Supplementary Material

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

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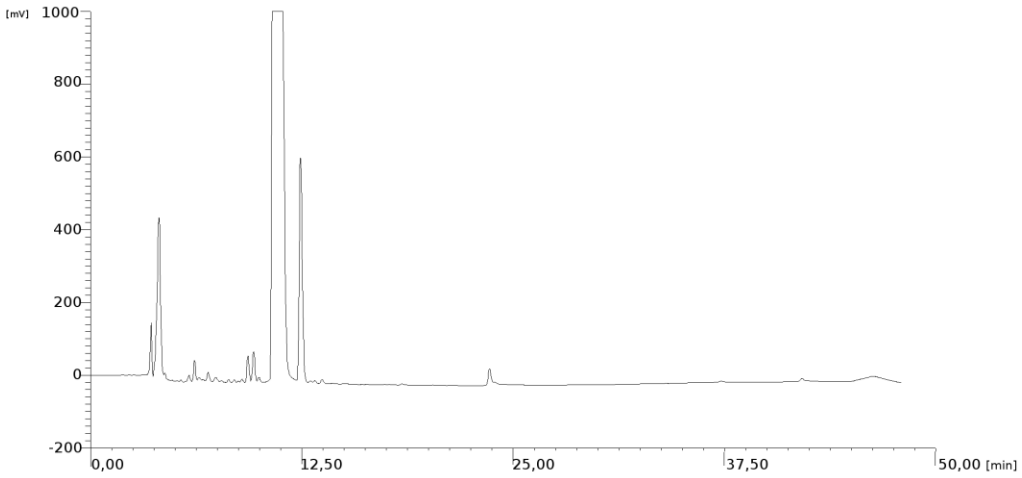
a)



b)

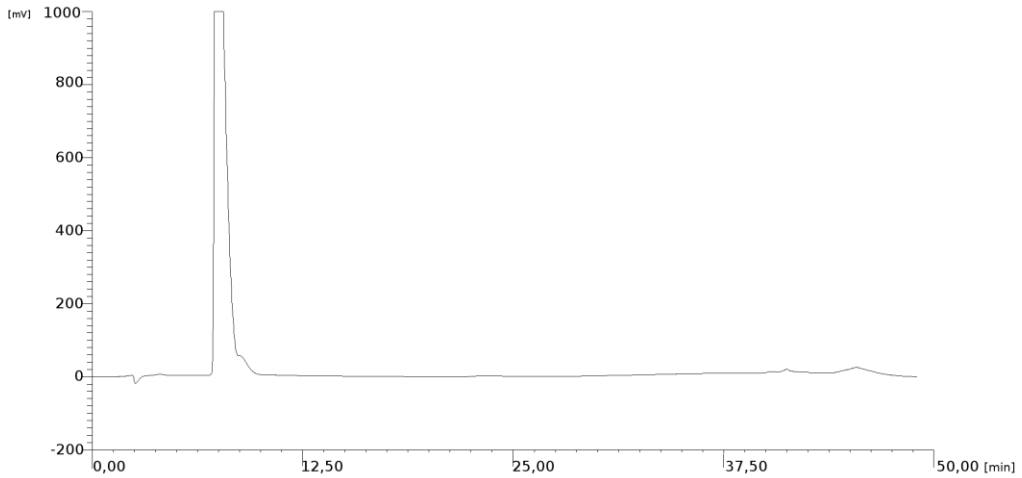


Figure S1. Isolation of the main component **5** from the product mixture obtained by the reaction of quinine (**1**) and CDMT (**2**). Panel a) after preparative chromatography; panel b) after recrystallization. Column Vydac C18 (250x4.6). Programme: 1) 0-5 min. isocratic acetonitrile / water 50 / 50%; 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.[7,8] Structure refinement details are summarized in **Table S1**. The molecular structure of compound **5** is shown in **Figure 1**. Program MERCURY[9] 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	$C_{30}H_{35}ClN_8O_6$
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 (Å^3)	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 [$I > 2\sigma(I)$] reflections	36943, 6330, 6186
R_{int}	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.024, 0.065, 1.04
No. of reflections	6330
No. of parameters	411
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (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	cosygpqf
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

