Chemical Exchange

Chris Waudby

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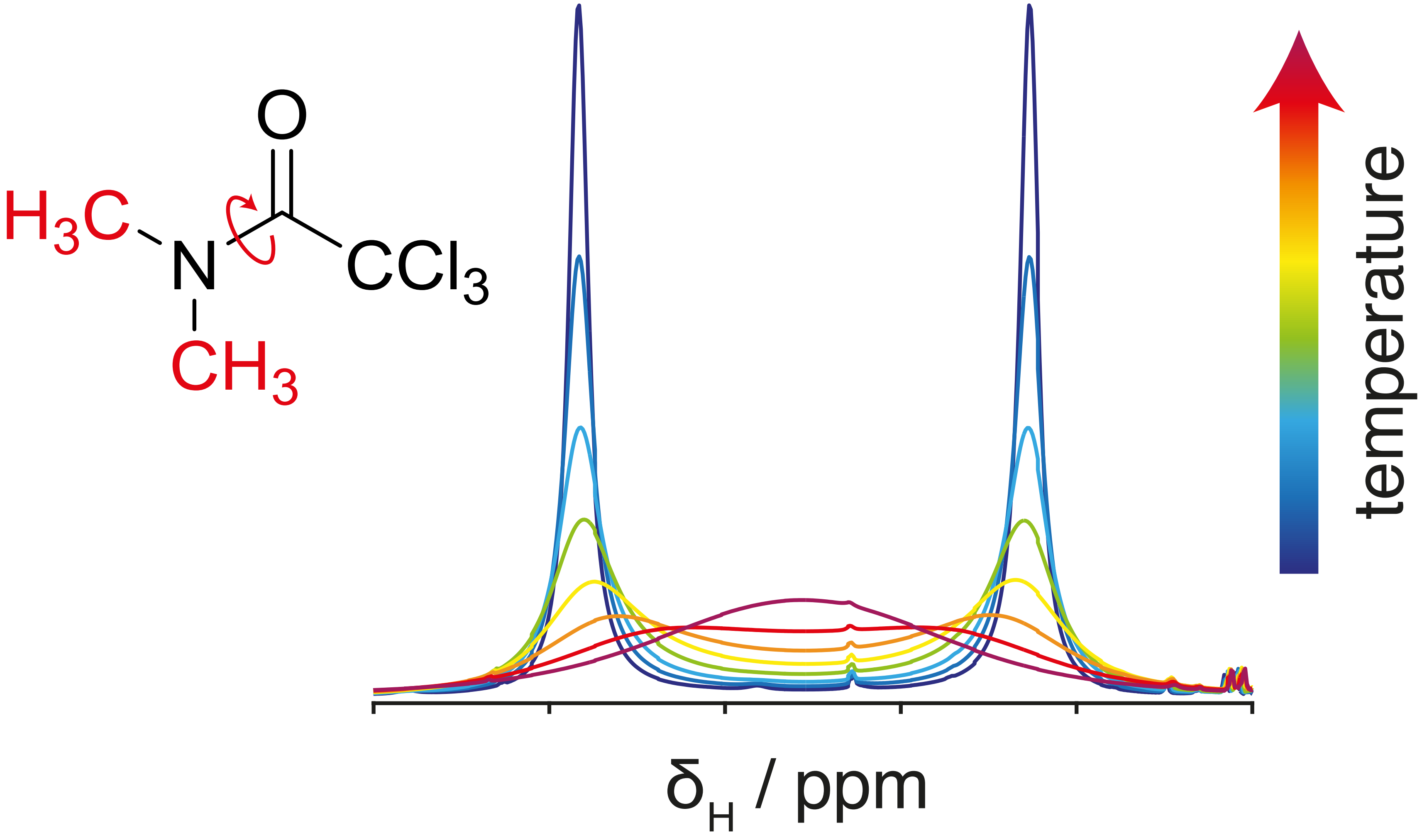
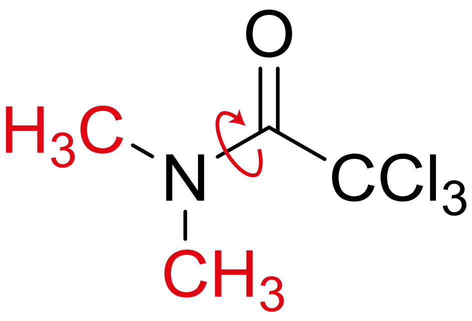
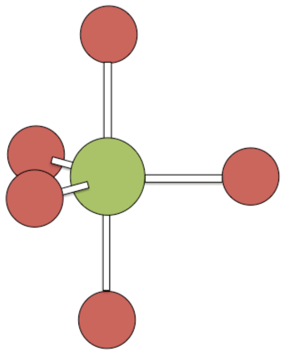


NMR Theory Club
10 Dec 2025

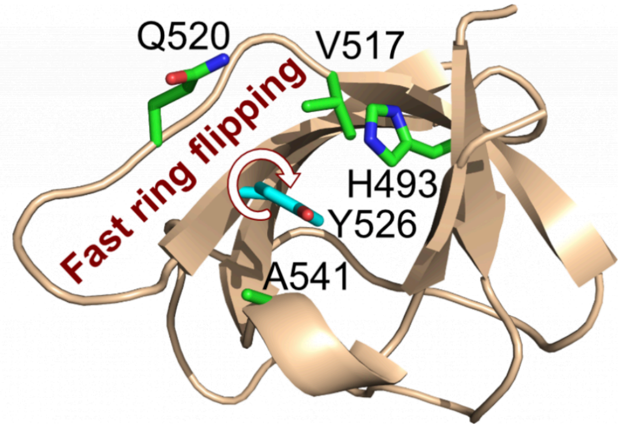
Chemical exchange is everywhere!



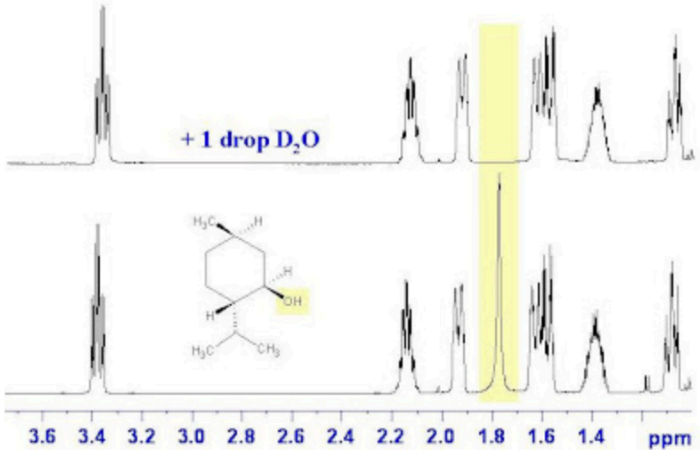
bond rotation



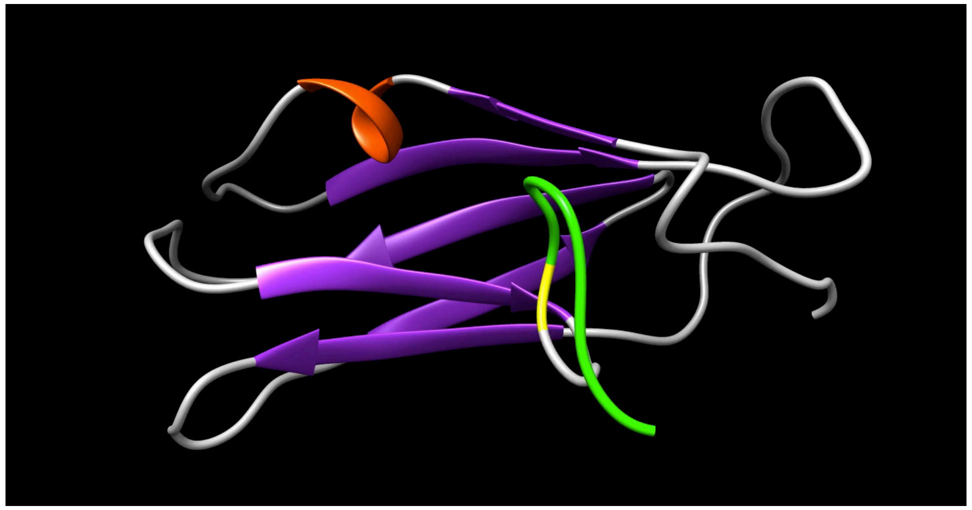
fluxionality



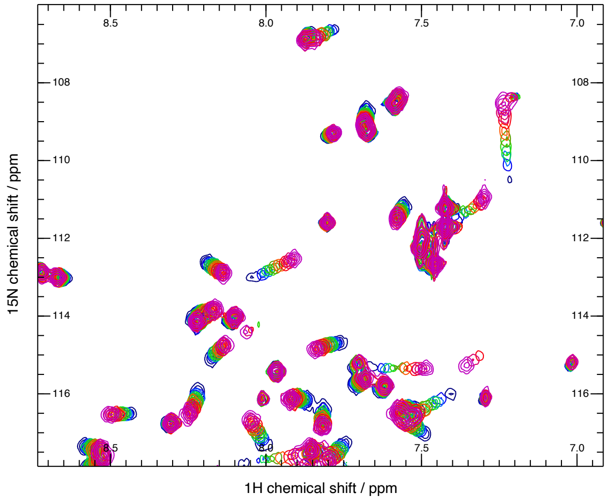
ring flips



hydrogen exchange



protein folding, unfolding and intermediate formation

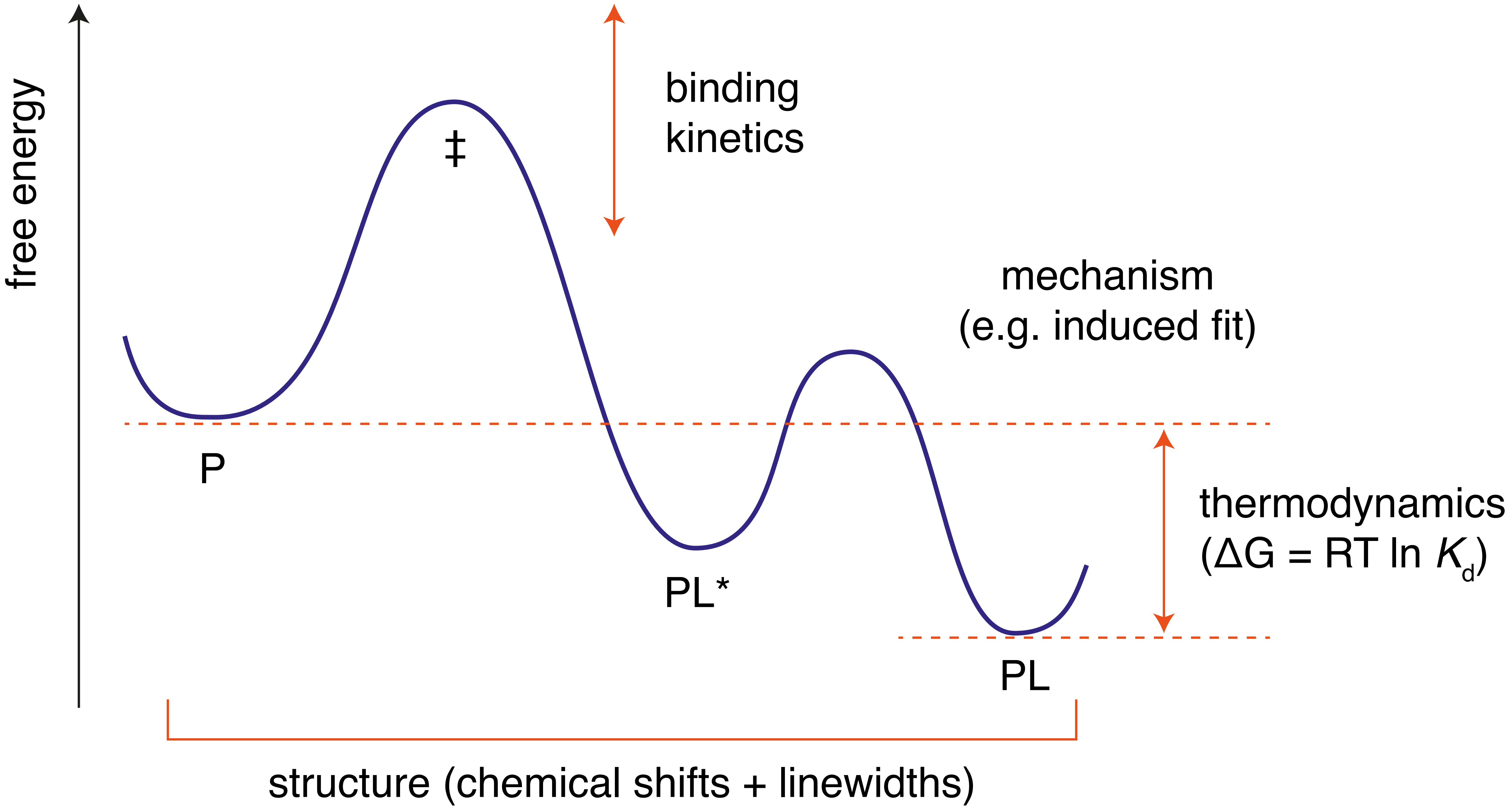


ligand binding /
host-guest recognition

$$\begin{tikzcd}
A + L \arrow[r, shift left, "k_{\mathrm{on,A}}"] \arrow[d, shift left, "k_{\mathrm{AB}}"] & AL \arrow[l, shift left, "k_{\mathrm{off,A}}"] \arrow[d, shift left, "k_{\mathrm{AB'}}"] \\
B + L \arrow[r, shift left, "k_{\mathrm{on,B}}"] \arrow[u, shift left, "k_{\mathrm{BA}}"] & BL \arrow[l, shift left, "k_{\mathrm{off,B}}"] \arrow[u, shift left, "k_{\mathrm{BA'}}"]
\end{tikzcd}$$

allostery

What information can NMR provide?



binding kinetics

mechanism (e.g. induced fit)

thermodynamics ($\Delta G = RT \ln K_d$)

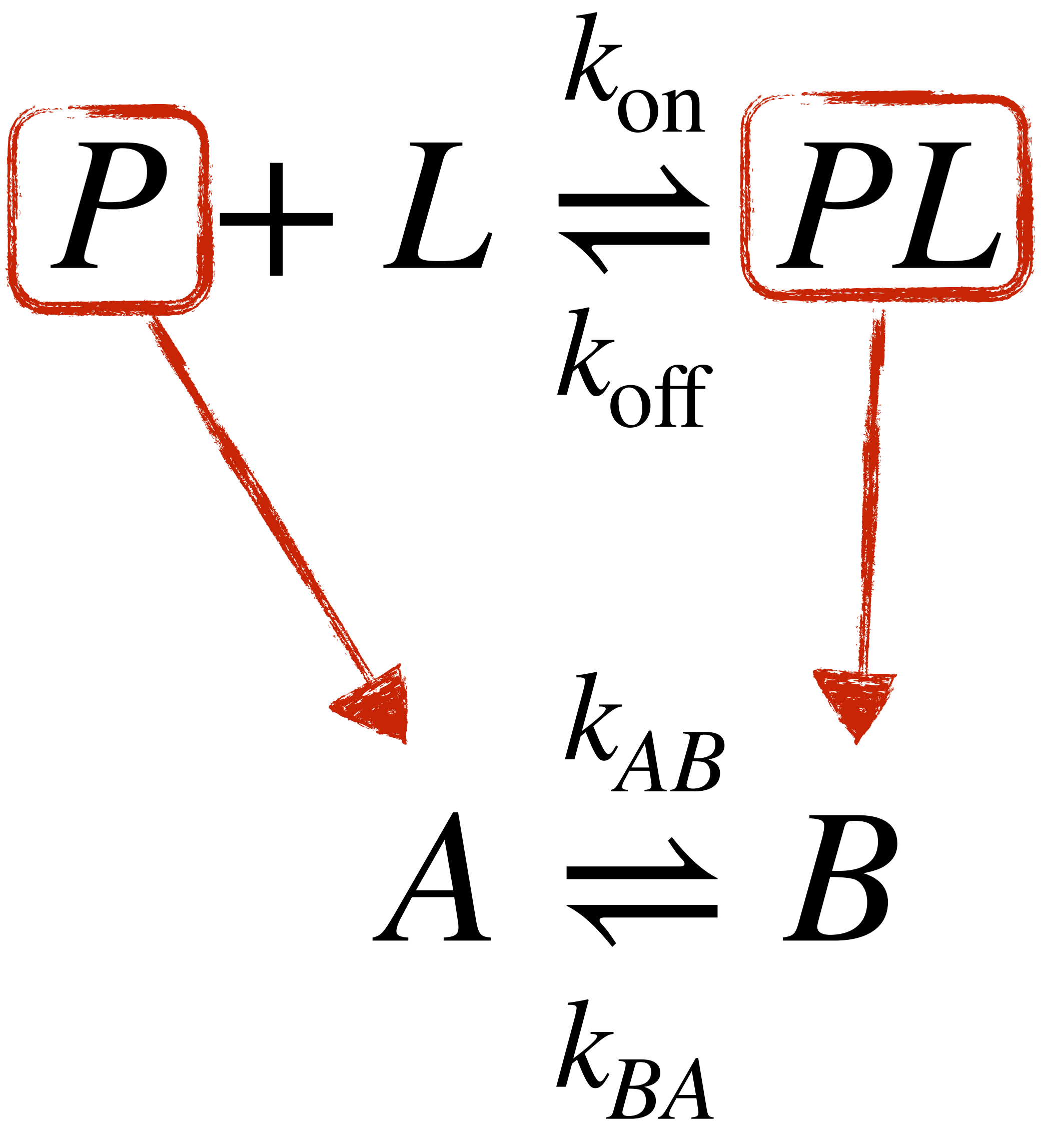
structure (chemical shifts + linewidths)

A note on units

linear frequencies = 2π x angular frequencies

measured in **Hz** (cycles per second = 1 / period)	measured in **s^{-1}** (**rad s^{-1}**, but radians are implicit)
usually written as **v**, **Δv**	usually written as **ω**, **Δω**
relaxation rates (R_1, R_2) are **not** measured in Hz and **cannot** be compared with angular frequency differences	**relaxation rates (R_1, R_2) are also measured in s^{-1}** and can be compared with angular frequency differences
first-order rate constants (e.g. k_{off}, k_{ex}) are **not** measured in Hz and **cannot** be compared with angular frequency differences	**first-order rate constants (e.g. k_{off}, k_{ex}) are also measured in s^{-1}** and can be compared with angular frequency differences

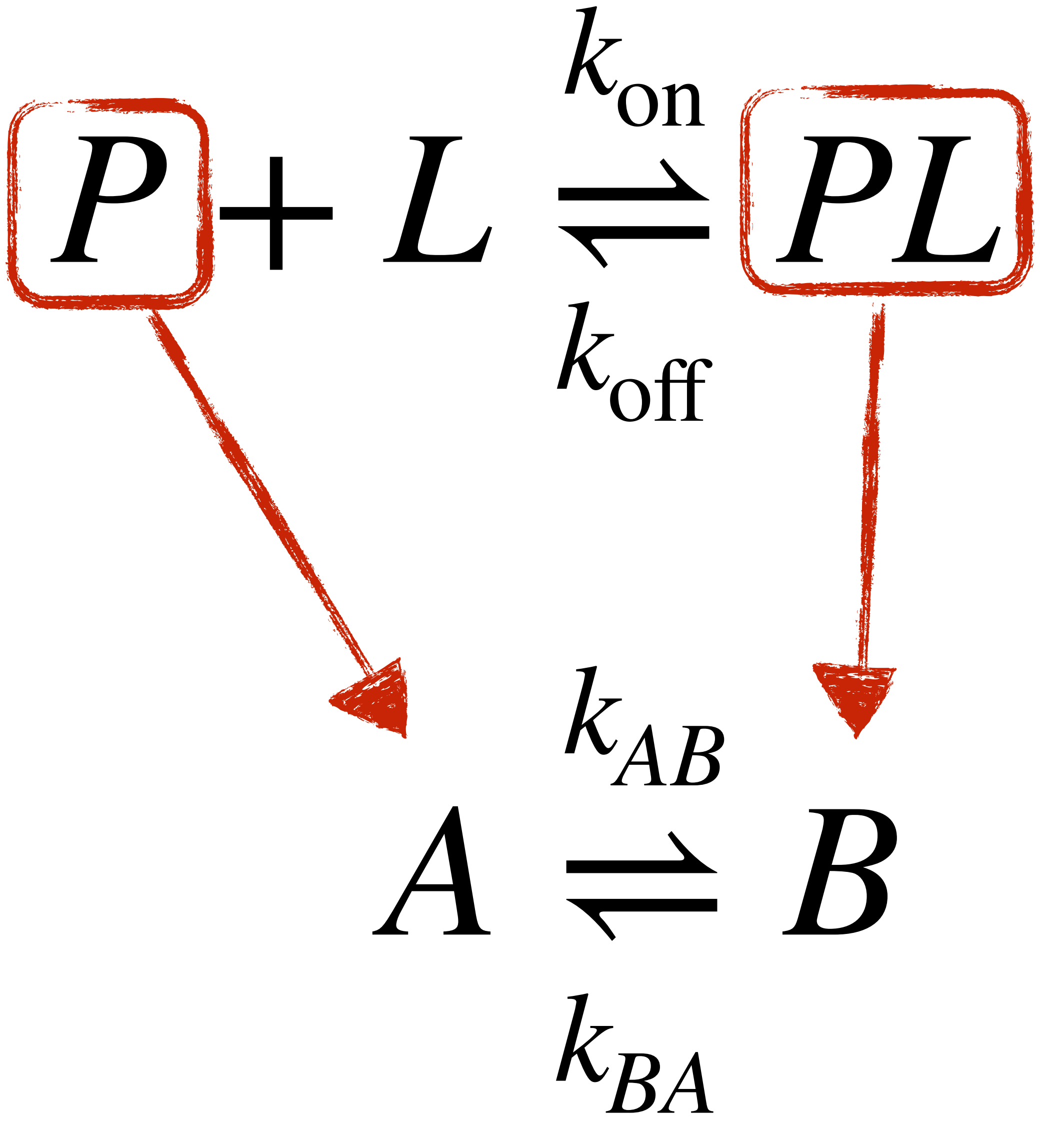
$$P + L \underset{k_{\mathrm{off}}}{\overset{k_{\mathrm{on}}}{\rightleftharpoons}} PL \qquad K_d = \frac{k_{\mathrm{off}}}{k_{\mathrm{on}}}$$



Molecules: $\boxed{P} + L \underset{k_{\text{off}}}{\overset{k_{\text{on}}}{\rightleftharpoons}} \boxed{PL}$

$$K_d = \frac{k_{\text{off}}}{k_{\text{on}}}$$

'P' nuclei: $A \underset{k_{BA}}{\overset{k_{AB}}{\rightleftharpoons}} B$



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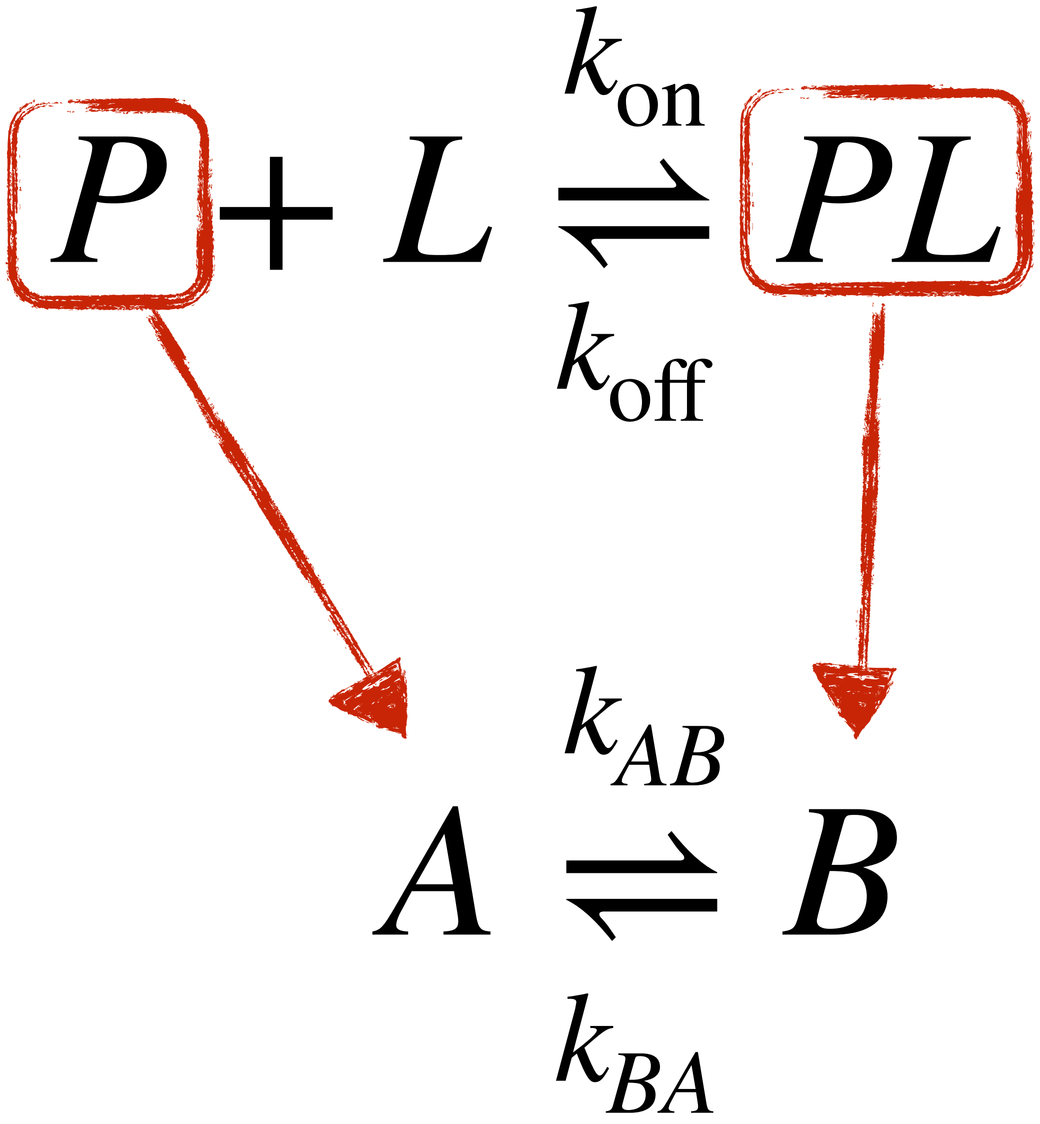

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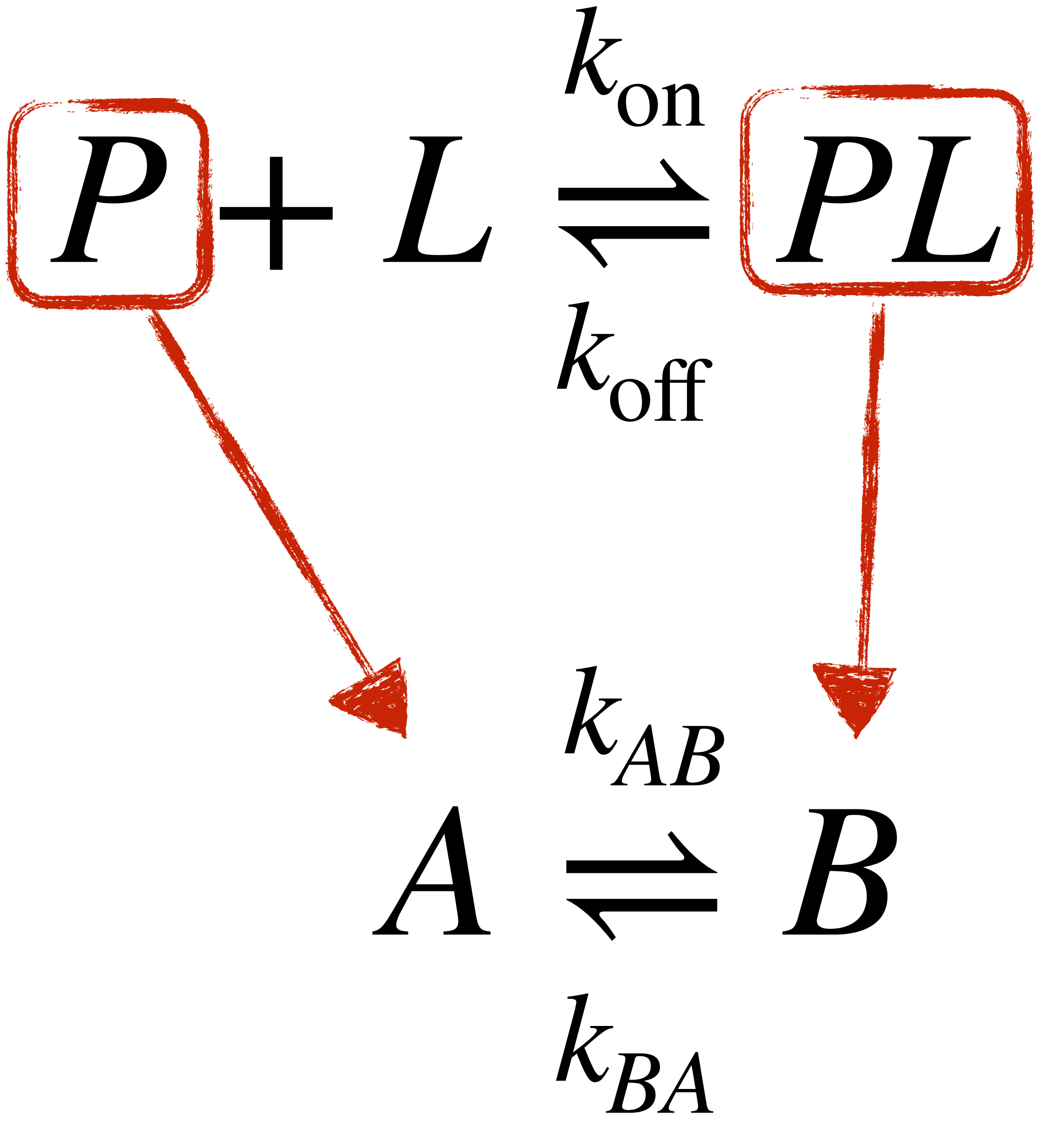
At dynamic equilibrium, chemical exchange processes are **always** first order (because perturbations from fluctuations are small)



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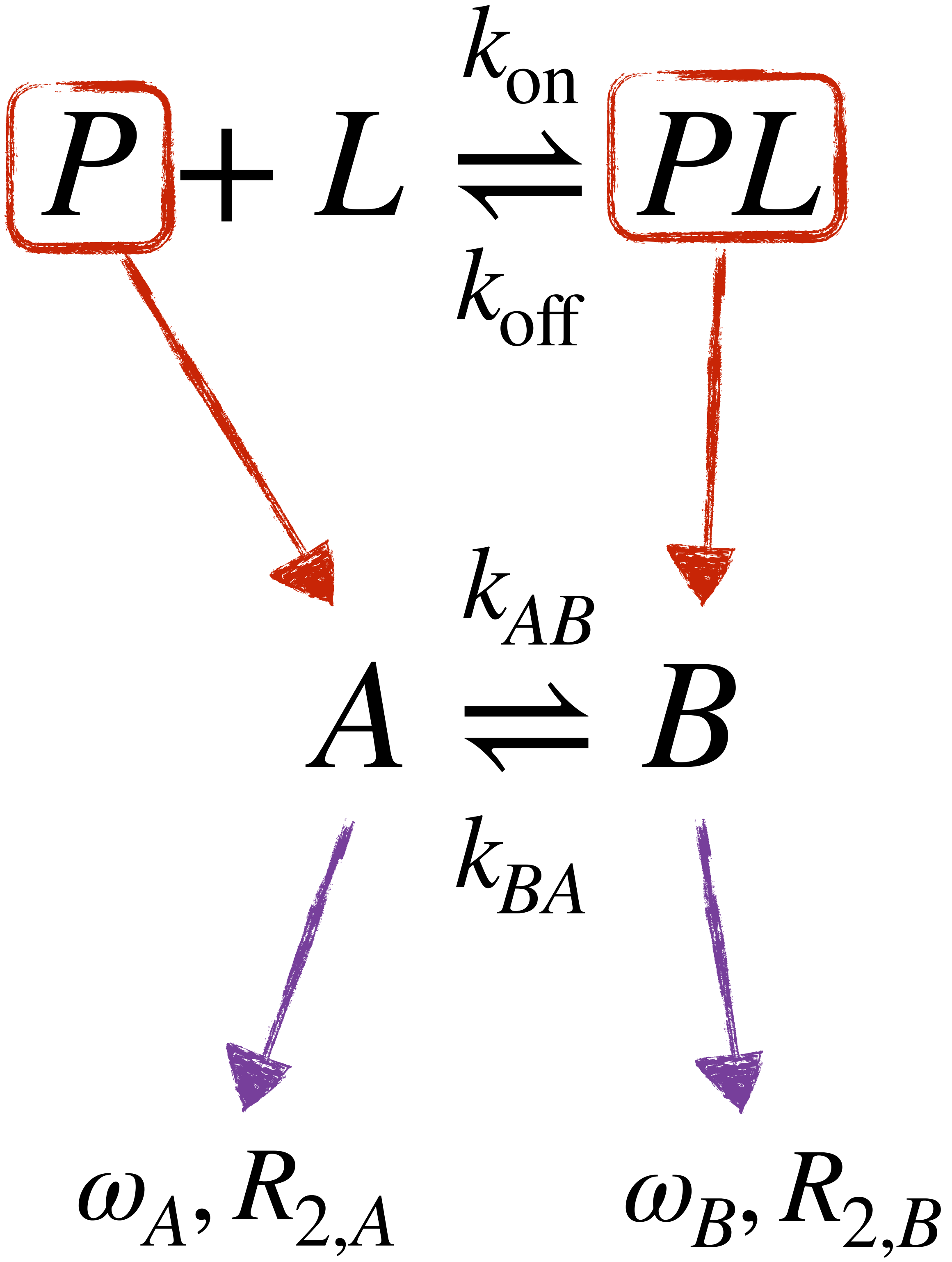
Equilibrium populations:

$$p_A = \frac{k_{BA}}{k_{AB} + k_{BA}} \qquad p_B = \frac{k_{AB}}{k_{AB} + k_{BA}}$$

At dynamic equilibrium, chemical exchange processes are **always** first order (because perturbations from fluctuations are small)



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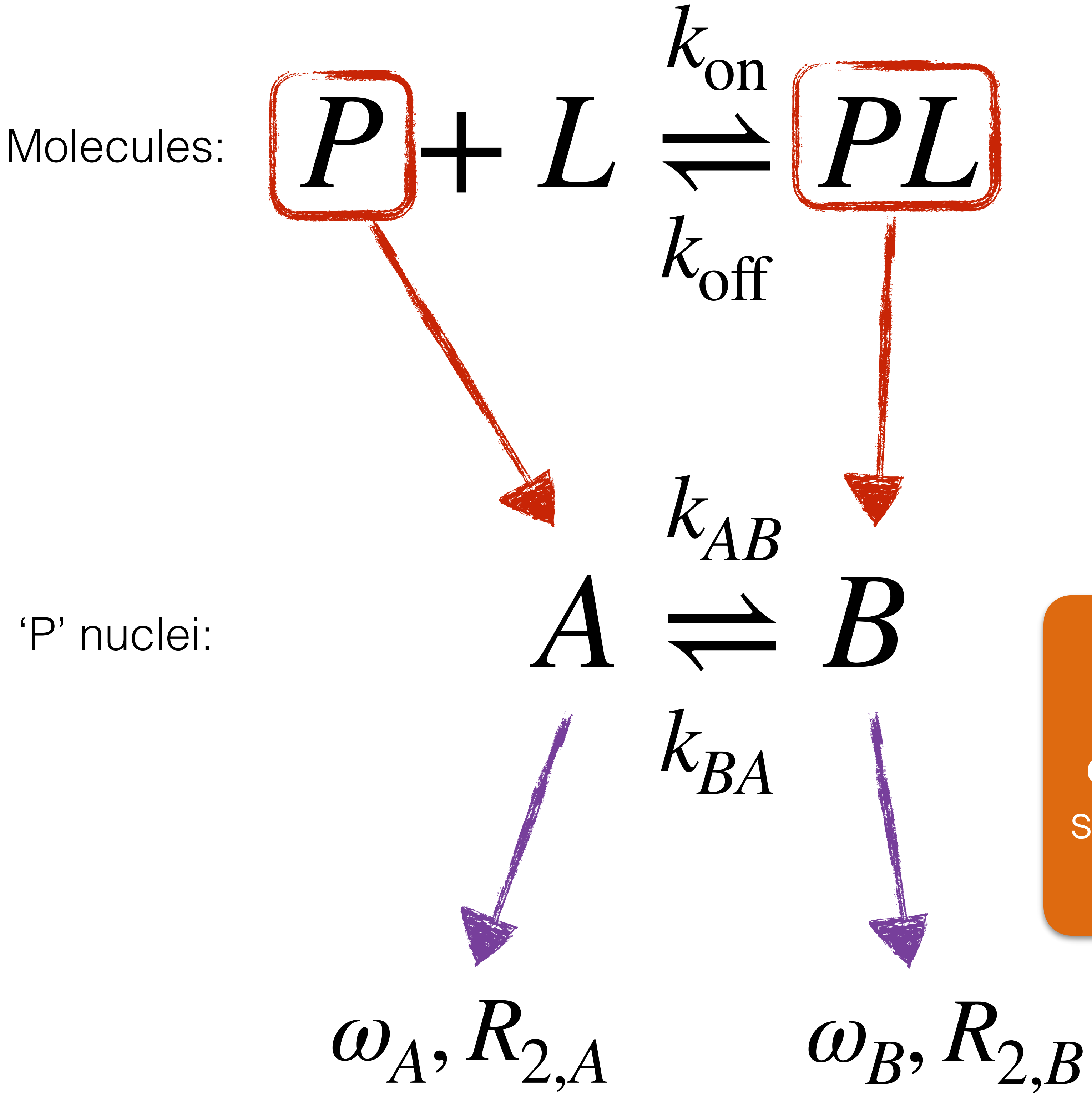
$\omega_A, R_{2,A}$

