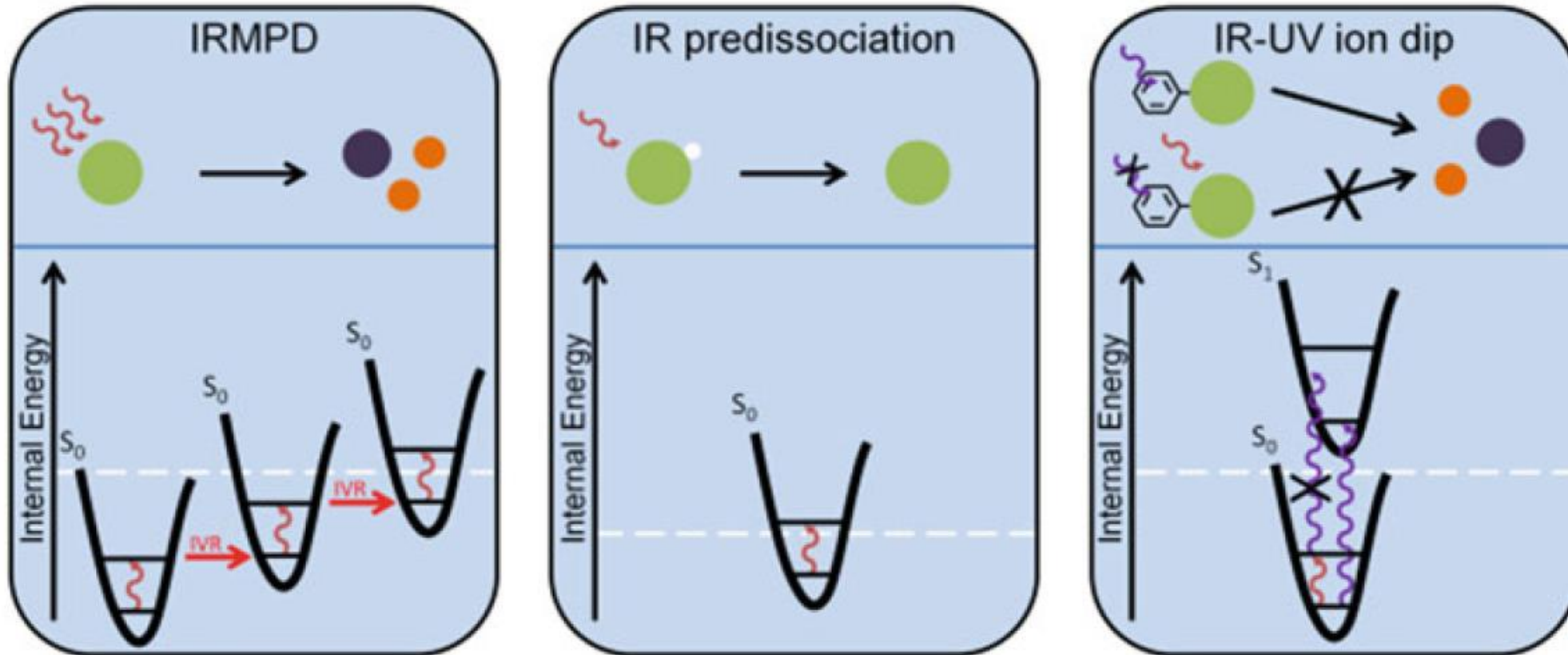


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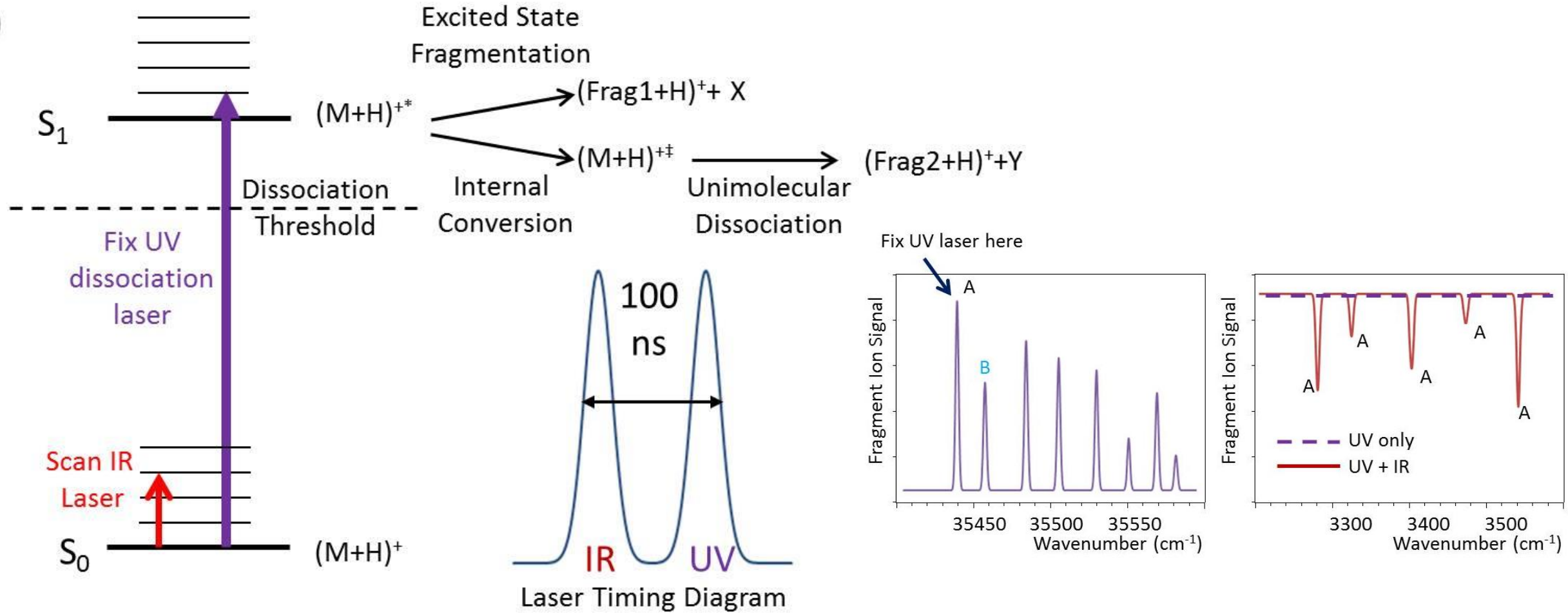
**Métodos híbridos para a diferenciação
de isômeros:
IMS, UVPD, FRET e múltiplos fótons**

Técnicas alternativas para aquisição de espectros IR



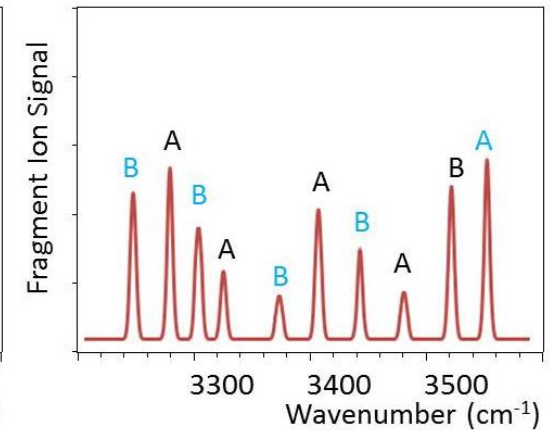
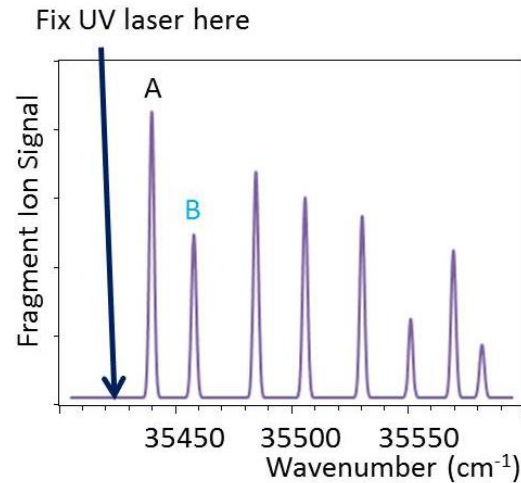
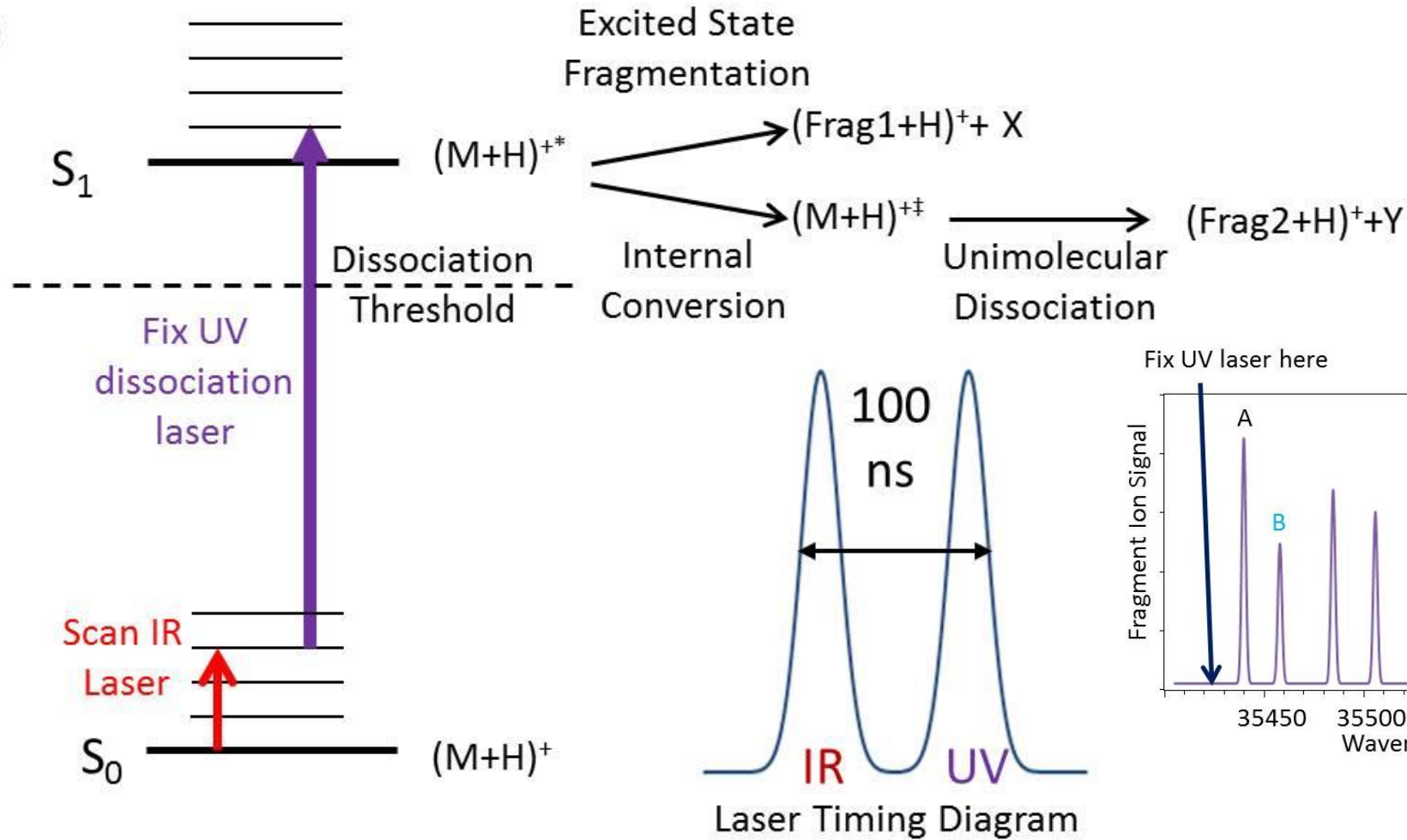
IR-UV depletion spectroscopy

