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Supporting information for article:

Two single-enantiomer amidophosphoesters: a database study on the chirality of (O)2P(O)(N)-based structures

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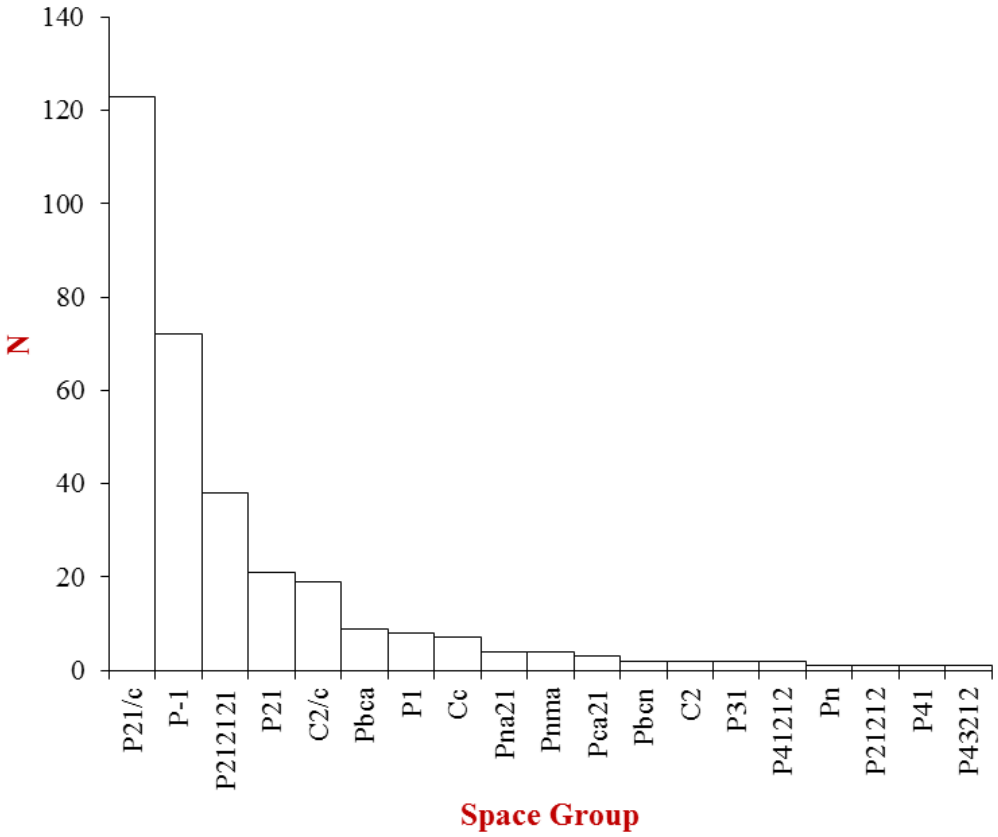


Figure S1. Populations of space groups in $(O)_2P(O)(N)$-based structures.

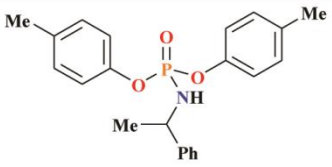
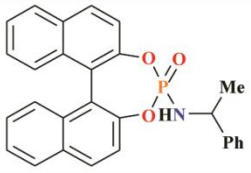
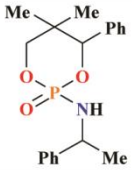
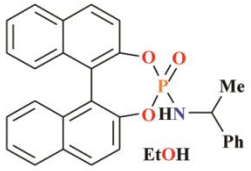
FIBROY		**MIWNUB**	
MAQPID		**TUKVOK**	

Figure S2. The chemical structures associated to the refcodes for typical compounds with a single-enantiomer $NHCH(CH_3)(C_6H_5)$ segment.