$\omega_B, R_{2,B}$



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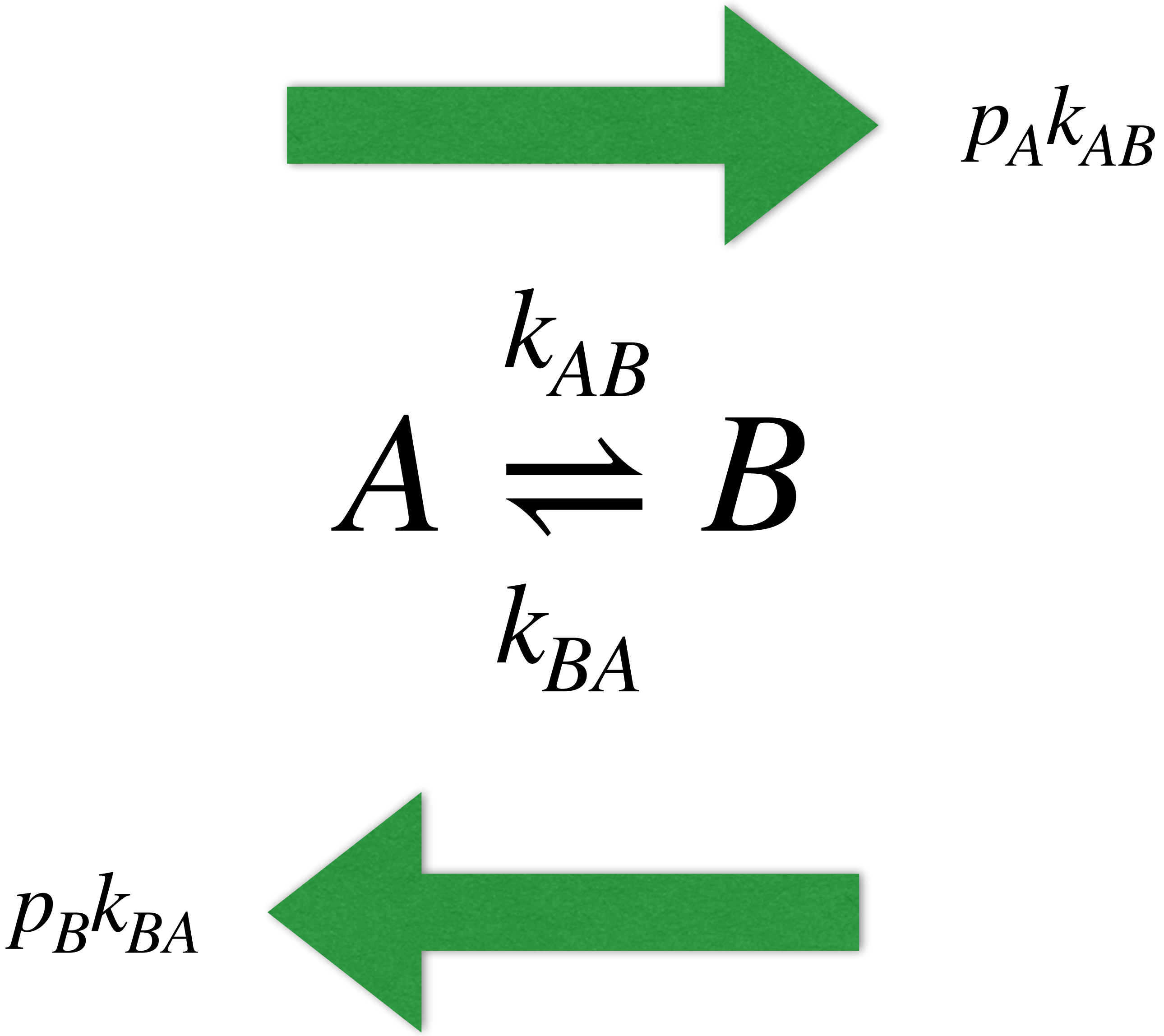
$\omega_A, R_{2,A}$

$\omega_B, R_{2,B}$

N.B. states are a global property

every spin in a molecule will exist in states A and B – but the difference in chemical shifts may be negligible

Forward and backward flux is equal at dynamic equilibrium

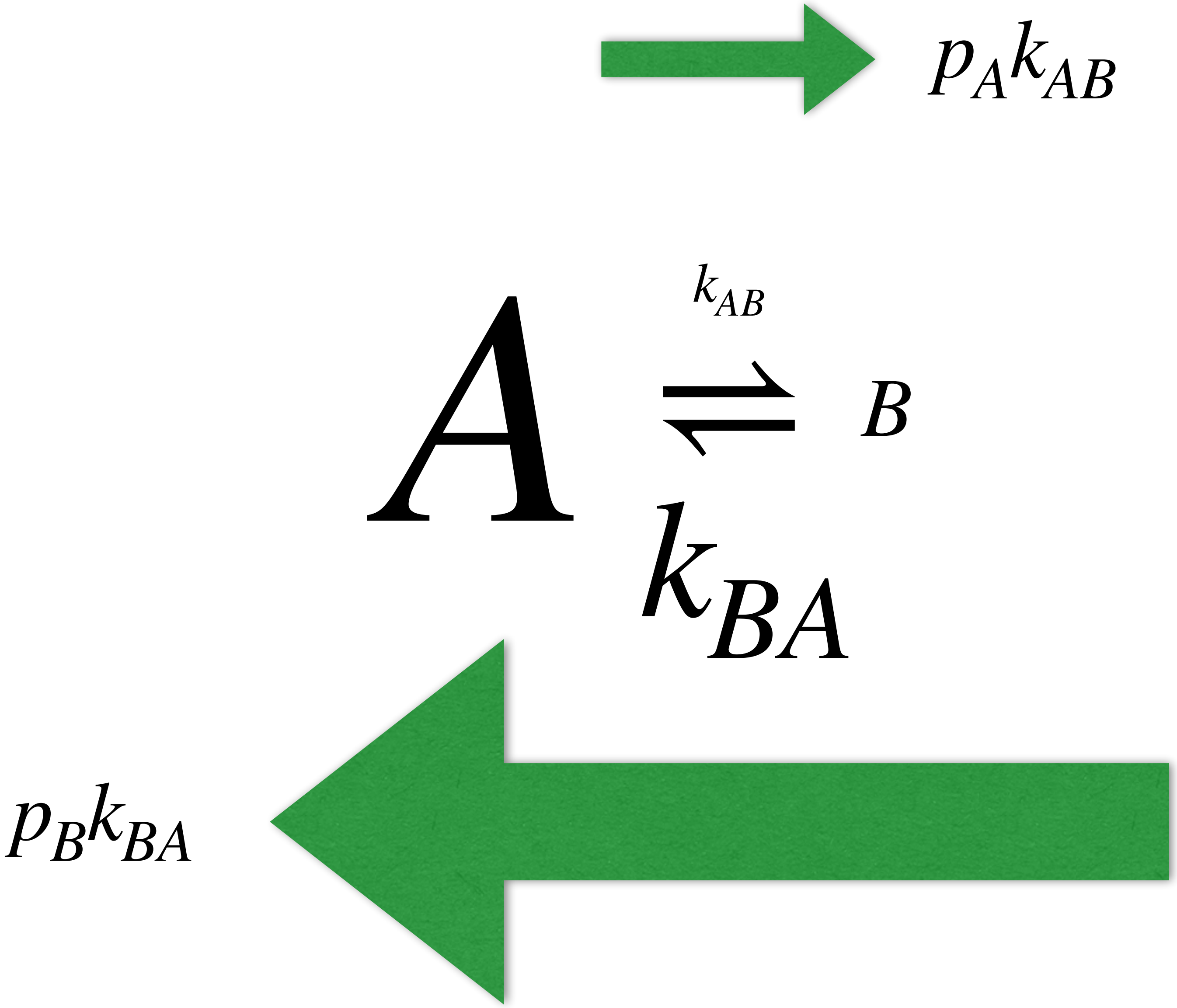


$p_A k_{AB}$

$$A \underset{k_{BA}}{\overset{k_{AB}}{\rightleftharpoons}} B$$

$p_B k_{BA}$

Forward and backward flux is equal at dynamic equilibrium



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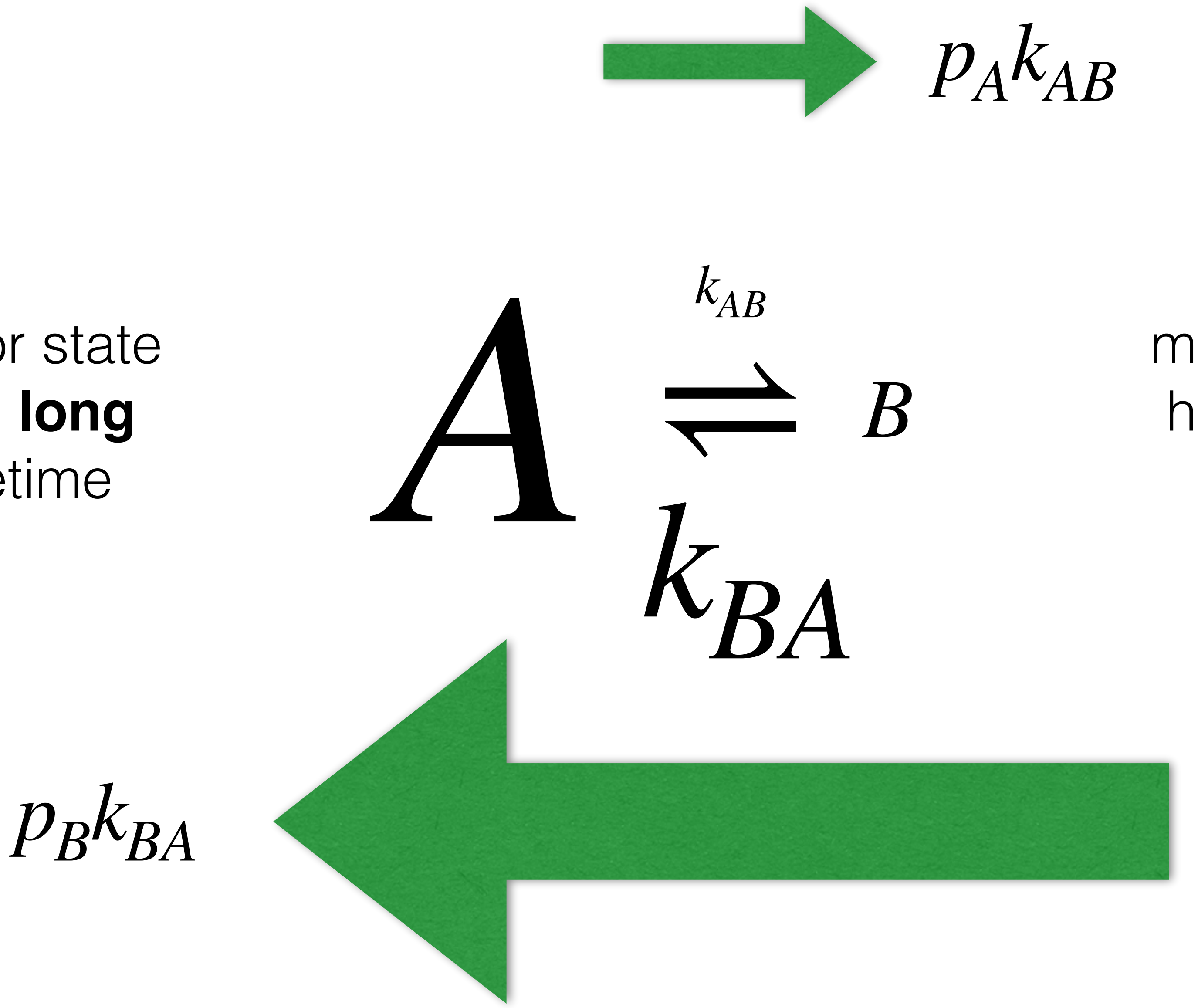

$p_A k_{AB}$

major state
has **long**
lifetime

$$A \underset{k_{BA}}{\overset{k_{AB}}{\rightleftharpoons}} B$$

minor state
has **short**
lifetime

$p_B k_{BA}$

Chemical exchange kinetics at dynamic equilibrium

$$A \underset{k_{BA}}{\overset{k_{AB}}{\rightleftharpoons}} B$$

We can write the rate equations:

$$\frac{dA}{dt} = -k_{AB}A + k_{BA}B$$
$$\frac{dB}{dt} = k_{AB}A - k_{BA}B$$

Chemical exchange kinetics at dynamic equilibrium

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$$\frac{dB}{dt} = k_{AB}A - k_{BA}B$$

Or more compactly using matrix notation:

$$\frac{d\vec{M}}{dt} = \frac{d}{dt}\begin{pmatrix}A\\B\end{pmatrix} = \begin{pmatrix}-k_{AB} & k_{BA}\\ k_{AB} & -k_{BA}\end{pmatrix}\cdot\begin{pmatrix}A\\B\end{pmatrix} = K\cdot\vec{M}$$

Chemical exchange kinetics at dynamic equilibrium

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The solution to this is:

$$\vec{M}(t) = e^{Kt} \cdot \vec{M}(0)$$

K is the **exchange operator** (or superoperator if you're being fancy!)

Eigenvalues of the exchange operator

$$A \underset{k_{BA}}{\overset{k_{AB}}{\rightleftharpoons}} B$$

The exchange operator, ***K***:

$$K = \begin{pmatrix} -k_{AB} & k_{BA} \\ k_{AB} & -k_{BA} \end{pmatrix}$$

has two eigenvalues:

$$\lambda = \left\{0,\, k_{AB} + k_{BA}\right\}$$

These represent the chemical relaxation rates of the system *(i.e. the rates of return to equilibrium following a perturbation)*

One eigenvalue is always zero – this just represents the equilibrium state that does not change over time

The second eigenvalue is often referred to as the exchange rate, $k_{\text{ex}} = k_{\text{AB}} + k_{\text{BA}}$.

Eigenvalues of the exchange operator

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The exchange operator, ***K***:

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Knowledge of the exchange rate is critical to understanding chemical exchange in NMR: It is the quantity against which differences in spectroscopic parameters are compared in order to define fast, intermediate and slow exchange regimes

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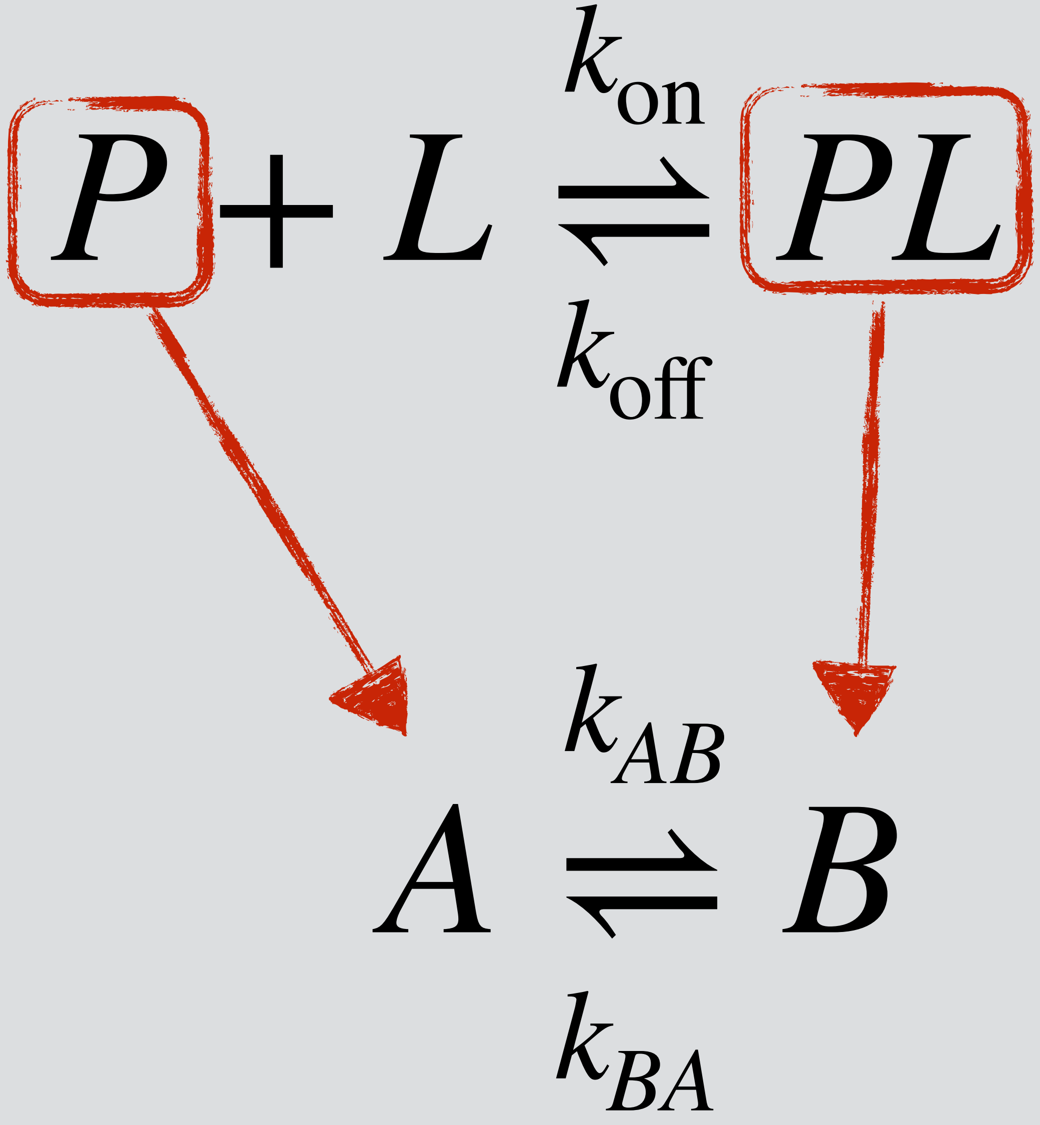
Example

$$k_{\text{ex}} = k_{AB} + k_{BA}$$

$$= k_{\text{on}}[L] + k_{\text{off}}$$

e.g. K_d = 20 μM
k_{off} = 1000 s^{-1}
=> k_{on} = 5 x 10^7 M^{-1} s^{-1}

$[P]_0$ = 100 μM
$[L]_0$ = 50 μM



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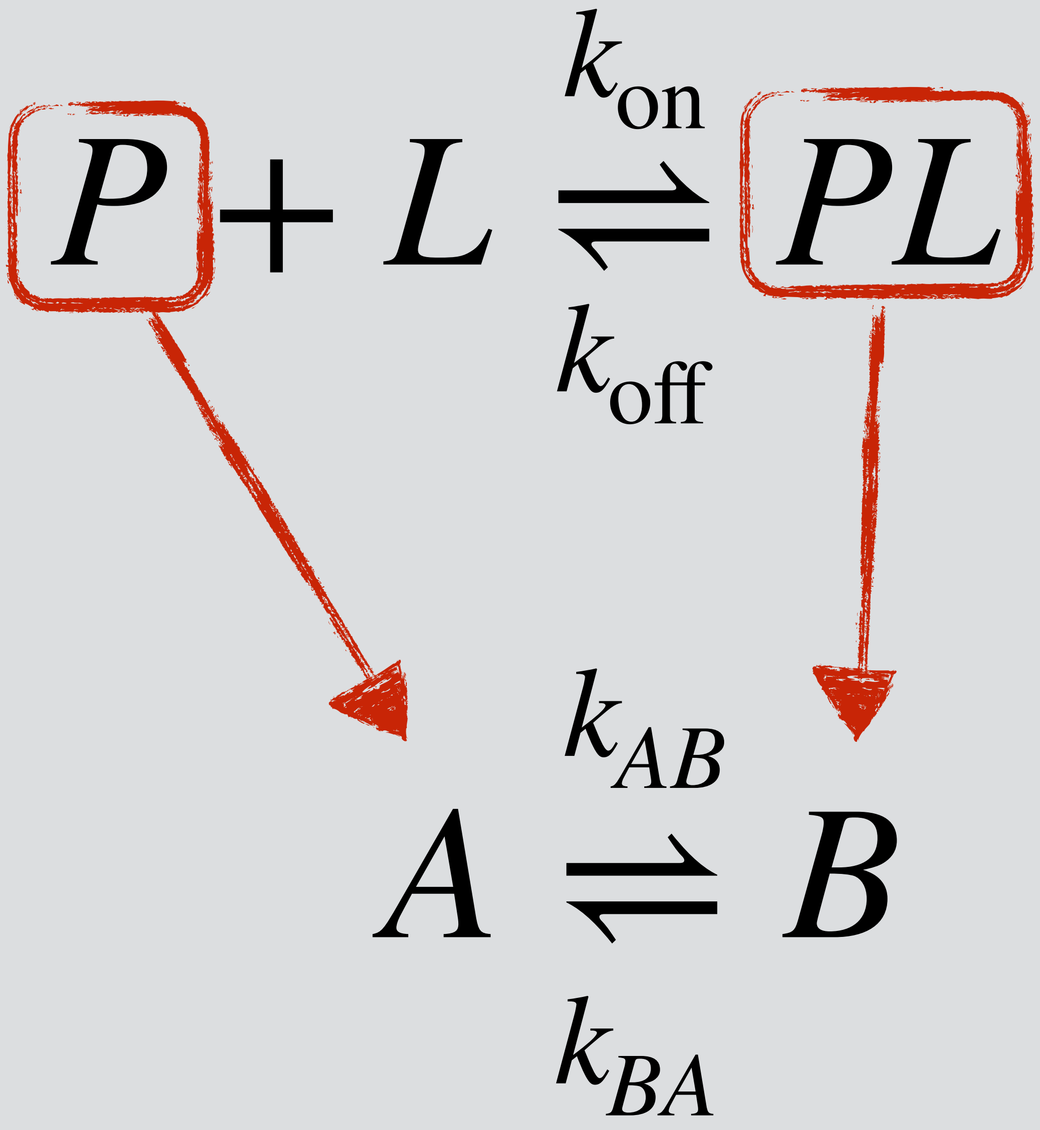
$[P]_0$ = 100 μM
$[L]_0$ = 50 μM

=> [L] = 12 μM
=> k_{AB} = k_{on}[L] = 600 s^{-1}

k_{ex} = 1600 s^{-1}



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Example

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$$\Delta\omega = \gamma B_0 \Delta\delta$$

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$[P]_0$ = 100 μM
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=> [L] = 12 μM
=> k_{AB} = k_{on}[L] = 600 s^{-1}

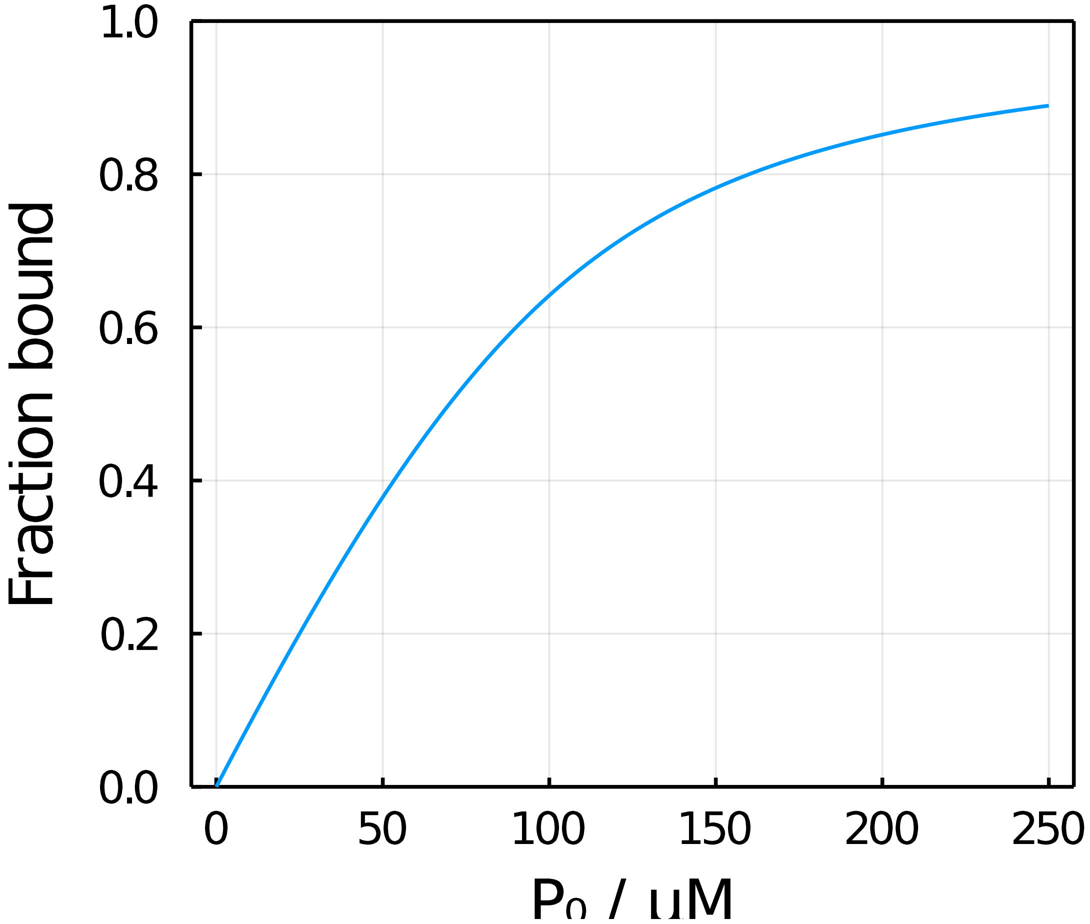
k_{ex} = 1600 s^{-1}

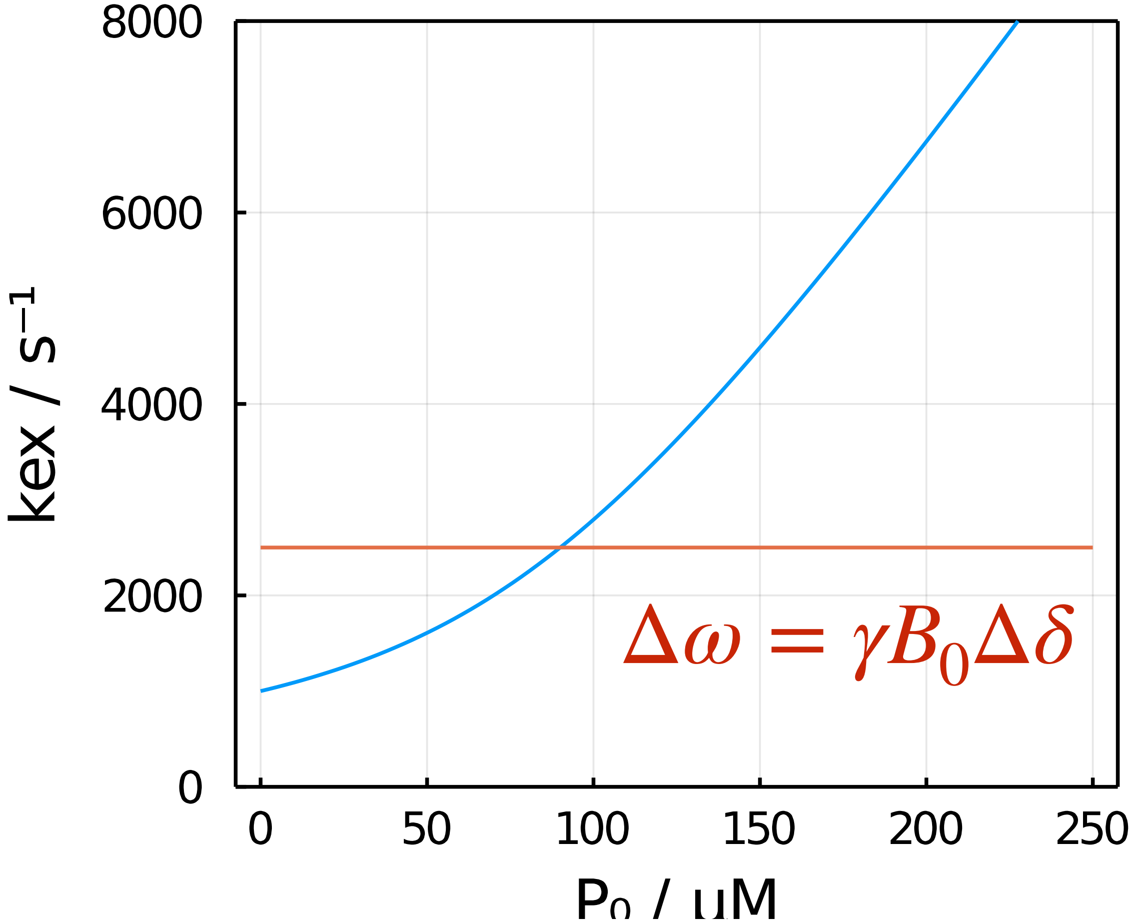
e.g. Δδ (^{1}H) = 0.5 ppm
800 MHz

Δν = 400 Hz
Δω = 2π Δν = 2500 s^{-1}

The exchange rate increases along a titration

$$k_{\mathrm{ex}} = k_{AB} + k_{BA}$$
$$= k_{\mathrm{on}}[L] + k_{\mathrm{off}}$$

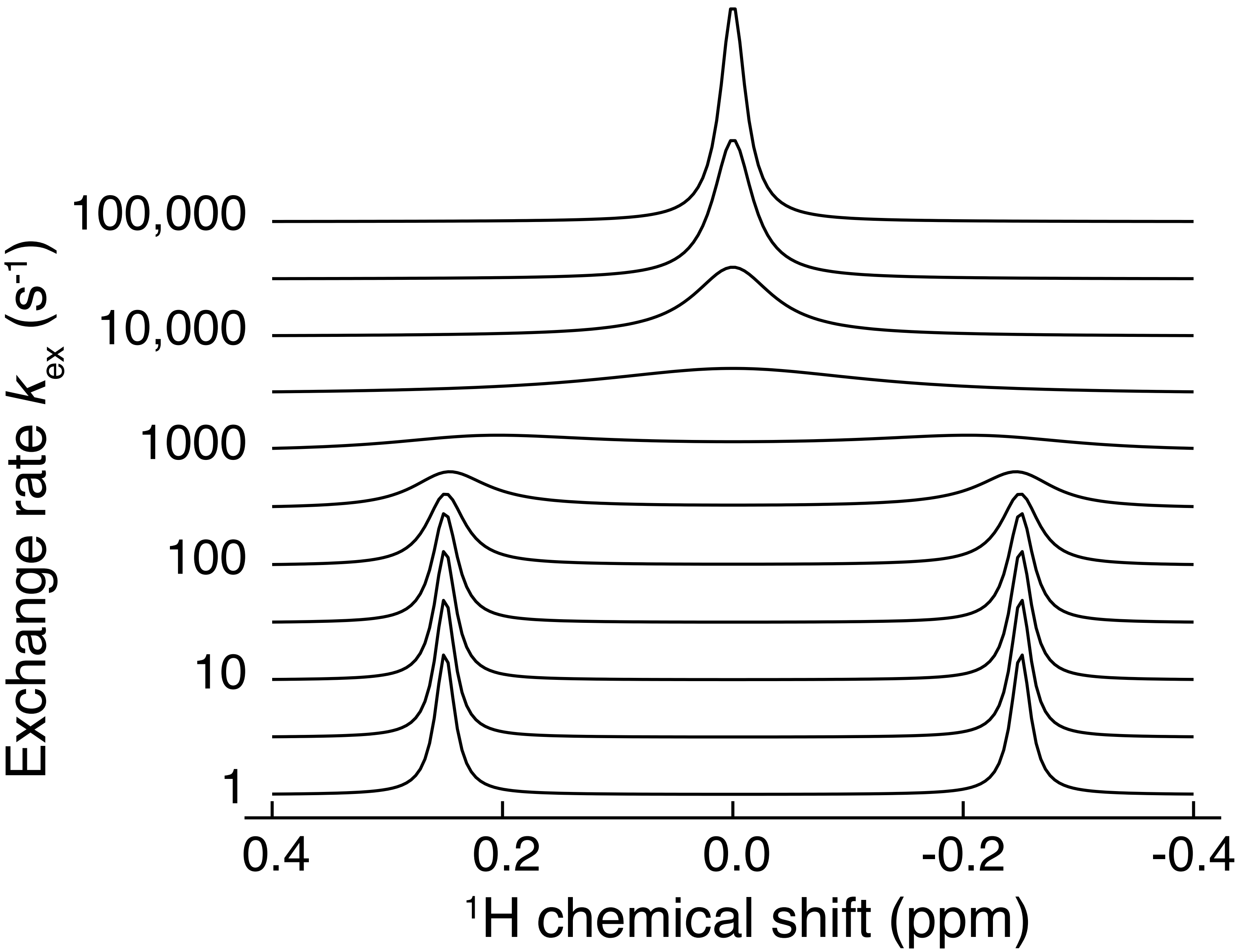




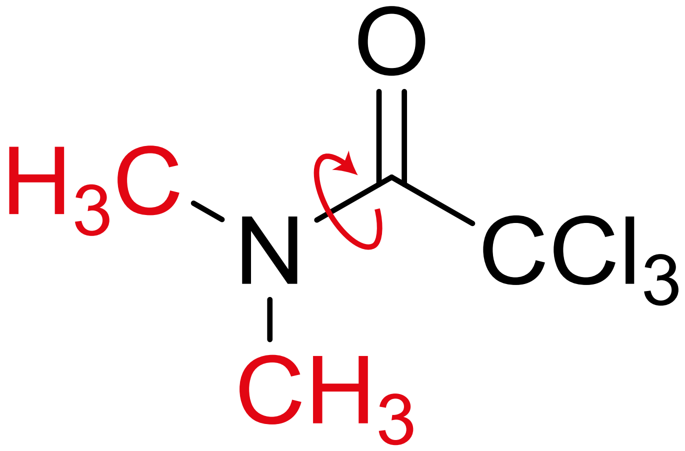
$$\Delta\omega = \gamma B_0 \Delta\delta$$

K_{d} = 20 μM
k_{off} = 1000 s^{-1}
$[\mathrm{P}]_0$ = 100 μM
Δδ (^{1}H) = 0.5 ppm (800 MHz)

Chemical exchange regimes

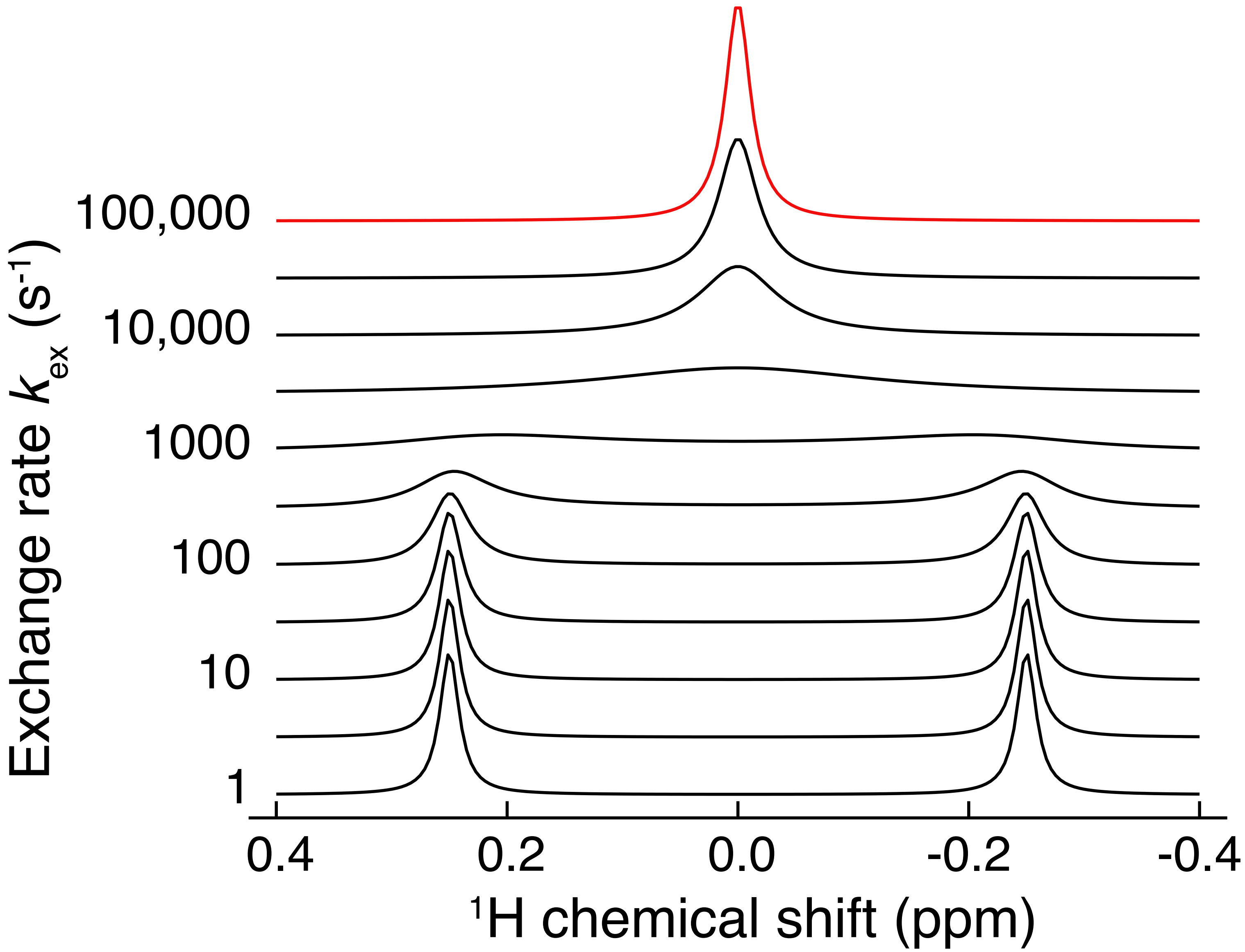


Simulated resonance line shapes for a ^{1}H chemical shift difference of 0.5 ppm at 800 MHz ($\Delta\omega = 2500$ s^{-1}) and the indicated exchange rate, k_{ex}



two sites, related by symmetry
=> equal populations

Chemical exchange regimes: fast exchange ($k_{ex} >> \Delta\omega$)

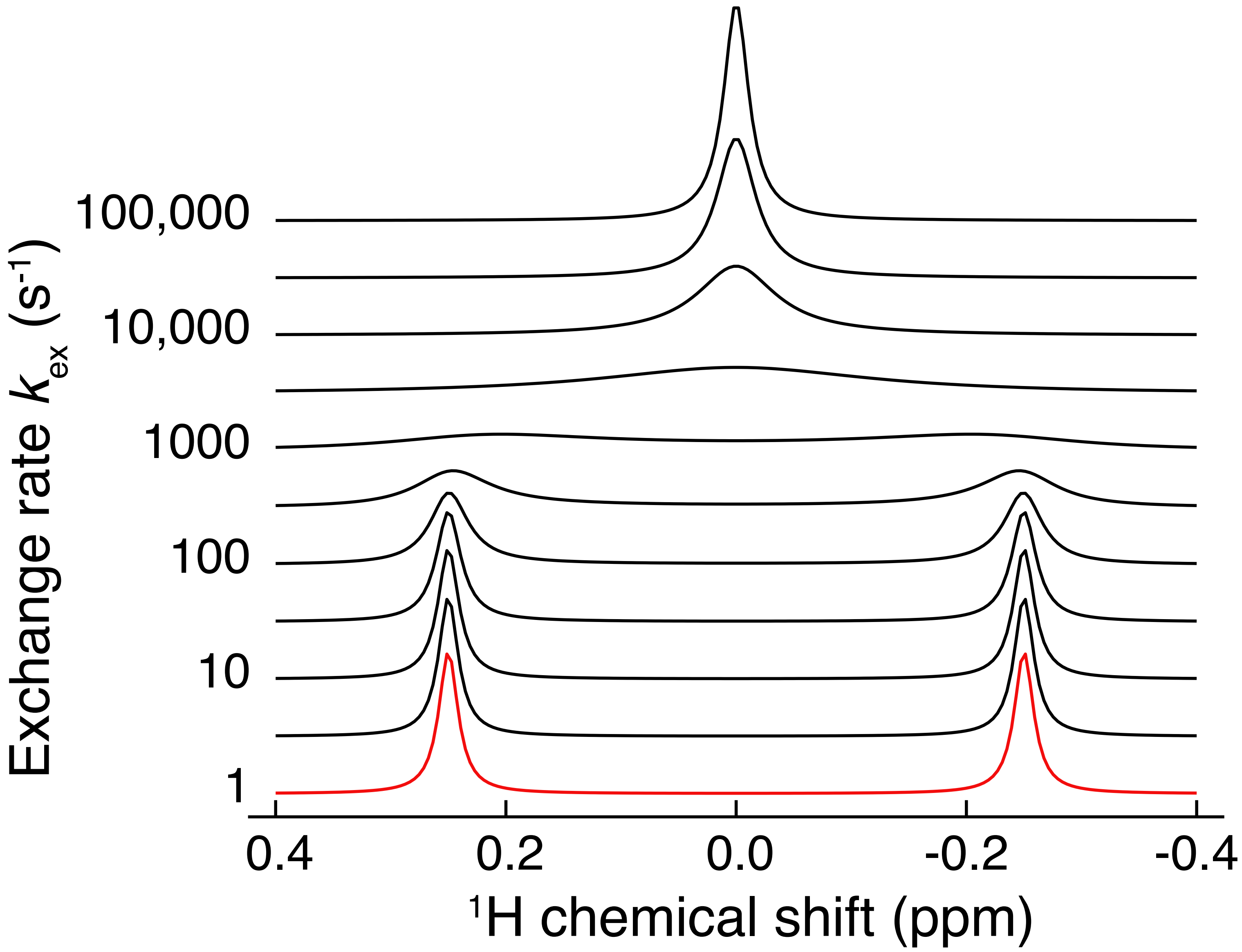


Molecules are jumping between states so rapidly that only a single averaged frequency can be detected

