

**Supporting Information: Table S4****List of reactions and their catalysts in ACS(18,27) (referred in Fig. 15 of main text)**

The table lists all the reactions with their respective catalysts and catalytic strengths in the example of a catalyzed chemistry, quoted in the main text, containing a cascade of partially overlapping ACSs for  $f = 2$  generated using Algorithm 5. The steady state concentrations for this chemistry are displayed in Fig. 15.

The catalyzed chemistry contains 10 generations of ACSs of lengths 3, 6, 10, 15, 19, 25, 30, 35, 40, and 45.

TABLE S4a: **List of reactions in the ACSs of different length and their catalysts.** ACSs of increasing length (using Algorithm 5) are added in the chemistry. The length of the ACS and the catalytic strength of the catalyst are mentioned in the table.

Reaction	Catalyst
<b>Generation 1 of length 3 (<math>\kappa = 1000</math>)</b>	
$(1, 0) + (1, 0) \rightleftharpoons (2, 0)$	$(3, 0)$
$(2, 0) + (1, 0) \rightleftharpoons (3, 0)$	$(3, 0)$
<b>Generation 2 of length 6 (<math>\kappa = 2000</math>)</b>	
$(1, 0) + (1, 0) \rightleftharpoons (2, 0)$	$(4, 2)$
$(0, 1) + (2, 0) \rightleftharpoons (2, 1)$	$(4, 2)$
$(2, 1) + (0, 1) \rightleftharpoons (2, 2)$	$(4, 2)$
$(2, 1) + (2, 1) \rightleftharpoons (4, 2)$	$(4, 2)$
<b>Generation 3 of length 10 (<math>\kappa = 4000</math>)</b>	
$(1, 0) + (0, 1) \rightleftharpoons (1, 1)$	$(4, 6)$
$(1, 1) + (1, 0) \rightleftharpoons (2, 1)$	$(4, 6)$
$(1, 1) + (1, 1) \rightleftharpoons (2, 2)$	$(4, 6)$
$(0, 1) + (2, 2) \rightleftharpoons (2, 3)$	$(4, 6)$
$(2, 3) + (2, 3) \rightleftharpoons (4, 6)$	$(4, 6)$
<b>Generation 4 of length 15 (<math>\kappa = 7000</math>)</b>	
$(0, 1) + (0, 1) \rightleftharpoons (0, 2)$	$(7, 8)$
$(0, 2) + (1, 0) \rightleftharpoons (1, 2)$	$(7, 8)$
$(1, 2) + (1, 0) \rightleftharpoons (2, 2)$	$(7, 8)$
$(2, 2) + (2, 2) \rightleftharpoons (4, 4)$	$(7, 8)$

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Reaction	Catalyst
$(1, 2) + (4, 4) \rightleftharpoons (5, 6)$	$(7, 8)$
$(5, 6) + (1, 2) \rightleftharpoons (6, 8)$	$(7, 8)$
$(5, 6) + (2, 2) \rightleftharpoons (7, 8)$	$(7, 8)$
<b>Generation 5 of length 19 (<math>\kappa = 10000</math>)</b>	
$(0, 1) + (1, 0) \rightleftharpoons (1, 1)$	$(7, 12)$
$(1, 1) + (0, 1) \rightleftharpoons (1, 2)$	$(7, 12)$
$(1, 2) + (1, 2) \rightleftharpoons (2, 4)$	$(7, 12)$
$(1, 1) + (2, 4) \rightleftharpoons (3, 5)$	$(7, 12)$
$(2, 4) + (3, 5) \rightleftharpoons (5, 9)$	$(7, 12)$
$(1, 1) + (5, 9) \rightleftharpoons (6, 10)$	$(7, 12)$
$(1, 2) + (6, 10) \rightleftharpoons (7, 12)$	$(7, 12)$
<b>Generation 6 of length 25 (<math>\kappa = 15000</math>)</b>	
$(0, 1) + (1, 0) \rightleftharpoons (1, 1)$	$(12, 13)$
$(1, 1) + (1, 0) \rightleftharpoons (2, 1)$	$(12, 13)$
$(2, 1) + (0, 1) \rightleftharpoons (2, 2)$	$(12, 13)$
$(2, 2) + (0, 1) \rightleftharpoons (2, 3)$	$(12, 13)$
$(1, 0) + (2, 3) \rightleftharpoons (3, 3)$	$(12, 13)$
$(2, 1) + (3, 3) \rightleftharpoons (5, 4)$	$(12, 13)$
$(2, 3) + (5, 4) \rightleftharpoons (7, 7)$	$(12, 13)$
$(7, 7) + (2, 2) \rightleftharpoons (9, 9)$	$(12, 13)$
$(7, 7) + (3, 3) \rightleftharpoons (10, 10)$	$(12, 13)$
$(9, 9) + (2, 3) \rightleftharpoons (11, 12)$	$(12, 13)$
$(11, 12) + (1, 1) \rightleftharpoons (12, 13)$	$(12, 13)$
<b>Generation 7 of length 30 (<math>\kappa = 20000</math>)</b>	
$(0, 1) + (1, 0) \rightleftharpoons (1, 1)$	$(13, 17)$
$(1, 1) + (0, 1) \rightleftharpoons (1, 2)$	$(13, 17)$
$(1, 2) + (1, 1) \rightleftharpoons (2, 3)$	$(13, 17)$
$(1, 0) + (2, 3) \rightleftharpoons (3, 3)$	$(13, 17)$
$(3, 3) + (1, 1) \rightleftharpoons (4, 4)$	$(13, 17)$
$(3, 3) + (1, 2) \rightleftharpoons (4, 5)$	$(13, 17)$
$(2, 3) + (4, 5) \rightleftharpoons (6, 8)$	$(13, 17)$
$(2, 3) + (6, 8) \rightleftharpoons (8, 11)$	$(13, 17)$
$(6, 8) + (4, 4) \rightleftharpoons (10, 12)$	$(13, 17)$
$(10, 12) + (2, 3) \rightleftharpoons (12, 15)$	$(13, 17)$
$(12, 15) + (1, 2) \rightleftharpoons (13, 17)$	$(13, 17)$
<b>Generation 8 of length 35 (<math>\kappa = 27000</math>)</b>	

