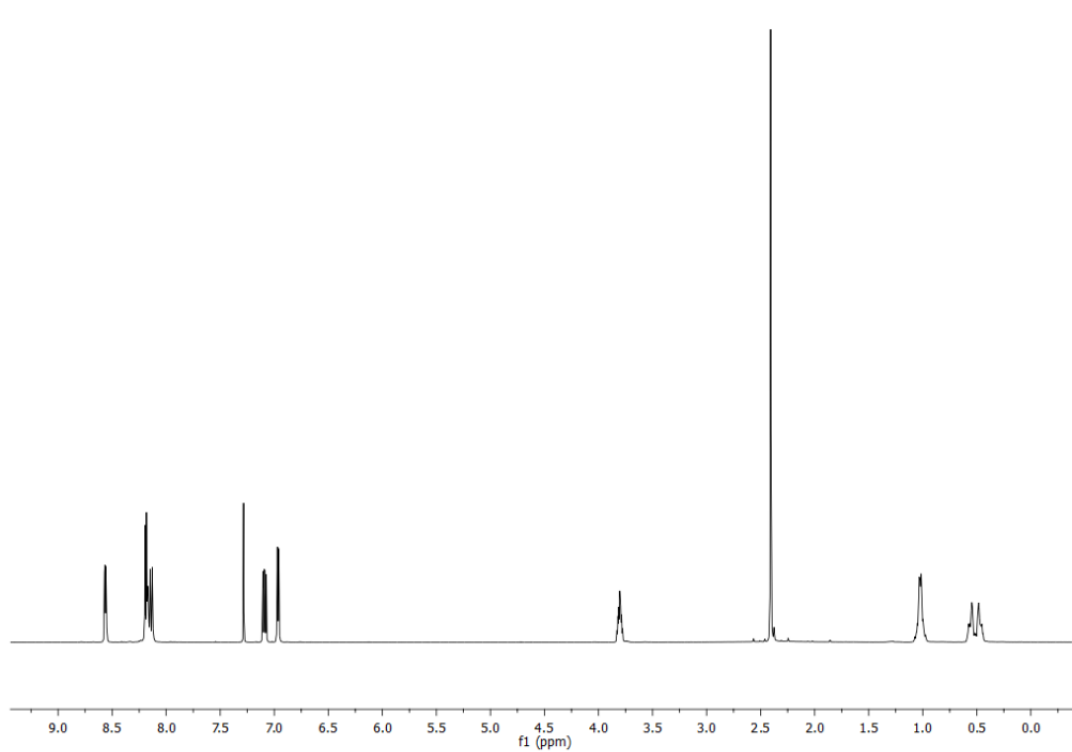


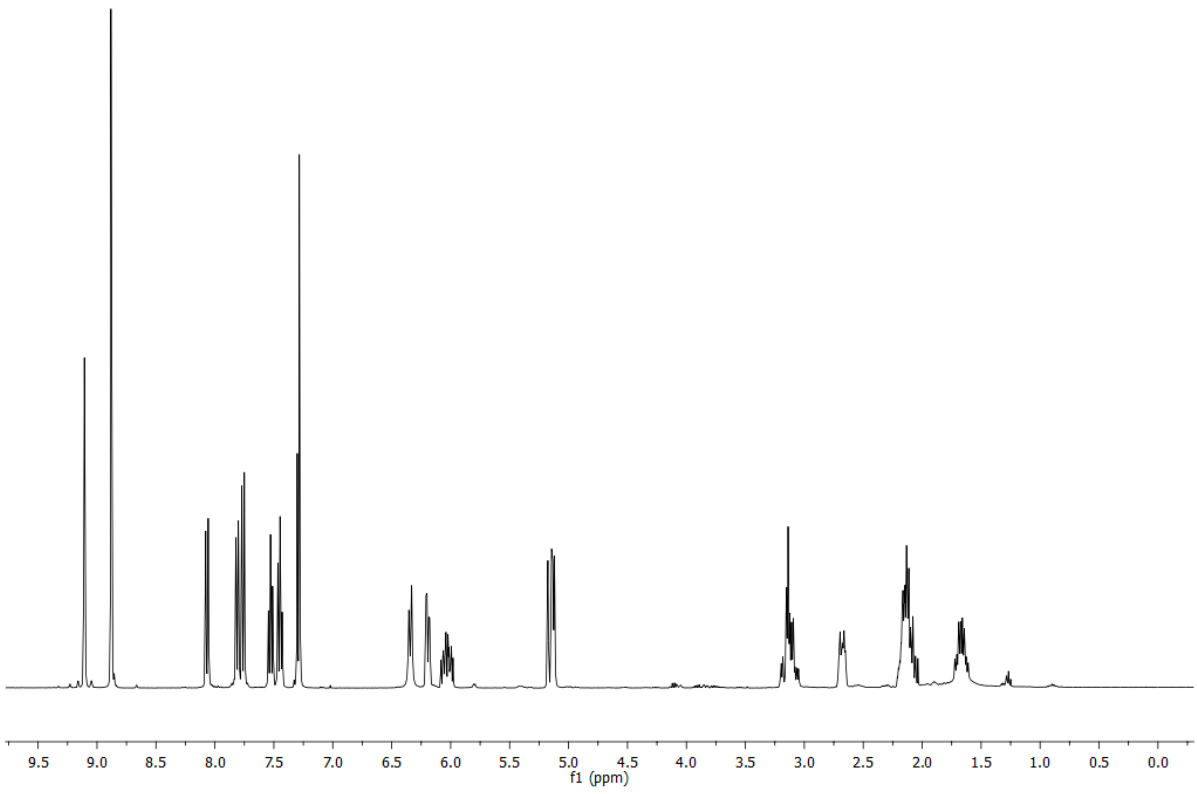
## Supporting information

### 1.NMR spectra

