

Supplementary Materials: Antidiabetic Activities and GC-MS Analysis of 4-Methoxychalcone

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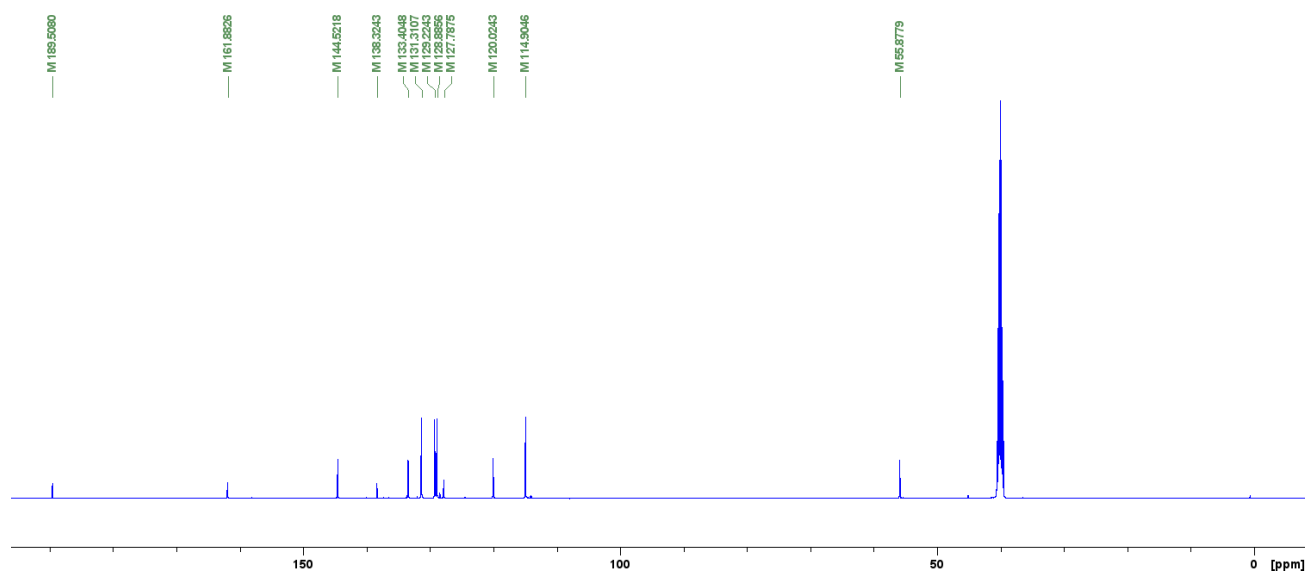


Figure S1. ^{13}C spectrum of MPP (125 Mz, DMSO- d_6).

