Supplementary Information

Semi-quantitative Evaluation of Molecular Meshing by Surface Analysis with Varying Probe Radius

Naru Tanaka,[1] Yi-Yang Zhan,[1] Yuka Ozawa,[1] Tatsuo Kojima,[1] Takuya Koide,[2] Takako Mashiko,[2] Umpei Nagashima,[3] Masanori Tachikawa[2] and Shuichi Hiraoka[1,*]

[1]Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro-ku, Tokyo 153-8902, Japan
[2]Quantum Chemistry Division, Graduate School of Science, Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa 236-0027, Japan
[3]Foundation for Computational Science (FOCUS), 7-1-28, Minatojimaminatomachi, Chuo-ku, Kobe, 650-0047, Japan

E-mail: chiraoka@mail.ecc.u-tokyo.ac.jp

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1. SAVPR (surface analysis with varying probe radius)

1.1 Method

Surface areas of the assembled and disassembled state, $A_{as}(D)$ and $A_{dis}(D)$, were calculated as the Connolly surface areas of the assembled and disassembled state with a probe sphere with a diameter of D, respectively, using Materials Studio software (version 8.0; Biovia Inc., USA). In this study, dD = 0.02 Å was adopted.

1.2 SAVPR for nanocubes

Geometry optimization for nanocubes **BM**, **PM**, **HM**, and **BD** in water and iodide ions was performed by molecular mechanics (MM) calculation with AMBER14 program package.[1] The initial coordinates for **PM** were used from the X-ray structure, while those for the other nanocubes were replaced by the substituents of the initial structure of **PM**. For the nanocubes, we employed the general AMBER force field[2] and restrained electrostatic potential charges,[3] based on the electrostatic potentials calculated with the HF/6-31G(d) method.[4] For water molecules and iodide ions, TIP4P/Ew force field[5] was used. The total numbers of water molecules were 10914, 10915, 10910, and 10930 for the **BM**, **PM**, **HM**, and **BD** systems, respectively, and the number of iodide ions was 12. Ten water molecules and one iodide ion were encapsulated in the nanocubes.

