

Supplementary material

Antimicrobial activity of *Annona emarginata* (Schltdl.) H. Rainer and the most active isolated compound, acting against clinically important bacteria. SAR study of structurally related compounds.

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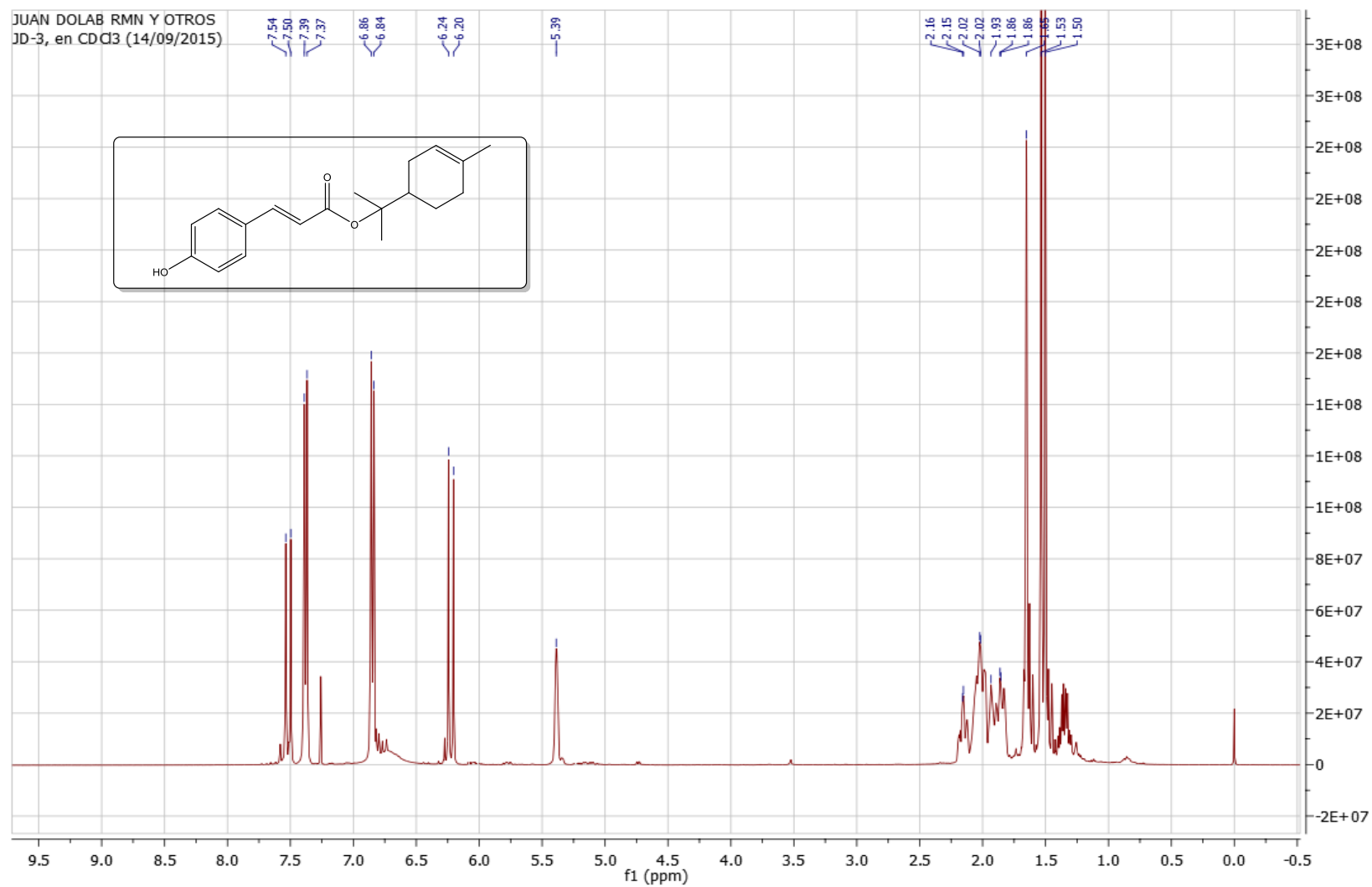
