Electronic Supplementary Material (ESI) for Dalton Transactions.

Open Metal Sites (OMSs) Inspired Investigation of Adsorption and Catalytic Functions in a Porous Metal-Organic Framework (MOF)

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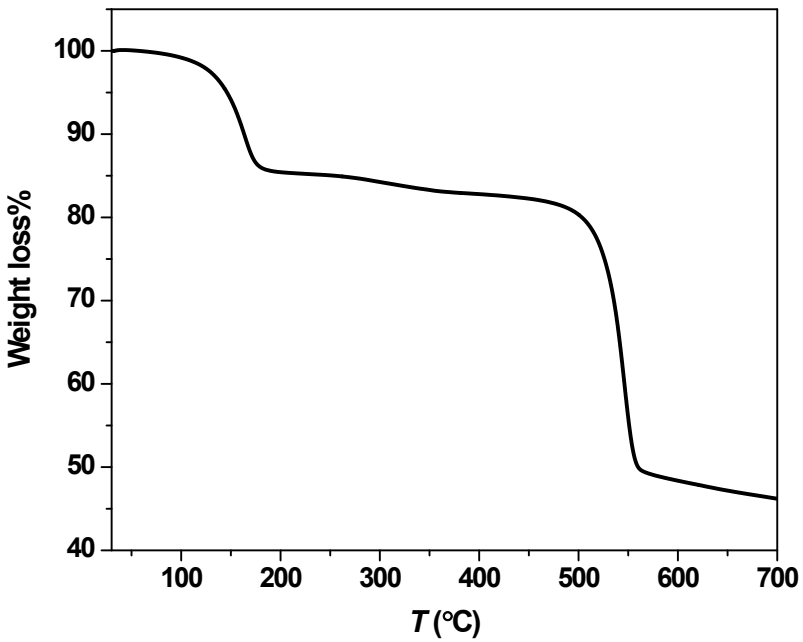

Fig. S1. TGA curve of compound **1** in the temperature range 30 - 700 °C (heating rate 5 °C/min under nitrogen).

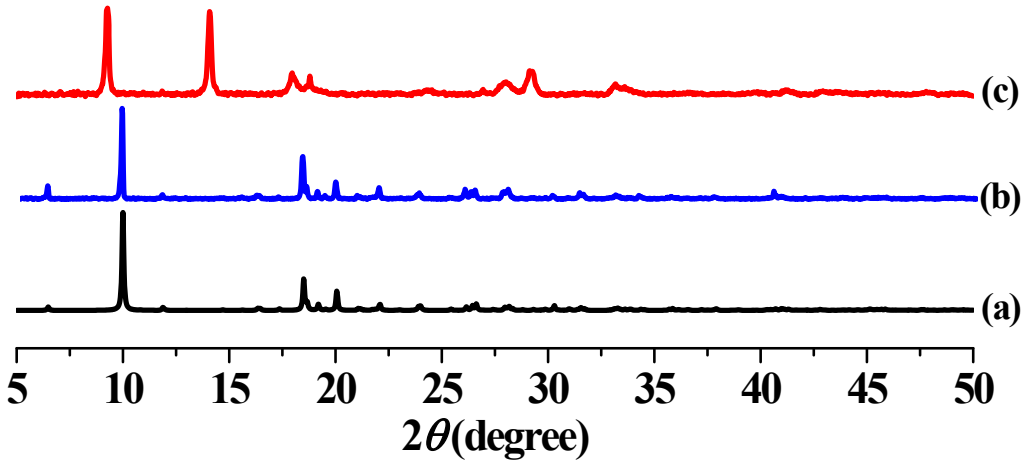

Fig. S2. Powder X-ray diffraction (PXRD) study of compound **1**. (a) simulated pattern; (b) assynthesized pattern and (c) desolvated pattern. Similarity of the assynthesized pattern with the simulated pattern indicates purity of the sample.

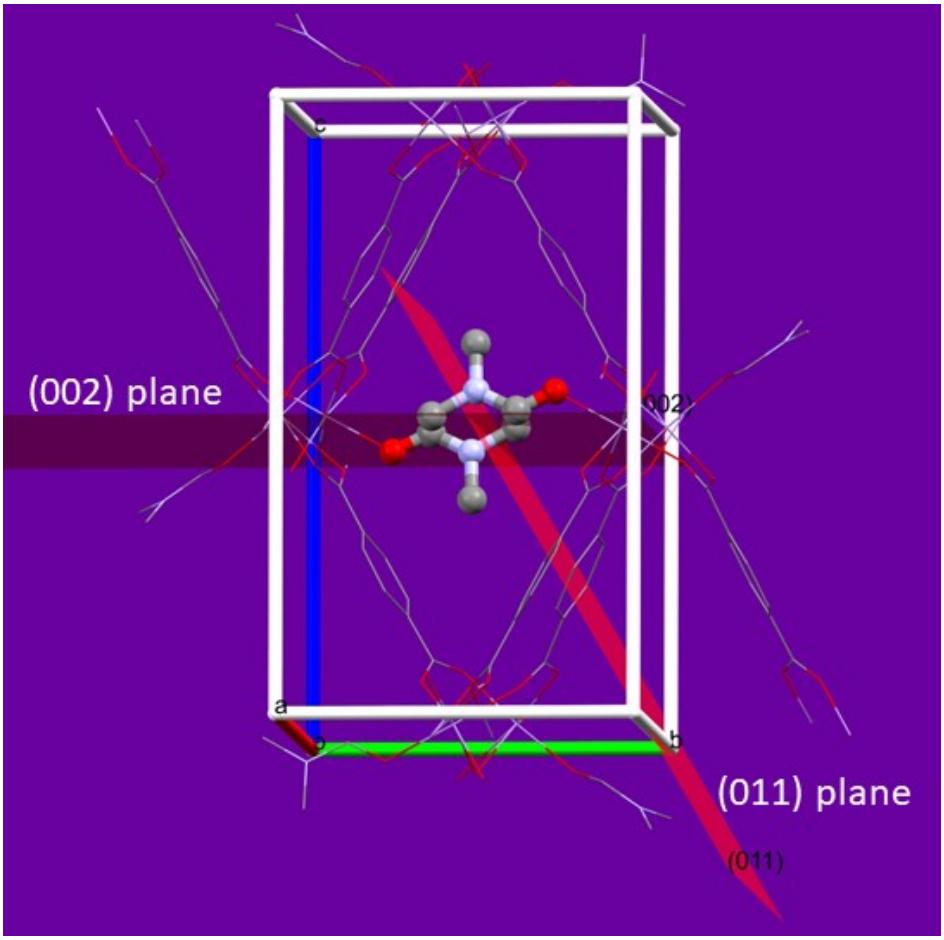

Fig. S3. View of the structure of compound **1** along the crystallographic *a* direction shows that (011) and (002) planes contains coordinated N,N-Dimethylformammide (DMF) molecules.

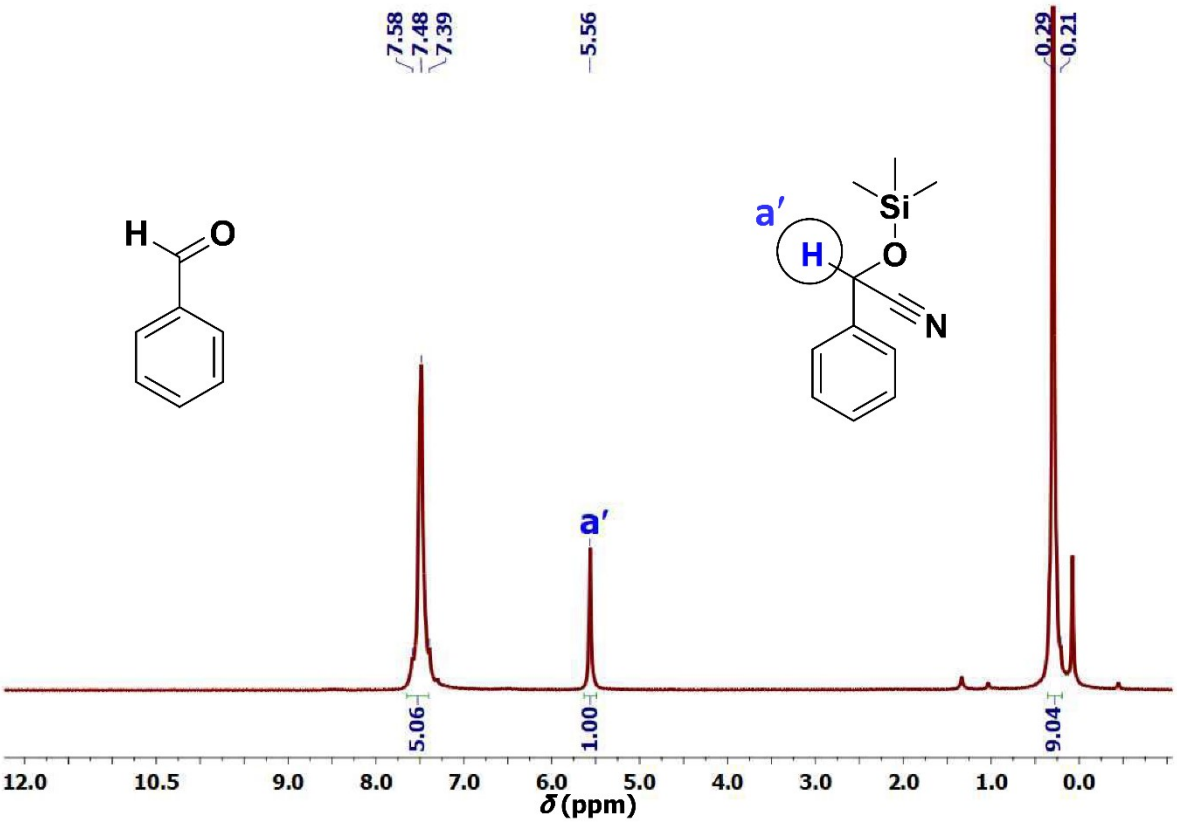

Fig. S4. ^{1}H NMR spectrum of the product 2-(phenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 1 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 100.

