Electronic Supplementary Material (ESI) for Analytical Methods.

Post-collection purity correction for internal standard correction - high performance liquid chromatography - quantitative nuclear magnetic resonance

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Supporting Information

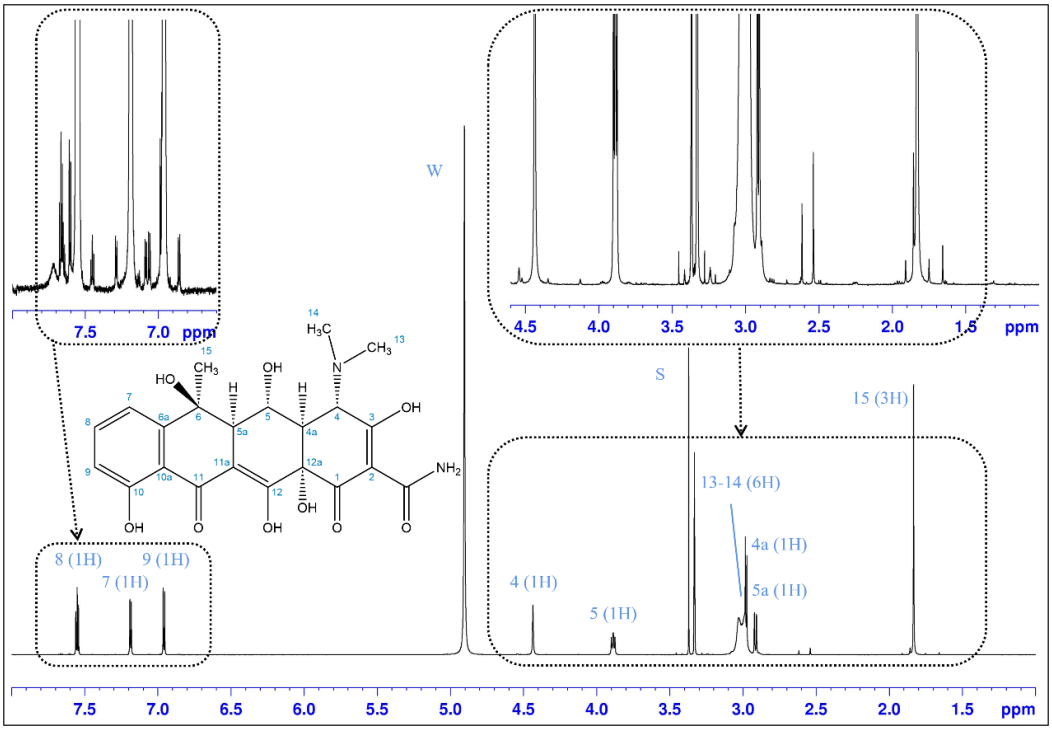

Fig. S1 ^{1}H NMR spectrum of the OTC in methanol-d_4. W: water peak; S: solvent residual peak

Table. S1 The longitudinal relaxation time (T_1) of the OTC and EP

chemical shift (ppm)	Analyte and IS	T_1(s)
7.887	EP(2H)	3.720
7.529	OTC(1H)	1.853
7.197	OTC(1H)	0.994
6.960	OTC(1H)	2.855
3.887	OTC(1H)	1.572
1.831	OTC(3H)	0.334
1.384	EP (3H)	2.630