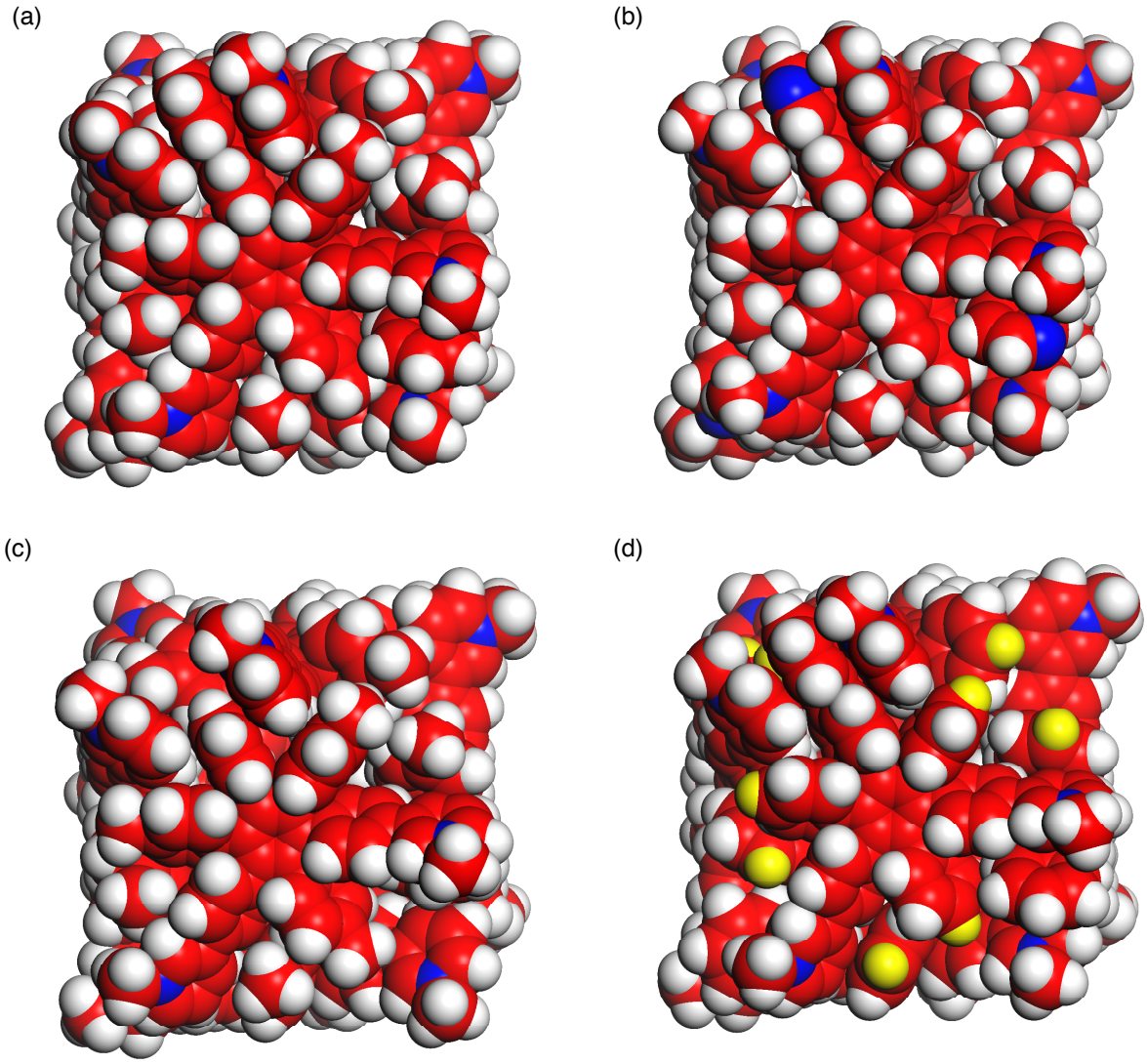

Figure S1. Optimized structures of nanocubes by MM calculation. (a) **BM**. (b) **PM**. (c) **HM**. (d) **BD**. Color labels: red, carbon; white, hydrogen; blue, nitrogen; yellow, deuterium.

1.3 SAVPR for 1:1 host-guest complexes

SAVPR for 1:1 host-guest complexes of CB[7] and α-CD hosts was conducted with the reported crystal structures[6–28] (Figures S2 and S3). In some crystals, there are several structures because of crystallographic independence or disorders of guest molecules. In such cases, all types of structures were adopted. Hydrogen atoms were attached manually to the atoms, when the structure lacks hydrogen atom(s). The positions of these attached H atoms were optimized by means of MM calculation with COMPASS II force field in Materials Studio software (version 8.0; Biovia Inc., USA).

The CB[7] complexes with guest **G1**, **G2**, **G3**, and **G4** lie much higher than eq. (1) on Figure 2 in the main text.

