



251ST ACS NATIONAL MEETING

SAN DIEGO, March 13–17

“COMPUTERS IN CHEMISTRY” is the theme of the ACS spring national meeting, which will be held in the San Diego Convention Center and contracted hotels.

Numerous events will support that theme, including a plenary session on Sunday, March 13, from 3 to 6 PM, featuring experts on self-assembly, proton-coupled electron transfer, protein design, and free-energy perturbation theory.

ACS President Donna J. Nelson will host 29 technical divisions and five committees in original programming over 1,028 half-day oral sessions and 141 poster sessions, including Sci-Mix. More than 12,000 papers and nearly 5,000 posters will be presented. There will also be more than 7,500 oral presentations.

Nelson will also host numerous events and symposia during the meeting, including a public outreach event, “Exploring Our World through Chemistry,” on Saturday, March 12, at 10 AM. Attendees can learn more about the world of chemistry through hands-on, age-appropriate activities.

This meeting offers programs for high school teachers, undergraduate and graduate students, postdocs, and chemical professionals. A range of professional development classes will be available; ACS Short Courses have a separate registration and fee. Job seekers can meet and interview with potential employers at the ACS Career Fair, find one-on-one career assistance, and pick among more than 20 career workshops.

The exposition will feature more than 250 companies that will showcase services, instruments, books, lab equipment, and much more in more than 400 booths.

The 2016 ACS national award winners will be recognized with a banquet on Tuesday, March 15, at 7:30 PM, and Mostafa El-Sayed, Regents’ Professor and Julius Brown Chair at Georgia Institute of Technology, will deliver the Priestley Medal Address. Although the banquet is a ticketed event, the Priestley Medal Address, at 9:30 PM, is free for all registered meeting attendees. The Arthur C. Cope Award winners will be recognized at the fall national meeting in Philadelphia.

San Diego boasts a range of dining and entertainment options. Visit the world-famous San Diego Zoo, tour the U.S.S.

Midway aircraft carrier and museum, get spooked at the haunted Whaley House, eat a kangaroo at Craze Burger, try to make out the tune on 25th Street’s musical bridge, or check out SeaWorld’s famous killer whale show before it shuts down later this year. —CRAIG BETTENHAUSEN

REGISTRATION CATEGORY	FEES
MEMBERS	
ACS member or society affiliate	\$500
Postdoctoral member	500
Emeritus or retired member	255
50-year member	No fee
Unemployed member (Dues waiver required)	No fee
Precollege teacher	105
Graduate student	210
Undergraduate	105
One-day registrant	255
NONMEMBERS	
Chemical scientist	\$880
Postdoctoral scientist	880
Visitor: Nonchemical scientist or chemical technician	500
Precollege teacher	105
Graduate student	415
Undergraduate	210
One-day registrant	500
Guest of registrant ^a	45
EXPOSITION-ONLY VISITORS	
Adult, exposition only	\$50
Student, exposition only	25

^a Registration is restricted to a spouse or family member of a registered attendee having no affiliation with the field of chemical science and who is not eligible to become an ACS member. Only one guest registration is allowed per registering attendee, and the guest registration must be completed and paid by the registering attendee at time of original registration.

MEETING INFO ON THE WEB
www.acs.org/sandiego2016

REGISTRATION

Early Registration. Attendees within the U.S. who registered prior to Jan. 24 will receive their badge credentials by mail before the meeting. International registrants must pick up their badge credentials at ACS Attendee Registration (this includes Canada and Mexico).

Standard & On-Site Registration. Attendees who register after Jan. 24 must pick up their badge credentials on-site at Attendee Registration.

Satellite Registration & On-Site Program Pick-Up. Printed copies of the On-Site Program Book will no longer be available for free. In support of ACS's sustainability efforts, we encourage the use of the ACS San Diego mobile app and digital program for quick access to the meeting's full technical program, maps, and search features.

Prefer a Printed On-Site Program? The On-Site Program Book will now be available for a **\$20** fee. Purchase your copy during the registration process or visit the locations listed below. Limited quantities will be available. Replacement copies also cost \$20.

San Diego Convention Center, Lobby D
Manchester Grand Hyatt, Coronado Ballroom Foyer
Hilton Bayfront, Sapphire North/West Foyer
Westin San Diego, Broadway Terrace

Satellite registration will also be available at those locations. Learn about ACS national meetings sustainability efforts at www.acs.org/greenermeetings.com. Questions? Contact nationalmeetings@acs.org.

TRAVEL

TRANSPORTATION DISCOUNTS. ACS has negotiated special travel discounts with the following partners. To get the best rates and avoid service fees, it is recommended to make reservations online (except Amtrak).

SUPERSHUTTLE. SuperShuttle service to and from the hotel can be arranged at www.supershuttle.com/default.aspx?GC=MFPQQ. The shared ride shuttle discount is \$1.00 one way, \$2.00 round trip. You can also book sedans. To reserve by

phone, call (800) blue-van (258-3826) and use the discount code MFPQQ.

AIRLINES:

Delta
(800) 328-1111
Discount code: NMMMK

United Airlines
(800) 426-1122
Discount code: ZWFB960724

Southwest Airlines
swabiz.com (online only)
Discount code: 99331750

TRAIN:

Amtrak
amtrak.com; (800) 872-7245
Discount code: X03V-918

RENTAL CARS

Avis
(800) 331-1600
Discount code: B923099

Hertz
(800) 654-2240
Discount code: CV# 02UZ0015

EVENTS & ACTIVITIES

A VARIETY of organizers will host special events during the meeting. Event participation is open to all interested registrants.

Some events require a ticket or registration to participate. The following

ACS BADGE REPRINT POLICY

1st Badge Reprint: No charge; upon proper identification and confirmation of registration payment, a duplicate badge is issued.

2nd Badge Reprint: Attendee completes a duplicate badge request, shows identification, a charge of \$25 is paid (cash/credit card), a duplicate badge is issued.

3rd Badge Reprint: Attendee completes a duplicate badge request, shows identification, a charge of \$50 is paid (cash/credit card), a duplicate badge is issued.

Beyond 3rd Badge Reprint: Attendee completes a duplicate badge request, shows identification, a charge of \$100 is paid (cash/credit card), a duplicate badge is issued.

