Supplementary Information

Design and Antibacterial Activity Assessment of "Green" Synthesized 1,4-disubstituted 1,2,3-triazoles via a Fe_3O_4/Silicalite-1/PVA/Cu(I) nanocomposite catalyzed three component reaction

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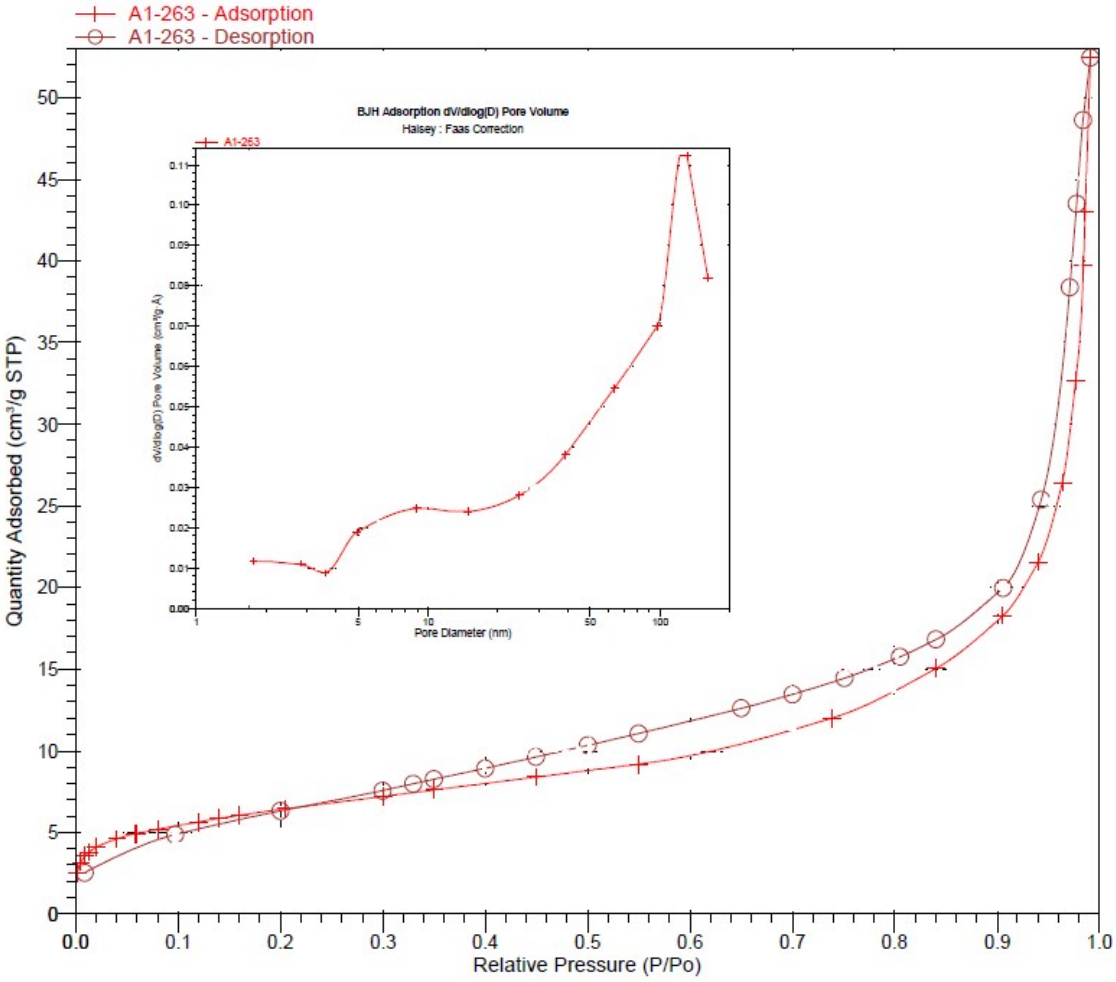
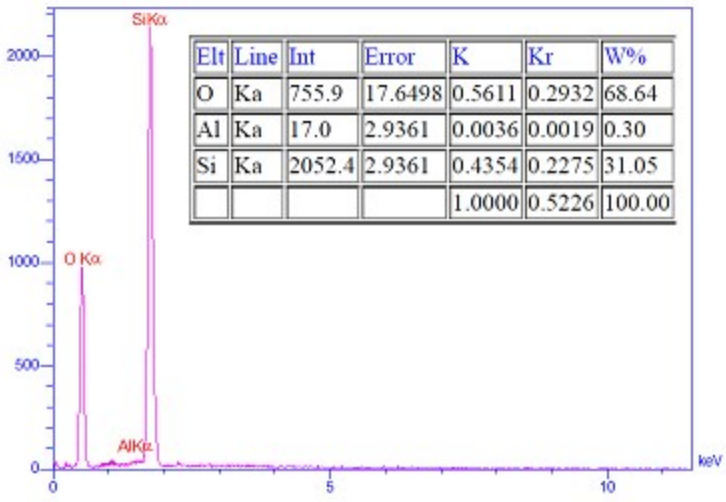


Figure S1. N_2 Adsorption-desorption isotherms and pore size distribution of Si-2.



Elt	Line	Int	Error	K	Kr	W%
O	Ka	755.9	17.6498	0.5611	0.2932	68.64
Al	Ka	17.0	2.9361	0.0036	0.0019	0.30
Si	Ka	2052.4	2.9361	0.4354	0.2275	31.05
				1.0000	0.5226	100.00

Figure S2. EDX data of Silicalite-1(Si-1) synthesized *via* sol-gel process.