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Reaction	Catalyst
$(1, 0) + (0, 1) \rightleftharpoons (1, 1)$	(15, 20)
$(0, 1) + (1, 1) \rightleftharpoons (1, 2)$	(15, 20)
$(1, 1) + (1, 2) \rightleftharpoons (2, 3)$	(15, 20)
$(1, 2) + (2, 3) \rightleftharpoons (3, 5)$	(15, 20)
$(3, 5) + (1, 1) \rightleftharpoons (4, 6)$	(15, 20)
$(1, 1) + (4, 6) \rightleftharpoons (5, 7)$	(15, 20)
$(3, 5) + (4, 6) \rightleftharpoons (7, 11)$	(15, 20)
$(7, 11) + (4, 6) \rightleftharpoons (11, 17)$	(15, 20)
$(1, 0) + (11, 17) \rightleftharpoons (12, 17)$	(15, 20)
$(1, 1) + (12, 17) \rightleftharpoons (13, 18)$	(15, 20)
$(13, 18) + (1, 2) \rightleftharpoons (14, 20)$	(15, 20)
$(1, 0) + (14, 20) \rightleftharpoons (15, 20)$	(15, 20)
<b>Generation 9 of length 40 (<math>\kappa = 35000</math>)</b>	
$(0, 1) + (0, 1) \rightleftharpoons (0, 2)$	(14, 26)
$(1, 0) + (0, 2) \rightleftharpoons (1, 2)$	(14, 26)
$(1, 2) + (1, 2) \rightleftharpoons (2, 4)$	(14, 26)
$(1, 2) + (2, 4) \rightleftharpoons (3, 6)$	(14, 26)
$(3, 6) + (1, 0) \rightleftharpoons (4, 6)$	(14, 26)
$(3, 6) + (2, 4) \rightleftharpoons (5, 10)$	(14, 26)
$(5, 10) + (1, 2) \rightleftharpoons (6, 12)$	(14, 26)
$(6, 12) + (2, 4) \rightleftharpoons (8, 16)$	(14, 26)
$(2, 4) + (8, 16) \rightleftharpoons (10, 20)$	(14, 26)
$(0, 1) + (10, 20) \rightleftharpoons (10, 21)$	(14, 26)
$(10, 21) + (0, 2) \rightleftharpoons (10, 23)$	(14, 26)
$(0, 2) + (10, 23) \rightleftharpoons (10, 25)$	(14, 26)
$(10, 23) + (1, 2) \rightleftharpoons (11, 25)$	(14, 26)
$(8, 16) + (5, 10) \rightleftharpoons (13, 26)$	(14, 26)
$(4, 6) + (10, 20) \rightleftharpoons (14, 26)$	(14, 26)
<b>Generation 10 of length 45 (<math>\kappa = 50000</math>)</b>	
$(0, 1) + (1, 0) \rightleftharpoons (1, 1)$	(18, 27)
$(0, 1) + (1, 1) \rightleftharpoons (1, 2)$	(18, 27)
$(1, 2) + (1, 0) \rightleftharpoons (2, 2)$	(18, 27)
$(1, 2) + (1, 1) \rightleftharpoons (2, 3)$	(18, 27)
$(1, 2) + (2, 2) \rightleftharpoons (3, 4)$	(18, 27)
$(2, 3) + (2, 3) \rightleftharpoons (4, 6)$	(18, 27)
$(4, 6) + (1, 1) \rightleftharpoons (5, 7)$	(18, 27)

