Charge-transfer interaction mediated organogels from 18β-glycyrrhetinic acid appended pyrene

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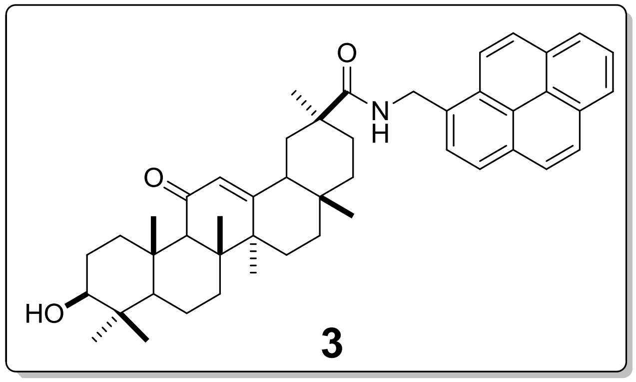
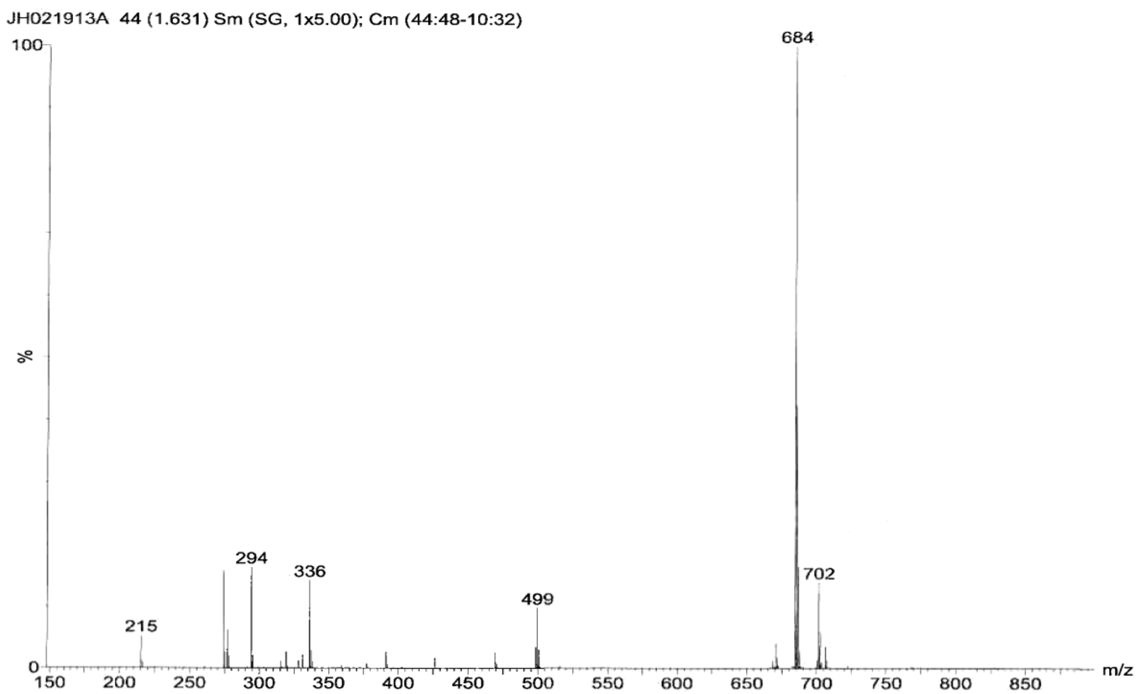
MS, ^{1}H NMR and ^{13}C NMR spectra of 18β-glycyrrhetinic acid appended pyrene 3 and 2,4,7-trinitrofluorenone (4); thermodynamic parameters of CT gel in various solvents

