Supplementary Information

Ultrasound-Assisted Diversion of Nitrobenzene Derivatives to their Aniline Equivalents through Heterogeneous Magnetic Ag/Fe_3O_4-IT Nanocomposite Catalyst

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Table S1. Applied materials and equipment in this project.

Material / equipment	Brand
Silver nitrate	Sigma Aldrich, ≥99.0%
Iron(II) chloride tetrahydrate	Sigma Aldrich, ≥99%
Iron(II)) chloride hexahydrate	Sigma Aldrich, ≥99%
5-Chloro-2-methyl-4-isothiazolin-3-one	Santa Cruz Biotechnology
Ammonia	Merck, 25%
APTES	Sigma Aldrich, 99%
Solvents	Merck
Nitrobenzene derivatives	Sigma Aldrich
Potassium carbonate	Sigma Aldrich, ≥99%
Silica gel for Column chromatography	Sigma Aldrich, 60
Glass tube	13 by 100 mm, equipped with a threaded cap
Glassware	Iso-Lab
Ultrasound bath	Cleaning bath KQ-250 DE
SEM analysis	ZEISS SIGMA
TEM analysis	Philips CM200
HRTEM	Hitachi S-5200 and Philips CM200
XRD	X-ray diffractometer operating at 40 mA, 40 kV,
DLS analysis	Horiba (SZ-100)
FT-IR analysis	Shimadzu-8400s
EDX analysis	VEGA-TESCAN-XMU
XPS analysis	K-Alpha
VSM analysis	Meghnatis Kavir Kashan Co.
NMR analysis	Varian Unity Inova 500 MHz
Melting point apparatus	Electrothermal 9100
TLC plate (silica)	Merck silica gel GF254 plates

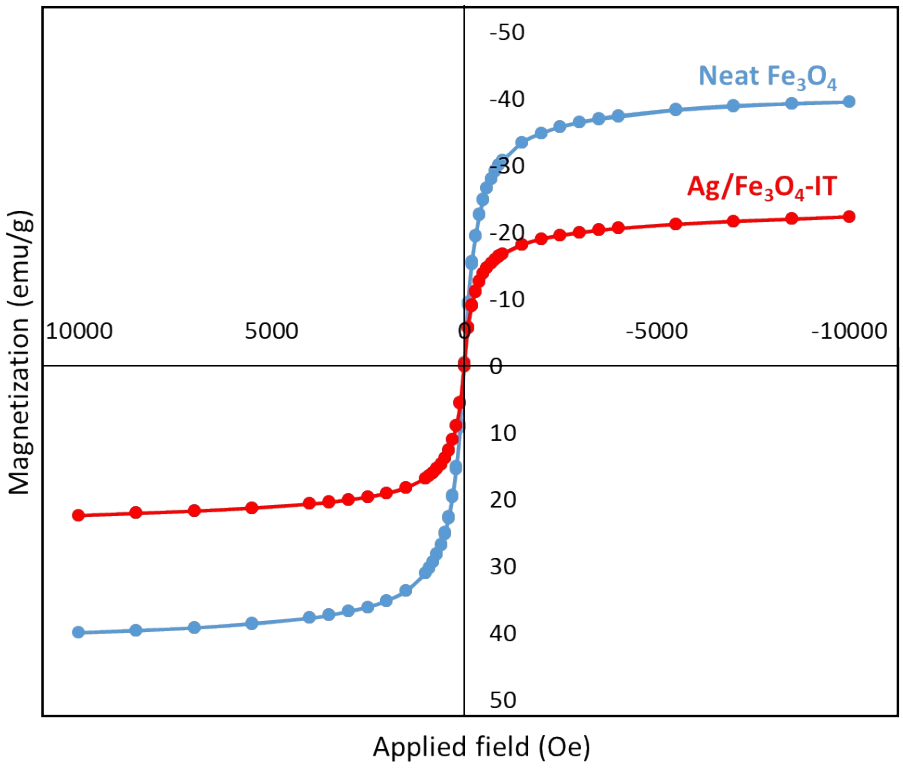

Figure S1. VSM M-H curves of IT-functionalized Ag/Fe_3O_4 nanocatalyst and the neat Fe_3O_4 NPs (recorded at room temperature).