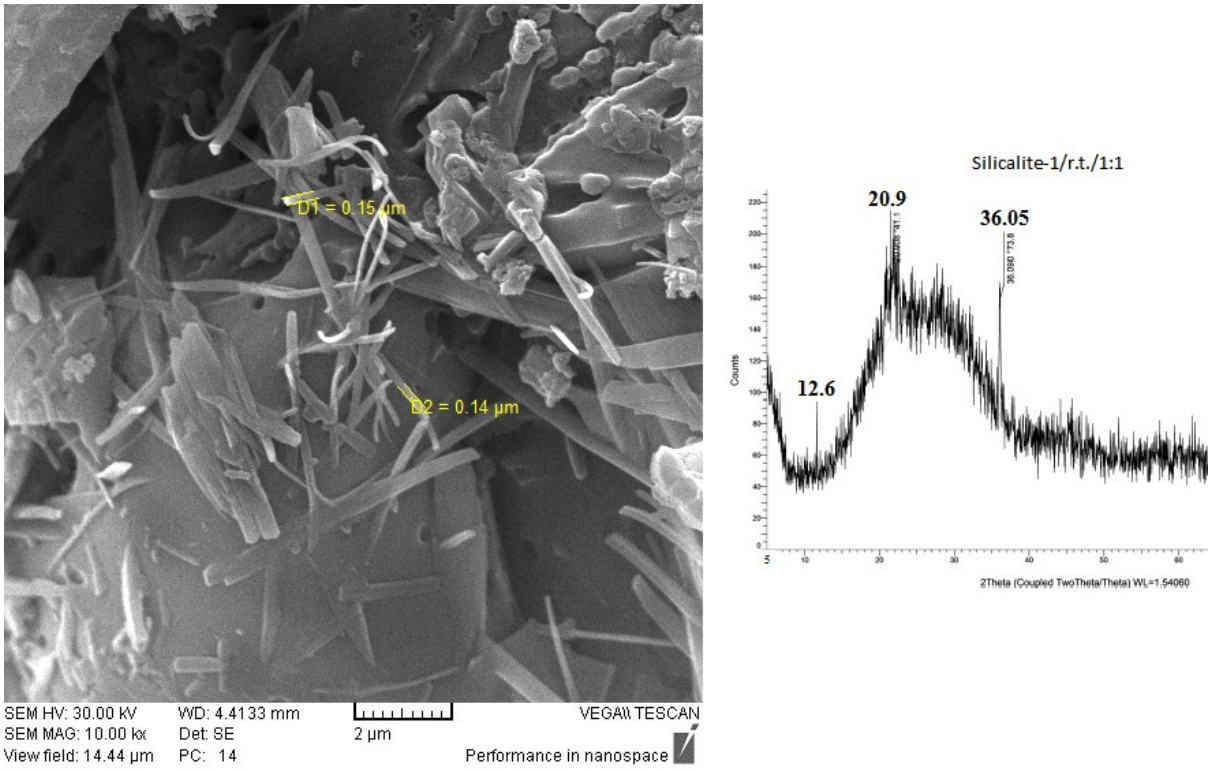
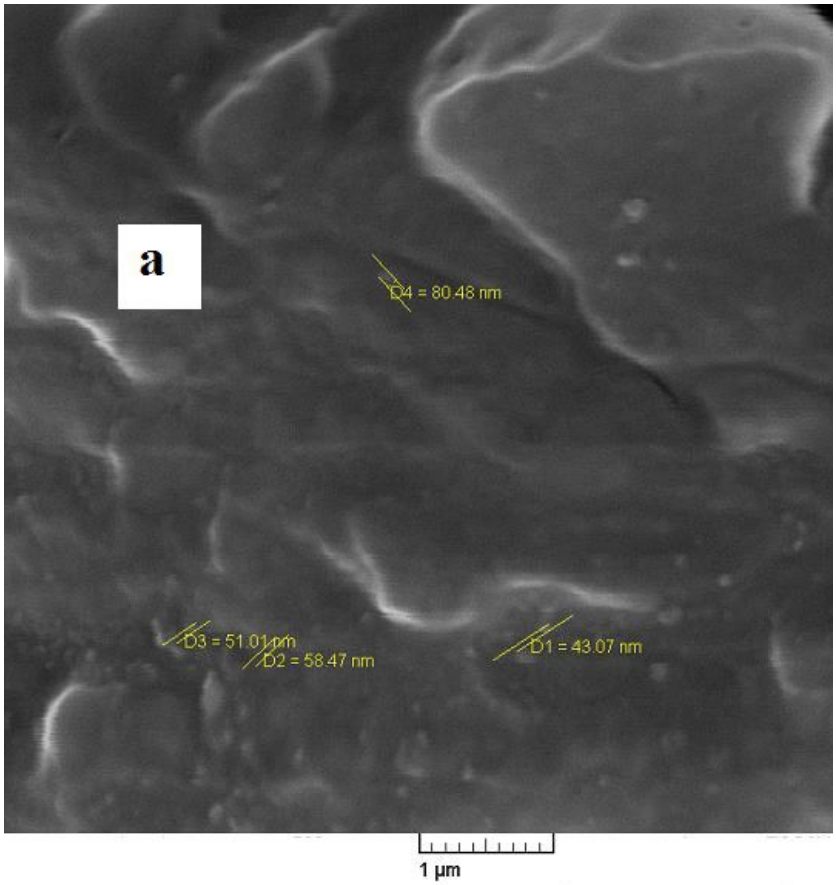
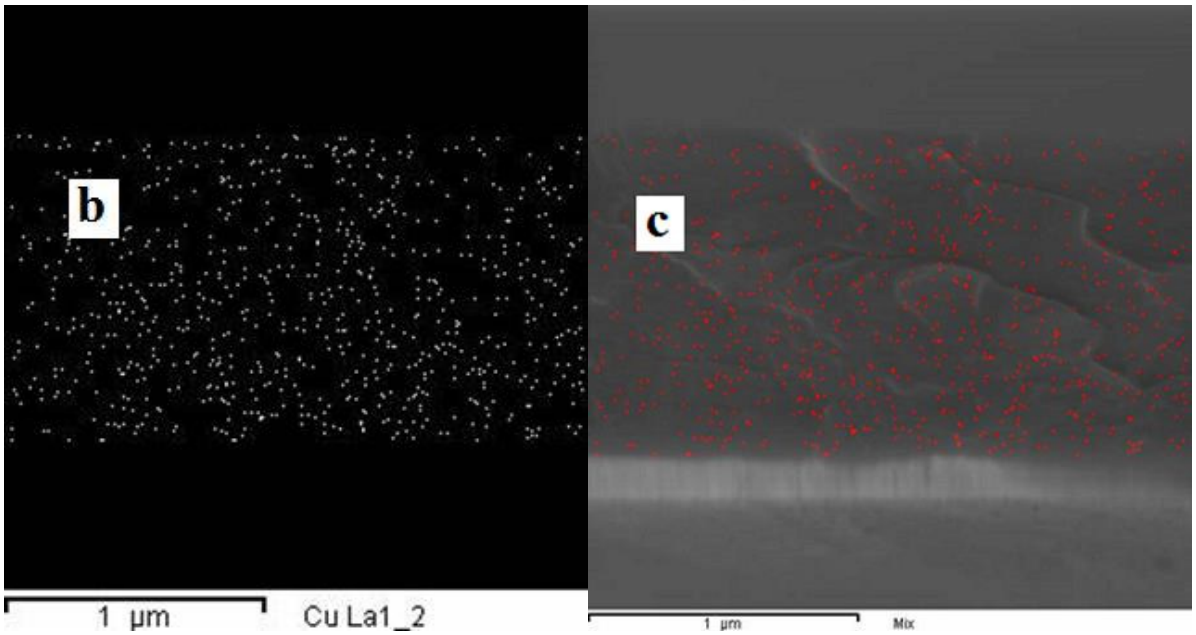


Figure S3. SEM image, EDX data and XRD of Silicalite-1(Si-2) synthesized *via* sol-gel process.