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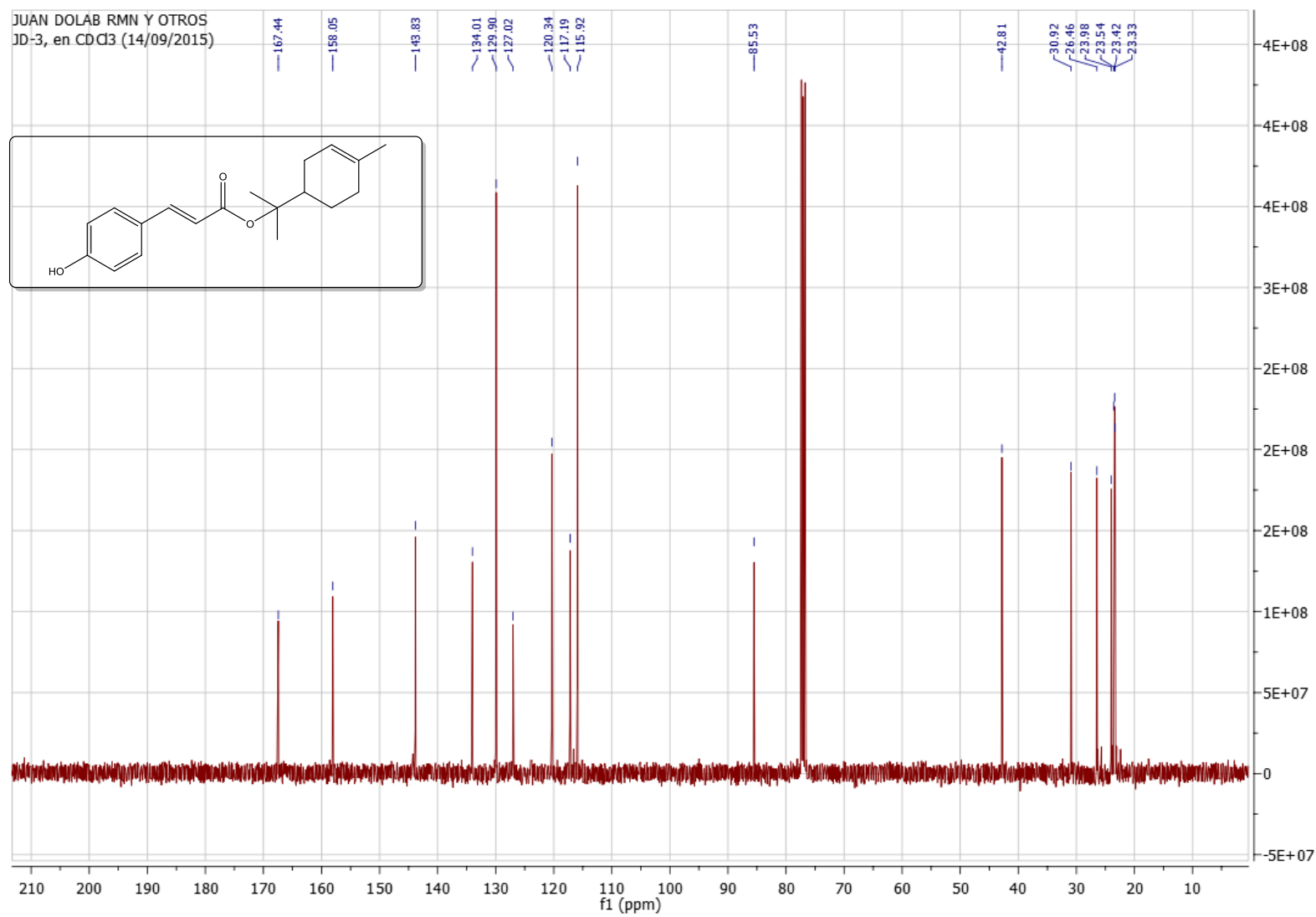
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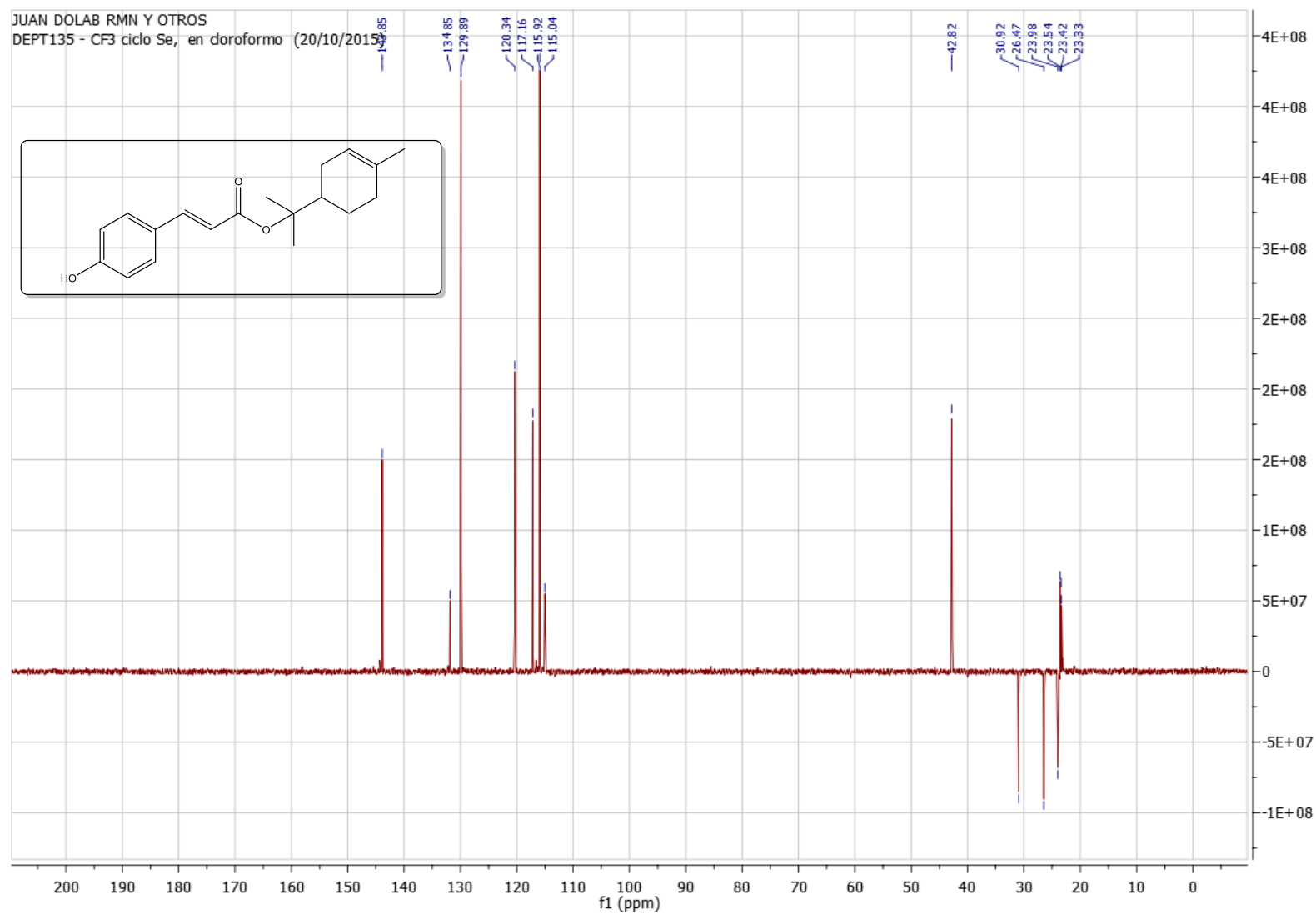
^1H NMR spectrum of (*R*)-2-(4-methylcyclohex-3-en-1-yl)propan-2-yl (*E*)-3-(4-hydroxyphenyl)acrylate (**1**)



