# COMPUTATIONAL STUDY OF THE INTERACTIONS OF COCAINE AND BENZOYLECGONINE WITH METHACRYLIC ACID IN MOLECULARLY IMPRINTED POLYMERS (MIPS).

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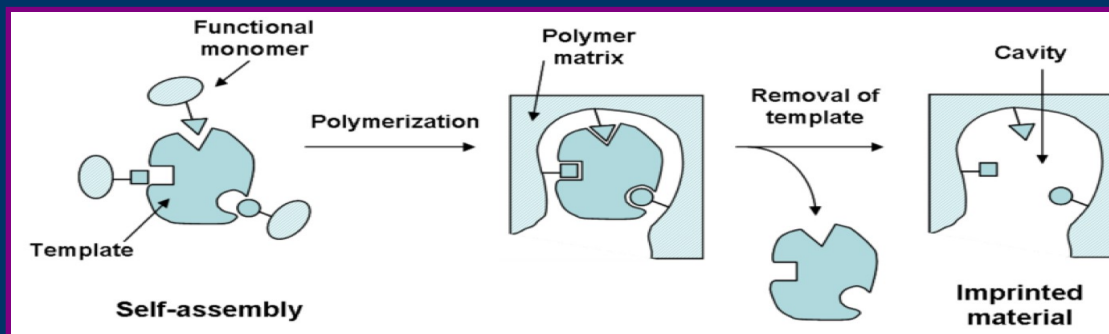
Molecularly imprinted polymers (MIPs) are a class of highly cross-linked polymer that can bind certain target compound with high specificity.

The knowledge of the interactions between the target (in this case, cocaine molecule) and the monomer seems to be very important in the design of this MIPs.

A DFT study was carried out in order to indicate if the methacrylic acid seems to be a good monomer in the recognize of benzoylecgonine and cocaine. The ratio template polymer and the effect of the environment were also analyzed.
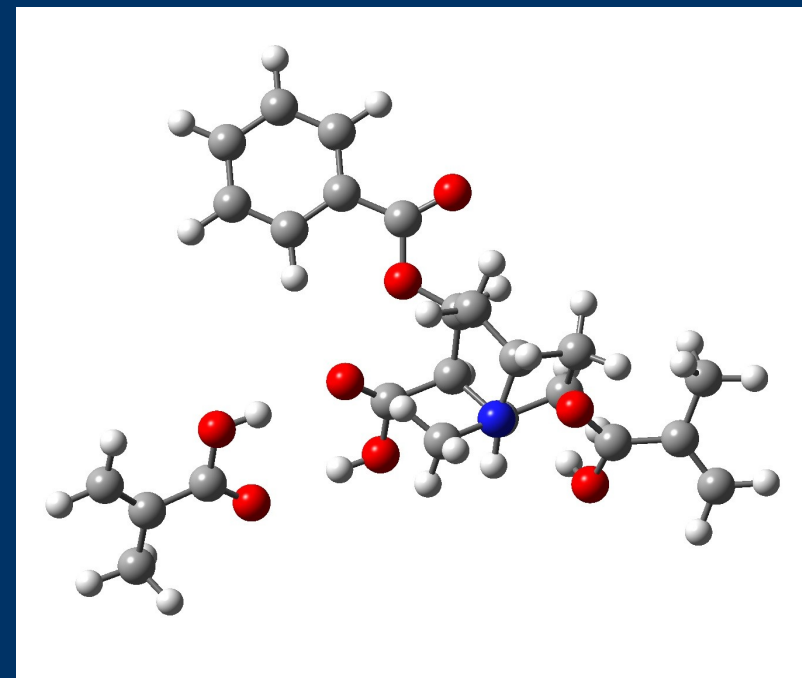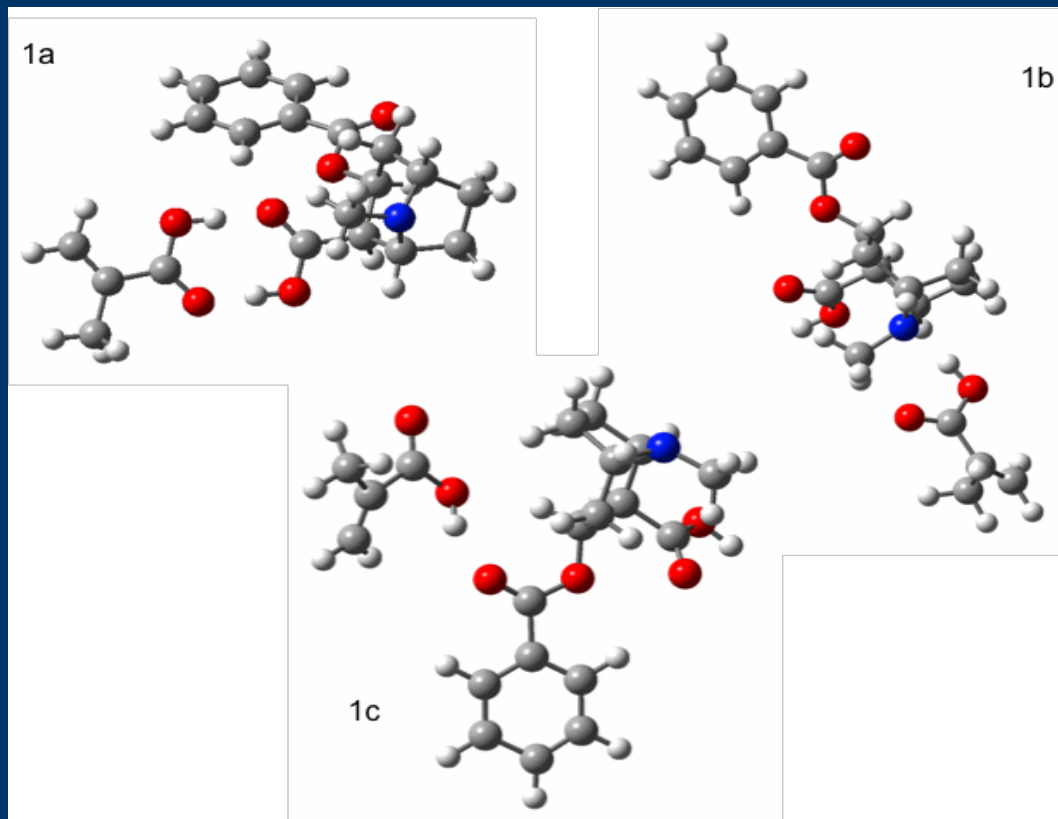
The energy for this complex is
-27,18 kcal/mol.

Structure	ΔE (kcal(mol)
1a	-16,66
1b	-10,56
1c	-6,67

Solvation effects have been treated by Conductorlike Screening Model (COSMO).