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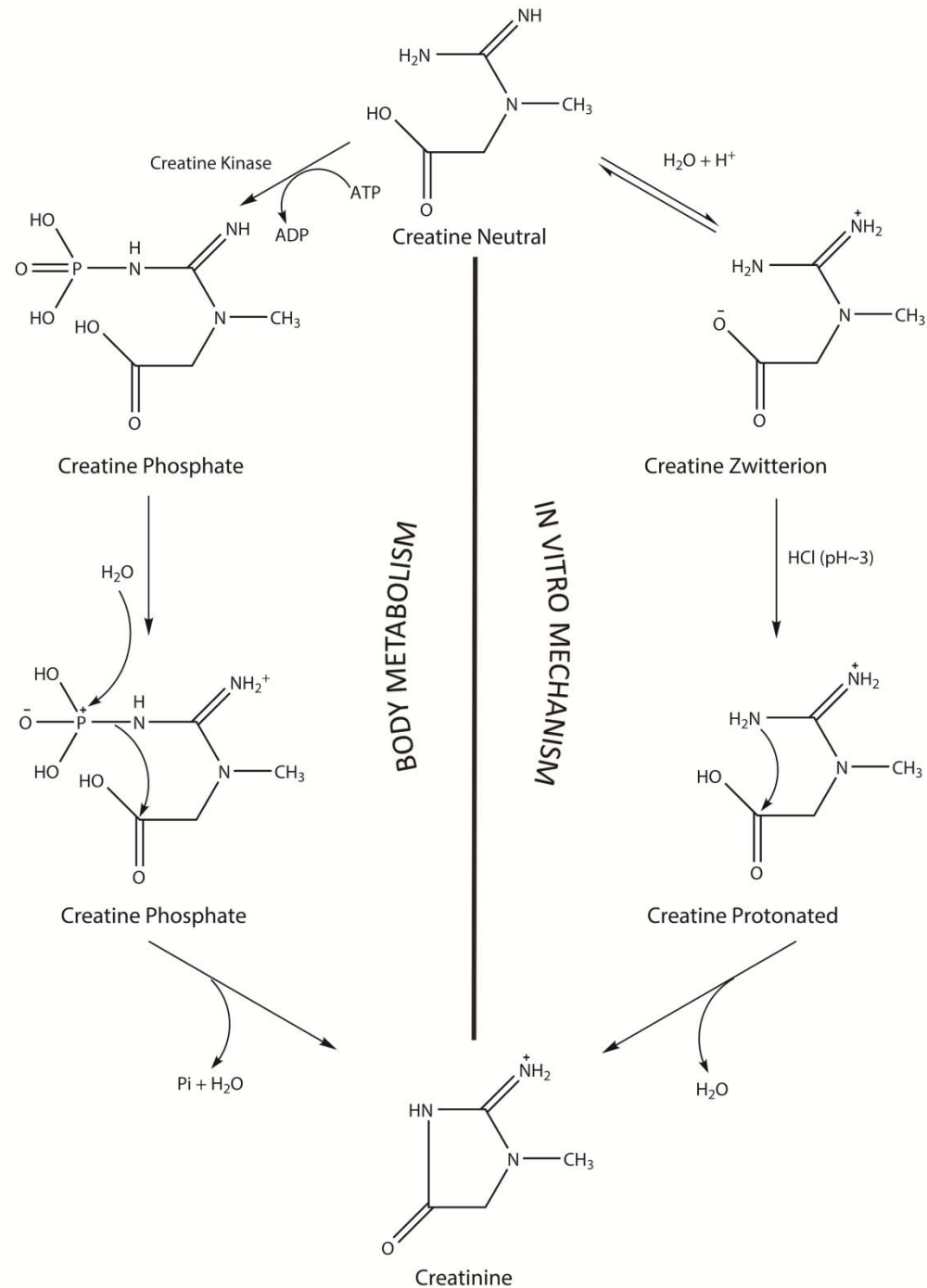
