



WATOC 2017

11th Triennial Congress of the World Association
of Theoretical and Computational Chemists

27 August – 1 September 2017

Munich, Germany



BOOK OF ABSTRACTS
WITH SCIENTIFIC PROGRAM



LUDWIG-
MAXIMILIANS-
UNIVERSITÄT
MÜNCHEN

www.watoc2017.com

Munich

2017

WATOC

SCIENTIFIC PROGRAM



Time	Foyer
12:00 – 15:00	REGISTRATION

Time	Philharmonic Hall
	OPENING CEREMONY <i>Chair: Christian Ochsenfeld</i>
15:00 – 15:50	Opening Schedule: <i>Christian Ochsenfeld</i> (Chair of WATOC2017) <i>Walter Thiel</i> (WATOC President) <i>Barbara Conrath</i> (Vice President of the University of Munich (LMU)) <i>Helmut Schwarz</i> (President of Humboldt Foundation (AvH)) Music Intermezzo by <i>Ville Kaila</i> (violin), <i>Lika Bibileishvili</i> (piano)
15:50 – 17:10	Plenary Session A <i>Chair: Peter Gill</i>
15:50 – 16:30	PL-1 <i>Todd Martinez</i> Ground and excited state dynamics on graphical processing units
16:30 – 17:10	PL-2 <i>Benedetta Mennucci</i> Present and future of multiscale approaches combining quantum chemistry and classical models: a personal overview
17:10 – 17:40	COFFEE BREAK
17:40 – 19:00	Plenary Session B <i>Chair: Leo Radom</i>
17:40 – 18:20	PL-3 <i>Trygve Helgaker</i> Quantum chemistry in magnetic fields
18:20 – 19:00	PL-4 <i>Helmut Schwarz</i> Mechanistic variants of metal-oxide mediated C-H bond activation: experiment and theory in concert

Time	Foyer
19:00 – 22:00	WELCOME RECEPTION – supported by BASF

Time	Philharmonic Hall		Carl-Orff Hall		Black Box		Small Concert Hall		Carl-Amery Hall		Multipurpose Room	
09:00 – 09:40	PL-5	Plenary Session C <i>Chair: Kenneth Ruud</i> Edward Valeev Reduced scaling and controlled precision: extending the reach of many-body electronic structure										
09:40 – 10:10	COFFEE BREAK											
10:10 – 12:15	Invited Session 1 <i>Chair: Thomas Jagau</i>		Invited Session 2 <i>Chair: Tim Clark</i>		Invited Session 3 <i>Chair: Tomasz Wesolowski</i>		Invited Session 4 <i>Chair: Hans Jørgen Aagaard Jensen</i>		Invited Session 5 <i>Chair: Manabu Sugimoto</i>		Invited Session 6 <i>Chair: Henry Rzepa</i>	
10:10	I-011	<i>Peter Gill</i> Strong correlation in electron gases	I-021	Peter Schwerdtfeger From graphene to graphyne, fullerenes, fulleroids, gaudienes and their golden duals	I-031	Lucas Visscher Subsystem and approximate DFT approaches for electronically excited states of complex molecular systems	I-041	Kenneth Ruud 4-component relativistic calculations with periodic boundary conditions	I-051	<i>Hiromi Nakai</i> Chemical reaction simulations on CO ₂ chemical absorption process	I-061	<i>Odile Eisenstein</i> Can carbon-13 NMR chemical shifts inform on reactivity in organometallic chemistry?
10:35	I-012	<i>Garnet Chan</i> Notes on the complexity of electronic structure theory	I-022	Kwang Soo Kim Graphene nanoribbon based electronics and spintronics	I-032	Neepa Maitra Confronting memory-dependence in time-dependent density functional theory	I-042	<i>Pekka Pyykkö</i> Recent results on compounds of heavy, and heaviest elements	I-052	<i>Nuria Lopez</i> New aspects in the simulations of heterogeneous catalysis	I-062	<i>Michael Buehl</i> Exploring NMR properties of paramagnetic Cu phenolic oxime complexes
11:00	I-013	<i>Jürgen Gauss</i> Beyond standard coupled-cluster theory and towards full configuration interaction	I-023	Jean-Luc Bredas Polymer/fullerene solar cells: characterization of the intermolecular interactions and interfacial charge-transfer states	I-033	Sharon Hammes-Schiffer Multicomponent density functional theory: integrating electronic and nuclear quantum effects	I-043	<i>Wenjian Liu</i> New Scenarios for Strongly Correlated Electrons	I-053	<i>Tore Brinck</i> σ -hole Bonding in the Catalysis of Nanostructured Metals: Surface Properties as Guides to Local Reactivity	I-063	<i>Gustavo Aucaer</i> NMR spectroscopic parameters of HB containing molecules and aggregates of DNA base pairs
11:25	I-014	<i>Poul Jørgensen</i> Cluster perturbation theory for energies and molecular properties	I-024	Marco Bernardi Advances in computing charge carrier dynamics from first principles	I-034	Eberhard Gross Potential-energy surfaces and Berry phases beyond the born-oppenheimer approximation: a new perspective on non-adiabatic dynamics	I-044	<i>Trond Saue</i> Variational perturbation theory in geochemistry	I-054	<i>Stuart Macgregor</i> Modelling alkane σ -Complexes in the solid state	I-064	<i>Ibon Alkorta</i> Anion-anion and cation-cation halogen and hydrogen bonded complexes
11:50	I-015	<i>Martin Head-Gordon</i> Some recent advances in variational energy decomposition analysis of electronic structure calculations	I-025	Jochen Blumberger Simulation of electron transfer on the nanoscale: from molecules to biomolecules to materials	I-035	Katarzyna Pernal Adiabatic connection approach toward including dynamic correlation for multireference wavefunctions	I-045	<i>Marcel Swart</i> Characterization of reactive high-valent transition-metal complexes	I-055	<i>Michelle Coote</i> Directionality and the role of polarization in electrostatic catalysis	I-065	<i>Sotiris Xantheas</i> Modeling of the spectroscopic signatures of water in different environments
12:15 – 13:45	LUNCH BREAK											

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
13:45 15:50	Invited Session 7 <i>Chair: Henrik Zipse</i>	Invited Session 8 <i>Chair: Martin Head-Gordon</i>	Invited Session 9 <i>Chair: Hiromi Nakai</i>	Invited Session 10 <i>Chair: H. Bernhard Schlegel</i>	Invited Session 11 <i>Chair: Oliver Kühn</i>	Invited Session 12 <i>Chair: Stefan Knippenberg</i>
13:45	I-071 <i>Jeremy Harvey</i> Modelling reaction mechanisms and kinetics in homogeneous catalysis: challenges and progress	I-081 Gustavo Scuseria Symmetry projected coupled cluster theory	I-091 Weitao Yang Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations	I-101 <i>Kurt Kremer</i> Open systems simulations of macromolecular solutes through adaptive resolutions simulations (AdResS)	I-111 <i>David Clary</i> Quantum dynamical and semi-classical calculations on chemical reactions with application to decomposition of nerve agents	I-121 <i>Benjamin Fingerhut</i> Numerical exact MACGIC-QUAPI simulations of electron transfer dynamics in <i>Drosophila</i> cryptochrome (dCRY)
14:10	I-072 <i>Peter Richard Schreiner</i> London dispersion effects in molecular chemistry – reconsidering steric effects[1]	I-082 Hans-Joachim Werner Accurate treatment of long-range correlation effects in large molecules using explicitly correlated local coupled-cluster methods	I-092 Peter Pulay Ultrafast quantum/molecular mechanics: thermodynamic integration and van der Waals parameters	I-102 <i>Florian Müller-Plathe</i> Multiscale molecular modelling of soft materials: the challenge of dynamics	I-112 <i>Irene Burghardt</i> High-dimensional quantum dynamics of functional organic polymer materials: Coherence, localization, and (dis)order	I-122 <i>Christel Marian</i> TADF efficiencies in coinage-metal coordination complexes and metal-free donor-acceptor systems
14:35	I-073 <i>Leo Radom</i> Impact of hydrogen bonding on the susceptibility of peptides to oxidation	I-083 Örs Legeza Tensor product methods and entanglement measures for strongly correlated molecular systems	I-093 Henry F. Schaefer Fast construction of the exchange operator in an atom-centered basis with concentric atomic density fitting	I-103 <i>Christoph Dellago</i> Exploring the mechanism and kinetics of nucleation processes: from crystallization to cavitation	I-113 <i>Roland Mitric</i> Light-induced nonadiabatic dynamics: from isolated molecules to molecular assemblies and light-harvesting nanostructures	I-123 <i>Ilaria Ciofini</i> New tools for the description of excited states of molecular systems in complex environment
15:00	I-074 <i>Yitzhak Apeloig</i> Isomerization mechanisms around E=E' (E,E'=C,Si) bonds. Experiment and theory	I-084 Jeppe Olsen Wave functions with several sets of optimized orbitals	I-094 Dage Sundholm Numerical electronic structure theory methods for massively parallel computations on molecules	I-104 <i>Christine Peter</i> A multiscale simulation perspective on mineralization processes	I-114 <i>Ivano Tavernelli</i> New strategies for non-adiabatic dynamics with trajectories	I-124 <i>Satoshi Maeda</i> Artificial force induced reaction (AFIR) method for automated search of adiabatic and non-adiabatic pathways
15:25	I-075 <i>Kendall Houk</i> Dynamics of pericyclic reactions	I-085 John Stanton Active thermochemical tables: what they are, why I care about them, and why you should	I-095 <i>Petr Čársky</i> Fourier transform of 1/r on graphical processing units – promising tool for applications in nanolithography	I-105 <i>Alexander Nemukhin</i> Computational modeling of molecular processes in proteins	I-115 <i>Graham Worth</i> Quantum dynamics simulations of photo-excited molecules using the MCTDH method	I-125 <i>Henrik Koch</i> The curious case of conical intersections in coupled cluster theory
15:50 16:20	COFFEE BREAK					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
16:20 18:25	Contributed Session 1 <i>Chair: David Tozer</i>	Contributed Session 2 <i>Chair: Sotiris Xantheas</i>	Contributed Session 3 <i>Chair: Jörn Manz</i>	Contributed Session 4 <i>Chair: William Hase</i>	Contributed Session 5 <i>Chair: Kaori Fukuzawa</i>	Contributed Session 6 <i>Chair: Henk Eshuis</i>
16:20	C-011 <i>Georg Schreckenbach</i> Modeling of two-dimensional (2D) materials: influence of chemical modifications	C-021 <i>Thomas Kühne</i> The name is bond - hydrogen bond	C-031 <i>Shirin Faraji</i> Utilizing light for repair of light-induced DNA damages: clever mode of action of DNA photolyases	C-041 <i>Manabu Sugimoto</i> First-principles molecular dynamics simulations on ammonia synthesis and decomposition	C-051 <i>Andreas Hauser</i> Carbon nanotubes immersed in superfluid helium: An incomplete flooding due to quantum effects	C-061 <i>Mercedes Alonso</i> Conductance switching in expanded porphyrins through aromaticity and topology changes
16:35	C-012 <i>Lorenzo Maschio</i> Local correlation for crystalline solids: dual basis sets by projection in the reciprocal space	C-022 <i>Tristan Beraud</i> High-throughput screening of drug-membrane thermodynamics	C-032 <i>Oliver Kühn</i> Ultrafast spin-flip dynamics in transition metal complexes triggered by soft X-ray light	C-042 <i>Tetsuya Taketsugu</i> Reaction-path bifurcation analyses based on Valley-Ridge transition and global reaction route mapping	C-052 <i>Raul Alvarez-Idaboy</i> The role of acid-base equilibria in formal hydrogen transfer reactions: uric acid with tryptophanyl radical	C-062 <i>Daniel Aravena</i> Spin-dependent transport and magnetoresistance in metalloporphyrin-based supramolecular wires at room temperature
16:50	C-013 <i>Marek Sierka</i> Density functional theory for periodic systems using density fitting and continuous fast multipole method	C-023 <i>Ragnar Björnsson</i> New insights into nitrogenase: QM/MM broken-symmetry DFT studies of FeMoco and the P-cluster	C-033 <i>Debashree Ghosh</i> Photoprotection mechanism in eumelanin	C-043 <i>Mark Waller</i> Retrosynthesis and reaction prediction with deep neural networks	C-053 <i>Albeiro Restrepo</i> Thermodynamics of the partition of Ibuprofen in a lipid bilayer	C-063 <i>Alexandre Magalhães</i> Catalyzing chemical reactions inside carbon nanotubes
17:05	C-014 <i>Joao B. L. Martins</i> Adsorption of glycerol and dihydroxyacetone on CaO and MgO surfaces	C-024 <i>Alister Page</i> Quantum chemical insights into polymer solvation and Hofmeister effects in aqueous and non-aqueous environments	C-034 <i>Daniel Roca-Sanjuán</i> Chemically-induced excited-state chemistry	C-044 <i>Seiji Mori</i> Graph theory approach in exploration of reaction path networks: Rh(I)BINAP-catalyzed isomerization of allylic amine	C-054 <i>Alessandro Contini</i> Automatization of the Nwat-MMGBSA method to rescore docking results in medium-throughput virtual screening applications	C-064 <i>Michal Straka</i> Theoretical calculations of endohedral fullerenes: from chemical bonding to single-molecule switches
17:20	C-015 <i>Wolfgang Heringer</i> Electronic structure of molecules at metal surfaces: recent results on organic molecules and coordination compounds	C-025 <i>Olaf Wiest</i> The past, present, and future of Q2MM	C-035 <i>Bo Durbeej</i> Exploiting excited-state aromaticity for the design of efficient light-driven rotary molecular motors	C-045 <i>Woo Youn Kim</i> Automated searching method for reaction paths using molecular graphs and chemical reaction network	C-055 <i>Przemyslaw Dopieralski</i> Stressed disulfide bonds in alkaline solution	C-065 <i>Matthias Lein</i> Structural and electronic properties of carbon nano-onions
17:35	C-016 <i>Ralf Tonner</i> Explaining organic chemistry at surfaces with energy decomposition analysis	C-026 <i>Dmitry Nerukh</i> Hybrid molecular dynamics - hydrodynamics modelling of liquid solutions: whole virus at atomistic resolution	C-036 <i>László Turi</i> Electronic excited state lifetimes of anionic water clusters: a quantized time correlation function approach	C-046 <i>Anoop Ayyappan</i> Exploring chemical evolution using tabu-search based automated reaction finding algorithm	C-056 <i>Joonkyung Jang</i> Wetting behavior of a surface decorated with periodic pillars	C-066 <i>Juan F. Espinal</i> Nickel effect on the spacing of 002 plane in a graphite-like structure
17:50	C-017 <i>Antti Karttunen</i> Crystal structure prediction of inorganic-organic coordination polymers	C-027 <i>Laurence Leherte</i> Reduced point charge models of proteins - influence of protein-solvent interactions	C-037 <i>Luca De Vico</i> How to control the absorption wavelength of light harvesting complexes	C-047 <i>Wolfgang Quapp</i> Patterns of moving saddle points in catalysis and mechanochemistry	C-057 <i>Petra Imhof</i> Communication in proteins and protein-substrate complexes	C-067 <i>Oscar Lung Wa Chung</i> Mechanistic insights on Ni-catalyzed selective C-O activation & Cu-catalyzed reductive CO ₂ coupling to form oxalate
18:05	C-018 <i>Jon M. Matxain</i> Transition metal doped magnetic Zn ₁₂ S ₁₂ nanoparticles	C-028 <i>Xabier Lopez</i> Insights into the structural toxicity of aluminum with biomolecules, using a computational approach	C-038 <i>Valérie Brenner</i> Excited states deactivation in model proteins chains: Nonadiabatic dynamics simulations and ab initio methods	C-048 <i>Michael Springborg</i> On the theoretical optimization of properties	C-058 <i>Wieslaw Nowak</i> Camphore's and Huperzine's adventures in proteinland	C-068 <i>Amalia I. Poblador Bahamonde</i> Mechanistic investigation on the Pd-catalyzed hydrogenation of 1,6-enynes: a DFT approach
18:20 20:00	DINNER BREAK					
20:00 22:00	Poster Session 1 – supported by ACS Energy Letters					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	PL-6 <i>Plenary Session D</i> <i>Chair: Josef Michl</i> <i>Giulia Galli</i> Electrochemistry meets condensed matter physics: first principles simulations of photocatalytic materials					
09:40 – 10:10	COFFEE BREAK					
10:10 – 12:15	Invited Session 13 <i>Chair: Teresa Head-Gordon</i>	Invited Session 14 <i>Chair: Arne Lüchow</i>	Invited Session 15 <i>Chair: Regina de Vivie-Riedle</i>	Invited Session 16 <i>Chair: Attila Császár</i>	Invited Session 17 <i>Chair: Roland Mitric</i>	Invited Session 18 <i>Chair: Christine Peter</i>
10:10	I-131 <i>Walter Thiel</i> Semiempirical quantum chemistry: methodology and excited-state dynamics	I-141 <i>Ali Alavi</i> Recent developments and applications of full configuration interaction quantum Monte Carlo	I-151 Leticia González Photostability and photodamage in DNA building blocks	I-161 <i>Joel Bowman</i> Many-body potentials for water and protonated water clusters and VSCF/VCI calculations of IR spectra	I-171 <i>Fernando Martin</i> Attochemistry: imaging and controlling electron dynamics in molecules	I-181 <i>Zexing Cao</i> Global simulation of cyanohydrin cleavage by hydroxynitrile lyases
10:35	I-132 <i>Stefan Grimme</i> Applications of the extended tight binding method (GFN-xTB)	I-142 <i>Seiichiro Ten-no</i> Multi-state effective Hamiltonian and size-consistency corrections for stochastic configuration interactions	I-152 Roland Lindh Non-adiabatic chemiluminescent dynamics of the methyl-substituted 1,2-dioxetanes	I-162 <i>Robert Berger</i> What molecules can reveal about fundamental interactions	I-172 <i>Shaul Mukamel</i> Novel multidimensional spectroscopy of conical intersections with X-ray pulses and quantum light	I-182 <i>Tim Clark</i> Metadynamics simulations of G-protein coupled receptors
11:00	I-133 <i>Frank Jensen</i> Developing improved force fields	I-143 <i>Roi Baer</i> Stochastic orbitals for electronic structure and quantum chemistry	I-153 <i>Chantal Daniel</i> Simulation of ultrafast excited state dynamics in transition metal complexes	I-163 <i>R. Benny Gerber</i> Computational vibrational spectroscopy: anharmonic algorithms and determination of 3D structures of biomolecular conformers	I-173 <i>H. Bernhard Schlegel</i> Angular dependence of ionization by short, intense pulses of linear and circularly polarized light	I-183 <i>Markus Meuwly</i> Quantitative atomistic simulations for chemical and biological applications
11:25	I-134 <i>Siewert-Jan Marrink</i> Computational microscopy of (bio) molecular processes	I-144 <i>David Tanner</i> New formulation of quantum mechanics using complex trajectories: application to nonadiabatic transitions and optical excitation	I-154 <i>George Schatz</i> Theories of SERS, TERS, electrochemistry and plasmon-enhanced energy transfer	I-164 <i>Lorenz S. Cederbaum</i> On systems with and without excess energy in environment ICD and other interatomic mechanisms	I-174 <i>Peter Saalfrank</i> Light-driven processes in molecular systems: from photophysics to photochemistry	I-184 <i>Sereina Riniker</i> Replica-exchange enveloping distribution sampling (RE-EDS) to calculate relative binding free energies
11:50	I-135 <i>Jan H. Jensen</i> Using semiempirical methods for fast and automated predictions	I-145 <i>Mark Gordon</i> Dispersion in intermolecular interactions	I-155 <i>Joseph Subotnik</i> Electrochemistry and non-adiabatic dynamics at metal surfaces: the importance of electron-electron correlation	I-165 <i>Sergey Yurchenko</i> Theoretical molecular line lists for atmospheric characterizations of exoplanets	I-175 <i>Peter Knowles</i> On the perturbative computation of ionization energies	I-185 <i>Xuhui Huang</i> Kinetics-controlled molecular self-assembly processes elucidated by kinetic network models
12:15 – 13:45	LUNCH BREAK					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
13:45 15:50	Invited Session 19 <i>Chair: Johan Åqvist</i>	Invited Session 20 <i>Chair: Trygve Helgaker</i>	Industry Session 1 - supported by BASF <i>Chair: Ansgar Schäfer</i>	Invited Session 21 <i>Chair: Markus Meuwly</i>	Invited Session 22 <i>Chair: Odile Eisenstein</i>	Invited Session 23 <i>Chair: Gregory Beran</i>
13:45	I-191 <i>Teresa Head-Gordon</i> New methods and models for condensed phase simulation	I-201 <i>Don Truhlar</i> Recent progress in density functional theories	IN-1 <i>Peter Deglmann</i> The challenge of chemical thermodynamics and kinetics for real world	I-211 <i>Michele Parrinello</i> Enhanced sampling for chemistry	I-221 <i>Elfi Kraka</i> A comprehensive view on the Claisen rearrangement of chorismate via a new quantum chemical toolbox	I-231 <i>Takeshi Yanai</i> Projector augmented wave method incorporated into Gauss-type atomic orbital based density functional theory
14:10	I-192 <i>Jiali Gao</i> Methods and applications of multistate density functional theory (MSDFT)	I-202 <i>Carlo Adamo</i> Non-empirical double-hybrid functionals: more theoretical constrains, better performances?	IN-2 <i>Christoph Taeschler</i> Mechanistic aspects of high temperature reactions of acetonitrile	I-212 <i>Ulf Ryde</i> Comparison of quantum-mechanical approaches to calculate ligand-binding affinities with free-energy perturbation	I-222 <i>Gabriel Merino</i> Massive search of planar hyper-coordinate carbon atoms	I-232 <i>Claudia Draxl</i> From evaluation of methodology to error bars in computational materials science
14:35	I-193 <i>Modesto Orozco</i> DNA. A fascinating multiscale problem	I-203 <i>Kieron Burke</i> Reliable DFT results for spin-crossover complexes	IN-3 <i>Michael Edmund Beck</i> Digging deep into binding modes in protein-ligand-complexes by quantum chemistry	I-213 <i>Zhipan Liu</i> Automated reaction pathway sampling using stochastic surface walking method for predicting chemical reactions	I-223 <i>Raghavan B. Sunoj</i> Non-covalent interactions in asymmetric catalysis: a mechanistic voyage from rationalizations to predictions	I-233 <i>Beate Paulus</i> The method of increments applied to weakly bound systems
15:00	I-194 <i>Shina Caroline Lynn Kamerlin</i> Dynamics, flexibility, cooperativity and the evolution of enzyme function	I-204 <i>G Narahari Sastry</i> Cooperativity of non-covalent interactions	IN-4 <i>Marcel Verdonk</i> The use of scoring functions for structure-based drug discovery	I-214 <i>GuanHua Chen</i> Time-dependent density-functional theory for open system and its applications	I-224 <i>Gopalan Rajaraman</i> Are single molecule magnets predictable? Learning from Ab-initio calculations on lanthanide and transition metal molecular-magnets	I-234 <i>Krzysztof Szalewicz</i> Physics-based intermolecular potentials for material design
15:25	I-195 <i>Helmut Grubmüller</i> Towards a mechanistic understanding of ribosomal function	I-205 <i>David Sherrill</i> Large datasets for benchmarking noncovalent interactions	IN-5 <i>Thomas Fox</i> Free energy calculations in drug design	I-215 <i>Michele Pavanello</i> Real and imaginary-time electron dynamics of open quantum subsystems	I-225 <i>Laura Gagliardi</i> Computationally guided discovery of metal-decorated metal-organic frameworks active for catalysis	I-235 <i>WanZhen Liang</i> Analytic energy gradient and hessian of TD-DFT/MM excited-state: implementation and applications
15:50 16:20	COFFEE BREAK					