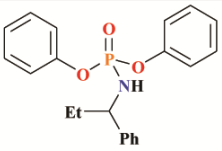
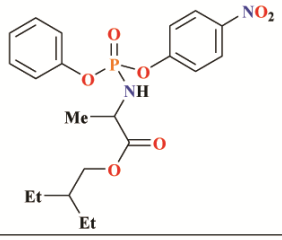
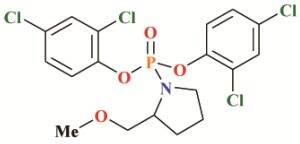
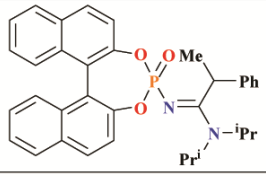
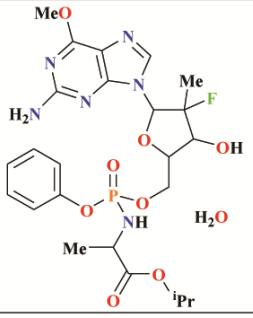
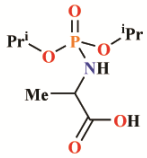
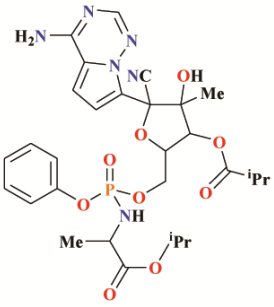
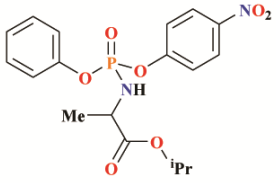
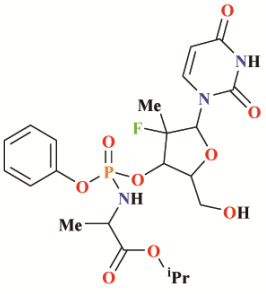
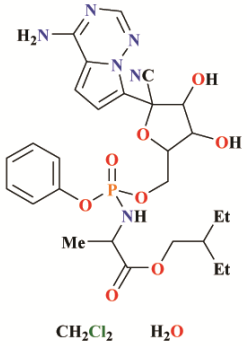
EXIQIM		**QABZIF**	
KEZTEO		**RITZEA**	
KUSCIM		**TAFHIR**	
MIYXAV		**UCIXUB**	
PARZIU		**ZARNAK**	

Figure S3. The chemical structures associated to the refcodes for compounds with chiral segments discussed in the subset "(b)". Typical examples of non-centrosymmetric cyclic hydrogen-bond motifs in this subset are $R_4^4(16)$ between one amidophosphoester molecule and one H_2O molecule (KUSCIM), $R_3^3(11)$ (ZARNAK), an $R_2^2(8)$ hetero-synthon including different conjunctions NH…O and NH…N (MIYXAV), a novel $R_2^2(10)$ including a C_2 axis (TAFHIR) instead of inversion element which usually found for such homo-synthon.

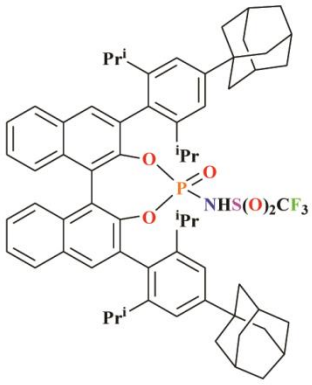


Figure S4. The chemical structure of CIYVOW, including a chiral aromatic diol. For the structures with refcodes MIWNUB and RITZEA, refer to Figures S2 and S3, respectively.

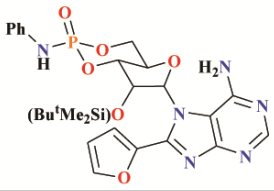
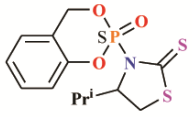
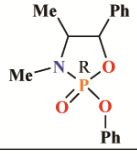
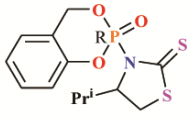
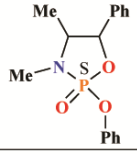
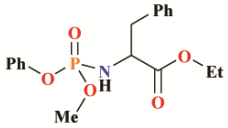
CIHDED		**OWUYEL**	
JOFPUP		**OWUYIP**	
JOFRAX		**PALPHS**	

Figure S5. The chemical structures of compounds with a dissymmetry P atom; also see MAQPID in Figure S2.

