Supporting Information

A novel homochiral metal–organic framework with expanded open cage based on (*R*)-3,3'-bis(6-carboxy-2-naphthyl)-2,2'-dihydroxy-1,1'binaphthyl: Synthesis, X-ray structure and efficient HPLC enantiomer separation

Koichi Tanaka,*^a Tomohiro Kawakita^a, Maja Morawiak,^b and Zofia Urbanczyk-Lipkowska^{*b}

^aDepartment of Chemistry and Materials Engineering, Faculty of Chemistry, Materials and Bioengineering, Kansai University, Suita, Osaka 564-8680, Japan. E-mail: ktanaka@kansai-u.ac.jp

^bInstitute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warszawa, Poland. Fax: +48 22 6326681; Tel: +48 22 3432207; E-mail: ocryst@icho.edu.pl.



Fig. S1 IR spectrum of (*R*)-3,3'-bis(6-methoxycarbonyl-2-naphthyl)-2,2'-bis(methoxymethoxy)-1,1'-binaphthyl



Fig. S2 ¹H-NMR spectrum of (R)-3,3'-bis(6-methoxycarbonyl-2-naphthyl)-2,2'-

bis(methoxymethoxy)-1,1'-binaphthyl



Fig. S3 ¹³C-NMR spectrum of (*R*)-3,3'-bis(6-methoxycarbonyl-2-naphthyl)-2,2'bis(methoxymethoxy)-1,1'-binaphthyl



Fig. S4 IR spectrum of (R)-3,3'-bis(6-methoxycarbonyl-2-naphthyl)-2,2'-dihydroxy-1,1'-binaphthyl



Fig. S5 ¹H-NMR spectrum of (R)-3,3'-bis(6-methoxycarbonyl-2-naphthyl)-2,2'-dihydroxy-



1,1'-binaphthyl

Fig. S6 ¹³C-NMR spectrum of (*R*)-3,3'-bis(6-methoxycarbonyl-2-naphthyl)-2,2'-dihydroxy-1,1'-binaphthyl



Fig. S7 IR spectrum of (R)-3,3'-bis(6-carboxy-2-naphthyl)-2,2'-dihydroxy-1,1'-binaphthyl



Fig. S8 ¹H-NMR spectrum of (*R*)-3,3'-bis(6-carboxy-2-naphthyl)-2,2'-dihydroxy-1,1'-binaphthyl



Fig. S9¹³C-NMR spectrum of (*R*)-3,3'-bis(6-carboxy-2-naphthyl)-2,2'-dihydroxy-1,1'-binaphthyl



Fig. S10 IR spectrum of (R)-CuMOF-2



Fig. S11 TG trace of (*R*)-CuMOF-2



Fig. S12 SEM image of (*R*)-CuMOF-**2**-silica



Compound 3 (MIDSIC)¹



Compound 8 (ZIHHAZ) ³



Compound 5 (OKOZAQ)²



Compound 13 (ITELOQ) 4

Fig. S13 X-ray structures and molecular dimensions of representative racemic compounds; the narrowest dimension does not exceed size of a phenyl ring, i.e. ca 4.7 Å.

References

- 1) MIDSIC: K. Kodama, Y. Kobayashi, K. Saigo, Cryst. Growth Des., 2007, 7, 935-939.
- 2) OKOZAQ: M. Akazome, A. Doba, S. Matsumoto, K. Ogura, J. Org. Chem., 2010, 75, 660-665.
- 3) ZIHHAZ: P. P. Korkas, E. Weber, M. Ctugler, G. Naray-Szaboc, Chem. Commun., 1995, 2229-2230.
- ITELOQ: D. Zhao, X.-H. Liu, Z.-Z. Shi, C.-D. Zhu, Y. Zhao, P. Wang, W.-Y. Sun, *Dalton Trans.*, 2016, 45, 14184-14190.