Time	Philharmonic Hall		Carl-Orff Hall		Black Box		Small Concert Hall		Carl-Amery Hall		Multipurpose Room	
16:20 18:20	Contributed Session 7 <i>Chair: Kieron Burke</i>		Contributed Session 8 <i>Chair: Max Holthausen</i>		Industry Session 2 - supported by BASF <i>Chair: Robert Franke</i>		Contributed Session 9 <i>Chair: Daniel Escudero</i>		Contributed Session 10 <i>Chair: Woo Youn Kim</i>		Contributed Session 11 <i>Chair: Iris Antes</i>	
16:20	C-071	<i>Mario Piris</i> NOF-MP2: a global method for the electron correlation	C-081	<i>Andrey Rogachev</i> Trianionic corannulene: tuning stability of supramolecular aggregates with alkali metal size	IN-6	<i>Glenn Jones</i> Industrial applications of first-principles modelling to obtain quality measures for screening of catalyst materials	C-091	<i>Masayoshi Nakano</i> Quantum master equation approach to singlet fission dynamics in molecular aggregates	C-101	<i>Mercè Deumal</i> Unraveling the magnetic transition temperature from changes in spin correlation	C-111	<i>Ferran Feixas</i> Accelerating metal-directed protein folding and molecular recognition with enhanced sampling techniques
16:35	C-072	<i>Heather Kulik</i> Recovering the flat plane condition in electronic structure theory at semi-local density functional theory cost	C-082	<i>Carsten Baldauf</i> About underappreciated, yet active conformations of thiourea organocatalysts			C-092	<i>Carmen Herrmann</i> Pathways in molecular conductance and spin coupling	C-102	<i>Nathalie Guihery</i> The magnetic couplings sensitivity to Fock exchange in DFT is not due to spin over-delocalization	C-112	<i>Snezana Zaric</i> Role of aromatic, aliphatic and backbone interactions in the stability of amyloids
16:50	C-073	<i>Pierre-François Loos</i> Dressing the CI matrix with explicit correlation	C-083	<i>Brian Yates</i> A new mechanism for gold catalysis	IN-7	<i>Hanne Falsig</i> A complete reaction mechanism for standard and fast SCR of NOx on VOx/TiO2(001) catalysts	C-093	<i>Takatoshi Fujita</i> Exciton dynamics in organic optoelectronic materials	C-103	<i>Annika Bande</i> Quantum dot inter-Coulombic decay governed by the quantum size effect	C-113	<i>Vladimir Palyulin</i> Design of AMPA receptor positive allosteric modulators: QSAR studies, virtual screening, and molecular dynamics simulations
17:05	C-074	<i>Henk Eshuis</i> Performance of the random phase approximation for first-row transition metal catalysis	C-084	<i>Hélène Bolvin</i> Magnetic coupling between F magnetic centers			C-094	<i>Paula Homem-de-Mello</i> Photophysical properties of macrocycles: a computational and experimental study	C-104	<i>Martin Rahm</i> Ternary gold hydrides: a new class of stable and potentially superconducting compounds	C-114	<i>José Pedro Cerón-Carrasco</i> AQUILES web server: open the eyes to blind docking
17:20	C-075	<i>Jiri Klimes</i> Highly accurate binding energies from the random phase approximation with singles corrections	C-085	<i>Masato Kobayashi</i> Study on metal nanocluster catalysts based on quantum chemical calculation and informatics	IN-8	<i>Martin Letz</i> Investigations on SiO2 glasses to answer the question: "What is a 'good' glass structure?"	C-095	<i>Tangui Le Bahers</i> Modeling the photochromism of sulphur-doped sodalites using DFT, TD-DFT and SAC-CI methods	C-105	<i>Ian Mackinnon</i> Density functional theory as a predictive tool for superconductivity	C-115	<i>Niels Hansen</i> Thermodynamics of self-assembly of perylene derivatives
17:35	C-076	<i>Eduard Matito</i> Separation of dynamic and nondynamic correlation	C-086	<i>Lubomir Rulíšek</i> Calibrating aurophilic interactions in weakly bound [L-Au-X]... [L'-Au-X] dimers by experiment and theory			IN-9	<i>Matthias Bremer</i> Increasing the polarity of liquid crystals - synthesis and computations	C-096	<i>Basile F. E. Curchod</i> Shedding light on the approximations underlying Ab initio multiple spawning	C-106	<i>Fernando Ruipérez</i> Design of new disulfide-based organic compounds for the improvement of self-healing materials
17:50	C-077	<i>Jan Řezáč</i> Describing non-covalent interactions in semiempirical QM methods: state of the art and future	C-087	<i>Zahra Jamshidi</i> Surface-enhanced Raman spectroscopy due to charge-transfer chemical mechanism: effect of surface and electric field	IN-10	<i>Thomas Eckl</i> Automated high-throughput DFT simulations for the development of enhanced energy storage and energy conversion materials			C-097	<i>William Glover</i> Polarizable QM/MM for excited-state dynamics	C-107	<i>Toyokazu Ishida</i> Computational modeling of thermal energy storage materials
18:05	C-078	<i>Ekaterina Pas</i> A new spin ratio scaled MP2 (SRS-MP2) method for the prediction of intermolecular interactions	C-088	<i>Jean Christophe Tremblay</i> Irreversible tautomerization in porphycene on Cu(111) induced by scanning tunnelling microscopy			C-098	<i>Matthias Stein</i> Hydrogen conversion in [NiFe]-enzymes and bio-inspired complexes	C-108	<i>Eliseo Ruiz</i> Spin crossover complexes: a challenge from theory to single-molecule devices	C-118	<i>Ole Swang</i> Towards reliable computed thermodynamic data for aqueous metal ions: the case of cadmium
18:20 20:00	DINNER BREAK											
20:00 22:00	Poster Session 2 – supported by <i>The Journal of Physical Chemistry</i>											

