Layered Double Hydroxides (LDHs): As Efficient Heterogeneous Catalyst for the Cyanosilylation of Aromatic Aldehydes

Javad Mokhtari,\*[a] Fahimeh Afi,[a] Fatemeh Tahoori\*[b]

aDepartment of Chemistry, Science and Research Branch, Islamic Azad University, P.O. Box 14515/775,Tehran, Iran.

bRazi Vaccine and Serum Research Institute, Agricultural Research and Extension Organization (AREEO), Karaj, Iran

E-mail: [j.mokhtari@srbiau.ac.ir](mailto:j.mokhtari@srbiau.ac.ir)

**Supplemental Materials**

Spectral data for compounds 3:

**2-phenyl-2-((trimethylsilyl)oxy)acetonitrile (3a) [1]:**

Yield: 95%; 1H NMR (500 MHz, CDCl3):*δ* 0.27 (s, 9H, -OSi(C**H**3)3), 5.55 (s, 1H, -C**H**CN), 7.40-7.51 (m, 5H, CH Ar).13C NMR (125 MHz, CDCl3):*δ*-0.1, 63.8, 119.4, 126.5, 129.1, 129.5, 136.5. Elemental Analysis: C, 64.34; H, 7.36; N, 6.82; found C, 64.32; H, 7.35; N, 6.81.

**2-(p-tolyl)-2-((trimethylsilyl)oxy)acetonitrile (3b) [1]:**

Yield: 96%; 1H NMR (500 MHz, CDCl3):*δ*0.21 (s, 9H, -OSi(C**H**3)3), 2.36 (s, 3H, Ph-C**H**3), 5.45 (s, 1H, -C**H**CN), 7.21 (d,*J*=8.5 Hz,2H, CH Ar), 7.35 (d,*J*=8 Hz,2H, CH Ar). Elemental Analysis: C, 65.71; H, 7.81; N, 6.39; found C, 65.69; H, 7.80; N, 6.37.

**2-(4-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile (3c) [2]:**

Yield: 92%; 1H NMR (500 MHz, CDCl3):*δ*0.26 (s, 9H, -OSi(C**H**3)3),5.58 (s, 1H, -C**H**CN), 7.65 (d,*J*=8.5 Hz,2H, CH Ar), 8.26 (d,*J*=8.5 Hz,2H, CH Ar). Elemental Analysis: C, 52.78; H, 5.64; N, 11.19; found C, 52.73; H, 5.60; N, 11.17.

**2-(4-methoxyphenyl)-2-((trimethylsilyl)oxy)acetonitrile (3d) [2]:**

Yield: 93%; 1H NMR (500 MHz, CDCl3):*δ*0.19 (s, 9H, -OSi(C**H**3)3), 3.81 (s, 3H, Ph-OC**H**3), 5.42 (s, 1H, -C**H**CN), 6.90 (d,*J*=9.0 Hz,2H, CH Ar), 7.36 (d,*J*=8.5 Hz, 2H, CH Ar). Elemental Analysis: C, 61.24; H, 7.28; N, 5.95; found C, 61.26; H, 7.25; N, 5.94.

**2-(4-chlorophenyl)-2-((trimethylsilyl)oxy)acetonitrile (3e) [2]:**

Yield: 95%;1H NMR (500 MHz, CDCl3) *δ*=0.05 (s, 9H, -OSi(C**H**3)3), 5.28 (s, 1H, -C**H**CN), 7.52 (d,*J*=3.5 Hz, 2H, CH Ar), 7.68 (d,*J*=3.5 Hz,2H, CH Ar). Elemental Analysis: C, 55.10; H, 5.89; N, 5.84; found C, 55.07; H, 5.86; N, 5.83.

**2-(o-tolyl)-2-((trimethylsilyl)oxy)acetonitrile (3f) [1]:**

Yield: 89%; Elemental Analysis: C, 65.71; H, 7.81; N, 6.39; found C, 65.69; H, 7.82; N, 6.37.

