SUPPORTING INFORMATION

Structural and spectroscopic characterization of TPGS micelles: disruptive role of cyclodextrins and kinetic pathways

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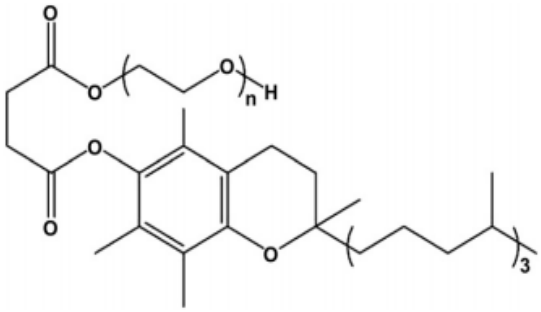
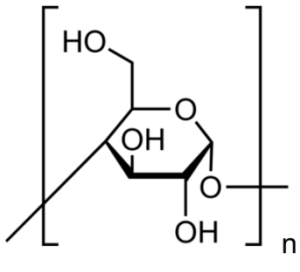
SUPPORTING INFORMATION

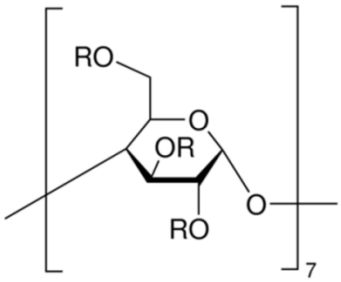


SI, Scheme 1. Chemical structure of TPGS.



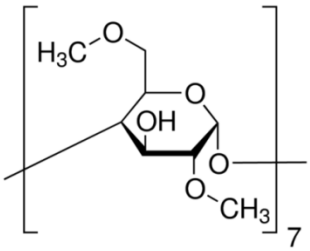
n = 6,7,8

α, β, γ-cyclodextrin

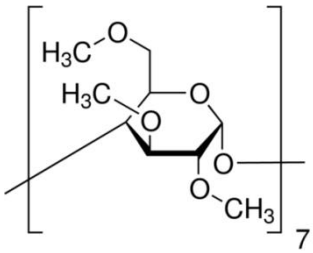


R = H or *−CH_3

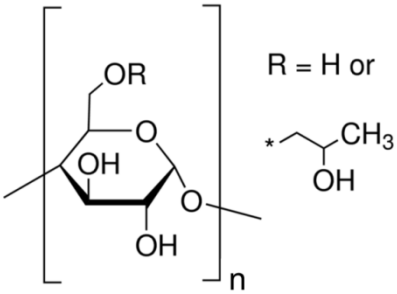
Randomly methylated β-cyclodextrin (RAMEB)



Heptakis(2,6-di-O-methyl)-β-cyclodextrin (DIMEB)



Heptakis(2,3,6-tri-O-methyl)-β-cyclodextrin (TRIMEB)



R = H or

n = 6,7,8

Hydroxypropyl-X-CD (HPXCD)

SI, Scheme 2. Structures of the repeating units of the cyclodextrin derivatives.

