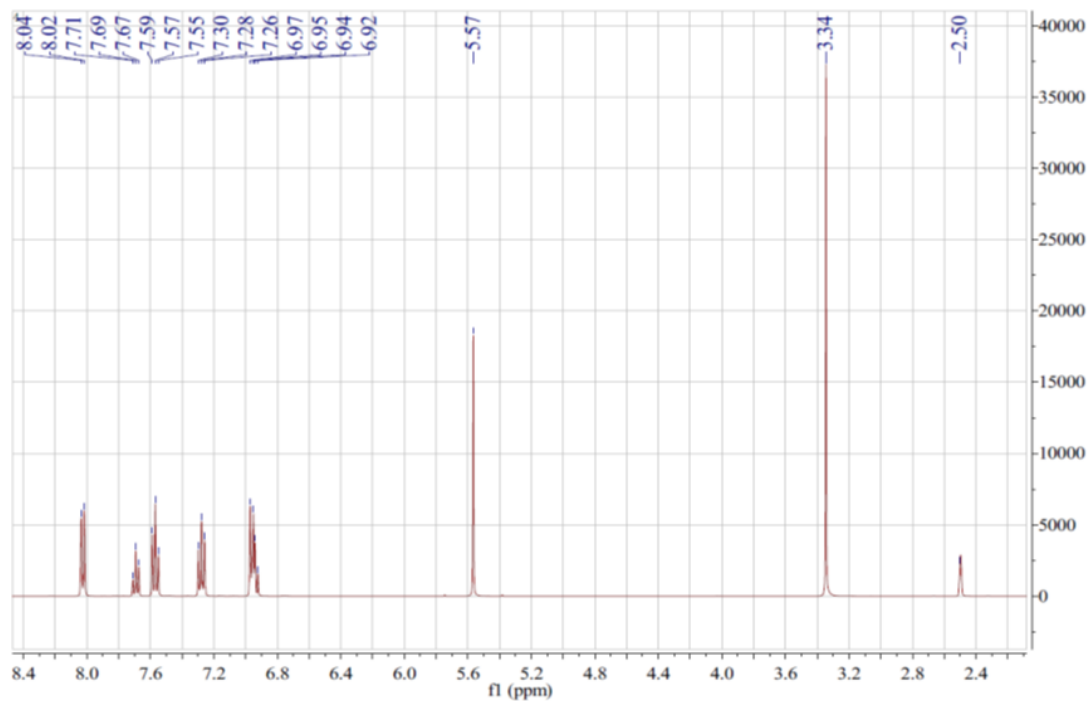
For the synthesis of 2-phenoxy-1-phenylethanone, a 150 mL round bottom flask equipped with a reflux condenser and a dropping funnel was charged with phenol (0.591 g, 6.28 mmol), 2-bromoacetophenone (1.000 g, 5.02 mmol) and K_2CO_3 (1.040 g, 7.54 mmol) in acetone (50 mL). The resulting suspension was stirred under reflux for 5 h, after the suspension was filtered and concentrated in vacuum. The crude product was purified by recrystallization from hexane/ethyl acetate solvent (100 mL, 3:1 Volume ratio) to give 2-phenoxy-1-phenylethanone as a white solid. For the synthesis of 2-phenoxy-1-phenethanol, A round bottom flask was charged with 2-phenoxy-1-phenylethanone (1.00 g, 4.71 mmol) in THF/ H_2O solvent (25 mL, 4:1 Volume ratio). Sodium borohydride (0.39 g, 10.41 mmol) was added to the solution in small portions at room temperature. After stirring for 6 h, the suspension was quenched with saturated aqueous NH_4Cl , followed by the addition of ethyl acetate. After separation, the organic phase was washed with H_2O , dried over Anhydrous $MgSO_4$, filtered and the solvent was evaporated under vacuum. The crude product was purified by recrystallization from hexane to give a white crystalline. For the other methoxyl substituted 2-phenoxy-1-phenylethanone and 2-phenoxy-1-phenethanol, the preparation procedure is the same as described above, except that using different starting materials. In addition, for the synthesis of 1-(3,4-dimethoxyphenyl)-3-hydroxy-2-(2-methoxyphenoxy)propan-1-one, K_2CO_3 (1.2 g, 8.6 mmol) and 1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy)ethanone (2.4 g, 8 mmol) were added in

ethanol: acetone (v/v=1:1, 40 mL) mixed solvent in a 100 mL round bottom flask under stirring at room temperature, then formaldehyde (36.5-38%) (1.2 mL, 14.6 mmol) was added and stirred for 4 h. subsequently, the reaction mixture was concentrated under vacuum to get a solid product. The solid was purified by column chromatography (pentane/ethyl acetate, 1:1) to yield 1-(3,4-dimethoxyphenyl)-3-hydroxy-2-(2-methoxyphenoxy)propan-1-one as yellow solid (2.40 g, 7.2 mmol) with 90% yield. For 1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol and guaiacylglycerol- β -guaiacyl ether, they are purchased from Aladdin reagent company (Shanghai, China). The NMR spectra of all above compounds, which were in accordance with theoretically predicted, were shown in below.

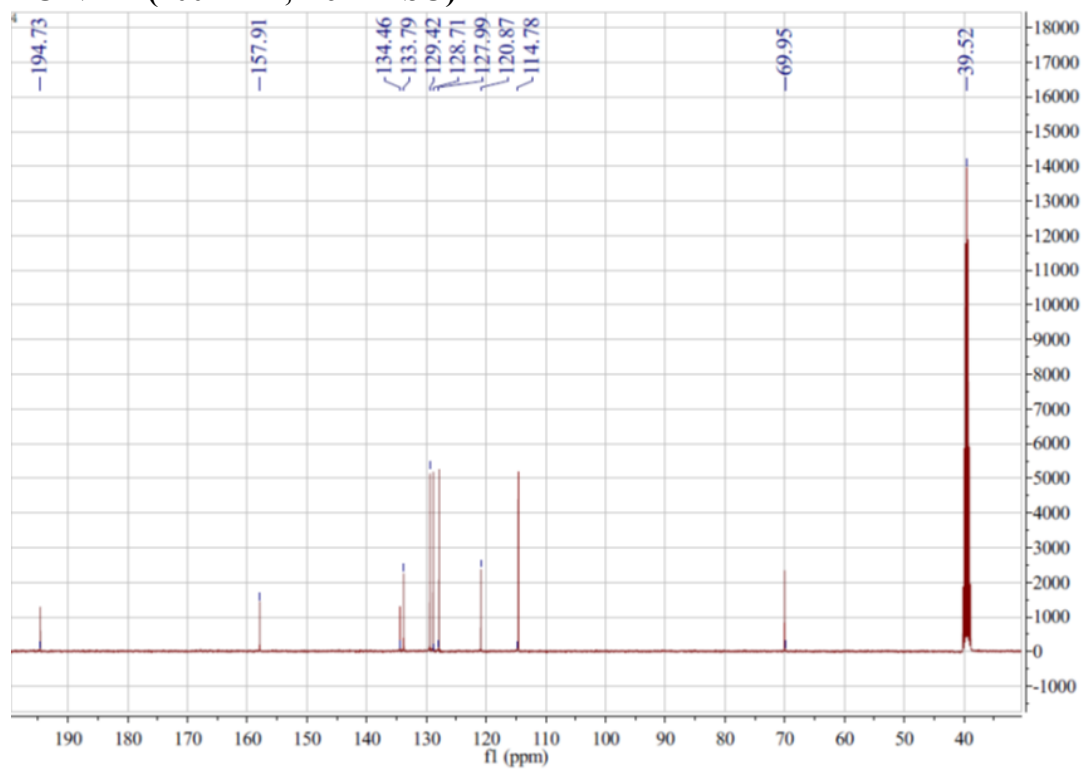
2-phenoxyacetophenone



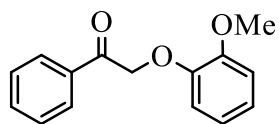
¹H NMR (400 MHz, D6-DMSO)



