

Department of Organic Chemistry, Faculty of Chemical Engineering and Technology, University of Zagreb,
Marulićev trg 20

Benzothiazole derivatives exhibit various biological activities such as antitumor, antimicrobial, antiviral and anti-inflammatory. [1] Among the azoles, 1,2,3- triazoles are biological active compounds and attract a lot of attention as pharmacophore. Besides, triazole ring represents an ideal linker due its physical and chemical properties and can interact with biological targets such as DNA and proteins. One of the most famous drug containing a triazole linker is Ribavirin which is used for antiviral treatment. Furthermore, 2-mercaptobenzothiazole and 1,2,3-triazole derivative demonstrated potent selective COX-2 inhibition comparable with the standard drug ibuprofen. [2] Nowadays, more attention is focused on the synthesis of new biologically active agents by ecofriendly methodologies such as microwave-assisted and mechanochemical syntheses.

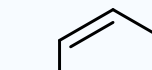
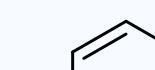
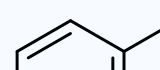
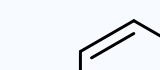
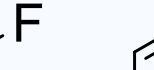
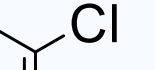
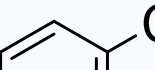
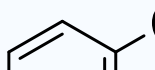
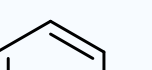
i
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 iii

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 5-36

R₁
 R₂-N₃

compd
 2
 3
 4
 R₁
 H
 Cl
 F

HEME 1. Reagents and conditions : (i) K_2CO_3 /ethanol/600W/40°C/30min/propargyl bromide/600W/90°C/90min (ii) $\text{Na}_2\text{S}_2\text{O}_5$ /DMF/reflux 2h (iii) corresponding 1-azidobenzene/ ethanol/ $\text{Cu}(\text{OAc})_2$ / 1.5 h- 2 h/ 30 Hz

		R ₂													
R ₁															
compd		5	6	7	8	9	10	11	12	13	14	15	16	17	
η/%	H	73,7	78,1	81,6	25,2	48,4	20,1	50,4	29,9	71,9	43	59,5	68,2	95	
compd		18	19	30	21	22	23	24	25	26	27	28	29	30	
η/%	F	61,1	89,8	87,1	83,5	55,5	75,2	75,3	67,2	81	89,2	96,8	79,6	51,2	
compd		31	32	33	34	35	36								
η/%	Cl	83,2	29	22	44,5	23,2	43,8								

Chemical structure of the compound is shown above the spectrum. The structure is a 1,2,3,4-tetrahydroquinoline derivative with a 2-chlorophenyl group attached to the nitrogen atom. The protons are labeled with numbers 1 through 10, corresponding to the peaks in the spectrum.

The spectrum shows the following peaks (from left to right):

- H-9' (singlet, ~8.8 ppm)
- H-2',6 (doublet, ~8.1 ppm)
- H-4 (singlet, ~7.9 ppm)
- H-7 (singlet, ~7.8 ppm)
- H-6'' (singlet, ~7.6 ppm)
- H-3'' (singlet, ~7.5 ppm)
- H-5'',4'',5,6 (multiplet, ~7.4 ppm)
- H-3,5' (doublet, ~7.2 ppm)

The chemical structure is a 1,2,3,4-tetrahydroquinoline derivative. The nitrogen atom is substituted with a 2-chlorophenyl group. The protons are labeled as follows: 1 (N-H), 2 (aromatic), 3 (aromatic), 4 (aromatic), 5 (aromatic), 6 (aromatic), 7 (aromatic), 8 (aromatic), 9 (aromatic), 10 (aromatic). The spectrum shows the following peaks (from left to right):

- H-9' (singlet, ~8.8 ppm)
- H-2',6 (doublet, ~8.1 ppm)
- H-4 (singlet, ~7.9 ppm)
- H-7 (singlet, ~7.8 ppm)
- H-6'' (singlet, ~7.6 ppm)
- H-3'' (singlet, ~7.5 ppm)
- H-5'',4'',5,6 (multiplet, ~7.4 ppm)
- H-3,5' (doublet, ~7.2 ppm)

