Supplementary Materials for:

Synthesis and Crystal Structure of Ethyl 5-(4-Bromophenyl)-7-methyl-3-oxo-2,3-dihidro-5*H*-thiazolo[3,2-*a*]pyrimidine-6-carboxylate

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Figure S1. ^{1}H NMR spectrum of compound **7** (DMSO-d$_6$, 500 MHz, 25^{0}C).

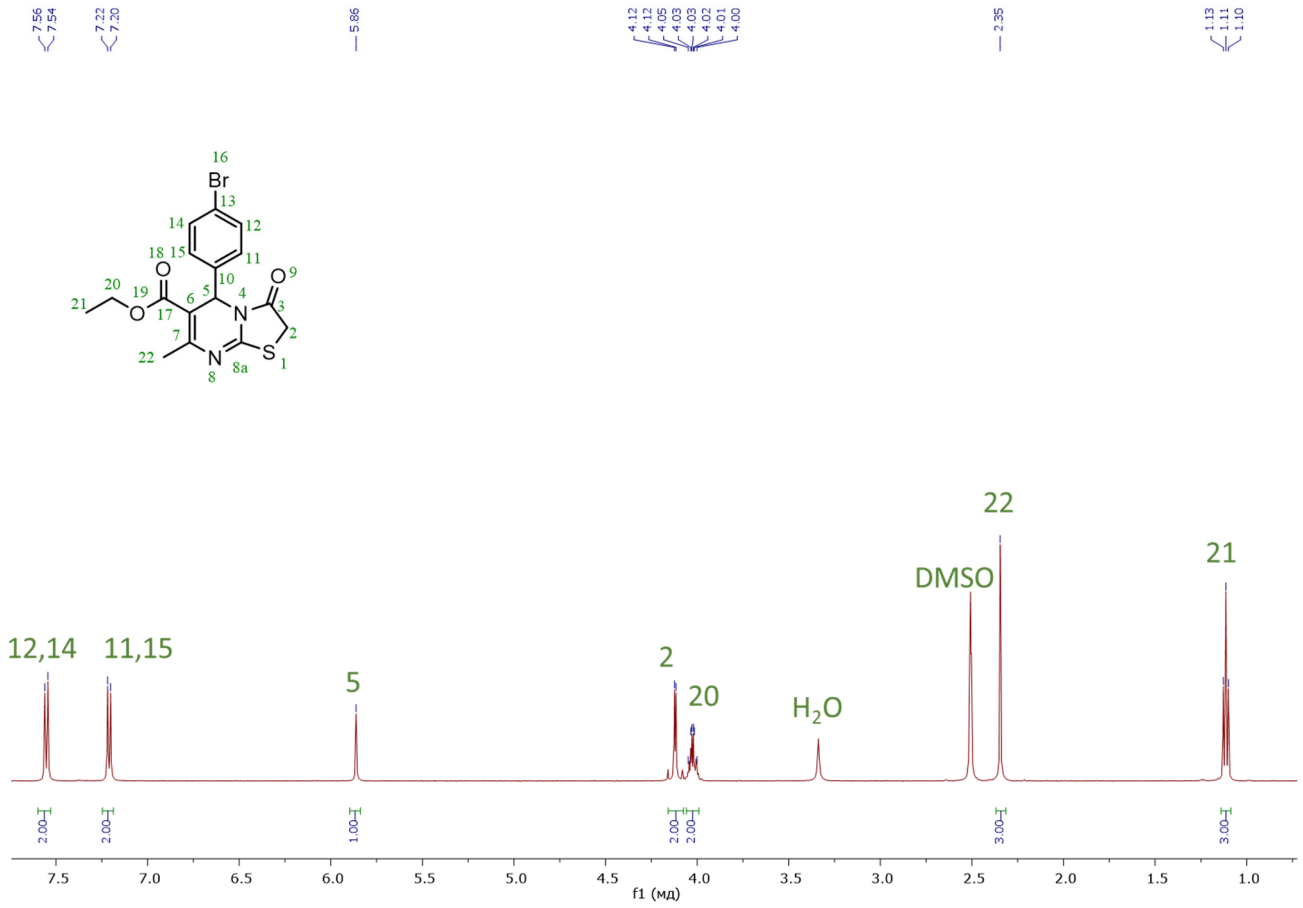

Figure S2. ^{13}C NMR spectrum of compound **7** (DMSO-d_6, 100 MHz, 25^{0}C).

