Electronic Supplementary Information (ESI)

for

Metal-metalloid bond containing complexes of bulky organotellurium ligand with palladium and ruthenium: applications in catalysis of C−O coupling and aldehyde to amide transformation reactions

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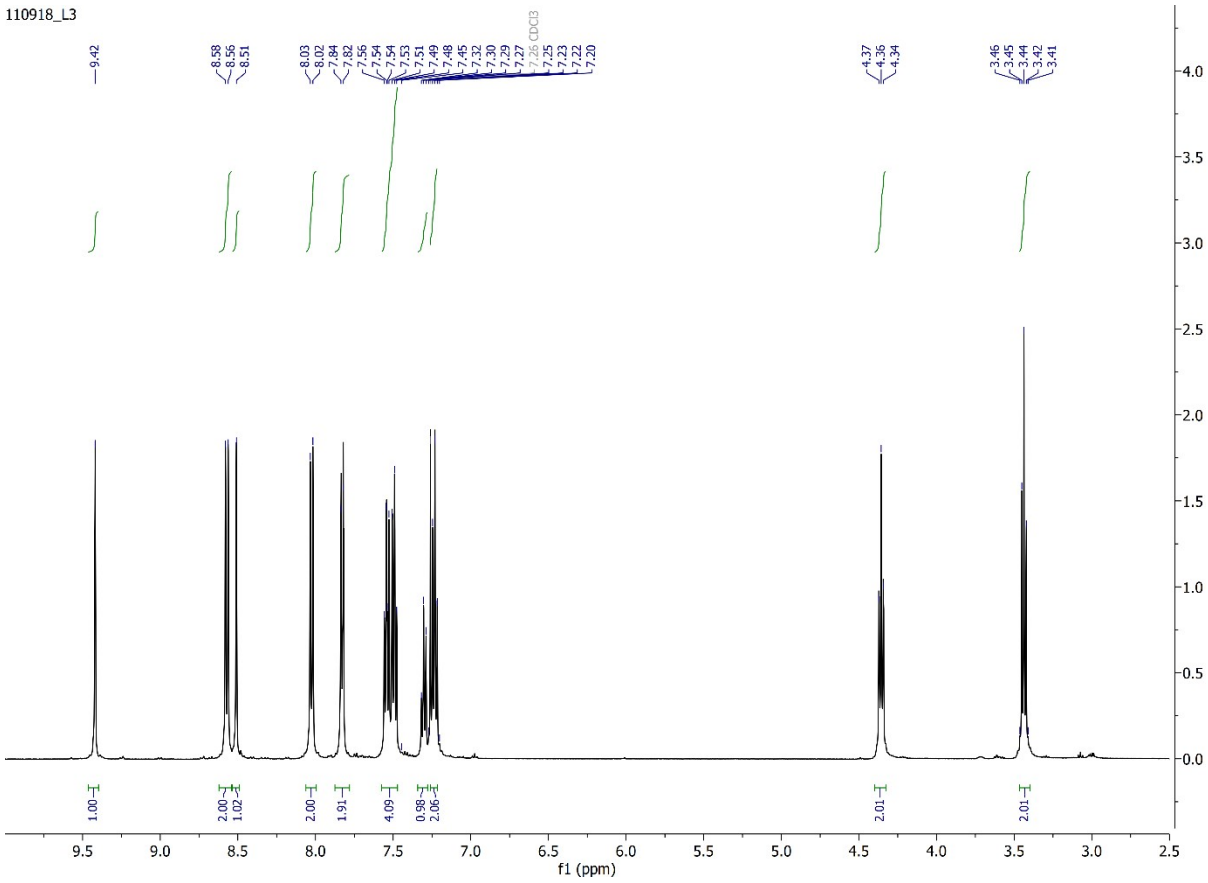


Fig. S1. ^{1}H NMR Spectrum of **L1** recorded in $CDCl_3$

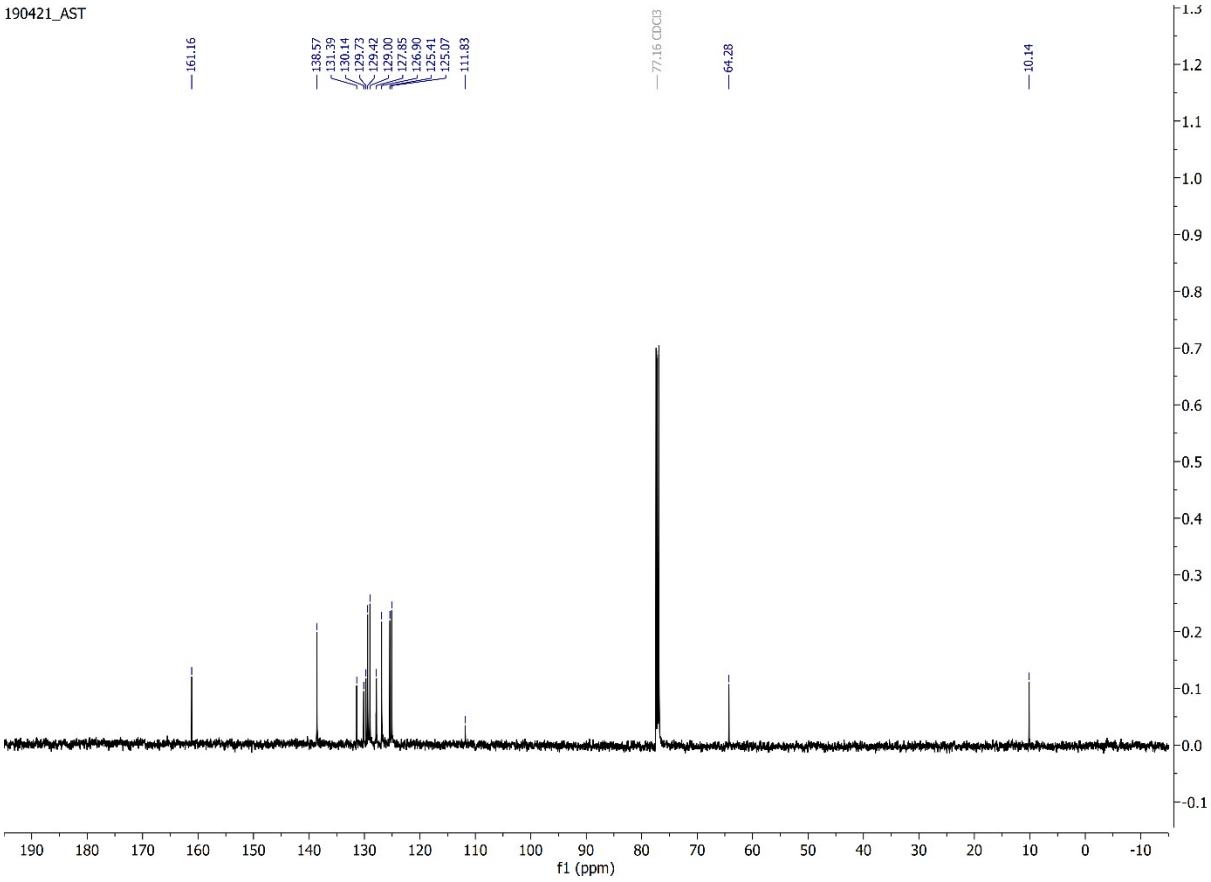


Fig. S2. $^{13}C\{^{1}H\}$ NMR Spectrum of **L1** recorded in $CDCl_3$

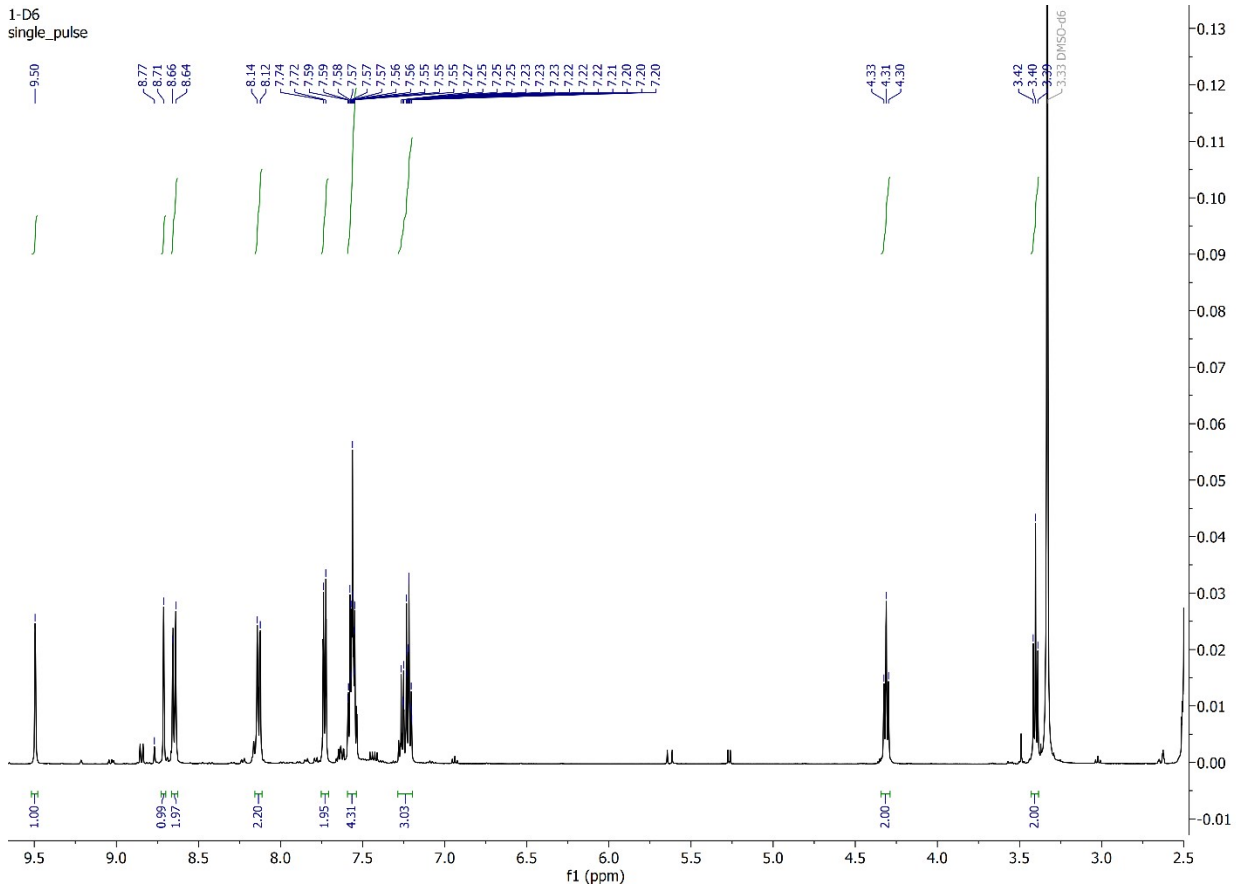


Fig. S3. ^{1}H NMR Spectrum of **L1** in DMSO-d^{6} after keeping it at room temperature for 12 h in DMSO-d^{6}