**2-(4-(dimethylamino)phenyl)-2-((trimethylsilyl)oxy)acetonitrile (3g) [3]:**

Yield: 92%; 1H NMR (500 MHz, CDCl3):*δ*0.18 (s, 9H, -OSi(C**H**3)3), 2.95 (s, 6H, -N(C**H**3)2), 5.38 (s, 1H, -C**H**CN), 6.69 (d,*J*=8.5 Hz, 2H, CH Ar), 7.29 (d,*J*=9 Hz, 2H, CH Ar). Elemental Analysis: C, 62.86; H, 8.12; N, 11.28; found C, 62.84; H, 8.09; N, 11.26.

**2-(4-bromophenyl)-2-((trimethylsilyl)oxy)acetonitrile (3h) [4]:**

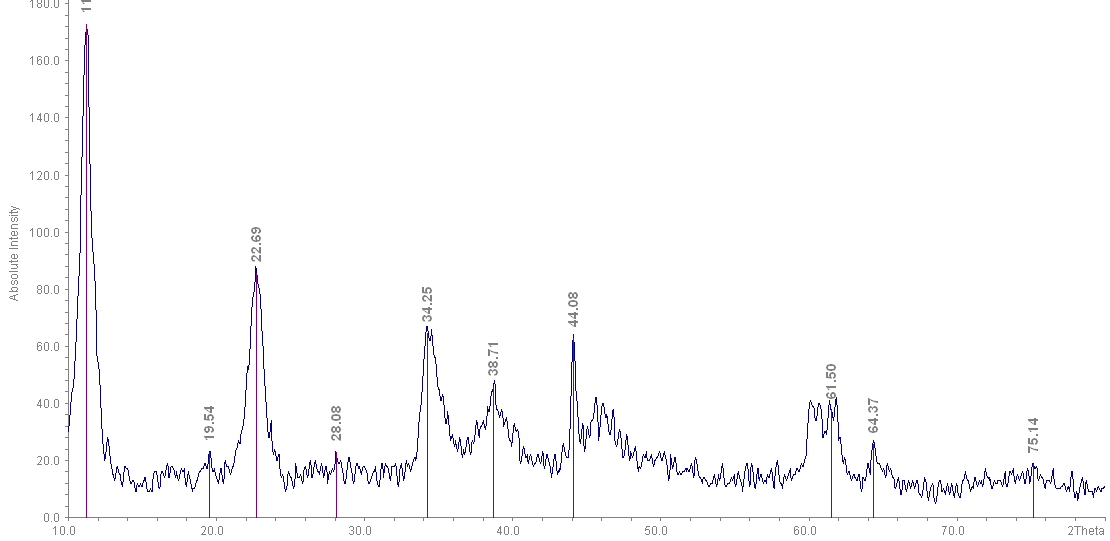
Yield: 92%; Elemental Analysis: C, 46.48; H, 4.96; N, 4.93; found C, 46.45; H, 4.94; N, 4.91.

**2-(2-chlorophenyl)-2-((trimethylsilyl)oxy)acetonitrile (3i) [1]:**

Yield: 88%; Elemental Analysis: C, 55.10; H, 5.89; N, 5.84; found C, 55.11; H, 5.88; N, 5.82