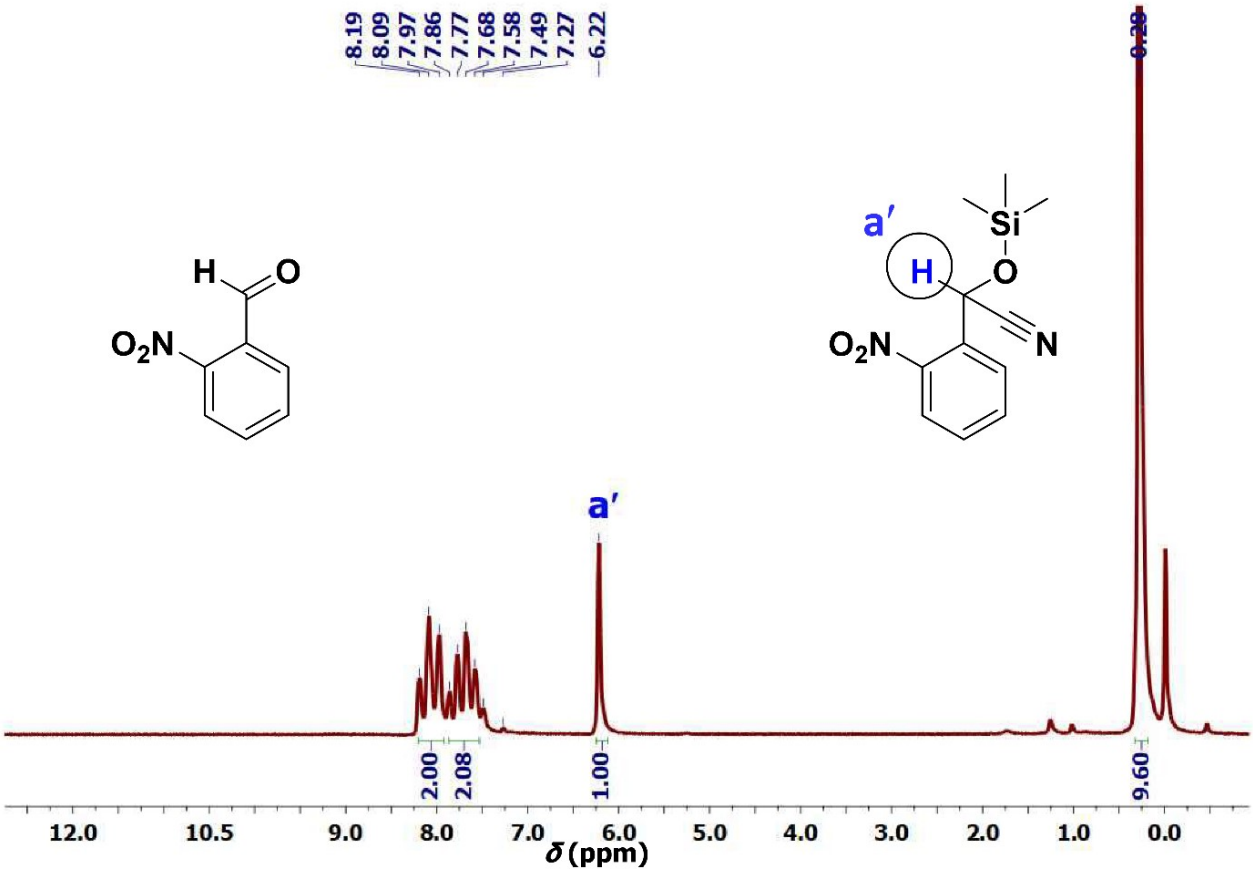

Fig. S5. ^{1}H NMR spectrum of the product 2-(2-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 2 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 100.

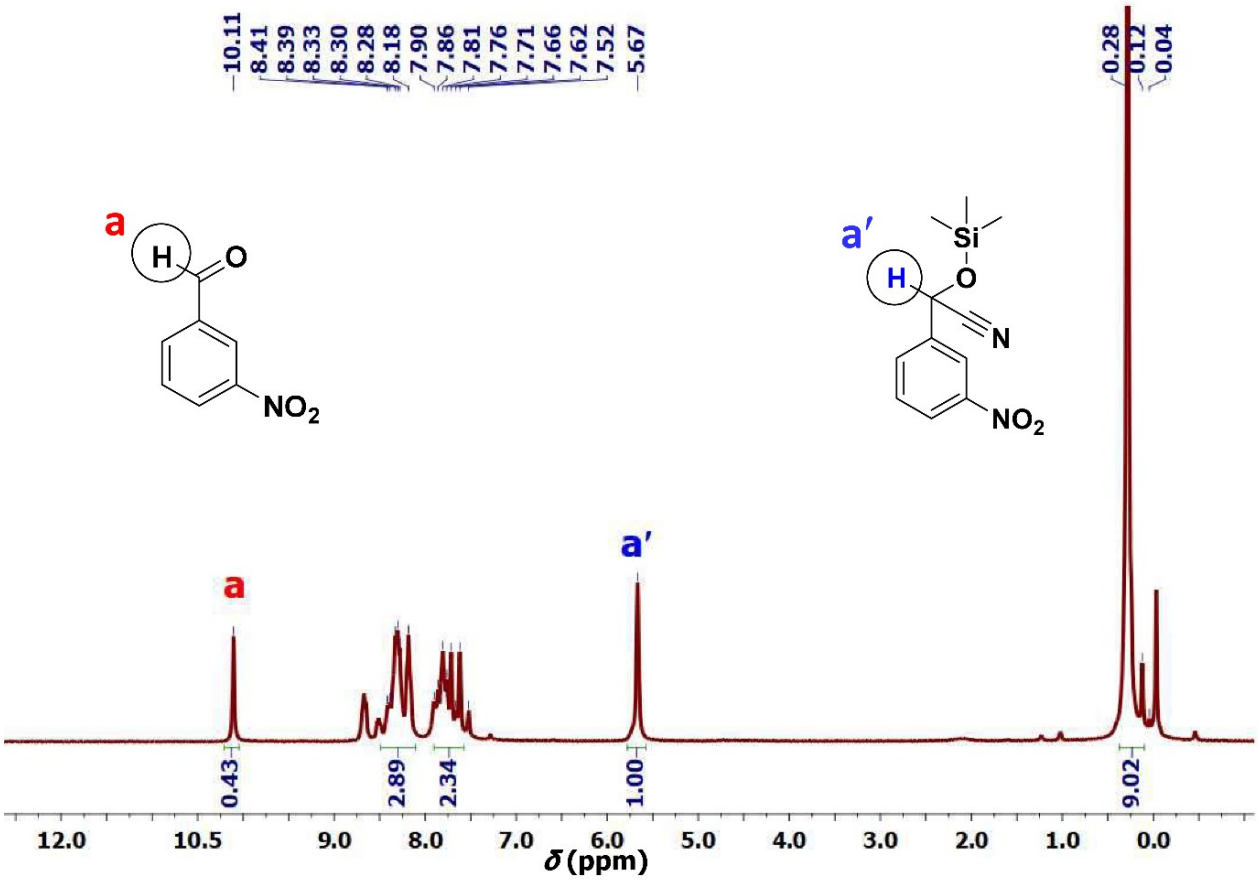

Fig. S6. ^{1}H NMR spectrum of the product 2-(3-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 3 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 69.9.

