Electronic Supplementary Material (ESI) for Chemical Science.

SUPPORTING INFORMATION

Catalytic Resonance Theory: Parallel Reaction Pathway Control

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Section S0. Visual interpretation of combined volcano plots

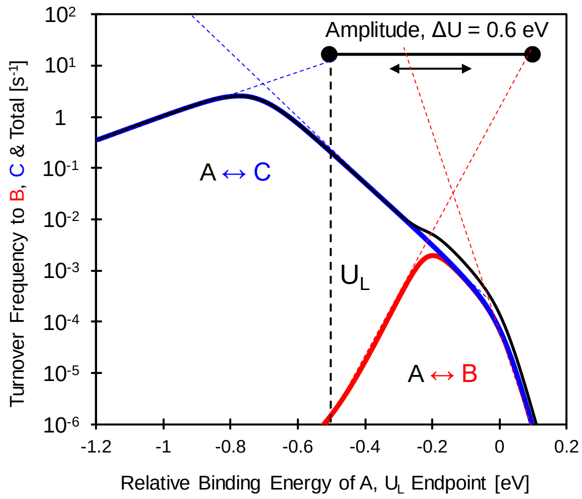

Figure S1. Sabatier volcano plot from Figure 3A. Volcano plot regimes are extrapolated to illustrate resonance frequencies for selectivity enhancement. **Conditions:** 150 °C, 100 bar A feed pressure, 1 % conversion of A. **Parameters:** $\Delta H_{ovr} \sim 0$ kJ mol^{-1} for both reactions, BEP parameters of $\alpha \sim 0.6$, $\beta \sim 100$ kJ mol^{-1}, surface binding ratios of $\gamma_{B\text{-}A} \sim 2.0$, $\gamma_{C\text{-}A} \sim 0.5$, and $\delta_{B\text{-}A} \sim 1.4$ eV, $\delta_{C\text{-}A} \sim 1.4$ eV. Relative binding energies of A can be converted to absolute binding energies of A by adding 1.4 eV to the independent axis.

Section S1. Matlab 2019a/b Code

Code S1a. Volcano Plot and Surface Coverage for A-to-B/A-to-C

```
% Remove prior data and runs
clear
clc

% Main program

% Constants:
% Gas constant
R = 8.31446261815324; % J/gmol-K
Rg = R*10^-2; % L-bar/gmol-K

% Conditions:
% Temperature
Tc = 150.0; % deg C
T = Tc + 273.15; % K
% Pressure (bar)
P(1) = 100.0;
P(2:3) = 0.0;
% Concentration (M)
Cf = P/(Rg*T);
% Adsorbed species (gmol)
Ns = zeros(3,1);
% Initial conditions
x0 = [Cf';Ns];

% Parameters:
% Number of active sites (gmol)
Nsites = 138.0/1000*20.0e-6;

% Reaction chemistry:
% Overall heat of reaction (J/gmol)
delHovr = zeros(1,2);
% Bronsted-Evans-Polanyi relationship
alpha(1:2) = 0.6; % unitless
beta(1:2) = 100.0e3; % J/gmol
% Linear scaling relationship
gamma(1) = 2.0; % unitless
gamma(2) = 0.5; % unitless
delta(1:2) = 1.4; % eV

% Initial binding energy (eV)
BEa0 = 1.4;

% Conversion target (mol %)
C = 1.0;

% Initial space velocity
```

```
qsdot = 50.0; % mL/min
qdot = qsdot/60000; % L/s
V = 138.0/1000*1/3.58*1/1000*1/(1 - 0.375); % L
SV0 = qdot/V; % 1/s

% ODE solver settings
tspan = [0 5.0e100]; % s
options = odeset('RelTol',1e-8,'AbsTol',1e-9);

% For loop bounds (eV)
is = -BEa0;
ii = 0.005;
ie = BEa0;

% Preallocate matrices
je = (ie - is)/ii + 1;
je = round(je);
delBEa = zeros(je,1);
TOFa = delBEa;
TOFb = TOFa;
TOFc = TOFb;
Theta_A_star = TOFc;
Theta_B_star = Theta_A_star;
Theta_C_star = Theta_B_star;

% Time volcano plot
tic

% Volcano plot generation
for i = is:ii:ie

  % Loop index
  j = (i - is)/ii + 1;
  j = round(j);

  % Relative binding energy (eV)
  delBEa(j) = i;

  % Obtain rate constants (1/bar-s or 1/s)
  k = rate_constants(BEa0,gamma,delta,delHovr,T,delBEa(j),alpha,beta);

  % Solver for space velocity (1/s)
  SV = fsolve(@(SV) targetfun(SV,Cf,k,T,x0,C),SV0(j));
  SV0(j + 1) = SV;

  % Generate optimal solution
  [t,x] = ode15s(@(t,x) xdot(t,x,SV,Cf,k,T),tspan,x0,options);

  % Store data
  TOFa(j) = (Cf(1) - x(end,1))*SV*V/Nsites;
  TOFb(j) = (x(end,2) - Cf(2))*SV*V/Nsites;
```

```
  TOFc(j) = (x(end,3) - Cf(3))*SV*V/Nsites;
  Theta_A_star(j) = x(end,4)/Nsites;
  Theta_B_star(j) = x(end,5)/Nsites;
  Theta_C_star(j) = x(end,6)/Nsites;

  % Remove prior data
  clear t x
end

% Stop timer
toc

% Plot results
semilogy(delBEa,[TOFa TOFb TOFc])
plot(delBEa,[Theta_A_star Theta_B_star Theta_C_star])

% Rate constants
function k = rate_constants(BEa0,gamma,delta,delHovr,T,delBEa,alpha,beta)

R = 8.31446261815324; % J/gmol-K

BE0(1) = BEa0; % A*
BE0(2:3) = gamma*BE0(1) + (1 - gamma).*delta + delHovr/96.485e3;

BE(1) = BE0(1) + delBEa; % A*
BE(2:3) = BE0(2:3) + gamma*delBEa;
% Restrict to positive values
BE = max(0,BE)*96.485e3;

delH(1) = -BE(1); % A(g) + * <--> A*
delH(2:2:5) = delHovr + BE(1) - BE(2:3);
delH(3:2:5) = BE(2:3);

K(1) = 1.0e-7*exp(-delH(1)/(R*T)); % A(g) + * <--> A*
K(2:2:5) = 1.0*exp(-delH(2:2:5)/(R*T));
K(3:2:5) = 1.0e7*exp(-delH(3:2:5)/(R*T));

A(1) = 1.0e6; % 1/bar-s
A(2:5) = 1.0e13; % 1/s

Ea(1) = 0.0e3; % A(g) + * --> A*
Ea(2:2:5) = alpha.*delH(2:2:5) + beta;
Ea(3:2:5) = delH(3:2:5);
% Restrict to positive values
Ea = max(0,Ea);

k(1:2:10) = A.*exp(-Ea/(R*T));
k(2:2:10) = k(1:2:10)./K;
end

% Target Function
```

```
function tf = targetfun(SV,Cf,k,T,x0,C)
tspan = [0 5.0e100]; % s
options = odeset('RelTol',1e-8,'AbsTol',1e-9);
[t,x] = ode15s(@(t,x) xdot(t,x,SV,Cf,k,T),tspan,x0,options);
tf = ((Cf(1) - x(end,1))/sum(Cf)*100 - C)^2;
end

% Derivative
function dx = xdot(t,x,SV,Cf,k,T)
R = 8.31446261815324; % J/gmol-K
Rg = R*10^-2; % L-bar/gmol-K
Nsites = 138.0/1000*20.0e-6; % gmol
V = 138.0/1000*1/3.58*1/1000*1/(1 - 0.375); % L
dx(1,1) = SV*(Cf(1) - x(1)) - k(1)*Rg*T*x(1)*(Nsites - sum(x(4:6)))/V + k(2)*x(4)/V; % M/s
dx(2,1) = SV*(Cf(2) - x(2)) - k(6)*Rg*T*x(2)*(Nsites - sum(x(4:6)))/V + k(5)*x(5)/V; % M/s
dx(3,1) = SV*(Cf(3) - x(3)) - k(10)*Rg*T*x(3)*(Nsites - sum(x(4:6)))/V + k(9)*x(6)/V; % M/s
dx(4,1) = k(1)*Rg*T*x(1)*(Nsites - sum(x(4:6))) - k(2)*x(4) - k(3)*x(4) + k(4)*x(5) - k(7)*x(4) +
  k(8)*x(6); % gmol/s
dx(5,1) = k(6)*Rg*T*x(2)*(Nsites - sum(x(4:6))) - k(5)*x(5) + k(3)*x(4) - k(4)*x(5); % gmol/s
dx(6,1) = k(10)*Rg*T*x(3)*(Nsites - sum(x(4:6))) - k(9)*x(6) + k(7)*x(4) - k(8)*x(6); % gmol/s
end
```

