Physico chemical studies of resveratrol, methyl-jasmonate and cyclodextrins interactions: an approach to resveratrol bioproduction optimization

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Supplementary Information

Figure S1: ESI (+) MS Spectra corresponding to RSV with maltoheptaose (a) and RSV with β-CD (b) in the same experimental conditions.

Figure S2: dedicated Job plots of (a) β-CD (up)/resveratrol (down) and (b) DIMEB (up)/resveratrol (down)

Figure S3: Plot of the relative intensity of each complex between CD and MeJA versus cone voltage.

Figure S4: Fit between experimental RSV solubility data (β-CD ■,and RAMEB ×) and theoretical values predicted by formation constants obtained by ITC (red line and blue line, respectively).

Figure S5: Fit between experimental MEJA solubility data (β-CD ■,and RAMEB ×) and theoretical values predicted by formation constants obtained by ITC (red line and blue line, respectively).

Table SI : Association constant values, K (M^{-1}) calculated from solubility data

Figure S6: Enlarged contour plot of a T-ROESY experiment (spin lock: 300 ms, 22 dB) performed at 600 MHz on a β-CD/RSV/MeJA mixture (4.6 mM of β-CD with RSV and MeJA at saturation in D_2O). Rectangles represent the absence of a correlation between RSV and MeJA and ovals the presence of correlations between β-CD/ RSV on one hand and β-CD/MeJA on the other hand

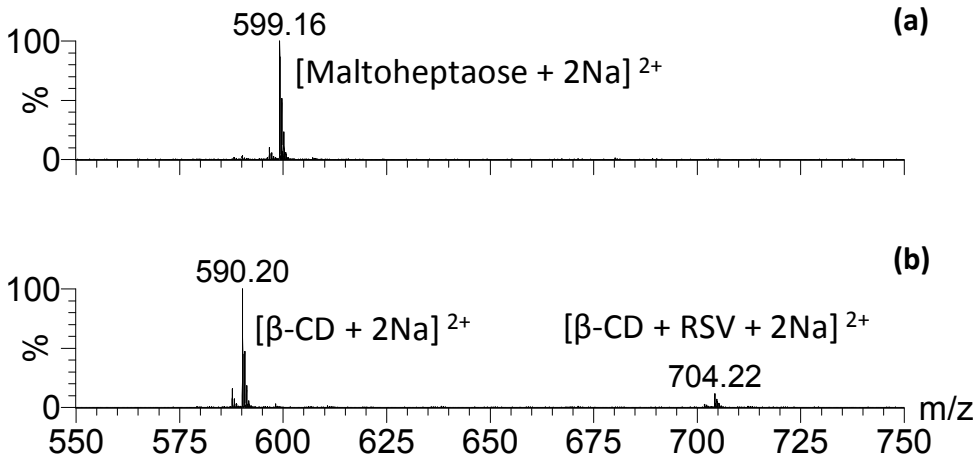
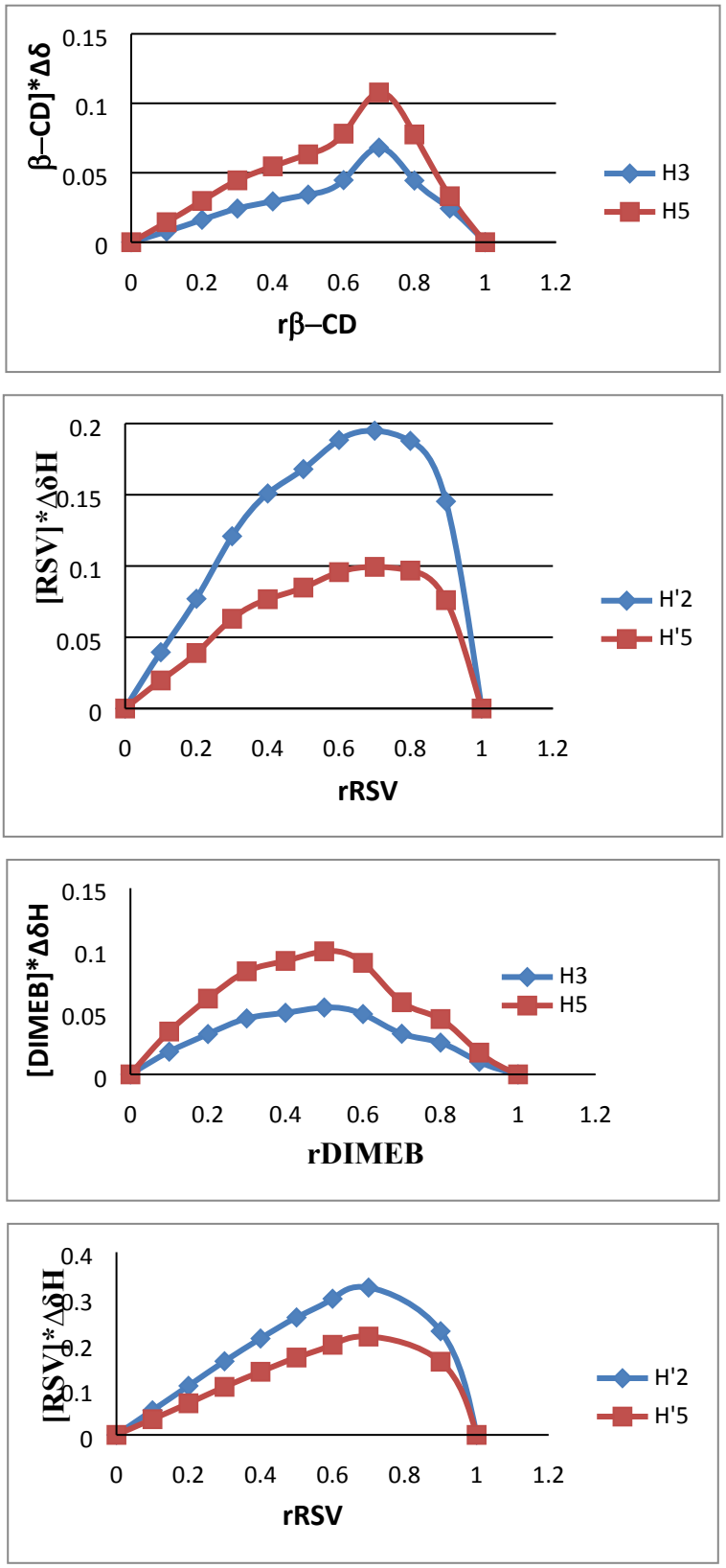