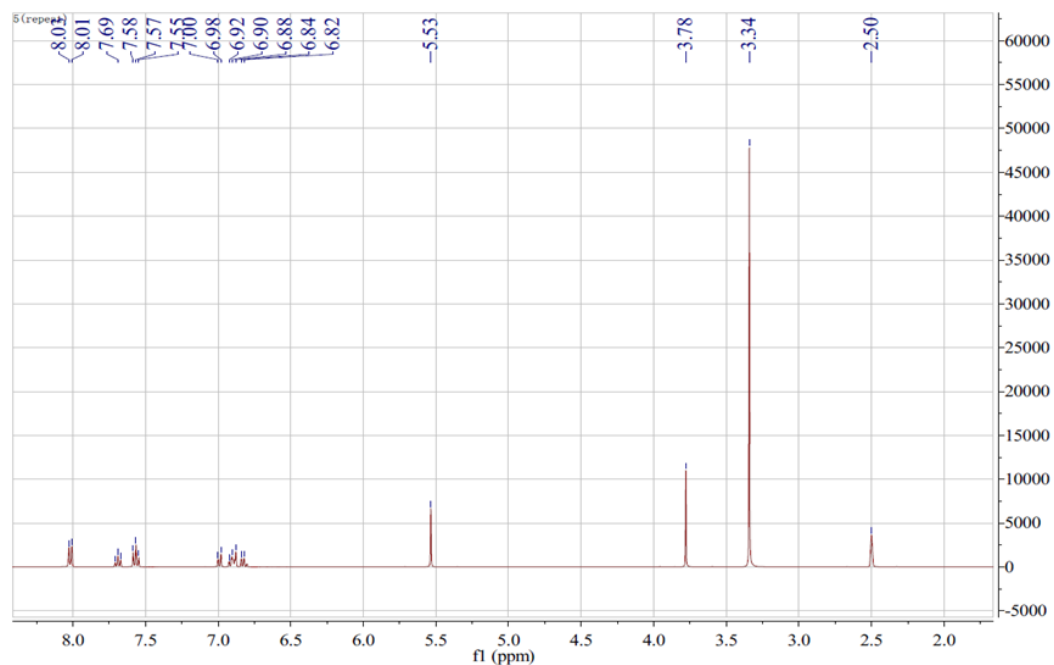
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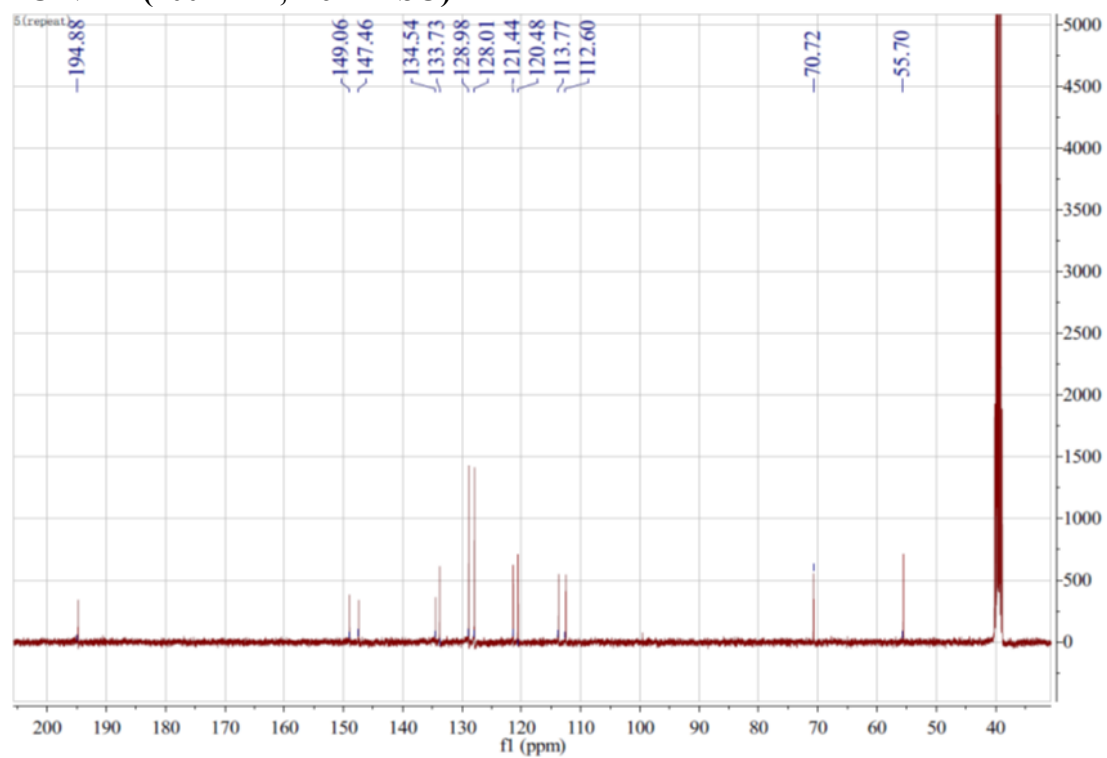
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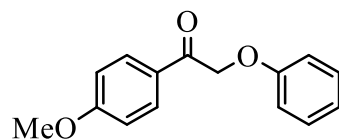
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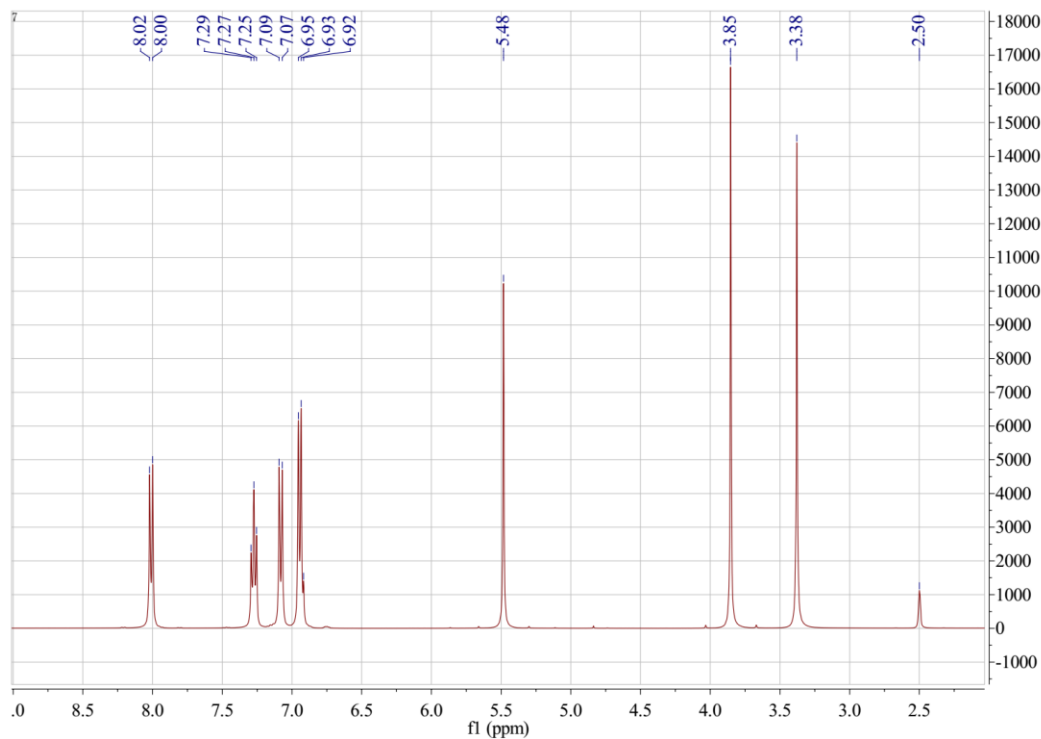
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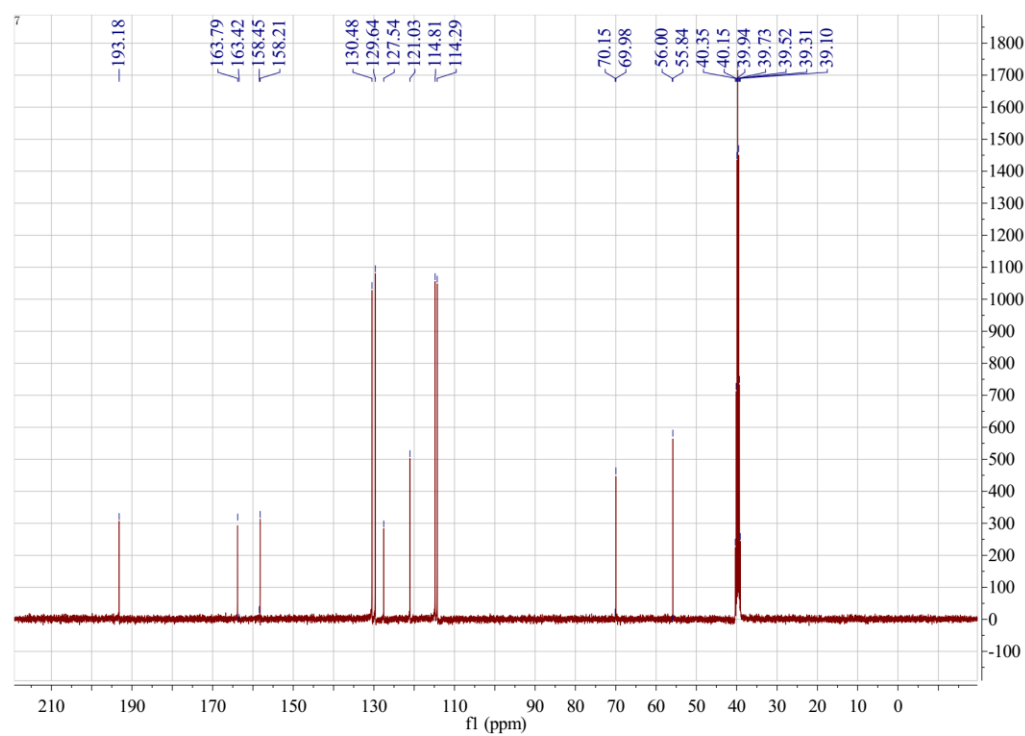
1-(4-methoxyphenyl)-2-phenoxyethan-1-one