Content

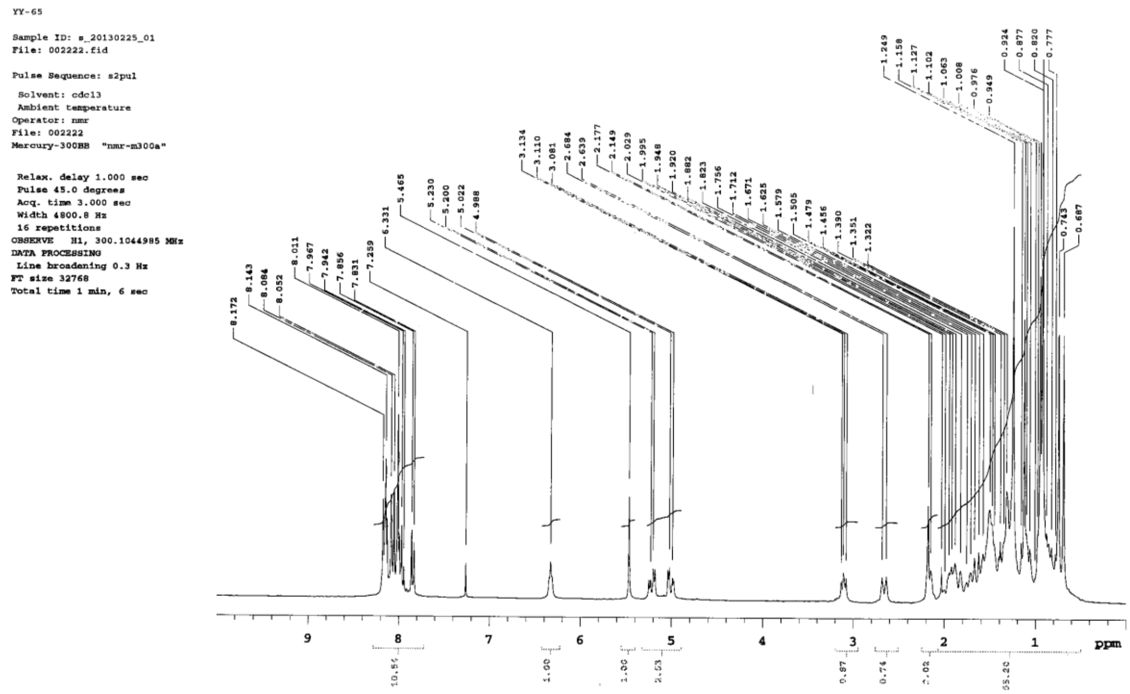
1. MS, ^{1}H NMR and ^{13}C NMR spectra of 18β-glycyrrhetinic acid appended pyrene (3)



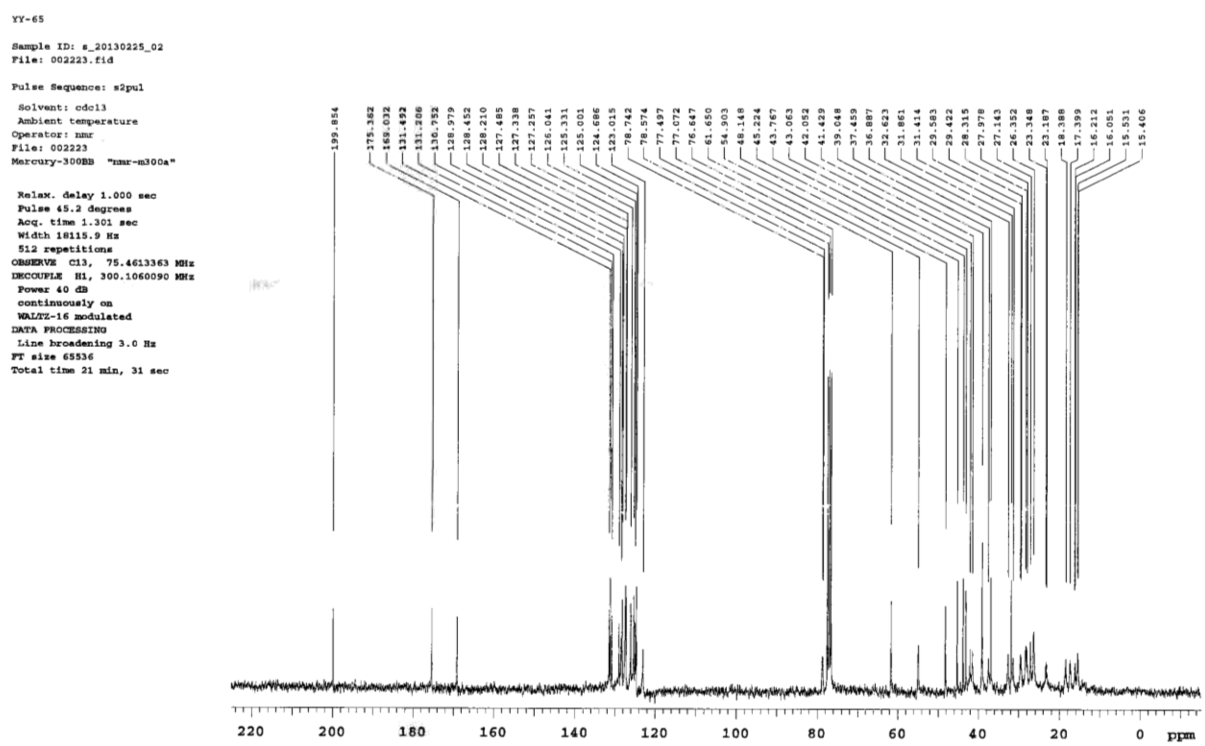
ESI-MS (+) Spectra of 18β-glycyrrhetinic acid appended pyrene **3**



