Supporting information for:

Mimicking Anaesthetic-Receptor Interaction: a Combined Spectroscopic and Computational study of Propofol···Phenol

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†Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/b000000x/

Figure S1. The five conformational isomers of propofol, with their relative stability in kJ/mol, as calculated at MP2/6-311++G(d,p) and at M06-2X/6-31+G(d) in parentheses. Atoms are coloured as follows: carbon: yellow, hydrogen: cyan and oxygen: red.

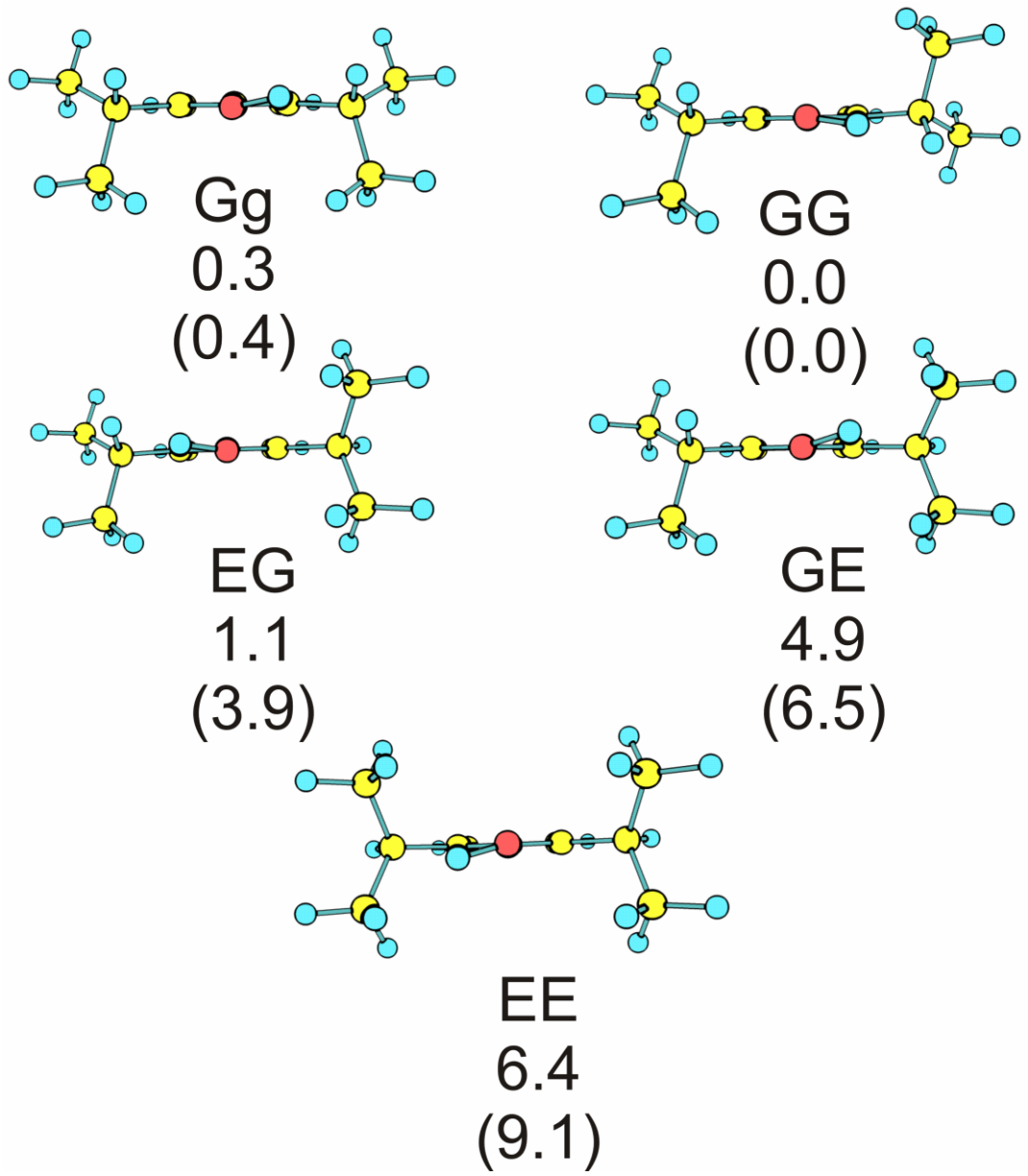


Figure S2. 18 most stable conformational isomers of propofol·phenol, with their relative stability in kJ/mol, as calculated at M06-2x/6-31+G(d). Atoms are coloured as follows: carbon: yellow, hydrogen: cyan and oxygen: red.