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 09:40	PL-7 Plenary Session E <i>Chair: Peter Richard Schreiner</i> Pavel Hobza Noncovalent interactions: theory and applications					
09:40 10:10	COFFEE BREAK					
10:10 12:15	Invited Session 24 <i>Chair: Mark Gordon</i>	Invited Session 25 <i>Chair: Gernot Frenking</i>	Invited Session 26 <i>Chair: Guan Hua Chen</i>	Invited Session 27 <i>Chair: Martin Kaupp</i>	Invited Session 28 <i>Chair: Qiang Cui</i>	Invited Session 29 <i>Chair: Dominika Zgid</i>
10:10	I-241 <i>Alán Aspuru-Guzik</i> Quantum computation for quantum chemistry	I-251 Sason Shaik Oriented electric fields as future smart reagents in chemistry	I-261 Karsten Reuter Refining first-principles photo-electrocatalysis	I-271 <i>David Tozer</i> Exchange-correlation functionals from density scaling	I-281 <i>Marcus Elstner</i> Multi-scale methods for electron and exciton transfer in biological and organic materials	I-291 <i>Bogumil Jeziorski</i> Theoretical determination of properties of helium for new temperature and pressure standards
10:35	I-242 <i>Michele Ceriotti</i> Machine-learning unifies the modelling of materials and molecules	I-252 Clémence Corminboeuf Bringing volcano plots as a tool to understand and predict homogenous catalysts	I-262 Fabrizia Negri Challenges in modeling electronic structure, optical and transport properties of conjugated molecular materials	I-272 <i>Hannes Jonsson</i> Self-interaction corrected energy functional applied to molecules and solids	I-282 <i>Elena Laura Coitiño Izaquirre</i> Sulfenic acid or sulfenate? A matter of protein environment and water access in oxidized Cysteine sites of physiological relevance	I-292 <i>Manuel Yáñez</i> Spontaneous generation of radicals and design of anion sponges through Beryllium bonds
11:00	I-243 <i>Markus Reiher</i> Interactive and automated exploration of reaction mechanisms	I-253 Julia Rice Nucleobases: from the prebiotic world to self-healing polymers	I-263 <i>Mariachiara Pastore</i> From dye-sensitized TiO ₂ to dye-sensitized NiO heterointerfaces: a new challenge for theory	I-273 <i>Julien Toulouse</i> Combining density-functional theory and many-body methods	I-283 <i>Matthias Heyden</i> Solvation and solvent-mediated driving forces: Spatially resolved information from detailed atomistic trajectories	I-293 <i>Johannes Kästner</i> Improvements of instanton theory to simulate atom tunneling in astrochemical reactions
11:25	I-244 <i>Matthias Scheffler</i> Big data of the chemical physics of materials: discovering interpretable patterns, correlations and causality	I-254 <i>Matthias Bickelhaupt</i> Rational design of chemical reactions	I-264 <i>Biswarup Pathak</i> Atomistic modeling of nanocluster based electrodes for fuel cell applications	I-274 <i>Erin R. Johnson</i> Dispersion interactions from the exchange-hole dipole moment	I-284 <i>Ville Kaila</i> Deciphering molecular mechanisms of energy-converting proteins from simulations across scales	I-294 <i>Eluvathingal D. Jemmis</i> Borophenes, borospherenes, boranes, 3D-boron allotropes and boron-rich solids
11:50	I-245 <i>Gregory Voth</i> Ultra-coarse-graining and its applications	I-255 William Hase Development and applications of direct Dynamics simulations	I-265 <i>Zhigang Shuai</i> Understanding intramolecular singlet fission process in D-A polymer from correlated wave-function perspective	I-275 <i>Matthias Ernzerhof</i> Factorizations of the exchange-correlation hole	I-285 <i>Holger Gohlke</i> Efficient approximation of configurational entropy changes upon binding to biomolecules	I-295 <i>Péter G. Szalay</i> On the accuracy of coupled-cluster-type methods describing excited states
12:15 13:00	LUNCH BREAK					
13:00 20:00	EXCURSIONS					
20:00 22:00	Löwenbräukeller (Address: Nymphenburger Str. 2) CONGRESS DINNER					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 09:40	PL-8 Plenary Session F <i>Chair: So Hirata</i> Hiroshi Nakatsuji Exact general theory for solving Schrödinger equations of atoms and molecules: Free-complement theory and applications					
09:40 10:10	COFFEE BREAK					
10:10 12:15	Invited Session 30 <i>Chair: Asbjörn Burow</i>	Invited Session 31 <i>Chair: Manuel Yáñez</i>	Invited Session 32 <i>Chair: Luca Frediani</i>	Invited Session 33 <i>Chair: Christof Hättig</i>	Invited Session 34 <i>Chair: Bogumil Jeziorski</i>	Invited Session 35 <i>Chair: Zexing Cao</i>
10:10	I-301 Filipp Furche Recent developments in random phase approximation methods	I-311 Josef Michl Oligosilanes: intuitive understanding of σ delocalization in loose and localization in tight helical conformations	I-321 Chiara Cappelli A fully polarizable embedding model for molecular spectroscopy of aqueous solutions	I-331 Anna Krylov Visualizing the contributions of virtual states to two-photon absorption cross-sections	I-341 Rodney J. Bartlett Quantitative molecular orbital theory	I-351 Pedro Fernandes Nanosecond-timescale conformational dynamics of enzymes, and its impact on reaction rates
10:35	I-302 Axel Becke Vertical excitation energies from the adiabatic connection	I-312 Gernot Frenking Aspects of chemical bonding	I-322 Jacob Kongsted Excited states in complex systems through polarizable (density) embedding	I-332 Xiaosong Li Two-component non-collinear time-dependent spin density functional theory for electronic dynamics and excited state calculations	I-342 Andreas Köhn Applications of interrenally contracted multireference coupled-cluster theory	I-352 Yiqin Gao Computer simulations of chemical reactions in solution
11:00	I-303 Eunji Sim Reliable DFT results with density correction	I-313 Marco Nascimento Are one-electron bonds any different from standard two-electrons covalent bonds?	I-323 Lyudmila Slipchenko Polarizable embedding and beyond: modeling photoactive proteins with the effective fragment potential method	I-333 Andreas Dreuw Algebraic diagrammatic construction - a versatile approach to excited states, ionization potentials and electron affinities	I-343 Shuhua Li Advances in Electronic Structure Methods for Strongly Correlated Systems and Condensed Phase Systems	I-353 Young Min Rhee Simulating photo-excited dynamics of biological complexes: overcoming present challenges with interpolated potentials
11:25	I-304 Andreas Görling Density-functional methods with the accuracy and wide applicability of high-level multi-reference approaches	I-314 Julia Contreras-García A new model for reference densities - really getting rid of interactions	I-324 Fred Manby Multiscale embedding methods for accurate quantum chemistry of complex systems	I-334 Spiridoula Matsika Theoretical studies of the interaction of uracil with low energy electrons	I-344 Jiri Pittner DMRG-externally-corrected local pair natural orbital based coupled cluster method	I-354 Carmay Lim How native and alien metal cations bind ATP
11:50	I-305 Paul Ayers Variational principle for partitioning molecules into atomic contributions	I-315 Russell J. Boyd Insight into hydrogen-bonded clusters and noncovalent interactions from changes in atomic energies	I-325 Kurt V. Mikkelsen Exploitation of solar energy	I-335 John Herbert First-principles exciton models, with application to singlet fission	I-345 Ove Christiansen Tensor decomposition and coupled cluster theory	I-355 David Smith A multiscale computational investigation of SILPCatalysis: the water-gas shift reaction
12:15 13:45	LUNCH BREAK					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
13:45 15:50	Invited Session 36 <i>Chair: Jiali Gao</i>	Invited Session 37 <i>Chair: Filipp Furche</i>	Invited Session 38 <i>Chair: Julien Toulouse</i>	Invited Session 39 <i>Chair: Francesco Aquilante</i>	Invited Session 40 <i>Chair: Andreas Dreuw</i>	Invited Session 41 <i>Chair: Brian Yates</i>
13:45	I-361 <i>Richard Henchman</i> Theory for the entropy of liquid mixtures of flexible molecules	I-371 <i>Marcel Nooijen</i> Towards a local coupled cluster theory for solids	I-381 <i>So Hirata</i> Many-body Green's function theory: algebraic recursions, linked- and irreducible-diagram theorems, and general-order algorithms	I-391 <i>Toru Shiozaki</i> On-the-fly CASPT2 surface hopping dynamics	I-401 <i>Patrick Norman</i> Response theory techniques to address X-ray spectroscopies	I-411 <i>Igor Alabugin</i> Reinventing cycloaromatization reactions: the diradical /zwitterion dichotomy
14:10	I-362 <i>Johan Åqvist</i> Entropy and enzyme catalysis	I-372 <i>Georg Kresse</i> The relation between the random phase approximation and GW and analytic forces for the RPA	I-382 <i>Dominika Zgid</i> Green's function embedding methods	I-392 <i>David Tew</i> Quantum dynamics on accurate electronic potentials	I-402 <i>Daniel Crawford</i> Streamlining coupled cluster response theory	I-412 <i>Miroslav Urban</i> DFT study of the Au-C bond formation in gold implanted polyethylene
14:35	I-363 <i>Qiang Cui</i> Understanding metalloenzyme catalysis with QM/MM free energy simulations	I-373 <i>Silke Biermann</i> Electronic structure calculations for correlated electron materials: a dynamical mean field perspective	I-383 <i>Denis Jacquemin</i> Is BSE/GW an effective method for modeling optical spectra of molecules?	I-393 <i>Yuki Kurashige</i> Ab initio modeling of inter-molecular electronic transition processes in molecular aggregates	I-403 <i>Benoît Champagne</i> Towards investigating the optical properties of molecular and ionic crystals using multi-scale approaches	I-413 <i>Attila Császár</i> Astructural molecules
15:00	I-364 <i>Pavel Jungwirth</i> Cell penetration and membrane fusion: two sides of the same coin	I-374 <i>Volker Blum</i> Affordable high numerical accuracy for large molecules and materials from numeric atom-centered basis functions	I-384 <i>Lucia Reining</i> Quasi-particles and satellites from a direct approach to the calculation of many-body Green's functions	I-394 <i>Hans Jørgen Aagaard Jensen</i> Open-shell MC-srDFT - a new way to describe high-spin, low-spin, intermediate spin states and more	I-404 <i>Sonia Coriani</i> Developing theoretical "beam-lines" for modern experiments	I-414 <i>Annia Galano</i> The role of acid-base equilibria in the antioxidant and pro-oxidant activity of phenolic compounds
15:25	I-365 <i>Gerhard Hummer</i> Molecular simulations of lipid membrane sensing and remodeling dynamics	I-375 <i>Gregory Beran</i> Ab initio molecular crystallography: Aiding and abetting experiment	I-385 <i>Wim Klopper</i> Using the GW and Bethe-Salpeter methods in molecular quantum chemistry	I-395 <i>Piotr Piecuch</i> Stochastic CC(P;Q) theory: converging high-level coupled-cluster energetics by Monte Carlo sampling and moment expansions	I-405 <i>Antonio Rizzo</i> Electronic nonlinear spectroscopies: recent contributions of theory and computational science	I-415 <i>Munir Skaf</i> Thermodynamic forces between plant cell wall constituents
15:50 16:20	COFFEE BREAK					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
16:20 18:20	Contributed Session 12 <i>Chair: David Tew</i>	Contributed Session 13 <i>Chair: Wolfgang Domcke</i>	Contributed Session 14 <i>Chair: Andy Teale</i>	Contributed Session 15 <i>Chair: Reinhold Fink</i>	Contributed Session 16 <i>Chair: Tanya K. Todorova</i>	Contributed Session 17 <i>Chair: Marco Nascimento</i>
16:20	C-121 <i>Jan M.L. Martin</i> Explicitly correlated benchmark study on water clusters: The right answer for the right reason?	C-131 <i>Nick Mayhall</i> Multiexcitons and strong correlation via single-excitation wavefunctions: applications and future directions	C-141 <i>Stella Stopkowitz</i> Accurate treatment for ground and excited states of atoms and molecules in strong magnetic fields	C-151 <i>Martin Kaupp</i> Mixed valency and local hybrid functionals	C-161 <i>Mark Iron</i> Computational insights into sulphur isotopic fractionation in carbonate-associated sulphate	C-171 <i>José Enrique Barquera-Lozada</i> Aromaticity from the point of view of the vorticity of the current density tensor
16:35	C-122 <i>Ricardo Mata</i> GoBench: a joint initiative for experimental benchmarking of quantum chemical methods	C-132 <i>Remco Havenith</i> The computation of dielectric constants	C-142 <i>Sandra Lubser</i> Recent advances in theoretical spectroscopy from ab initio molecular dynamics	C-152 <i>Lars Goerigk</i> Double-hybrid density functionals: is there anything new to tell?	C-162 <i>Silvia Simon</i> Tailoring resonance assisted hydrogen bonds	C-172 <i>Fabio Pichierri</i> Cesium cation- π interactions: DFT and QTAIM studies
16:50	C-123 <i>Peter Nagy</i> Approaching CCSD(T)/CBS energies for large molecules with the linear-scaling local natural orbital CCSD(T) method	C-133 <i>Andrzej L. Sobolewski</i> Organic photovoltaics with p-f-n junctions: computational study of ferroelectric columnar molecular clusters	C-143 <i>Malgorzata Biczysko</i> Anharmonic effects on vibrational spectra intensities: infrared, Raman, vibrational circular dichroism, and Raman optical activity	C-153 <i>Sergei Vyboishchikov</i> Exchange-Correlation Potentials and Energy Densities in Spherically Confined Atoms	C-163 <i>Ulrike Salzner</i> Effect of biradical character of organic molecules on Opto electronic properties	C-173 <i>András Stirling</i> Hypervalency and reactivity from Wannier orbitals
17:05	C-124 <i>Graham Fletcher</i> Large-scale valence bond applications: excitons and transition metal complexes	C-134 <i>Thomas Koerzdoerfer</i> Accurate ionization potentials, electron affinities, and photoelectron spectra of molecules from first principles	C-144 <i>Takeshi Iwasa</i> Infrared absorption spectroscopy beyond the dipole approximation based on the multipolar Hamiltonian: Theory and application	C-154 <i>Arindam Chakraborty</i> Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states	C-164 <i>Hong-Xing Zhang</i> Computationally driven design of efficient photosensitizer for dye-sensitized solar cell applications	C-174 <i>Leonardo Belpassi</i> Charge-displacement analysis: a simple tool to reveal charge transfer effects throughout the whole periodic table
17:20	C-125 <i>Jean-Philip Piquemal</i> Scalable polarizable molecular dynamics using Tinker-HP: millions of atoms on thousands of cores	C-135 <i>Emanuele Coccia</i> Dissipation and dephasing for molecules close to plasmonic nanoparticles: an ab initio approach	C-145 <i>Franco Egidi</i> Toward the accurate simulation of vibrationally-resolved spectra for spin-forbidden transitions	C-155 <i>István Mayer</i> Local spins	C-165 <i>Martial Boggio-Pasqua</i> Computational studies of the photoswitching mechanisms in photochromic ruthenium complexes	C-175 <i>Apostolos Kalemos</i> The nature of the chemical bond in Be containing molecules: Be $2^{+}, 0, -$, Be 3 , BeO $0, -$, BeOBe $+, 0, -$
17:35	C-126 <i>Joonsuk Huh</i> Vibronic boson sampling	C-136 <i>Robert Góra</i> Microhydration induces qualitative changes in the photochemistry of biomolecular building blocks	C-146 <i>Sergei Ivanov</i> Nuclear correlation effects in X-ray spectroscopy from a time-domain perspective	C-156 <i>Fan Wang</i> Spin-orbit coupling effects of open-shell systems with coupled-cluster theory	C-166 <i>Aurélie Perrier</i> Photosensitizing properties of functionalized thiolate-protected gold nanoclusters: insights from theory	C-176 <i>David Wilson</i> Theoretical investigation of a strong cis-effect in an imidazole-imidazolium substituted alkene
17:50	C-127 <i>Luca Frediani</i> PCMSolver: a modern, modular approach to include solvation in any quantum chemistry code	C-137 <i>Isabelle Navizet</i> Role of the environment in bioluminescence emission: QM/MM study	C-147 <i>Stjepan Sklenak</i> DFT calculations of NMR parameters of framework and extra-framework atoms in silicon-rich zeolites	C-157 <i>Mikael P. Johansson</i> Can spin-state energetics of transition metal complexes be accurate at single reference level?	C-167 <i>David Henry</i> Modifying the reactivity of gallium nanoclusters with ligands	C-177 <i>Ignacy Cukrowski</i> Fragment attributed molecular system energy change (FAMSEC) in the study of interactions and molecular stability
18:05	C-128 <i>Sebastian Höfener</i> Combining frozen-density embedding with the conductor-like screening model using Lagrangian techniques	C-138 <i>Stefan Knippenberg</i> Investigation of optical probes for membrane phase recognition	C-148 <i>Alfonso Hernández-Laguna</i> Elastic behavior of White Micas solid solutions as a function of the pressure	C-158 <i>Ran Friedman</i> Specific ion interactions with biomolecules: molecular dynamics simulations and energy decomposition analysis	C-168 <i>Thibaud Étienne</i> Orbital relaxation and electronic transitions - what is the nature of Handy's Z-vector?	C-178 <i>Hugo Gattuso</i> Efficiently modeling the electronic circular dichroism of amino and nucleic acids ensembles
18:20 20:00	DINNER BREAK					
20:00 22:00	Poster Session 3 – supported by ACS Publications					

Time	Philharmonic Hall	
09:00 10:20	Plenary Session G <i>Chair: David Sherrill</i>	
09:00 09:40	PL-9	<i>Francesco Evangelista</i> Multireference coupled cluster theory, infinities and renormalization
09:40 10:20	PL-10	<i>Johannes Neugebauer</i> Subsystem density-functional theory for properties and spectra of complex chemical systems
10:20 10:50	COFFEE BREAK	
10:50 12:10	Plenary Session H <i>Chair: Walter Thiel</i>	
10:50 11:30	PL-11	<i>Ursula Roethlisberger</i> Next generation first-principles based multiscale simulations: computational chemistry meets artificial intelligence
11:30 12:10	PL-12	<i>Frank Neese</i> Wavefunction based correlation methods for large molecules: recent developments, applications and limitations
12:10 12:50	CLOSING CEREMONY AND POSTER AWARDS	

Munich

2017

WATOC

AUTHOR INDEX



A

Aav R.	PO3-131		
Abbott A.	PO3-123		
Abe M.	PO3-98		
Abramov P.	PO1-85		
Abudoukadeer A.	PO1-103		
Acher E.	PO3-188		
Acke G.	PO1-39		
Adamo C.	I-202 , PO2-163		
Agee M.M.	I-301, PO3-183		
Agostini F.	I-114		
Aguilar-Galindo F.	PO2-158		
Aguilera-Porta N.	PO1-99		
Aguzzi C.	PO2-155		
Ahlrichs R.	PO3-84		
Ahlstrand E.	C-023		
Ahn-Furudate M.	PO3-193		
Ajani H.	PO2-290		
Akiyama H.	PO1-135		
Alabugin I.	I-411		
Alarco J.	C-105		
Alavi A.	I-141 , PO3-202, PO3-230, PO3-295		
Alcamí M.	PO1-262		
Aldongarov A.	PO2-106		
Alessandri R.	C-132, PO3-167		
Alessio M.	PO2-150		
Aliaga-Alcalde N.	C-062		
Alikhani E.	PO1-49		
Alimonti A.	PO1-132		
Alizadeh Sanati D.	PO2-102		
Alkorta I.	I-064		
Allgäuer S. D.	PO2-141		
Almeida A.L.d.	C-014		
Almora Díaz C.X.	PO3-143		
Alonso G.	PO1-50		
Alonso M.	C-061		
Altun Z.	PO1-114, PO1-71		
Álvarez D.	PO2-12		
Álvarez Barcia S.	PO2-16		
Alvarez-Idaboy R.	C-052		
Alves T.	PO2-43		
Alves de Castro A.	PO3-226		
Amaral de Faria J.	PO3-226		
Amgoune A.	PO1-118, PO1-237		
Amine B.	PO2-226		
Amitay Z.	PO1-200		
Anas S.	PO2-76		
Anda A.	C-037		
Andrada D.	PO2-148		
Andrae D.	PO1-226		
Andrikopoulos P.C.	PO1-22 , C-086, PO2-289		
Andris E.	C-086		
Andruniów T.	PO1-119		
Andrushchenko V.	C-064		
Andrzejak M.	PO1-201		
Añez R.	PO1-147		
Ang S.J.	PO1-76		
Antalik A.	I-344, PO3-230		
Antes I.	PO3-120 , PO3-222, PO3-25, PO3-43		
Antipov S.	PO3-110, PO3-116		
Antol I.		PO2-5	
Antonietti M.		PO1-27	
Antonio F.C.T.	PO1-107, PO2-55 , C-094		
Antony J.		PO3-210	
Antušek A.		I-412	
Aoki S.		PO1-247	
Aoki Y.		PO1-141	
Aono C.M.		PO1-100	
Apeloig Y.		I-074	
Apfel U.-P.		PO3-239	
Aquino A.J.A.		PO1-120	
Åqvist J.		I-362	
Aradi B.		PO3-105	
Aragó J.		PO1-53	
Aragonès A.		C-062	
Aranda Moratalla J.		PO2-152	
Aravena D.		C-062	
Arbuznikov A.V.		PO2-51	
Arismendi Arrieta D.J.		PO1-102	
Arnarson L.		IN-7	
Aroua S.		PO2-135	
Arpa González E.M.		PO1-185	
Artukhin D.		PO1-170	
Arulmozhiraja S.		PO3-53	
Arvanitidis A.		PO3-191	
Asahara H.		PO2-141	
Ásgeirsson V.		PO3-164 , PO2-265	
Ashcroft N.W.		C-104	
Aspuru-Guzik A.	I-241 , PO3-146, PO3-150		
Assfeld X.		C-178, PO3-294	
Assilbekova A.		PO2-106	
Atanasov M.		PO3-213	
Atlam F.		PO1-37, PO1-38	
Attia A.		PO1-34, PO2-107	
Aucar G.A.		I-063 , PO3-21, PO3-284	
Aucar M.G.		PO3-155	
Auth T.		PO2-105	
Avanzini F.		PO2-142	
Aviyente V.		PO3-247	
Awad M.		PO1-37 , PO1-38	
Ayers P.		I-305 , PO2-230	
Ayub R.		PO2-90	
Ayyappan A.		C-046	
Azarias C.		PO1-263	
Aziz E.F.		C-103	
Aziz S.		PO3-242	
Azizi S.		PO3-261	
Azofra L.M.		PO1-180	
B			
Bacchus M.-C.		PO1-42	
Bae H.		PO1-106	
Baek H.		PO2-195	
Baer R.		I-143 , PO1-12, PO1-219	
Bagherpoor Helabad M.		C-057	
Bahamón D.		PO1-50, PO3-299	
Bahlke M.P.		PO2-219	
Bahmann H.		PO2-51	
Bai L.		C-056	
Bai S.		PO1-212	