Code S1b. Dynamic Catalysis in an A-to-B System with Square Waveform

```
% Remove prior runs and data
clear
clc

% Step test for Model 1 - CSTR

% Constants:
% Gas constant (L-bar/gmol-K)
Rg = 8.31446261815324e-2;

% Conditions:
% Temperature
Tc = 150.0; % deg C
T = Tc + 273.15; % K

% Parameters:
% Feed pressure (bar)
Pf(1) = 100.0; % A(g)
Pf(2) = 0.0; % B(g)
% Feed concentration (M)
Cf = Pf/(Rg*T);

% Volumetric flowrate
qsdot = 50.0; % mL/min
qdot = qsdot/60000; % L/s
% Number of active sites (gmol)
Nsites = 138.0/1000*20.0e-6;
```

```
% CSTR volume (L)
V = 138.0/1000*1/3.58*1/1000*1/(1 - 0.375);
% Space velocity (1/s)
SV = qdot/V;

% Steady State Initial Conditions for the States
C_ss = Cf'; % M
N_ss = zeros(2,1); % gmol
x_ss = [C_ss;N_ss];

% Reaction chemistry:
% Heat of reaction (J/gmol)
delHovr = 0.0;
% Bronsted-Evans-Polanyi relationship
alpha = 0.6; % unitless
beta = 100.0e3; % J/gmol
% Linear scaling relationship
gamma = 2.0; % unitless
delta = 1.4; % eV

% Initial binding energy of A (eV)
BEa0 = mean(delta);

% Dynamic catalysis:
% Oscillation time constants (s)
tau(1) = 5e5;
taur = 1.0;
tau(2) = taur*tau(1);
% Oscillation frequency (Hz)
fosc = 1/sum(tau);
% Number of oscillations (unitless)
Nosc = max(11,fosc);

% Oscillation amplitude (eV)
delU = 0.6;
% Oscillation endpoints (eV)
UL = -0.20;
UR = UL + delU;
% Obtain rate constants (1/bar-s or 1/s)
kR = cstr1_constants(BEa0,gamma,delta,delHovr,UR,T,alpha,beta);
kL = cstr1_constants(BEa0,gamma,delta,delHovr,UL,T,alpha,beta);

% Solver options
options = odeset('RelTol',1e-8,'AbsTol',1e-9);

% Time Matlab code
tic

% Iterate until convergence
for n = 1:inf
  % Empty matrices
```

```
tsvm = [];
xsvm = [];
tsve = [];
xsve = [];
% Simulate all oscillations
for i = 1:Nosc

    % Odd numbered runs
    if mod(i,2) == 1

    % Generate ODE solution
    [t,x] = ode23tb(@(t,x) cstr1(t,x,SV,Cf,kR,T),[0 tau(1)],x_ss(:,i),options);
    % Store data
    if i == 1
            tsv = t;
            xsv = x;
    else
            if round(i) == round(Nosc/2.0) || round(i) == round(Nosc/2.0 + 1.0)
            tsv = [tsv;t + tsv(end)];
            xsv = [xsv;x];
            tsvm = [tsvm;t + tsv(end)];
            xsvm = [xsvm;x];
            else
            if round(i) == round(Nosc - 1.0) || round(i) == round(Nosc)
            tsv = [tsv;t + tsv(end)];
            xsv = [xsv;x];
            tsve = [tsve;t + tsv(end)];
            xsve = [xsve;x];
            else
            tsv = [tsv;t + tsv(end)];
            xsv = [xsv;x];
            end
            end
    end
    x_ss(:,i + 1) = x(end,:)';

    % Clean up matrices
    clear t x

    % Even numbered runs
    else

    % Generate ODE solution
    [t,x] = ode23tb(@(t,x) cstr1(t,x,SV,Cf,kL,T),[0 tau(2)],x_ss(:,i),options);
    % Store data
    if round(i) == round(Nosc/2.0) || round(i) == round(Nosc/2.0 + 1.0)
            tsv = [tsv;t + tsv(end)];
            xsv = [xsv;x];
            tsvm = [tsvm;t + tsv(end)];
            xsvm = [xsvm;x];
    else
```

```
            if round(i) == round(Nosc - 1.0) || round(i) == round(Nosc)
            tsv = [tsv;t + tsv(end)];
            xsv = [xsv;x];
            tsve = [tsve;t + tsv(end)];
            xsve = [xsve;x];
            else
            tsv = [tsv;t + tsv(end)];
            xsv = [xsv;x];
            end
        end
        x_ss(:,i + 1) = x(end,:)';

        % Clean up matrices
        clear t x
        end
    end

    % Parse out the state values (M)
    Casvm = xsvm(:,1); % A(g)
    Casve = xsve(:,1); % A(g)

    % Measure reactor performance (mol %)
    Xasvm = (Cf(1) - Casvm)/sum(Cf)*100;
    Xasve = (Cf(1) - Casve)/sum(Cf)*100;

    % Midpoint Riemann sums
    Xainte = zeros(size(tsve));
    Xaintm = zeros(size(tsvm));
    for k = 2:size(Xainte,1)
        Xainte(k) = (tsve(k) - tsve(k - 1))*mean([Xasve(k),Xasve(k - 1)]);
    end
    for l = 2:size(Xaintm,1)
        Xaintm(l) = (tsvm(l) - tsvm(l - 1))*mean([Xasvm(l),Xasvm(l - 1)]);
    end

    % Time averaged conversion
    Xaavge = sum(Xainte)*fosc;
    Xaavgm = sum(Xaintm)*fosc;

    % Converge on C conversion of A (mol %)
    C = 1.0;
    if abs(Xaavge - Xaavgm) > 0.01
        plot(tsv,xsv)
        x_ss(:,1) = xsv(end,:)';
        nt = n;
        nt
        clear tsv xsv Casvm Casve Xasvm Xasve
    else
        if abs(Xaavge - C) > 0.01
        SV = SV*Xaavge/C;
        x_ss(:,1) = [C_ss;N_ss];
```

```
      nq = n;
      nq
      clear tsv xsv Casvm Casve Xasvm Xasve
      else
      toc
      break
      end
  end
end

% Parse out the state values (M)
Cbsve = xsve(:,2); % B(g)

% Measure reactor performance (1/s)
TOFae = (Cf(1) - Casve)*SV*V/Nsites;
TOFbe = (Cbsve - Cf(2))*SV*V/Nsites;

% Midpoint Riemann sums
TOFaint = zeros(size(tsve));
TOFbint = TOFaint;
for m = 2:size(TOFaint,1)
  TOFaint(m) = (tsve(m) - tsve(m - 1))*mean([TOFae(m),TOFae(m - 1)]);
  TOFbint(m) = (tsve(m) - tsve(m - 1))*mean([TOFbe(m),TOFbe(m - 1)]);
end

% Time averaged TOF (1/s)
TOFaavg = sum(TOFaint)*fosc;
TOFbavg = sum(TOFbint)*fosc;

% Check data visually
plot(tsv,xsv)

% Collect results
Results = [SV,TOFaavg,TOFbavg];
```

Code S1c. Dynamic Catalysis in a Parallel A-to-B/A-to-C System with Square Waveform

```
% Remove prior runs and data
clear
clc

% Step test for Model 1 - CSTR

% Constants:
% Gas constant (L-bar/gmol-K)
Rg = 8.31446261815324e-2;

% Conditions:
% Temperature
Tc = 150.0; % deg C
T = Tc + 273.15; % K
```

```
% Parameters:
% Feed pressure (bar)
Pf(1) = 100.0; % A(g)
Pf(2:3) = 0.0;
% Feed concentration (M)
Cf = Pf/(Rg*T);

% Volumetric flowrate
qsdot = 50.0; % mL/min
qdot = qsdot/60000; % L/s
% Number of active sites (gmol)
Nsites = 138.0/1000*20.0e-6;
% CSTR volume (L)
V = 138.0/1000*1/3.58*1/1000*1/(1 - 0.375);
% Space velocity (1/s)
SV = qdot/V;

% Steady State Initial Conditions for the States
C_ss = Cf'; % M
N_ss = zeros(3,1); % gmol
x_ss = [C_ss;N_ss];

% Reaction chemistry:
% Heat of reaction (J/gmol)
delHovr = zeros(1,2);
% Bronsted-Evans-Polanyi relationship
alpha(1:2) = 0.6; % unitless
beta(1:2) = 100.0e3; % J/gmol
% Linear scaling relationship
gamma(1) = 2.0; % unitless
gamma(2) = 0.5; % unitless
delta(1:2) = 1.4; % eV

% Initial binding energy of A (eV)
BEa0 = 1.4;

% Dynamic catalysis:
% Oscillation time constants (s)
tau(1) = 5e5;
taur = 1.0;
tau(2) = taur*tau(1);
% Oscillation frequency (Hz)
fosc = 1/sum(tau);
% Number of oscillations (unitless)
Nosc = max(11,fosc);

% Oscillation amplitude (eV)
delU = 0.60;
% Oscillation endpoints (eV)
UL = -0.50;
```

```
UR = UL + delU;
% Obtain rate constants (1/bar-s or 1/s)
kR = parallel_cstr1_constants(BEa0,gamma,delta,delHovr,UR,T,alpha,beta);
kL = parallel_cstr1_constants(BEa0,gamma,delta,delHovr,UL,T,alpha,beta);

% Solver options
options = odeset('RelTol',1e-8,'AbsTol',1e-9);

% Time Matlab code
tic

% Iterate until convergence
for n = 1:inf
  % Empty matrices
  tsvm = [];
  xsvm = [];
  tsve = [];
  xsve = [];
  % Simulate all oscillations
  for i = 1:Nosc

      % Odd numbered runs
      if mod(i,2) == 1

      % Generate ODE solution
      [t,x] = ode23tb(@(t,x) parallel_cstr1(t,x,SV,Cf,kR,T),[0 tau(1)],x_ss(:,i),options);
      % Store data
      if i == 1
              tsv = t;
              xsv = x;
      else
              if round(i) == round(Nosc/2.0) || round(i) == round(Nosc/2.0 + 1.0)
              tsv = [tsv;t + tsv(end)];
              xsv = [xsv;x];
              tsvm = [tsvm;t + tsv(end)];
              xsvm = [xsvm;x];
              else
              if round(i) == round(Nosc - 1.0) || round(i) == round(Nosc)
              tsv = [tsv;t + tsv(end)];
              xsv = [xsv;x];
              tsve = [tsve;t + tsv(end)];
              xsve = [xsve;x];
              else
              tsv = [tsv;t + tsv(end)];
              xsv = [xsv;x];
              end
              end
      end
      x_ss(:,i + 1) = x(end,:)';

      % Clean up matrices
```

```
        clear t x

        % Even numbered runs
        else

        % Generate ODE solution
        [t,x] = ode23tb(@(t,x) parallel_cstr1(t,x,SV,Cf,kL,T),[0 tau(2)],x_ss(:,i),options);
        % Store data
        if round(i) == round(Nosc/2.0) || round(i) == round(Nosc/2.0 + 1.0)
                tsv = [tsv;t + tsv(end)];
                xsv = [xsv;x];
                tsvm = [tsvm;t + tsv(end)];
                xsvm = [xsvm;x];
        else
                if round(i) == round(Nosc - 1.0) || round(i) == round(Nosc)
                tsv = [tsv;t + tsv(end)];
                xsv = [xsv;x];
                tsve = [tsve;t + tsv(end)];
                xsve = [xsve;x];
                else
                tsv = [tsv;t + tsv(end)];
                xsv = [xsv;x];
                end
        end
        x_ss(:,i + 1) = x(end,:)';

        % Clean up matrices
        clear t x
        end
    end

    % Parse out the state values (M)
    Casvm = xsvm(:,1); % A(g)
    Casve = xsve(:,1); % A(g)

    % Measure reactor performance (mol %)
    Xasvm = (Cf(1) - Casvm)/sum(Cf)*100;
    Xasve = (Cf(1) - Casve)/sum(Cf)*100;

    % Time averaged conversion
    Xaavge = trapz(tsve,Xasve)*fosc;
    Xaavgm = trapz(tsvm,Xasvm)*fosc;

    % Converge on C conversion of A (mol %)
    C = 1.0;
    if abs(Xaavge - Xaavgm) > 0.01
        plot(tsv,xsv)
        x_ss(:,1) = xsv(end,:)';
        nt = n;
        error = abs(Xaavge - Xaavgm)/max([Xaavge,Xaavgm])*100;
        nt
```

```
        error
        clear tsv xsv Casvm Casve Xasvm Xasve
    else
        if abs(Xaavge - C) > 0.01
        SV = SV*Xaavge/C;
        x_ss(:,1) = [C_ss;N_ss];
        nq = n;
        conversion = Xaavge;
        nq
        conversion
        clear tsv xsv Casvm Casve Xasvm Xasve
        else
        toc
        break
        end
    end
end

% Parse out the state values (M)
Cbsve = xsve(:,2); % B(g)
Ccsve = xsve(:,3); % C(g)

% Measure reactor performance (1/s)
TOFae = (Cf(1) - Casve)*SV*V/Nsites;
TOFbe = (Cbsve - Cf(2))*SV*V/Nsites;
TOFce = (Ccsve - Cf(3))*SV*V/Nsites;

% Time averaged TOF (1/s)
TOFaavg = trapz(tsve,TOFae)*fosc;
TOFbavg = trapz(tsve,TOFbe)*fosc;
TOFcavg = trapz(tsve,TOFce)*fosc;

% Check data visually
plot(tsv,xsv)

% Collect results
Results = [SV,TOFaavg,TOFbavg,TOFcavg];
```

Section S2. Matlab ODE Solver Performance

ODE45 is Matlab's general purpose solver and we attempted to use it for both static and dynamic catalysis in the parallel reaction system. Since ODE45 was slow, stiff solvers including ODE15s, ODE23s, ODE23t, and ODE23tb were used to compare performance. A relative tolerance of 10^{-8} and absolute tolerance of 10^{-9} were used throughout the performance tests.

Trial S2a. Solver Performance for Static Catalysis

Stats for ode15s:
632 successful steps
9 failed attempts
774 function evaluations
3 partial derivatives
149 LU decompositions
752 solutions of linear systems
Elapsed time is 0.034665 seconds.