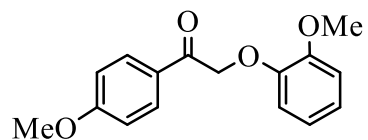
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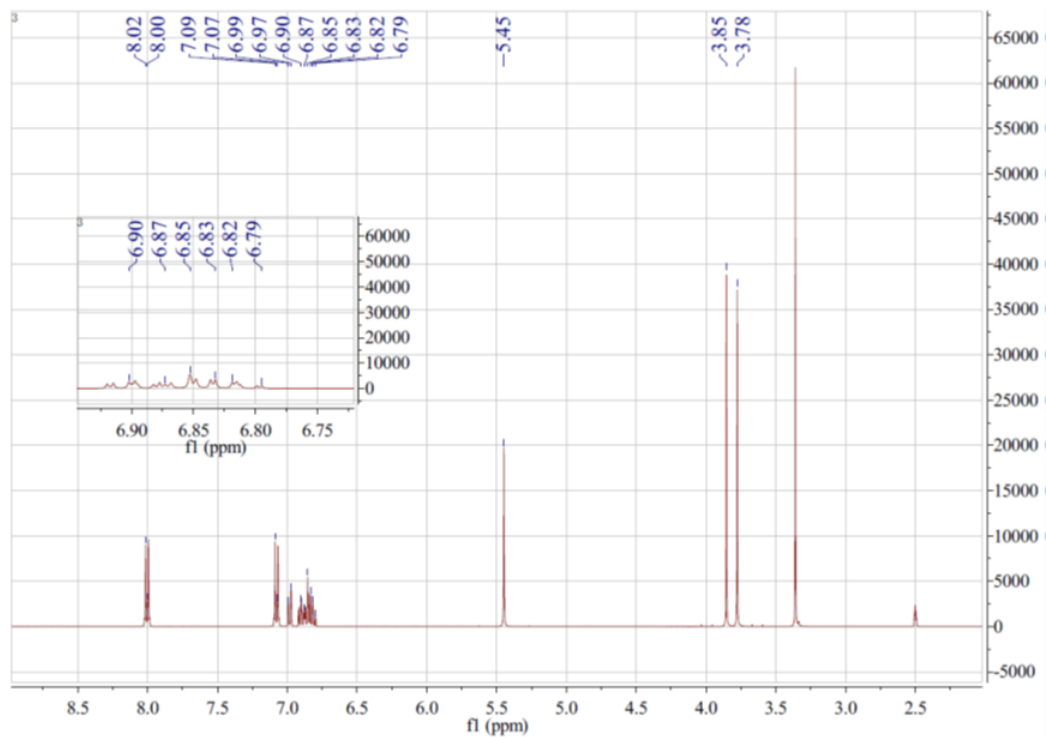
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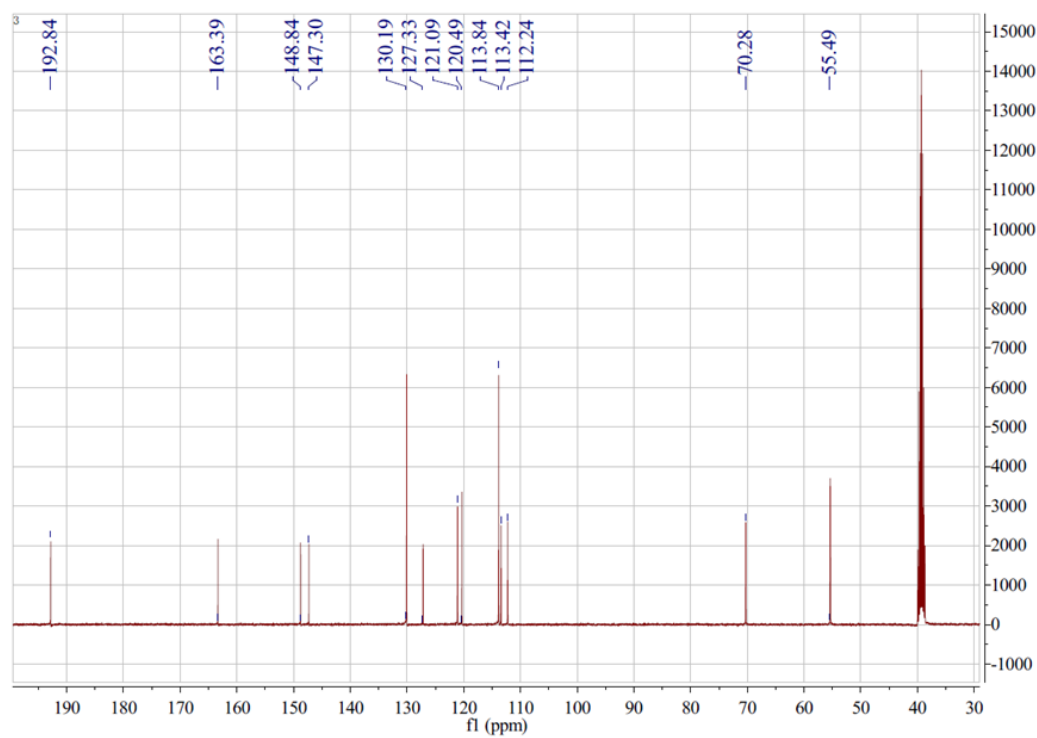
2-(2-methoxyphenoxy)-1-(4-methoxyphenyl)ethan-1-one



¹H NMR (400 MHz, D6-DMSO)

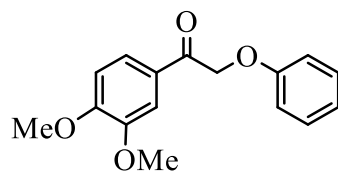


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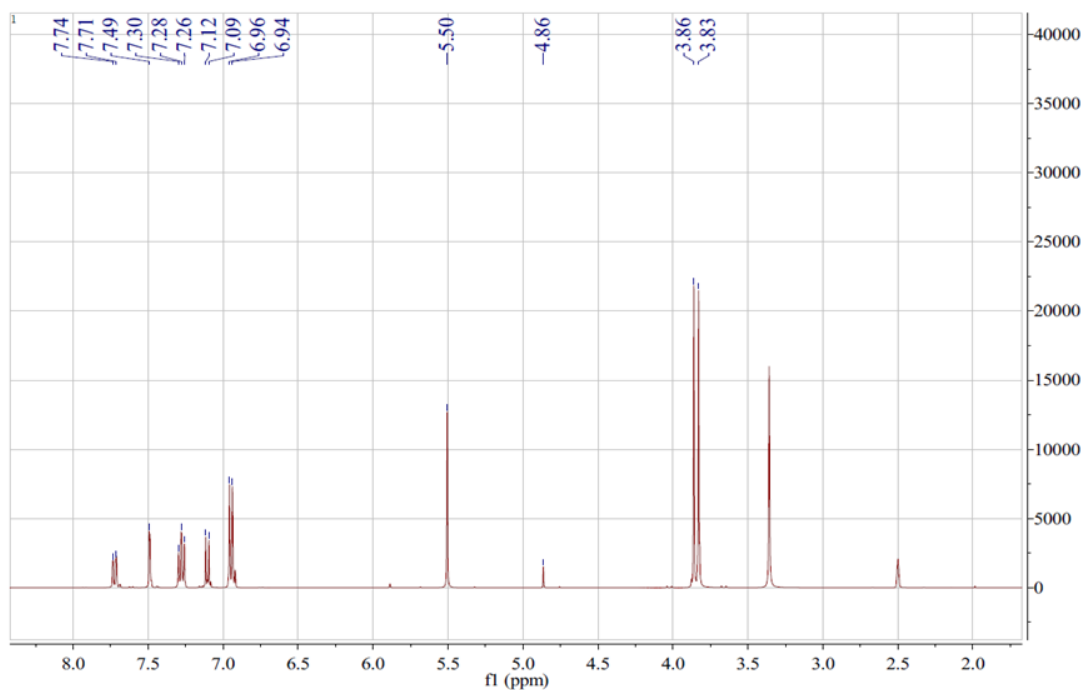


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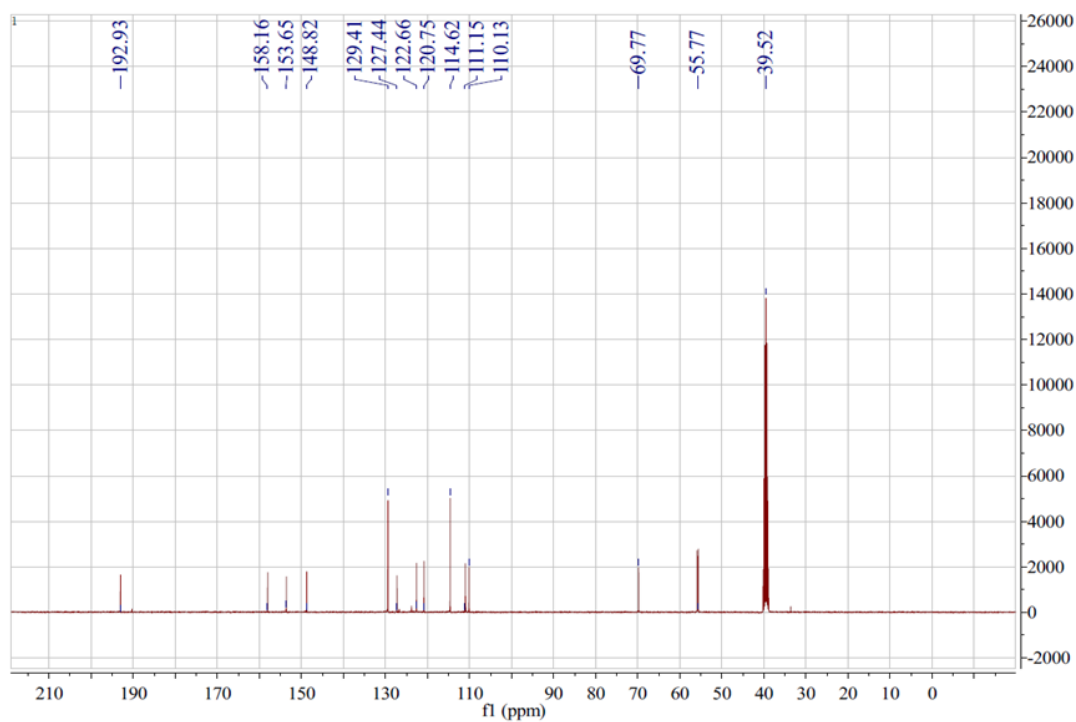
(3,4-dimethoxyphenyl)-2-phenoxyethan-1-one