a
D4 = 80.48 nm
D3 = 51.01 nm
D2 = 58.47 nm
D1 = 43.07 nm
1 µm


b
1 µm
Cu La1_2
c
1 µm
Mix

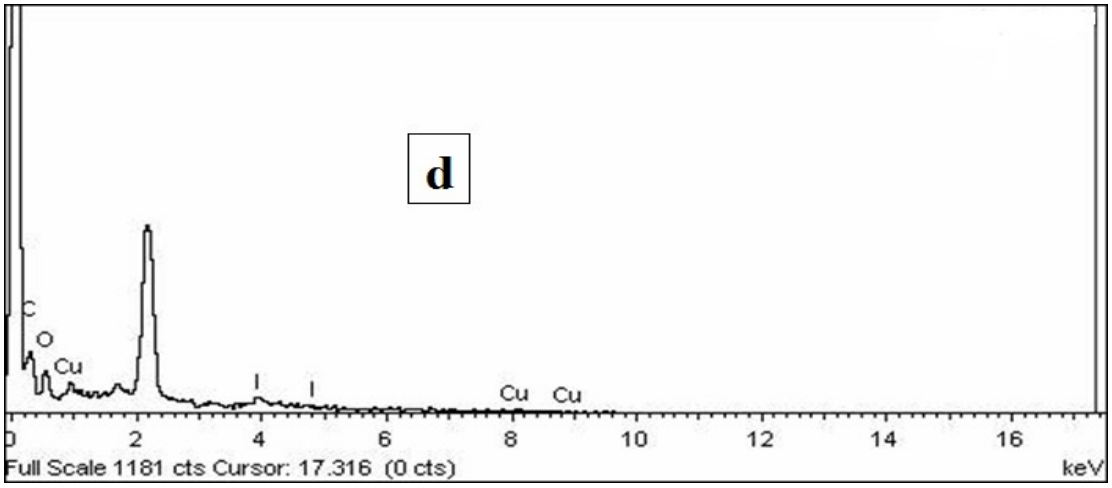
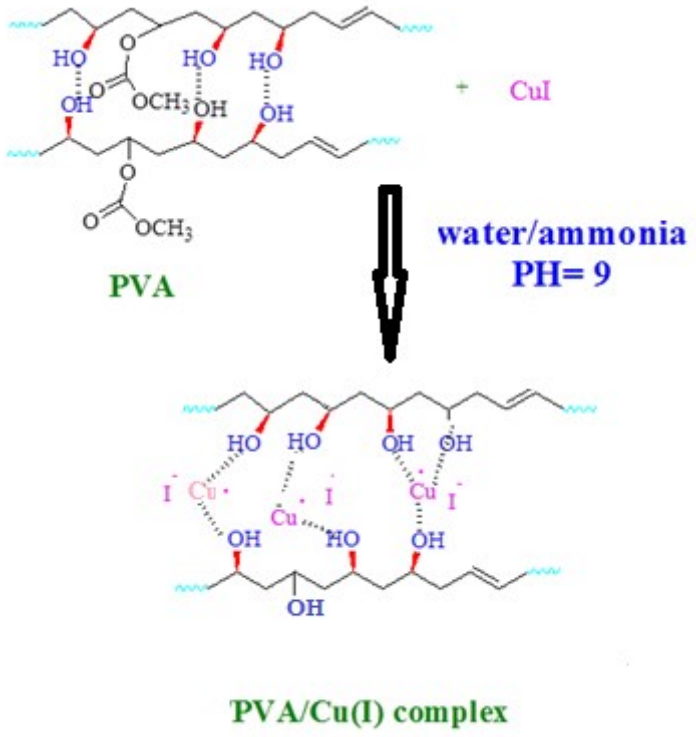


Figure S4. SEM image of PVA/Cu(I) catalyst (a), dispersion of PVA/Cu(I) catalyst (b and c) and EDX data of PVA/Cu(I) (d).



Scheme S1. Mechanism of reaction between PVA and CuI in formation of PVA/Cu(I) nanocomposite.

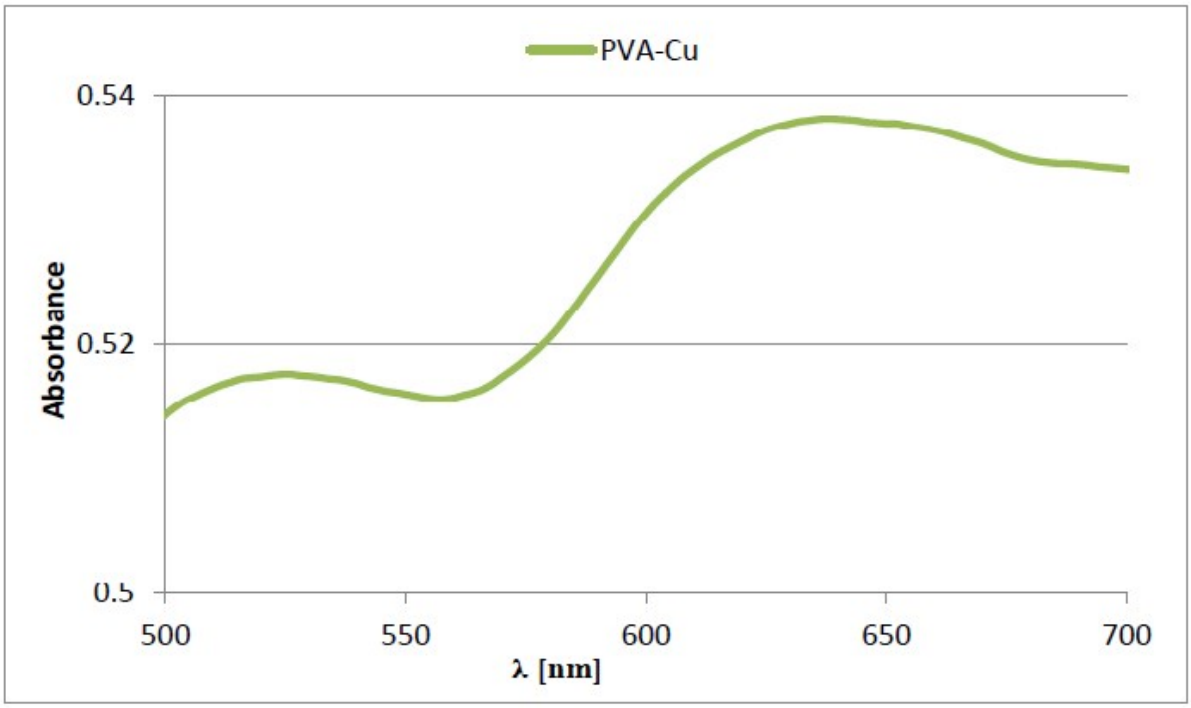


Figure S5. UV-Vis spectrum of PVA/Cu(I) nanocatalyst.

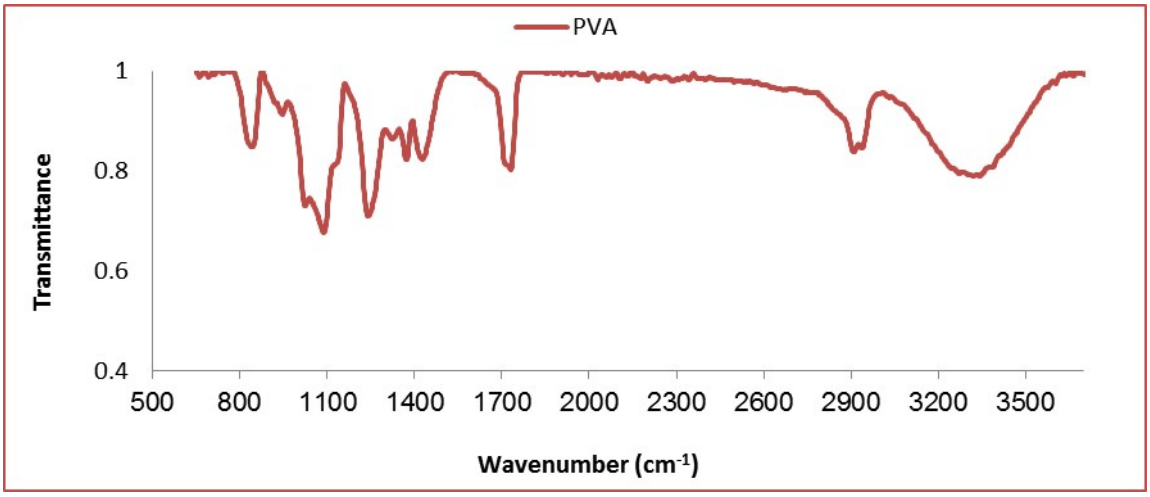


Figure S6. FT-IR spectrum of PVA.