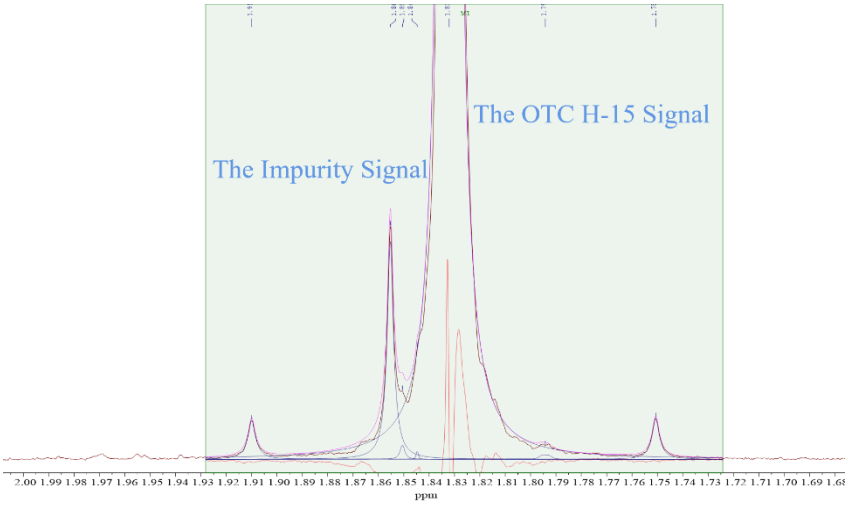

Fig. S2 The deconvolution spectrum of H-15

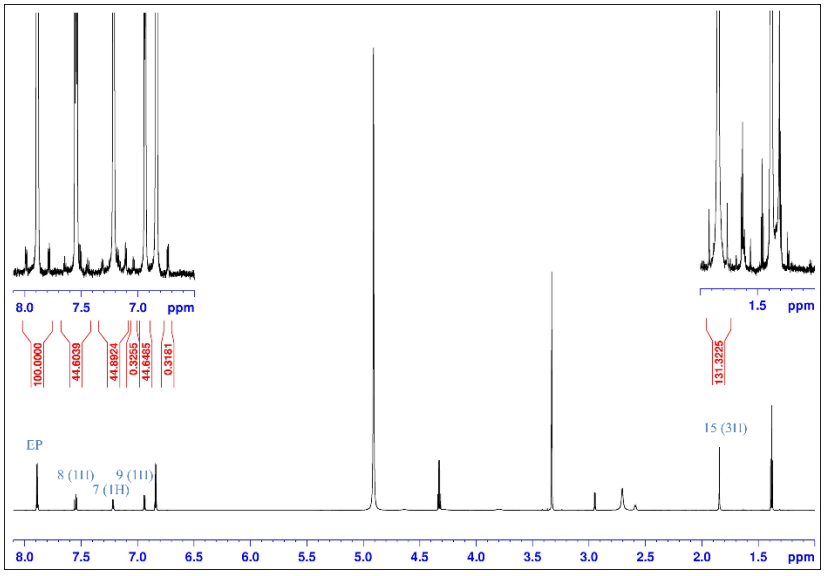

Fig. S3 Schematic of the integration of solution C using the ISC-HPLC-qNMR method (H-9: the corresponding quantitative peak area can be obtained by integrating the area of the EP satellite peak on the other side and subtracting it)

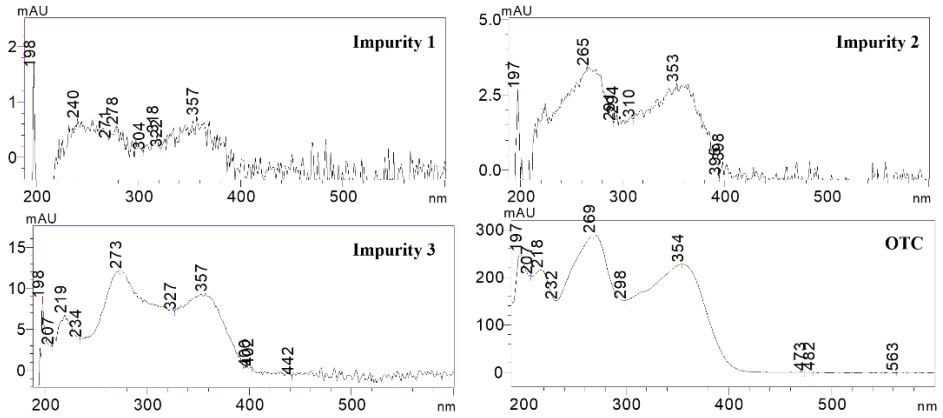

Fig. S4 The UV spectrograms of OTC and the impurities

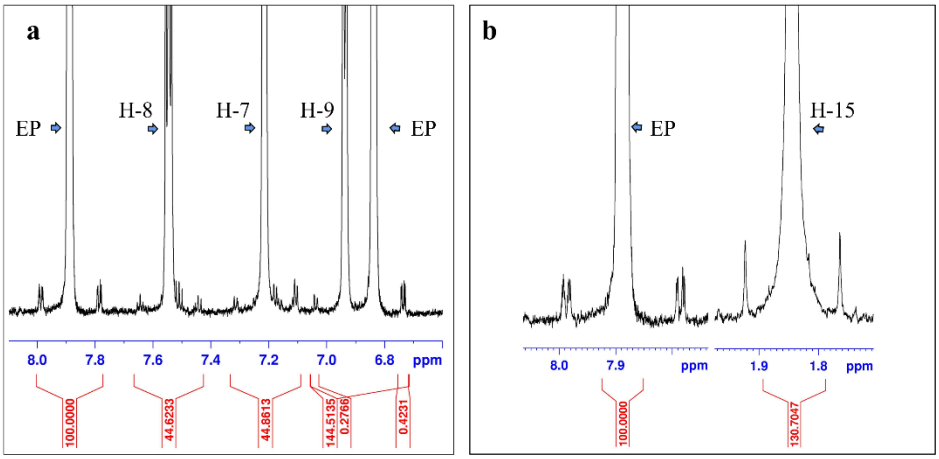

Fig. S5 Schematic of the integration of solution C using the post-collection purity correction for ISC-HPLC-qNMR method. (**a**: include the satellite peaks in benzene rings region; H-9: same as Fig. S3; **b**: methyl region; not include the satellite peaks)