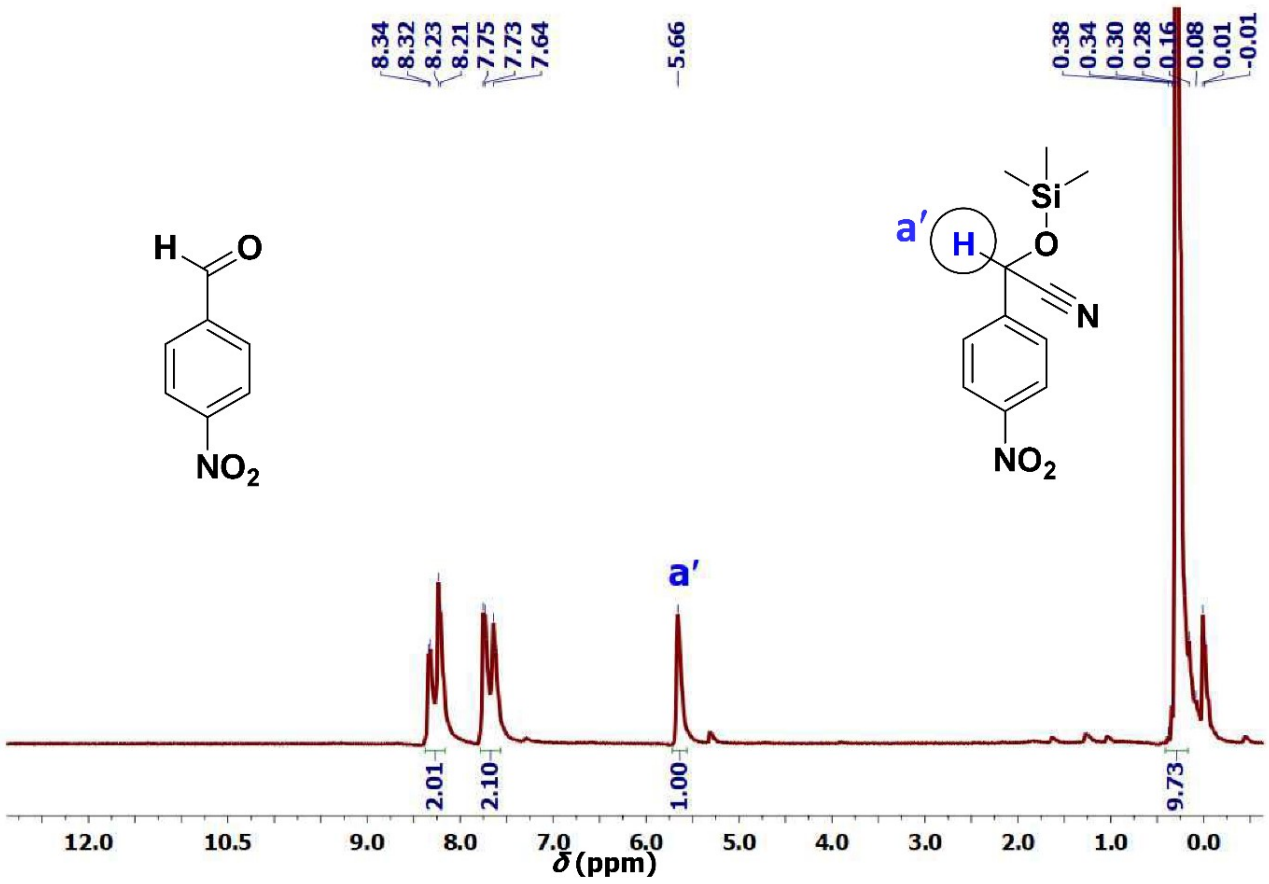

Fig. S7. ^{1}H NMR spectrum of the product 2-(4-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 4 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 100.

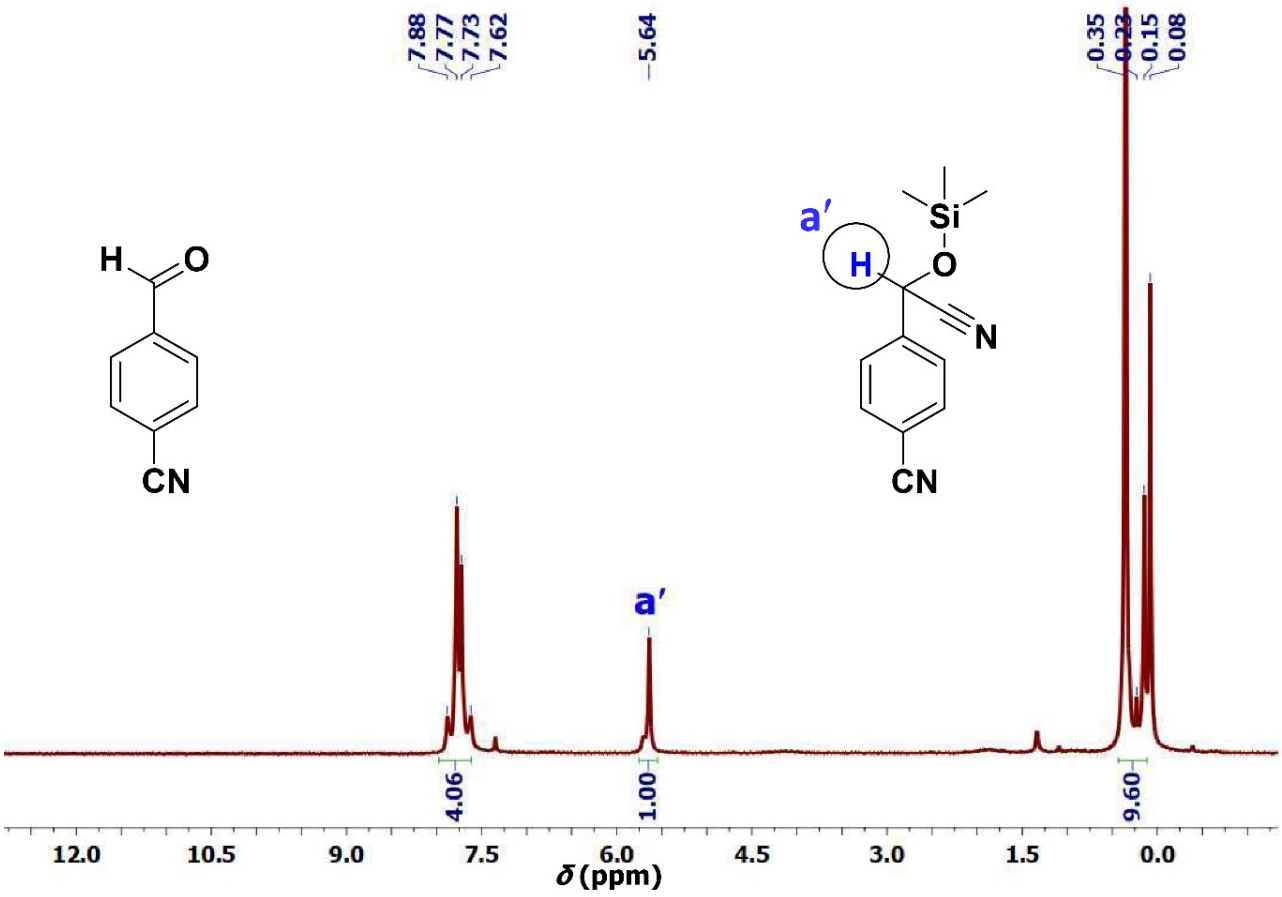

Fig. S8. ^{1}H NMR spectrum of the product 4-(cyano((trimethylsilyl)oxy)methyl)benzonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 5 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 100.

