Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Molecular dynamics approaches to the design and synthesis of PCB targeting molecularly imprinted polymers: interference to monomer-template interactions in imprinting of 1, 2, 3-trichlorobenzene

Dougal Cleland,[a] Gustaf D. Olsson,[b] Björn C. G. Karlsson,[b] Ian A. Nicholls,[c] and Adam McCluskey[a*]

[a] *Chemistry, Centre for Chemical Biology, The University of Newcastle, Callaghan, NSW 2308, Australia. Fax:+61 2 4921 5472; Tel: +61 2 4921 5472; E-mail: Adam.McCluskey@Newcastle.edu.au*

[b] *Bioorganic and Biophysical Chemistry Laboratory, Linnæus University Centre for Biomaterials Chemistry, Linnæus University, Kalmar, SE-391 82 Kalmar, Sweden*

[c] *Department of Chemistry-BMC, Uppsala University, Box 576, SE-751 23 Uppsala, Sweden*

Supplementary Data

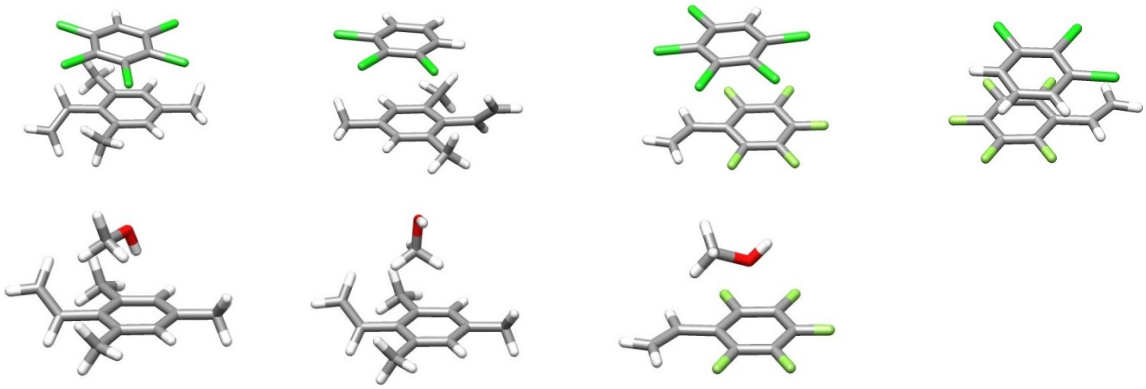

Figure S1. EFP energy optimised configurations and intermolecular separation of (**A**) TMS-**1** in a π-π stacking interaction; 3.6 Å separation; (**B**) TMS-**2** in a π-π stacking interaction; 3.6 Å separation; (**C**) PFS-**1** in a π-π stacking interaction; 3.5 Å separation; (**D**) PFS-**2** in a π-π stacking interaction; 3.5 Å separation; (E) TMS-MeOH in a hydrogen bond configuration; 2.5 Å separation $MeOH_{H2}$-TMS_{C1}; 3.4 Å separation $MeOH_{O2}$-TMS_{C1}; 3.8 Å separation $MeOH_{C1}$-TMS_{C1}; (F) TMS-MeOH in a perpendicular configuration; 3.5 Å separation $MeOH_{C1}$-TMS_{C1} and (G) PFS-MeOH in a lone pair–π orbital interaction; 3.1 Å separation $MeOH_{O1}$-PFS_{C1}. Atom colours; grey = carbon, white = hydrogen and green = chlorine.

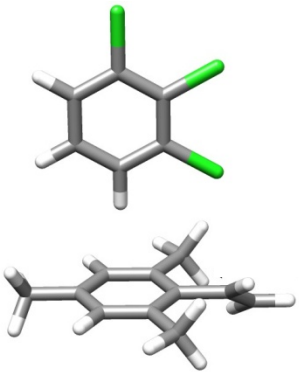

Figure S2: T-shape interaction between **2** and TMS.

