

## Supplementary Material

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

Angelika Thurner<sup>a</sup>, Bernadett Vas-Feldhoffer<sup>b</sup>, Éva Bottka<sup>b</sup>, Tamás Holczbauer<sup>c</sup>,  
Miklós Nyerges<sup>d</sup> and Ferenc Faigl<sup>a,b\*</sup>

<sup>a</sup> MTA-BME Organic Chemical Technology Research Group, Hungarian Academy of Sciences,  
H-1111 Budapest, Budafoki út 8., Hungary

<sup>b</sup> Department of Organic Chemistry and Technology, Budapest University of Technology and  
Economics, H-1111 Budapest, Budafoki út 8., Hungary

<sup>c</sup> Institute of Structural Chemistry, Hungarian Academy of Sciences, 1117 Budapest, Magyar  
tudósok körútja 2., Hungary

<sup>d</sup> Servier Research Institute of Medicinal Chemistry, H-1031 Budapest, Záhony u. 7., Hungary  
E-mail: [ffaigl@mail.bme.hu](mailto:ffaigl@mail.bme.hu)

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

Empirical formula	C <sub>16</sub> H <sub>17</sub> NO <sub>4</sub>
Formula weight	287.31
Temperature	295(2)
Radiation and wavelength	Mo-K $\alpha$ , $\lambda$ = 0.71075 Å
Crystal system	orthorhombic
Space group	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell dimensions	<i>a</i> = 8.1717(6) Å
	<i>b</i> = 8.9080(7) Å
	<i>c</i> = 21.0551(18) Å
	$\alpha$ = 90.00°
	$\beta$ = 90.00°
	$\gamma$ = 90.00°
Volume	1532.7(2) Å <sup>3</sup>
<i>Z</i> , <i>Z'</i>	4, 1
Density (calculated)	1.245 Mg/m <sup>3</sup>
Absorption coefficient, $\mu$	0.090 mm <sup>-1</sup>
<i>F</i> (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
$\theta$ -range for data collection	3.00 ≤ $\theta$ ≤ 22.21°
Index ranges	-8 ≤ <i>h</i> ≤ 8; -9 ≤ <i>k</i> ≤ 9; -22 ≤ <i>l</i> ≤ 22
Reflections collected	21813
Completeness to 2 $\theta$	0.997
Independent reflections	1935 [ <i>R</i> (int) = 0.0423]
Reflections <i>I</i> > 2 $\sigma$ ( <i>I</i> )	1609
Refinement method	full-matrix least-squares on <i>F</i> <sup>2</sup>
Data / restraints / parameters	1935 / 0 / 192
Final <i>R</i> indices [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0415, <i>wR</i> <sup>2</sup> = 0.1017
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.0511, <i>wR</i> <sup>2</sup> = 0.1058
Max. and mean shift/esd	0.000; 0.000
Largest diff. peak and hole	0.10 and -0.10 e.Å <sup>-3</sup>

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](mailto:deposit@ccdc.cam.ac.uk).