Stats for ode23s:
1621 successful steps
1131 failed attempts
16853 function evaluations
1621 partial derivatives
2752 LU decompositions
8256 solutions of linear systems
Elapsed time is 0.228154 seconds.

Stats for ode23t:
699 successful steps
5 failed attempts
1041 function evaluations
3 partial derivatives
243 LU decompositions
1019 solutions of linear systems
Elapsed time is 0.041602 seconds.

Stats for ode23tb:
543 successful steps
6 failed attempts
1278 function evaluations
3 partial derivatives
208 LU decompositions
1803 solutions of linear systems
Elapsed time is 0.019131 seconds.

ODE23tb was used throughout the manuscript for static catalysis simulation (i.e. volcano plots and surface coverage) because it required the fewest number of steps and was the fastest to converge.

Trial S2b. Solver Performance for Dynamic Catalysis

Stats for ode15s:
101 successful steps
1 failed attempts
144 function evaluations
1 partial derivatives
22 LU decompositions
135 solutions of linear systems
Elapsed time is 9.699912 seconds

Stats for ode23s:
295 successful steps
166 failed attempts
2990 function evaluations
295 partial derivatives
461 LU decompositions
1383 solutions of linear systems
Elapsed time is 63.131786 seconds

Stats for ode23t:
148 successful steps
0 failed attempts
191 function evaluations
1 partial derivatives
34 LU decompositions
182 solutions of linear systems
Elapsed time is 15.923910 seconds

Stats for ode23tb:
109 successful steps
0 failed attempts
266 function evaluations
1 partial derivatives
30 LU decompositions
366 solutions of linear systems
Elapsed time is 5.758628 seconds

ODE23tb was used throughout the manuscript for dynamic catalysis simulation because it required few steps and was the fastest to converge.

Section S3. Example CSTR Time-on-Stream Data

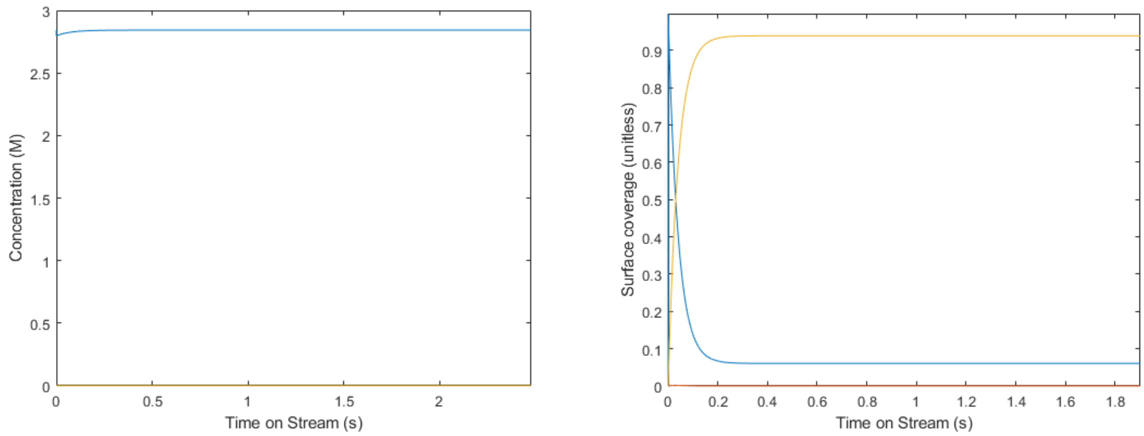

Figure S2. Time on Stream Data for a Parallel Reaction System. Gas phase concentrations ([=] M) for A, B, and C are shown on the left. Surface coverage for A*, B*, and C* are displayed on the right panel.

Section S4. Raw Data for Manuscript Heatmaps

Table S1. Raw data for Figure 3C, heatmap for the selectivity of B ([=] mol %). Conditions: T of 150 ^{o}C, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 2.0, $\gamma_{C\text{-}A}$ of 0.5, $\delta_{B\text{-}A}$ of 1.4 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), oscillation frequency (Hz)	-1.64	-1.58	-1.52	-1.46	-1.40	-1.34	-1.28	-1.22	-1.16	-1.10	-1.04	-0.98	-0.92	-0.86	-0.80	-0.74	-0.68	-0.62	-0.56	-0.50	-0.44	-0.38	-0.32	-0.26	-0.20	-0.14	-0.08	-0.02	0.04	0.10	0.16
1.00E-06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.03	0.01	0.00	0.00	0.01	0.14	1.76	16.62	43.66	49.50	49.97	50.00	50.00	50.00	50.00
3.16E-06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.03	0.01	0.00	0.00	0.02	0.15	1.79	16.65	43.67	49.50	49.97	50.00	50.00	50.00	50.00
1.00E-05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.03	0.01	0.01	0.01	0.03	0.19	1.87	16.76	43.70	49.50	49.97	50.00	50.00	50.00	50.00
3.16E-05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.03	0.02	0.01	0.03	0.09	0.31	2.12	17.10	43.81	49.52	49.97	50.00	50.00	50.00	50.00
1.00E-04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.03	0.02	0.03	0.10	0.24	0.67	2.91	18.14	44.13	49.58	49.99	50.00	50.00	50.00	50.00
3.16E-04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.03	0.03	0.10	0.31	0.75	1.80	5.31	21.28	45.11	49.77	50.02	50.01	50.01	50.00	50.00
1.00E-03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.03	0.06	0.31	0.96	2.29	5.21	12.14	29.73	48.02	50.35	50.15	50.05	50.02	50.01	50.01
3.16E-03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.04	0.16	0.98	2.98	6.86	14.50	28.29	47.53	55.57	52.16	50.54	50.15	50.06	50.03	50.02
1.00E-02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.11	0.06	0.06	0.46	3.00	8.79	18.73	34.54	54.56	70.90	69.62	57.09	51.73	50.48	50.18	50.09	50.06
3.16E-02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.07	0.10	0.06	0.13	1.41	8.81	23.11	41.89	62.34	78.94	87.93	84.85	67.66	55.19	51.50	50.57	50.29	50.18
1.00E-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.07	0.10	0.07	0.35	4.17	23.03	48.46	69.41	83.93	92.20	95.78	94.18	82.01	63.68	54.60	51.82	50.92	50.56
3.16E-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.05	0.08	0.11	0.96	11.78	48.37	74.77	87.77	94.31	97.41	98.63	98.07	92.12	78.25	63.42	56.00	53.03	51.80
1.00E+00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.04	0.07	0.21	2.79	27.05	72.07	90.06	95.78	98.15	99.18	99.58	99.43	97.85	92.41	81.89	69.42	60.52	56.12
3.16E+00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.04	0.08	0.48	5.16	34.76	78.50	94.56	98.29	99.37	99.75	99.88	99.87	99.62	98.73	96.07	89.56	79.10	69.45
1.00E+01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.09	0.60	4.76	28.71	73.69	94.31	98.73	99.65	99.90	99.97	99.98	99.95	99.85	99.50	98.32	95.02	88.47
3.16E+01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.06	0.31	2.01	13.05	48.56	88.63	98.22	99.70	99.94	99.99	99.99	99.99	99.97	99.91	99.75	99.25	97.80
1.00E+02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.12	0.73	4.93	29.72	80.27	97.82	99.79	99.97	100.00	100.00	100.00	99.99	99.97	99.93	99.81	99.52
3.16E+02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.06	0.38	3.09	24.83	78.82	97.90	99.83	99.99	100.00	100.00	100.00	100.00	99.99	99.98	99.94	99.84
1.00E+03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.05	0.31	2.86	23.72	78.78	97.95	99.84	99.99	100.00	100.00	100.00	100.00	100.00	99.99	99.98	99.95
3.16E+03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.04	0.31	2.83	24.21	78.82	97.97	99.85	99.99	100.00	100.00	100.00	100.00	100.00	100.00	99.99	99.98
1.00E+04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.04	0.31	2.83	24.21	78.83	97.98	99.85	99.99	100.00	100.00	100.00	100.00	100.00	100.00	100.00	99.99