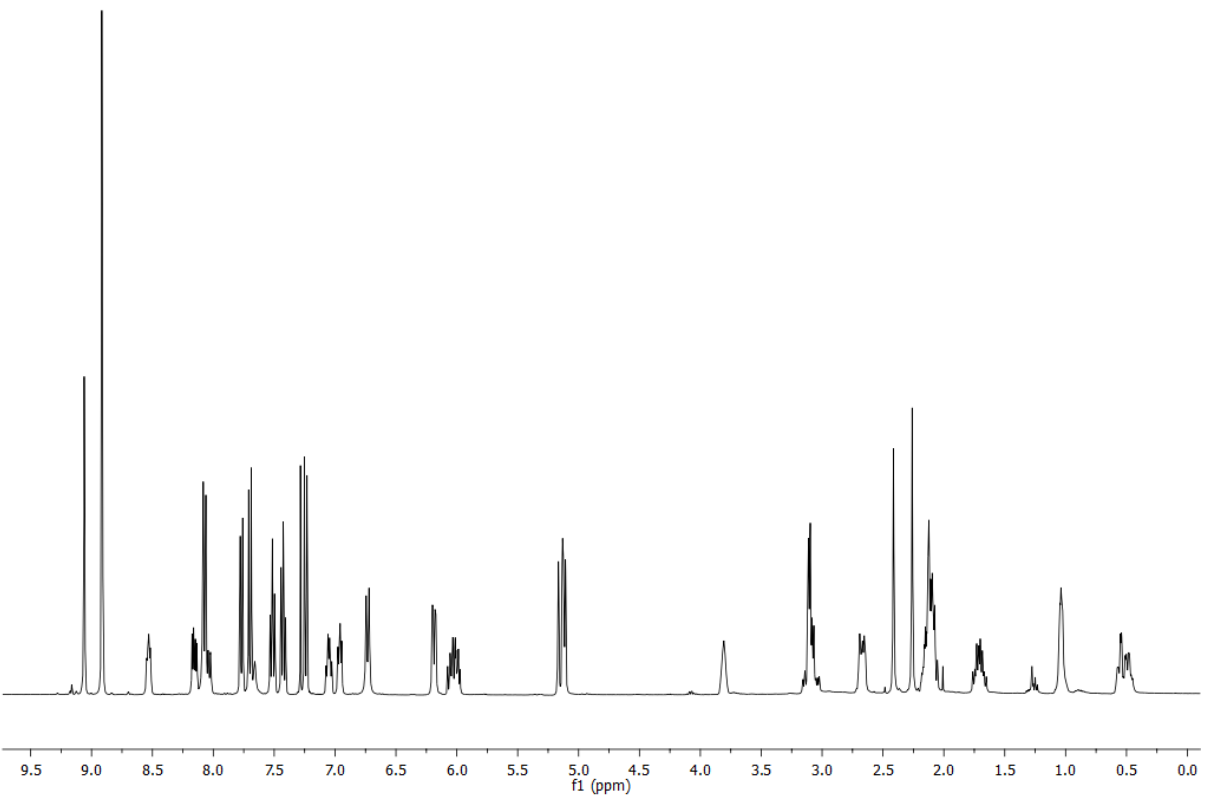
$^1\text{H}$ NMR nevirapine



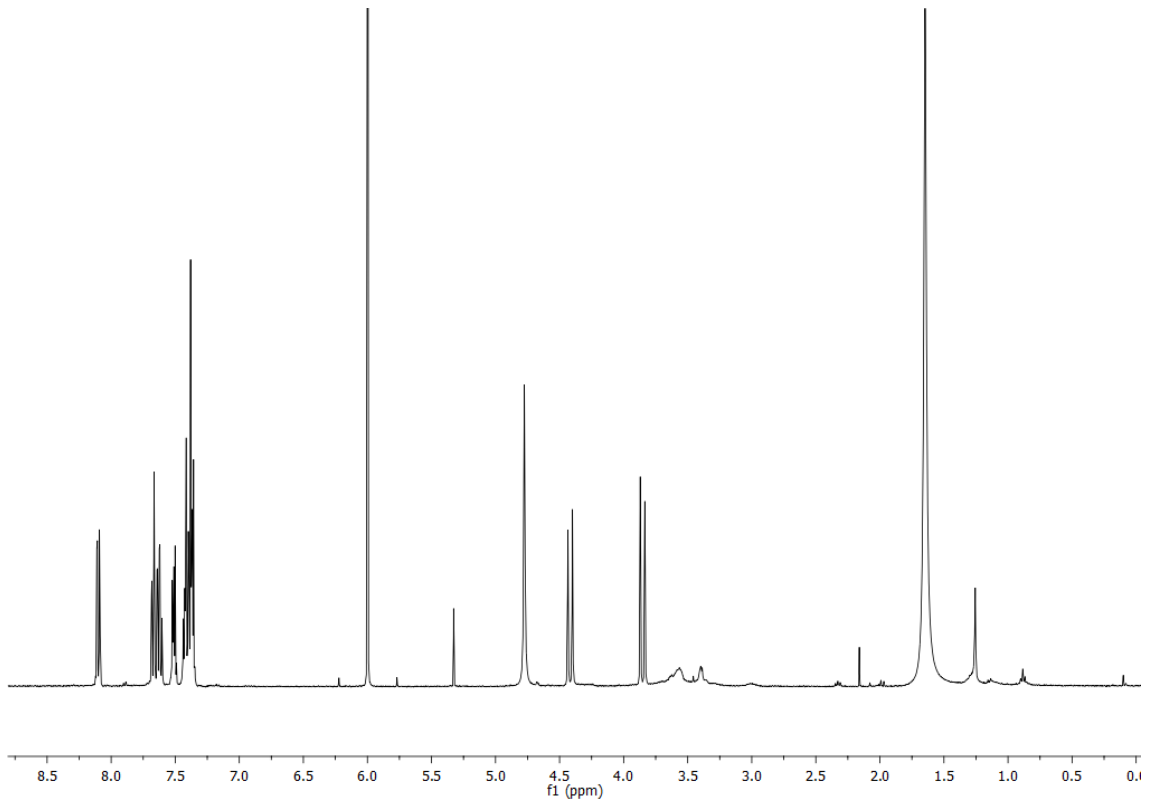
$^1\text{H}$ NMR (R,R)WhelkO1