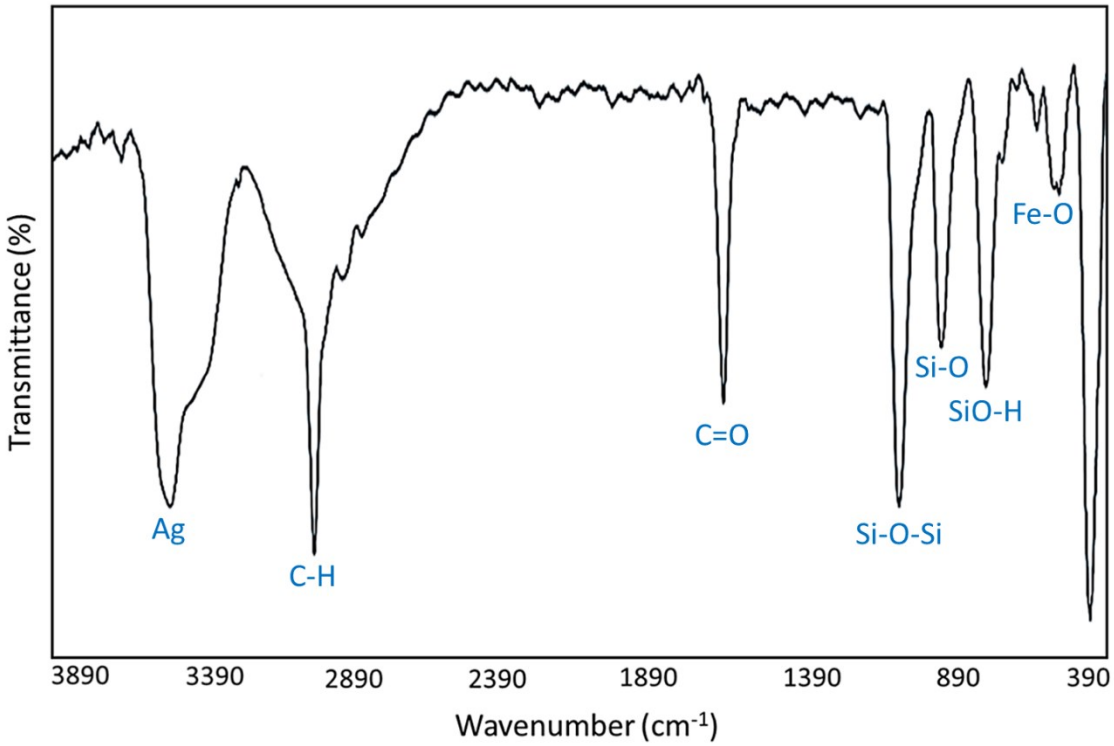

Figure S2. FT-IR spectrum of recovered IT-functionalized Ag/Fe_3O_4 nanocatalyst.

A sharp peak at 3500 cm^{-1} is related to Ag NPs, a sharp peak at 2950 cm^{-1} is related to C─H (sp3), a sharp peak at 1690 cm^{-1} is related to C=O (present in the IT ring), a sharp peak at 1100 cm^{-1} is related to Si─O─Si (stretching vibration), a peak at 1000 cm^{-1} is related to Si─O (stretching vibration), a peak around 860 cm^{-1} is related to SiO─H (stretching vibration), and the peak appeared at around 580 cm^{-1} coming from Fe─O bond.

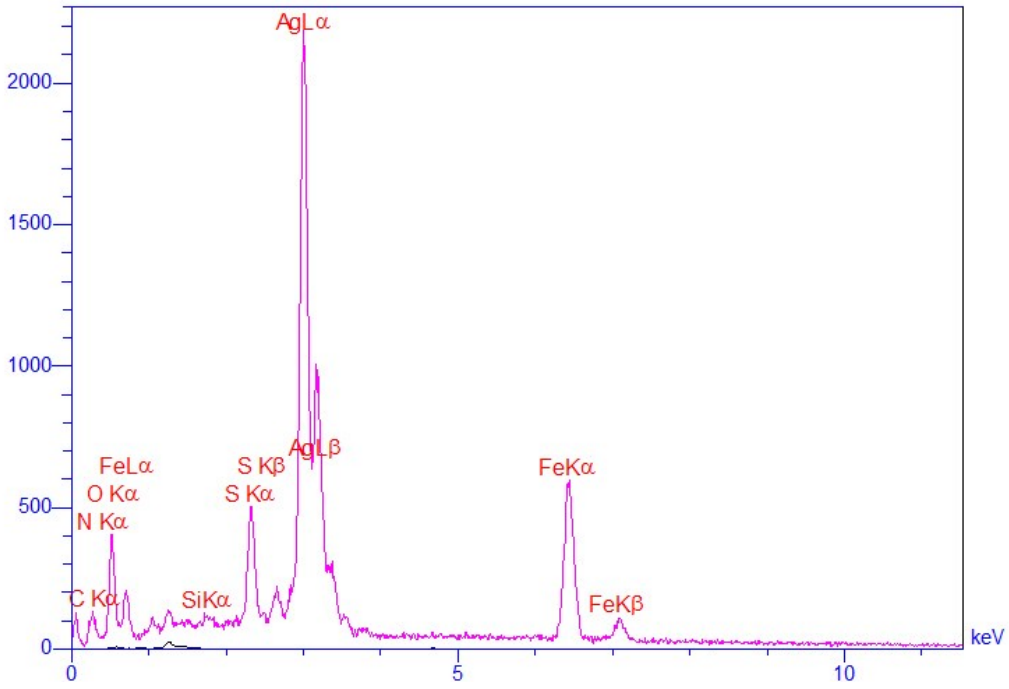

Figure S3. EDX spectrum of recovered IT-functionalized Ag/Fe_3O_4 nanocatalyst.

C: 10.6 wt%

N: 5.4 wt%

O: 20.3 wt%

Si: 0.3 wt%

S: 3.5 wt%

Fe: 14.4 wt%

Ag: 45.5 wt%

Per 100 g of catalyst, there are 0.26 mol Fe and 0.42 mol of Ag elements. It means that the molar ratio of Fe/Ag in 100 g of catalyst is: **0.61**