Baiardi A.	C-145, PO3-107	Berraud-Pache R.	C-137, PO2-160
Baik M.-H.	PO1-11	Berry J.	PO1-87
Bajaj A.	C-072	Berski S.	PO1-131
Bakó I.	PO2-2 , PO2-268	Berta D.	PO2-268
Baldauf C.	C-082	Besley E.	PO3-46
Baldofski M.	PO2-214	Besley N.	PO3-46
Baldoni M.	PO3-46	Beton P.	PO3-46
Balta B.	PO2-73, PO3-247	Beuerle M.	PO2-273
Bande A.	C-103	Beyle F.	PO3-221
Bandeira N.A.G.	PO3-292	Beyle F.E.	PO3-252
Banerjee S.	I-174	Bhalodia P.	PO3-245
Bannwarth C.	PO2-72	Bhat H.	PO1-2
Baptista L.	PO1-147, PO2-61, PO3-80	Bhati A.P.	PO1-36
Baranek P.	PO2-94	Bhattacharyya D.	C-046
Barbatti M.	PO2-117, PO2-292, PO3-101	Bickelhaupt F.M.	I-254 , PO1-84, PO2-78
Barca G.	PO3-94	Biczysko M.	C-143
Barcza G.	I-083, PO3-178	Bieberle-Hütter A.	PO1-6
Bargholz A.	PO3-48	Biele R.	PO2-239
Baric D.	PO2-248	Bielewicz T.	PO2-280
Barnard A.	PO2-192	Biermann S.	I-373
Barone V.	C-145, PO3-107	Bieske E.	C-176
Barquera-Lozada J.E.	C-171	Bilgin N.	PO3-247
Barrales-Martínez C.	PO2-60	Bilonda M.K.	PO1-285
Barroso J.	PO1-296	Bim D.	PO1-306
Bartlett R.	I-341	Binder R.	I-112
Barton D.	PO1-153	Bisha I.	PO3-222
Bassi A.	PO3-140	Bistoni G.	PO1-234
Batebi H.	PO3-165	Bjornsson R.	C-023
Battaglia S.	PO1-226	Blanco-Rey M.	C-088
Battistini F.	PO2-164	Blase X.	PO1-263
Bauer C.	PO2-265	Blaško M.	I-412
Bauer F.	PO2-33	Blatter S.P.	PO3-284
Bauer P.	PO1-43	Bleda E.A.	PO1-114 , PO1-71
Bauerfeldt G.F.	PO3-78 , PO3-79, PO3-80	Bleiziffer P.	PO3-220
Bayne M.	C-154	Bley M.	PO2-88
Baz J.	C-115	Bloino J.	C-143, C-145
Bazhenov A.S.	PO3-142 , PO1-80	Blum V.	I-374
Bearpark M.J.	PO1-126	Blumberger J.	I-025 , PO1-60, PO1-160
Beattie N.	PO2-144	Bo C.	PO3-292
Beaumont C.	PO1-239	Bochenkova A.	PO3-119
Beck A.K.	PO2-246	Bock L.V.	I-195
Beck M.E.	IN-3	Böckers M.	PO1-153
Becke A.	I-302 , PO3-266	Bocola M.	PO3-23
Becker M.	PO2-30	Bodenstein T.	PO2-169, PO3-5
Begic I.	C-078	Boereboom J.	PO3-236
Begusic T.	PO3-134	Boese A.D.	PO2-97
Belinassi A.R.	PO2-43	Bofill J.M.	C-047, PO1-218
Bellili A.	PO3-100	Bogdanov N.	PO3-202 , PO3-295
Bellinger D.	PO2-36 , PO3-162	Boggio-Pasqua M.	C-165 , PO2-45
Belpassi L.	C-174	Boguslawski K.	PO1-133
Ben Amor N.	C-038	Bohle F.	PO3-176
Benda Z.	PO2-224	Bois J.	PO1-220
Benediktsson B.	C-158	Boisson J.-C.	I-314, PO3-113, PO3-135
Ben-Shalom I.	I-285	Bokarev S.	PO3-233 , PO3-242
Beran G.	I-375 , PO1-93	Bold B.	PO3-252
Bereau T.	C-022 , PO2-206	Bollini M.	PO3-155
Berger D.	I-355	Bols M.	PO1-68
Berger R.	I-162 , PO1-157, PO1-301, PO1-97	Bolvin H.	C-084
Bernardi M.	I-024	Borge J.	C-101
Bernasconi L.	PO1-155	Borges-Martinez M.	PO3-72

Borgis D.	C-036	Buyadzhi V.	PO3-255
Borisov A.	PO2-158	Byon H.-R.	PO1-11
Borovik A.S.	I-045		
Borrego-Sánchez A.	PO2-155	C	
Borrego-Varillas R.	PO3-128	Cabellos J.L.	PO1-66
Borschevsky A.	PO3-257	Caffarel M.	C-073
Bortoli M.	PO2-78	Cafiero M.	PO1-57, PO1-58, PO1-59, PO1-63, PO1-65
Bottoni A.	PO2-120	Calatayud M.	PO1-188
Bouaouli S.	PO3-254	Calbo J.	PO1-53
Boulanger E.	PO3-17	Caldeweyher E.	PO2-137
Bouledroua M.	PO1-4	Calhorda M.J.	PO3-169
Bourissou D.	PO1-118, PO1-237	Call A.	PO1-142
Bouteloup R.	PO2-250	Calvaresi M.	PO2-120
Bowman J.	I-161	Calvelo Souto M.	PO3-38
Boyd R.	I-315	Calvo F.	PO3-296
Boyle P.D.	PO1-196	Campetella M.	PO3-228
Boz E.	PO2-118	Canola S.	I-262, PO2-124
Brabec J.	I-344, PO3-136 , PO3-225	Cantatore V.	PO3-96
Braeuer A.	PO2-131	Canuto S.	PO1-109, PO2-305
Braïda B.	PO1-39	Cao X.	PO3-64
Brakestad A.M.	I-152	Cao Z.	C-156, I-181
Brandão I.	PO3-234	Cappelli C.	I-321 , PO3-208
Brandbyge M.	PO2-274	Caprasecca S.	PO2-80, PO3-228
Brandejs H.	I-083	Carazo E.	PO2-155
Brandenburg G.	PO1-13	Cárdenas Morales D.J.	PO1-185
Branzanic A.	PO1-229	Cardenas-Jiron G.	PO2-194 , PO3-72
Brauer C.-A.	PO1-202	Cardoso C.	PO3-80
Bredas J.-L.	I-023	Carneiro J.W.d.M.	PO1-84, PO1-206
Breher F.	PO3-34	Carniato S.	PO2-35
Brehm M.	PO2-11	Carof A.	PO1-160, PO1-60
Bremer M.	IN-9	Carsky P.	I-095
Brenner V.	C-038	Casademont Reig I.	PO1-142
Brickel S.	PO1-184	Casadevall C.	PO1-142
Brinck T.	I-053	Casado J.	PO2-76
Brinkmeier A.	PO2-256	Casanova D.	PO1-136, PO1-190
Brites G.	PO3-80	Casasnovas R.	PO3-145
Brkljača Z.	PO3-256	Cassam-Chenaï P.	PO2-20
Broer R.	C-132, PO1-24	Cassera M.	PO3-274
Brothers E.	C-112, PO3-200	Castro A.C.	PO2-229
Brown J.	PO1-300	Castro M.A.	PO3-234
Browne W.R.	I-045	Castro R.	PO3-78
Browning N.J.	PO2-277	Castro Ramalho T.	PO3-67
Brüggemann J.	PO1-258	Catak S.	PO2-296, PO3-81
Bruno Goncalves P.F.	PO2-117	Caux J.-S.	PO2-230
Brzęk F.	PO1-133	Cavalli A.	PO1-132
Buehl M.	I-062	Cavallo L.	PO1-180
Bulo R.	PO3-236	Cavasotto C.N.	PO3-155
Bultinck P.	PO1-39, PO1-86	Ceccato A.	PO2-130
Buma W.J.	PO2-77	Cederbaum L.S.	I-164
Bumüller D.	PO3-84	Cederquist H.	PO3-103
Bunge C.F.	PO3-143	Celestino A.	PO2-269
Bunting P.	PO3-213	Cembran A.	PO2-283
Burghardt I.	I-112 , PO3-264	Ceriotti M.	I-242
Burke K.	I-203	Cerón-Carrasco J.P.	C-114
Burow A.M.	C-013, PO2-153	Cerqueira N.M.F.S.A.	PO1-239
Burrows A.	PO1-167	Cerullo G.	PO3-128
Bursch M.	PO1-186	Cervinka C.	PO1-93
Burton H.	PO3-76	Ceulemans A.	PO3-215
Buš V.	PO3-60	Cezar H.	PO1-109
Busch M.	I-252	Chadwick F.M.	PO3-52



Chakrabarty S.	PO1-179		
Chakraborty A.	C-154		
Chalasinski G.	PO3-281		
Champagne B.	I-403 , PO1-298, PO2-191		
Champion J.	PO1-288		
Chan B.	I-073, PO1-246, PO1-91		
Chan C.H.	PO3-102		
Chan G.	I-012		
Chang H.	PO1-112		
Chang M.-W.	PO1-182		
Changotra A.	PO1-72		
Chaumont A.	PO3-279		
Chavarot-Kerlidou M.	PO2-42		
Chedid J.	C-074		
Cheeseman J.R.	PO3-208		
Chen G.	I-214 , PO3-183		
Chen G.P.	I-301		
Chen J.	PO1-132		
Chen L.	PO3-249		
Chen P.	PO3-240		
Chen Q.	PO2-141		
Chen W.-C.	PO1-254		
Cheng Y.C.	PO1-166		
Chermette H.	PO1-81		
Chiş V.	PO2-98		
Chibotaru L.F.	PO1-252		
Chilton N.F.	PO3-219		
Chitpakdee C.	PO2-223		
Chiu C.-C.	PO1-35		
Chołuj M.	PO2-203		
Choi H.	PO1-106		
Choi S.	PO2-182, PO2-228, PO2-70		
Chou C.-P.	PO1-233, PO1-305, PO2-68		
Christian M.	PO2-176		
Christiansen O.	I-345 , PO2-209, PO2-210, PO2-236, PO2-79, PO3-198		
Chug O.L.W.	C-067		
Chunchen L.	PO1-190		
Chung L.W.	PO1-110		
Ciarlariello N.	PO2-124		
Cid Mora F.A.	PO3-271		
Çifci G.	PO3-247		
Cilpa-Karhu G.	PO2-204		
Ciofini I.	I-123		
Cirera J.	C-108		
Civalleri B.	PO2-94		
Claeys P.	PO2-230		
Clark T.	I-182		
Clary D.	I-111		
Clavaguera C.	PO1-259		
Clavaguera C.	PO2-278		
Coccia E.	C-135		
Cochrane B.	PO1-240		
Coelho M.	PO1-124		
Coitiño Izaguirre E.L.	I-282		
Colebatch A.	PO2-144		
Coles J.	PO3-211		
Colombi Ciacchi L.	PO3-36		
Comas-Vives A.	PO3-115		
Comba P.	PO2-212, PO2-298, PO2-304, PO3-15, PO3-207		
Goncalves T.P.	PO3-301		
Condic-Jurkic K.	PO2-197		
Conic D.	PO1-303		
Conti I.	PO3-128		
Contini A.	C-054 , PO1-264		
Contreras-García J.	I-314 , PO3-113		
Cooper A.	PO1-253		
Coote M.	I-055		
Copéret C.	I-061, PO3-115		
Corentin L.	I-314		
Coriani S.	I-404		
Corminboeuf C.	I-252 , PO2-159, PO2-46		
Cornard J.P.	PO3-192		
Corni S.	C-135, PO1-260		
Corno M.	PO2-171		
Corral I.	PO1-239, PO1-99		
Corral Pérez I.	PO1-185		
Correa J.D.	C-066		
Correia A.N.	PO1-127		
Cortés-Arriagada D.	PO1-146, PO2-60		
Cortese R.	PO1-14		
Cossi M.	PO2-171		
Cossío F.P.	PO2-58, PO3-203		
Costa França T.C.	PO3-67		
Coto P.B.	PO2-4 , PO2-50		
Coughtrie D.	PO1-284		
Coutinho K.	PO1-109		
Coveney P.V.	PO1-36		
Cowley R.E.	PO1-22		
Cozar I.B.	PO2-98		
Crawford T.D.	I-402 , PO2-156, PO3-175, PO3-273, PO3-274, PO3-51		
Crespo-Otero R.	PO2-119, PO2-161		
Crestoni M.E.	PO3-37		
Cristina de Assis L.	PO3-226		
Cristofol-Clough M.	PO3-114		
Crnković L.	PO2-5		
Croce R.	PO2-225		
Crovetto A.	PO2-274		
Csaszar A.	I-413		
Cui Q.	I-363		
Cukrowski I.	C-177 , PO2-108		
Cunha A.	PO3-118		
Cupellini L.	PO3-174, PO3-228		
Curchod B.F.E.	C-096		
Curutchet A.	C-095		
Custer T.	PO3-95		
Cytter Y.	PO1-219		
Czapla M.	PO1-25		
D			
Da Silveira E.F.	PO1-147		
Dabjartsdóttir F.B.	PO3-164		
Dai Y.	PO2-124, PO3-274		
Dalal S.	PO3-274		
Dale S.	PO3-266		
D'Amore L.	PO2-256		
Dang T.T.M.	PO1-244		

Dang Y.	PO2-188	Dognon J.-P.	PO1-113
D'Angelo G.	PO3-103	Dohm S.	PO3-231
Daniel C.	I-153 , PO2-109	Dokainish H.	PO1-249
Dans P.D.	PO2-164	Dolbundalchok P.	C-103
Darre L.	PO2-164	Dolg M.	PO3-64
Daru J.	C-116 , PO3-11	Dolgonos G.A.	PO2-97
Das S.	PO2-167	Domcke W.	PO1-30, PO2-101, PO2-175
Davari M.D.	PO3-23	Domingues Coutinho-Neto M.	PO2-149
David G.	C-102, PO2-262	Dominguez A.	PO3-105
Dawid A.	PO2-247	Domínguez M.M.	PO1-306
Daza M.	C-053	Dommett M.	PO2-119 , PO2-161
De Azevedo Santos L.	PO2-179 , PO2-180	Domratcheva T.	PO1-149
De Baerdemacker S.	PO1-39, PO2-230	Dong Y.	PO2-13
De Brito Sá É.	PO3-35	Dononelli W.	PO3-88
De Bruin T.	PO1-250	Dopieralski P.	C-055 , PO2-258
De Castro Ramalho T.	PO2-179, PO3-226	Doran A.E.	I-381
De Costa S.	PO2-197	Dornbach M.	PO3-205
De Cózar A.	PO3-203	Doublet M.-L.	PO1-287
De Lange J.H.	C-177, PO2-108	Dragelj J.	PO2-40
De Lara-Castells M.P.	C-051	Dragičević I.	PO2-248
De Lima-Neto P.	PO1-127	Dral P.O.	PO3-62 , PO2-85
De Mesmaeker A.	PO2-296, PO3-81	Draxl C.	I-232
De Oliveira Silva D.	PO2-49	Dresselhaus T.	PO1-153
De Vico L.	C-037	Dreuw A.	I-333 , PO1-292, PO2-140, PO2-162, PO3-196, PO3-29
De Vivie-Riedle R.	PO1-279, PO2-121, PO2-125, PO2-127, PO2-157, PO2-201	Driant T.	PO1-43 , PO2-128
De Vries A.H.	PO3-167	Du Y.	PO3-274
DeBeer S.	PO1-46	Dube H.	PO2-157
Dedecek J.	C-147	Duboué-Dijon E.	PO1-62
Deeth R.J.	PO3-180	Dubrovskaya Y.	PO3-255
Deffner M.	PO2-251	Duca D.	PO1-14
Deglmann P.	IN-1	Duchemin I.	PO1-263
Dehnen S.	PO3-50	Dufrêche J.-F.	PO2-88
Delgado-Alonso C.	PO3-250, PO3-268	Dumon A.S.	PO2-133
Dellago C.	I-103	Dumont E.	PO3-102
Delle Piane M.	PO3-36	Dums J.	PO2-136
Delor M.	PO3-216	Duran M.	C-162
Demel O.	I-344, I-371, PO3-225	Durán R.	PO1-146, PO1-178
Denzel A.	PO1-261	Durbeej B.	C-035
Derat E.	PO1-43, PO2-128	Dutta A.K.	PO2-170
Desch S.	PO1-299	Dutta Banik S.	PO3-111
Deumal M.	C-101	Dutton J.	C-176
Deustua J.E.	I-395	Duvail M.	PO2-88
Dhoke G.V.	PO3-23	Dvorak M.	PO2-147
Di Luca A.	PO3-121	Dyduch K.	PO1-217
Di Remigio R.	C-127, C-128	Dziedzic J.	PO3-273
Diamantis P.	PO1-199		
Diaz N.	PO1-32	E	
Díaz L.	PO1-147 , PO2-307	East A.	C-117
Díaz-Tendero S.	PO2-158	Easton C.	I-073
Diefenbach M.	PO2-105, PO2-241	Ebata T.	PO1-29
Diestler D.J.	PO1-164	Eckhardt A.K.	PO1-145
Dietl N.	PL-4	Eckl T.	IN-10
Dietschreit J.	PO3-26	Eda M.	PO1-140
Dietzek B.	PO2-42	Edwards B.	PO3-219
Díez-Pérez I.	C-062	Egidi F.	C-145 , PO3-208
Dimitrova M.	PO3-190	Ehara M.	PO1-29
Dina N.E.	PO2-98	Ehrmaier J.	PO1-138
Dmitriev A.	PO1-85	Eisenstein O.	I-061
Dobi Z.	PO2-116	Eisert J.	I-083