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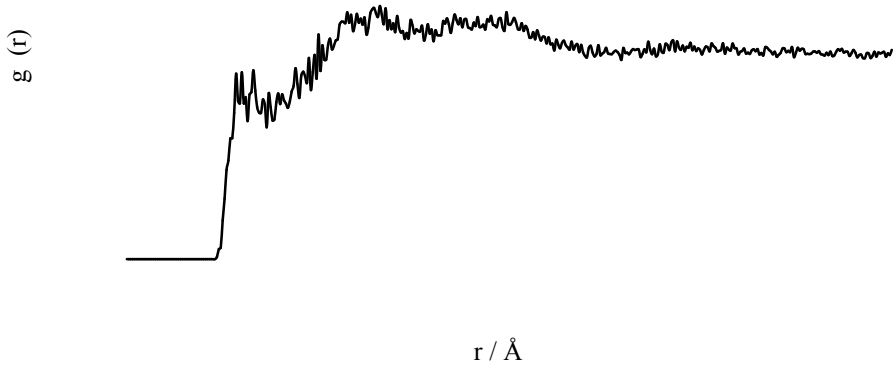

Figure S3: RDF showing the density of $\mathbf{2}_{H1}$ as a function of the distance from TMS_{C1} during S2.

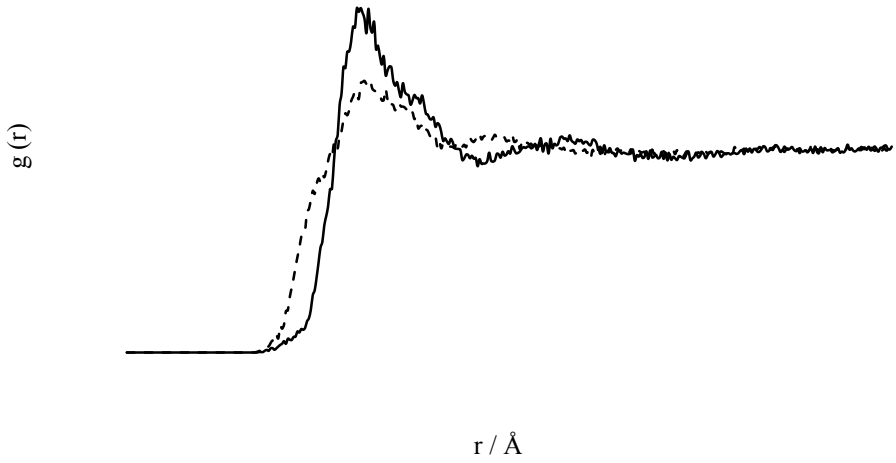

Figure S4: RDFs showing the density of TMS_{C1} as a function of the distance from TMS atoms during S2. TMS_{C1} –TMS_{C4} (- - -) and TMS_{C1} –TMS_{C1} (—).

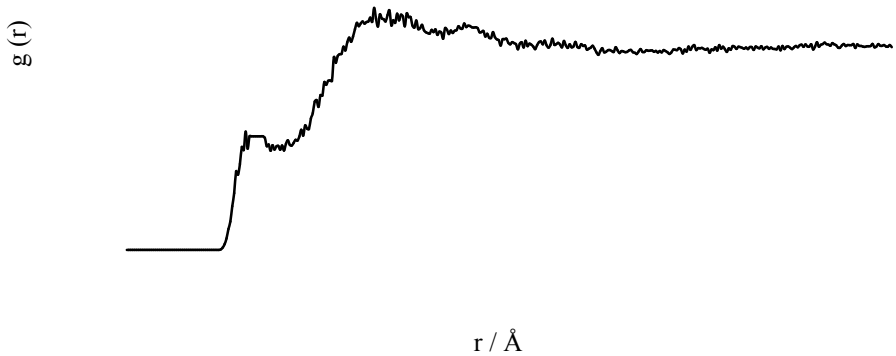

Figure S5: RDF showing the density of TMS_{H3} as a function of the distance from TMS_{C1} during S2.