Single resonance observed at average of individual chemical shifts

Linewidth (R_2) is average of individual resonances

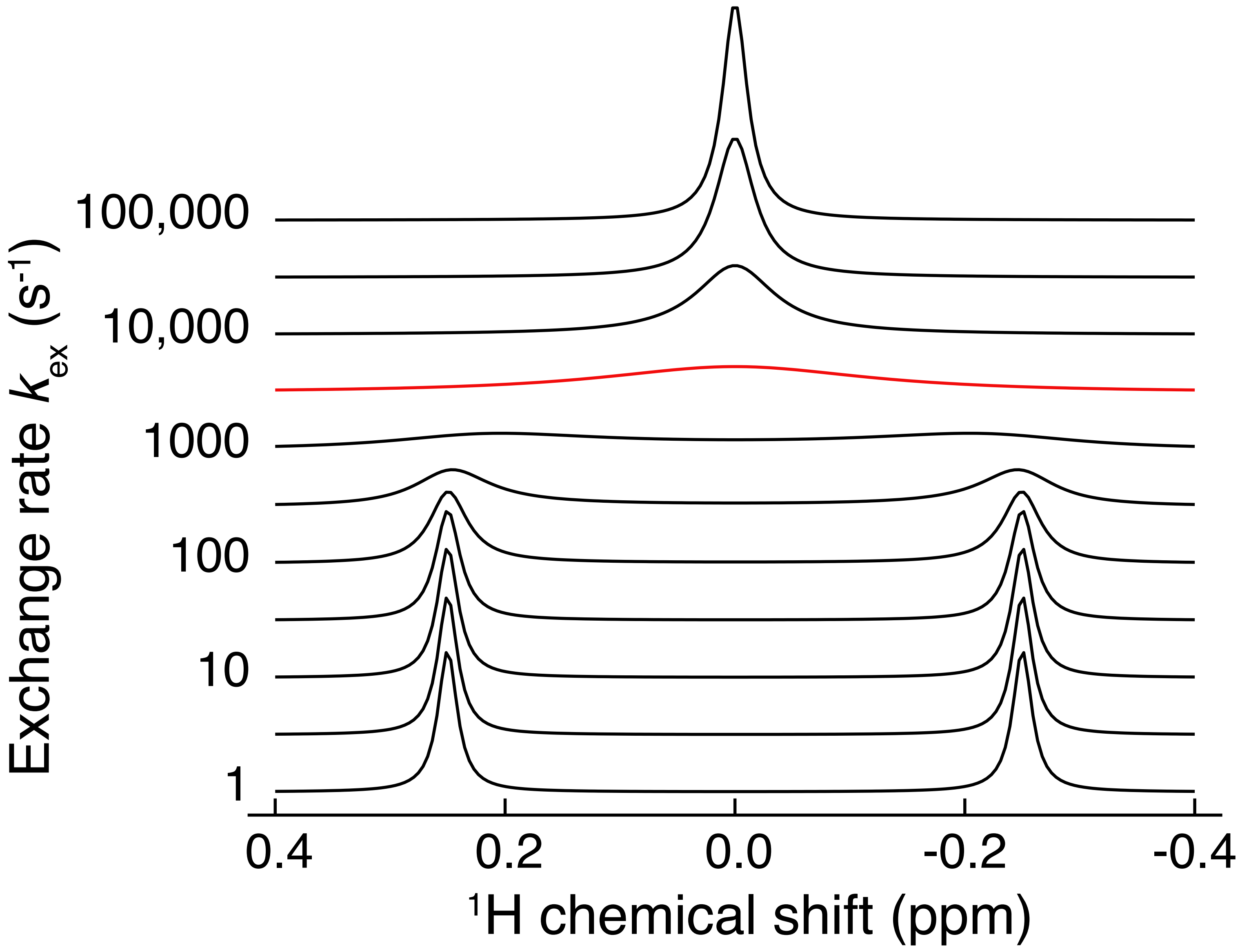
Chemical exchange regimes: slow exchange ($k_{ex} \ll \Delta\omega$)



Molecules effectively never exchange during free induction decay – like two separate chemical species

Individual resonances observed

Chemical exchange regimes: intermediate exchange ($k_{ex} \approx \Delta\omega$)

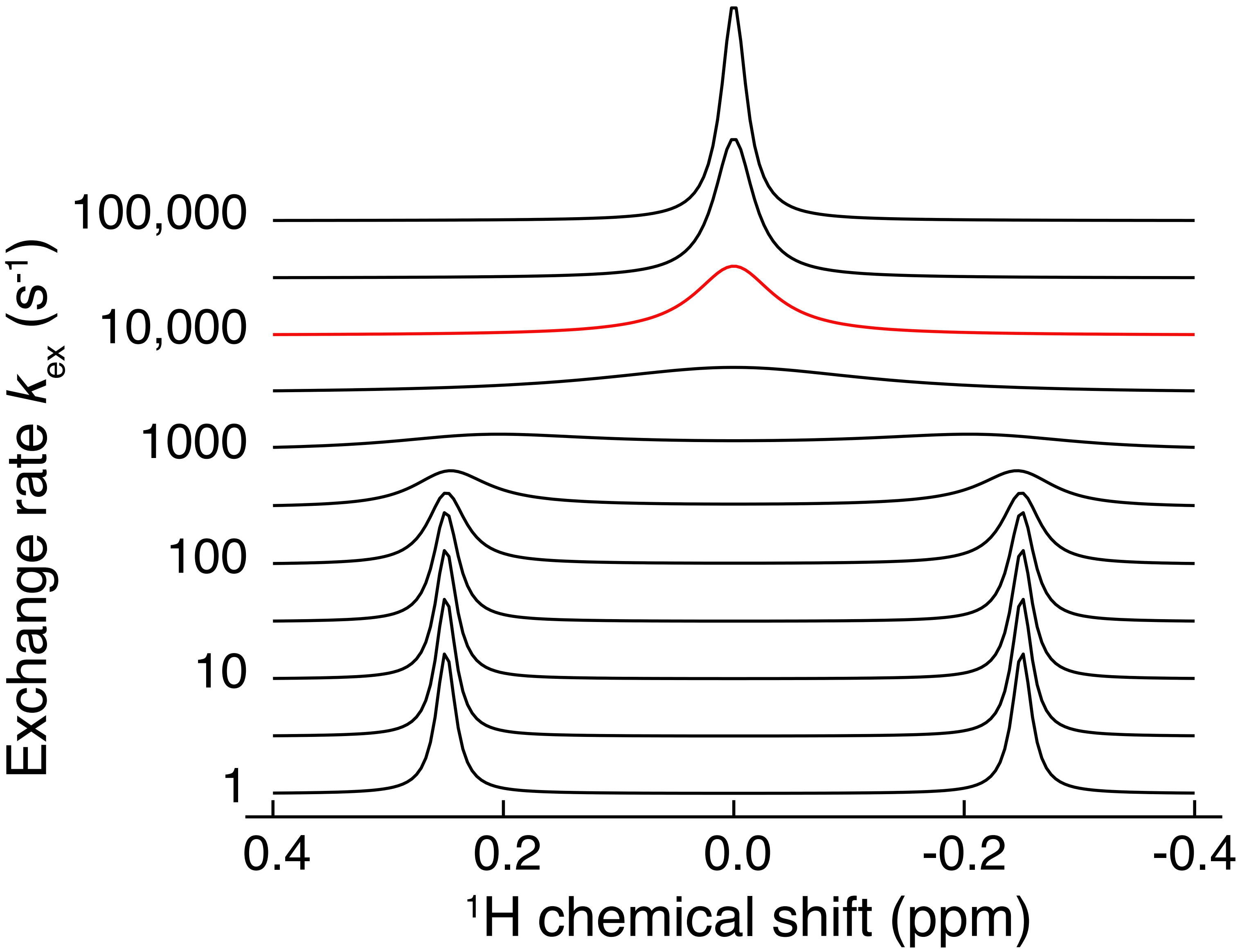


Severe line broadening results when the exchange rate is comparable to the frequency difference – the intermediate exchange regime

The coalescence point, defined by vanishing first and second derivates, occurs when $k_{ex} = |\Delta\omega| / \sqrt{2}$

Identification of the coalescence point provides a simple way to determine exchange rates – but more sophisticated approaches are available!

Chemical exchange regimes: fast-intermediate exchange ($k_{\mathrm{ex}} > \Delta\omega$)



As a signal in fast exchange approaches the coalescence point, its line width increases and intensity decreases due to **exchange broadening**:

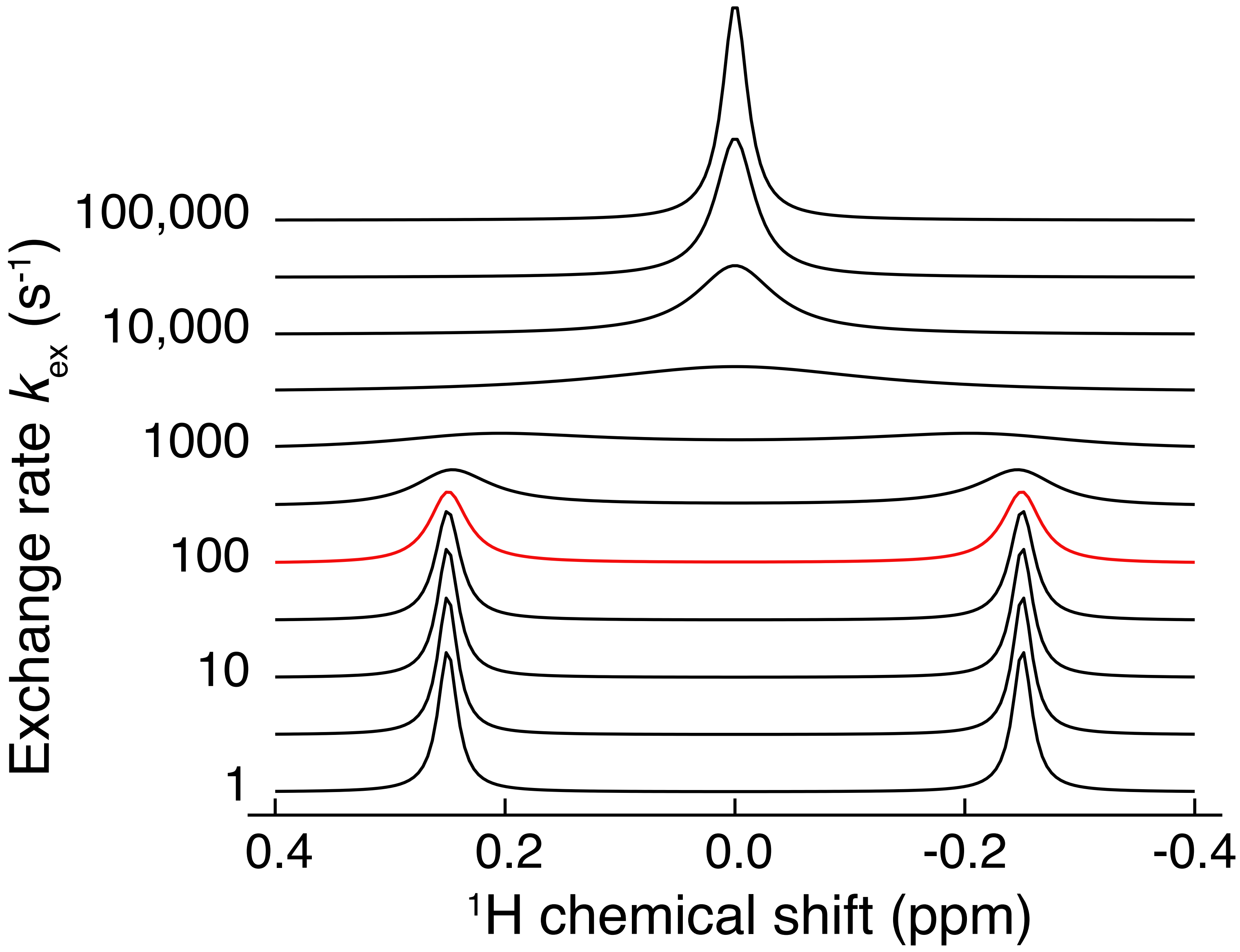
$$R_{2,\mathrm{obs}} = R_{2,0} + R_{\mathrm{ex}}$$

The exchange broadening contribution depends on the populations, exchange rate and frequency difference:

$$R_{\mathrm{ex}} = \frac{p_A p_B \Delta\omega^2}{k_{\mathrm{ex}}}$$

Note that the frequency difference is also proportional to the magnetic field strength – exchange broadening is more severe at higher field strengths

Chemical exchange regimes: slow-intermediate exchange ($k_{ex} < \Delta\omega$)



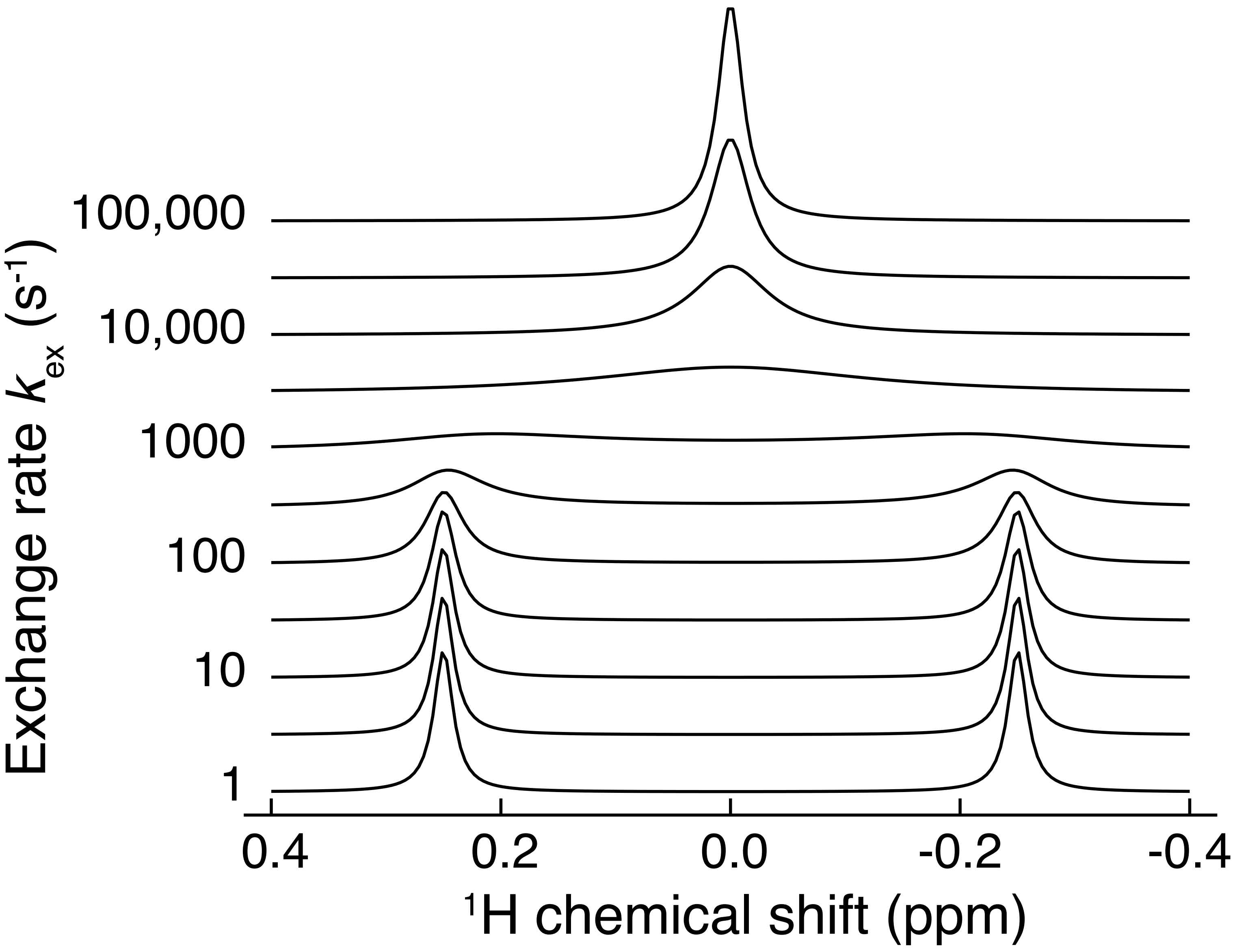
Resonances in slow exchange approaching the coalescence point also experience **lifetime line broadening**:

$$R_{\text{ex,A}} = k_{AB}$$

This arises from the irreversible loss of magnetisation from spins exchanging during the FID

Lifetime line broadening is independent of the chemical shift difference, population and magnetic field strength

Chemical exchange regimes: how sensitive is NMR?



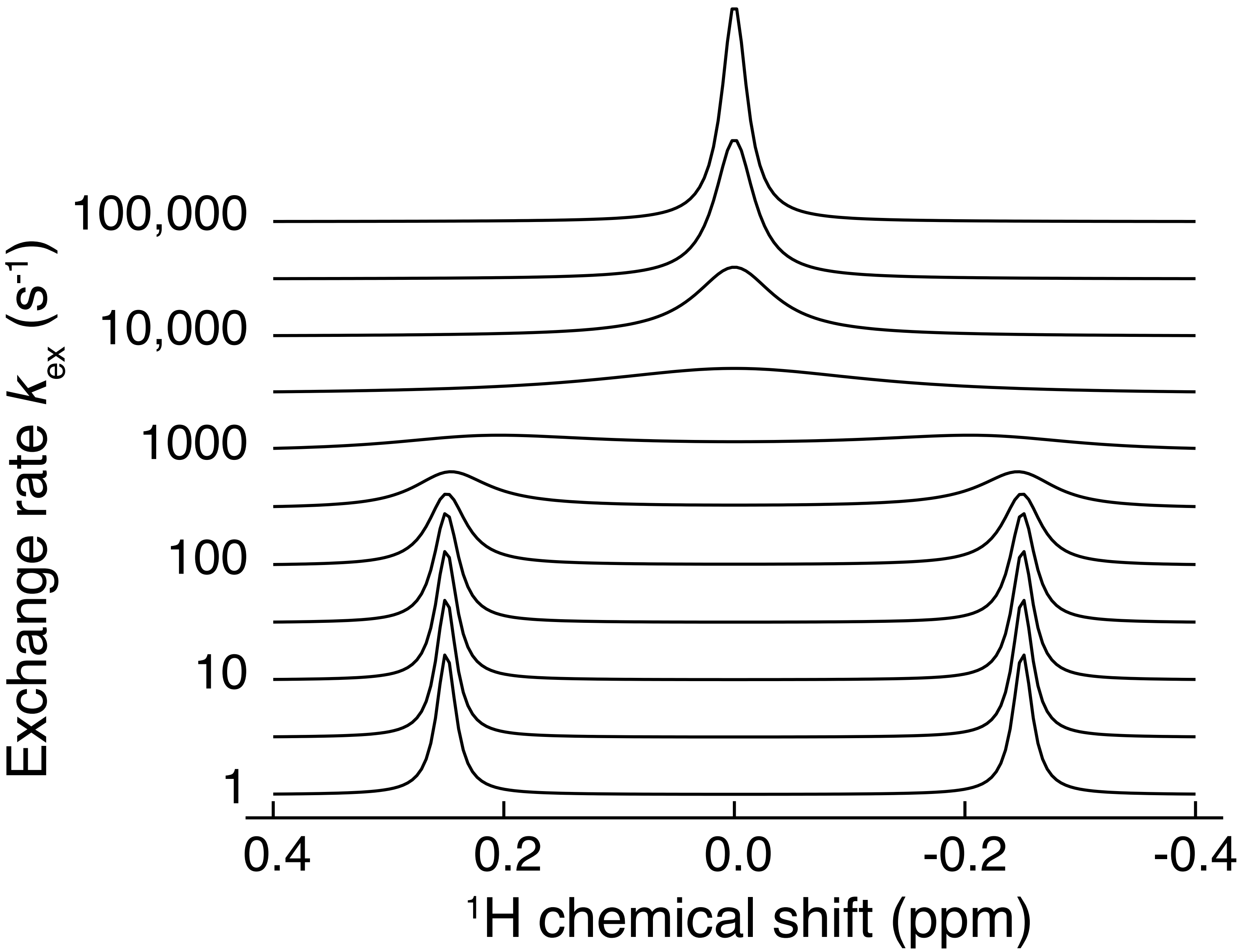
Spectra are most sensitive to exchange in the vicinity of the coalescence point

Line broadening effects can be observed over a wide range of parameter space, approximately:

$\Delta\omega / 50 < k_{ex} < 50\,\Delta\omega$

Different spins within a molecule can also have difference $\Delta\omega$, bringing sensitivity to an even wider range of exchange rates!

Chemical exchange regimes: why is NMR unique?



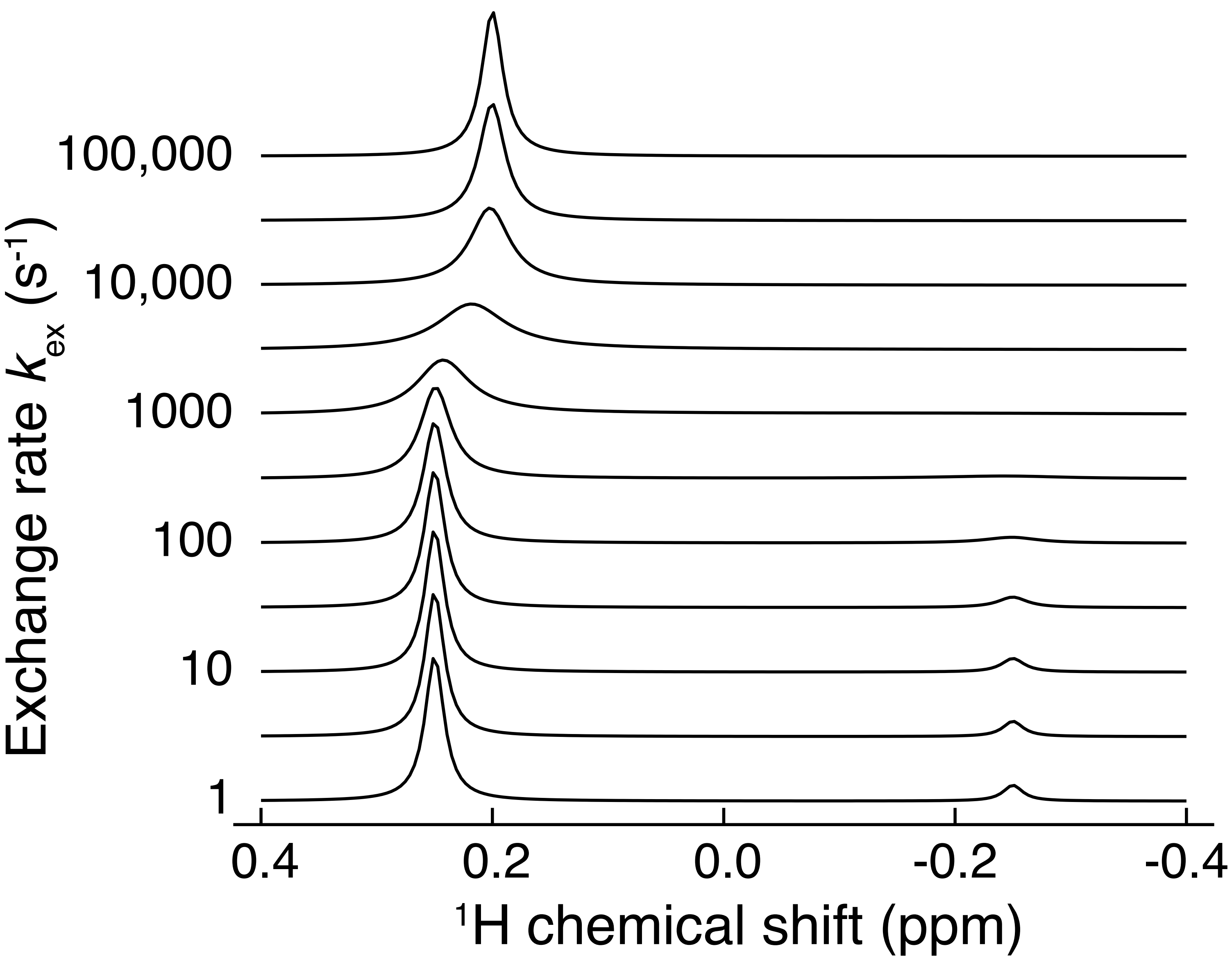
Why do other forms of spectroscopy (e.g. CD, UV, IR, fluorescence) not see similar chemical exchange effects?

…because the relevant frequency differences are **much** bigger!

e.g. two species absorbing at 500 nm and 520 nm have frequencies of
6×10^{14} Hz and 5.8×10^{14} Hz

=> $\Delta\omega \approx 1.2 \times 10^{14}\ s^{-1}$!

Chemical exchange regimes: unequal populations

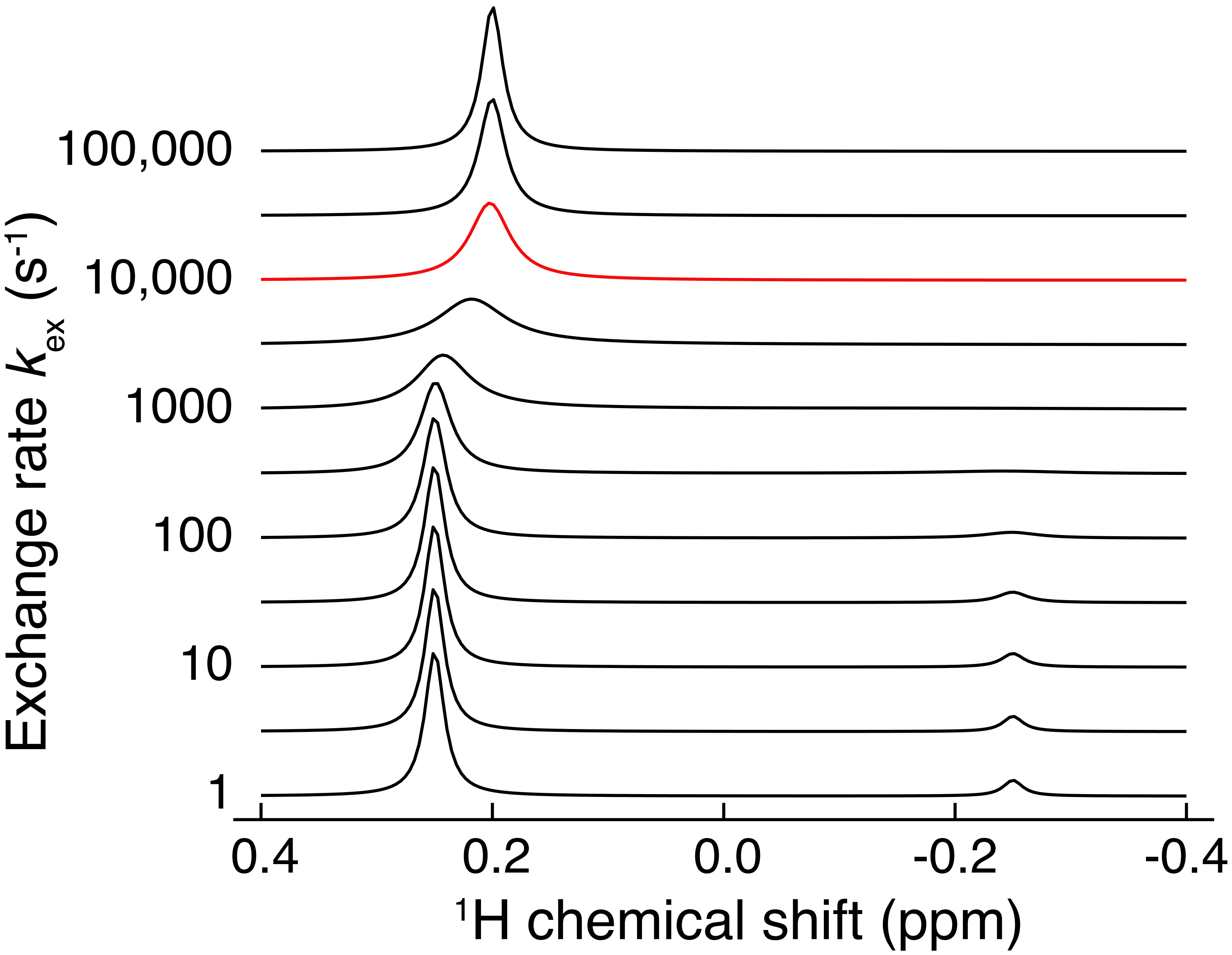


Simulated resonance line shapes for unequal populations (90% / 10%)

Unequal populations can arise in many circumstances:

- early stages of a titration
- sparsely populated intermediates in biomolecules
- spins in exchange with the solvent (solvent is the major state!)

Chemical exchange regimes: unequal populations



Simulated resonance line shapes for unequal populations (90% / 10%)

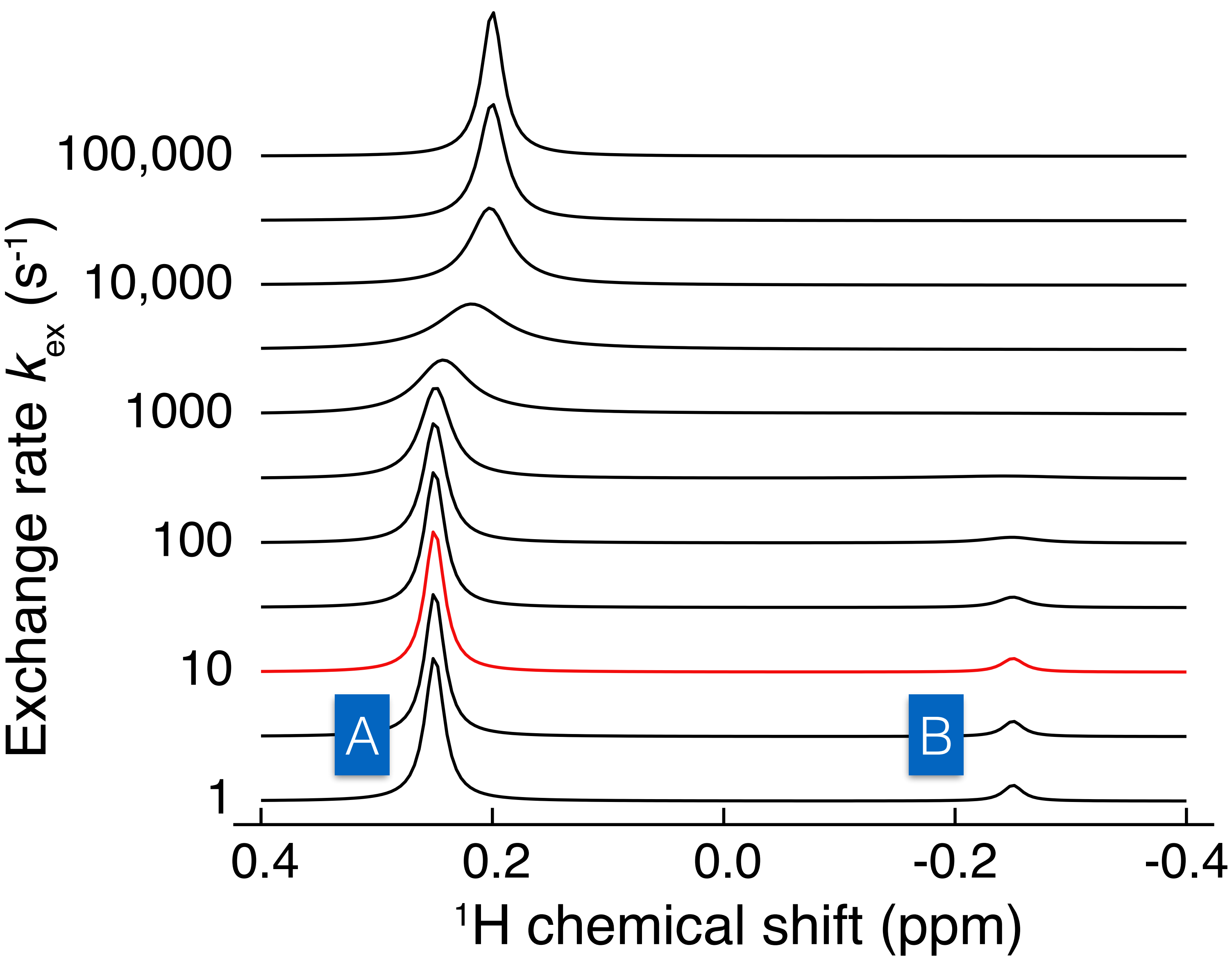
In fast exchange, we observe a single resonance at the population-weighted average frequency:

$$\omega_{obs} = p_A\omega_A + p_B\omega_B$$

with exchange broadening as for symmetric populations:

$$R_{\mathrm{ex}} = \frac{p_A p_B \Delta\omega^2}{k_{\mathrm{ex}}}$$

Chemical exchange regimes: unequal populations



Simulated resonance line shapes for unequal populations (90% / 10%)

In slow exchange, we observe two resonances with population-weighted **amplitudes**

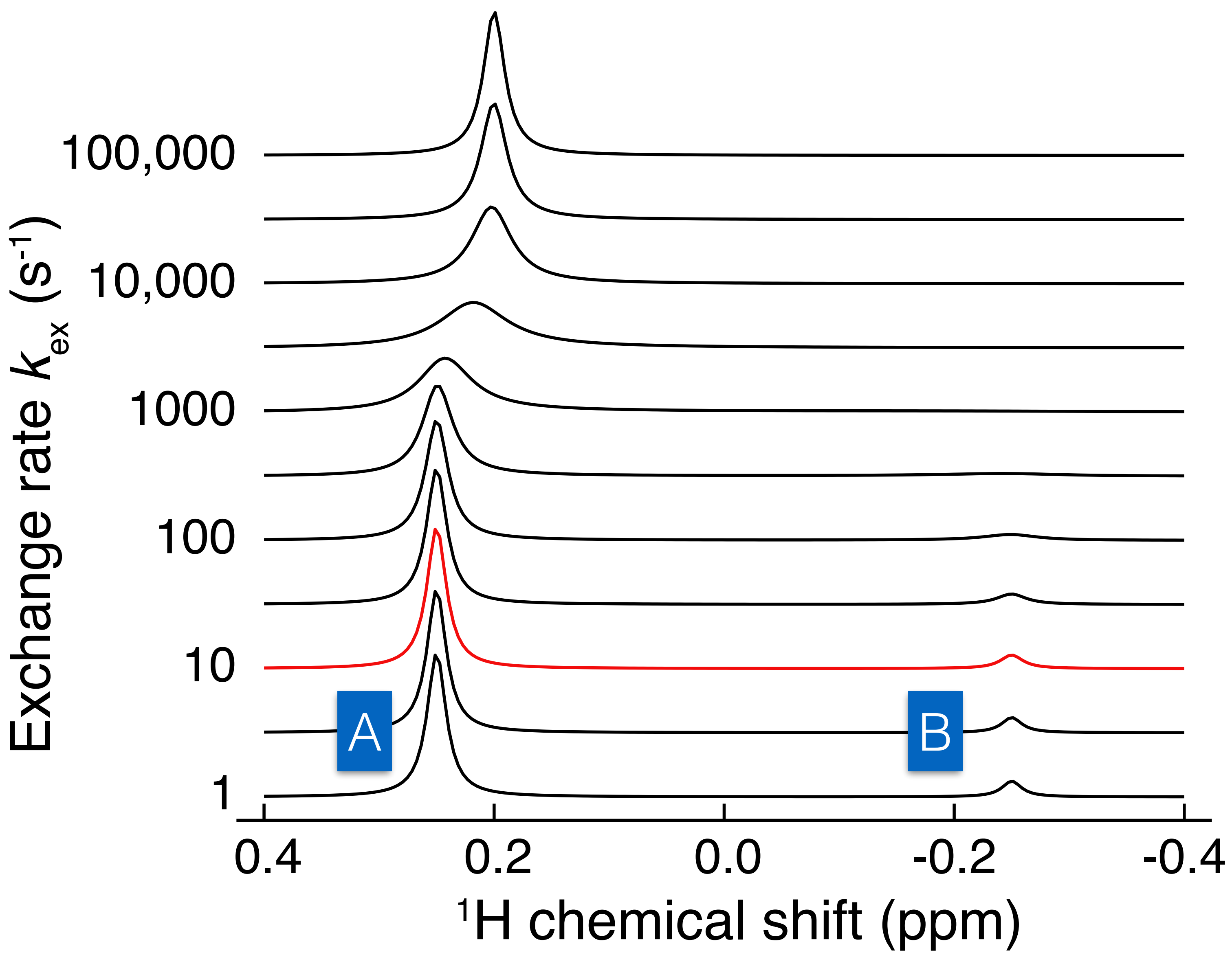
Major and minor peaks both exhibit **lifetime line broadening**, but the impact of this is very different for the two peaks

$R_{\mathrm{ex,A}} = k_{AB}$ small

$R_{\mathrm{ex,B}} = k_{BA}$ **LARGE**

$$\text{intensity} \sim \frac{\text{amplitiude}}{R_{2,0} + R_{\mathrm{ex}}}$$

Chemical exchange regimes: unequal populations



Simulated resonance line shapes for unequal populations (90% / 10%)

In slow exchange, we observe two resonances with population-weighted **amplitudes**

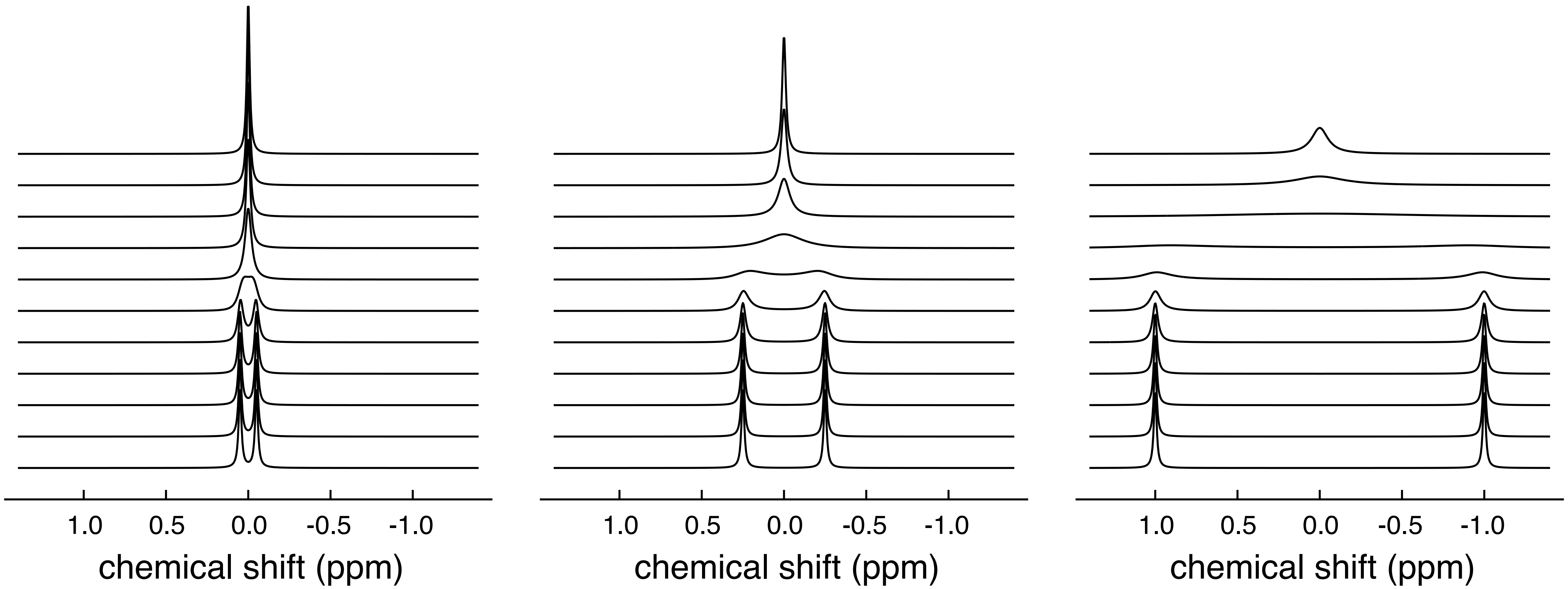
Major and minor peaks both exhibit **lifetime line broadening**, but the impact of this is very different for the two peaks

$$R_{\mathrm{ex,A}} = k_{AB}$$ small

$$R_{\mathrm{ex,B}} = k_{BA}$$ **LARGE**

Minor states are often effectively 'invisible' and experiments such as CEST and CPMG may be required to detect and probe them