Table S2. Raw data for Figure 3D, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, γ_{B-A} of 2.0, γ_{C-A} of 0.5, δ_{B-A} of 1.4 eV, and δ_{C-A} of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), oscillation frequency (Hz)	-1.64	-1.58	-1.52	-1.46	-1.40	-1.34	-1.28	-1.22	-1.16	-1.10	-1.04	-0.98	-0.92	-0.86	-0.80	-0.74	-0.68	-0.62	-0.56	-0.50	-0.44	-0.38	-0.32	-0.26	-0.20	-0.14	-0.08	-0.02	0.04	0.10	0.16
1.00E-06	7.33E-01	9.88E-01	1.19E+00	1.42E+00	1.56E+00	1.58E+00	1.23E+00	8.05E-01	5.44E-01	4.41E-01	4.49E-01	5.43E-01	7.07E-01	9.21E-01	1.11E+00	1.09E+00	7.93E-01	4.39E-01	2.10E-01	9.51E-02	4.21E-02	1.85E-02	8.22E-03	4.20E-03	2.65E-03	1.21E-03	4.48E-04	1.23E-04	1.50E-05	8.01E-07	3.37E-08
3.16E-06	7.33E-01	9.51E-01	1.19E+00	1.42E+00	1.56E+00	1.58E+00	1.23E+00	8.05E-01	5.44E-01	4.41E-01	4.49E-01	5.43E-01	7.07E-01	9.21E-01	1.11E+00	1.09E+00	7.93E-01	4.39E-01	2.10E-01	9.51E-02	4.21E-02	1.85E-02	8.22E-03	4.21E-03	2.66E-03	1.21E-03	4.49E-04	1.23E-04	1.51E-05	7.86E-07	4.10E-08
1.00E-05	7.33E-01	9.66E-01	1.19E+00	1.42E+00	1.56E+00	1.58E+00	1.23E+00	8.05E-01	5.44E-01	4.41E-01	4.49E-01	5.43E-01	7.07E-01	9.21E-01	1.11E+00	1.09E+00	7.93E-01	4.39E-01	2.10E-01	9.51E-02	4.21E-02	1.85E-02	8.23E-03	4.21E-03	2.66E-03	1.21E-03	4.49E-04	1.23E-04	1.52E-05	8.23E-07	6.18E-08
3.16E-05	7.33E-01	9.51E-01	1.19E+00	1.42E+00	1.56E+00	1.58E+00	1.23E+00	8.05E-01	5.44E-01	4.41E-01	4.49E-01	5.43E-01	7.07E-01	9.21E-01	1.11E+00	1.09E+00	7.93E-01	4.39E-01	2.10E-01	9.51E-02	4.21E-02	1.85E-02	8.25E-03	4.23E-03	2.66E-03	1.21E-03	4.50E-04	1.24E-04	1.51E-05	9.00E-07	1.29E-07
1.00E-04	7.33E-01	9.51E-01	1.19E+00	1.42E+00	1.56E+00	1.58E+00	1.23E+00	8.05E-01	5.44E-01	4.41E-01	4.49E-01	5.43E-01	7.08E-01	9.21E-01	1.11E+00	1.09E+00	7.93E-01	4.39E-01	2.10E-01	9.52E-02	4.22E-02	1.86E-02	8.33E-03	4.29E-03	2.68E-03	1.21E-03	4.52E-04	1.25E-04	1.54E-05	1.09E-06	9.18E-07
3.16E-04	7.33E-01	9.52E-01	1.19E+00	1.42E+00	1.56E+00	1.58E+00	1.23E+00	8.05E-01	5.44E-01	4.41E-01	4.49E-01	5.44E-01	7.08E-01	9.22E-01	1.11E+00	1.10E+00	7.94E-01	4.39E-01	2.11E-01	9.54E-02	4.24E-02	1.89E-02	8.56E-03	4.48E-03	2.74E-03	1.22E-03	4.55E-04	1.27E-04	1.62E-05	1.80E-06	1.01E-06
1.00E-03	7.34E-01	9.52E-01	1.19E+00	1.42E+00	1.56E+00	1.58E+00	1.23E+00	8.05E-01	5.44E-01	4.42E-01	4.50E-01	5.45E-01	7.09E-01	9.23E-01	1.11E+00	1.10E+00	7.94E-01	4.40E-01	2.11E-01	9.61E-02	4.32E-02	1.96E-02	9.28E-03	5.06E-03	2.91E-03	1.24E-03	4.63E-04	1.29E-04	1.83E-05	3.91E-06	3.13E-06
3.16E-03	7.37E-01	9.54E-01	1.19E+00	1.42E+00	1.56E+00	1.59E+00	1.23E+00	8.05E-01	5.45E-01	4.43E-01	4.53E-01	5.48E-01	7.12E-01	9.26E-01	1.12E+00	1.10E+00	7.95E-01	4.41E-01	2.13E-01	9.83E-02	4.55E-02	2.19E-02	1.15E-02	6.83E-03	3.42E-03	1.32E-03	4.67E-04	1.32E-04	2.52E-05	8.66E-05	9.94E-06
1.00E-02	7.45E-01	9.61E-01	1.19E+00	1.42E+00	1.57E+00	1.59E+00	1.23E+00	8.04E-01	5.46E-01	4.48E-01	4.61E-01	5.58E-01	7.23E-01	9.37E-01	1.13E+00	1.10E+00	7.99E-01	4.44E-01	2.18E-01	1.05E-01	5.27E-02	2.89E-02	1.83E-02	1.24E-02	4.98E-03	1.46E-03	4.79E-04	1.55E-04	4.66E-05	3.18E-05	3.13E-05
3.16E-02	7.71E-01	9.86E-01	1.21E+00	1.44E+00	1.58E+00	1.59E+00	1.22E+00	8.02E-01	5.50E-01	4.62E-01	4.85E-01	5.88E-01	7.56E-01	9.69E-01	1.15E+00	1.12E+00	8.09E-01	4.53E-01	2.35E-01	1.27E-01	7.45E-02	5.06E-02	3.96E-02	2.98E-02	9.86E-03	1.94E-03	5.95E-04	2.24E-04	1.14E-04	9.96E-05	9.83E-05
1.00E-01	8.55E-01	1.05E+00	1.27E+00	1.49E+00	1.61E+00	1.60E+00	1.22E+00	7.92E-01	5.62E-01	5.05E-01	5.56E-01	6.76E-01	8.52E-01	1.07E+00	1.24E+00	1.18E+00	8.43E-01	4.80E-01	2.84E-01	1.91E-01	1.42E-01	1.19E-01	1.07E-01	8.50E-02	2.55E-02	3.95E-03	9.00E-04	2.23E-04	1.08E-04	9.94E-05	9.86E-05
3.16E-01	1.07E+00	1.23E+00	1.42E+00	1.62E+00	1.72E+00	1.63E+00	1.20E+00	7.73E-01	5.88E-01	5.81E-01	6.79E-01	8.44E-01	1.06E+00	1.29E+00	1.45E+00	1.33E+00	9.11E-01	5.36E-01	4.28E-01	3.91E-01	3.55E-01	3.34E-01	3.19E-01	2.59E-01	7.49E-02	8.26E-03	1.90E-03	2.28E-04	9.98E-05	9.92E-05	9.88E-05
1.00E+00	1.31E+00	1.44E+00	1.64E+00	1.86E+00	1.93E+00	1.70E+00	1.17E+00	7.58E-01	6.01E-01	6.25E-01	7.61E-01	9.90E-01	1.28E+00	1.58E+00	1.73E+00	1.48E+00	9.49E-01	6.40E-01	7.89E-01	9.90E-01	1.02E+00	1.01E+00	9.91E-01	8.11E-01	2.31E-01	2.51E-02	4.98E-03	2.18E-04	1.04E-04	9.90E-05	9.86E-05
3.16E+00	1.33E+00	1.50E+00	1.74E+00	2.00E+00	2.07E+00	1.75E+00	1.18E+00	7.65E-01	6.12E-01	6.32E-01	8.06E-01	1.03E+00	1.34E+00	1.67E+00	1.79E+00	1.45E+00	9.08E-01	6.65E-01	9.92E-01	1.78E+00	2.47E+00	2.85E+00	3.00E+00	2.53E+00	7.23E-01	7.48E-02	1.42E-02	2.01E-04	9.80E-05	9.88E-05	9.84E-05
1.00E+01	1.36E+00	1.53E+00	1.82E+00	2.14E+00	2.20E+00	1.87E+00	1.25E+00	7.99E-01	6.85E-01	6.97E-01	8.63E-01	1.05E+00	1.37E+00	1.61E+00	1.66E+00	1.36E+00	8.48E-01	5.71E-01	7.41E-01	1.61E+00	3.18E+00	4.92E+00	6.39E+00	6.44E+00	2.00E+00	1.38E-01	3.78E-02	2.09E-04	1.04E-04	1.04E-04	1.04E-04

3.16E+01	1.41E+00	1.66E+00	1.98E+00	2.35E+00	2.47E+00	2.07E+00	1.39E+00	8.45E-01	6.56E-01	6.50E-01	7.67E-01	9.63E-01	1.18E+00	1.45E+00	1.52E+00	1.25E+00	7.94E-01	4.58E-01	3.73E-01	8.39E-01	2.30E+00	5.64E+00	1.01E+01	1.50E+01	3.68E+00	2.13E-01	3.54E-02	2.82E-04	1.40E-04	1.39E-04	1.40E-04
1.00E+02	1.60E+00	1.96E+00	2.53E+00	3.12E+00	3.38E+00	2.80E+00	1.75E+00	9.95E-01	6.74E-01	6.01E-01	6.92E-01	8.71E-01	1.12E+00	1.35E+00	1.47E+00	1.20E+00	7.55E-01	4.05E-01	3.35E-01	4.82E-01	1.87E+00	7.94E+00	2.43E+01	4.20E+01	5.05E+00	2.34E-01	3.39E-02	2.79E-04	2.53E-04	2.51E-04	2.53E-04
3.16E+02	2.06E+00	2.91E+00	4.17E+00	5.57E+00	6.23E+00	5.11E+00	2.83E+00	1.28E+00	6.80E-01	5.57E-01	6.39E-01	8.14E-01	1.06E+00	1.32E+00	1.42E+00	1.18E+00	7.30E-01	3.95E-01	2.62E-01	4.51E-01	1.94E+00	9.82E+00	4.22E+01	7.98E+01	5.71E+00	2.47E-01	3.32E-02	2.54E-04	2.52E-04	2.51E-04	2.52E-04
1.00E+03	3.60E+00	5.93E+00	9.18E+00	1.30E+01	1.49E+01	1.03E+01	4.22E+00	1.50E+00	7.07E-01	5.45E-01	6.44E-01	8.01E-01	1.07E+00	1.32E+00	1.45E+00	1.18E+00	7.47E-01	3.94E-01	3.15E-01	4.50E-01	1.99E+00	1.07E+01	5.28E+01	9.14E+01	5.91E+00	2.49E-01	3.32E-02	2.54E-04	2.52E-04	2.52E-04	2.52E-04
3.16E+03	8.51E+00	1.52E+01	2.54E+01	3.72E+01	3.52E+01	1.55E+01	5.03E+00	1.62E+00	7.13E-01	5.40E-01	6.19E-01	7.97E-01	1.04E+00	1.31E+00	1.41E+00	1.18E+00	7.29E-01	3.94E-01	2.60E-01	4.51E-01	2.01E+00	1.10E+01	5.59E+01	9.29E+01	5.94E+00	2.50E-01	3.33E-02	2.54E-04	2.52E-04	2.51E-04	2.52E-04
1.00E+04	2.36E+01	4.51E+01	7.79E+01	1.01E+02	5.50E+01	1.81E+01	5.34E+00	1.65E+00	7.14E-01	5.39E-01	6.18E-01	7.95E-01	1.04E+00	1.31E+00	1.41E+00	1.18E+00	7.29E-01	3.94E-01	2.60E-01	4.51E-01	2.02E+00	1.11E+01	5.63E+01	9.30E+01	5.94E+00	2.50E-01	3.33E-02	2.54E-04	2.52E-04	2.51E-04	2.52E-04

Table S3. Raw data for Figure 3E, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 °C, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 2.0, and $\delta_{B\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation frequency (Hz), oscillation endpoint (eV)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	9.87E-04	7.09E-04	1.08E-04	8.46E-05	2.23E-04	2.57E-03	1.20E-02	1.90E-02	8.52E-04	2.31E-04	1.59E-03	1.13E-02	1.88E-02	8.19E-04	8.55E-06	1.63E-08
1E-05	9.87E-04	7.09E-04	1.08E-04	8.46E-05	2.23E-04	2.57E-03	1.20E-02	1.90E-02	8.53E-04	2.38E-04	1.60E-03	1.13E-02	1.88E-02	8.20E-04	8.67E-06	2.23E-08
1E-04	9.87E-04	7.09E-04	1.08E-04	8.46E-05	2.23E-04	2.57E-03	1.20E-02	1.90E-02	8.67E-04	3.06E-04	1.69E-03	1.14E-02	1.89E-02	8.25E-04	8.66E-06	8.23E-08
1E-03	9.87E-04	7.09E-04	1.08E-04	8.46E-05	2.23E-04	2.58E-03	1.20E-02	1.90E-02	9.67E-04	9.81E-04	2.59E-03	1.23E-02	1.91E-02	8.37E-04	9.30E-06	6.80E-07
1E-02	9.54E-04	7.09E-04	1.08E-04	8.46E-05	2.23E-04	2.58E-03	1.21E-02	1.93E-02	1.87E-03	7.73E-03	1.15E-02	2.12E-02	2.14E-02	8.48E-04	1.53E-05	6.65E-06
1E-01	6.80E-04	4.18E-04	7.19E-05	4.96E-05	2.23E-04	2.55E-03	1.21E-02	1.95E-02	1.09E-02	7.52E-02	1.00E-01	1.10E-01	4.21E-02	1.01E-03	7.44E-05	6.63E-05
1E+00	6.80E-04	5.55E-05	7.19E-05	4.96E-05	2.80E-04	1.96E-03	1.26E-02	2.22E-02	1.00E-01	7.48E-01	9.89E-01	9.94E-01	2.48E-01	2.71E-03	6.73E-04	6.65E-04
1E+01	6.80E-04	5.55E-05	7.19E-05	4.96E-05	2.80E-04	1.33E-03	1.86E-02	4.80E-02	4.60E-01	3.31E+00	9.47E+00	9.84E+00	2.15E+00	1.30E-02	6.66E-03	6.64E-03
1E+02	6.80E-04	5.55E-05	7.19E-05	4.96E-05	2.80E-04	1.33E-03	3.75E-02	1.01E-01	6.10E-01	4.25E+00	2.70E+01	8.81E+01	5.35E+00	3.39E-02	2.53E-02	2.53E-02
1E+03	6.80E-04	5.55E-05	7.19E-05	4.96E-05	2.80E-04	1.33E-03	3.43E-02	1.07E-01	6.25E-01	4.36E+00	3.10E+01	1.99E+02	5.97E+00	3.32E-02	2.52E-02	2.52E-02
1E+04	6.80E-04	5.55E-05	7.19E-05	4.96E-05	2.80E-04	1.33E-03	2.92E-02	1.08E-01	6.27E-01	4.37E+00	3.15E+01	2.12E+02	5.99E+00	3.33E-02	2.52E-02	2.52E-02