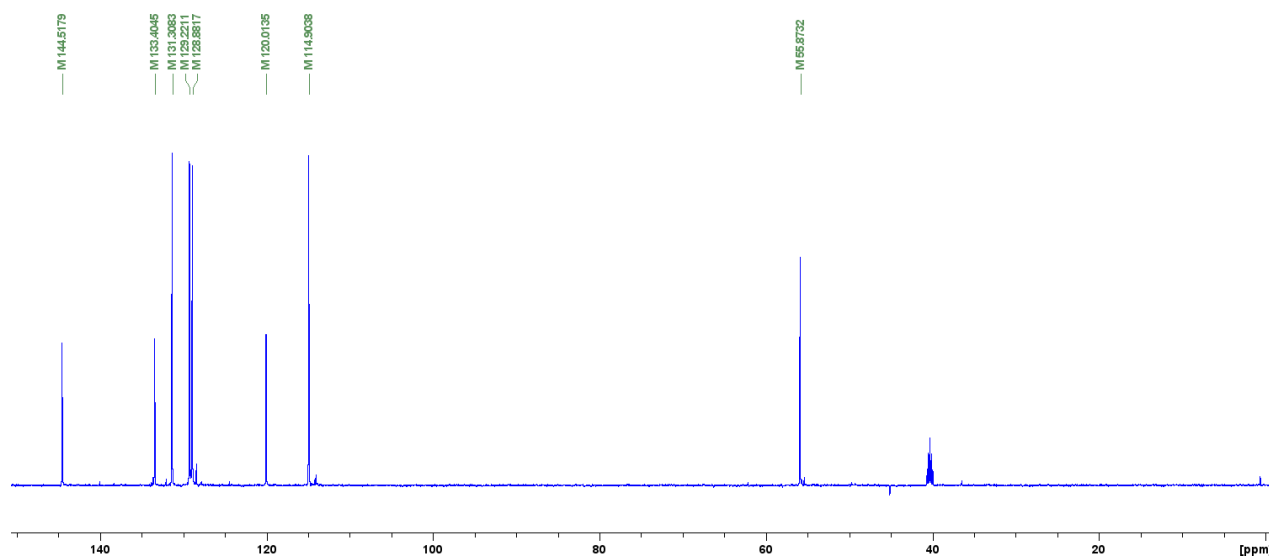


Figure S2. DEPT-135 spectrum of MPP (125 Mz, DMSO- d_6).

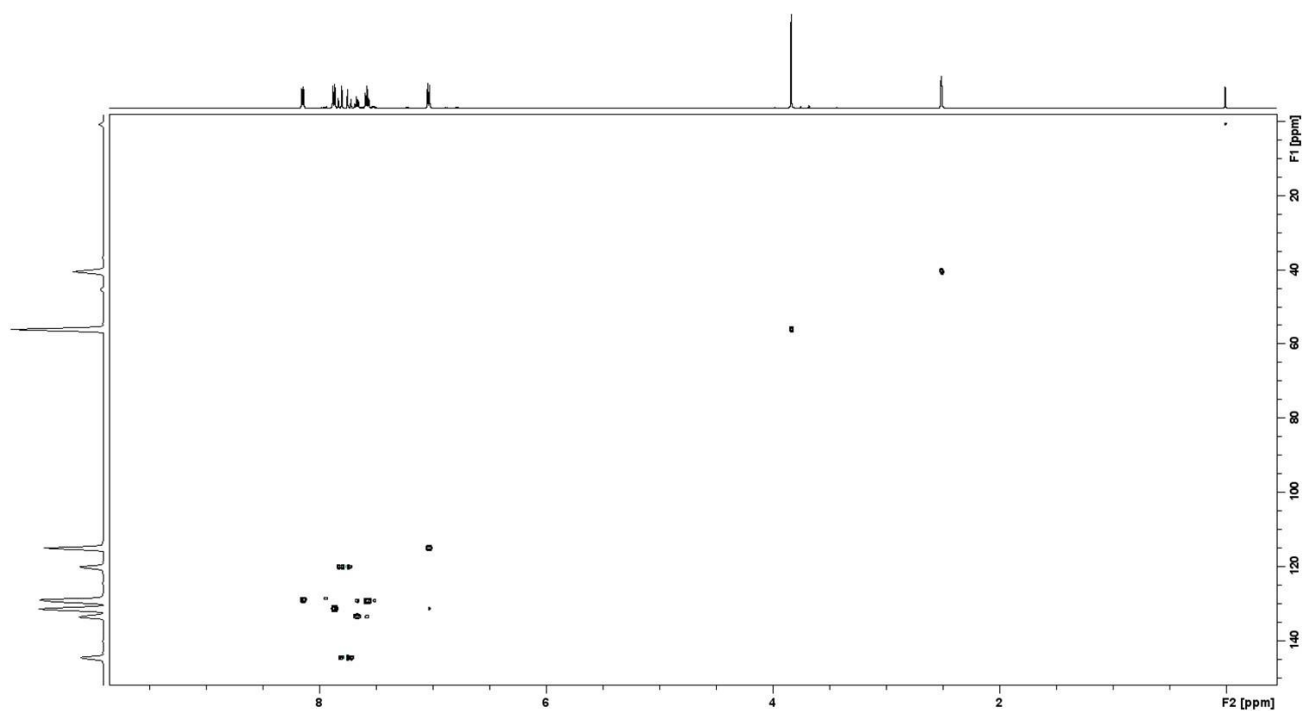


Figure S3. ^1H - ^{13}C HSQC of MPP (11.74 T, $\text{DMSO-}d_6$).