El Bakouri O.	PO2-76, PO2-90	Ferrari A.	PO1-132
Eliav E.	PO3-168	Ferraro Gómez F.	PO3-39
Elleuchi S.	PO3-169	Ferré N.	C-102, PO2-262
Elm J.	PO2-300	Ferreira de Moraes L.H.	PO2-49
Elsen H.	PO1-77	Feskov S.	PO3-56
Elstner M.	I-281 , PO1-203, PO3-105, PO3-221, PO3-252	Feyrer A.	PO3-34
Embry C.	PO1-65	Fingerhut B.	I-121
Eng J.	I-153	Fink K.	PO2-169 , PO3-34
Engels B.	PO3-162, PO3-199	Fink R.	PO2-124, PO3-147
Ensing B.	PO3-7	Finkelmann A.	PO1-205
Epifanovsky E.	PO1-297, PO3-248	Finzel K.	PO1-86
Ercan S.	PO3-247	Fiorot R.	PO1-206
Erdmannsdörfer J.	PO3-162	Fischer J.M.	PO2-200
Eriksen J.J.	PO2-297	Fischer R.A.	PO1-51
Erlebach A.	PO1-210	Fischermeier D.	PO2-136
Ernst W.E.	PO1-158	Flambaum V.	PO3-257
Ernzerhof M.	I-275	Fletcher G.	C-124
Escamilla-Roa E.	PO2-26	Fleurat-Lessard P.	PO3-236
Escudero D.	PO1-176	Fliegl H.	PO2-222 , PO3-190
Eshuis H.	C-074	Florindo C.	PO3-140
Espinal J.F.	C-066	Flöser B.	PO1-82
Espinosa E.	I-064	Földes T.	PO2-116
Espinosa de Oliveira T.	PO1-274	Folkestad S.D.	PO3-265
Esser B.	PO3-176	Föllner J.	I-122
Estep M.	PO3-71 , PO3-77	Fonseca T.L.	PO3-234
Esteves da Silva J.C.G.	PO1-242	Fontecave M.	PO2-135
Estevez L.	PO1-118	Fontes Ferreira da Cunha E.	PO2-179, PO3-226
Etienne M.	PO2-53	Foppa L.	PO3-115
Etienne T.	C-168 , PO1-287, PO3-294	Formoso E.	PO1-111
Etinski M.	PO3-7	Förster M.	PO2-134
Eulenstein A.	PO3-50	Fouroutan-Nejad C.	C-064
Evangelista F.	PL-9	Fox T.	IN-5
Evangelisti S.	PO1-226	Franck O.	PO3-69
Evans R.	PO1-63	Franco L.R.	PO3-234
Eveleens C.	PO1-129	Frank I.	PO1-144
Eyrilmez S.M.	PO3-277	Frank M.	PO3-189
F			
Fabian M.D.	PO1-12	Franke R.	PO1-174
Faginas-Lago N.	PO1-226	Franzoni I.	C-068
Falahati K.	PO3-264	Frau J.	PO3-145
Falsig H.	IN-7	Frauenheim T.	PO3-105
Faltermeier D.	PO2-304	Frediani L.	C-127 , C-128, PO3-276
Fan C.	PO1-172	Fregoni J.	PO1-260
Fanfrlík J.	PO2-87 , PO2-290, PO3-277	Freitag L.	PO2-269
Fantuzzi F.	PO3-129, PO3-61	Frenking G.	I-312 , PO1-47, PO1-51, PO2-148
Faraji S.	C-031	Freund M.S.	C-011
Fasshauer E.	PO3-184	Frezzato D.	PO2-130
Fässler T.F.	PO2-136	Friedman R.	C-158
Feixas F.	C-111 , PO2-76	Friese D.H.	PO3-181
Feldt J.	PO1-243	Fujie T.	PO2-226
Feldt M.	PO2-245	Fujinami M.	PO1-280
Fennimore M.	I-334	Fujioka A.	PO2-23
Fensterbank L.	PO2-128	Fujita T.	C-093
Ferch L.S.	C-011	Fujiyoshi J.	PO1-298
Ferenc D.	PO1-15 , PO2-268	Fukushima T.	PO1-269
Ferenczy G.G.	PO2-82	Fukuzawa K.	PO3-86 , PO3-87
Fernandes P.A.	I-351 , PO1-116	Fumagalli V.	C-054
Fernandez I.	PO1-31	Fumanal M.	I-153, PO2-109
Ferrara N.	C-074	Furche F.	I-301 , PO3-149, PO3-183
		Fuse M.	C-145

G

Gagliardi L.	I-225	Gill P.M.W.	I-011 , PO1-294, PO1-297
Gajsek O.	PO2-301	Gillet N.	PO1-203
Galano A.	C-052, I-414 , PO1-101	Gil-Mestres A.	PO3-169
Galembeck S.E.	PO2-77	Gilmour J.	PO2-63
Galland N.	PO1-288, PO2-28	Giménez X.	PO3-299 , PO1-50
Gallandi L.	PO2-14	Gimferrer M.	C-111
Gallego J.	C-066	Gindensperger E.	I-153
Galli G.	PL-6	Ginsbach J.	PO1-22
Galván I.F.	I-152	Giovannini T.	PO3-208
Gamallo P.	PO1-50, PO3-299	Giraldo Nohra F.	PO1-256
Gamarnik A.V.	PO3-155	Giribet C.	PO3-21
Gámez V.	PO1-101	Giussani A.	PO2-287
Gamiz-Hernandez A.P.	PO2-103 , PO1-137	Glaser M.	PO3-120
Ganesh Balasubramani S.	I-301	Glasovac Z.	PO2-5
Gani T.Z.H.	C-072	Glebko N.	PO2-99
Ganzer L.	PO3-128	Glenn R.	PO3-175
Gao J.	I-192	Gloaguen E.	C-038
Gao M.	C-085, PO2-291	Glover W.	C-097
Gao Y.	I-352	Glushkov A.	PO3-251 , PO3-255, PO3-258, PO3-259
Garavelli M.	PO3-128, PO3-174	Godtliobsen I.H.	PO3-198
García S.P.	PO1-218	Goerigk L.	C-152 , PO1-295
Garcia Meseguer R.	PO3-160	Goetz M.	PO3-274
Garcia-Borràs M.	C-111	Gogan O.M.	PO1-8
Garcia-Hernandez R.J.	PO3-308	Gohlke H.	I-285
Garcia-Iriepa C.	C-137	Golding B.T.	PO2-248
Garcia-Rodeja Y.	PO1-31	Goldmann D.	PO1-205
Garniron Y.	C-073	Göllner A.H.	PO1-205 , PO2-54
Garofalo M.	PO1-132	Golze D.	PO2-286
Gaston N.	PO2-64	Gómez H.	PO2-164 , PO2-152
Gatchell M.	PO3-103	Gomez Pech C.	PO2-28
Gattuso H.	C-178 , PO2-109	Gomez Rodriguez S.	PO2-240
Gaul K.	PO1-97	Gonthier J.F.	PO3-137
Gauld J.W.	PO3-194	González L.	I-151 , PO2-45, PO2-109, PO2-113, PO2-140, PO2-240, PO2-301
Gauss J.	I-013 , PO2-297	Gonzalez Campos A.	C-062
Gebhard L.G.	PO3-155	Gonzalez Herrero L.	PO2-95
Geerke D.	PO2-123	Gopalakrishna T.Y.	PO1-190
Geerke D.P.	PO2-303	Góra R.W.	C-136 , PO2-146, PO3-224
Geiß A.	PO3-199	Gordon M.	I-145
Geng C.	PL-4	Görling A.	I-304
Georg H.	PO3-234	Gorritz R.	C-057
Gerber R.B.	I-163 , PO1-221, PO1-302, PO3-159	Goto H.	PO2-17
Gerbig D.	PO1-145, PO1-299	Götte L.	PO1-174
Geronimo I.	PO1-235	Gourlaouen C.	PO3-272
Ghafarian Shirazi R.	PO1-286	Govind N.	PO3-136
Ghane T.	C-057	Grabarek D.	PO1-119
Gherman A.M.R.	PO2-98	Grad J.-N.	PO3-49
Ghorai S.	PO1-278	Gräfe S.	PO2-42
Ghose K.K.	PO1-293	Graham C.M.E.	PO1-196
Ghosh D.	C-033	Grande Aztatzi R.	PO1-282
Ghuman K.	PO1-194	Granucci G.	PO1-260, PO1-99
Giacomozzi L.	PO3-103	Grazioso G.	PO1-132
Giampapa R.	PO1-59	Grebenschikov S.Y.	PO2-175
Giannini S.	PO1-160	Green M.	PO2-57
Gianotti E.	PO2-171	Gregory K.	C-024, PO2-69
Gierada M.	PO1-216	Gregson M.	PO2-197
Giereth R.	PO1-284	Grell G.	PO3-260
Giesen S.M.	PO1-301	Grimme S.	I-132 , PO1-186, PO2-265, PO2-54, P O2-72, PO3-176, PO3-231
Gilbert A.	PO2-196	Gritsan N.	PO1-21, PO1-85
Gilbert A.T.B.	PO1-297		

Groenhof G.	PO1-115	Hansen M.B.	PO2-236
Groll M.	PO2-131	Hansen N.	C-115
Gronowski M.	PO3-95	Hansen O.	PO2-274
Gross E.K.U.	I-114, I-034 , PO3-291	Hansen T.	C-037
Grotjahn R.	PO2-41	Hansmann A.-K.	PO1-157
Grubmüller H.	I-195	Hanulikova B.	PO1-281
Grübner I.	PO2-105	Hanževački M.	PO1-257
Gruden M.	PO2-217	Hao Y.	PO3-257
Grundeis M.	PO2-153	Hapka M.	PO3-281
Grüneis A.	PO1-163	Harabuchi Y.	C-042, PO1-29
Gryn'ova G.	I-055	Harding M.	PO3-267
Gsänger S.	PO1-18	Harish H.	PO2-141
Guarnetti Prandi I.	PO3-67	Harris A.	PO2-57
Gückel S.	C-151	Harrison E.	PO1-56
Guggolz L.	PO3-50	Harting J.	I-355
Gui X.	PO3-45	Hartke B.	PO2-221, PO2-38
Guido C.A.	PO3-127 , PO3-228	Harvey J.N.	I-071 , PO2-245, PO3-17, PO3-19
Guihéry N.	C-102 , PO2-262	Hase W.L.	I-255 , PO3-37
Guilbaud P.	PO2-88	Hashmi M.A.	PO1-304
Guillaumont D.	PO3-188	Hatanaka M.	PO3-90
Gül Ş.	PO3-247	Hättig C.	PO1-198, PO2-213, PO3-109, PO3-189
Gunnarsson O.	PO3-202	Hauser A.W.	C-051 , PO1-158, PO3-297
Gunst T.	PO2-274	Havenith R.W.A.	C-132 , PO1-24, PO3-167
Guo N.	PO1-288	Hayami M.	PO1-268
Guo Y.	PO1-23 , PO3-252	Hayamizu K.	PO3-53
Gupta A.K.	PO1-168	Head-Gordon M.	I-015 , PO3-137, PO3-269, PO3-290
Gupta P.K.	C-116, PO3-11	Head-Gordon T.	I-191
Gupta T.	PO2-298	Hecht S.	C-082
Guthmuller J.	PO1-265 , PO2-154, PO2-285	Hegely B.	C-123
Gutierrez O.	PO3-89	Hegemann P.	PO3-252
Gutierrez de Teran H.	PO3-307	Hehn A.-S.	PO3-84
Gutiérrez-Flores J.	PO2-65	Heidar-Zadeh F.	I-305
Gutiérrez-Oliva S.	PO1-146, PO2-60, PO3-182, PO3-271	Heilos A.	PO3-199
Gutten O.	PO2-232	Heimermann A.	PO2-169
Guzmán-Angel D.	PO3-182	Heindl M.	PO2-95
Gwee E.	PO1-248	Heine T.	PO1-104
H			
Haasler M.	PO2-51	Heinz N.	PO3-64
Hada M.	PO3-98	Heiska J.	C-017
Hadad C.	C-053	Hekal H.	PO1-37
Hagebaum-Reignier D.	PO3-193	Helgaker T.	PL-3
Hahn D.F.	PO3-40	Helmich-Paris B.	PO3-74
Hahn R.	PO3-176	Henchman R.	I-361
Haines B.	C-025	Hénin J.	PO2-211
Häkkinen H.	PO1-80	Hénon E.	I-314, PO3-113 , PO3-135
Haldar S.	PO2-290	Henry D.	C-167
Hall M.	C-112, PO3-200	Henschel H.	PO1-173
Hallaert S.	PO1-68	Heras-Domingo J.	PO3-18
Hamann J.	PO2-212	Herbert J.	I-335
Hamerton I.	PO1-33	Hermann G.	PO1-164, PO3-99
Hammerschmidt L.	PO2-64	Hermann M.	PO1-47
Hammes-Schiffer S.	I-033	Hermansson K.	C-023
Hammoutène D.	PO3-85	Hermesen M.	PO2-212
Hamza A.	PO2-32	Hernandes Barrozo A.	PO2-166
Han N.	PO3-195	Hernández-Haro N.	C-148
Handzlik J.	PO1-216	Hernández-Laguna A.	C-148
Hanni M.	PO1-173	Hernández-Lemus E.	PO2-65
Hansen E.	C-025	Hernando J.	PO1-139
		Herrera B.	PO1-178
		Herrmann C.	C-092 , PO1-266, PO2-237, PO2-251, PO2-280

Herrmann N.	PO3-64	Hühn C.	PO2-27
Heuer M.A.	PO1-117	Huix-Rotllant M.	PO3-264
Heuser J.	C-128, PO2-86	Hummel F.	PO1-163
Heyda J.	PO3-44	Hummer G.	I-365
Heyden M.	I-283	Hünenberger P.H.	PO3-40
Hidalgo Cardenuto M.	PO2-305	Husch T.	PO2-246
Hieringer W.	C-015	Huwig K.	PO1-172, PO2-13
Higham J.	I-361	Huynh H.M.	PO3-9
Hilal R.	PO3-101	Hwang S.-Y.	PO2-182, PO2-228, PO3-24
Hildebrand N.	PO3-36	Hynes J.T.	PO3-160
Hinkley J.	PO1-293		
Hiraga K.	PO1-268	I	
Hirata S.	I-381	Iannuzzi M.	PO3-115
Hirshberg B.	PO3-159	Iffland L.	PO3-239
Hitzenberger M.	PO2-264	Ikabata Y.	PO1-268 , PO1-269
Hiyama M.	PO1-135	Imamura Y.	PO3-54
Hnyk D.	PO3-277	Imberti S.	PO1-155
Ho E.	PO1-287	Imhof P.	C-057 , PO3-165, PO3-91
Hobza P.	PL-7 , PO2-290, PO3-277	Ingolfsson H.I.	PO3-6
Hochlaf M.	PO3-100	Ingr M.	PO3-60
Hodecker M.	PO2-162	Irgibaeva I.	PO2-106
Höfener S.	C-128 , PO2-86	Irle S.	PO1-129, PO1-152
Hoffmann D.	PO3-49	Iron M.	C-161
Hoffmann F.	PO2-151	Ishida T.	C-107
Hoffmann K.	PO1-164	Ishii T.	PO2-23
Hoffmann R.	C-104	Ishimura K.	PO2-189
Hofierka J.	PO2-253	Işık M.	PO3-247
Hogan C.	C-176	Islas R.	PO2-165
Hollas D.	PO3-282	Ito K.	PO1-228
Holm C.	PO2-281	Ito S.	C-091, PO3-53
Hölscher M.	PO1-69	Ivanov S.	C-146
Holthausen M.C.	PO2-134, PO2-241, PO2-294, PO2-48, PO2-81	Ivashchenko D.	PO1-239
Holub D.	PO1-203, PO3-158	Iwahara N.	PO1-252
Holzer C.	PO2-138 , PO3-45	Iwasa T.	C-085, C-144
Holzmann N.	PO1-155	Iwata S.	PO1-223
Homem-de-Mello P.	C-094 , PO1-100, PO1-107, PO1-127, PO2-55	Iwata T.	PO1-249
Hong K.	PO2-182	Izgorodina E.	PO1-248
Honkala K.	PO1-80	Izsák R.	PO2-170
Honma T.	PO3-87		
Hooper J.	PO3-12	J	
Hornung J.	PO1-51	Jackson C.	PO3-197
Hough M.A.	PO1-204	Jacob C.R.	PO1-123, PO1-202, PO1-258, PO3-293
Houk K.	I-075 , PO1-1, PO2-229	Jacquemin D.	I-383 , PO1-263
Howard J.C.	PO3-273	Jagau T.-C.	PO2-44 , PO2-224
Howlin B.J.	PO1-33	Jahn B.O.	PO2-76
Hoyau S.	C-038	Jahn E.	PO2-289
Høyvik I.-M.	PO3-265	Jahn U.	PO2-289
Hrnčířik J.	PO3-60	Jalife-Jacobo S.	PO1-79
Hršák D.	PO2-132	James A.M.	PO3-51 , PO3-175
Hsu C.-P.	PO2-218	Jamshidi Z.	C-087
Hu X.	C-054, PO1-264	Janet J.P.	C-072
Huang B.-J.	PO1-35	Jang J.	C-056
Huang G.-T.	PO1-9	Jani Thaviligadu D.	PO3-192
Huang P.	PO2-76	Janicki M.	C-136, PO2-146
Huang R.	PO1-110	Janoš P.	PO3-133
Huang X.	C-025, I-185	Jansen G.	PO1-256
Huber L.	PO2-157	Jansen T.L.C.	PO3-118
Huh J.	C-126	Jaoul A.	PO1-259, PO2-278
		Jaque P.	PO3-286
		Jarraya K.	PO3-169



