Supporting Information
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Entropic Separations of Mixtures of Aromatics by Selective Face-to-Face Molecular Stacking in One-Dimensional Channels of Metal–Organic Frameworks and Zeolites

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Entropic Separations of Mixtures of Aromatics by Selective Face-to-Face Molecular Stacking in One-Dimensional Channels of Metal-Organic Frameworks and Zeolites
Single component isotherms in AFI zeolite at 433K

Figure S1: Single component isotherms in AFI zeolite at 433K. At saturation conditions, benzene and o-xylene can reach higher loadings because of molecular reorientation. This can be exploited as a separation mechanism in liquid conditions.
Single component isotherms in MAZ zeolite at 433K

Figure S2: Single component isotherms in MAZ zeolite at 433K. The smaller channel of MAZ compared to AFI allows for a better reorientation of benzene.
Heat of adsorption in AFI and MAZ zeolite

Figure S3: Infinite dilution heat of adsorption of benzene, o-, m-, p-xylene and ethylbenzene in AFI (left) and MAZ (right) zeolites at different temperatures. For AFI zeolite, our results agree qualitatively with the experimental results of Chiang et al. [1]. In the Henry regime, benzene is the least strongly adsorbed species in both zeolites.
Langmuir-Freundlich parameters for pure component aromatics at 433K in AFI

Table S1: Dual-site Langmuir-Freundlich parameters for pure component xylene isomers at 433 K in AFI. The saturation capacities are expressed in molecules per unit cell; these numbers need to be multiplied by the conversion factor of 1.082 to get mol kg$^{-1}$.

$$q_i = q_{i,A,sat} \frac{b_{i,A} f_i^{\nu_{i,A}}}{1 + b_{i,A} f_i^{\nu_{i,A}}} + q_{i,B,sat} \frac{b_{i,B} f_i^{\nu_{i,B}}}{1 + b_{i,B} f_i^{\nu_{i,B}}}$$ (4.1)
Figure S4: Fe$_2$(BDP)$_3$ variant with a 4,4$'$-bis(1H-pyrazol-4-yl)biphenyl instead of a BDP linker. The topology of the metal organic framework is the same as the Fe$_2$(BDP)$_3$, triangular 1D channels running in the z-direction, but the size of the channels is larger due to the extra aromatic molecule in the linker. Color code: organic linker (cyan), iron (brown), nitrogen (blue).
Single component isotherms of trichlorobenzene isomers

**Figure S5:** Single component isotherms of 1,3,5-/1,2,4- and 1,2,3-trichlorobenzene in Fe$_2$(BDP)$_3$ variant at 433K. The 1,3,5-trichlorobenzene is the only isomer that can reorient within the metal-organic framework channels, which permits a higher saturation capacity.

<table>
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<th>Isomer</th>
<th>$q_{i,A,\text{sat}}$ [mol. kg$^{-1}$]</th>
<th>$b_{i,A}$ [Pa$^{-\nu_{i,A}}$]</th>
<th>$\nu_{i,A}$ [-]</th>
<th>$q_{i,B,\text{sat}}$ [mol. kg$^{-1}$]</th>
<th>$b_{i,B}$ [Pa$^{-\nu_{i,B}}$]</th>
<th>$\nu_{i,B}$ [-]</th>
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<td>0.41</td>
<td>2.1</td>
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<td>0.44</td>
<td>2.2</td>
<td>$2.2 \times 10^{-2}$</td>
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</tbody>
</table>

**Table S1:** Dual-site Langmuir-Freundlich parameters for pure component trichlorobenzene isomers at 433 K in Fe$_2$(BDP)$_3$ variant. The saturation capacities are expressed in mol kg$^{-1}$.