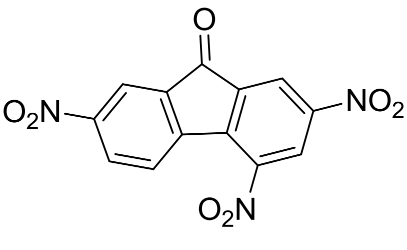
^{1}H NMR Spectra ($CDCl_3$, 300 MHz) of 18β-glycyrrhetinic acid appended pyrene **3**



^{13}C NMR Spectra ($CDCl_3$, 75 MHz) of 18β-glycyrrhetinic acid appended pyrene **3**

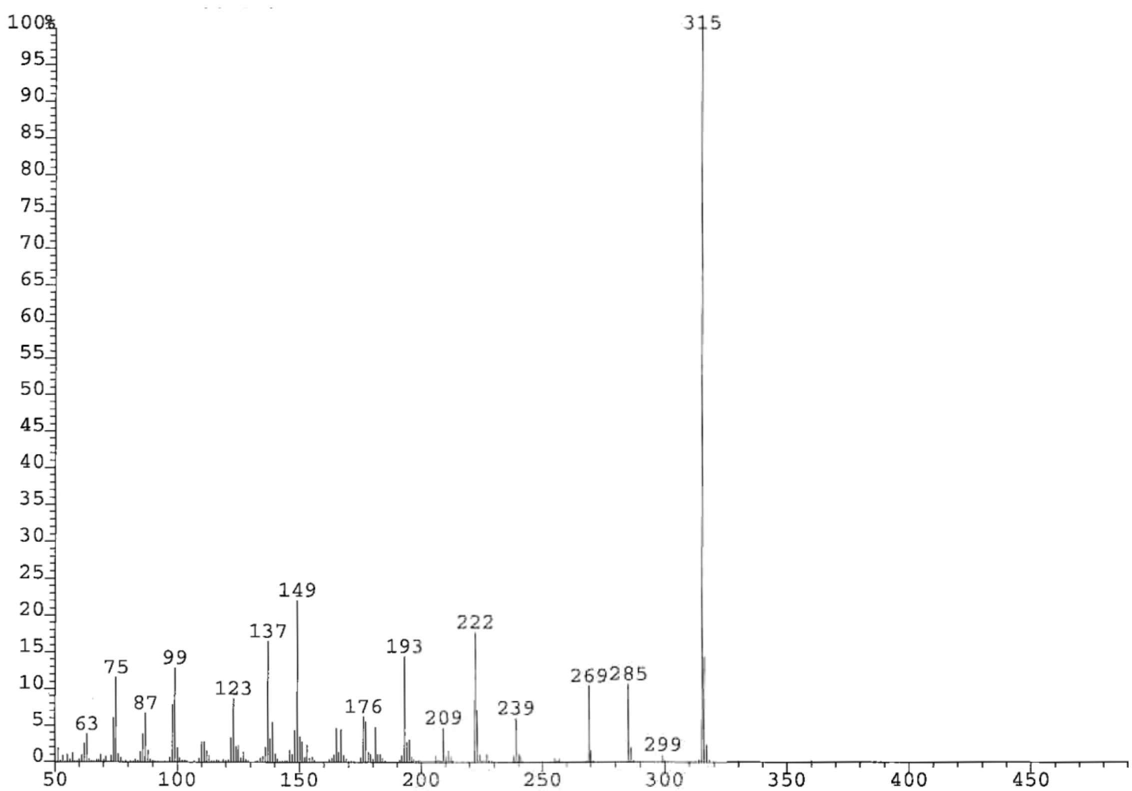


2. MS, ^{1}H NMR and ^{13}C NMR spectra of 2,4,7- trinitrofluorenone (4)

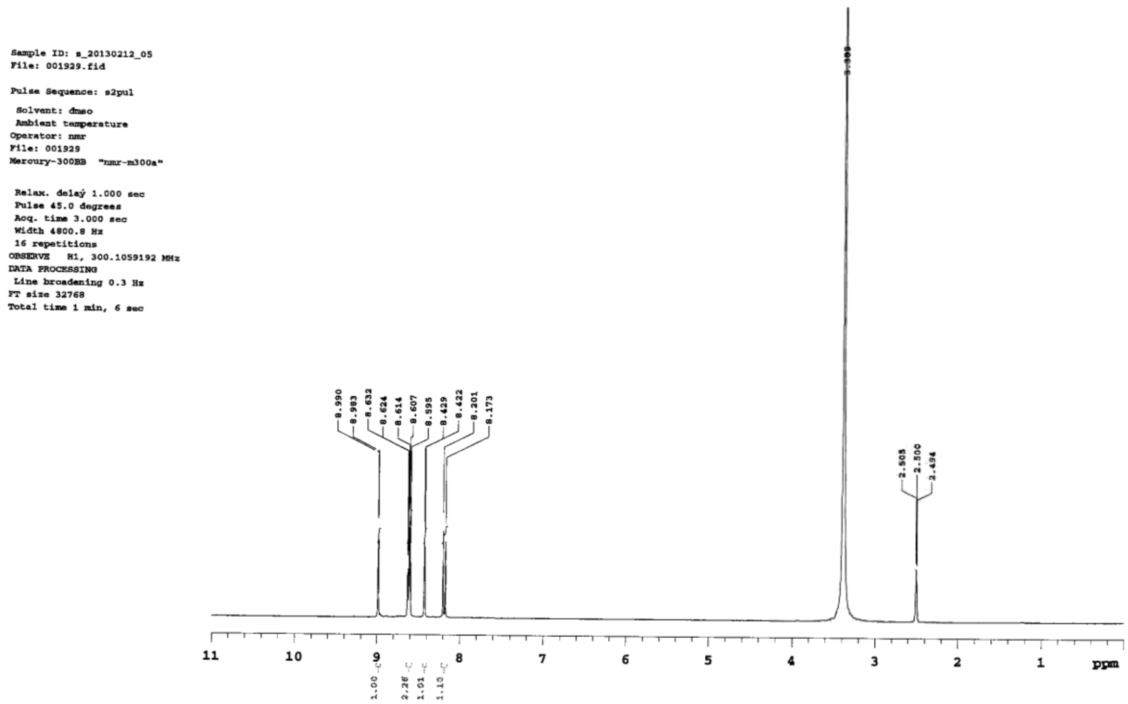


4

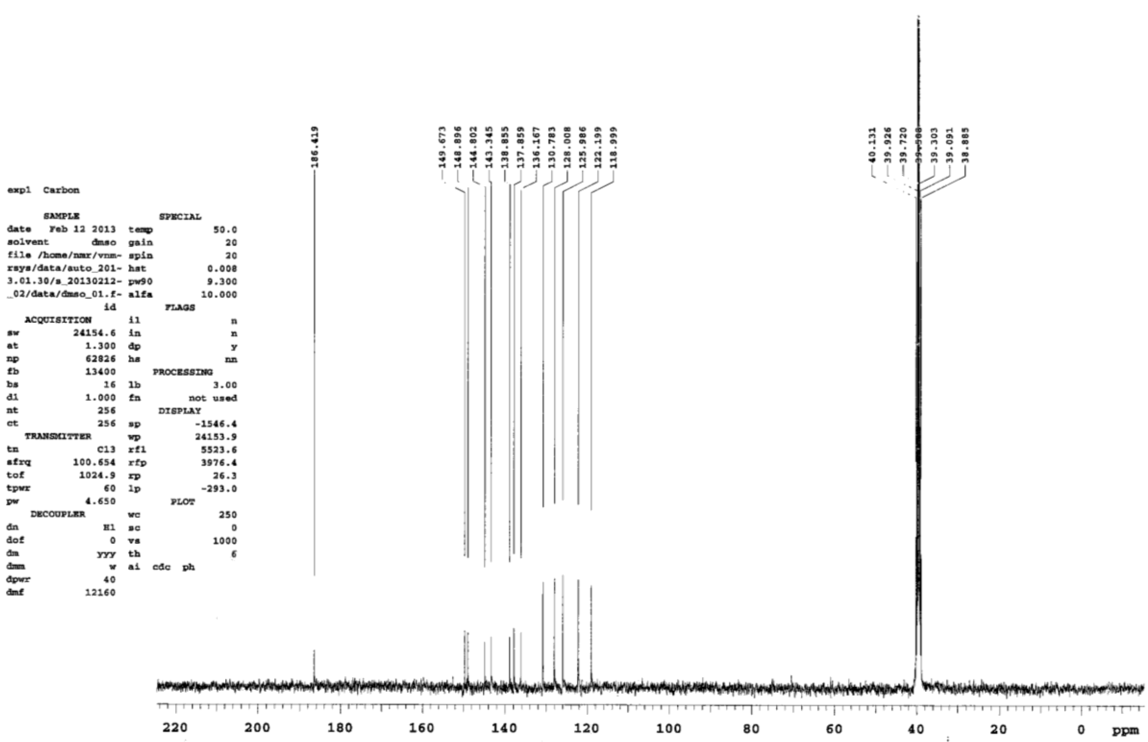
EI-MS (+) Spectra of 2, 4, 7-trinitrofluorenone (**4**)