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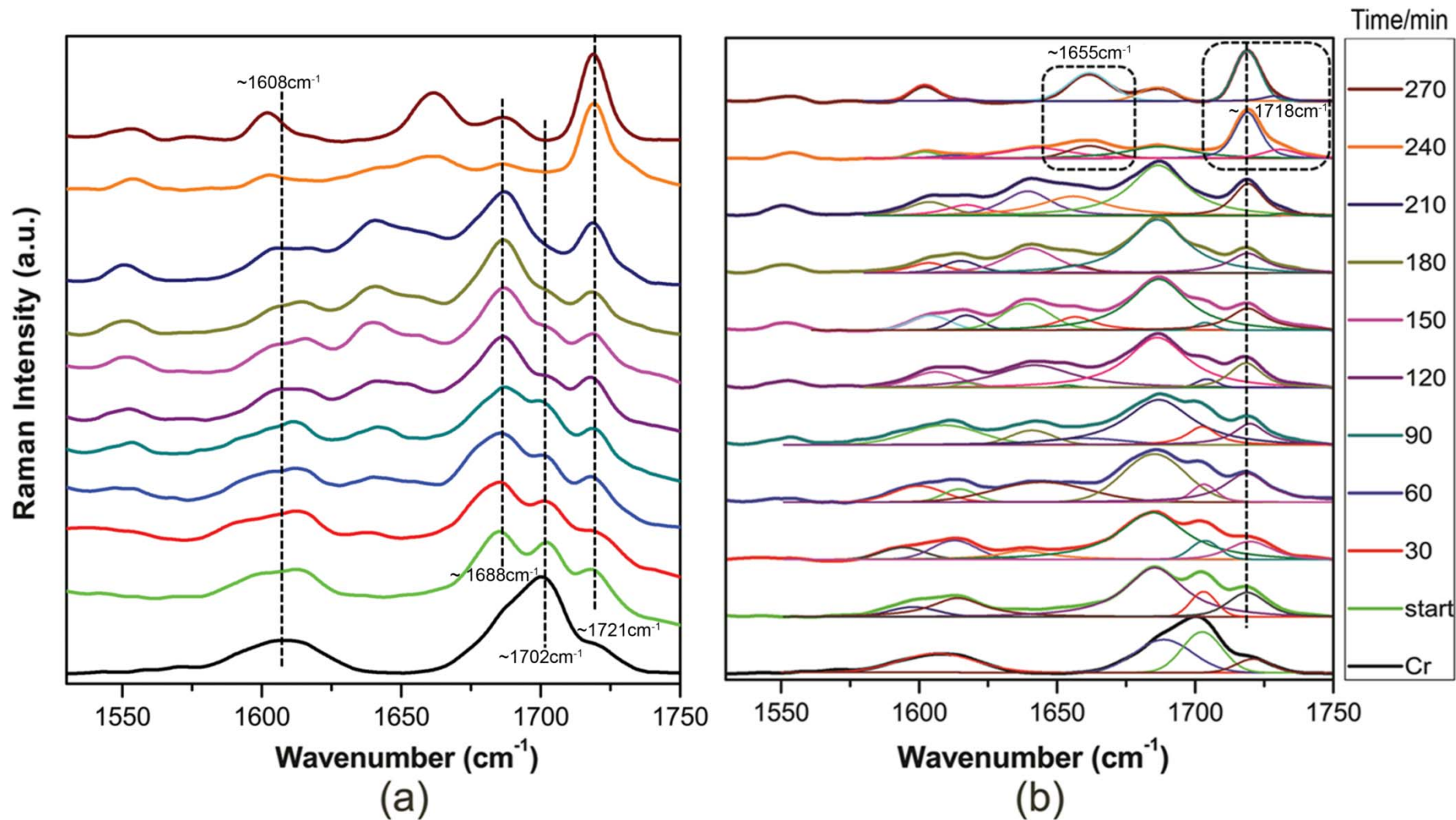
Date: 05/11/2025
Time: 10: 00 am

