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Supplementary Material

1*H*,4*H*-Piperazine-diium Dichlorosulfonate: Structure Elucidation and its Dual Solvent-Catalyst Activity for the Synthesis of New Dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine Scaffolds

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Figure S1. Photo of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ at 20 °C.

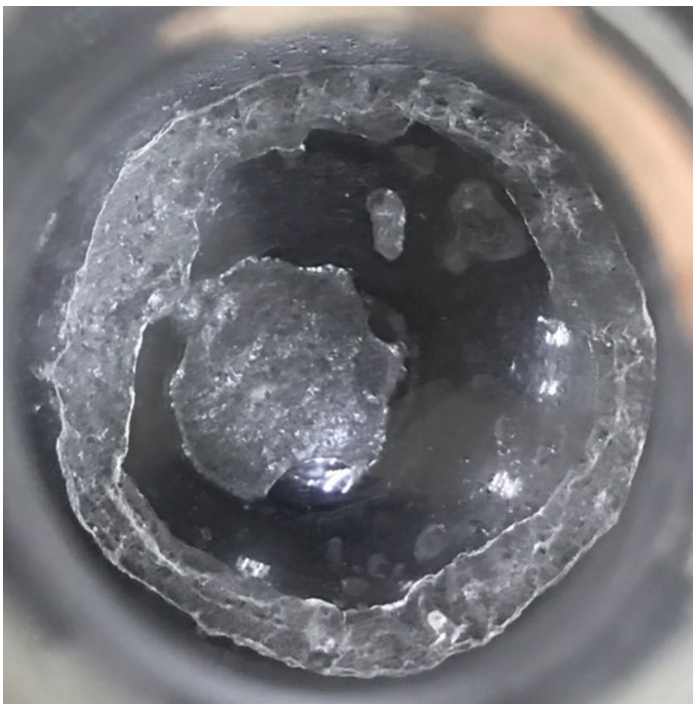


Figure S2. ^{1}H NMR of piperazine (600 MHz, DMSO-d_6).

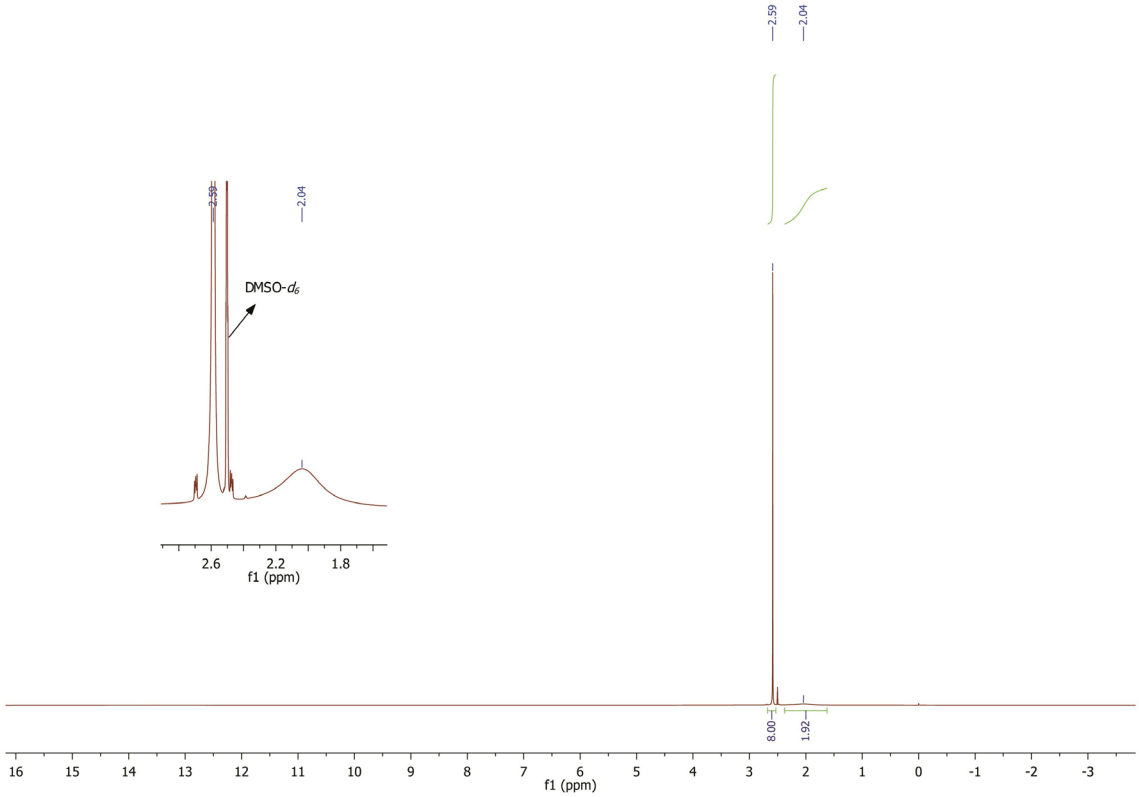


Figure S3. ^{13}C NMR of piperazine (600 MHz, DMSO-d_6).

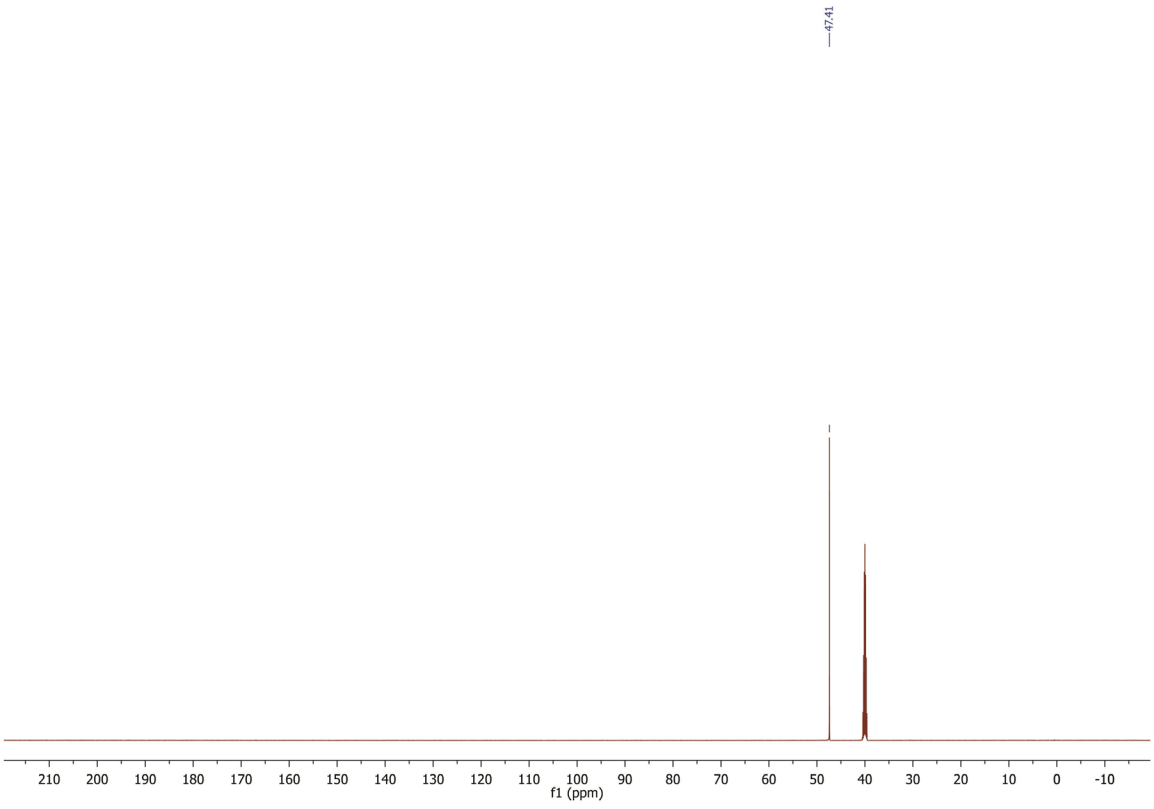


Figure S4. ^{1}H NMR of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (600 MHz, DMSO-d_6).

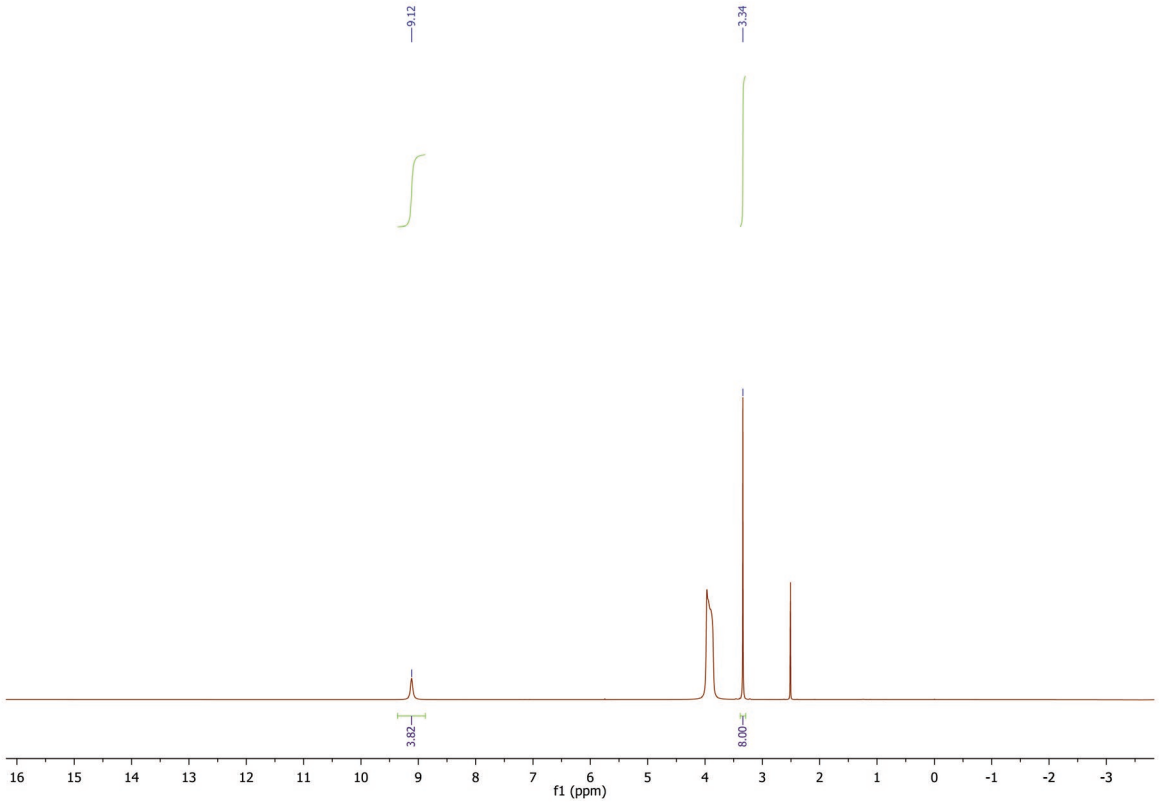


Figure S5. ^{13}C NMR of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (150 MHz, CDMSO-d_6).