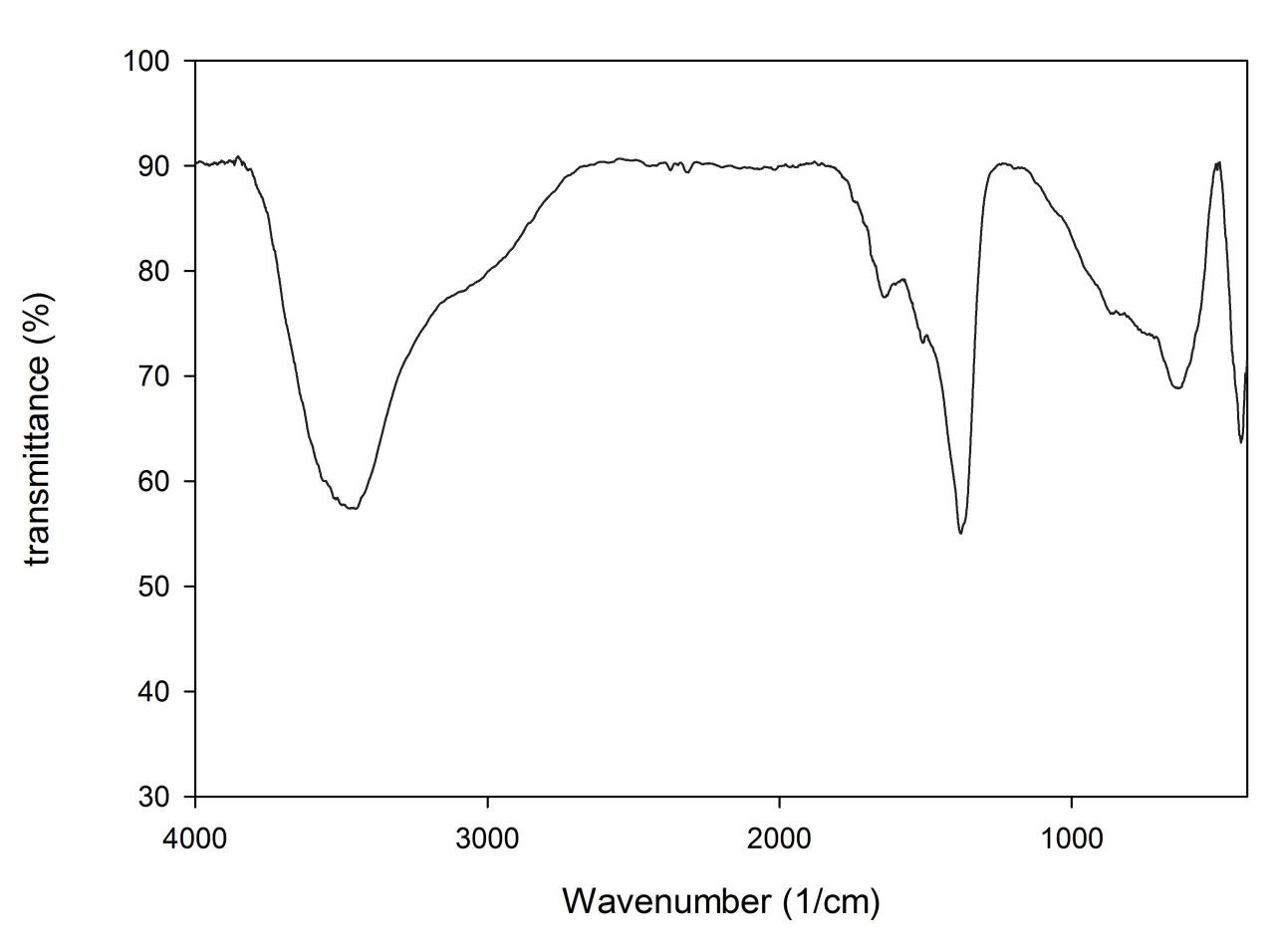
**2-(2-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile (3j) [4]:**

Yield: 90%; Elemental Analysis: C, 52.78; H, 5.64; N, 11.19; found C, 52.75; H, 5.62; N, 11.16.