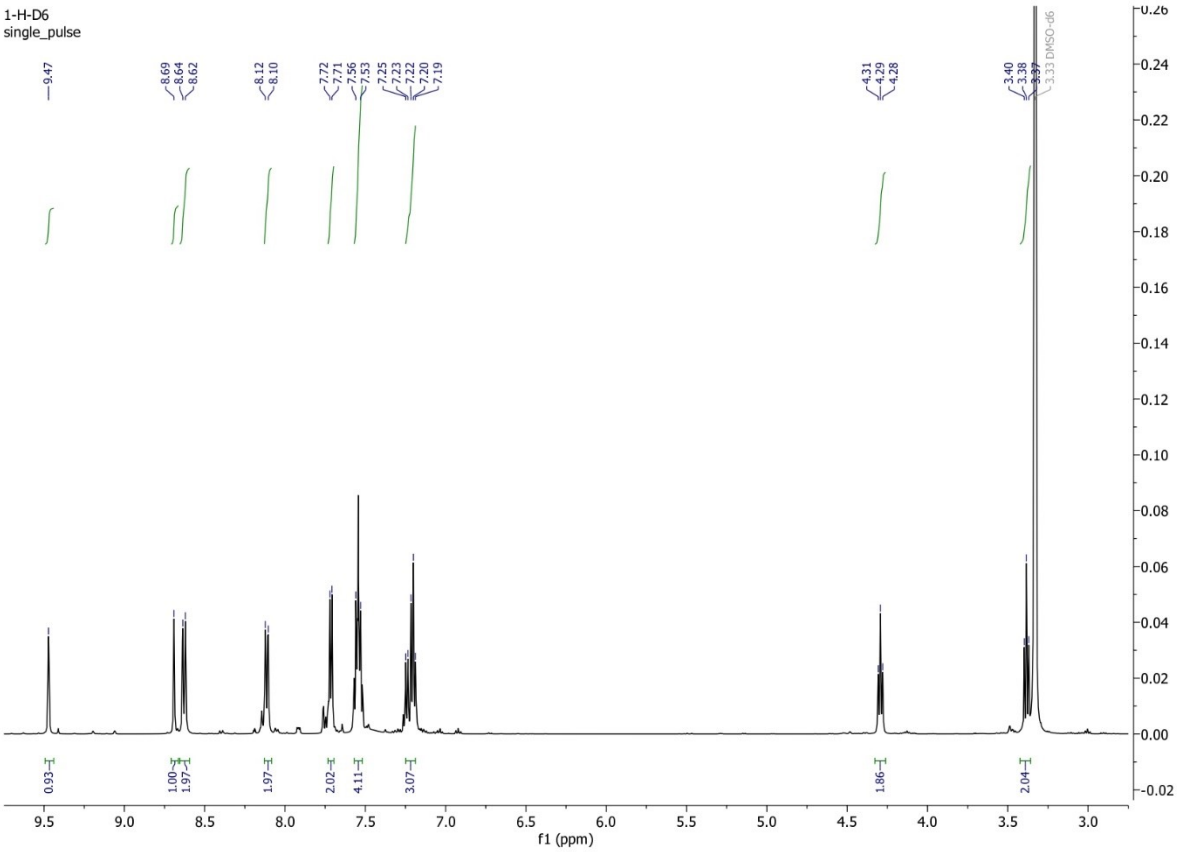


Fig. S4. ^{1}H NMR Spectrum of **L1** in DMSO-d^{6} after keeping it at 110 ˚C for 12 h in DMSO-d^{6}

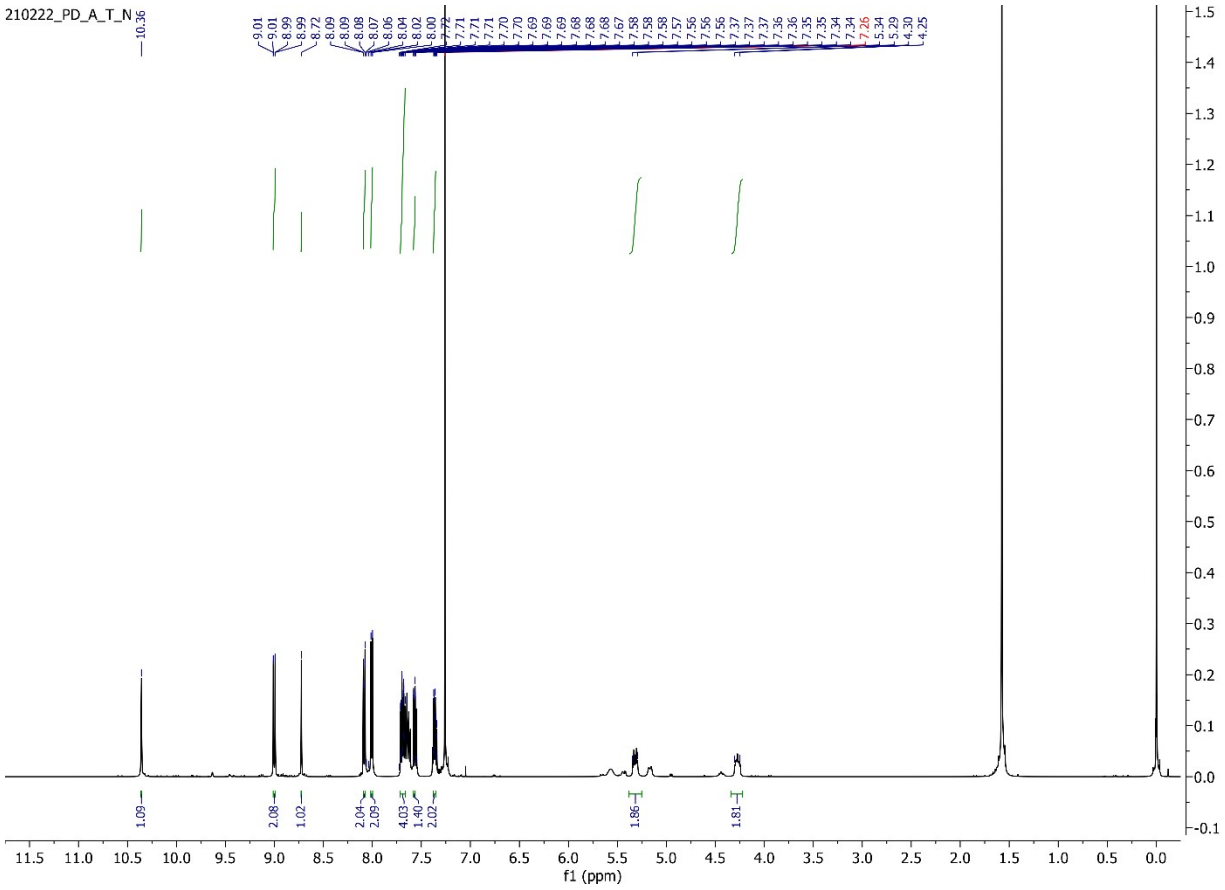


Fig. S5. ^{1}H NMR of Pd(II) complex **1** recorded in $CDCl_3$

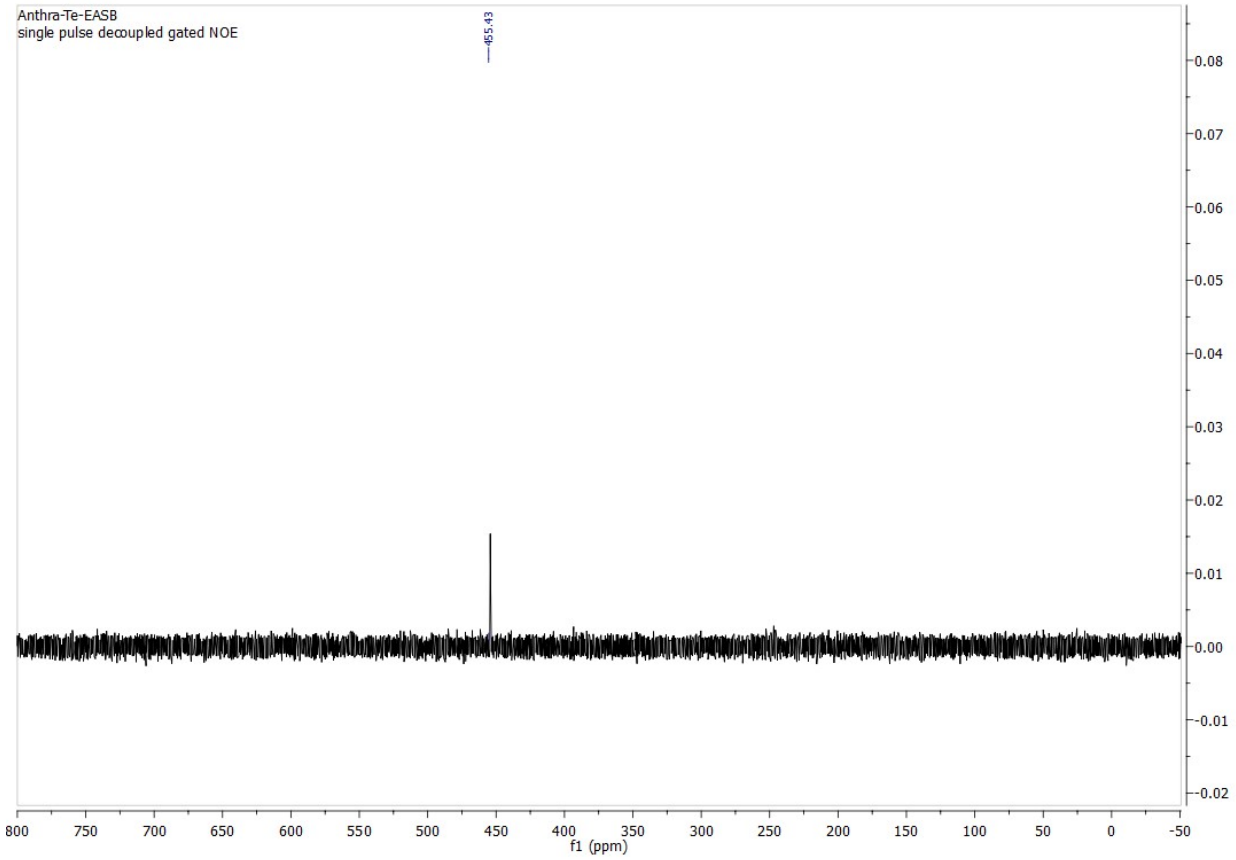


Fig. S6. $^{125}Te\{^{1}H\}$ NMR Spectrum of **L1** recorded in $CDCl_3$

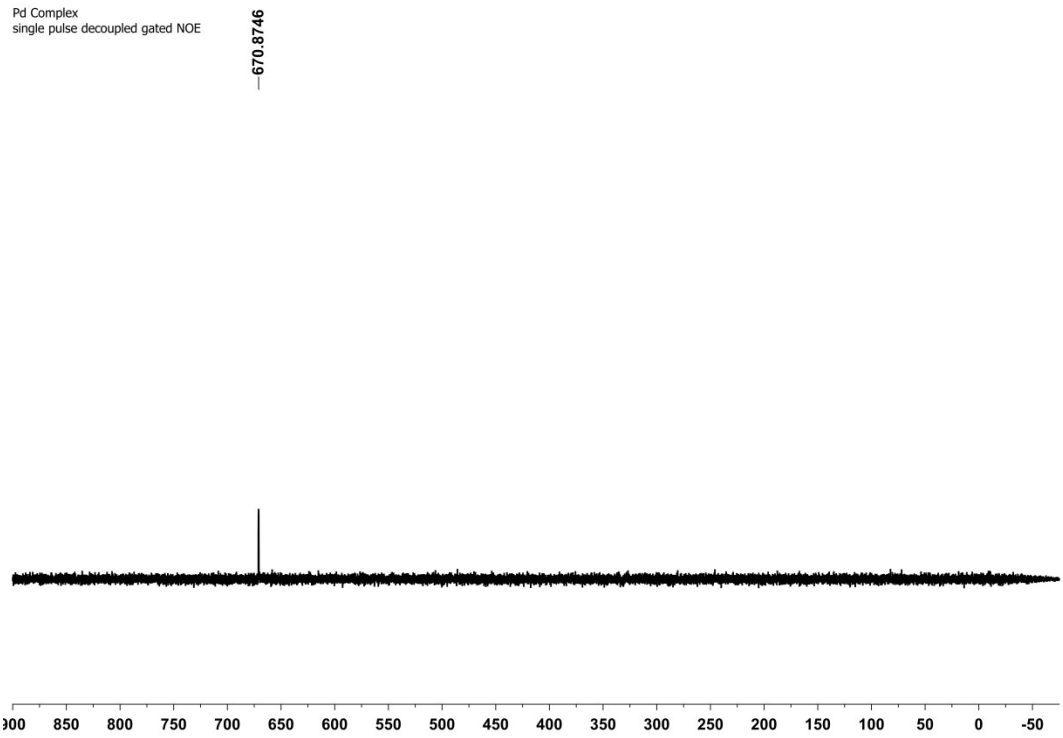


Fig. S7. $^{125}Te\{^{1}H\}$ NMR Spectrum of palladium(II) complex **1** recorded in DMSO-d^6

