



**ACERT 2015 Computational Methods Workshop, Speakers'  
Agenda *Final Draft, June 3, 2015***

**Tuesday June 9**

5:45pm – 7:00pm	Welcome Cocktail Hour Appetizers and Beverages (Cash Bar)	Kilpatrick's, Hilton Garden Inn
7:30pm	Dinner for Speakers and Advisory Board (Budil, Mattar, Saxena)	Madeline's, The Commons

**Wednesday June 10**

7:30 – 8:30am	Welcome, Registration & Coffee/Continental Breakfast	Baker Portico
8:30 – 9:15	Welcome and Talk 1: <b>Jack Freed</b> <i>Introduction to Computational ESR and to Producing Noiseless Spectra from Noisy Ones</i>	Baker 119
9:15 – 9:55	Talk 2: <b>Stefan Stoll</b> , <i>EasySpin</i>	Baker 119
9:55 – 10:15	Coffee Break	Baker Portico
10:15 – 10:55	Talk 3: <b>Christian Altenbach</b> , <i>EPR Data Analysis for the Rest of Us</i>	Baker 119
10:55 – 11:35	Talk 4: <b>Yevhen Polyhach</b> , <i>Coarse-grained Simulation Approaches for Rotamer Libraries</i>	Baker 119
11:35 – 12:15	Talk 5: <b>Peter Fajer</b> , <i>Simulations of the Rotamer Structure of Spin Labels</i>	Baker 119
12:15 – 2:00pm	Buffet Lunch / TECH Help Break	PSB 401
2:00 – 2:40pm	Talk 6: <b>Zhichun Liang</b> , <i>Motional Dynamics for 1 and 2 Nitroxides by Two-Dimensional ESR</i>	Baker 119
2:40 – 3:20	Talk 7: <b>Keith Earle</b> , <i>Multi-Frequency ESR and a New Tool for Simulating Saturated Spectra in the Slow-Motional Regime</i>	Baker 119
3:20 – 3:40	Coffee Break	Baker Portico
3:40 – 4:20	Talk 8: <b>Alex Nevzorov</b> , <i>Many-Body Theory of Electron-Electron and Electron-Nucleus Relaxation</i>	Baker 119
4:20 – 5:00	Talk 9: <b>Saba Mattar</b> , <i>Theory and Computation of hf and g Tensors by DFT</i>	Baker 119
5:15pm [sharp]	Shuttle Bus Departs from near the Clark Breezeway Exit to Winery Dinner	Clark Breezeway
6:15 – 9:00pm	Winery Dinner – Wagner Winery, Seneca Lake (optional)	Wagner Vineyard

Thank You for the Generous Support



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## Thursday June 11

7:30 – 8:30am	Coffee/Tea / Continental Breakfast / Posters	Clark Atrium
8:30 – 9:10	Talk 10: <b>Ilya Kuprov</b> , <i>Large-Scale Magnetic Resonance Simulations</i>	PSB 120
9:10 – 9:50	Talk 11: <b>Deniz Sezer</b> , <i>Biomolecular ESR and DNP ... in SILICO</i>	PSB 120
9:50 – 10:30	Talk 12 <b>Antonino Polimeno</b> , <i>Stochastic Modeling of Flexible Systems in Solution</i>	PSB 120
10:30 – 12:00	Coffee Break / Posters Session	Clark Atrium
12:00 – 1:30pm	Buffet Lunch	Clark Atrium
1:30 – 2:15	Demo 1 : <b>Stefan Stoll</b> , <i>EasySpin</i>	PSB 120
2:15 – 3:00	Demo 2 : <b>Christian Altenbach</b> , <i>MultiComponent and LongDistances</i>	PSB 120
3:00 – 3:45	Demo 3 : <b>John Franck</b> , <i>Making NLSL Accessible to the Next Generation of Scientists</i>	PSB 120
3:45 – 4:05	Coffee Break / Posters	Clark Atrium
4:05 – 5:15	Demo 4 and 5: <b>Yevhen Polyhach</b> , <i>MMM and Coarse-grained Simulation Approaches for Rotamer Libraries</i> and <b>Stephan Pribitzer</b> , <i>SPIDYAN</i>	PSB 120
5:15pm	Tour of ACERT labs (optional)	ACERT Labs
5:15 – 6:00pm	Poster Sessions	Clark Atrium
6:15 – 8:00pm	Conference Dinner	Baker Portico

## Friday June 12

7:30 – 8:30am	Coffee /Tea / Continental Breakfast	Clark Atrium
8:30 – 9:15	DEMO 6: <b>Saba Mattar</b> , <i>ORCA Software to Calculate the Magnetic Properties of Nitroxides</i>	PSB 120
9:15 – 10:00	DEMO 7: <b>Peter Fajer</b> , <i>CHARMM</i>	PSB 120
10:00 – 10:20	Coffee Break / Poster	Clark Atrium
10:20 – 11:05	DEMO 8: <b>Antonino Polimeno</b> , <i>Stochastic Approach for Flexible Molecules (SALEM)</i>	PSB 120
11:05 – 11:50	DEMO 9: <b>Ilya Kuprov</b> , <i>Spinach</i>	PSB 120
11:50 – 12:10	Workshop Closing Discussion and Concluding Remarks by Jack Freed	PSB 120
12:15 – 2:00pm	Buffet Lunch	Clark Atrium
2:00pm	Workshop Ends	