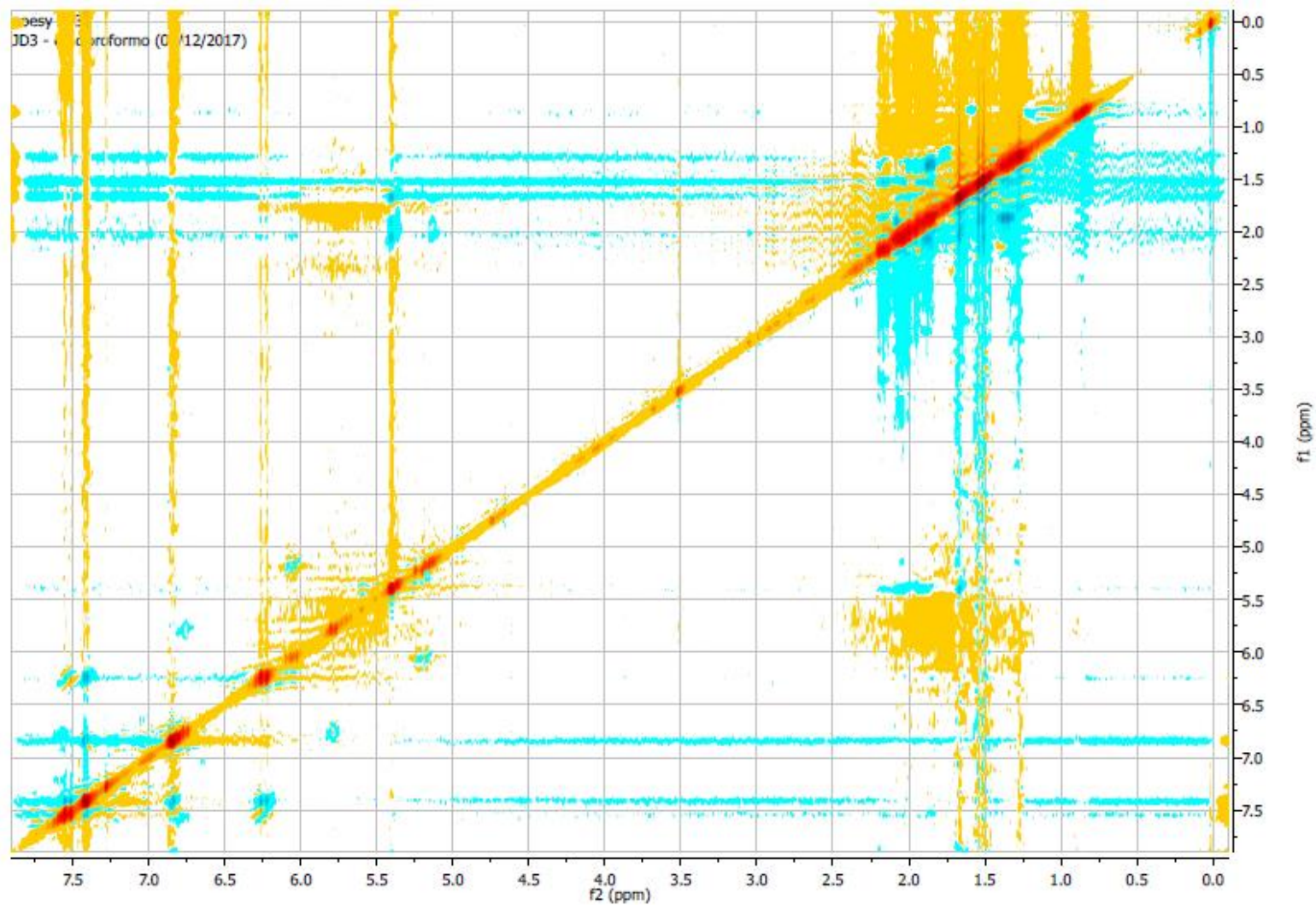
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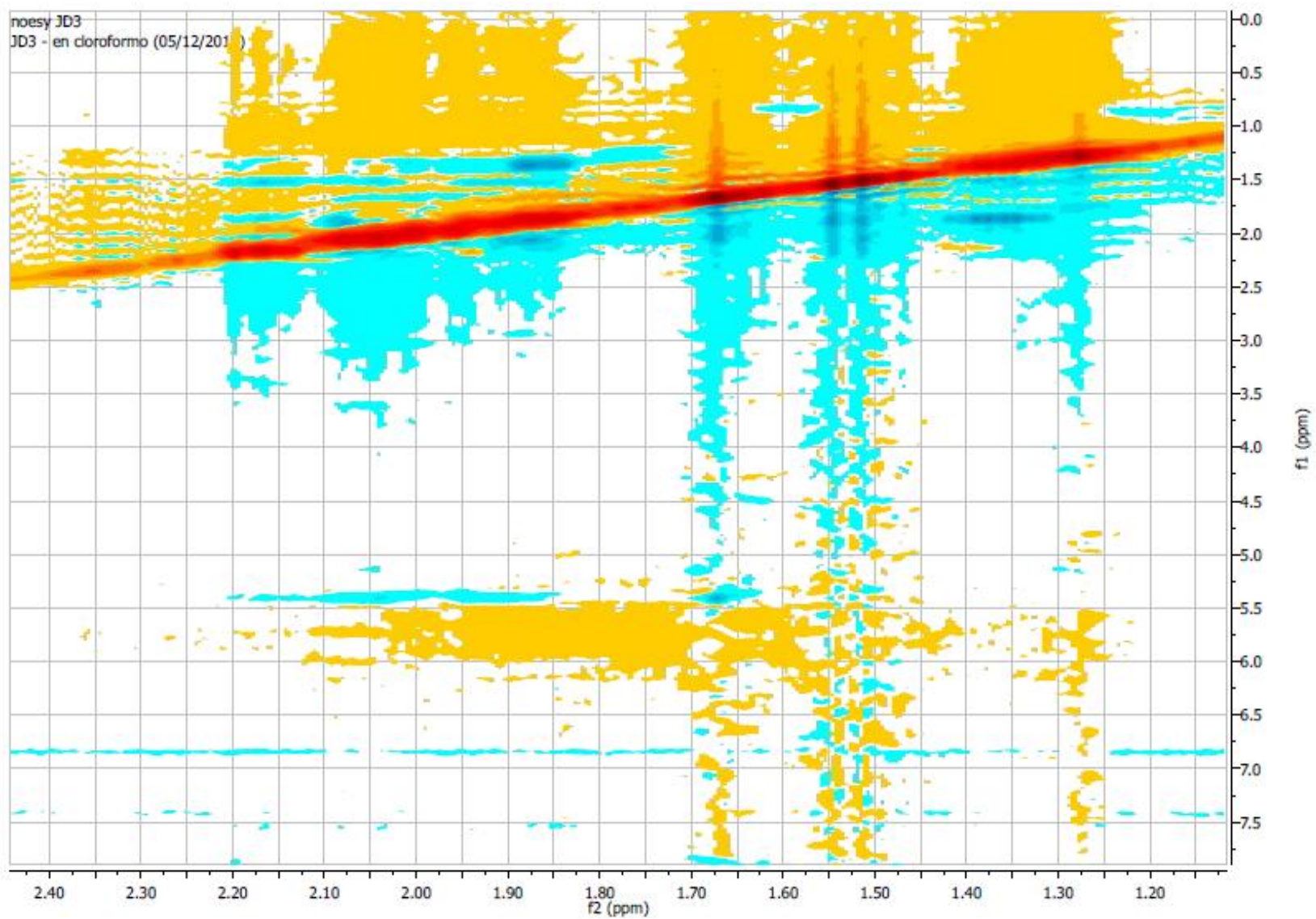
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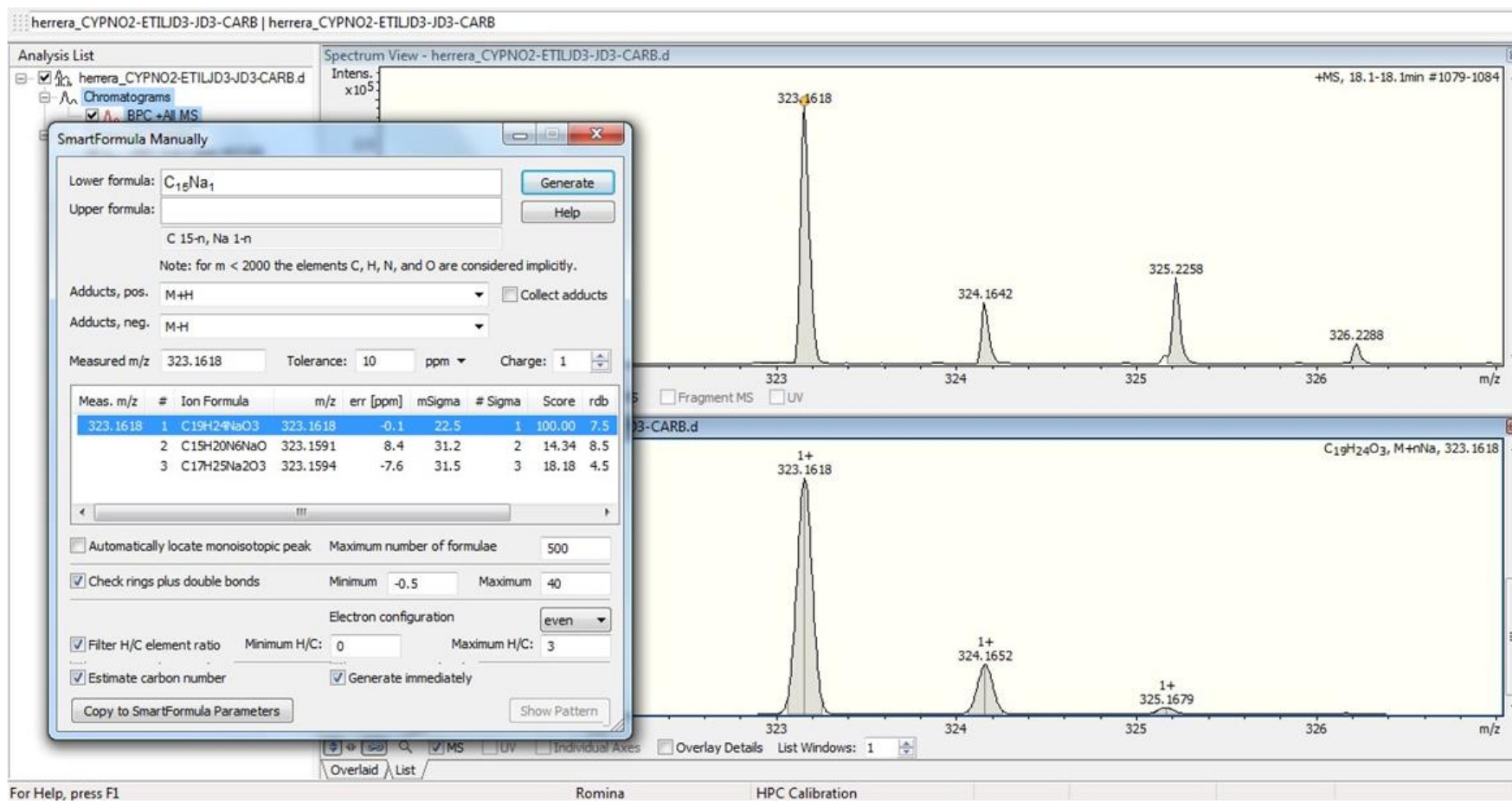