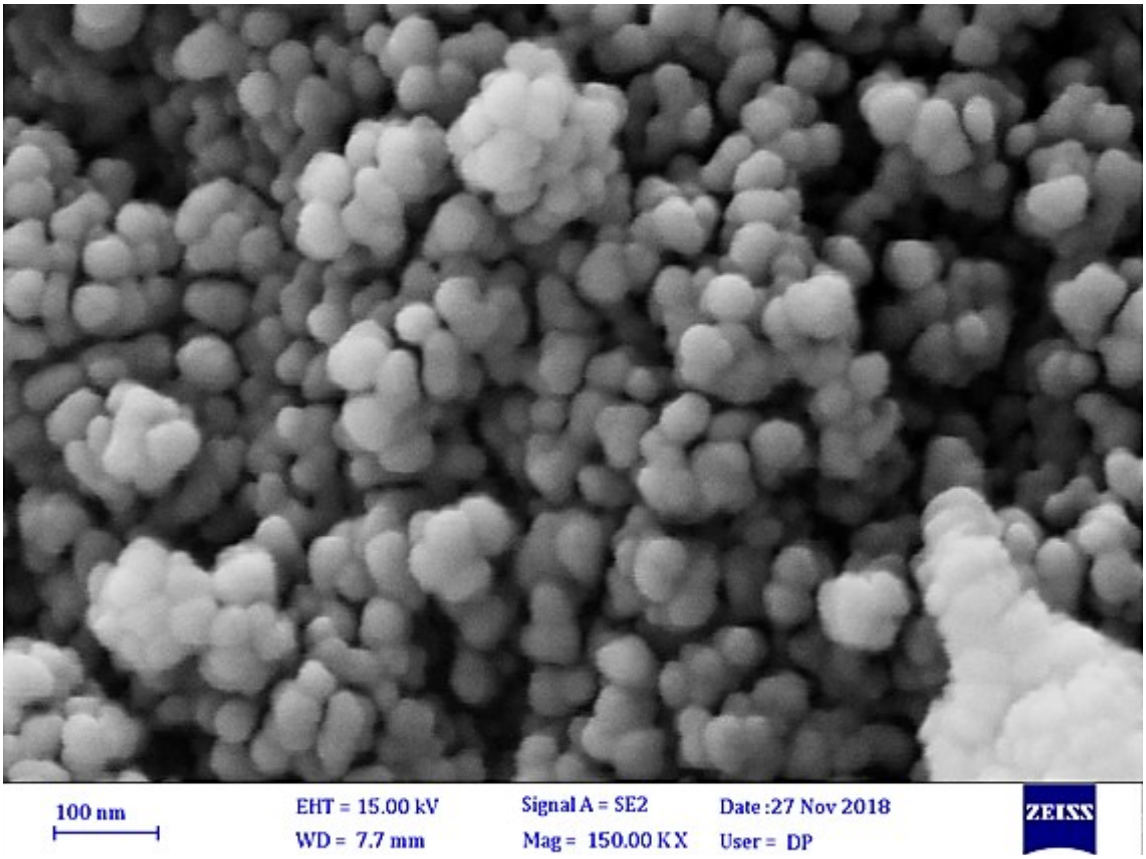

Figure S4. SEM image of recovered IT-functionalized Ag/Fe_3O_4 nanocatalyst.

Benzene-1,4-diamine (**Table 2 – Entry 2)**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.59 (s, 4 H), 3.36 (s, 4 H). ^{13}C NMR (500 MHz, $CDCl_3$) δ 138.75, 116.87.

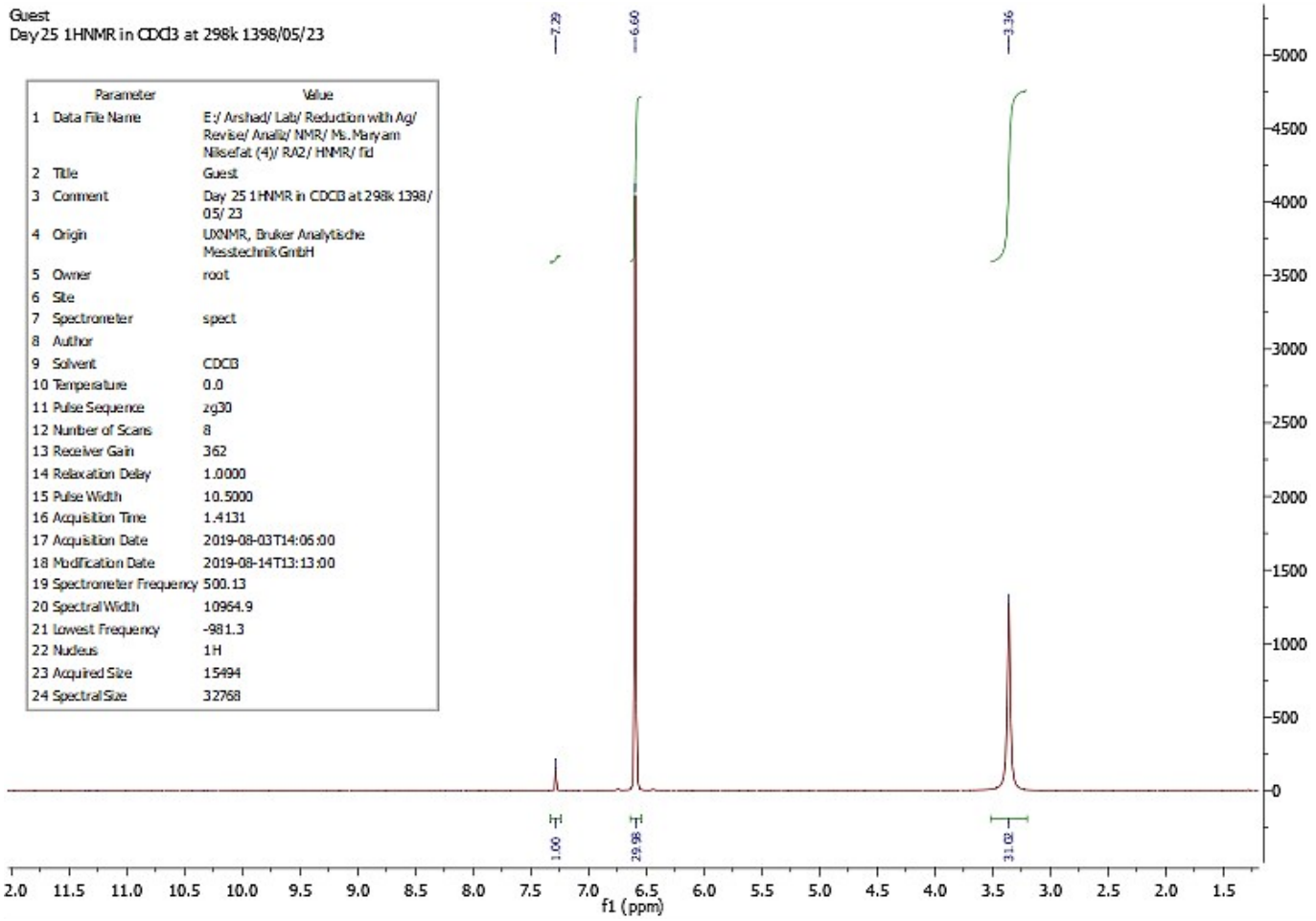

Figure S5. Spectral data and ^{1}H-NMR spectrum of benzene-1,4-diamine.