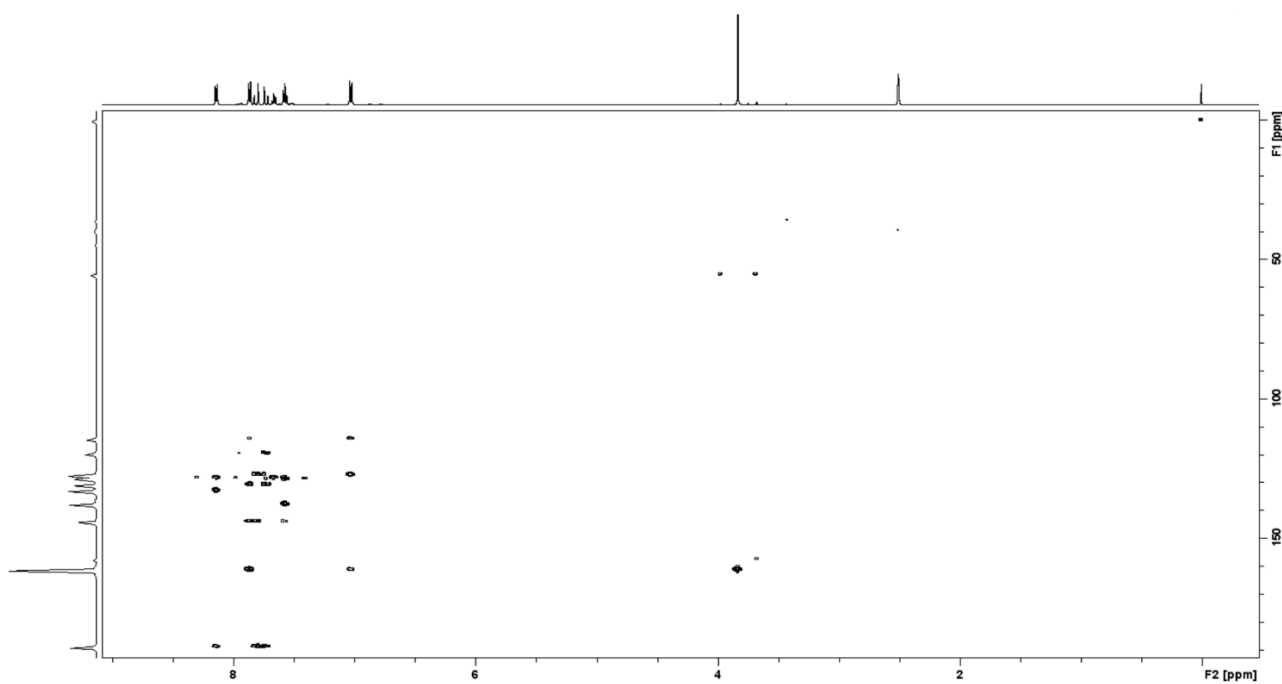


Figure S4. ^1H - ^{13}C HMBC of MPP (11.74 T, $\text{DMSO-}d_6$).

MA5_emerson#50 RT: 0,88 AV: 1 NL: 6,71E6
T: + c ESI Full ms2 239,000 [100,000-242,000]

