

### Supporting Information: Table S3

#### List of reactions and their catalysts in ACS(36,28) (referred in Fig. 14 of main text)

The table lists all the reactions with their respective catalysts in the example of a catalyzed chemistry, quoted in the main text, containing a cascade of nested ACSs for  $f = 2$  generated using Algorithm 4. The steady state concentrations for this chemistry are displayed in Fig. 14. This chemistry was generated with  $g = 7$  and  $n_k = 3$ .

The molecules in various generations are as follows:  $P_0 = \{(1, 0), (0, 1)\}$ ,  $P_1 = \{(1, 1), (0, 2), (2, 0)\}$ ,  $P_2 = \{(1, 3), (2, 2), (3, 0)\}$ ,  $P_3 = \{(2, 6), (2, 3), (5, 2)\}$ ,  $P_4 = \{(4, 6), (7, 4), (7, 8)\}$ ,  $P_5 = \{(8, 12), (6, 12), (14, 8)\}$ ,  $P_6 = \{(14, 24), (22, 20), (11, 12)\}$ ,  $P_7 = \{(29, 28), (36, 28), (24, 26)\}$ .

The catalyst for a reaction listed under generation  $P_k$  is added at step  $k$  of algorithm. It is apparent from the reaction table that the ACSs are maximally overlapping, *i.e.*, any ACS of generation  $k$  contains all the reactions of generation  $k - 1$ .

Reaction	Catalyst added in generation						
	$P_1$	$P_2$	$P_3$	$P_4$	$P_5$	$P_6$	$P_7$
$(0, 1) + (0, 1) \rightleftharpoons (0, 2)$	(1, 1)	(1, 3)	(2, 3)	(7, 4)	(8, 12)	(11, 12)	(29, 28)
$(0, 1) + (1, 0) \rightleftharpoons (1, 1)$	(0, 2)	(1, 3)	(2, 6)	(4, 6)	(14, 8)	(22, 20)	(36, 28)
$(1, 0) + (1, 0) \rightleftharpoons (2, 0)$	(1, 1)	(3, 0)	(5, 2)	(7, 4)	(14, 8)	(14, 24)	(29, 28)
$(1, 0) + (2, 0) \rightleftharpoons (3, 0)$		(2, 2)	(5, 2)	(4, 6)	(14, 8)	(14, 24)	(24, 26)
$(1, 1) + (0, 2) \rightleftharpoons (1, 3)$		(1, 3)	(2, 6)	(7, 8)	(8, 12)	(14, 24)	(24, 26)
$(0, 2) + (2, 0) \rightleftharpoons (2, 2)$		(1, 3)	(2, 6)	(7, 8)	(6, 12)	(22, 20)	(29, 28)
$(0, 1) + (2, 2) \rightleftharpoons (2, 3)$			(2, 6)	(7, 4)	(14, 8)	(22, 20)	(24, 26)
$(3, 0) + (2, 2) \rightleftharpoons (5, 2)$			(2, 3)	(7, 8)	(6, 12)	(11, 12)	(29, 28)
$(1, 3) + (1, 3) \rightleftharpoons (2, 6)$			(5, 2)	(7, 8)	(14, 8)	(22, 20)	(24, 26)
$(2, 0) + (2, 6) \rightleftharpoons (4, 6)$				(4, 6)	(14, 8)	(22, 20)	(36, 28)
$(2, 2) + (5, 2) \rightleftharpoons (7, 4)$				(7, 4)	(6, 12)	(14, 24)	(36, 28)
$(5, 2) + (2, 6) \rightleftharpoons (7, 8)$				(7, 4)	(14, 8)	(14, 24)	(36, 28)
$(2, 6) + (4, 6) \rightleftharpoons (6, 12)$					(14, 8)	(11, 12)	(29, 28)
$(4, 6) + (4, 6) \rightleftharpoons (8, 12)$					(14, 8)	(22, 20)	(36, 28)
$(7, 4) + (7, 4) \rightleftharpoons (14, 8)$					(8, 12)	(11, 12)	(36, 28)
$(3, 0) + (8, 12) \rightleftharpoons (11, 12)$						(22, 20)	(36, 28)

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Reaction	Catalyst in generation						
	$P_1$	$P_2$	$P_3$	$P_4$	$P_5$	$P_6$	$P_7$
$(8, 12) + (6, 12) \rightleftharpoons (14, 24)$						(22, 20)	(24, 26)
$(14, 8) + (8, 12) \rightleftharpoons (22, 20)$						(11, 12)	(29, 28)
$(2, 6) + (22, 20) \rightleftharpoons (24, 26)$							(29, 28)
$(7, 8) + (22, 20) \rightleftharpoons (29, 28)$							(29, 28)
$(14, 8) + (22, 20) \rightleftharpoons (36, 28)$							(29, 28)