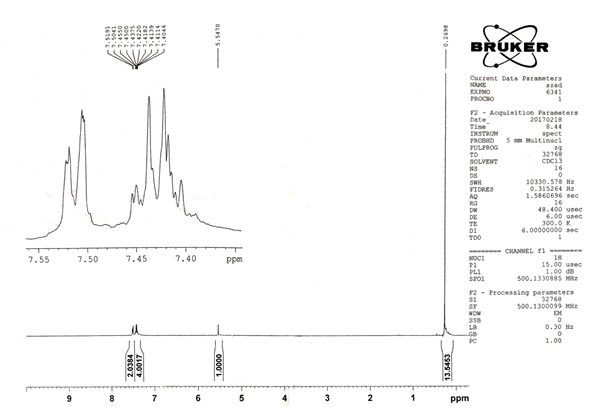


**Figure S 1.** XRD patterns of Mg-Al-Cu-LDH

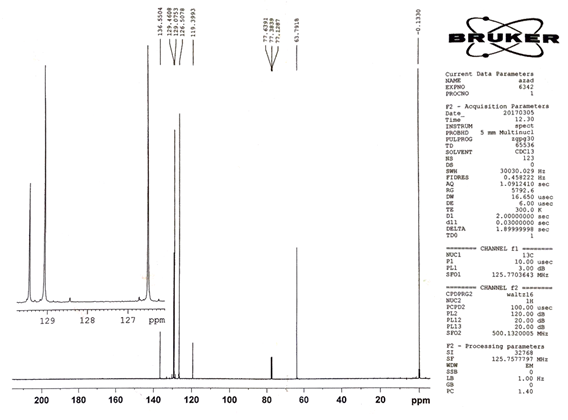
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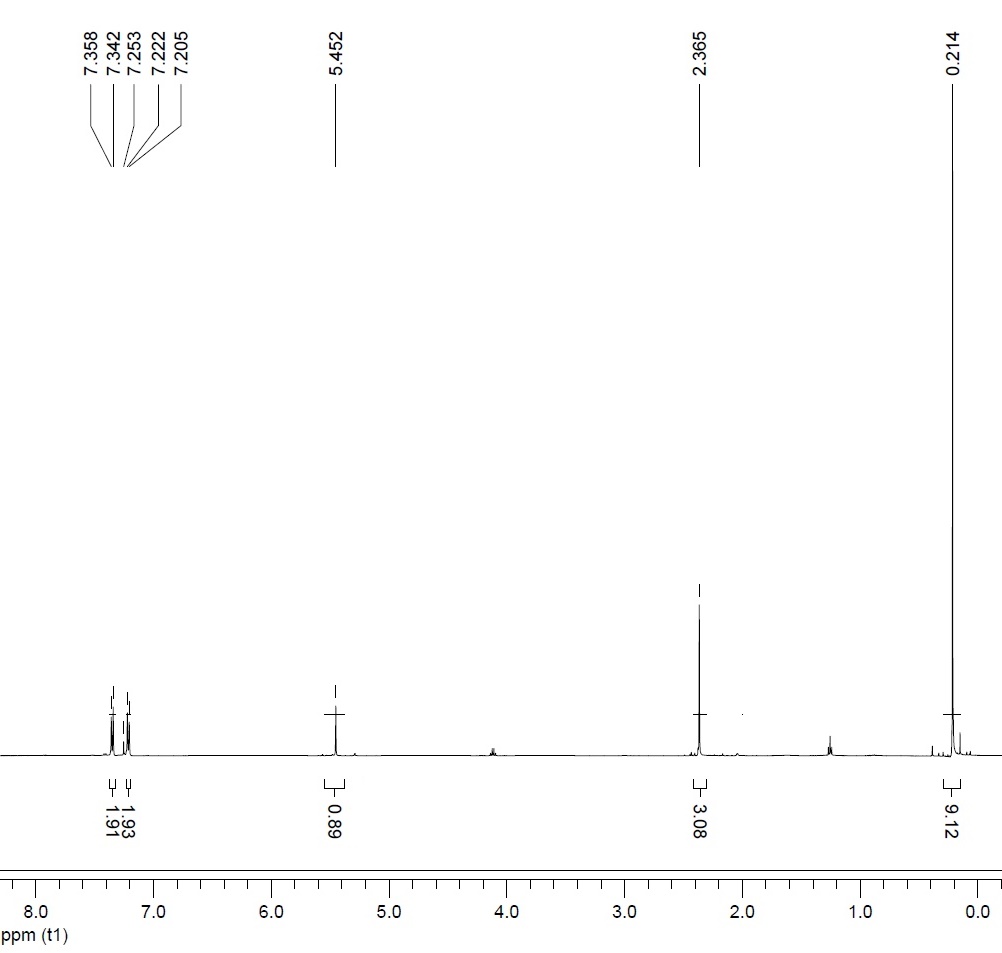
**Figure S 2.** IR Spectra of Mg-Al-Cu-LDH