a)

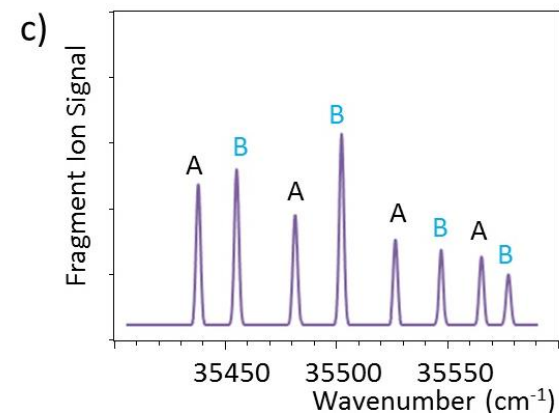
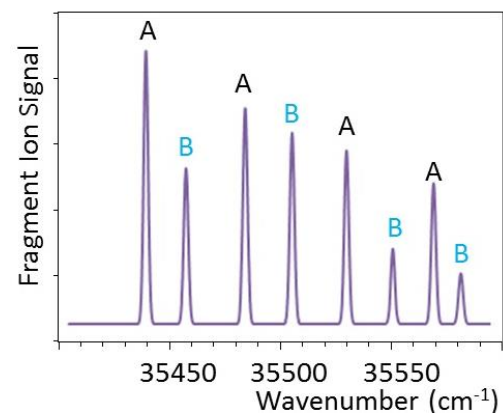
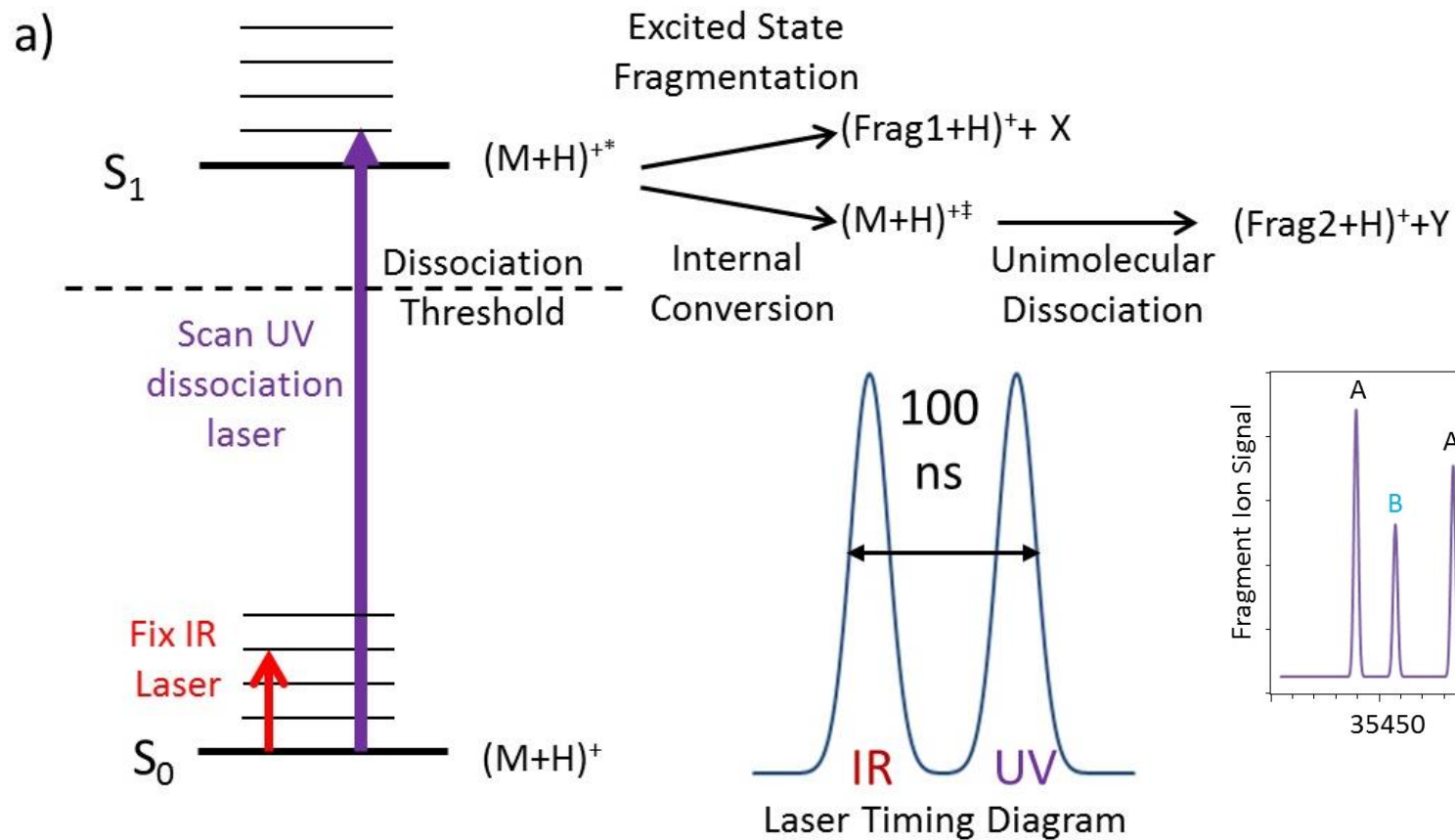


IR-UV Gain Spectroscopy

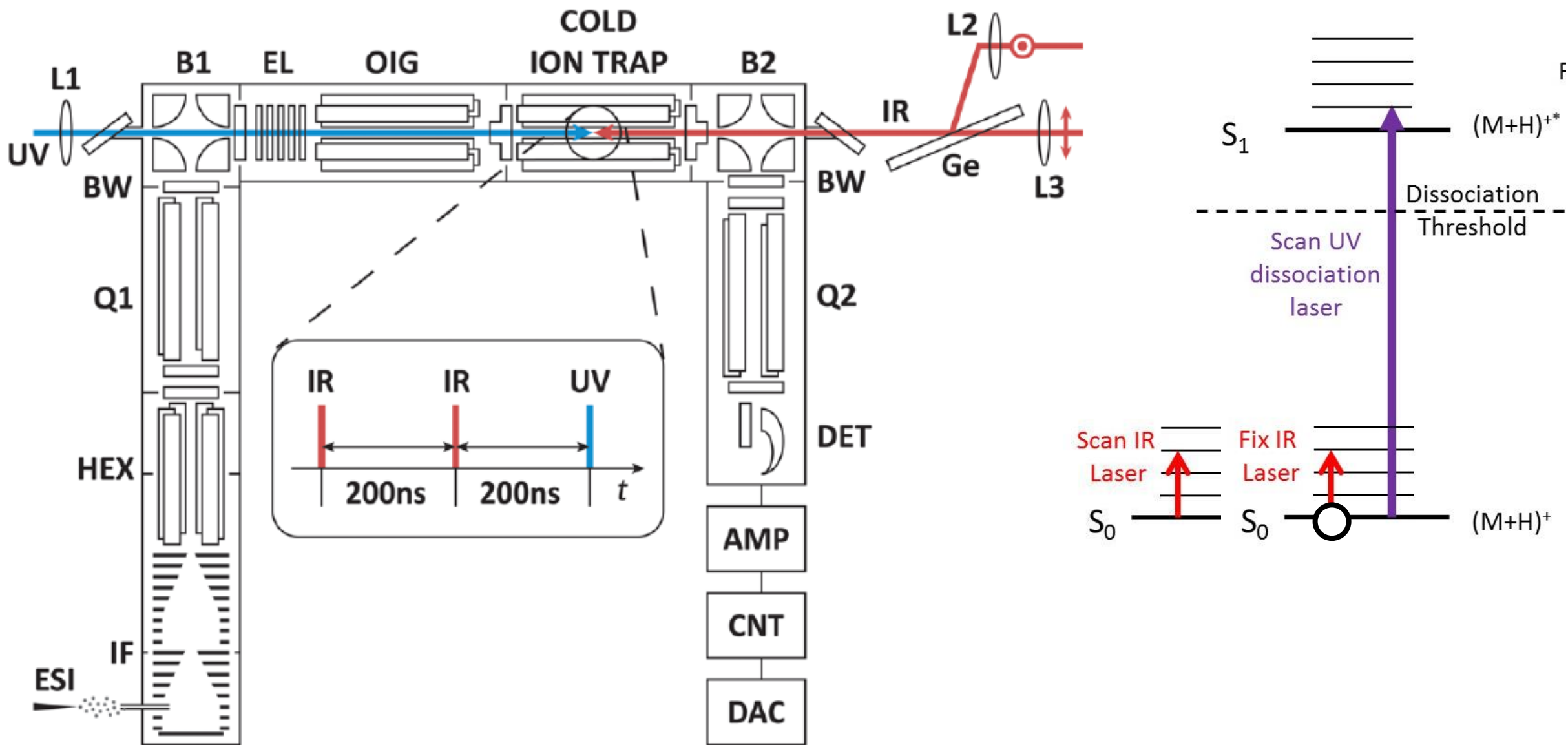
a)



