Supplementary Material

Synthesis of new, optically active 1-(substituted aryl)pyrrole derivatives via atropisomerism directed diastereoselective metalation

Angelika Thurner[a], Bernadett Vas-Feldhoffer[b], Éva Bottka[b], Tamás Holczbauer[c], Miklós Nyerges[d] and Ferenc Faigl[a,b]*

[a] *MTA-BME Organic Chemical Technology Research Group, Hungarian Academy of Sciences, H-1111 Budapest, Budafoki út 8., Hungary*
[b] *Department of Organic Chemistry and Technology, Budapest University of Technology and Economics, H-1111 Budapest, Budafoki út 8., Hungary*
[c] *Institute of Structural Chemistry, Hungarian Academy of Sciences, 1117 Budapest, Magyar tudósok körútja 2., Hungary*
[d] *Servier Research Institute of Medicinal Chemistry, H-1031 Budapest, Záhony u. 7., Hungary*
E-mail: ffaigl@mail.bme.hu

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Table S1. Summary of crystallographic data, data collection, structure determination and refinement for crystal (*R*$_a$,*S*)-(+)-**7a**

Empirical formula	$C_{16}H_{17}NO_4$
Formula weight	287.31
Temperature	295(2)
Radiation and wavelength	Mo-Kα, λ =0.71075 Å
Crystal system	orthorhombic
Space group	*P* 2_1 2_1 2_1
Unit cell dimensions	*a* = 8.1717(6)Å
	b = 8.9080(7)Å
	c = 21.0551(18)Å
	α = 90.00°
	β = 90.00°
	γ = 90.00°
Volume	1532.7(2)Å^3
Z, Z'	4, 1
Density (calculated)	1.245 Mg/m^3
Absorption coefficient, μ	0.090 mm^{-1}
F(000)	608
Crystal colour	colourless
Crystal description	prism
Crystal size	0.45 x 0.45 x 0.30 mm
Absorption correction	numerical
Max. and min. transmission	0.98 and 0.96
θ–range for data collection	3.00 ≤ θ ≤ 22.21°
Index ranges	-8 ≤ *h* ≤8; -9≤ *k* ≤9; -22 ≤ *l* ≤22
Reflections collected	21813
Completeness to 2θ	0.997
Independent reflections	1935 [*R*(int) =0.0423]
Reflections *I*>2σ(*I*)	1609
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	1935 /0 /192
Final *R* indices [*I*>2σ(*I*)]	R_1 = 0.0415, wR^2 = 0.1017
R indices (all data)	R_1 = 0.0511, wR^2 = 0.1058
Max. and mean shift/esd	0.000; 0.000
Largest diff. peak and hole	0.10 and -0.10 e.Å^{-3}

Crystallographic data (including structure factors) for the structure in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC 1032325. E-mail: deposit@ccdc.cam.ac.uk).