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Reaction	Catalyst
$(4, 6) + (3, 4) \rightleftharpoons (7, 10)$	(18, 27)
$(7, 10) + (7, 10) \rightleftharpoons (14, 20)$	(18, 27)
$(0, 1) + (14, 20) \rightleftharpoons (14, 21)$	(18, 27)
$(14, 21) + (2, 2) \rightleftharpoons (16, 23)$	(18, 27)
$(2, 3) + (16, 23) \rightleftharpoons (18, 26)$	(18, 27)
$(14, 21) + (4, 6) \rightleftharpoons (18, 27)$	(18, 27)

TABLE S4b: **List of reactions in the catalyzed chemistry and their catalysts.** The table lists all the reactions that are part of the catalyzed chemistry with all its catalysts. The catalysts that belong to different generations ( $G_1$  to  $G_{10}$ ) have been separated in different columns. It is easy to see from this table the amount of overlap between any two nested ACSs. For example, between the ACSs  $G_5$  and  $G_6$  which contain, respectively, 7 and 11 reactions, only one is common.

Reaction	Catalyst									
	$G_1$	$G_2$	$G_3$	$G_4$	$G_5$	$G_6$	$G_7$	$G_8$	$G_9$	$G_{10}$
$(0, 1) + (0, 1) \rightleftharpoons (0, 2)$				(7,8)					(14,26)	
$(1, 0) + (0, 1) \rightleftharpoons (1, 1)$			(4,6)		(7,12)	(12,13)	(13,17)	(15,20)		(18,27)
$(1, 0) + (1, 0) \rightleftharpoons (2, 0)$	(3,0)	(4,2)								
$(0, 2) + (1, 0) \rightleftharpoons (1, 2)$				(7,8)					(14,26)	
$(1, 1) + (0, 1) \rightleftharpoons (1, 2)$					(7,12)		(13,17)	(15,20)		(18,27)
$(0, 1) + (2, 0) \rightleftharpoons (2, 1)$		(4,2)								
$(1, 1) + (1, 0) \rightleftharpoons (2, 1)$			(4,6)			(12,13)				
$(2, 0) + (1, 0) \rightleftharpoons (3, 0)$	(3,0)									
$(2, 1) + (0, 1) \rightleftharpoons (2, 2)$		(4,2)				(12,13)				
$(1, 1) + (1, 1) \rightleftharpoons (2, 2)$			(4,6)							
$(1, 2) + (1, 0) \rightleftharpoons (2, 2)$				(7,8)						(18,27)
$(0, 1) + (2, 2) \rightleftharpoons (2, 3)$			(4,6)			(12,13)				
$(1, 2) + (1, 1) \rightleftharpoons (2, 3)$							(13,17)	(15,20)		(18,27)
$(1, 2) + (1, 2) \rightleftharpoons (2, 4)$					(7,12)				(14,26)	
$(1, 0) + (2, 3) \rightleftharpoons (3, 3)$						(12,13)	(13,17)			
$(2, 1) + (2, 1) \rightleftharpoons (4, 2)$		(4,2)								
$(1, 2) + (2, 2) \rightleftharpoons (3, 4)$										(18,27)
$(1, 1) + (2, 4) \rightleftharpoons (3, 5)$					(7,12)					
$(1, 2) + (2, 3) \rightleftharpoons (3, 5)$								(15,20)		
$(2, 2) + (2, 2) \rightleftharpoons (4, 4)$				(7,8)						

