iScience, Volume *26*

Supplemental information

Siderophore-mediated iron partition promotes dynamical coexistence between cooperators and cheaters

Jiqi Shao, Nan Rong, Zhenchao Wu, Shaohua Gu, Beibei Liu, Ning Shen, and Zhiyuan Li

Table S1. Symbos for our model, related to the STAR methods.

Chemostat parameters	
$R_{\mathrm{iron,supply}}$	Iron supply.
d	Dilution rate.
Chemostat variables	
R_{sid}	Concentration of public siderophores.
R_{iron}	Concentration of the iron.
m_σ	Biomass density of microbe σ.
species-specific quantities	
$\vec{\alpha}_\sigma = \left(\alpha_{\sigma,\mathrm{growth}}, \alpha_{\sigma,\mathrm{private}}, \alpha_{\sigma,\mathrm{public}}\right)$	Resource allocation strategy of microbe σ, defined by the fractions of resources being located to growth ($\alpha_{\sigma,\mathrm{growth}}$), production of private siderophores$\left(\alpha_{\sigma,\mathrm{private}}\right)$, and production of public siderophores ($\alpha_{\sigma,\mathrm{public}}$)
$g(R_{\mathrm{sid}}, R_{\mathrm{iron}}, \vec{\alpha}_\sigma)$	Growth rate as a function of $R_{\mathrm{sid}}, R_{\mathrm{iron}},$ and $\vec{\alpha}_\sigma$.
$I_\sigma = I\left(R_{\mathrm{sid}}, R_{\mathrm{iron}}, \vec{\alpha}_{\sigma_i}\right)$	Iron intake rate per biomass of the microbe σ_i.
$v_{\mathrm{m}}, v_{\mathrm{l}}$	Uptake coefficients for private and public siderophores, respectively. “m” stands for “membrane”, and “l” stands for “liquid”
$K_{\mathrm{m}}, K_{\mathrm{l}}$	Affinity constants for private and public siderophores, respectively
γ	Species growth coefficient.
β	Production coefficient of private siderophores.
ϵ	Production coefficient of public siderophores.
p	Consumption ratio of public siderophores when microbes uptake iron.
r	Relative biomass concentration in the cell compared to its microenvironment, set to be a constant of 100.

Table S2. The Routh-Hurwitz table for criterion, related to the STAR methods.

Term ID	Values
Term 0	a_0
Term 1	a_1
Term 2	$\frac{a_1 a_2 - a_0 a_3}{a_1}$
Term 3	$\frac{(a_1 a_2 - a_0 a_3) a_3 - a_1^2 a_4}{a_1 a_2 - a_0 a_3}$
Term 4	a_4

Table S3. Parameters used for different figures, related to Figure 1, Figure 2, Figure 3, Figure 4, and the STAR methods.