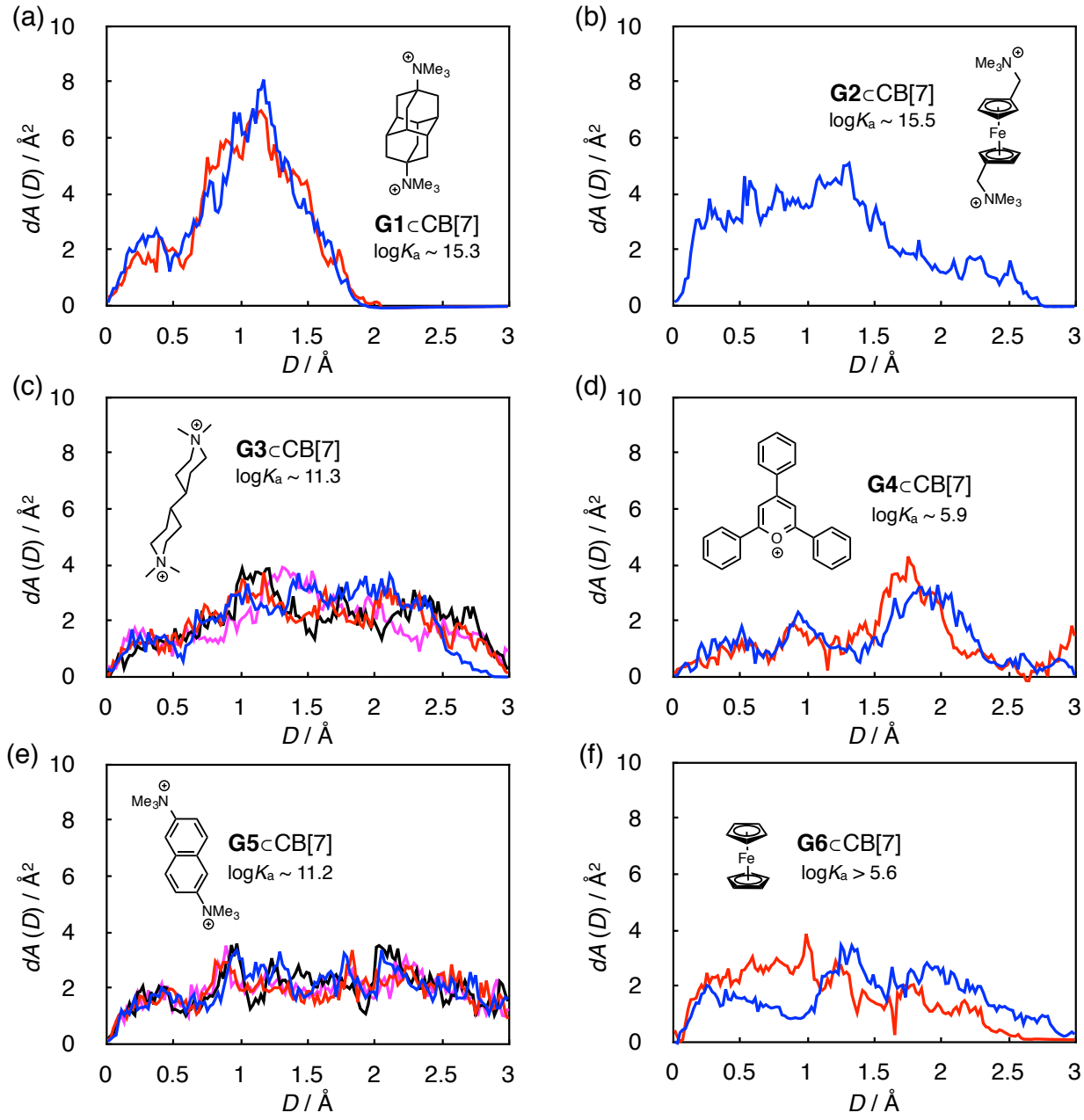

Figure S2. (a)–(i) SAVPR for 1:1 complexes of CB[7] with guest **G1**–**G9**.