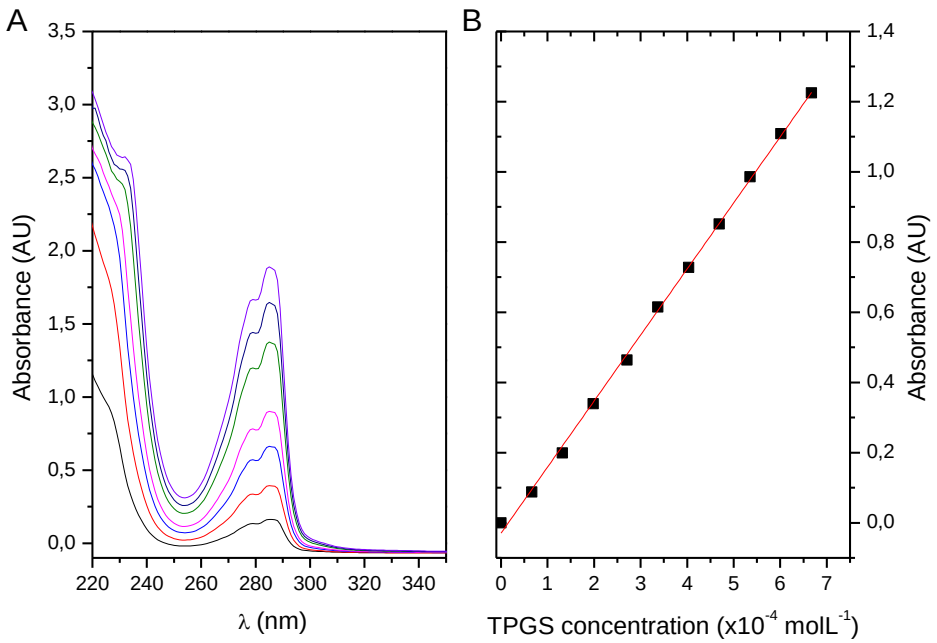


Figure S1. a) Absorption spectrum of TPGS at varying concentrations up to 0.1%; b) Beer-Lambert plot for the determination of TPGS molar absorptivity (λ_{max} = 285 nm).

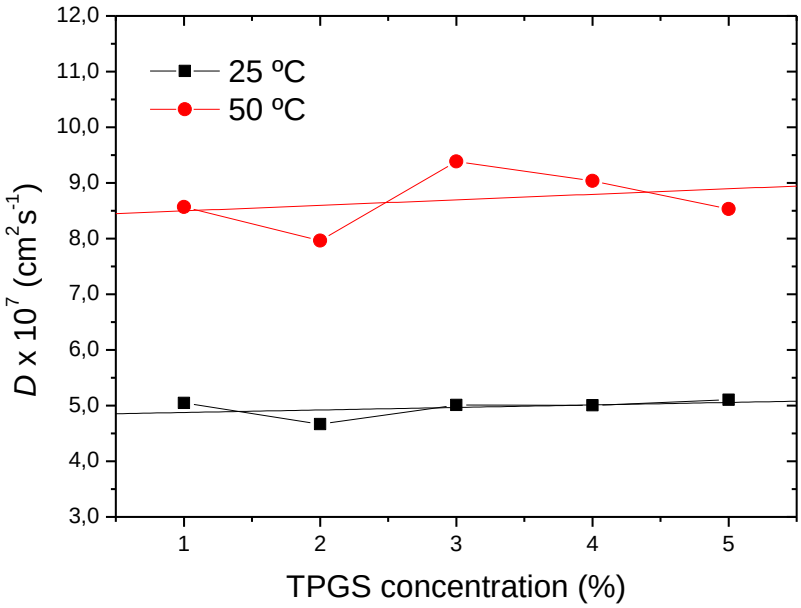


Figure S2. Diffusion coefficients of TPGS as a function of concentration and temperature.

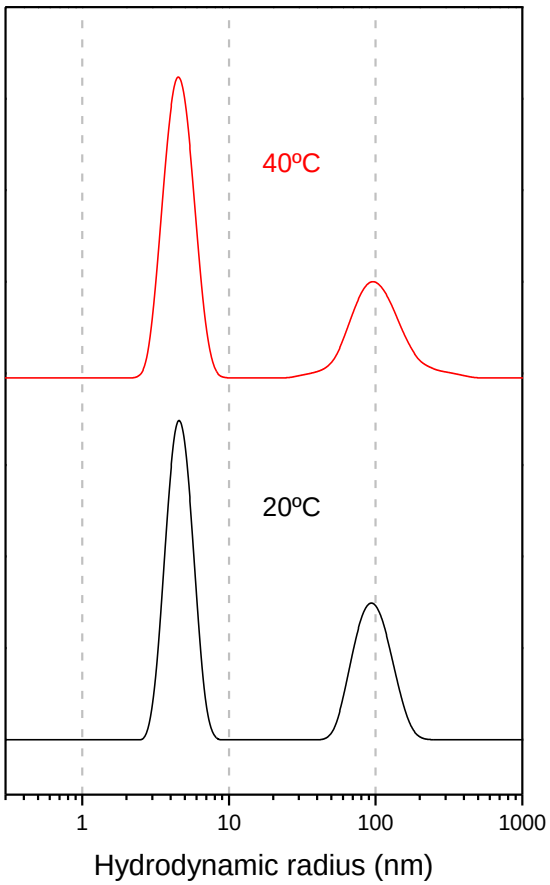


Figure S3. a) Intensity size distribution obtained by DLS at 20ºC and 40ºC of mixtures of 1% TPGS with 5% αCD in water (solutions filtered by 0.2 μm filters).