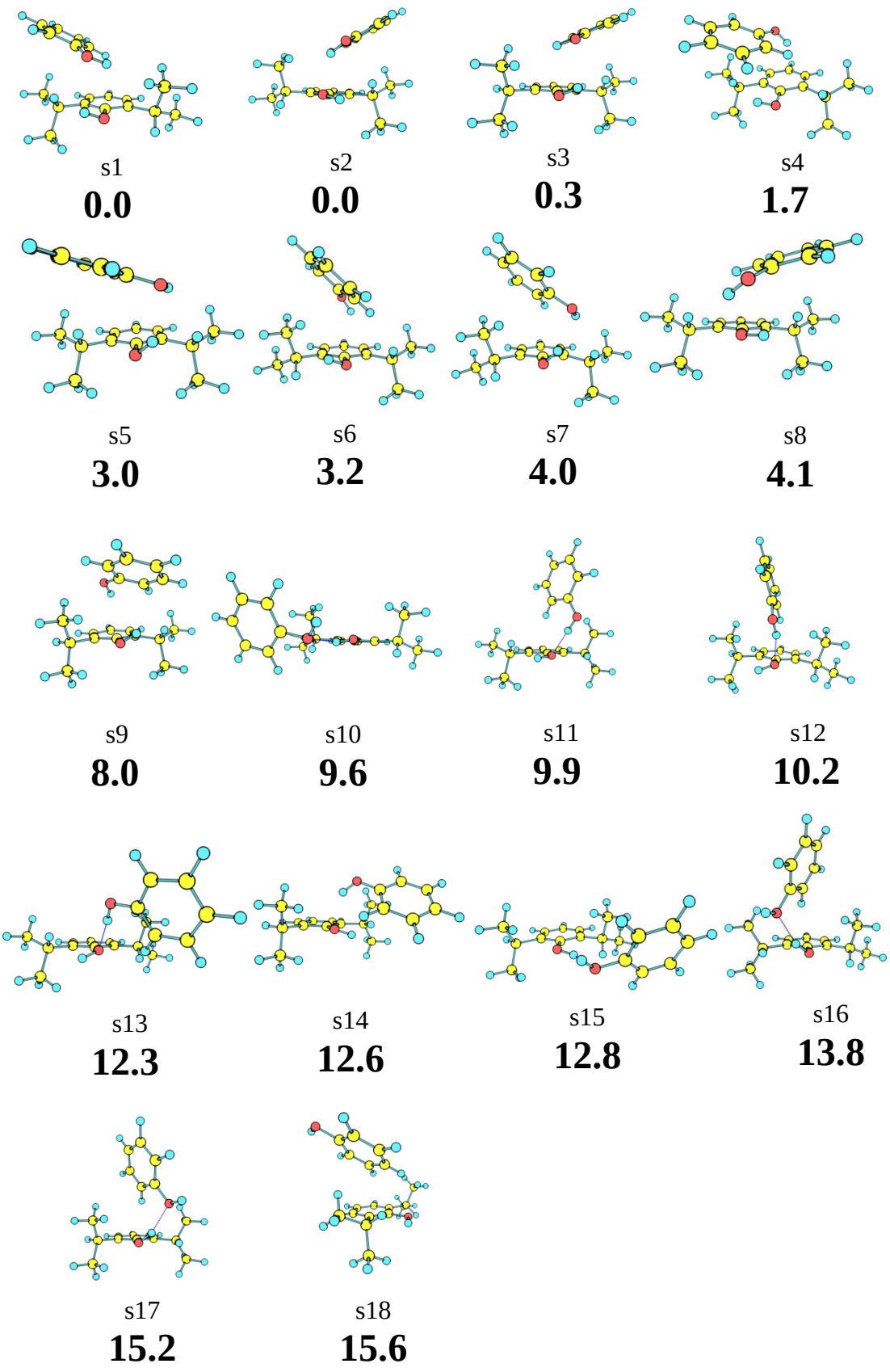


Figure S3. Comparison between the S_0 IRID spectra of the six detected propofol···phenol conformers and the IR spectra for the calculated structures.