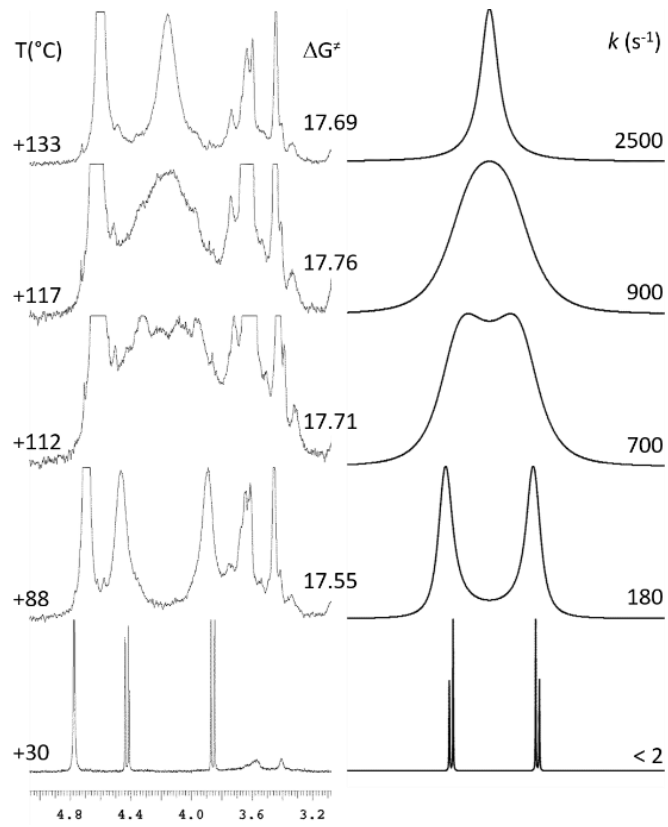
<sup>1</sup>HNMR Nevirapine + saturated solution of (R,R)whelk01



<sup>1</sup>HNMR Oxcarbazepine