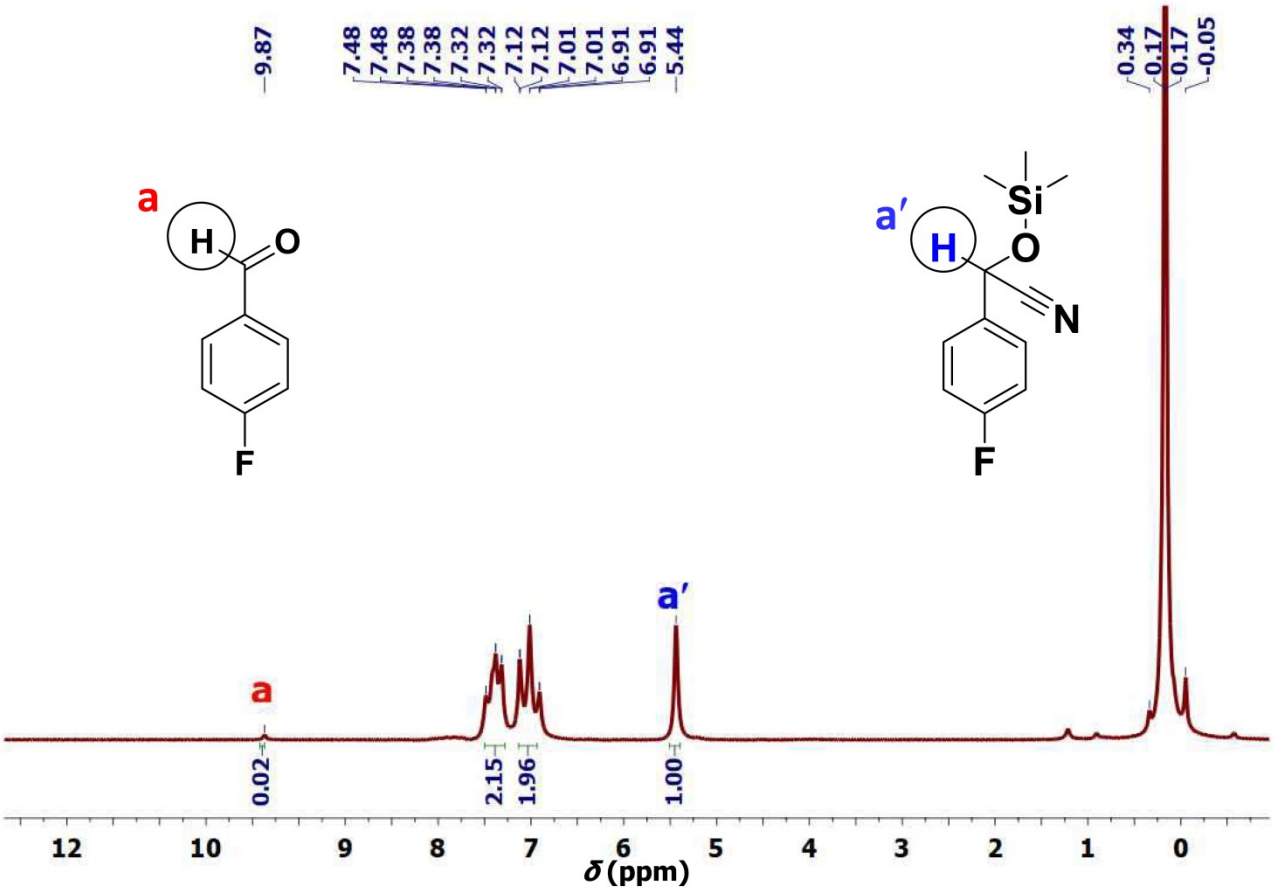

Fig. S9. ^{1}H NMR spectrum of the product 2-(4-flurophenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 6 in Table 3) recorded in $CDCl_3$. The percentage conversion calculated for the product is 98.

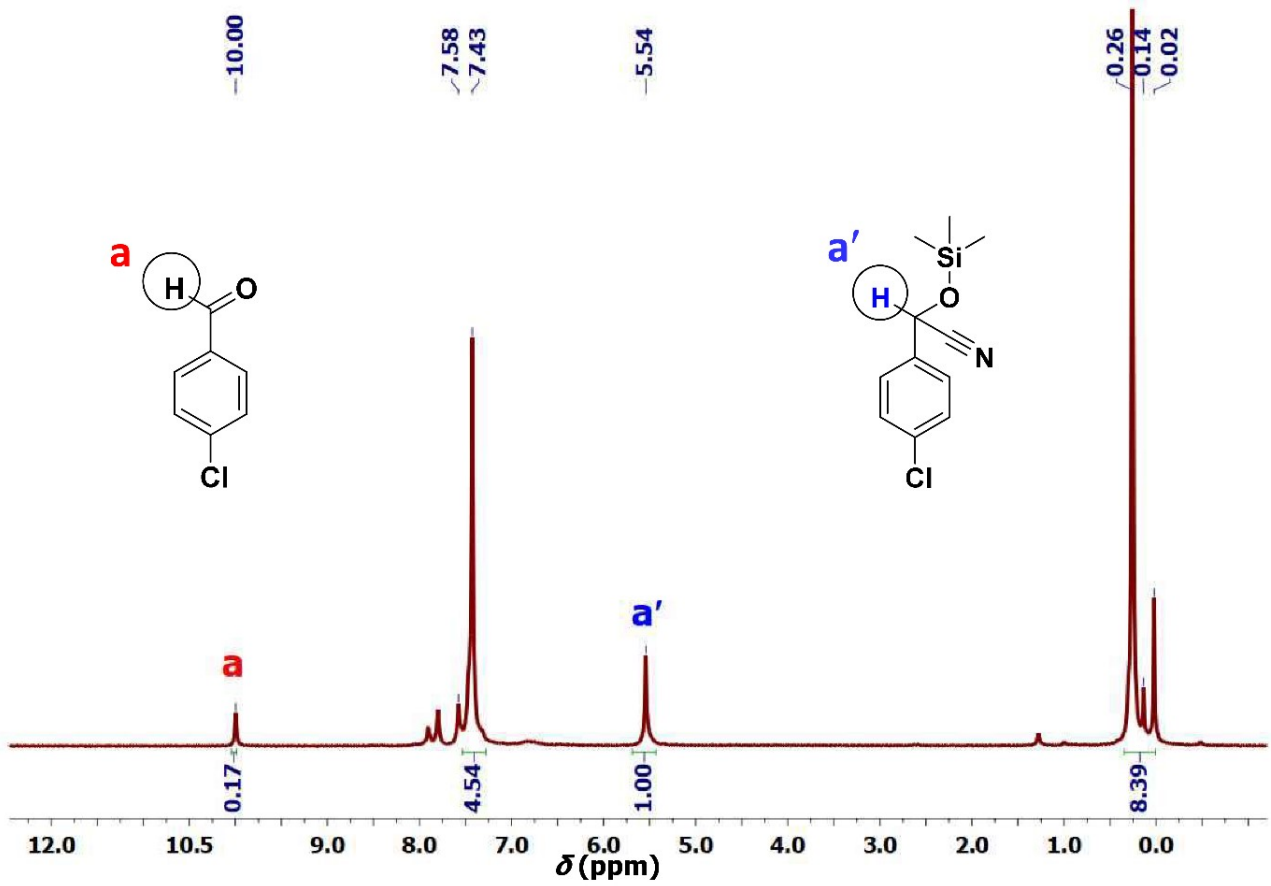

Fig. S10. ^{1}H NMR spectrum of the product 2-(4-chlorophenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 7 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 85.4.

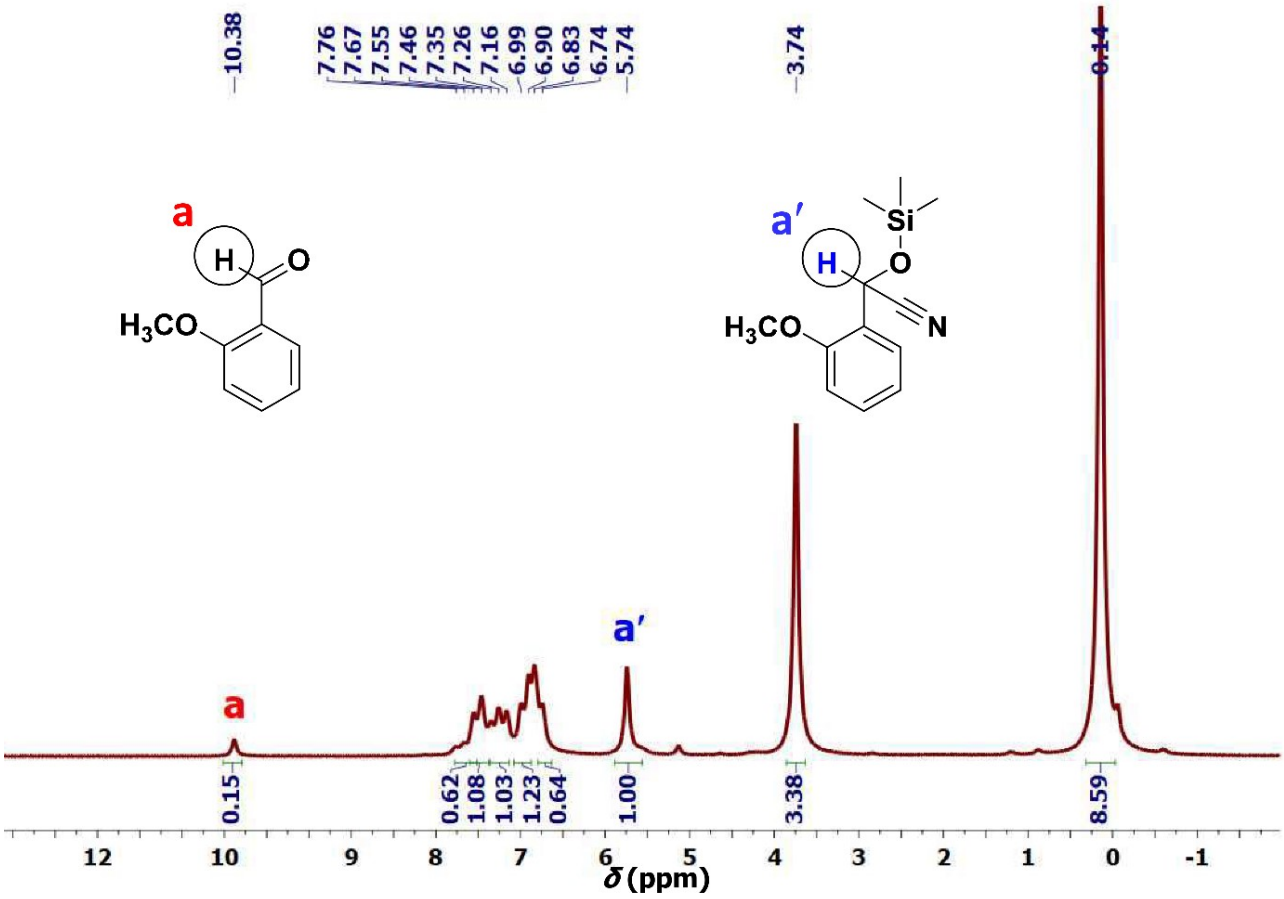

Fig. S11. ^{1}H NMR spectrum of the product 2-(2-methoxyphenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 8 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 86.9.