Term	Parameter values
Basic Parameter	$\beta = 1,\ \gamma = 10,\ \epsilon = 1,\ K_\mathrm{m} = 1,\ K_\mathrm{l} = 0.1,\ v_\mathrm{m} = 1,\ v_\mathrm{l} = 1.$
Initial value	In dynamical simulations, we generally set the initial value [$m_\mathrm{cooperator,0}$, $m_\mathrm{cheater,0}$, $R_\mathrm{sid,0}$, $R_\mathrm{iron,0}$] as [50, 50, 0, $R_\mathrm{iron,supply}$]. In bifurcation simulations, we generally set the initial value [$m_\mathrm{cooperator,0}$, $m_\mathrm{cheater,0}$, $R_\mathrm{sid,0}$, $R_\mathrm{iron,0}$] as [1, 1, 0.5, $R_\mathrm{iron,supply}$]. $R_\mathrm{sid,0} = 0.5$ is set to avoid early extinction due to the high dilution rate.
Figure 1	$d = 0.5,\ R_\mathrm{iron,supply} = 1.5;$ E: Pure cooperator: $\vec{\alpha} = (0.6, 0, 0.4);$ F: Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2).$
Figure 2	A: Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2),\ d = 0.5,\ R_\mathrm{iron,supply} = 0.5;$ B: Partial cooperator: $\vec{\alpha} = (0.6, 0.39, 0.01),\ d = 0.5,\ R_\mathrm{iron,supply} = 0.5;$ D: Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2),\ R_\mathrm{iron,supply} = 0.5;$ E: Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2),\ d = 0.5.$
Figure 3	Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2),\ d = 0.5$ B: $R_\mathrm{iron,supply} = 0.3$; C: $R_\mathrm{iron,supply} = 0.4$; D: $R_\mathrm{iron,supply} = 0.6$
Figure 4	$d = 0.5,\ R_\mathrm{iron,supply} = 0.5,$ Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2).$ B: start strain: $\vec{\alpha} =$ (0.6, 0.2, 0.2), middle strain: $\vec{\alpha} = (1, 0, 0)$, end strain: $\vec{\alpha} = (0.65, 0.35, 0)$
S2	Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2),\ \epsilon = 1$
S3	Partial cooperator: $\vec{\alpha} = (0.8, 0.1, 0.1),$ Pure cooperator $\vec{\alpha} = (0.99, 0, 0.01).$ B: $R_\mathrm{iron,supply} = 0.1$; C: $R_\mathrm{iron,supply} = 0.16$; D: $R_\mathrm{iron,supply} = 0.18$; E: $R_\mathrm{iron,supply} = 0.25$
S4	$d = 0.5,\ R_\mathrm{iron,supply} = 0.5$
S5	$d = 0.5,\ R_\mathrm{iron,supply} = 0.5$
S6	$d = 0.5,\ R_\mathrm{iron,supply} = 1$ Partial cooperator: $\vec{\alpha} = (0.6, 0.2, 0.2)$
S7	$d = 0.5,\ R_\mathrm{iron,supply} = 1$

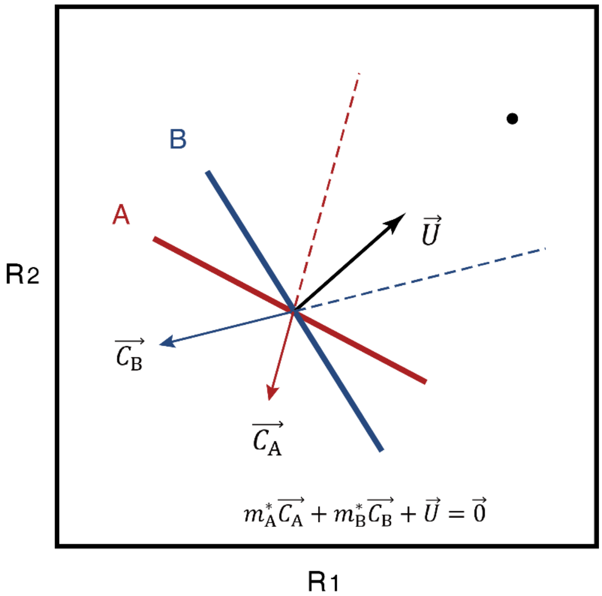

Figure S1. Diagram of the Tilman's graphical tools on the classical consumer resource model, related to the STAR methods. In the chemical space expanded by two resources $\boldsymbol{R_1}$ and $\boldsymbol{R_2}$, The Tilman's graphical tool in analyzing resource competition model contains: (1) resource supply point $[\boldsymbol{R_{1,supply}}, \boldsymbol{R_{2,supply}}]$ (black dot) , which sets the maximal possible concentration of $\boldsymbol{R_1}$ and $\boldsymbol{R_2}$ that can occur at steady state; (2) resource supply vector $\vec{\boldsymbol{U}}$ (black arrow), which denotes the environmental supply rate of resources and $\vec{\boldsymbol{U}} = \boldsymbol{d}\begin{bmatrix}\boldsymbol{R_{1,supply}} - \boldsymbol{R_1^*} \\ \boldsymbol{R_{2,supply}} - \boldsymbol{R_2^*}\end{bmatrix}$ at steady state; (3) zero net growth isocline(ZNGI), or growth contour $\left\{(\boldsymbol{R_1}, \boldsymbol{R_2})\middle| \frac{\boldsymbol{dm_i}}{\boldsymbol{dt}} = \boldsymbol{0}\right\}$, for each strain (strain A: red line; strain B: blue line), which shows the contour where growth rate equals to death or dilution rate; (4) consumption vector (red and blue arrows for that of strain A $\overrightarrow{\boldsymbol{C_A}}$, and stain B $\overrightarrow{\boldsymbol{C_B}}$, respectively), which indicates the total consumption rate of resources for the species. When two species reach a steady state, $\boldsymbol{m_A^*}\overrightarrow{\boldsymbol{C_A}} + \boldsymbol{m_B^*}\overrightarrow{\boldsymbol{C_B}} + \vec{\boldsymbol{U}} = \vec{\boldsymbol{0}}$. The consumption vectors and growth contours in this figure show that each of species A and species B consumes more of the one resource which more limits its own growth rate, leading to stable coexistence.