Table S4. Raw data for Figure 3F, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 ^{o}C, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{C\text{-}A}$ of 0.5, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation frequency (Hz), oscillation endpoint (eV)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.49E-01	7.07E-01	1.11E+00	7.93E-01	2.10E-01	4.21E-02	8.07E-03	1.48E-03	2.28E-04	2.20E-05	1.16E-06
1E-05	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.49E-01	7.07E-01	1.11E+00	7.93E-01	2.10E-01	4.21E-02	8.07E-03	1.48E-03	2.29E-04	2.20E-05	1.16E-06
1E-04	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.49E-01	7.07E-01	1.11E+00	7.93E-01	2.10E-01	4.21E-02	8.08E-03	1.49E-03	2.32E-04	2.20E-05	1.22E-06
1E-03	7.34E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.50E-01	7.09E-01	1.11E+00	7.94E-01	2.10E-01	4.22E-02	8.13E-03	1.51E-03	2.33E-04	2.24E-05	1.83E-06
1E-02	7.45E-01	1.19E+00	1.57E+00	1.23E+00	5.46E-01	4.61E-01	7.23E-01	1.12E+00	7.98E-01	2.11E-01	4.26E-02	8.23E-03	1.51E-03	2.37E-04	2.81E-05	7.67E-06
1E-01	8.55E-01	1.27E+00	1.61E+00	1.22E+00	5.62E-01	5.56E-01	8.52E-01	1.23E+00	8.39E-01	2.17E-01	4.28E-02	8.19E-03	1.56E-03	2.95E-04	8.76E-05	6.74E-05
1E+00	1.31E+00	1.64E+00	1.93E+00	1.17E+00	6.01E-01	7.61E-01	1.28E+00	1.72E+00	9.18E-01	2.07E-01	4.09E-02	8.37E-03	1.63E-03	8.55E-04	6.77E-04	6.65E-04
1E+01	1.36E+00	1.81E+00	2.18E+00	1.22E+00	6.11E-01	7.62E-01	1.28E+00	1.63E+00	7.64E-01	1.75E-01	4.17E-02	1.30E-02	7.30E-03	6.71E-03	6.66E-03	6.65E-03
1E+02	1.60E+00	2.53E+00	3.37E+00	1.75E+00	6.58E-01	6.73E-01	1.09E+00	1.44E+00	7.31E-01	1.94E-01	6.20E-02	3.15E-02	1.31E-02	2.53E-02	2.53E-02	2.53E-02
1E+03	3.60E+00	9.18E+00	1.49E+01	4.22E+00	7.08E-01	6.24E-01	1.05E+00	1.41E+00	7.26E-01	1.94E-01	6.16E-02	3.13E-02	2.57E-02	2.51E-02	2.52E-02	2.51E-02
1E+04	2.36E+01	7.79E+01	5.50E+01	5.34E+00	7.14E-01	6.18E-01	1.04E+00	1.41E+00	7.26E-01	1.94E-01	6.16E-02	3.13E-02	2.57E-02	2.51E-02	2.51E-02	2.52E-02

Table S5. Raw data for Figure 5B, heatmap for the selectivity of B ([=] mol %). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 2.0, $\gamma_{C\text{-}A}$ of 0.5, $\delta_{B\text{-}A}$ of 1.4 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation amplitude and frequency. The oscillation midpoint is fixed at the volcano peak for B production.

Oscillation amplitude (eV), oscillation frequency (Hz)	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
1.00E-06	40.68	36.25	25.53	14.56	7.19	3.27	1.41	0.57	0.21	0.07	0.02	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3.16E-06	40.68	36.25	25.53	14.56	7.19	3.27	1.41	0.57	0.21	0.07	0.02	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1.00E-05	40.68	36.25	25.53	14.56	7.19	3.27	1.41	0.58	0.22	0.08	0.03	0.02	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3.16E-05	40.68	36.25	25.53	14.56	7.19	3.28	1.42	0.59	0.24	0.10	0.06	0.04	0.03	0.02	0.01	0.01	0.01	0.01	0.00	0.00	0.00
1.00E-04	40.68	36.25	25.53	14.56	7.20	3.29	1.45	0.63	0.30	0.18	0.14	0.11	0.08	0.06	0.05	0.03	0.03	0.02	0.01	0.01	0.01
3.16E-04	40.68	36.25	25.52	14.56	7.21	3.33	1.53	0.77	0.50	0.43	0.39	0.33	0.26	0.20	0.15	0.11	0.08	0.06	0.05	0.04	0.03
1.00E-03	40.68	36.24	25.50	14.55	7.26	3.46	1.78	1.20	1.13	1.20	1.19	1.03	0.82	0.62	0.46	0.34	0.25	0.19	0.15	0.12	0.10
3.16E-03	40.68	36.23	25.48	14.58	7.42	3.87	2.57	2.51	3.05	3.56	3.61	3.18	2.55	1.94	1.44	1.07	0.80	0.60	0.47	0.38	0.32
1.00E-02	40.68	36.24	25.54	14.82	8.06	5.19	4.97	6.42	8.59	10.26	10.48	9.34	7.59	5.85	4.40	3.28	2.46	1.87	1.46	1.19	1.01
3.16E-02	40.68	36.34	25.80	15.65	10.06	9.18	11.88	16.93	22.52	26.30	26.77	24.32	20.39	16.24	12.55	9.57	7.28	5.60	4.40	3.59	3.05
1.00E-01	40.66	36.63	26.91	18.41	15.98	19.87	28.34	38.70	47.71	52.89	53.47	50.19	44.46	37.63	30.77	24.58	19.39	15.29	12.23	10.04	8.58
3.16E-01	40.67	37.10	29.09	25.30	30.12	41.54	54.94	66.47	74.21	77.98	78.38	76.07	71.60	65.46	58.16	50.27	42.43	35.22	29.11	24.35	20.89
1.00E+00	40.73	38.37	35.69	41.21	54.27	68.01	78.34	84.91	88.65	90.47	90.92	90.21	88.38	85.41	81.27	75.99	69.70	62.68	55.42	48.53	42.60
3.16E+00	40.69	41.91	48.40	60.45	71.72	79.80	85.13	88.58	90.73	92.22	93.04	93.35	93.14	92.37	90.98	88.92	86.12	82.57	78.31	73.46	68.33
1.00E+01	41.97	47.78	58.23	66.76	73.06	77.80	80.29	83.43	85.13	87.32	89.06	90.37	91.25	91.72	91.77	91.35	90.44	89.03	87.20	85.02	82.62
3.16E+01	41.51	51.71	62.53	67.77	70.51	72.30	73.70	75.06	75.27	78.30	79.11	80.90	83.01	84.91	86.48	87.64	88.31	88.52	88.27	87.67	86.88
1.00E+02	41.67	51.80	63.68	67.62	69.77	70.46	70.73	70.84	71.14	71.46	71.94	73.12	74.10	75.43	76.44	78.37	80.39	82.31	83.96	85.26	86.19
3.16E+02	41.68	52.44	63.94	68.55	70.13	70.63	70.73	70.65	70.59	70.53	70.60	70.78	71.14	71.71	72.46	73.49	74.79	76.40	78.22	80.26	82.42
1.00E+03	41.67	52.44	63.96	68.20	70.25	70.73	70.78	70.68	70.59	70.50	70.55	70.70	71.01	71.51	72.17	73.09	74.22	75.66	77.26	79.11	81.16
3.16E+03	41.68	52.44	63.21	68.62	70.27	70.76	70.80	70.70	70.60	70.52	70.56	70.72	71.03	71.55	72.23	73.18	74.34	75.83	77.48	79.38	81.46
1.00E+04	41.67	52.44	67.20	68.62	70.27	70.77	70.81	70.70	70.61	70.52	70.57	70.73	71.05	71.58	72.27	73.23	74.42	75.93	77.61	79.55	81.67

Table S6. Raw data for Figure 5C, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 °C, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, γ_{B-A} of 2.0, γ_{C-A} of 0.5, δ_{B-A} of 1.4 eV, and δ_{C-A} of 1.4 eV. Dynamics: various oscillation amplitude and frequency. The oscillation midpoint is fixed at the volcano peak for B production.

