

Supplementary Material

Synthesis of a Pyrrolo[1,2-*a*]quinazoline-1,5-dione Derivative by Mechanochemical Double Cyclocondensation Cascade

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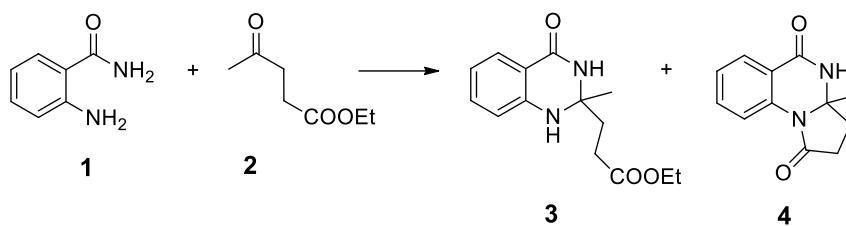
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General formulae

Reaction of anthranilamide (**1**) and ethyl levulinate (**2**):



The conversions and the selectivities were calculated with the formulas given below using the relative concentrations determined by gas chromatography.

$$\text{Conv} = \frac{c_{0,1} - c_1}{c_{0,1}} \times 100 (\%)$$

$$\text{S3} = \frac{c_3}{c_{0,1} - c_1} \times 100 (\%)$$

$$\text{S4} = \frac{c_4}{c_{0,1} - c_1} \times 100 (\%)$$

where:

Conv: conversion, **S3**: selectivity of product **3**, **S4**: selectivity of product **4**;

$c_{0,1}$: initial concentration of **1**; c_1 : concentration of the unreacted **1**;

c_3 : concentration of the resulted **3**; c_4 : concentration of the resulted **4**.

Effect of temperature on the reaction of anthranilamide (1) with ethyl levulinate (2) in the batch system

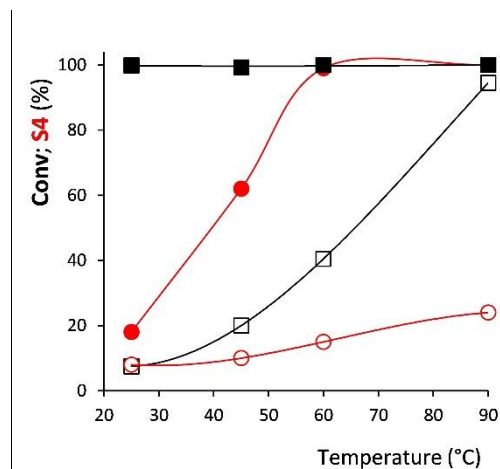


Figure S1. Effect of the reaction temperature with (■, ●) and without (□, ○) catalyst. Reaction conditions: 100 mg as received Amberlyst® 15, 1 mmol anthranilamide (1), 1.5 mmol ethyl levulinate (2), 24 h, magnetic stirring 600 rpm; conversion: ■, □; selectivity of 4 (S4): ●, ○.

Effect of the catalyst amount on the reaction of anthranilamide (1) with ethyl levulinate (2) in the batch system

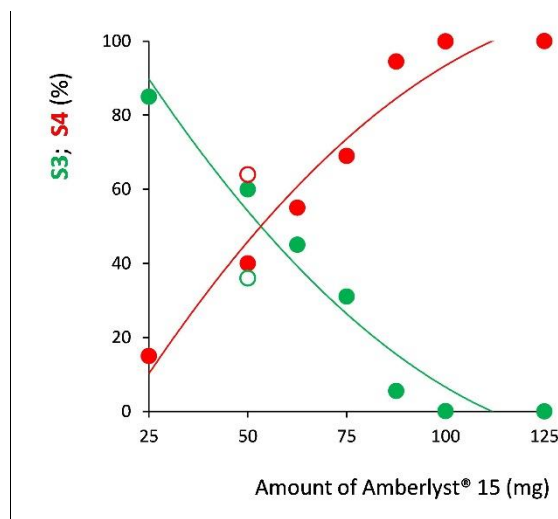
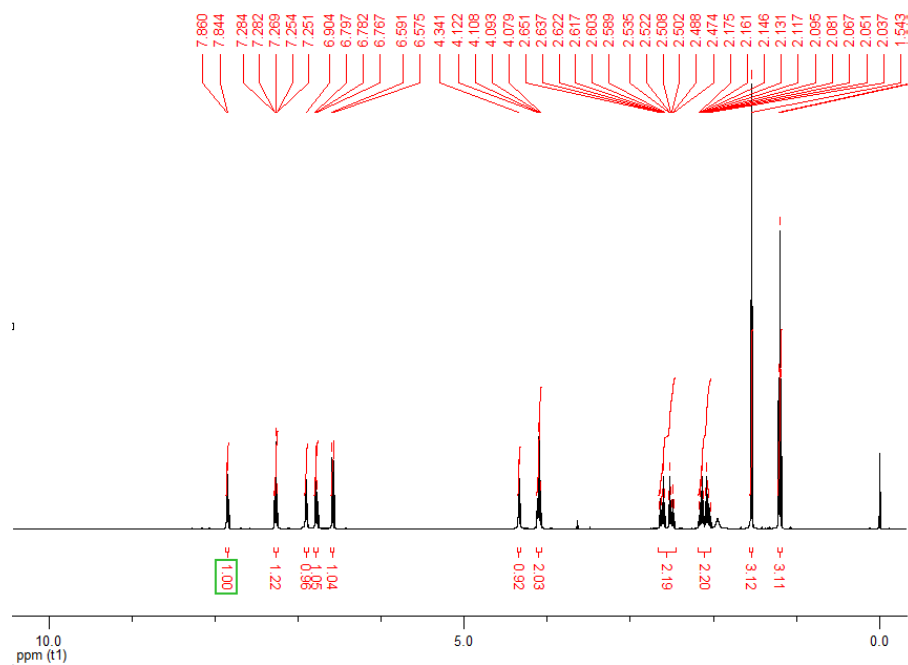