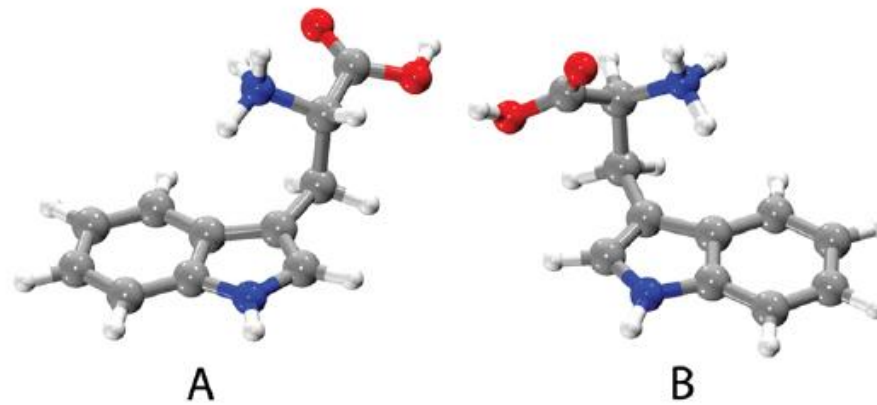
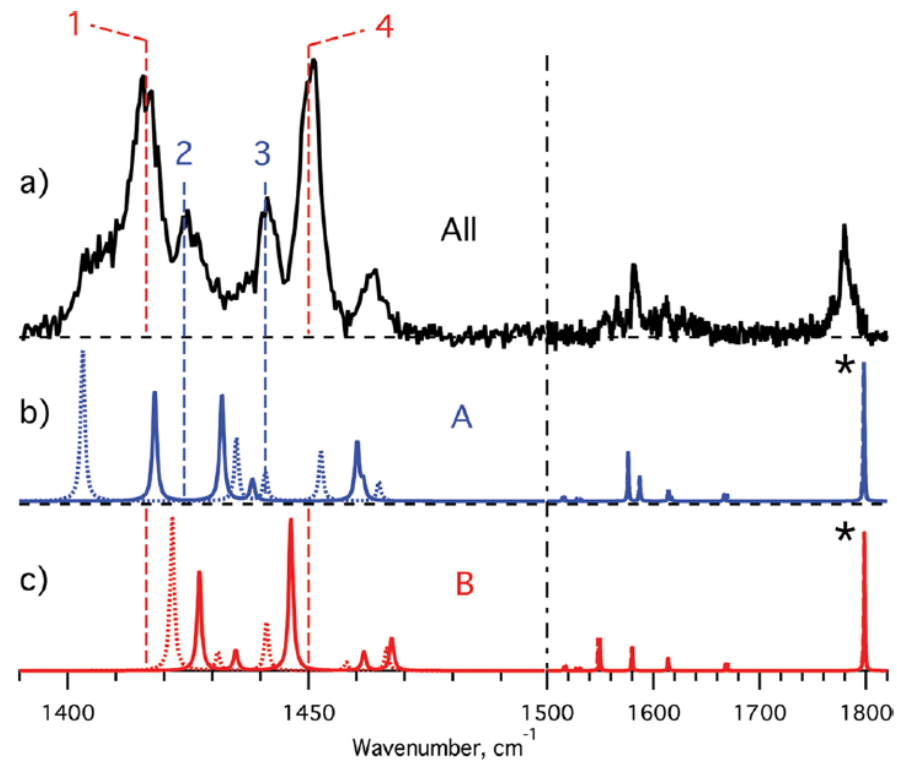
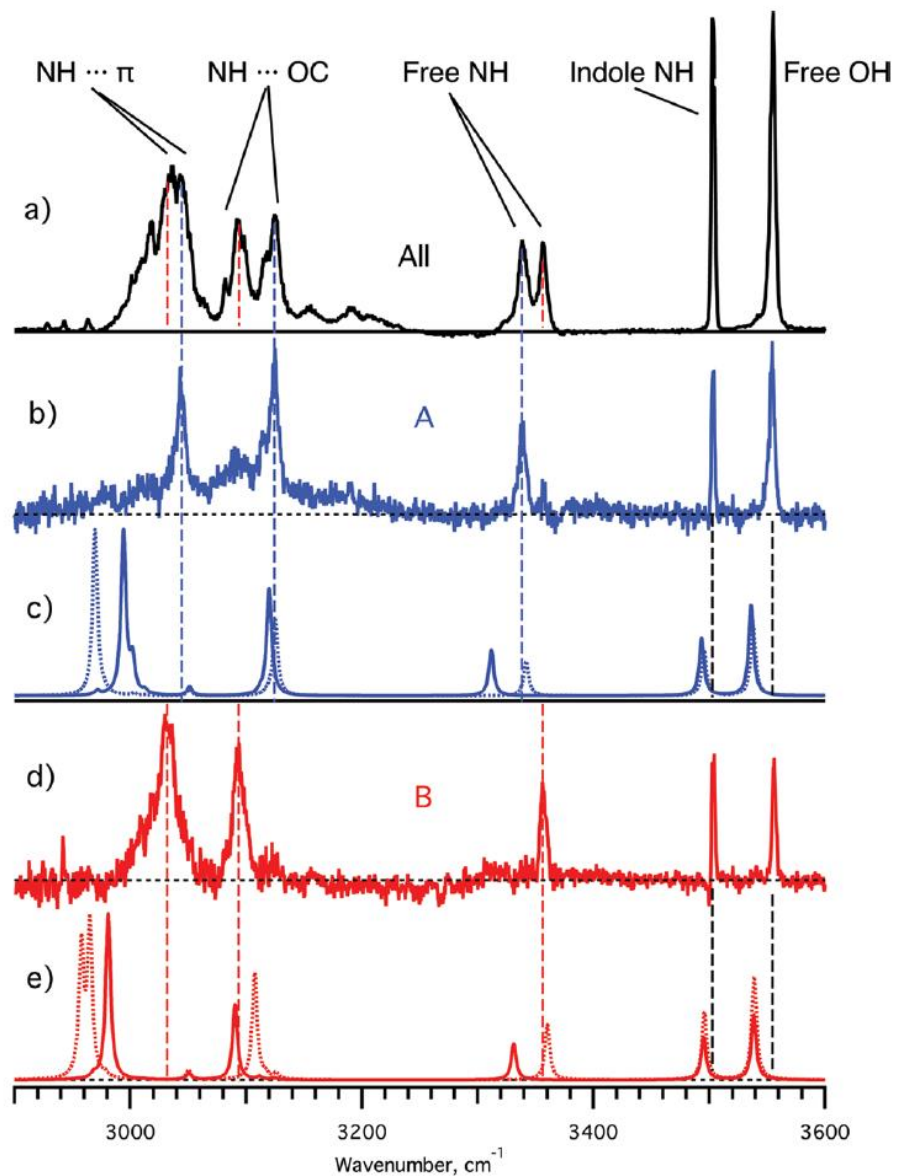
IR-UV Holeburning