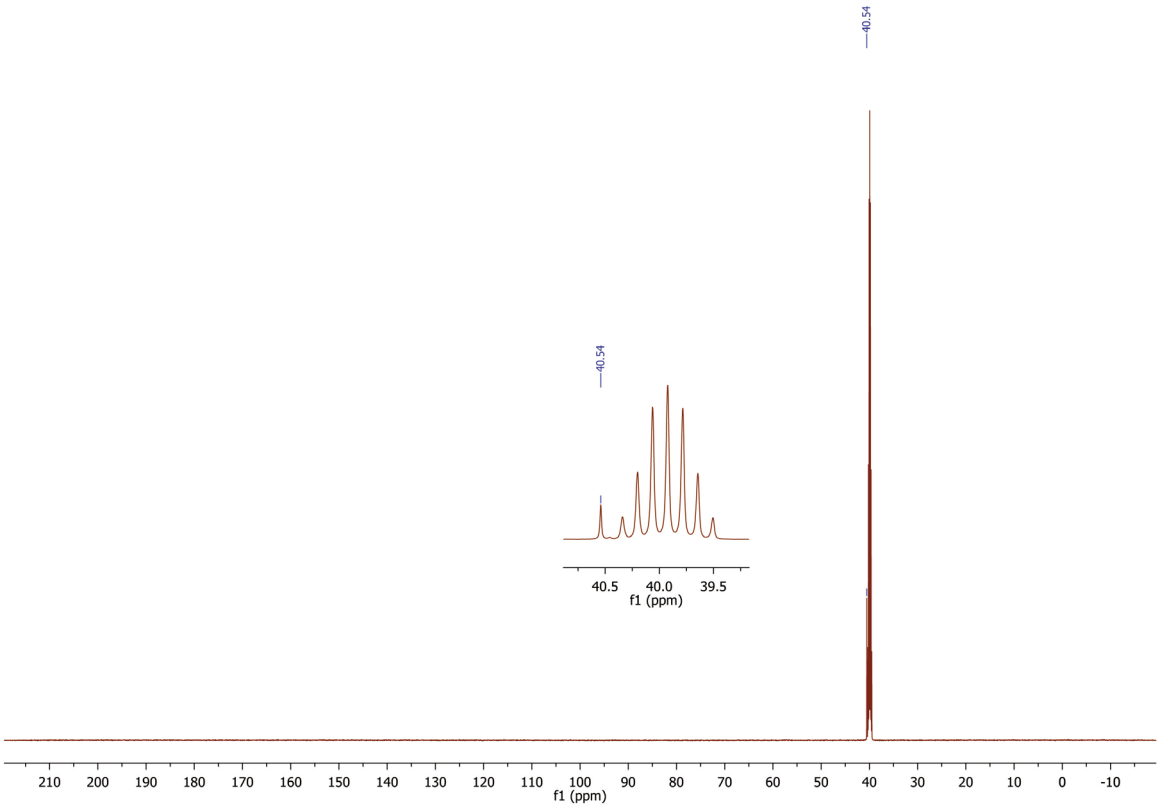


Figure S6. ^{1}H NMR of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (600 MHz, DMSO-d_6).

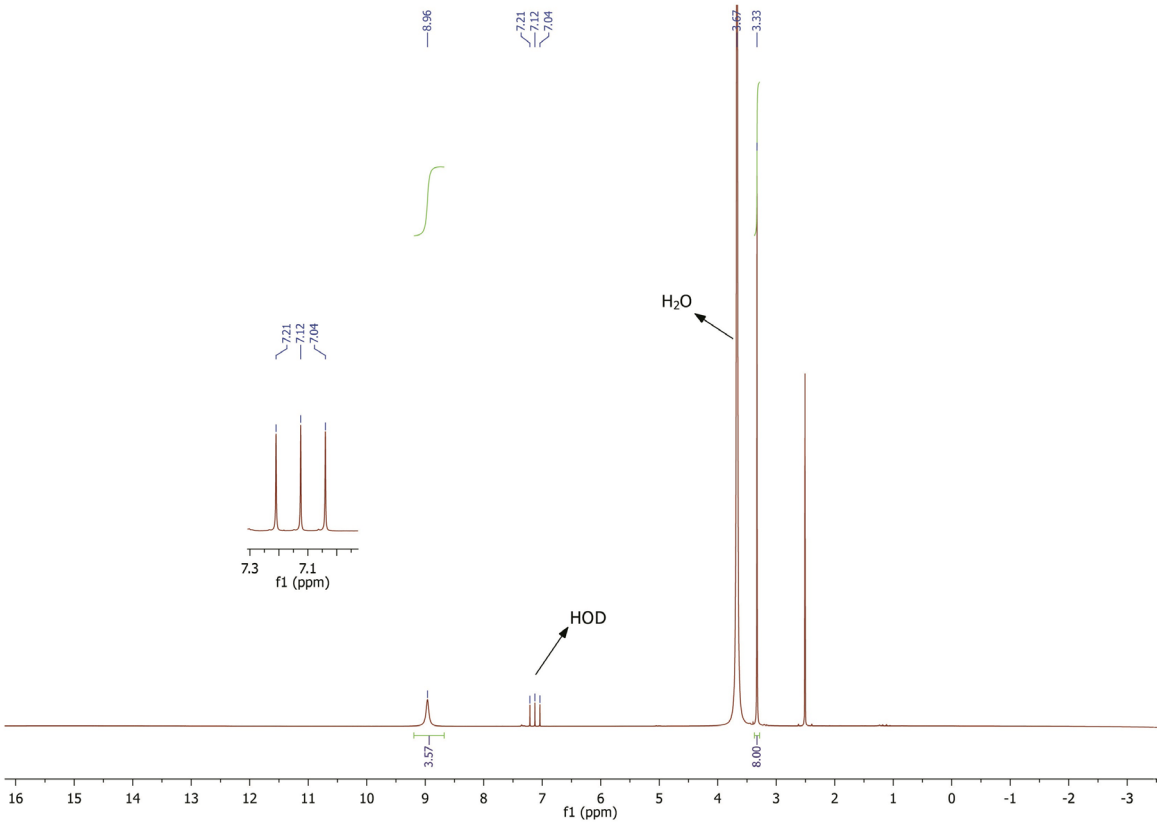


Figure S7. ^{1}H NMR of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (600 MHz, D_2O).

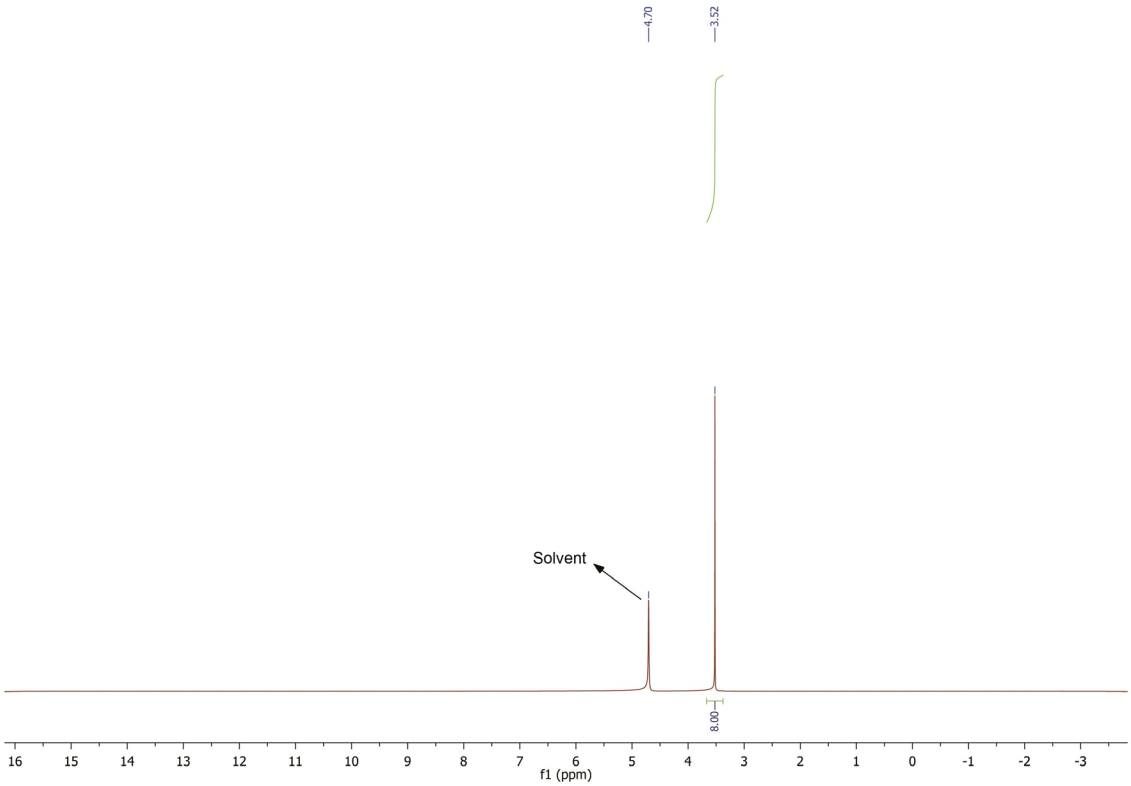


Figure S8. ^{1}H,^{1}H-COSY of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_4]^{2+}[ClSO_3^-]_2$ (600 MHz, CDMSO-d_6).

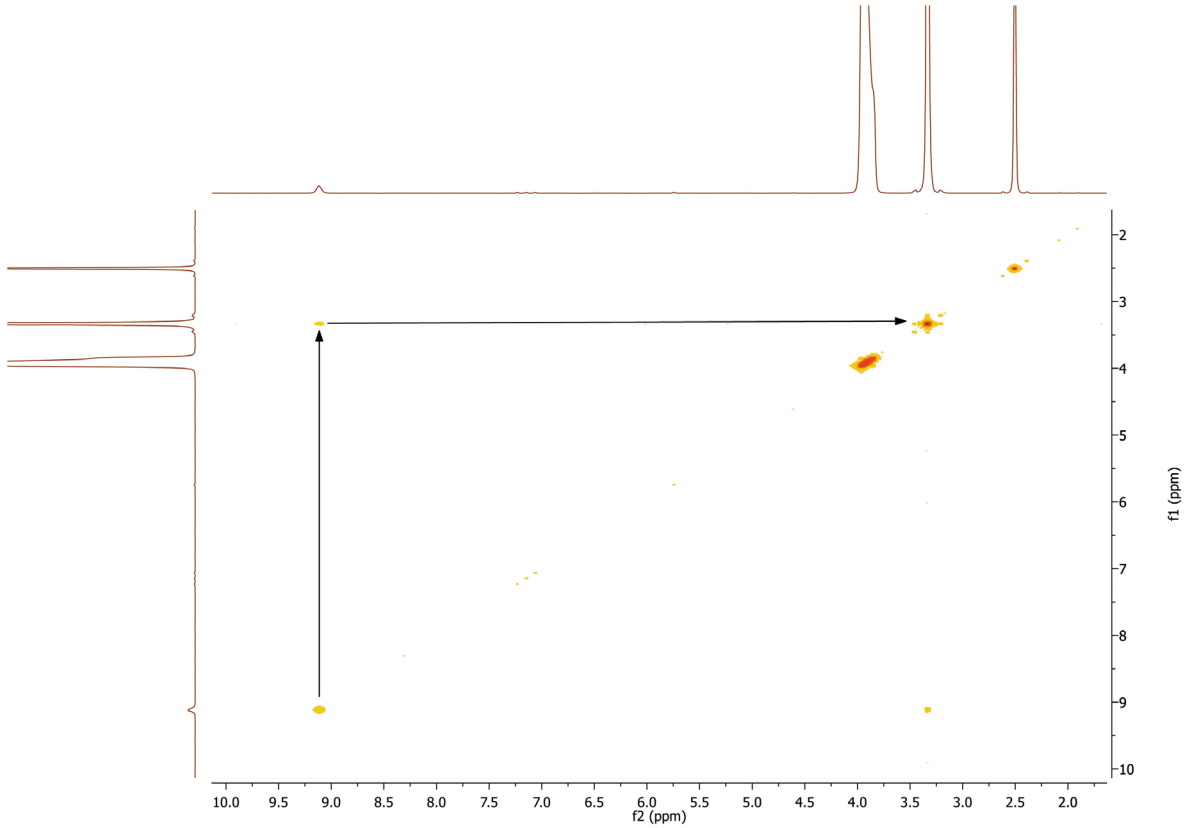


Figure S9. $^{1}H,^{13}C$-HMBC of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_4]^{2+}[ClSO_3^-]_2$ (600 MHz, CDMSO-d_6).