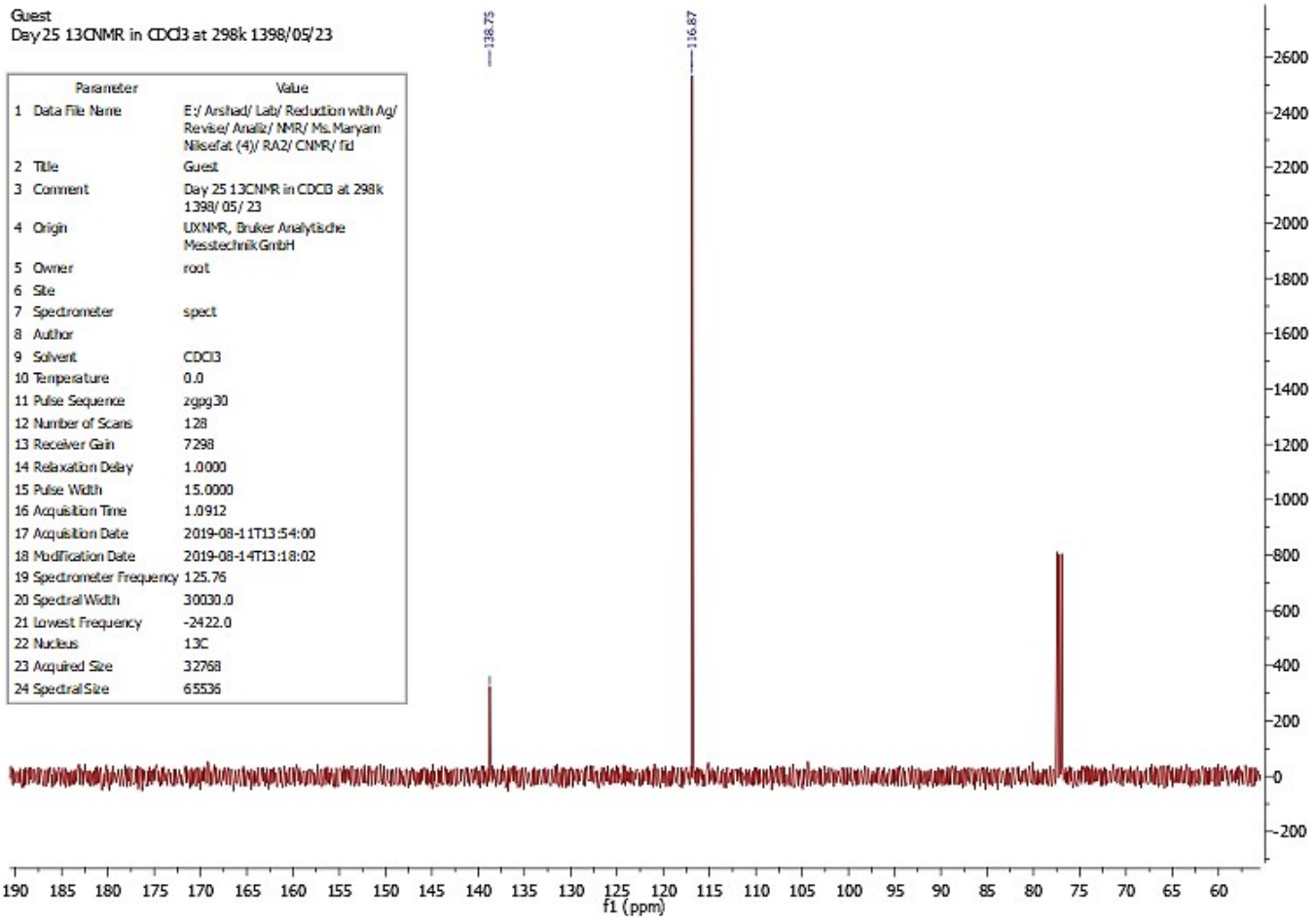

Figure S6. ^{13}C-NMR spectrum of benzene-1,4-diamine.

Benzene-1,3-diamine (**Table 2 – Entry 3)**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.96-6.99 (m, 1 H), 6.15–6.13 (d, J = 7.8 Hz, 2 H), 6.03 (s, 1 H), 3.59 (s, 4 H). ^{13}C NMR (500 MHz, $CDCl_3$) δ 147.78, 130.34, 106.25, 102.18.