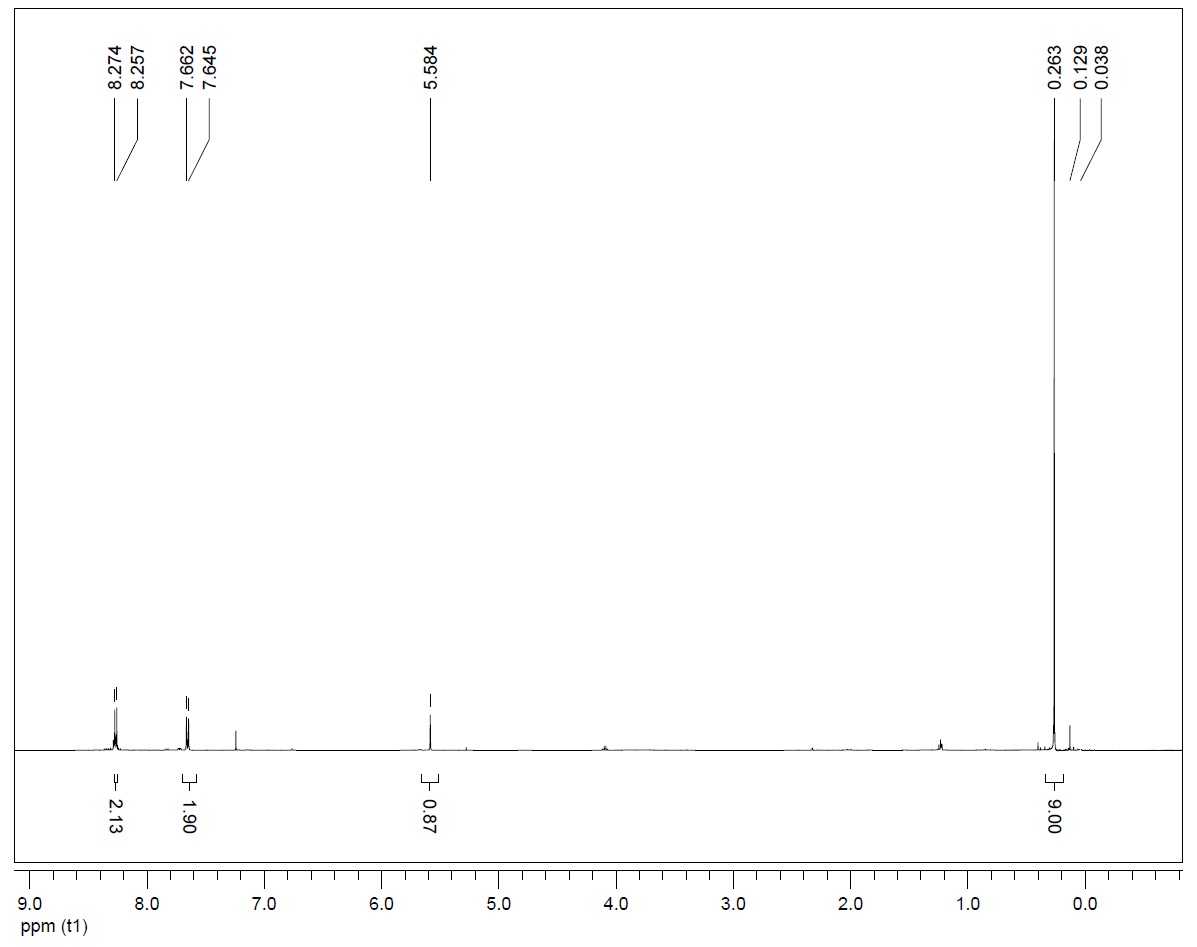
**Figure S 3.** 1H NMR of 2-phenyl-2-((trimethylsilyl)oxy)acetonitrile