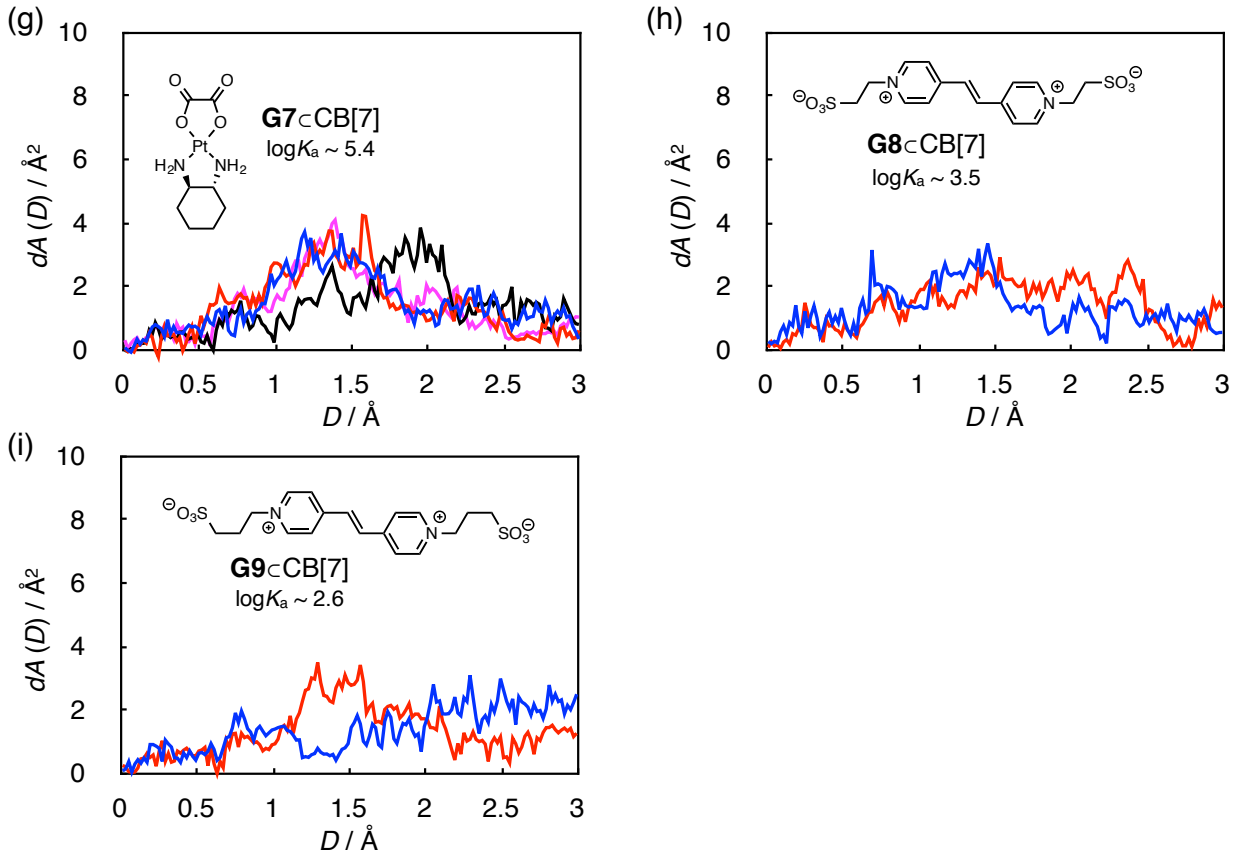

Figure S2. (*continued*).