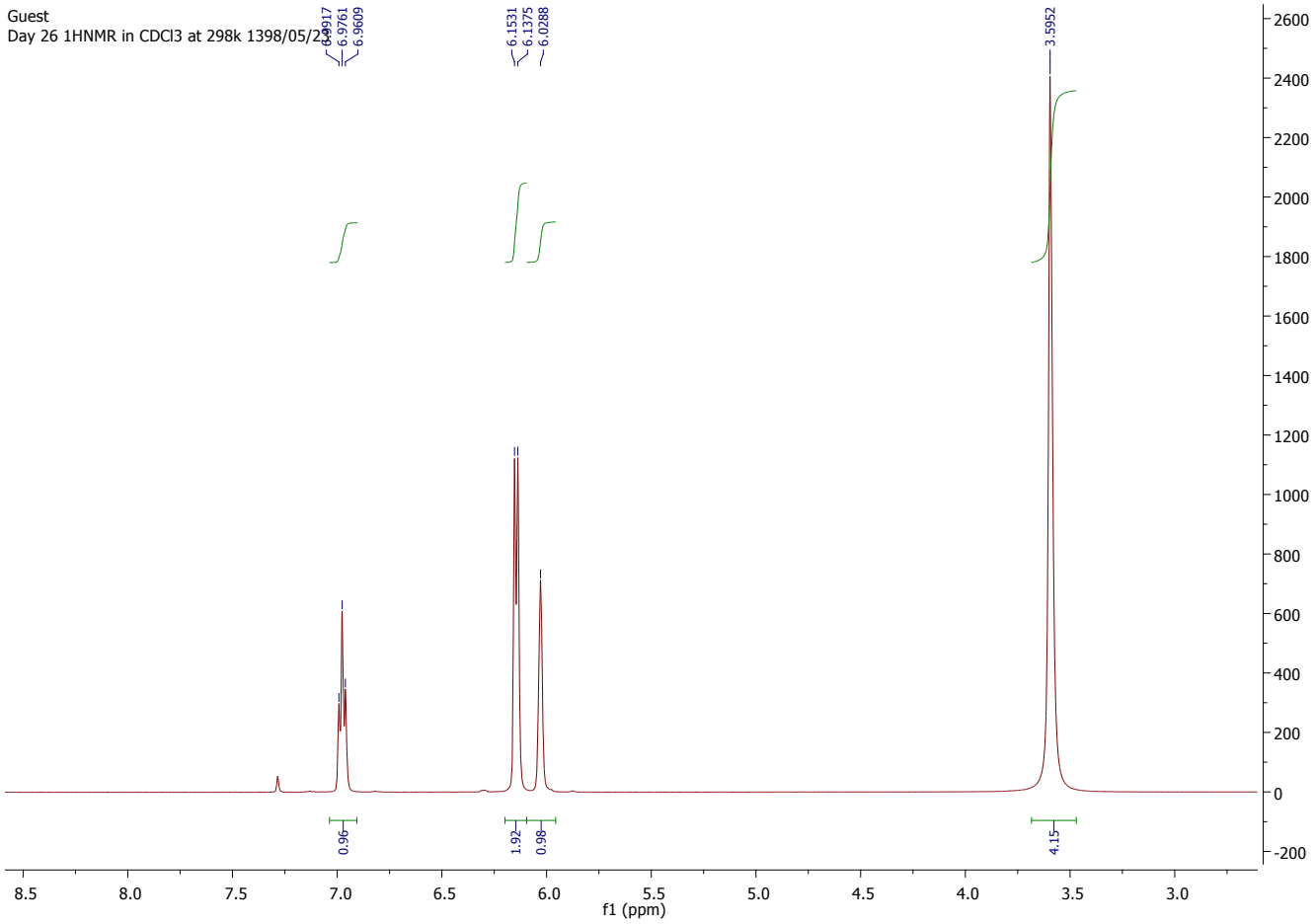

Figure S7. Spectral data and ^{1}H-NMR spectrum of benzene-1,3-diamine.