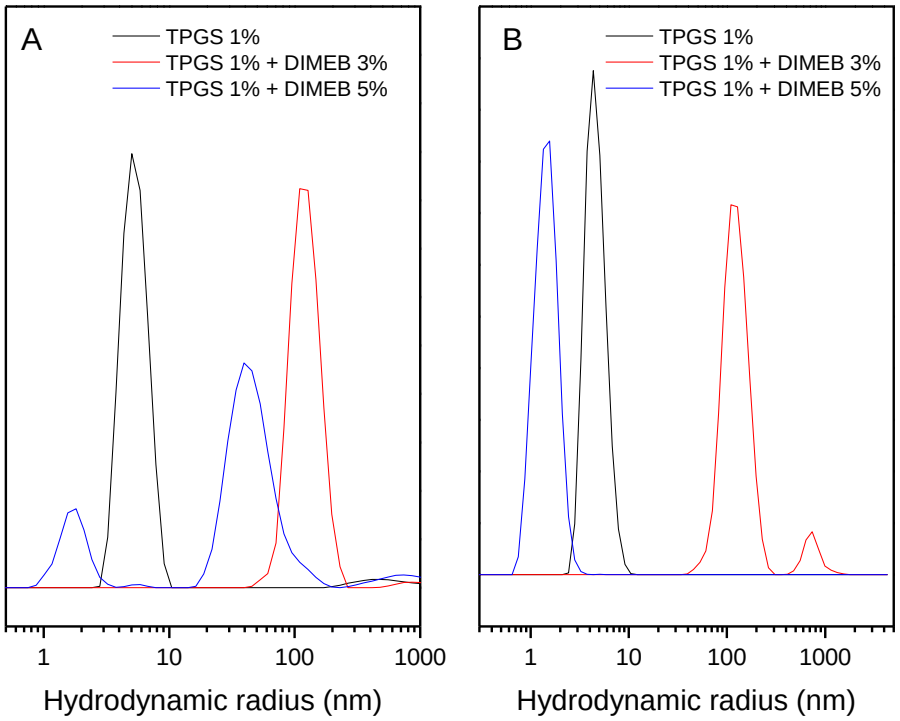


Figure S4. DLS intensity size (A) and volume (B) distributions in D_2O of 1% TPGS alone (black), and with the addition of 3% DIMEB (red) or 5% DIMEB (blue), at 20ºC.

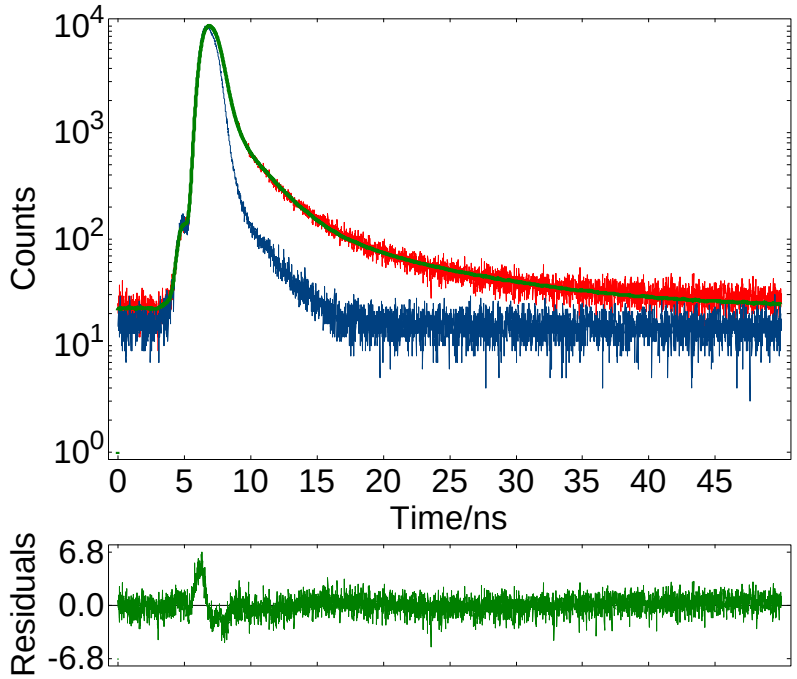


Figure S5. Fluorescence decays (λ_{ex}=295 nm, λ_{em}=320 nm) of a 0.01% TPGS with DIMEB 3% solution (red line) and fit to a double exponential. In blue, the response of the instrument (IR) for curve deconvolution.