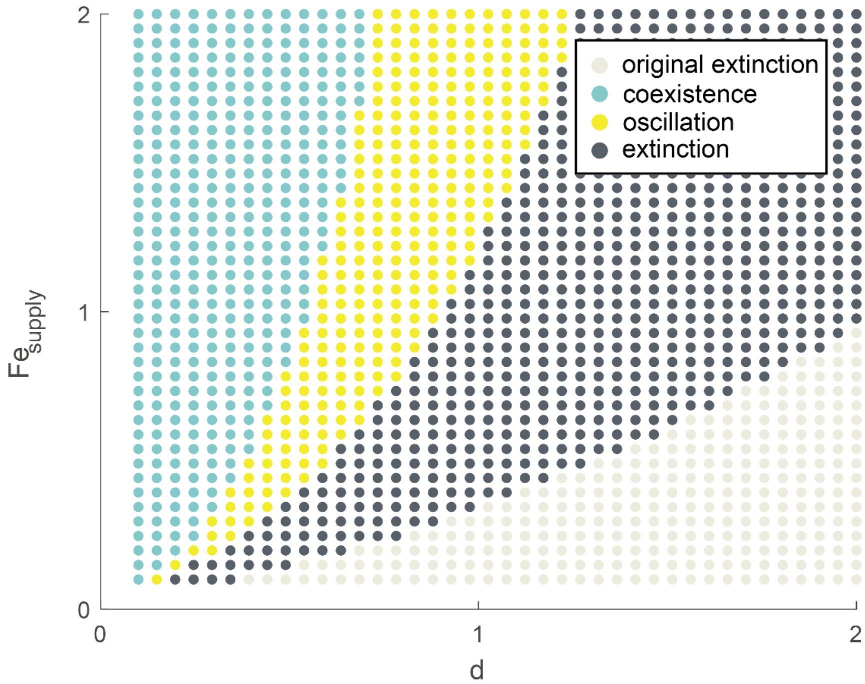

Figure S2. Cheaters accelerate the collapse of the system when invading partial cooperators, related to Figure 2. Consequence of the pure cheater invading the partial cooperator $\vec{\alpha} = (0.6, 0.2, 0.2)$ under various chemostat conditions. Light gray denotes chemostat conditions in which the partial cooperator cannot survive even on its own. Deep gray indicates regions where partial cooperators can exist on their own, yet the invasion of cheaters drives them to extinction. The yellow dots represent oscillatory dynamics, while the blue zone represents coexistence.