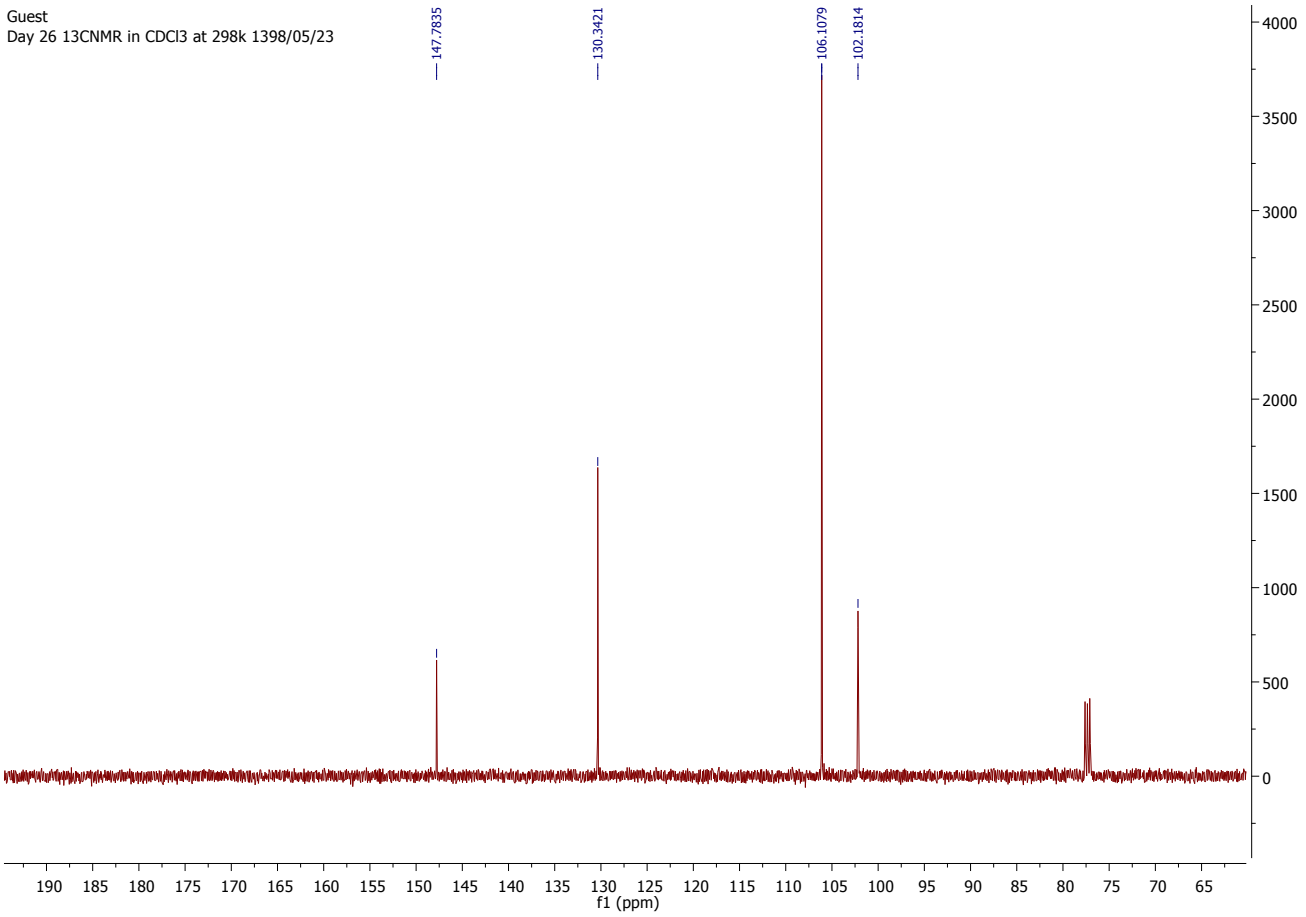

Figure S8. ^{13}C-NMR spectrum of benzene-1,3-diamine.

4-Aminophenol (**Table 3, Entry 6**): white solid, ^{1}H NMR (500 MHz, DMSO): δ (ppm) = 4.38 (2H, s, NH_2), 6.42–6.44 (2H, d, J=10 Hz, H–Ar), 6.48–6.50 (2H, d, J=10 Hz, H–Ar), 8.37 (1H, s, OH). ^{13}C NMR (500 MHz, DMSO) δ 168.09, 153.70, 131.82, 113.18.

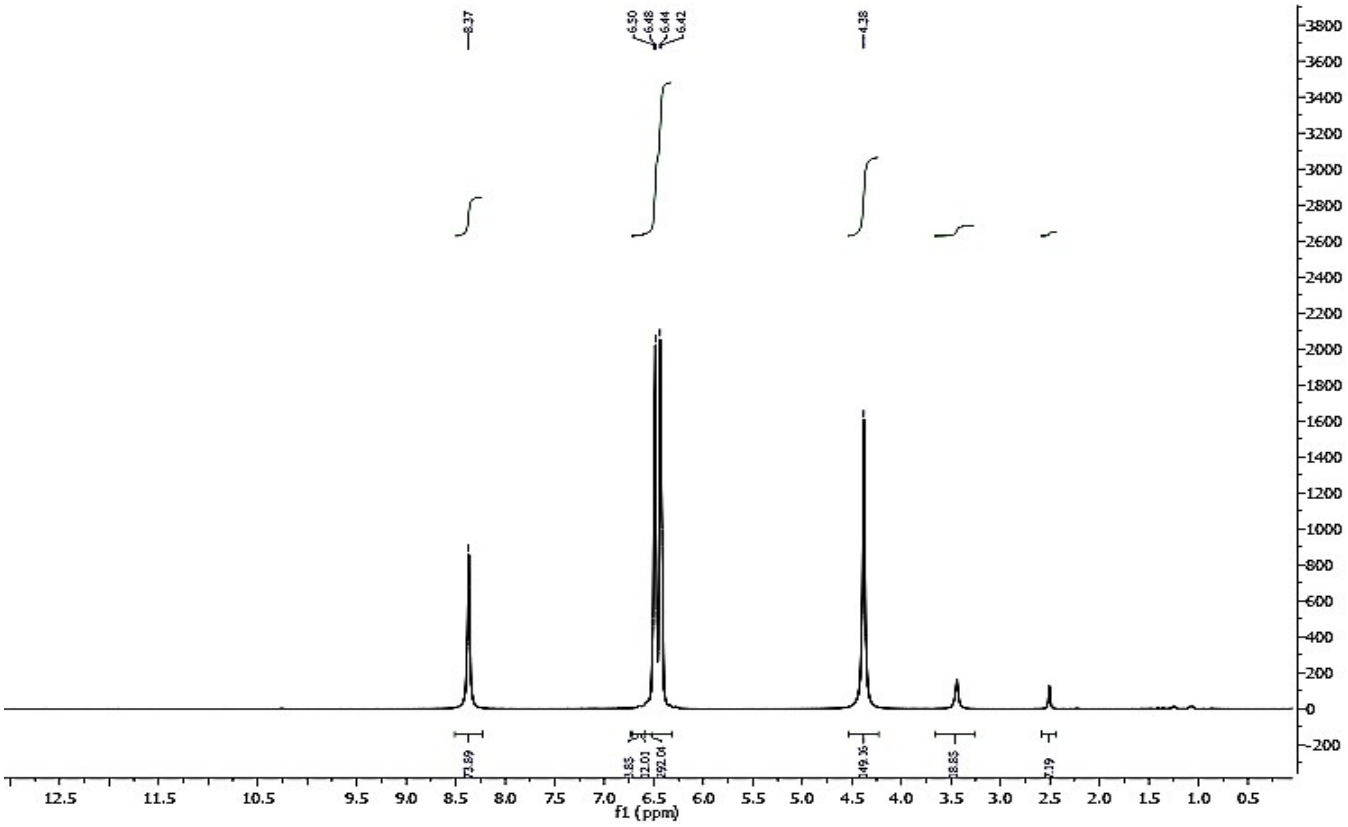

Figure S9. Spectral data and ^{1}H-NMR spectrum of 4-aminophenol.