FOR UP-TO-DATE EVENT LISTINGS, VISIT
www.acs.org/sandiego2016

events are coded to indicate what is required to participate: **(R)** registration, and payment when applicable, required; **SE-##** ticket required. **All nonticketed events require a visible registration badge for entry.**

Tickets are sold on a first-come, first-served basis. Ticket sales will close at 6 PM the evening prior to the event. Some event organizers may offer a limited number of tickets for sale at the door of the events. Cancellations or refund requests are not accepted after March 6.

Locations and times are subject to change. To learn more about these events and to buy tickets or register, visit www.acs.org/sandiego2016.

FRIDAY, MARCH 11

CHAS Workshop: Laboratory Waste Management

7:30 AM to 4 PM, San Diego Convention Center, Room 31B

CHAS Workshop: Laboratory Safety

7:30 AM to 5 PM, San Diego Convention Center, Room 31A

SATURDAY, MARCH 12

CHAS Workshop: How To Be a More Effective Chemical Hygiene Officer

7:30 AM to 5 PM, San Diego Convention Center, Room 31C

CHAS Workshop: Reactive Chemical Management for Laboratories & Pilot Plants

7:30 AM to 5 PM, San Diego Convention Center, Room 31B

CHAS Workshop: Meeting Chemical Safety Expectations in Instructional Laboratories

7:30 AM to 5 PM, San Diego Convention Center, Room 31A

CHAS Workshop: Cannabis Extraction & Analysis

7:30 AM to 5 PM, San Diego Convention Center, Room 32A

DIGITAL MEETING PROGRAM AVAILABLE AT

<http://cenm.ag/sandiego2016fp>

COACH Workshop: COACH Leadership & Advanced Negotiations

8:30 AM to 5 PM, Hilton Gaslamp Quarter, Marina A

Presidential Outreach Event: Exploring Our World Through Chemistry

1 to 4 PM, San Diego Central Library, 330 Park Blvd., San Diego

In collaboration with the San Diego Festival of Science & Engineering, this event will feature hands-on experiments to engage kids and the community in chemistry.

COACH Reception

5 to 7 PM, Hilton Gaslamp Quarter, Marina B

SUNDAY, MARCH 13

Undergraduate Hospitality Center

8 AM to 5 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

Undergraduate Digital Café

8 AM to 5 PM, Marriott Marquis San Diego Marina, Carlsbad

Undergraduate Workshop: Making the Most of Your First National Meeting

9 to 9:45 AM, Marriott Marquis San Diego Marina, San Diego Ballroom B

Undergraduate Workshop: Graduate School Reality Check, Part I: Getting In

10 to 11:15 AM, Marriott Marquis San Diego Marina, San Diego Ballroom A

ACS Career Fair Workshops: Career Pathway Workshop

10 AM to 5 PM, San Diego Convention Center, Room 24A

Undergraduate Workshop: Chem Demo Exchange

11 AM to 12:30 PM, San Diego Convention Center, Sails Pavillon

Leading Without Authority

11 AM to 5 PM, Embassy Suites San Diego Downtown Bay, Monterey I

Undergraduate Workshop: Graduate School Reality Check, Part II: You're In—Now What?

11:15 AM to 12:30 PM, Marriott Marquis San Diego Marina, San Diego Ballroom A

SCHB & PROF Luncheon

11:30 AM to 1:30 PM, Marriott Marquis San Diego Marina, Oceanside Room

ACS Board Open Session & Luncheon

(Open to staff and attendees)

11:45 AM to 1 PM, San Diego Convention Center, Room 20D

CHED High School/College Interface Luncheon/SE-01/\$45

(Included at no charge with high school teacher registration)

Noon to 1 PM, Manchester Grand Hyatt San Diego, Harbor Ballroom A

BIOT Lunch Seminars

12:30 to 2 PM, Westin San Diego, Topaz Room

CTA National Technician Award Luncheon/SE-02/\$45

1 to 3 PM, Hilton San Diego Bayfront, Indigo 204A

Undergraduate Workshop: Networking Social with Graduate School Recruiters

1 to 5 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

ACS Career Fair Workshops: Career Pathways I

1:30 to 5:30 PM, San Diego Convention Center, Room 23A

ACS Career Fair Workshops: Career Pathways II

1:30 to 5:30 PM, San Diego Convention Center, Room 23B

ACS Career Fair Workshops: Career Pathways III

1:30 to 5:30 PM, San Diego Convention Center, Room 23C

Event codes indicate what is required to participate: **(R)** registration, and payment when applicable, required; **SE-##** ticket required; all nonticketed events require a visible registration badge for entry. View an updated listing of events and activities at www.acs.org/sandiego2016.

Undergraduate Workshop: Effective Chemistry Demos for Community Outreach

2:45 to 4 PM, San Diego Convention Center, Sails Pavillon

Graduate & Postdoctoral Scholars Workshop: Faculty & Postdoc Afternoon Networking Coffee Break

3 to 5 PM, San Diego Convention Center, Sails Pavillon

Ten Million Thanks (invitation only)