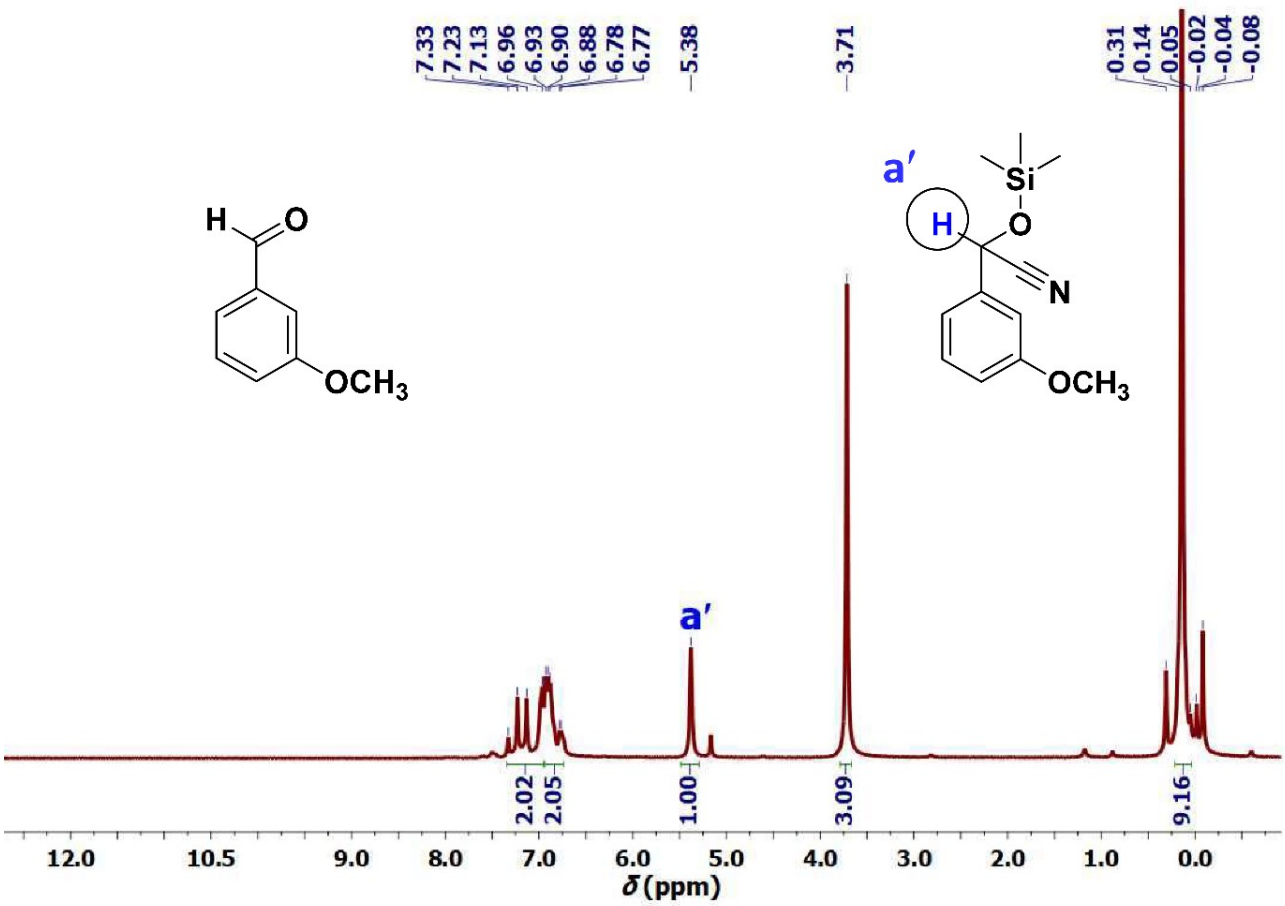

Fig. S12. ^{1}H NMR spectrum of the product 2-(3-methoxyphenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 9 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 100.

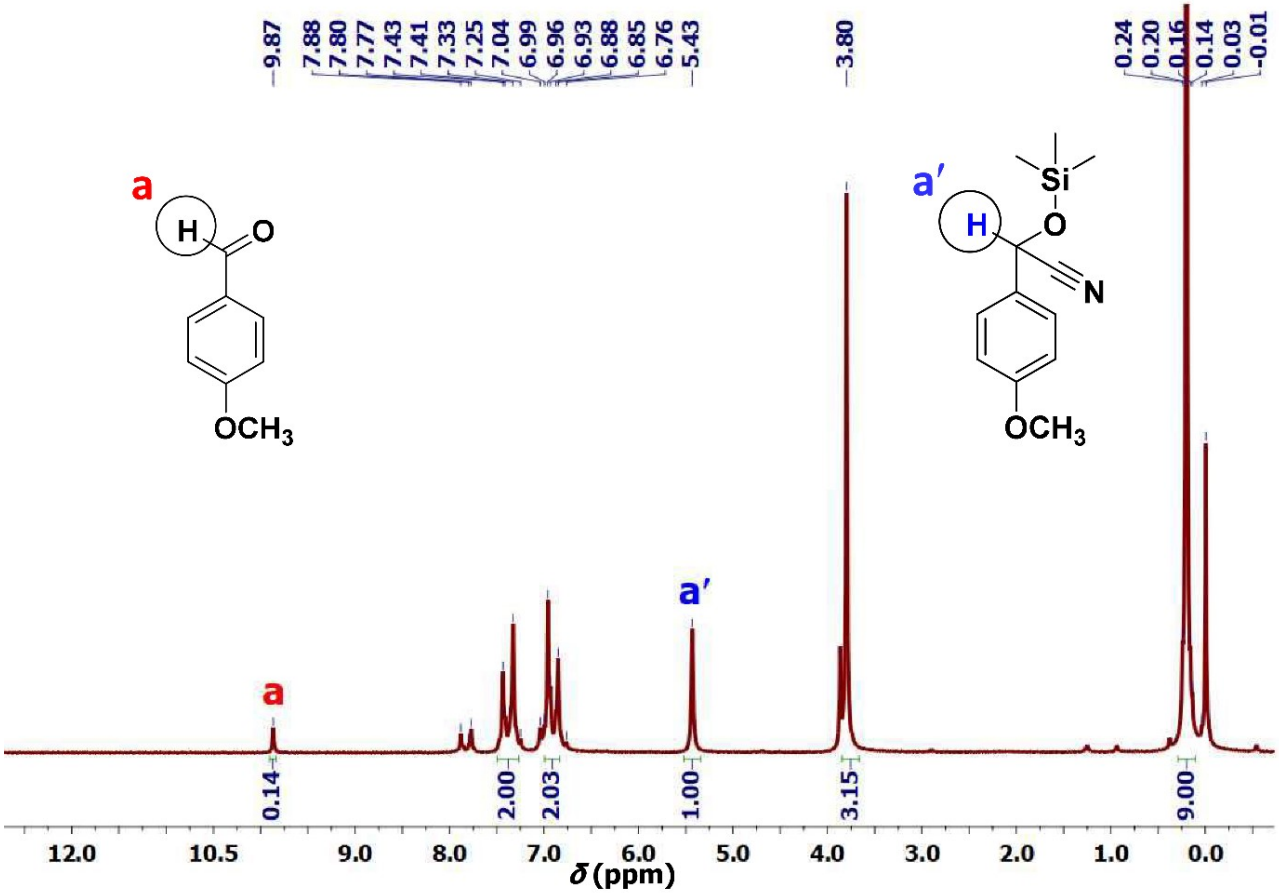

Fig. S13. ^{1}H NMR spectrum of the product 2-(4-methoxyphenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 10 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 87.7.

