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Kinetics and possible mechanism of chlorogenic acid-water complexes formation

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1. External calibration for molecular weight determination in DMSO-d_6 using NMR DOSY

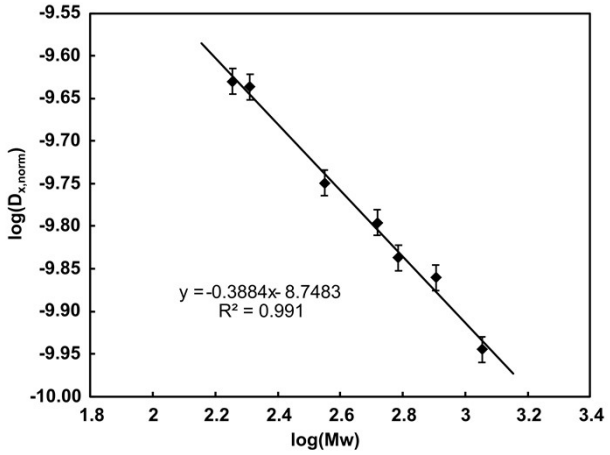

Figure S1. External calibration curve constructed for molecular weight estimation of polyphenolic compounds in DMSO-d_6.

2. Determination of 5-CQA∗H_2O molecular weight using external calibration curve in DMSO-d_6 and NMR DOSY

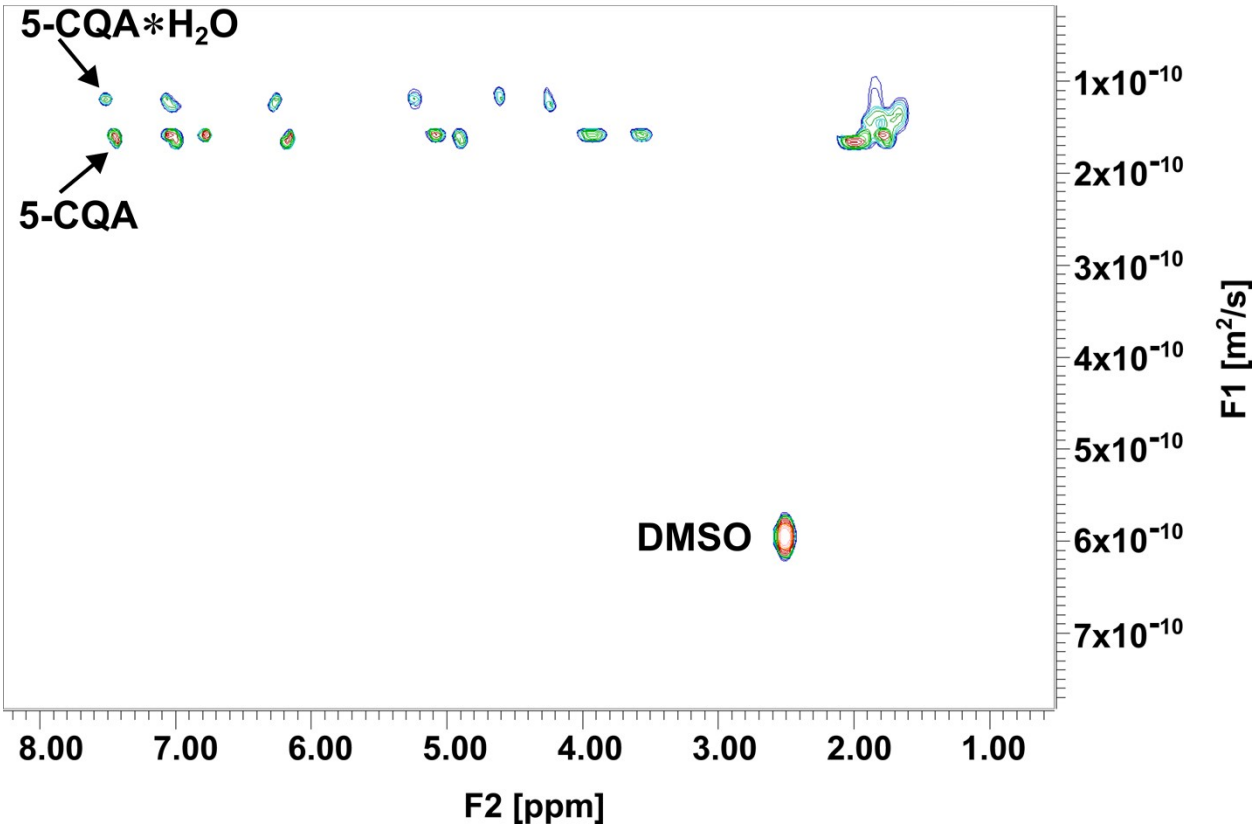

Figure S2. ^{1}H DOSY spectrum of dry residue obtained from incubated 5-CQA water solution dissolved in DMSO-d_6.

TABLE S1. Results of the molecular weight estimation of 5-CQA∗H_2O complexes in DMSO-d_6 using NMR DOSY measurements and external calibration method.

Average value of diffusion coefficient of 5-CQA∗H_2O[a] [m^2/s]	$1.20 \bullet 10^{-10}$
Logarithm of normalized diffusion coefficient of 5-CQA∗H_2O	-9.877
Determined molecular weight of 5-CQA∗H_2O [g/mol]	805.42
Theoretical molecular weight of 5-CQA∗H_2O [g/mol]	744.65

[a] Average was calculated over all non-overlapping signals of 5-CQA∗H_2O-1 and 5-CQA∗H_2O-2 as the differences in diffusion coefficients of both 5-CQA∗H_2O did not exceed experimental error for the employed method for determination of diffusion coefficients.