III/MPHYCC10 Atomic and Molecular Physics

Raman spectroscopic approach to monitor the in vitro cyclization of creatine → creatinine

- The **creatine → creatinine cyclization reaction** can be initiated in vitro at acidic pH.





(a) Room temperature Raman spectra of 0.01M aqueous Cr solution at pH 3 at different time intervals in the range $1530 - 1750\text{ cm}^{-1}$

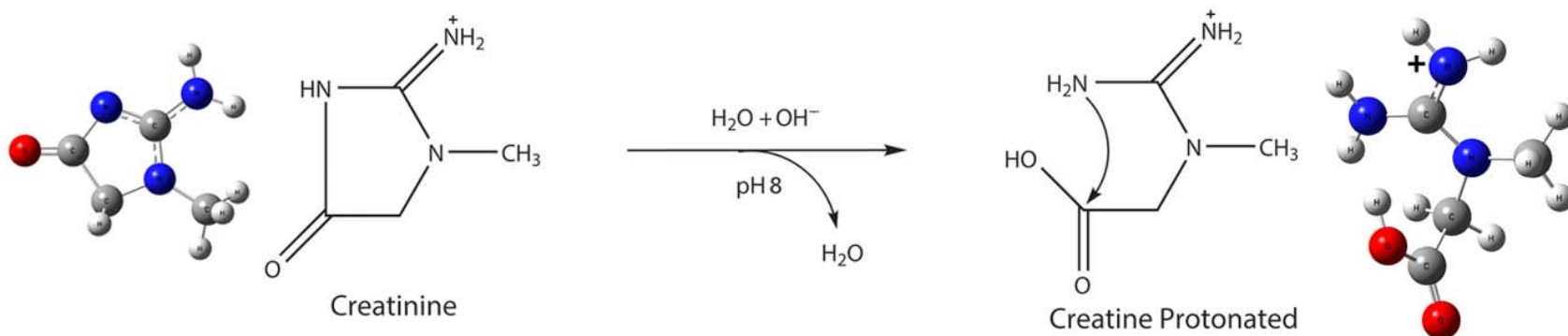
(b) Deconvoluted spectra of the Raman bands in the range $1530 - 1750\text{ cm}^{-1}$

- The equilibrium composition of neutral, zwitterionic and protonated microspecies of creatine has been monitored with time as the reaction proceeds.
- Time series Raman spectra show clear signature of creatinine formation at pH 3 after ~240 min at room temperature and reaction is faster at higher temperature.
- The spectra at pH 1 and pH 5 do not show such signature up to 270 min implying faster reaction rate at pH 3.

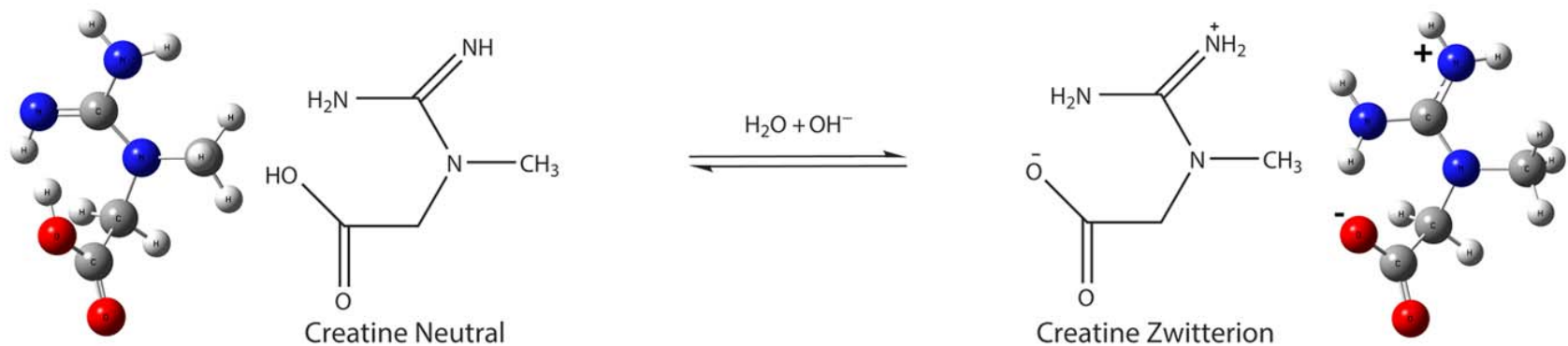
Decyclization of CRN: toxic substance converted to a beneficial product CR.

Since acidic pH supports cyclization, there is a possibility that a basic pH buffer might cause the decyclization of CRN to yield CR, as this reaction has been found to be reversible at neutral and basic pH.