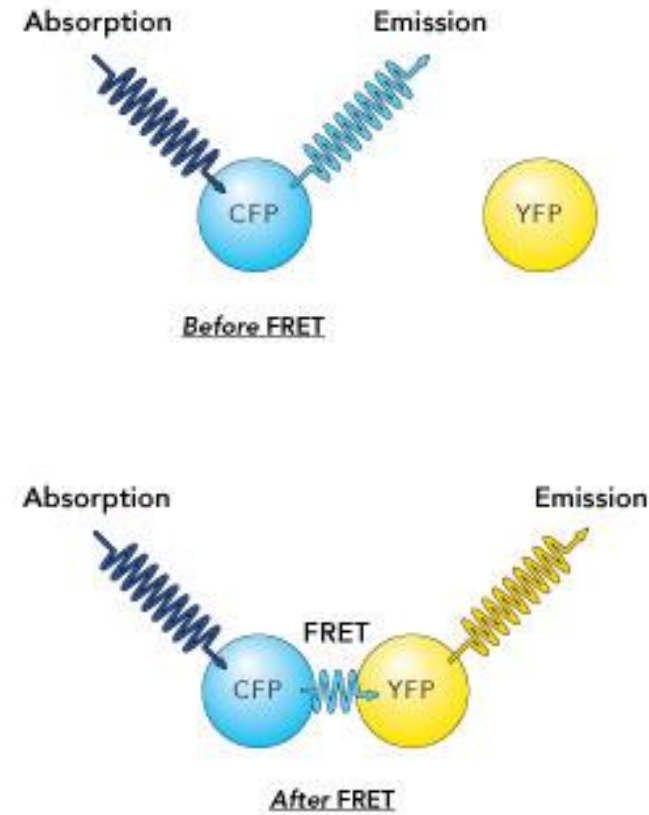
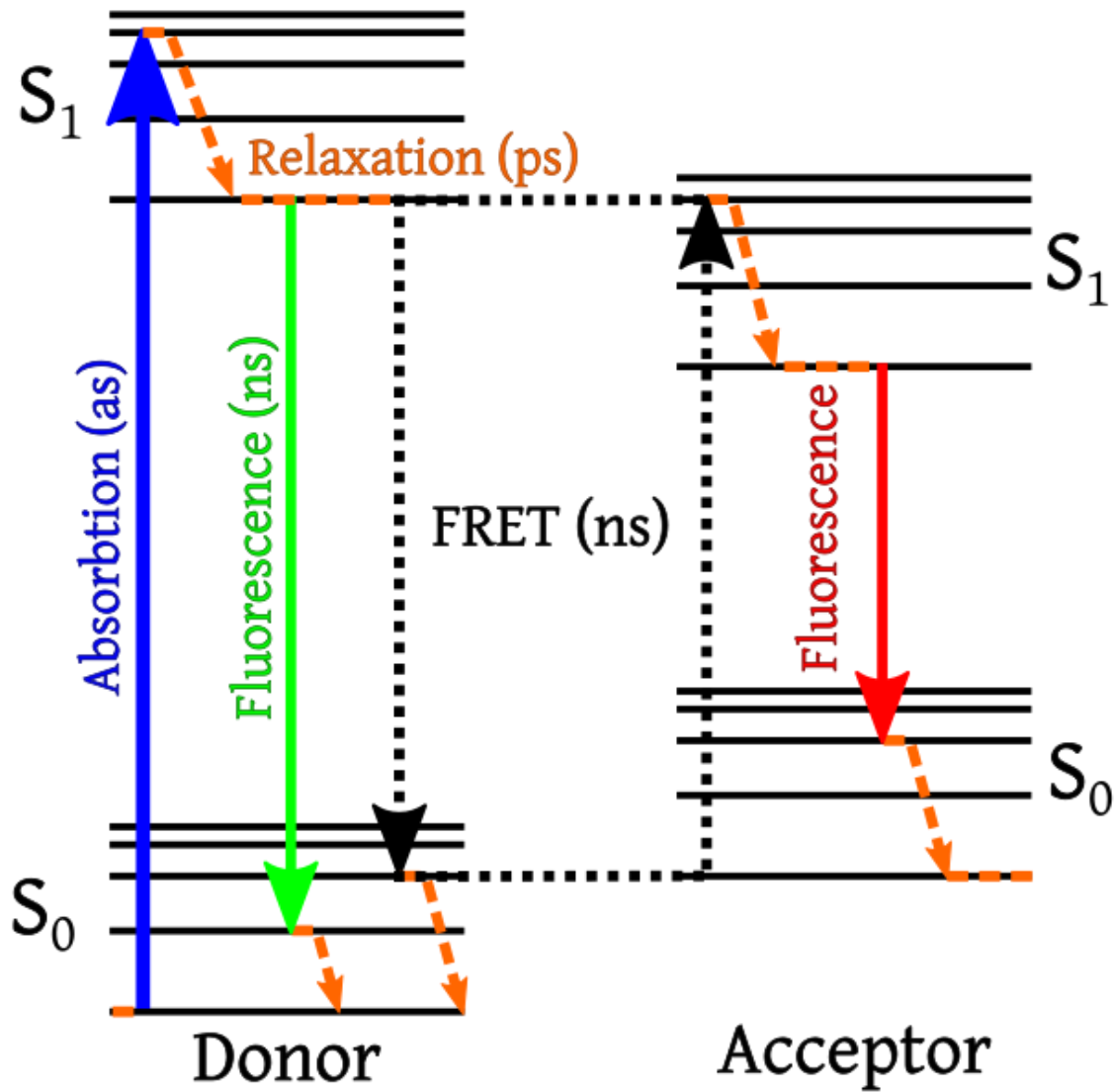
Hole burning IR-IR-UV spectroscopy



Seleção de isômeros específicos



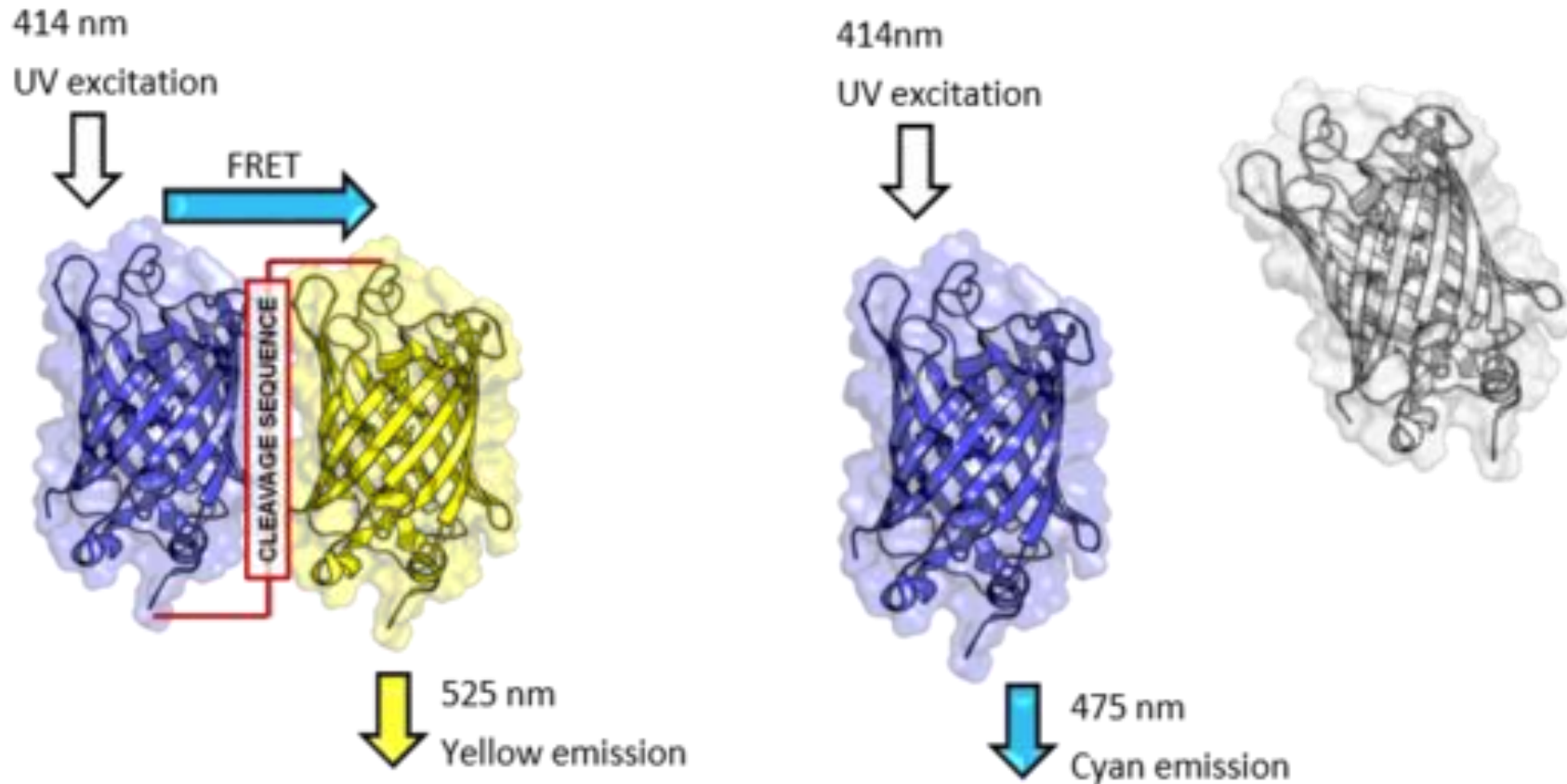
FRET - Förster (Fluorescence) resonance energy transfer



FRET distance dependence

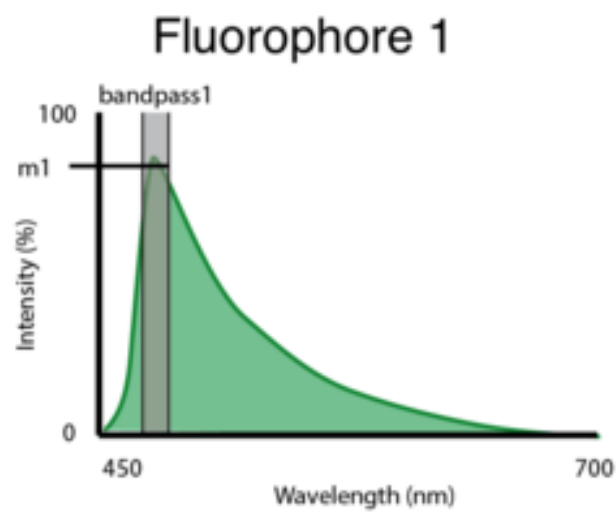
$$E = \frac{k_{\text{ET}}}{k_f + k_{\text{ET}} + \sum k_i}$$

$$E = \frac{1}{1 + (r/R_0)^6}$$

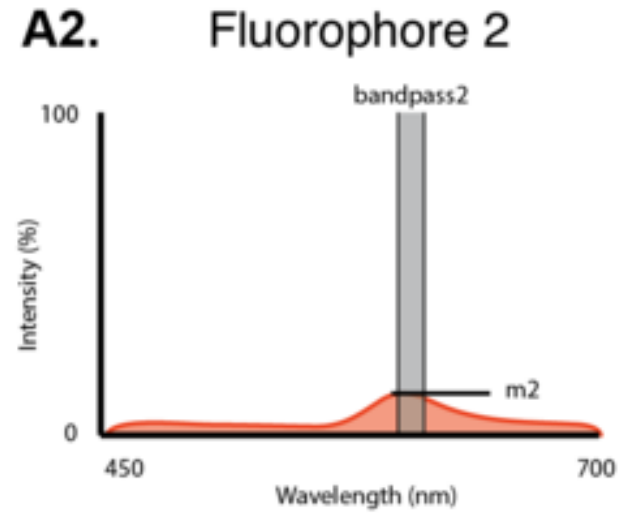


FRET in solution

A1.



A2.