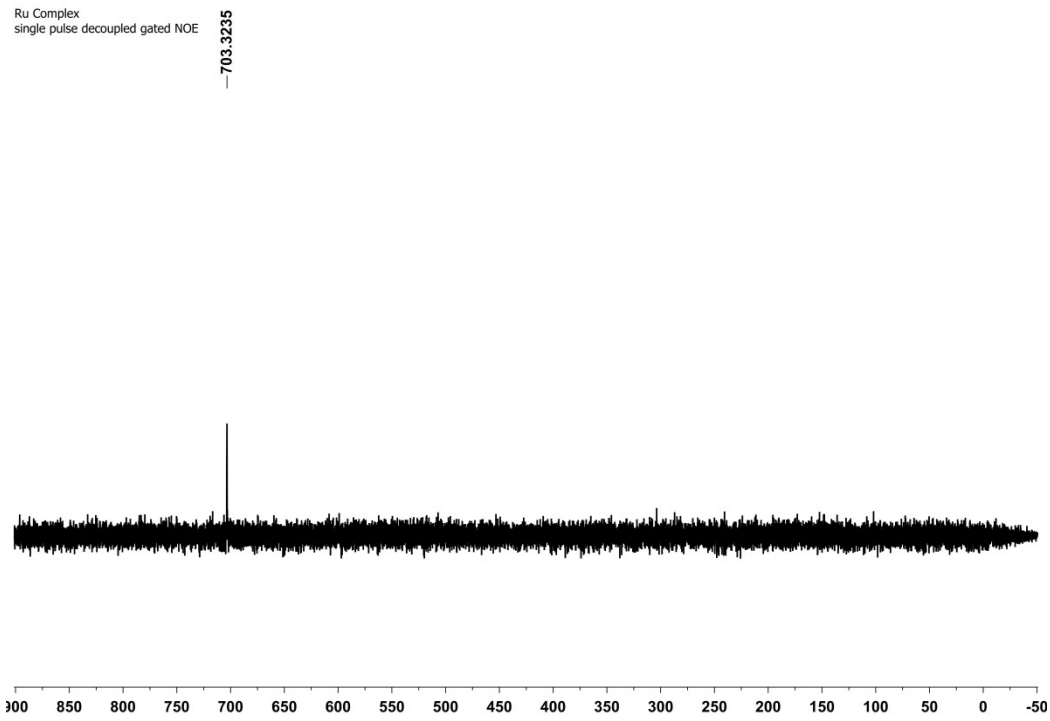


Fig. S8. $^{125}Te\{^{1}H\}$ NMR spectrum of ruthenium(II) complex **2** recorded in DMSO-d^6

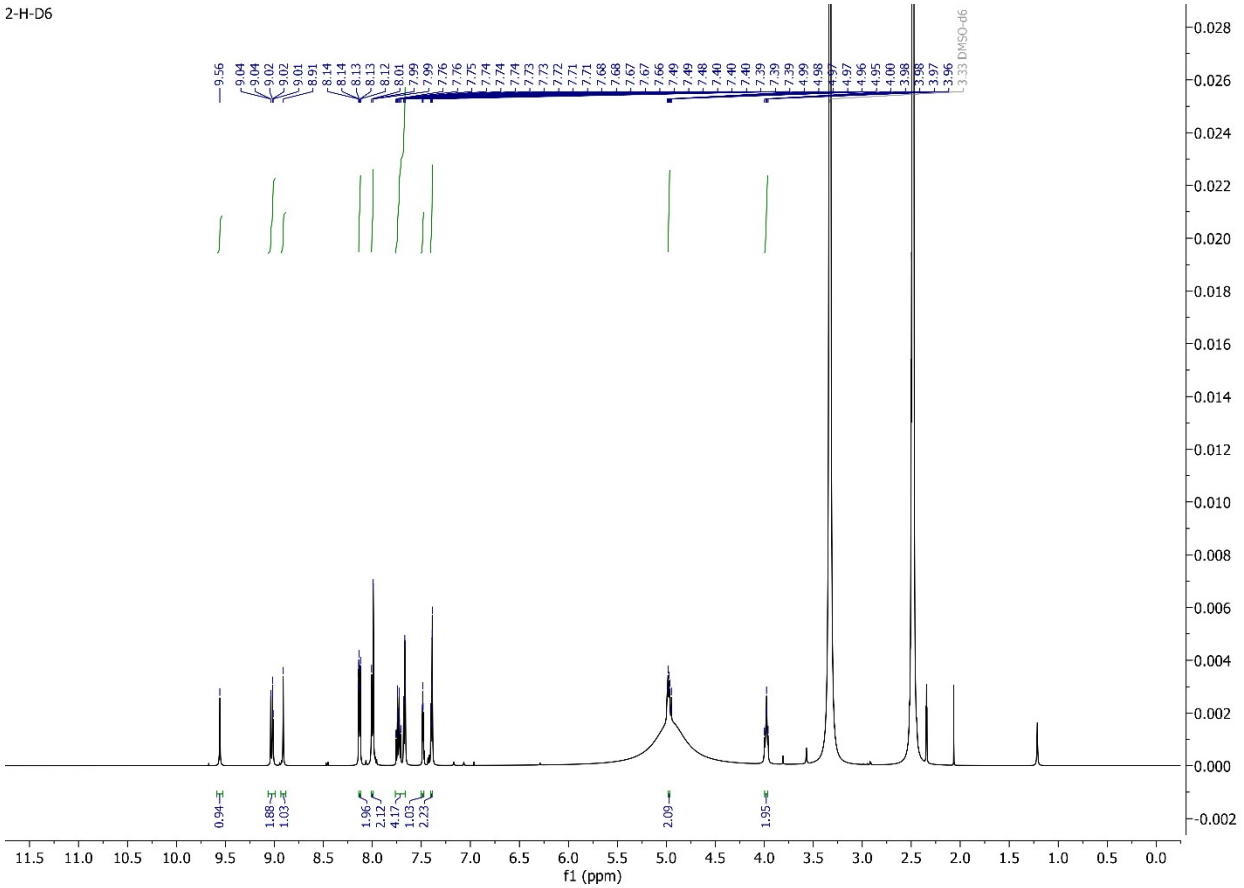


Fig. S9. ^{1}H NMR Spectrum of complex **1** in DMSO-d^{6} after keeping it at room temperature for 12 hours in DMSO-d^{6}

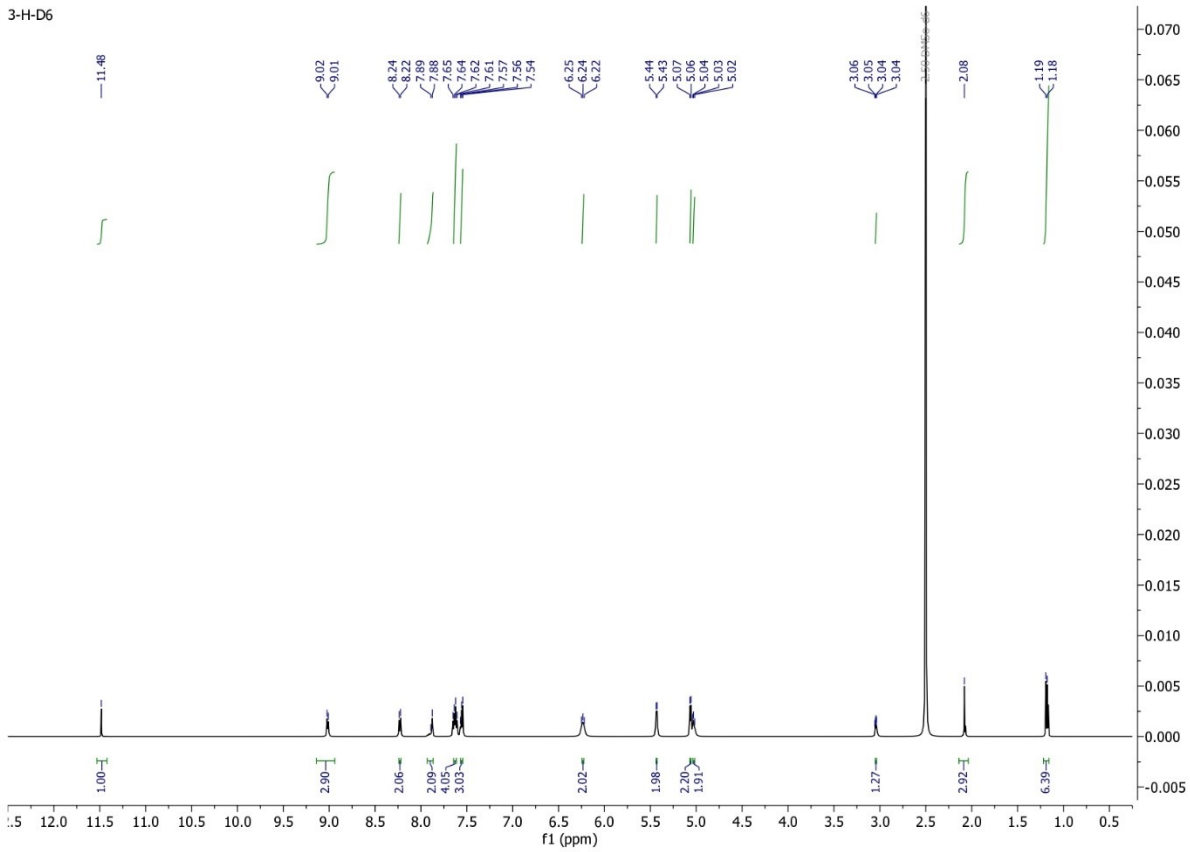


Fig. S10. ^{1}H NMR Spectrum of complex **2** in DMSO-d^{6} after keeping it at room temperature for 12 hours in DMSO-d^{6}