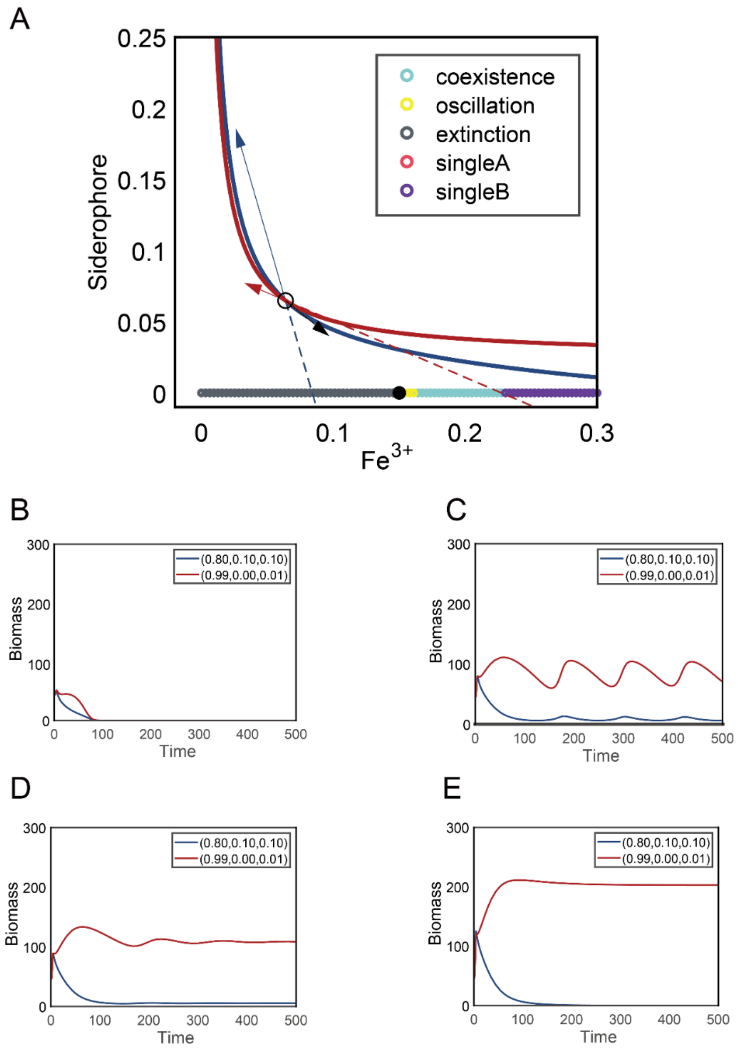

Figure S3. Competition between two cooperators under different Fe supply, related to Figure 3, and the STAR methods. Similar as Figure 3 in the main text, but the system consists of two cooperators competing for iron. The strategies of the partial cooperator A is $\vec{\boldsymbol{\alpha}}_A$ =(0.8,0.1,0.1), and the nearly-pure cooperator B is $\vec{\boldsymbol{\alpha}}_B$ =(0.99,0,0.01). (A) As the iron supply increases, the systems dynamics experiences extinction, oscillation, coexistence, and strain B excluding strain A, respectively. The interior of the reverse extension of the consumption vector covers the supply region where coexistence is possible, while the exterior is the region where exclusion occurs and the cooperator B survives alone. (B-E) Time-courses of the competition dynamics between strain A and strain B under increasing iron supply, as shown in (A). (B): $\boldsymbol{R}_{\text{iron,supply}} = \mathbf{0.1}$; (C): $\boldsymbol{R}_{\text{iron,supply}} = \mathbf{0.16}$; (D): $\boldsymbol{R}_{\text{iron,supply}} = \mathbf{0.18}$; (E): $\boldsymbol{R}_{\text{iron,supply}} = \mathbf{0.25}$.