Figure S1: ESI (+) MS Spectra corresponding to RSV with maltoheptaose (a) and RSV with β-CD (b) in the same experimental conditions.

a



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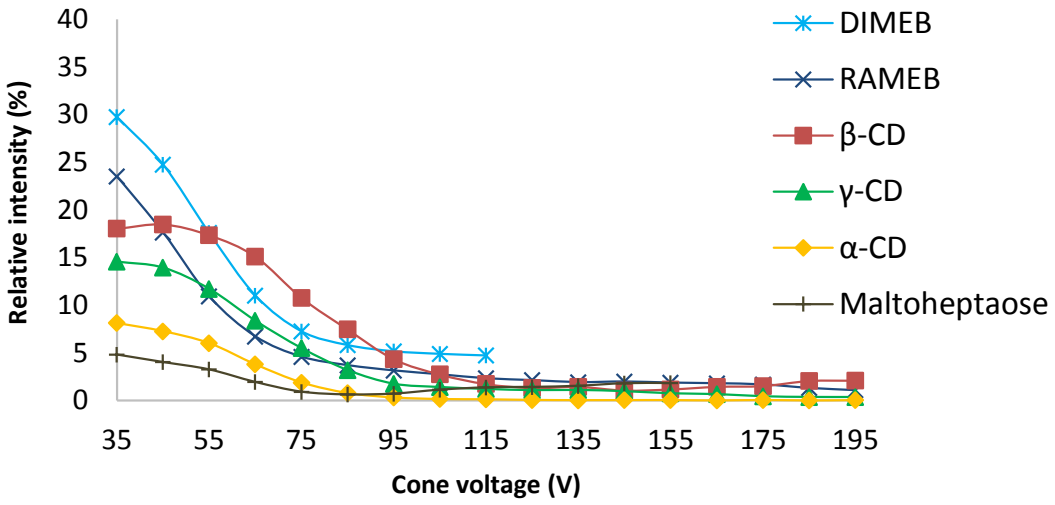


Figure S3: Plot of the relative intensity of each complex between CD and MeJA versus cone voltage.