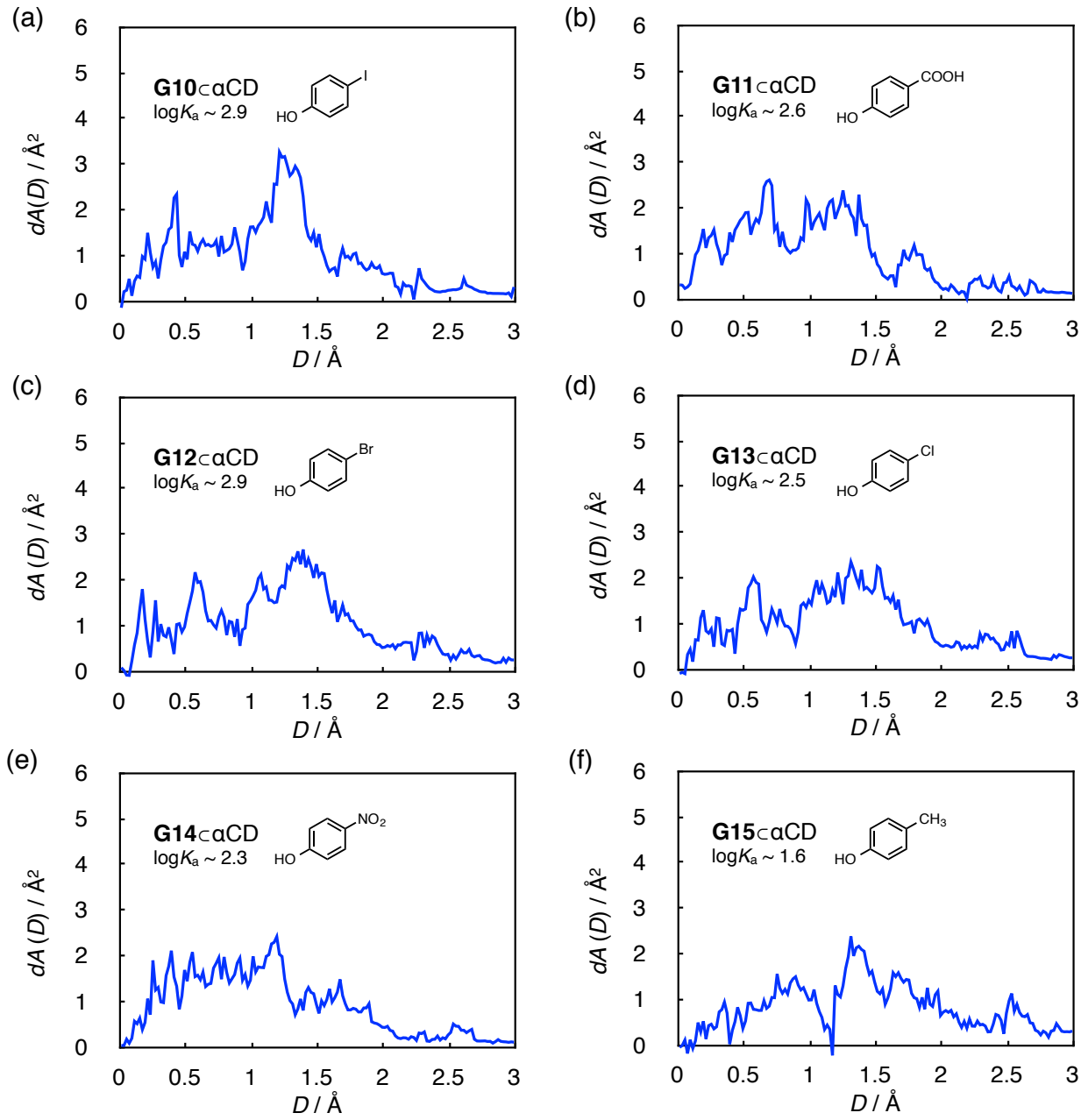

Figure S3. (a)–(r) SAVPR for 1:1 complexes of α-CD with guest **G10**–**G27**.

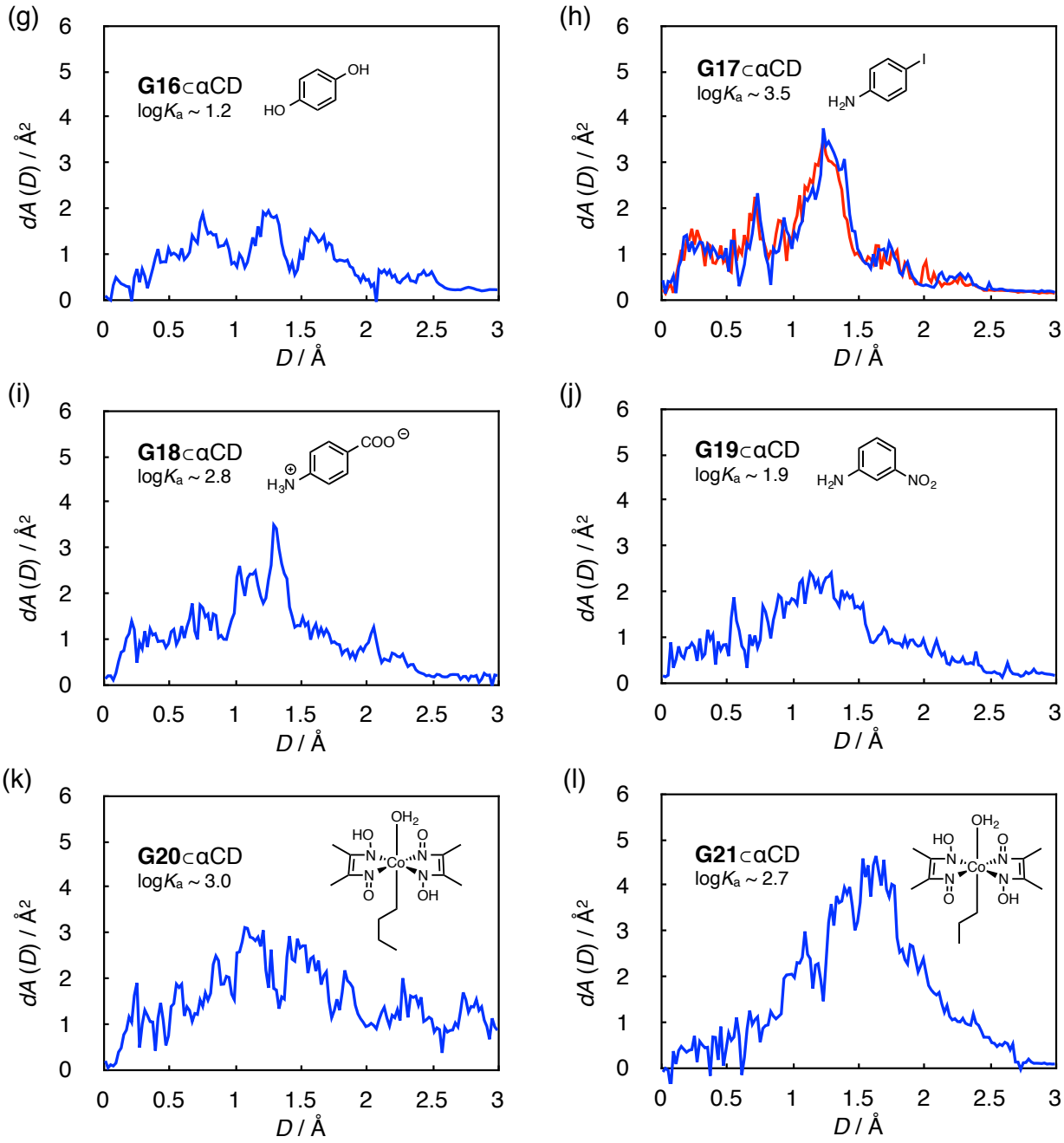

Figure S3. (*continued*).

