Molecular Dynamics and Structure on Biology

High-field NMR facility in Life Science

850/600/500 MHz

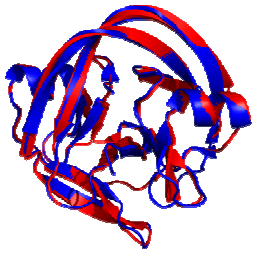
850 MHz Nuclei Magnetic Resonance Spectrum-scope with Cryo/regular probe

600 MHz Nuclei Magnetic Resonance Spectrum-scope with regular probe

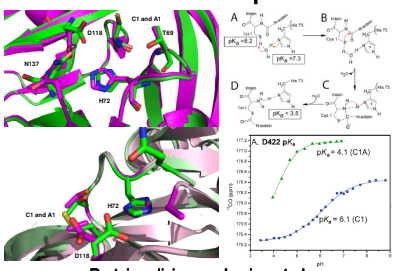
500 MHz Nuclei Magnetic Resonance Spectrum-scope with BBO/regular probe

Group leader and Group member

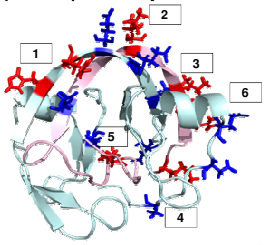
Protein trans-splicing (PTS) in membrane protein ligation: Structure basis of detergent/denaturant-resistant split intein



*Npu*DanE split intein Crystal structure



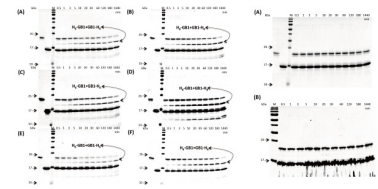
Protein splicing mechanism study



Electrostatics distribution on assemble interface

pair number	positive	negative
1	H48	D118
	R50	
2	K113	E52
		E54
3	K109	E57
4	K104	D98
5	K130	D62
		E7
6	R108	E91
		D93

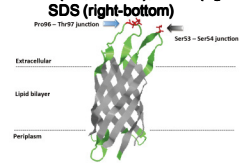
Salt-bridge list on assemble interface



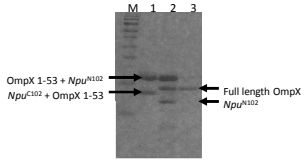
PTS-assay in Urea (left, 1M~6M), CTAB (right-top) and SDS (right-bottom)

Detergent Category	Abbreviated Name	Fraction of Ligation (%)	K trans (s⁻¹)	T ½ (min)
Ionic	SDS	N.A.	N.A.	N.A.
	CTAB	N.A.	N.A.	N.A.
Non-ionic	Brij35	63.9 ± 2.9	(6.0 ± 1.4) × 10⁻²	1.9
	DDM	67.1 ± 3.2	(4.5 ± 0.8) × 10⁻²	2.6
	Digitonin	80.0 ± 4.0	(9.1 ± 2.3) × 10⁻²	1.3
	OG	65.4 ± 3.7	(2.6 ± 0.5) × 10⁻²	0.5
	Triton X-100	70.0 ± 4.9	(7.3 ± 3.0) × 10⁻²	1.6
	Tween 20	68.4 ± 3.7	(5.6 ± 1.4) × 10⁻²	2.1
Zwitterion	Chaps	73.5 ± 3.0	(1.0 ± 0.2) × 10⁻²	1.2
	DHPC	70.2 ± 4.0	(1.2 ± 0.4) × 10⁻²	1.0
	LDAO	89.1 ± 3.6	(5.0 ± 1.4) × 10⁻²	2.1
Control		74.6 ± 1.5	(5.8 ± 1.5) × 10⁻²	2.0

PTS-assay result in series detergent/lipid

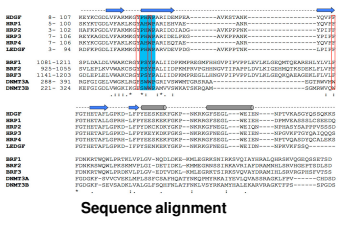


Outer membrane protein X split site design

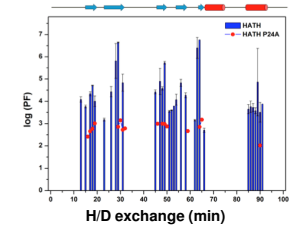


In vitro ligation of OmpX via PTS

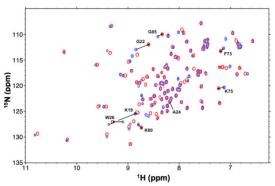
The first residue of PWWP motif modulates Hepatoma- Derived Growth Factor binding and stability