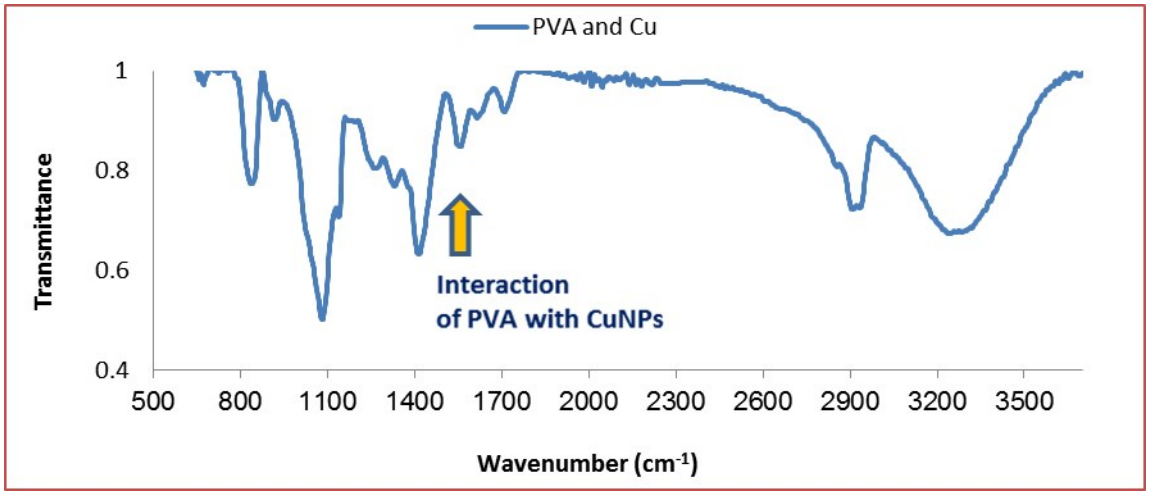


Figure S7. FT-IR spectrum of PVA/Cu(I).

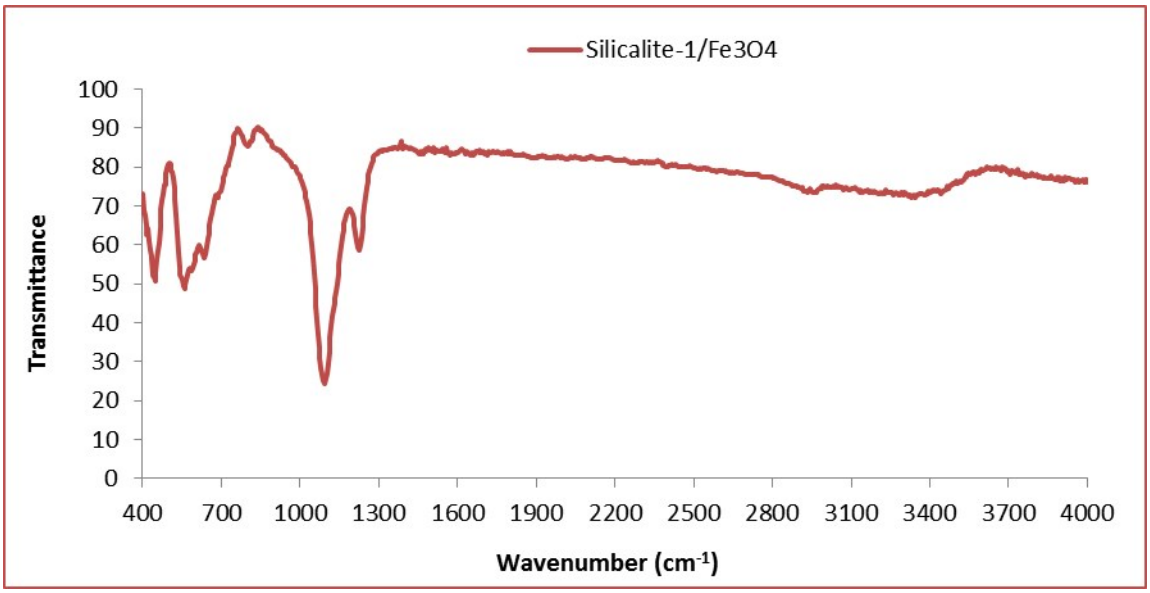


Figure S8. FT-IR spectrum of Fe_3O_4/Silicalite-1 nanocomposite.

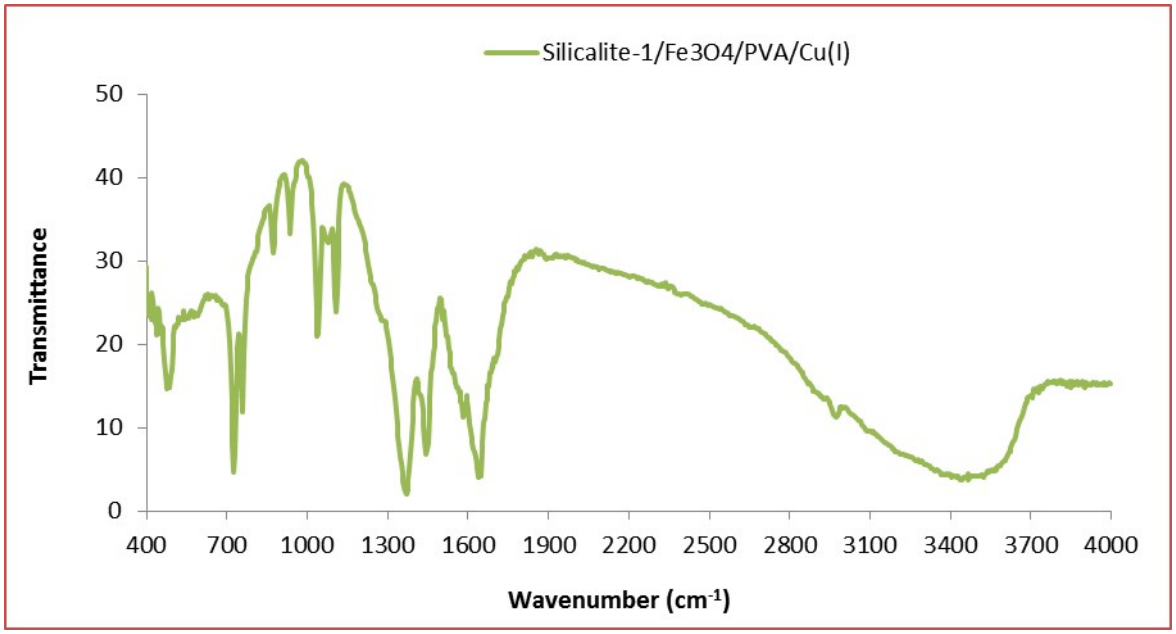


Figure S9. FT-IR spectrum of Fe_3O_4/Silicalite-1/PVA/Cu(I).