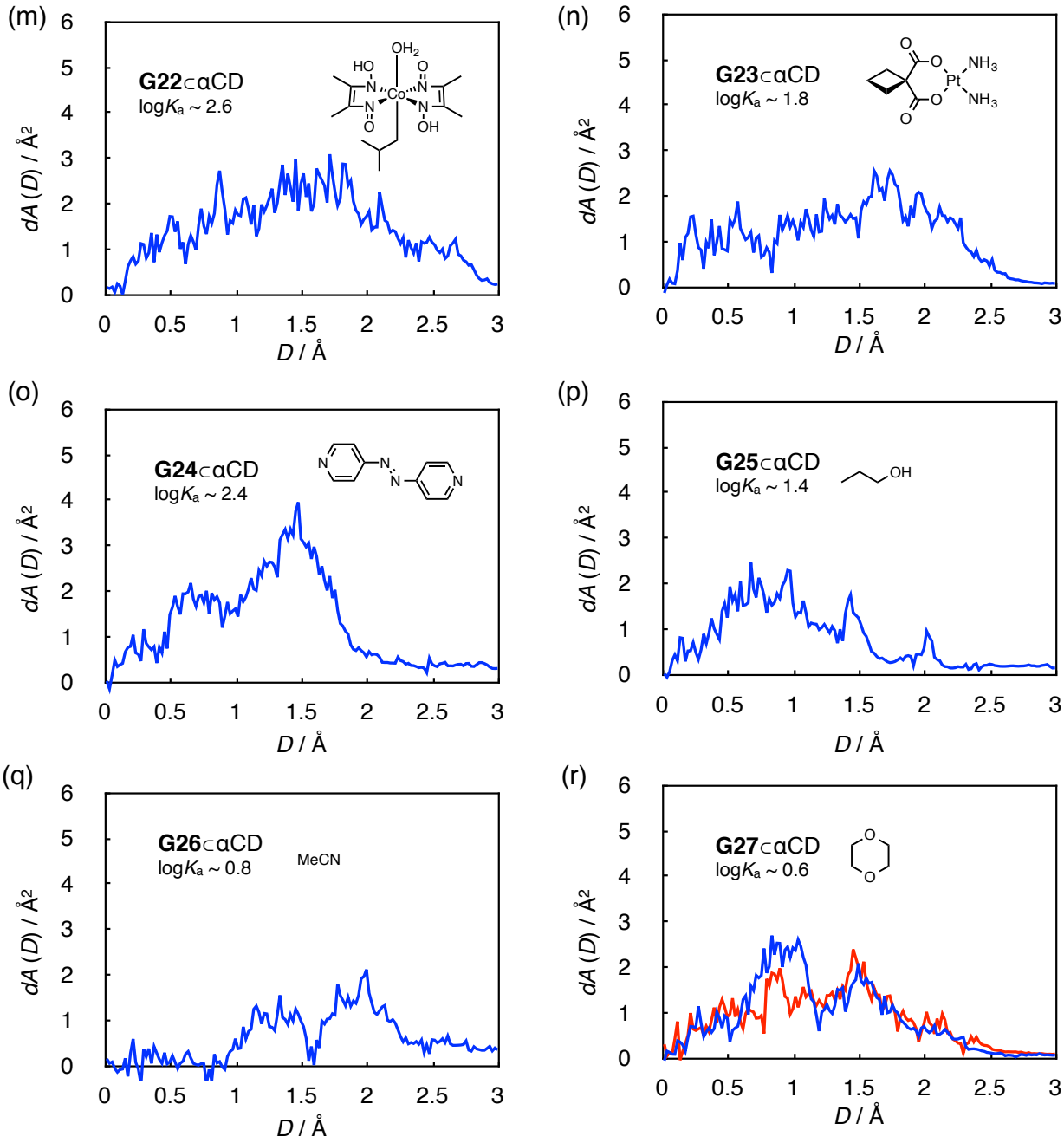

Figure S3. (*continued*).

2. References

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