A tribute to all who made possible the success of the ACS Scholars Program

3:30 to 5:30 PM, Hilton San Diego Bayfront, Indigo Ballroom D

International Networking Event

4 to 5:30 PM, Hilton San Diego Bayfront, Aqua 300A/B

Undergraduate Workshop: Networking 101 Workshop

4 to 5:30 PM, Marriott Marquis San Diego Marina, San Diego Ballroom A

Nominees Town Hall Meeting

4:30 to 5:30 PM, Hilton San Diego Bayfront, Indigo Ballroom A

ACS Diversity Reception

5 to 7 PM, Hilton San Diego Bayfront, Aqua Salon D

University of Wisconsin, Madison, Alumni & Friends

5 to 7 PM, Hilton Gaslamp Quarter, Pacific Room

Chemistry at Illinois Alumni & Friends Reception

5 to 8 PM, Westin San Diego, Topaz Room

CHED Social Reception

5:30 to 7 PM, Manchester Grand Hyatt San Diego, Coronado Foyer

International Welcome Reception/SE-03/no charge

5:30 to 7:30 PM, Hilton San Diego Bayfront, Sapphire Ballroom A/B & E/F

Joint Research Corporation/Petroleum Research Fund Reception

5:30 to 7:30 PM, Hilton San Diego Bayfront, Indigo Ballroom C/G

COLL Social Hour/Poster Session/Open Business Meeting

5:30 to 8 PM, San Diego Convention Center, Hall E

District II Councilor Caucus

6 to 7 PM, Hilton San Diego Bayfront, Indigo 202B

District IV Councilor Caucus

6 to 7 PM, Hilton San Diego Bayfront, Indigo 204A

District V Councilor Caucus

6 to 7 PM, Hilton San Diego Bayfront, Indigo 204B

District VI Councilor Caucus

6 to 7 PM, Hilton San Diego Bayfront, Indigo 206

Mid-Atlantic Councilor Caucus

6 to 7 PM, Hilton San Diego Bayfront, Indigo 202A

CELL & FLUO Poster Sessions

6 to 8 PM, San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

INOR Poster Sessions

6 to 8 PM, San Diego Convention Center, Hall D

Expo Attendee Welcome Reception

6 to 8:30 PM, San Diego Convention Center, Halls B–C

CINF Welcoming Reception & Poster Session

6:30 to 8:30 PM, San Diego Convention Center, Room 3

ACS Student Chapter Awards Ceremony

7 to 8:30 PM, San Diego Convention Center, Ballroom 20 A/C

ANYL Poster Session

7 to 9 PM, San Diego Convention Center, Sails Pavilion

CHED Poster Session

7 to 9 PM, San Diego Convention Center, Hall D

MEDI & BIOL Poster Session

7 to 9 PM, San Diego Convention Center, Hall F

ORGN Poster Session

8 to 10 PM, San Diego Convention Center, Hall D

Presidential Poster Session

8 to 10 PM, San Diego Convention Center, Hall D

Undergraduate Research Social

8:30 to 11 PM, San Diego Convention Center, Ballroom 20D

MONDAY, MARCH 14

YCC 5K Fun Run/SE-04/\$25 (regular)/SE-04A/\$15 (student)

6:45 to 8:30 AM, San Diego Convention Center, Lobby D

WCC Women in the Chemical Enterprise Breakfast/SE-05/\$40 (regular)/SE-05A/\$20 (student)

7:30 to 9 AM, Hilton San Diego Bayfront, Indigo Ballroom C/G

(A limited number of student tickets are available. Students may purchase regular tickets if student tickets are sold out.)

Engaging Colleagues in Dialogue

8 AM to noon, Embassy Suites San Diego Downtown Bay, Monterey I

Undergraduate Hospitality Center

8 AM to 5 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

Undergraduate Digital Café

8 AM to 5 PM, Marriott Marquis San Diego Marina, Carlsbad Room

ACS Career Fair Workshop: Career Pathways I

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23A

ACS Career Fair Workshop: Career Pathways II

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23B

ACS Career Fair Workshop: Career Pathways III

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23C

ACS Exposition

9 AM to 5 PM, San Diego Convention Center, Halls B/C

Undergraduate Workshop: Chemists Celebrate Earth Day (cosponsored by Committee on Community Activities)

9:45 to 11 AM, San Diego Convention Center, Room 30C/D

Chem Ambassadors Game & Cafe

10:30 to 11:30 AM, Marriott Marquis San Diego Marina, Carlsbad Room XX

Diversity Women Chemist of Color Networking Event/SE-06/no charge

10:30 AM to Noon, Hilton San Diego Bayfront, Aqua Salon A/B

Committee on Minority Affairs Luncheon/SE-07/\$50 (regular)/SE-07A/\$25 (student)

11:30 AM to 1:30 PM, Hilton San Diego Bayfront, Sapphire Ballroom A/B

SCHB & PROF Luncheon

11:30 AM to 1:30 PM, Marriott Marquis San Diego Marina, Vista Room

CHAL Drug & Power Luncheon/SE-08/\$40

Noon to 1:30 PM, San Diego Convention Center, Room 20D

Undergraduate Poster Session

12 to 2 PM, San Diego Convention Center, Hall D/E

Purdue University Chemistry Luncheon/SE-09/\$10

12 to 2 PM, Manchester Grand Hyatt San Diego, Coronado E

BIOT Lunch Seminars

12:30 to 2 PM, Westin San Diego, Topaz Room

Fostering Innovation

1 to 5 PM, Embassy Suites San Diego Downtown Bay, Monterey I

ENFL Poster Session

2 to 4 PM, San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

Undergraduate Workshop: Speed Networking with Chemistry Professionals

3:45 to 5:15 PM, Marriott Marquis San Diego Marina, San Diego Ballroom B

The Kavli Foundation Emerging Leader in Chemistry Lecture

4 to 5:10 PM, San Diego Convention Center, Ballroom 20 A/C

Just Cocktails, WCC Open Meeting

4 to 5:30 PM, Hilton San Diego Bayfront, Aqua Salon D

The Fred Kavli Innovations in Chemistry Lecture

5:15 to 6:30 PM, San Diego Convention Center, Ballroom 20 A/C

CHAL Reception

6 to 8 PM, San Diego Convention Center, Room 22

Chinese American Chemical Society Dinner Banquet/SE-10/\$35

6 to 9 PM, Panda Inn Mandarin Cuisine, 506 Horton Plaza

University of Pennsylvania Alumni Reception

6:30 to 8:30 PM, Cafe Sevilla, 335 5th Ave.

CARB Award Dinner/SE-11/\$60

6:30 to 9:30 PM, Rockin' Baja Lobster—Gaslamp, 310 5th Ave.

ACS Graduate & Postdoctoral Scholars Reception

7 to 8:30 PM, San Diego Convention Center, Room 20D

Sci-Mix Interdivisional Poster Session & Mixer

(Drink ticket included with registration)
8 to 10 PM, San Diego Convention Center, Hall D/E

TUESDAY, MARCH 15

Senior Chemists Committee Breakfast/SE-12/\$20

7:30 to 9:30 AM, Hilton San Diego Bayfront, Indigo Ballroom D/H

University of Minnesota Alumni & Friends Breakfast/SE-13/\$5.00

7:30 to 9:30 AM, San Diego Convention Center, Room 20D

Coaching & Feedback

8 AM to noon, Embassy Suites San Diego Downtown Bay, Monterey I

ACS Career Fair Workshop: Career Pathways I

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23A

ACS Career Fair Workshop: Career Pathways II

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23B

ACS Career Fair Workshop: Career Pathways III

8:30 AM to 5:30 PM, San Diego Convention Center, Room 23C

ACS Exposition

9 AM to 5 PM, San Diego Convention Center, Halls B–C

Eli Lilly Travel Award Poster Session

11 AM to noon, Hilton San Diego Bayfront, Indigo Ballroom D/H

Alpha Chi Sigma Fraternity Luncheon

11:30 AM to 1:30 PM, San Diego Pier Café, 889 West Harbor Dr.