parametry	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

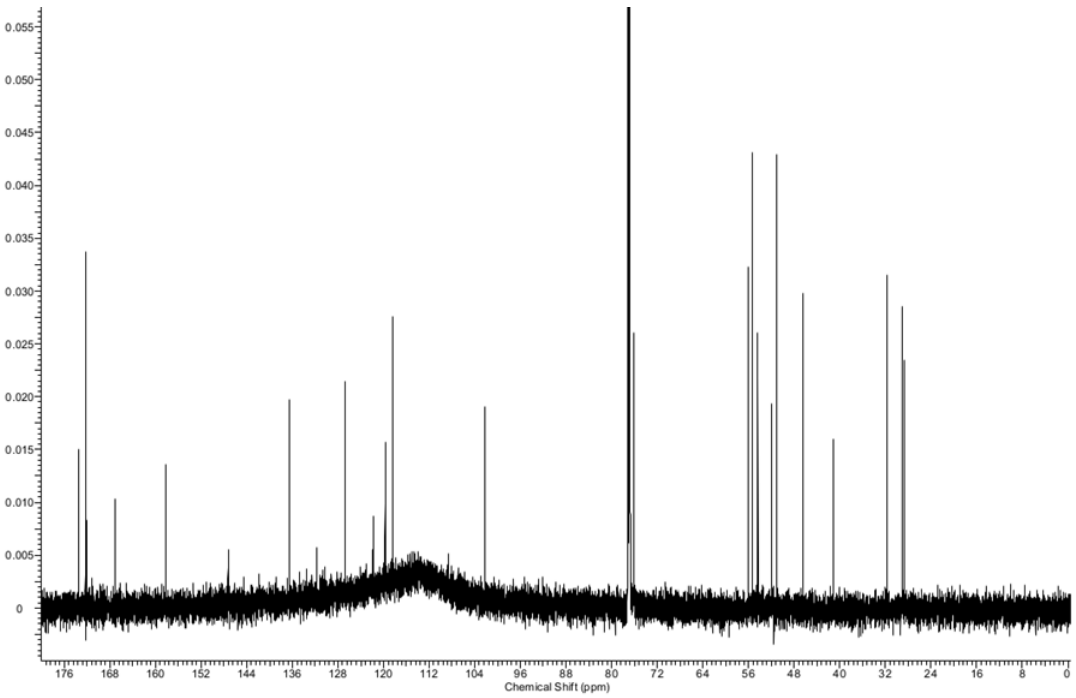


Figure S2. ^{13}C NMR spectrum of the main product **5** formed in reaction of quinine with CDMT.

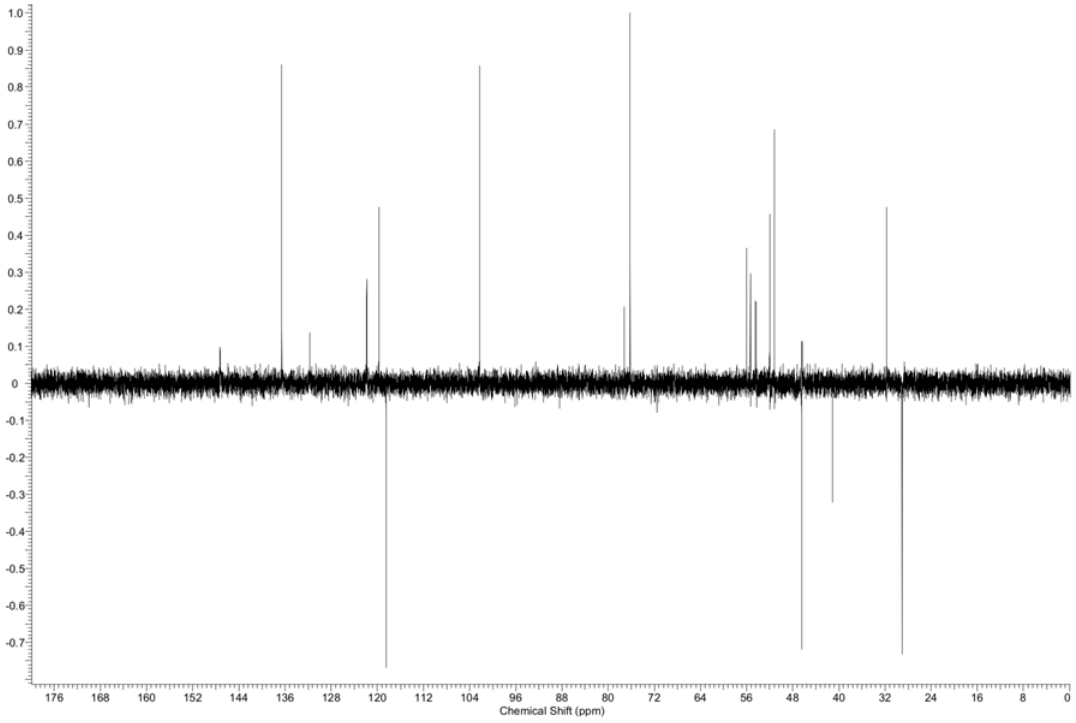


Figure S3, DEPT-135 spectrum in $CDCl_3$ of the main product **5** formed in reaction of quinine with CDMT.