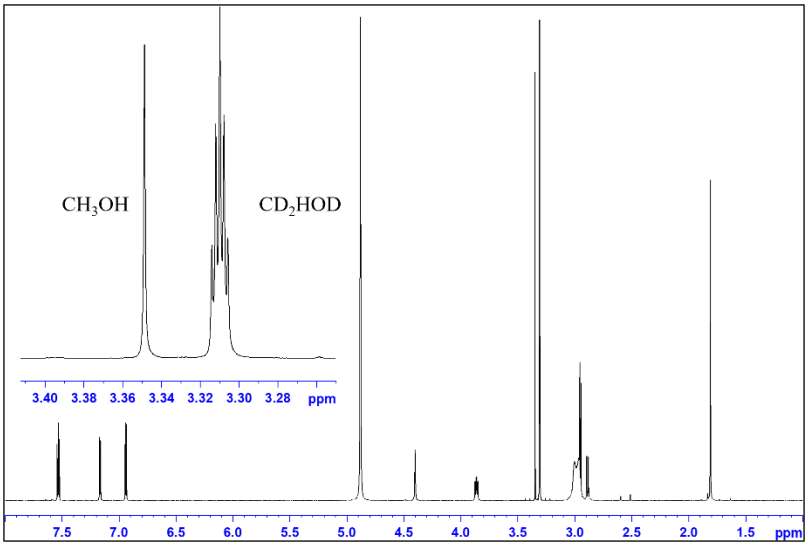

Fig. S6 The NMR spectrum of the OTC (in methanol-d_4 solvent): the signal peak at chemical shift 3.348 for a methyl peak on the residual methanol

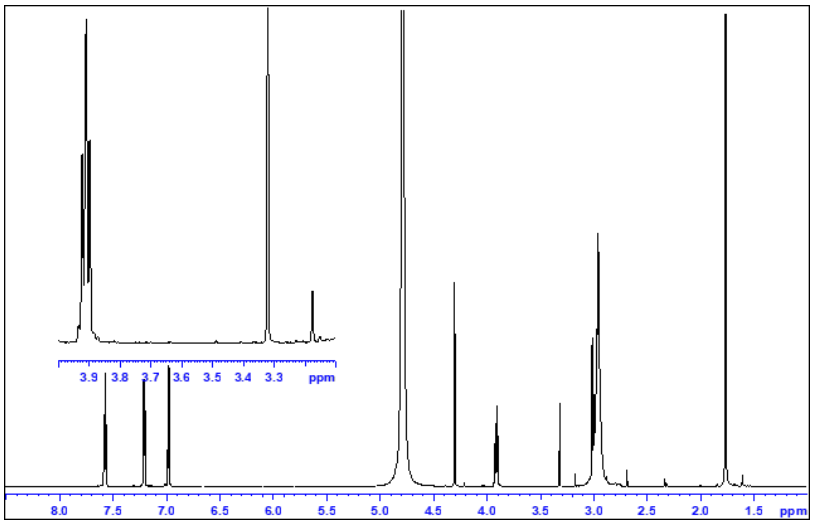

Fig. S7 The NMR spectrum of the OTC (in D_2O solvent): the signal peak at chemical shift 3.33 for a methyl peak on the residual methanol

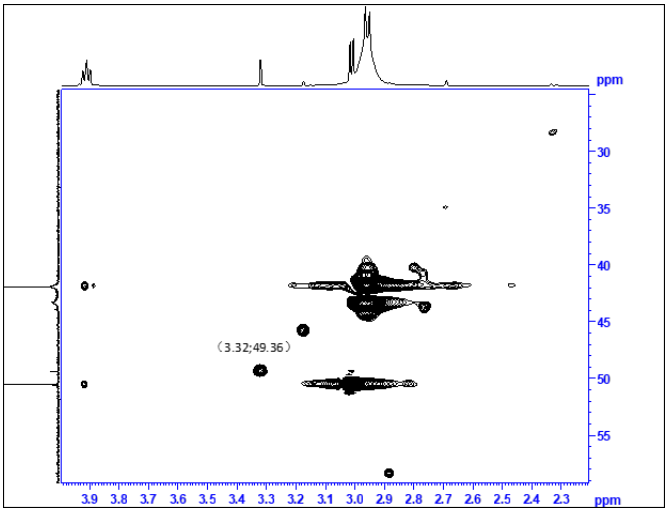

Fig. S8 HSQC spectra of methanol peak

Table S1 Chemical shifts of hydrogen and carbon in the methanol signal in the HSQC spectrum of the OTC sample studied (in D_2O solvent)

	Literature Value	Actual Value
Chemical Shift (^1H)	3.36 ppm (CH_3; s)	3.32 ppm (CH_3; s)
Chemical Shift (^{13}C)	49.50 ppm (CH_3)	49.36 ppm (CH_3)

Table S2 Quantitative results of residual methanol in OTC

Result						Mean	RSD
0.68%	0.62%	0.58%	0.65%	0.57%	0.63%	0.62%	6.70%