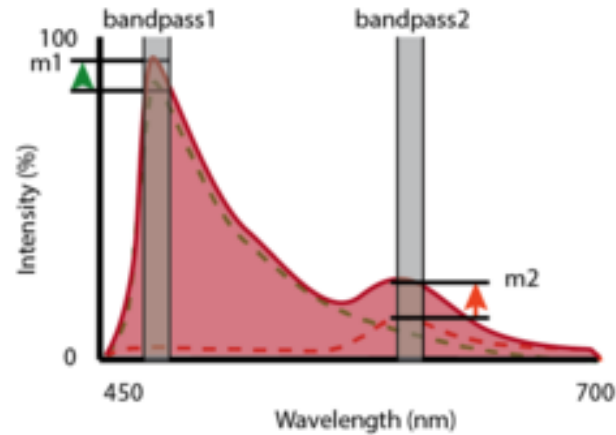


combine solution

— Donor
— Acceptor
— Donor + Acceptor

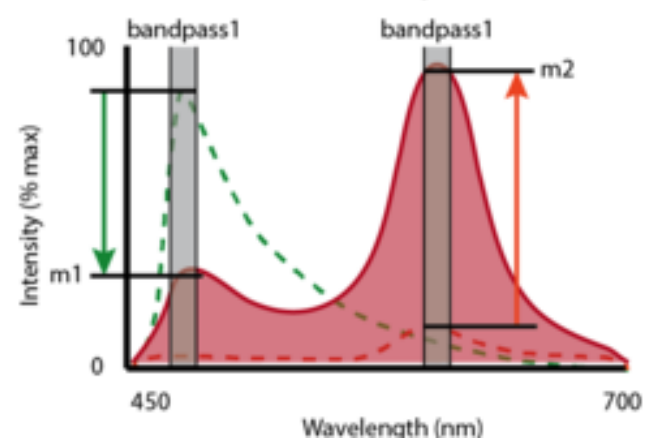
B1.

low concentration (no FRET)
distance between fluorophores is large

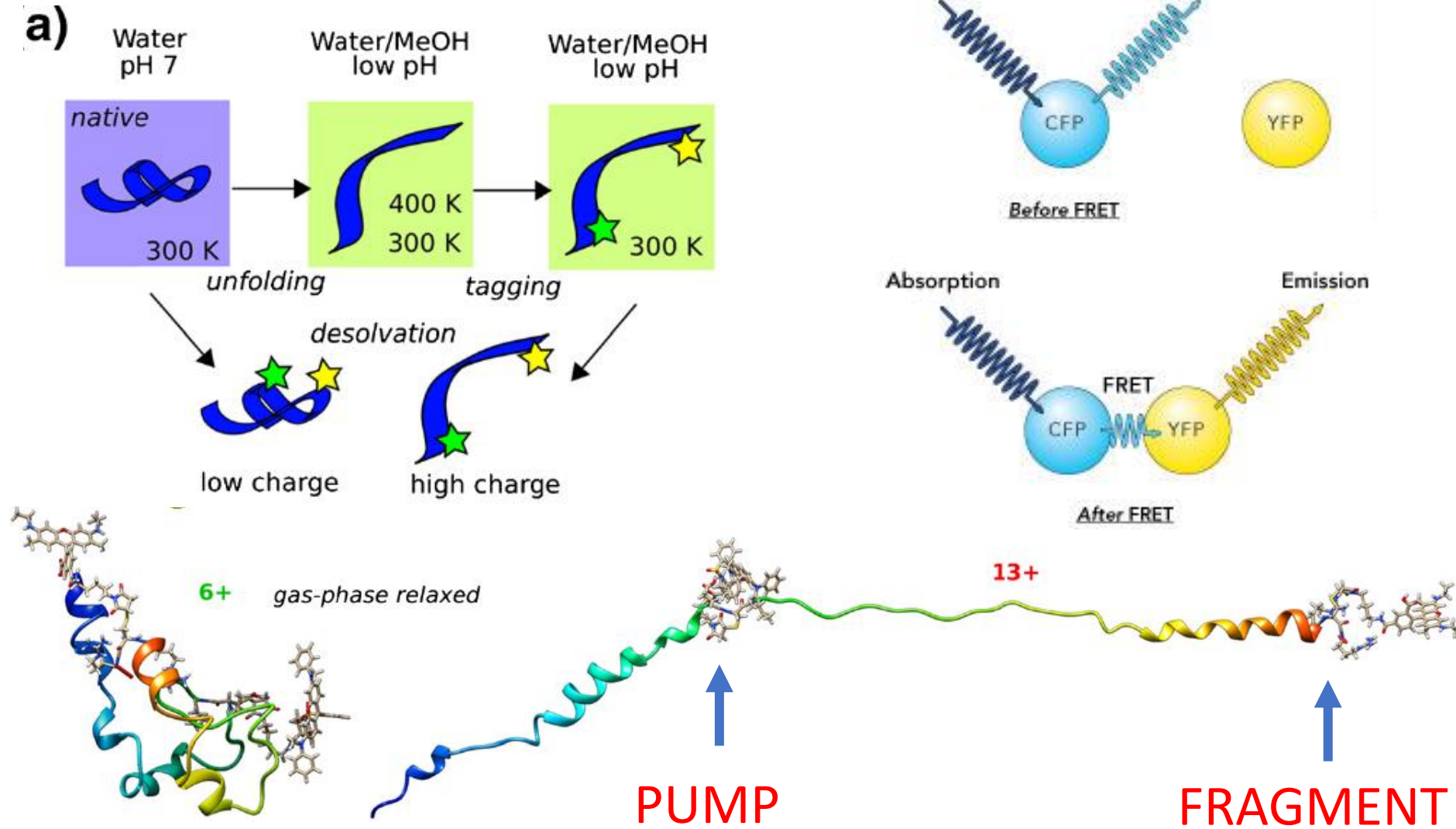


B2.

high concentration (FRET)
distance between fluorophores is small



Action FRET



Ubiquitin unfolding vs. charge state and solution nature

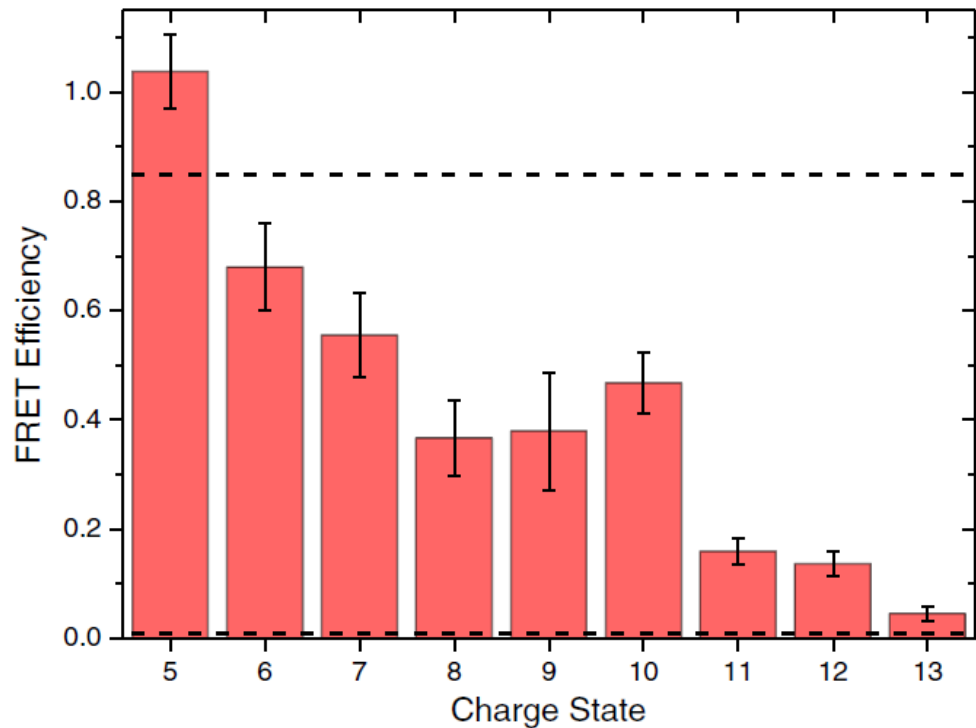


Figure 5. FRET efficiency as a function of the charge state of $[\text{d-UBI-a} + (z-2)\text{H}]^{z+}$ cations produced by ESI from a 1:1 solution of $\text{H}_2\text{O}:\text{CH}_3\text{OH}$ with 1% acetic acid by volume. The dashed lines indicate estimated FRET efficiencies for the native (N) and A-states of doubly grafted ubiquitin