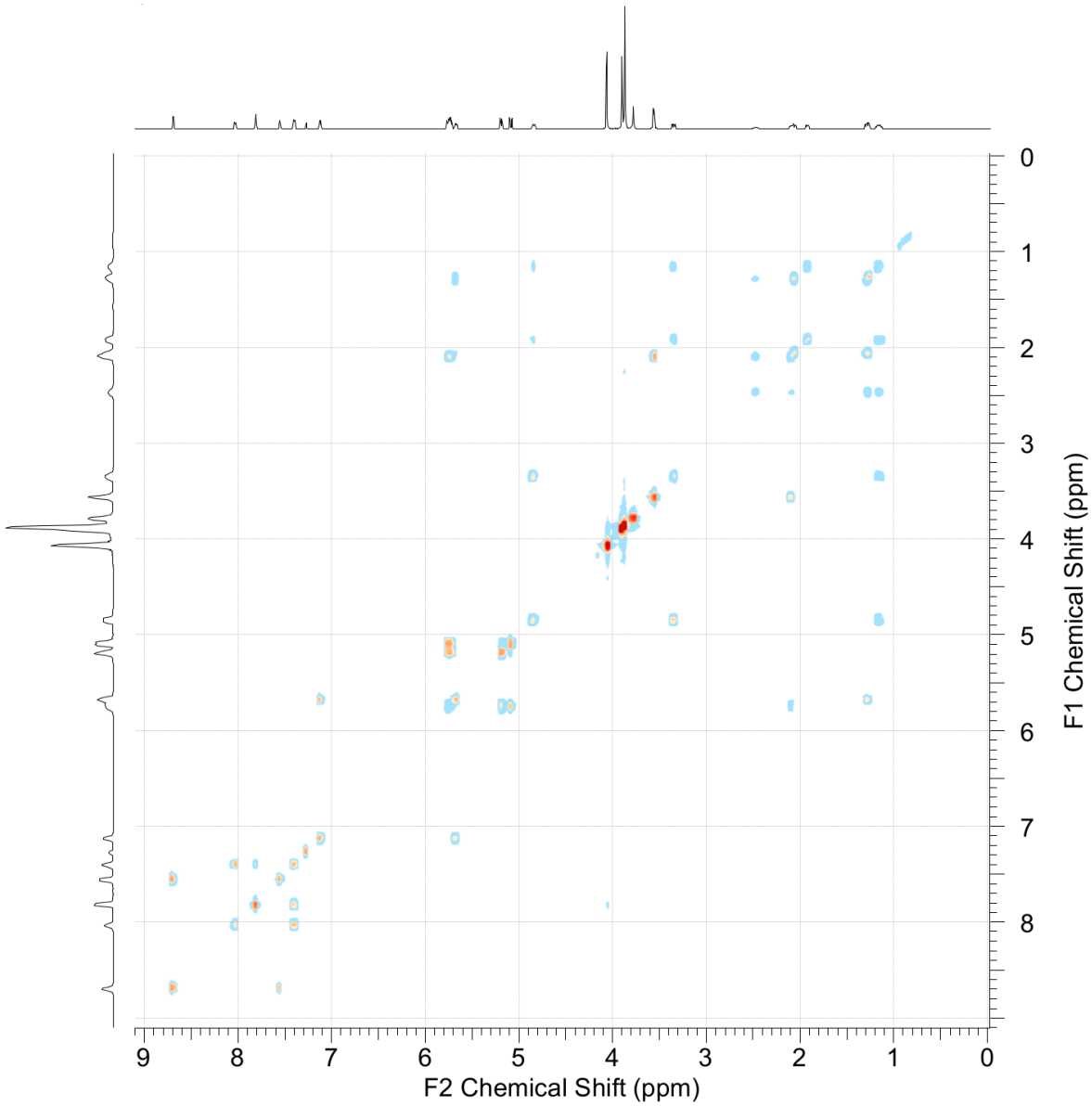


Figure S4. COSY spectrum of the main product **5** formed in reaction of quinine with CDMT.