The solubility of a guest G in the presence of CD (leading to a CD-G complex with a formation constant K), can be calculated as follows:

$[G]_T = [G] + [CD\text{-}G]$ (1)

$[CD]_T = [CD] + [CD\text{-}G]$ (2)

$K = [CD\text{-}G] / ([CD]*[G])$ (3)

Combining equation (3) with equation (2):

$[CD\text{-}G] = K * ([CD]_T - [CD\text{-}G]) * [G]$ (4)

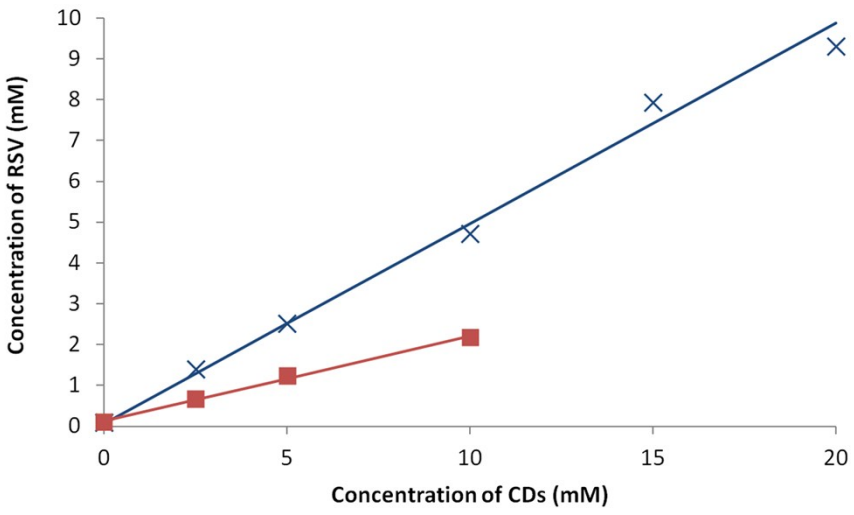
In phase solubility experiments, [G] is equal to the intrinsic G solubility S_0, thus:

$[CD\text{-}G] = (K*[CD]_T*S_0) / (1+K*S_0)$ (5)

As a result, the total guest concentration (ie. its solubility in the presence of CD) is equal to:

$[G]_T = [G] + [CD\text{-}G] = S_0 + (K*[CD]_T*S_0) / (1+K*S_0)$ (6)

Accordingly, formation constants obtained by ITC were used to simulate the RSV and MEJA solubility in the presence of β-CD and RAMEB. Least square fitting between experimental and theoretical data were then realized (Figure S4 and S5, for RSV and MEJA, respectively), with a floating value for the intrinsic guest solubility.



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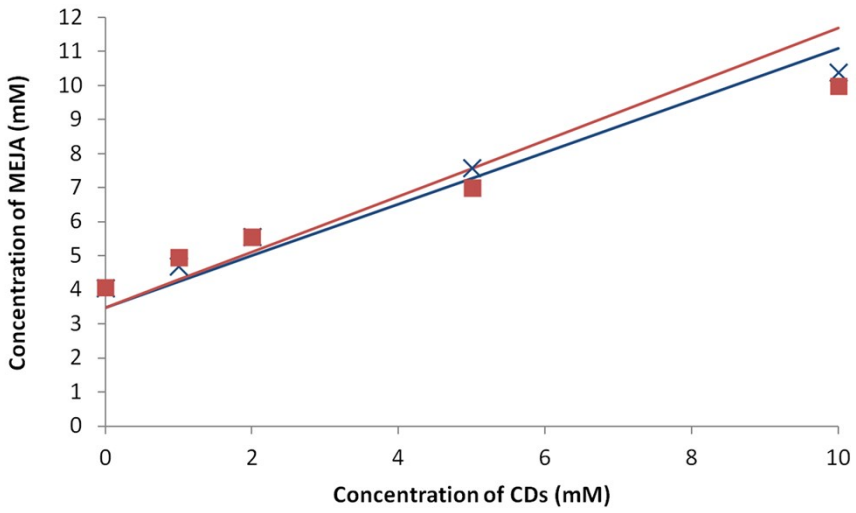

Figure S5: Fit between experimental MeJA solubility data (β-CD ■ and RAMEB ×) and theoretical values predicted by formation constants obtained by ITC (red line and blue line, respectively).