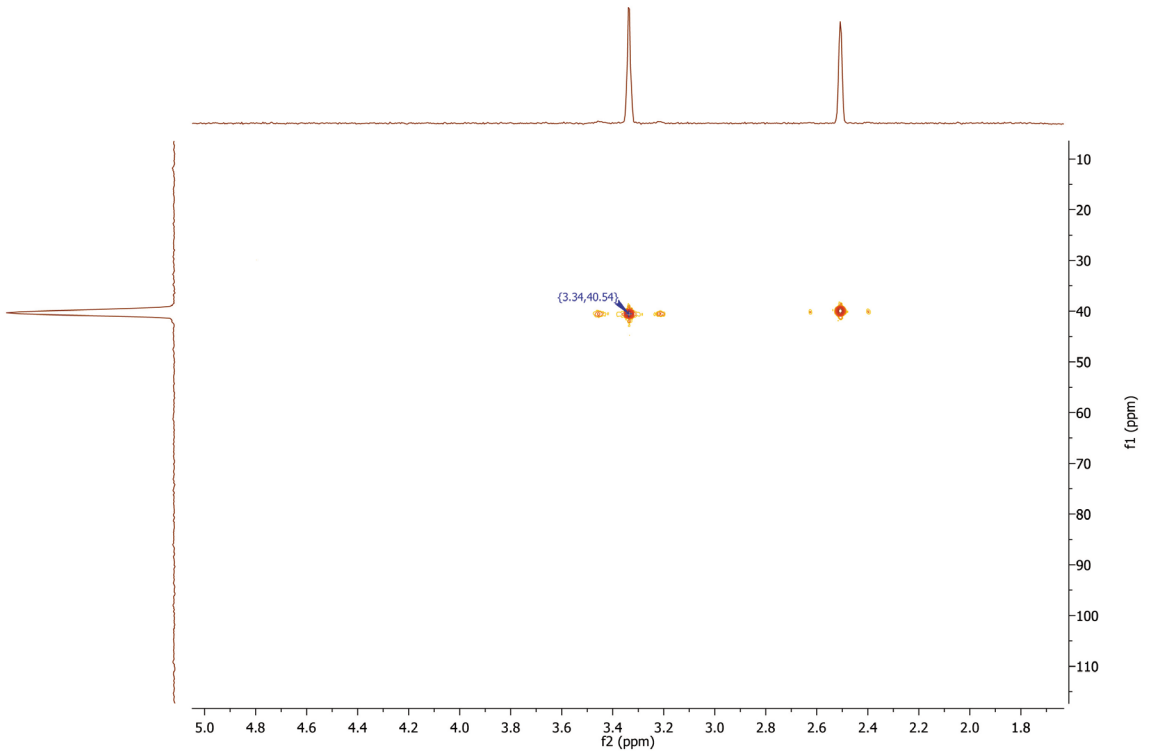


Figure S10. $^{1}H,^{15}N$-HMBC of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_4]^{2+}[ClSO_3^-]_2$ (600 MHz, CDMSO-d_6).

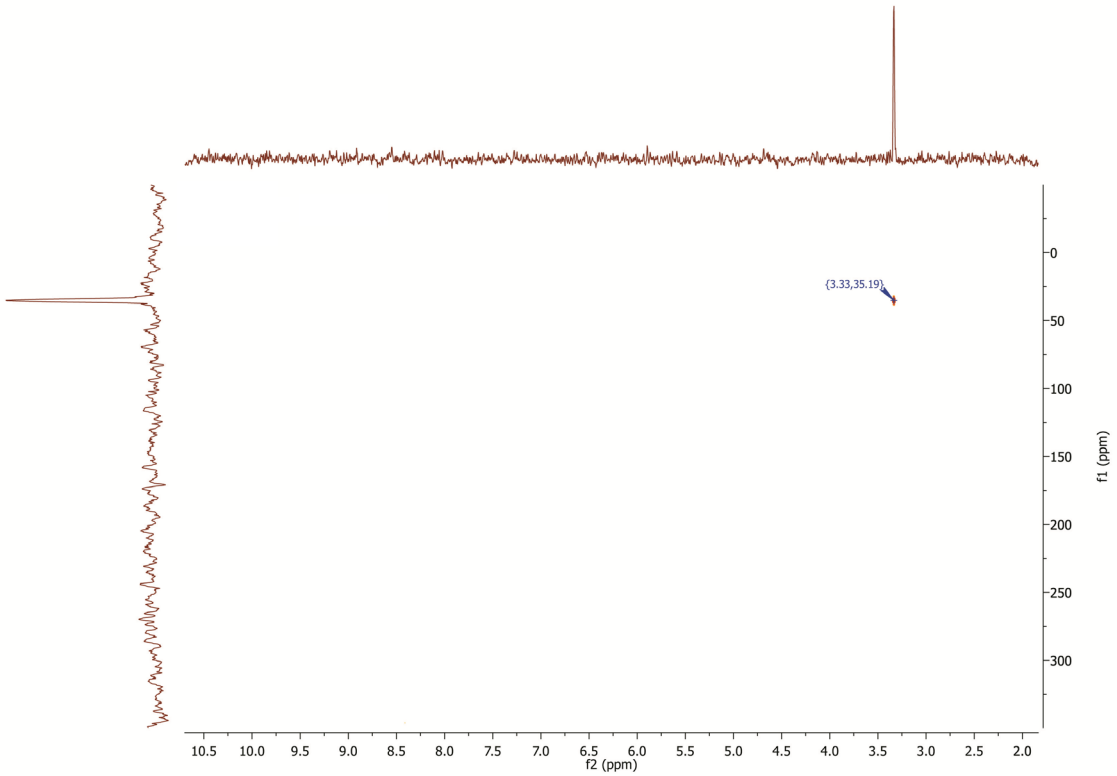


Figure S11. The FTIR of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (in the range of 4000-400 cm^{-1}).

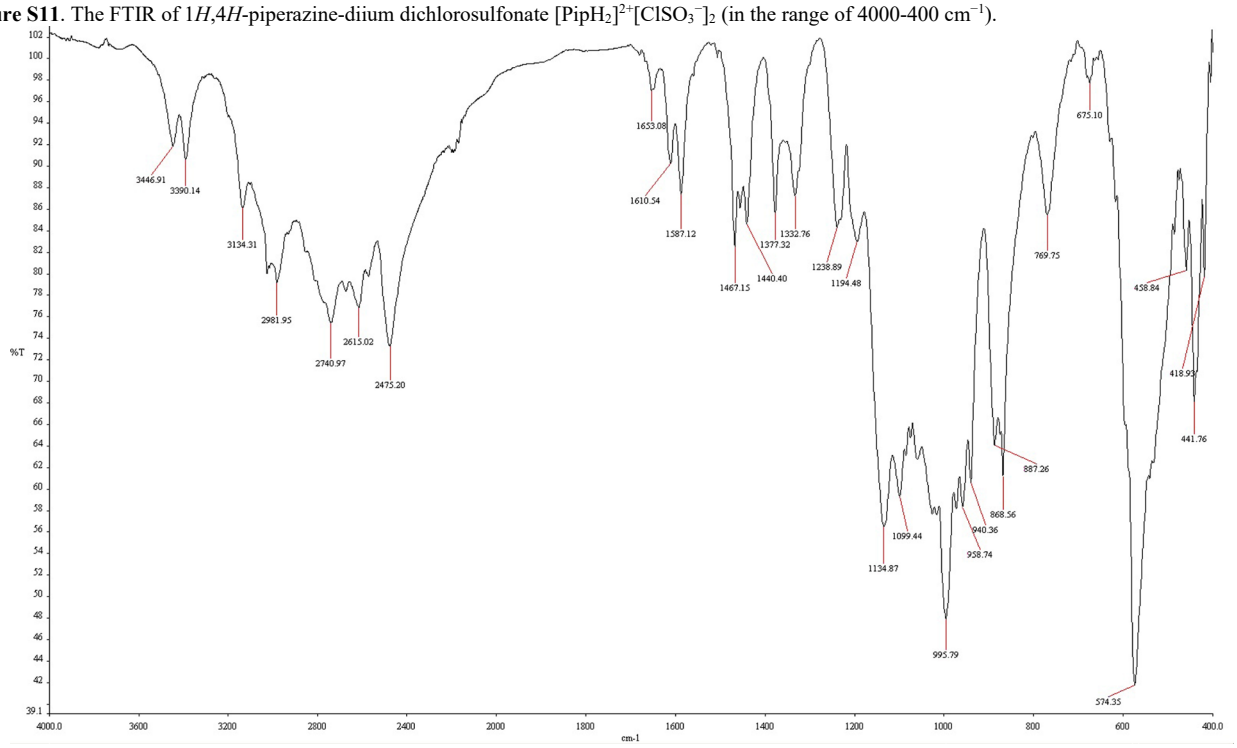


Figure S12. The Raman spectrum of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (in the range of 3200-100 cm^{-1} at 514 nm).

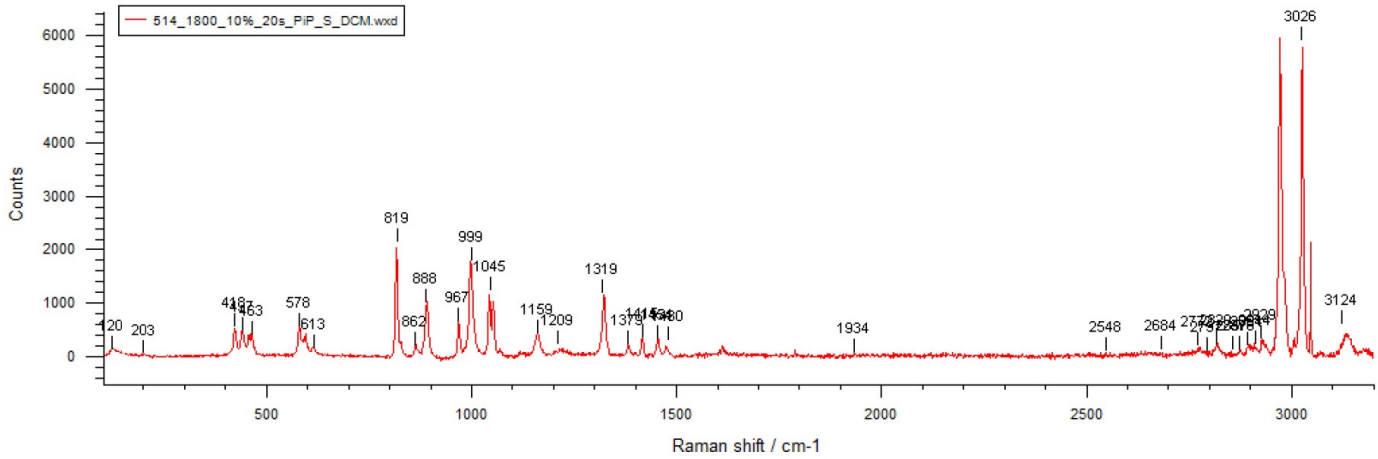


Figure S13. The DSC of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (in two cycles at a temperature ranges 30-300 and 30-500 °C).