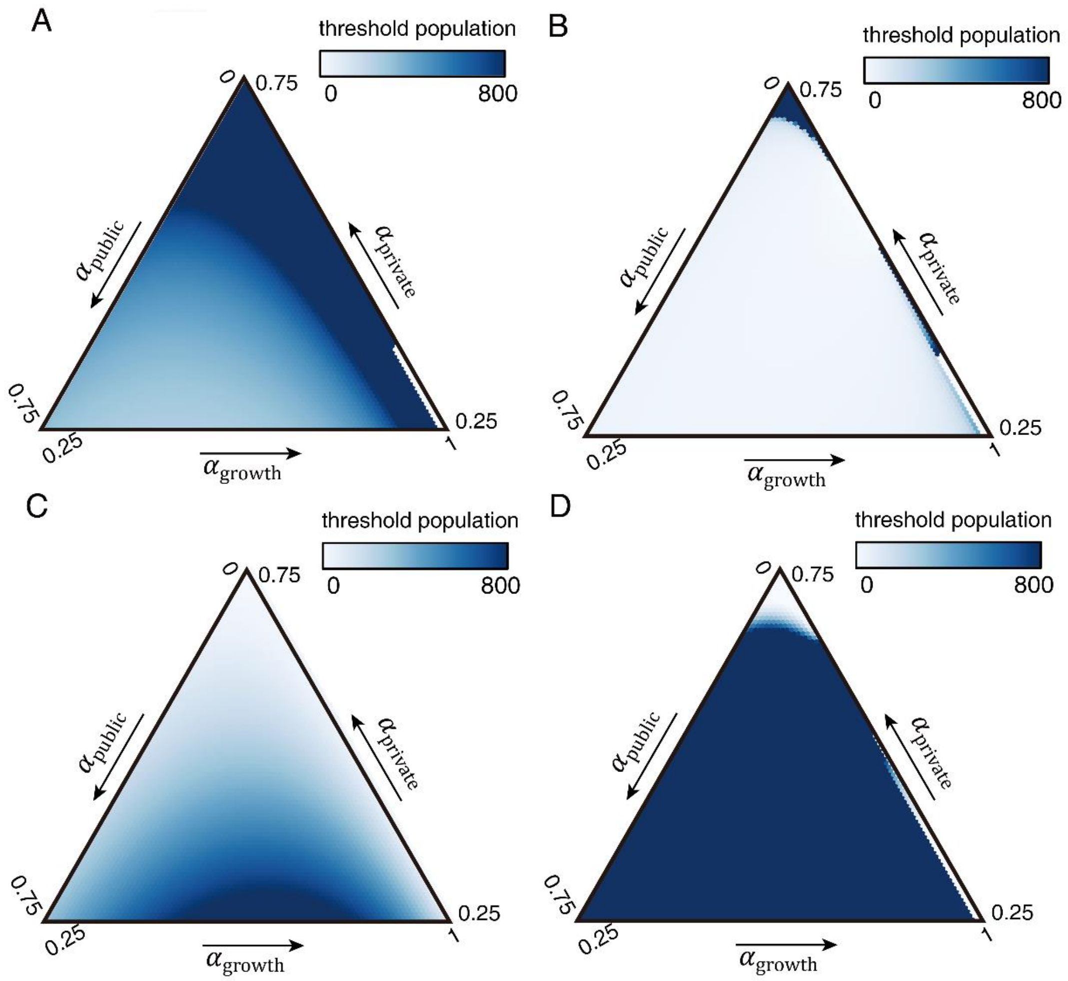

Figure S4. The invasion from another species with non-overlapping siderophores, related to Figure 4. To assess a species' resistance to invasion by other species with different forms of siderophores, we modeled a second species with the same parameters but non-sharable siderophore. To assist the differentiation, we refer to the native species as species 1 and the invading species as species 2. (A) The minimum population required for all strategies of species 2 to invade a native species 1 under the partial cooperator strategy ($\vec{\boldsymbol{\alpha}}_1$ =(0.6,0.2,0.2)). (B) The minimum population required for all strategies of species 2 to invade a native species 1 under the self-supplier strategy ($\vec{\boldsymbol{\alpha}}_1$ =(0.6, 0.4, 0)). (C) The minimum population required for a species 2 under the partial cooperator strategy(($\vec{\boldsymbol{\alpha}}_2$ =(0.6,0.2,0.2)) to invade all strategies of species 1. (D) The minimum population required for a species 2 under the self-supplier strategy ($\vec{\boldsymbol{\alpha}}_2$ =(0.6, 0.4, 0)) to invade all strategies of species 1.