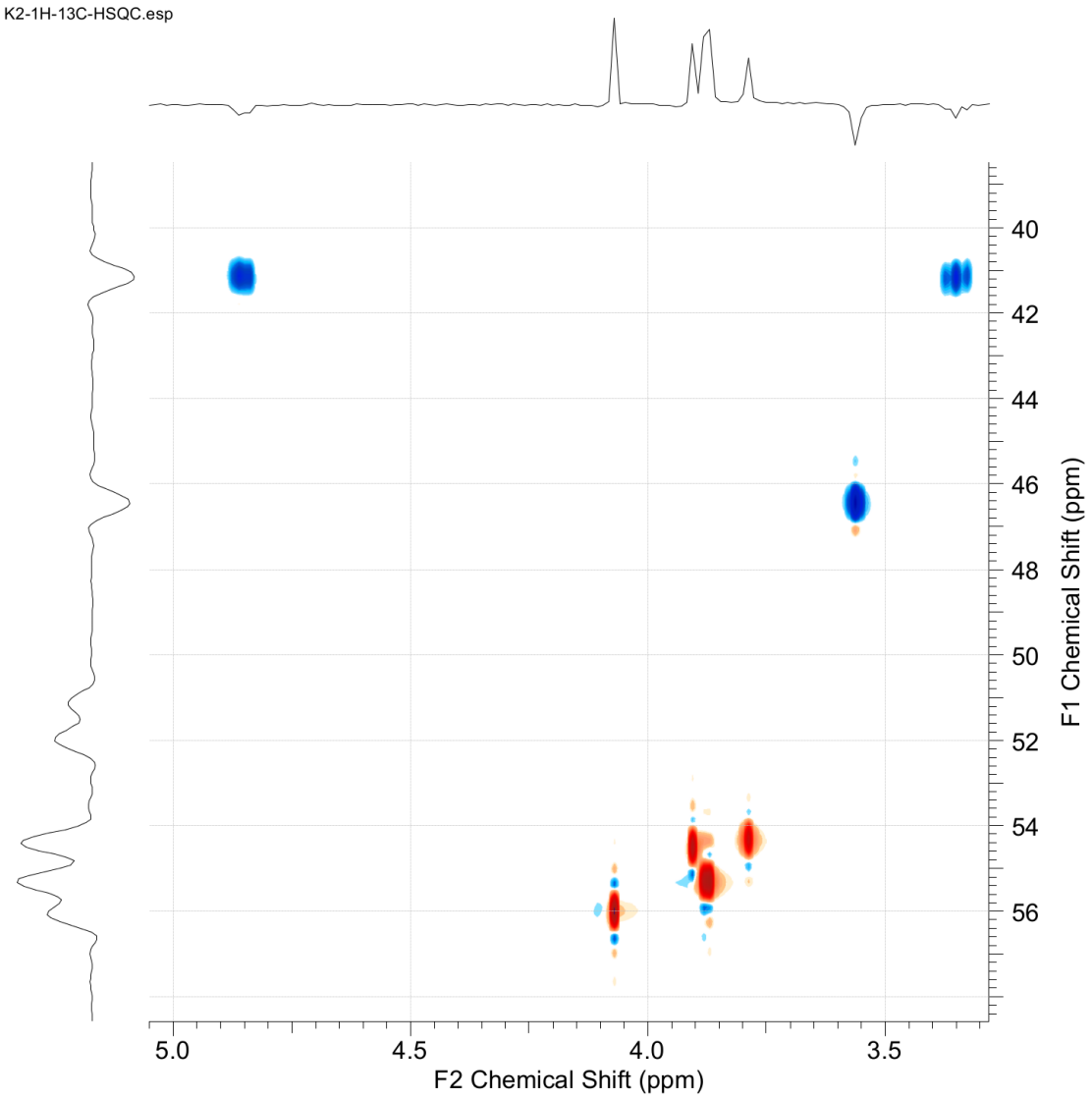


Figure S5. HSQC spectrum of fragment 3.30 – 5.00 ppm.