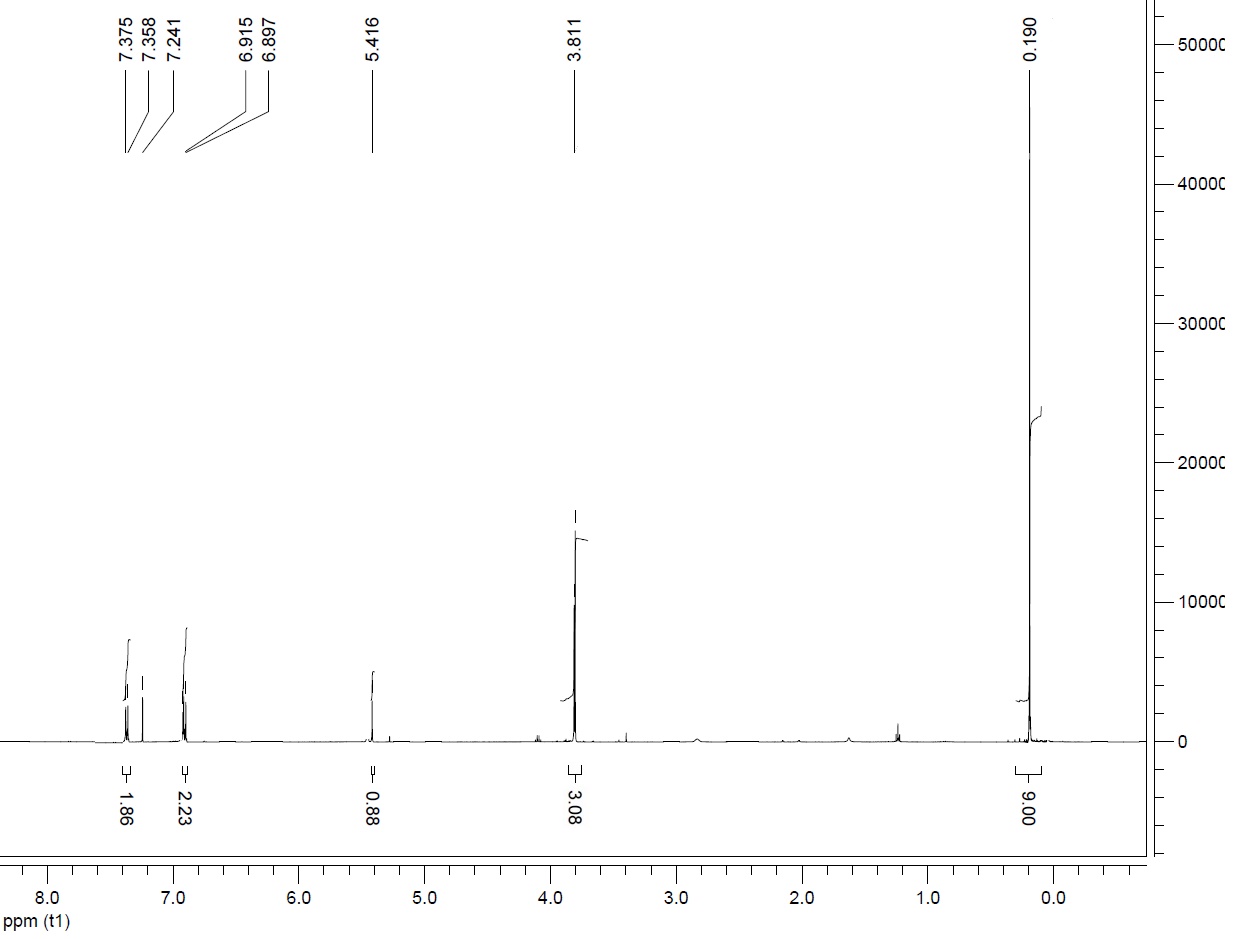
**Figure S 4.** 13C NMR of 2-phenyl-2-((trimethylsilyl)oxy)acetonitrile