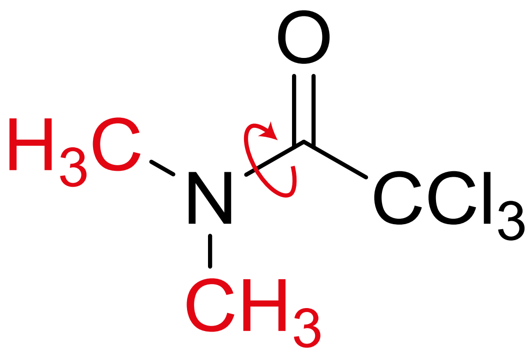
Modulating chemical exchange regimes



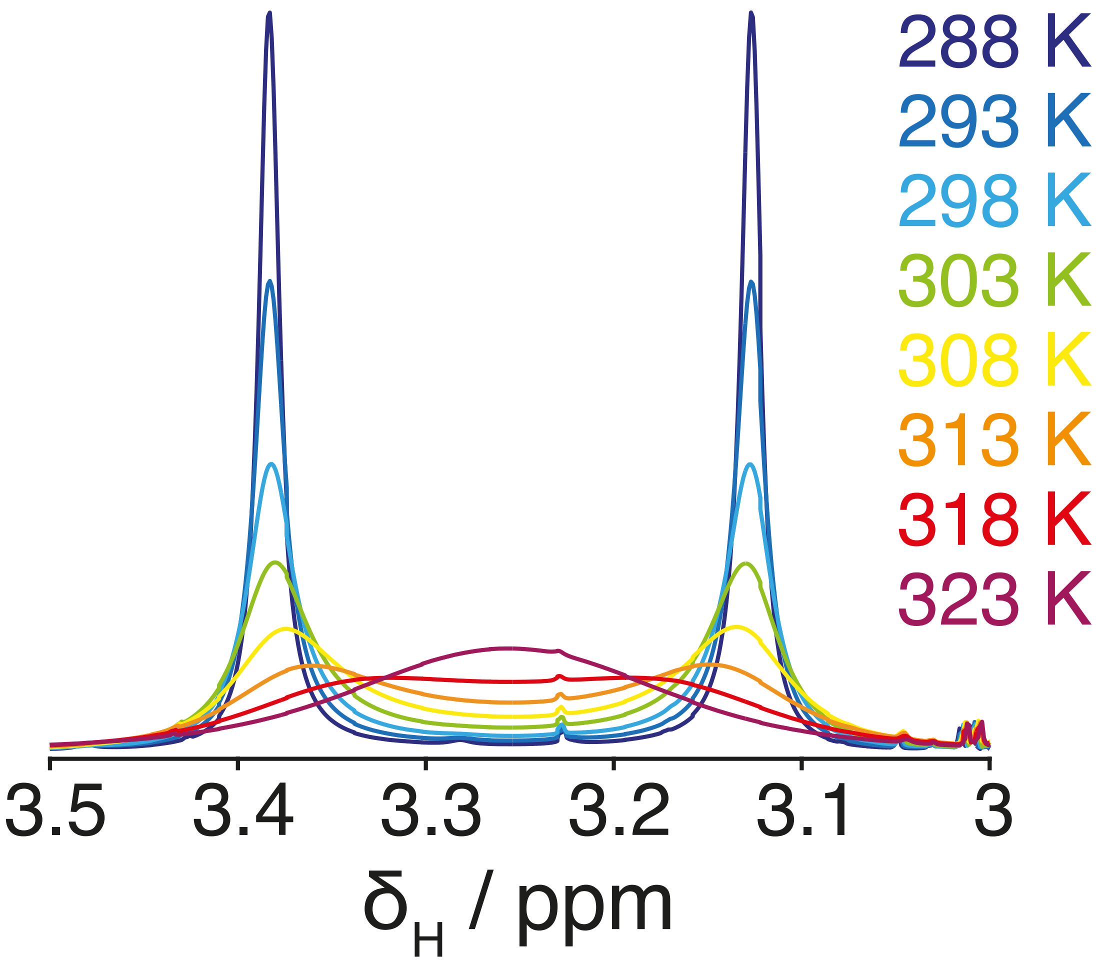
Varying the magnetic field strength will vary $\Delta\omega = \gamma\Delta\delta B_0$

Alternatively, most molecules will contain a range of spins that experience a variety of chemical shift changes between states

Modulating chemical exchange regimes

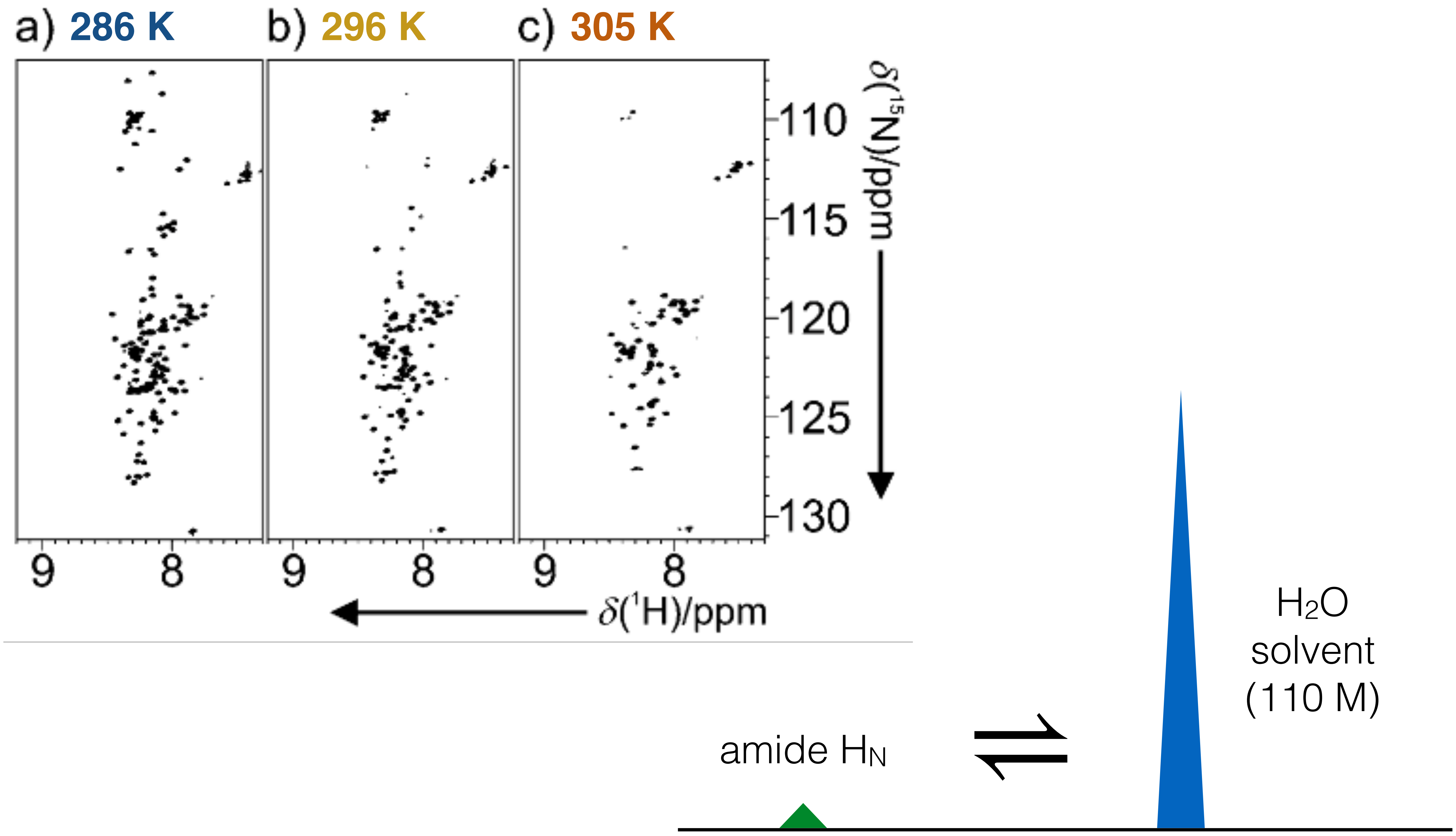


$\Delta\delta_H = 0.26$ ppm
$\Delta\delta_C = 0.62$ ppm
${}^1J_{CH} = 140$ Hz
$k_{ex} = 125\ \mathrm{s}^{-1}$
(298 K)



Changing the temperature can change the kinetics of the exchange process

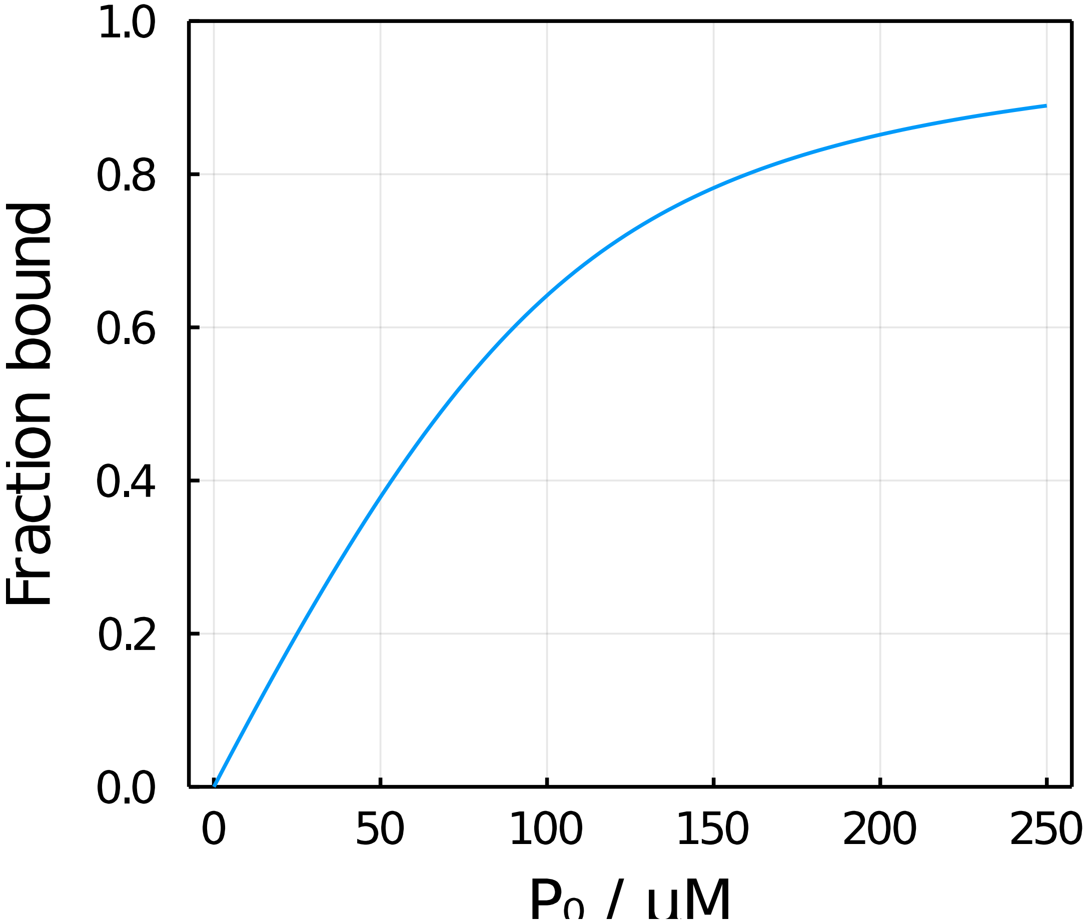
Application of VT NMR to intrinsically disordered proteins

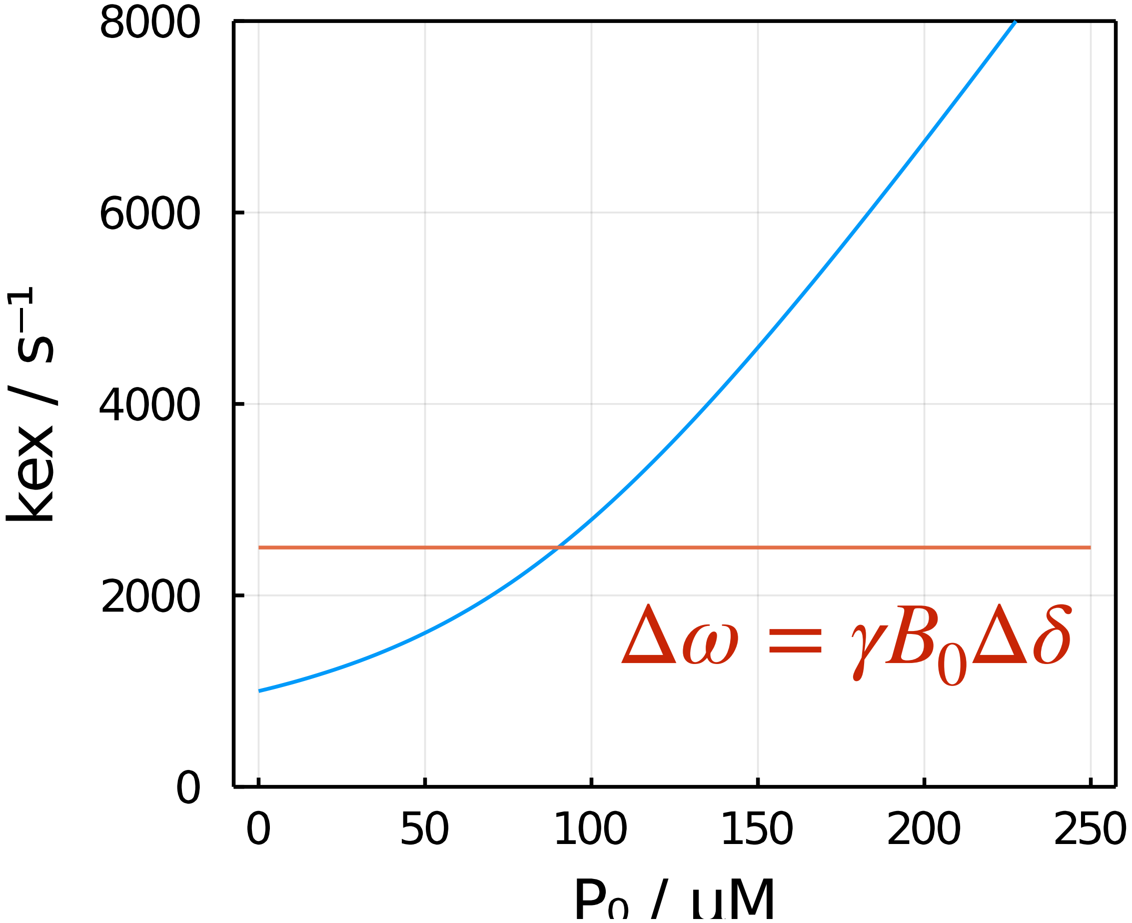


lifetime line broadening due to solvent hydrogen exchange of amide minor state leads to loss of resonances in 2D spectra

Titration experiments

$$k_{\mathrm{ex}} = k_{AB} + k_{BA}$$
$$= k_{\mathrm{on}}[L] + k_{\mathrm{off}}$$

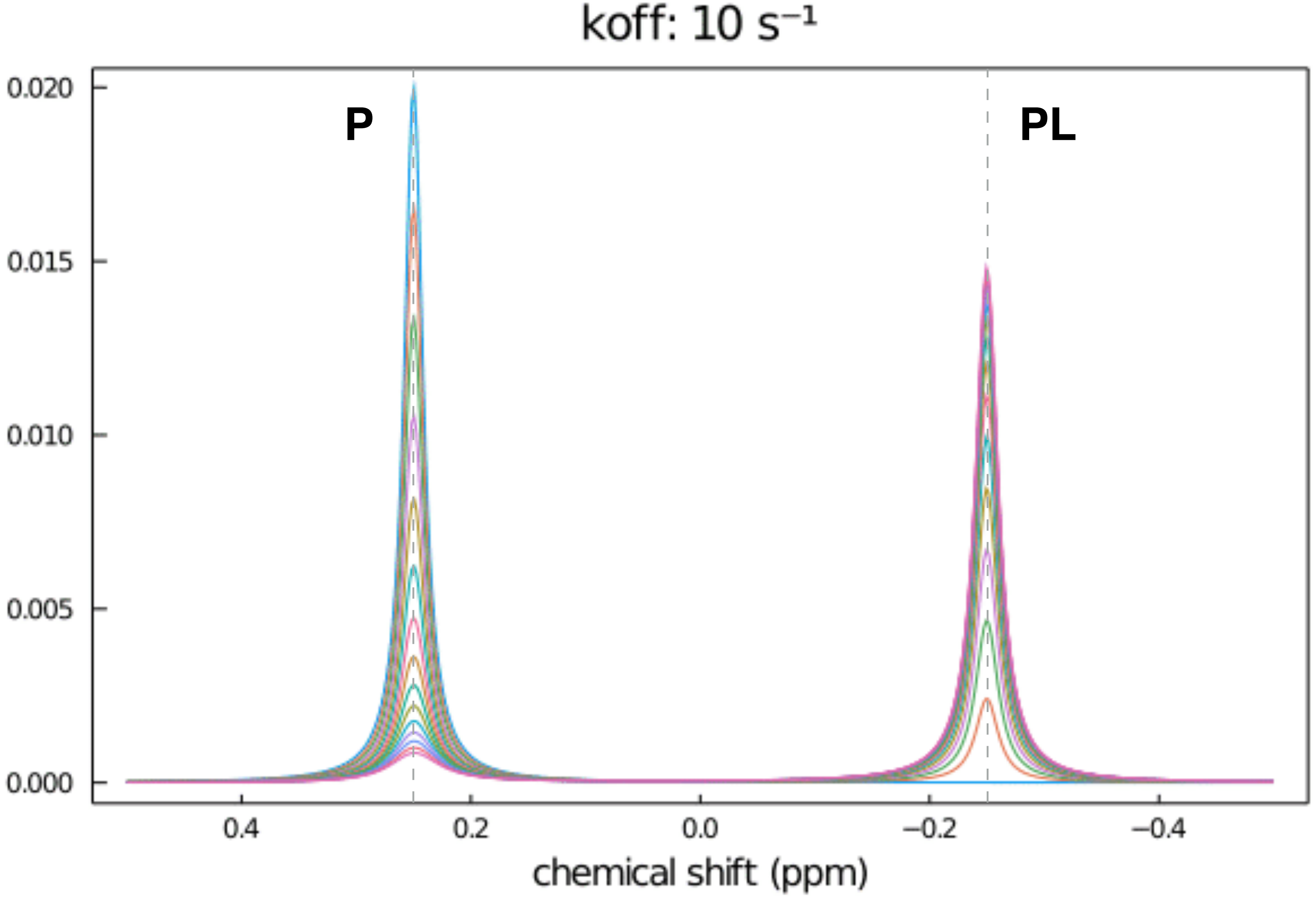




$$\Delta\omega = \gamma B_0 \Delta\delta$$

K_d = 20 μM
k_{off} = 1000 s^{-1}
$[P]_0$ = 100 μM
Δδ (^{1}H) = 0.5 ppm (800 MHz)

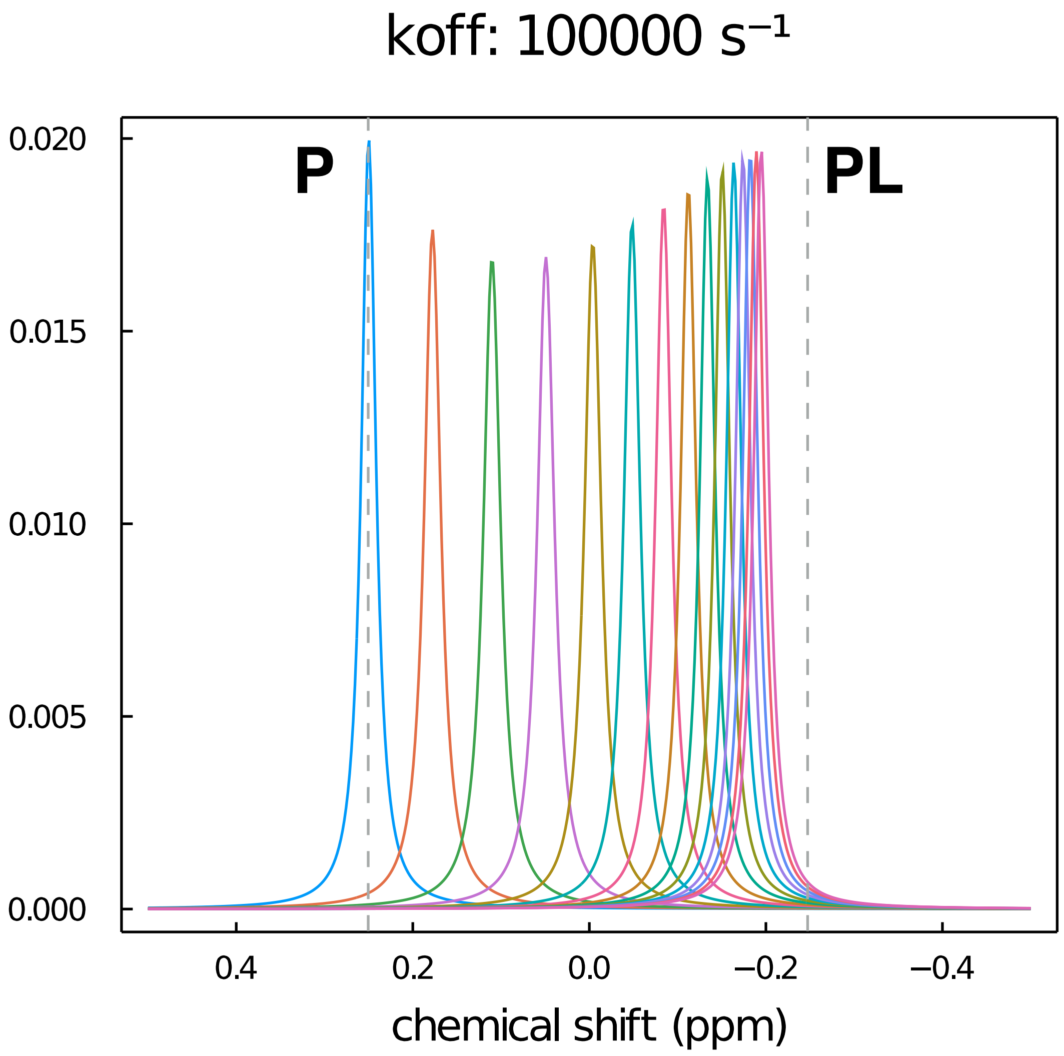
Titration experiments: effect of varying dissociation rate



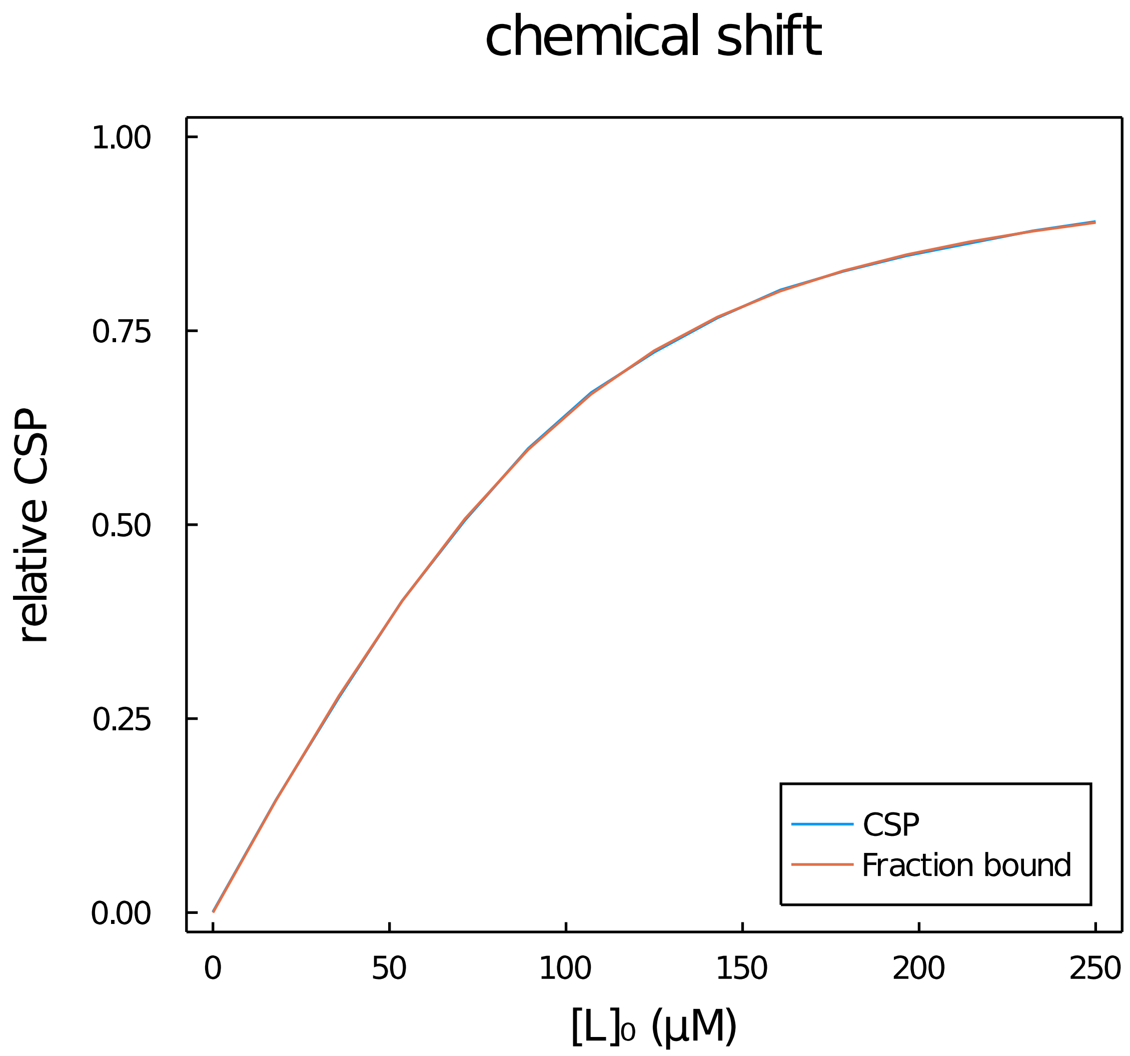
$\Delta\delta$ (^{1}H) = 0.5 ppm (800 MHz)
$\Delta\omega$ = 2500 s^{-1}
K_d = 20 μM

$[P]_0$ = 100 μM
$[L]_0$ = 0 – 250 μM

Titration experiments: fast exchange



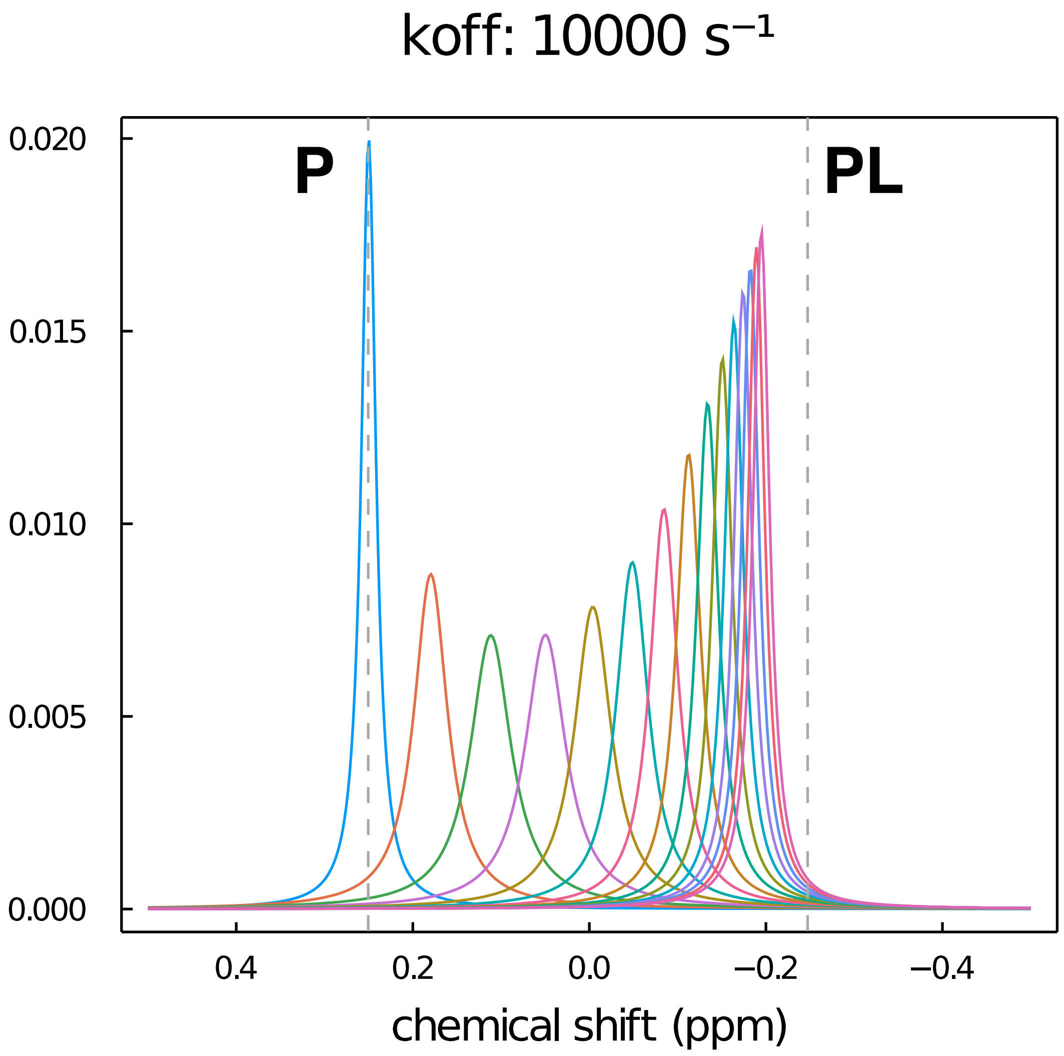
koff: 100000 s^{-1}

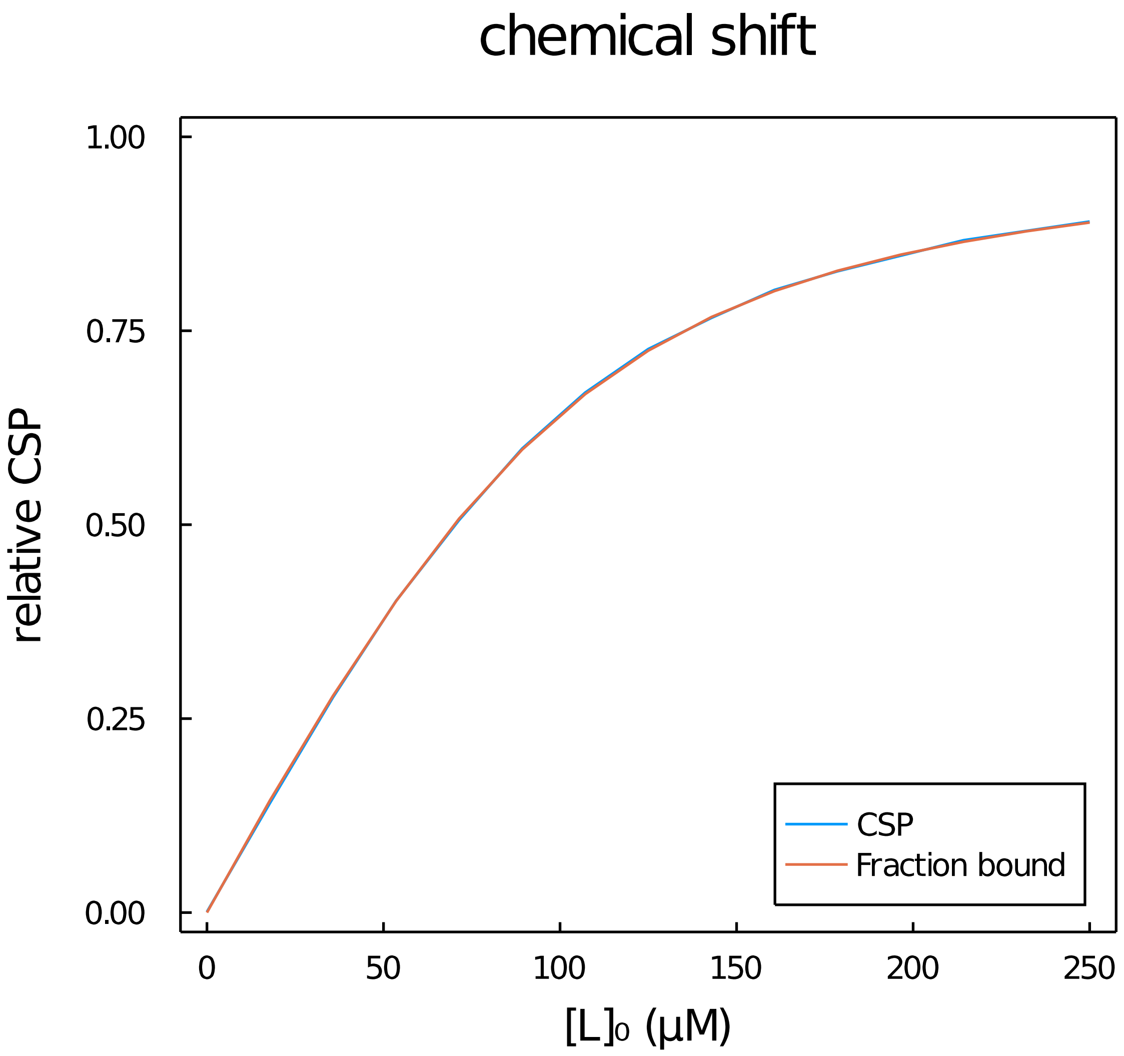


chemical shift

CSPs strongly correlated with fraction bound (easy to analyse)

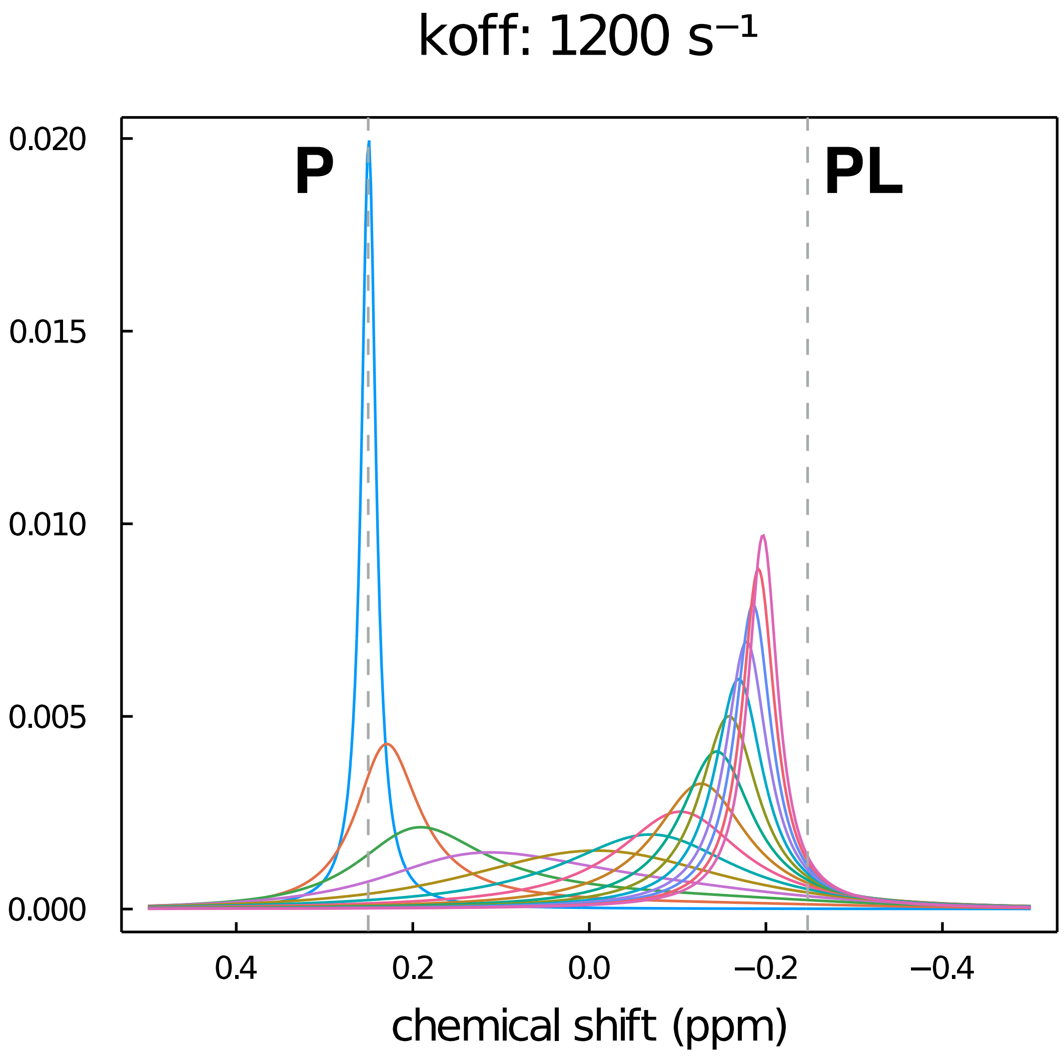
Titration experiments: fast exchange

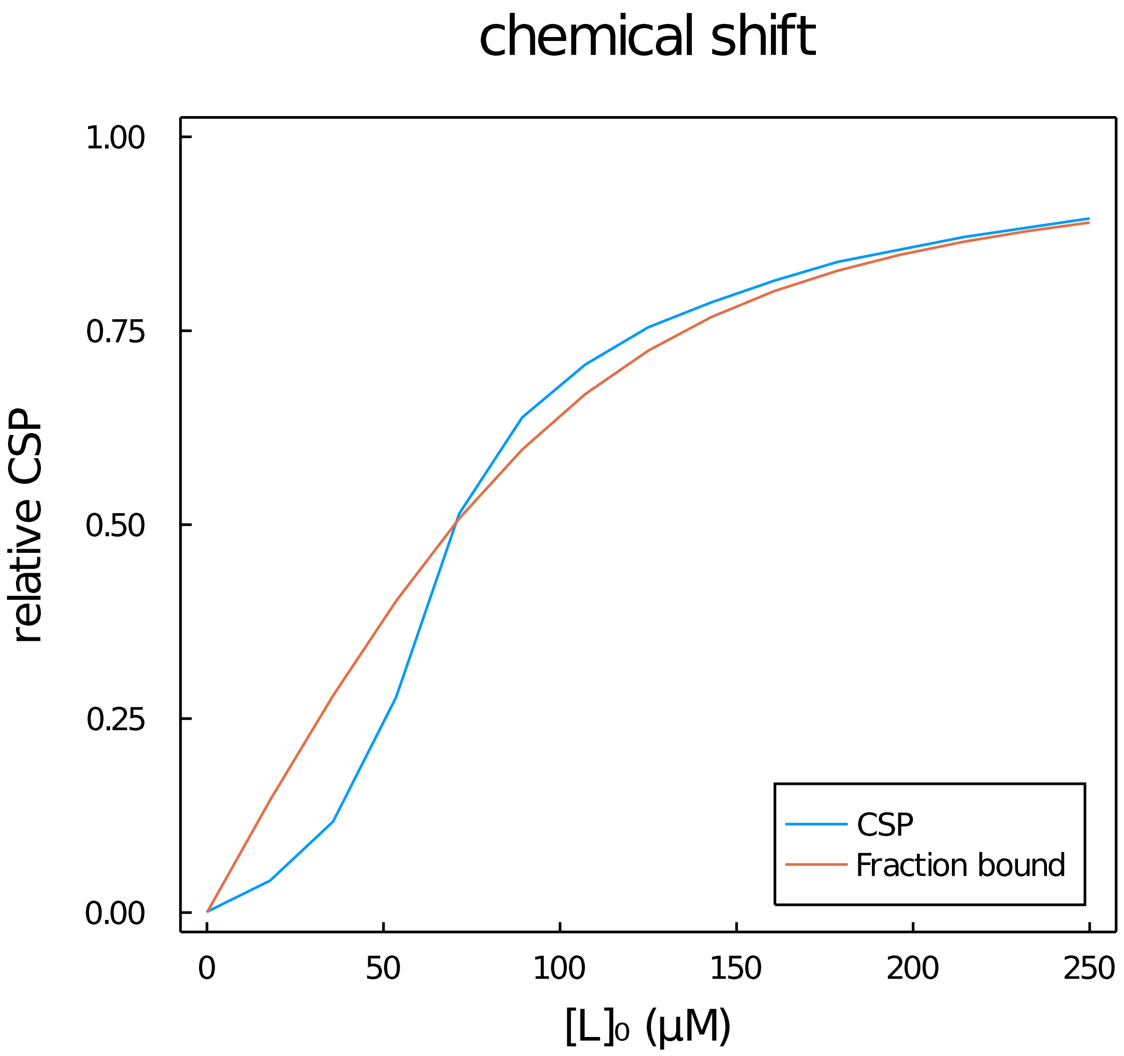




Exchange broadening $R_{\text{ex}} = \dfrac{p_A p_B}{k_{\text{ex}}} \Delta\omega^2$