SCHB & PROF Luncheon

11:30 AM to 1:30 PM, Marriott Marquis San Diego Marina, Vista Room

CINF Luncheon/SE-14/\$20 (regular member)/SE-14A/\$25 (nonmember)/SE-14B/\$15 (student)

Noon to 1:30 PM, San Diego Convention Center, Room 20D

COLL Luncheon/SE-18/\$45

Noon to 1:30 PM, San Diego Convention Center, Room 20B/C

WCC Luncheon/SE-15/\$50 (regular)/SE-15A/\$25 (student)

Noon to 1:30 PM, Hilton San Diego Bayfront, Indigo Ballroom D/H

Committee on Environmental Improvement (CEI) Film Series

Noon to 2 PM, San Diego Convention Center, Room 8

BIOT Lunch Seminars

12:30 to 2 PM, Westin San Diego, Topaz Room

Strategic Planning

1 to 5 PM, Embassy Suites San Diego Downtown Bay, Monterey I

AGFD C⁴ Communicating Chemistry: Caribbean Cuisine/SE-21/\$10

2:30 to 4:30 PM, San Diego Wine & Culinary Event Center, 200 Harbor Dr.

AGFD Poster Session

3 to 5 PM, San Diego Convention Center, Exposition, Exhibit Halls B/C, Town Center (#100A)

Local Section Officers, Outreach Coordinator & Speakers Reception

3:30 to 5:30 PM, Hilton San Diego Bayfront, Indigo 204A/B

Division Councilors & Division Officers Caucus & Reception

4 to 6:30 PM, San Diego Convention Center, Room 24A

I&EC Poster Session

5 to 7 PM, San Diego Convention Center, Hall D

UCLA Research Showcase

5 to 7 PM, San Diego Convention Center, Room 20A

District I Councilor Caucus

5:30 to 7 PM, Hilton San Diego Bayfront, Indigo 202A

Geochemistry Division Reception

5:30 to 7:30 PM, Omni San Diego Hotel, Grand Ballroom E

ENFL Energy & Fuel Dinner/SE-16/\$60

6 to 9 PM, The Prado at Balboa Park, 1549 El Prado

PMSE/POLY Joint Poster Session

6 to 8 PM, San Diego Convention Center, Hall F

INOR Poster Session

6 to 8 PM, San Diego Convention Center, Hall D

COMP Poster & Awards Session

6 to 8 PM, San Diego Convention Center, Hall E

BIOT Poster Session

6 to 9 PM, San Diego Convention Center, Hall E

ENVR Division Reception/SE-19/\$20

6:30 to 8 PM, Meze Greek Fusion Restaurant, 345 5th Ave.

**ACS National Awards Reception,
Banquet Ceremony & General Meeting of
the Society/SE-17/\$130**

6:30 to 10 PM, Manchester Grand Hyatt
San Diego, Harbor Ballroom D-I

CELL Awards Banquet/SE-20/\$65

6:30 to 10 PM, Fogo de Chao, 668 6th Ave.

BIOL Poster Sessions

7 to 9 PM, San Diego Convention Center,
Hall E

CARB Poster Session

7 to 9 PM, San Diego Convention Center,
Hall D

CATL & ORGN Poster Session

8 to 10 PM, San Diego Convention Center,
Hall D

WEDNESDAY, MARCH 16

**ACS Career Fair Workshop: Career
Pathways I**

8:30 AM to 5:30 PM, San Diego Convention
Center, Room 23A

**ACS Career Fair Workshop: Career
Pathways II**

8:30 AM to 5:30 PM, San Diego Convention
Center, Room 23B

**ACS Career Fair Workshop: Career
Pathways III**

8:30 AM to 5:30 PM, San Diego Convention
Center, Room 23C

POLY/PMSE Awards Reception

5:30 to 8:30 PM, Marriott Marquis San
Diego Marina, San Diego Ballroom B

ENVR & PHYS Poster Sessions

6 to 8 PM, San Diego Convention Center,
Hall D

GEOC Poster Session

8 to 10 PM, San Diego Convention Center,
Hall D

Joint MED & ORGN Poster Session

7 to 10 PM, San Diego Convention Center,
Hall F



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EXPOSITION

SEE WHAT'S NEW INSIDE THE EXPOSITION.

Visit the ACS National Exposition at the San Diego Convention Center (SDCC), Halls B/C, from Sunday, March 13, through Tuesday, March 15. The show hours will be Sunday, 6 to 8:30 PM, and Monday and Tuesday, 9 AM to 5 PM.

Companies will showcase services, instruments, books, computer hardware, scientific software, and an array of chromatographic, lab, and safety equipment. Technical personnel will give demonstrations, answer questions, and discuss your needs and interests.

You can also visit the ACS Career Fair Recruiters Row inside the exposition, where employers will showcase their products and services. Also, join us at the ACS Booth in the middle of the exposition floor, where ACS staff members will present the many benefits, services, products, and merchandise offered by ACS.

Online Exposition. The Online Exposition is a component within the Exhibitor Directory that enables attendees to view videos, press releases, brochures, and flyers of participating exhibitors. Access the Online Exposition at www.acs.org/sandiego2016 to learn more about exhibiting companies and download product information that meets your needs.

Free Exhibitor Workshops. Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the San Diego Convention Center. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity. Register at www.acs.org/sandiego2016 to reserve your seat.

Presentations & Special Events. Join us on Sunday from 6 to 8:30 PM for the Attendee Welcome Reception. Also, visit the Town Center inside the exposition for poster sessions, to connect with colleagues, and to relax during the Tuesday

afternoon break from 3 to 5 PM. Refreshments available while supplies last.

Internet & Technology. Get free Internet access and leave messages for one another at the Meeting Mail terminals inside the Town Center. Enjoy free Wi-Fi service at designated areas in the San Diego Convention Center.