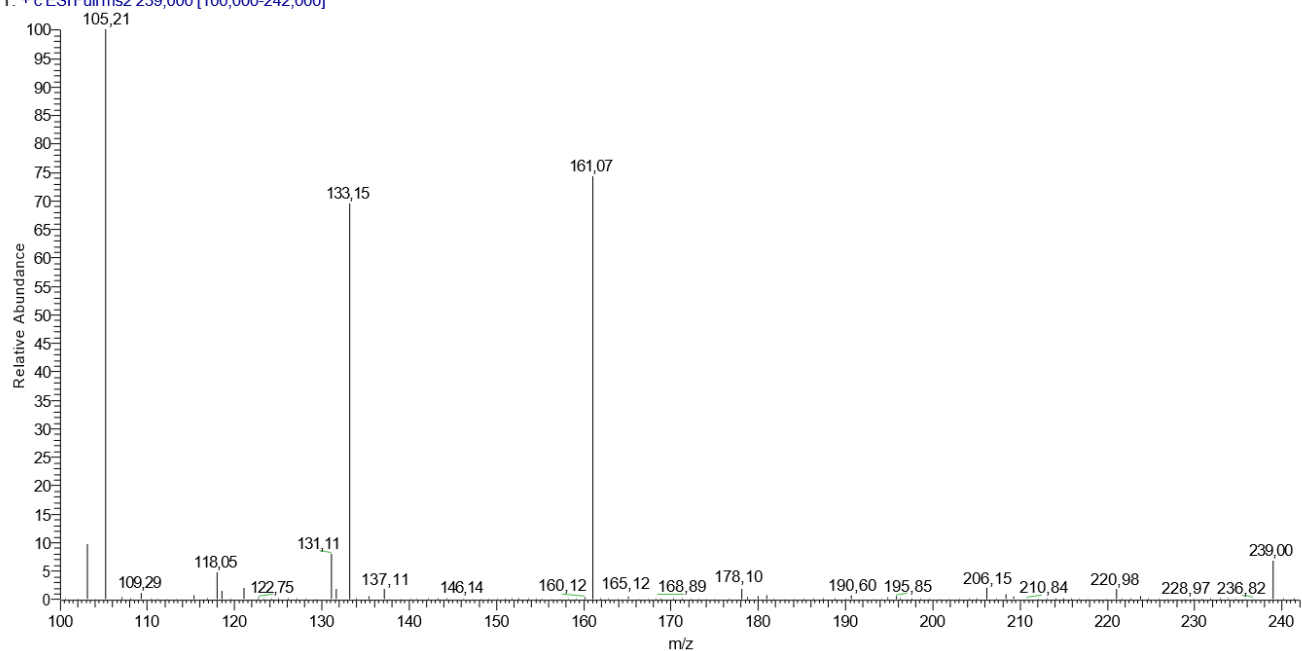


Figure S5. ESI-MS/MS spectra in positive mode of m/z 239.