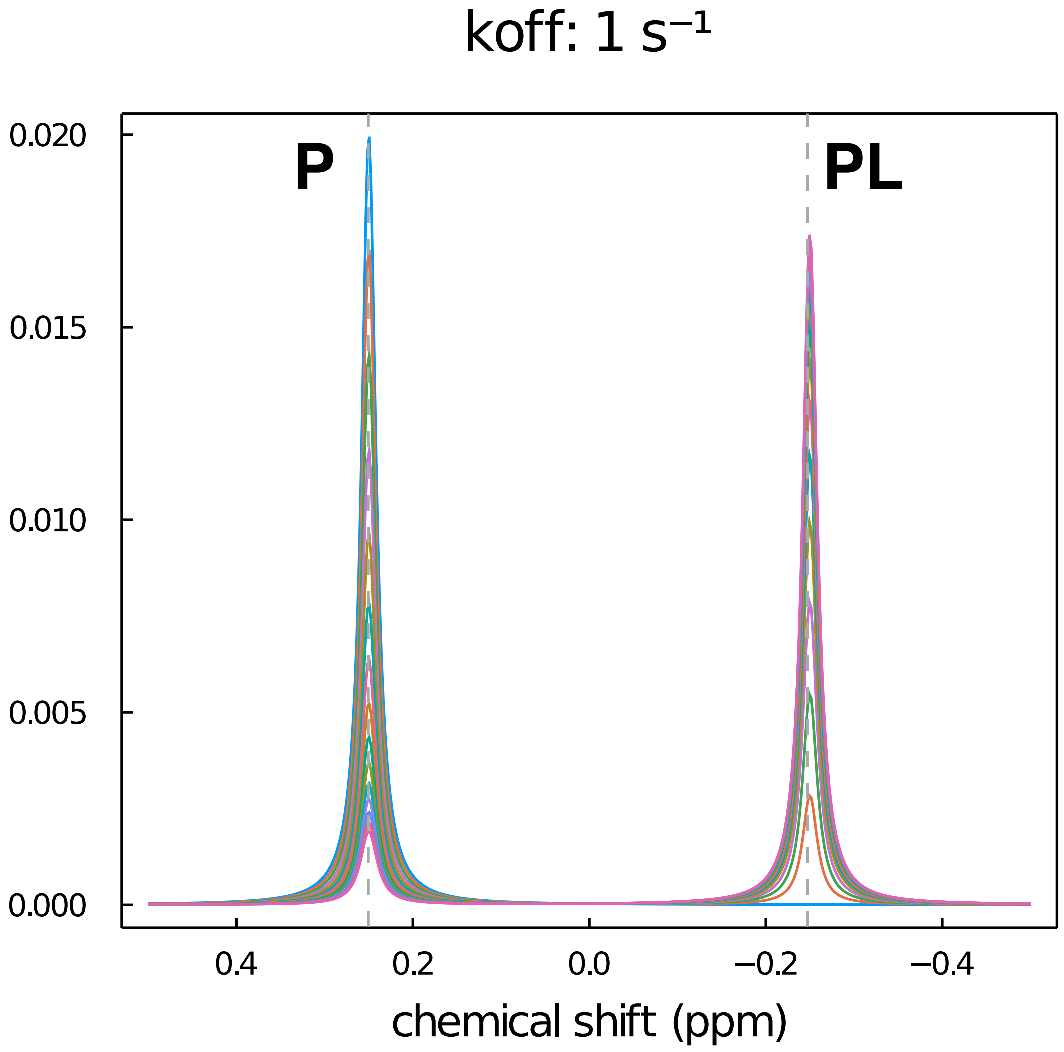
Titration experiments: intermediate exchange

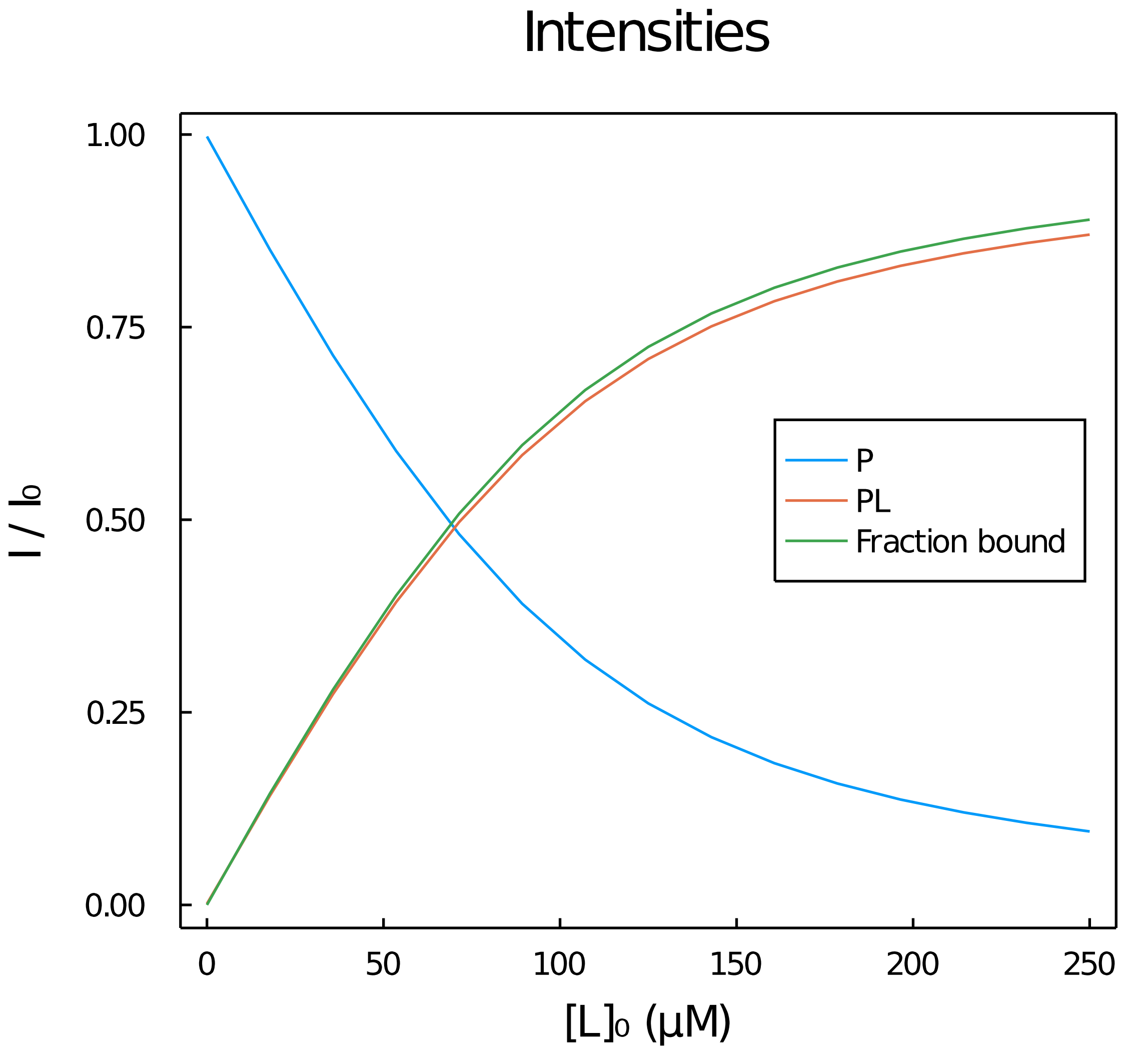




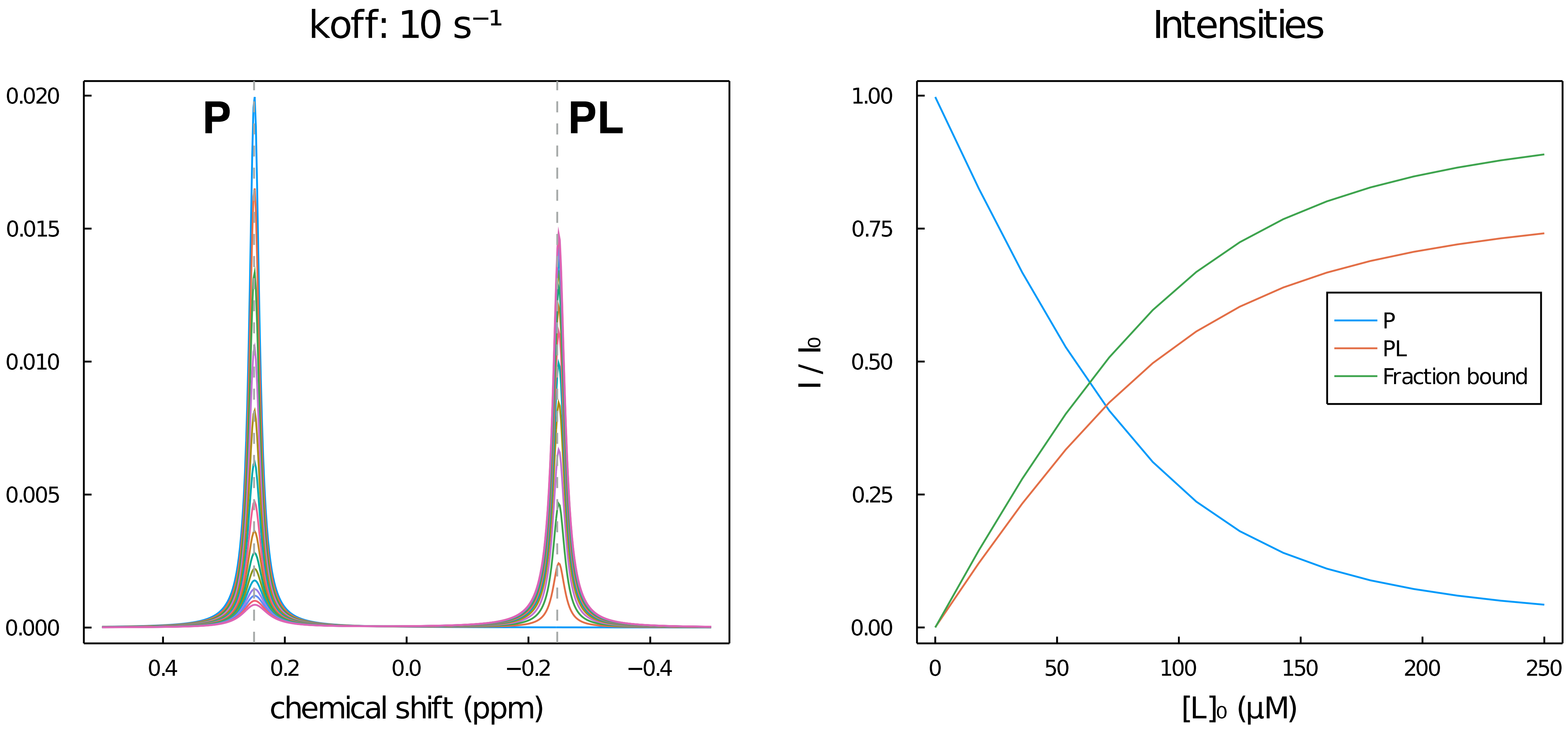
CSPs are no longer a good reporter of fraction bound

Titration experiments: slow exchange



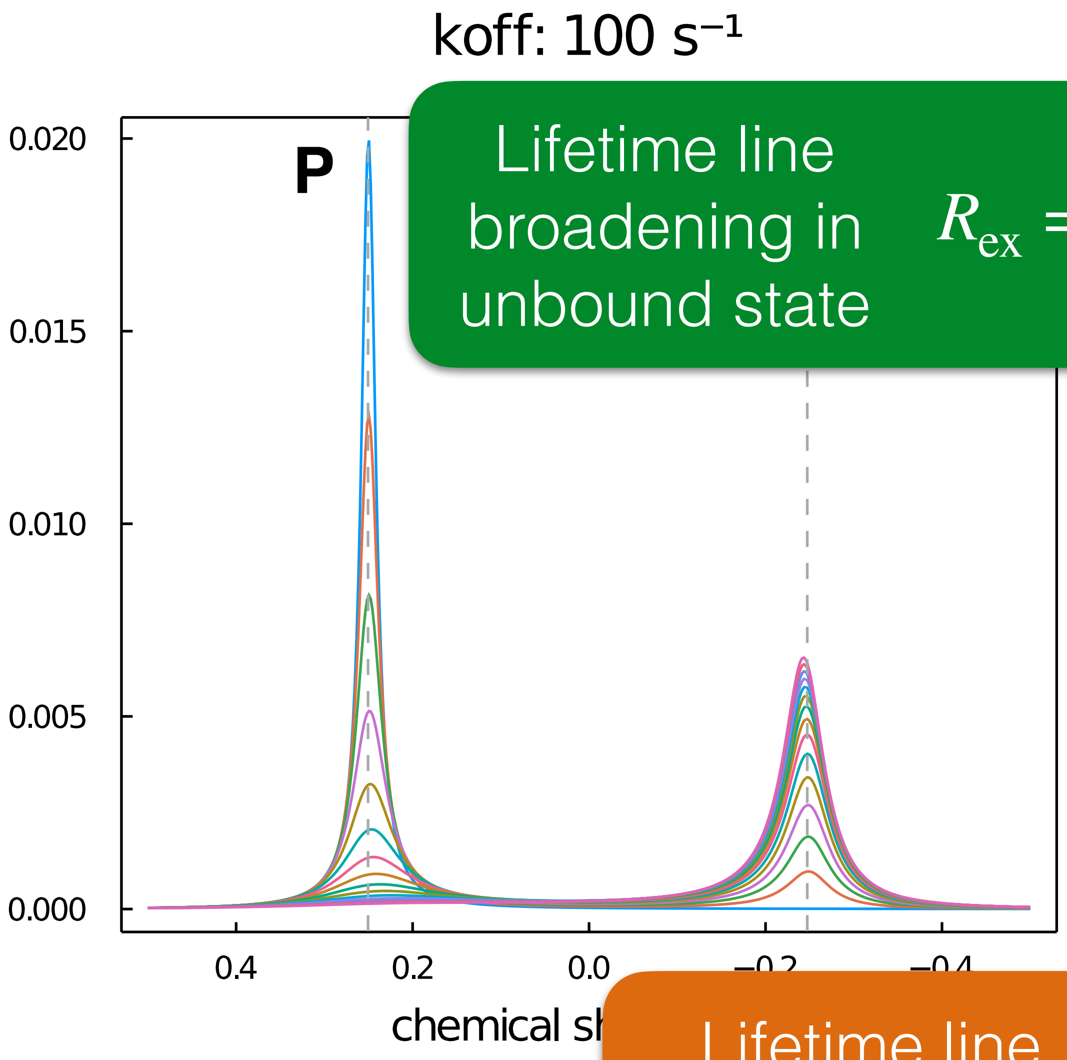


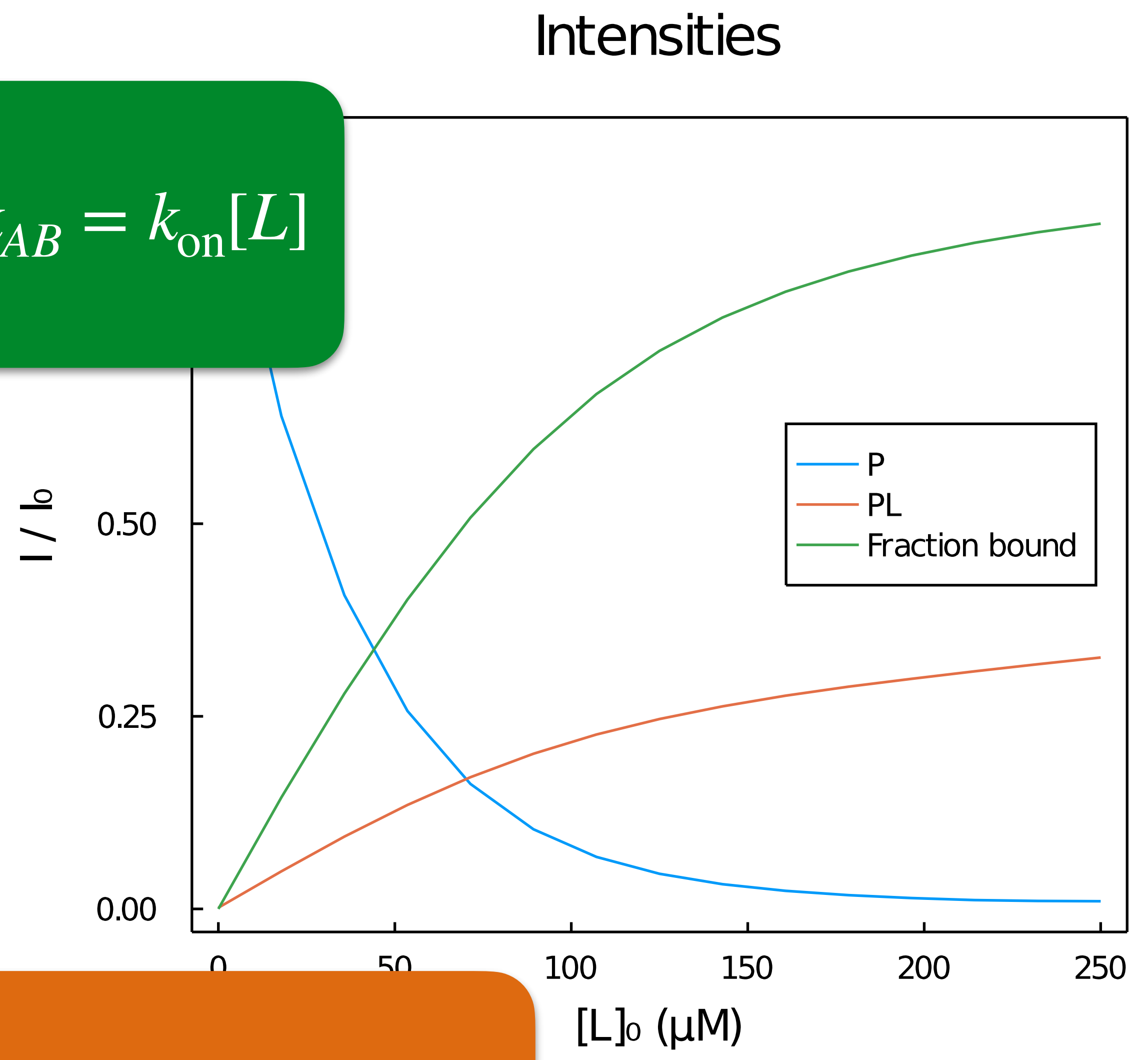
Titration experiments: slow exchange



Peak intensities may not be a good measure of fraction bound

Titration experiments: slow exchange

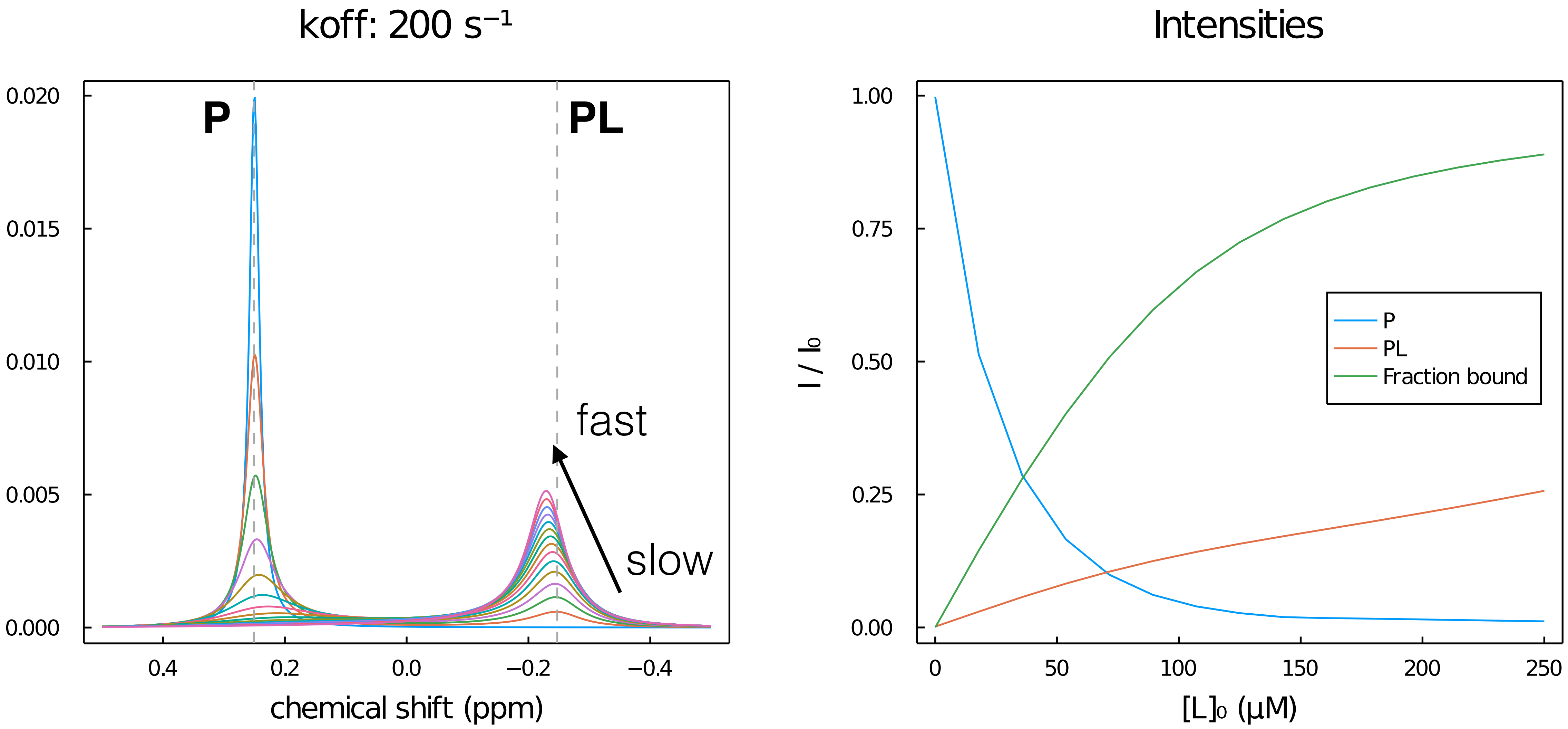




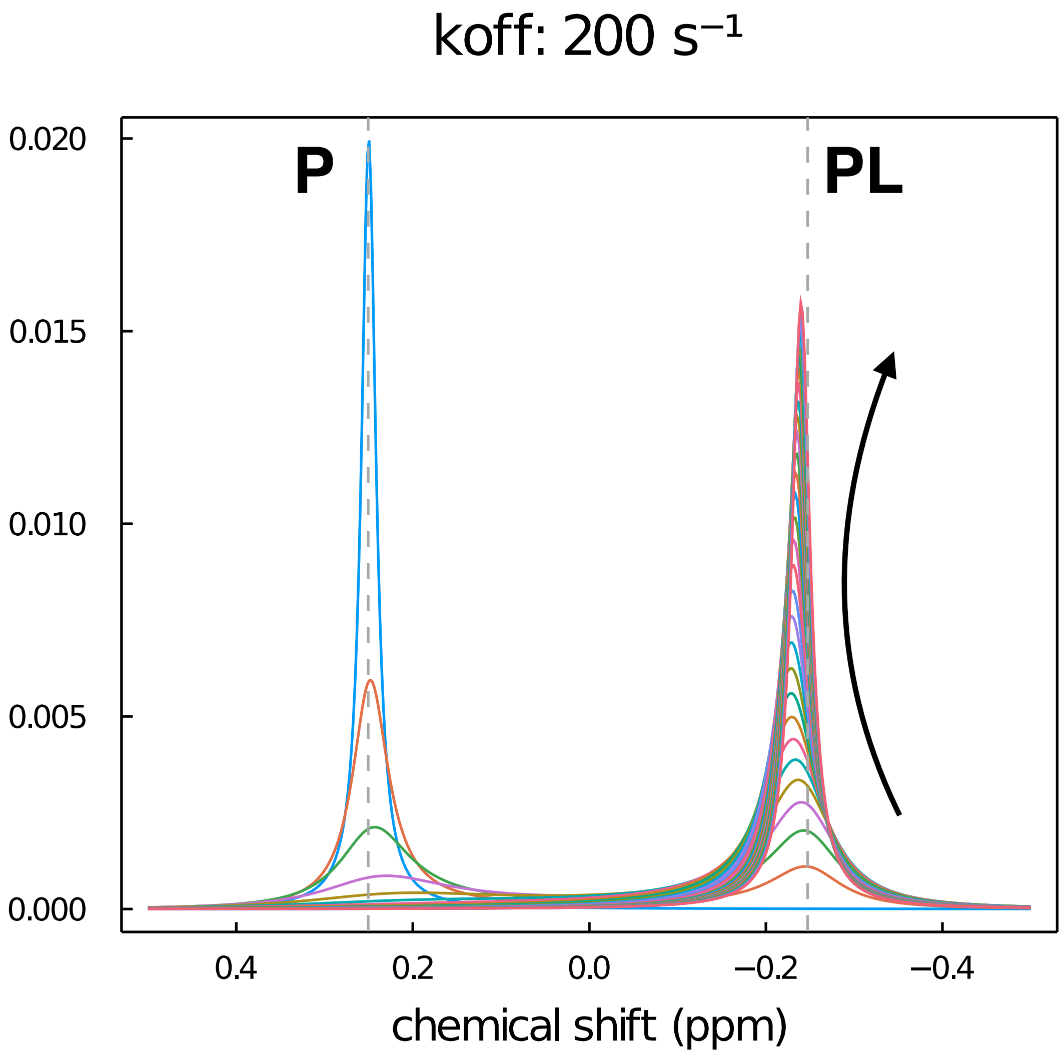
Lifetime line broadening in unbound state $R_{\mathrm{ex}} = k_{AB} = k_{\mathrm{on}}[L]$

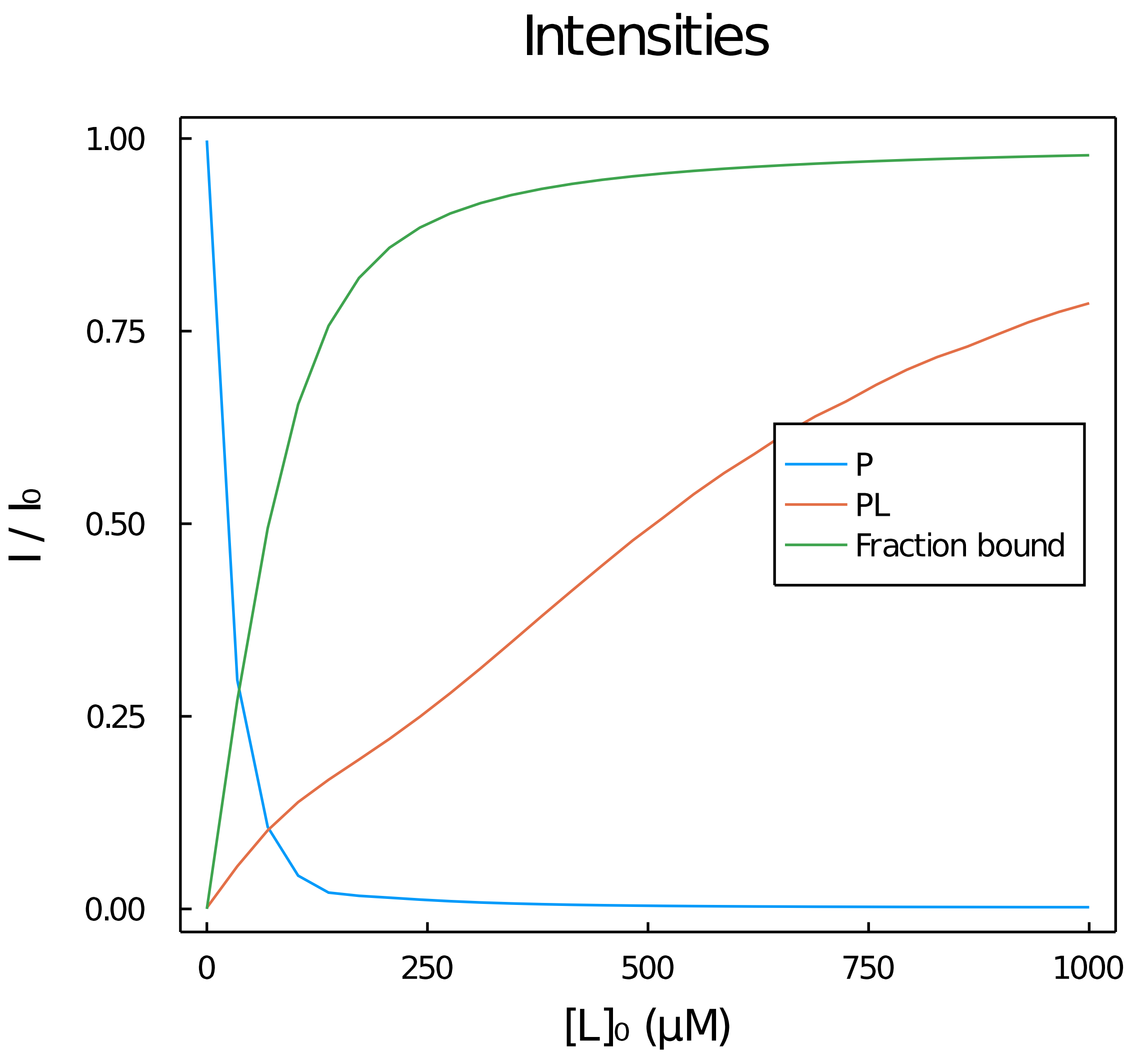
Lifetime line broadening in bound state $R_{\mathrm{ex}} = k_{BA} = k_{\mathrm{off}}$

Titration experiments: cross-over effects

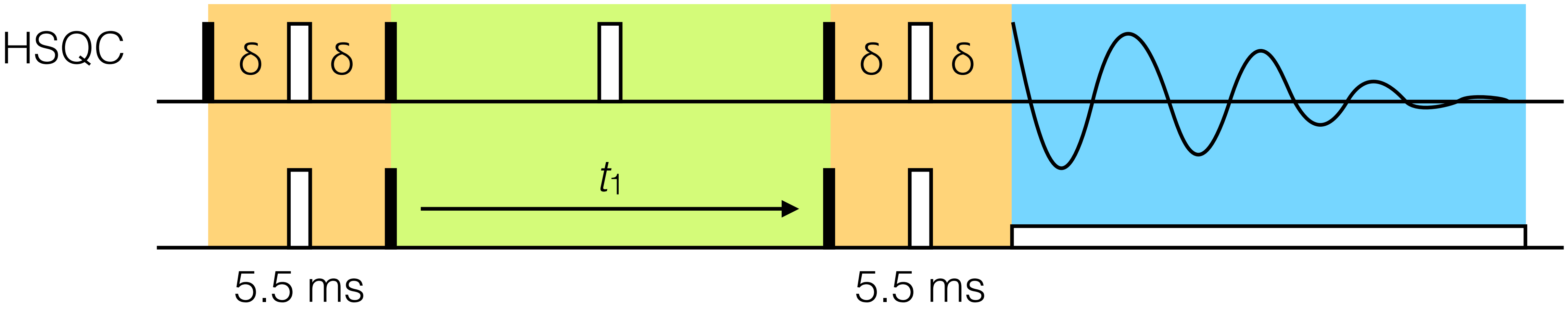


Titration experiments: cross-over effects

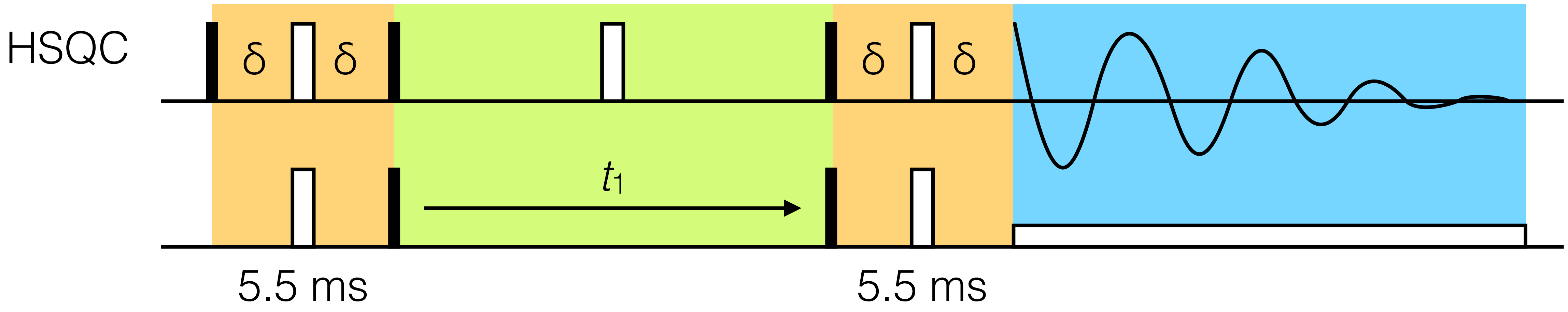




Chemical exchange in 2D experiments



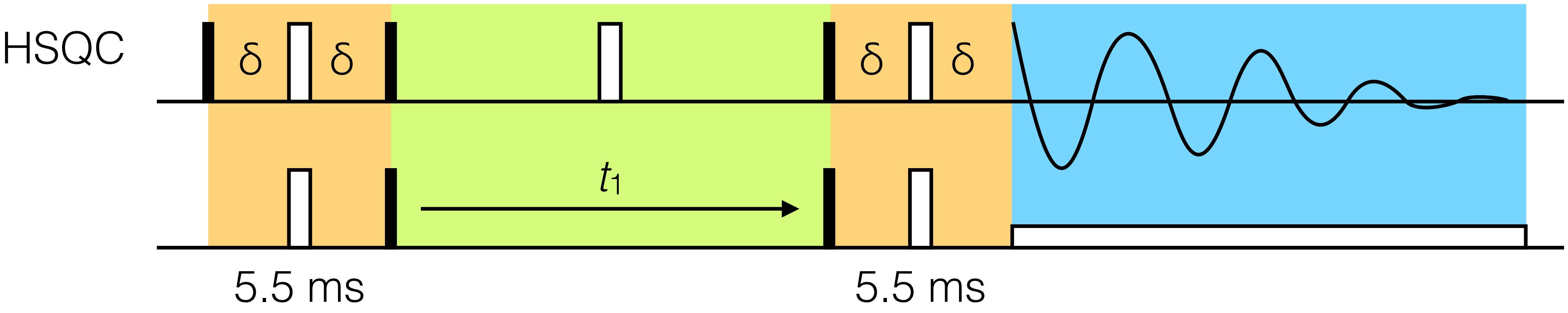
Chemical exchange in 2D experiments



Impact of chemical exchange on cross peak intensities is more significant than in 1D experiments – twice as many opportunities to lose signal!

$$I = I_0 \cdot \text{(relaxation loss during CTPs)} \cdot \frac{1}{R_{2,0}^{\text{indirect}} + R_{ex}^{\text{indirect}}} \cdot \frac{1}{R_{2,0}^{\text{direct}} + R_{ex}^{\text{direct}}}$$

Chemical exchange in 2D experiments



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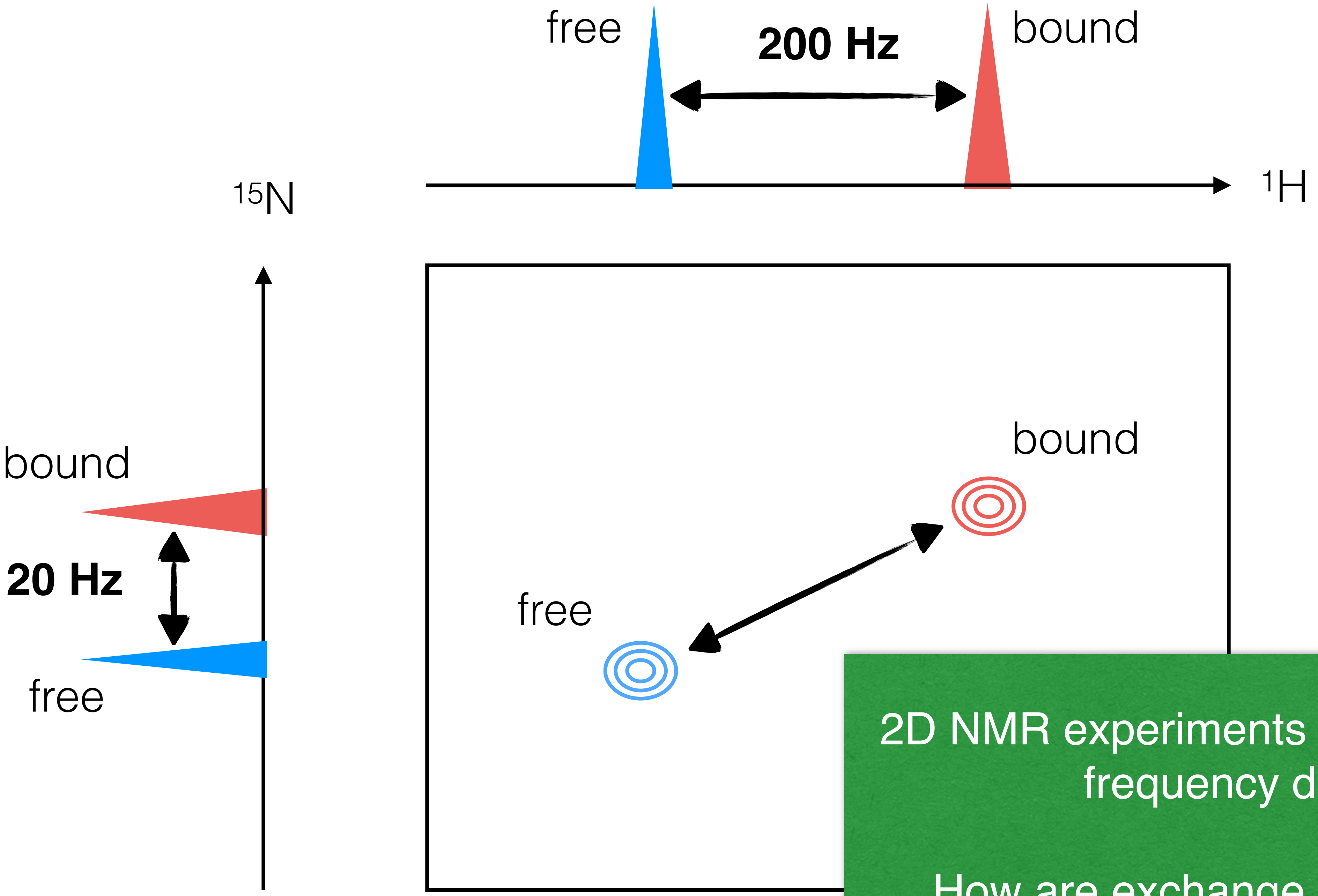
conversely – 2D experiments can be much more sensitive probes of exchange

