

Supporting information of:

“Molecular Recognition in Gas Phase: Benzocaine-Phenol as a Model of The Anesthetic-Receptor Interaction”,

By

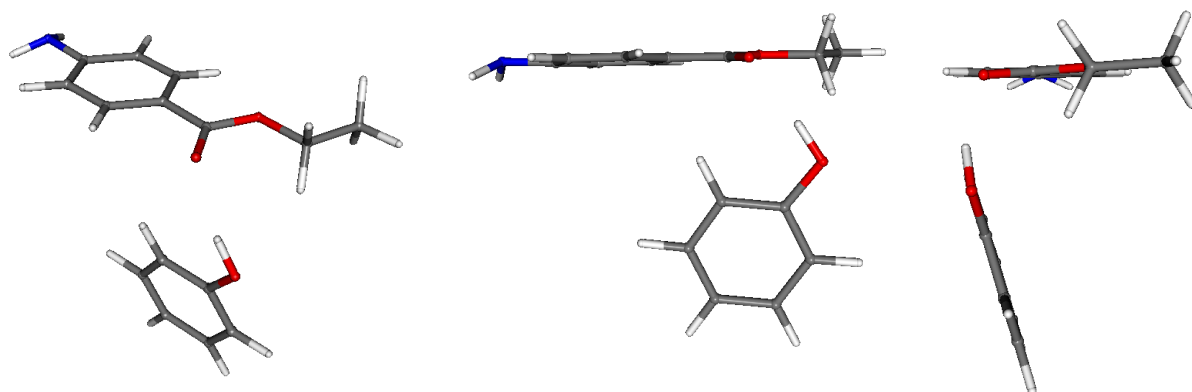
Edurne Aguado,¹ Iker León,¹ Emilio J. Cocinero,¹ Alberto Lesarri,² José A Fernández^{1} and Fernando Castaño¹*

¹Departamento de Química Física, Universidad del País Vasco, Apdo. 644, Bilbao 48080. Spain

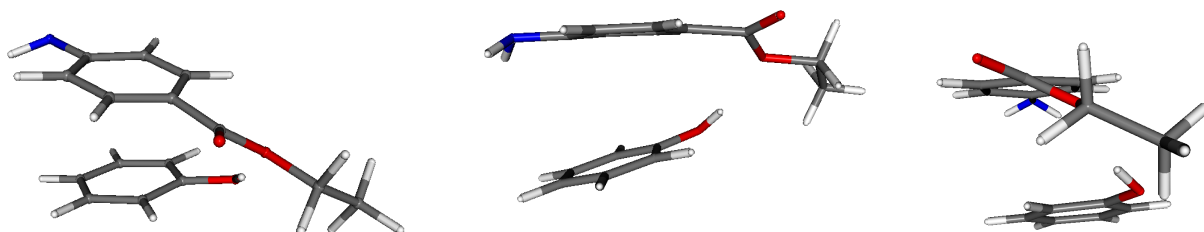
² Departamento de Química Física y Química Inorgánica; Facultad de Ciencias, Universidad de Valladolid, E-47005 Valladolid, Spain,

Supporting Figure S1. Benzocaine-phenol structures calculated at MP2/6-31g(d) level.