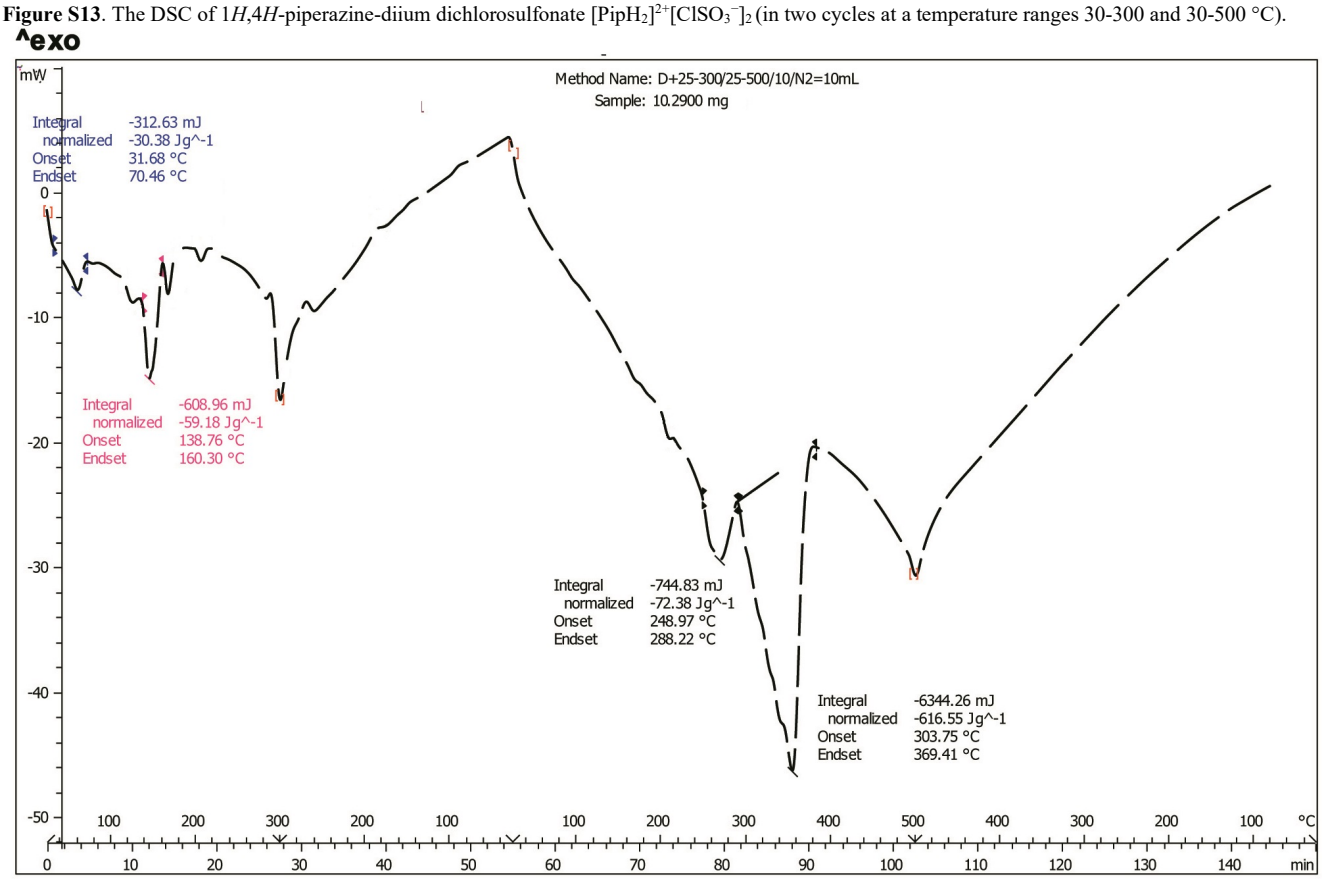
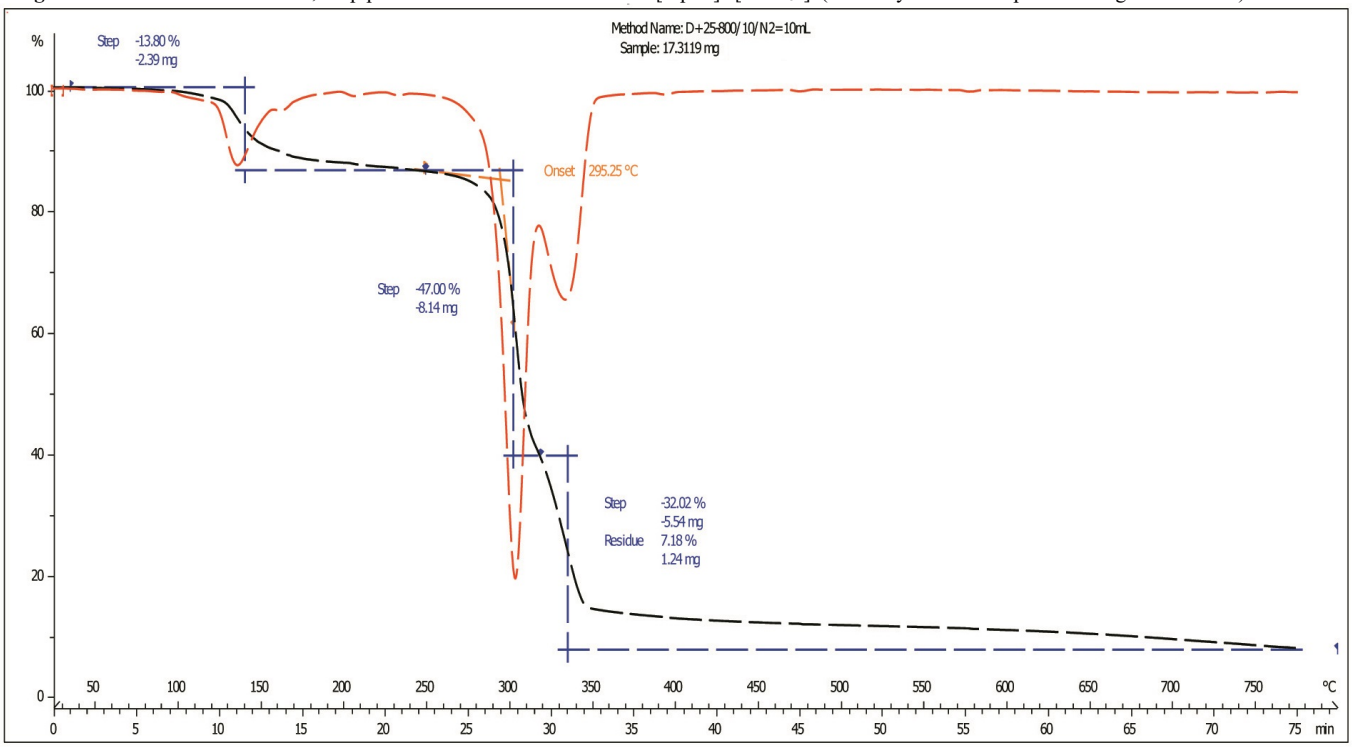
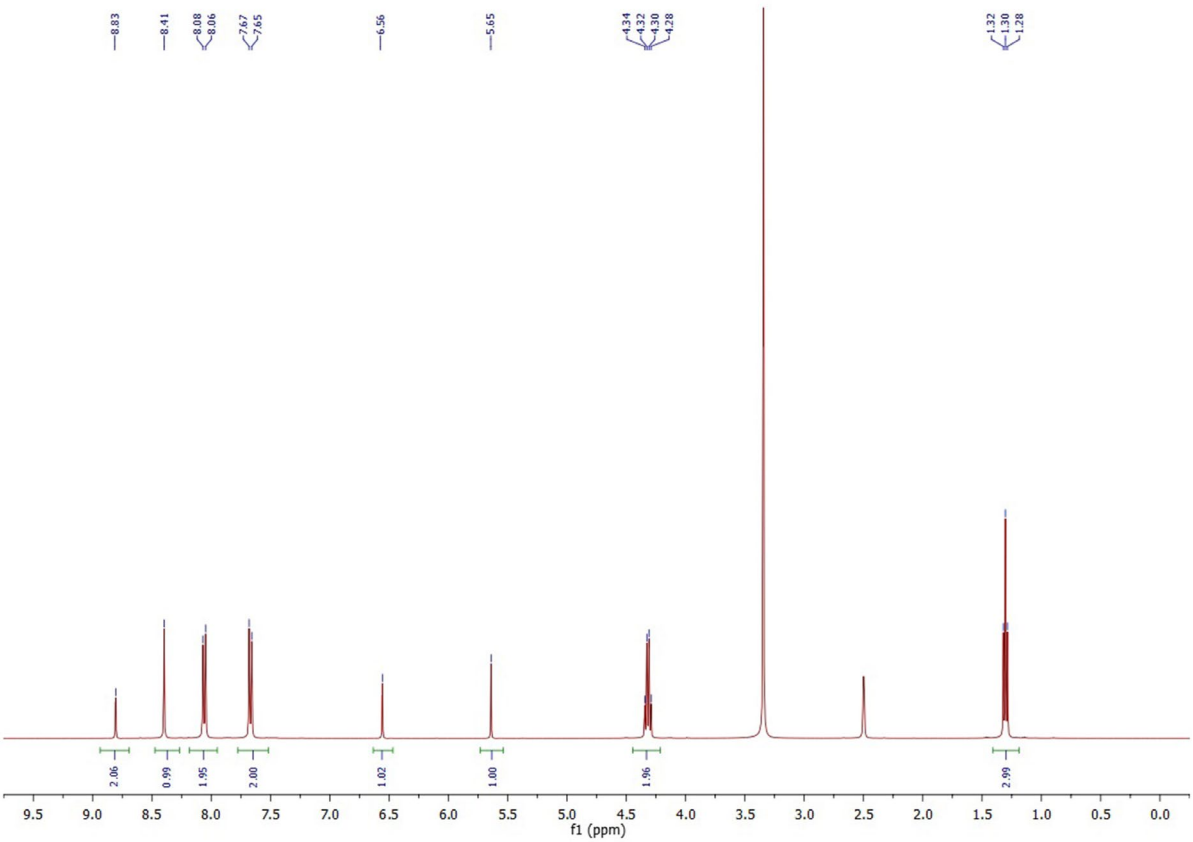


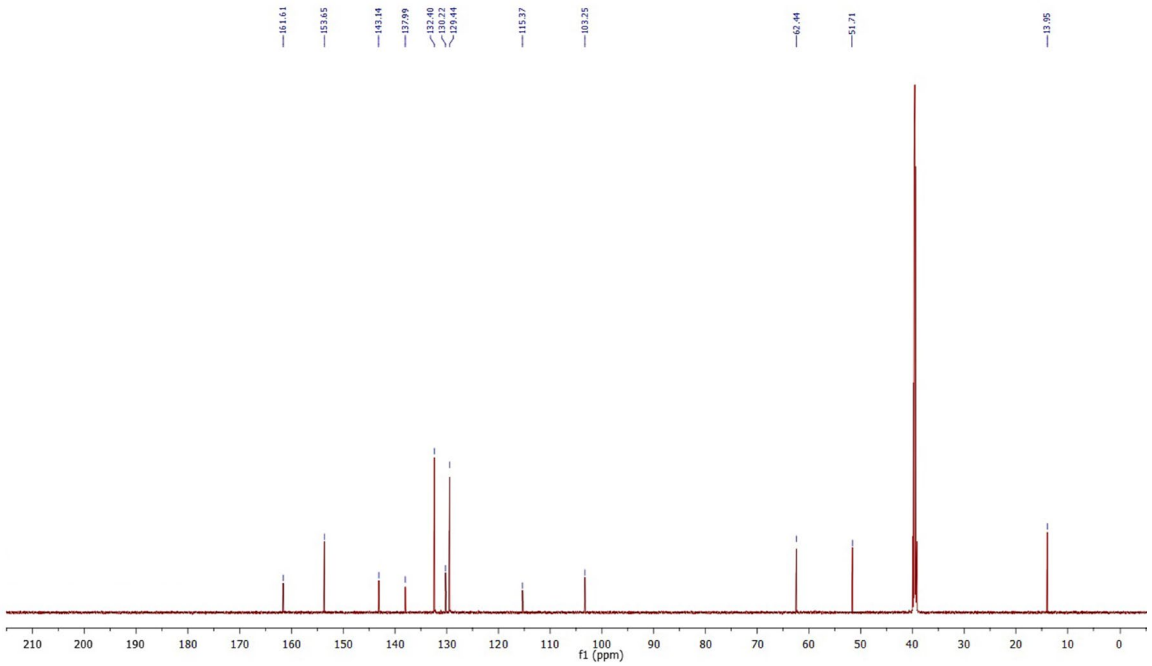
Figure S14. The TGA/DTA of 1*H*,4*H*-piperazine-diium dichlorosulfonate $[PipH_2]^{2+}[ClSO_3^-]_2$ (in two cycles at a temperature ranges 30-800 °C).