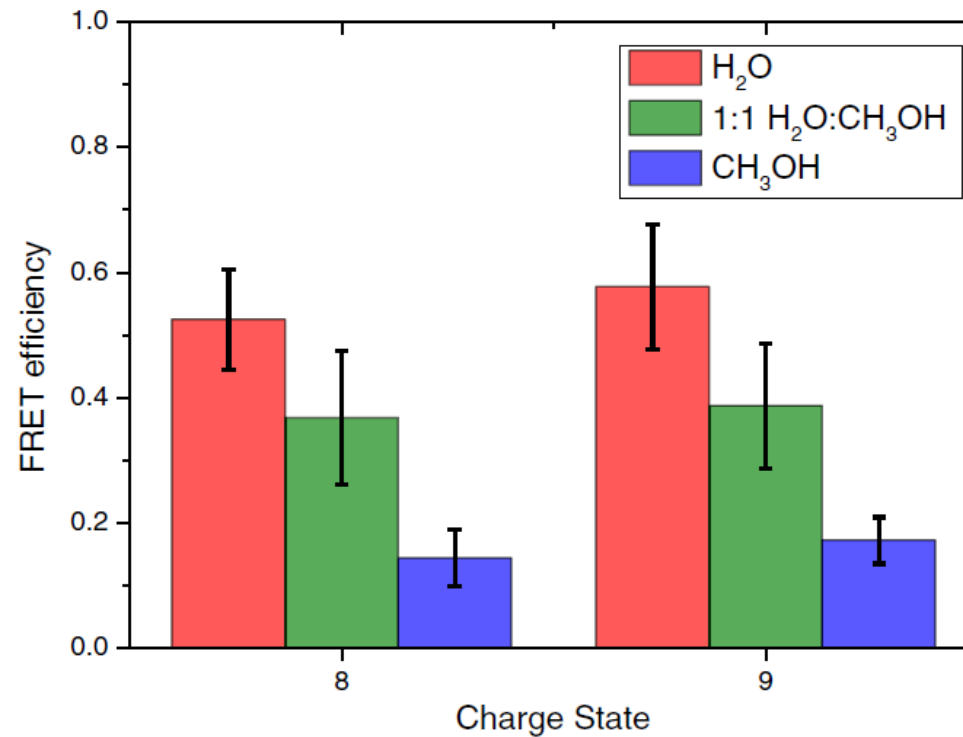
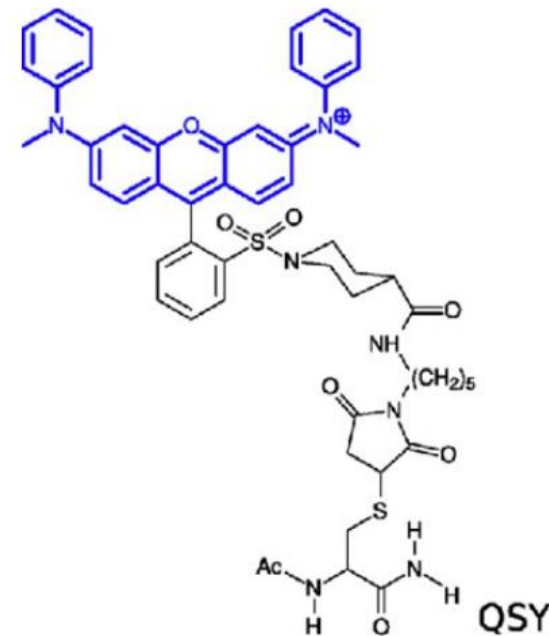
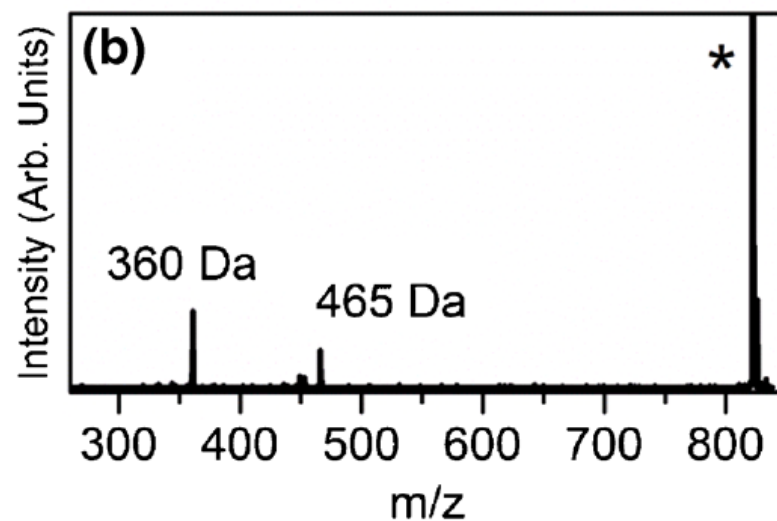
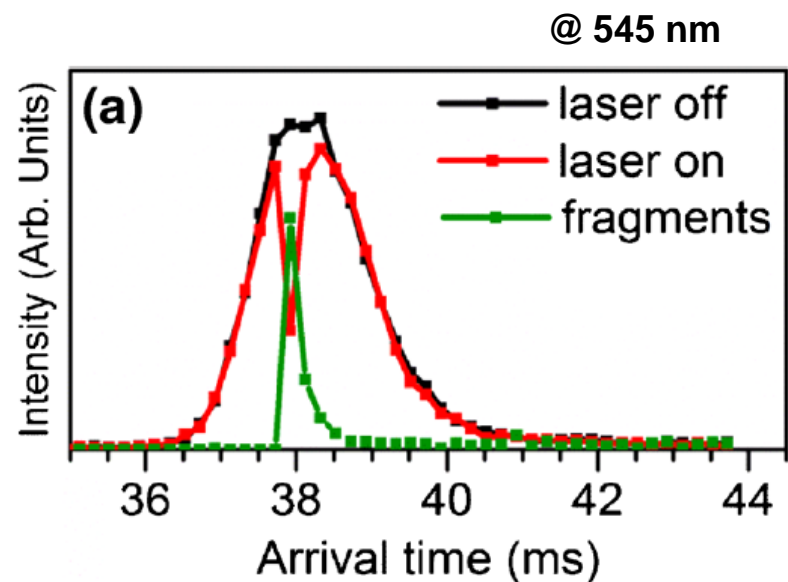
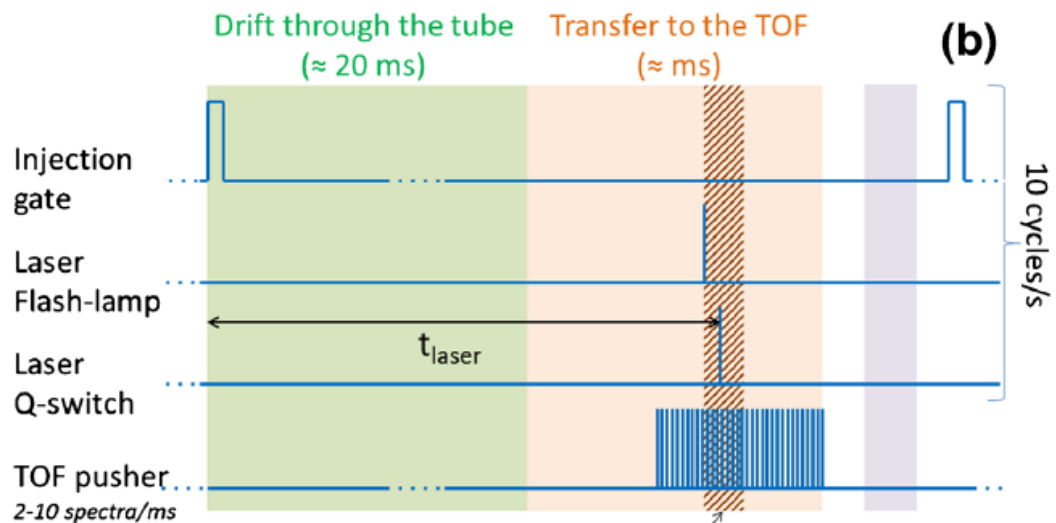
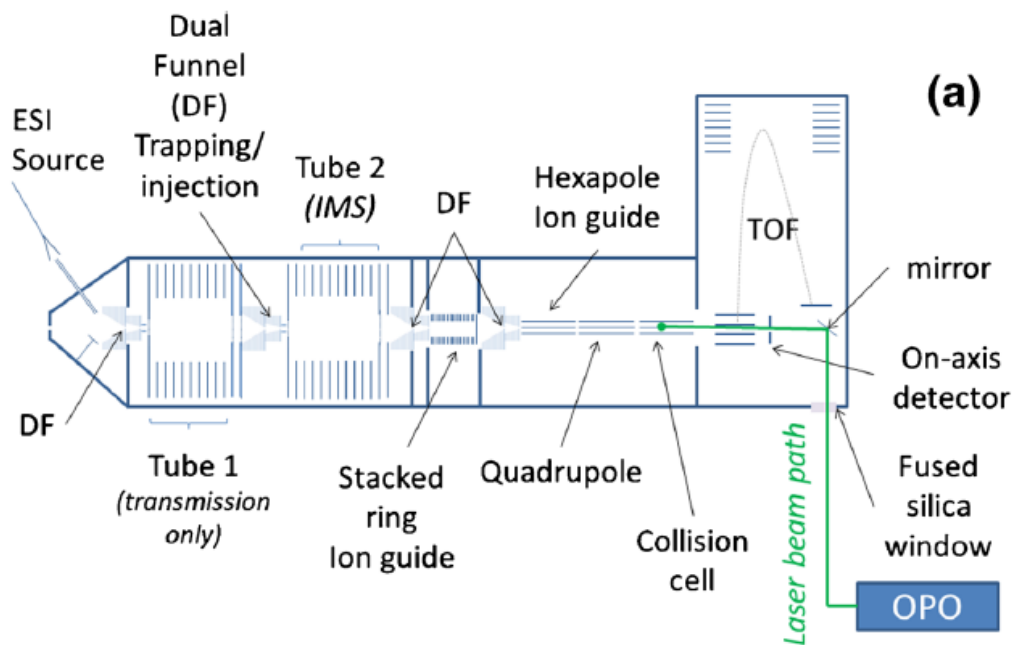