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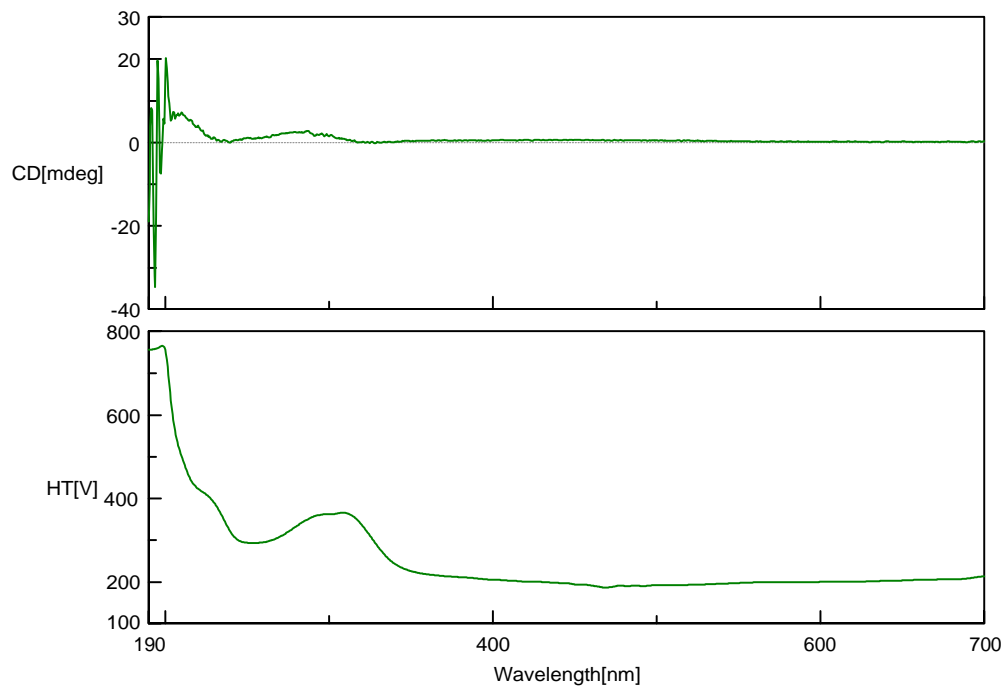
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HRMS spectrum of (R)-2-(4-methylcyclohex-3-en-1-yl)propan-2-yl(E)-3-(4-hydroxyphenyl)acrylate (1)