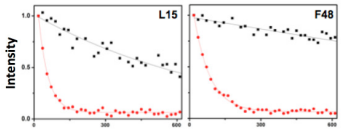
Sequence alignment



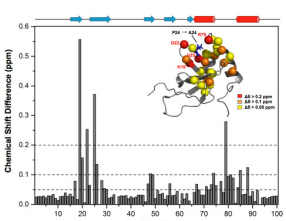
H/D exchange (min)



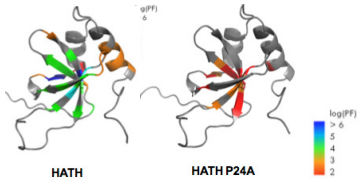
^{1}H-^{15}N Heteronuclear Single Quantum Coherence



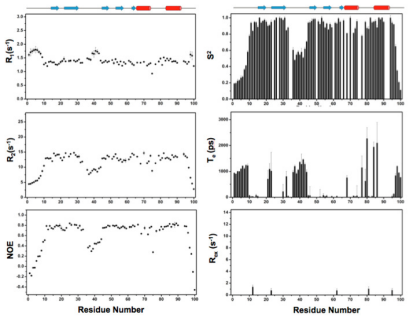
H/D exchange (min)

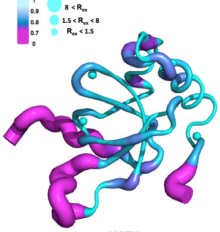


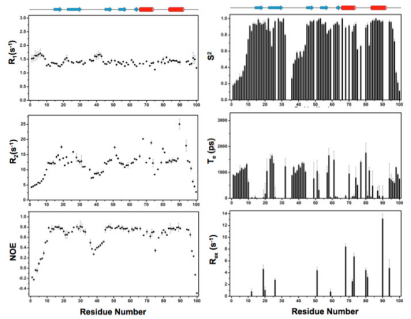
Chemical Shift Perturbation

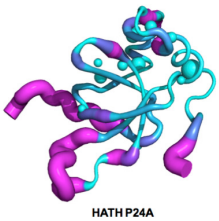


Hydrogen protecting factor









Atomic-resolution solution structure dynamics via Nucleus Magnetics Resonance spectrum scope

1. Hung YL, Lin YJ, & Sue SC (2015) (13)C, (15)N and (1)H resonance assignments of receiver domain of ethylene receptor ETR1. *Biomol NMR Assign* 9(1):119-122.
2. Hung YL, *et al.* (2015) The First Residue of the PWWP Motif Modulates HATH Domain Binding, Stability, and Protein-Protein Interaction. *Biochemistry* 54(26):4063-4074.
3. Lee YZ, Lee YT, Lin YJ, Chen YJ, & Sue SC (2014) A streamlined method for preparing split intein for NMR study. *Protein Expr Purif* 99:106-112.
4. Chiu LY, Hung KW, Tjong SC, Chiang YW, & Sue SC (2014) NMR characterization of the electrostatic interaction of the basic residues in HDGF and FGF2 during heparin binding. *Biochim Biophys Acta* 1844(10):1851-1859.
5. Chen YC, Cheng CS, Tjong SC, Yin HS, & Sue SC (2014) Case study of hydrogen bonding in a hydrophobic cavity. *J Phys Chem B* 118(50):14602-14611.
6. Kuo JH, *et al.* (2013) Alternative C-terminal helix orientation alters chemokine function: structure of the anti-angiogenic chemokine, CXCL4L1. *J Biol Chem* 288(19):13522-13533.
7. Lee YT, Su TH, Lo WC, Lyu PC, & Sue SC (2012) Circular permutation prediction reveals a viable backbone disconnection for split proteins: an approach in identifying a new functional split intein. *PLoS One* 7(8):e43820.
8. Chen FF, *et al.* (2012) Significance of heparin binding to basic residues in homologous to the amino terminus of hepatoma-derived growth factor and related proteins. *Glycobiology* 22(5):649-661.