[1]H NMR Spectra (DMSO, 300 MHz) of 2, 4, 7-trinitrofluorenone (**4**)



[13]C NMR Spectra (DMSO, 75 MHz) of 2, 4, 7-trinitrofluorenone (**4**)



3. Thermodynamic parameters of CT gel in various solvents [1,2]

The thermoreversible melting of a two component gel can be expressed as:

Gel $\rightleftharpoons$ liquid

For one component gel, the equilibrium constant can be expressed as:

K = [Gelator] / [Gel]

Assuming unit activity of the gel and taking the concentration of the solution to be equal to the dissolved concentration of the gelator, the equilibrium constant can be expressed as:

K = [Gelator].

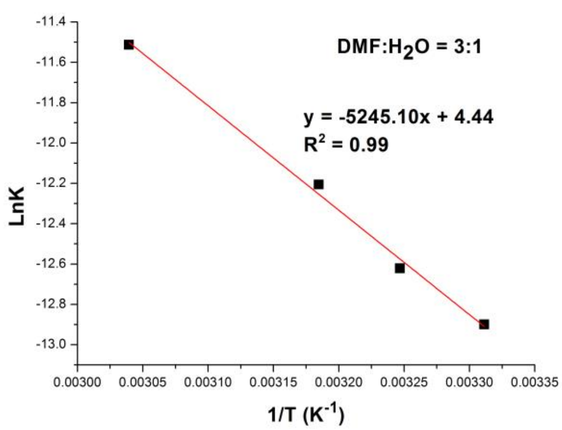
The Gibbs free energy change during gel melting can be expressed as:

$\Delta G^{o} = -\Delta RT\ln K = \Delta H^{o} - T\Delta S^{o}$,

Hence, $\ln K = -\Delta H^{o} / R\ (1/T) + T\Delta S^{o} / R$

The gel melting temperature (T_{gel}) increases with the concentration of the "solutes". A plot of ln$K$ vs 1/T allowed us to calculate the thermodynamic parameters.