Järvinen T.	PO2-258	Kar T.	PO1-241
Jaworska M.	PO2-252	Karadeniz U.	PO3-81
Jelinek S.	PO1-57	Karancsiné Menyhárd D.	PO2-82
Jemmis E.	I-294	Karandashev K.	PO3-235
Jena N.K.	C-138	Karbalaei Khani S.	PO2-213
Jensen F.	I-133 , PO1-183	Karlovs D.	C-113
Jensen H.J.A.	I-394	Karlsson H.O.	I-152
Jensen J.H.	I-135	Karmodak N.	PO1-275
Jensen S.R.	PO3-276	Karppinen M.	C-017
Jerabek P.	PO1-51, PO2-181	Karsili T.N.V.	I-334, PO2-101
Jesus D.	PO3-80	Karton A.	C-151, PO1-151, PO1-246, PO2-104, PO3-55
Jeung G.-H.	PO3-193	Karttunen A.J.	C-017 , PO2-110, PO2-99, PO2-136
Jeziorski B.	I-291	Kasamatsu S.	PO2-10, PO2-83
Jha P.	PO1-2	Kashef Ol Gheta S.	PO3-217
Ji L.	PO3-232	Kästner J.	I-293 , PO1-253, PO1-41, PO2-16, PO2-19
Jia D.	PO1-164	Kato T.	PO2-83
Jiang F.	PO3-209	Katoh K.	PO2-8
Jiao H.	PO3-152	Katouda M.	PO3-54
Jimenez-Oses G.	PO1-1	Kats D.	PO3-41
Johansson M.P.	C-157	Kaupp M.	C-151 , PO2-41, PO2-51, PO2-52
Johnson E.R.	I-274 , PO1-211, PO2-176, PO3-163, PO3-266	Kawasaki A.	PO2-29
Jones C.	PO1-47	Keal T.W.	PO1-204
Jones G.	IN-6 , PO1-1	Keane T.	PO3-216
Jónsson H.	I-272 , PO2-275, PO3-164	Keefer D.	PO2-125 , PO2-127
Jorgensen P.	I-014	Keremu A.	PO1-88
Jorner K.	PO2-76 , PO2-90	Kerfoot J.	PO3-46
Jornet-Somoza J.	C-101, PO2-239	Kesharvani M.K.	PO3-55
Jovanovic M.	I-311, PO3-83	Keshavarz F.	PO3-299
Judd M.	PO2-199	Keskin F.E.	PO2-73
Juhasz G.	PO2-187	Khartabil H.	I-314, PO3-113, PO3-135
Jungwirth P.	I-364 , PO1-62	Khazaei S.	PO2-295
Junkaew A.	PO2-223	Khedkar A.	PO3-239
Jurásková V.	PO3-275	Khetselius O.	PO3-251, PO3-253 , PO3-255, PO3-258
Jurinovich S.	PO3-174, PO3-228	Khomyakov P.	PO2-275
K			
Kaczmarek-Kedziera A.	PO1-267 , PO3-125	Kılıç M.	PO2-277
Kadek M.	I-041	Kim C.S.	PO2-190
Kähler S.	PO2-22	Kim C.W.	PO2-202
Kaila V.R.I.	I-284 , PO1-137, PO2-131, PO3-13, PO3-222	Kim H.W.	C-056, PO1-112
Kaiser D.	PO2-301, PO3-162	Kim J.	PO2-182 , PO2-183, PO2-195, PO2-228, PO2-70
Kaldre D.	PO2-301	Kim K.S.	I-022
Kalemos A.	C-175	Kim W.Y.	C-045 , PO2-182, PO2-228, PO2-70, PO3-24
Kallay M.	C-123	Kim Y.-H.	PO2-184
Kalmykov S.	PO2-18	King R.B.	PO1-34, PO2-107
Kaloni T.P.	C-011	Kingston D.G.I.	PO3-274
Kaltsoyannis N.	PO3-219	Kinzel D.	PO2-154
Kalvet I.	PO2-284	Kipouros I.	PO1-22
Kamerlin S.C.L.	I-194 , PO1-43	Kiran Y.B.	PO1-206
Kaminský J.	C-064	Kiselev V.	PO1-21
Kamisaka K.	PO3-87	Kishi R.	C-091, PO1-298, PO2-191
Kamorzin B.	PO3-119	Kiss D.J.	PO2-82
Kandori H.	PO1-249	Kitagawa Y.	C-091, PO1-247, PO2-8
Kanekal K.	C-022	Kitao A.	PO1-249
Kang S.	PO2-182, PO2-228	Kitaoka Y.	PO1-140
Kanger T.	PO2-111	Klahr K.	PO1-153, PO1-171
Kannath S.	PO1-61	Klamroth T.	I-174
Kappes M.M.	PO3-84	Klein A.	PO2-177
Kar M.	PO1-165	Klimes J.	C-075 , PO2-253
		Klinke C.	PO2-280
		Klinting E.L.	PO2-299
		Klöffel T.	PO2-173

Klopper W.	I-385 , PO2-138, PO3-45	Kühne T.D.	C-021 , PO3-66
Klüner T.	PO1-161, PO1-162, PO1-7, PO3-88	Kuklin M.S.	PO1-80
Knapp E.-W.	PO2-40	Kukułka M.	PO1-201
Knecht S.	PO2-269, PO3-74	Kulik H.	C-072
Knippenberg S.	C-138	Kumar A.	PO2-156
Knowles P.J.	I-175 , I-381, PO1-270	Kumar K.	PO2-178
Ko Y.-K.	PO2-190	Kumawat A.	PO1-179
Koča J.	PO3-133	Kundu A.	PO2-143
Kolos R.	PO3-95	Kuniyil R.	PO3-309
Kobayashi M.	C-085 , PO2-218	Kunz L.	IN-10
Koch C.P.	PO1-200	Kuo J.-L.	PO1-35
Koch H.	I-125	Kupfer S.	PO2-154, PO2-42
Koenis M.	PO2-77	Kurashige Y.	I-393
Koeppl C.	PO1-195	Kuritka I.	PO1-281
Koerzdoerfer T.	C-134	Kuroda Y.	PO2-218
Koga N.	PO1-135	Kurtén T.	PO2-300
Kohaut S.	PO3-34	Kussmann J.	PO2-220 , PO2-273, PO3-28
Kohguchi H.	PO1-29	Kutáľková E.	PO3-60
Kohls E.	PO2-266	Kuznetsova A.	PO3-251, PO3-253
Köhn A.	I-342 , PO1-175, PO1-284, PO2-24, PO2-33, PO3-48	Kvasikova A.	PO3-258
Koistinen O.-P.	PO3-164	Kwon S.-K.	PO2-184
Kolar M.H.	I-195		
Kolleth A.	PO2-296, PO3-81	L	
Kollmar C.	PO2-89	Laage D.	PO3-1, PO3-160
Komorovsky S.	I-041	Laasonen K.	PO2-172, PO2-204
Konecny L.	PO3-303	Labat S.	PO2-53
Kongsted J.	I-322 , PO2-132	Lafond F.	PO2-94
König C.	PO2-210, PO2-79	Lagardère L.	PO2-80
Köppl C.	I-082	Lagones T.A.	PO2-199
Köprülüoğlu C.	PO2-290	Laio A.	PO3-222
Korolokov V.	PO3-46	Lamberts T.	PO1-41
Körzdörfer T.	PO1-220, PO2-14	Lan J.	C-067
Kosloff R.	PO1-200	Lang L.	PO2-1
Kosłowski A.	PO2-85	Langer R.	PO1-64
Kossoski F.	PO2-292	Lankau T.	PO1-214
Koszinowski K.	PO2-105	Lans I.	C-053
Kovačević B.	PO2-248	Larrañaga O.	PO3-203
Kovács Á.	PO1-15	Larsson H.R.	PO2-38
Kozłowska M.	PO2-173, PO3-125	Lasorne B.	PO1-287
Kozmon S.	PO3-133	Lauritsen J.	IN-7
Kraemer T.	I-054, PO3-52	Lautens M.	C-068
Krai P.	PO3-274	Lavrov M.	C-113
Kraka E.	I-221	Łazarski R.	C-013
Kranz J.J.	PO3-105	Le T.A.	PO2-122
Krause P.	I-173, I-174	Le Bahers T.	C-095
Kreisbeck C.	PO3-146	Le Bras L.	PO2-163
Kremer K.	C-022, I-101 , PO2-206	Leal E.S.	PO3-155
Kreplin D.A.	PO1-270	LeBlanc L.	PO1-211
Kreppel A.	PO3-20	Lecours M.	I-371
Kresse G.	I-372	Ledendecker M.	PO1-27
Kříž K.	PO2-255	Lee K.	PO1-83
Kruegener M.	C-057	Lee M.E.	PO2-275
Krumnow C.	I-083	Lee S.G.	PO1-83 , PO2-190
Kruse H.	PO3-16	Lefebvre C.	PO3-113
Krylov A.	I-331	Lefebvre J.-F.	PO2-42
Krzemińska A.	PO1-17	Legault C.	PO3-68
Kubas A.	PO2-75	Legeza Ö.	I-083 , I-344, PO2-7, PO3-230
Kubo T.	C-091	Leherte L.	C-027
Kühn O.	C-032 , PO3-242	Lei J.	C-025
		Lein M.	C-065 , PO1-304

Leininger T.	PO1-226	Lu B.	PO2-205
Lelièvre T.	PO2-211	Lu L.	PO1-230
Lepšík M.	PO2-290, PO3-277	Luber S.	C-142
Lesiuk M.	PO3-280	Lüchow A.	PO1-117
Letz M.	IN-8	Ludwig M.	PO2-242
Levandowski B.	PO1-1	Luis J.M.	PO1-208 , PO3-126, PO3-250
Levin L.	PO1-200	Lumbroso A.	PO2-296, PO3-81
Levine D.S.	PO3-290	Lundell J.	PO2-258
Lewenstein M.	PO2-247	Lupan A.	PO1-34
Lewis C.	PO3-229 , PO3-57	Lutsker V.	PO3-105
Li J.	PL-4, PO1-10, PO1-5	Luy J.-N.	PO2-139
Li J.-H.	PO3-238	Luyt A.S.	PO1-95
Li J.-W.	PO3-82	Lyalin A.	C-085, PO3-97
Li S.	I-343	Lyskov I.	I-122
Li T.	PO3-172	Lyu P.	C-168
Li W.	I-173, PO2-205		
Li X.	I-332 , PO2-186, PO2-188	M	
Li Z.	PO2-141	Ma Q.	I-082, PO1-195
Li Manni G.	PO3-202, PO3-295	Ma Y.	PO2-269
Liakos D.G.	PO3-288	Macaluso V.	PO3-37
Liang W.	I-235	Macgregor S.A.	I-054 , PO2-144, PO3-52
Liao Q.	I-173	Machado F.B.C.	PO1-120
Liedl K.R.	PO2-234	Machado G.	PO3-78
Liégeois V.	PO1-298	Maciel C.	PO2-149
Ligouri N.	PO2-225	Mackinnon I.	C-105
Lim C.	I-354	Madarász Á.	PO1-15, PO2-116, PO2-268
Lim J.	PO2-182, PO2-228, PO2-70	Mader S.	PO2-131
Lima M.A.P.	PO2-292	Madsen A.Ø.	C-037
Limacher P.A.	PO3-305	Madsen D.	PO2-210 , PO2-79
Limpouchová Z.	PO3-130	Madsen N.K.	PO3-198
Lin K.-H.	PO2-46	Maeda S.	C-042, C-044, C-085, I-124 , PO1-143, PO1-159, PO1-29, PO2-293, PO3-106
Linderberg J.	PO3-171	Maffucci I.	C-054
Lindh R.	I-152	Magalhães A.	C-063 , PO1-239
Lindner J.	PO3-8	Magalhães C.	PO1-242
Linguerrí R.	PO3-100	Maganas D.	PO3-289
Linnera J.	C-017, PO2-110	Magee C.	PO1-58 , PO1-65
Lins I.A.	PO2-43	Magistrato A.	PO3-222
Lipparini F.	PO2-297, PO2-80	Mahata A.	I-264, PO1-134
Lischka H.	PO1-120, PO3-51	Mai S.	PO2-109 , PO2-140
Liu C.	PO1-154 , PO3-186	Maier T.M.	PO2-41, PO2-51 , PO2-52
Liu W.-J.	I-043 , PO2-124	Maitra N.	I-032
Liu Z.-P.	I-213 , PO2-283, PO2-309	Mak A.M.	PO1-76
Lloret J.	PO1-142	Maldonado A.F.	PO3-284
Loboda O.A.	PO2-97	Maldonado-Dominguez M.	PO3-223
Loco D.	PO2-80	Malenov D.	C-112
Lode A.U.J.	PO3-184	Malhado J.P.	PO1-126
Loffreda D.	PO3-102	Mammino L.	PO1-285
Loher C.	PO2-34	Manby F.	I-324
Löhle A.	PO1-255	Mandal D.	I-251
Long J.R.	PO3-213	Manrique-Moreno M.	C-053
Longo E.	PO1-92	Mansarliysky V.	PO3-253
Loos P.-F.	C-073	Mansikkamäki A.	PO1-252
Lopes L.J.S.	PO2-211	Manz J.	PO1-164
Lopez N.	I-052	Marazzi M.	C-178, PO3-252
Lopez X.	C-028 , PO1-111	Marchese L.	PO2-171
López R.	PO2-12 , PO2-194	Mardyukov A.	PO1-73
López Carballeira D.	PO1-136	Marefat Khah A.	PO3-109
Lopez-Tarifa P.	I-031, PO2-225	Marforio T.D.	PO2-120
Lotfikatooli L.	PO3-58	Margetić D.	PO2-5
Low P.J.	C-151		

Margraf J.	PO2-243	Meijer A.	PO3-216
Margreiter M.A.	PO1-207	Meisner J.	PO2-19
Marian C.	I-122	Meister P.	PO3-194
Mariani Silla J.	PO2-180	Melo A.	PO3-148
Marín Pérez M.D.C.	PO1-197 , PO3-215	Melse O.	PO3-120, PO3-43
Marin-Luna M.	PO2-71	Menche M.	PO2-81
Marion A.	PO3-120, PO3-25 , PO3-43	Mendoza C.I.	PO2-65
Markmeyer M.	PO2-39	Menegon Arantes G.	PO2-49
Marković M.	PO2-145 , PO2-34	Menéndez Rodríguez M.I.	PO1-209 , PO2-12
Markussen T.	PO2-274	Meng L.	PO2-186 , PO2-205
Marques C.	PO1-274	Menger M.	PO1-215
Marrink S.-J.	I-134 , PO3-6, PO3-167	Menichetti R.	C-022
Marsoner Steinkasserer L.E.	PO2-249	Mennucci B.	PL-2 , PO2-80, PO3-174
Martin A.	C-108	Mera-Adasme R.	PO3-72
Martin B.	PO3-207	Merieux G.	PO3-135
Martin F.	I-171	Merino G.	I-222 , PO1-66
Martin J.M.L.	C-121 , PO2-104, PO3-55	Mester D.	C-123
Martinez F.	I-063	Metin D.	PO2-198
Martinez T.	PL-1	Metsala A.	PO2-111
Martinez-Nunez E.	PO3-37	Metthews D.A.	I-295
Martín-Rodríguez A.	C-062	Meuwly M.	I-183 , PO1-122, PO1-184, PO1-251
Martins J.B.L.	C-014 , PO1-92	Mewes J.-M.	PO1-292
Martin-Somer A.	PO3-33	Mewes S.A.	PO2-140
Martin-Torres J.	PO2-26	Meyer B.	PO1-18, PO1-27, PO2-173, PO3-42
Martynow M.	PO2-285	Meyer F.	PO2-256
Maruszczyk A.	IN-10	Meyer L.	PO2-48
Marx D.	C-116, PO3-11, PO3-31	Meyer R.	PO1-158, PO3-297
Maryasin B.	PO2-301	Meyerhenke H.	PO1-123
Maschio L.	C-012	Michalak A.	PO1-217
Masella M.	PO3-188	Michels B.	PO3-162
Mason P.E.	PO1-62	Michl J.	I-311 , PO2-41, PO3-83
Massolle A.	PO2-37	Mihaylov T.	PO3-227
Mata I.	I-064	Mikkelsen K.V.	I-325
Mata R.A.	C-122 , PO1-243, PO1-271, PO2-21, PO2-245, PO2-74	Miletto I.	PO2-171
Mathieu D.	PO2-250	Millán L.	PO3-21
Matito E.	C-076 , PO1-142, PO1-44, PO3-126	Mills D.P.	PO3-219
Matsika S.	I-334	Min S.K.	I-114
Matsui H.	PO2-191	Miqueu K.	PO1-118 , PO1-237, PO2-53
Matsunaga S.	PO1-140	Miriyala V.M.	PO2-235
Matsuzaki Y.	PO1-181	Mitchell I.	PO1-152
Matveev P.	PO2-18	Mitchell J.	PO3-197
Matxain J.M.	C-018	Mitric R.	I-113 , PO3-8
Matz O.	PO1-188	Mitrofanov A.	PO2-18
Maulide N.	PO2-301	Mitzinger S.	PO3-50
Maurer M.	PO2-242	Miyazaki Y.	PO1-29
Maurice R.	PO1-288 , PO2-28	Mo L.	PO2-186
Maximowitsch E.	PO1-149	Modrzejewski M.	PO3-281
Mayer I.	C-155 , PO2-2	Moe S.	PO2-283
Mayhall N.	C-131	Mohr S.	PO3-66
Mayr H.	PO2-141	Moiseyev N.	PO2-177
Mazumdar A.	PO3-6	Molins E.	I-064
McCaslin L.	PO1-221	Møller K.B.	PO3-59
McConnell S.	PO2-9	Monari A.	C-178, PO2-109, PO3-294
McDonald A.R.	I-045	Moncho S.	PO3-200
McKay A.I.	PO3-52	Moncomble A.	PO3-192
McKemmish L.	PO3-22	Mondragón-Solórzano G.	PO1-296
McKenzie S.	PO1-297	Mons M.	C-038
McLean B.	PO1-130	Montavon G.	PO1-288
Medina F.	PO1-116	Montero M.	I-063
		Mookherjee M.	C-148