Figure S2. Effect of the catalyst amount on the selectivity of 3 (S3: ●) and selectivity of 4 (S4: ●) using as received Amberlyst® 15, and on the selectivity of 3 (S3: ○) and the selectivity of 4 (S4: ○) using pre-milled Amberlyst® 15; Reaction conditions: 1 mmol 1, 1.5 mmol 2, 60°C, 24 h, magnetic stirring 600 rpm, the conversion of 1 was >99% in all these reactions.

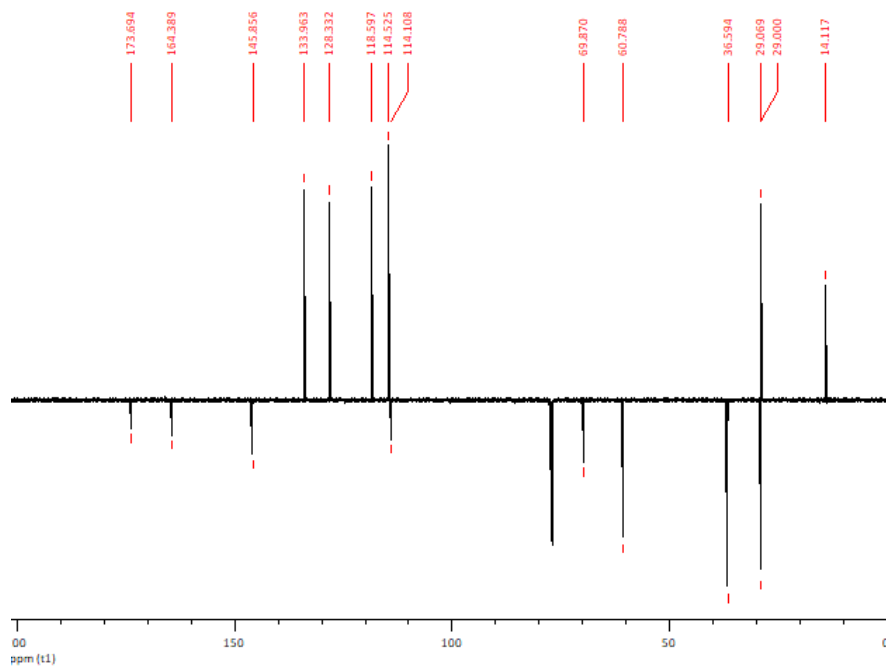
^1H and ^{13}C NMR spectra of the isolated products

Ethyl 3-(2-methyl-4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)propanoate (**3**)

^1H NMR (500 MHz, CDCl_3)