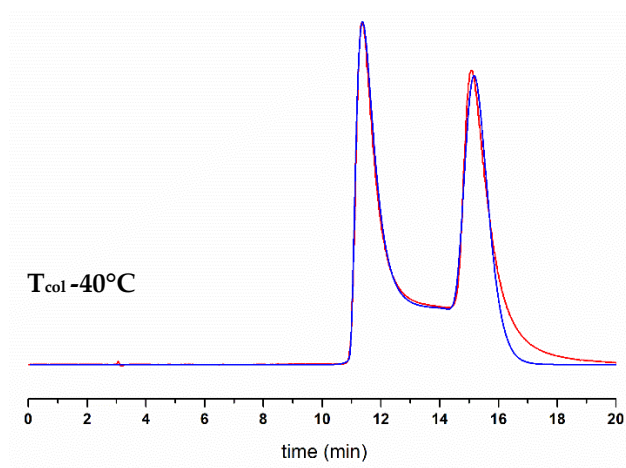
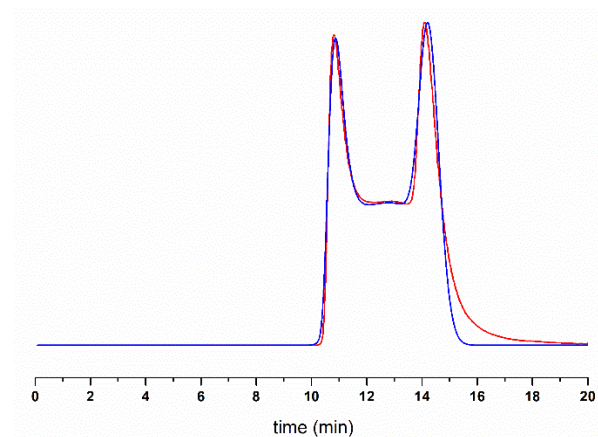
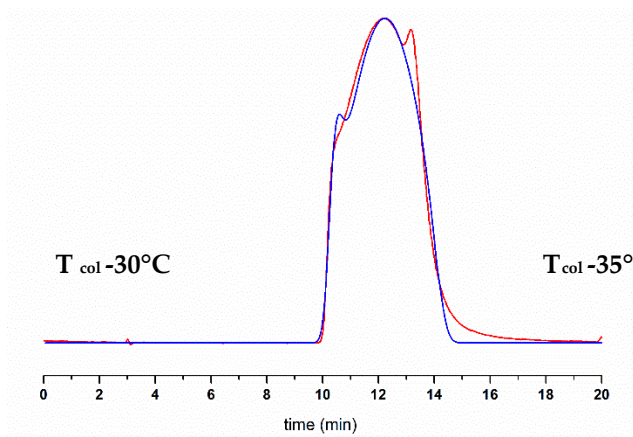