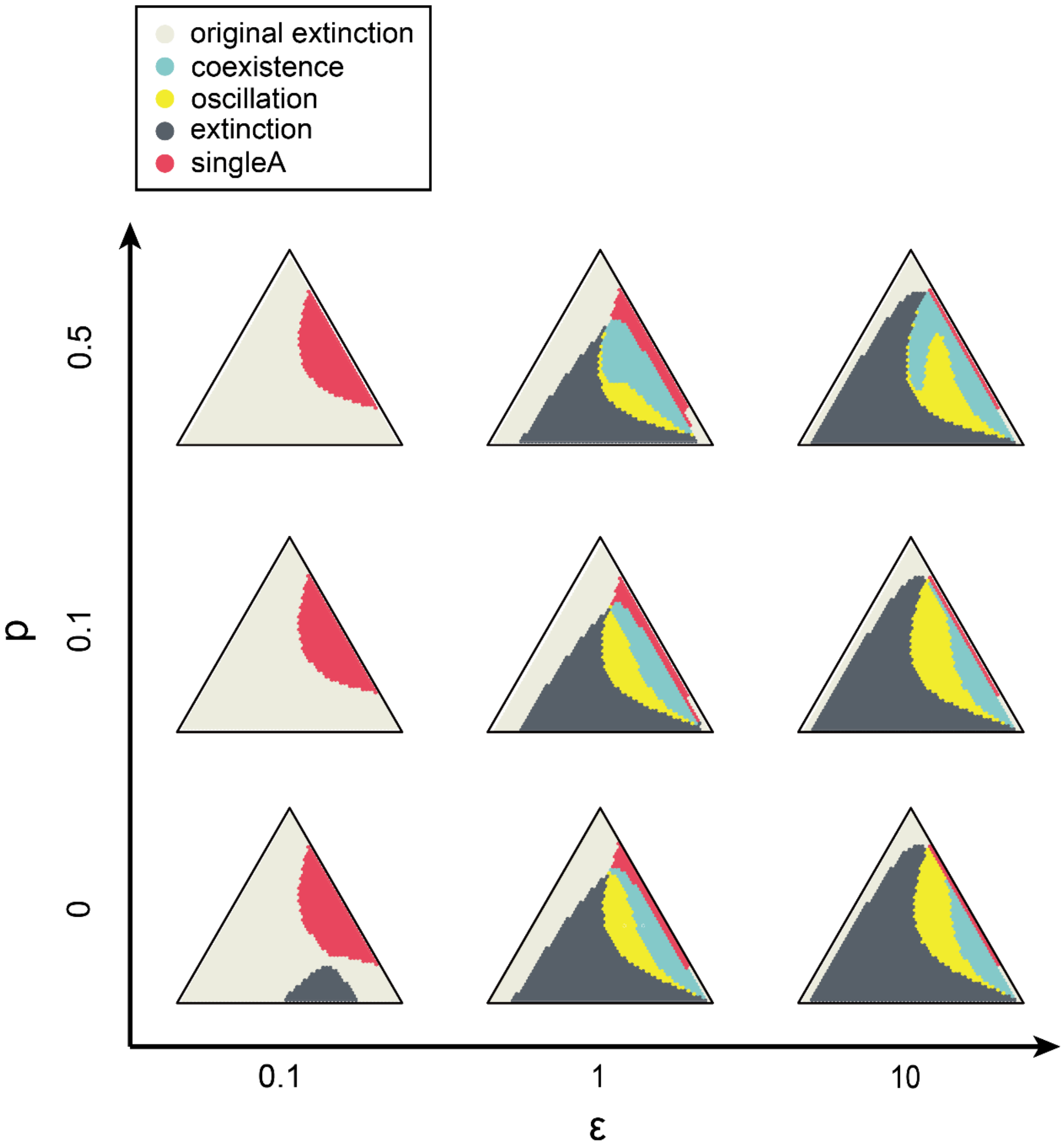

Figure S5. The impact of consumption, production, and recycle rate of public siderophores on strategies' interaction consequences with the pure cheater, related to Figure 4, and the STAR methods. To quantify the effects of siderophores' production cost (represented by ϵ) and recycle rate (represented by p) on its coexistence with the cheater, here we set up different combinations of ϵ and p to reproduce Figure 4A. Along the x-axis, decreasing the production cost of public siderophores, i.e., larger ϵ, helps to substantially enlarge the area of oscillation (yellow) and stable coexistence (blue) instead of exclusion (red). Along the y-axis, increased siderophore consumption, i.e., larger p, slightly increased the area of stable coexistence.