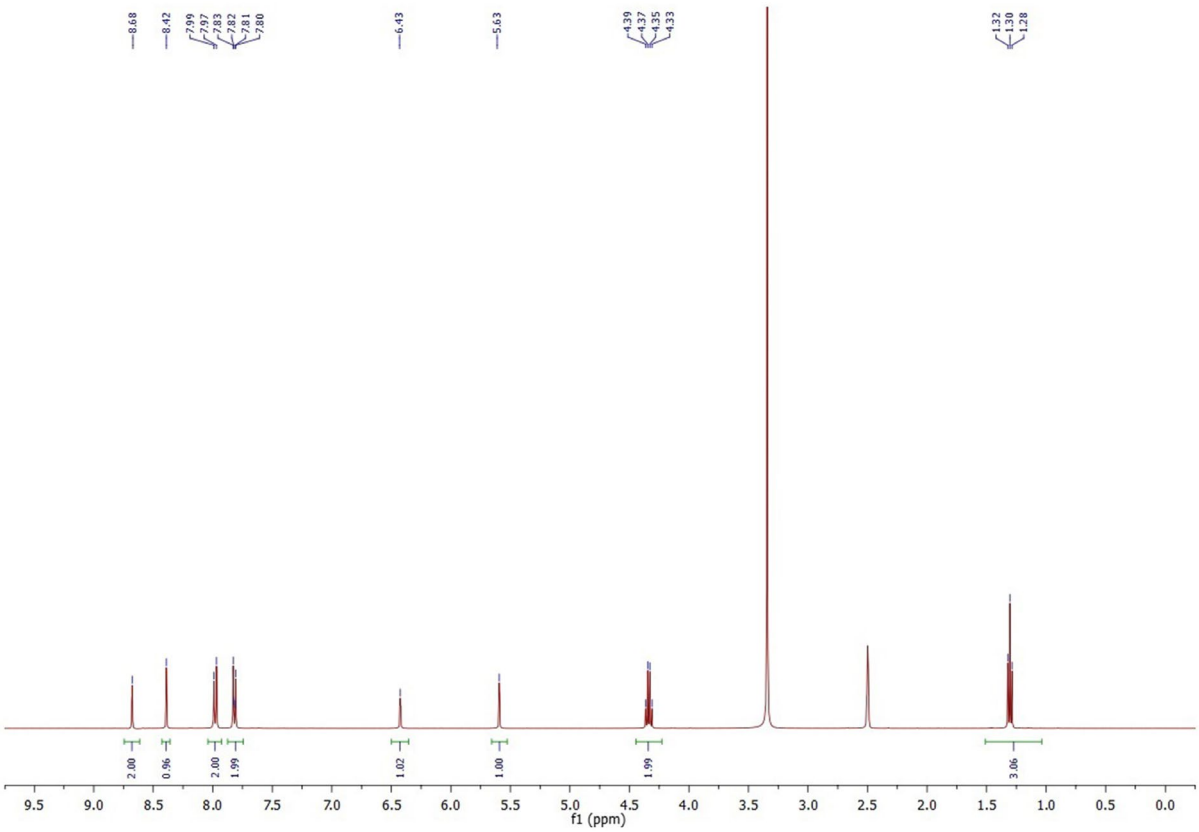
^{1}H and ^{13}C NMR spectra copies of the dihydro-[1,2,4]triazolo[1,5-a]pyrimidines recorded with Bruker Avance instruments (400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR in DMSO-d_6).

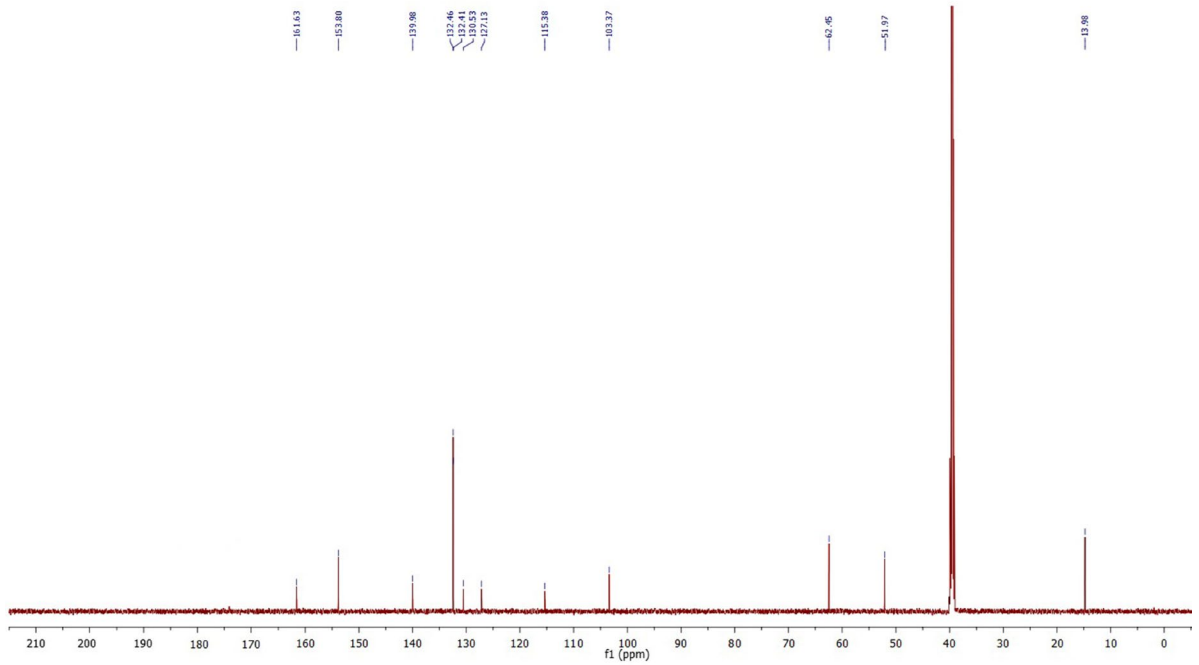
Ethyl 5-amino-7-(4-chlorophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2a**)



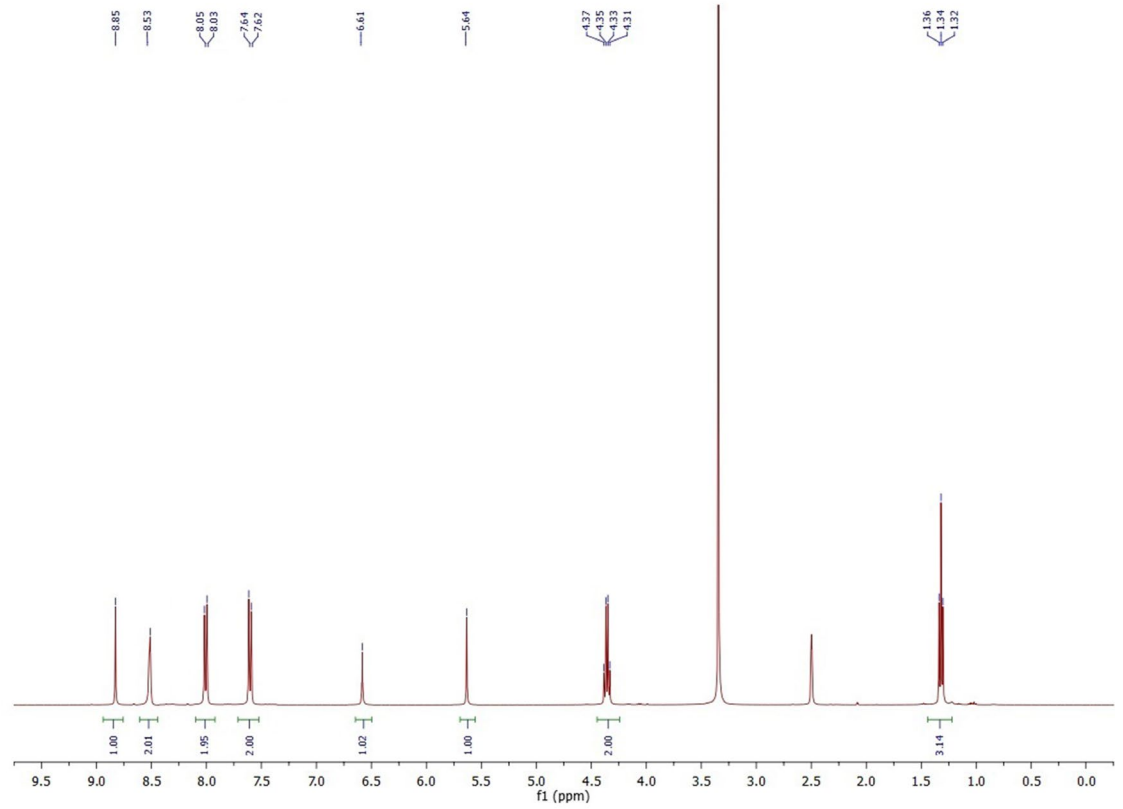


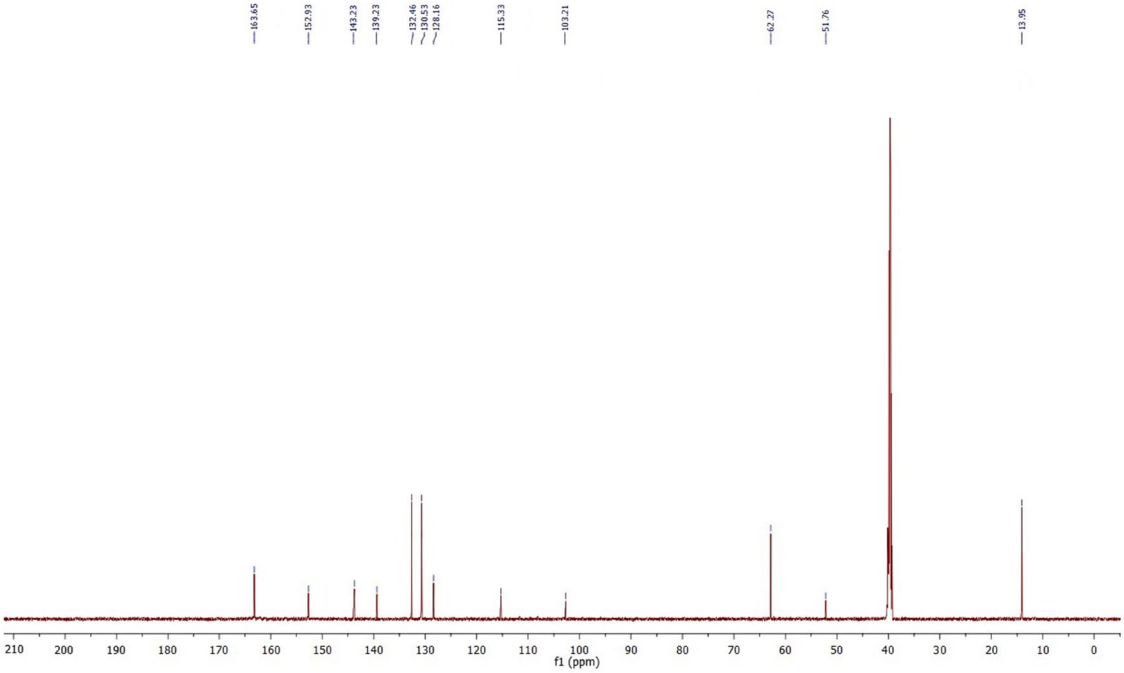
Ethyl 5-amino-7-(4-bromophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2b**)