Moon J.	PO2-183	Natori Y.	PO1-247 , PO2-8
Moore K.	PO3-123	Natrajan L.	PO3-219
Mora A.	PO3-144	Naumkin F.	PO1-240
Morais S.	PO1-127	Nava P.	PO2-270
Moran D.	I-073	Navizet I.	C-137 , PO2-160
Moraru I.-T.	PO2-259	Nazarikatouli F.	PO3-58
Mori S.	C-044 , PO2-23	Neale S.	PO2-31
Moro G.J.	PO2-142	Neese F.	I-344, PL-12 , PO1-23, PO1-245, PO1-286, PO1-46, PO2-1, PO2-170, PO2-47, PO3-225, PO3-27, PO3-288, PO3-289
Morokuma K.	C-044, PO1-143	Negri F.	I-262 , PO2-124
Morozov D.	PO1-115	Nemes G.	PO2-259
Morris M.	PO1-57	Nemukhin A.	I-105
Morrison A.	I-335	Nenadovič M.	I-412
Morshedi M.	PO2-199	Nenov A.	PO3-128
Moses P.G.	IN-7	Nerukh D.	C-026
Moskaleva L.	PO3-88	Neto A.D.M.	C-014
Moszynski R.	PO3-280	Netz P.A.	PO2-61 , PO1-274
Mougel V.	PO2-135	Neugebauer J.	PL-10 , PO1-153, PO1-171, PO2-37
Mráziková K.	PO3-16	Neuhauser D.	PO1-12, PO1-219
Mück-Lichtenfeld C.	PO3-206	Neves R.P.P.	PO1-116
Mühlbach A.	PO2-272	Nguyen Q.N.	PO2-207
Mukamel S.	I-172 , PO3-128	Nicolini P.	PO2-130
Müller C.	PO3-243	Nicu P.V.	PO2-77
Müller-Plathe F.	I-102	Niehaus T.	PO3-101, PO3-105
Munarriz J.	PO3-218	Nieminen M.T.	PO1-173
Munejiri S.	PO1-307	Nikiforidis G.	PO1-11
Muñoz F.	PO3-145	Nikšić-Franjić I.	PO3-179
Muñoz-Muriedas J.	PO1-99, PO1-239	Ning A.	PO3-232
Muñoz-Rugeles L.	C-052	Ninkovic D.	C-112, PO3-200
Muñoz-Santiburcio D.	C-148, PO3-31	Nishimoto Y.	PO1-26
Murdachaew G.	PO2-172	Nishimura Y.	PO1-225 , PO1-305
Murugan N.A.	C-138	Nisula M.	C-017
Mustalahti S.	PO1-115	Nizovtsev A.	PO3-46
Mutapčić I.	PO2-145	Noble B.	PO3-92
Muuronen M.J.	PO2-308 , I-301	Nocton G.	PO1-259, PO2-278
Myllyperkio P.	PO1-115	Noga P.	I-412
Myllys N.	PO2-300	Noguchi Y.	PO1-135, PO1-224
N			
Nachtigall P.	C-168	Nogueira Perez J.J.	PO2-95 , PO2-113, PO2-140
Nadj A.	PO2-48	Nooijen M.	I-371
Nagami T.	C-091, PO1-298	Norman P.	I-401 , PO3-29
Nagaoka M.	PO2-226	Norrby P.-O.	C-025
Nagase S.	PO3-87	Novko D.	C-088
Nagy P.	C-123	Novoa J.J.	C-101
Najibi A.	PO1-295	Nowak W.	C-058 , PO1-227
Nakahara M.	C-085	Nyvang A.	PO3-213
Nakai H.	I-051 , PO1-225, PO1-233, PO1-268, PO1-269, PO1-280, PO1-305, PO2-68	O	
Nakakoji K.	PO1-223	Oakley M.	PO2-59
Nakano M.	C-091 , PO1-247, PO1-276, PO1-298, PO2-191, PO2-8	Oberli S.	PO2-35
Nakano S.	PO3-53	Ochsenfeld C.	PO2-242, PO2-244, PO2-273, PO3-157, PO3-177, PO3-20, PO3-26, PO3-28
Nakatsuji H.	PL-8	Oda T.	PO1-223
Namuangruk S.	PO2-223, PO2-66	Odriozola-Gimeno M.	PO2-58
Nandi S.	C-046	Oesterling S.	PO2-157
Narevicius E.	PO2-177	Ofial R. A.	PO2-141
Naruse Y.	PO1-3	Ohmiya H.	PO2-23
Narva T.	PO3-131	Ohno K.	PO1-223
Nascimento M.	I-313 , PO3-61	Okiyama Y.	PO3-87
Natarajan U.	PO1-168	Okoshi M.	PO1-233

Oláh J.	PO2-82	Pareek M.	PO1-75
Olenius T.	PO2-300	Pareras G.	C-162
Olinto G.	PO1-92	Park J.H.	PO2-190
Oliveira Jr R.R.	PO3-129	Park J.W.	PO3-63
Olivucci M.	PO3-215	Park J.Y.	PO1-11
Ollitrault P.J.	PO3-137	Parker K.	PO2-53
Olsen J.M.H.	I-014, I-084 , PO2-22, PO2-132 PO3-213, PO3-5	Parker S.	PO3-149
Olsson M.A.	I-212	Parrinello M.	I-211 , PO3-241
Olszówka M.	PO3-208	Partos B.	I-295
O'Mara M.L.	PO1-150, PO2-199, PO3-197	Pas E.	C-078
Ong T.-G.	PO2-218	Pascual M.J.	PO3-155
Onitsuka Y.	PO1-29	Pasteka L.F.	PO3-257
Ono Y.	C-042	Pastore M.	I-263 , PO3-294
Oostenbrink C.	PO2-62	Patel A.	PO1-1
Oppel M.	PO2-240	Patel H.	PO3-245
Orian L.	PO2-78	Pathak B.	I-264 , PO1-134
Oriana A.	PO3-128	Pathak H.	PO1-90
Ornellas F.R.	PO2-43	Pathak S.	PO2-1
Orozco M.	I-193 , PO2-152, PO2-164	Pati S.K.	PO2-167
Ortega D.E.	PO1-146	Patkowski K.	PO3-156
Ortega-Castro J.	C-148	Paton R.	PO1-108
Ortí E.	PO1-53	Patoz A.	PO3-134
Ortiz J.V.	I-381	Patschinski P.	PO2-71
Ortiz de Luzuriaga I.	C-018	Paukku Y.	PO1-289
Ortiz-Chi F.	PO1-66	Paulikat M.	PO2-21
Ortu F.	PO3-219	Paulus B.	I-233 , PO1-164, PO2-249, PO2-6, PO2-7
Oruganti B.	C-035	Pavanello M.	I-215
Osella S.	C-138	Pavosevic F.	PO3-27
Osipov V.A.	C-037	Pawlak M.	PO2-177
Ostermeir K.	PO2-54	Pawlowski F.	I-014
Osuna S.	PO2-229	Pearce K.C.	PO3-274
Ota Y.	PO1-74	Peccati F.	PO1-139
Otero de la Roza A.	PO1-211, PO2-176	Pecher L.	C-016, PO2-238
Ottosson H.	PO2-76, PO2-90	Peláez D.	C-103
Overgaard J.	PO3-213	Peltzer R.	PO3-214
Oyama T.	PO1-268	Pendás Á.M.	PO1-39
Ozmaldar A.	PO2-91	Penfold T.J.	PO3-59
P			
Pacchioni G.	PO1-80, PO2-96	Peng C.	PO1-52 , PO3-27
Page A.J.	C-024 , PO1-128, PO1-129, PO1-130, PO1-152, PO1-246, PO1-293, PO1-300, PO2-69	Peng Q.	PO3-2
Pahl E.	PO1-167 , PO2-181, PO3-296	Perchik M.	PO1-59
Palacino-González E.	PO3-244	Pereira R.	PO1-242
Palikot E.	PO3-262	Peres J.	PO1-124
Palsgaard M.	PO2-274	Perez M.A.S.	PO2-277
Palusiak M.	C-162	Pérez del Valle C.	C-148
Palyulin V.	C-113 , PO3-93	Pernal K.	I-035
Pan X.	PO1-193	Perrier A.	C-166 , PO2-163
Panas I.	PO3-96	Persico M.	PO1-24, PO1-260
Paneth P.	PO1-17	Peschel M.	PO2-15
Pantaleone S.	PO1-139	Peschina J.	PO2-294
Pantazis D.A.	PO1-46, PO1-245, PO1-286	Peter C.	I-104
Papadakis R.	PO2-76	Peters L.D.M.	PO3-28
Papai M.	PO3-59	Petersen T.	PO1-162
Pápai I.	PO2-116, PO2-3 , PO2-32	Peterson K.A.	PO2-104, PO2-181
Parasuk V.	PO1-232 , PO1-40, PO2-67	Peterson L.	PO1-57, PO1-58, PO1-59, PO1-63, PO1-65
Parasuk W.	PO1-40, PO2-67	Petrone D.A.	C-068
Paredes K.	PO1-291	Petrov V.	PO2-18
		Petrovic P.	C-112, PO3-200
		Petterson M.	PO1-115
		Petuker A.	PO3-239
		Pfeifer R.	PO3-129

Pham L.N.	PO1-277
Phung Q.	PO1-148
Piccini G.	PO3-241
Piccinin S.	I-263
Picconi D.	PO2-175
Pichierri F.	C-172
Pieck F.	PO2-238, PO2-279
Piecuch P.	I-395
Pierloot K.	PO1-148, PO1-68
Pilmé J.	PO2-28
Pinheiro Jr M.	PO1-120
Pinski P.	PO2-47
Pinto da Silva L.	PO1-242
Piquemal J.-P.	C-125 , PO2-80
Piris M.	C-071
Pisarek J.	PO2-115
Pittner J.	I-083, I-344 , PO3-225, PO3-230
Pižl M.	PO3-44
Pla P.	PO1-262
Plasser F.	PO2-109, PO2-140 , PO3-101
Platts J.A.	PO3-180
Ploetz E.A.	PO3-6
Pluharova E.	PO3-1
Poblador Bahamonde A.I.	C-068
Podewitz M.	PO2-234
Pohl M.	PO3-282
Pohl V.	PO1-164, PO2-254 , PO3-99
Poier P.P.	PO1-183
Poisson L.	PO3-100
Polkehn M.	I-112
Polly R.	PO1-169
Polo V.	PO2-260 , PO3-218
Polozij M.	C-168
Pomelli C.S.	PO1-290
Postils V.	PO3-268
Postils Ribó V.	PO3-250
Postnikov A.	PO2-94
Pototschnig J.V.	PO1-158
Potter T.	PO1-28
Prager S.	PO3-196
Prats Garcia H.	PO1-50
Prem M.	PO3-162
Prestianni A.	PO1-14
Price A.	PO3-163
Pritchard T.E.	PO1-196
Prlj A.	PO2-46
Procházka K.	PO3-130
Proppe J.	PO1-177
Prosmi R.	PO1-102
Puchta R.	PO3-300
Puggina de Freitas M.	PO2-180
Pulay P.	I-092
Puripat M.	PO1-40
Putau A.	PO2-105
Puthenkalathil R.	PO3-7
Puzzarini C.	PO3-100
Pyykkö P.	I-042
Q	
Qu C.	I-161
Quanz H.	PO3-246
Quapp W.	C-047 , PO1-218
Quinn T.	C-025
Quiñonero D.	I-064, PO1-238
R	
Rabani E.	PO1-12, PO1-219
Radadiya A.	PO3-245
Radchenko E.	C-113, PO3-93
Radom L.	I-073 , PO1-91
Radon M.	PO1-191
Radu L.-F.	PO2-84
Raeker T.	PO2-221
Ragogna P.J.	PO1-196
Rahm M.	C-104
Rajabi N.A.	PO3-170
Rajagopala Reddy S.	PO2-50
Rajaraman G.	I-224
Ramanan R.	I-251
Rambabu G.	PO1-206
Ramek M.	PO2-145, PO2-34
Ramin Moayed M.M.	PO2-280
Ramírez Solís A.	PO3-143
Ramos E.	PO2-65
Ramos M.J.	PO1-116
Ramos-Cordoba E.	C-076, PO1-44, PO1-142, PO3-269
Randall S.	PO3-219
Rao A.G.	PO3-161
Rasmussen S.	IN-7
Ratanasak M.	PO1-232
Rawat K.S.	PO1-134
Raybaud P.	PO2-133
Raynaud C.	I-061
Réal F.	PO3-188
Reddy S.R.	PO2-4
Rehn D.R.	PO3-29 , PO2-162
Reich D.	PO1-200
Reidelbach M.	PO3-91
Reiher M.	I-243 , PO1-177, PO1-187, PO2-174, PO2-246, PO2-269, PO3-107, PO3-166
Reining L.	I-384
Reiter K.	PO2-302
Reiter S.	PO2-127 , PO2-201
Rekhroukh F.	PO1-118
Ren T.	PO3-4
Renevey A.	PO1-16
Renger T.	PO3-228
Repisky M.	I-041, PO3-74
Restrepo A.	C-053 , PO1-66
Reta D.	PO3-219
Reuter K.	I-261 , PO2-243
Révész Á.	PO2-116
Reynaud S.	PO3-110
Řezáč J.	C-077 , PO2-235, PO2-255
Rhee Y.M.	I-353 , PO2-202
Ribas J.	PO1-218
Ribas X.	PO1-208
Ribas-Arino J.	C-047

Ribeiro A.	C-094	Ruiz-Barragan S.	PO3-31
Ricardi N.	PO3-196	Rulišek L.	C-086 , PO1-22, PO1-306, PO2-289
Ricci G.	PO2-124	Rungnim C.	PO2-66
Rice J.	I-253 , PO1-1	Rusu T.	PO1-8
Richards N.	PO3-245	Ruud K.	I-041
Richter M.	C-032	Rybak L.	PO1-200
Rickmeyer K.	PO2-224	Rybarczyk M.	PO2-261
Riedle E.	PO2-157	Ryde U.	I-212 , PO1-229
Riipinen I.	PO2-300	Rydzewski J.	C-058, PO1-227
Riniker S.	I-184 , PO1-16, PO3-114, PO3-220	Ryu S.	PO2-182, PO2-228
Rinke P.	PO2-147, PO2-286		
Riplinger C.	PO3-306	S	
Rivera M.	PO2-119, PO2-161	Saalfrank P.	I-174
Rivera-Arrieta H.I.	PO3-124	Saavedra-Torres M.	PO2-194
Rivero U.	PO1-122	Sabolović J.	PO2-34 , PO2-145
Rivilla I.	PO2-58	Sadeghian K.	PO3-157
Rivlin T.	PO3-22	Sagarik K.	PO3-304
Rizzo A.	I-405	Sainz-Díaz C.I.	PO2-26 , C-148, PO2-155
Robb M.A.	C-101, PO1-126	Sairi M.	PO1-33
Roberts A.	PO1-239, PO3-15	Saita K.	PO3-106
Roca-Sanjuán D.	C-034	Saito T.	PO2-288
Rocca D.	I-263	Saitow M.	PO3-225
Roch L.	PO3-150	Sakata K.	PO1-140
Rocha V.	PO3-78	Sakellaris C.	PO3-293
Rodrigues Silva D.	PO2-179, PO2-180	Sakti A.W.	PO1-305
Rodríguez J.F.	C-068	Sakuma S.	PO1-307
Rodríguez Mayorga M.A.	PO1-98 , C-076, PO1-44	Salama R.	PO1-38
Rodríguez Segundo R.	PO1-102	Salvador M.A.	PO1-127
Rodríguez-Santiago L.	PO3-35	Salvador P.	C-076, C-111, PO3-268 , PO3-250
Rodziewicz P.	PO2-173, PO3-125	Salzner U.	C-163
Roemelt M.	PO3-239	Samanta P.	PO1-175
Roethlisberger U.	PL-11	Sami S.	C-132
Rogachev A.	C-081	Samu G.	C-123
Rogozina M.	PO1-236	Sánchez O.	PO3-299
Röhr M.I.S.	PO3-8	Sánchez-Navas A.	C-148
Roithova J.	C-086	Sancho-García J.C.	PO1-53
Rojas-Valencia N.	C-053	Sandberg L.	PO3-139
Róldan-Gómez S.	PO1-208	Sandoval A.B.	PO1-293
Romero A.	PO2-229, PO2-282	Sandoval-Salinas M.E.	PO1-190 , PO1-296
Romero J.	PO3-187	Santa Cruz T.	PO3-151
Romerosa A.	PO1-155	Santiso E.	PO3-186
Rommel J.	PO2-263	Santos J.	PO1-92
Roos M.K.	PO2-121, PO2-201	Sanz F.	C-062
Rossetti G.	PO1-207	Sanz Matias A.	PO3-19
Rossky P.J.	C-036	Sarkar A.	PO2-112
Rothlisberger U.	PO1-199, PO2-277	Sarrami Foroushani F.	PO1-151
Rott F.	PO2-15, PO2-157	Sastre S.	PO3-145
Roulet J.	PO3-117	Sastry G.N.	I-204
Rovira M.	PO1-208	Satoh H.	PO1-223
Roy L.	PO1-94	Saue T.	I-044
Rozgonyi T.	PO3-59	Sauer J.	PO2-143, PO2-150, PO2-214
Rubes M.	PO3-204	Sauer S.	PO3-162
Rubez G.	PO3-113	Saura P.	PO3-13
Rubio A.	PO2-239	Savasci G.	PO2-267
Rudek B.	PO3-61	Sawamura M.	C-044, PO2-23
Rudolph J.	PO1-202	Sawatlon B.	PO2-159
Rudzinski J.	PO2-206	Sayós R.	PO1-50, PO3-299
Rüger R.	I-031, PO1-104	Scalambra F.	PO1-155
Ruipérez F.	C-106 , PO1-136	Scalmani G.	PO3-208
Ruiz E.	C-062, C-108	Scarbath-Evers L.K.	PO2-56