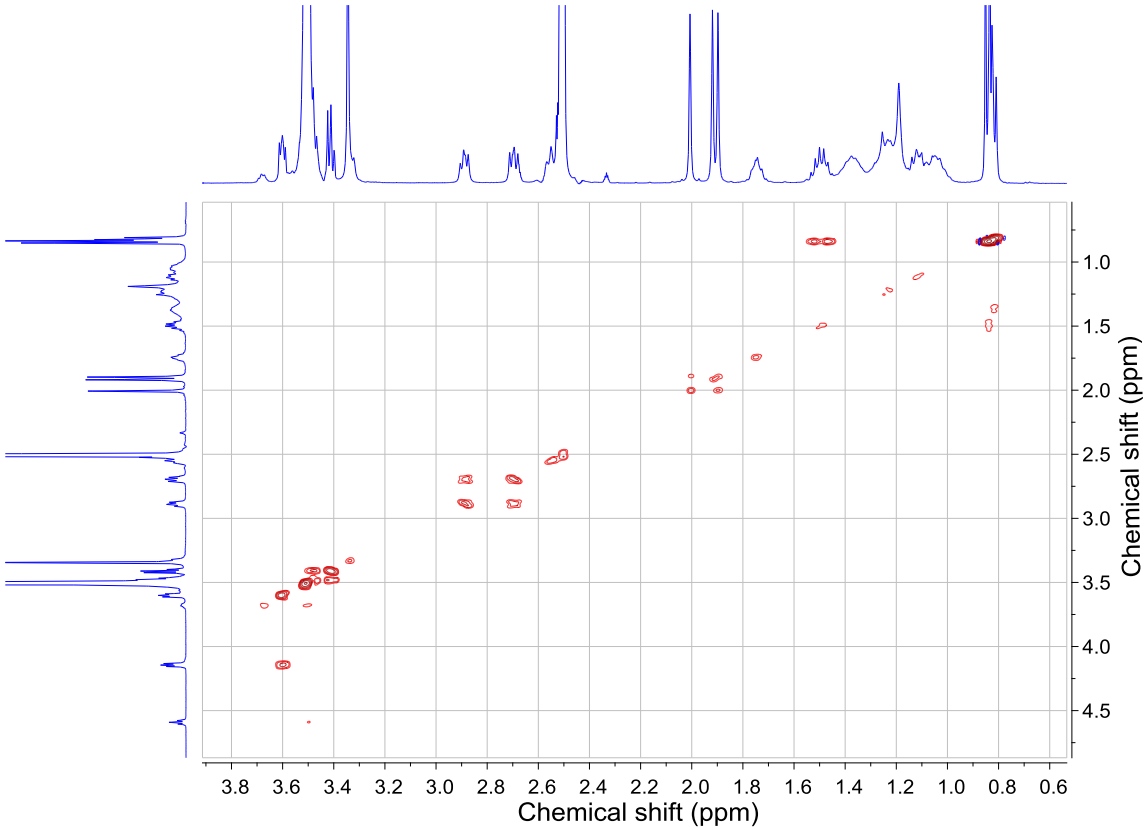


Figure S6A. ^{1}H-COSY spectrum of TPGS in DMSO.