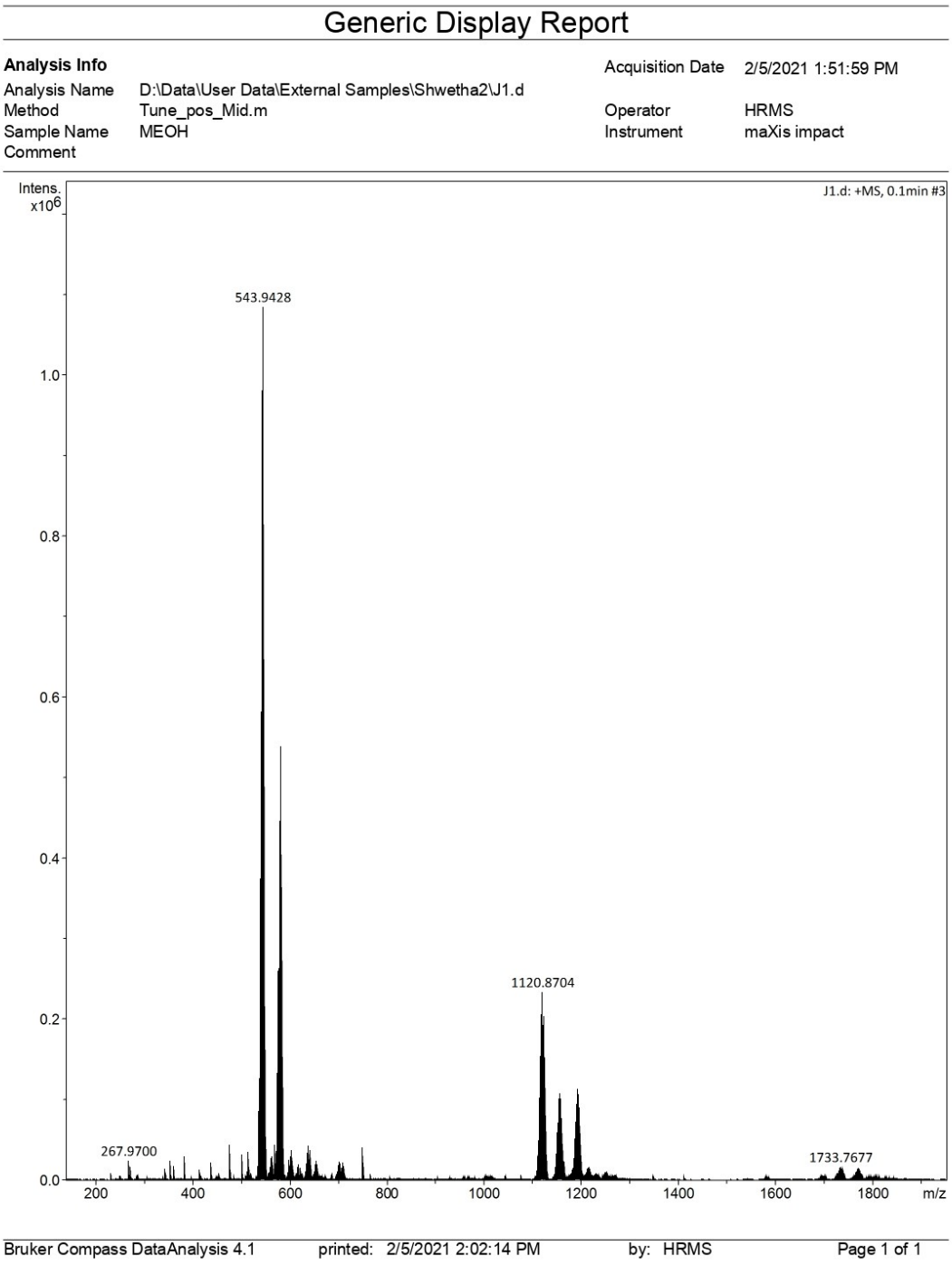


Fig. S11. High resolution mass spectrum (HRMS) of complex **1**.

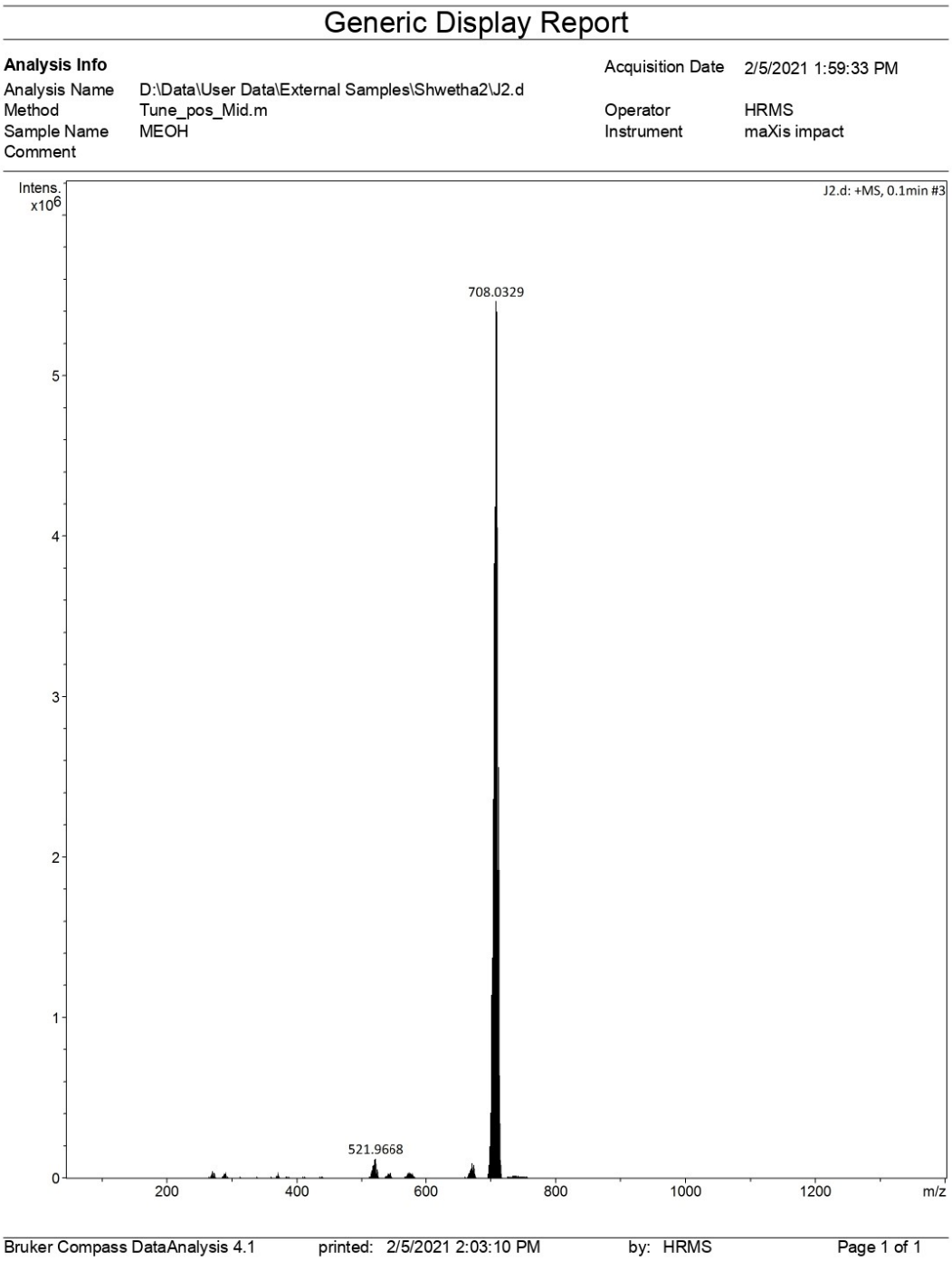


Fig. S12. High resolution mass spectrum (HRMS) of complex **2**.

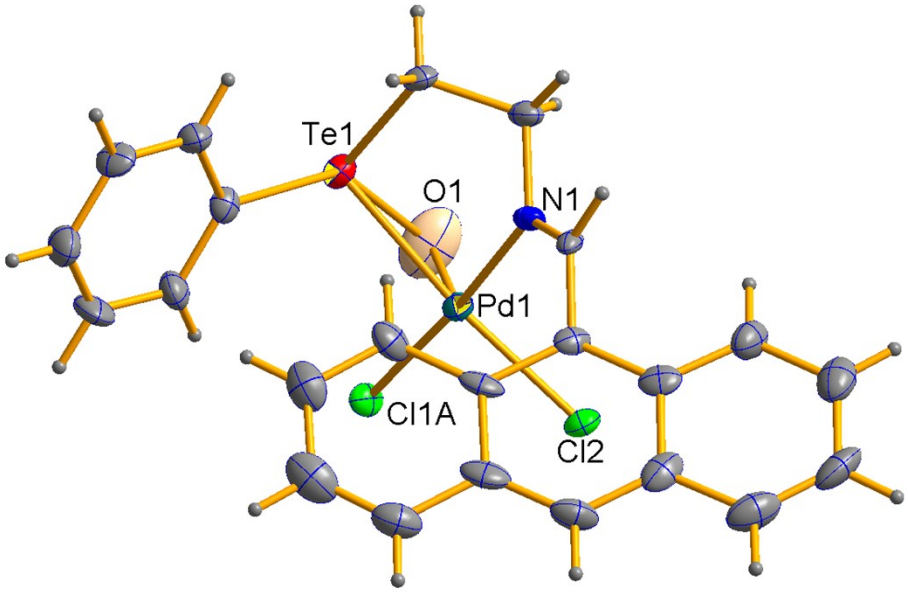


Fig. S13. Molecular structure of complex **1** with crystallized water molecule

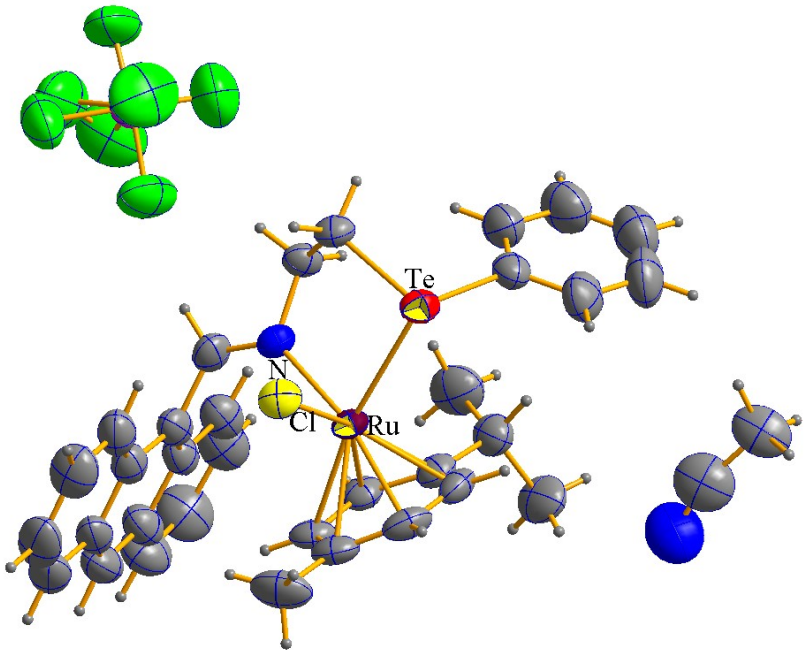
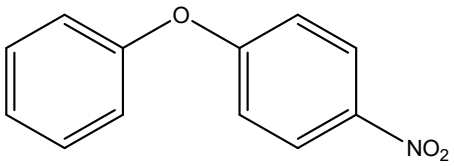
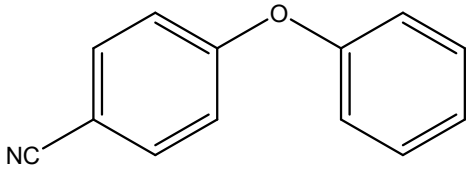