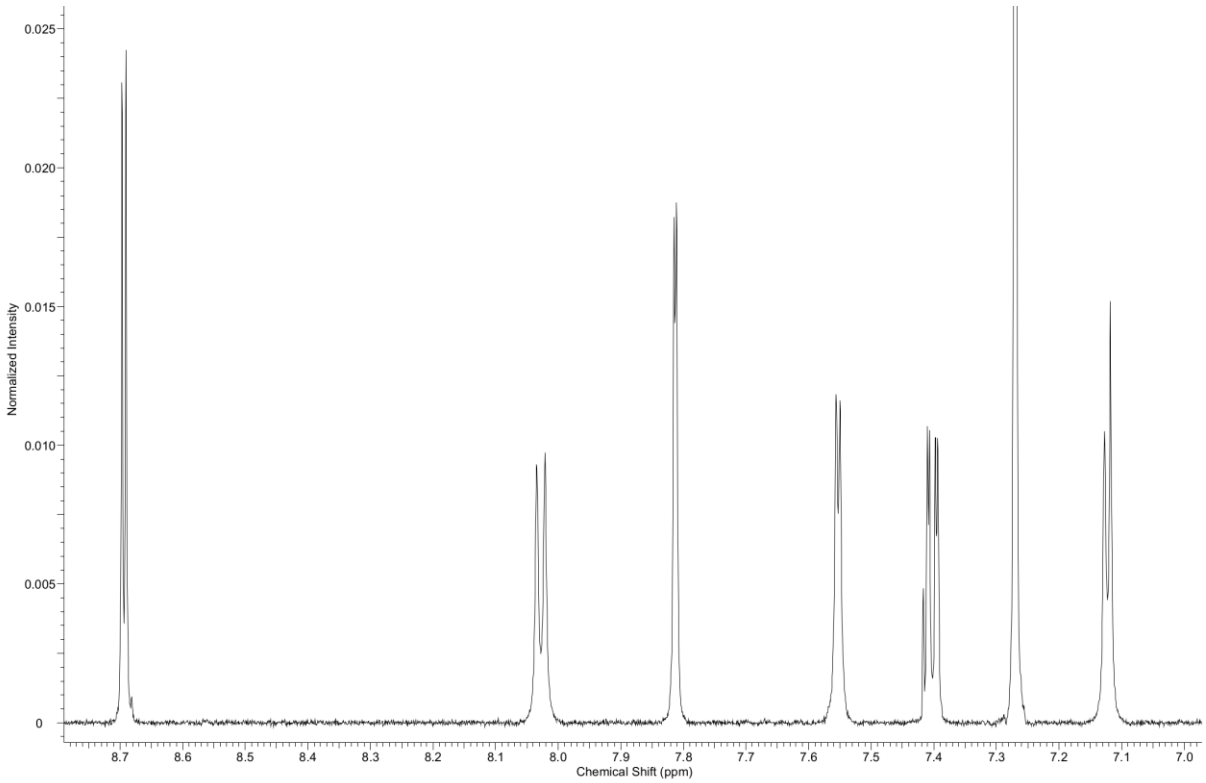


Figure S6. Fragment 7.00-8.75 ppm of ^{1}H NMR spectrum of product **5** formed in reaction of quinine with CDMT.