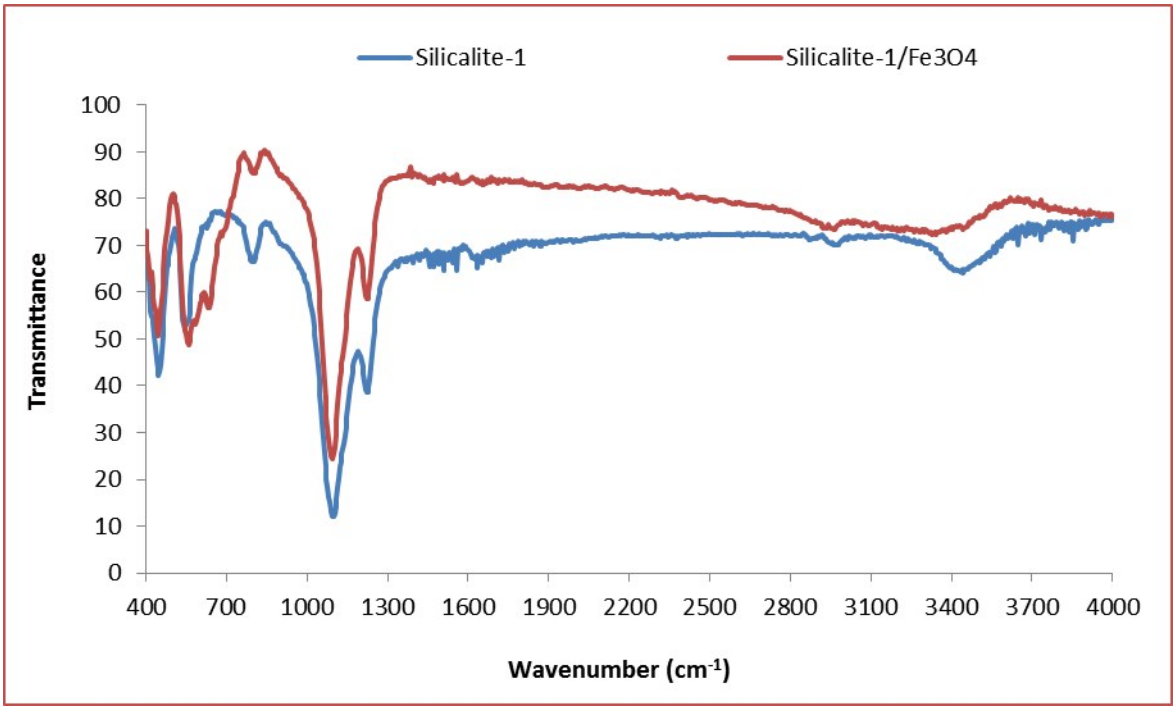


Figure S10. FT-IR spectra of Fe_3O_4/Silicalite-1 nanocomposite and Fe_3O_4/Silicalite-1/PVA/Cu(I).

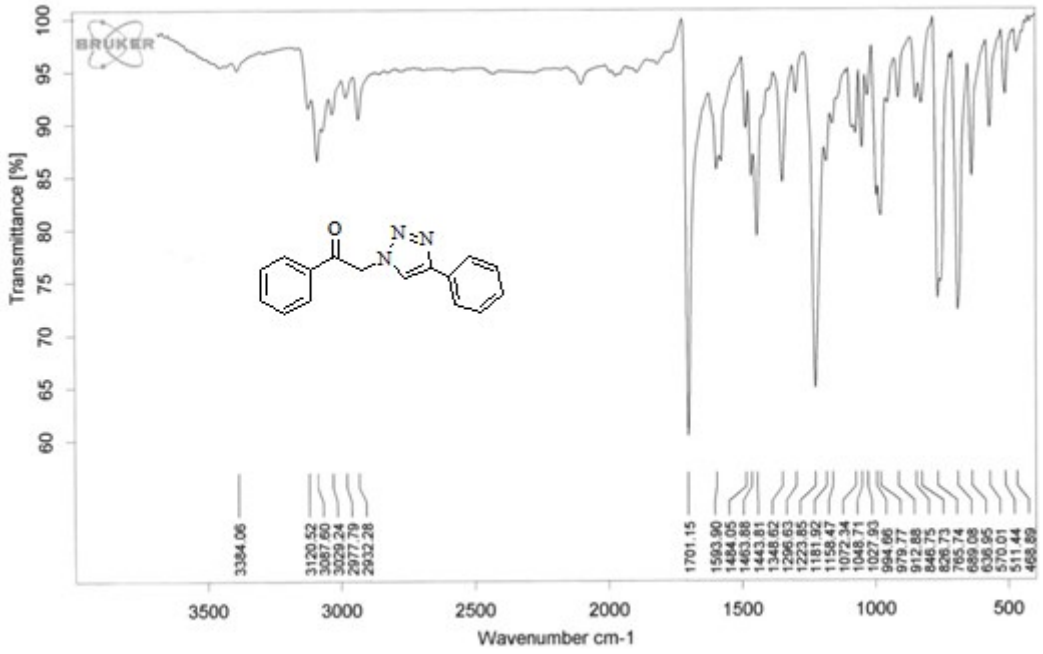


Figure S11. IR Spectrum of 1-Phenyl-2-(4-phenyl-[1,2,3]triazol-1-yl)ethanone **5a**.

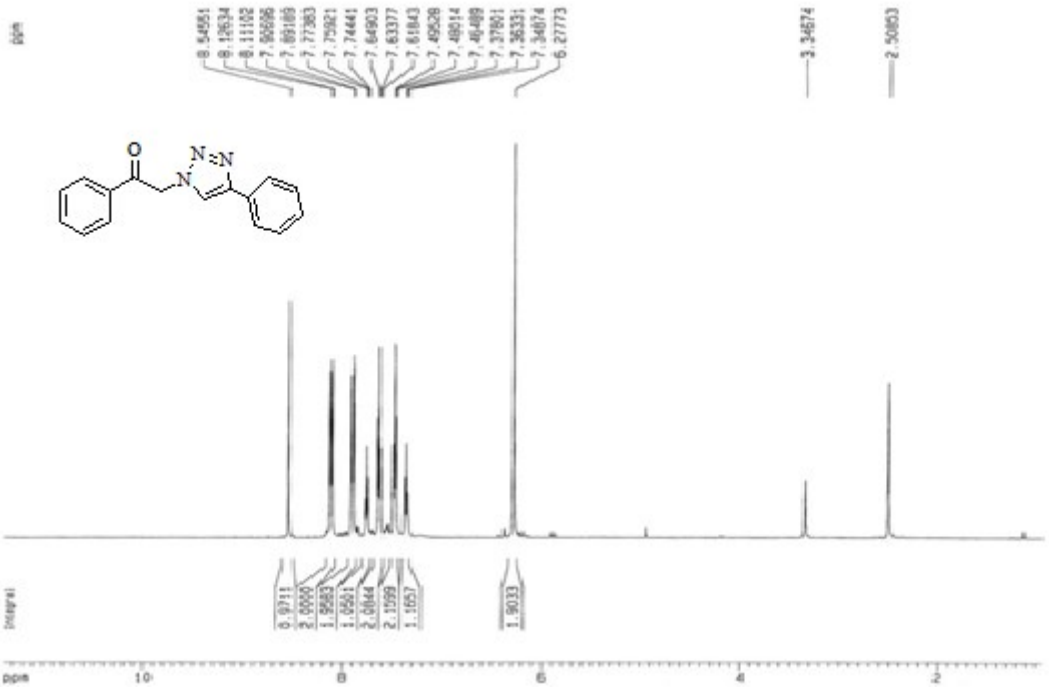


Figure S12. [1]HNMR Spectrum of 1-Phenyl-2-(4-phenyl-[1,2,3] triazol-1-yl) ethanone **5a**.

