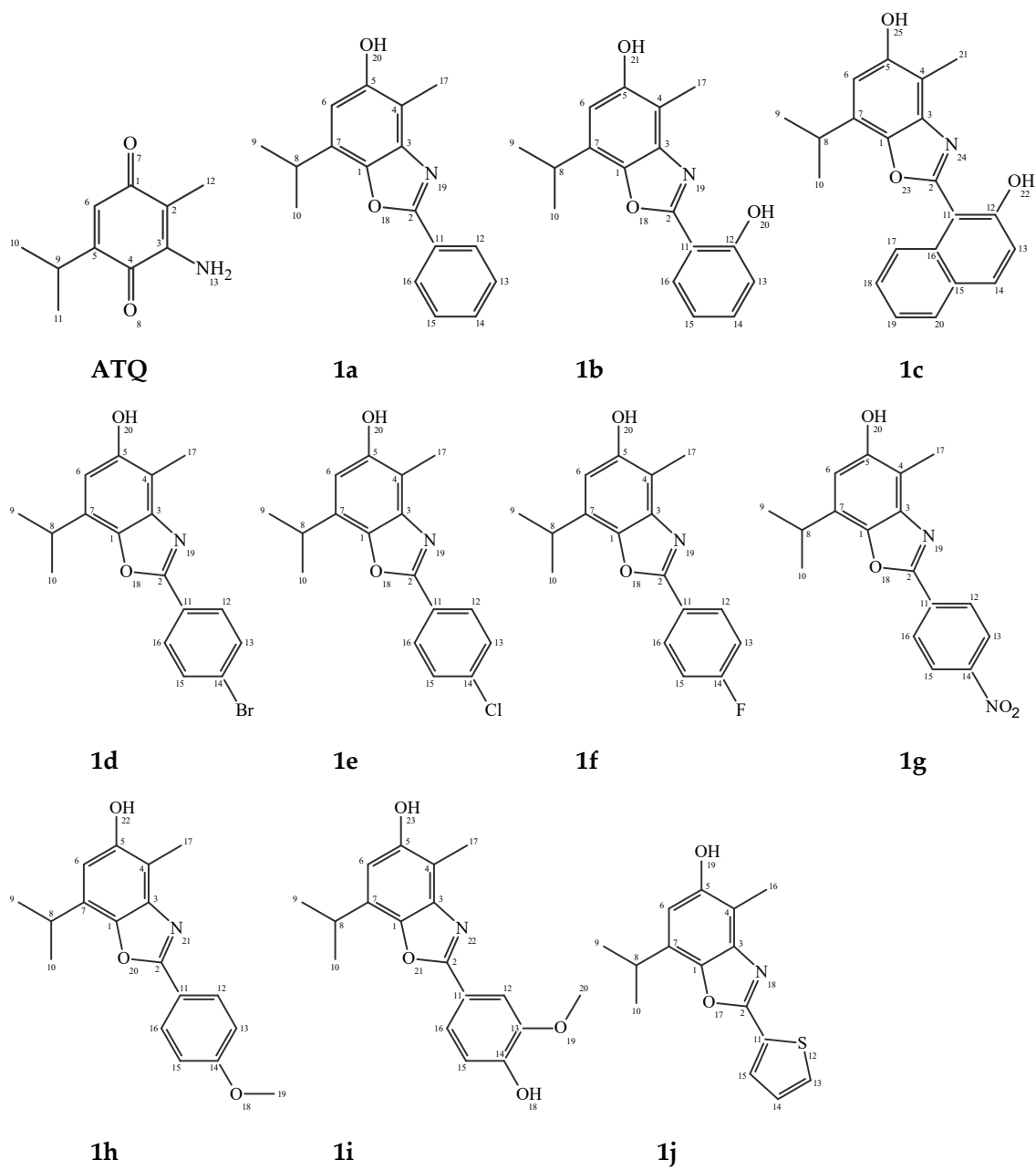


Supplementary material for the article:

Glamočlija, U.; Padhye, S.; Špirtović-Halilović, S.; Osmanović, A.; Veljović, E.; Roca, S.; Novaković, I.; Mandić, B.; Turel, I.; Kljun, J.; et al. Synthesis, Biological Evaluation and Docking Studies of Benzoxazoles Derived from Thymoquinone. *Molecules* **2018**, *23* (12).

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Scheme S1. Numbering scheme for 3-aminothymoquinone (ATQ) and series of benzoxazoles (1a–1j).

Table S1. The crystal structure data of compound **1a**.

Empirical Formula	C ₁₇ H ₁₇ NO ₂
M _w	267.31
T, K	150(2)
Crystal system	<i>monoclinic</i>
Space group	<i>P 2₁/n</i>
a, Å	7.7624 (2)
b, Å	18.3338 (5)
c, Å	10.0202 (3)
α, deg.	90
β, deg.	105.809 (3)
γ, deg.	90
V, Å ³	1372.08 (7)
Z	4
D _{calc} , g/cm ³	1.294
μ, mm ⁻¹	0.676
F (000)	568
Crystal size, mm	0.60 × 0.60 × 0.40
Color	colorless
Data collected/unique	5041/2687
R _{int}	0.0178
Restraints/parameters	0/186
S	1.021
R ₁ , wR ₂ [I > 2σ(I)]	0.0382/0.1026
R ₁ , wR ₂ (all data)	0.0416/0.1056
Larg. diff. peak/hole (e·Å ⁻³)	0.23/-0.19

Table S2. Mobile phases used in purification of compounds **1a-1j**.

Compound	Mobile Phase
1a	<i>n</i> -hexane: Dichloromethane (DCM): Tetrahydrofuran (THF) = 50:50:1.4, gradually increasing quantity of THF until final concentration of 10% THF in combination
1b	<i>n</i> -hexane, then <i>n</i> -hexane: Diethyl ether (DEE) = 30:5
1c	<i>n</i> -hexane: DCM = 1:1, then <i>n</i> -hexane: DCM = 8:12, and at the end DCM 100%
1d	<i>n</i> -hexane, then <i>n</i> -hexane: THF = 12:1
1e	<i>n</i> -hexane: DCM: THF = 50:50:4
1f	<i>n</i> -hexane: DCM: THF = 50:50:2, and after that content of <i>n</i> -hexane and DHM are decreased while content of THF is increased in ratios 30:30:3 and 20:20:4
1g	<i>n</i> -hexane, after that DEE is gradually added with increasing ratios <i>n</i> -hexane: DEE = 30:1, 30:2, 30:3, 30:5, 30:10 and 30:15
1h	<i>n</i> -hexane: DCM: THF = 50:50:3, after that content of THF is increased 50:50:4, 50:50:5, 50:50:8, 50:50:10, 50:50:11 and 50:50:12
1i	<i>n</i> -hexane: DEE = 2:1
1j	<i>n</i> -hexane: DCM: THF = 50:50:2.5