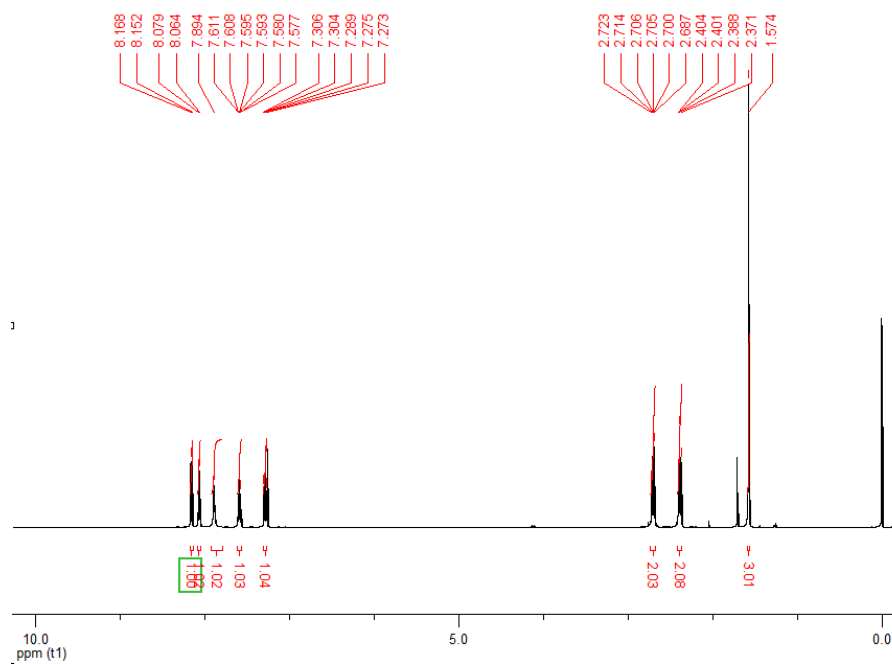


^{13}C NMR (500 MHz, CDCl_3)

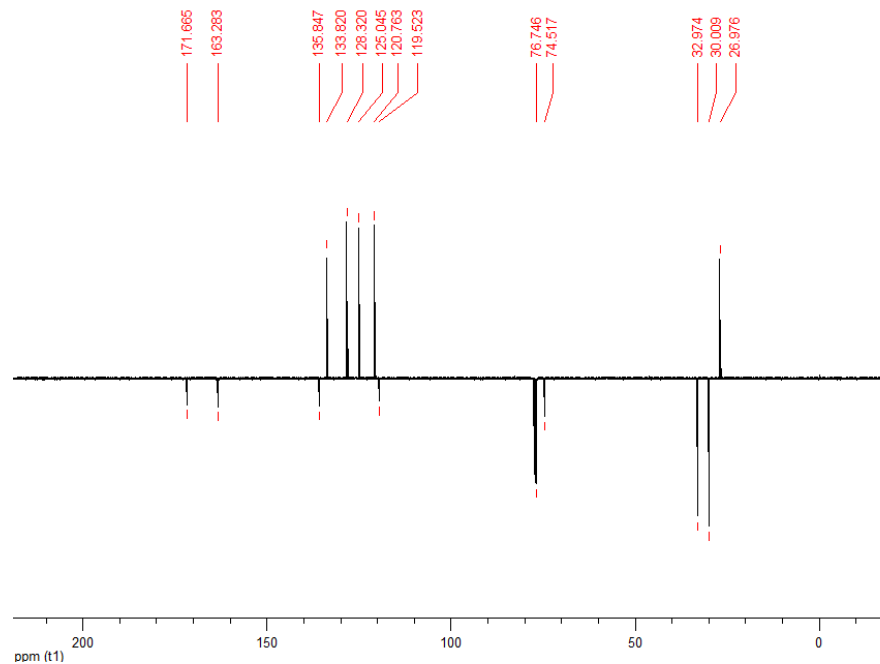


3a-Methyl-2,3,3a,4-tetrahydropyrrolo[1,2-*a*]quinazoline-1,5-dione (**4**)

^1H NMR (500 MHz, CDCl_3)



^{13}C NMR (500 MHz, CDCl_3)



Chromatograms and mass spectra of the products (GC-FID and GC-MSD)

