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Methodological Keys For Accurate $pK_a^\star$ Simulations: Supplementary Information

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1 Absorption and emission wavelenghts of the training set

Table S1: Maximum absoption wavelengh (in nm) of protonated/deprotonated forms of the training set (See Figure 2 of the main manuscript) using the IE-TD-DFT/PBE0 level of theory

	LR		*c*LR		SS		Exp.
	eq	neq	eq	neq	eq	neq	
1	305/364	299/356	303/373	300/362	315/394	301/364	380/445[?]
2	306/362	301/354	302/362	300/355	304/371	300/356	-
3	340/430	333/420	343/450	336/429	361/475	338/475	337/371[?]
4	318/378	311/365	315/376	311/364	322/377	311/365	338/360[?]
5	340/423	335/415	343/440	337/423	355/465	338/426	350/380[?]
6	340/420	333/406	340/422	334/409	352/433	335/410	342/382[?]

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Table S2: Maximum emission wavelengh (in nm) of the training set (See Figure 2 of the main manuscript) using the IE-TD-DFT/PBE0 level of theory

	LR(eq)	cLR(eq)	SS(eq)	SS(neq)	Exp.
1	347/411	352/443	366/472	366/472	350/550[1]
2	299/396	335/410	330/423	302/423	358/415[2]
3	382/492	396/548	417/587	417/587	430/630[3]
4	350/410	353/426	360/435	360/435	360/500[3]
5	374/475	383/517	397/554	397/554	380/530[3]
6	374/461	383/494	396/510	396/510	410/510[3]

2 pK_a results for hydroxystilbenes

Table S3 gathered PBE0 and M06-2X pK_a results for hydroxystilbenes as only M06-2X data are shown in the main manuscript . We observe that results using IE solvent model give a rather small deviation between PBE0 and M06-2X functionals, as for the training set.

Table S3: Computed pK_a values of hydroxystilbenes

	PBE0		M06-2X			Exp.
	PCM	IE	PCM	SMD	IE	
7	13.8	10.8	13.3	11.9	11.2	10.1[4]
8	11.0	9.7	12.1	11.4	9.0	9.3[4]

References

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