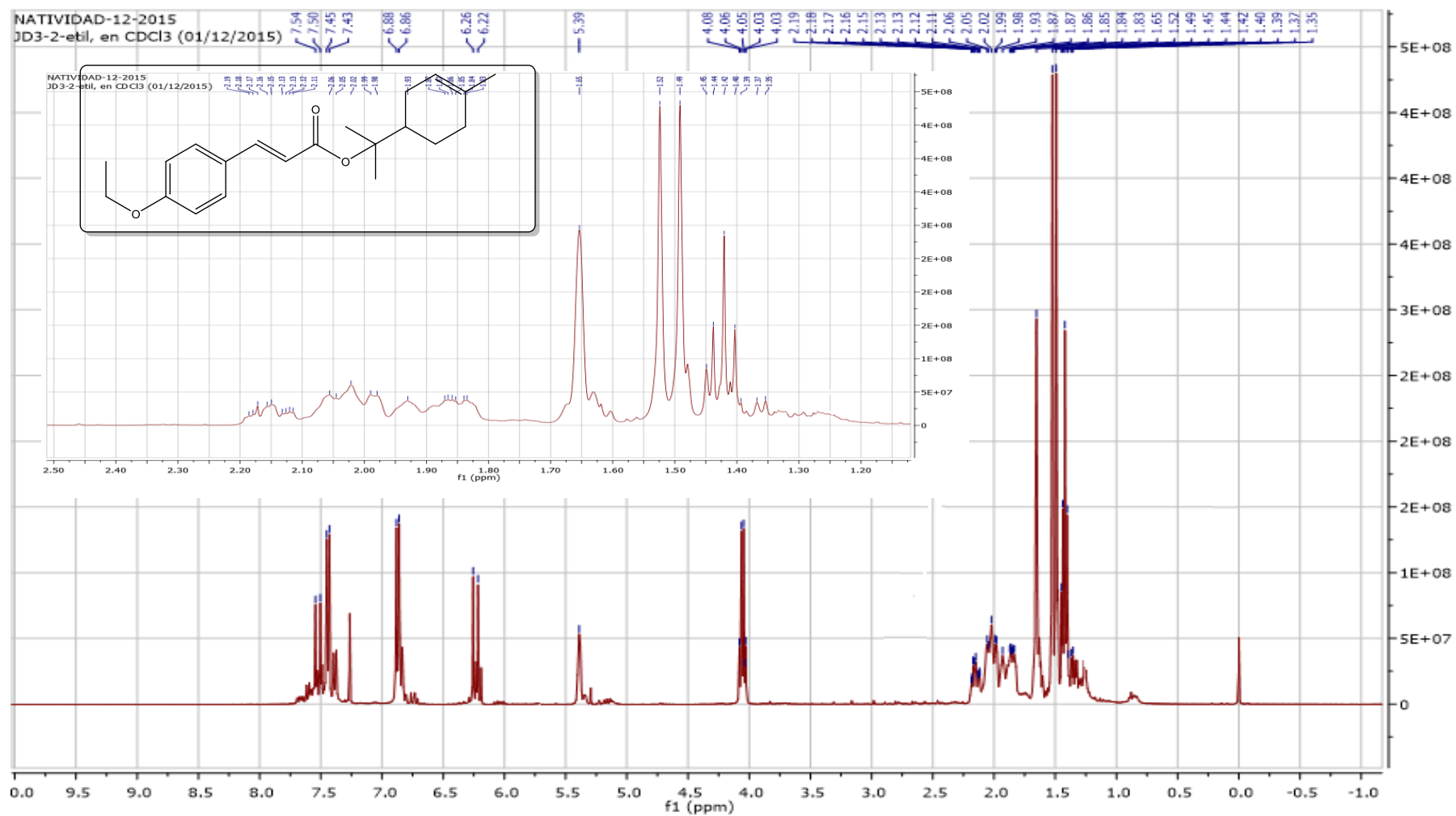


Circular Dichroism spectra of (R)-2-(4-methylcyclohex-3-en-1-yl)propan-2-yl(E)-3-(4-hydroxyphenyl)acrylate (1)