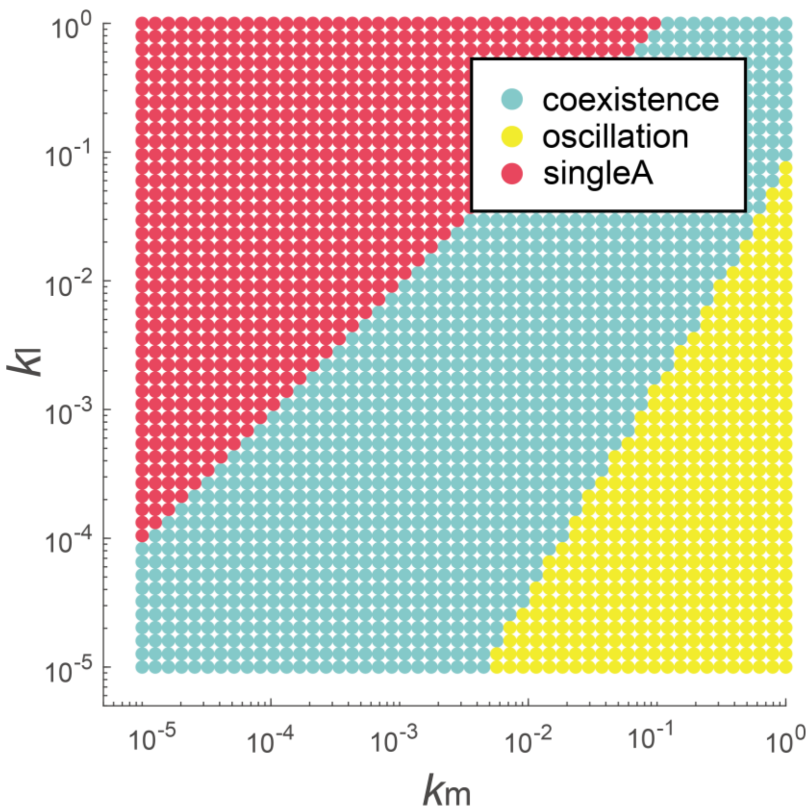

Figure S6. The impact of iron affinity of private and public siderophores on coexistence between the partial cooperator and the pure cheater, related to Figure 4, and the STAR methods. K_m and K_l denote iron affinity of private and public siderophores, respectively. The consequence of the pure cheater invading a partial cooperator ($\vec{\alpha}_A$ =(0.6,0.2,0.2), termed as “strain A”) under different levels of K_m and K_l were mapped to dot colors in the phase plane. Partial cooperators can stably coexist with pure cheaters in a wide range of parameter combinations, when K_m balances with K_l (blue dots). When K_l decreases and K_m increases, i.e., public siderophores increase affinity for iron, the system is more likely to oscillate (yellow dot). When K_l increases and K_m decreases, the partial cooperator is more likely to exclude the cheater (red dots denoted as “single A”).

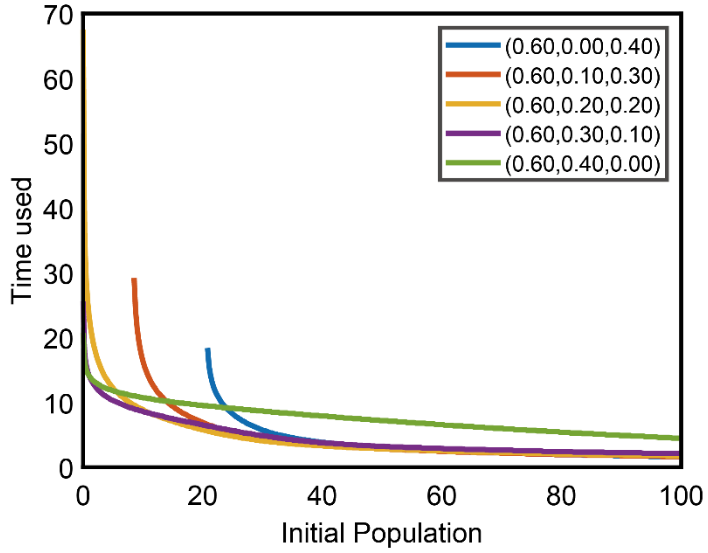

Figure S7. Speed of reaching a population's steady-state size for various strategies and initial populations, related to Figure 4. In order to measure the speed of population establishment, we quantified the time used between introducing the initial population and reaching the steady-state population. Assuming constant $\boldsymbol{\alpha}_{\mathbf{growth}}$, self-suppliers and partial cooperators that allocate more resources to private siderophores can establish a population faster with a smaller initial population size, whereas strategies that allocate more resources to public siderophores can achieve the same or even faster results when the initial population size increases.