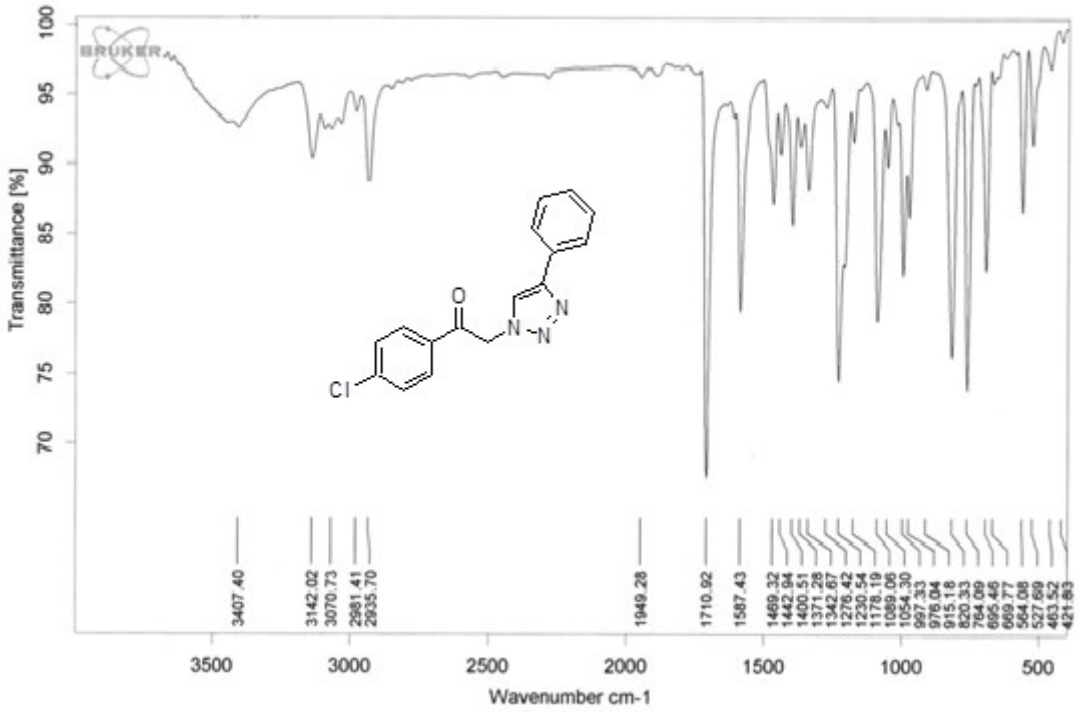


Figure S13. IR Spectrum of 1-(4-Chlorophenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone **5d**.

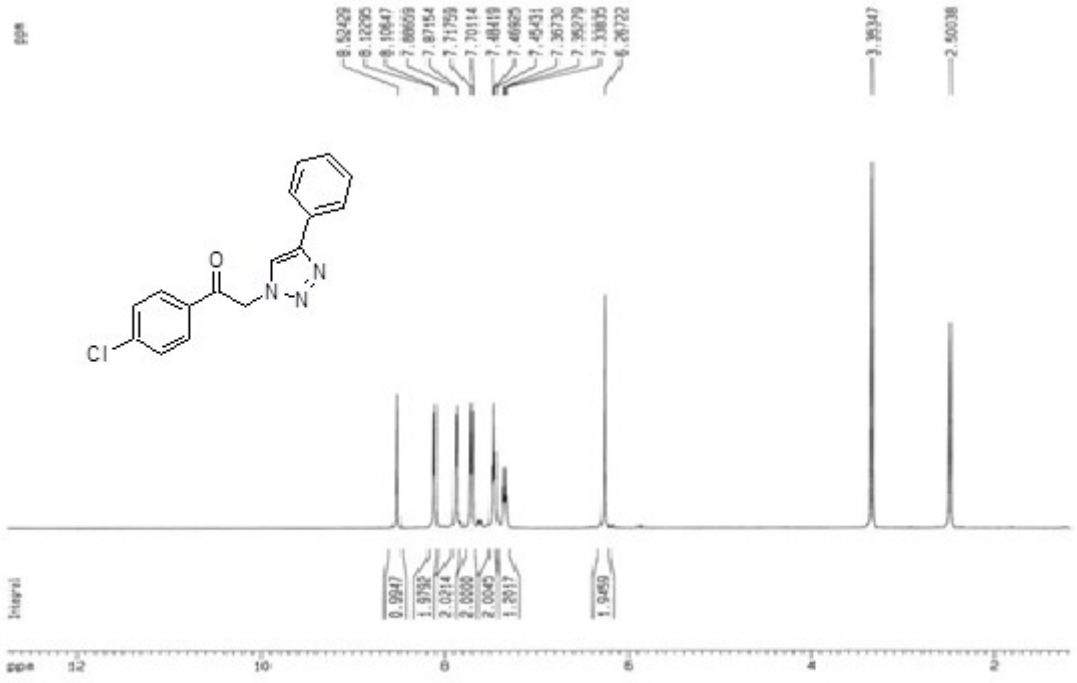


Figure S14. [1]HNMR Spectrum of 1-(4-Chlorophenyl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethanone **5d**.

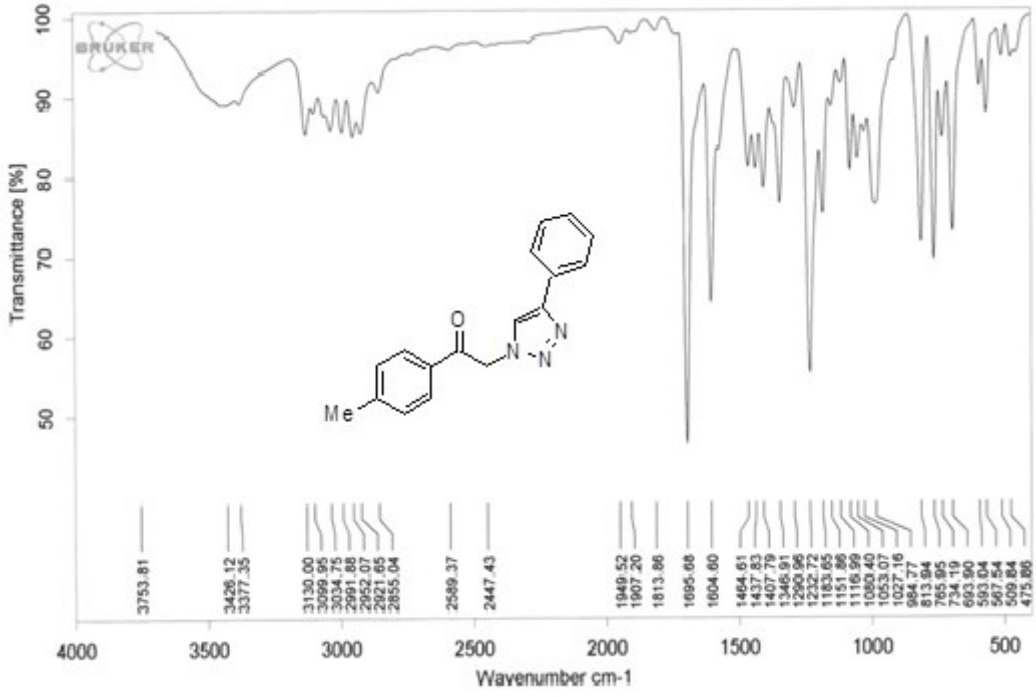


Figure S15. IR Spectrum of 2-(4-Phenyl-1H-1,2,3-triazol-1-yl)-1-p-tolyl-ethanone **5e**.

