

SMASH 2000 Preliminary Schedule

[[Sunday](#)] [[Monday](#)] [[Tuesday](#)] [[Wednesday](#)]

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Sunday, July 16th		
12:00-5:00	Registration	APS Lobby
6:00-7:00	Dinner	Argonne Guest House
7:00-8:00	Plenary Speaker	Ad Bax - NIH <i>"NMR of Very Small Proteins in a Medium of Very Small Solvent Molecules."</i>
8:00-10:00	Mixer	Argonne Guest House
Monday, July 17th		
7:00-8:15	Breakfast	Argonne Guest House
8:25-8:30	Opening Remarks	Gary Martin
8:30-10:30	NMR of Natural Products	Chair: P.J. Sidebottom <ul style="list-style-type: none"> • Scott K. Smith - Merck & Co., Rahway, NJ <u>"The use of NMR Chemical Shift Libraries for the Dereplication of Natural Products."</u> • Antony Williams, Kirill Blinov, Mikhail Elyashberg and Eduard Martirosian - ACD Laboratories <i>"Recent Advances in the Use of NMR Prediction and Automated Structure Elucidation Software for Natural Product Characterization"</i> • David J. Russell, Chad E. Hadden, Gary E. Martin, Steven M. Musser, and Robert L. Dickey - Pharmacia Corp. <i>"Characterization of Submicromole Quantities of Marine Polyether (Red Tide) Toxins"</i> • G. Bringmann - Institut fuer Organische Chemie <i>"The use of hyphenated techniques for the elucidation of full absolute stereostructures of natural products directly from crude extracts"</i>
10:30-11:00	Break	APS - Gallery
11:00-12:30	Pulse Sequences	Chair: V.V. Krishnamurthy <ul style="list-style-type: none"> • Haruo Seto and K. Furihata - University of Tokyo <i>"Modified HMBC techniques useful for structural studies of natural products"</i>

		<ul style="list-style-type: none"> • Thomas Williamson, Brian L. Marquez, and William H. Gerwick - Oregon State University <u>"Survey of Methods for the Analysis of Long-Range Heteronuclear Couplings"</u> • Brian Antalek - Kodak <u>"The PGSE NMR Diffusion Experiment: A powerful tool for mixture analysis"</u> <u>ENC Varian Users Meeting Talk</u> • Krish Krishnamurthy - Varian <i>"Pulse Sequence Development - A LEGO Approach."</i>
12:30-2:00	Lunch	APS - Gallery
2:00-3:30	Graduate Student and Post Doc Session	<p>Chair: R.T. Williamson</p> <ul style="list-style-type: none"> • Brian Marquez, R. Thomas Williamson, William H. Gerwick - Oregon State University <i>"Application and Development of New NMR Techniques to Facilitate the Structure Elucidation of Small Molecule Natural Products"</i> • Jochen Junker, M. Kock, T. Linde - University of Frankfurt, Germany <i>"Why a Computer's Help is Needed for Structure Determination"</i> • Mari A. Smith and A. J. Shaka - University of California <i>"Improved Broadband Inversion Performance"</i>
3:30-5:00	Workshop (APS)	<ul style="list-style-type: none"> • G. Chmurny, D.J. Russell <i>Structure Elucidation</i> <p>[Send Suggestions for Discussion Topics]</p>
4:00-5:00	Tour	<ul style="list-style-type: none"> • Advanced Photon Source
6:00-7:00	Dinner	Argonne Guest House
7:00-8:00	Plenary Speaker	Cynthia Jameson - University of Illinois, Chicago <i>"The NMR Chemical Shift"</i>
8:00-10:00	Mixer	Argonne Guest House
<p>Tuesday, July 18th [top]</p>		
7:00-8:15	Breakfast	Argonne Guest House

8:30-10:30	Metabolism and NMR	<p>Chair: J.P. Shockcor</p> <ul style="list-style-type: none"> • Michael Reily, Donald G. Robertson, Robert E. Sigler, Dale Wells, David Patterson and Timothy Braden, - Warner Lambert <i>"Flow NMR as a Tool to Rapidly Evaluate Toxicity in Vivo"</i> • Paul E. Fagerness - Pharmacia <i>"Novel NMR Applications in Drug Metabolism"</i> • R. Duncan Farran, Valerie Walker, Graham A. Mills, John M. Mellor, G. John Langley - GlaxoWellcome <i>"Comatose with Proline: Pyridoxal Phosphate Deactivation by Pyrroline-5-carboxylate: Increased Risk of Vitamin B₆ Deficiency and Fits in Hyperprolomaemia Type II"</i>
10:30-11:00	Coffee Break	APS - Gallery
11:00-12:30	Solid State NMR of Small Molecules	<p>Chair A. Swanson</p> <ul style="list-style-type: none"> • Robin Harris - University of Durham, UK <i>"NMR Crystallography?"</i> • S. R. Byrn, J. G. Stowell, P. Tishmack, and R. Te - Purdue University <i>"Setting up Region-Selected Heteronuclear Correlation Experiments"</i> • Harald Günther*, Martin Kühnen, and Andreas Pepels - University of Siegen, Germany <i>"Solid State NMR of Organolithium Compounds: Structural Information from Quadrupolar ⁷Li Coupling"</i>
12:30-2:00	Lunch	APS - Gallery
2:00-3:30	Workshop (APS)	<ul style="list-style-type: none"> • A. Swanson, S.R. Maple <i>LC/NMR</i> <p>[Send Suggestions for Discussion Topics]</p>
3:30-5:00	Workshop (APS)	<ul style="list-style-type: none"> • G. Bruahman, G. Nemeth <i><u>Direct Injection NMR</u></i> <p>[Send Suggestions for Discussion Topics]</p>

4:00-5:00	Tour	<ul style="list-style-type: none"> Advanced Photon Source
6:00-11:00	Poster Session and Buffet Dinner	Chair: D. Lankin [Poster Submittal Information]
Wednesday, July 19th [top]		
7:00-8:15	Breakfast	Argonne Guest House
8:30-10:30	Tips & Techniques	Chair: D. Lankin <ul style="list-style-type: none"> Janice K. Gard, Marty Pagel, Shengtian Yang - Monsanto <u>"Quantitative NMR"</u> Bruce D. Hilton - Pharmacia <i>"Practical Aspects of Excitation and Spin Locking in 1D-TOCSY and Related Experiments"</i> Eugene P. Mazzola - US-FDA <i>"Beware Analogs"</i> Daneen T. Angwin and Chad E. Hadden. - Pharmacia <i>"How Not to Miss Direct Correlation Responses in Your GHSQC or GHMQC Spectra"</i> Ronald C. Crouch, Krish Krishnamurthy -Varian NMR Systems <i>"Setting up Region-Selected Heteronuclear Correlation Experiments"</i>
10:30-11:00	Coffee Break	APS - Gallery
11:00-12:30	Forensic NMR	Co-Chairs: J. Meyers & P. Hays <ul style="list-style-type: none"> Pr. Gérard Martin - Eurofins Scientific <i>"Application of SNIF-NMR and other isotopic techniques in the fight against counterfeiting of fine chemicals and pharmaceuticals"</i> Thomas Schäfer, Torsten Schönberger, - <i>"Analysis and Profiling of Ecstasy Tablets: The NMR Approach"</i> John Meyers and Patrick Hays - Drug Enforcement Administration (DEA) <i>"DEA's Use of NMR in the Analysis of Drugs"</i>

12:30-12:45	Closing Remarks	APS
12:45	Box lunch & departure	APS - Gallery