Scemama A.	C-073	Selles P.	PO2-35
Schaefer H.F.	I-093 , PO3-71, PO3-77, PO3-123, PO3-124	Selner E.	PO1-58, PO1-65
Schäfer A.	PO2-212	Sels B.	PO1-68
Schapiro I.	PO3-161, PO3-221	Sen K.	PO1-204
Schattenberg C.J.	PO2-52	Sen S.	PO2-225 , PO3-108
Schatz G.	I-154	Senami M.	PO1-228
Schaub T.	PO2-212	Senjean B.	PO3-32
Scheffler M.	I-244	Serga I.	PO3-258
Scheiner S.	PO1-241	Sergentu D.-C.	PO1-288, PO2-28
Scherbinin A.	PO3-119	Serwatka T.	PO2-6
Scherrer C.	IN-8	Sethio D.	PO1-48
Schieschke N.	C-128	Sgrignani J.	PO1-132
Schild A.	PO3-291	Shagam Y.	PO2-177
Schimmenti R.	PO1-14	Shah A.	PO3-245
Schlangen M.	PL-4, PO1-10	Shah N.J.	PO1-207
Schlegel H.B.	I-173	Shahsavand A.	PO3-58
Schlott H.	PO1-27	Shaik S.	I-251 , PL-4
Schlüns D.	PO1-171	Shalashilin D.	PO2-240
Schmid P.	PO3-199	Shalom M.	PO1-27
Schmidt A.-C.	PO2-212	Shang C.	PO2-309
Schmitt-Monreal D.	PO1-258	Shao M.	PO3-136
Schmitz G.	PO2-209 , PO3-189	Sharapa D.	PO2-306
Schnabel J.	PO2-24	Sharma S.	PO3-202
Schnappinger T.	PO1-279	Shemesh D.	PO1-231
Schneider G.L.	PO1-22, PO1-205	Shen J.	I-395
Schnieders D.	PO1-153, PO1-222	Sherrill D.	I-205
Schnitzer T.	PO3-26	Sheu S.-Y.	PO1-54 , PO1-55
Schoenebeck F.	PO2-284	Sheu W.-S.	PO1-182
Schönborn B.	I-174	Shiga M.	PO1-135, PO1-74
Schoonheydt R.	PO1-68	Shigemitsu Y.	PO1-156
Schooss D.	PO3-84	Shih P.	PO1-166
Schreckenbach G.	C-011	Shiozaki T.	I-391 , PO3-63
Schreiner P.R.	I-072 , PO1-145, PO1-299, PO3-246	Shoji Y.	PO1-269
Schröder B.	PO2-261	Shpiro B.	PO1-12
Schröder H.	PO2-25	Shuai Z.	I-265 , PO3-2
Schulz C.	PO1-46	Sibaev M.	PO1-294
Schulz J.B.	PO1-207	Sidler D.	PO3-114
Schumann-Gillett A.	PO1-150	Siegmann M.	PO2-129
Schüppel F.	PO2-121	Siemering R.	PO1-279
Schurkus H.	PO2-244	Sierka M.	C-013 , PO1-210, PO2-27, PO2-30
Schwabe T.	PO2-25	Sierraalta A.	PO2-307
Schwaninger A.	PO3-114	Silaghi-Dumitrescu R.	PO1-229
Schwarz H.	PL-4 , PO1-10, PO1-5	Sillar K.	PO2-143
Schwarzer M.C.	PO2-23	Silva J.C.F.	C-014
Schweizer J.I.	PO2-48, PO2-81	Silvani A.	PO1-132
Schwell M.	PO3-100	Sim E.	I-303
Schwerdtfeger P.	I-021 , PO1-167, PO2-181, PO3-257, PO3-296	Simm G.	PO1-187
Schwilk M.	I-082, PO1-195	Simmermacher M.	PO3-237
Scott C.J.C.	PO3-65	Šindelka K.	PO3-130
Scuderì D.	PO3-37	Singh A.	PO1-105
Scuseria G.	I-081	Sinha V.	PO1-78
Sebald P.	PO2-261	Sirohiwal A.	PO1-245
Sebastiani D.	PO2-295	Sisourat N.	PO2-35
Seebach D.	PO2-246	Sitkiewicz S.	PO3-126
Segarr-Marti J.	PO3-128	Sivalingam K.	PO1-23
Segatta F.	PO3-128, PO3-174	Skaf M.	I-415
Seibert J.	PO2-72	Skitnevskaya A.	PO2-100
Seino J.	PO1-268, PO1-269, PO1-280	Sklenak S.	C-147
		Skomorowski W.	PO1-200
		Skyllaris C.-K.	PO3-273

Sladek V.	PO3-53	Sulzer S.	PO2-296, PO3-81
Slaviček P.	PO3-275, PO3-282	Sumiya Y.	PO2-293
Slipchenko L.	I-323	Summerfield A.	PO3-46
Smeu M.	PO3-70	Sun Y.	PO1-19
Smiatek J.	PO2-281	Sunaga A.	PO3-98
Smidstrup S.	PO2-275	Sundholm D.	I-094 , PO1-137, PO3-190
Smirnova A.	PO2-18	Sunoj R.B.	I-223
Smith A.-S.	I-355, PO3-256	Suomivuori C.-M.	PO1-137
Smith D.M.	I-355 , PO2-233, PO2-248, PO3-256	Supady A.	C-082
Smits O.	PO2-181	Suzuki K.	PO1-143 , PO1-181
Smyrnova D.	PO3-215	Suzumura T.	PO2-17
Sobolewski A.L.	C-133 , PO2-101	Svatek S.	PO3-46
Sochorová Vokáčová Z.	PO3-1	Svinarenko A.	PO3-259
Sodupe M.	PO1-139, PO3-35	Swang O.	C-118
Sokkar P.	PO3-104	Swart M.	I-045 , PO2-229, PO2-256, PO2-282
Solà M.	C-162, PO2-76, PO2-90, PO2-257	Swope W.C.	PO2-123
Solans-Monfort X.	PO1-139, PO3-35	Sylvetsky N.	PO2-104
Sollogoub M.	PO2-128	Symonds C.	PO2-240
Solomon E.I.	PO1-22	Szabla R.	C-136, PO2-146, PO3-224
Song L.	PO3-278	Szalay P.G.	I-295
Sosa Carrizo E.D.	PO1-237 , PO2-53	Szalay S.	I-083
Sotiropoulos J.-M.	PO2-53	Szalewicz K.	I-234
Sousa C.P.	PO1-127	Szatyłowicz H.	PO1-272
Sousa S.	PO1-124	Szczesniak M.	PO3-281
Souza T.	C-094	Szilvási T.	I-083
Spezia R.	PO3-37		
Sponer J.	PO3-16, PO3-224	T	
Springborg M.	C-048 , PO1-172, PO2-13	Taenzler P.	PO3-157
Srebro-Hooper M.	PO1-217	Taeschler C.	IN-2
Srnec M.	PO1-306, PO3-223	Taft C.	PO1-92
Staemmler V.	PO1-174	Taioli S.	PO3-174
Staniszewska M.	PO2-154	Tajti A.	I-295
Stanke M.	PO3-262, PO3-47	Takagi M.	C-085, PO1-159
Stanton J.F.	I-085 , I-295	Takamuku S.	PO1-276 , PO2-191
Stasyuk A.	PO2-257	Takano Y.	PO2-288
Steenbergen K.G.	PO3-296	Takaya D.	PO3-87
Steenbock T.	PO1-266	Takenaka M.	C-144
Stefanovic R.	C-024, PO1-128	Takenaka N.	PO2-226
Steffen J.	PO1-189	Taketsugu T.	C-042 , C-044, C-085, C-144, PO1-29, PO2-218, PO3-97
Stein C.	PO2-174 , PO3-107	Talbot P.	C-105
Stein M.	C-098 , PO2-118, PO2-266	Talhi F.	PO1-4
Steinmetzer J.	PO2-216	Talotta F.	PO2-45
Stemmle C.	PO2-7	Tamayo T.	PO3-146
Štěpánek M.	PO3-130	Tamm T.	PO3-131
Stepic R.	I-355, PO3-256	Tamura H.	I-112
Stirling A.	C-173	Tan Y.S.	PO1-192 , C-078
Stojanovic L.	PO3-101	Tannor D.J.	I-144 , PO2-38
Stokbro K.	PO2-274, PO2-275	Tanriver G.	PO2-296 , PO3-81
Stopkowicz S.	C-141	Tapavicza E.	PO3-154
Stradi D.	PO2-275	Tarumi M.	PO1-181
Straka M.	C-064	Tashiro M.	PO3-54
Strange R.W.	PO1-204	Tavşanlı A.	PO2-73
Stroet M.	PO2-92	Tavares da Costa L.	PO3-226
Suarez D.	PO1-20 , PO1-32	Tavernelli I.	I-114
Subotnik J.	I-155	Tecmer P.	PO1-133
Sugimoto M.	C-041	Teixeira Mancini D.	PO3-226
Sugino O.	PO1-135, PO1-224, PO2-10, PO2-29, PO2-83	Tejero T.	PO3-79
Suksumolrat N.	PO2-67	Tellgren E.	PO3-108
Sullivan M.B.	PO1-76	Ten-no S.	I-142 , PO2-208
Sulskus J.	PO2-168		

Tennyson J.	I-165, PO3-22	Uno T.	PO1-223
Teodoro T.	PO2-77	Unsleber J.	PO1-153
Teramae H.	PO1-141	Uosaki K.	PO3-97
Ternovsky E.	PO3-259	Uranga J.	PO1-45
Ternovsky V.	PO3-258	Uranga O.	PO3-122
Teusch T.	PO1-161	Urban M.	I-412
Teuteberg T.	PO2-74	Urbanek P.	PO1-281
Tew D.P.	I-392 , C-075	Uta M.-M.	PO2-107
Teze D.	PO1-288	Uusitalo J.J.	PO3-167
Thallmair S.	PO2-15, PO3-6		
Thiel W.	I-131 , PO2-193, PO2-85, PO3-62	V	
Thom A.J.W.	PO3-65	Vacher M.	I-152, PO1-126
Thomas M.	PO2-11, PO2-199	Vaiana A.C.	I-195
Thompson T.H.	PO3-177	Vala H.	PO3-245
Thomsen M.	PO3-213	Valeev E.F.	PL-5 , PO1-23, PO3-27, PO3-57, PO3-229
Þórhallsson A.	C-158	Valjus J.	PO1-196
Thoss M.	PO2-4, PO2-50	Vallejo W.	PO1-213
Titov E.	I-174	Vallet V.	PO3-188
Todorova T.K.	PO2-135	Valsson O.	PO2-227
Tokiwa H.	PO3-53	Van de Sanden M.C.M.	PO1-6
Toldo J.M.	PO2-117	Van Dijk M.	PO2-303
Tomaschun G.	PO1-7	Van Gastel M.	PO3-239
Tomza M.	PO2-247	Van Lenthe E.	PO1-104
Tonner R.	C-016 , PO2-238, PO2-279	Van Neck D.	PO1-39, PO2-230
Töpfer K.	PO2-93	Van Niekerk D.	PO2-108
Toro-Labbé A.	PO1-146, PO1-178, PO3-182, PO3-271	Van Niekerk D.M.E.	C-177
Torrent Sucarrat M.	PO2-58	Van Sittert C.G.C.E.	PO1-95
Tosoni S.	PO1-80, PO2-96	Van Wüllen C.	PO2-169
Tóth G.	PO2-82	Vanelderden P.	PO1-68
Tóth Z.	PO3-75	Vaniček J.	PO3-110, , PO3-116 PO3-117, PO3-134, PO3-235
Toulouse J.	I-273	Vankó G.	PO3-59
Tozer D.	I-271	Varella M.T.d.N.	PO2-292
Traber P.	PO2-42	Varga S.	PO2-116
Tran D.H.	PO3-173 , C-078	Varga Z.	PO1-289
Tremblay J.C.	C-088 , PO1-164, PO2-254, PO2-6, PO2-93, PO3-99	Vargas A.	PO1-66
Trindle C.	PO1-114, PO1-71	Varner M.E.	PO1-302
Trnka T.	PO3-133	Vaucher A.	PO3-166
Trofimov A.	PO2-100	Vecharynski E.	PO3-136
Truhlar D.	I-201 , PO1-289	Vehkamäki H.	PO2-300
Tsatsoulis T.	PO1-163	Vehtari A.	PO3-164
Tsuchimochi T.	PO2-208	Veiros L.F.	PO3-292
Tsutsumi T.	C-042	Veis L.	I-083, I-344, PO3-230
Tucholska A.	PO3-280	Vej-Hansen U.G.	PO2-274 , PO2-275
Tuczek F.	PO1-82	Vercauteren D.P.	C-027
Tuna D.	PO2-193	Verdonk M.	IN-4
Tuñón I.	PO3-160	Verstraete F.	I-083
Tuononen H.M.	PO1-196	Very T.	C-038
Turi L.	C-036	Via Nadal M.	PO1-44 , C-076
Turner M.	PO3-180	Vícha J.	C-064, PO1-273
Turney J.M.	PO3-124	Vidal-Daza I.	C-148
Turupcu A.	PO2-62	Vieira T.F.	PO1-124
Tuvi-Arad I.	PO3-185	Vila Verde A.	PO3-217
Tvaroška I.	PO3-133	Vilhena F.D.S.	PO1-84
		Villegas-Escobar N.	PO1-146
U		Viseras C.	PO2-155
Ueno-Noto K.	PO2-185	Visscher K.M.	PO2-303 , PO2-123
Uhlig F.	PO2-281	Visscher L.	I-031 , PO1-104, PO2-225, PO2-77, PO3-74
Unnikrishnan A.	PO1-70	Vlček Jr. A.	PO3-44

Author Index

Vogler S.	PO2-242	Wesolowski T.A.	PO3-196
Vöhringer-Martinez E.	PO1-125	Weßing J.	PO1-51
Voigt A.	PO1-207	White N.G.	PO2-199
Voigt B.A.	PO2-237	Whitfield J.H.	PO3-197
Volkenandt S.	C-057	Wibowo M.	PO1-24
Von Looz M.	PO1-123	Wick C.	I-355, PO2-233
Vondung L.	PO1-64	Wiebeler C.	PO3-161
Voora V.K.	I-301	Wiebeler H.	PO3-66
Voronina E.	PO2-271	Wiest O.	C-025
Voth G.	I-245	Wilcken R.	PO2-157
Vucemilovic-Alagic N.	I-355	Willitsch S.	PO1-122
Vyboishchikov S.	C-153	Wilson D.	C-176

W

Waigel W.	PO3-199	Wilson M.	PO1-28
Waite S.	PO1-246	Winpenny R.E.P.	PO3-219
Waite C.	C-074	Wipff G.	PO3-279
Waldt E.	PO3-84	Wirsing S.	PO3-162
Wales D.J.	PO3-65	Witasek R.	PO3-60
Waller M.	C-043	Witek H.A.	PO1-201
Walsh J.P.S.	PO3-213	Witek J.	PO2-114
Wan S.	PO1-36	Wodrich M.D.	I-252, PO2-159
Wang C.-Y.	PO1-35	Wolff W.	PO3-61
Wang D.	PO3-10	Wolter M.	PO1-123
Wang F.	C-156	Womack J.C.	PO3-273
Wang G.	PO1-96	Won J.S.	PO2-190
Wang H.	PO3-242	Wong M.W.	PO1-76
Wang J.	C-035	Wood B.	PO1-248
Wang K.	I-161	Wood G.	PO3-186
Wang Q.	PO1-269	Woody A.	PO1-57
Wang T.	PO3-201	Worth G.A.	I-115 , PO2-240, PO2-287
Wang W.	PO2-188	Wouters S.	PO1-148
Wang X.	PO1-193 , PO3-57	Wright D.W.	PO1-36
Wang Y.	I-161, PO1-262, PO1-96	Wu H.-N.	PO3-209
Wang Z.	C-156	Wu J.	PO1-190
Wanless E.	PO2-69	Wu X.	PO2-101 , PO2-85
Warnau J.	PO1-283	Wu Y.-D.	C-067, PO3-209
Wasif Baig M.	PO3-30	Wuttke A.	PO2-231
Watanabe C.	PO3-87	Wylie L.	C-078
Watanabe H.	PO3-87		
Watanabe K.	C-091, PO1-298	X	
Watanabe Y.	PO3-53	Xantheas S.	I-065
Webb A.	PO1-239	Xavier N.	PO3-80
Webber G.B.	PO1-128, PO1-130, PO2-69	Xie W.	PO1-30
Weber F.	C-103	Xiong X.-G.	I-231
Weber M.	PO3-91	Xu L.	C-067
Wei Z.	PO3-141	Xu X.	PO3-132
Weidman J.	PO3-77	Xu Z.-H.	PO1-251
Weigend F.	PO2-302		
Weinstein J.	PO3-216	Y	
Weiske T.	PL-4	Yamada D.	PO1-249
Wellendorff J.	PO2-274, PO2-275	Yamada S.	PO3-53
Weller A.S.	PO2-144, PO3-52	Yamamoto Y.	PO2-10 , PO3-53
Wells B.	PO2-192	Yamane M.	C-091, PO1-298
Welz E.	PO3-263	Yamasaki M.	PO1-307
Wender J.H.	PO2-241	Yamashita M.	PO2-8
Wennemers H.	PO3-26	Yamazaki K.	PO1-29
Werner H.-J.	I-082 , PO1-195, PO1-270, PO1-284, PO3-205	Yanai T.	I-231
Werner M.	PO1-271	Yáñez M.	I-292
		Yang C.	PO1-11, PO3-136
		Yang D.-Y.	PO1-54, PO1-55
		Yang K.	PO2-184

Author Index

Yang T.	PO1-87	Żuchowski P.	PO1-133
Yang W.	I-091		
Yang Y.	PO1-164		
Yates B.	C-083		
Yavuz I.	PO3-302		
Ye J.	C-068		
Yepes D.	PO1-146, PO3-283		
Yimieraishan M.	PO1-89		
Yönder Ö.	PO1-198		
Yong C.W.	PO1-204		
Yoshimura T.	C-044		
Yoshino T.	PO1-140		
Yu C.	PO1-214		
Yu H.	PO1-193, PO3-10		
Yu J.-S.K.	PO1-9		
Yu Q.	I-161		
Yuan Y.Y.	PO1-121		
Yudanov V.	PO3-270		
Yung M.-H.	C-126		
Yurchenko S.	I-165		
Z			
Zacharias M.	PO2-264		
Zaichenko A.	PO2-215		
Zakay I.	PO1-302		
Záliš S.	PO3-44		
Zanotto M.	C-094, PO1-107 , PO2-55		
Žari S.	PO2-111		
Zaric S.	C-112 , PO3-200		
Zauleck J.P.P.	PO1-279, PO2-15		
Zech A.	PO3-196		
Zefirov N.	C-113, PO3-93		
Zeman J.	PO2-281		
Zeng J.	PO1-52		
Zeng Y.	PO2-186, PO2-205		
Zettergren H.	PO3-103		
Zgid D.	I-382		
Zhang H.	PO1-230		
Zhang H.-X.	C-164		
Zhang J.	I-352		
Zhang W.H.	PO3-197		
Zhang X.	C-067, PO1-108 , PO1-6 , PO3-2		
Zhang X.-J.	PO2-309		
Zhang Y.	PO2-42		
Zhang Z.	C-056		
Zhao L.	PO1-47 , PO3-4		
Zhao Q.	C-072		
Zheng C.	PO3-120		
Zhong R.	PO3-4		
Zhou J.-K.	PO1-54		
Zhou M.	PO2-13		
Zhou Q.	PO1-110		
Zhou S.	PL-4, PO1-10		
Zhu J.	PO1-49		
Ziebarth B.	IN-10		
Zins E.-L.	PO1-49		
Zipse H.	PO2-141, PO2-71		
Zlatar M.	PO2-217		
Zobel P.	PO2-113		
Zöllner M.S.	PO2-251, PO2-280		