DMF/H_2O (3:1, v/v)



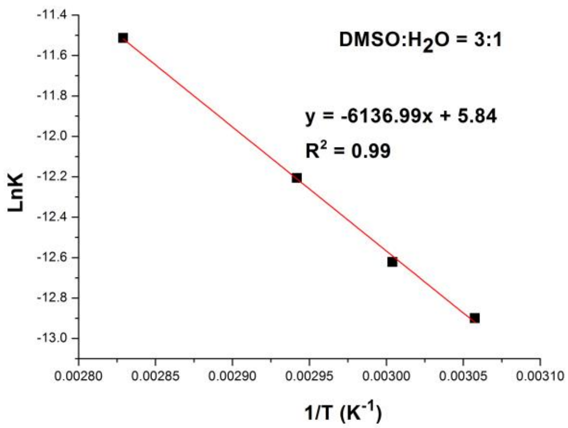
$\ln K = -5245.10 \times (1/T) + 4.44$, $R^2 = 0.99$

$\Delta H^{o}/R = 5245.10$, $\Delta H^{o} = 43.1$ kJ/mol;

$\Delta S^{o}/R = 4.44$, $\Delta S^{o} = 36.9$ J/mol/K

$\Delta G^{o} = \Delta H^{o} - T\Delta S^{o} = 43.1 - 298 \times 0.0369 = 32.1$ kJ/mol

$DMSO/H_2O$ (3:1, v/v)



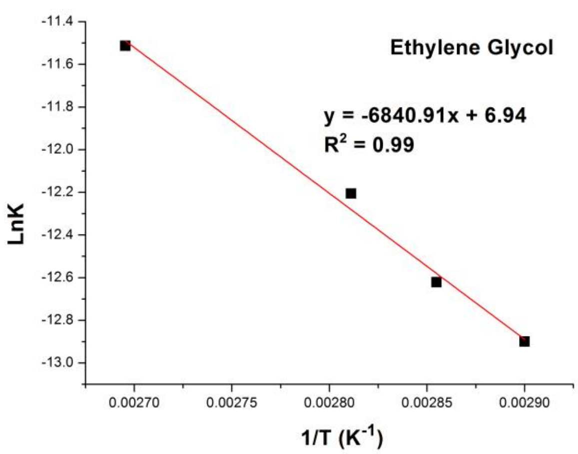
Ln*K* = −6136.99 × (1/*T*) + 5.84, R^2 = 0.99

$\Delta H^o/R$ = 6136.99, ΔH^o = 51.0 kJ/mol;

$\Delta S^o/R$=5.84, ΔS^o = 48.5 J/mol/K

ΔG^o=$\Delta H^o - T\Delta S^o$ = 51.0 – 298 × 0.0485 = 36.5 kJ/mol

Ethylene Glycol



Ln*K* = −6840.91 × (1/*T*) + 6.94, R^2 = 0.99

$\Delta H^o/R$ = 6840.91, ΔH^o = 56.8 kJ/mol;

$\Delta S^o/R$ = 6.94, ΔS^o = 57.6J/mol/K

$\Delta G^o = \Delta H^o - T\Delta S^o$ = 56.8 – 298 × 0.0576 = 39.6 kJ/mol

References

1 D. Rizkov, J. Gun, O. Lev, R. Sicsic and A. Melman, *Langmuir,* **2005,** *21,* 12130.

2 J. Hu, M. Zhang and Y. Ju, *Soft Matter*, **2009**, *5*, 4971.