Chemical structure of the compound is shown above the spectrum. The structure is a 1,3,5-trisubstituted benzene ring with a 4-phenyl-1,3,5-trisubstituted benzene ring at position 1, a 4-phenyl-1,3,5-trisubstituted benzene ring at position 3, and a 4-phenyl-1,3,5-trisubstituted benzene ring at position 5. The protons are labeled with numbers 1 through 12. The ¹H NMR spectrum (400 MHz, CDCl₃) shows peaks at 8.3 (d, 1H, H-9'), 8.2 (d, 1H, H-4), 8.1 (d, 1H, H-7,2',6'), 8.0 (d, 1H, H-7,2',6'), 7.9 (d, 1H, H-7,2',6'), 7.8 (d, 1H, H-7,2',6'), 7.7 (d, 1H, H-7,2',6'), 7.6 (d, 1H, H-7,2',6'), 7.5 (d, 1H, H-7,2',6'), 7.4 (d, 1H, H-7,2',6'), 7.3 (d, 1H, H-7,2',6'), 7.2 (d, 1H, H-7,2',6'), 7.1 (d, 1H, H-7,2',6'), 7.0 (d, 1H, H-7,2',6'), 6.9 (d, 1H, H-7,2',6'), 6.8 (d, 1H, H-7,2',6'), 6.7 (d, 1H, H-7,2',6'), 6.6 (d, 1H, H-7,2',6'), 6.5 (d, 1H, H-7,2',6'), 6.4 (d, 1H, H-7,2',6'), 6.3 (d, 1H, H-7,2',6'), 6.2 (d, 1H, H-7,2',6'), 6.1 (d, 1H, H-7,2',6'), 6.0 (d, 1H, H-7,2',6'), 5.9 (d, 1H, H-7,2',6'), 5.8 (d, 1H, H-7,2',6'), 5.7 (d, 1H, H-7,2',6'), 5.6 (d, 1H, H-7,2',6'), 5.5 (d, 1H, H-7,2',6'), 5.4 (d, 1H, H-7,2',6'), 5.3 (d, 1H, H-7,2',6'), 5.2 (d, 1H, H-7,2',6'), 5.1 (d, 1H, H-7,2',6'), 5.0 (d, 1H, H-7,2',6'), 4.9 (d, 1H, H-7,2',6'), 4.8 (d, 1H, H-7,2',6'), 4.7 (d, 1H, H-7,2',6'), 4.6 (d, 1H, H-7,2',6'), 4.5 (d, 1H, H-7,2',6'), 4.4 (d, 1H, H-7,2',6'), 4.3 (d, 1H, H-7,2',6'), 4.2 (d, 1H, H-7,2',6'), 4.1 (d, 1H, H-7,2',6'), 4.0 (d, 1H, H-7,2',6'), 3.9 (d, 1H, H-7,2',6'), 3.8 (d, 1H, H-7,2',6'), 3.7 (d, 1H, H-7,2',6'), 3.6 (d, 1H, H-7,2',6'), 3.5 (d, 1H, H-7,2',6'), 3.4 (d, 1H, H-7,2',6'), 3.3 (d, 1H, H-7,2',6'), 3.2 (d, 1H, H-7,2',6'), 3.1 (d, 1H, H-7,2',6'), 3.0 (d, 1H, H-7,2',6'), 2.9 (d, 1H, H-7,2',6'), 2.8 (d, 1H, H-7,2',6'), 2.7 (d, 1H, H-7,2',6'), 2.6 (d, 1H, H-7,2',6'), 2.5 (d, 1H, H-7,2',6'), 2.4 (d, 1H, H-7,2',6'), 2.3 (d, 1H, H-7,2',6'), 2.2 (d, 1H, H-7,2',6'), 2.1 (d, 1H, H-7,2',6'), 2.0 (d, 1H, H-7,2',6'), 1.9 (d, 1H, H-7,2',6'), 1.8 (d, 1H, H-7,2',6'), 1.7 (d, 1H, H-7,2',6'), 1.6 (d, 1H, H-7,2',6'), 1.5 (d, 1H, H-7,2',6'), 1.4 (d, 1H, H-7,2',6'), 1.3 (d, 1H, H-7,2',6'), 1.2 (d, 1H, H-7,2',6'), 1.1 (d, 1H, H-7,2',6'), 1.0 (d, 1H, H-7,2',6'), 0.9 (d, 1H, H-7,2',6'), 0.8 (d, 1H, H-7,2',6'), 0.7 (d, 1H, H-7,2',6'), 0.6 (d, 1H, H-7,2',6'), 0.5 (d, 1H, H-7,2',6'), 0.4 (d, 1H, H-7,2',6'), 0.3 (d, 1H, H-7,2',6'), 0.2 (d, 1H, H-7,2',6'), 0.1 (d, 1H, H-7,2',6').

Chemical shifts (ppm): 167.403, 163.005, 162.998, 161.906, 156.129, 143.396, 134.795, 133.988, 133.986, 129.798, 129.796, 126.463, 126.461, 123.798, 123.796, 123.040, 123.038, 122.302, 122.300, 118.805, 118.803.

Peak assignments: C-2, C-4', C-4a, C-8', C-1', C-1'', C-7a, C-6,5,7,4,9', C-2',6', C-3',5''.

13C NMR spectrum of compound 1 in CDCl₃. The x-axis represents the chemical shift in ppm, ranging from 55 to 165. The spectrum shows several sharp peaks. Key peaks are labeled: C-2 at ~163 ppm, C-4' at ~154 ppm, C-4a at ~151 ppm, C-8' at ~138 ppm, C-1', 7a, 2'' at ~135 ppm, C-3'', 7'' at ~132 ppm, C-2', 6', 5'', 6, 9', 7, 4 at ~128 ppm, C-4'', 6'' at ~125 ppm, C-3', 5' at ~115 ppm, C-7'' at ~60 ppm, and CH₂ at ~55 ppm. A list of chemical shifts is provided on the right side of the spectrum.

Chemical Shift (ppm)
163.941
160.906
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Figure 6. ^{13}C -NMR spectrum of compound **17**

[1] S.G. Agalave, S.R. Maujan, S. Vandana, Click Chemistry, Asian J. Chem. 6 (2011) 2696

[2] S. Shafi, M. Mahboob Alam, N. Mulakayala, C. Mulakayala, G. Vanaja, A.M. Kalle, M.S. Alam, Eur. J. Med. Chem. 49 (2012) 324

O-propargylated benzaldehyde (1) was prepared by S_N2 reaction of 4-hydroxybenzaldehyde and propargyl bromide using K₂CO₃ as a base. Propargylated benzothiazole derivatives (2-4) were prepared by cyclization reaction of *O*-propargyl benzaldehyde and different substituted aminothiophenol in DMF using oxidizing agent Na₂S₂O₅. Target 1,2,3-triazolyl derivatives of benzothiazole (5-36) were prepared by mechanochemical Huisgen 1,3-dipolar cycloaddition reaction. Structures of all newly prepared benzothiazole derivatives were confirmed by ¹H and ¹³C-NMR spectroscopy.

Financial support from the Croatian Science Foundation under the project IP-2018-01-4682.