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Corrigendum

Corrigendum to "A multicomponent access to 1,3-thiazine-6-phenylimino-5-carboxylates" [Tetrahedron Lett. 57 (2016) 3256–3259]

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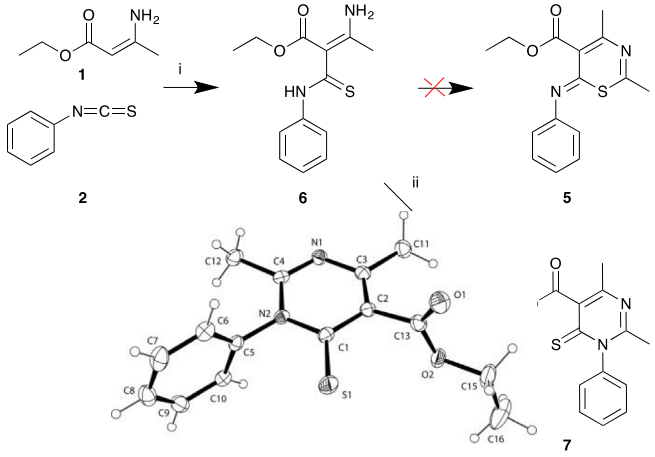
In recent studies on the multicomponent route described in our original submission [1], we gained access to crystalline material suitable for X-ray analysis (Scheme 1). This revealed that our original structural assignment based on NMR, IR and MS evidence was incorrect. The product arising from the multicomponent reaction of ethyl 3-aminocrotonate (**1**), phenylisothiocyanate (**2**) and acetic anhydride (**3**) was not ethyl (*Z*)-2,4-dimethyl-6-(phenylimino)-6*H*-1,3-thiazine-5-carboxylate (**5**), but the thioamide isomer, ethyl 2,4-dimethyl-1-phenyl-6-thioxo-1,6-dihydropyrimidine-5-carboxylate (**7**) (Scheme 1 and insert).

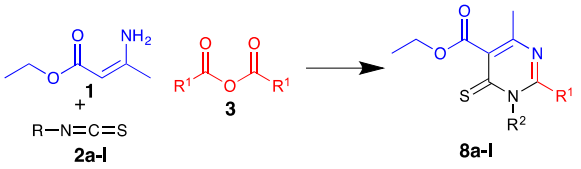
The structure of thioamide (**7**), and related analogues, is consistent with the NMR and IR data presented in our original submission. Using the compound numbering from the original manuscripts, analogues **8a**–**l**, are the equivalent thioamides as shown in Table 1.

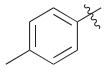
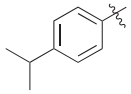
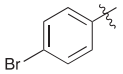
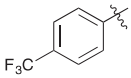
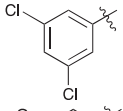
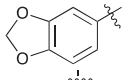
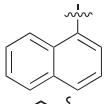
Re-examination of the reaction mechanism based on this data supports a N to S anion resonance with the charge intercepted by acetic anhydride at the nitrogen anion stage [1,2]. As previously



Scheme 1. Reagents and conditions: (i) rt, solvent free, N_2, overnight; (ii) acetic anhydride, CH_3CN, rt, 24 h. Insert: ORTEP 3D view of **7** (30% ellipsoids shown).

Table 1
Synthesis of substituted 1,3-thiazin-6-imino-5-carboxylates **8a–l**.



Entry	R^1	R^2	Product	Yield (%)
1	CH_3		**8a**	65
2	CH_3		**8b**	19
3	CH_3		**8c**	50
4	CH_3		**8d**	64
5	CH_3		**8e**	35
6	CH_3		**8f**	20
7	CH_3		**8g**	29
8	CH_3		**8h**	29
9	CH_3		**8i**	15
10	CH_3CH_2		**8j**	29
11			**8k**	4
12	CF_3		**8l**	12

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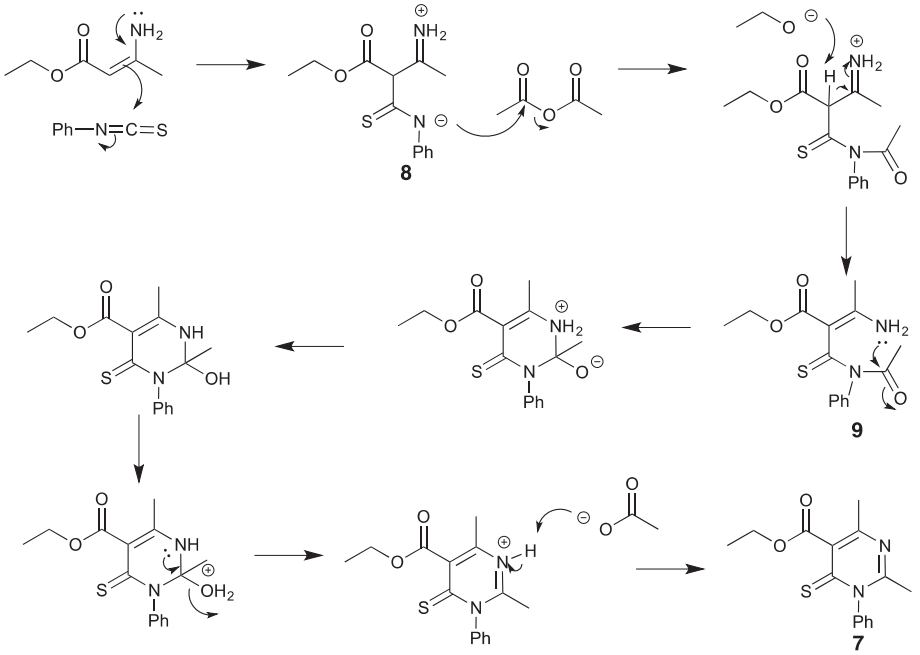
https://doi.org/10.1016/j.tetlet.2018.07.018



Scheme 2. Revised mechanism for the 3-component MCR reaction of 3-aminocrotonate, phenyl isothiocyanate (**2**) and acetic anhydride to give ethyl 2,4-dimethyl-1-phenyl-6-thioxo-1,6-dihydropyrimidine-5-carboxylate (**7**), not ethyl (*Z*)-2,4-dimethyl-6-(phenylimino)-6*H*-1,3-thiazine-5-carboxylate (**5**).

proposed, ensuing acetate loss and H-abstraction affords the ene-amine **9** which effects an intramolecular condensation with the *N*-acyl carbonyl moiety. Loss of water and acetate removal of the proton yields ethyl 2,4-dimethyl-1-phenyl-6-thioxo-1,6-dihydropyrimidine-5-carboxylate (Scheme 2). This mechanism differs only in the interception of the nitrogen anion rather than the sulfur anion by acetic anhydride, but this re-working is necessitated by the structure confirmed herein by X-ray crystallography.

We regret any inconvenience this may have caused readers and sincerely apologize for this error.

References

[1] N.T. Trinh, A. McCluskey, Tetrahedron Lett. 56 (2016) 3256–3259.
[2] H.B. Jalani, J.C. Kaila, A.B. Baraiya, A.N. Pandya, V. Sudarsanam, K.K. Vasu, Tetrahedron Lett. 51 (2010) 5686–5689.