VT-NMR of oxcarbazepine



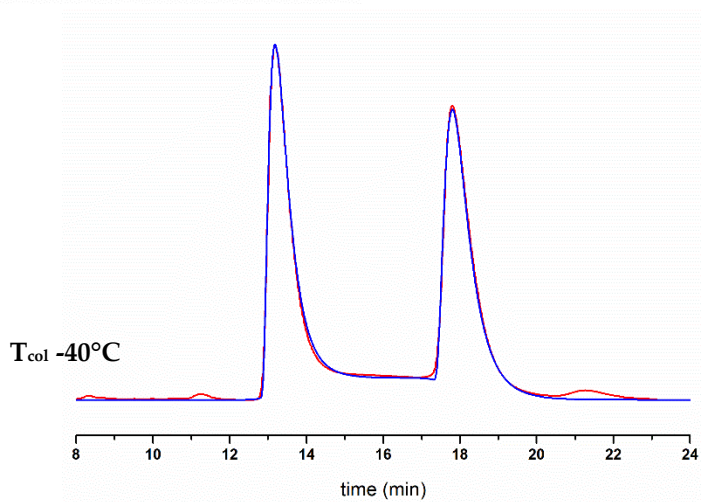
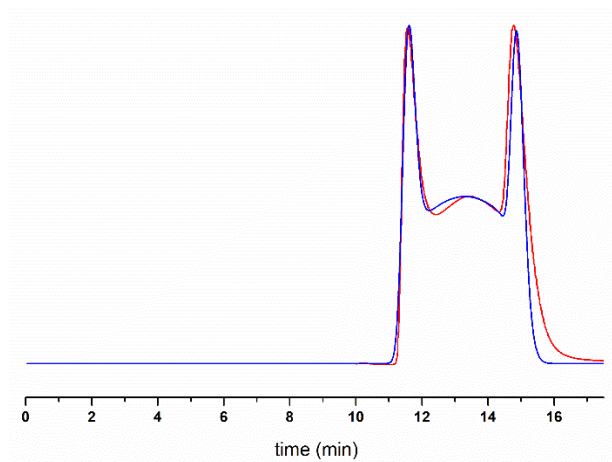
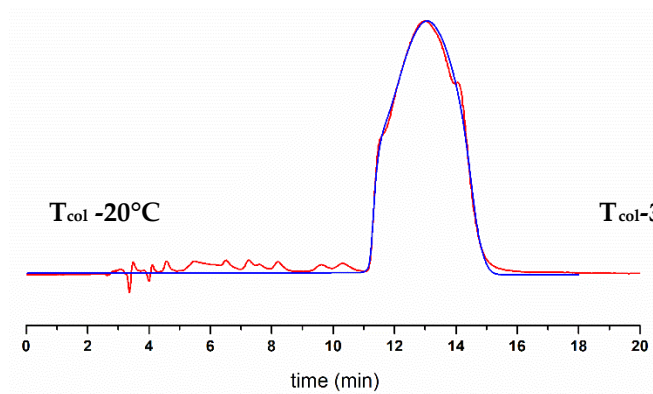
## 2. Simulated VT-HPLC profiles