	RSV	MeJA
β-CD	3 053	481
RAMEB	10 700	570

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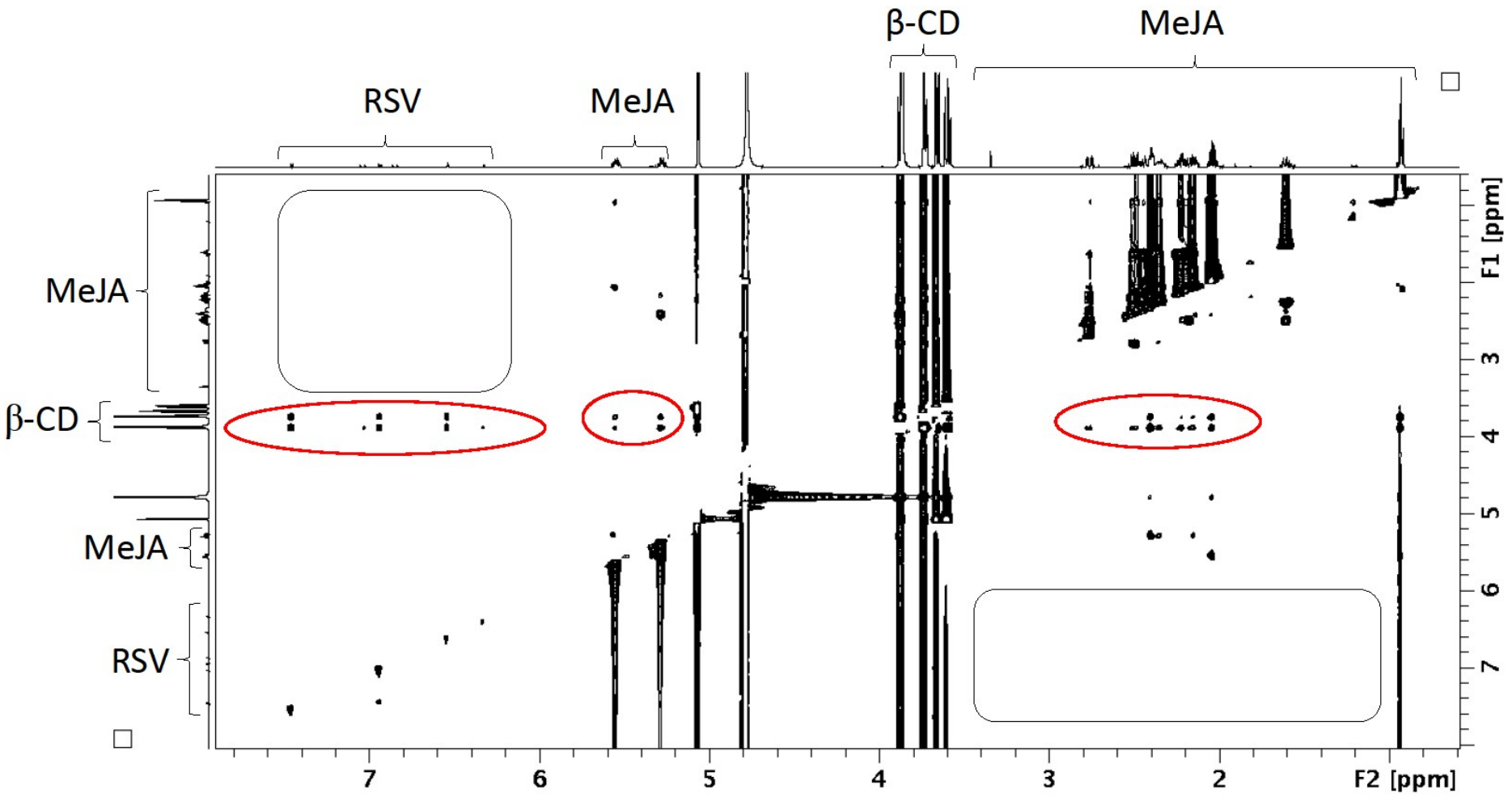

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