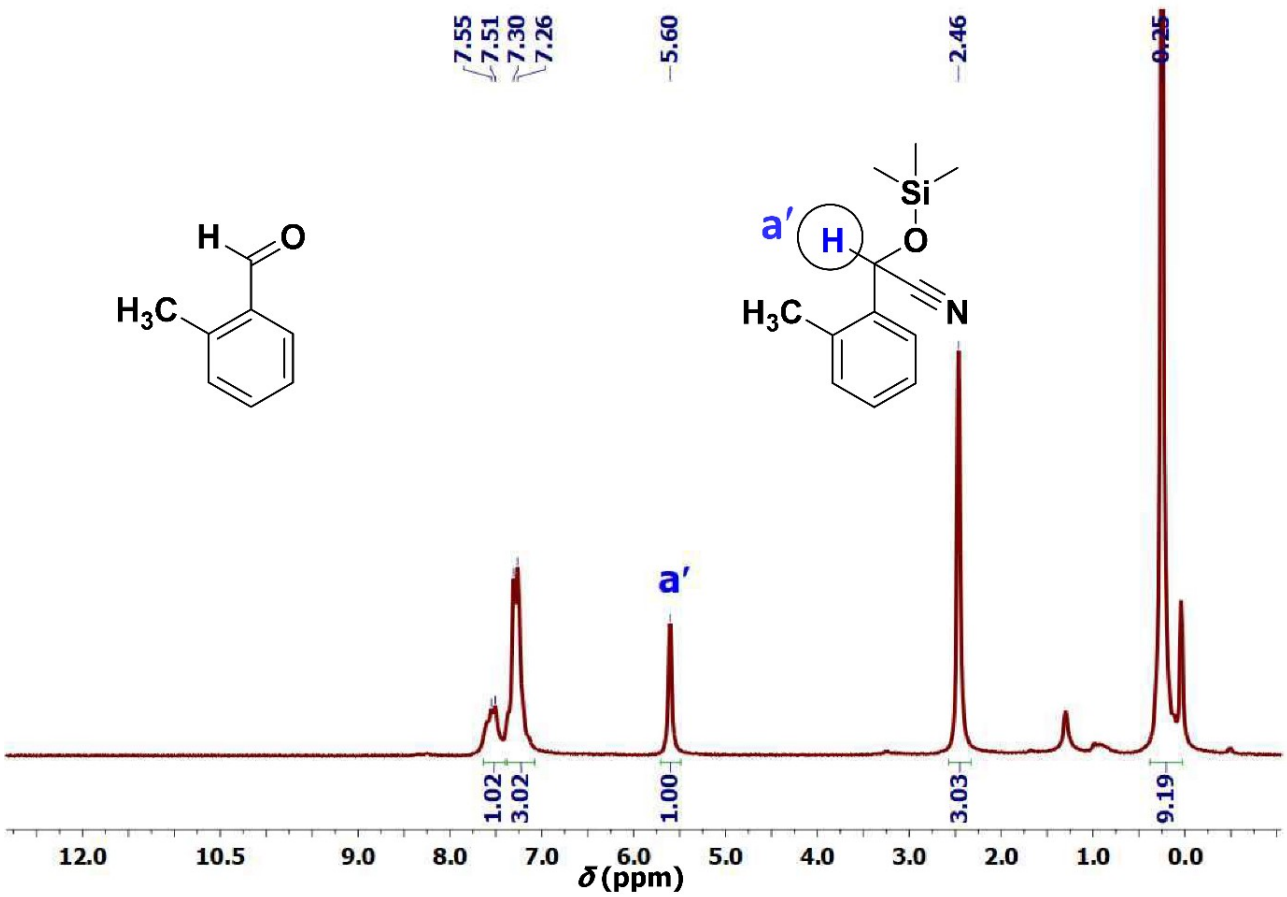

Fig. S14. ^{1}H NMR spectrum of the product 2-(2-methylphenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 11 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 100.

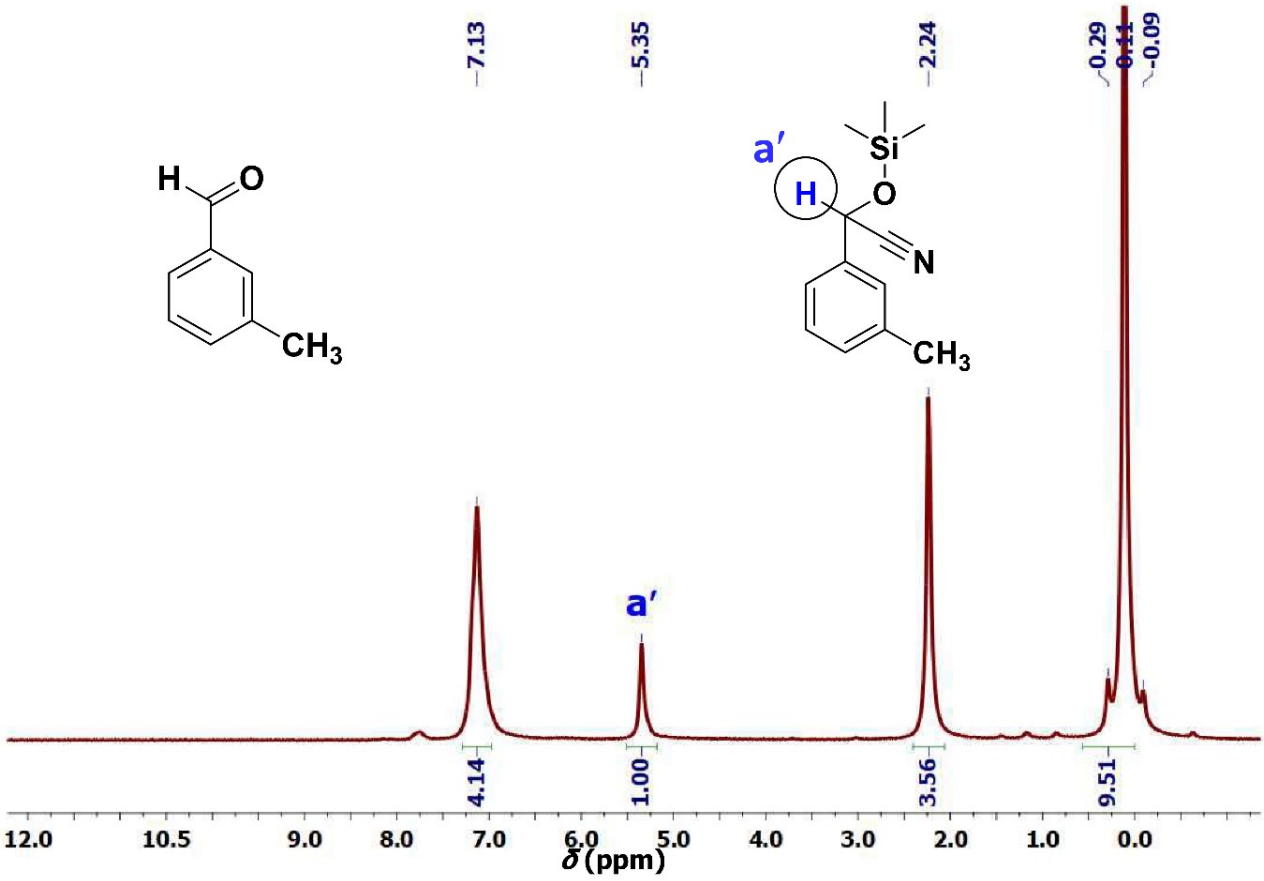

Fig. S15. ^{1}H NMR spectrum of the product 2-(3-methylphenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 12 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 100.

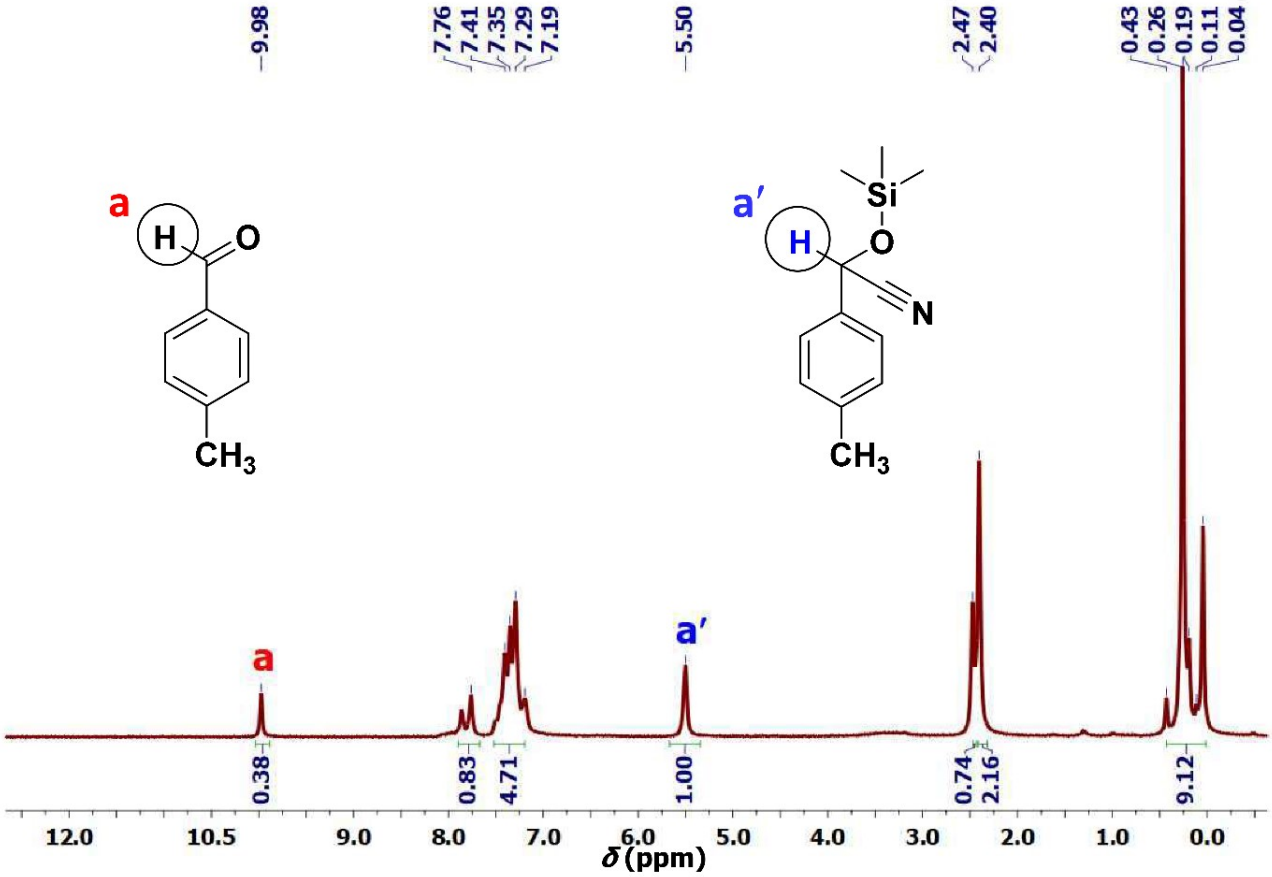

Fig. S16. ^{1}H NMR spectrum of the product 2-(4-methylphenyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 13 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 72.4.