### 2.1 Nevirapine



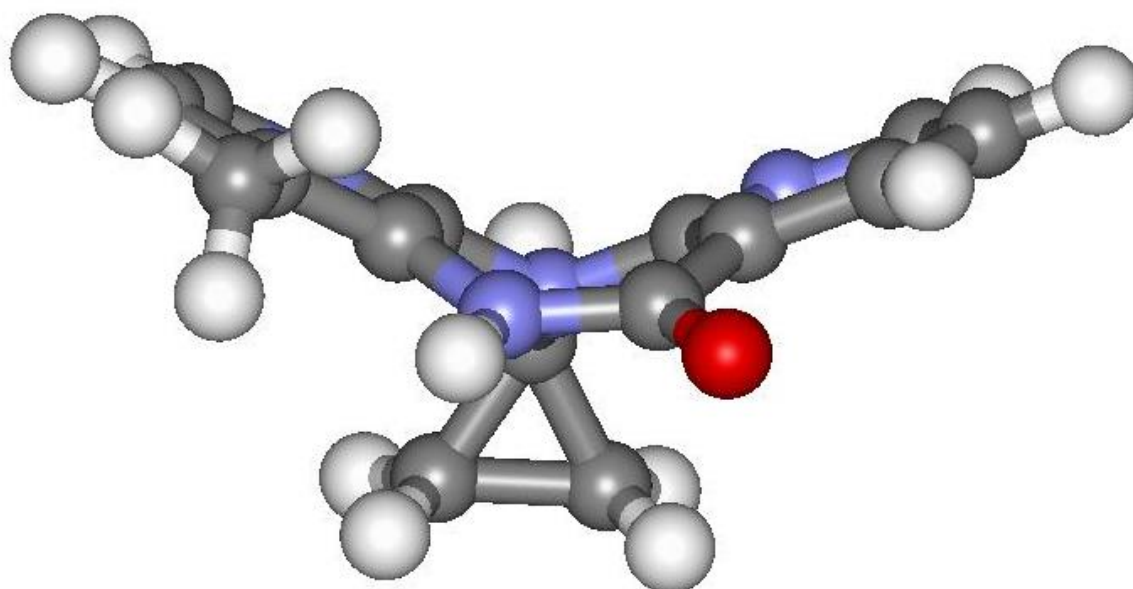
T°C	$k_{app\ 1,2}$ (min <sup>-1</sup> )	$k_{app\ 2,1}$ (min <sup>-1</sup> )	$\Delta G_{app}^\ddagger_{1,2}$ (kcal/mol)	$\Delta G_{app}^\ddagger_{2,1}$ (kcal/mol)
-30	0,231	0.171	16.82	16.96
-35	0.073	0.055	17.01	17.14
-40	0.076	0.057	17.08	17.22

## 2.1 Oxcarbazepine

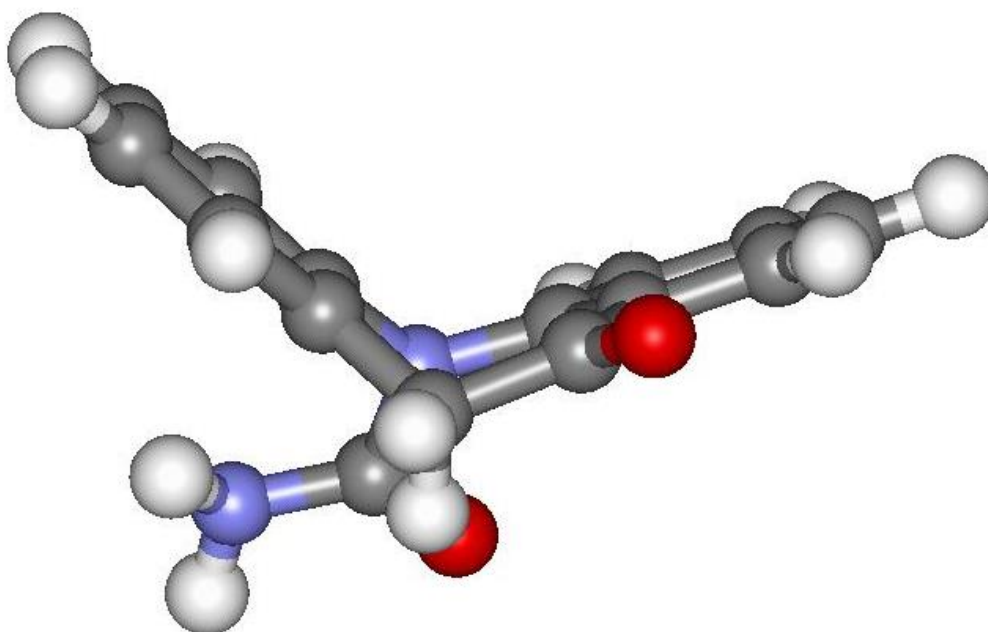


$T^{\circ}\text{C}$	$k_{app\ 1,2} (\text{min}^{-1})$	$k_{app\ 2,1} (\text{min}^{-1})$	$\Delta G_{app\ 1,2}^{\ddagger} (\text{kcal/mol})$	$\Delta G_{app\ 2,1}^{\ddagger} (\text{kcal/mol})$
-20	0.216	0.196	17.55	17.68
-30	0.096	0.075	17.45	17.45
-40	0.014	0.010	17.39	17.53