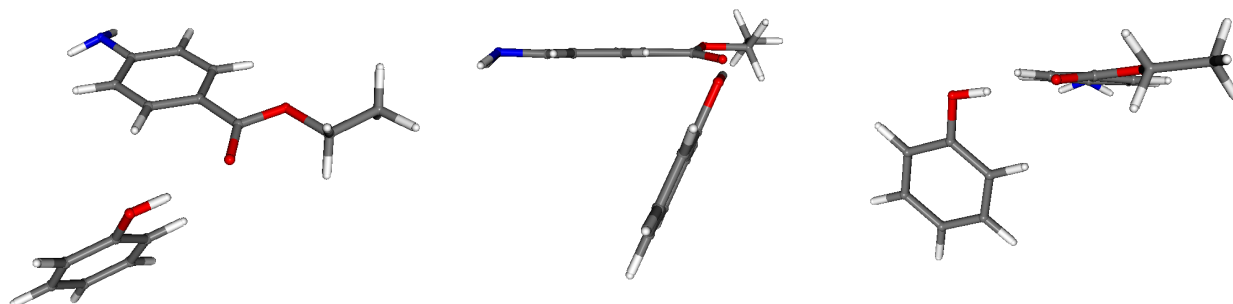
t-BzPhOH 1



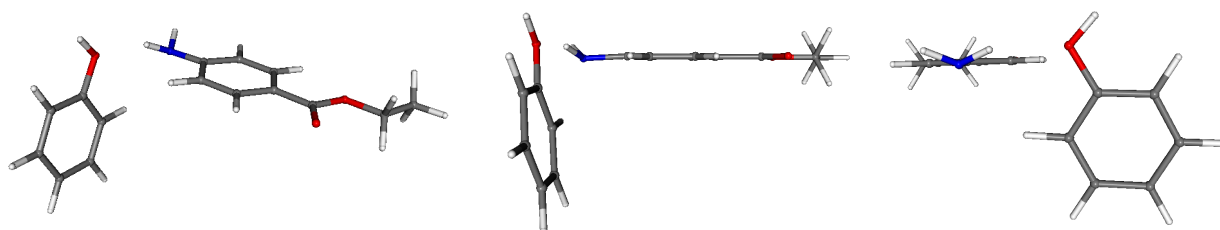
t-BzPhOH 2



t-BzPhOH 3

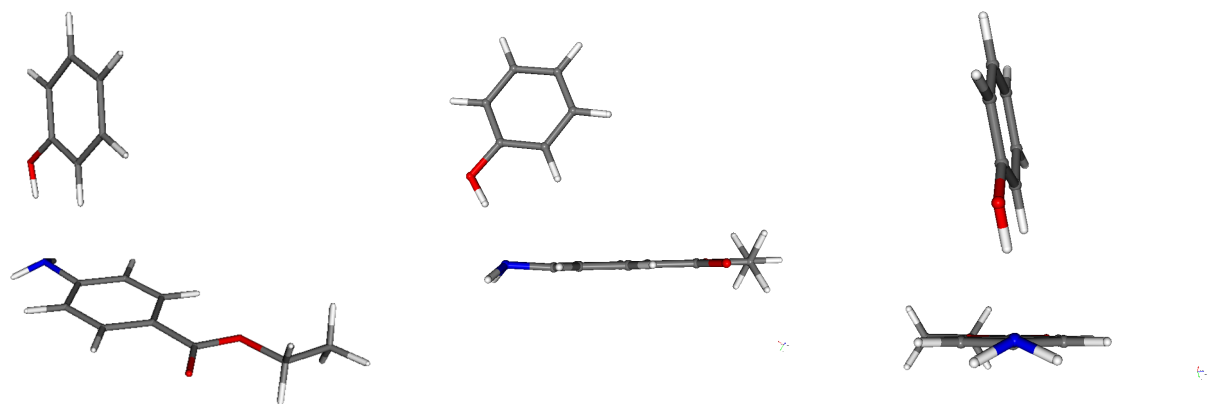


t-BzPhOH 4

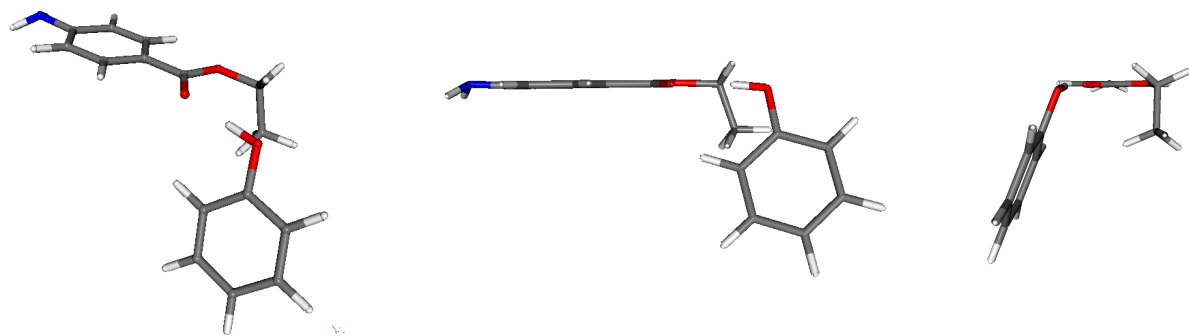


Supporting Figure 1 (cont.)