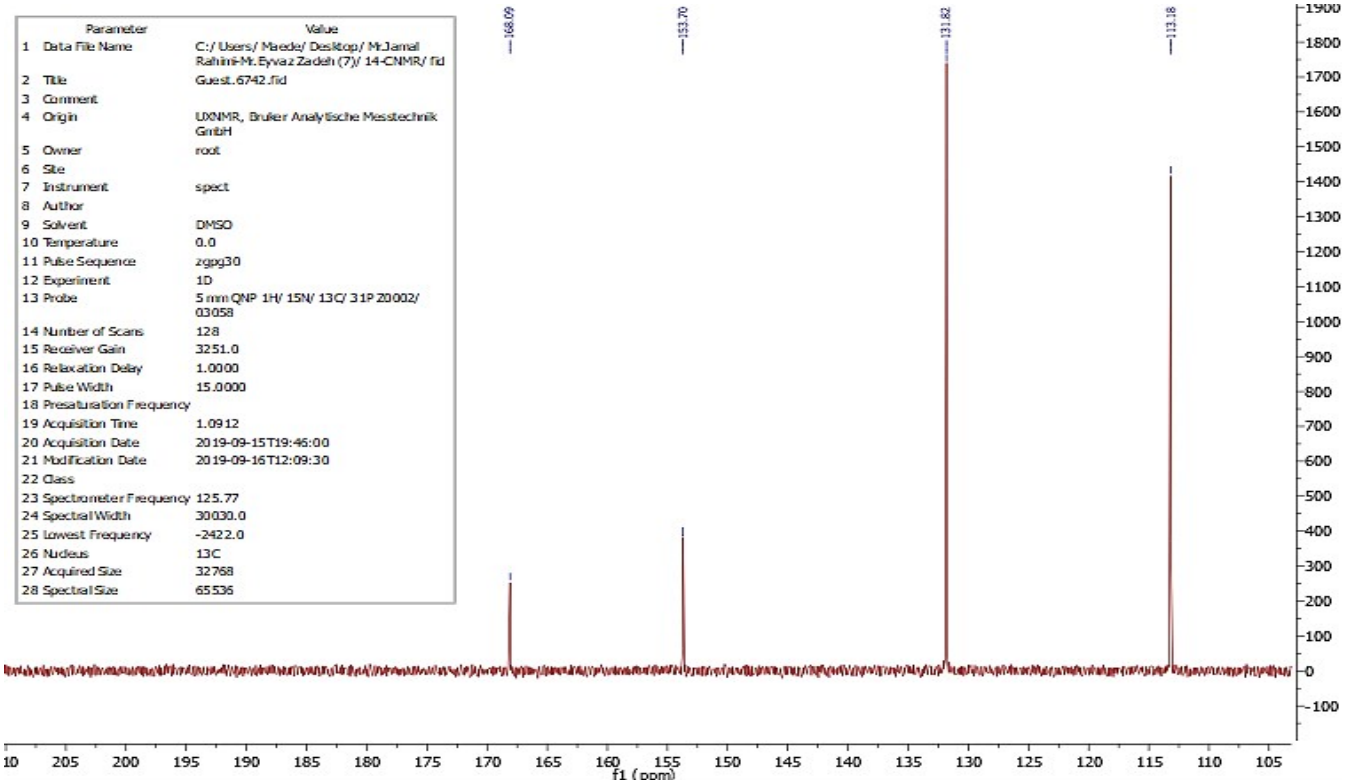

Figure S10. ^{13}C-NMR spectrum of 4-aminophenol.

3,4-Diaminobenzoic acid (**Table 2 – Entry 9):** ^{1}H NMR (500 MHz, DMSO) δ 5.37 (s, 4H), 6.51-6.53 (d, J = 10 Hz, 1H), 7.10-7.12 (d, J = 10 Hz, 1H), 7.17 (s, 1H). ^{13}C NMR (500 MHz, DMSO) δ 168.63, 140.76, 134.24, 121.09, 118.99, 116.04, 113.36.