Admission Requirements & Expo-Only Registration. Exposition admission is complimentary for all national meeting registrants; however, you are required to wear your badge. Individuals who want to visit the exhibits without registering for the technical component of the national meeting can obtain an expo-only badge for \$60. Students with school identification can obtain an expo-only badge for \$30. Registration can be handled online or in person at ACS Attendee Registration in the San Diego Convention Center, Lobby D, and at our satellite registration areas at the Manchester Grand Hyatt, Hilton San Diego Bayfront, and Westin San Diego.

EXHIBITOR WORKSHOPS

EXHIBITING COMPANIES will host free education sessions for attendees to introduce new products and services, build skills with specific tools and techniques, and highlight applications for existing instrumentation. Visit www.acs.org/sandiego2016 to register for workshops.

SUNDAY, MARCH 13

Flow Chemistry Seminar. *Sponsor:* ThalesNano Nanotechnology, 3:30 to 6 PM, SDCC, Room 12. Join our seminar for a glimpse into the latest advances in continuous-flow reactor technology, and see how it can benefit your chemistry. Information is also available at the ThalesNano booth, #1121.

MONDAY, MARCH 14

Innovative Technologies To Improve Your Students' Learning Experience. *Sponsor:* McGraw-Hill Education, 9:30 AM to noon, SDCC, Room 15B. 9:30 to 10:30 AM—*Adaptive Learning To Help Prepare & Engage Your Students for Success.* Adaptive technology is at the fore-

front of the evolution of digital teaching, allowing instructors to teach and students to learn in ways never before possible. But what does this really mean? And how can you make it work for you and your students? Get answers to these questions from instructors who have years of experience using adaptive technology, including SmartBook and LearnSmart Prep. 11 AM to noon—*Revolutionizing the Lab Experience: Introducing LearnSmart Labs for General Chemistry.* LearnSmart Labs provides an adaptive, interactive, personalized lab experience that encourages students to theorize and experiment like scientists do. In the realistic LearnSmart Labs environment, students can practice the scientific method, safely develop and test hypotheses, and think critically about their findings before ever setting foot in a physical lab.

Waters Technical Workshops. *Sponsor:* Waters, 9:30 AM to noon, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. Join Waters for two educational workshops designed to help improve laboratory effectiveness in your organization. 9:30 to 10:30 AM—*Transforming Sample Preparation.* Waters has developed a new, water-wettable, reversed-phase sorbent and an easy-to-use, streamlined approach that produces high recoveries, improved

sample flow capabilities, and reduced matrix effects. Don't miss this discussion on a new, novel sorbent for small-molecule sample preparation that is easier to use and produces cleaner samples in less time with fewer steps.

10:30 to 11:30 AM—*Empowering Solutions.* We will explore the new features of Empower 3 FR3 in this session. Topics covered will include mass spectrometric peak tracking, new peak labeling options, new component summary reporting options, location fields, new custom field capabilities, Waters's data manager, and qualification and performance enhancements.

CAS Solutions. *Sponsor:* CAS, 9:30 AM to 3 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 1. Visit CAS in the Exhibitor Workshop to learn more about our products and solutions.

ACS on Campus. *Sponsor:* ACS Store, 12:30 to 3 PM, SDCC, Room 15B. Learn from ACS editors and experts in the field about how to maximize your research, get published, and build the skills you need to gain that competitive edge for your career. The event is free, including complimentary food, drinks, and giveaways. The event is open to undergraduates, graduate students, researchers, faculty, and librarians.

Solutions for Innovation: From Composition to Structure. *Sponsor:* JEOL USA, 12:30 to 3 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. In your element: SEM/EDS. Find your formula: ambient ionization mass spectrometry. Verify your structure: NMR. Learn how the latest innovations from JEOL integrate to enhance your science.

Seamless Integration of 2-D & 3-D SAR To Guide MultiParameter Optimization.

Sponsor: Optibrium, 3:30 to 6 PM, SDCC, Room 15B. In this hands-on workshop, we will explore how the combination of two-dimensional structure-activity relationships (SARs) with 3-D structure-based design can be used to guide the optimization of high-quality compounds. Practical examples will illustrate how analyses such as activity-cliff detection and matched molecular pair analysis in StarDrop's Card View system can be linked with a 3-D view of a compound binding to a therapeutic target. We will also use the SeeSAR software platform to demonstrate how 2-D quantitative structure-activity relationship (QSAR) models of key absorption, distribution, metabolism, and excretion (ADME) properties can monitor potential risks, and we will consider strategies to improve binding affinity using SeeSAR's visual HYDE scoring approach.

TUESDAY, MARCH 15

Innovative Technologies To Improve Your Students' Learning Experience.

Sponsor: McGraw-Hill Education, SDCC, Room 15B. 9:30 to 10:30 AM—*The Rewards of Technology in Organic Chemistry.* With digital tools designed to streamline tasks and improve student outcomes, educators are free to focus on what matters most: teaching. Help your students come to class more prepared and engaged, increase course retention, study smarter, and get better grades. 11 AM to noon—*Moving Beyond Traditional Homework with ALEKS.* Jack Eichler from the University of California, Riverside, will present his research findings from his *Journal of Chemical Education* article "Online Homework Put to the Test" (2013, DOI: 10.1021/ed3006264). In his study, Eichler compared two separate online learning systems, ALEKS (responsive-adaptive) and MasteringChemistry (responsive), and measured the impact of each online learning system on student final exam scores for a general chemistry course. Eichler will share his results and as well as his experiences using online homework.

Introduction to Protein & Peptide HPLC (Part I) and State-of-the-Art Protein & Peptide Reversed-Phase Separations by UHPLC (Part II). *Sponsor:* MilliporeSigma (Sigma-Aldrich), 9:30 AM to noon, SDCC, Room 12. Join MilliporeSigma for a two-part workshop focusing on bioanalytical HPLC separations. Learn about the latest technologies, enjoy complimentary refreshments, and be entered to win a free HPLC column for your evaluation.

CAS Solutions. *Sponsor:* CAS, 9:30 AM to 3 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 1. See page EXPO-1.