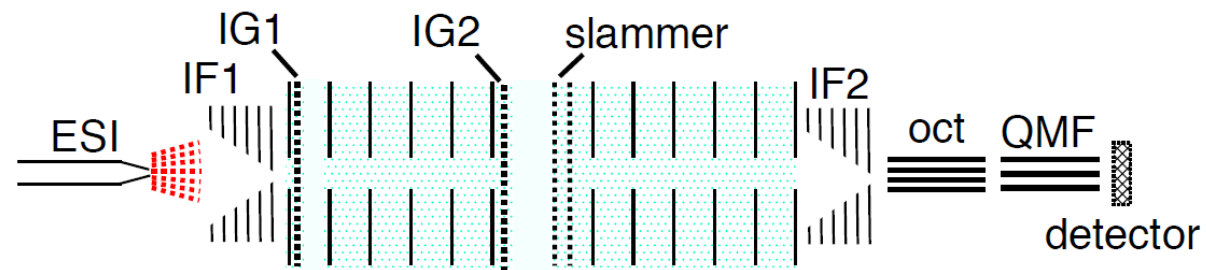
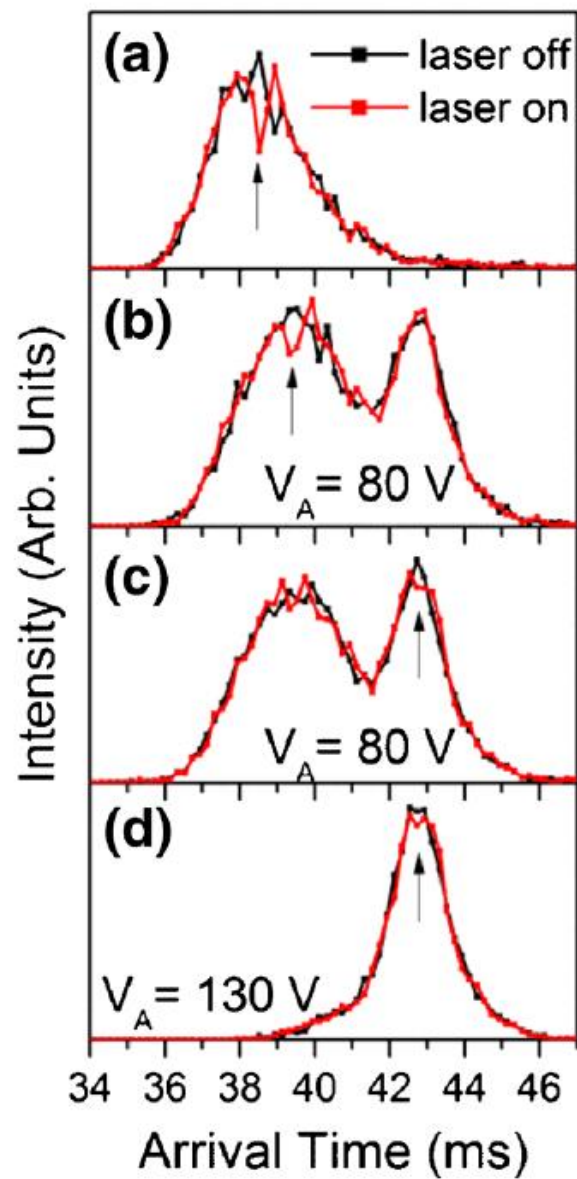
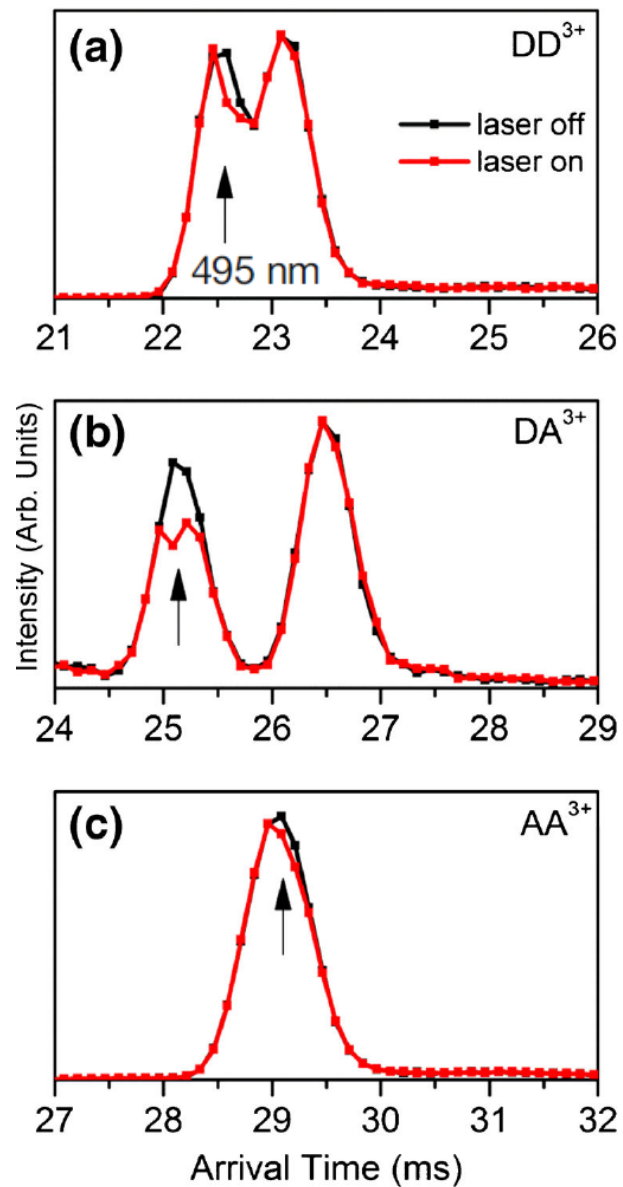
Figure 6. FRET efficiencies of $[\text{d-UBI-a} + 6\text{H}]^{8+}$ and $[\text{d-UBI-a} + 7\text{H}]^{9+}$ following ESI from either H_2O (red), 1:1 $\text{H}_2\text{O}:\text{CH}_3\text{OH}$ (green) or CH_3OH (blue) solutions with 1% acetic acid by volume

IMS - Action FRET

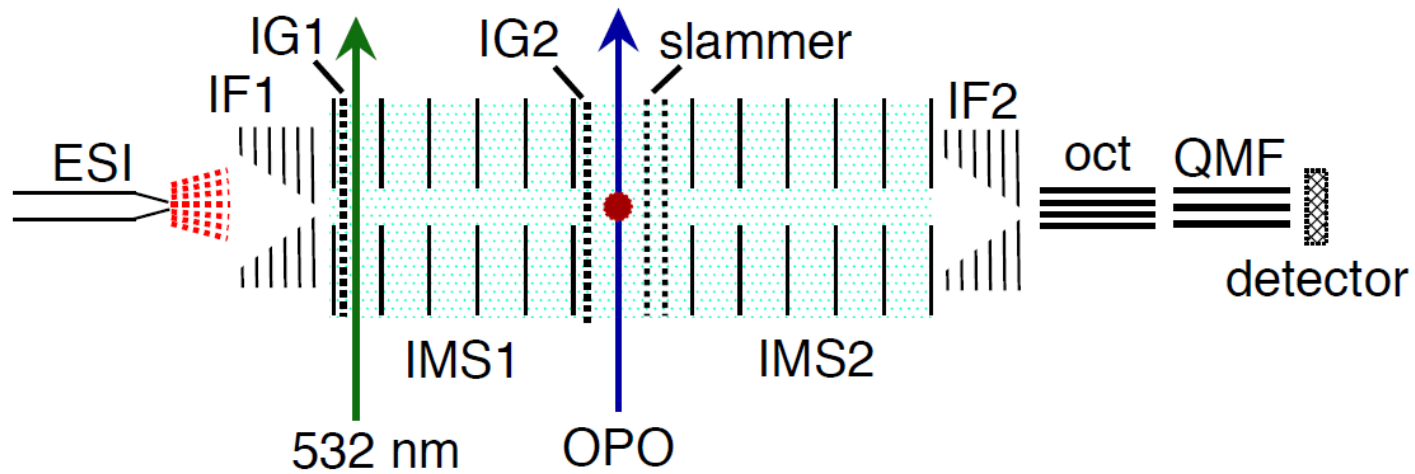
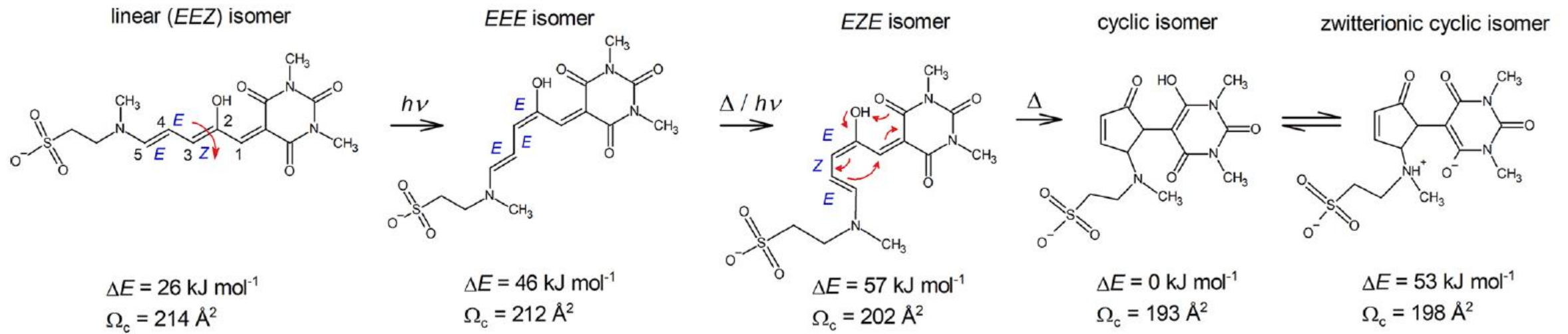