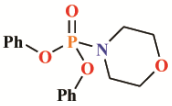
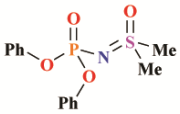
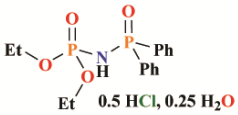
BILCAC		**DAXGIS**		**WIYFAL**	

Figure S6. The chemical structures associated to the refcodes of typical chiral structures obtained from achiral molecules.

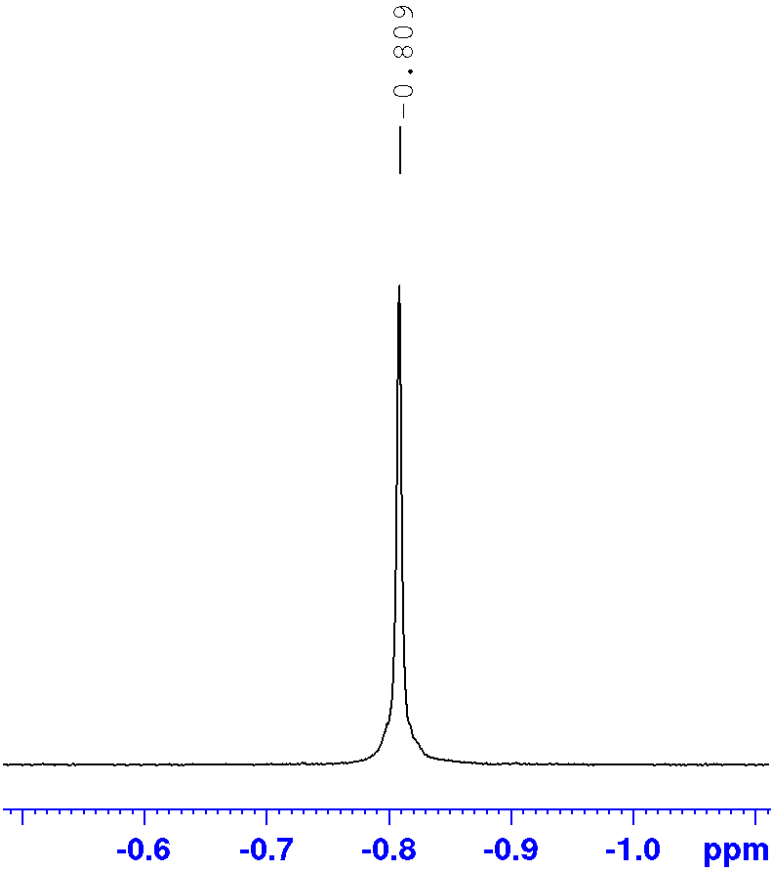


Figure S7. The $^{31}P\{^{1}H\}$ NMR spectrum of $(C_6H_5O)_2P(O)[NH\text{-}R\text{-}(+)CH(CH_3)(C_6H_5)]$ in DMSO-d_6.