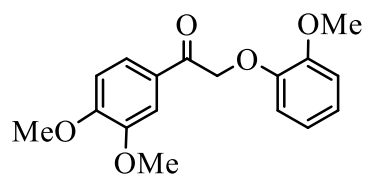
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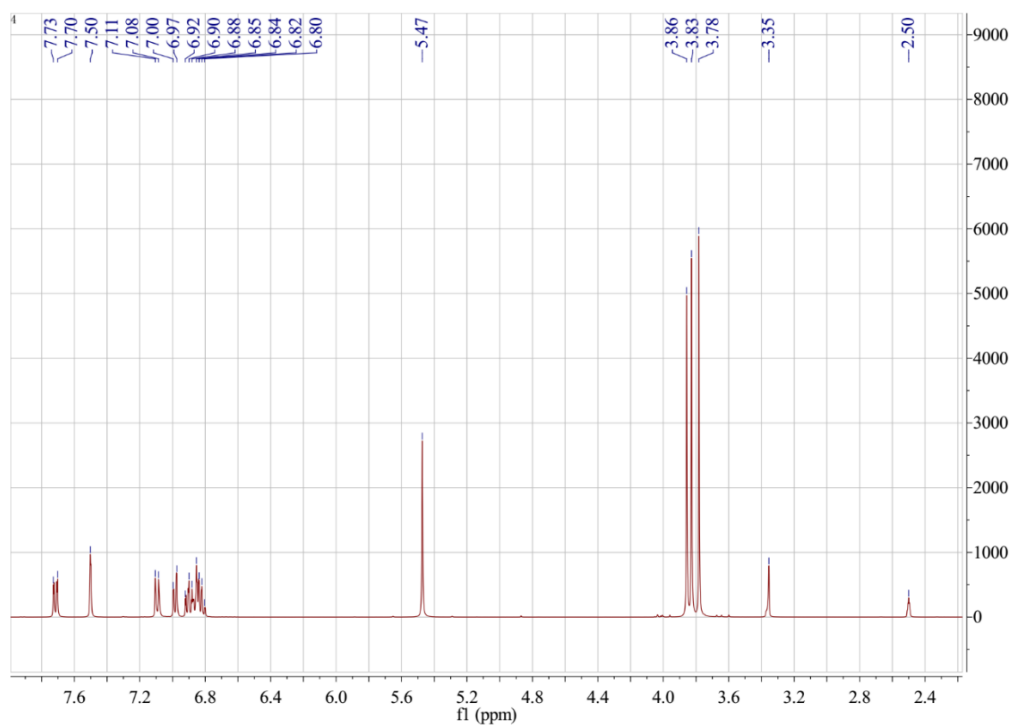
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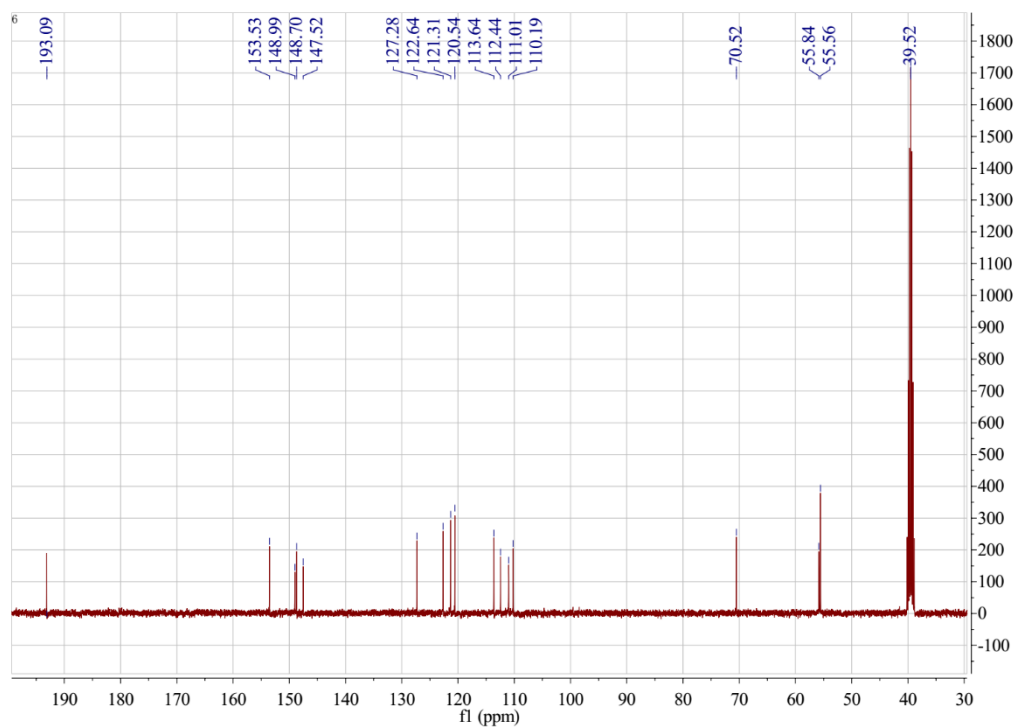


^1H NMR (400 MHz, D₆-DMSO)

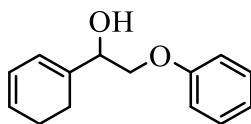


^{13}C

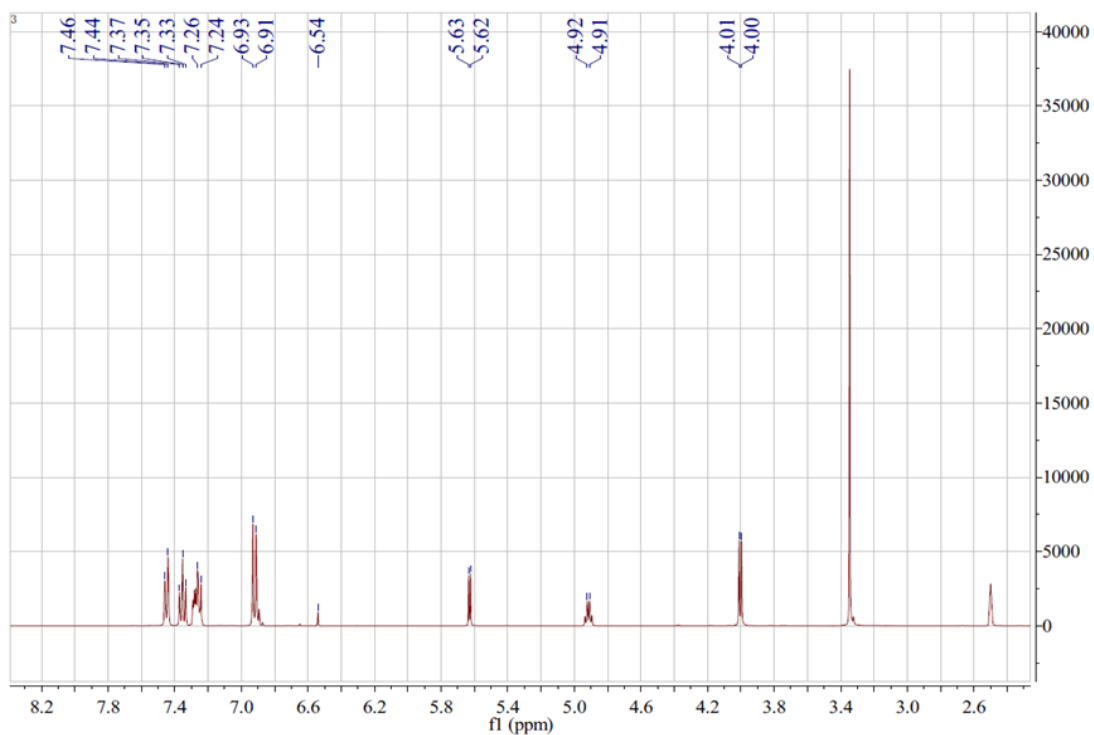
NMR (400 MHz, D₆-DMSO)



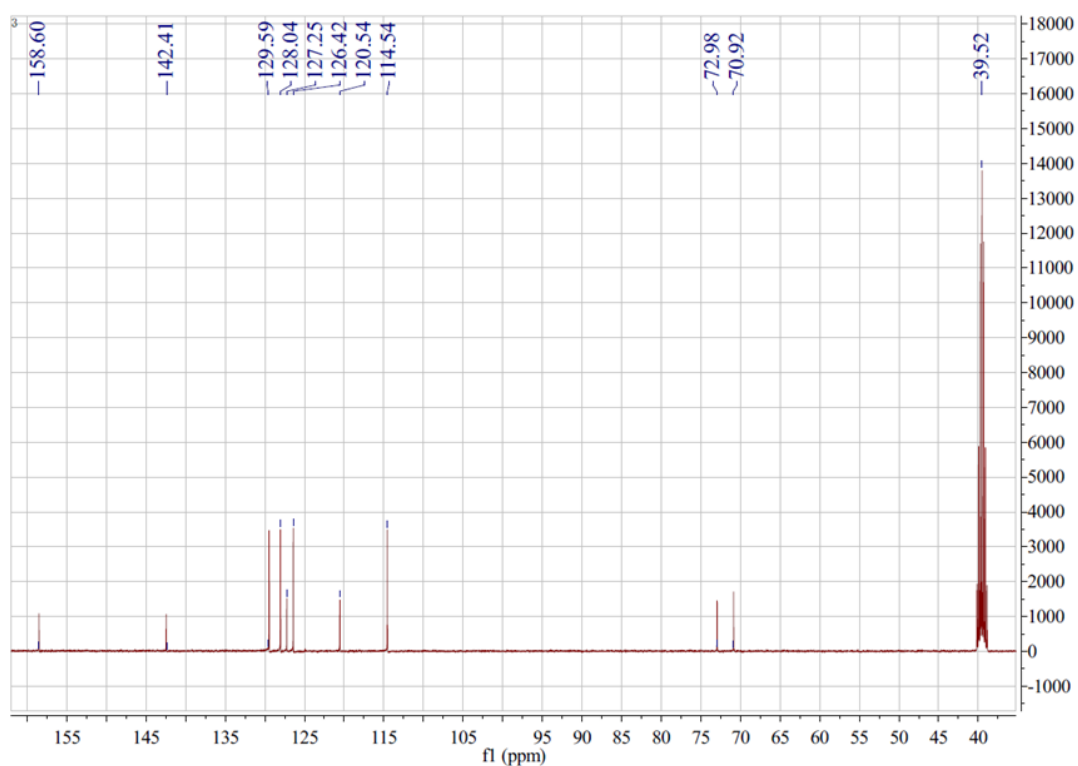
2-phenoxy-1-phenylethanol



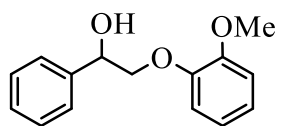
^1H NMR (400 MHz, D6-DMSO)