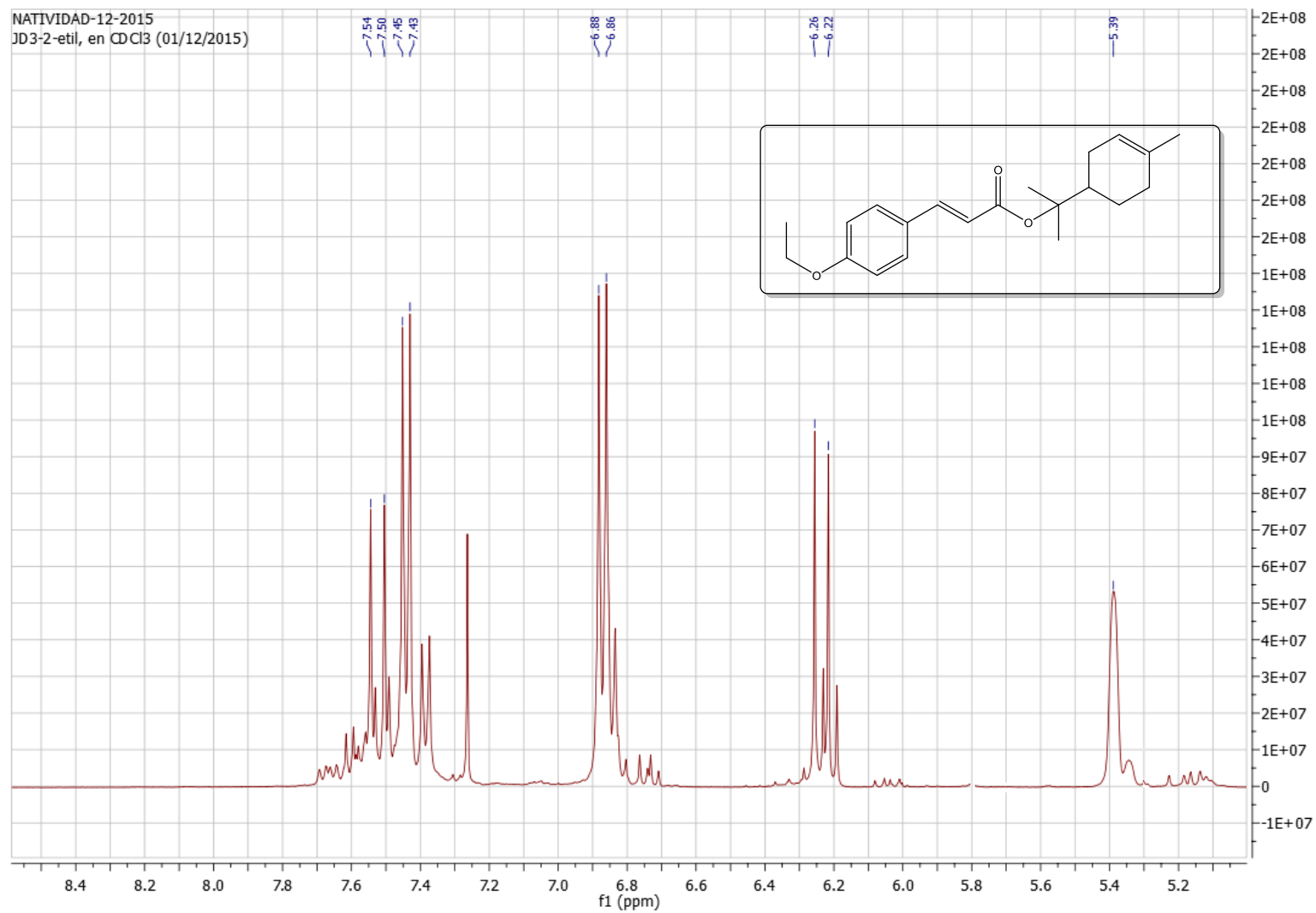


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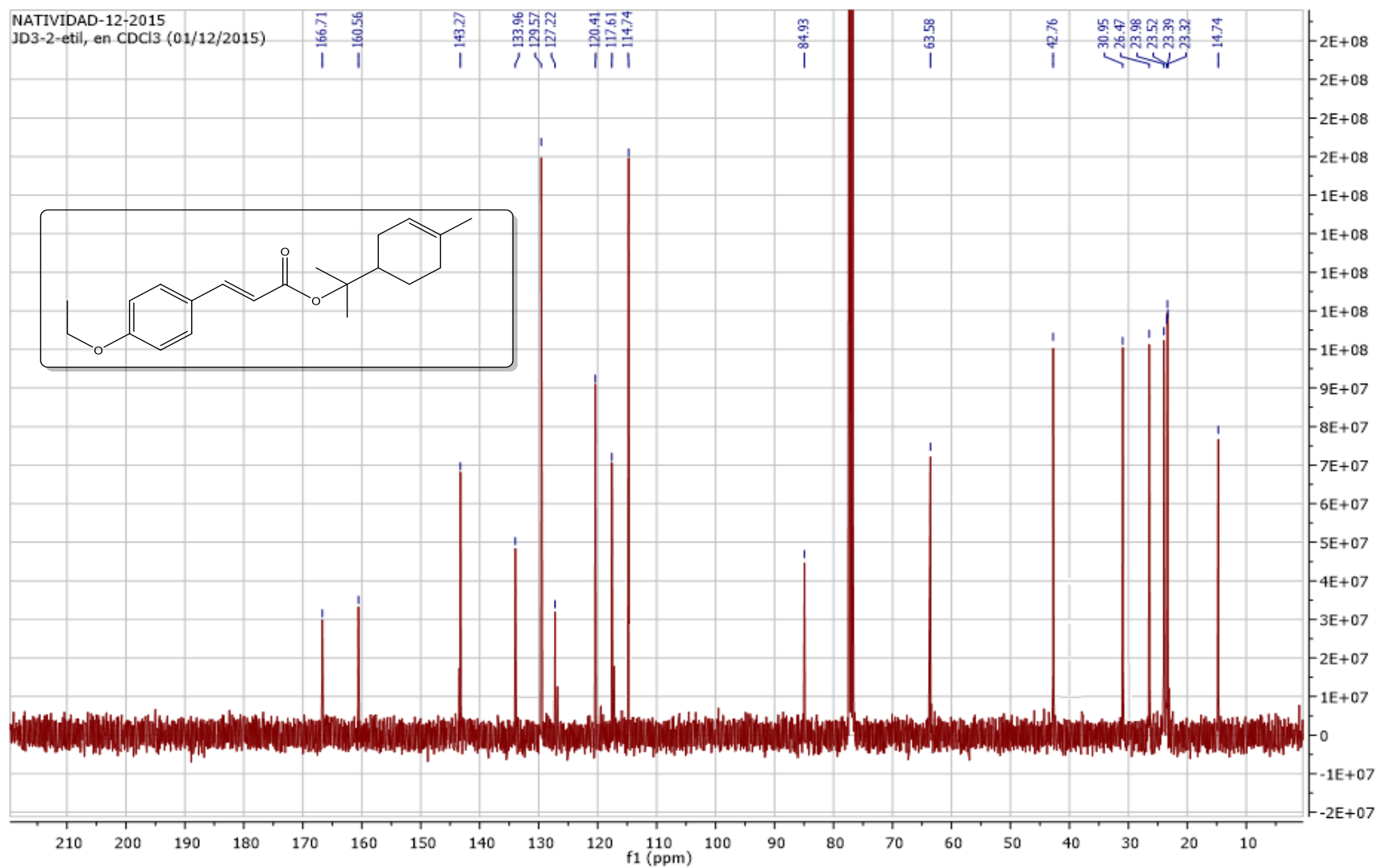
¹H NMR spectrum of (R)-2-(4-methylcyclohex-3-en-1-yl)propan-2-yl (E)-3-(4-ethoxyphenyl) acrylate (2)