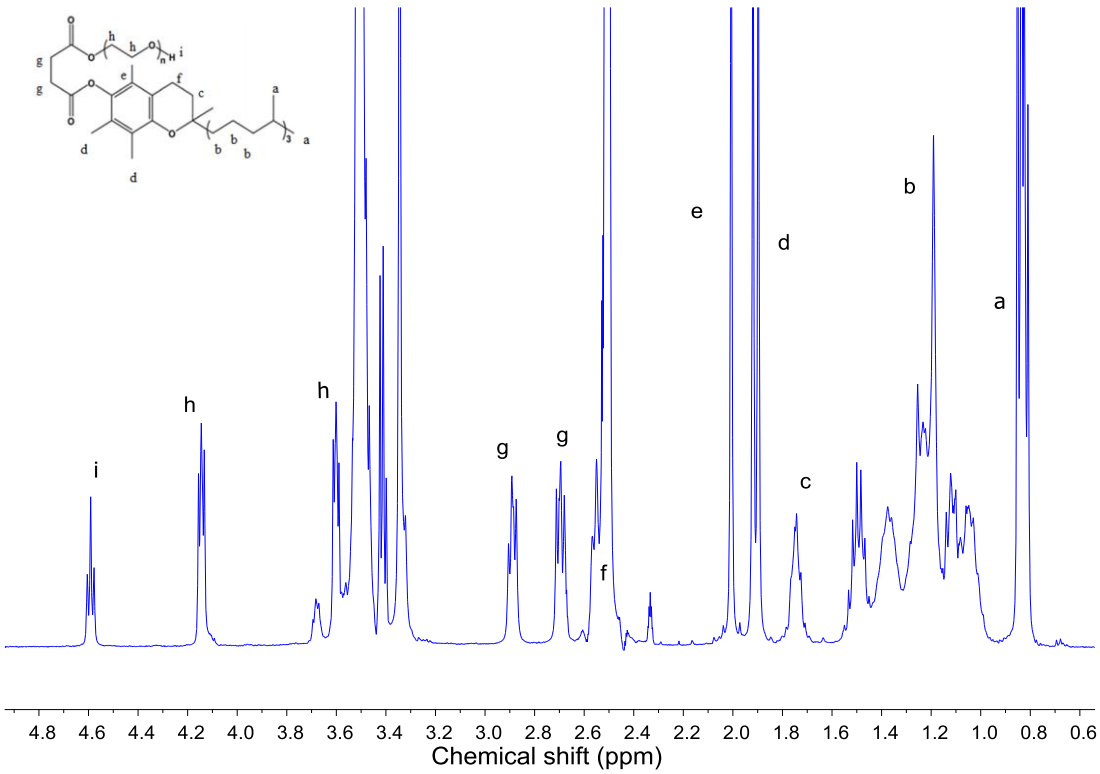


Figure S6B. ^{1}H-NMR spectrum of TPGS in DMSO, showing signal assignation.