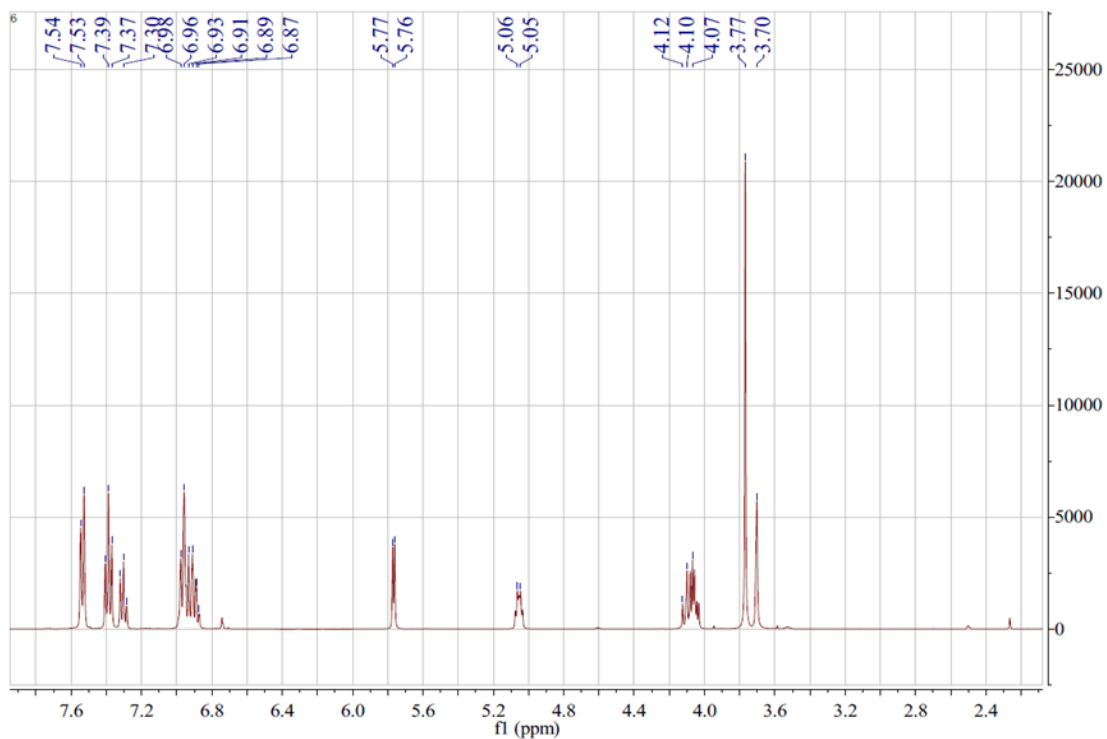
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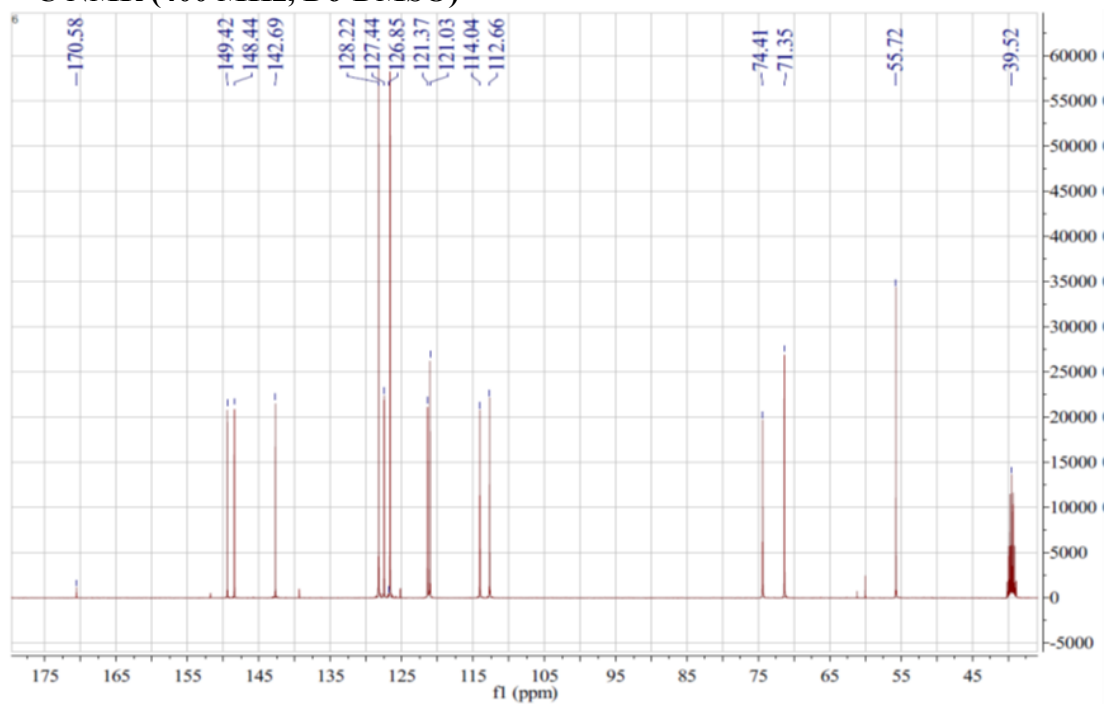
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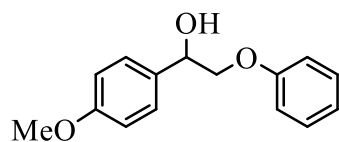
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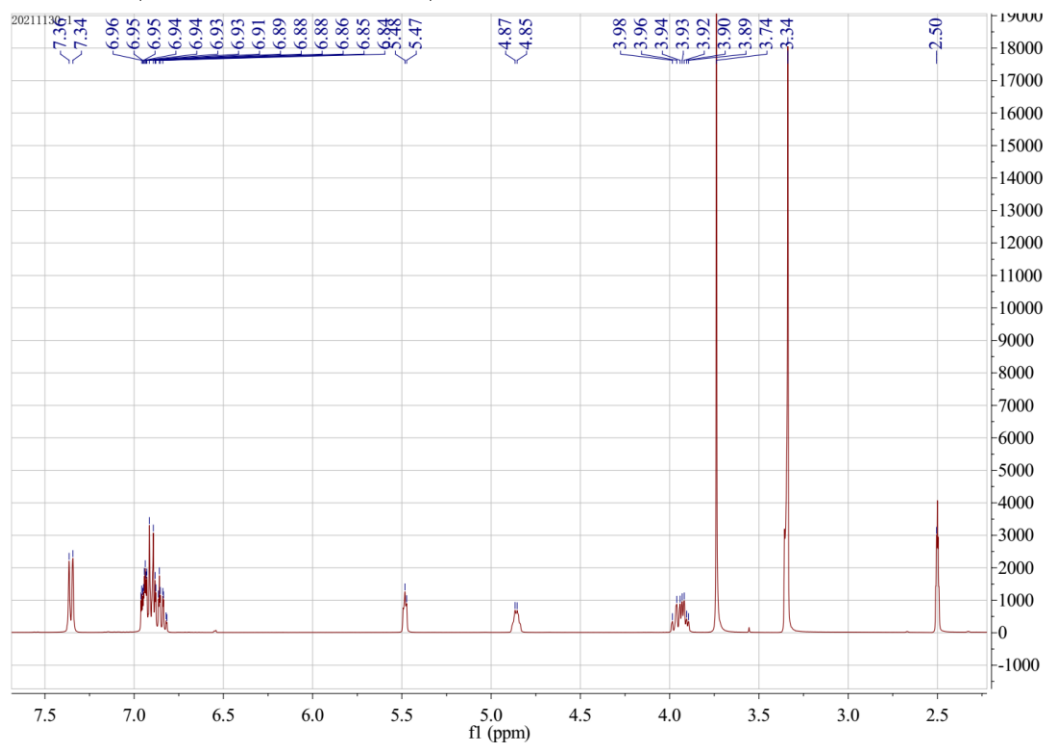
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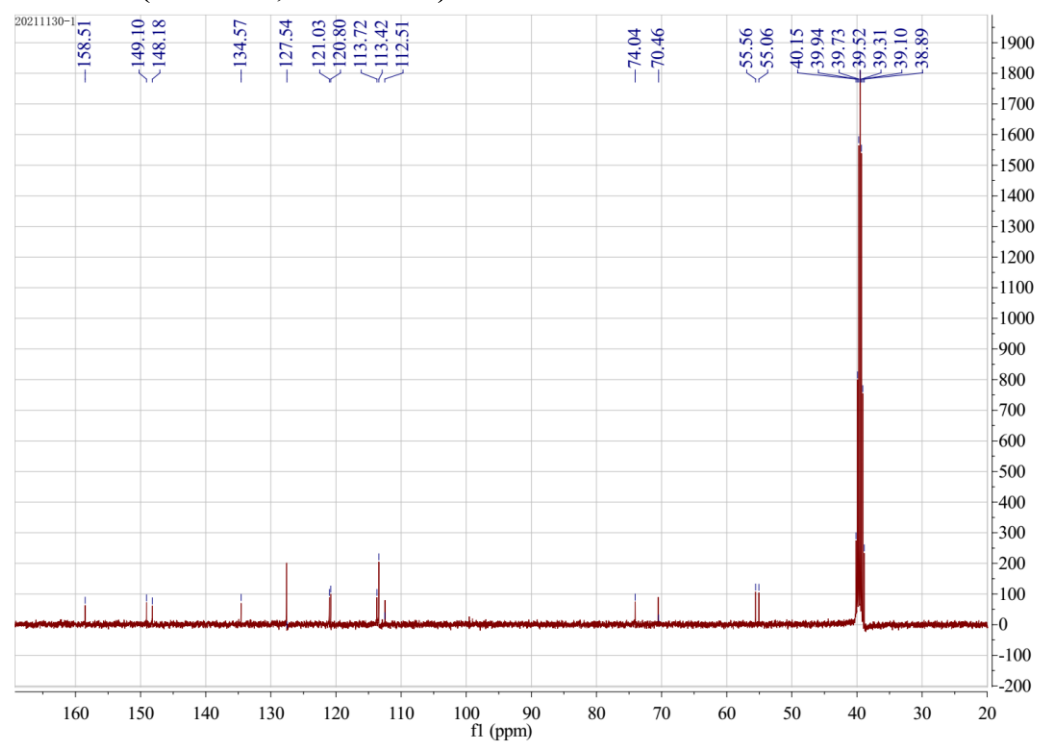
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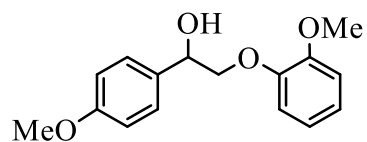