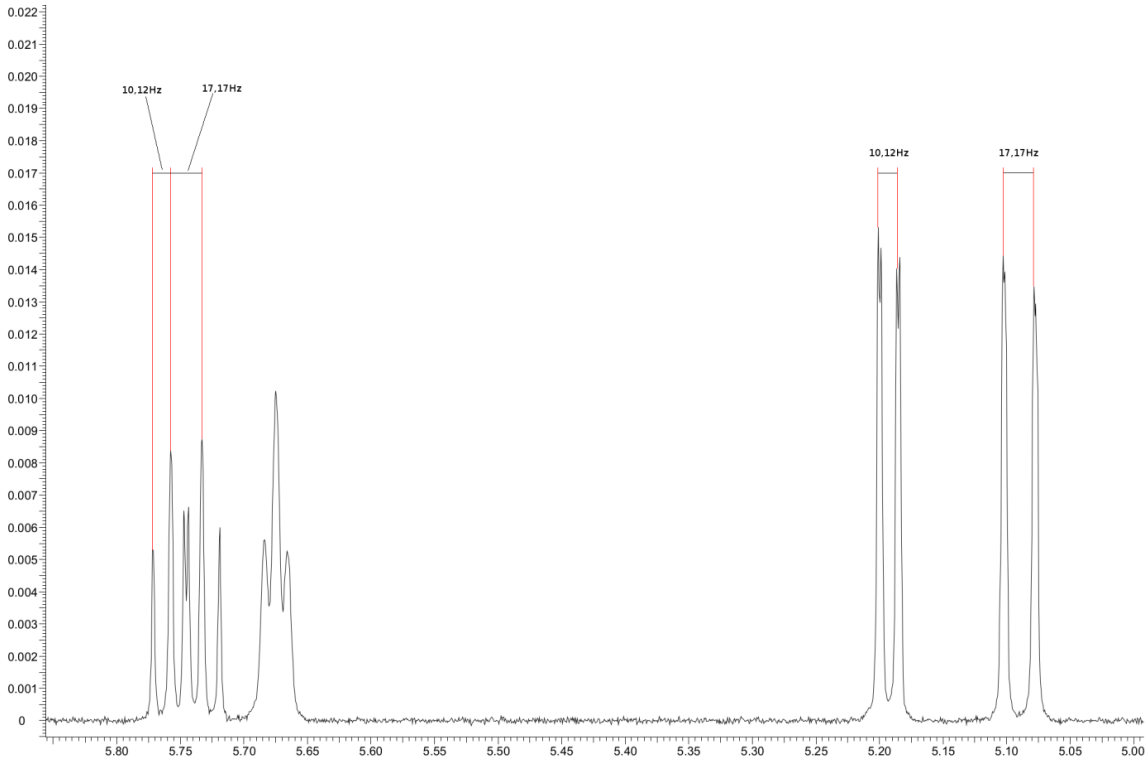


Figure S7. Fragment 5.00-5.80 ppm of ^{1}H NMR spectrum of **5** formed in reaction of quinine with CDMT.

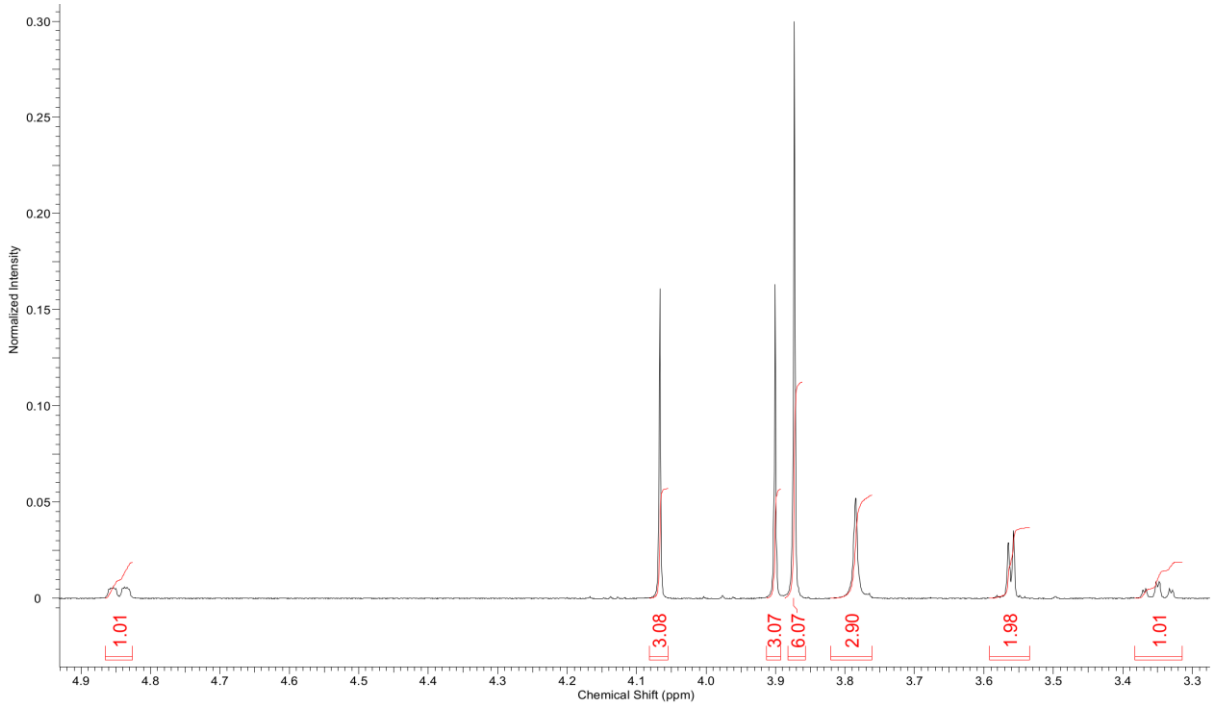


Figure S8. Fragment 3,30 to 4,90 ppm of ^{1}H NMR spectrum of product **5** formed in reaction of quinine with CDMT.