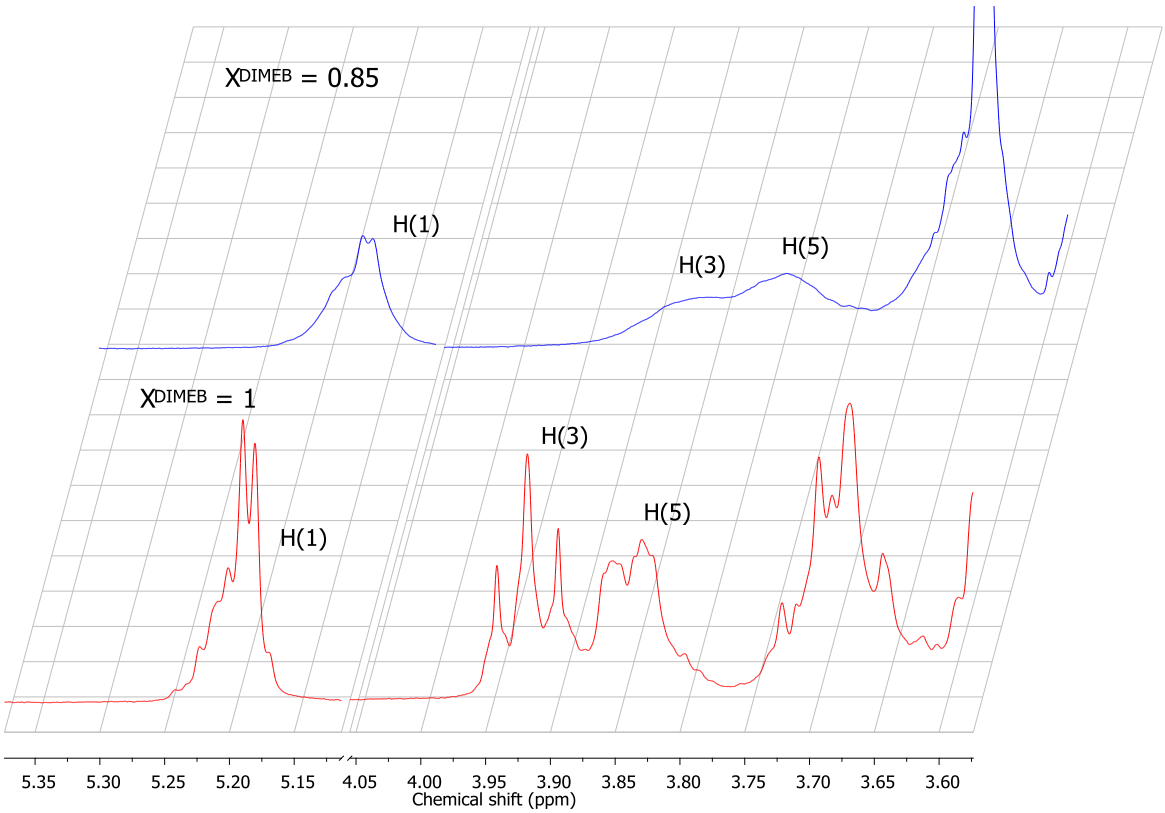


Figure S7. ^{1}H-NMR spectra of selected DIMEB protons of DIMEB alone (red) and a mixture of DIMEB and TPGS (blue).

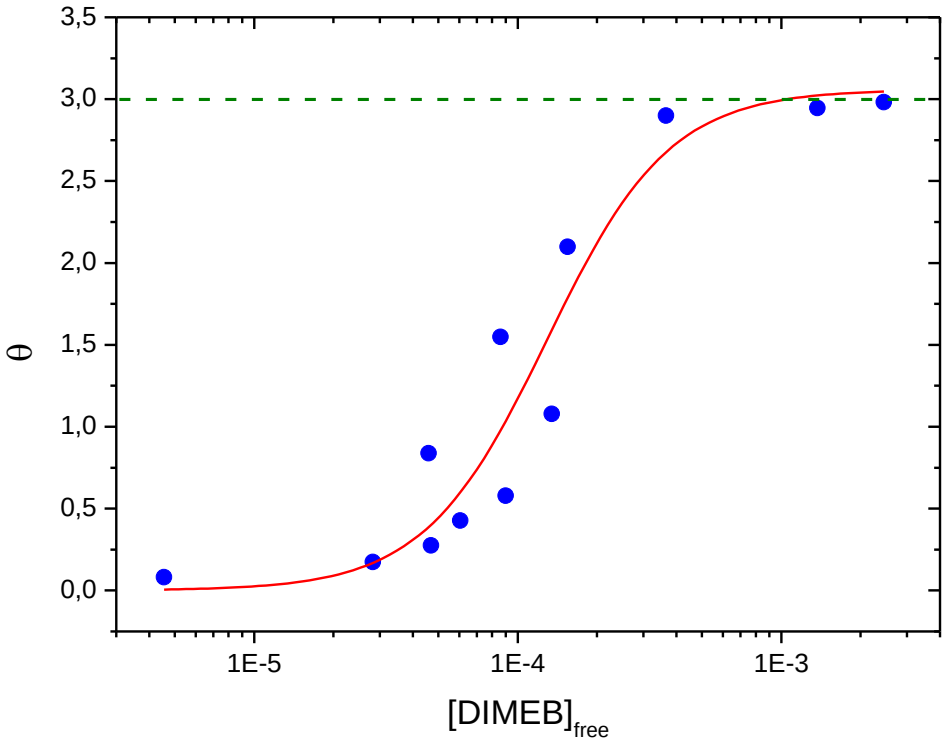


Figure S8. Hill's plot obtained from the shifts in H(1), H(3), H(5) and Me(6) protons of DIMEB. The limit of θ at high concentrations indicates the stoichiometry of the complex.

Table T1. Parameters obtained from the fit of the fluorescence decays of TPGS as a function of the surfactant concentration. Fluorescence lifetimes of TPGS in unimer form (τ_1), micelle form (τ_2), and fraction of the overall emission due to the micelles (F_{mic}/F_T).

%TPGS	F_{mic}/F_T	τ_1(ns)	τ_2(ns)
0.005	0.179	0.410	2.211
0.010	0.192	0.445	2.196
0.020	0.200	0.474	2.194
0.040	0.250	0.487	2.188
0.080	0.273	0.541	2.243
0.120	0.286	0.566	2.225