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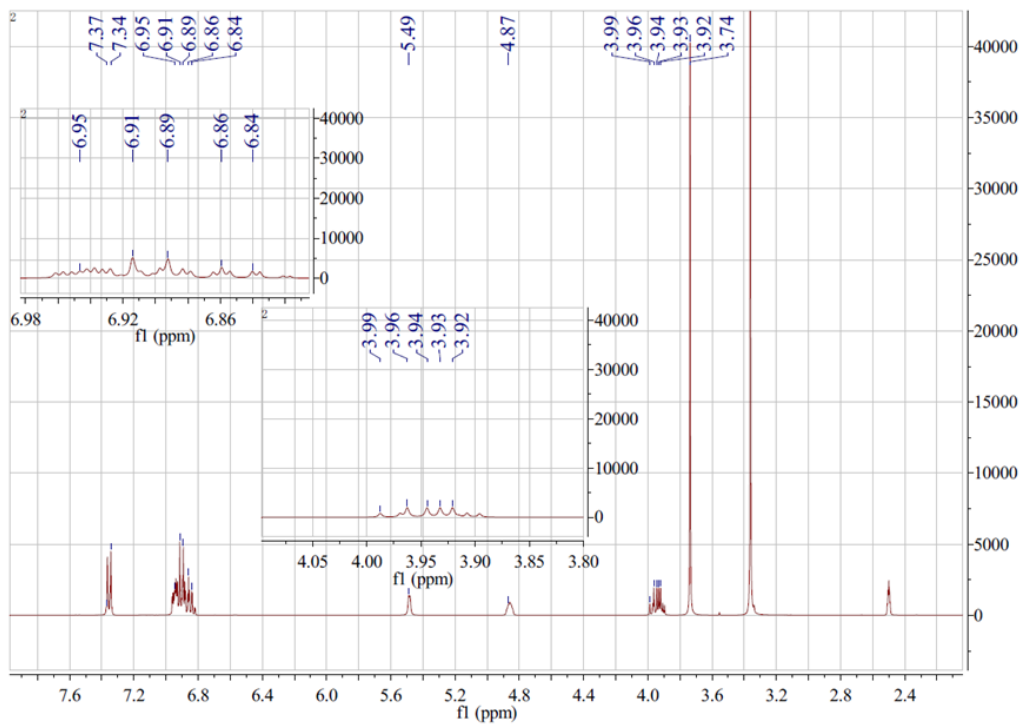
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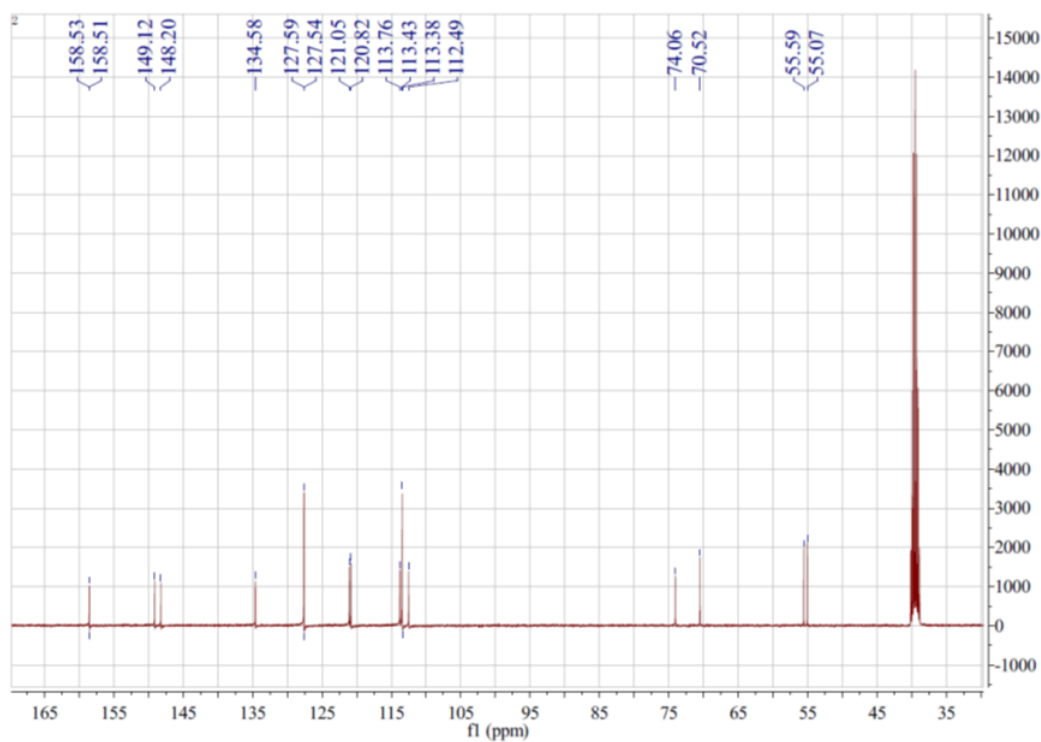
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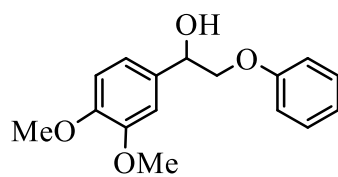
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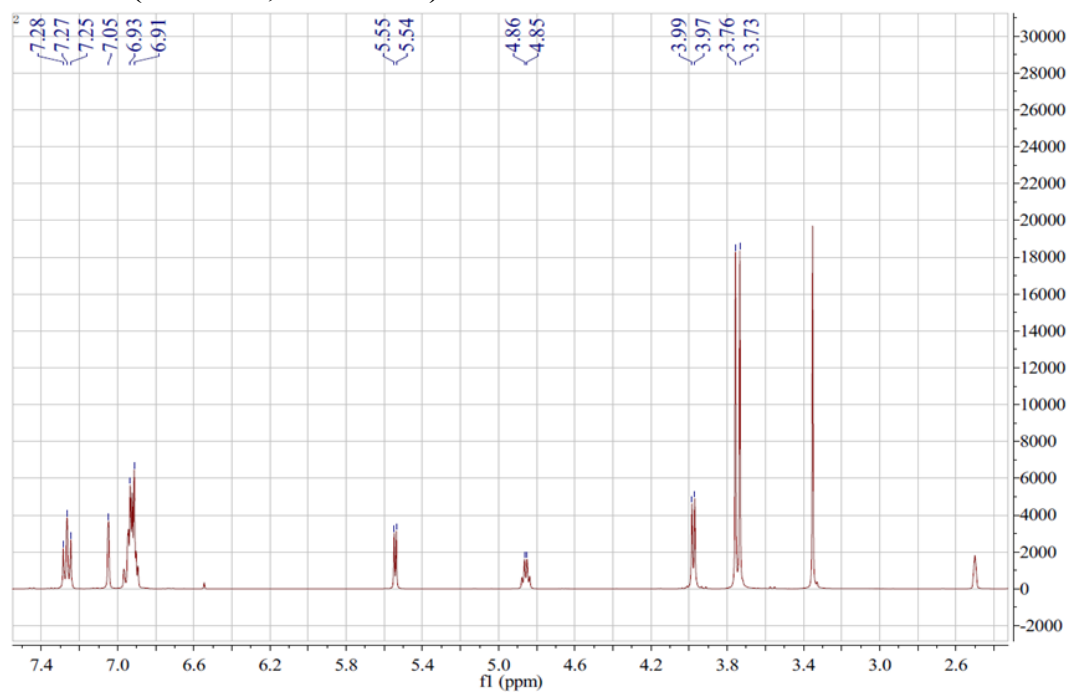
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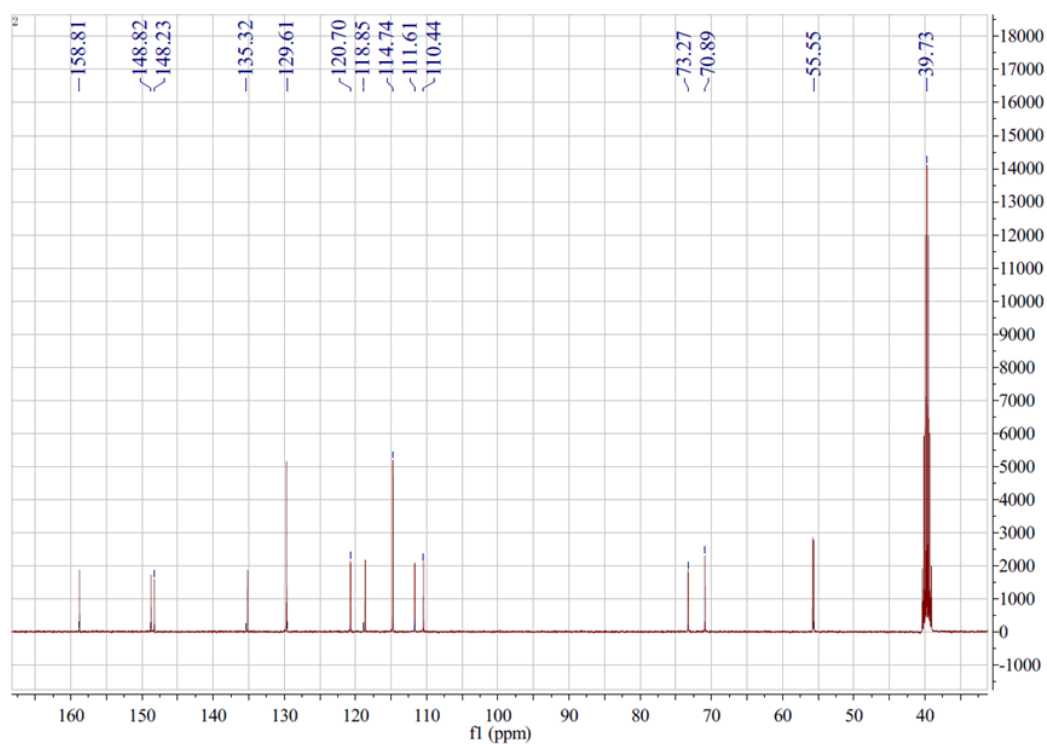
1-(3,4-dimethoxyphenyl)-2-phenoxyethan-1-ol