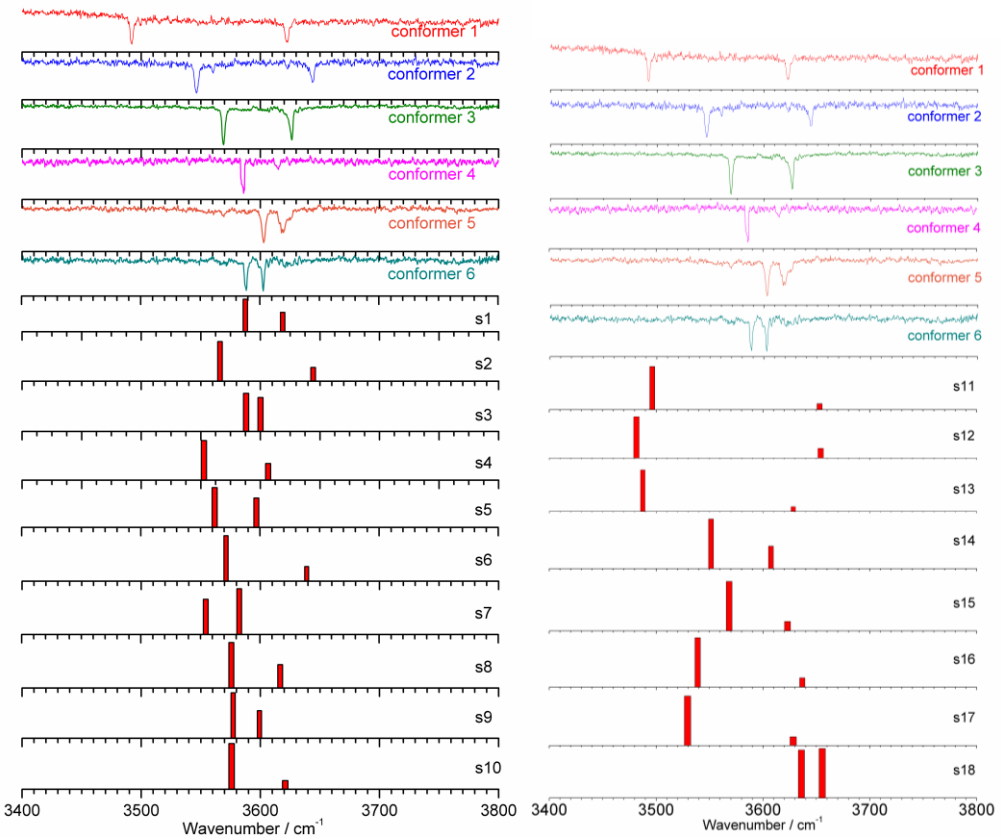
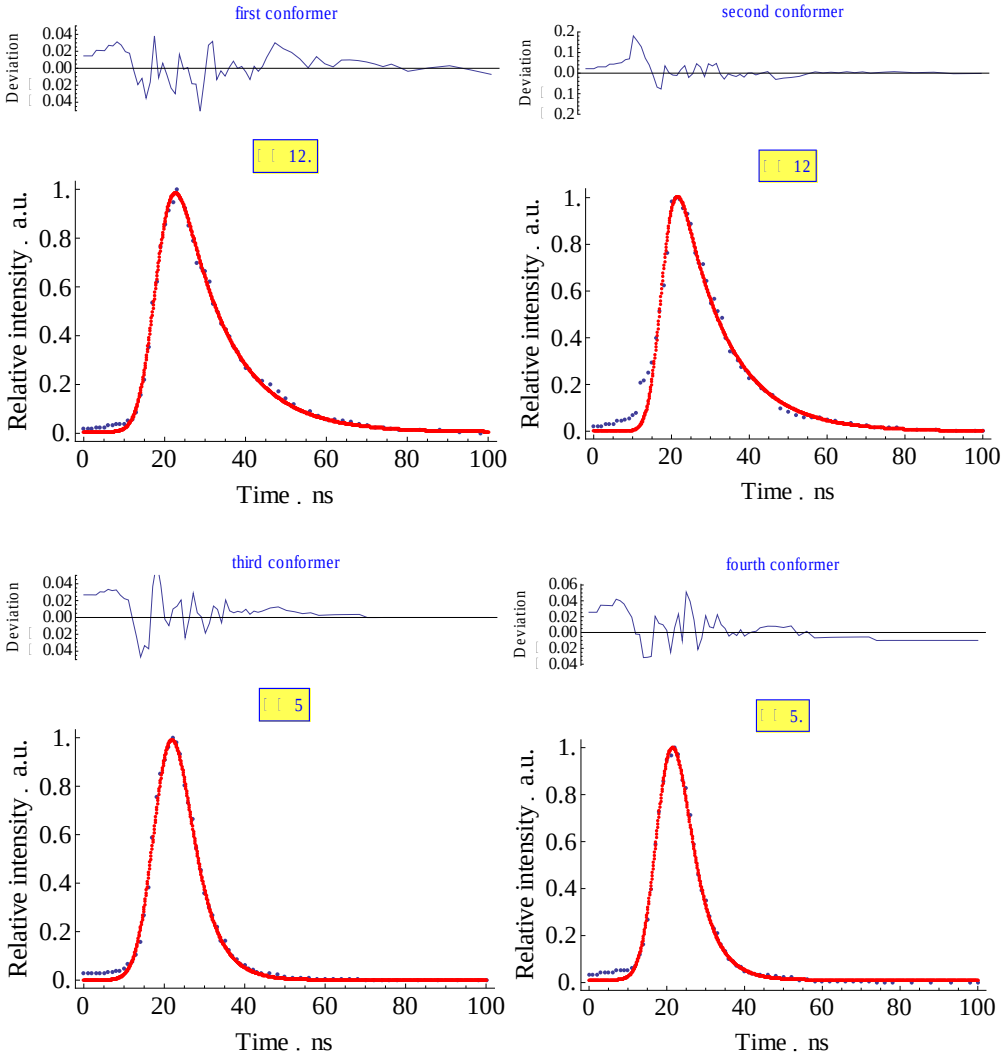