Oscillation amplitude (eV), oscillation frequency (Hz)	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
1.00E-06	5.92E-03	5.84E-03	5.89E-03	6.53E-03	8.02E-03	1.06E-02	1.44E-02	2.00E-02	2.80E-02	3.94E-02	5.53E-02	7.76E-02	1.09E-01	1.52E-01	2.10E-01	2.89E-01	3.91E-01	5.19E-01	6.68E-01	8.24E-01	9.71E-01
3.16E-06	5.92E-03	5.84E-03	5.89E-03	6.53E-03	8.02E-03	1.06E-02	1.44E-02	2.00E-02	2.80E-02	3.94E-02	5.53E-02	7.76E-02	1.09E-01	1.52E-01	2.10E-01	2.89E-01	3.91E-01	5.19E-01	6.68E-01	8.24E-01	9.71E-01
1.00E-05	5.92E-03	5.84E-03	5.89E-03	6.53E-03	8.02E-03	1.06E-02	1.44E-02	2.00E-02	2.80E-02	3.94E-02	5.53E-02	7.76E-02	1.09E-01	1.52E-01	2.10E-01	2.89E-01	3.91E-01	5.19E-01	6.68E-01	8.24E-01	9.71E-01
3.16E-05	5.92E-03	5.84E-03	5.89E-03	6.53E-03	8.02E-03	1.06E-02	1.44E-02	2.00E-02	2.80E-02	3.94E-02	5.53E-02	7.77E-02	1.09E-01	1.52E-01	2.10E-01	2.89E-01	3.91E-01	5.19E-01	6.68E-01	8.24E-01	9.71E-01
1.00E-04	5.92E-03	5.84E-03	5.89E-03	6.53E-03	8.03E-03	1.06E-02	1.44E-02	2.00E-02	2.81E-02	3.94E-02	5.54E-02	7.77E-02	1.09E-01	1.52E-01	2.10E-01	2.89E-01	3.91E-01	5.19E-01	6.68E-01	8.24E-01	9.71E-01
3.16E-04	5.92E-03	5.84E-03	5.90E-03	6.54E-03	8.04E-03	1.06E-02	1.44E-02	2.01E-02	2.81E-02	3.95E-02	5.55E-02	7.79E-02	1.09E-01	1.52E-01	2.11E-01	2.89E-01	3.92E-01	5.19E-01	6.69E-01	8.25E-01	9.71E-01
1.00E-03	5.92E-03	5.85E-03	5.90E-03	6.56E-03	8.07E-03	1.06E-02	1.45E-02	2.02E-02	2.84E-02	3.99E-02	5.61E-02	7.86E-02	1.10E-01	1.53E-01	2.12E-01	2.90E-01	3.92E-01	5.20E-01	6.70E-01	8.26E-01	9.73E-01
3.16E-03	5.92E-03	5.85E-03	5.92E-03	6.59E-03	8.14E-03	1.08E-02	1.47E-02	2.06E-02	2.91E-02	4.10E-02	5.77E-02	8.05E-02	1.12E-01	1.55E-01	2.14E-01	2.93E-01	3.95E-01	5.23E-01	6.73E-01	8.30E-01	9.77E-01
1.00E-02	5.92E-03	5.85E-03	5.93E-03	6.62E-03	8.22E-03	1.10E-02	1.52E-02	2.17E-02	3.11E-02	4.45E-02	6.26E-02	8.66E-02	1.19E-01	1.63E-01	2.22E-01	3.01E-01	4.04E-01	5.33E-01	6.84E-01	8.43E-01	9.92E-01
3.16E-02	5.92E-03	5.86E-03	5.95E-03	6.69E-03	8.41E-03	1.15E-02	1.65E-02	2.45E-02	3.70E-02	5.47E-02	7.74E-02	1.05E-01	1.40E-01	1.85E-01	2.46E-01	3.27E-01	4.32E-01	5.63E-01	7.17E-01	8.81E-01	1.04E+00
1.00E-01	5.92E-03	5.91E-03	6.01E-03	6.93E-03	8.90E-03	1.29E-02	2.03E-02	3.33E-02	5.49E-02	8.59E-02	1.23E-01	1.61E-01	2.03E-01	2.53E-01	3.17E-01	4.02E-01	5.13E-01	6.52E-01	8.17E-01	9.96E-01	1.17E+00
3.16E-01	5.92E-03	6.29E-03	6.32E-03	7.68E-03	1.10E-02	1.77E-02	3.22E-02	6.08E-02	1.11E-01	1.84E-01	2.64E-01	3.36E-01	3.98E-01	4.59E-01	5.31E-01	6.22E-01	7.41E-01	8.95E-01	1.08E+00	1.30E+00	1.51E+00
1.00E+00	5.92E-03	7.31E-03	8.12E-03	1.09E-02	1.76E-02	3.29E-02	6.71E-02	1.35E-01	2.52E-01	4.23E-01	6.26E-01	8.18E-01	9.71E-01	1.09E+00	1.19E+00	1.29E+00	1.42E+00	1.59E+00	1.80E+00	2.06E+00	2.35E+00
3.16E+00	5.92E-03	1.07E-02	1.05E-02	1.59E-02	2.80E-02	5.16E-02	9.56E-02	1.75E-01	3.05E-01	5.12E-01	8.07E-01	1.19E+00	1.63E+00	2.06E+00	2.44E+00	2.78E+00	3.09E+00	3.40E+00	3.73E+00	4.09E+00	4.48E+00
1.00E+01	5.92E-03	1.05E-02	1.19E-02	1.47E-02	3.91E-02	5.42E-02	7.32E-02	1.18E-01	1.87E-01	3.09E-01	5.05E-01	8.08E-01	1.25E+00	1.86E+00	2.62E+00	3.49E+00	4.39E+00	5.27E+00	6.15E+00	7.04E+00	7.95E+00
3.16E+01	5.92E-03	9.50E-03	1.06E-02	1.86E-02	4.39E-02	5.44E-02	6.99E-02	9.29E-02	1.15E-01	1.83E-01	2.58E-01	3.96E-01	6.25E-01	9.86E-01	1.54E+00	2.35E+00	3.44E+00	4.81E+00	6.38E+00	8.03E+00	9.72E+00
1.00E+02	5.92E-03	8.20E-03	1.25E-02	1.80E-02	4.93E-02	5.89E-02	7.21E-02	9.06E-02	1.05E-01	1.44E-01	1.98E-01	2.92E-01	4.09E-01	5.84E-01	8.49E-01	1.26E+00	1.88E+00	2.83E+00	4.18E+00	6.02E+00	8.27E+00
3.16E+02	5.92E-03	8.21E-03	1.24E-02	1.69E-02	4.93E-02	5.91E-02	7.22E-02	9.02E-02	1.17E-01	1.52E-01	2.05E-01	2.74E-01	3.78E-01	5.17E-01	7.23E-01	1.00E+00	1.40E+00	1.94E+00	2.72E+00	3.82E+00	5.37E+00
1.00E+03	5.92E-03	8.20E-03	1.30E-02	1.86E-02	4.94E-02	5.89E-02	7.22E-02	9.02E-02	1.17E-01	1.52E-01	2.04E-01	2.78E-01	3.76E-01	5.13E-01	7.15E-01	9.85E-01	1.36E+00	1.86E+00	2.55E+00	3.47E+00	4.70E+00

3.16E+03	5.92E-03	8.14E-03	1.19E-02	1.69E-02	4.95E-02	5.89E-02	7.23E-02	9.02E-02	1.17E-01	1.52E-01	2.05E-01	2.78E-01	3.76E-01	5.14E-01	7.17E-01	9.89E-01	1.37E+00	1.88E+00	2.59E+00	3.54E+00	4.84E+00
1.00E+04	5.92E-03	8.13E-03	1.27E-02	1.69E-02	4.95E-02	5.89E-02	7.23E-02	9.03E-02	1.17E-01	1.52E-01	2.05E-01	2.79E-01	3.76E-01	5.14E-01	7.17E-01	9.91E-01	1.37E+00	1.89E+00	2.61E+00	3.59E+00	4.94E+00

Table S7. Raw data for Figure 6C, heatmap for the selectivity of B ([=] mol %). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 0.25, $\gamma_{C\text{-}A}$ of 0.50, $\delta_{B\text{-}A}$ of 1.4 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), oscillation frequency (Hz)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	98.94	98.11	96.69	94.08	89.54	91.87	95.16	94.61	89.82	71.81	53.93	50.38	50.03	50.00	50.00	50.00
1E-05	98.94	98.11	96.68	94.08	89.54	91.87	95.16	94.60	89.80	71.79	53.92	50.38	50.03	50.00	50.00	50.00
1E-04	98.94	98.11	96.68	94.08	89.56	91.88	95.13	94.53	89.57	71.56	53.88	50.37	50.03	50.00	50.00	50.00
1E-03	98.93	98.10	96.66	94.05	89.73	91.98	94.93	93.79	87.40	69.37	53.45	50.28	50.01	50.00	50.00	50.00
1E-02	98.86	98.00	96.43	93.80	90.79	92.42	93.08	87.39	70.50	52.73	49.17	49.37	49.78	49.96	50.01	50.02
1E-01	98.76	97.87	96.29	93.49	90.17	87.34	77.87	52.00	23.55	14.89	27.86	41.76	47.61	49.57	50.09	50.16
1E+00	98.72	97.83	96.07	92.94	88.10	79.16	54.46	18.09	4.85	5.37	16.32	29.88	39.46	46.79	50.99	51.86
1E+01	98.68	97.02	91.55	93.21	88.59	76.20	48.13	18.52	6.97	11.12	16.16	22.69	33.56	44.11	52.43	58.63
1E+02	98.68	96.34	94.29	93.19	88.50	78.74	59.67	35.40	19.94	16.71	16.81	16.98	17.25	19.45	29.87	49.36
1E+03	98.69	97.59	95.51	93.19	87.62	75.80	78.60	51.84	24.35	17.67	16.82	16.74	16.74	16.75	16.93	18.19
1E+04	98.61	97.70	96.21	84.07	91.80	92.28	83.10	54.86	24.66	17.71	16.82	16.74	16.74	16.72	16.72	16.73

Table S8. Raw data for Figure 6D, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 0.25, $\gamma_{C\text{-}A}$ of 0.50, $\delta_{B\text{-}A}$ of 1.4 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), oscillation frequency (Hz)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	3.24E-02	4.03E-02	2.86E-02	1.95E-02	1.87E-02	2.53E-02	3.16E-02	2.29E-02	1.18E-02	6.57E-03	3.73E-03	1.65E-03	6.37E-04	2.01E-04	3.40E-05	2.25E-06
1E-05	3.24E-02	4.03E-02	2.86E-02	1.95E-02	1.87E-02	2.53E-02	3.16E-02	2.29E-02	1.18E-02	6.57E-03	3.73E-03	1.65E-03	6.37E-04	2.01E-04	3.43E-05	2.26E-06
1E-04	3.24E-02	4.04E-02	2.86E-02	1.95E-02	1.88E-02	2.54E-02	3.17E-02	2.29E-02	1.19E-02	6.60E-03	3.74E-03	1.65E-03	6.41E-04	2.03E-04	3.45E-05	2.51E-06
1E-03	3.26E-02	4.04E-02	2.84E-02	1.94E-02	1.91E-02	2.62E-02	3.24E-02	2.33E-02	1.23E-02	6.85E-03	3.80E-03	1.67E-03	6.47E-04	2.04E-04	3.76E-05	5.43E-06
1E-02	3.44E-02	4.11E-02	2.71E-02	1.86E-02	2.18E-02	3.28E-02	3.81E-02	2.65E-02	1.55E-02	9.04E-03	4.12E-03	1.70E-03	6.53E-04	2.33E-04	6.62E-05	3.30E-05
1E-01	3.74E-02	4.24E-02	2.65E-02	1.85E-02	2.31E-02	4.05E-02	5.10E-02	4.55E-02	4.55E-02	2.91E-02	6.78E-03	2.25E-03	9.80E-04	5.06E-04	1.73E-04	3.13E-04
1E+00	4.05E-02	4.54E-02	2.95E-02	2.17E-02	2.79E-02	4.81E-02	7.34E-02	1.24E-01	1.85E-01	6.57E-02	6.60E-03	5.59E-03	3.83E-04	3.27E-04	3.15E-05	3.10E-04
1E+01	4.16E-02	6.17E-02	6.18E-02	2.08E-02	2.60E-02	9.17E-02	1.08E-01	1.30E-01	1.54E-01	4.93E-02	4.09E-03	3.37E-03	3.18E-04	3.12E-04	3.11E-04	3.12E-04
1E+02	4.17E-02	7.72E-02	4.07E-02	2.07E-02	2.53E-02	3.96E-02	7.70E-02	6.07E-02	7.17E-02	5.01E-02	3.57E-03	2.88E-03	1.31E-04	2.53E-04	1.26E-04	2.54E-04
1E+03	4.48E-02	5.47E-02	3.56E-02	1.85E-02	1.24E-02	1.26E-02	5.63E-02	5.92E-02	6.40E-02	4.90E-02	1.56E-03	1.58E-03	2.55E-04	2.51E-04	2.51E-04	2.51E-04
1E+04	8.80E-02	9.83E-02	5.30E-02	1.71E-02	9.04E-03	1.17E-02	1.16E-01	5.73E-02	4.85E-02	4.89E-02	1.56E-03	1.57E-03	2.55E-04	2.52E-04	2.51E-04	2.52E-04