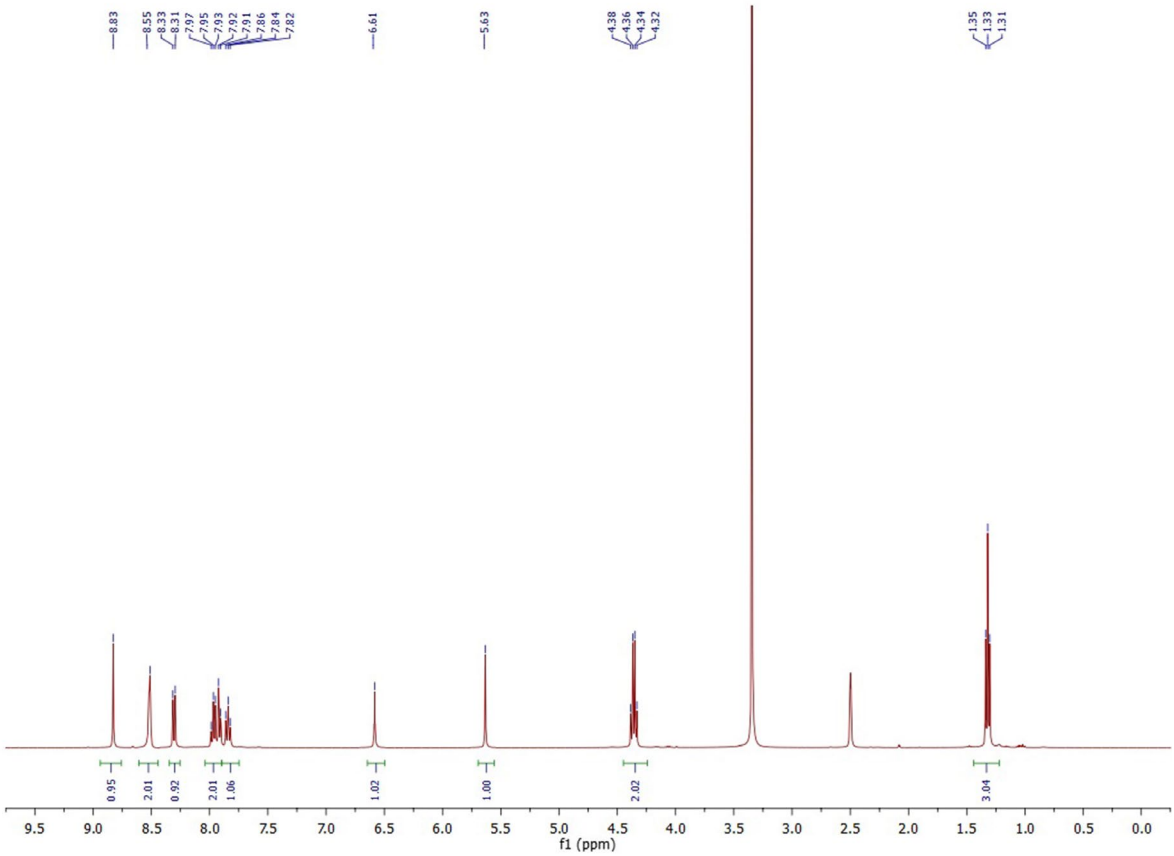


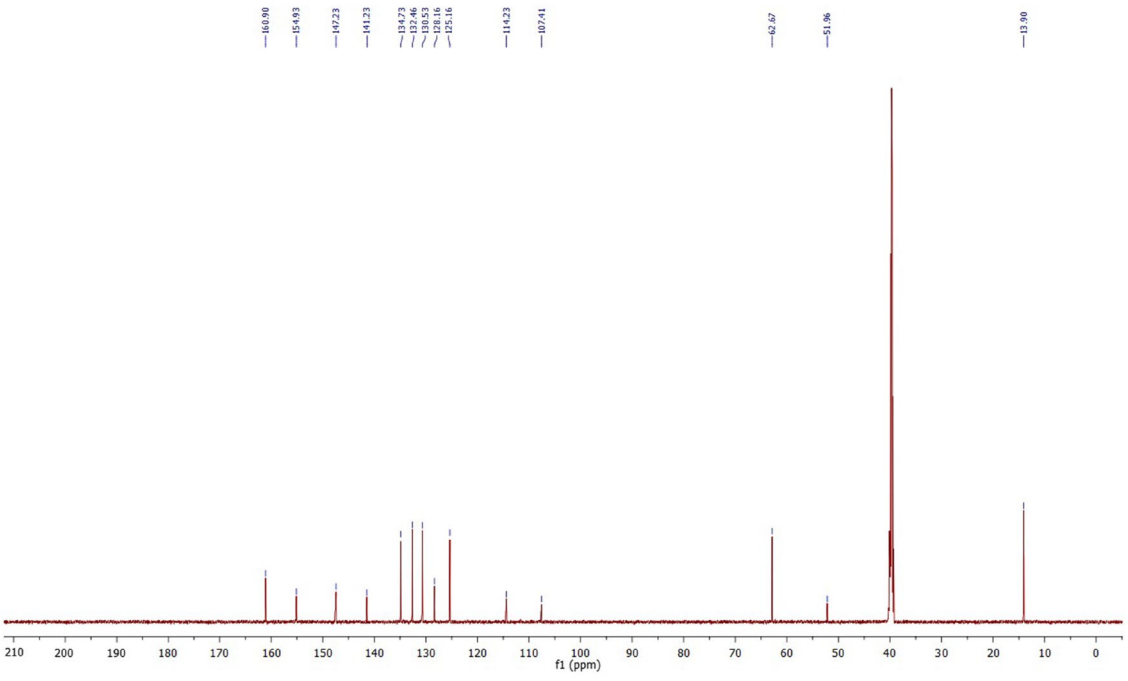
Ethyl 5-amino-7-(4-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2c**)



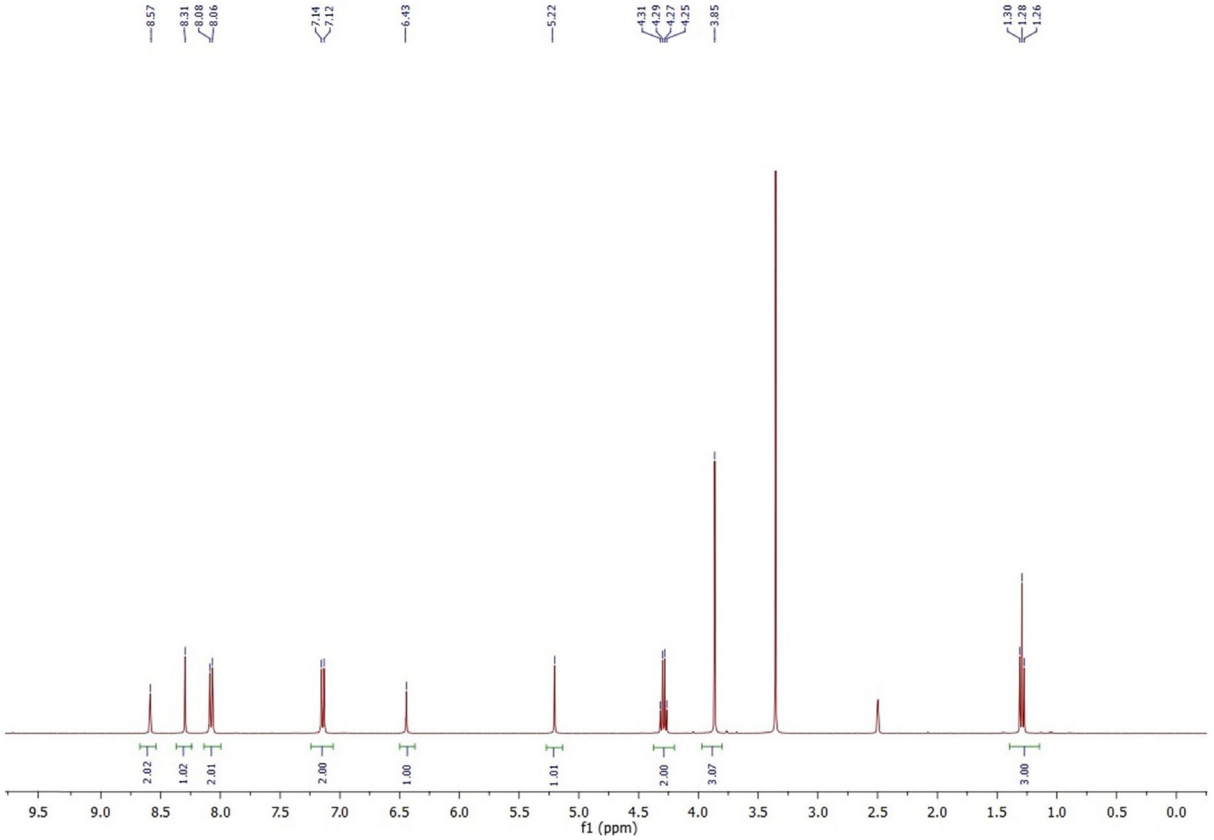


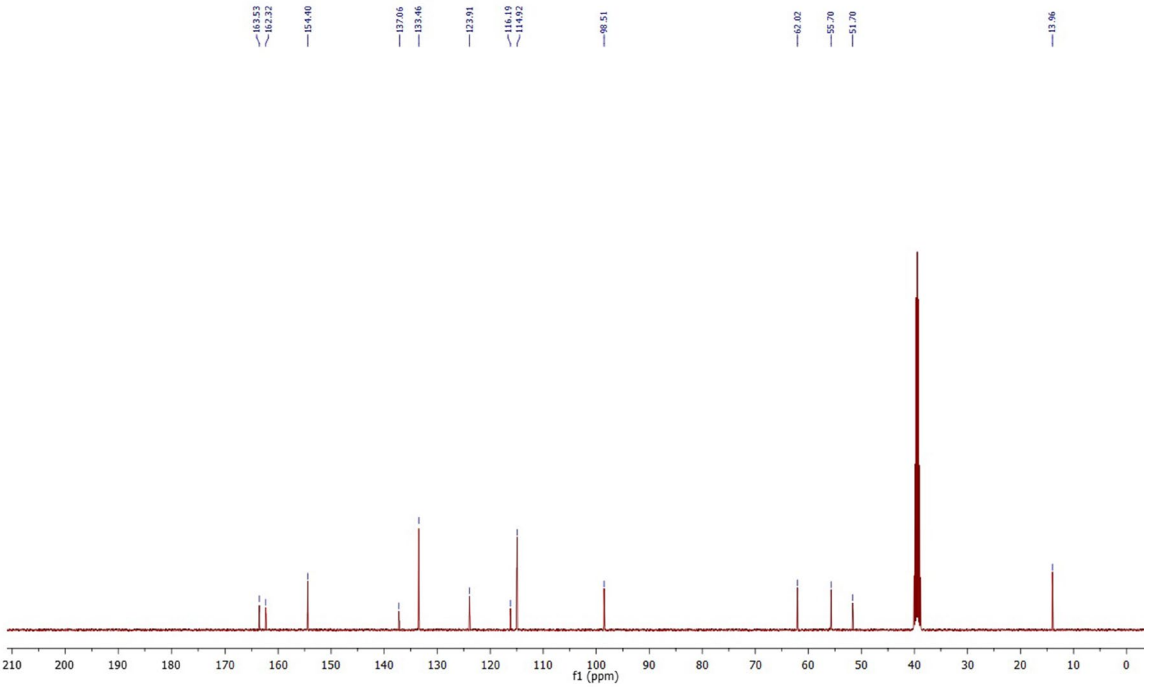
Ethyl 5-amino-7-(2-nitrophenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2d**)



