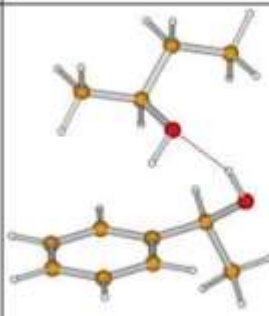
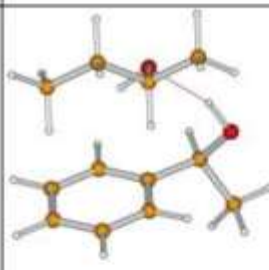
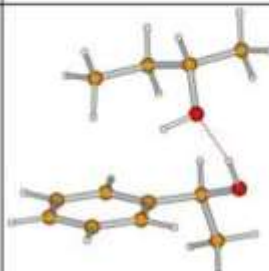
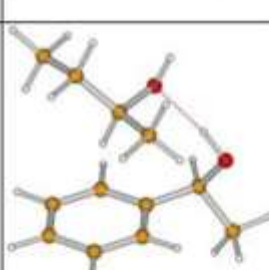
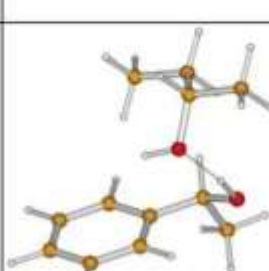


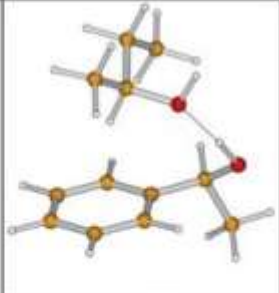
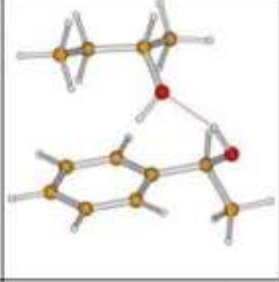
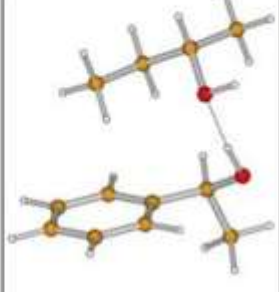
SUPPLEMENTARY INFORMATION

D-B3LYP/6-31++G** structures, relative energies (kcal/mol) $\nu_{\text{O}^{\text{bu}}\text{H}}$ and $\nu_{\text{O}^{\text{H}}}$ frequencies of the So ground state of the complexes of oFE_S , pFE_S and E_R with butan-2-ol.

Non-fluorinated complexes: homochiral

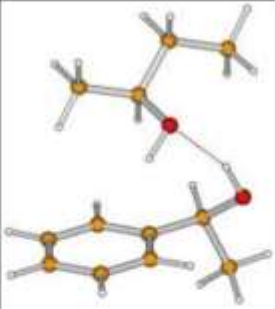
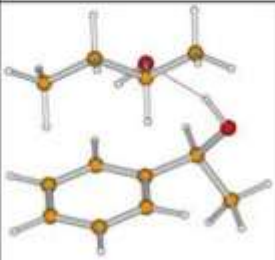
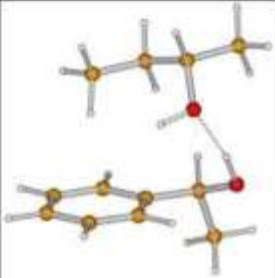
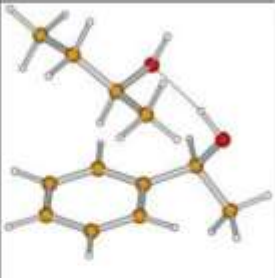
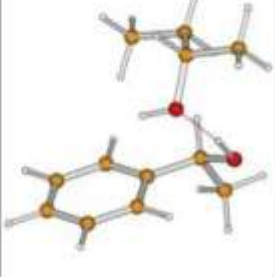
$\text{E}_S\text{-Bu}_S$ (all frequencies are scaled by 0.96)