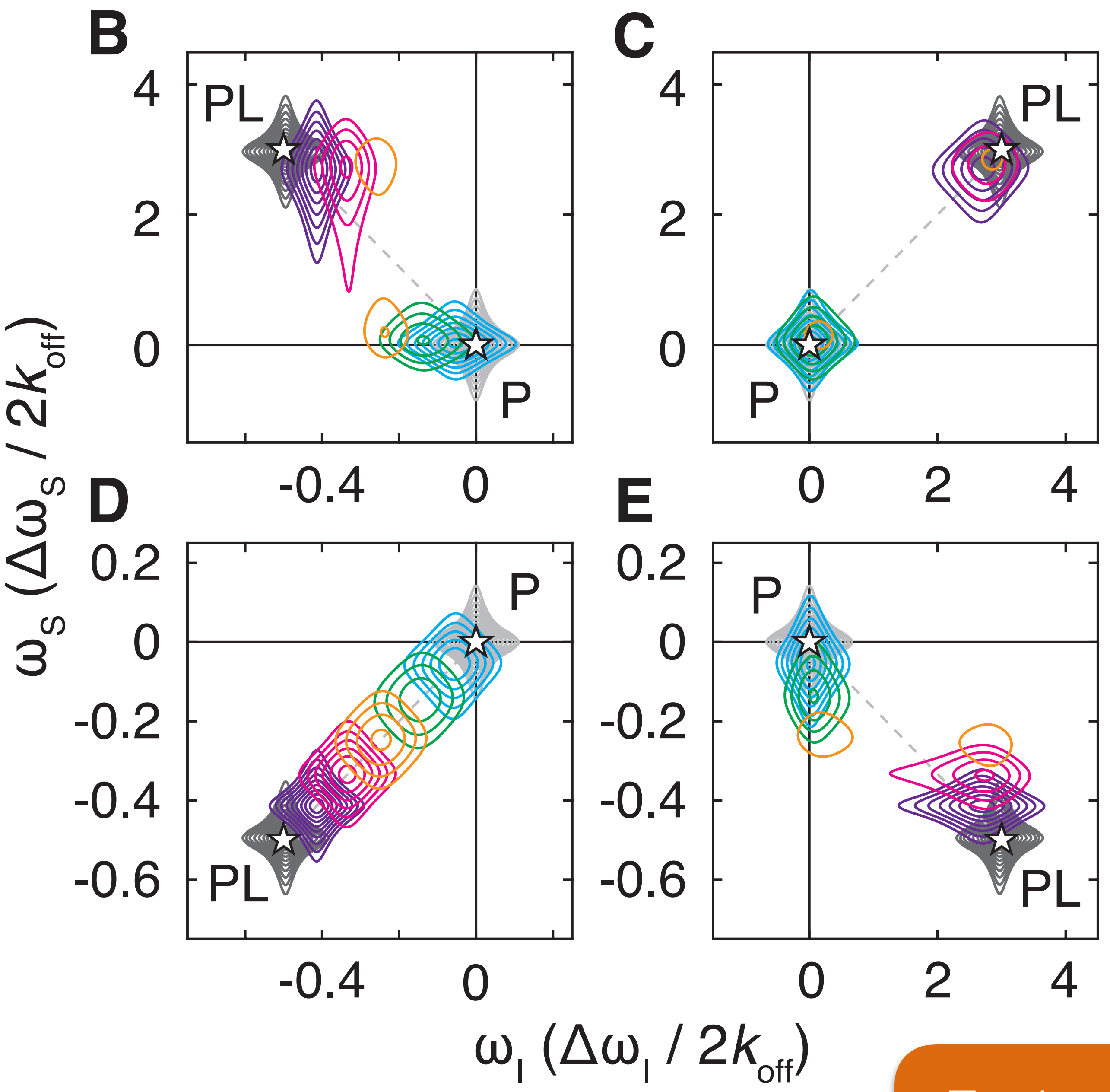
Chemical exchange regimes in 2D experiments



2D NMR experiments involve two different frequency differences

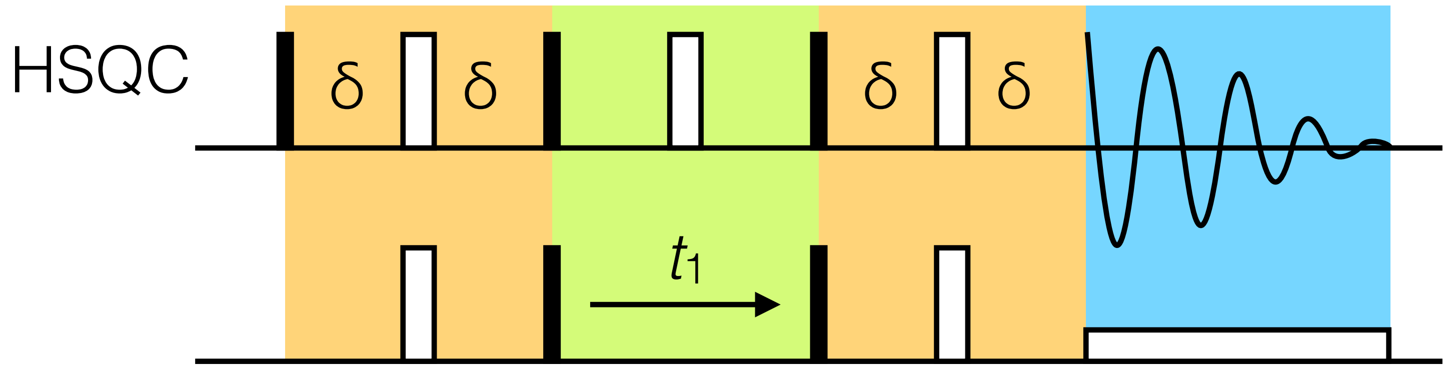
How are exchange regimes defined?

Chemical exchange regimes in HSQC experiments



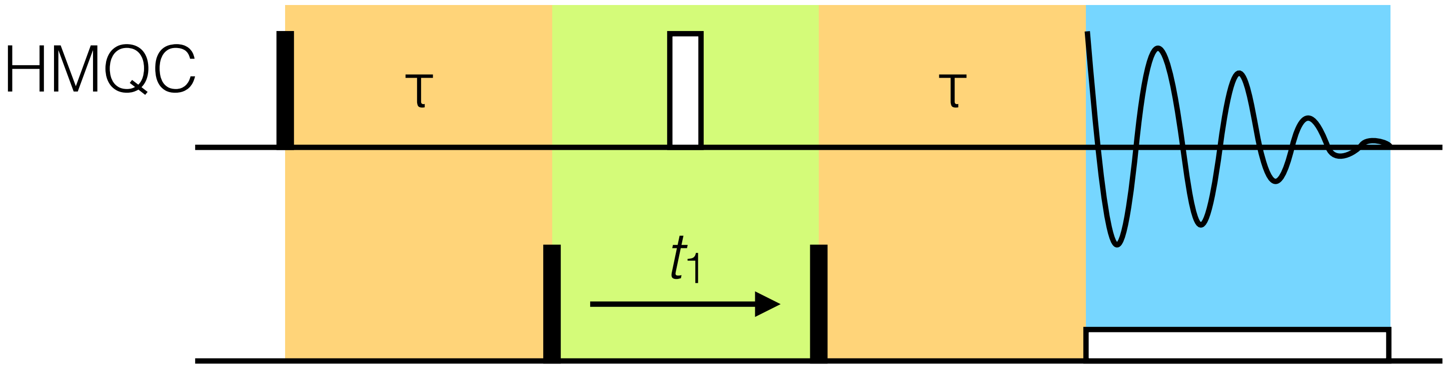
Exchange can be fast or slow with respect to both direct and indirect chemical shift differences

Different pulse programs have different exchange effects



Magnetisation is SQ during t_1

=> chemical exchange effects depend on $\Delta\omega^{SQ}$ vs k_{ex}

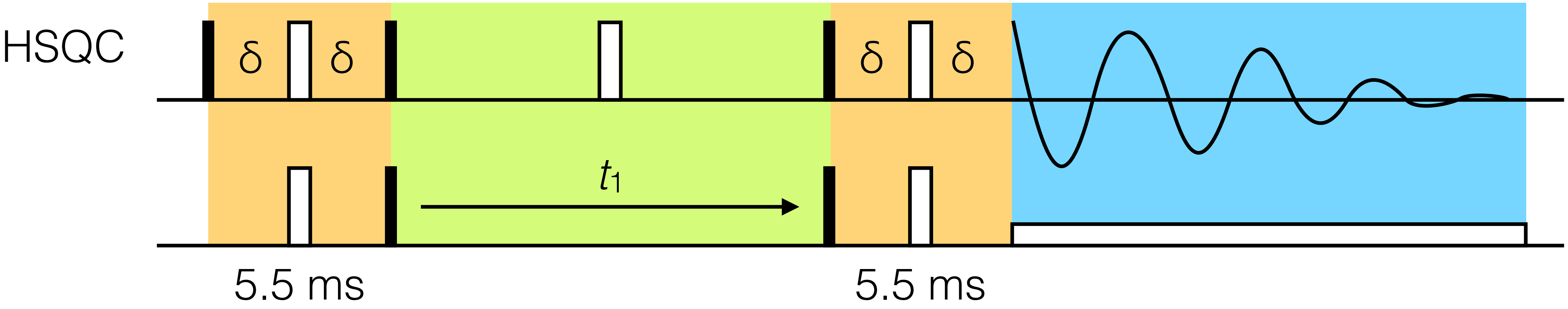


Magnetisation is a mixture of ZQ and DQ coherences during t_1

=> chemical exchange effects depend on *both* $\Delta\omega^{ZQ}$ and $\Delta\omega^{DQ}$ vs k_{ex}

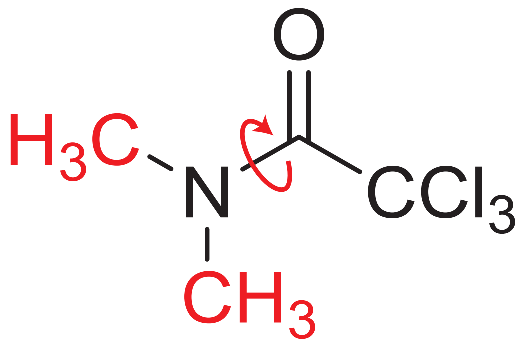
In general, HMQC is more sensitive to chemical exchange than HSQC

Unexpected exchange cross-peaks in 2D experiments

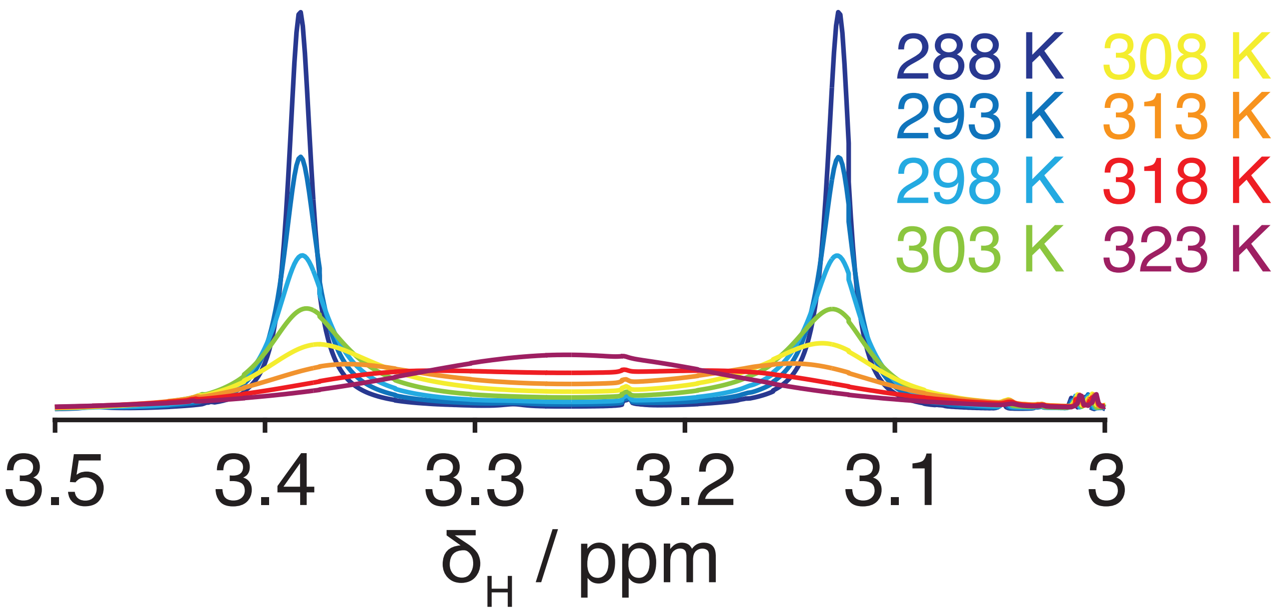


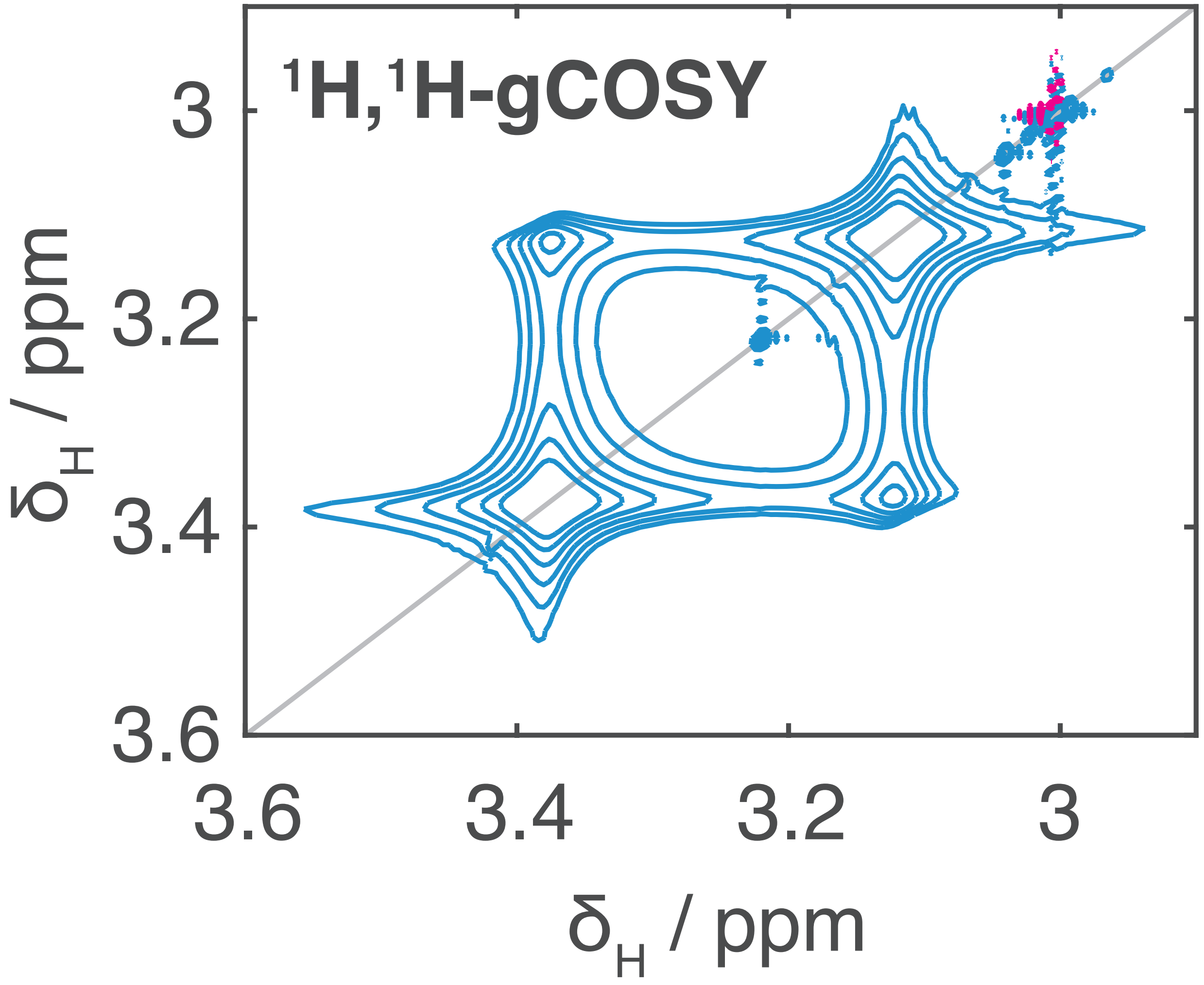
Chemical exchange during successive evolution periods or during coherence transfer periods can give rise to unexpected cross-peaks in 2D experiments

Unexpected exchange cross-peaks in 2D experiments

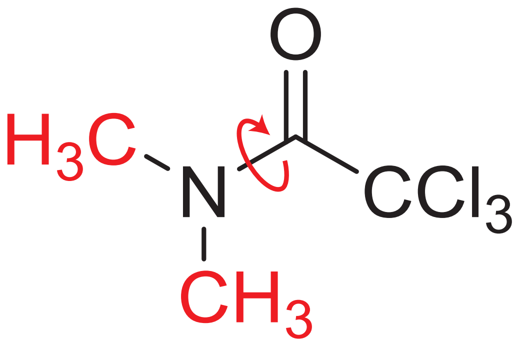


$\Delta\delta_H = 0.26$ ppm
$\Delta\delta_C = 0.62$ ppm
${}^1J_{CH} = 140$ Hz
$k_{ex} = 125\ s^{-1}$
(298 K)





Unexpected exchange cross-peaks in 2D experiments



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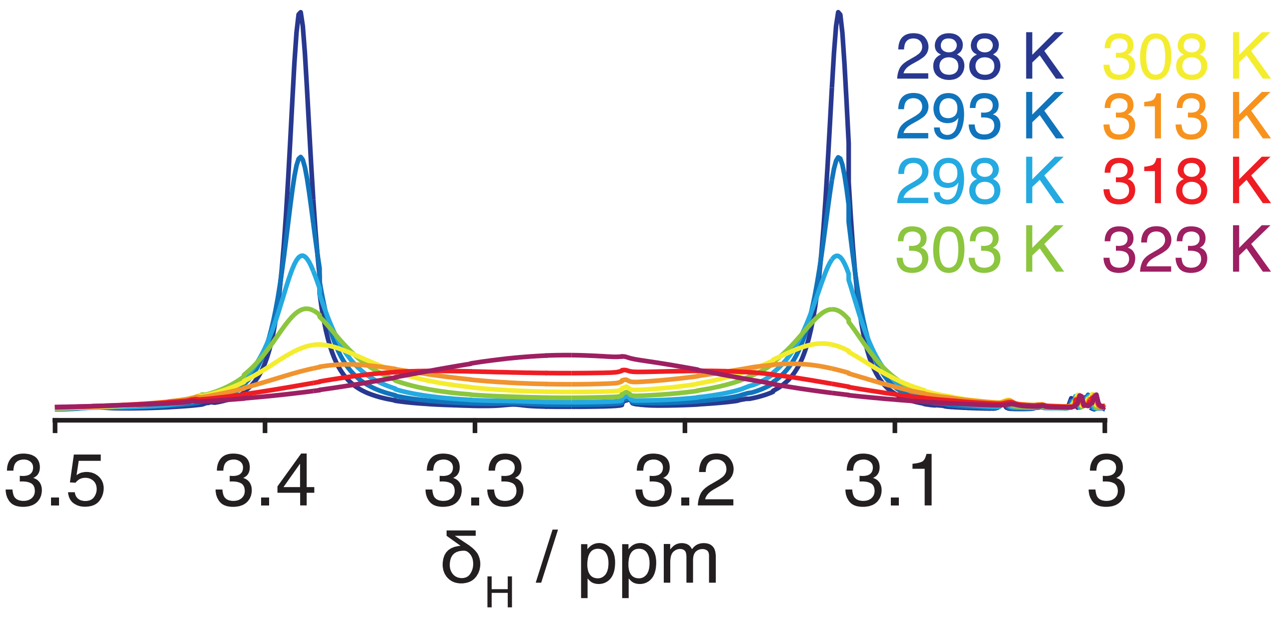
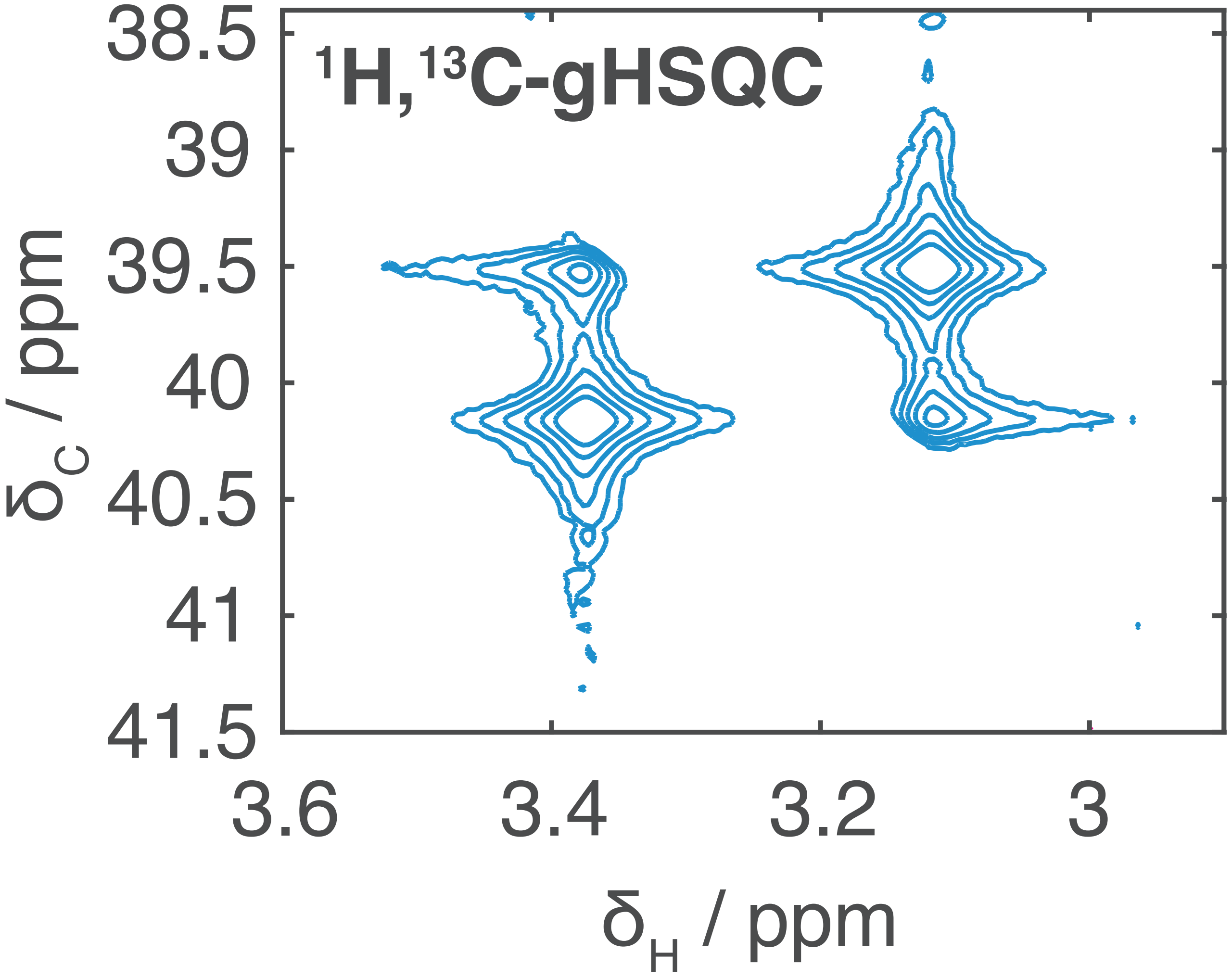
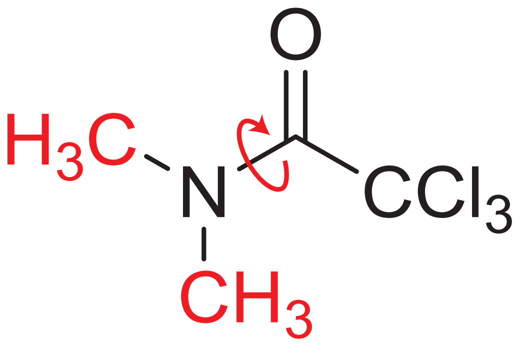




Unexpected exchange cross-peaks in 2D experiments



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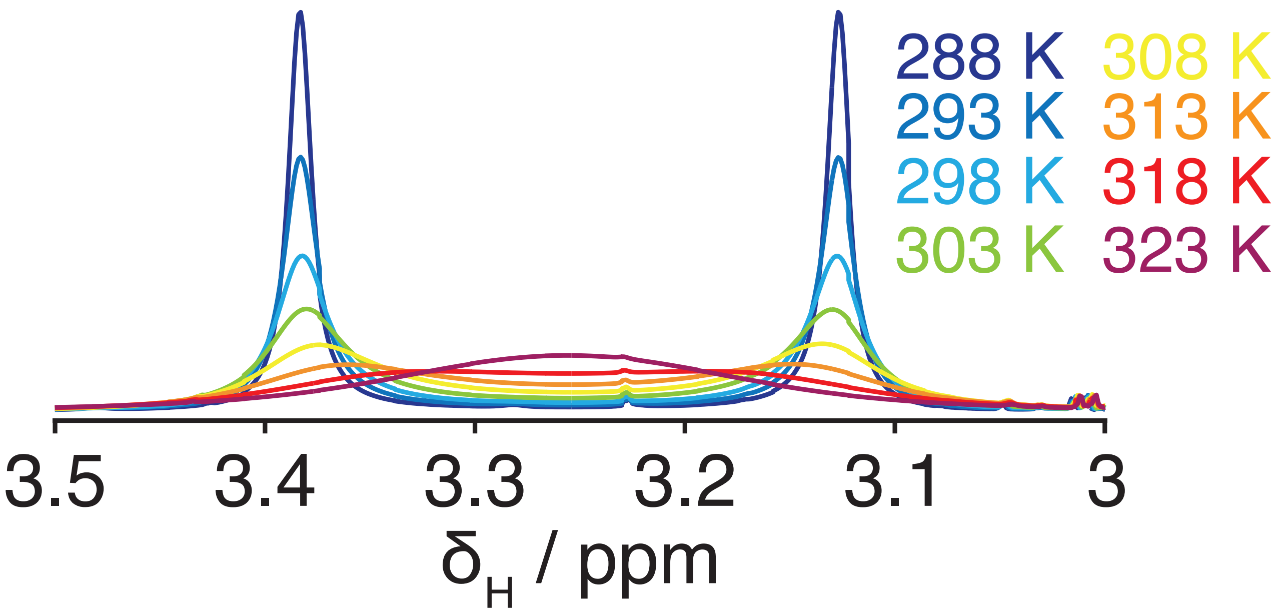
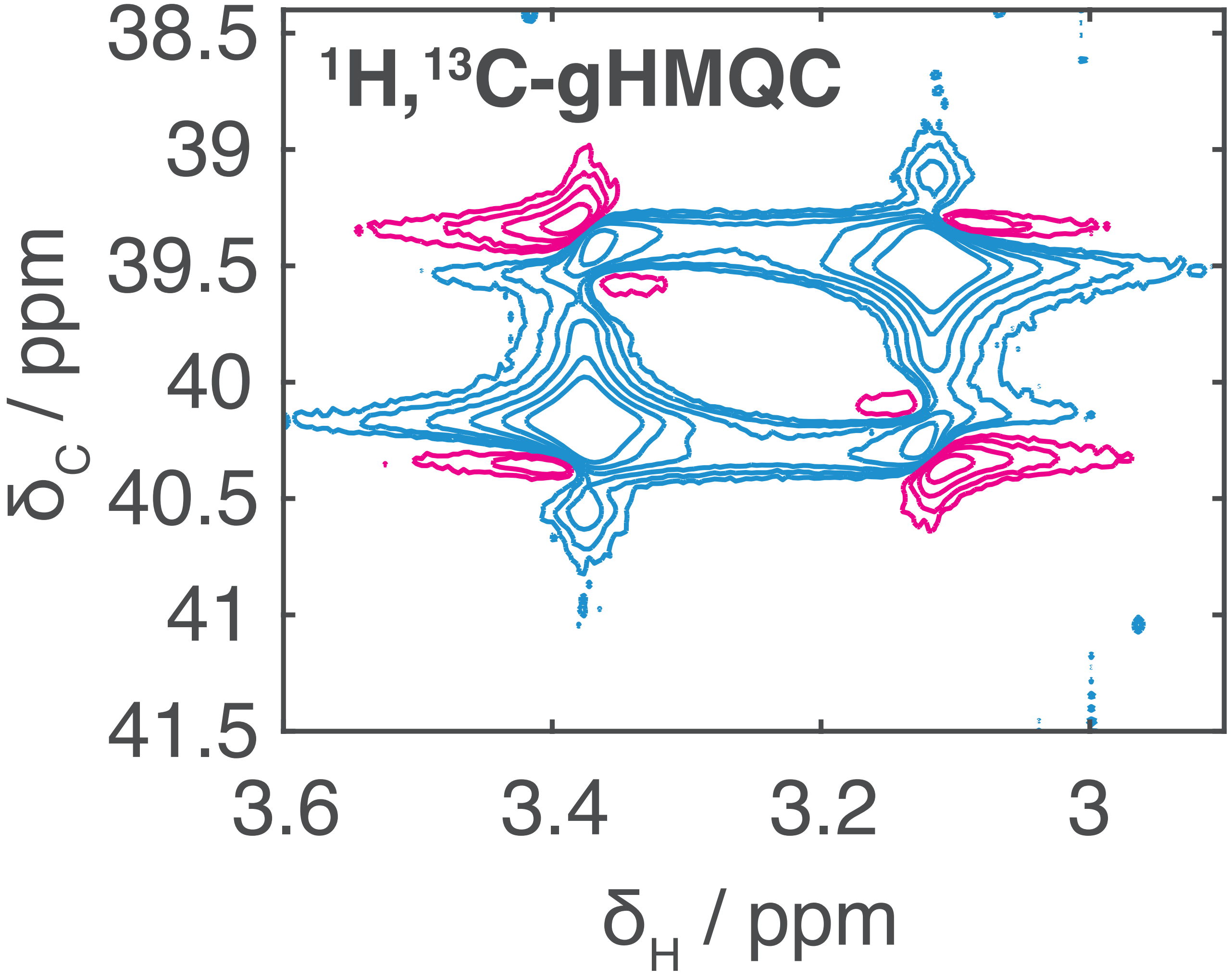
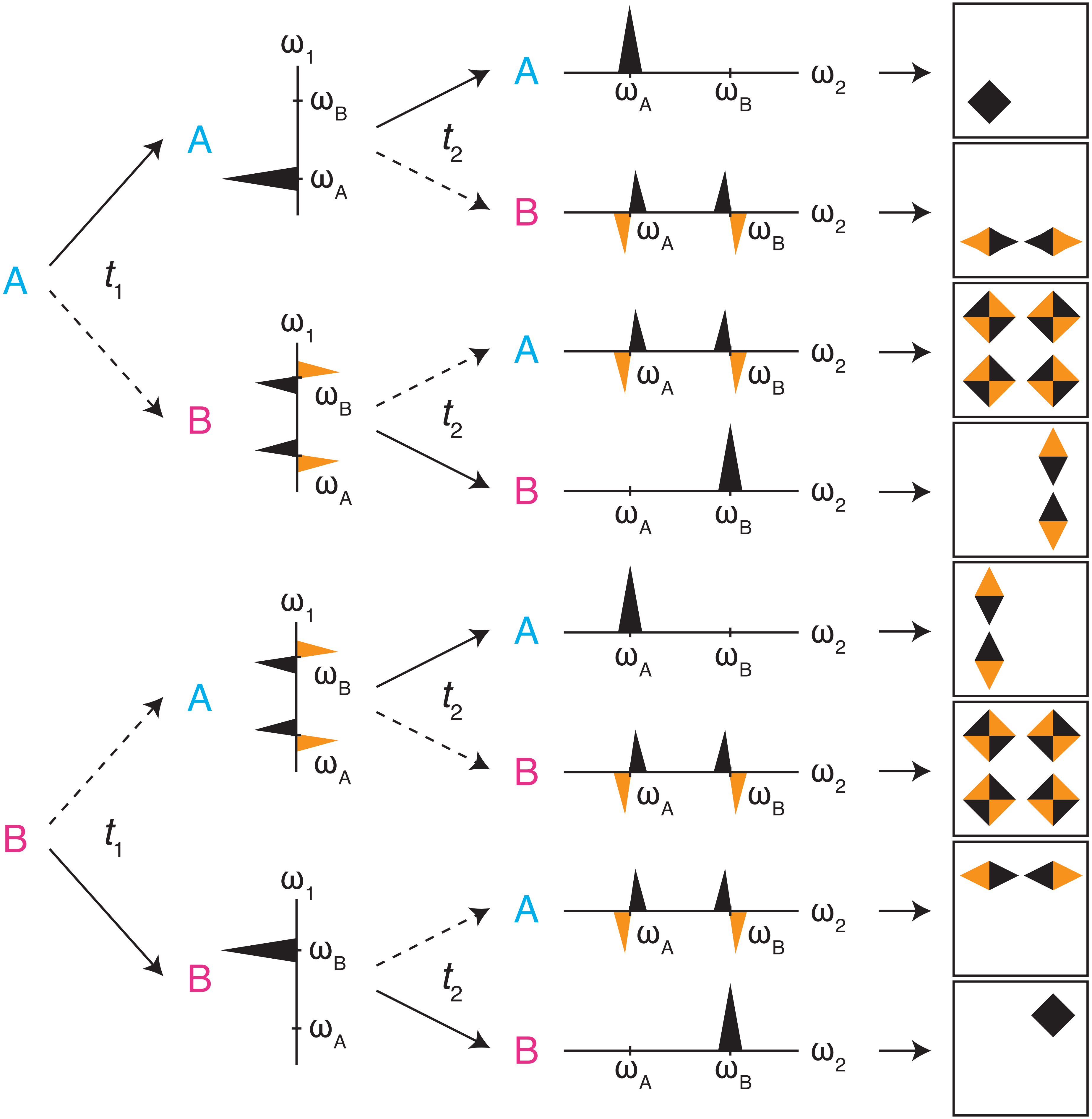
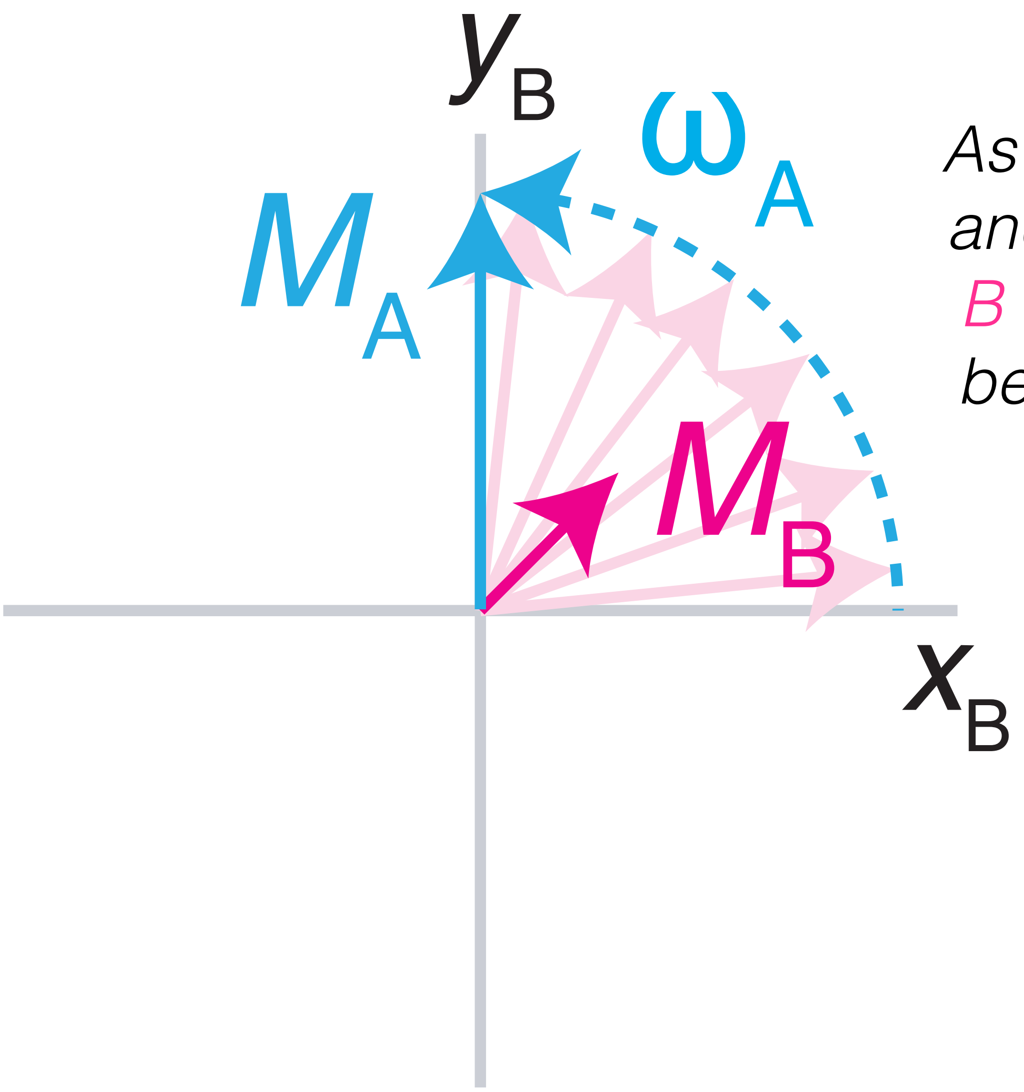