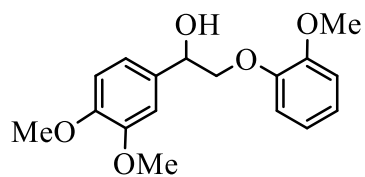
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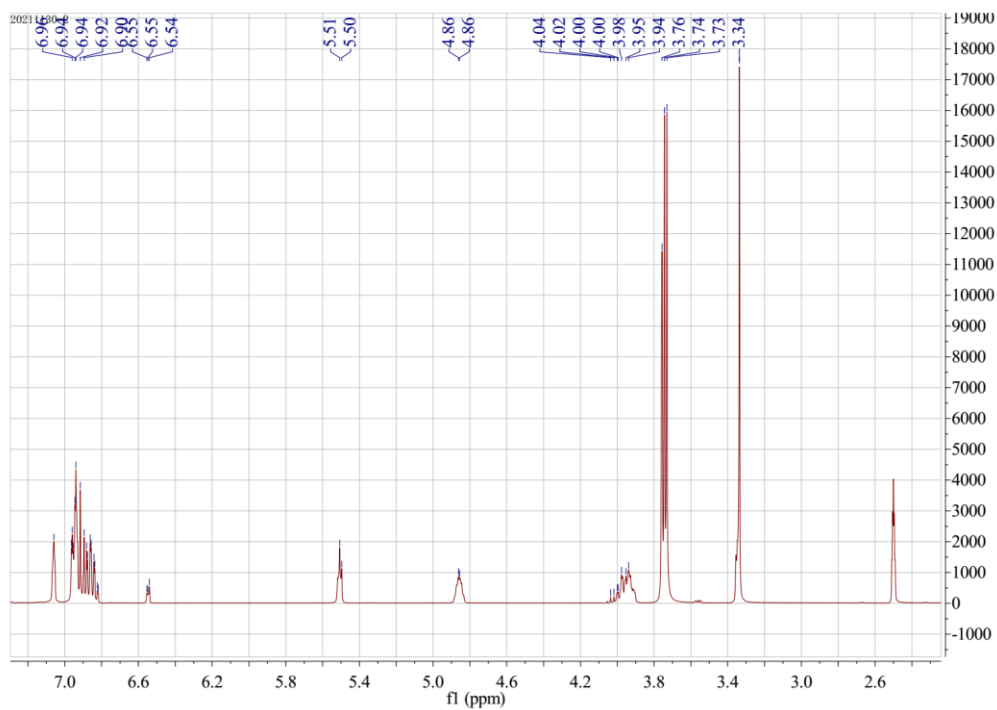
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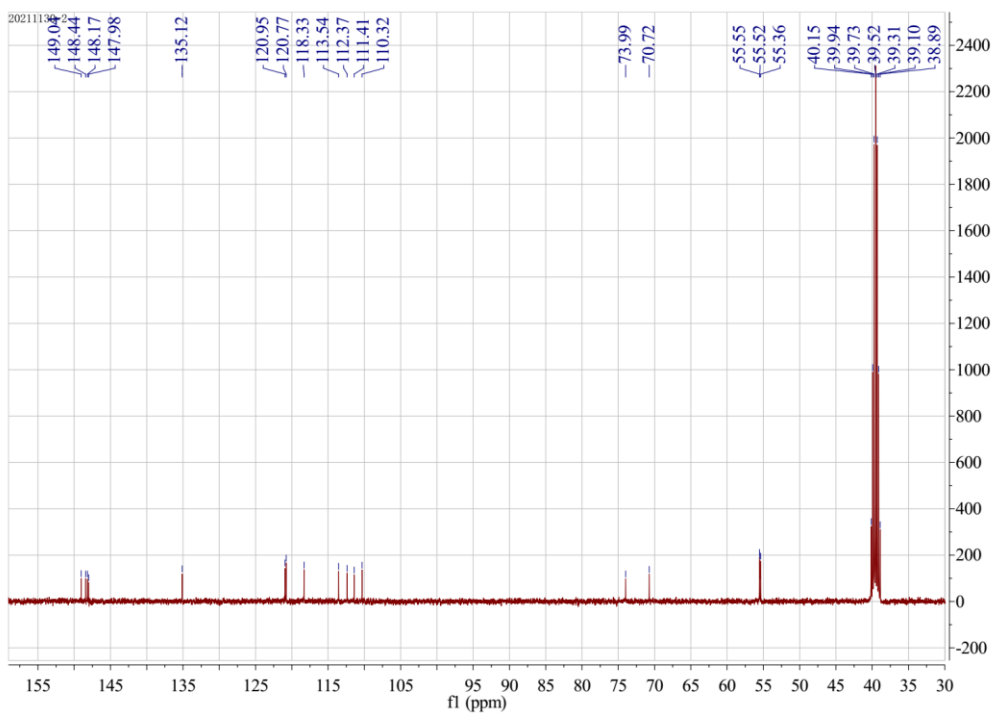
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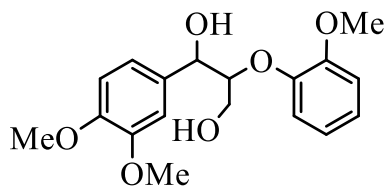
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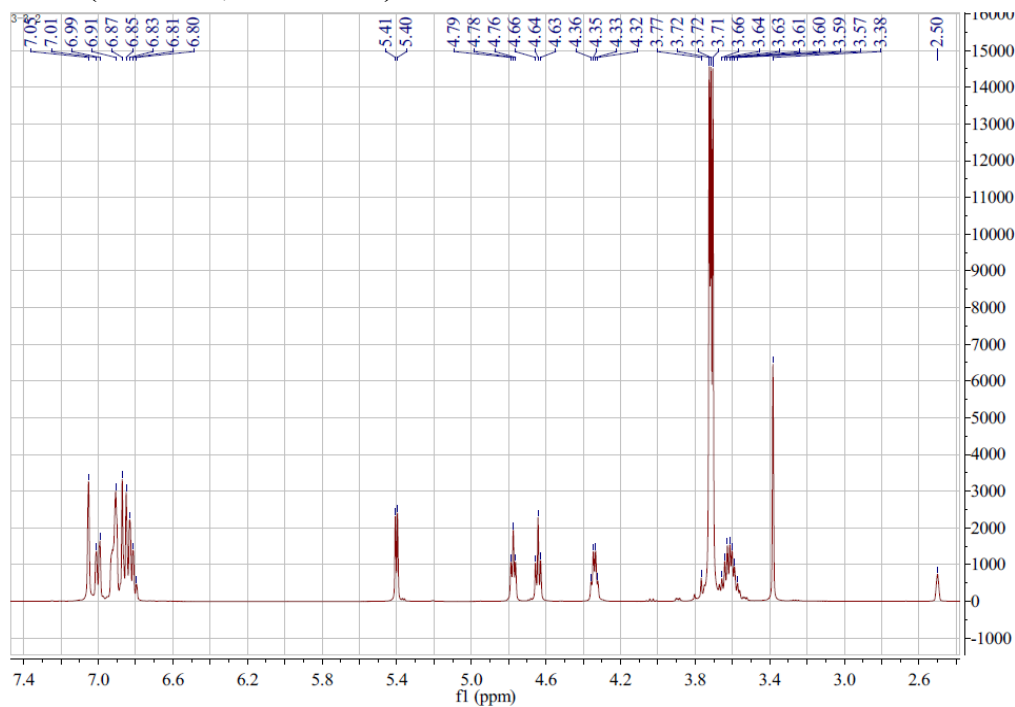
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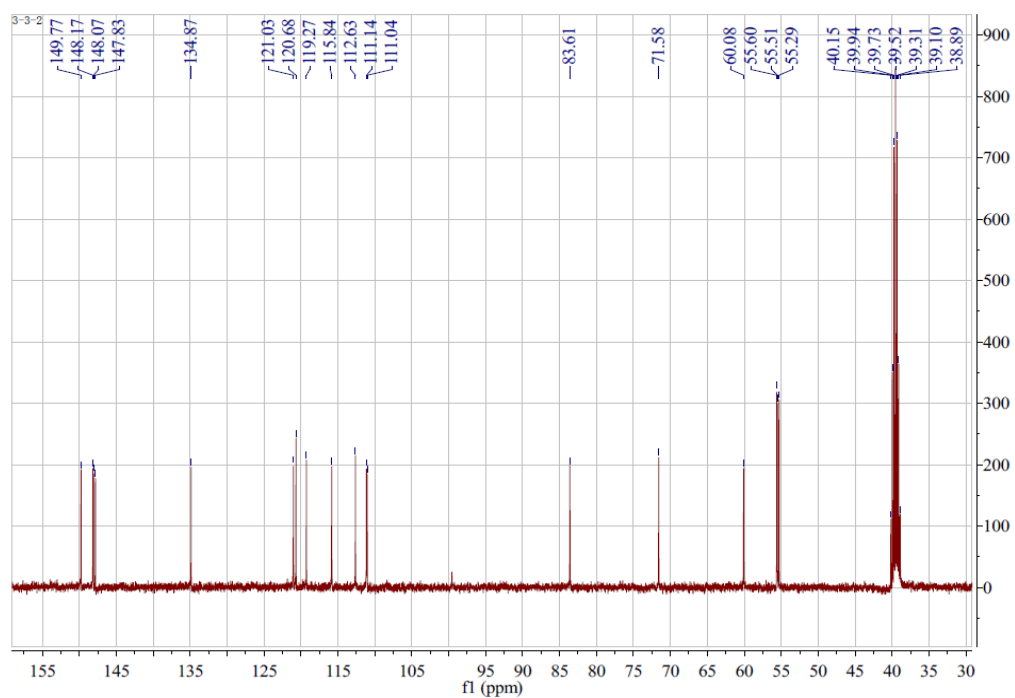
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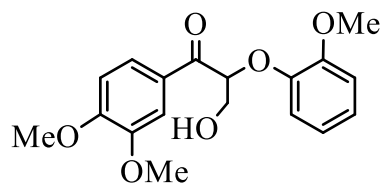
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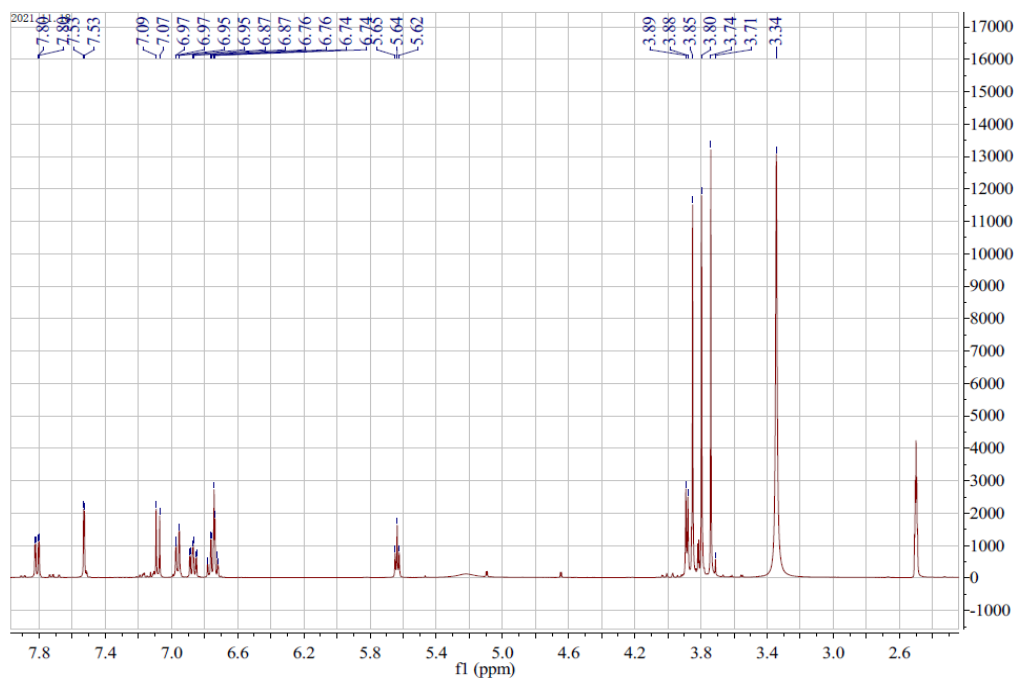
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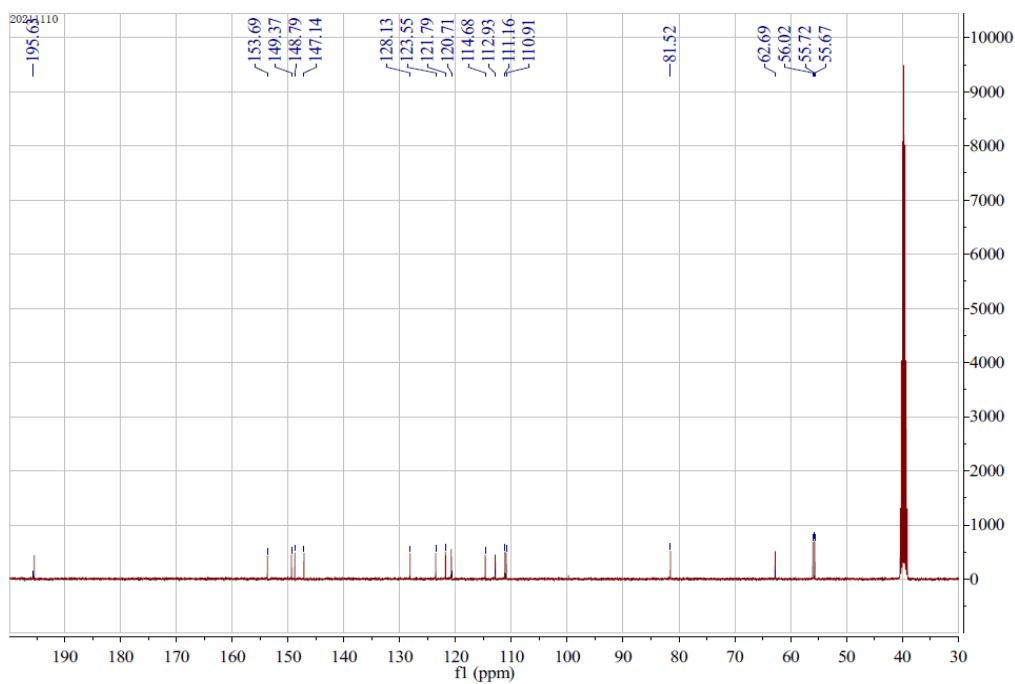
1-(3,4-dimethoxyphenyl)-3-hydroxy-2-(2-methoxyphenoxy)propan-1-one