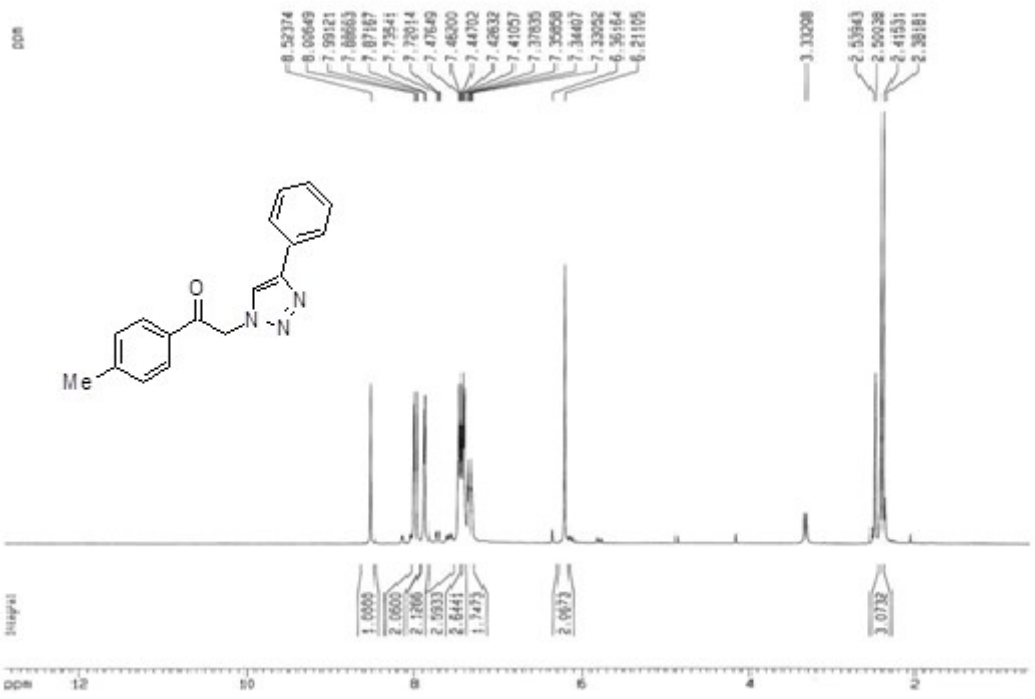


Figure S16. [1]HNMR Spectrum of 2-(4-Phenyl-1H-1,2,3-triazol-1-yl)-1-p-tolyl-ethanone **5e**.

Materials and equipment used in this study

All starting chemicals and reagents were commercially available and were utilized without further purification. Melting points were obtained through an Electrothermal 9100 apparatus. Fourier transform infrared spectroscopy (FT-IR) spectra were recorded by the film without KBr with a Shimadzu IR-470 spectrometer. Scanning electron micrograph (SEM) images were taken with a VEGA-TESCAN microscope with an attached camera. Energy-dispersive X-ray (EDX) analysis recorded by Numerix DXP-X10P. The XRD measurements were carried out by using a DRON-8 X-ray diffractometer, thermal analysis (TGA) was done by using of Bahr-STA 504 instrument under an argon atmosphere, and the magnetic properties of the sample were detected at room temperature using a VSM (Meghnatis Kavir Kashan Co., Kashan, Iran. Analytical thin-layer chromatography (TLC) was performed using

Merck silica gel GF254 plates. The surface areas of the catalyst sample were measured by N_2 adsorption at −195 °C with Autosorb-1 (Quanta Chrome), the BET equation being applied to the isotherm. The external surface area was obtained from a t-plot.

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References

1. S. Alfaro, M. A. Valenzuela and P. Bosch, *Journal of Porous Materials*, 2009, **16**, 337-342.
2. J. A. Thompson, N. A. Brunelli, R. P. Lively, J. Johnson, C. W. Jones and S. Nair, *The Journal of Physical Chemistry C*, 2013, **117**, 8198-8207.
3. A. Nanoti, S. Dasgupta, N. Biswas, A. N. Goswami, M. O. Garg, S. Divekar and C. Pendem, *Industrial & Engineering Chemistry Research*, 2012, **51**, 13765-13772.
4. L. R. Rad, A. Momeni, B. F. Ghazani, M. Irani, M. Mahmoudi and B. Noghreh, *Chemical Engineering Journal*, 2014, **256**, 119-127.
5. X. Yang, L. Huang, J. Li, X. Tang and X. Luo, *RSC Advances*, 2017, **7**, 12224-12230.
6. Z. Zhang, M. Sadakane, T. Murayama, N. Sakaguchi and W. Ueda, *Inorganic chemistry*, 2014, **53**, 7309-7318.
7. A. M. Abdel-Mageed, S. Eckle, H. Anfang and R. Behm, *Journal of catalysis*, 2013, **298**, 148-160.
8. N. K. Kanellopoulos, *Recent advances in gas separation by microporous ceramic membranes*, Elsevier, 2000.
9. D. W. Breck, *Zeolite molecular sieves: structure, chemistry and use*, Krieger, 1984.
10. S. Alfaro, C. Rodriguez, M. Valenzuela and P. Bosch, *Materials Letters*, 2007, **61**, 4655-4658.
11. C.-H. Cheng and D. F. Shantz, *The Journal of Physical Chemistry B*, 2005, **109**, 13912-13920.
12. R. M. Barrer, *Hydrothermal chemistry of zeolites*, Academic press, 1982.
13. E. R. Parnham and R. E. Morris, *Accounts of Chemical Research*, 2007, **40**, 1005-1013.
14. Y. K. Hwang, J. S. Chang, S. E. Park, D. S. Kim, Y. U. Kwon, S. H. Jhung, J. S. Hwang and M. S. Park, *Angewandte Chemie International Edition*, 2005, **44**, 556-560.
15. J. Guth, H. Kessler, J. Higel, J. Lamblin, J. Patarin, A. Seive, J. Chezeau and R. Wey, ACS Publications, 1989.
16. J. Sun, C. Bonneau, Á. Cantín, A. Corma, M. J. Díaz-Cabañas, M. Moliner, D. Zhang, M. Li and X. Zou, *Nature*, 2009, **458**, 1154.
17. E.-P. Ng, D. Chateigner, T. Bein, V. Valtchev and S. Mintova, *Science*, 2012, **335**, 70-73.
18. J. Jiang, J. L. Jorda, J. Yu, L. A. Baumes, E. Mugnaioli, M. J. Diaz-Cabanas, U. Kolb and A. Corma, *Science*, 2011, **333**, 1131-1134.
19. H. Kalipcilar and A. Culfaz, *Crystal Research and Technology: Journal of Experimental and Industrial Crystallography*, 2000, **35**, 933-942.
20. M. Nawab, S. Barot and R. Bandyopadhyay, *Journal of Chemical Sciences*, 2019, **131**, 2.
21. D. Astruc, F. Lu and J. R. Aranzaes, *Angewandte Chemie International Edition*, 2005, **44**, 7852-7872.
22. I. S. Park, M. S. Kwon, Y. Kim, J. S. Lee and J. Park, *Organic letters*, 2008, **10**, 497-500.