A
t_1
B
A
B
A
B
ω_1
ω_B
ω_A
t_2
A
B
A
B
A
B
A
B
ω_A
ω_B
ω_2

Origin of exchange-induced crosspeaks

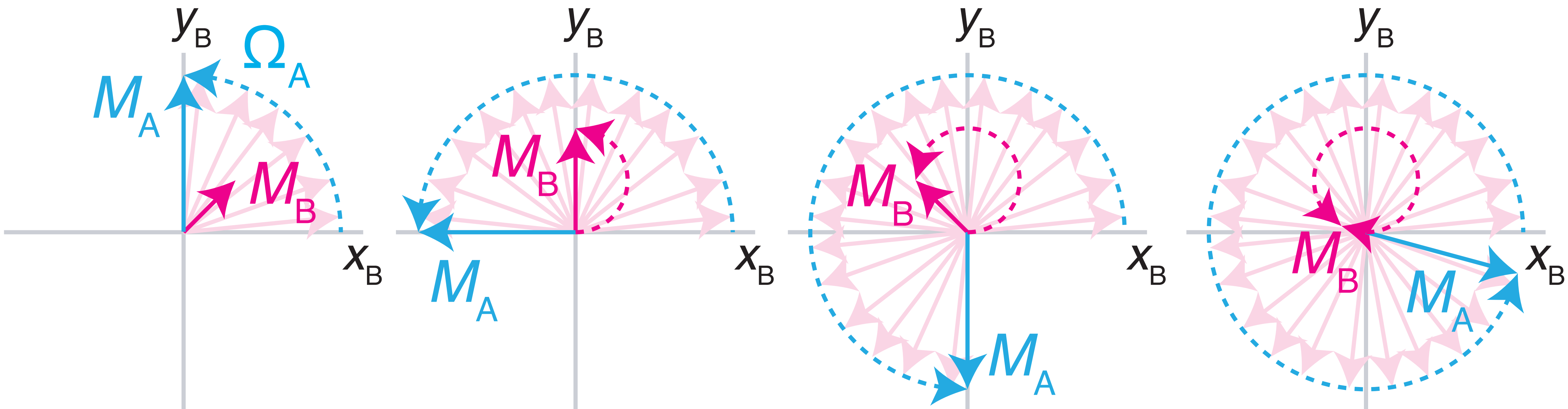


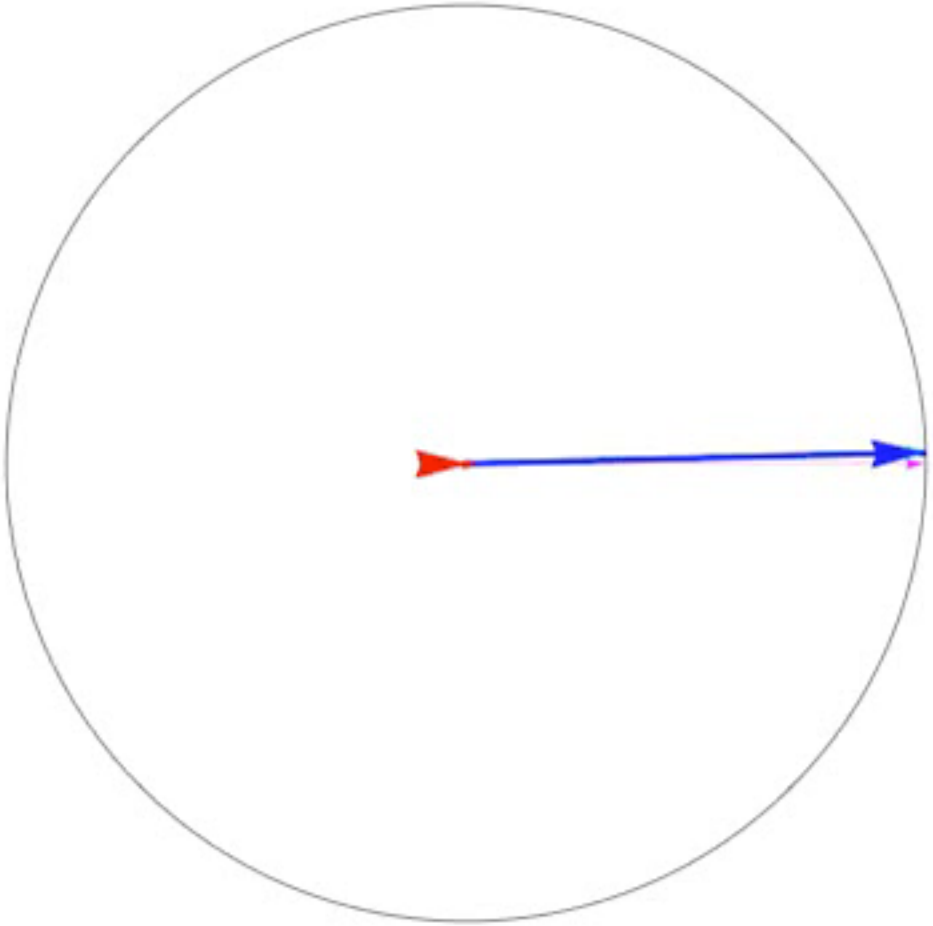
As A chemically reacts and exchanges into B, B spins are 'dropped' behind the evolving A magnetisation

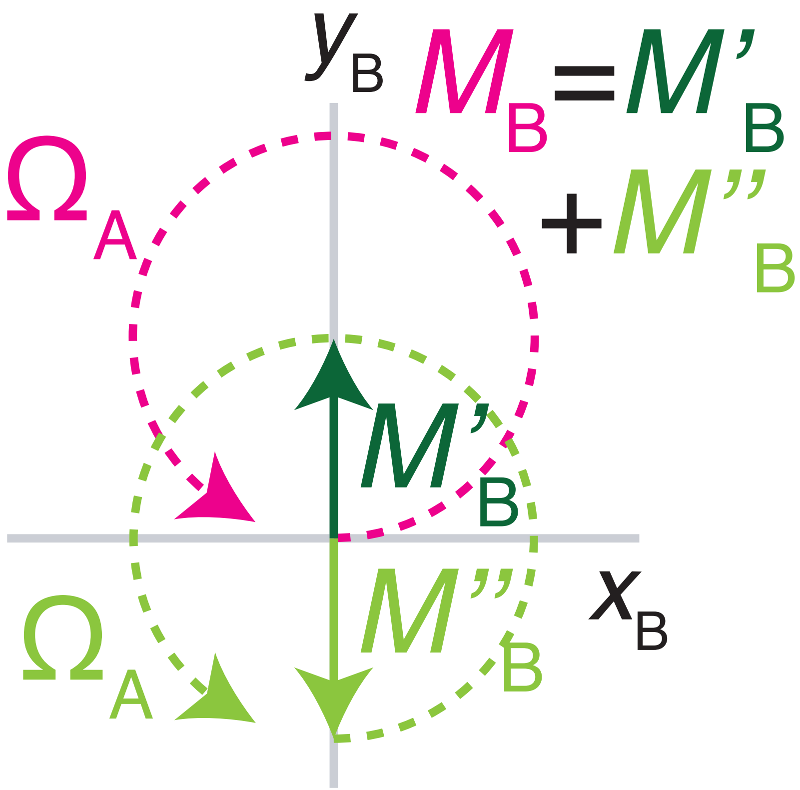
Diagram shown in rotating frame of spin B

Chris Waudby, NMR Theory Club, 10 Dec 2025

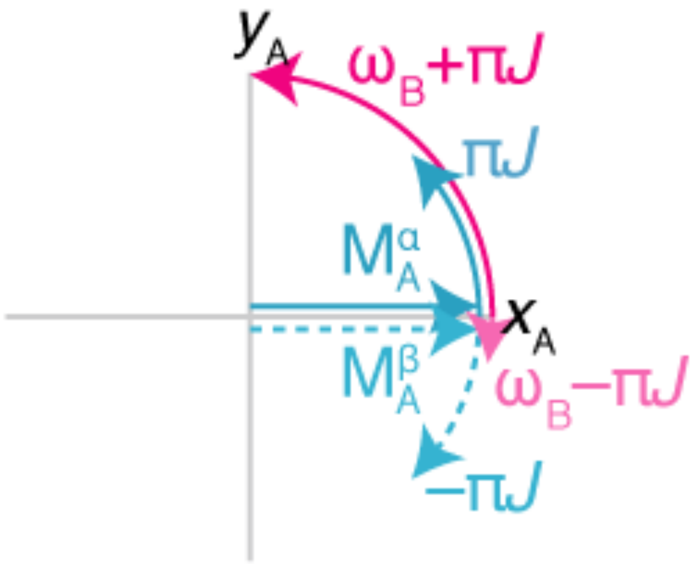
Origin of exchange-induced crosspeaks

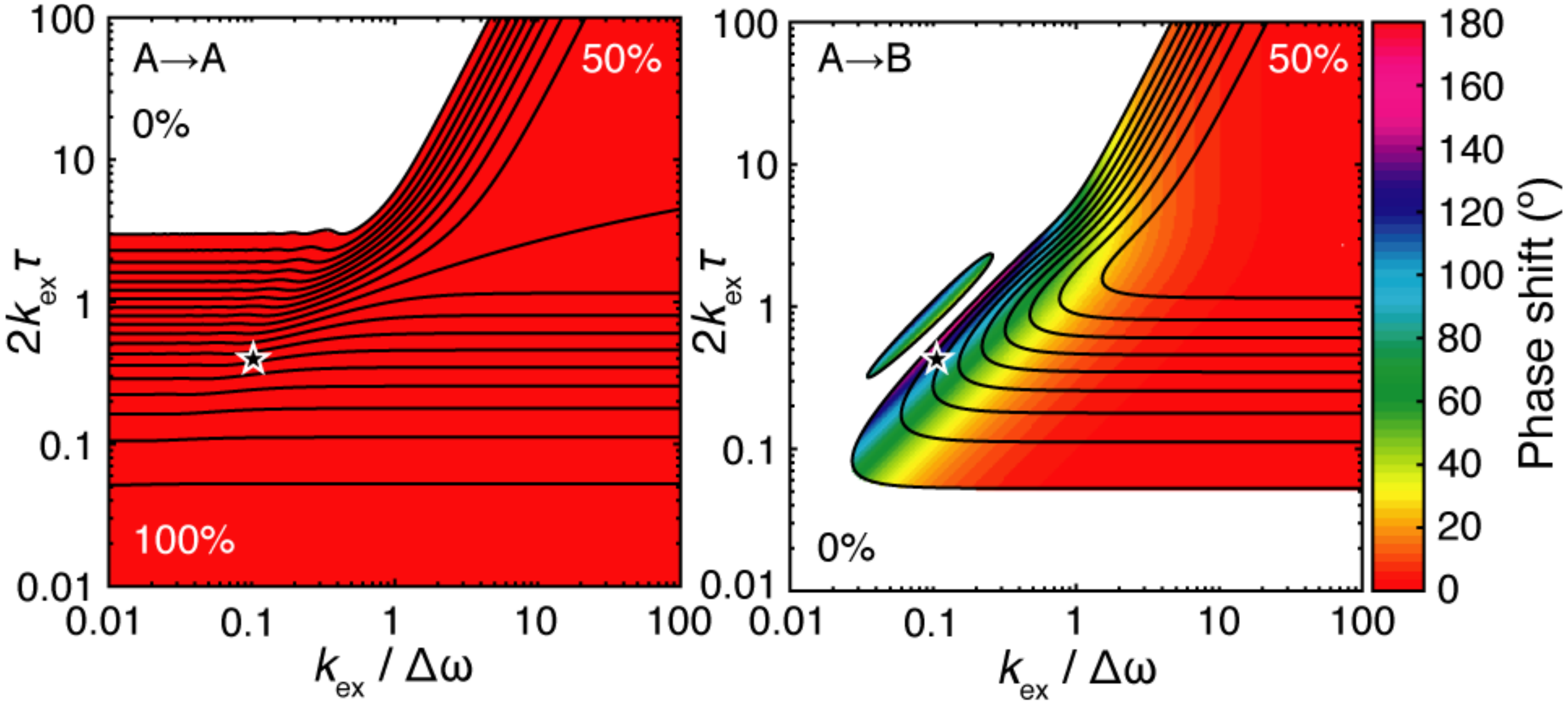




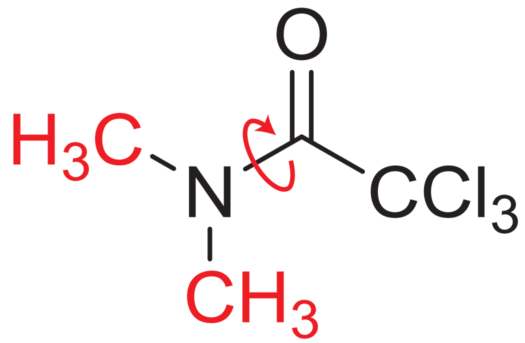


Exchange during INEPT coherence transfer periods





Unexpected exchange cross-peaks in 2D experiments



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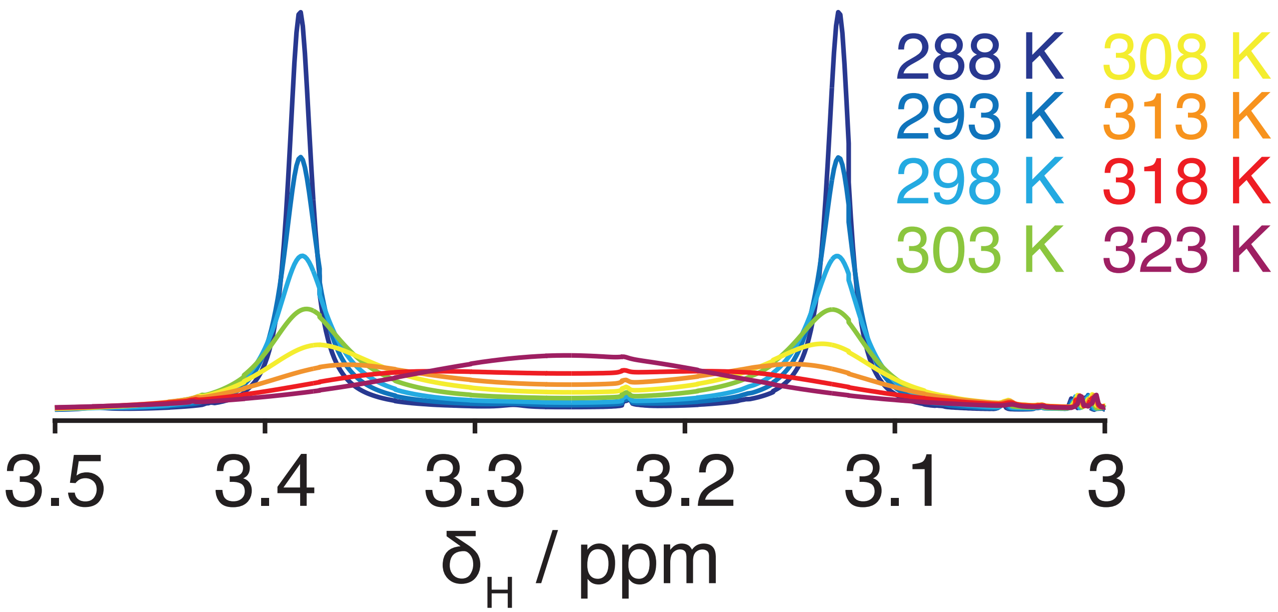
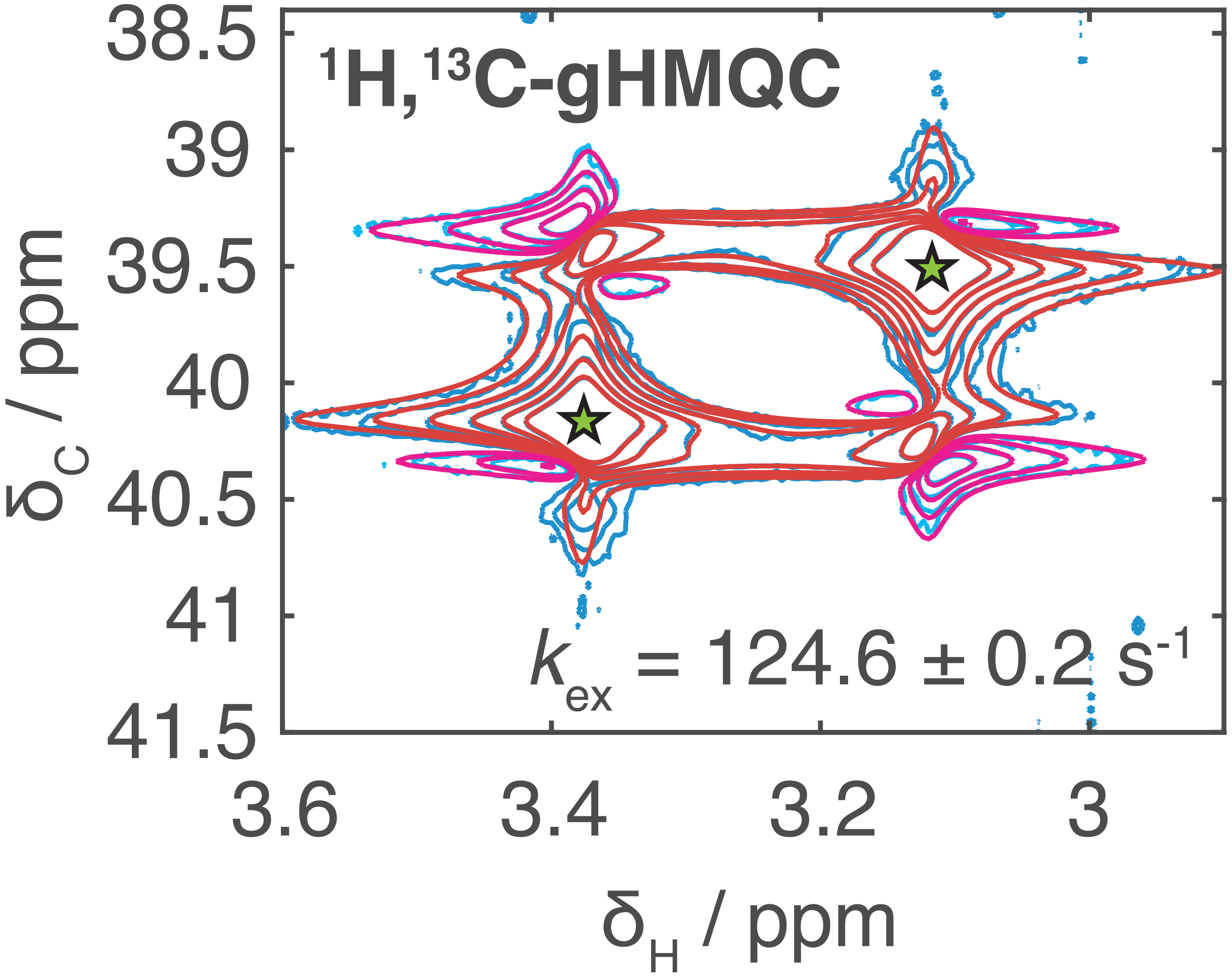
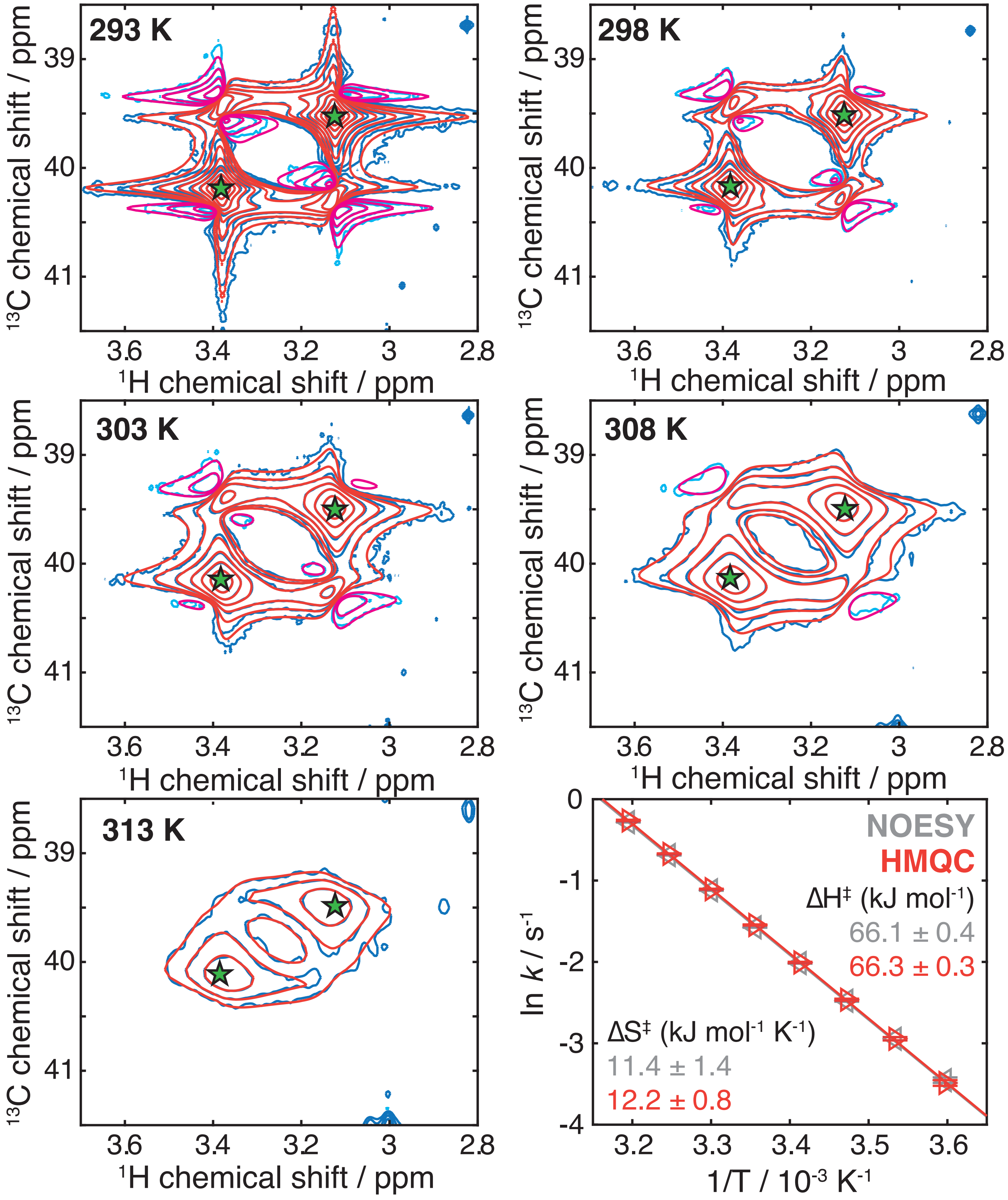
$k_{ex} = 125\ s^{-1}$
(298 K)



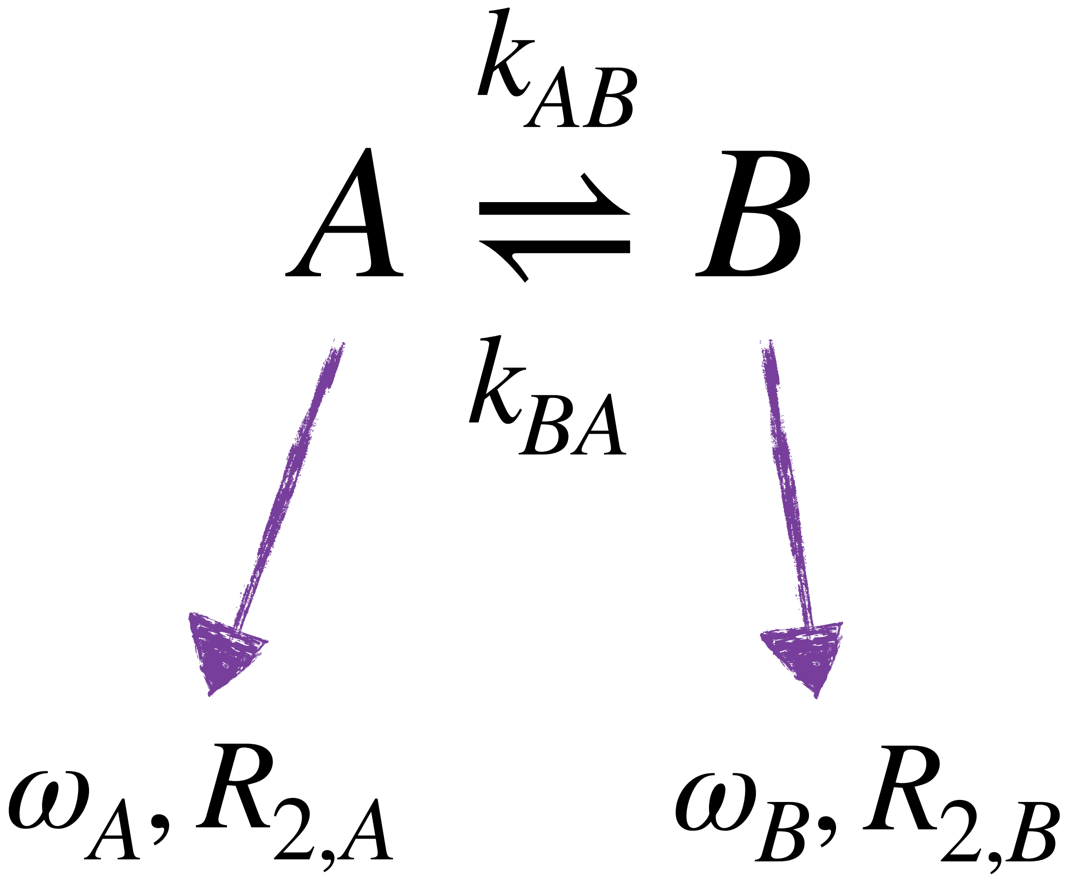


$k_{ex} = 124.6 \pm 0.2\ s^{-1}$

Unexpected exchange cross-peaks in 2D experiments



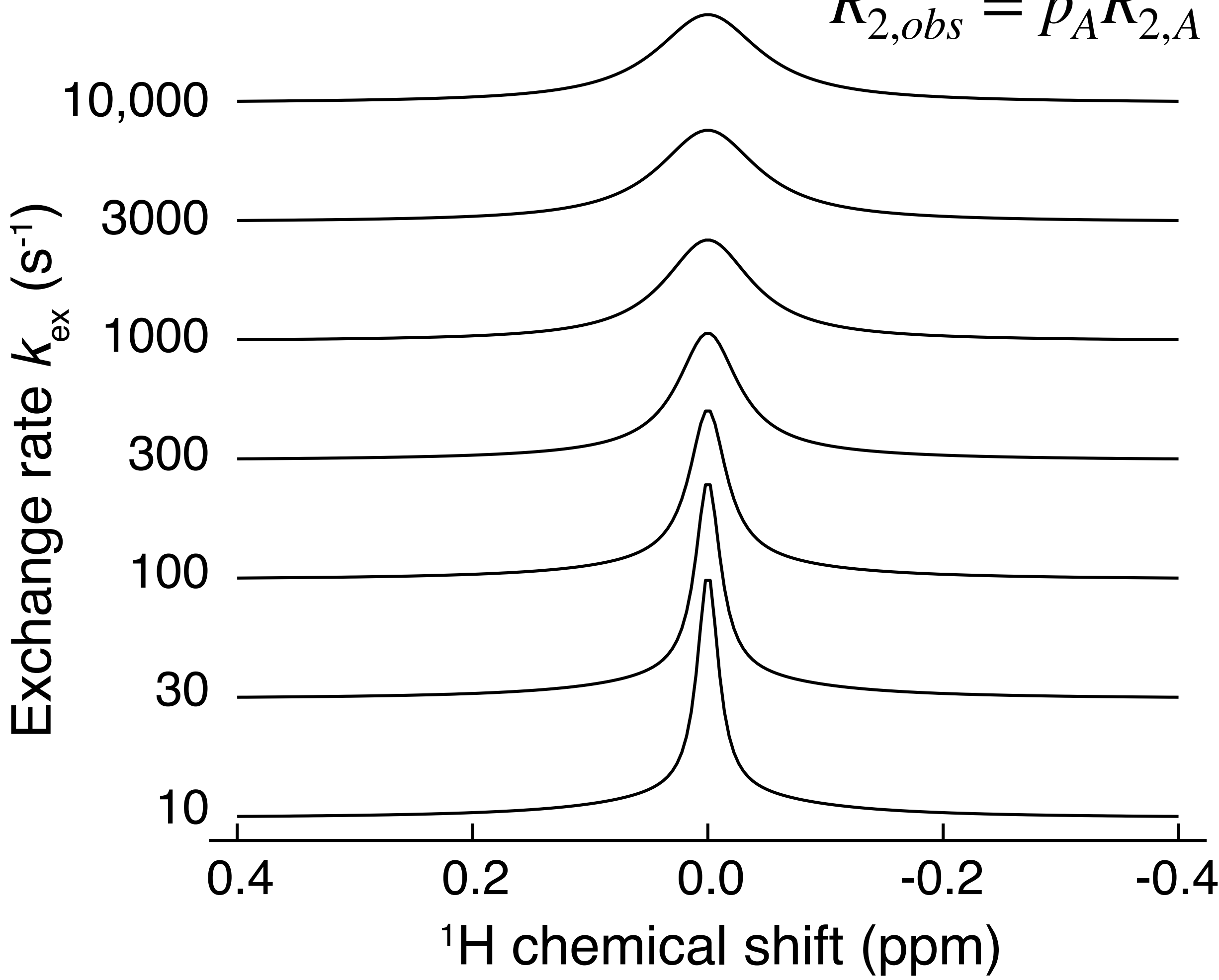
Exchange beyond the chemical shift: relaxation



$$A \underset{k_{BA}}{\overset{k_{AB}}{\rightleftharpoons}} B$$

$$\omega_A, R_{2,A} \qquad \omega_B, R_{2,B}$$

$$R_{2,obs} = p_A R_{2,A} + p_B R_{2,B}$$

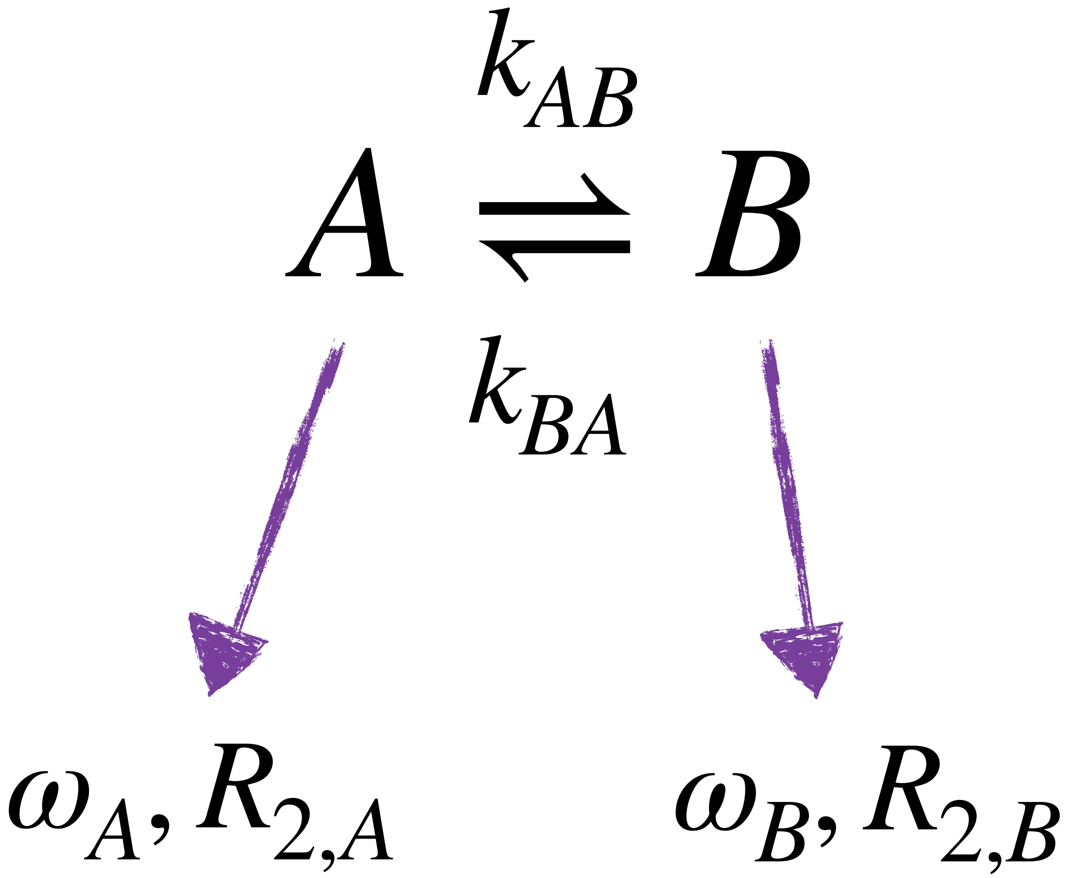


Chemical exchange effects can also arise between states that differ only in linewidth (R_2)

The observed spectrum will depend on the exchange rate relative to

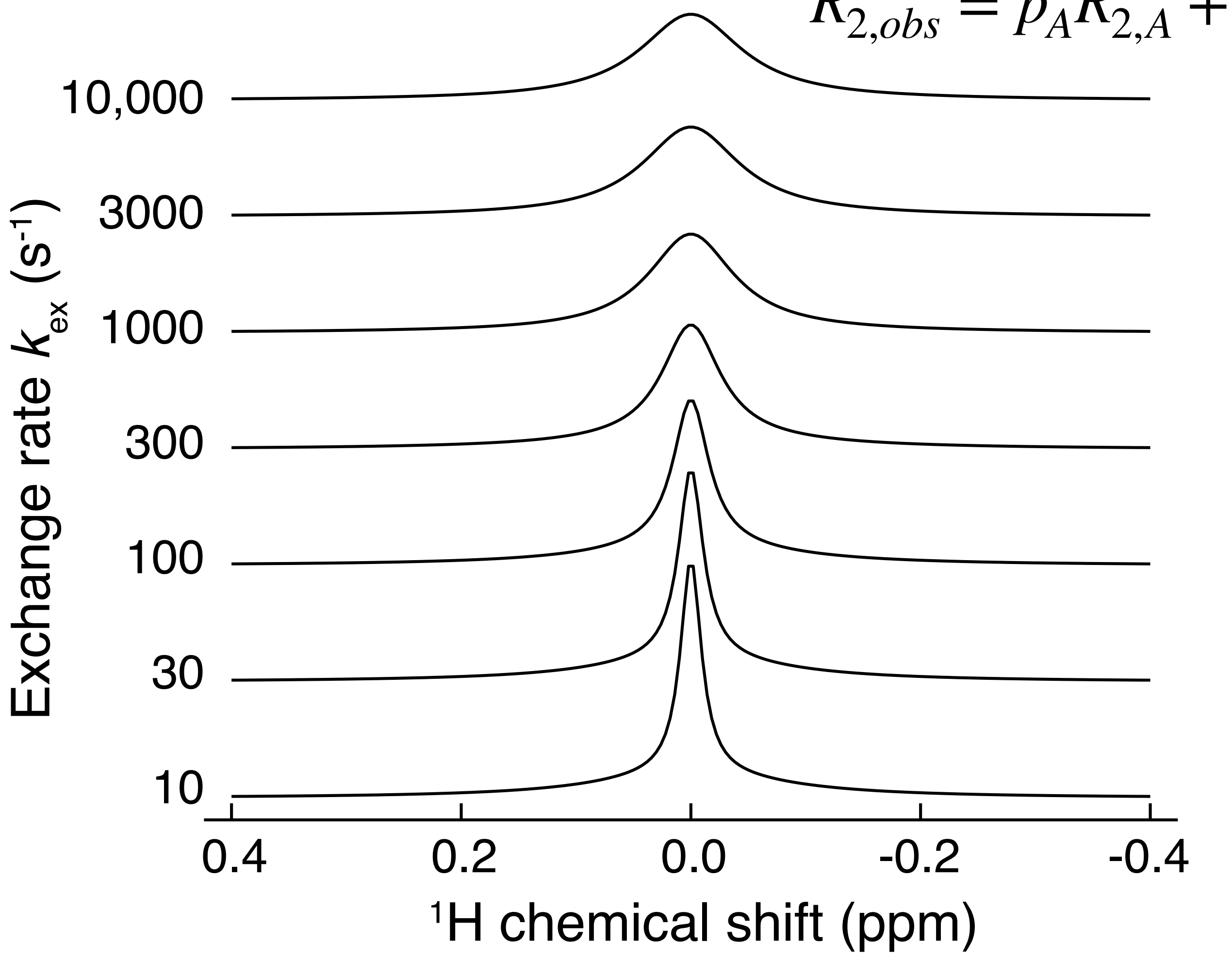
$$\Delta R_2 = \left| R_{2,A} - R_{2,B} \right|$$

Exchange beyond the chemical shift: relaxation



$$\begin{tikzcd} A \arrow[r, shift left, "k_{AB}"] \arrow[d] & B \arrow[l, shift left, "k_{BA}"] \arrow[d] \\ \omega_A, R_{2,A} & \omega_B, R_{2,B} \end{tikzcd}$$

$$R_{2,obs} = p_A R_{2,A} + p_B R_{2,B}$$

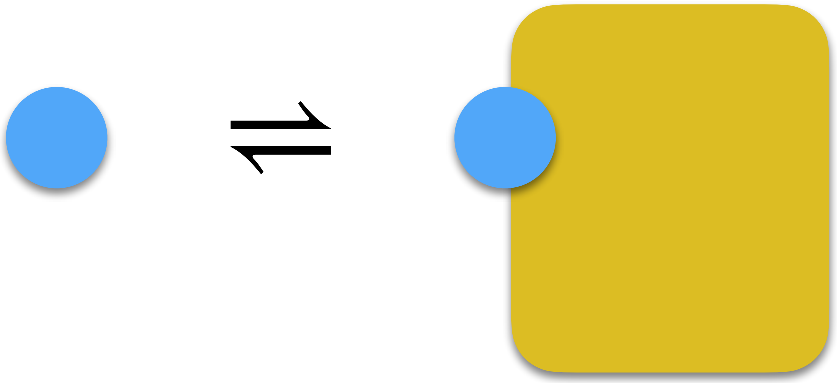


More generally, if both the frequency and linewidth change, the relevant quantity is:

$$\left| i\Delta\omega + \Delta R_2 \right| = \sqrt{\Delta\omega^2 + \Delta R_2^2}$$

Exchange beyond the chemical shift: relaxation

Transferred relaxation through ligand binding:

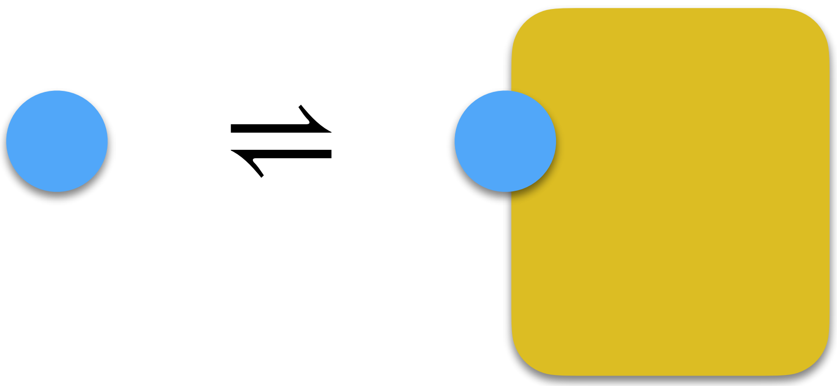


$$R_{2,obs} = p_A R_{2,A} + p_B R_{2,B}$$

If relaxation in the bound state is rapid, even a small bound population can have a large effect on the appearance of the free ligand