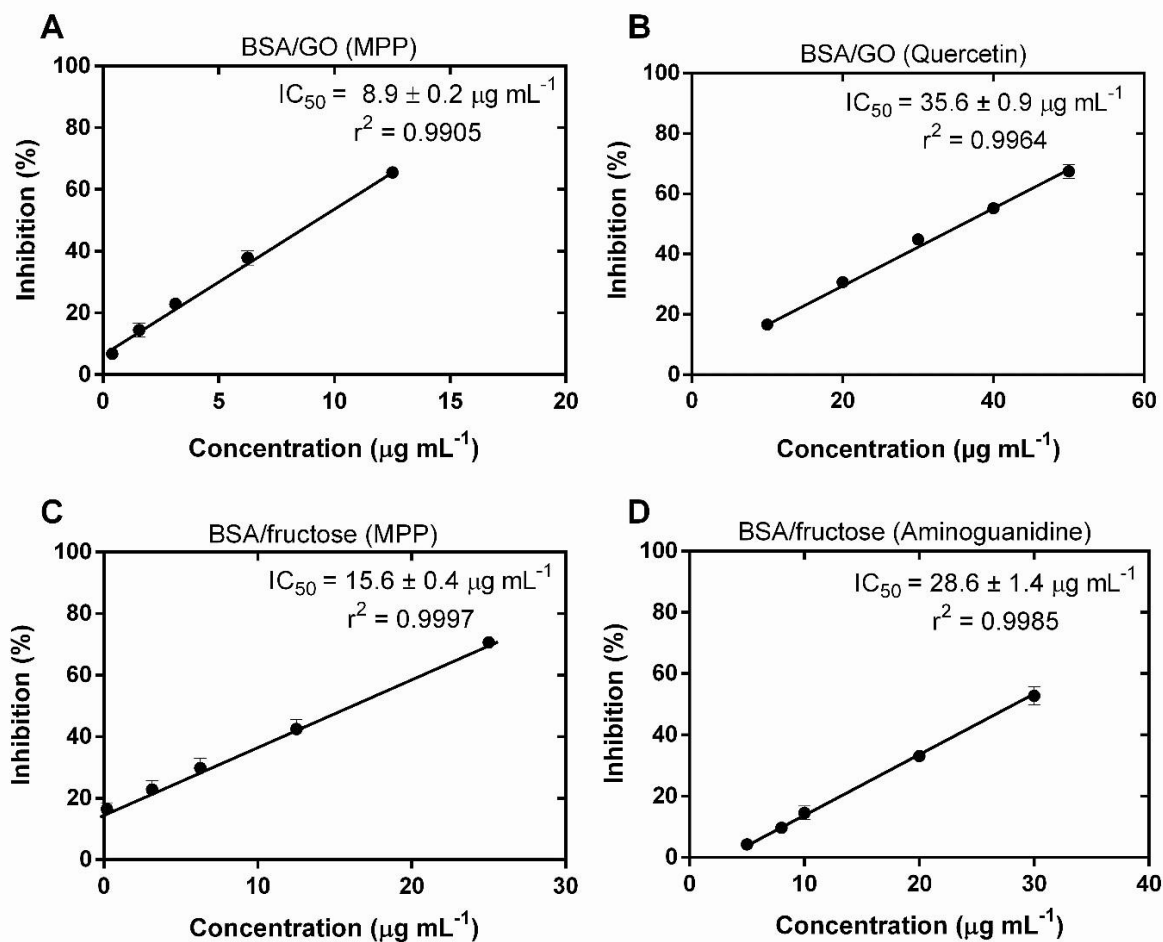


Figure S6. Antiglycant activity of MPP (A) and Quercetin (B) by the BSA/Glyoxal method. Antiglycant activity of MPP (C) and Aminoguanidine (D) by the BSA/fructose method. Results as mean \pm standard deviation of triplicates, concentration % inhibition: 100 $\mu g mL^{-1}$. IC_{50} : 50% Inhibitory capacity in $\mu g mL^{-1}$.

Quantitative NMR acquisition data.

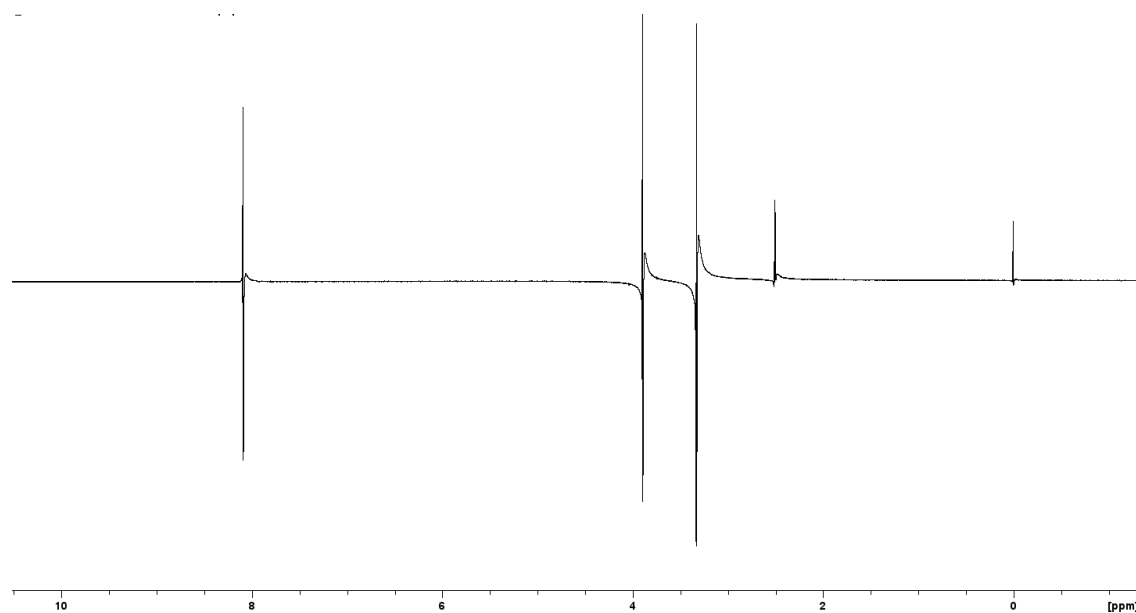


Figure S7. The 90° pulse experiment (zg) calibrated for the signal at δ 8.08 (s, 4H) of dimethyl terephthalate standard.