Fig. S14. Molecular structure of complex **2** with PF_6 anion and acetonitrile molecule

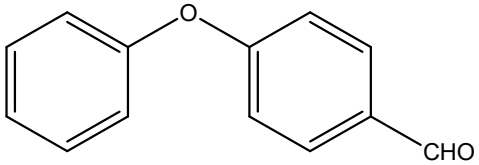
S1. NMR data of cross-coupled products obtained in C-O coupling reactions of aryl halides and phenol or derivatives of phenol



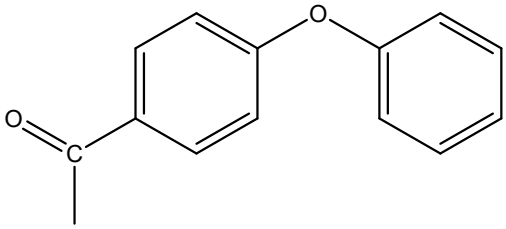
1-Nitro-4-phenoxy benzene: Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 8.11-8.14 (d, 2H), 7.34-7.40 (t, 2H), 7.16-7.21 (t, 1H), 7.01-7.03 (d, 2H), 6.92-6.95 (d, 2H).+



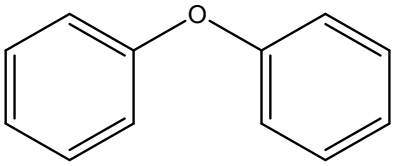
4-Phenoxybenzonitrile: Colourless solid. ^{1}H NMR (500 MHz, $CDCl_3$), δ(ppm): 7.55 (d, 2H), 7.43 (t, 2H), 7.20 (t, 1H), 7.00 (d, 2H), 6.95 (d, 2H).



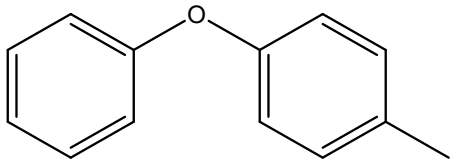
4-Phenoxybenzaldehyde: Yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 9.92 (s, 1H), 7.84-7.86 (d, 2H), 7.40-7.45 (t, 2H), 7.20-7.26 (m, 1H), 7.05-7.11 (t, 4h).



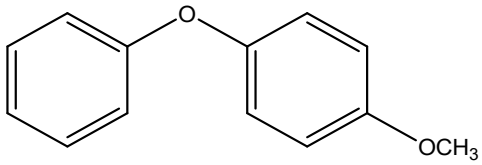
1-(4-phenoxyphenyl)ethanone: Colourless solid. ^{1}H NMR (500 MHz, $CDCl_3$), δ(ppm): 7.93 (m, 2H), 7.37-7.41 (m, 2H), 7.18-7.21 (t, 1H), 7.08-7.06 (m, 2H), 6.98-7.00 (m, 2H), 2.57 (s, 3H).



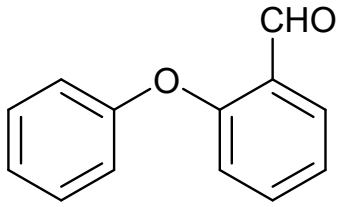
Diphenyl ether: Colorless liquid. ^{1}H NMR (500 MHz, $CDCl_3$), δ(ppm): 7.25 (t, 4H), 6.93 (t, 2H), 7.37 (d, 4H).



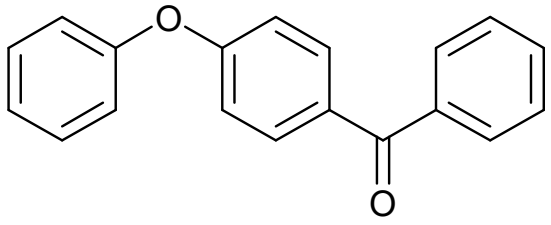
1-Methyl-4-phenoxybenzene: Colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 7.46-7.48 (m, 2H), 7.23-7.26 (t, 2H), 7.06-7.07 (m, 1H), 6.98-7.04 (m, 2H), 6.89-6.91 (m, 2H), 2.26 (s, 3H).



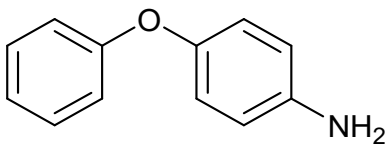
1-Methoxy-4-phenoxybenzene: Colorless liquid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 7.25-7.32 (m, 2H), 7.01-7.06 (t, 1H), 6.93-7.01 (m, 4H), 6.86-6.90 (m, 2H), 3.81 (s, 3H).



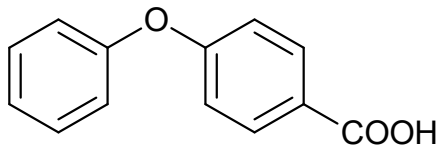
2-Phenoxybenzaldehyde: Yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 10.45 (s, 1H), 7.85-7.88 (d, 1H), 7.41-7.47 (t, 1H), 7.30-7.35 (t, 2H), 7.10-7.14 (t, 2H), 6.98-7.01 (d, 2H), 6.81-6.84 (d, 1H).



4-phenoxybenzophenone: Yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 7.81-7.80 (d, 2H), 7.77-7.75 (d, 2H), 7.55-7.528 (t, 1H), 7.46-7.43 (t, 2H), 7.39-7.36 (t, 2H), 7.19-7.16 (t, 1H), 7.09-7.05 (m, 3H)



4-phenoxyaniline: Yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 7.26-7.29 (t, 2H), 7.01-6.92 (m, 3H), 6.87-6.75 (d, 2H), 6.67-6.51 (d, 2H).



4-phenoxybenzoic acid: Yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$, 25°C vs TMS), δ(ppm): 8.10-8.08 (d, 2H), 7.41-7.36 (t, 2H), 7.21-7.17 (t, 1H), 7.09-7.03 (m, 4H).

S2. NMR spectra of cross-coupled products obtained in C-O coupling reactions of aryl halides and phenol or derivatives of phenol