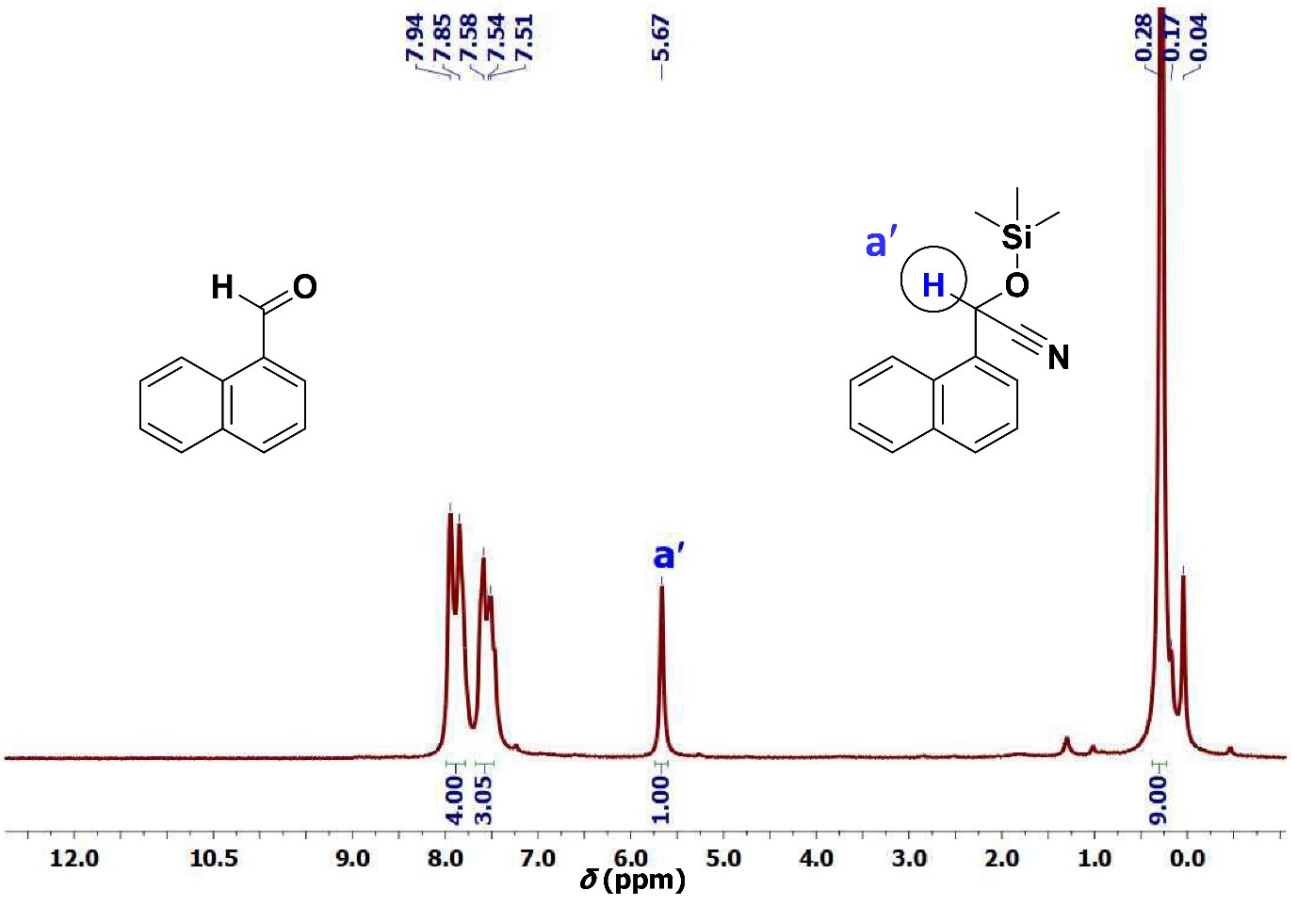

Fig. S17. ^{1}H NMR spectrum of the product 2-(napthyl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 14 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is100.

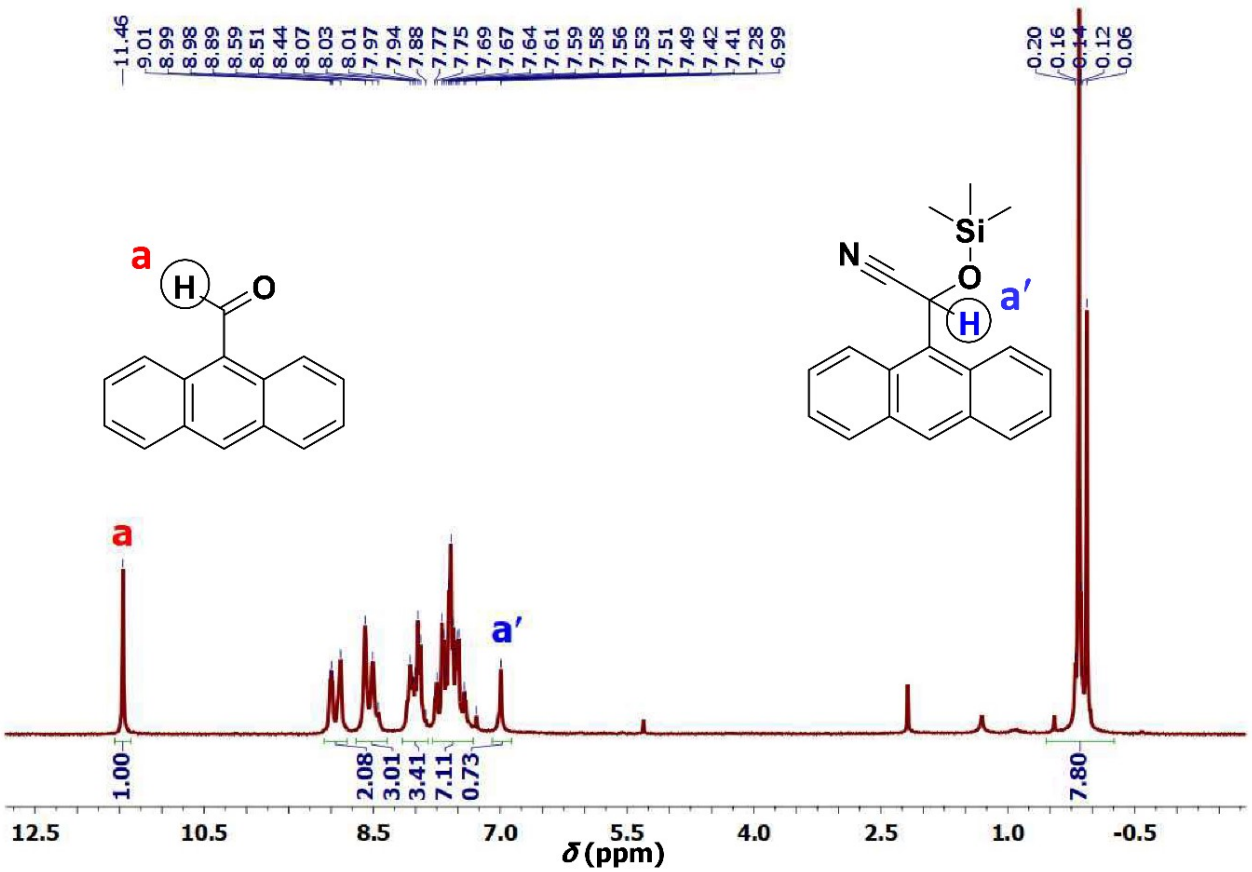

Fig. S18. ^{1}H NMR spectrum of the product 2-(9-anthryl)-2-((trimethylsilyl)oxy)acetonitrile obtained *via* cyanosilylation reaction of benzaldehyde (Entry 15 in Table 2) recorded in $CDCl_3$. The percentage conversion calculated for the product is 42.1.