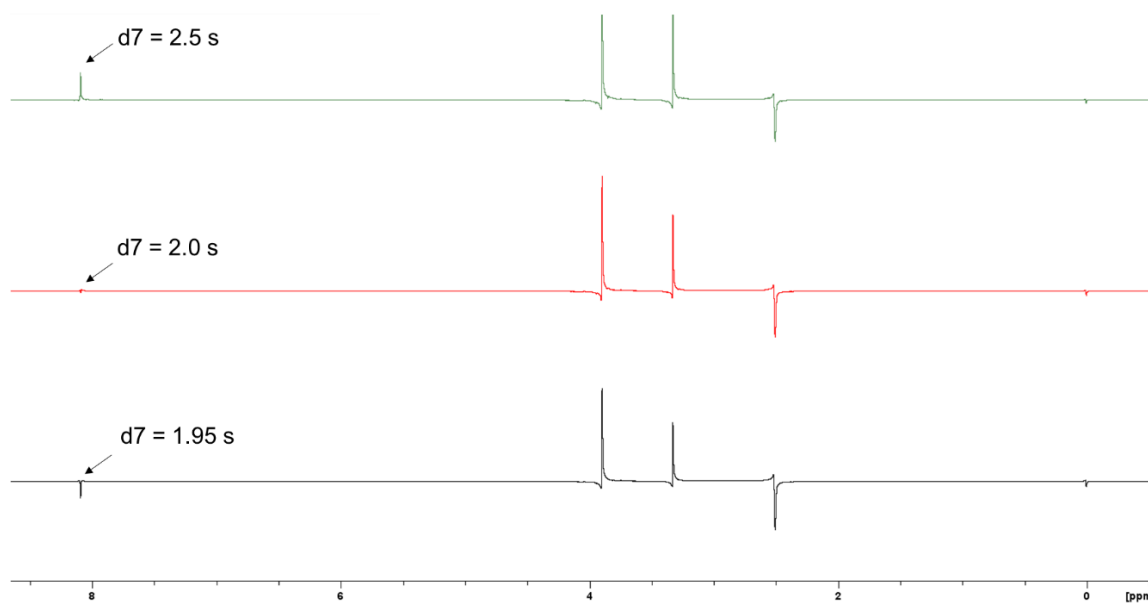


Figure S8. The Inversion-Recovery experiment (t1ir1d) for the signal at δ 8.08 (s, 4H) of dimethyl terephthalate standard (d1=22s).

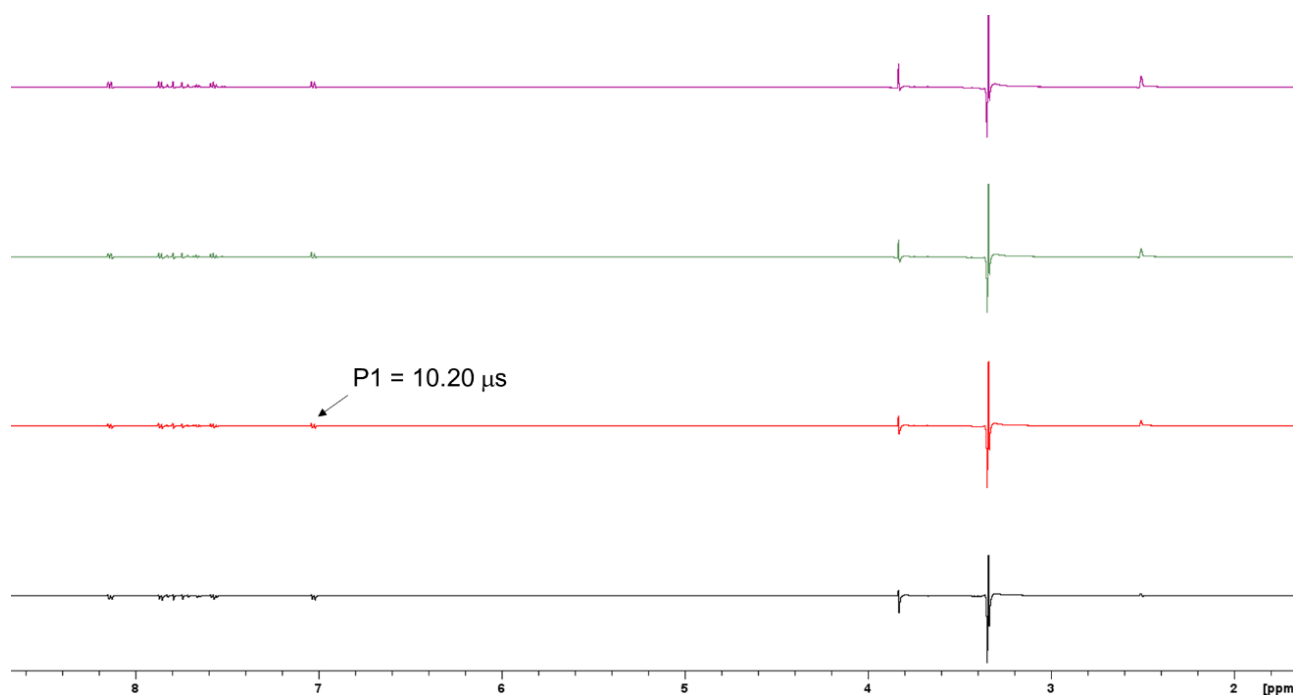


Figure S9. The 90° pulse experiment (zg) calibrated for the signal at δ 7.03 (*d*, 2H) of MPP (360° pulse).