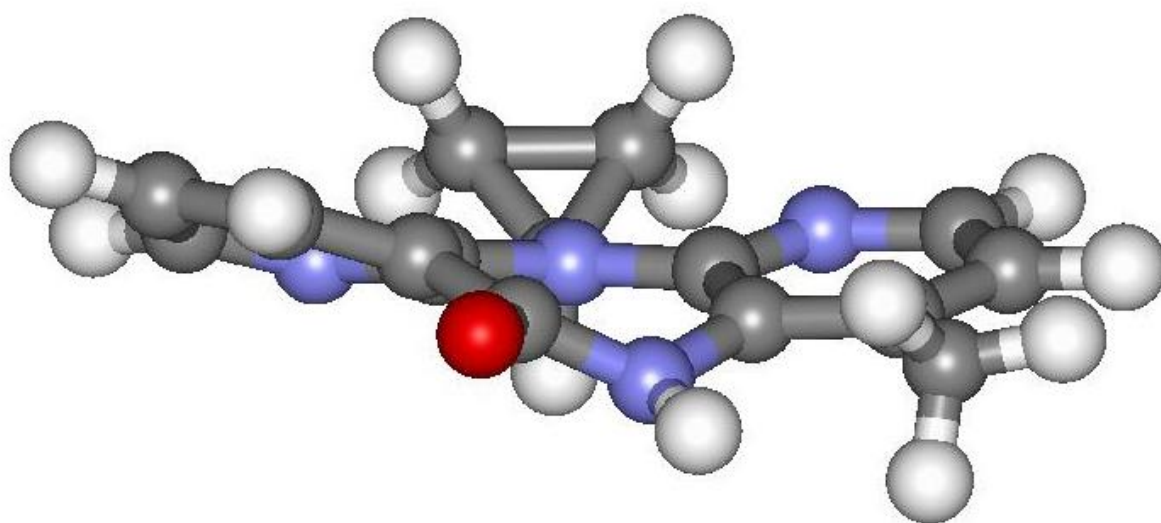
### 3. Geometries of ground state and transition state for NVP and OXC