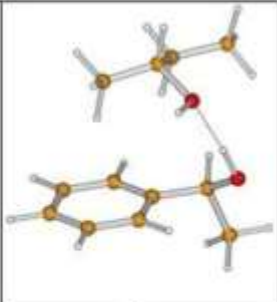
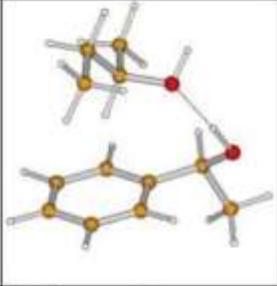
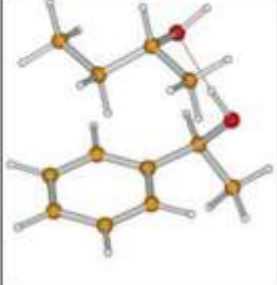
	E_{rel} (Kcal/mol)	Low Frequency (cm^{-1})	High Frequencies (cm_1)	
A	0.00	28.2	3463.6 3624.1	
B	0.06	23.4	3455.2 3633.9	
C	0.06	25.2	3423.6 3651.8	
D	0.54	18.1	3442.0 3647.9	
E	0.67	18.0	3423.9 3647.9	

F	0.87	16.2	3456.2 3653.4	
G	0.91	17.1	3461.9 3612.6	
H	1.58	14.5	3433.1 3673.8	

Non-fluorinated complexes: heterochiral


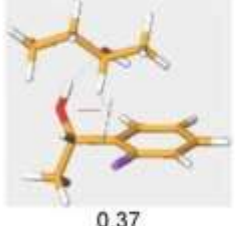
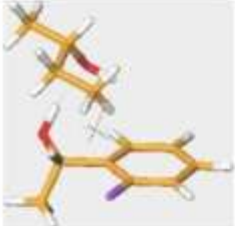


Es-BUR (All frequencies are scaled by 0.96)


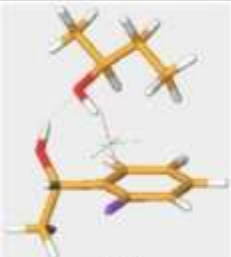
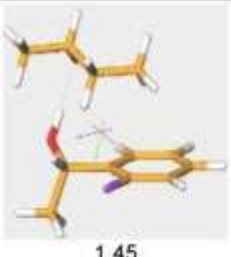

	E_{rel} (Kcal/mol)	Low Frequency (cm^{-1})	High Frequencies (cm^{-1})	
A	0.00	29.0	3442.7 3634.4	
B	0.28	28.5	3473.2 3627.2	
D	0.68	21.7	3482.6 3601.9	
C	0.68	15.3	3441.7 3673.0	
E	0.68	11.2	3449.8 3637.9	

F	1.05	29.2	3444.8 3683.5	
G	1.08	25.6	3446.6 3650.9	
H	1.26	21.7	3441.3 3678.3	

Ortho-fluorinated complexes: homochiral

$o\text{FE}_s\text{-B}_s$

	ZPE_{rel} (Kcal/mol)	Low Frequencies (cm ⁻¹)	High Frequencies (cm ⁻¹)
A	 <p style="text-align: center;">0.00</p>	40 53 62 67 83 96	3433 3661
B	 <p style="text-align: center;">0.37</p>	25 36 50 61 77 84	3471 3635
C	 <p style="text-align: center;">0.57</p>	28 41 49 55 77 90	3421 3652
D	 <p style="text-align: center;">1.04</p>	17 46 55 78 87	3462 3655
E	 <p style="text-align: center;">1.14</p>	12 31 51 56 77 86	3491 3659

F	 1.19	7 37 46 52 69 81	3500 3684
G	 1.42	18 34 48 60 69 87	3472 3650
H	 1.45	23 41 57 60 77	3426 3675
I	 1.51	22 49 60 66 82 92	3468 3617