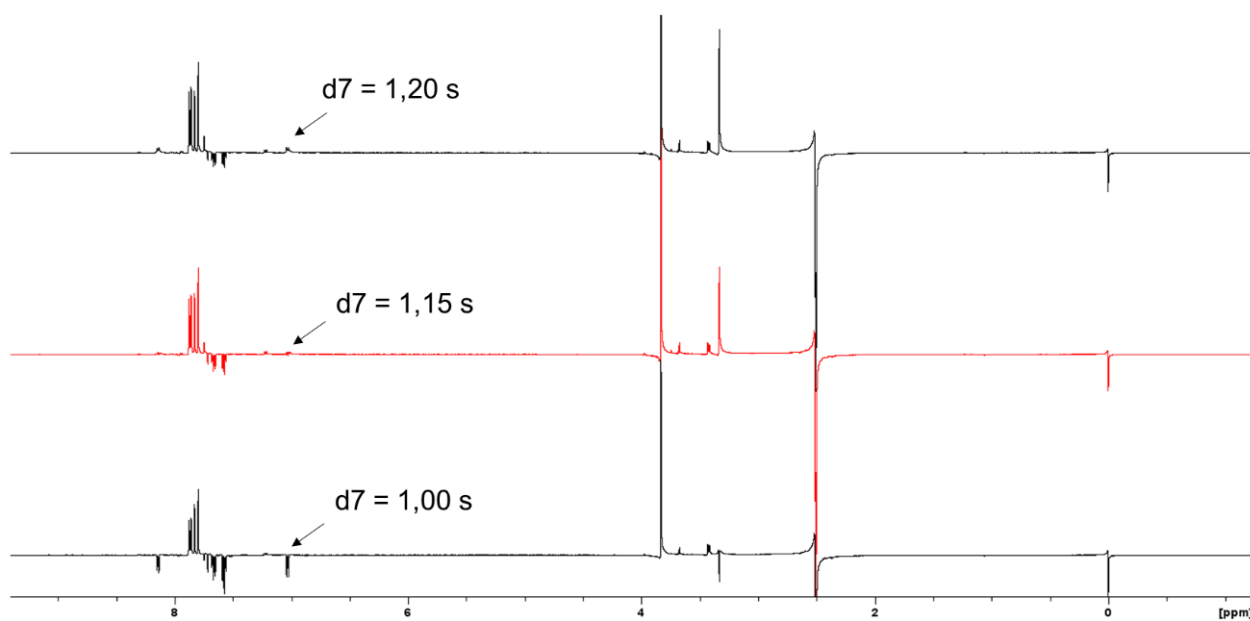


Figure S10. The Inversion-Recovery experiment (t1ir1d) for the signal at δ 7.03 (*s*, 2H) of MPP (d1=15s).

Table S1. MPP purity obtained by qNMR ^1H and with the values of the absolute integrals of the TD and MPP standard; proton numbers for TD (4H) and MPP (2H); molar mass of the TD standard ($194.1834 \text{ g mol}^{-1}$) and MPP ($238.0993 \text{ g mol}^{-1}$); and purity of the TD standard (99.988%).

	Replicata	Weight of TD Standard (mg)	TD Standard Integral [abs]	Weight of MPP (mg)	MMP Integral [abs]	Calculated Purity	% RSD
Samples	1	2.94	108,914.89	4.80	73,402.33	97.14%	
	2	2.95	110,596.59	4.82	73,605.85	95.99%	
	3	3.01	115,618.23	4.80	73,709.48	95.84%	
Average						96.32%	0.73%

TD: tereftalato de dimetila external standard. MPP: (*E*)-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one.

Table S2. Pharmacokinetic parameters of MPP.

Physical Chemical Properties	Result	Parameters
Molecular weight	238.28g/mol	<500
Number of heavy atoms	18	
Aroma number. heavy atoms	12	
Number of rotating titles	4	≤10
Number H-bond acceptors	2	≤10
Number H-bond donors	0	≤5
TPSA	26.30Å	≤140 Å
Csp3 fraction	0.06	
Log P o/w	3.27	≤5
Log S (SILICOS-IT)	Moderately soluble	
Gastrointestinal Absorption	High	
BBB permeant	Yes	
P-gp substrate	No	
Bioavailability score	55%	