Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis of Metapristone through an Efficient *N*-Demethylation of Mifepristone

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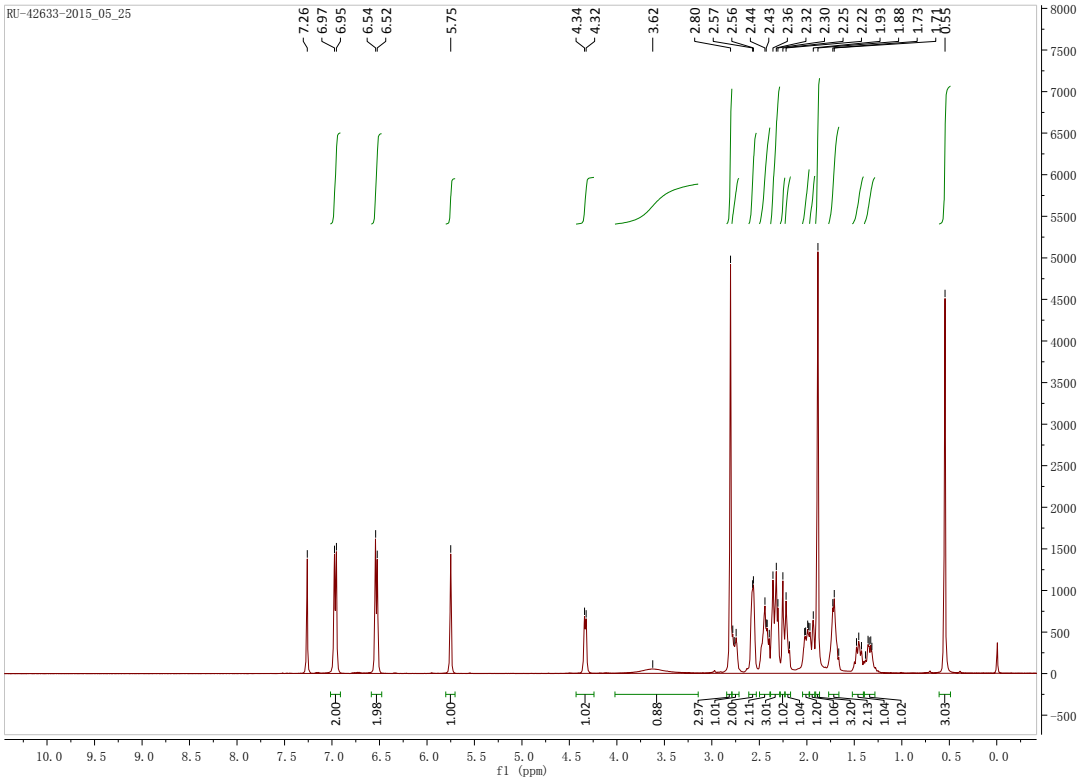
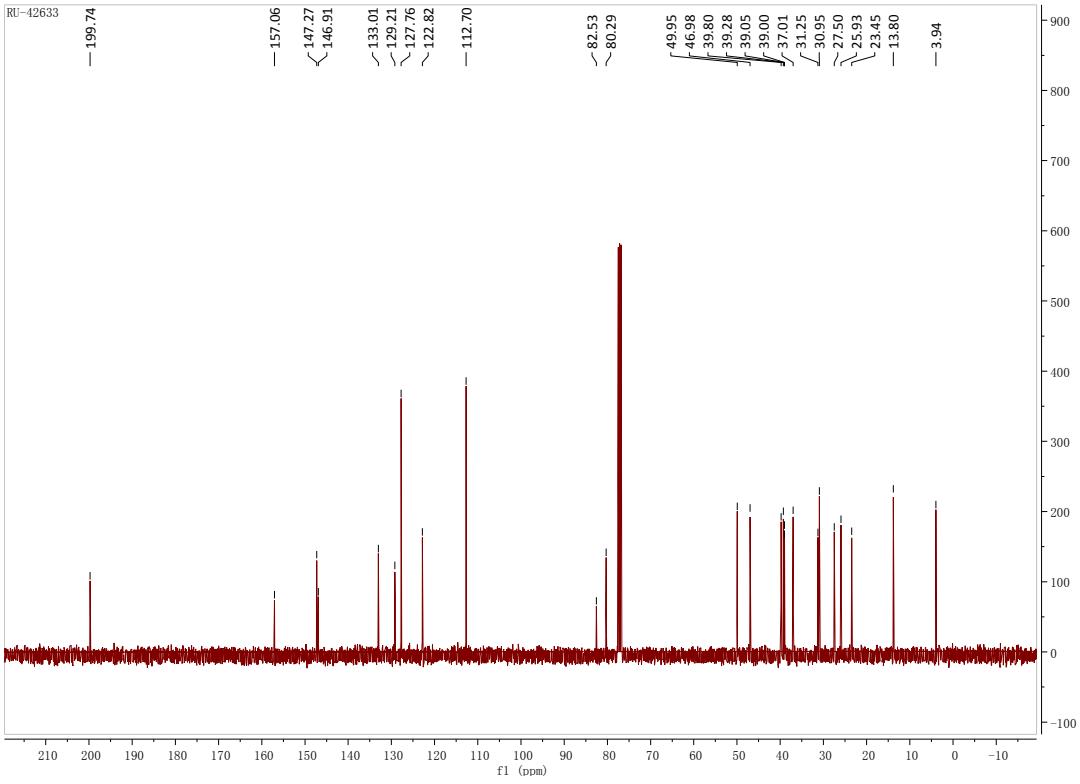
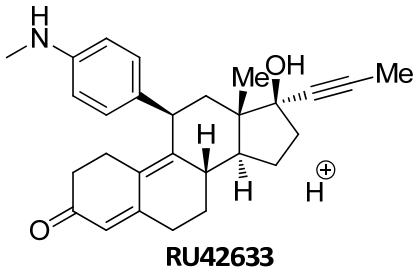
1. Copies of ^{1}H and ^{13}C NMR spectra of RU-42633





