Supplementary Material

Reactions of quinine with 2-chloro-4,6-dimethoxy-1,3,5-triazine

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Figure S1. Isolation of the main component 5 from the product mixture obtained by the reaction of quinine (1) and CDMT (2). Panel a) after preparative chromatography; panel b) after recrystallization. Column Vydac C18 (250x4.6). Programme: 1) 0-5 min. isocratic acetonitrile / water 50 / 50%; 2) 5-35 min. gradient acetonitrile / water 50-97%; 3) 35-40 min. isocratic acetonitrile/water 97/3%; 4) 40-50 min. isocratic acetonitrile / water 50 / 50. Note shortening of R_t after recrystallization.
2. Crystal structure data

The intensity data was collected on the Bruker SMART APEX II CCD diffractometer equipped with a Cu Kα (1.54178 Å) radiation source. Crystal structure refinement was carried out with SHELX. Structure refinement details are summarized in Table S1. The molecular structure of compound 5 is shown in Figure 1. Program MERCURY was used for molecular graphics. CCDC: 2027177 contains the supplementary crystallographic data for this paper. The data is provided free of charge by The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Table S1. Structure refinement and experimental details

| Crystal data                                                                 |                                                                 |
|----------------------------------------------------------------------------|------------------------------------------------------------------|
| Chemical formula                                                           | C_{30}H_{35}ClN_{8}O_{6}                                          |
| M_r                                                                        | 639.11                                                           |
| Crystal system, space group                                               | Orthorhombic, P2\_12\_12\_1                                      |
| Temperature (K)                                                           | 100                                                              |
| a, b, c (Å)                                                                | 7.7702 (2), 10.6624 (3), 38.4161 (10)                             |
| V (Å³)                                                                    | 3182.73 (15)                                                     |
| Z                                                                         | 4                                                                |
| Radiation type                                                            | Cu Kα                                                            |
| μ (mm⁻¹)                                                                  | 1.53                                                             |
| Crystal size (mm)                                                         | 0.60 × 0.07 × 0.04                                               |

| Data collection                                                            |                                                                 |
|----------------------------------------------------------------------------|------------------------------------------------------------------|
| Diffractometer                                                            | Bruker SMART APEX CCD                                            |
| T_{min}, T_{max}                                                           | 0.643, 0.754                                                     |
| No. of measured, independent and observed [I > 2σ (I)] reflections        | 36943, 6330, 6186                                                |
| R_{int}                                                                    | 0.025                                                            |
| (sin θ/λ)_{max} (Å⁻¹)                                                      | 0.619                                                            |
| Refinement                                                                |                                                                  |
| R[F^2 > 2σ (F^2)], wR(F^2); S                                             | 0.024, 0.065, 1.04                                              |
| No. of reflections                                                        | 6330                                                             |
| No. of parameters                                                         | 411                                                              |
| Δρ_{max}, Δρ_{min} (e Å⁻³)                                                 | 0.21, -0.19                                                     |
Table S2. Parameters of $^1$H MNR, $^{13}$C NMR and DEPT-135 spectra

| parameters          | $^1$H     | $^{13}$C   | DEPT-135 |
|---------------------|-----------|-----------|----------|
| Acquisition Time (sec) | 2.2719   | 0.7864   | 0.7864   |
| Frequency (MHz)     | 700.08   | 176.04   | 176.04   |
| Nucleus             | $^1$H     | $^{13}$C   | $^{13}$C   |
| Number of Transients | 128      | 12288    | 8192     |
| Original Points Count | 32768   | 32768    | 32768    |
| Points Count        | 32768    | 32768    | 32768    |
| Receiver Gain       | 2050.00  | 2050.00  | 2050.00  |
| SW(cyclical) (Hz)    | 14423.08 | 41666.67 | 41666.67 |
| Solvent             | CDCl$_3$ | CDCl$_3$ | CDCl$_3$ |
| Spectrum Offset (Hz) | 4308.0820 | 17607.8320 | 17600.0859 |
| Sweep Width (Hz)    | 14422.64 | 41665.39 | 41665.39 |
| Temperature (degree C) | 27.000  | 27.100   | 27.000   |

Table S3. Parameters of COSY spectra

| parameters          | COSY     |
|---------------------|----------|
| Acquisition Time (sec) | (0.2433, 0.0609) |
| Frequency (MHz)     | (700.08, 700.08) |
| Nucleus             | (1H, 1H) |
| Number of Transients | 24      |
| Original Points Count | (2048, 512) |
| Points Count        | (2048, 1024) |
| Pulse Sequence      | cosygppqf |
| Solvent             | CDCl$_3$ |
| Spectrum Offset (Hz) | COSY    |
| Sweep Width (Hz)    | (8413.40, 8392.81) |
| Temperature (degree C) | 27.000  |

Table S3. Parameters of HSQC spectra

| parameter          | HSQC     |
|--------------------|----------|
| Acquisition Time (sec) | (0.1217, 0.0171) |
| Frequency (MHz)     | (700.08, 176.05) |
| Nucleus             | (1H, 13C) |
| Number of Transients | 32      |
| Original Points Count | (1024, 512) |
| Points Count        | (1024, 2048) |
| Pulse Sequence      | hsqcedetgpsisp2.2.pp |
| Solvent             | CHLOROFORM-d |
| Spectrum Offset (Hz) | HSQC    |
| Sweep Width (Hz)    | (8409.29, 29913.78) |
| Temperature (degree C) | 27.200  |
Figure S2. $^{13}$C NMR spectrum of the main product 5 formed in reaction of quinine with CDMT.

Figure S3. DEPT-135 spectrum in CDCl$_3$ of the main product 5 formed in reaction of quinine with CDMT.
Figure S4. COSY spectrum of the main product 5 formed in reaction of quinine with CDMT.
Figure S5. HSQC spectrum of fragment 3.30 – 5.00 ppm.
**Figure S6.** Fragment 7.00-8.75 ppm of $^1$H NMR spectrum of product 5 formed in reaction of quinine with CDMT.

**Figure S7.** Fragment 5.00-5.80 ppm of $^1$H NMR spectrum of 5 formed in reaction of quinine with CDMT.
Figure S8. Fragment 3.30 to 4.90 ppm of $^1$H NMR spectrum of product 5 formed in reaction of quinine with CDMT.

Figure S9. Fragment 1.20 to 2.50 ppm of $^1$H NMR spectrum of product formed in reaction of quinine with CDMT.
**Figure S10.** Mass spectrum (ESI⁻) of the main product 5 formed in reaction of quinine with CDMT isolated after crystallization from ethyl acetate / n-heptane.

**Figure S11.** IR spectrum of the main product 5 formed in reaction of quinine with CDMT isolated after crystallization from ethyl acetate / n-heptane.