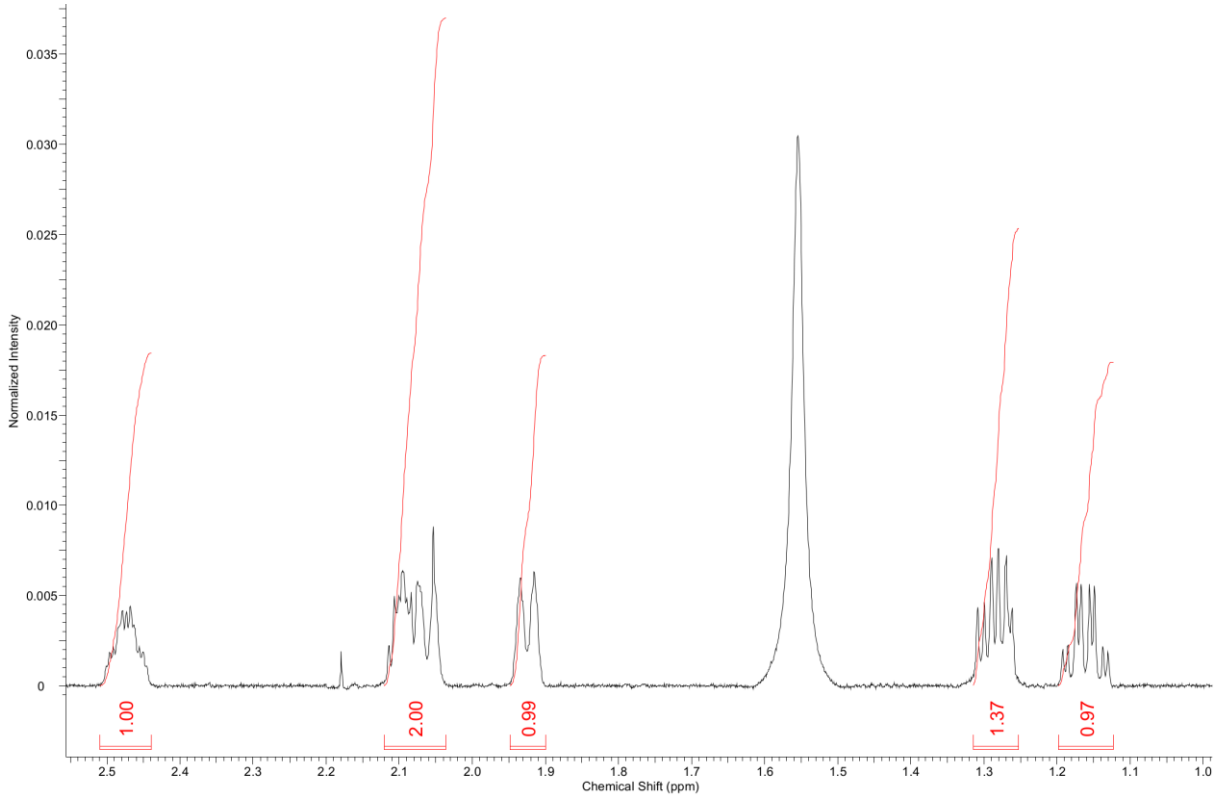


Figure S9. Fragment 1.20 to 2.50 ppm of ^{1}H NMR spectrum of product formed in reaction of quinine with CDMT.

