

IDENTIFYING THE PERFECT METHOD

NEW SOLUTION FROM CAS PROVIDES HOPE FOR ANALYTICAL SCIENTISTS

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Robust and reproducible experimental and analytical techniques are the backbone of the scientific endeavor. However, for many researchers, the search for useful and relevant protocols turns into a frustrating and often fruitless scavenger hunt through the literature. Much of this process is guesswork—attempting to predict the contents of a methods section based on clues from the title and abstract. “Right now, the only way to do it is to go back and read all those papers,” says Zachary Schultz, Associate Professor of Chemistry and Biochemistry at the University of Notre Dame.

In February 2016, CAS, a division of the American Chemical Society, launched MethodsNow, a first-of-its-kind resource that aims to provide a shortcut in the search for analytical methods. Scientists extract critical methodological information from peer-reviewed publications into a standardized template that can easily be searched and compared. “Rather than spending two hours to look for a piece of information and having to go through that and refine it and go back and forth, we’re finding that with our solution it might take only 15 or 20 minutes to find exactly what you’re looking for,” says Matthew J. Toussant, senior vice president of Content and Product Operations at CAS.

CAS has positioned itself as a hub for chemistry and related scientific information for more than a century. Among other resources, the company produces SciFinder, which launched in 1995 as an end-user tool for researching chemical information. Since

then, SciFinder has expanded considerably to encompass more detailed content information found in publications and provided better functionality to search for chemical structures and synthetic reactions.

“When I was a grad student, I lived and died by SciFinder,” Schultz says. This service is highly leveraged by organic chemists who are engaged in synthesis and related research. It also serves the broader community of scientists who need chemical substance, literature and related information. According to sales director Steve Morris, a consistent opportunity emerged in discussions between CAS and its customers. “It was clear that analytical chemists, in particular, wanted more than SciFinder was able to do,” Morris says, “and the existing tools that people mentioned were exceedingly narrowly focused and fairly costly.”

This need would ultimately fuel the development and launch of MethodsNow. The foundational data for this platform is the semi-automated identification of journal articles based on criteria pertaining to methodological quality and relevance. “We look at the highly cited work that people are already widely using in research,” Toussant says, “but we’ve also tried to focus on the cutting edge and get things into our content collection that are from reputable laboratories, in highly regarded journals, and that have early citations from other authors.”

The method template is highly structured, breaking down each protocol in terms of

key information including the analyte being characterized, the sample matrices from which the analyte can be isolated, and the equipment required. This design makes it simple to search and filter techniques based on a user’s interests—for example, homing in quickly on immunoassays for measuring disease-related metabolites in human blood. Furthermore, this structured design makes it simple to perform direct comparisons across protocols, allowing users to examine the requirements and capabilities of as many as three methods simultaneously. “Because of the granularity we’ve created, we can align about 15 different components of each method,” Toussant says. Such comparisons might uncover alternative experimental strategies that employ instruments and reagents that are more readily available, or which are optimized for different types of specimens or achieve a superior limit of detection.

In the early months following the product’s launch, the uptake has been greatest in the private sector—particularly amongst small-, medium- and large-scale pharmaceutical, agricultural, and chemical manufacturing companies with robust analytical divisions. Toussant also notes that the product has proven highly popular at contract research laboratories. The service has not yet made major inroads into the academic world, although there are clear signs that this tool could become popular in this community as well. “It looks like an interesting idea—I’m going to want to play around with this a bit,” Schultz says. Morris notes that several university consortia are currently testing the

CAS Solutions - METHODSNow A CAS SOLUTION carbamazepine

Return to Results

Compare Methods

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Title	Analysis of Phenobarbital in Blood plasma by Solid phase extraction	Analysis of Carbamazepine in Blood plasma by Solid phase extraction	Analysis of Carbamazepine in Blood plasma by Reversed-phase HPLC
CAS Method Number	1-101-CAS-66910	1-101-CAS-133183	1-101-CAS-60070
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Solid phase extraction; UV radiation; HPLC	Solid phase extraction; UV-visible spectroscopy; HPLC; Liquid-liquid microextraction	Solid phase extraction; Reversed-phase HPLC
Analyte	<i>trans</i> -10,11-Dihydroxy-10,11-dihydrocarbamazepine; Carbamazepine; Lamotrigine; View All	Carbamazepine	Licarbazepine; Oxcarbazepine; Eslicarbazepine acetate; <i>trans</i> -10,11-Dihydroxy-10,11-; View All
Matrix	Blood plasma	Drinking waters; Urine; Blood plasma	Blood plasma
Other Materials	Methanol; Acetonitrile; Phosphoric acid; C18 column (55 mm x 4 mm; 3 µm particle size)	Acetonitrile; Acetone; Chloroform; Methanol; Spherisorb ODS2 column (250 mm x 4.6 mm; with 5.0 µm); View All	Oasis® HLB (30 mg, 1 ml) cartridges; LICHRO-CART® Purospher® Star (C ₁₈ , 3 µm, 55 mm x 4 mm)
Equipment Used	Liquid chromatograph, BAS-480	Binary HPLC pump, 1525, Waters, Massachusetts, USA; UV/Vis detector, 2487, Waters; Vacuum pump; View All	liquid chromatograph, BAS-480, Bioanalytical systems, West Lafayette, IN, USA
Conditions	Chromatographic: Mobile phase - water:methanol:acetonitrile:TEA	Instrument: detection wavelength: 237 nm; mobile phase: mixture of	

A screenshot from the Compare Methods tool for the analysis of carbamazepine in the MethodsNow platform.

product to see how well it fits the needs of their researchers.

The MethodsNow data collection has steadily accumulated content since launch—the number of protocols has doubled over the past several months, and new updates are scheduled to occur on a monthly basis in 2017.

Each of these methods is assigned a unique number. For now, this is used solely in the context of MethodsNow, but in time this could feed back into the research publishing

world to become a more broadly-used identifier for use in journal articles. “Our CAS Method Number could be like a CAS Registry Number, and an easy way to reference back to our methods,” says Sabine Kuhn, manager of content projects at CAS, “And there have been discussions between CAS and ACS Publications on how to integrate CAS Method Numbers into ACS journals prior to publication.”

This first iteration of MethodsNow is broadly targeted to appeal to the greatest number

of early adopters, which means that some subfields and highly-focused applications remain underrepresented. “We’ve been asked to become a collection house for government standards and analytical equipment standards and things like that,” Morris says. “This is important for groups doing more specialized work like water treatment, for example.” These areas may be targeted for inclusion in the future, but for the time being Morris concludes that smaller analytical companies may find that “this is more tool than they need.”

Over the longer term, the platform’s breadth and depth could expand considerably. For example, Toussant is intrigued by the possibility of crossing disciplinary boundaries to include techniques related to genomic analysis and metabolomics experiments. Schultz is also hopeful that future iterations might throw computational methods into the mix as well. “It would be extremely useful to have something like this for data analysis,” he says. “Especially when you’re talking about big datasets, and there’s a number of different multivariate approaches that you can use.”

For now, however, the lofty goal of creating a consolidated, one-stop shop for scientific methods remains on the horizon, and CAS is setting its immediate priorities based on the feedback gathered from its first-generation customers. “We need to understand how they’re using it so we can learn what is missing,” Kuhn says, and to “separate the nice-to-haves from the need-to-haves to ensure the most optimal experience in the evaluation of methods and protocols.”

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