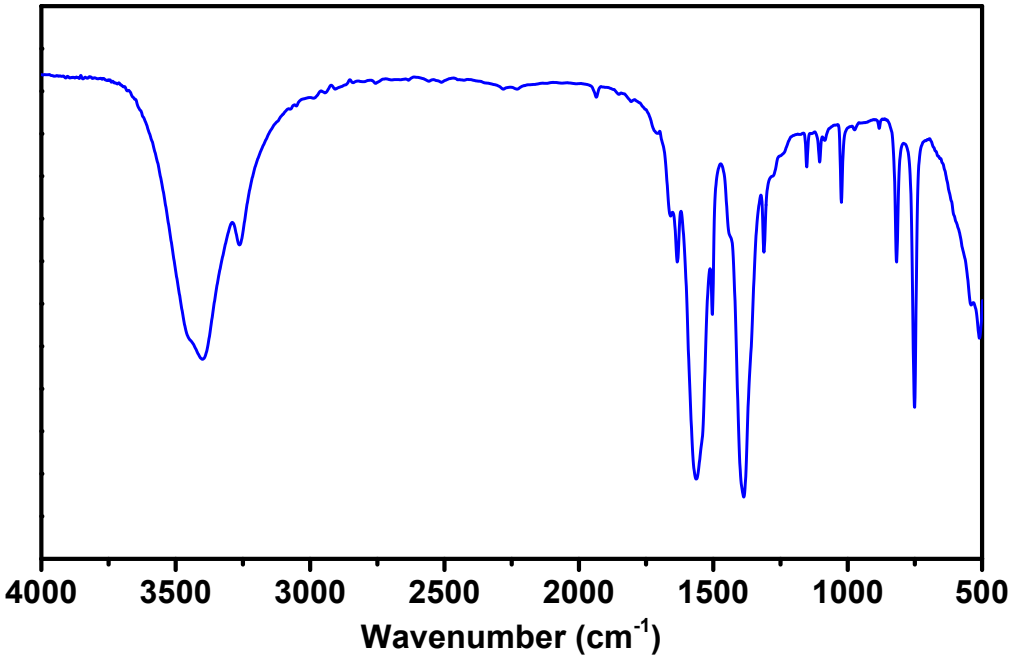

Fig. S19. FTIR spectrum of compound **1**.

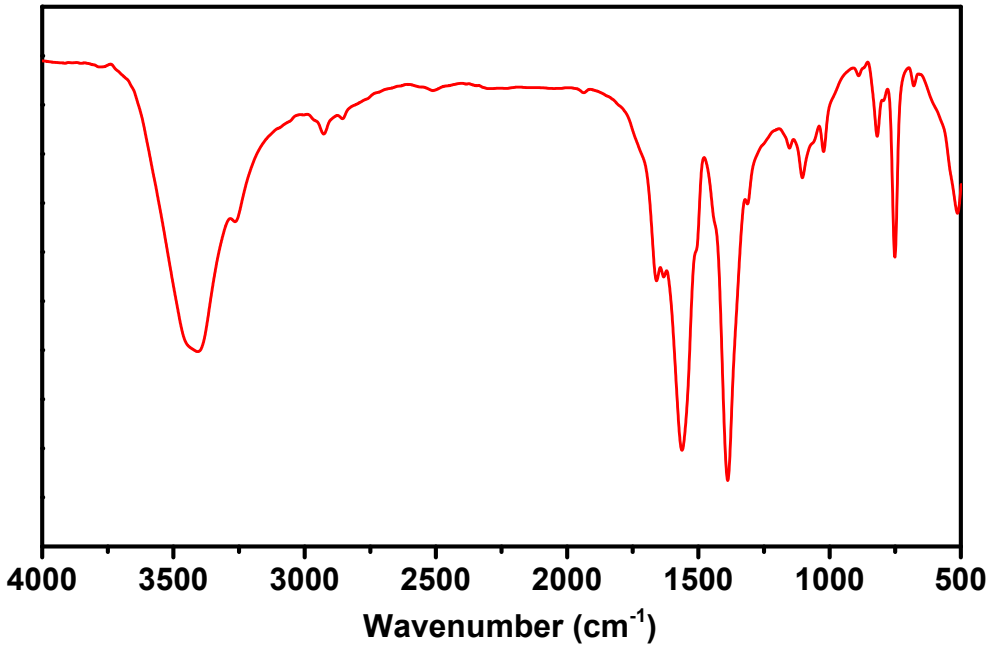

Fig. S20. FTIR spectrum of compound **1′**.

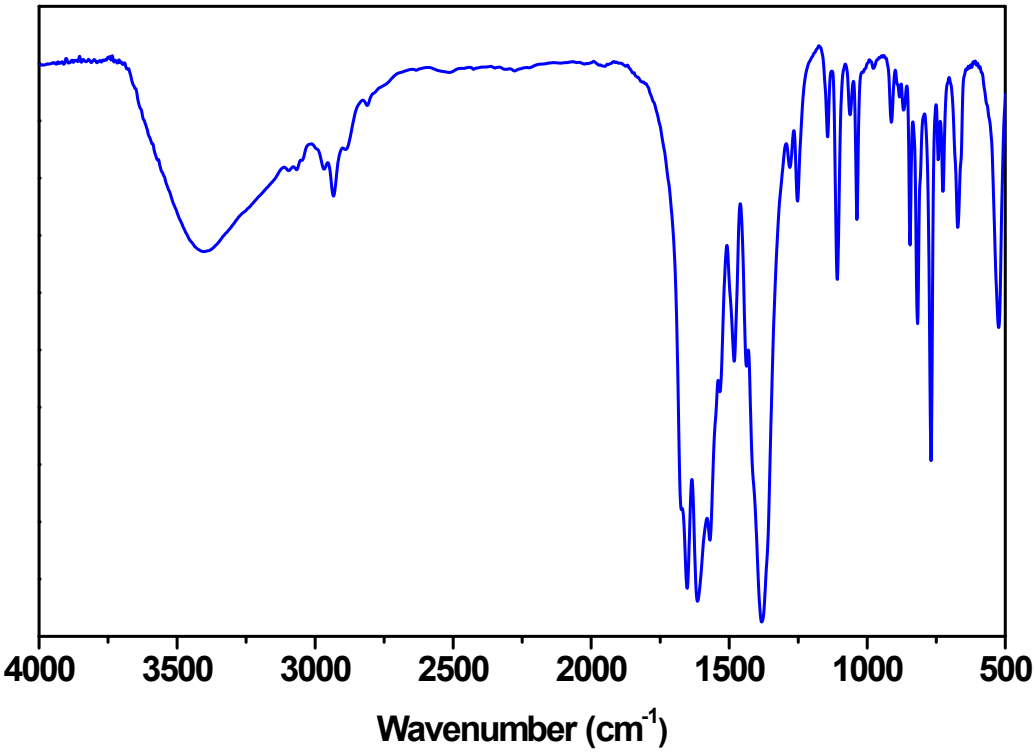

Fig. S21. FTIR spectrum of compound **2**.

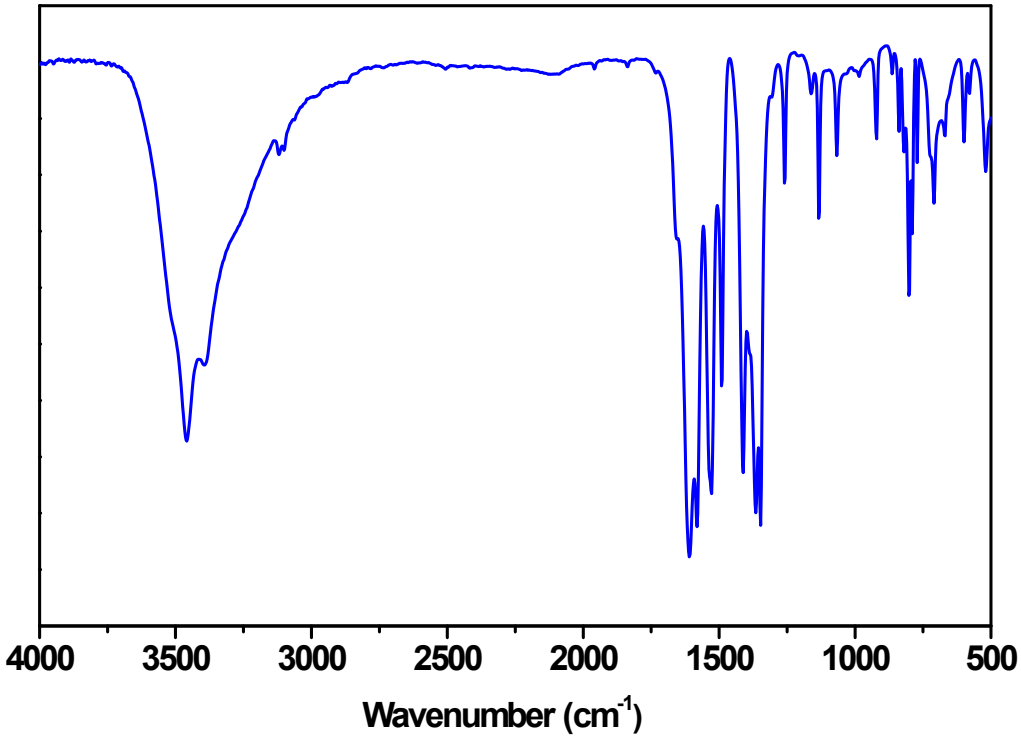

Fig. S22. FTIR spectrum of compound **3**.