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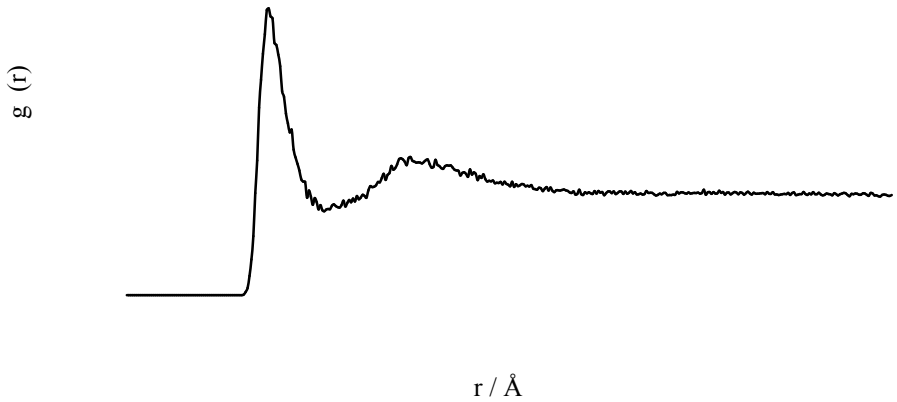

Figure S6: RDF showing the density of PFS_{C1} as a function of the distance from PFS_{C1} during S4.

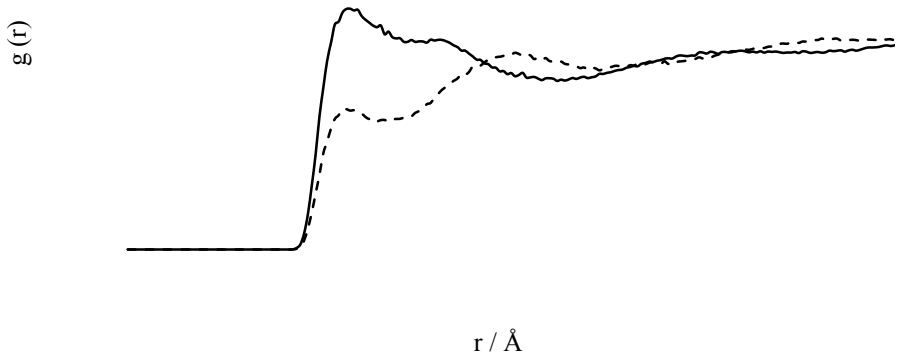

Figure S7: RDFs showing the density of $EGDMA_{-O5}$ atoms as a function of the distance from PFS atoms during S4. $EGDMA_{O5}$ –PFS_{H5} (- - -) and $EGDMA_{O5}$ –PFS_{H6} (—).

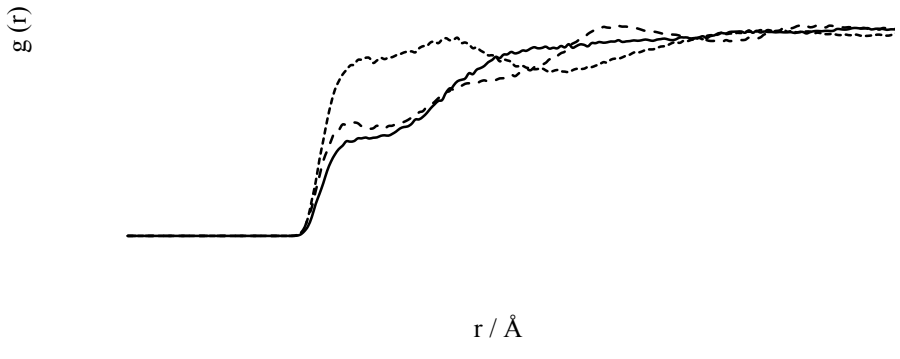

Figure S8: RDFs showing the density of $EGDMA_{-O5}$ atoms as a function of the distance from TMS atoms during S2. $EGDMA_{O5}$ –TMS_{H3} (- - -), $EGDMA_{O5}$ –TMS_{H5} (⋯) and $EGDMA_{O5}$ –TMS_{H6} (—)