* All frequencies are scaled by 0.96

Ortho-fluorinated complexes: heterochiral


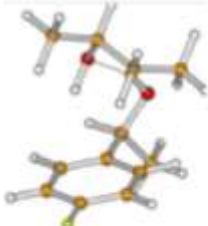
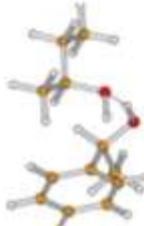
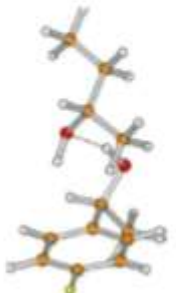
oFE_S-Bu_R


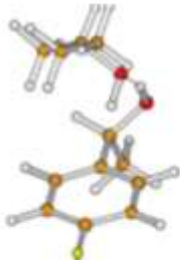
	ΔE_{rel} (Kcal/mol) -	Low Frequency (cm ⁻¹)	High Frequency (cm ⁻¹)	
A	0.00	19.9	3452 3643	
B	0.75	30.1	3454 3684	
C	0.77	30.5	3459 3653	
D	0.95	29.2	3446 3675	
E	1.11	32.6	3500 3600	
F	1.14	26.8	3479 3661	
G	1.21	11.2 / 29.0	3465 3681	
H	1.28	13.8 / 34.4	3484 3640	
I	1.42	19.3	3428 3654	

* All frequencies are scaled by 0.96

Para-fluorinated complexes: homochiral

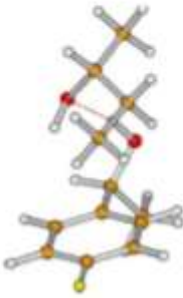
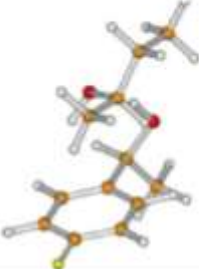
pFE₅-Bu₅

	E_{REL} (kcal/mol)	
A	+ 0.00	
B	+0.32	
C	+0.47	
D	+0.98	

E	+0.99	
F	+1.34	

Para-fluorinated complexes: heterochiral

pFE_SBu_R

	E _{REL} (kcal/mol)	
A	+ 0.00	
B	+0.06	

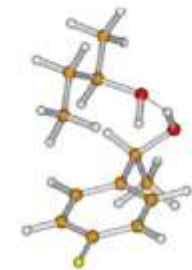

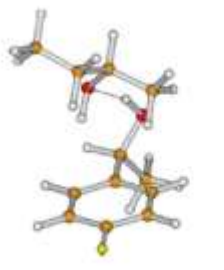
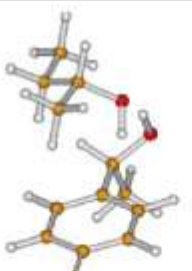
C	+0.24	
D	+0.63	
E	+0.70	
F	+1.04	

Table S1: energy components analysis: contribution of hydrogen bond, CH... π , OH... π , CH...F interactions to the total energy as calculated by MM3 force field at the D-B3LYP/6-31++G** minimum energy geometries.

Conformer	OH...O	CH... π	OH... π	CH...F
oA_{hetero}	3.18	0.57	0.79	0.25
oB_{hetero}	3.12	0.60	0.02	0.11
oA_{homo}	2.95	0.11	0.57	0.19
oB_{homo}	3.32	0.16	0.90	0.14
pA_{hetero}	3.10	0.22	0.77	0.16
pB_{hetero}	3.40	0.54	1.05	0.15
pC_{hetero}	3.07	0.59	0.80	0.12
pA_{homo}	3.27	0.78	0.99	0.2
pB_{homo}	3.43	0.82	1.06	0.12
A_{hetero}	3.06	0.62	0.82	
B_{hetero}	3.42	0.57	1.07	
C_{hetero}	3.26	0.32	0.30	
D_{hetero}	3.39	0.79	1.07	
A_{homo}	3.26	0.29	0.98	
B_{homo}	3.25	0.88	0.95	
D_{homo}	3.16	0.63	0.13	