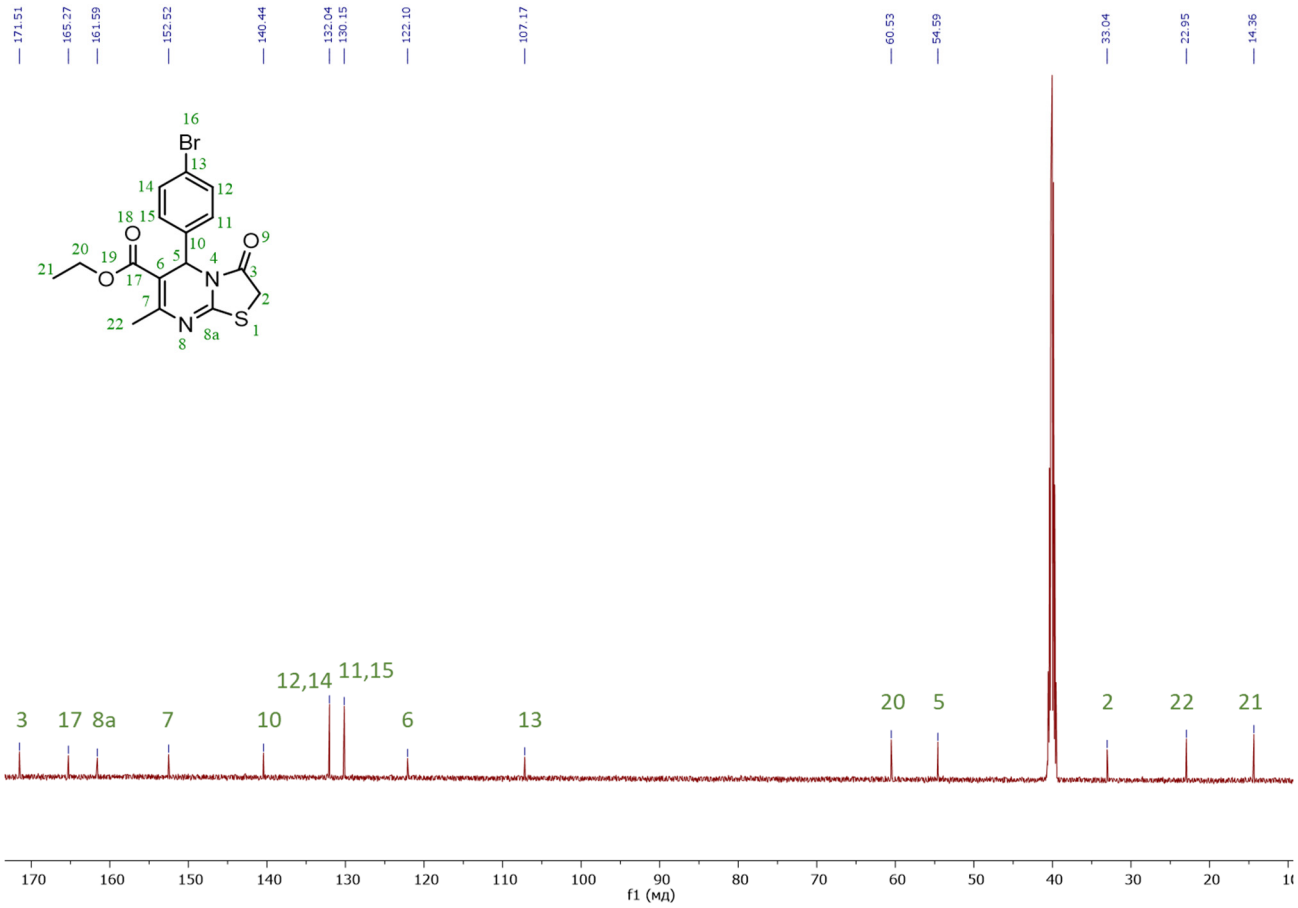

Figure S3. ESI MS spectrum of compound **7** (Ion Polarity: Positive).