Spinsolve Benchtop NMR for Industry & Academia. *Sponsor:* Magritek, 10 AM to noon, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. Magritek presents the latest developments with the Spinsolve benchtop NMR spectrometer. Join us to learn about the extended and improved capabilities of this high-performance NMR instrument, including applications in a range of practical problems of interest for industry and academia.

WebAssign 101: Getting Started with WebAssign. *Sponsor:* WebAssign, 3:30 to 6 PM, SDCC, Room 12. This workshop is ideal for new WebAssign users or active users who want to learn more about how to use WebAssign's features to save time, better engage your students, and assess student performance. Join WebAssign's Brad Spiker for a lively and informative introduction to WebAssign. You'll learn how to create a course, build an assignment, and schedule assignments, and you'll get some of Brad's favorite tips for enriching your chemistry classroom experience. You won't want to miss this workshop for a painless way to jump-start your success with WebAssign.

Reverse Engineering of Materials & Polymers Using Infrared & Raman Spectroscopy. *Sponsor:* Bruker, 12:30 to 3 PM, SDCC, Room 15B. Product development in the industrial world can be a long and expensive process. In a competitive market, the window of opportunity for significant revenue can close before a new product even exits the development cycle. The obvious solution to keeping up in a competitive market is to acquire the product in question, disassemble it, and analyze it. This reverse engineering process can greatly expedite the immediate introduction of competitive products into the marketplace. The chemical properties can be readily de-

termined by utilizing analytical tools such as gas-phase chromatography and atomic absorption spectroscopy. Molecular spectroscopy (infrared and Raman) is among the most powerful tools in the reserve-engineering process. Each molecule has a unique infrared and Raman signature that provides great specificity in the identification process.

New in the Field of Chromatography from Thermo Fisher Scientific *Sponsor:* Thermo Fisher Scientific, 12:30 to 3 PM, SDCC, Exhibit Halls B/C, Exhibitor Workshop Room 2. **Part I: A New & Exciting Line of High-Pressure Ion Chromatography (HPIC) Instruments.** Ion chromatography is a well established and accepted analytical technique used for a wide diversity of sample matrices such as foods and beverages, industrial chemicals, and ultra-high-purity water. Learn faster and more cost-effective methods that use a new line of high-pressure-capable IC systems. Examples will include the determination of common ionic pollutants found in environmental samples—organic acids, anions, cations, and carbohydrates in food and beverage matrices—as well as ionic compound determinations in pharmaceutical and biotechnology samples. **Part II: Advances in UHPLC Instrumentation.** Learn how the Vanquish UHPLC system's novel detectors, method transfer tools, and dedicated columns help you solve your toughest scientific challenges.

Characterizing Structure & Chemistry of Functional Nanomaterials by Advanced Electron Microscopy. *Sponsor:* FEI, 12:30 to 3 PM, SDCC, Room 12. The development of technologies for efficient resource usage, energy conversion, transportation, environmental protection, and other applications relies heavily on the development of new and improved nanostructures and nanomaterials. Characterization of these materials down to the subnanometer scale—while focusing on structural evolution with a link to the nanomaterial's performance—plays a crucial role in obtaining detailed knowledge about the relationship among structure, unique properties, and function in these systems. FEI's solutions can help you to visualize and analyze structure and morphology as well as the chemical composition of those materials under a variety of conditions. In this workshop, we will profile use cases in nanostructure characterization—including 2-D materials, catalysts, and polymers—and take you through different electron microscopy

characterization methods that will enable you to get more insight.

Exploiting Matched Molecular Pairs in Drug Discovery. *Sponsor:* Simulations Plus, 3:30 to 6 PM, SDCC, Room 15B. This hands-on workshop will guide attendees through the design of potential BACE1 inhibitors using state-of-the-art ADMET Predictor 8.0 software. BACE1 is a classic target for Alzheimer's disease, a progressive neurodegenerative disorder. The binding site of BACE1 contains two acidic amino acids (Asp32 and Asp228) where inhibitors that contain a basic moiety can form salt bridge/hydrogen binding interactions. Modification of the ligand's pKa is important not only for binding to the enzyme but also because it affects the ligand's ability to penetrate the blood-brain barrier. The initial step in the design phase is to analyze the available data for structure-activity relationships (SARs). The attendees will learn how to cluster compounds according

to their maximum common substructure, create R tables, and use matched molecular pair analysis to extract SARs. Presenters will demonstrate a QSAR model that predicts BACE1 enzymatic inhibition. Virtual libraries containing amidine-like functionality will be generated and then be filtered based on their predicted BACE1 inhibition, solubility, permeability, metabolic stability, and other ADMET properties using an ADMET liability scoring function. The workshop will conclude with physiological-based pharmacokinetic (PBPK) simulations for the filtered analogs.

WEDNESDAY, MARCH 16

Inhibitor Design Using MOE Structure-Based Drug Design Applications. *Sponsor:* Chemical Computing Group, 3:30 to 6 PM, SDCC, Room 15B. This hands-on workshop will cover in silico structure-based drug design (SBDD) meth-

ods for the rational design of EGFR kinase inhibitors. Starting with raw PDB protein-ligand 3-D structures, all the steps required to initiate and advance an SBDD modeling study will be covered: preparing PDB structures for modeling, binding pocket visualization, and 2-D and 3-D protein-ligand contact analyses. We will cover advanced topics such as pharmacophore query generation, protein-ligand docking, protein alignments for binding-site comparative analysis and SAR evaluation, and combinatorial synthesis. In silico ligand modification and derivatization will also be covered in the context of ligand optimization.

Automated HPLC & LCMS Workflows Implemented in Complex Analytical Challenges. *Sponsor:* Agilent Technologies, 9:30 AM to noon, SDCC, Room 12.

Elemental Impurity & Extractables and Leachables. *Sponsor:* Agilent Technologies, 12:30 PM to 3 PM, SDCC, Room 12.