2. HRMS spectra of RU-42633

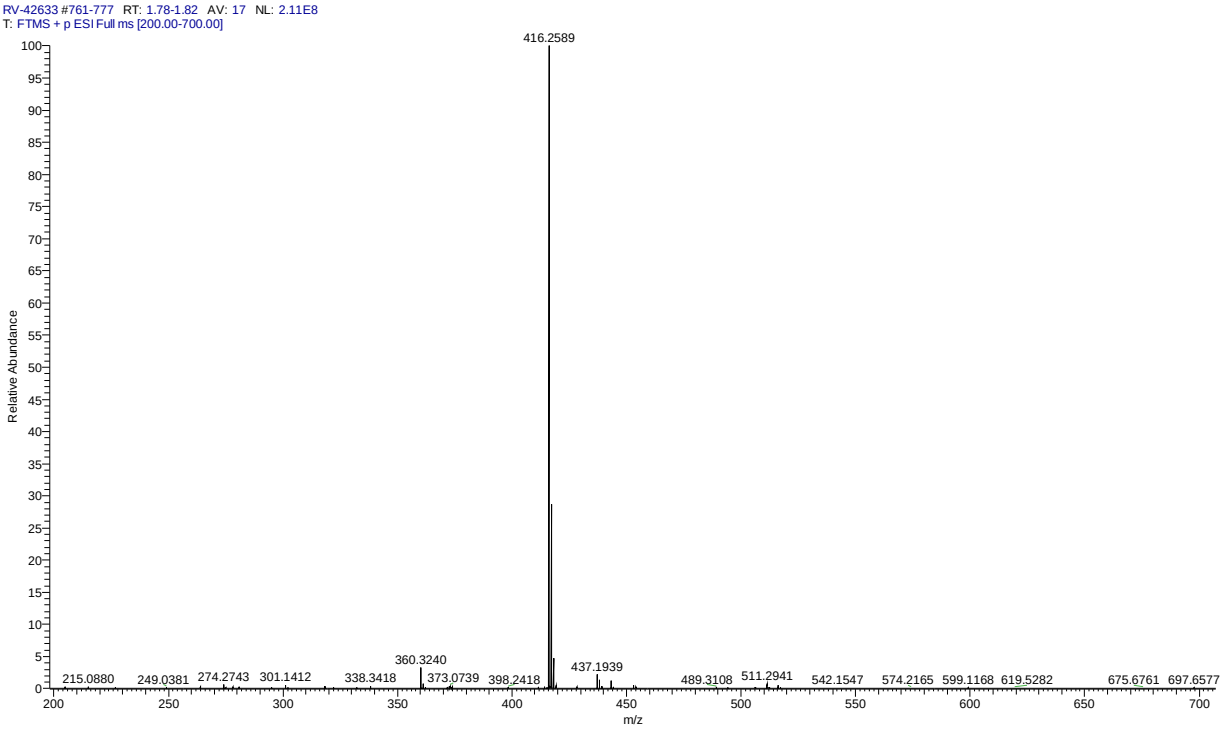


RU42633

Chemical Formula: $C_{28}H_{34}NO_2^+$

Exact Mass: 416.2584

Found:416.2589



3. Photographic guide for the synthesis of RU-42633 (grams scale)

Fig. S1. Left: Materials and reagents. Right: To a solution of mifepristone (2.5 g) and LiOAc (1.92 g) in 90 mL THF was added I_2/MeOH (46 mL) at 0 ^{o}C.

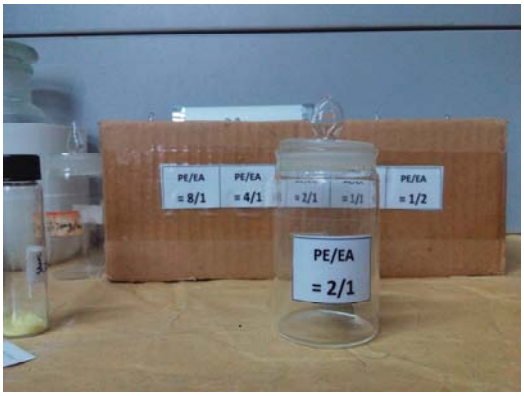



Fig. S2. Left: The reaction was stirred at r.t. under argon atmosphere. Right: The reaction was monitored by TLC (PE/EA = 2/1).


Fig. S3. Left: TLC plate, the reaction mixture was stirred for 24 h. Right: The reaction was quenched by 5% $Na_2S_2O_3$ (aq) at 0 ^{o}C.


Fig. S4. Left: The organic layer was concentrated under reduced pressure after extraction (EA/H_2O). Right: The crude product was dissolved by CH_2Cl_2.


Fig. S5. Left: The residue was purified by a silica gel column (PE/EA = 1/1). Right: The desired product RU-42633 (2.22 g, 92% yield) was obtained as a yellow solid.