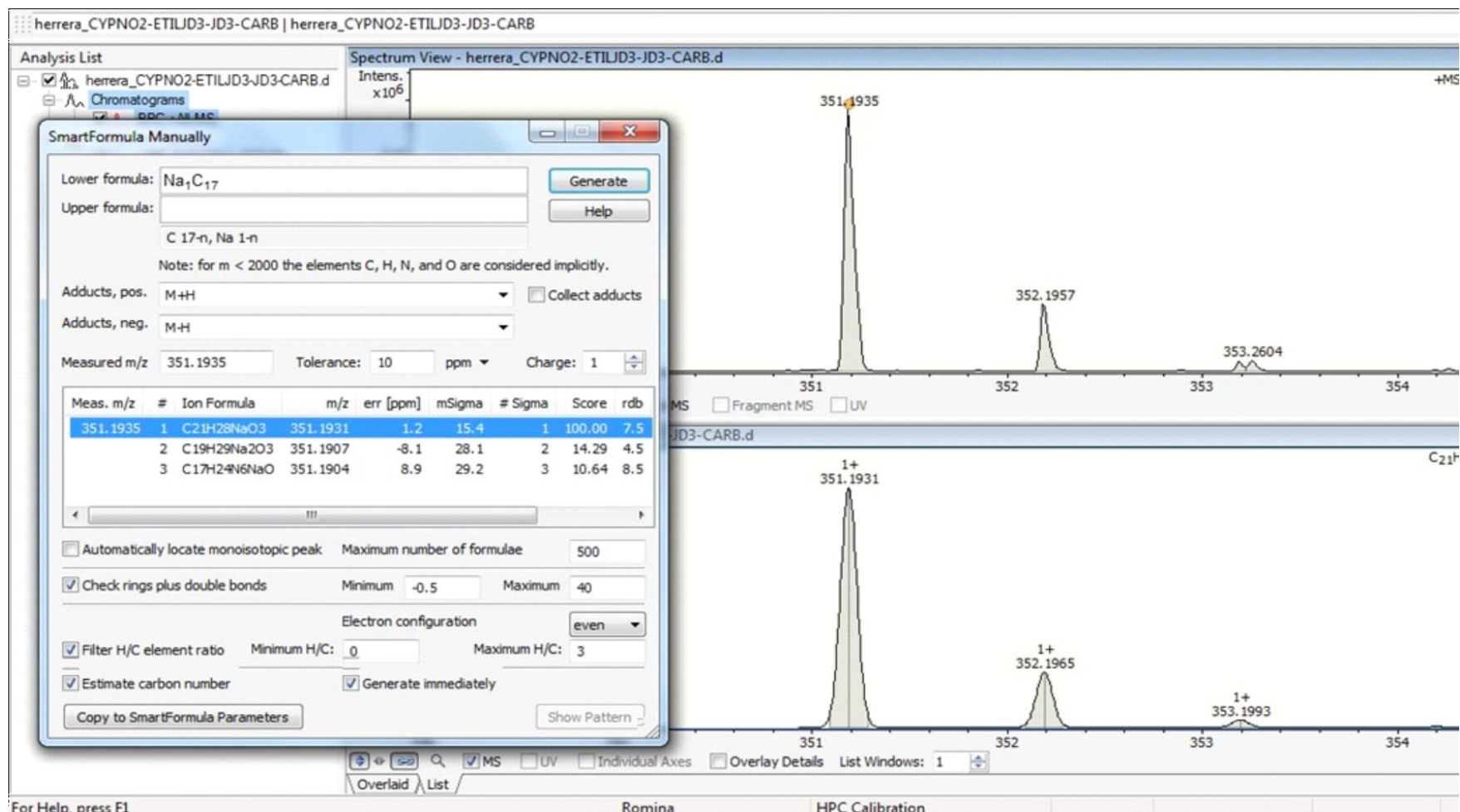
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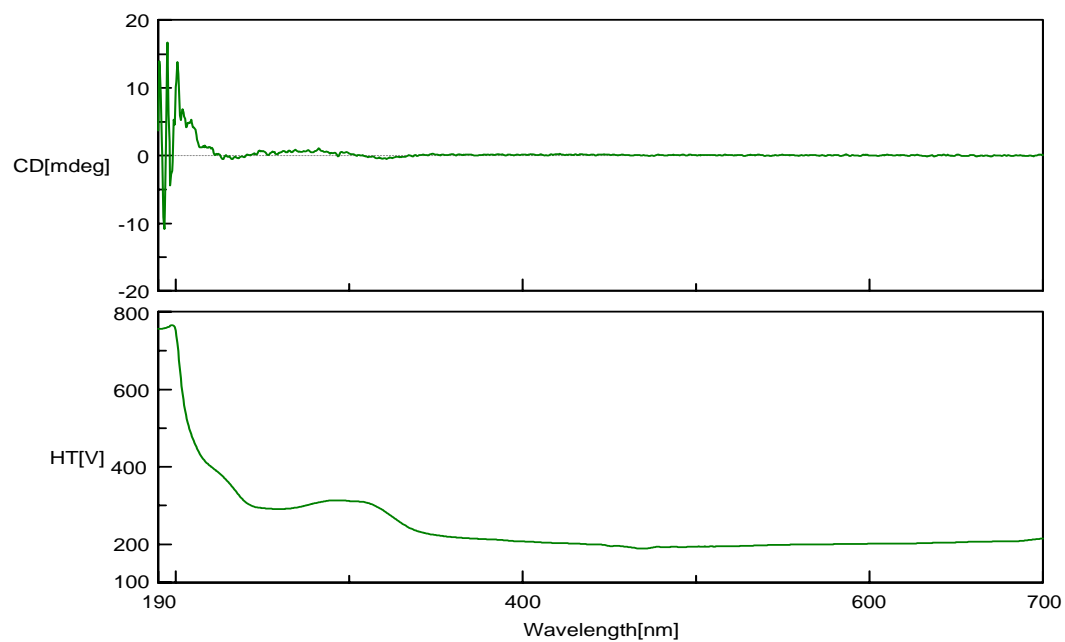
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HRMS spectrum of (R)-2-(4-methylcyclohex-3-en-1-yl)propan-2-yl (E)-3-(4-ethoxyphenyl) acrylate (2)



Circular Dichroism spectra of (R)-2-(4-methylcyclohex-3-en-1-yl)propan-2-yl (E)-3-(4-ethoxyphenyl) acrylate (2)



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| Sample name | cata fer |
| Operator | DC |
| Comment | |

Figure 1S. Potential Energy Curve (PEC) obtained for torsional angle ϕ_1 of compound 1. PEC was calculated at B3LYP/6-31G (d) level of theory.