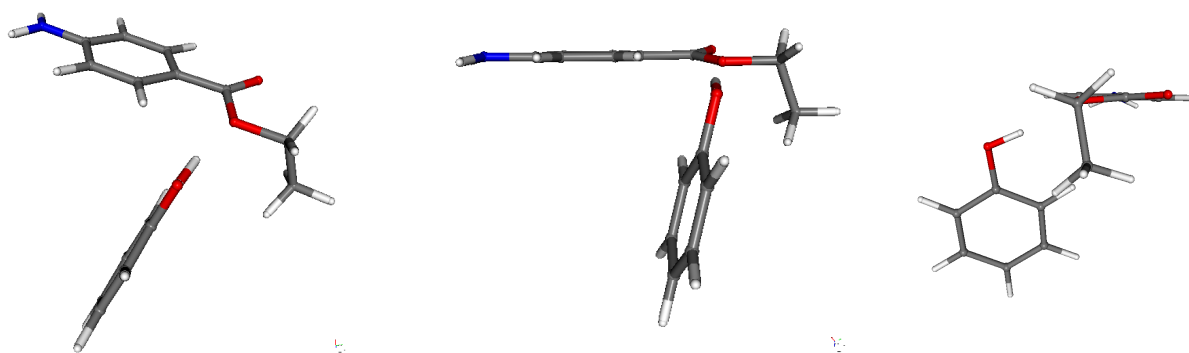
t-BzPhOH 5



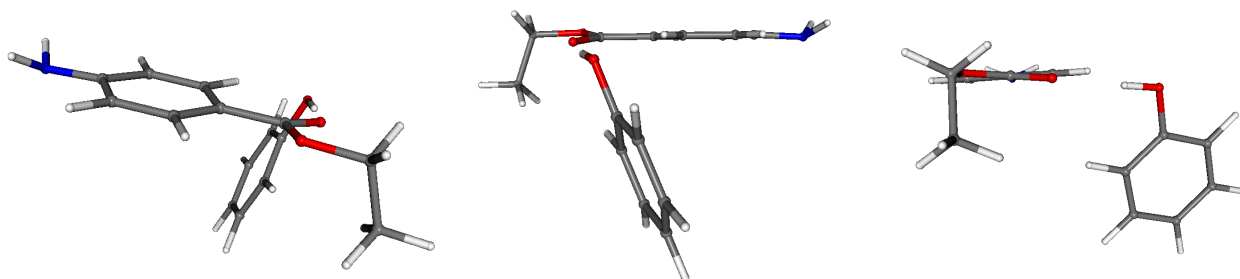
g-BzPhOH SS1



g-BzPhOH SS2

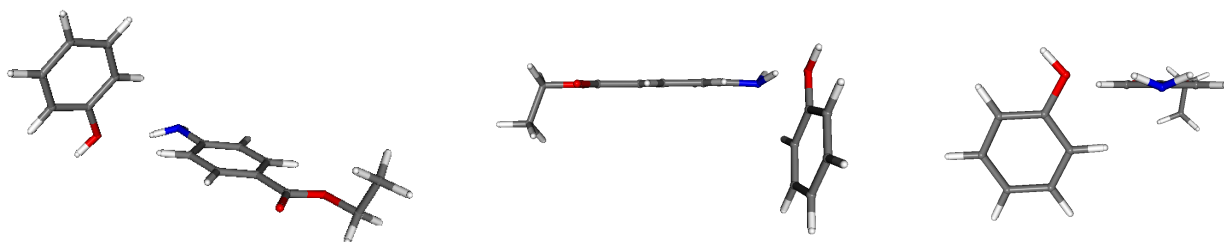


g-BzPhOH SS3

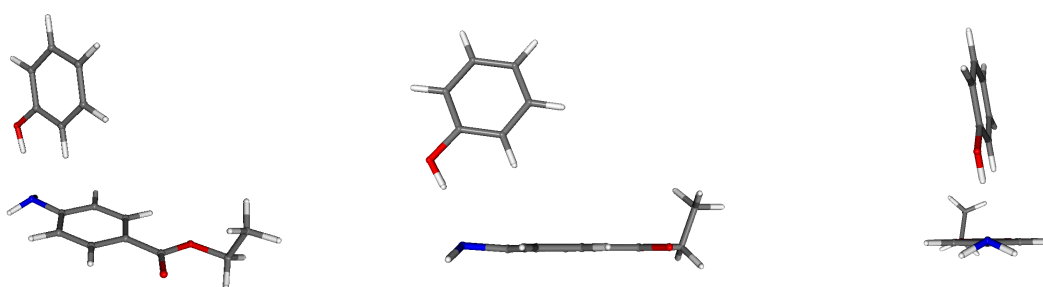


Supporting Figure 1 (cont.)

