Electronic Supplementary Information

Multi-objective *de novo* molecular design of organic structure-directing agents for zeolites using nature-inspired ant colony optimization

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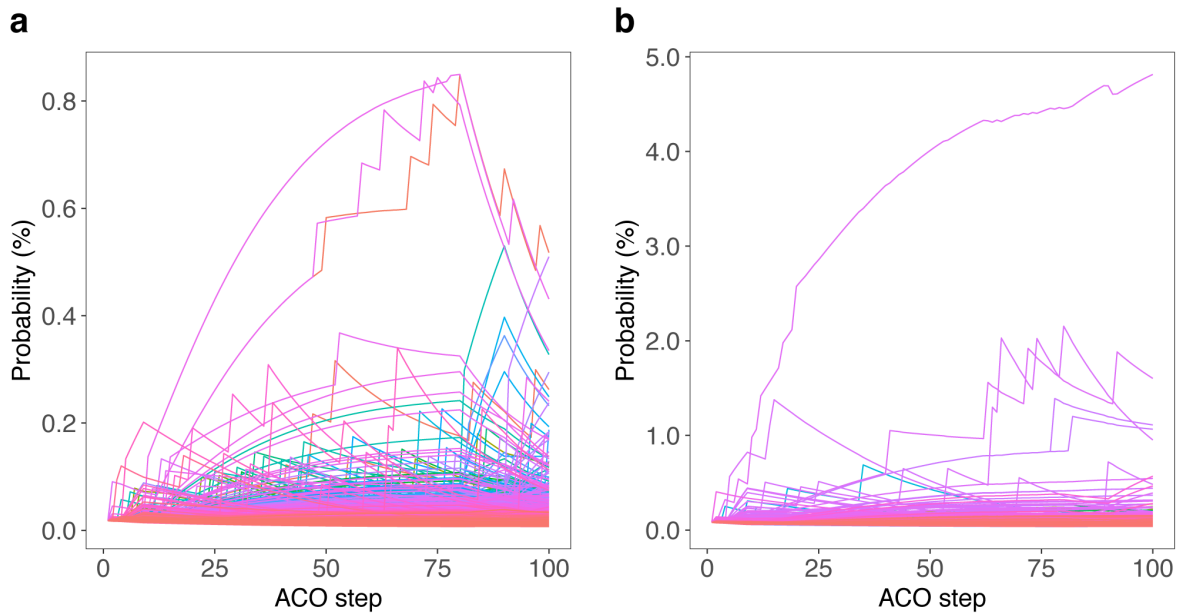
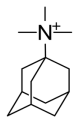
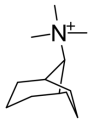
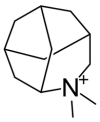
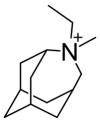
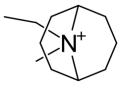
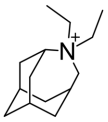
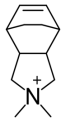
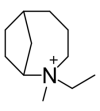
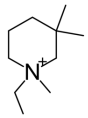


Figure S1. Typical trajectory of normalized amount of pheromone (*i.e.*, probability) deposited on chemicals for a single run for **CHA** without considering the cost of chemicals (a cost adjustable parameter, β = 0) during first 100 steps. a) Trajectory of probability that an amine is selected. b) Trajectory of probability that a halide is selected.

Table S1. Experimentally proven OSDAs for the synthesis of aluminosilicate **CHA** zeolite and their corresponding stabilization energies.

	OSDA	E_s (kJ mol_{Si}^{-1})	
1		−16.8	[1]
31		−16.5	[2]
32		−15.6	[3]
33		−15.2	[3]
34		−15.1	[2]
35		−14.8	[3]
36		−14.5	[3]
37		−14.4	[2]
38		−13.7	[3]
39		−13.5	[3]
40		−13.4	[4]

41		−12.6	[3]
42		−12.1	[3]
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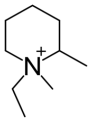
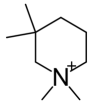
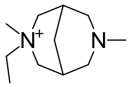
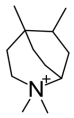
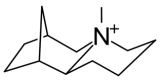
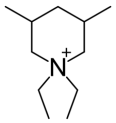
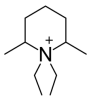
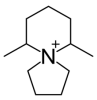
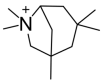
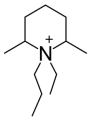
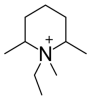
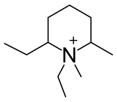
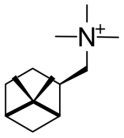
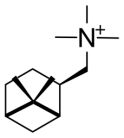
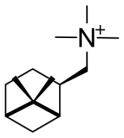
44		−11.9	[3]
45		−11.9	[3]
46		−11.2	[3]
47		−10.3	[4]
48		−9.9	[3]
49		−9.4	[4]

Table S2. Experimentally proven OSDAs for the synthesis of aluminosilicate **AEI** zeolite and their corresponding stabilization energies.[5]

	OSDA	E_s (kJ mol_{Si}^{-1})
50		−16.9
19		−16.2
51		−15.7
52		−15.5
53		−15.5
54		−15.3
55		−15.0
56		−14.9
57		−14.9
58		−14.8
59		−14.4

60		−14.0
61		−13.2

Table S3. Experimentally proven OSDAs for the synthesis of aluminosilicate **CON** zeolite and their corresponding stabilization energies.

	OSDA	OSDA/u.c.	E_s (kJ/mol$_{Si}$)
25		2	−6.1
25		3	−8.2
25		4	−11.4

References

[1] S. I. Zones, US Patent 4,544,538, 1985.

[2] Y. Kubota, M. M. Helmkamp, S. I. Zones and M. E. Davis, *Microporous Mater.*, 1996, **6**, 213–229.

[3] P. Wagner, Y. Nakagawa, G. S. Lee, M. E. Davis, S. Elomari, R. C. Medrud and S. I. Zones, *J. Am. Chem. Soc.*, 2000, **122**, 263–273.

[4] A. W. Burton, G. S. Lee and S. I. Zones, *Microporous Mesoporous Mater.*, 2006, **90**, 129–144.

[5] J. E. Schmidt, M. W. Deem, C. Lew and T. M. Davis, *Top. Catal.*, 2015, **58**, 410–415.