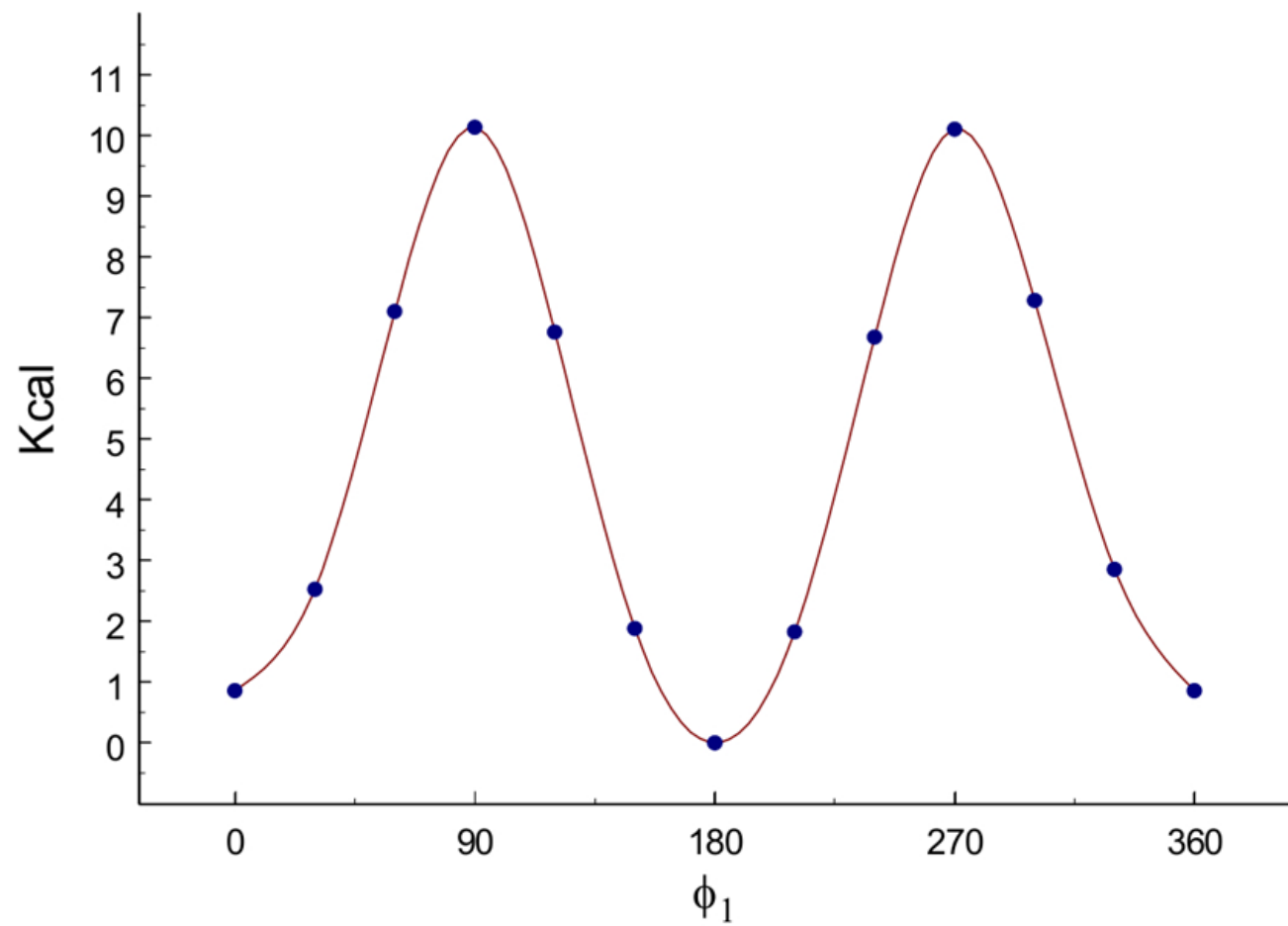


Figure 2S. Contour graphic of Potential Energy Surface (PES) obtained for compound 1 from RHF/3-21G calculations. Full cycle of rotation (from 0° to 360°) is shown for variables ϕ_2 vs ϕ_3 . The iso-energy curves included in an energy window of 4 Kcal/mol are denoted in red.

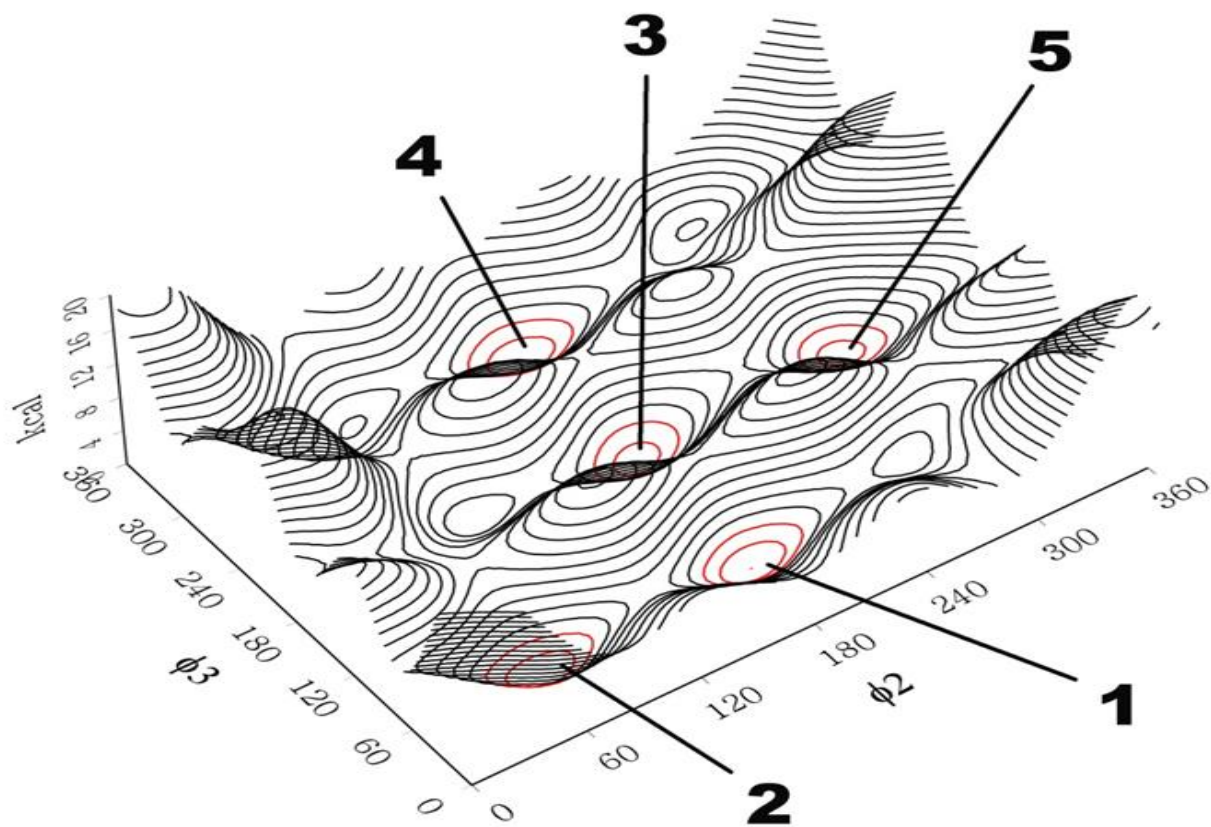


Table 1S. Different conformers obtained for compound 1. Torsional angles corresponds to those shown in Figure 1.

| Conformer | Φ_1 | Φ_2 | Φ_3 | $\Delta Kcal/mol$ |
|------------------|----------------------------|----------------------------|----------------------------|-------------------------------------|
| 1 | 179,57 | -179,9 | 63,72 | 0 |
| 2 | 179,6 | 65,31 | 57,42 | 0,16140812 |
| 3 | -179,9 | 179,97 | 179,67 | 0,45619349 |
| 4 | 178,95 | 179,34 | -60,173 | 0,02813127 |
| 5 | -179,86 | -63,13 | -170,68 | 0,37493095 |