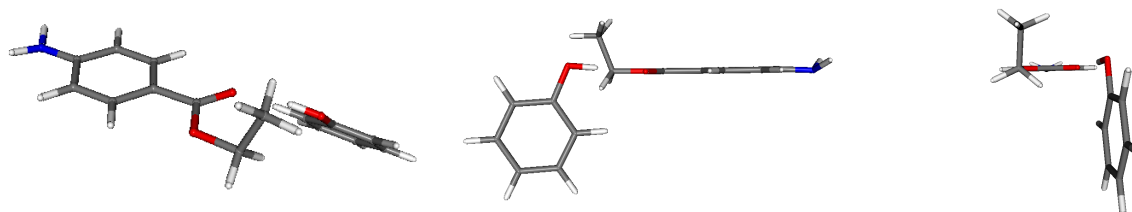
g-BzPhOH SS4



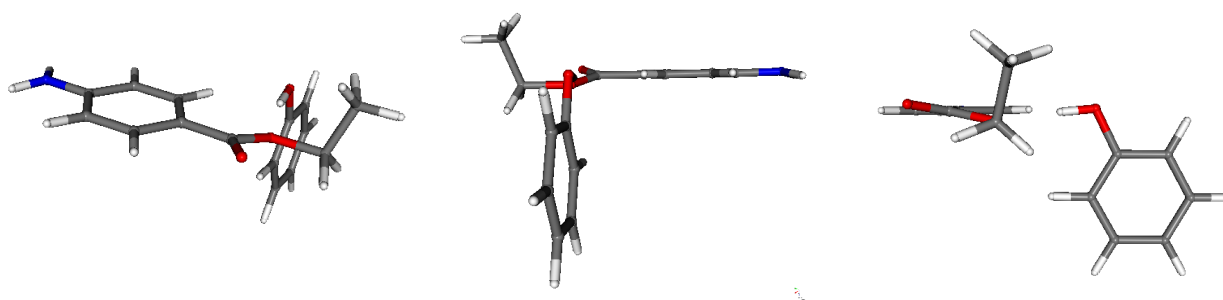
g-BzPhOH SS5



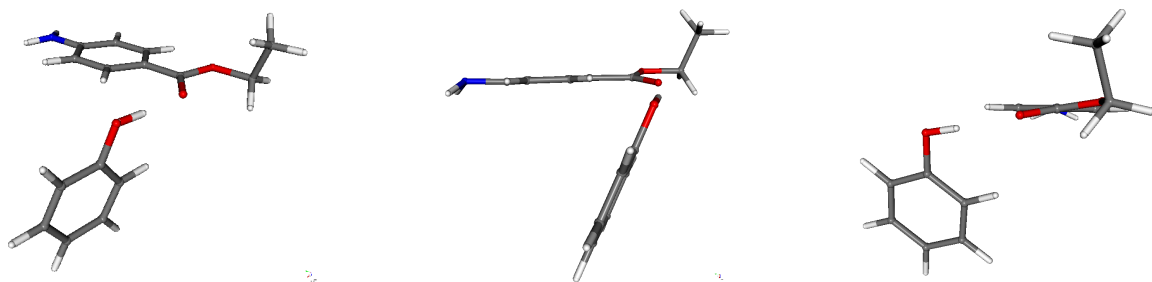
g-BzPhOH OS1



g-BzPhOH OS2

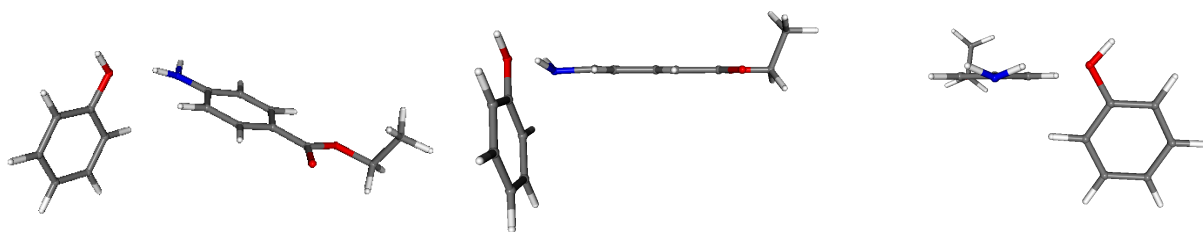


g-BzPhOH OS3

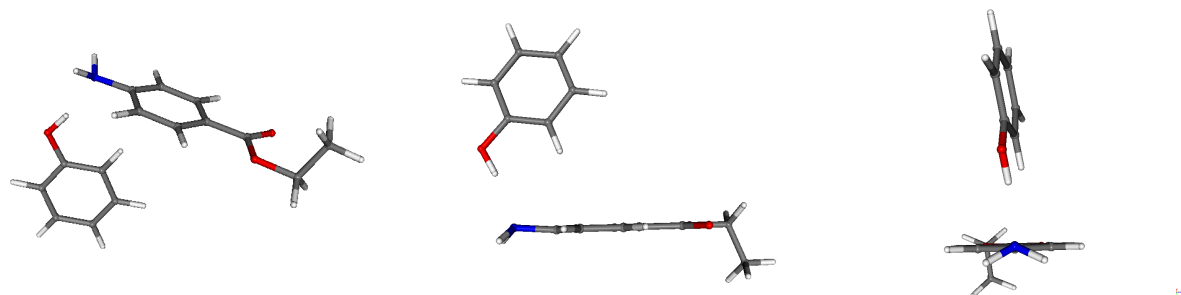


Supporting Figure 1 (cont.)

g-BzPhOH OS4



g-BzPhOH OS5



Supporting Fig. S2. Bz ionization thresholds obtained using 1+1' REMPI and Bz-PhOH ionization and fragmentation threshold obtained by scanning the ionization laser in a 2-color REMPI experiment, setting the pump laser on the origin band at 34129 cm^{-1} and integrating either the $[\text{Bz-PhOH}]^+$ (ionization) or the Bz^+ mass channel (fragmentation, red trace).