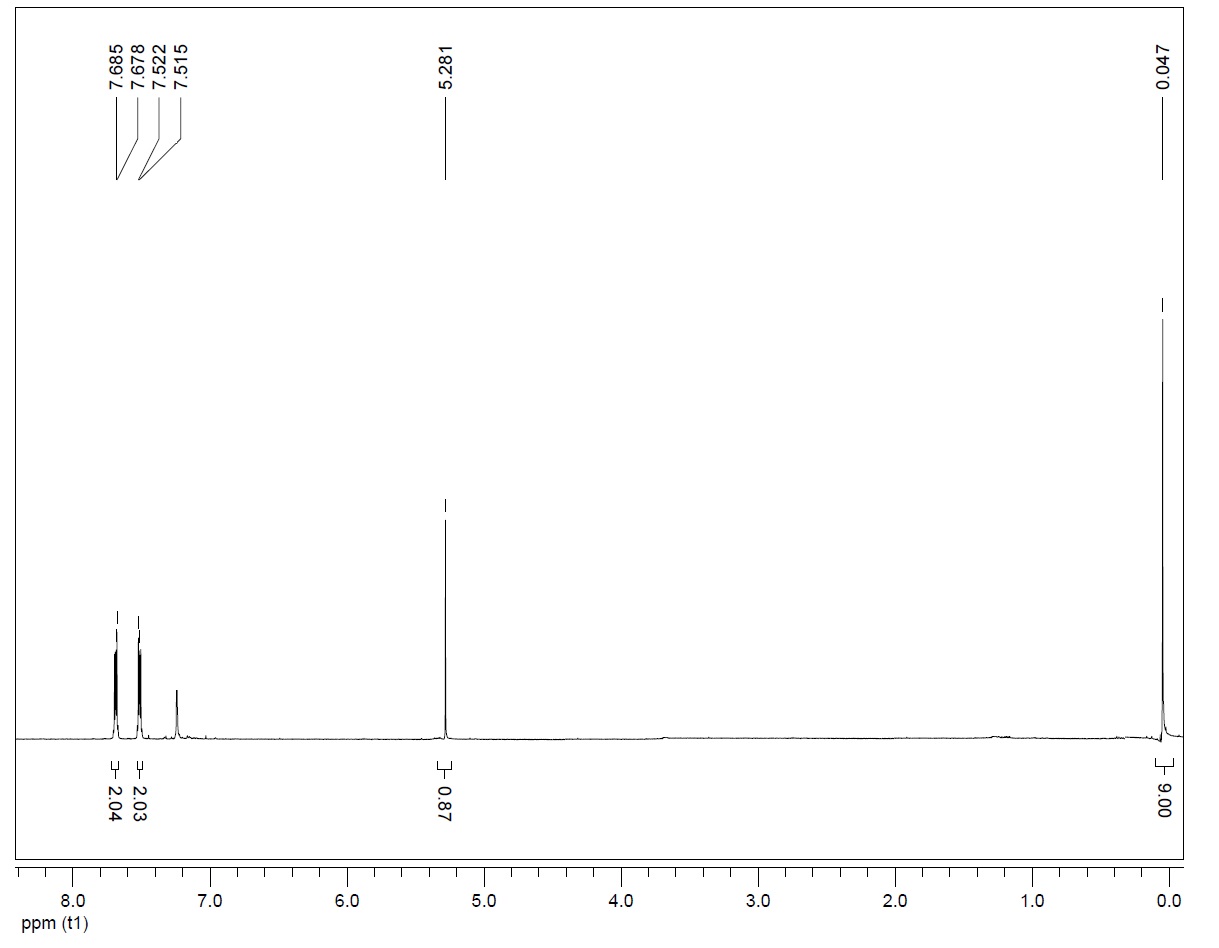
**Figure S 5.** 1H NMR of 2-(p-tolyl)-2-((trimethylsilyl)oxy)acetonitrile