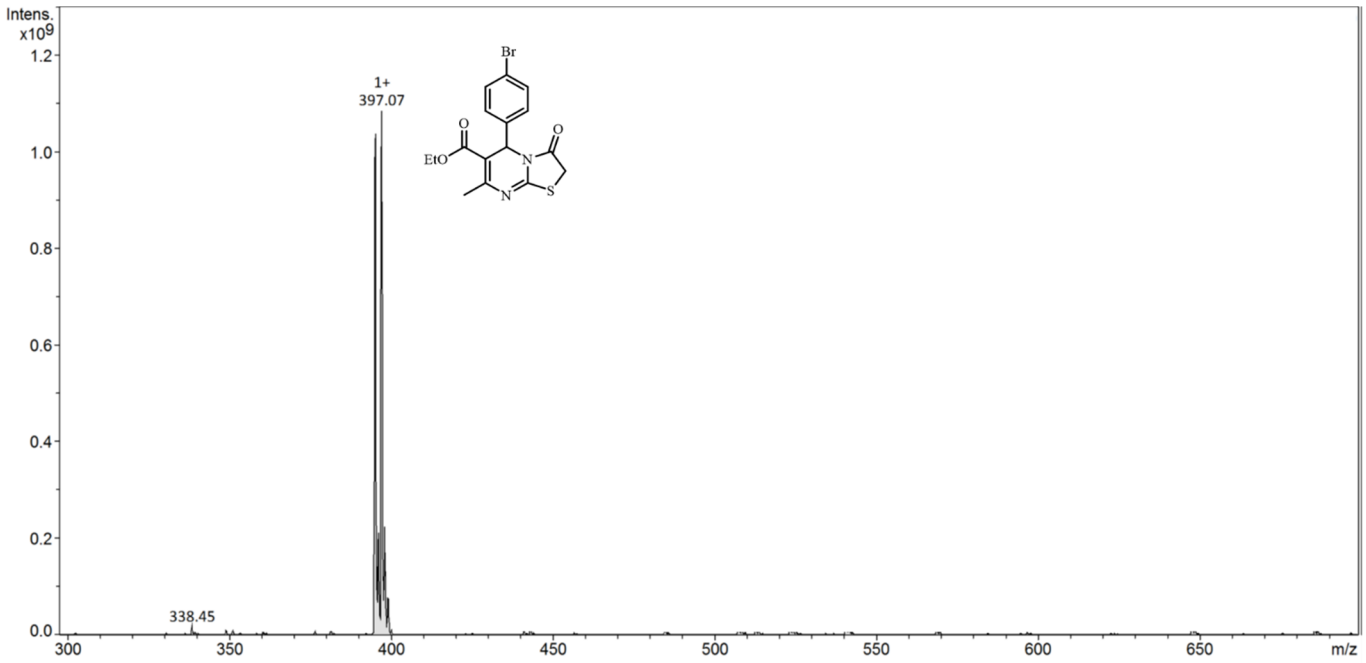

Table S1. Crystallographic data for compound **7**.

Molecular formula	$C_{16}H_{15}BrN_2O_3S$
Sum Formula	$C_{16}H_{15}BrN_2O_3S$
Formula Weight	395.26
Crystal System	monoclinic
Space group	*P2(1)/c*
Temp. of measurement, K	110(2)
Cell parameters	*a* = 10.3465(4) Å, *b* = 8.2938(4) Å, *c* = 19.3950(9) Å; β = 100.981(2)°
V [Å3]	1633.85(13)
Z and Z′	4 and 1
D(calc) [g/cm3]	1.607
λ (Å)	(MoKα) 0.71073
μ [/mm]	2.659
F(000)	800
Theta Min-Max [Deg]	2.0–32.0°
Reflections measured	66335
Independent reflections	5669
Observed reflections [I > 2σ(I)]	5046
Goodness of fit	1.023
R [I > 2σ(I)]	*R*1 = 0.0271, *wR*2 = 0.0659
R (all reflections)	*R*1 = 0.0326, *wR*2 = 0.0681
Max. and Min. Resd. Dens. [e/Å−3]	0.68 and – -0.44
Depositor numbers in CCDC	2232755

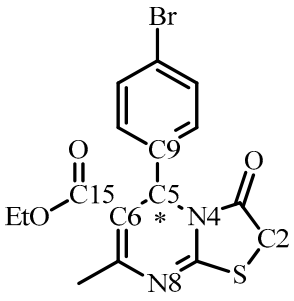

Table S2. Bond distances and angles of asymmetric C5 atom in studied compounds established by SCXRD for **7**.

Compound	**1**
d(C5-C6), Å	1.518(2)
d(N4-C5), Å	1.475(1)
d(N4-C3), Å	1.384(1)

d(C5-C9), Å	1.520(2)
∠C6-C5-N4, ⁰	108.40(9)
∠C6-C5-C9, ⁰	112.77(9)
∠N4-C5-C9, ⁰	108.88(9)

Table S3. Selected bond distances and dihedral angles for studied compound **7** established by SCXRD.

Compound	Dihedral angle between thiazolopyrimidine and the carbonyl group at C6 atom π-systems, ⁰	Dihedral angle between two different 4-bromophenyl fragment, ⁰	d(C6-C15), Å
7	15.46	56.40	1.478(2)

Table S4. The distances between the bromine atom and the 4-bromophenyl fragment present in the crystals of the studied compound.

Compound	1
d(Br- π), Å	3.339(1)