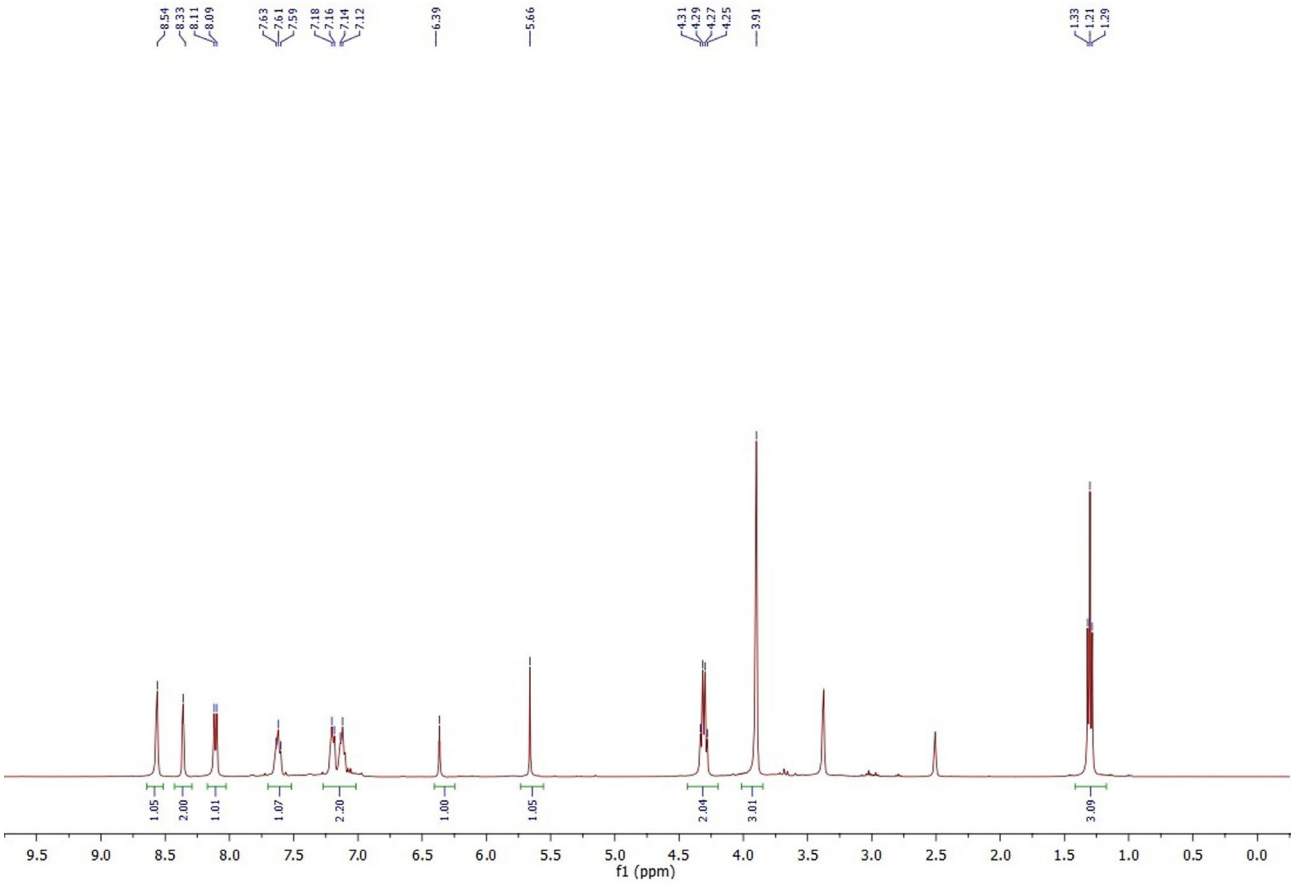


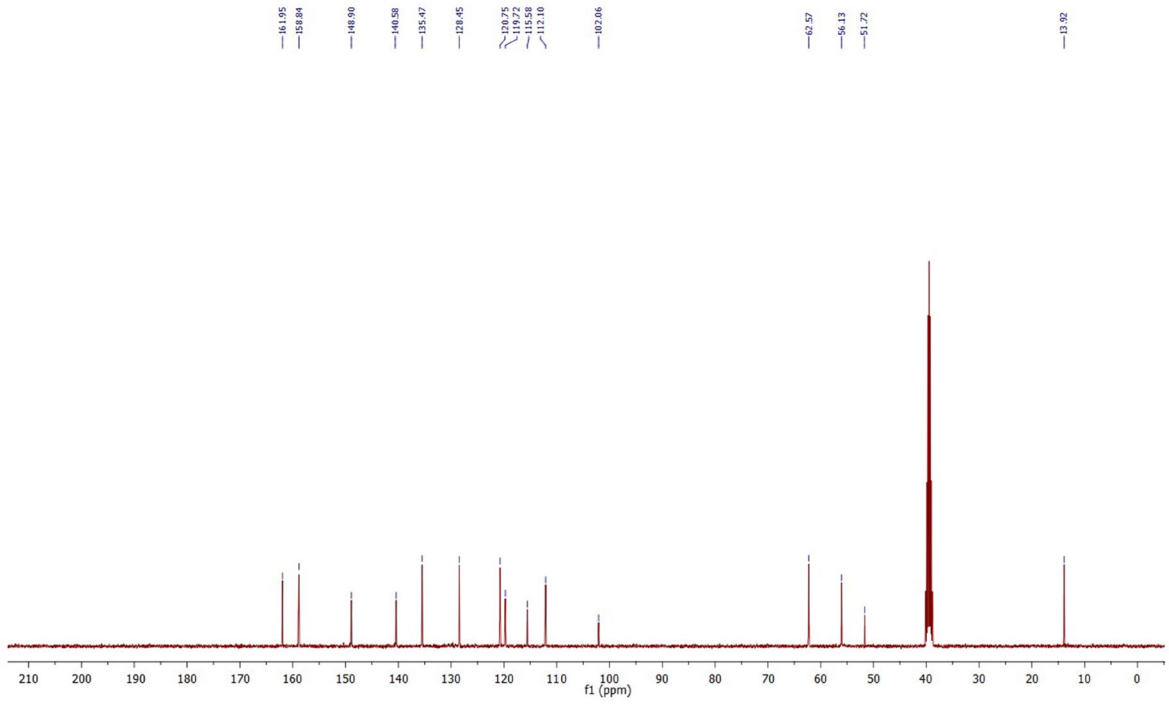
Ethyl 5-amino-7-(4-methoxyphenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2e**)



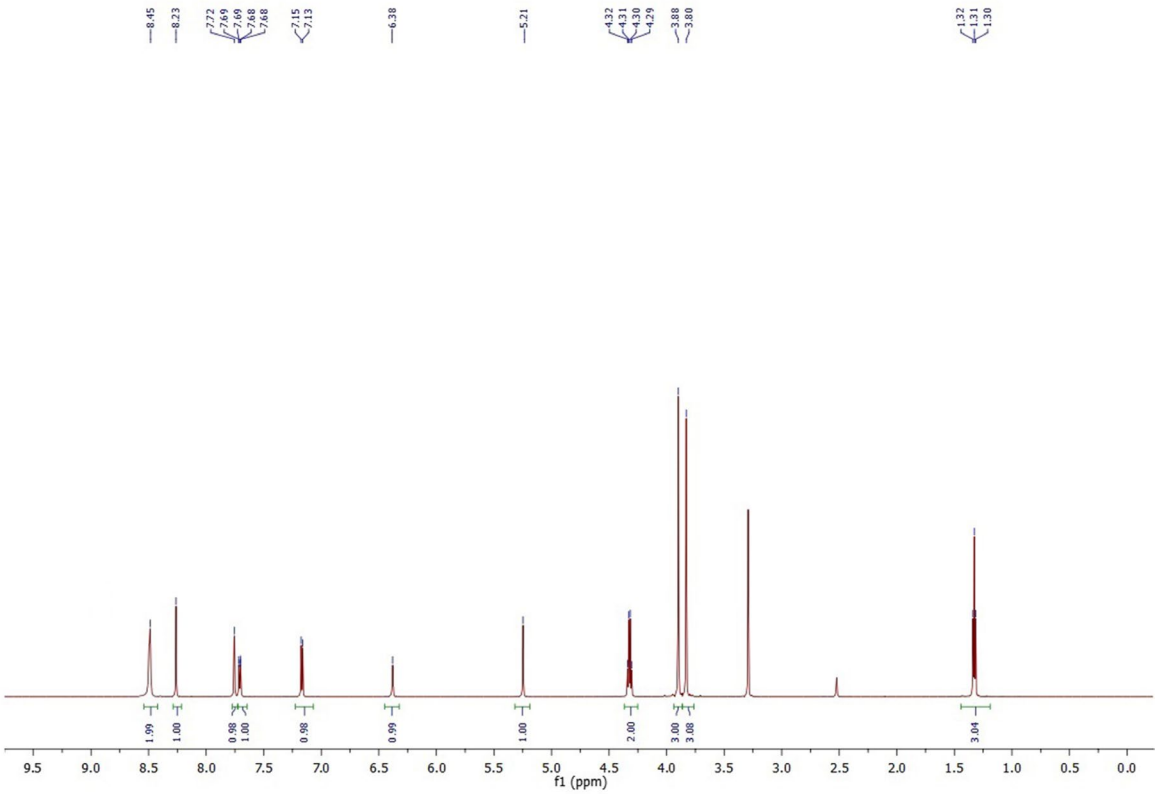


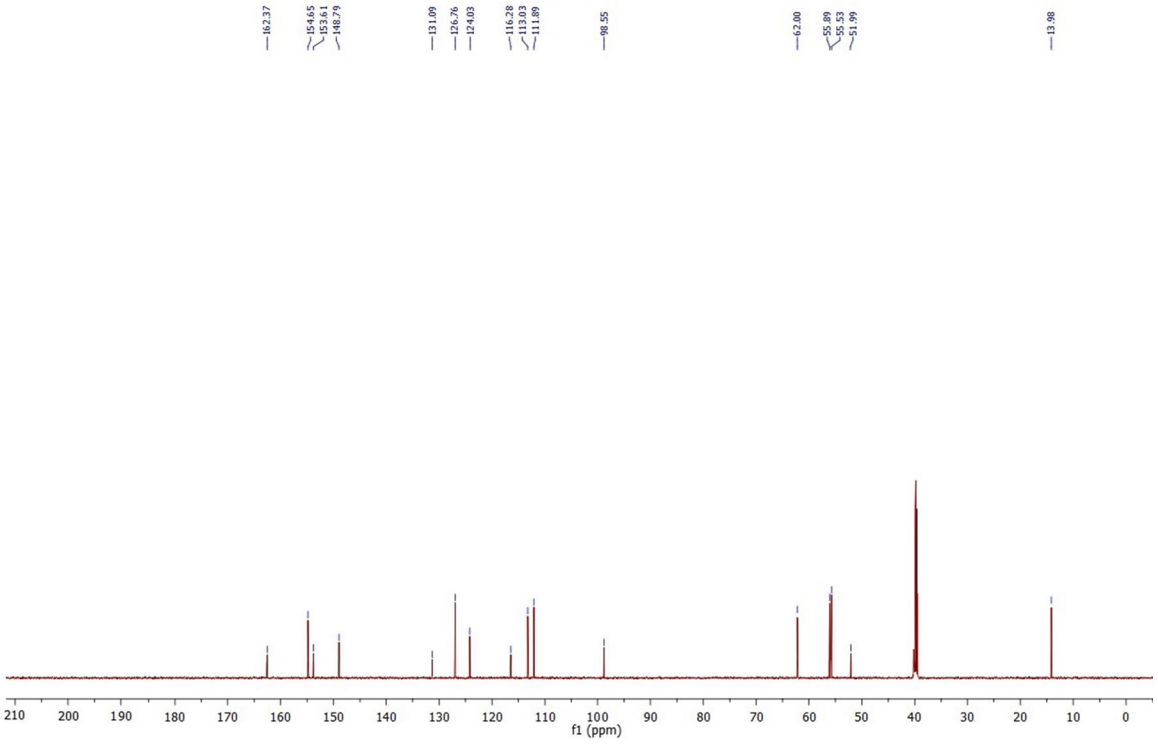
Ethyl 5-amino-7-(2-methoxyphenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2f**)