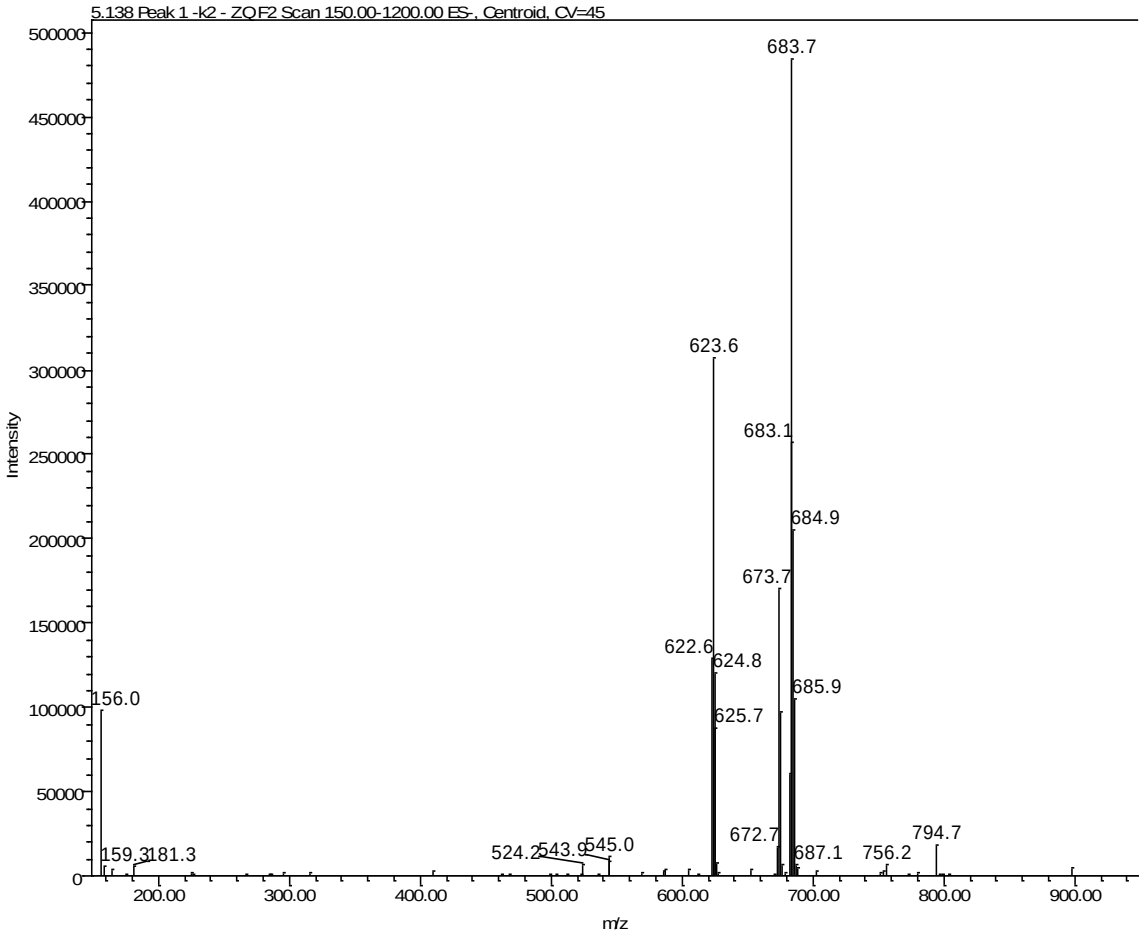


Figure S10. Mass spectrum (ESI$^-$) of the main product **5** formed in reaction of quinine with CDMT isolated after crystallization from ethyl acetate / n-heptane

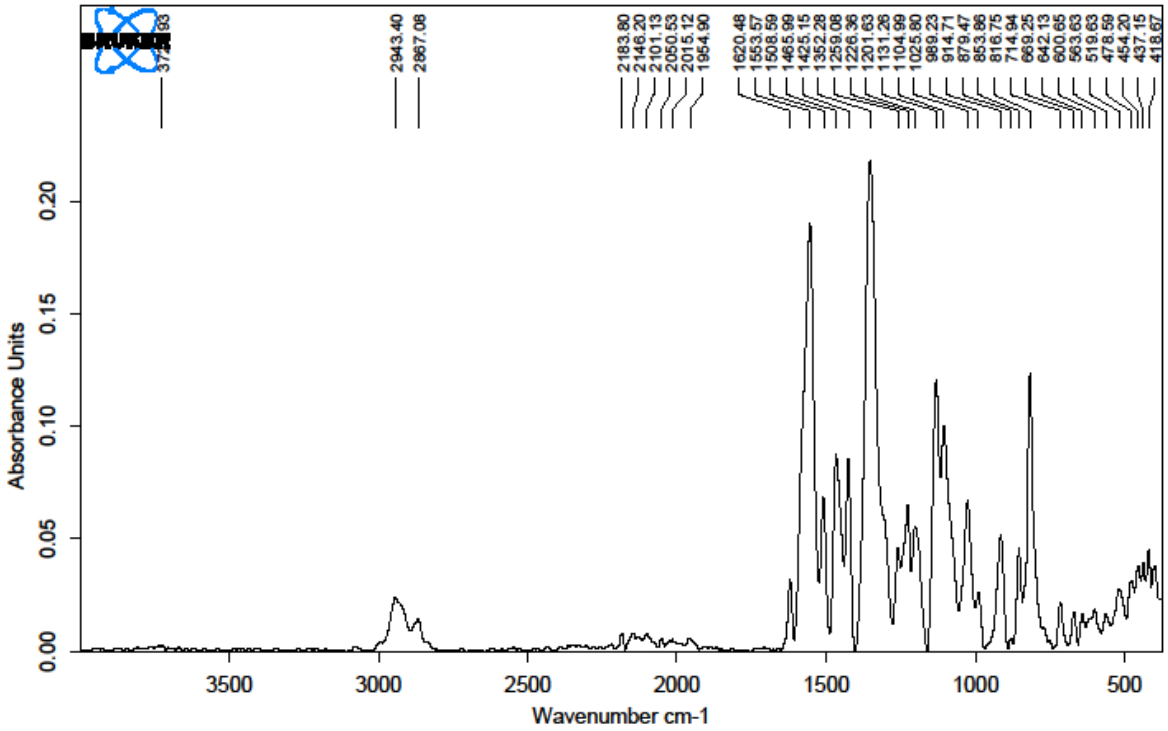


Figure S11. IR spectrum of the main product **5** formed in reaction of quinine with CDMT isolated after crystallization from ethyl acetate / n-heptane.