Ground state geometry found for Nevirapine NVP

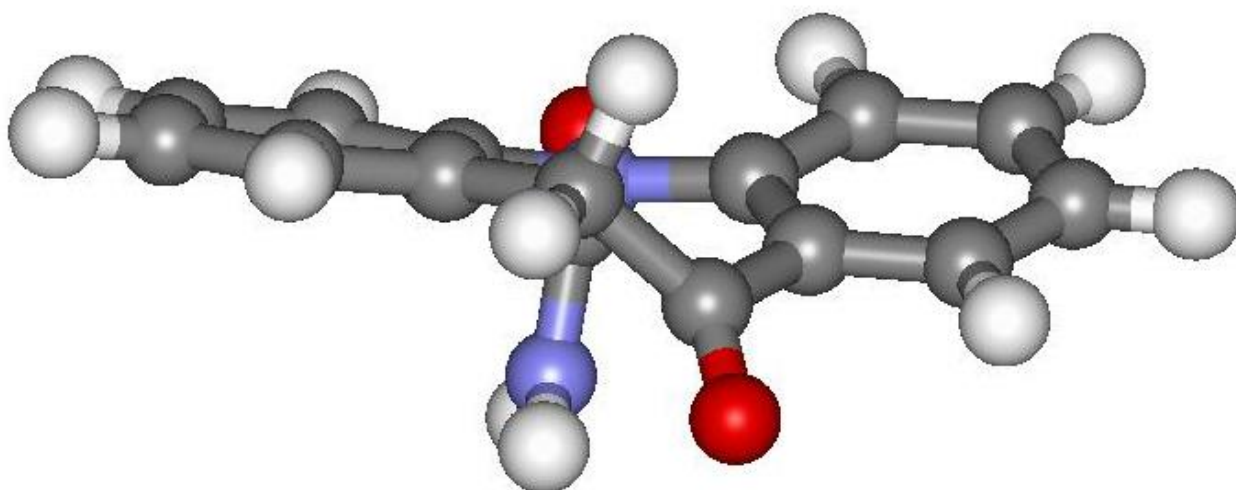


Ground state geometry found for Oxacarbazepine OXC

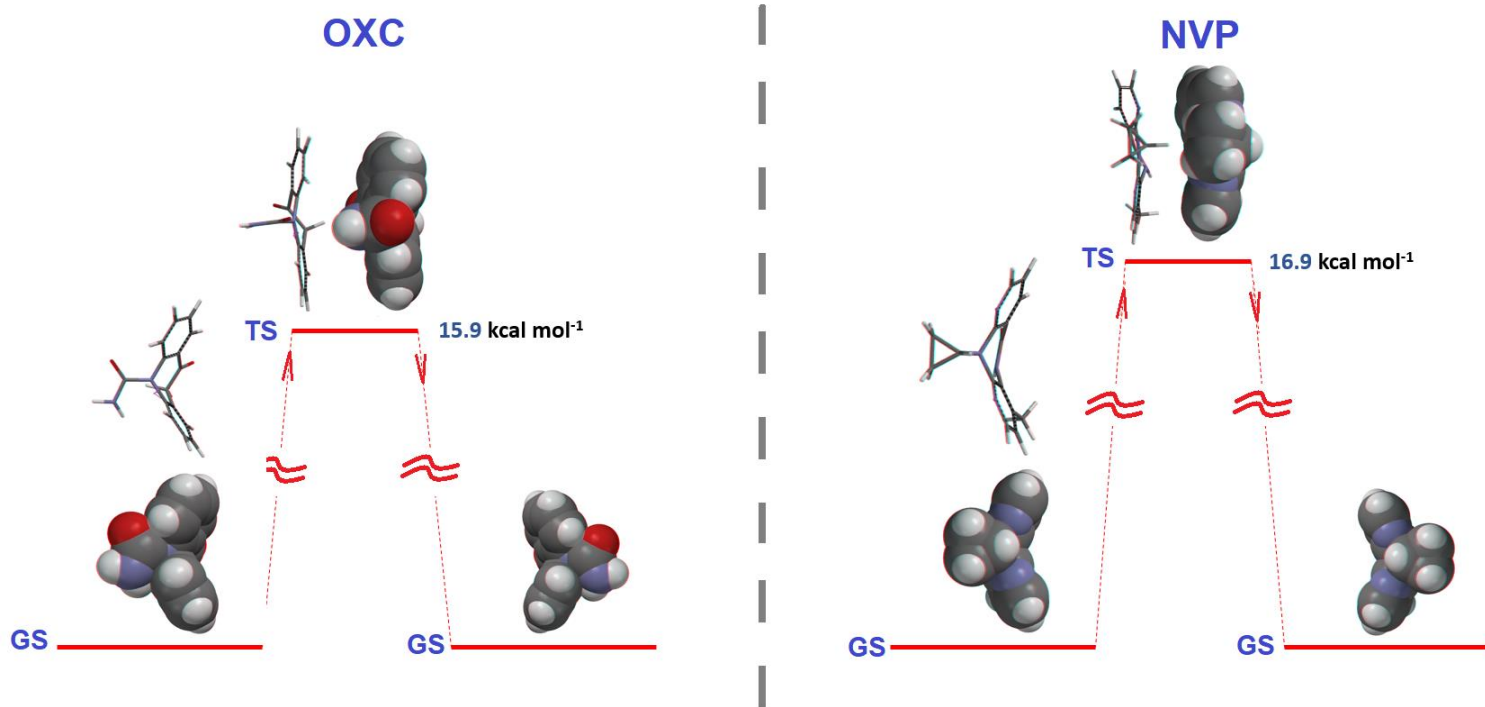


**Transition state geometry found for Nevirapine NVP enantiomerization**





Transition state geometry found for Oxacarbazepine OXC enantiomerization



Enantiomerization barriers found for Oxacarbazepine OXC (left) and Nevirapine NVP (right)