Table 1: Calculated surface areas (m^2/g) for the 13 MOFs with GCMC isotherms. Cases where a software does not find a surface area are denoted by N/A. Zeo++ calculations are conducted with the same CIF files used to generate GCMC isotherms, and a 1.67 Å radius probe N_2 molecule, the high accuracy flag, and 2,000 Monte Carlo samples per atom are used. All other software take as input the GCMC isotherms.

	SESAMI 1 (BET)	SESAMI 1 (BET+ESW)	SESAMI 2 (LASSO)	BETSI	pyGAPS	BEaTmap	Zeo++
HKUST-1	2001	1933	2089	1962	1902	1980	2397
IRMOF-1	3502	3543	3123	3519	3504	N/A	3722
MIL-100 (Cr)	2107	1853	2111	1799	1852	2094	1957
MIL-100 (Fe)	2386	2438	2203	2426	82	2423	1933
MIL-101	3828	2862	2944	2879	2939	3331	3164
MIL-53 (Al)	1221	1168	1405	1164	1183	1212	1510
MOF-74 (Mg)	1828	1834	1902	1815	1839	1791	1796
MOF-808	44	N/A	1275	1172	N/A	1147	1690
NU-1000	2439	2181	2633	2082	2144	2672	3050
NU-1200	2711	934	2601	1077	1073	2930	3192
NU-1500 (Fe)	3543	3594	3111	3756	3758	3492	3944
UiO-66	1239	1239	1443	1201	1242	1304	1289
ZIF-8	1429	1386	1575	1381	1390	1414	1588

Table 2: Comparison between calculated surface areas from software for isotherm to surface area calculation and from Zeo++, over the 13 MOFs with GCMC isotherms. The mean absolute percent error and Pearson correlation coefficient are taken with respect to Zeo++ calculations for each software, over all successful surface area calculations for that software.

Surface area calculation software	Mean absolute percent error (MAPE)	Pearson correlation coefficient	Successful calculations (out of 13)
SESAMI 1 (BET)	19.4	0.85	13
SESAMI 1 (BET+ESW)	17.9	0.72	12
SESAMI 2 (LASSO)	12.4	0.95	13
BETSI	18.7	0.77	13
pyGAPS	23.0	0.75	12
BEaTmap	12.6	0.93	12

Table 3: Calculated surface areas (m^2/g) for the 9 MOFs with experimental isotherms. All software take as input the experimental isotherms.

	SESAMI 1 (BET)	SESAMI 1 (BET+ESW)	SESAMI 2 (LASSO)	BETSI	pyGAPS	BEaTmap
HKUST-1	1505	1466	1668	1500	1495	1498
MOF-74 (Mg)	1580	1467	1692	1575	1574	1565
MOF-808	1998	900	1727	1021	2439	1752
NU-1000	2154	2090	2385	2229	2654	2459
NU-1200	2893	2718	2781	2758	3917	3069
NU-1500 (Fe)	3305	3409	2809	3328	3413	3227
SIFSIX-3 (Ni)	356	201	716	355	355	353
UiO-66	1251	1228	1413	1250	1249	1246
ZIF-8	1092	910	1214	1082	1082	1047