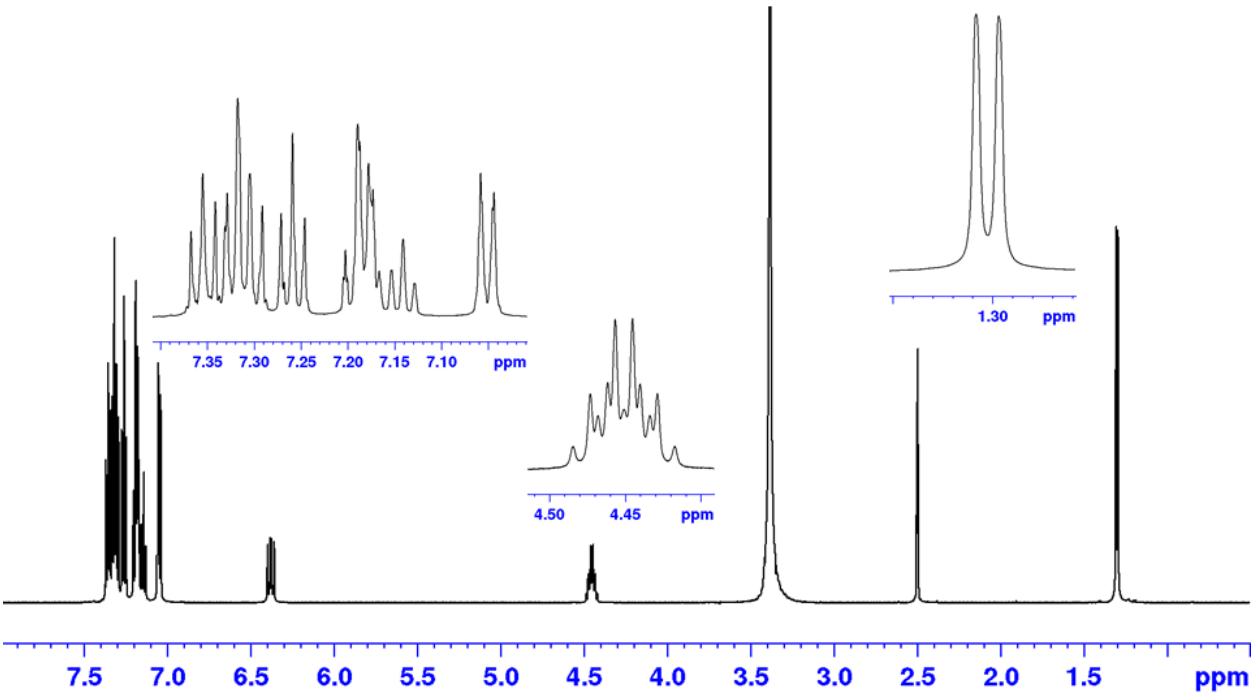


Figure S8. The ^{1}H NMR spectrum of $(C_6H_5O)_2P(O)[NH\text{-}R\text{-}(+)CH(CH_3)(C_6H_5)]$ in DMSO-d_6.