23. S. Ma, S. Zhan, Y. Jia and Q. Zhou, *ACS applied materials & interfaces*, 2015, **7**, 21875-21883.
24. A. Maleki, E. Akhlaghi and R. Paydar, *Applied Organometallic Chemistry*, 2016, **30**, 382-386.
25. K. Dobrovolný, P. Ulbrich, M. Švecová, S. Rimpelová, J. Malinčík, M. Kohout, J. Svoboda and V. Bartůněk, *Journal of Alloys and Compounds*, 2017, **697**, 147-155.
26. M. T. Razzak and D. Darwis, *Radiation Physics and Chemistry*, 2001, **62**, 107-113.
27. S. M. Kuo, S. J. Chang and Y. J. Wang, *Journal of Polymer Research*, 1999, **6**, 191-196.
28. P. Molyneux, *Water-Soluble synthetic polymers: Properties and Behavior. Volume I*, CRC Press, 1983.
29. T. Hirai, Y. Asada, T. Suzuki, S. Hayashi and M. Nambu, *Journal of applied polymer science*, 1989, **38**, 491-502.
30. H. C. Kolb, M. Finn and K. B. Sharpless, *Angewandte Chemie International Edition*, 2001, **40**, 2004-2021.
31. R. Huisgen, *Journal*, 1984.
32. C. W. Tornøe, C. Christensen and M. Meldal, *The Journal of organic chemistry*, 2002, **67**, 3057-3064.
33. V. V. Rostovtsev, L. G. Green, V. V. Fokin and K. B. Sharpless, *Angewandte Chemie International Edition*, 2002, **41**, 2596-2599.
34. H. A. Stefani, D. M. Leal and F. Manarin, *Tetrahedron Letters*, 2012, **53**, 6495-6499.
35. S. Mohammed, A. K. Padala, B. A. Dar, B. Singh, B. Sreedhar, R. A. Vishwakarma and S. B. Bharate, *Tetrahedron*, 2012, **68**, 8156-8162.
36. B.-Y. Lee, S. R. Park, H. B. Jeon and K. S. Kim, *Tetrahedron letters*, 2006, **47**, 5105-5109.
37. K. Fehér, J. Balogh, Z. Csók, T. Kégl, L. Kollár and R. Skoda-Földes, *Steroids*, 2012, **77**, 738-744.
38. J. E. Hein and V. V. Fokin, *Chemical Society Reviews*, 2010, **39**, 1302-1315.
39. M. Vincent, P. Hartemann and M. Engels-Deutsch, *International journal of hygiene and environmental health*, 2016, **219**, 585-591.
40. M. Vincent, R. E. Duval, P. Hartemann and M. Engels-Deutsch, *Journal of applied microbiology*, 2018, **124**, 1032-1046.
41. H. Palza, M. Nuñez, R. Bastías and K. Delgado, *International journal of antimicrobial agents*, 2018, **51**, 912-917.
42. U. Bogdanovic, V. Vodnik, M. Mitric, S. Dimitrijevic, S. D. Skapin, V. Zunic, M. Budimir and M. Stoiljkovic, *ACS applied materials & interfaces*, 2015, **7**, 1955-1966.
43. N. Cioffi, L. Torsi, N. Ditaranto, G. Tantillo, L. Ghibelli, L. Sabbatini, T. Bleve-Zacheo, M. D'Alessio, P. G. Zambonin and E. Traversa, *Chemistry of Materials*, 2005, **17**, 5255-5262.
44. D. N. Bikiaris and K. S. Triantafyllidis, *Materials Letters*, 2013, **93**, 1-4.
45. D. Green, S. Jayasundara, Y.-F. Lam and M. Harris, *Journal of non-crystalline solids*, 2003, **315**, 166-179.
46. J. Qi, T. Zhao, X. Xu, F. Li and G. Sun, *Journal of Porous Materials*, 2011, **18**, 509-515.
47. Y. F. Yeong, A. Z. Abdullah, A. L. Ahmad and S. Bhatia, *Journal of Membrane Science*, 2009, **341**, 96-108.
48. J. Lin and M. Yates, *Langmuir*, 2005, **21**, 2117-2120.
49. B. Tokay, M. Somer, A. Erdem-Şenatalar, F. Schüth and R. W. Thompson, *Microporous and Mesoporous Materials*, 2009, **118**, 143-151.
50. Y. Dong, Y. Peng, G. Wang, Z. Wang and Y. Yan, *Industrial & Engineering Chemistry Research*, 2012, **51**, 3646-3652.
51. J. Rahimi, R. Taheri-Ledari, M. Niksefat and A. Maleki, *Catalysis Communications*, 2020, **134**, 105850.
52. Y. Gan, S. Bai, S. Hu, X. Zhao and Y. Li, *RSC advances*, 2016, **6**, 56728-56737.
53. R. Mirsafaei, M. M. Heravi, S. Ahmadi, M. H. Moslemin and T. Hosseinnejad, *Journal of Molecular Catalysis A: Chemical*, 2015, **402**, 100-108.
54. M. Daraie and M. M. Heravi, *International journal of biological macromolecules*, 2019, **140**, 939-948.

55. F. Ebrahimpour-Malamir, T. Hosseinnejad, R. Mirsafaei and M. M. Heravi, *Applied Organometallic Chemistry*, 2018, **32**, e3913.
56. E. Hashemi, Y. S. Beheshtiha, S. Ahmadi and M. M. Heravi, *Transition Metal Chemistry*, 2014, **39**, 593-601.
57. A. T. Kal-Kashvandi, M. M. Heravi, S. Ahmadi and T. Hosseinnejad, *Journal of Inorganic and Organometallic Polymers and Materials*, 2018, **28**, 1457-1467.
58. A. Pourjavadi, A. Motamedi, S. H. Hosseini and M. Nazari, *RSC Advances*, 2016, **6**, 19128-19135.
59. N. Pourmohammad, M. M. Heravi, S. Ahmadi and T. Hosseinnejad, *Applied Organometallic Chemistry*, 2019, **33**, e4967.
60. B. Movassagh and N. Rezaei, *Tetrahedron*, 2014, **70**, 8885-8892.
61. A. Akbari, N. Arsalani, M. Amini and E. Jabbari, *Journal of Molecular Catalysis A: Chemical*, 2016, **414**, 47-54.
62. D. D. Díaz, D. Kühbeck and R. J. Koopmans, *Chemical Society Reviews*, 2011, **40**, 427-448.
63. M. Heravi and S. Sadjadi, *Journal of the Iranian Chemical Society*, 2009, **6**, 1-54.
64. A. Azam, A. S. Ahmed, M. Oves, M. S. Khan, S. S. Habib and A. Memic, *International journal of nanomedicine*, 2012, **7**, 6003.
65. T. Pandiyarajan, R. Udayabhaskar, S. Vignesh, R. A. James and B. Karthikeyan, *Materials Science and Engineering: C*, 2013, **33**, 2020-2024.
66. M. Balouiri, M. Sadiki and S. K. Ibnsouda, *Journal of pharmaceutical analysis*, 2016, **6**, 71-79.