Title: Coupling Between the Microscopic Dynamics of Solute and Solvent: Universal Picture of the Dynamical Transition
Proposal Number: B32-04; **Unique ID:** 19987; **Time Received:** Oct 1, 2014
Proposer Surname: SHARMA; **Instrument Requested:** NG-2 -- HFBS, High-flux backscattering spectrometer (CHRNS)

Reviewer: Reviewer 1
Rating: E-VG
The proposal aims at unraveling the coupling between the microscopic dynamics of solute and solvent on polystyrene-tolune model systems with a particular focus on a dynamical transition as evidenced by fixed-window scans on the backscattering spectrometer HFBS. The proposal further aims at showing that such a dynamic transition as it is commonly also observed in biomolecular systems is universal in the sense that it is a purely solvent driven phenomenon. The authors carried out preliminary work using molecular dynamics simulations on the here proposed systems with which they back-up there argument. What is missing is experimental verification which they here propose. The choice of systems and temperatures to be studied is well motivated.

Reviewer: Reviewer 2
Rating: E-VG
The study of coupling between solute and solvent dynamics in is an interesting one. Neutrons and backscattering spectroscopy is an appropriate approach for this study and a careful consideration is given in the proposal as to how deuteration can be used to good effect. One may in fact wonder if the full range of solute/solvent combinations is fully necessary. This makes the study thorough, but perhaps some instrument time could be saved by limiting the number of combinations.

Reviewer: Reviewer 3
Rating: E (Excellent)
The proposal aims to give an experimental proove of the coupling between solute and solvent dynamics even in absence of aqueous solvent and hydrogen bonding. This experiment is highly relevant for deep understanding of the famous and strongly discussed dynamical transition in hydrated proteins at about 220 K. MD simulation of the proposed experiment has been already performed which gives a solid base for defining the experimental conditions, i.e. temperature range and toluene/styrene ratios.

Reviewer: Reviewer 4
Rating: VG (Very Good)
This proposal aims to shed light on the so-called dynamical transition, which has been conceived in studies of protein dynamics. Here a simple model system of a solution of 2 glass formers will be studied. The phase diagram of this mixture in respect to temperature and solvent concentration will be characterised by elastic window scans.
Extensive MD simulations already exist to compare to. To unravel the different contributions to the dynamics 3 concentrations with different isotopic labelling are necessary. The beamtime request seems realistic. Certainly an interesting study in mixtures of complex liquids, which might provide some insight into the dynamics of biological molecules as well.

Reviewer: Reviewer 5
Rating: VG (Very Good)
In the search for a universal, solvent driven transition in solute dynamics the model system of polystyrene (PS) solvated with toluene was studied in a systematic molecular dynamics (MD) simulation. The results displayed in Fig.1 give reason to expect a successful experiment on HFBS.

Technical Review
Reviewer: Reviewer 6
Instrument Requested: NG-2 -- HFBS, High-flux backscattering spectrometer (CHRNS)
Days Requested: 7.0
Days Recommended: 7
Comments: For the proposed 17 fixed-window scans, 7 days are reasonable.

BTAC Review
Days Alloc.: 7.0
Comments: The BTAC recommends 7 days of beamtime. BTAC suggests to reduce the number of samples and complete a dynamics study, rather than only fixed-window scans.