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TABLE S4b

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Reaction	Catalyst									
	$G_1$	$G_2$	$G_3$	$G_4$	$G_5$	$G_6$	$G_7$	$G_8$	$G_9$	$G_{10}$
$(3, 3) + (1, 1) \rightleftharpoons (4, 4)$							(13,17)			
$(1, 2) + (2, 4) \rightleftharpoons (3, 6)$									(14,26)	
$(3, 3) + (1, 2) \rightleftharpoons (4, 5)$							(13,17)			
$(2, 1) + (3, 3) \rightleftharpoons (5, 4)$						(12,13)				
$(2, 3) + (2, 3) \rightleftharpoons (4, 6)$			(4,6)							(18,27)
$(3, 5) + (1, 1) \rightleftharpoons (4, 6)$								(15,20)		
$(3, 6) + (1, 0) \rightleftharpoons (4, 6)$									(14,26)	
$(1, 2) + (4, 4) \rightleftharpoons (5, 6)$				(7,8)						
$(1, 1) + (4, 6) \rightleftharpoons (5, 7)$								(15,20)		(18,27)
$(2, 4) + (3, 5) \rightleftharpoons (5, 9)$					(7,12)					
$(5, 6) + (1, 2) \rightleftharpoons (6, 8)$				(7,8)						
$(2, 3) + (4, 5) \rightleftharpoons (6, 8)$							(13,17)			
$(2, 3) + (5, 4) \rightleftharpoons (7, 7)$						(12,13)				
$(3, 6) + (2, 4) \rightleftharpoons (5, 10)$									(14,26)	
$(5, 6) + (2, 2) \rightleftharpoons (7, 8)$				(7,8)						
$(1, 1) + (5, 9) \rightleftharpoons (6, 10)$					(7,12)					
$(4, 6) + (3, 4) \rightleftharpoons (7, 10)$										(18,27)
$(5, 10) + (1, 2) \rightleftharpoons (6, 12)$									(14,26)	
$(3, 5) + (4, 6) \rightleftharpoons (7, 11)$								(15,20)		
$(7, 7) + (2, 2) \rightleftharpoons (9, 9)$						(12,13)				
$(1, 2) + (6, 10) \rightleftharpoons (7, 12)$					(7,12)					
$(2, 3) + (6, 8) \rightleftharpoons (8, 11)$							(13,17)			
$(7, 7) + (3, 3) \rightleftharpoons (10, 10)$						(12,13)				
$(6, 8) + (4, 4) \rightleftharpoons (10, 12)$							(13,17)			
$(9, 9) + (2, 3) \rightleftharpoons (11, 12)$						(12,13)				
$(6, 12) + (2, 4) \rightleftharpoons (8, 16)$									(14,26)	
$(11, 12) + (1, 1) \rightleftharpoons (12, 13)$						(12,13)				
$(10, 12) + (2, 3) \rightleftharpoons (12, 15)$							(13,17)			
$(7, 11) + (4, 6) \rightleftharpoons (11, 17)$								(15,20)		
$(1, 0) + (11, 17) \rightleftharpoons (12, 17)$								(15,20)		
$(2, 4) + (8, 16) \rightleftharpoons (10, 20)$									(14,26)	
$(12, 15) + (1, 2) \rightleftharpoons (13, 17)$							(13,17)			
$(0, 1) + (10, 20) \rightleftharpoons (10, 21)$									(14,26)	
$(1, 1) + (12, 17) \rightleftharpoons (13, 18)$								(15,20)		
$(10, 21) + (0, 2) \rightleftharpoons (10, 23)$									(14,26)	

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TABLE S4b

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Reaction	Catalyst									
	$G_1$	$G_2$	$G_3$	$G_4$	$G_5$	$G_6$	$G_7$	$G_8$	$G_9$	$G_{10}$
$(13, 18) + (1, 2) \rightleftharpoons (14, 20)$								(15,20)		
$(7, 10) + (7, 10) \rightleftharpoons (14, 20)$										(18,27)
$(0, 2) + (10, 23) \rightleftharpoons (10, 25)$									(14,26)	
$(0, 1) + (14, 20) \rightleftharpoons (14, 21)$										(18,27)
$(1, 0) + (14, 20) \rightleftharpoons (15, 20)$								(15,20)		
$(10, 23) + (1, 2) \rightleftharpoons (11, 25)$									(14,26)	
$(8, 16) + (5, 10) \rightleftharpoons (13, 26)$									(14,26)	
$(14, 21) + (2, 2) \rightleftharpoons (16, 23)$										(18,27)
$(4, 6) + (10, 20) \rightleftharpoons (14, 26)$									(14,26)	
$(2, 3) + (16, 23) \rightleftharpoons (18, 26)$										(18,27)
$(14, 21) + (4, 6) \rightleftharpoons (18, 27)$										(18,27)