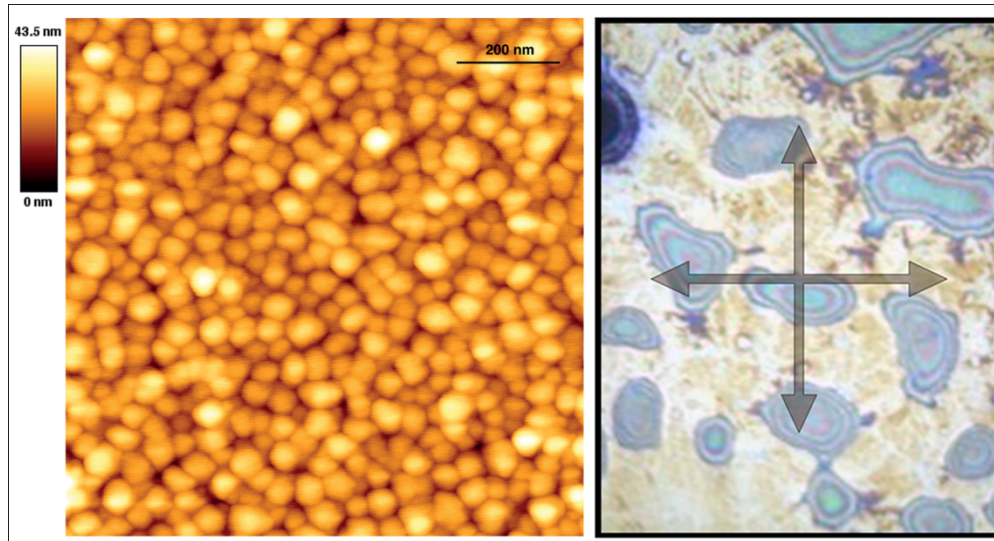
Reaction mechanism of in vitro decyclization of creatinine → creatine