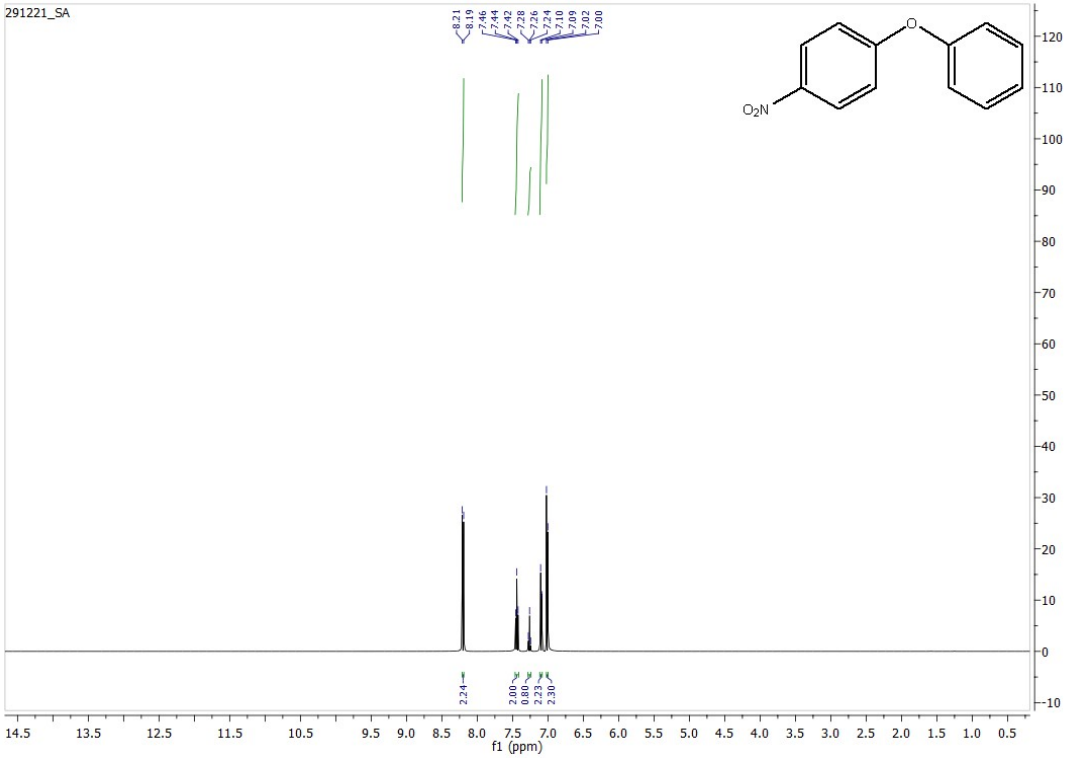


Fig. S15. ^{1}H NMR of 1-nitro-4-phenoxy benzene recorded in $CDCl_3$

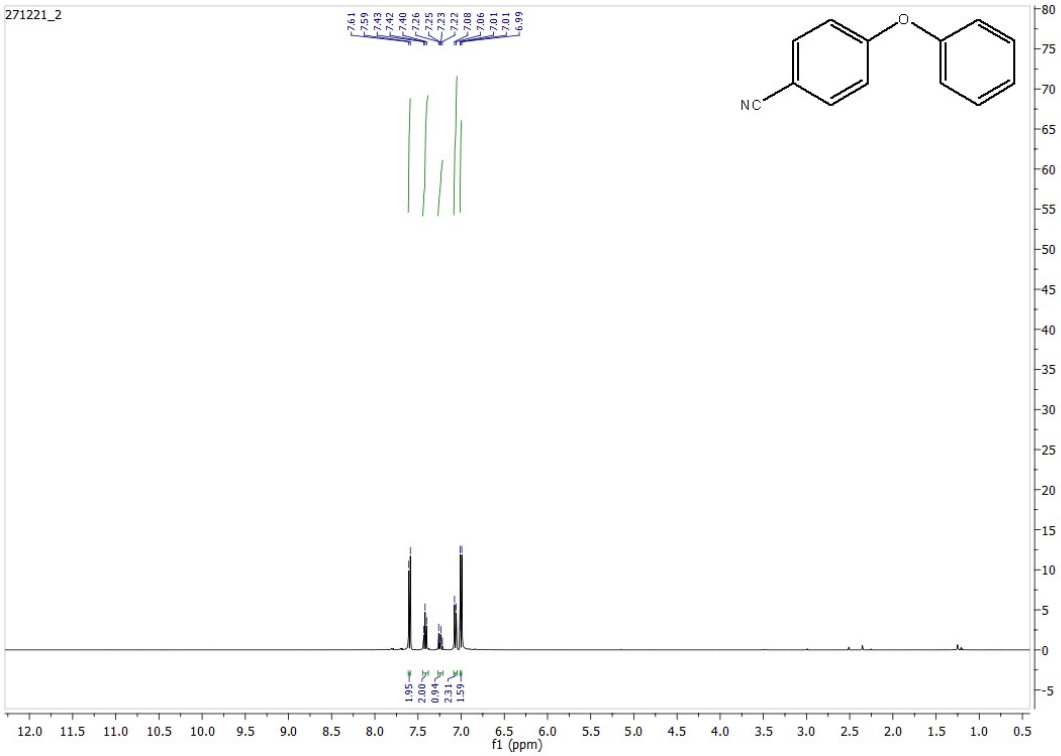


Fig. S16. ^{1}H NMR of 4-phenoxybenzonitrile recorded in $CDCl_3$

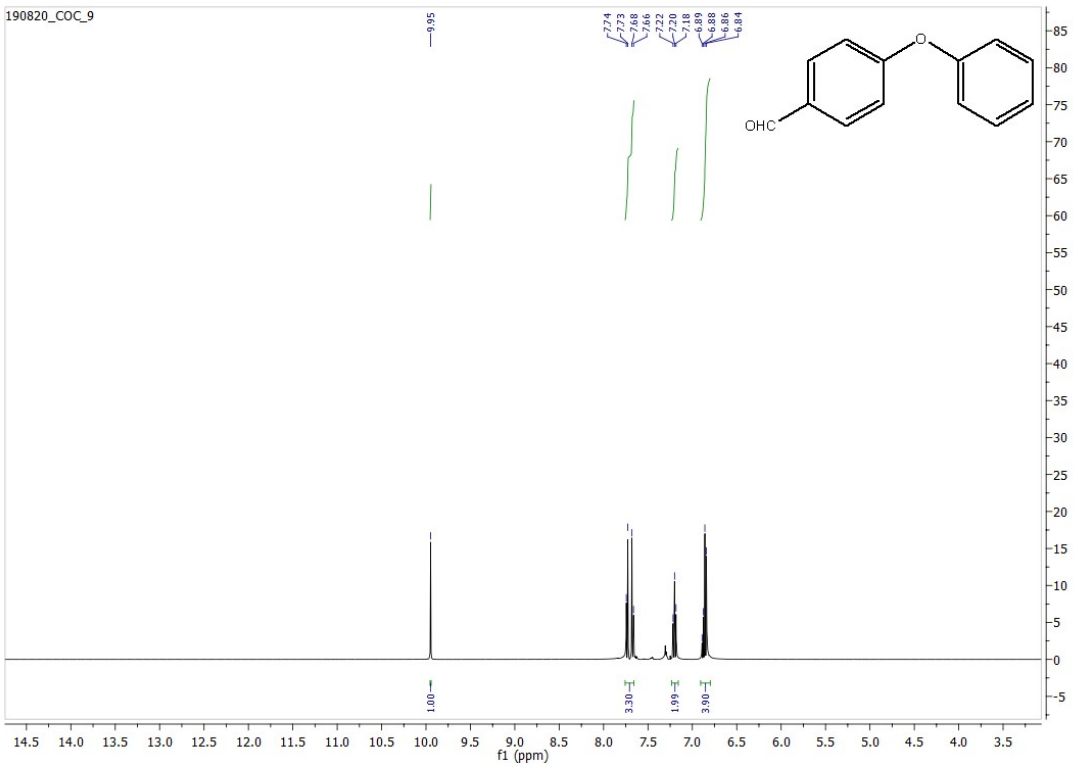


Fig. S17. ^{1}H NMR of 4-phenoxy benzaldehyde recorded in $CDCl_3$

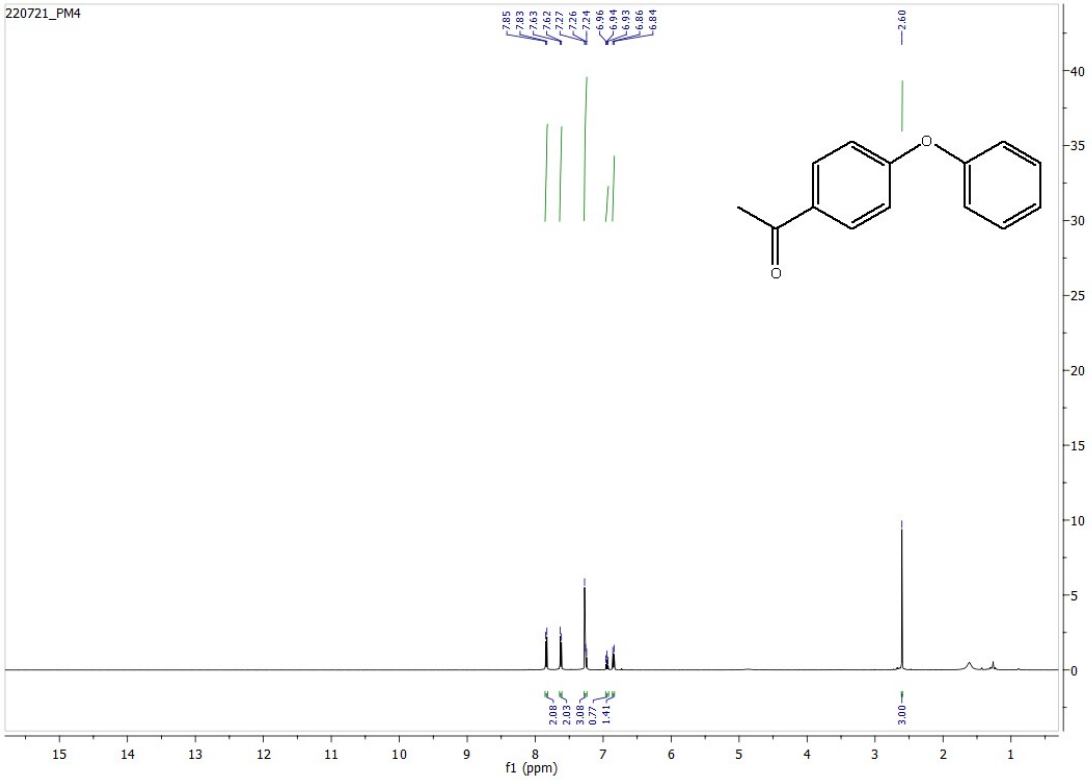


Fig. S18. ^{1}H NMR of 4-acetyl diphenylether recorded in $CDCl_3$

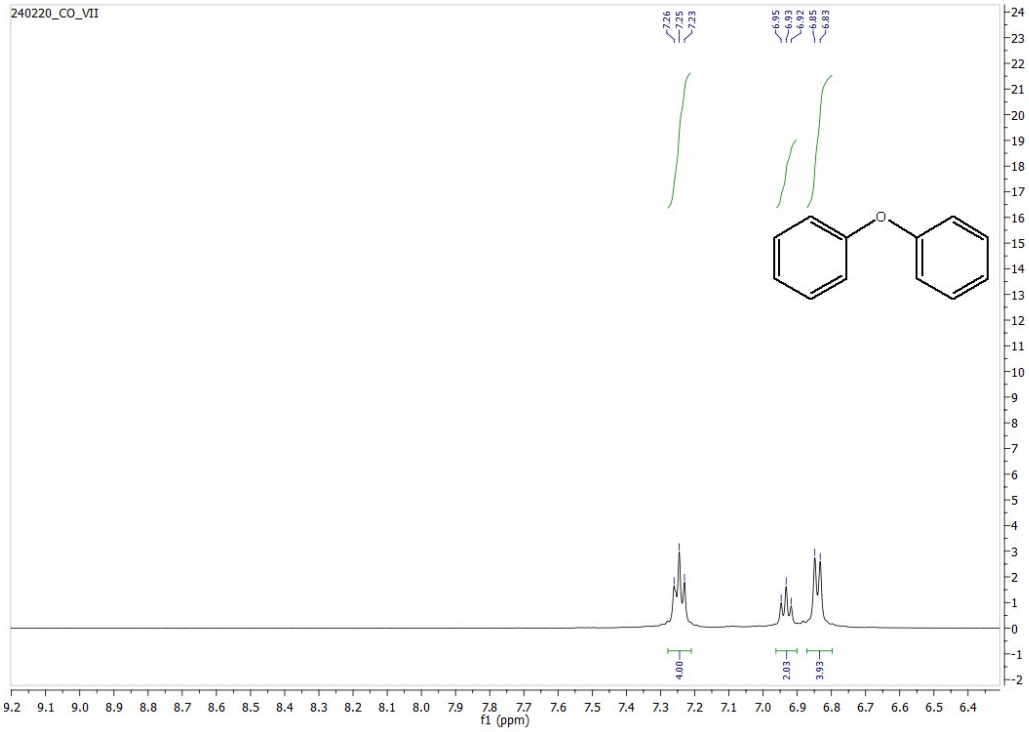


Fig. S19. ^{1}H NMR of diphenyl ether recorded in $CDCl_3$

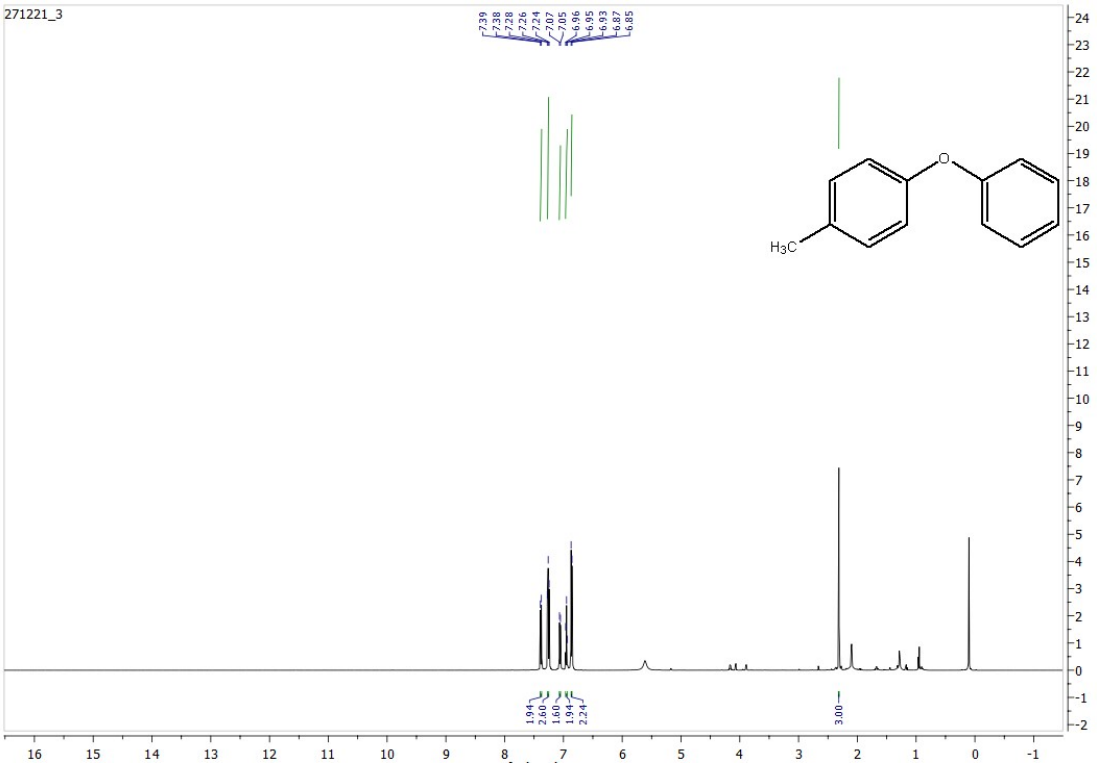


Fig. S20. ^{1}H NMR of 4-methyl diphenylether recorded in $CDCl_3$

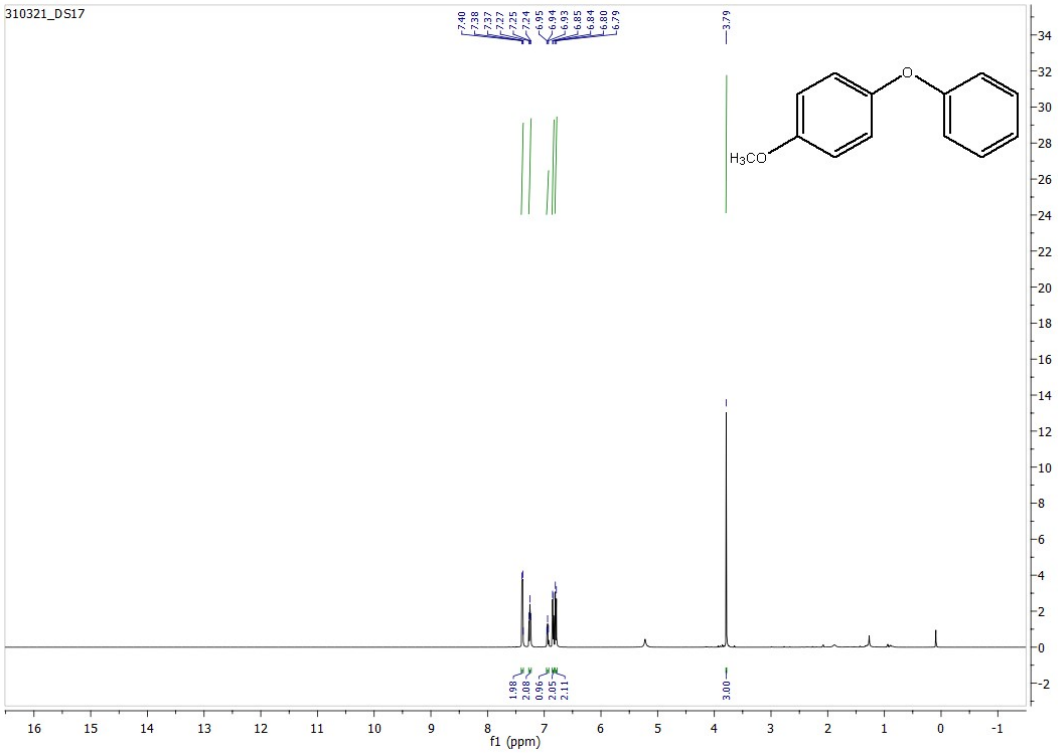
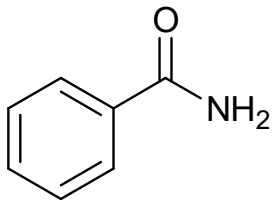
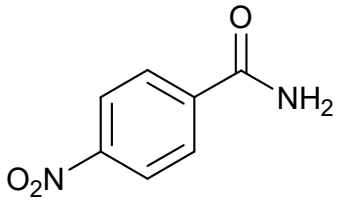


Fig. S21. ^{1}H NMR of 4-methoxy diphenylether recorded in $CDCl_3$

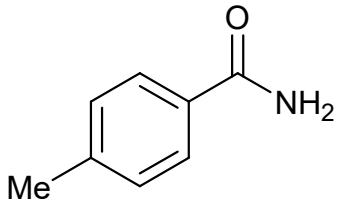
S3. NMR data of products obtained in Aldehyde to amide reactions of aryl aldehyde and hydroxylamine hydrochloride.



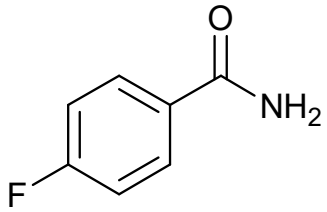
Benzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 7.816 (d, 2H, *J* = 7.6 Hz), 7.528 (t, 1H, *J* = 7.4 Hz), 7.4439 (t, 2H, *J* = 7.6 Hz), 6.2237 (br s, 2H).



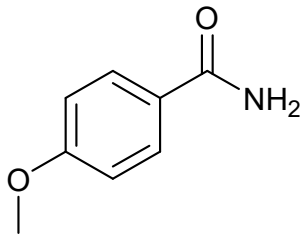
4- Nitrobenzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 8.15 (d, J = 9.2 Hz, 2H), 7.96 (d, J = 8.8 Hz, 2H), 7.45 (br s, 1H), 6.31 (br s, 1H).



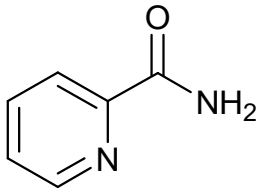