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Yamazen Science, Inc., 1455 Rollins Road, Burlingame, CA, United States 94010, 650-347-7750, fax: 650-347-6496, e-mail: info@yamazenusa.com, Internet: www.yamazenscience.com Yamazen manufactures Japan's Leading Automated Flash Purification Systems & High Resolution Columns with 45 years of Chromatography experience. US Patented software (GREEN FLASH) gearing toward GREEN CHEMISTRY: Fast (4CV) & Predictable Streamlined Advanced Chromatography & Low Solvent Usage. W-Prep: Parallel - can run two columns simultaneously. ELSD & TLC Reader as add-ons **1201**

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CrystalViewer 9.2
CrystalDiffra 6.5
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Booth # 1304
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Booth # 327
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Quark Glass
Booth # 1106
DrySyn
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Booth # 1118
PEG silanes
TentaGel XV

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AR5 Refractometer
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Ampac
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Booth # 1120
Repaglinide
Trospium Chloride
Teriflunomide
Eprosartan Mesylate
Methyl Pipecolinate Hydrochloride

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AAPS (Amer Assoc. of Pharm Sci.)	1203
ACS Education	427
ACS Green Chemistry Institute	426
Active Spectrum Inc.	1441
BioChromato (Amuza Inc.)	329
CONFLEX Corp.	215
Cresset	127
Elsevier	235
Gaussian	719
GlycoSurface LLC	1341
InfoChem GmbH	815
Inst. of Chemical Biology and Nanomedicine (Hunan University)	1726
Maruzen Co., Ltd.	411
Materials Design, Inc.	1104
McGraw-Hill Education	903
Mettler-Toledo AutoChem, Inc.	206
MicroLAB, Inc.	226
Nanalysis Corp.	802
NT-MDT Co.	936
OpenStax	1339
Oxford University Press	705
Pearson	1005
Pine Research Instrumentation	220
Royal Society of Chemistry	601
Royal Society Publishing	303
Scilligence Corporation	1306
Semichem	717
Specac, Ltd.	1035
ThalesNano Nanotechnology Inc.	1121
Thermo Scientific	816,817
Thieme Chemistry	200
Trivedi Chemistry	1440
University Science Books	904
Vernier Software & Technology	1001
W.W. Norton	710
WebAssign	1204
Wiley	500

Accessible Products

AdValue Technology	1200
BioChromato (Amuza Inc.)	329
Cedarlane	1207
CONFLEX Corp.	215
CP Lab Safety	916
Cresset	127
Elsevier	235
Nananalysis Corp.	802
Piercan USA Inc.	1416
Pine Research Instrumentation	220
Thermo Scientific	816,817

Analytical Research

Active Spectrum Inc.	1441
Anton Paar USA	1013
BioChromato (Amuza Inc.)	329
Biolin Scientific	100
Cedarlane	1207
CONFLEX Corp.	215
Elsevier	235
Grace Discovery Sciences	417
Gaussian	719
Hidden Analytical Inc.	1312
Japan Analytical Industry Co. Ltd.	1338
Knauer	211

Magritek Inc.	418,419
Manta Instruments Inc.	1415
Metrohm USA, Inc.	918
Minesoft	310
Nacalai USA, Inc.	1433
Nananalysis Corp.	802
NIST	221
Northernchem Inc.	1536
NT-MDT Co.	936
Park Systems, Inc.	708
Parr Instrument Co.	1401
Particle Sizing Systems	1304
PerkinElmer Inc.	835
PIKE Technologies	1009
Pine Research Instrumentation	220
PROTO Manufacturing	327
Scilligence Corporation	1306
Semichem	717
Simulations Plus, Inc.	1216
SNKV Services, Inc.	1343
Specac, Ltd.	1035
Thermo Scientific	816,817
Vernier Software & Technology	1001
Waters Corp.	912
Wiley	500
Wyatt Technology Corp.	305
YMC America, Inc.	128

Business Management & Services

ACS Division of Small Chemical Businesses (SCHB)	1235
Lab Manager	126
Scilligence Corporation	1306

Career Development & Training

AAPS (Amer Assoc. of Pharm Sci.)	1203
ACS Education	427D
ACS Green Chemistry Institute	426
GlycoSurface LLC	1341
Lab Manager	126
Wiley	500

Chemicals / Reagents / Raw Materials

abcr GmbH	1521
Accela ChemBio Co. Ltd.	304
ACS Division of Small Chemical Businesses (SCHB)	1235
ACS Green Chemistry Institute	426
Advanced ChemBlocks Inc.	330
AK Scientific, Inc.	1438
Ark Pharm, Inc.	804
Avantor Performance Materials	714
Berry & Associates	930
Cedarlane	1207
ChemBridge Corp.	416
Chemshuttle	312
Combi-Blocks, Inc.	1407
CombiPhos Catalysts, Inc.	805
Enamine LLC	1314
Frontier Scientific, Inc.	306
Materia, Inc.	1117
Metrohm USA, Inc.	918
Northernchem Inc.	1536
Oakwood Products Inc.	1404
Oxchem Corporation	1129
Particle Sizing Systems	1304
Rapp Polymere GMBH	1118
Scilligence Corporation	1306
Spectrum Chemical Mfg Corp.	317
TCI America	1120
Thermo Scientific	816,817
WuXi AppTec (Shanghai) Co. Ltd.	207

Laboratory Equipment & Services

ACS Division of Small Chemical Businesses (SCHB)	1235
Active Spectrum Inc.	1441
Agilent Technologies	112,113
AGI USA Inc.	1221
Anasazi Instruments Inc.	318
Anton Paar USA	1013
Asylum Research, an Oxford Instruments Company	1010
BioChromato (Amuza Inc.)	329
Biolin Scientific	100
BrandTech Scientific	917
B&W Tek	1310
Camag Scientific, Inc.	121
Chemrus Inc.	1334
CONFLEX Corp.	215
CP Lab Safety	916
Delong America	1414
Ecodyst, Inc.	1442
Edinburgh Instruments	801
FEI Company	1518
Gamry Instruments	800
GlycoSurface LLC	1341
Grace Discovery Sciences	417
Harrick Scientific	1418
Heidolph North America	1218
Hidden Analytical Inc.	1312
Hielscher Ultrasonics	813
HORIBA Scientific	1016
IKA Works, Inc.	900
Inert	212
Interchim Inc.	1006
J-KEM Scientific	1027
Japan Analytical Industry Co. Ltd.	1338
JULABO	1018
Kimble Chase LLC	908
Knauer	211
KNF Neuberger	1026
Lab Manager	126
Magna-Safe International	107
Magritek Inc.	418,419
Malvern Instruments, Inc.	1410
Manta Instruments Inc.	1415
Maruzen Co., Ltd.	411
Metrohm USA, Inc.	918
Mettler-Toledo AutoChem, Inc.	206
MicroLAB, Inc.	226
Microtrac Inc.	219
Molymod Models - Spiring Ltd	210
Nacalai USA, Inc.	1433
Nananalysis Corp.	802
Netzsch Instruments North America, LLC	1326
NT-MDT Co.	936
Park Systems, Inc.	708
Parr Instrument Co.	1401
Particle Sizing Systems	1304
PerkinElmer Inc.	835
Piercan USA Inc.	1416
PIKE Technologies	1009
Pine Research Instrumentation	220
PROTO Manufacturing	327
Quark Glass	1106
Scilligence Corporation	1306
SHEL LAB (Sheldon Manufacturing, Inc.)	213
Shimadzu Scientific Instruments Inc.	609
Specac, Ltd.	1035
Spectrum Chemical Mfg Corp.	317
ThalesNano Nanotechnology Inc.	1121
Thermo Scientific	816,817
Vacuubrand, Inc.	301
Vacuum Atmospheres Co.	300
Vernier Software & Technology	1001
Vigor Tech USA, LLC	901
Waters Corp.	912
Wyatt Technology Corp.	305
Yamazen Science, Inc.	1201
YMC America, Inc.	128