Exchange beyond the chemical shift: relaxation

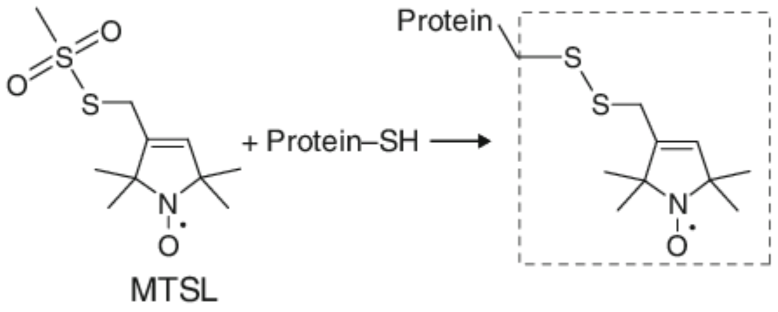
Transferred relaxation through ligand binding:

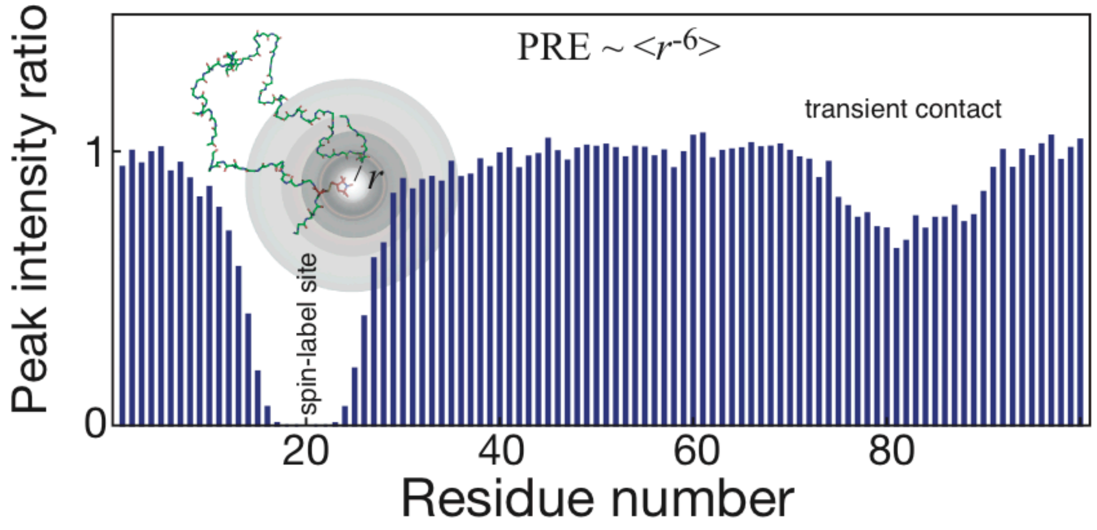


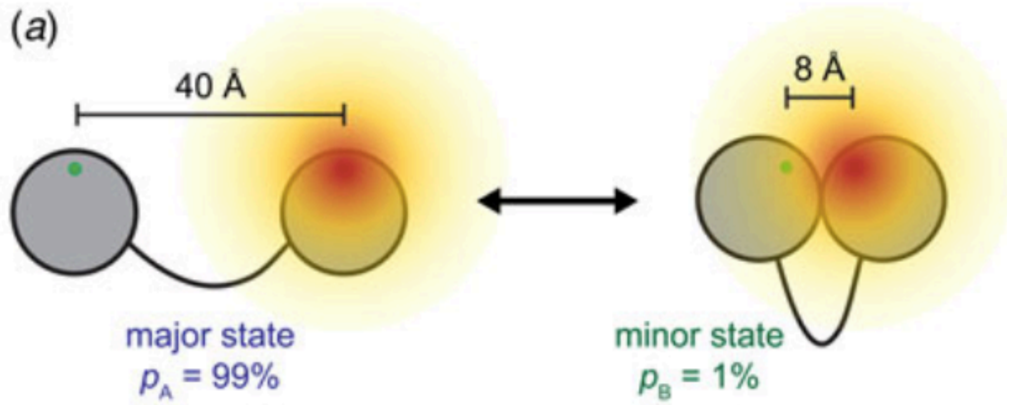
$$R_{2,obs} = p_A R_{2,A} + p_B R_{2,B}$$

If relaxation in the bound state is rapid, even a small bound population can have a large effect on the appearance of the free ligand

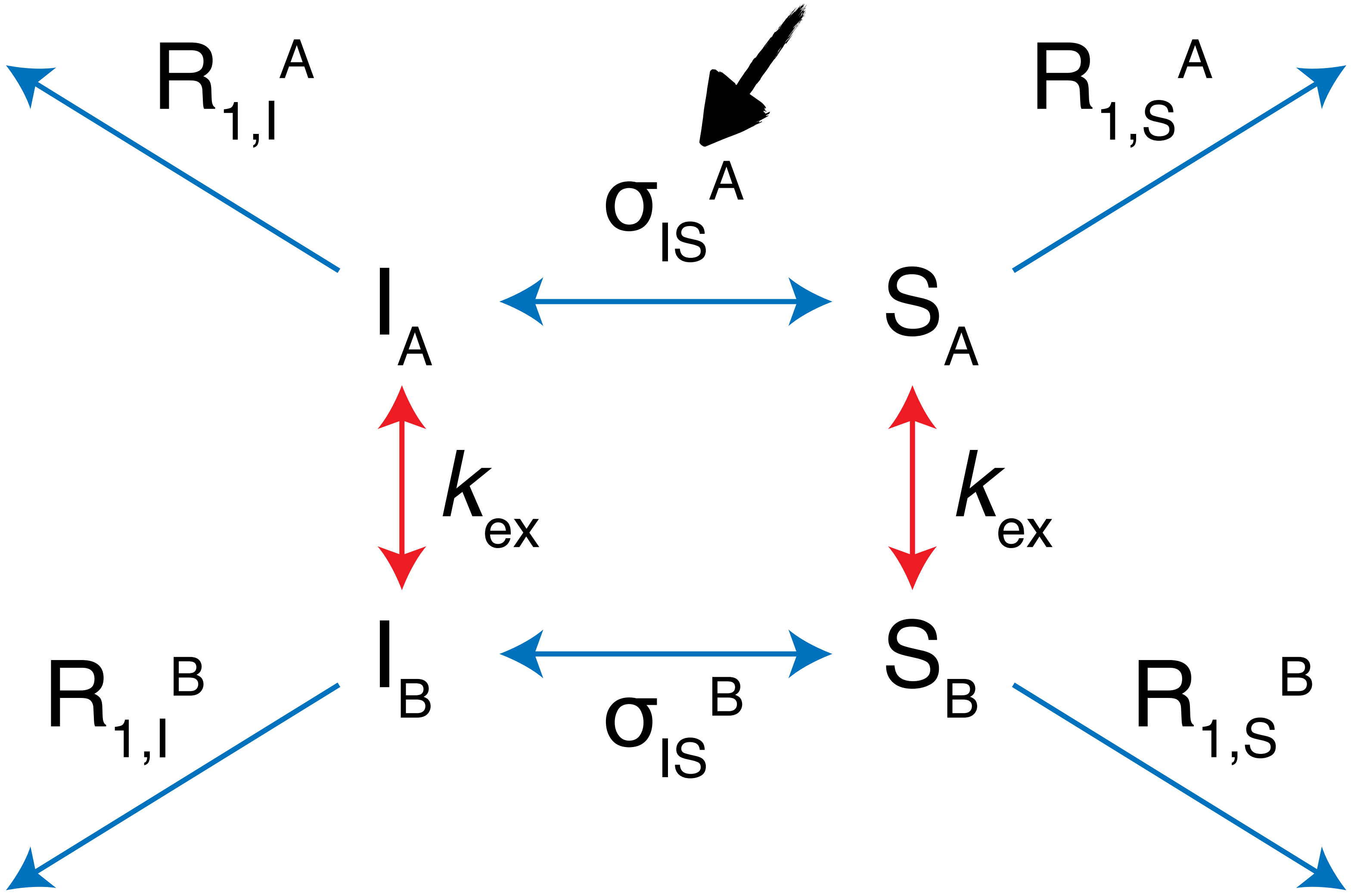
Paramagnetic relaxation enhancements (PREs):







Exchange beyond the chemical shift: cross-relaxation



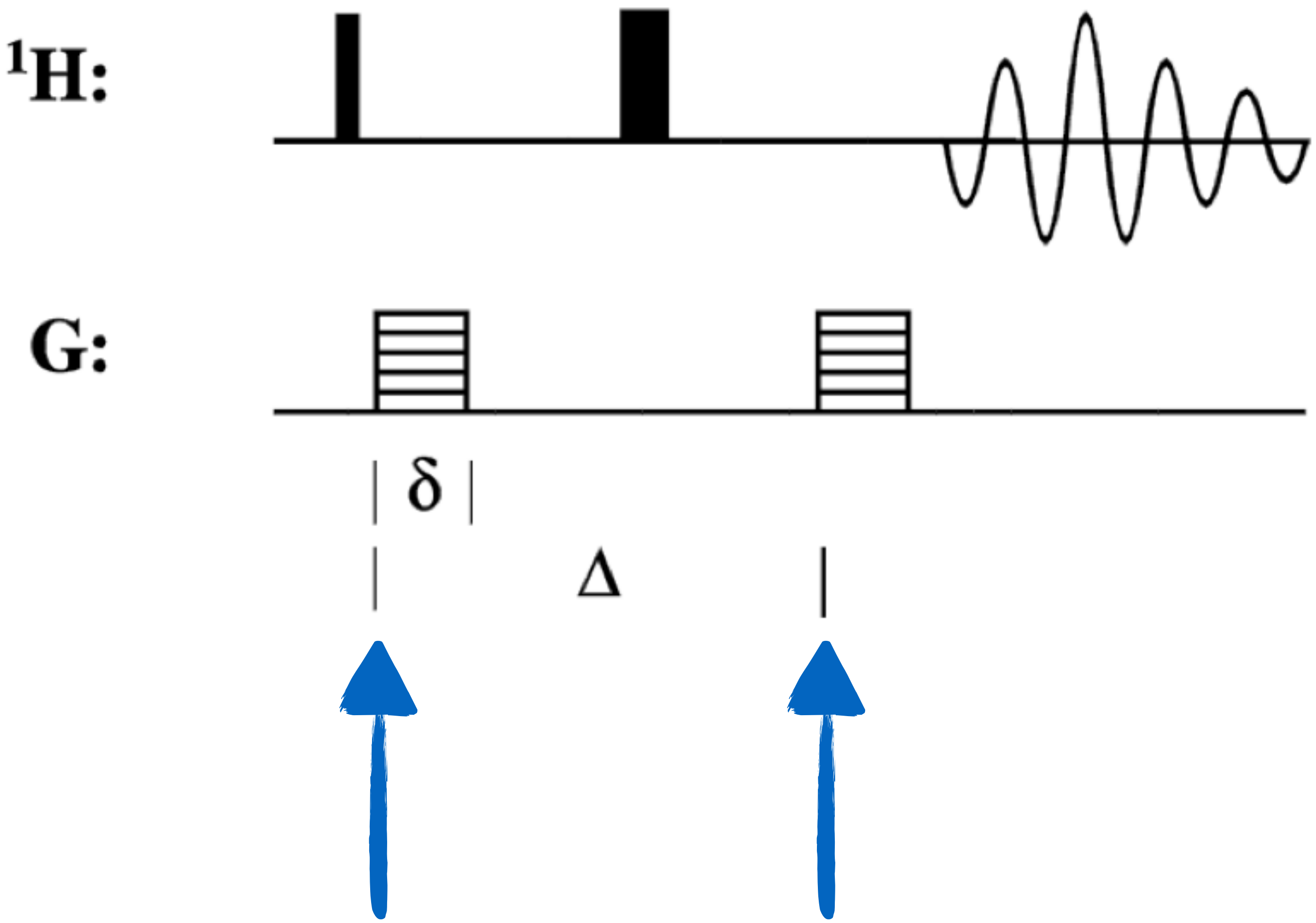
cross-relaxation rate (NOE) ~ r_{IS}^{-6}

In fast exchange ($\Delta\sigma << k_{ex}$), a population-weighted average cross-relaxation rate is observed:

$$\sigma_{obs} = p_A \sigma_A + p_B \sigma_B$$

Exchange beyond the chemical shift: diffusion

Pulsed gradient spin echo experiment

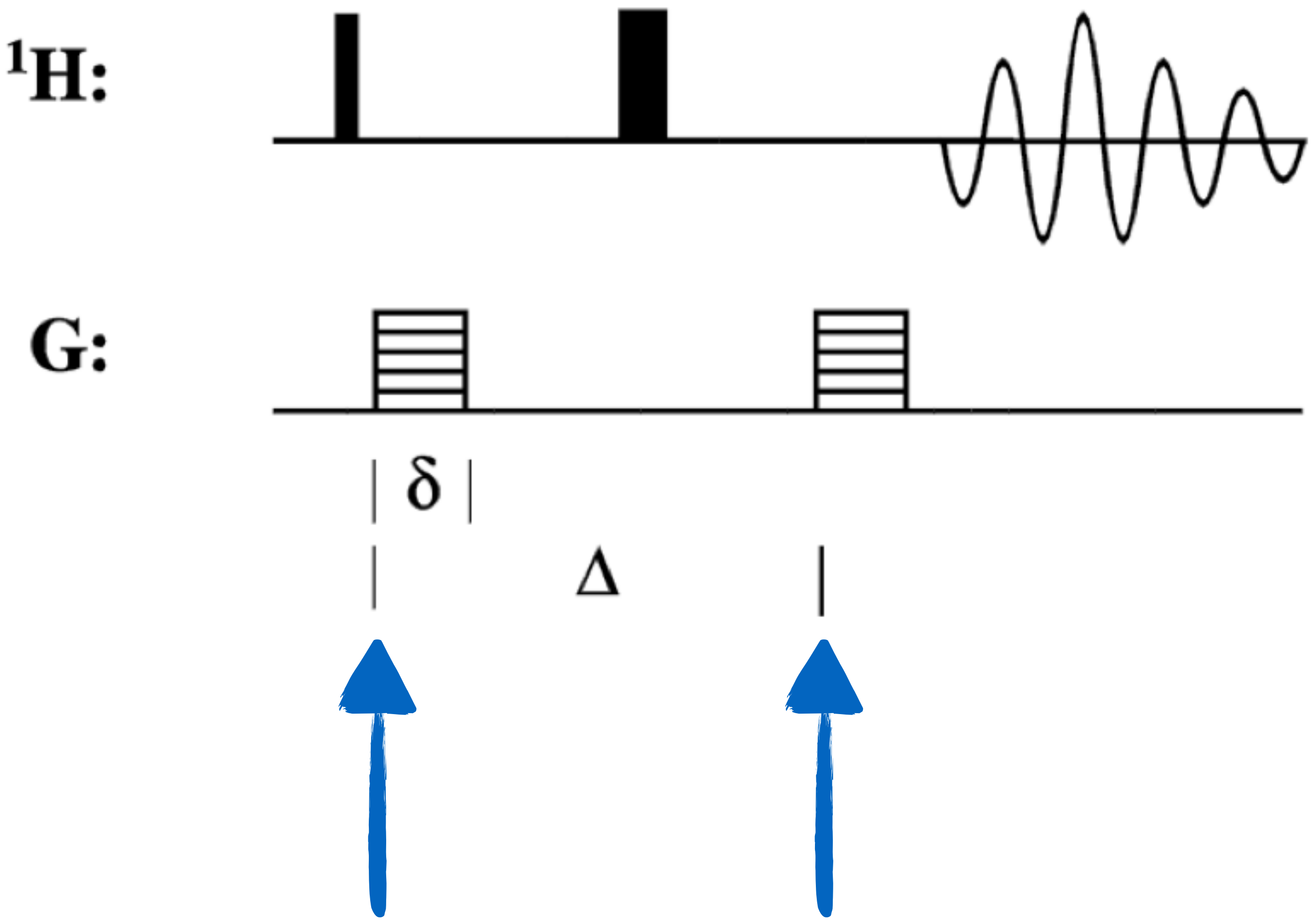


Pairs of gradient pulses encode and decode the position of spins along the *z* axis

Diffusion during the intervening period, Δ, leads to a loss of signal that can be analysed to measure the diffusion coefficient

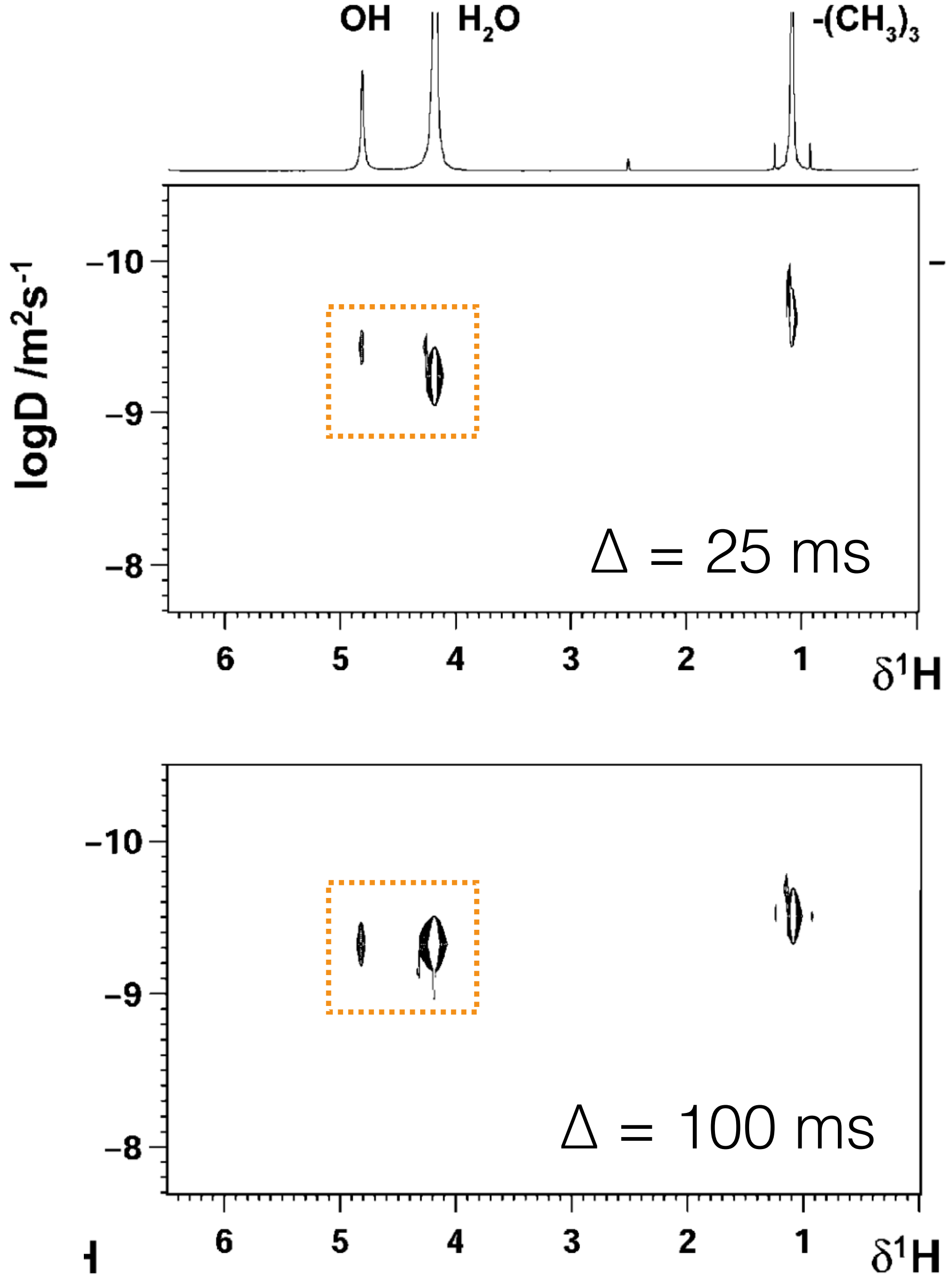
Exchange beyond the chemical shift: diffusion

Pulsed gradient spin echo experiment



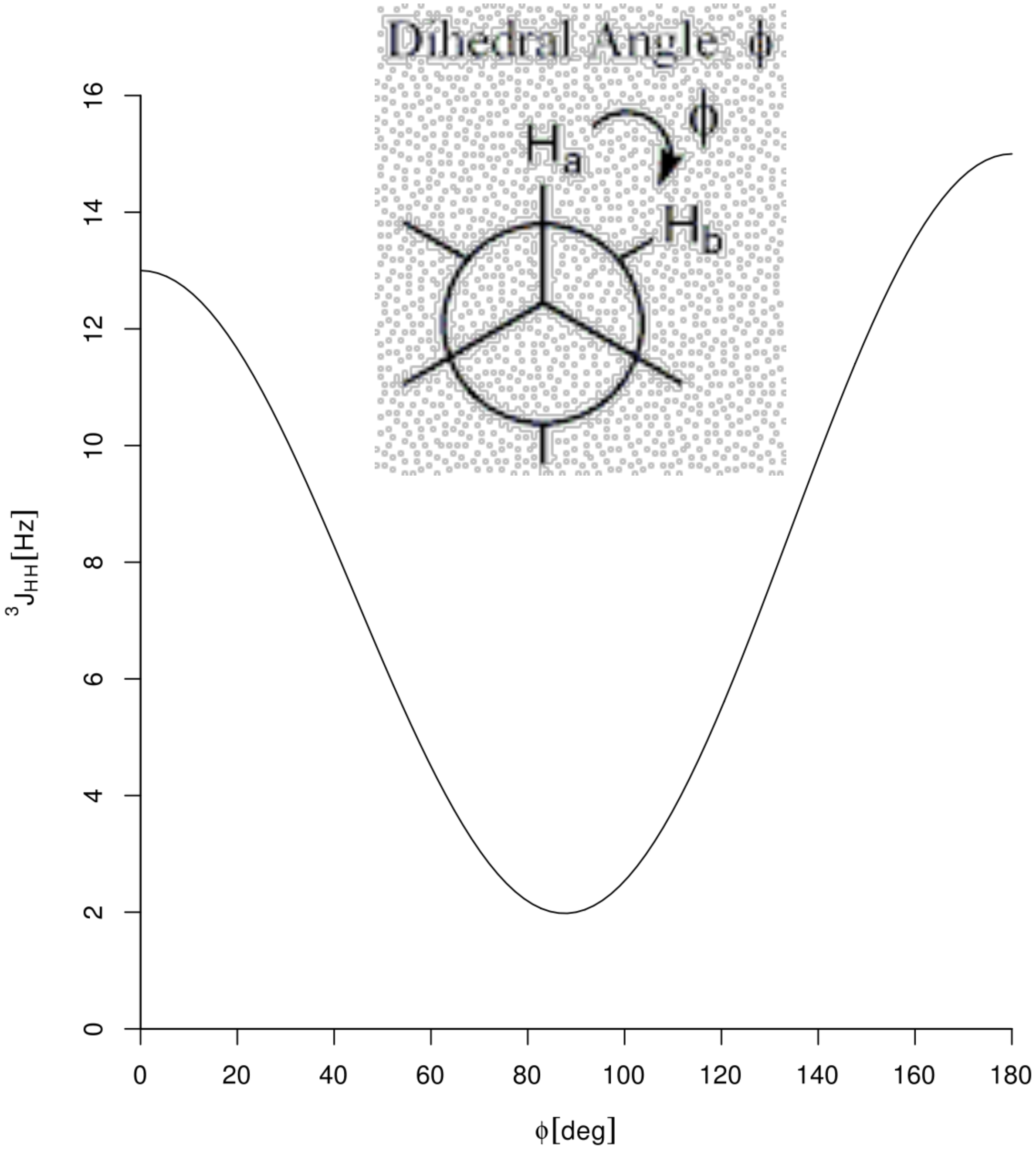
Pairs of gradient pulses encode and decode the position of spins along the *z* axis

Diffusion during the intervening period, Δ, leads to a loss of signal that can be analysed to measure the diffusion coefficient



Chemical exchange during Δ leads to averaging of the observed diffusion coefficient

Exchange beyond the chemical shift: scalar couplings



Karplus equation: $J = A\cos^2\phi + B\cos\phi + C$

Intramolecular exchange
e.g. sidechain rotamers

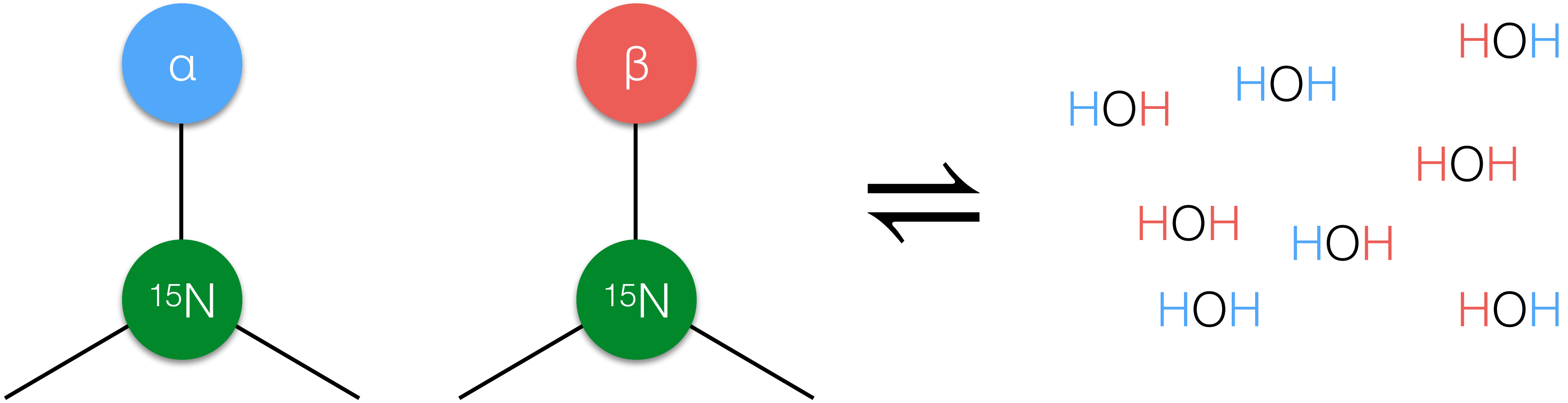
The dependence of the $^3J_{HH}$ scalar coupling on dihedral angle is described by a Karplus equation

Different rotamers will be associated with different coupling constants, but provided exchange between rotamers is rapid:

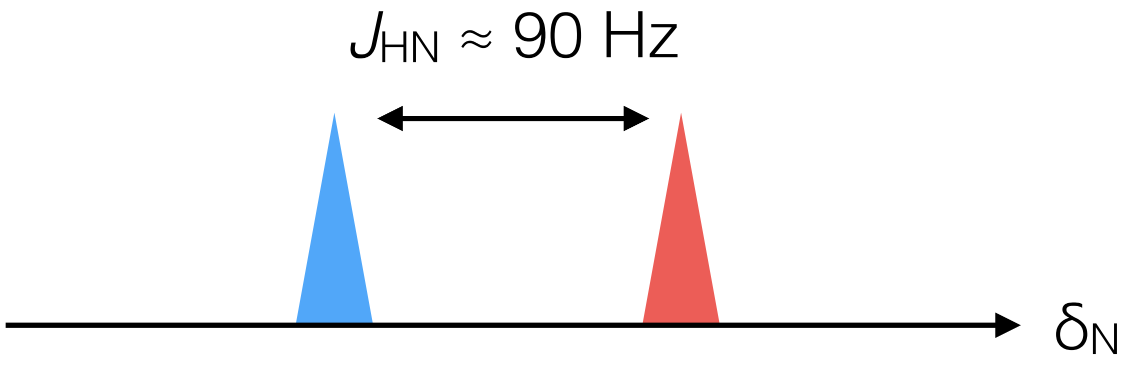
$$\Delta J << k_{ex}$$

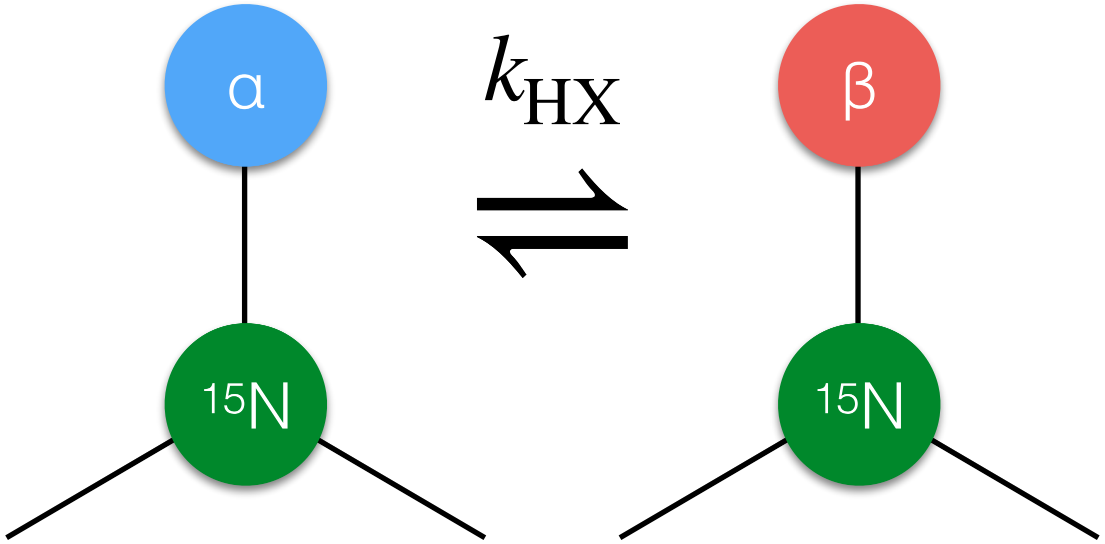
then a single coupling constant will be observed corresponding to the population-weighted average

Scalar couplings and intermolecular exchange

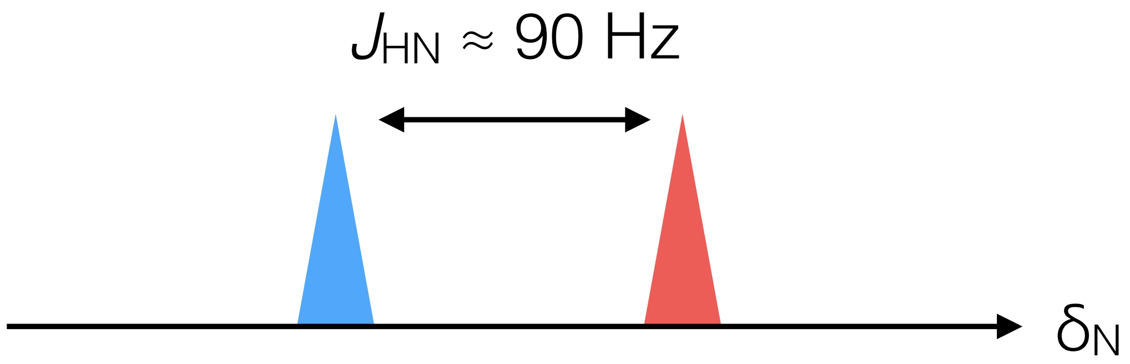


Chemical exchange of the coupled proton with the solvent randomises its spin state, which appears like exchange between α and β lines of doublet:





Scalar couplings and intermolecular exchange



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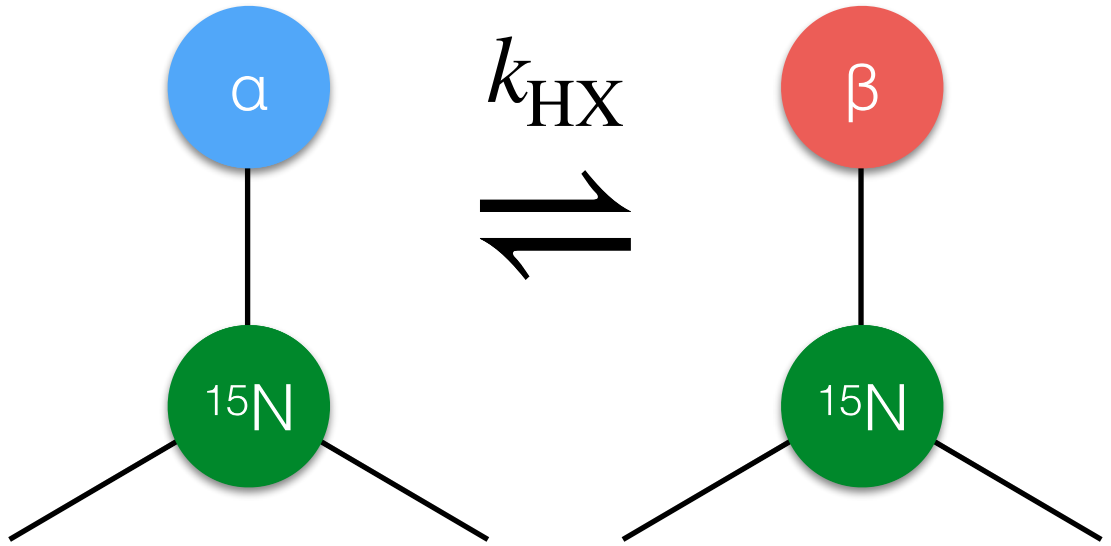
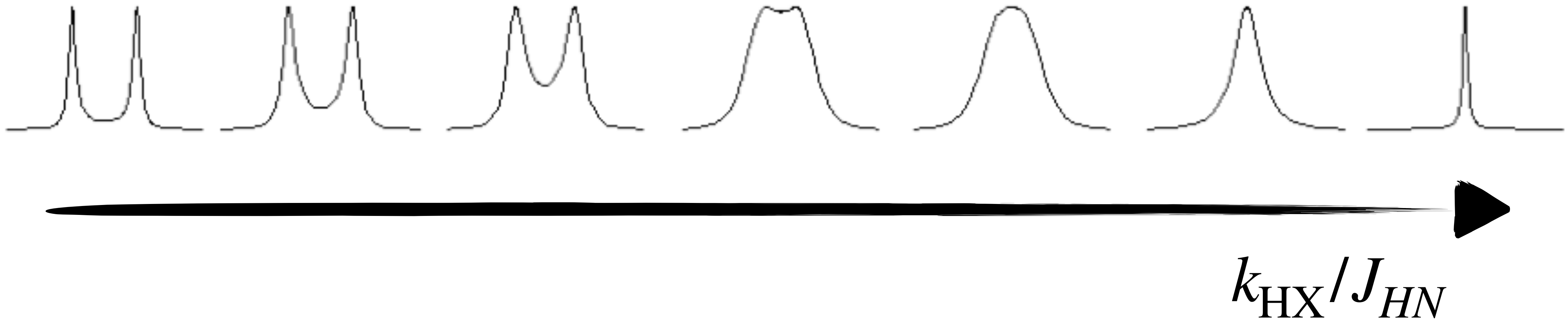
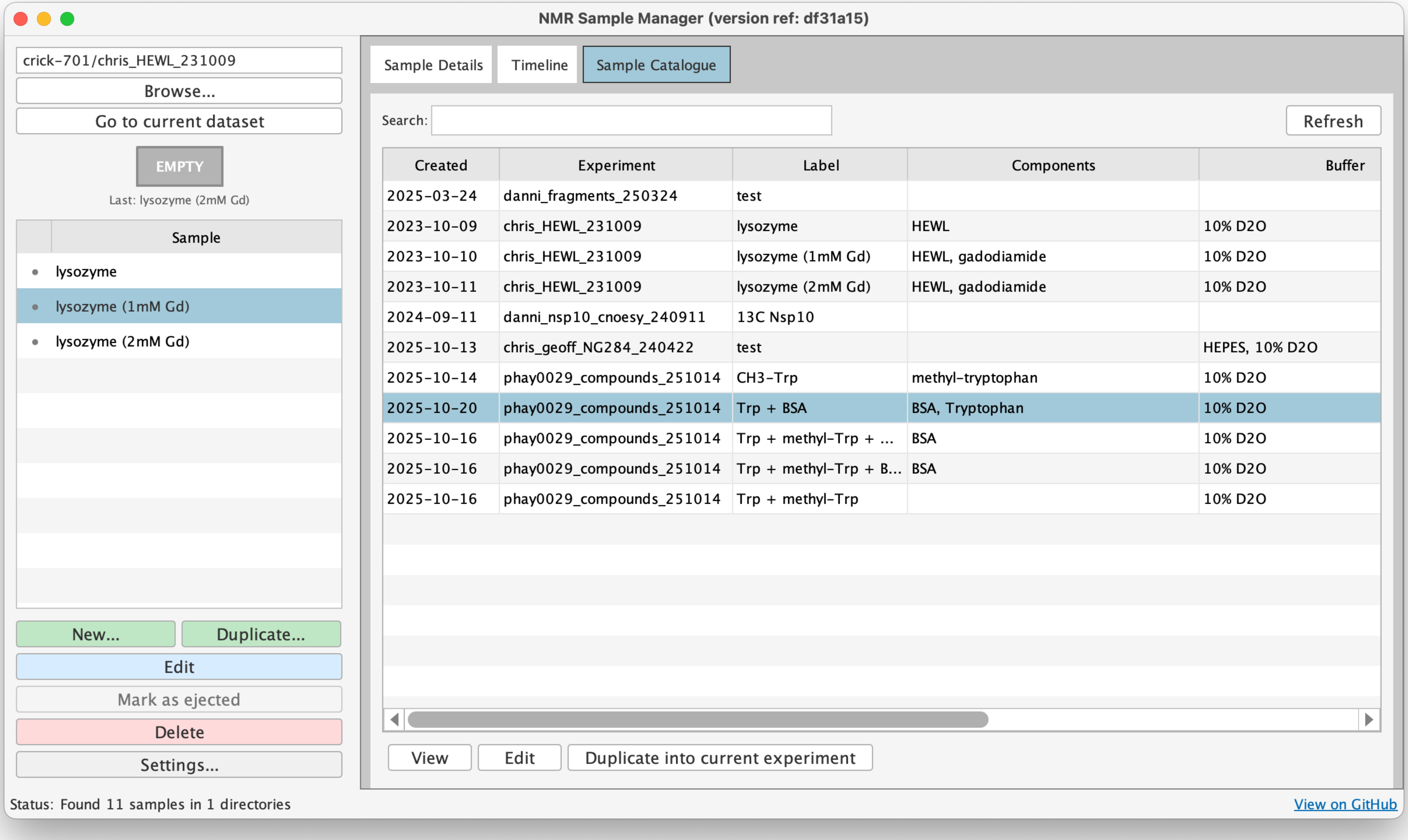




NMR Sample Management

waudbylab.org/topspin-samples



NMR Sample Manager (version ref: df31a15)

crick-701/chris_HEWL_231009

Last: lysozyme (2mM Gd)

Sample
lysozyme
lysozyme (1mM Gd)
lysozyme (2mM Gd)

Search:

Created	Experiment	Label	Components	Buffer
2025-03-24	danni_fragments_250324	test		
2023-10-09	chris_HEWL_231009	lysozyme	HEWL	10% D2O
2023-10-10	chris_HEWL_231009	lysozyme (1mM Gd)	HEWL, gadodiamide	10% D2O
2023-10-11	chris_HEWL_231009	lysozyme (2mM Gd)	HEWL, gadodiamide	10% D2O
2024-09-11	danni_nsp10_cnoesy_240911	13C Nsp10		
2025-10-13	chris_geoff_NG284_240422	test		HEPES, 10% D2O
2025-10-14	phay0029_compounds_251014	CH3-Trp	methyl-tryptophan	10% D2O
2025-10-20	phay0029_compounds_251014	Trp + BSA	BSA, Tryptophan	10% D2O
2025-10-16	phay0029_compounds_251014	Trp + methyl-Trp + ...	BSA	10% D2O
2025-10-16	phay0029_compounds_251014	Trp + methyl-Trp + B...	BSA	10% D2O
2025-10-16	phay0029_compounds_251014	Trp + methyl-Trp		10% D2O

Status: Found 11 samples in 1 directories