4-Methylbenzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 7.71 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H), 6.06 (br s, 1H), 5.78 (br s, 1H), 2.41 (s, 3H).



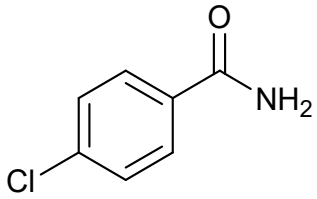
4-Fluorobenzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 7.845-7.816 (m, 2H), 7.129 (t, 2H), 6.052-5.830 (br s, 2H).



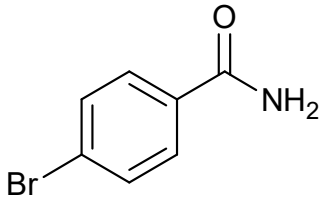
4-Methoxybenzmide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 7.782 (d, 2H, *J* = 8.7 Hz), 6.935 (d, 2H, *J* = 8.8 Hz), 6.004-5.709 (br s, 2H), 3.857 (s, 3H).



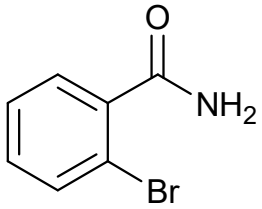
Picolinamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 8.56 (d, J = 2.0 Hz, 1H), 8.18 (d, J = 7.6 Hz, 1H), 7.84 (t, J = 7.6, 1.6 Hz, 2H), 7.45-7.42 (m, 1H), 5.73 (br s, 1H)



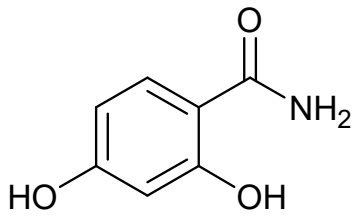
4-Chlorobenzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 7.755 (d, 2H, *J*= 8.4 Hz), 7.432 (d, 2H, *J* = 7.7 Hz), 6.040 (br s, 1H), 5.721 (br s, 1H).



4-Bromobenzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 7.648 (d, 2H, *J*= 8.4 Hz), 7.596 (d, 2H, *J* = 8.4 Hz), 6.041 (br s, 1H), 5.697 (br s, 1H).



2-Bromobenzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 7.65 (d, J = 8.0, 1.2 Hz, 1H), 7.58-7.46 (m, 3H), 6.35 (br s, 1H), 6.19 (br s, 1H)



2,4-dihydroxybenzamide: ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm): 13.26 (s, 1H), 10.04 (s, 1H), 8.08 (br s, 1H), 7.67 (d, J = 7.5, 1H), 7.55(br s, 1H), 6.26-6.21 (m, 2H)

S4. NMR spectra of products obtained in Aldehyde to amide reactions of aryl aldehyde and hydroxylamine hydrochloride.