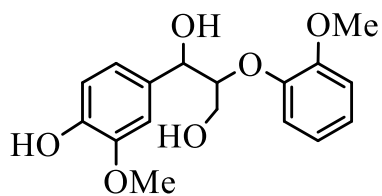
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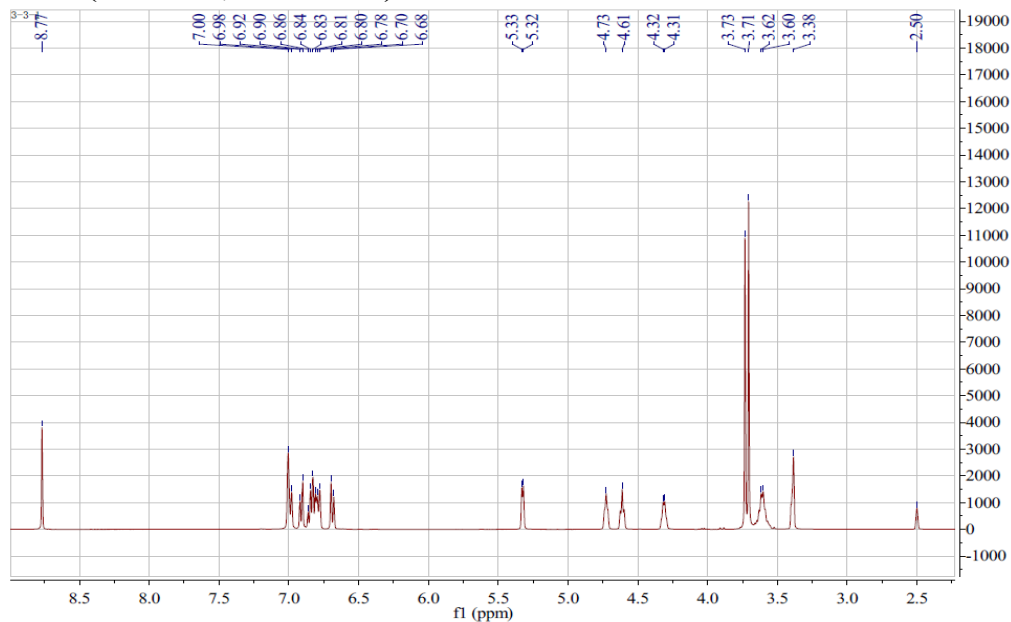
¹³C NMR (400 MHz, D6-DMSO)



Guaiacylglycerol-guaiacyl ether



¹H NMR (400 MHz, D₆-DMSO)



¹³C NMR (400 MHz, D₆-DMSO)