Other

AAPS (Amer Assoc. of Pharm Sci.)	1203
ACS Division of Small Chemical Businesses (SCHB)	1235

EXPOSITION

ACS Meetings & Expositions	427
ACS Member Insurance Program	427
ACS Office of Public Affairs	827
ACS Web Strategy & Operations	427
Advanced Clustering Technologies	1527
AIP Publishing – The Journal of Chemical Physics	432
BioChromato (Amuza Inc.)	329
Chemshuttle	312
CP Lab Safety	916
Cresset	127
Hielscher Ultrasonics	813
JEOL USA, Inc.	1000
Knobbe Martens Olson and Bear, LLP	1626
Metrohm USA, Inc.	918
MilliporeSigma (Sigma-Aldrich)	919
Nature Publishing Group	101
NIST	221
Optibrium Ltd.	1227
Paraza Pharma Inc.	1034
Simulations Plus, Inc.	1216
Wyatt Technology Corp.	305

R&D and Manufacturing Services

abcr GmbH	1521
Accela ChemBio Co. Ltd.	304
ACS Division of Small Chemical Businesses (SCHB)	1235
Advanced ChemBlocks Inc.	330
Ark Pharm, Inc.	804
Cedarlane	1207
Combi-Blocks, Inc.	1407
CONFLEX Corp.	215
Cresset	127
Frontier Scientific, Inc.	306
Gaussian	719
Grace Discovery Sciences	417
Hidden Analytical Inc.	1312
Hielscher Ultrasonics	813
J-KEM Scientific	1027
Lilly USA, LLC	935
Materia, Inc.	1117
Mettler-Toledo AutoChem, Inc.	206
Northernchem Inc.	1536
NT-MDT Co.	936
Oakwood Products Inc.	1404
Ocean Nanotech	1342
Oxchem Corporation	1129
Particle Sizing Systems	1304
PerkinElmer Inc.	835

PharmAgra Labs, Inc.	1336
Piercan USA Inc.	1416
PROTO Manufacturing	327
Rapp Polymere GMBH	1118
Scientific Computing & Modelling NV	833
Scilligence Corporation	1306
Semichem	717
Simulations Plus, Inc.	1216
Specac, Ltd.	1035
ThalesNano Nanotechnology Inc.	1121
The Chemistry Research Solution LLC	1426
Tosoh Bioscience LLC	1301
Waters Corp.	912
WuXi AppTec (Shanghai) Co. Ltd.	207
YMC America, Inc.	128

Scientific Computer & Data Management

ACS Division of Small Chemical Businesses (SCHB)	1235
Cambridge Crystallographic Data Ctr.	926
ChemAxon LLC	328
Collaborative Drug Discovery	333
CONFLEX Corp.	215
CrunchYard	1437
CrystalMaker Software Ltd.	831
Gaussian	719
InfoChem GmbH	815
Integrated Chemistry Design, Inc.	1427
Materials Design, Inc.	1104
Minesoft	310
NIST	221
PerkinElmer Inc.	835
Schrodinger, Inc.	1300
Scientific Computing & Modelling NV	833
Scilligence Corporation	1306
Semichem	717
Waters Corp.	912
Wavefunction, Inc.	405

Technical Literature / Websites / Databases

De Gruyter	942
Elsevier	235
Grace Discovery Sciences	417
InfoChem GmbH	815
NIST	221

Royal Society of Chemistry	601
Royal Society Publishing	303
Scilligence Corporation	1306

Testing & Measurement Instrumentation

ACS Division of Small Chemical Businesses (SCHB)	1235
Active Spectrum Inc.	1441
Anton Paar USA	1013
Asylum Research, an Oxford Instruments Company	1010
Biolin Scientific	100
Brookhaven Instruments Corp.	1135
Delong America	1414
Extrel CMS	510
FEI Company	1518
Gamry Instruments	800
Grace Discovery Sciences	417
Hidden Analytical Inc.	1312
HORIBA Scientific	1016
J-KEM Scientific	1027
Kimble Chase LLC	908
Knauer	211
Magritek Inc.	418,419
Malvern Instruments, Inc.	1410
Manta Instruments Inc.	1415
Metrohm USA, Inc.	918
Mettler-Toledo AutoChem, Inc.	206
MicroLAB, Inc.	226
Micromeritics Instrument Corp.	320
Microtrac Inc.	219
Nanalysis Corp.	802
NIST	221
NT-MDT Co.	936
Park Systems, Inc.	708
Parr Instrument Co.	1401
Particle Sizing Systems	1304
Piercan USA Inc.	1416
PIKE Technologies	1009
PROTO Manufacturing	327
Reichert Technologies	1316
Specac, Ltd.	1035
Thermo Scientific	816,817
Vacuum Atmospheres Co.	300
Vernier Software & Technology	1001
Waters Corp.	912
Wiley	500
Wilmad-LabGlass	1526
Wyatt Technology Corp.	305

251st American Chemical Society National Exposition

Meeting - March 13-17, 2016
Exposition - March 13-15, 2016
San Diego Convention Center - Halls B&C
San Diego, California