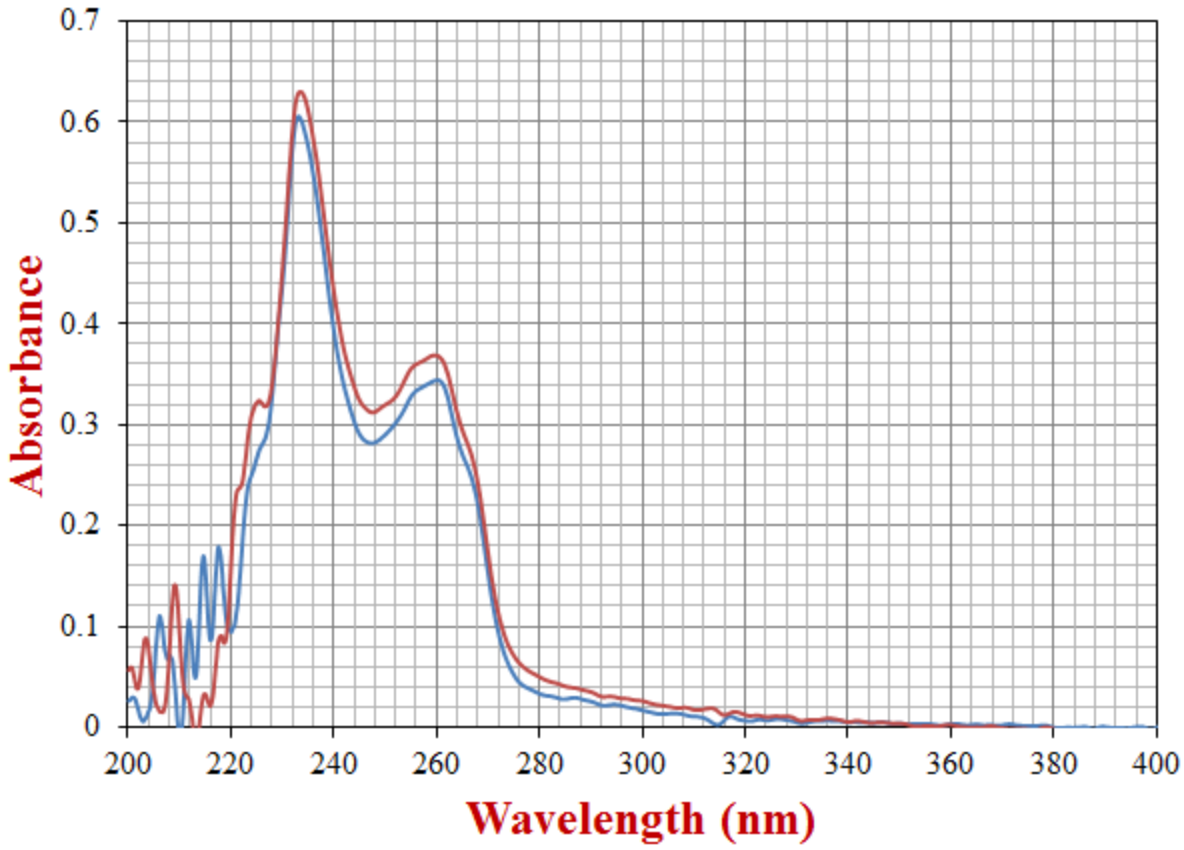


Figure S9. The UV spectra of $(C_6H_5O)_2P(O)[NH\text{-}R\text{-}(+)CH(CH_3)(C_6H_5)]$ (blue) and $(C_6H_5O)_2P(O)[NH\text{-}S\text{-}(–)CH(CH_3)(C_6H_5)]$ (red) in CH_3CN.

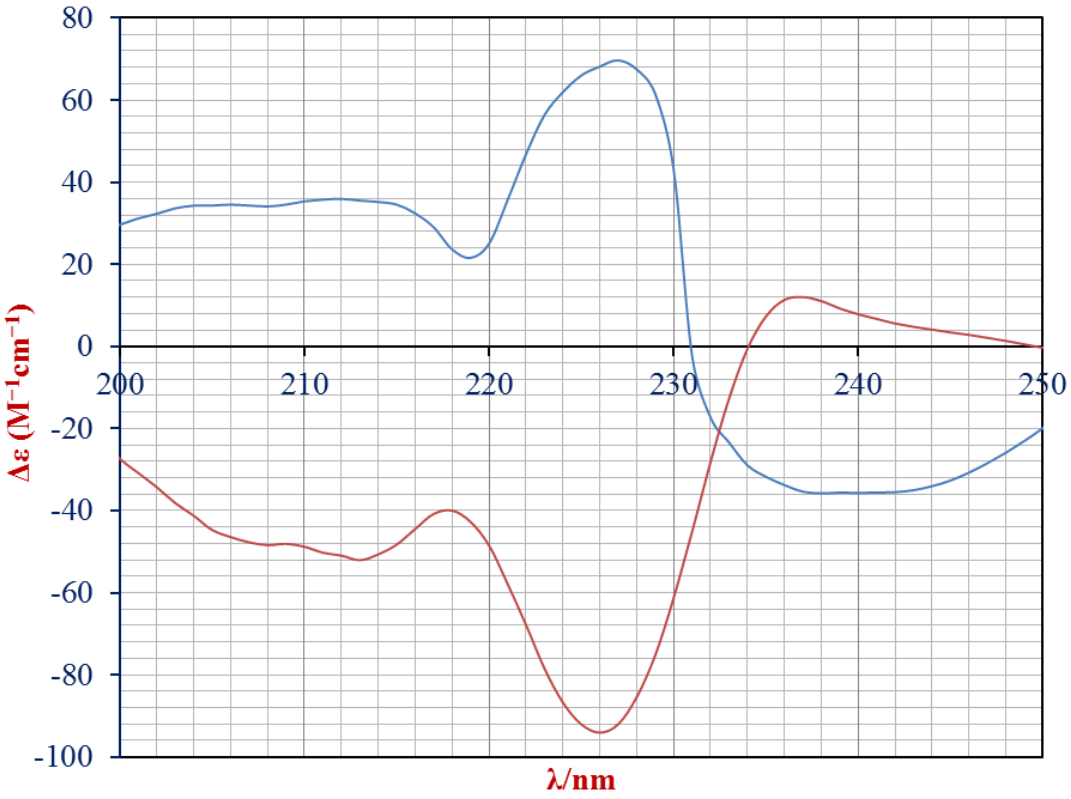


Figure S10. CD spectra of (I) (blue) and (II) (red) in $CHCl_3$ solution.