Figure S4. S_1 state lifetimes, for five of the six detected propofol·phenol complexes, determined as in dicated in Ware, W. R. et al., *J. Phys. Chem.* 1973, **77,** 2038-2048; Schulman, S. G.and Capomacchia, A. C. *J. Phys. Chem.* 1975, **79,** 1337-1343. The blue dots in the graphics represent the experimental data, while the dotted red line is the best fit. The lifetime in ns is indicated in an insert for each species.



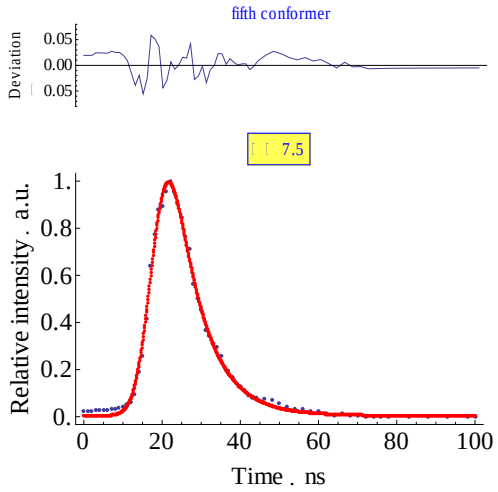


Table S1. Relative energies, BSSE and ZPE contributions for the 18 propofol·phenol structures, calculated at M06-2X/6-31G(d) level.

Structure	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*D_0 (kJ/mol)*	*BSSE (kJ/mol)*
s1	0.00	0.00	-35.21	6.28
s2	0.80	0.01	-34.90	6.59
s3	0.34	0.27	-38.60	6.33
s4	2.67	1.69	-33.94	6.28
s5	2.70	3.01	-31.93	6.97
s6	4.38	3.17	-32.28	6.04
s7	5.54	3.95	-30.47	7.08
s8	4.19	4.12	-31.57	6.22
s9	9.34	8.00	-30.93	6.28
s10	8.64	9.56	-27.23	5.11
s11	8.82	9.94	-24.07	7.49
s12	9.92	10.18	-30.12	7.38
s13	12.11	12.30	-22.77	6.43
s14	11.84	12.64	-26.24	6.33
s15	11.50	12.75	-27.37	5.08
s16	14.20	13.81	-21.33	6.36
s17	16.44	15.22	-23.58	6.41
s18	17.02	15.65	-22.22	3.63