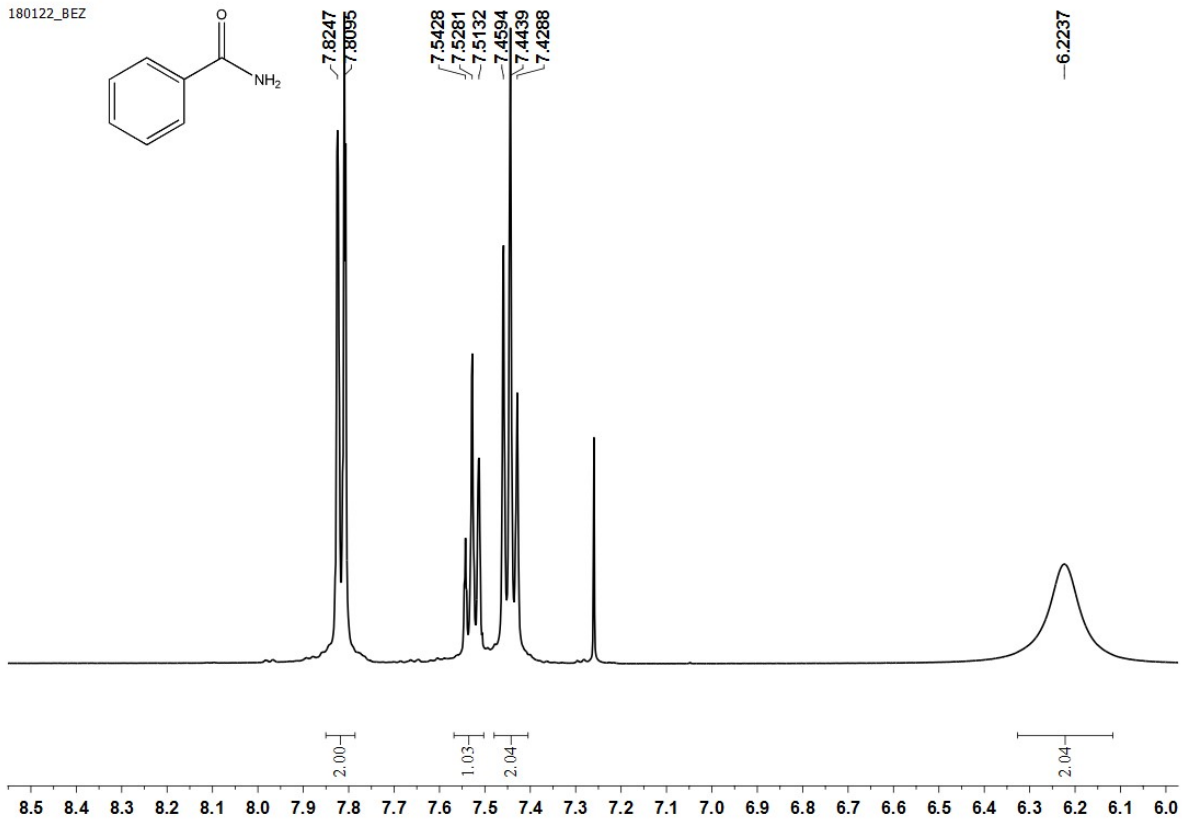


Fig. S22. ^{1}H NMR of Benzamide recorded in $CDCl_3$

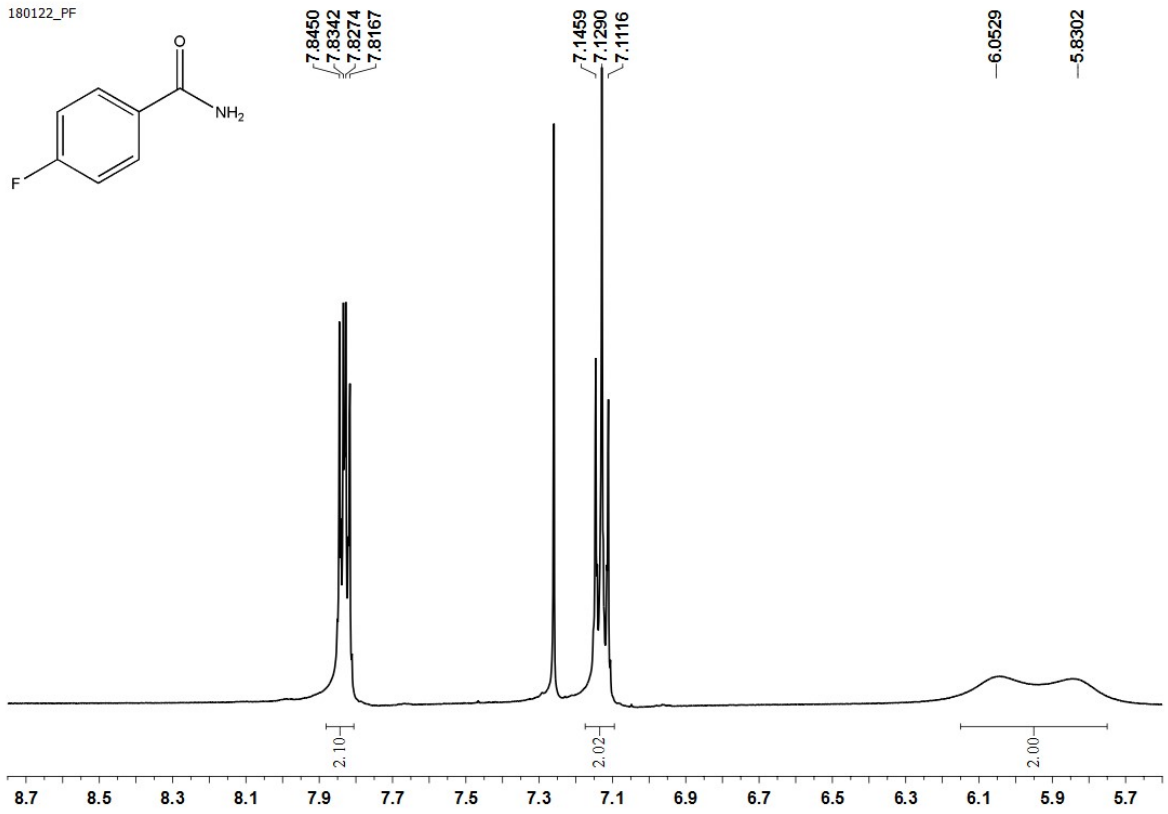


Fig. S23. ^{1}H NMR of 4-Fluorobenzamide recorded in $CDCl_3$

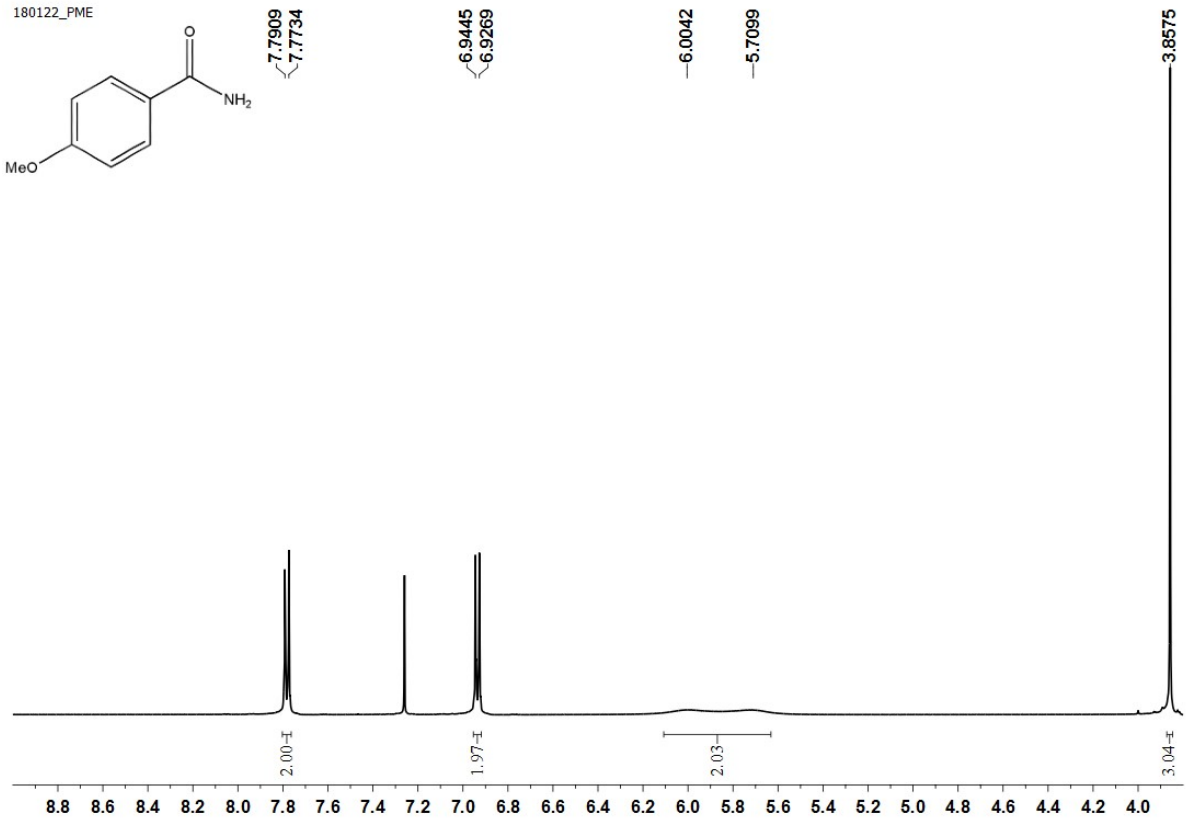


Fig. S24. ^{1}H NMR of 4-methoxybenzamide recorded in $CDCl_3$

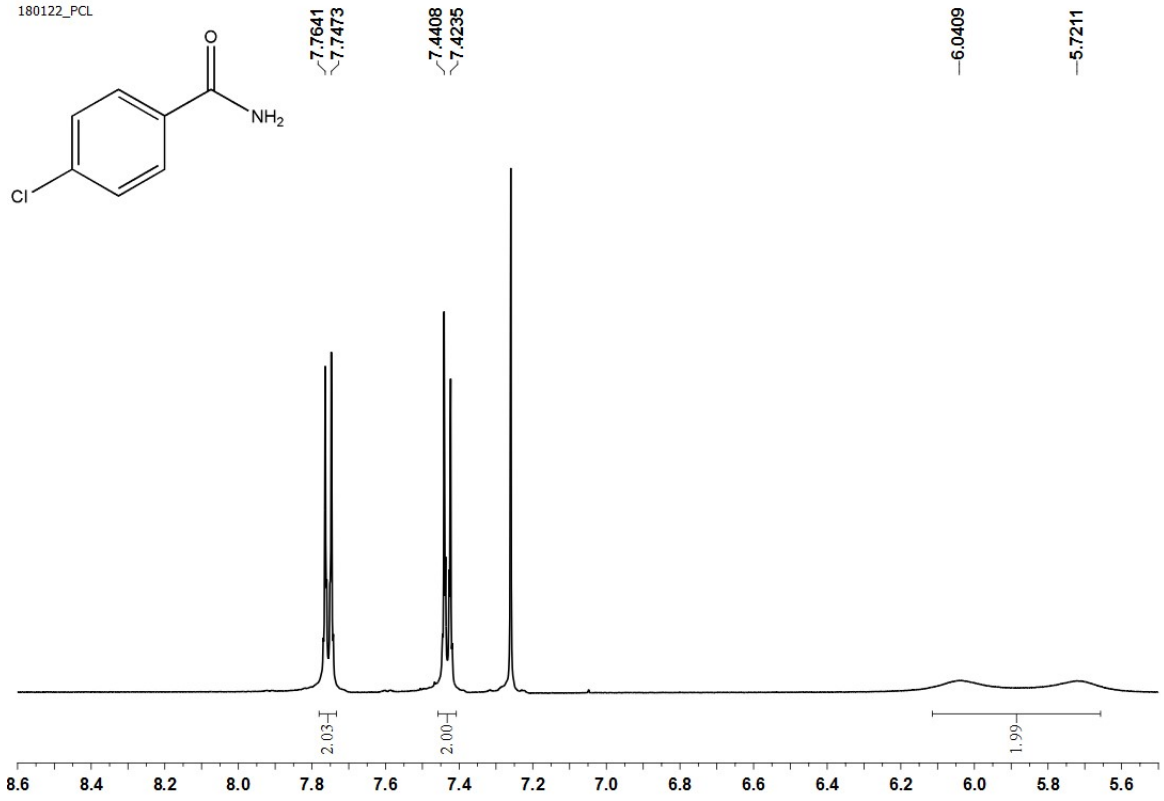


Fig. S25. ^{1}H NMR of 4-chlorobenzamide recorded in $CDCl_3$

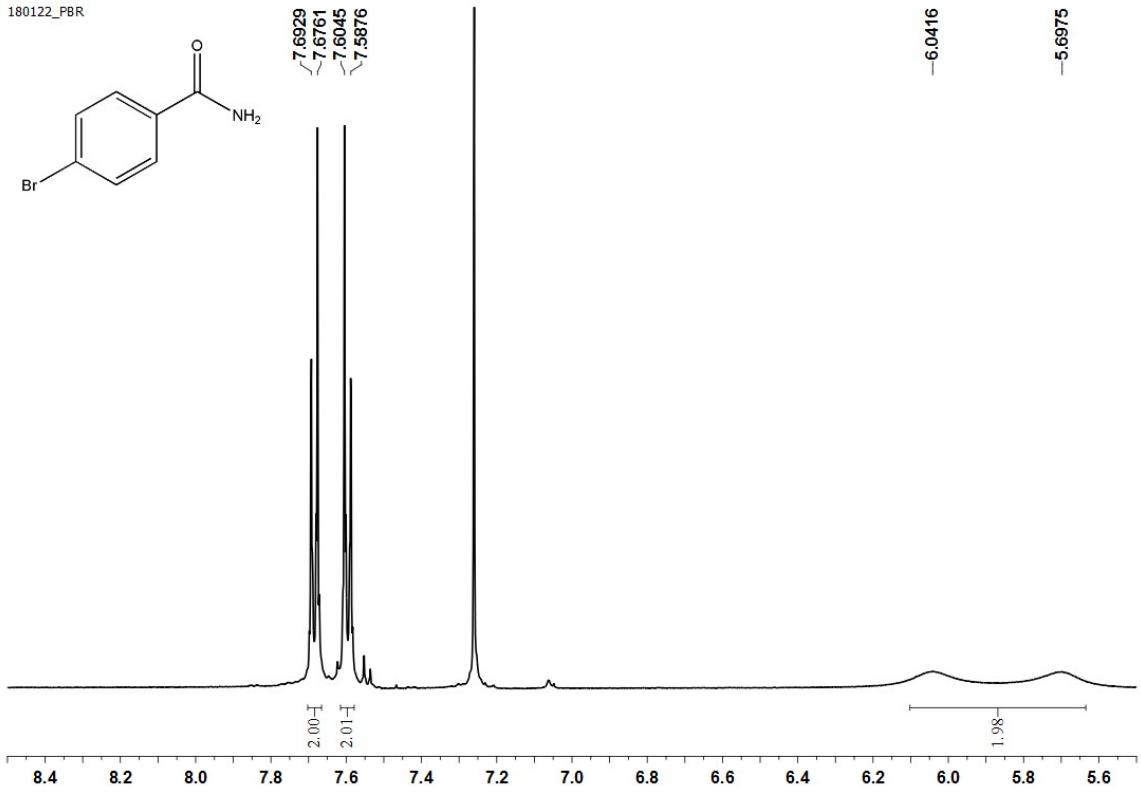


Fig. S26. ^{1}H NMR of 4-bromobenzamide recorded in $CDCl_3$