In vitro
Creatinine $\rightarrow$ Creatine

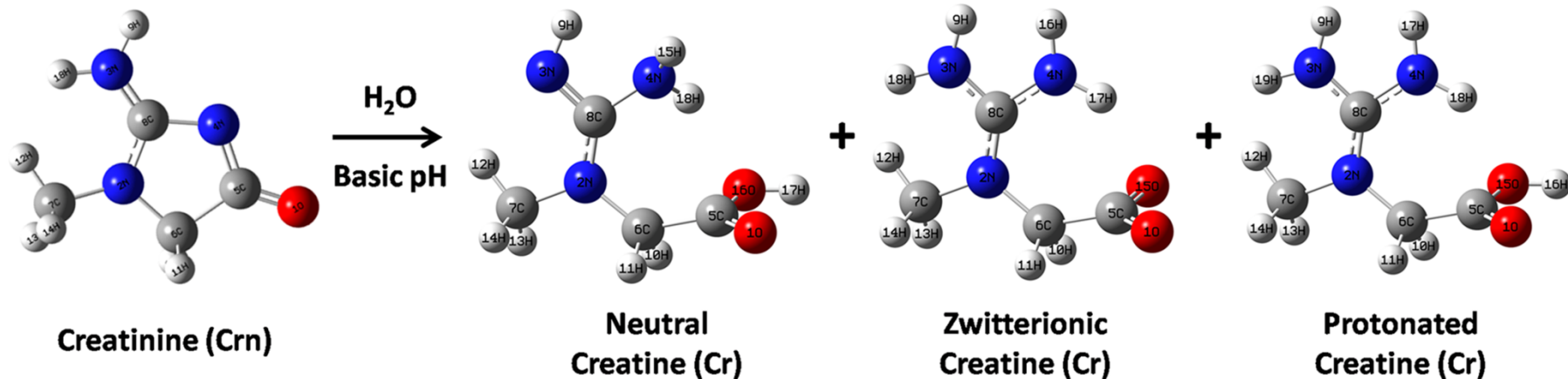
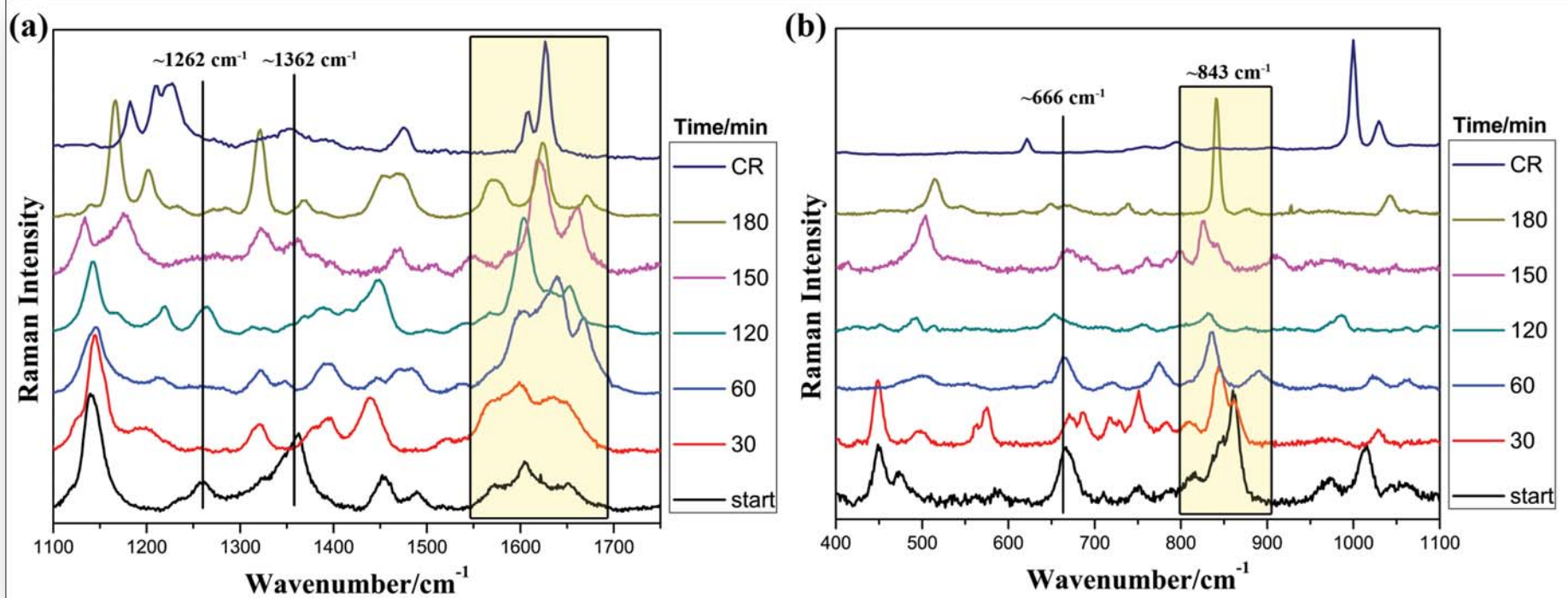


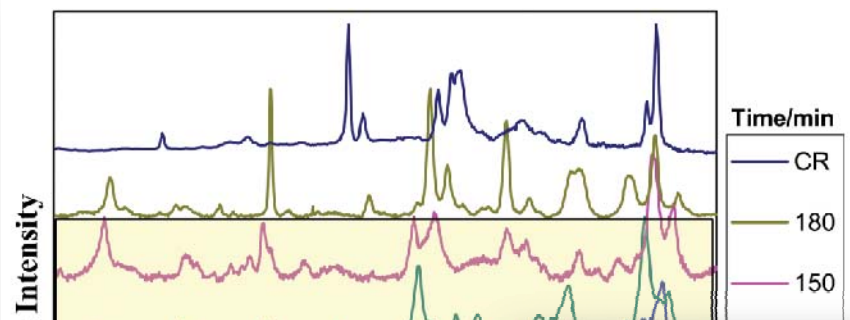
SILVER ISLAND FILM



- Ag island films prepared by the method used by Stöckle *et al.* (Appl. Spectrosc. 2000; 54, 1577) were used as SERS substrates.
- AFM tip (NSG10, NT-MDT) was used to obtain the topographic image of silver island film, showing average grain size ~ 40 nm.
- The time series SERS spectra on Renishaw inVia Raman spectrometer (532 nm line of a diode pumped solid state laser).

TIME SERIES SERS SPECTRA





120 min

- ❖ The Raman signatures for decyclization at room temperature are observed after 120 min at pH 8, 60 min at pH 10 and 30 min at pH 12.
- ❖ At higher pH values, although decyclization occurs faster, the reversibility is also more pronounced.

30 min