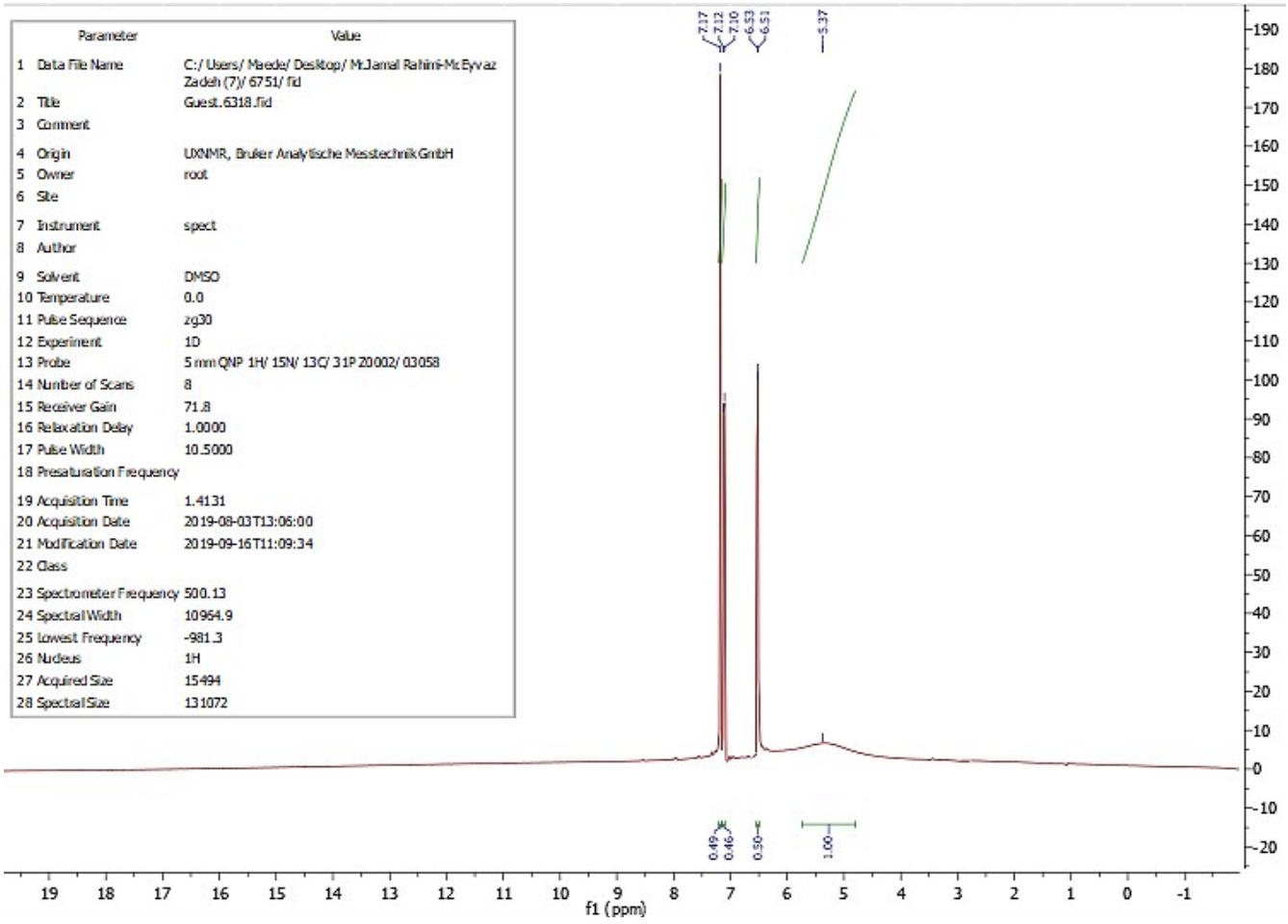

Figure S11. Spectral data and ^{1}H-NMR spectrum of 3,4-diaminobenzoic acid.

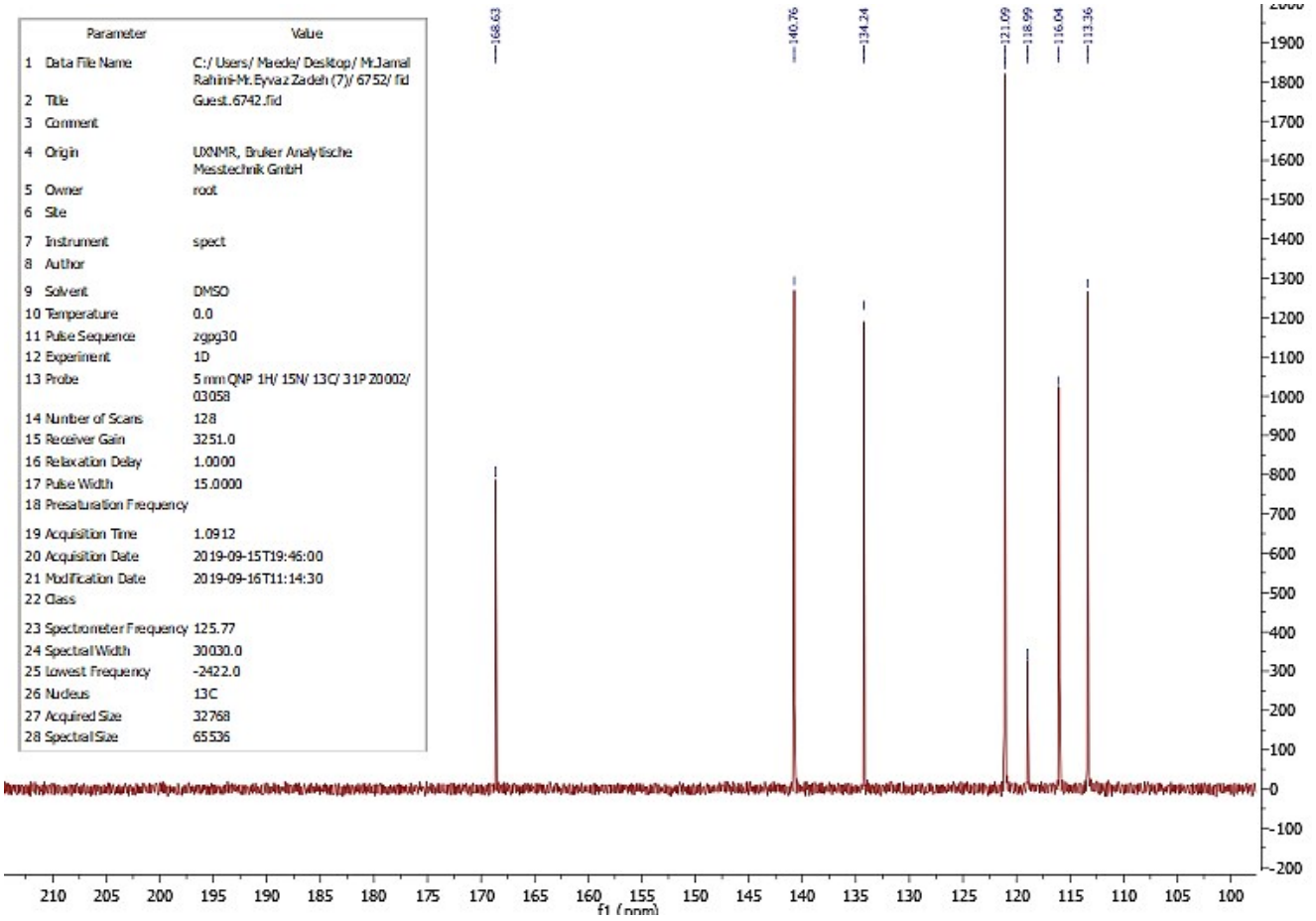

Figure S12. ^{13}C-NMR spectrum of 3,4-diaminobenzoic acid.