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 x]) 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 x]) and theoretical values predicted by formation constants obtained by ITC (red line and blue line, respectively).

Table SI: Association constant values, K (M\textsuperscript{-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\textsubscript{2}O). 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.
Figure S2: dedicated Job plots of (a) $\beta$-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.
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:

\[
[G]_T = [G] + [\text{CD-G}] \tag{1}
\]

\[
[\text{CD}]_T = [\text{CD}] + [\text{CD-G}] \tag{2}
\]

\[
K = \frac{[\text{CD-G}]}{([\text{CD}] \times [G])} \tag{3}
\]

Combining equation (3) with equation (2):

\[
[\text{CD-G}] = K \times ([\text{CD}]_T - [\text{CD-G}]) \times [G] \tag{4}
\]

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

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

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

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

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.

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 x) and theoretical values predicted by formation constants obtained by ITC (red line and blue line, respectively).
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<thead>
<tr>
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<th>RSV</th>
<th>MeJA</th>
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<tr>
<td>β-CD</td>
<td>3053</td>
<td>481</td>
</tr>
<tr>
<td>RAMEB</td>
<td>10700</td>
<td>570</td>
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</table>

Table SI: Association constant values, $K \text{(M}^{-1}\text{)}$ 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 D₂O). 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.