Table S9. Raw data for Figure 6E, heatmap for the selectivity of B ([=] mol %). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 1.0, $\gamma_{C\text{-}A}$ of 0.5, $\delta_{B\text{-}A}$ of 1.4 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), oscillation frequency (Hz)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	0.02	0.04	0.12	0.28	0.59	1.29	0.96	0.27	0.42	1.47	12.08	44.12	49.78	50.00	50.00	50.00
1E-05	0.02	0.04	0.12	0.28	0.59	1.29	0.96	0.27	0.42	1.47	12.09	44.12	49.78	50.00	50.00	50.00
1E-04	0.02	0.04	0.12	0.28	0.59	1.29	0.96	0.27	0.42	1.49	12.16	44.17	49.79	50.00	50.00	50.00
1E-03	0.02	0.04	0.12	0.28	0.59	1.29	0.96	0.28	0.44	1.65	12.87	44.59	49.90	50.03	50.01	50.01
1E-02	0.02	0.04	0.12	0.28	0.59	1.26	0.95	0.32	0.67	3.24	19.33	48.50	50.94	50.33	50.12	50.05
1E-01	0.02	0.04	0.12	0.29	0.57	1.05	0.89	0.70	2.73	16.33	53.72	70.34	59.66	53.28	51.22	50.53
1E+00	0.02	0.05	0.13	0.32	0.54	0.77	1.05	2.86	15.22	61.44	91.09	94.93	87.09	73.53	62.11	55.60
1E+01	0.02	0.05	0.13	0.33	0.60	0.89	1.73	3.22	16.69	56.98	92.35	97.10	95.86	93.37	88.57	81.22
1E+02	0.02	0.05	0.14	0.34	0.57	0.46	0.53	0.94	3.70	27.62	85.44	96.00	96.44	96.42	96.33	95.89
1E+03	0.02	0.05	0.14	0.36	0.59	0.22	0.20	0.46	2.27	24.58	85.08	95.99	96.45	96.46	96.46	96.45
1E+04	0.02	0.05	0.14	0.36	0.59	0.19	0.16	0.43	2.24	24.54	85.08	95.99	96.47	96.46	96.46	96.46

Table S10. Raw data for Figure 6F, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 ^{o}C, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, γ_{B-A} of 1.0, γ_{C-A} of 0.5, δ_{B-A} of 1.4 eV, and δ_{C-A} of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), oscillation frequency (Hz)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	7.33E-01	1.19E+00	1.57E+00	1.23E+00	5.49E-01	4.60E-01	7.20E-01	1.12E+00	7.97E-01	2.14E-01	4.80E-02	1.44E-02	2.81E-03	3.69E-04	2.66E-05	1.23E-06
1E-05	7.33E-01	1.19E+00	1.57E+00	1.23E+00	5.49E-01	4.60E-01	7.20E-01	1.12E+00	7.97E-01	2.14E-01	4.80E-02	1.44E-02	2.81E-03	3.69E-04	2.69E-05	1.23E-06
1E-04	7.33E-01	1.19E+00	1.57E+00	1.23E+00	5.49E-01	4.60E-01	7.20E-01	1.12E+00	7.98E-01	2.14E-01	4.81E-02	1.45E-02	2.82E-03	3.72E-04	2.70E-05	1.53E-06
1E-03	7.34E-01	1.19E+00	1.57E+00	1.23E+00	5.49E-01	4.61E-01	7.22E-01	1.12E+00	7.98E-01	2.14E-01	4.85E-02	1.46E-02	2.85E-03	3.75E-04	2.98E-05	4.40E-06
1E-02	7.45E-01	1.19E+00	1.57E+00	1.23E+00	5.51E-01	4.71E-01	7.36E-01	1.13E+00	8.05E-01	2.19E-01	5.30E-02	1.59E-02	2.91E-03	4.01E-04	5.79E-05	3.22E-05
1E-01	8.55E-01	1.27E+00	1.62E+00	1.22E+00	5.67E-01	5.65E-01	8.65E-01	1.25E+00	8.68E-01	2.61E-01	9.33E-02	2.71E-02	3.74E-03	6.95E-04	1.65E-04	3.12E-04
1E+00	1.31E+00	1.64E+00	1.94E+00	1.17E+00	6.06E-01	7.75E-01	1.30E+00	1.79E+00	1.11E+00	5.66E-01	4.71E-01	1.30E-01	1.07E-02	3.61E-03	3.14E-03	3.10E-03
1E+01	1.37E+00	1.81E+00	2.19E+00	1.23E+00	6.58E-01	8.14E-01	1.40E+00	1.72E+00	9.82E-01	4.77E-01	5.25E-01	1.90E-01	4.10E-02	3.14E-02	3.11E-02	3.13E-02
1E+02	1.60E+00	2.53E+00	3.38E+00	1.76E+00	6.63E-01	6.78E-01	1.13E+00	1.47E+00	7.69E-01	2.77E-01	2.90E-01	1.52E-01	3.58E-02	2.57E-02	1.27E-02	2.53E-02
1E+03	3.60E+00	9.19E+00	1.49E+01	4.25E+00	7.15E-01	6.26E-01	1.05E+00	1.42E+00	7.49E-01	2.66E-01	2.84E-01	1.51E-01	3.55E-02	2.55E-02	2.52E-02	2.52E-02
1E+04	2.37E+01	7.80E+01	5.52E+01	5.37E+00	7.22E-01	6.20E-01	1.05E+00	1.42E+00	7.49E-01	2.66E-01	2.84E-01	1.51E-01	2.28E-02	2.55E-02	2.52E-02	2.51E-02

Table S11. Raw data for Figure 7C, heatmap for the selectivity of B ([=] mol %). Conditions: T of 150 °C, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, γ_{B-A} of 2.0, γ_{C-A} of 0.5, δ_{B-A} of 0.8 eV, and δ_{C-A} of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation frequency (Hz), Oscillation endpoint (eV)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04
1E-06	0.00	0.00	0.00	0.08	1.13	5.98	0.04	0.01	0.11	2.78	43.61	50.45	50.05	50.01	50.00
1E-05	0.00	0.00	0.00	0.08	1.13	5.98	0.05	0.01	0.11	2.78	43.62	50.45	50.05	50.01	50.00
1E-04	0.00	0.00	0.00	0.08	1.13	5.98	0.06	0.01	0.12	2.82	43.65	50.46	50.06	50.01	50.00
1E-03	0.00	0.00	0.00	0.08	1.13	5.98	0.18	0.10	0.23	3.23	43.98	50.53	50.09	50.02	50.01
1E-02	0.00	0.00	0.00	0.08	1.12	5.97	1.37	0.88	1.34	7.07	47.09	51.18	50.39	50.18	50.09
1E-01	0.00	0.00	0.00	0.08	1.09	6.02	9.45	7.17	10.51	32.80	68.65	58.43	53.62	51.78	50.90
1E+00	0.00	0.00	0.00	0.09	1.02	6.95	17.13	21.70	43.67	81.21	95.70	86.74	77.16	67.86	60.02
1E+01	0.00	0.00	0.01	0.09	1.14	8.68	20.53	28.13	60.16	92.04	98.79	97.16	95.75	93.29	88.60
1E+02	0.00	0.00	0.01	0.09	1.07	5.20	16.76	30.34	62.71	94.94	99.38	98.03	96.77	96.53	96.38
1E+03	0.00	0.00	0.01	0.10	1.12	2.58	9.78	43.25	82.22	99.21	99.92	99.63	98.22	96.83	96.58
1E+04	0.00	0.00	0.01	0.10	1.13	2.15	7.86	54.43	96.53	99.92	99.99	99.96	99.10	97.11	96.73

Table S12. Raw data for Figure 7D, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 2.0, $\gamma_{C\text{-}A}$ of 0.5, $\delta_{B\text{-}A}$ of 0.8 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation frequency (Hz), Oscillation endpoint (eV)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04
1E-06	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.53E-01	4.91E-01	6.92E-01	1.11E+00	7.94E-01	2.17E-01	6.57E-02	5.88E-04	8.64E-07	2.45E-09	1.25E-09
1E-05	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.53E-01	4.91E-01	6.92E-01	1.11E+00	7.94E-01	2.17E-01	6.57E-02	5.88E-04	8.78E-07	1.36E-08	1.26E-08
1E-04	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.53E-01	4.91E-01	6.92E-01	1.11E+00	7.94E-01	2.17E-01	6.57E-02	5.92E-04	1.18E-06	1.26E-07	1.26E-07
1E-03	7.34E-01	1.19E+00	1.56E+00	1.23E+00	5.53E-01	4.92E-01	6.95E-01	1.11E+00	7.96E-01	2.18E-01	6.60E-02	5.96E-04	3.95E-06	1.25E-06	1.25E-06
1E-02	7.45E-01	1.19E+00	1.57E+00	1.23E+00	5.55E-01	5.04E-01	7.27E-01	1.14E+00	8.12E-01	2.28E-01	6.92E-02	6.03E-04	3.16E-05	1.25E-05	1.25E-05
1E-01	8.55E-01	1.27E+00	1.61E+00	1.22E+00	5.71E-01	6.06E-01	9.96E-01	1.40E+00	9.61E-01	3.27E-01	9.72E-02	8.32E-04	3.11E-04	1.25E-04	1.25E-04
1E+00	1.31E+00	1.64E+00	1.93E+00	1.17E+00	6.11E-01	8.36E-01	1.71E+00	2.44E+00	1.76E+00	1.18E+00	1.89E-01	1.61E-03	3.13E-03	1.25E-03	1.25E-03
1E+01	1.37E+00	1.82E+00	2.18E+00	1.22E+00	6.62E-01	8.81E-01	1.77E+00	2.72E+00	2.38E+00	2.72E+00	2.41E-01	3.14E-02	3.12E-02	1.25E-02	1.25E-02
1E+02	1.60E+00	2.53E+00	3.37E+00	1.75E+00	6.67E-01	7.51E-01	1.58E+00	2.83E+00	2.61E+00	4.25E+00	2.45E-01	1.29E-02	2.53E-02	1.26E-02	1.26E-02
1E+03	3.60E+00	9.18E+00	1.49E+01	4.23E+00	7.21E-01	6.55E-01	1.32E+00	4.05E+00	6.02E+00	2.42E+01	2.50E-01	2.55E-02	2.52E-02	1.25E-02	1.25E-02
1E+04	2.36E+01	7.79E+01	5.50E+01	5.35E+00	7.28E-01	6.44E-01	1.26E+00	5.89E+00	3.32E+01	1.02E+02	2.51E-01	2.54E-02	2.52E-02	1.25E-02	1.25E-02

Table S13. Raw data for Figure 7E, heatmap for the selectivity of B ([=] mol %). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 2.0, $\gamma_{C\text{-}A}$ of 0.5, $\delta_{B\text{-}A}$ of 2.0 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), Oscillation frequency (Hz)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.02	3.25	46.60	50.00
1E-05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.02	3.60	47.70	50.15
1E-04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.05	6.93	56.89	51.62
1E-03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.29	30.91	84.39	62.64
1E-02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.02	2.67	80.69	97.90	88.61
1E-01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.18	21.39	97.68	99.79	98.59
1E+00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	1.85	74.46	99.80	99.98	99.88
1E+01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.07	13.35	97.64	99.99	100.00	100.00
1E+02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.11	25.77	98.81	99.99	100.00	100.00
1E+03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.23	31.73	98.91	99.99	100.00	100.00
1E+04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	32.46	98.92	99.99	100.00	100.00