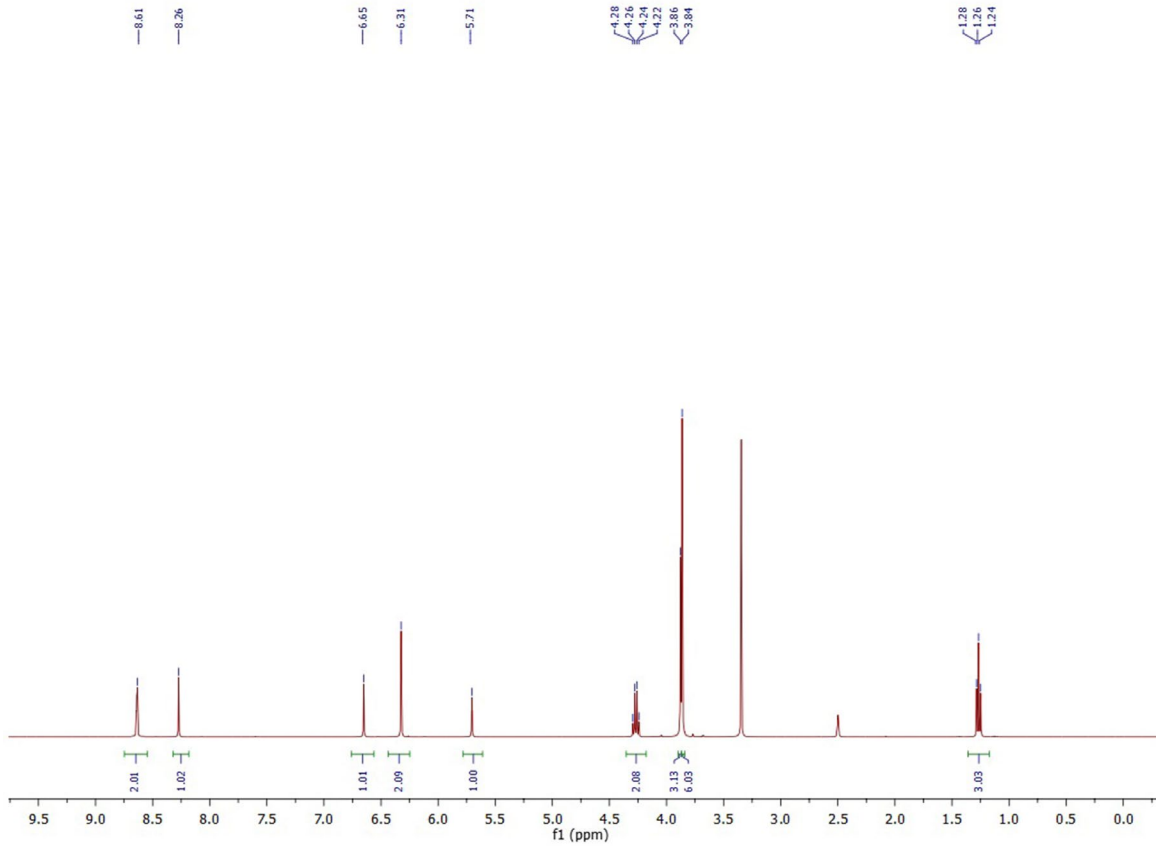


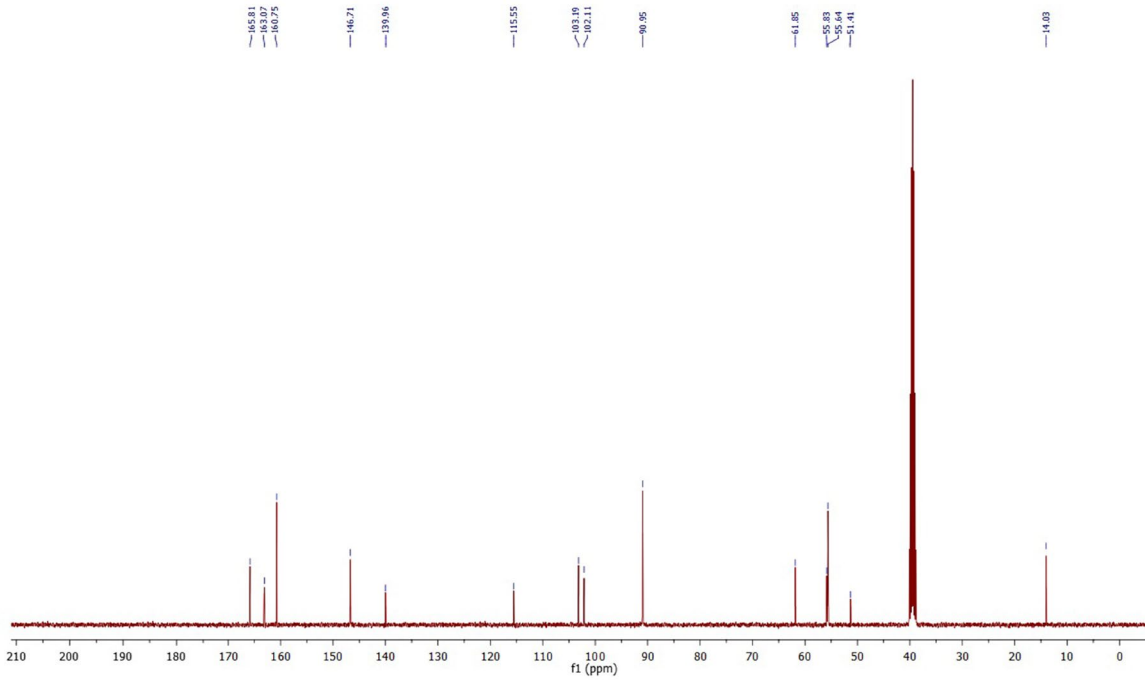
Ethyl 5-amino-7-(3,4-dimethoxyphenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2g**)



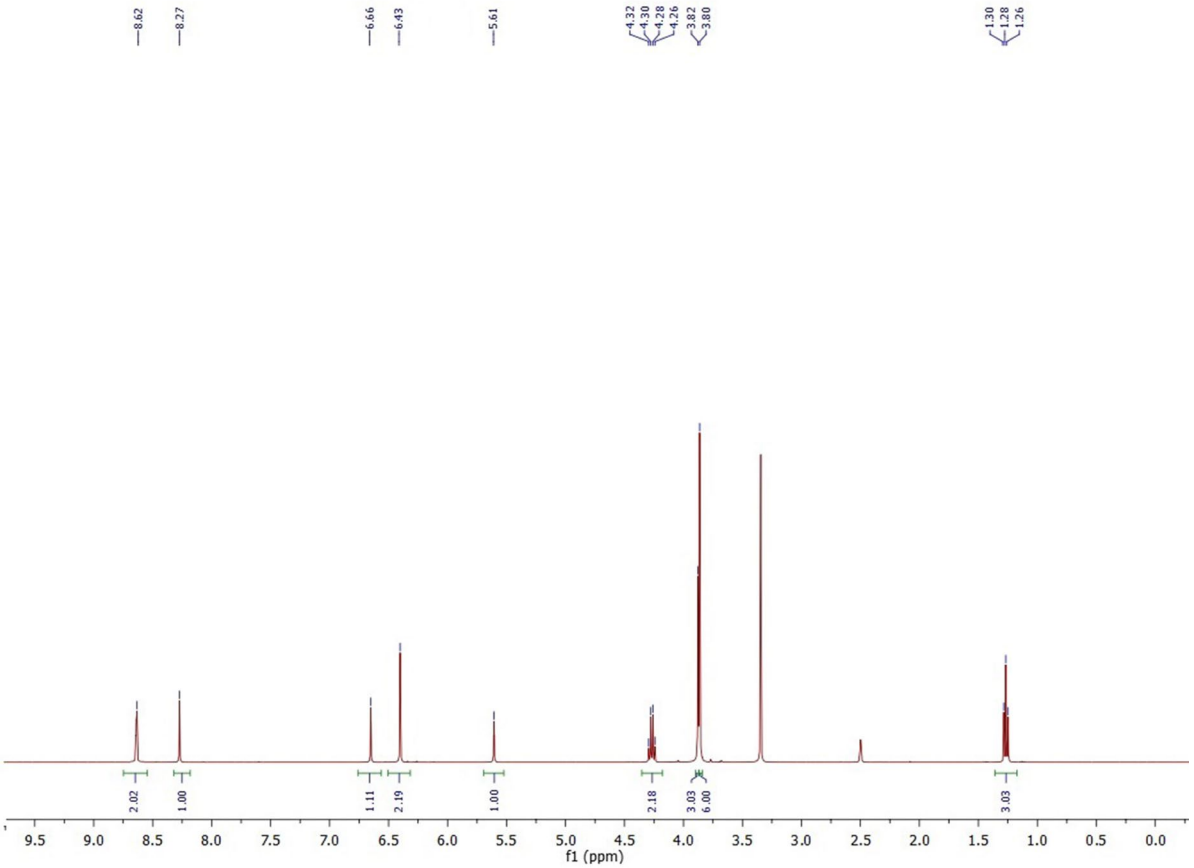


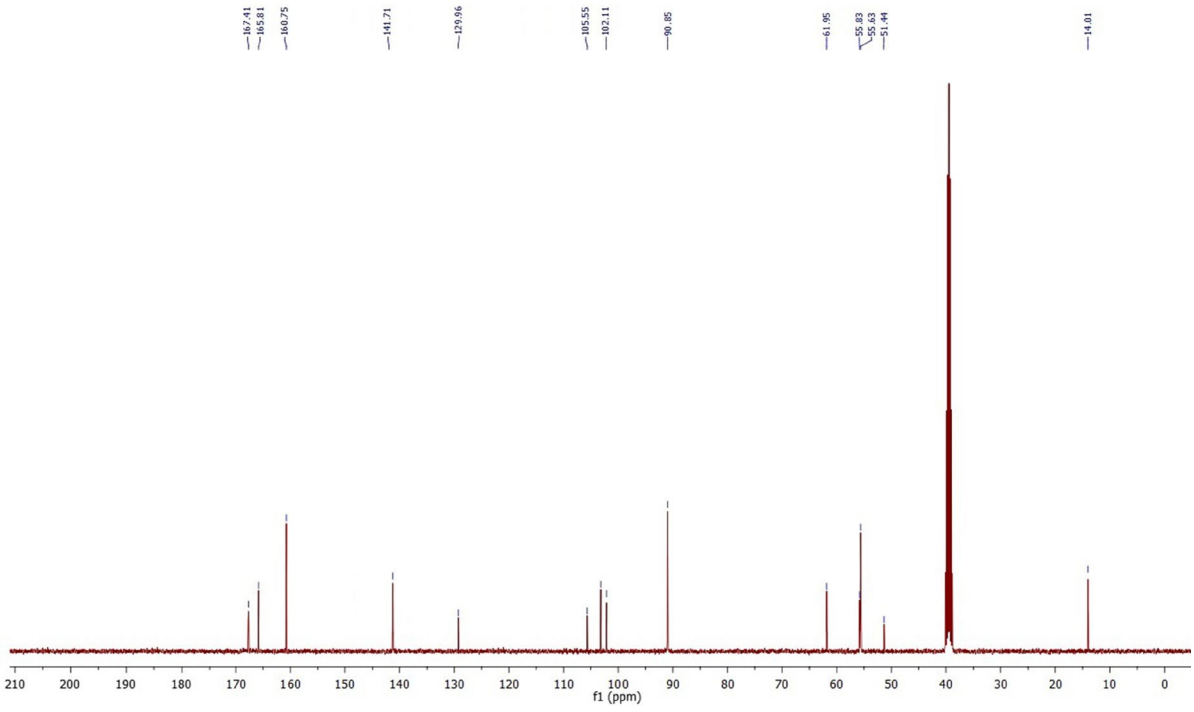
Ethyl 5-amino-7-(2,4,6-trimethoxyphenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2h**)





Ethyl 5-amino-7-(3,4,5-trimethoxyphenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2i**)





Ethyl 5-amino-7-(4-(dimethylamino)phenyl)-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate (**2j**)