IMS - Action FRET

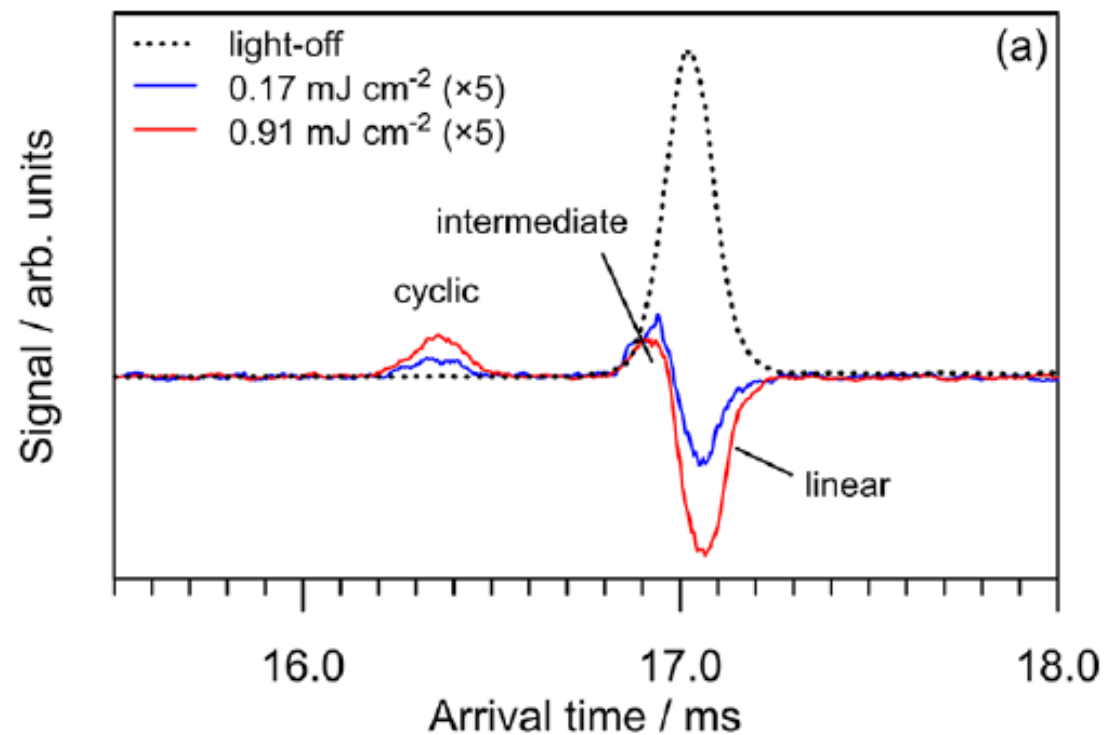
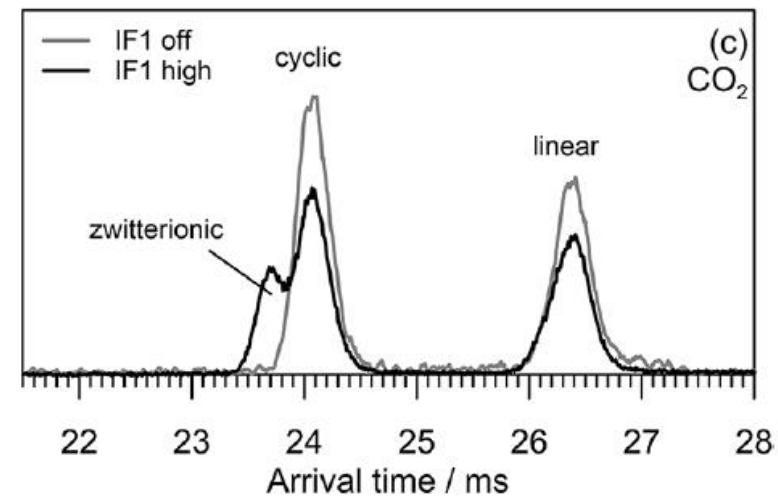
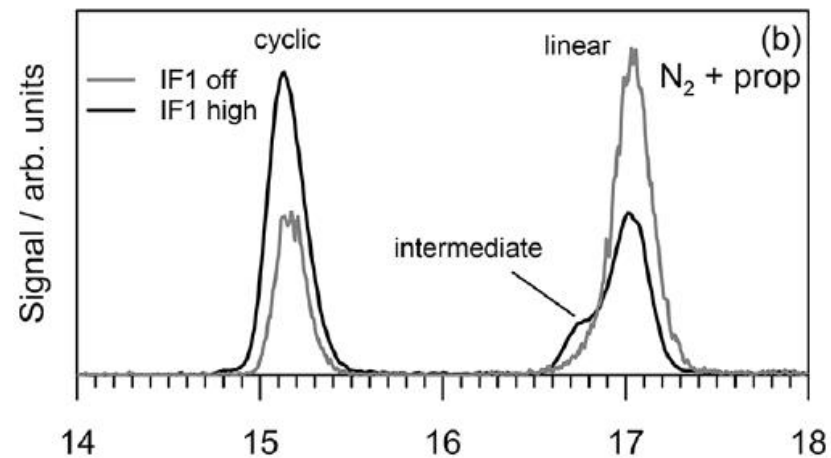
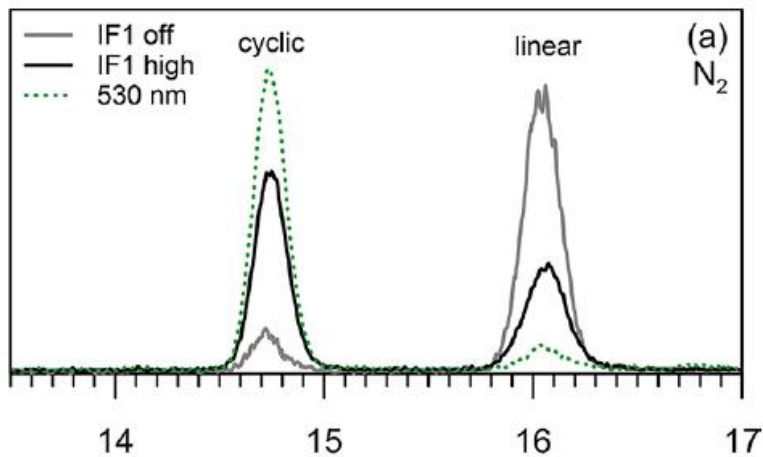
doubly tagged ace-CAAKAAC-NH₂



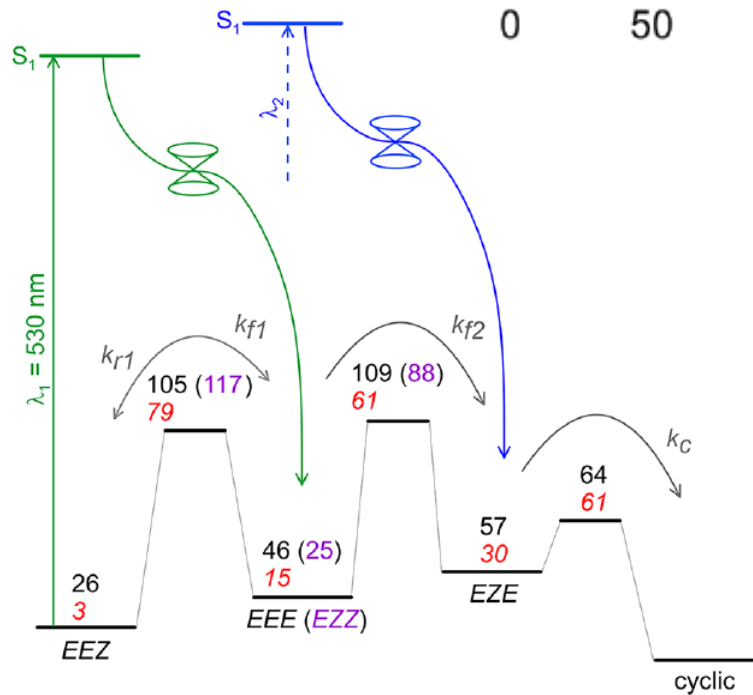
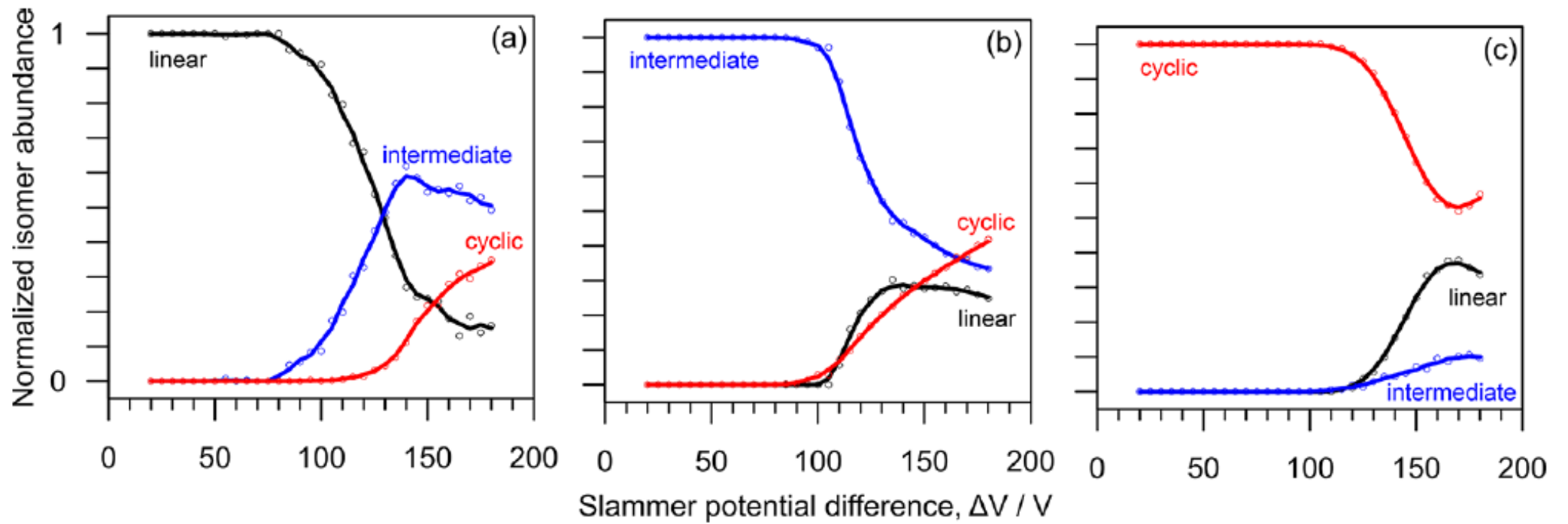
Photoisomerization Action Spectroscopy

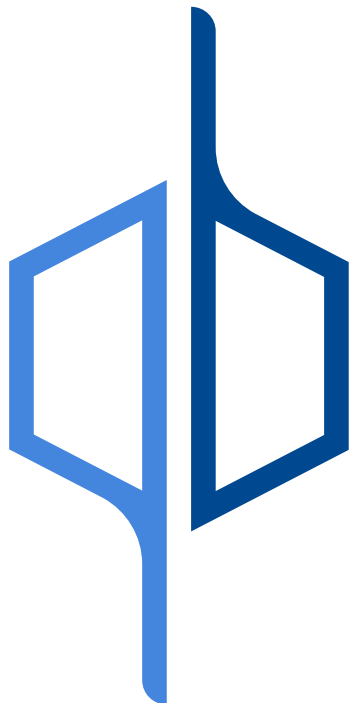


Photoisomerization Action Spectroscopy



Post IMS ion activation





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