Table S14. Raw data for Figure 7F, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, γ_{B-A} of 2.0, γ_{C-A} of 0.5, δ_{B-A} of 2.0 eV, and δ_{C-A} of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation endpoint (eV), Oscillation frequency (Hz)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.49E-01	7.07E-01	1.11E+00	7.93E-01	2.10E-01	4.21E-02	8.07E-03	1.48E-03	2.36E-04	4.07E-05	2.32E-06
1E-05	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.49E-01	7.07E-01	1.11E+00	7.93E-01	2.10E-01	4.21E-02	8.07E-03	1.48E-03	2.37E-04	4.19E-05	2.34E-06
1E-04	7.33E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.49E-01	7.07E-01	1.11E+00	7.93E-01	2.10E-01	4.21E-02	8.08E-03	1.49E-03	2.49E-04	5.12E-05	2.63E-06
1E-03	7.34E-01	1.19E+00	1.56E+00	1.23E+00	5.44E-01	4.50E-01	7.09E-01	1.11E+00	7.94E-01	2.11E-01	4.22E-02	8.13E-03	1.51E-03	3.38E-04	1.43E-04	6.13E-06
1E-02	7.45E-01	1.19E+00	1.57E+00	1.23E+00	5.46E-01	4.61E-01	7.23E-01	1.12E+00	7.98E-01	2.11E-01	4.26E-02	8.24E-03	1.57E-03	1.19E-03	1.04E-03	4.08E-05
1E-01	8.55E-01	1.27E+00	1.61E+00	1.22E+00	5.62E-01	5.56E-01	8.52E-01	1.23E+00	8.39E-01	2.17E-01	4.28E-02	8.42E-03	2.23E-03	9.92E-03	1.01E-02	3.93E-04
1E+00	1.31E+00	1.64E+00	1.93E+00	1.17E+00	6.01E-01	7.61E-01	1.28E+00	1.72E+00	9.18E-01	2.06E-01	4.35E-02	1.10E-02	8.55E-03	9.71E-02	1.00E-01	3.88E-03
1E+01	1.37E+00	1.82E+00	2.18E+00	1.22E+00	6.53E-01	8.06E-01	1.37E+00	1.63E+00	8.05E-01	2.16E-01	7.02E-02	3.89E-02	6.04E-02	4.39E-01	4.64E-01	3.89E-02
1E+02	1.60E+00	2.53E+00	3.37E+00	1.75E+00	6.58E-01	6.73E-01	1.09E+00	1.44E+00	7.31E-01	1.94E-01	6.20E-02	3.41E-02	7.47E-02	5.32E-01	5.75E-01	4.64E-02
1E+03	3.60E+00	9.18E+00	1.49E+01	4.22E+00	7.08E-01	6.24E-01	1.05E+00	1.41E+00	7.26E-01	1.94E-01	6.17E-02	3.37E-02	7.86E-02	5.45E-01	5.95E-01	4.76E-02
1E+04	2.36E+01	7.79E+01	5.50E+01	5.34E+00	7.14E-01	6.18E-01	1.04E+00	1.41E+00	7.26E-01	1.94E-01	6.17E-02	3.39E-02	7.88E-02	5.46E-01	5.96E-01	4.74E-02

Table S15. Raw data for Figure 7G, heatmap for the selectivity of B ([=] mol %). Conditions: T of 150 ^{o}C, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 2.0, $\gamma_{C\text{-}A}$ of 2.0, $\delta_{B\text{-}A}$ of 1.0 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation frequency (Hz), Oscillation endpoint (eV)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	50.00	50.00	95.69	99.48	99.66	99.76	97.15	94.15	99.86	99.86	99.85	98.15	56.39	50.04	50.00	50.00
1E-05	50.00	50.00	95.69	99.48	99.66	99.76	97.15	94.16	99.86	99.86	99.85	98.15	56.40	50.04	50.00	50.00
1E-04	50.00	50.00	95.70	99.48	99.66	99.76	97.16	94.31	99.86	99.86	99.85	98.15	56.46	50.04	50.00	50.00
1E-03	50.00	50.00	95.72	99.48	99.66	99.76	97.19	95.48	99.86	99.86	99.85	98.15	56.49	50.04	50.00	49.97
1E-02	50.00	50.00	95.76	99.49	99.66	99.76	97.49	98.50	99.90	99.87	99.85	98.16	56.52	50.02	49.90	49.55
1E-01	50.00	50.00	95.84	99.51	99.67	99.76	98.71	99.78	99.97	99.91	99.86	98.20	56.49	49.73	48.79	45.71
1E+00	50.00	50.00	95.76	99.54	99.68	99.76	99.68	99.95	99.99	99.95	99.87	98.20	55.72	46.88	39.91	25.54
1E+01	50.00	50.00	95.77	99.49	99.70	99.77	99.84	99.95	99.92	99.88	99.86	98.16	48.84	29.71	13.80	4.42
1E+02	50.00	50.00	95.77	99.49	99.67	99.77	99.85	99.88	99.87	99.86	99.85	98.15	50.66	33.32	17.16	5.81
1E+03	50.00	50.00	95.77	99.49	99.67	99.77	99.86	99.86	99.86	99.86	99.85	98.15	50.66	33.29	17.16	5.81
1E+04	50.00	50.00	95.77	99.49	99.65	99.77	99.86	99.86	99.86	99.86	99.85	98.15	50.66	33.27	17.14	5.81

Table S16. Raw data for Figure 7H, heatmap for the consumption of A ([=] 1/s). Conditions: T of 150 ºC, P of 100 bar, 1 % conversion of A. Parameters: ΔH_{ovr} of 0 kJ/mol, α of 0.6, β of 100 kJ/mol, $\gamma_{B\text{-}A}$ of 2.0, $\gamma_{C\text{-}A}$ of 2.0, $\delta_{B\text{-}A}$ of 1.0 eV, and $\delta_{C\text{-}A}$ of 1.4 eV. Dynamics: various oscillation endpoints and frequency. Fixed oscillation amplitude of 0.6 eV.

Oscillation frequency (Hz), Oscillation endpoint (eV)	-1.64	-1.52	-1.40	-1.28	-1.16	-1.04	-0.92	-0.80	-0.68	-0.56	-0.44	-0.32	-0.20	-0.08	0.04	0.16
1E-06	1.96E-03	1.44E-03	3.21E-03	2.23E-02	1.60E-01	1.05E+00	6.81E-02	3.36E-03	2.22E-02	1.60E-01	1.05E+00	6.67E-02	1.81E-04	2.89E-07	3.56E-09	3.10E-09
1E-05	1.96E-03	1.43E-03	3.22E-03	2.23E-02	1.60E-01	1.05E+00	6.81E-02	3.37E-03	2.22E-02	1.60E-01	1.05E+00	6.67E-02	1.82E-04	3.13E-07	3.14E-08	3.10E-08
1E-04	1.96E-03	1.44E-03	3.21E-03	2.23E-02	1.60E-01	1.05E+00	6.82E-02	3.46E-03	2.23E-02	1.60E-01	1.05E+00	6.67E-02	1.83E-04	5.95E-07	3.11E-07	3.12E-07
1E-03	1.98E-03	1.44E-03	3.24E-03	2.24E-02	1.60E-01	1.05E+00	6.91E-02	4.36E-03	2.32E-02	1.61E-01	1.05E+00	6.67E-02	1.82E-04	1.54E-06	3.12E-06	3.10E-06
1E-02	1.97E-03	1.45E-03	3.23E-03	2.25E-02	1.60E-01	1.05E+00	7.77E-02	1.33E-02	3.23E-02	1.70E-01	1.06E+00	6.72E-02	2.08E-04	3.15E-05	3.13E-05	3.11E-05
1E-01	1.69E-03	1.17E-03	2.96E-03	2.26E-02	1.62E-01	1.06E+00	1.58E-01	1.03E-01	1.22E-01	2.60E-01	1.14E+00	6.81E-02	4.93E-04	3.10E-04	3.13E-04	3.13E-04
1E+00	7.19E-04	1.81E-04	2.02E-03	2.01E-02	1.61E-01	1.07E+00	9.55E-01	9.99E-01	1.02E+00	1.16E+00	1.96E+00	6.94E-02	3.26E-03	3.13E-03	3.13E-03	3.10E-03
1E+01	8.40E-04	2.89E-04	9.21E-04	1.03E-02	1.33E-01	1.09E+00	5.49E+00	9.94E+00	1.00E+01	1.02E+01	1.00E+01	8.63E-02	3.13E-02	3.11E-02	3.12E-02	3.12E-02
1E+02	8.40E-04	2.89E-04	7.38E-04	1.00E-02	1.39E-01	1.11E+00	8.06E+00	4.56E+01	9.88E+01	1.00E+02	4.15E+01	8.88E-02	2.55E-02	2.54E-02	2.53E-02	2.53E-02
1E+03	8.40E-04	2.89E-04	7.38E-04	1.02E-02	1.37E-01	1.13E+00	8.40E+00	5.91E+01	3.55E+02	9.57E+02	5.31E+01	8.91E-02	2.55E-02	2.51E-02	2.52E-02	2.52E-02
1E+04	8.40E-04	2.89E-04	7.38E-04	1.02E-02	1.21E-01	1.13E+00	8.44E+00	6.07E+01	4.29E+02	2.69E+03	5.45E+01	8.91E-02	2.55E-02	2.51E-02	2.52E-02	2.51E-02

Section S5. Derivation of Linear Scaling Relationship Parameters

1. Nomenclature:
    a. General reactant (R) and product (P)
    b. Manuscript specific reactant (A) and products (B and C)
    c. **Note:** this derivation is valid for any reaction system where two products are referenced to one other reactant or product

2. ɣ definition

$$\frac{dBE_P}{dBE_R} \equiv \gamma_{P-R} \quad \text{(S1)}$$

3. δ definition

In words: when $BE_R = \delta_{P-R}$, $BE_P = \delta_{P-R} + \Delta H_{P-R}$

In equations: $\frac{dBE_P}{dBE_R} \equiv \gamma_{P-R}$

Integrating the definition of ɣ: $BE_P = \gamma_{P-R} BE_R + constant$ (S2)

Using the definition of δ: $\delta_{P-R} + \Delta H_{P-R} = \gamma_{P-R}\delta_{P-R} + constant$ (S3)

Rearranging: $constant = (1 - \gamma_{P-R})\delta_{P-R} + \Delta H_{P-R}$

Therefore: $BE_P = \gamma_{P-R} BE_R + (1 - \gamma_{P-R})\delta_{P-R} + \Delta H_{P-R}$ (S4)

4. $\delta_{B\text{-}C}$ derivation

We can substitute in symbols for our specific reactant (A) and products (B and C) to complete the derivation.

For product B: $BE_B = \gamma_{B-A} BE_A + (1 - \gamma_{B-A})\delta_{B-A} + \Delta H_{B-A}$ (S5)

For product C: $BE_C = \gamma_{C-A} BE_A + (1 - \gamma_{C-A})\delta_{C-A} + \Delta H_{C-A}$ (S6)

In words: when $BE_C = \delta_{B\text{-}C}$, $BE_B = \delta_{B\text{-}C} + \Delta H_{B\text{-}C}$

Plug in: $\gamma_{B-A} BE_A + (1 - \gamma_{B-A})\delta_{B-A} + \Delta H_{B-A} - \Delta H_{B-C} = \gamma_{C-A} BE_A + (1 - \gamma_{C-A})\delta_{C-A} + \Delta H_{C-A}$ (S7)

Rearranging: $(\gamma_{B-A} - \gamma_{C-A}) \ BE_A = (1 - \gamma_{C-A})\delta_{C-A} - (1 - \gamma_{B-A})\delta_{B-A} + \Delta H_{C-A} - \Delta H_{B-A} + \Delta H_{B-C}$

Simplifying: $BE_A = \frac{(1-\gamma_{C-A})\delta_{C-A} - (1-\gamma_{B-A})\delta_{B-A}}{\gamma_{B-A} - \gamma_{C-A}}$ (S8)

5. **Final answer**

At $\delta_{B\text{-}C}$: $\boldsymbol{BE_A = \frac{(1-\gamma_{C-A})\delta_{C-A} - (1-\gamma_{B-A})\delta_{B-A}}{\gamma_{B-A} - \gamma_{C-A}}}$