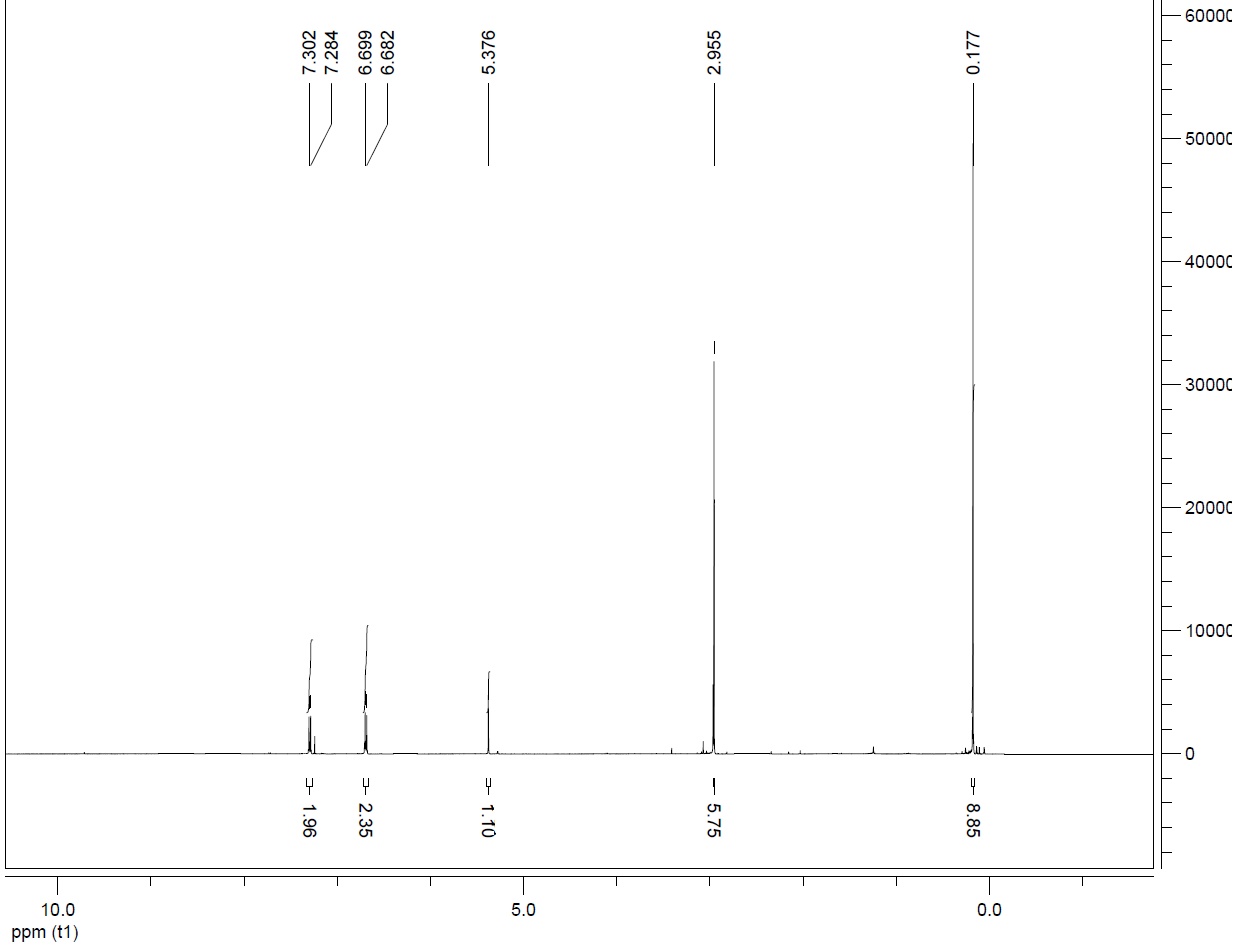
**Figure S 6.** 1H NMR of 2-(4-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile



**Figure S 7.** 1H NMR of 2-(4-methoxyphenyl)-2-((trimethylsilyl)oxy)acetonitrile



**Figure S 8.** 1H NMR of 2-(4-chlorophenyl)-2-((trimethylsilyl)oxy)acetonitrile



**Figure S 9.** 1H NMR of 2-(4-(dimethylamino)phenyl)-2-((trimethylsilyl)oxy)acetonitrile

**References**:

1. Kurono, N.; Arai, K.; Uemura, M.; Ohkuma, T. [Ru(phgly)2(binap)]/Li2CO3: A Highly Active, Robust, and Enantioselective Catalyst for the Cyanosilylation of Aldehydes. *Angew. Chem. Int. Ed.* **2008**, *47*, 6643-6646. DOI: 10.1002/anie.200801501.
2. Strappaveccia, G; Lanari, D.; Gelman, D.; Pizzo, F.; Rosati, O.; Curinib, M.; Vaccaro, L. Efficient synthesis of cyanohydrin trimethylsilyl ethers via 1,2-chemoselective cyanosilylation of carbonyls. *Green Chem*., **2013**, *15*, 199-204. DOI: 10.1039/C2GC36442E.
3. Pourmousavi, S. A.; Salahshornia, H. Efficient, Rapid and Solvent-free Cyanosilylation of Aldehydes and Ketones Catalyzed by SbCl3. *Bull. Korean Chem. Soc*. **2011**, *32*, 1575-1578. DOI:10.5012/bkcs.2011.32.5.1575.
4. Dekamin, M. G; Mokhtari, J.; Naimi-Jamal, M. R. Organocatalytic cyanosilylation of carbonyl compounds by tetrabutylammonium phthalimide-N-oxyl. *Catal. Commun.* **2009**, 10, 582-585. DOI: 10.1016/j.catcom.2008.10.036.