Separation of the products using GC-FID, chromatograms of raw products

Table 5, entry 4

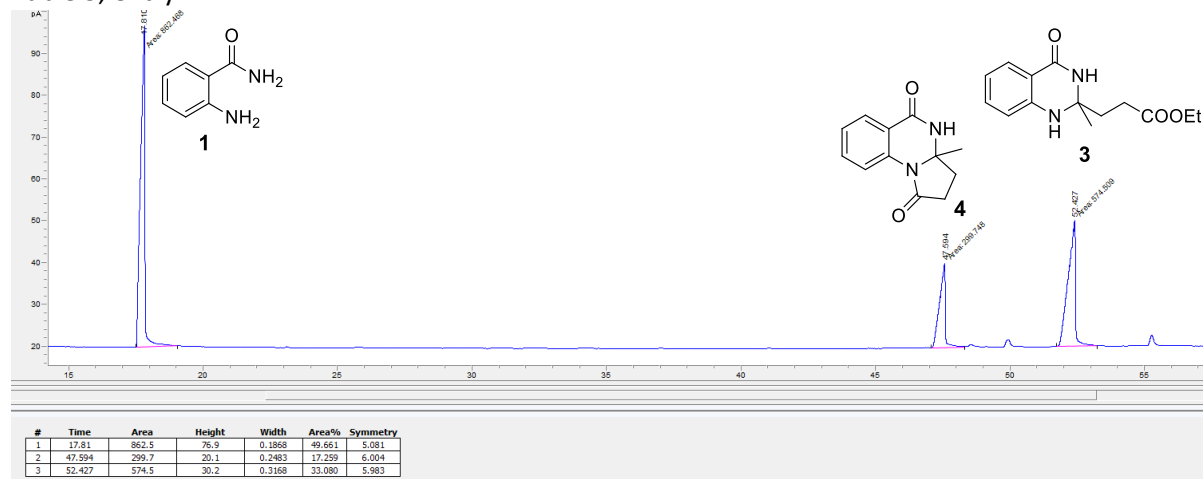


Table 2, entry 4

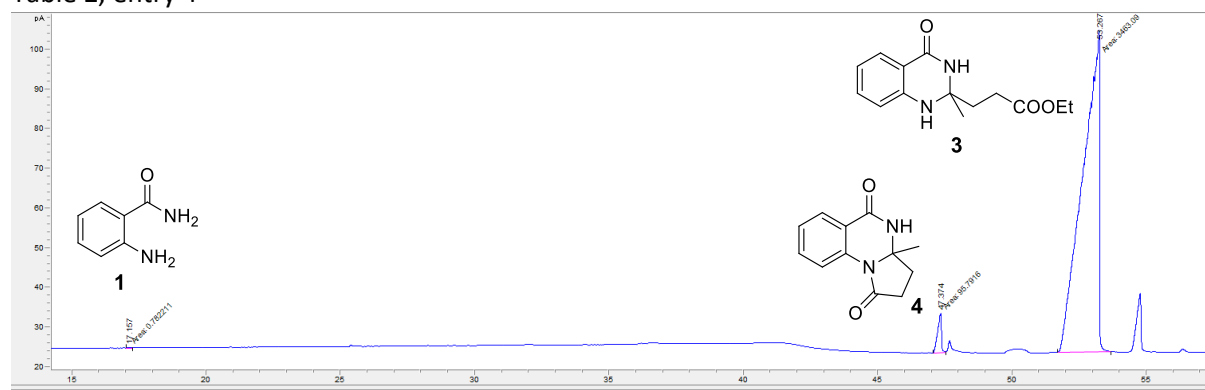
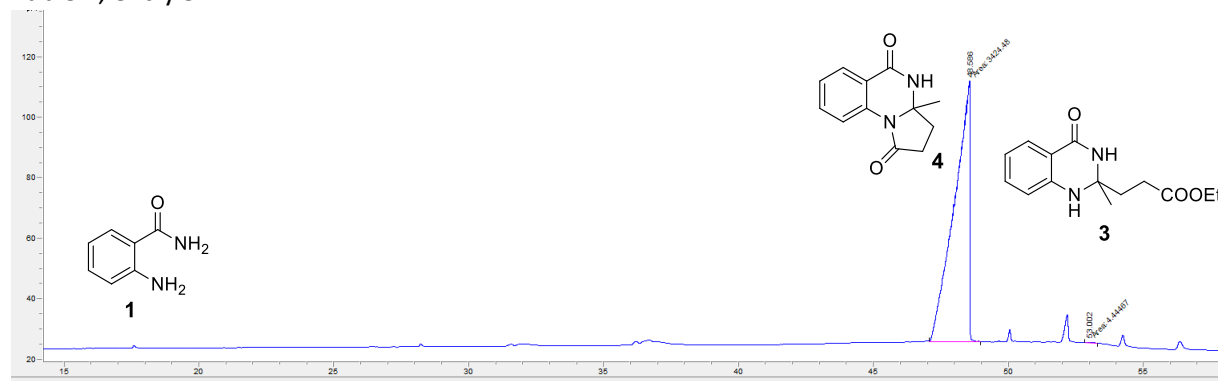


Table 2, entry 5



Retention times: $R_t(1) = 17.8$ min, $R_t(3) = 47.6$ min, $R_t(4) = 52.4$ min

Identification of the products by GC-MSD, EI-MS mass spectra of the purified products

