SYNTHESIS

▶ Mechanism-based screening accelerates photocatalysis research

Screening strategies to discover new catalysts or types of reactions typically count hits by the number of new products that turn up in crude reaction mixtures. Frank Glorius and colleagues of the University of Münster have decided to try a different approach: They only screen molecules for their ability to take part in a single step of a reaction. If an interaction occurs, the molecule is considered a hit. What's more, each molecule tested is taken as a representative of an entire class of molecules, which greatly expands the scope of the screen. Once a target molecule is acquired, the researchers flip the screen to use the molecule with various catalysts to identify the optimal catalyst for the job at hand (*Angew. Chem. Int. Ed.* 2016, DOI: 10.1002/anie.201600995). The Münster team tested this approach by looking at excited-state catalyst quenching by an organic reactant, which is the key step common to all photocatalytic reactions. If an interaction occurs, which the researchers determine via spectroscopy, a reactive radical species forms that is capable of following different downstream reaction pathways to form various products. The team's screen of 100 compounds identified benzotriazoles and phenols as two new molecule classes that interact with iridium catalysts in denitrogenation and bromination reactions, respectively.—STEVE RITTER

DRUG DEVELOPMENT

▶ Forecasting liver toxicity before the damage is done

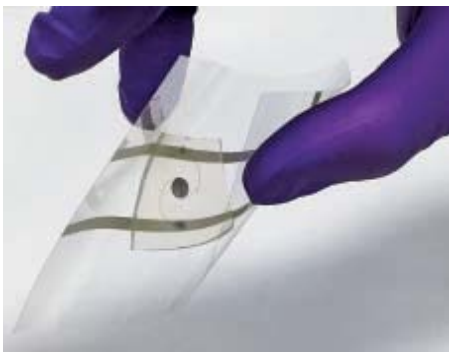
The liver takes the brunt of the job clearing drugs from the body. Now, researchers have developed a computational model that predicts which drug candidates will prove toxic to the organ (*Chem. Res. Toxicol.* 2016, DOI: 10.1021/acs.chemrestox.5b00465). Denis Mulliner of Sanofi and his team developed a model that incorporated human and animal toxicity data from 3,712 compounds—three or more times the number used in most earlier models—organizing the data based on each chemical's molecular properties and mechanism of liver toxicity. The model looks for common chemical and structural properties that lead to a particular type of toxicity. The team then tested its model with 269 proprietary compounds not included in the database. The liver toxicity of these compounds had been tested in animals, and the new model correctly identified 72% of the hepatotoxic compounds. The researchers are sharing this database, along with the model's source code, with the scientific community "to advance the field of predictive toxicology," Mulliner says.—ERIKA GEBEL BERG, special to C&EN

ELECTRONIC MATERIALS

▶ Pressure sensors gaining durability

Researchers in Singapore have done what most materials scientists can only dream about: They ran their project over with a car. But this act wasn't born of frustration. Rather, it demonstrated the durability of pressure sensors made from eutectic gallium indium, or eGaIn, a metal that's liquid at room temperature (*ACS Sens.* 2016, DOI: 10.1021/acssensors.6b00115). To create their device, researchers at the National University of Singapore dispense electrically conductive eGaIn into a cavity they have patterned within a silicone elastomer. They then seal the device with a flexible polyethylene terephthalate film that also supports two electrodes made from screen-printed silver. Squishing a device redistributes the liquid metal and alters the resistance between the electrodes, converting pressure changes to electrical signals. The sensor is durable enough to stomp on, but soft and flexible enough to wear inside a shoe, the researchers report. They could even discern whether it was worn inside a sneaker or a high heel. Such sensors have many potential

Within this flexible sensor, eutectic gallium indium is confined in an *S*-shaped channel and connected to two printed silver bands.



CHEMICAL COMMUNICATION

How beetle moms tell mates to bug off

Nicrophorus vespilloides

Caring for newborns is tough for all kinds of new parents. The burying beetles *Nicrophorus vespilloides,* for example, have to juggle their responsibility of feeding carrion to hungry larvae and their drive to make more offspring. Tending to existing young, rather than making new ones, is the more successful strategy for this beetle. Now, researchers led by Sandra Steiger of the University of Ulm have discovered that the female *N. vespilloides* manages this balancing act by being infertile in her brood's early days. What's more, the scientists found females give off a volatile compound that lets males know nothing will come from efforts to copulate (*Nat. Commun.* 2016, DOI: 10.1038/ncomms11035). By using deuterium labeling, the researchers learned that the hormone that makes the female infertile and the antiaphrodisiac pheromone—methyl geranate—arise from the same biosynthetic precursor. "There can be intense conflicts between males and females over mating rate or how much each sex should invest in raising the young," the authors note. "Our results uncover mechanisms underlying parental care decisions, and illustrate how a physiological interplay between hormone and pheromone systems guarantees that both parents draw their attention towards the existing young as long as they are needy."—BETHANY HALFORD

JOHANNES STÖKL (BEETLE); *ACS SENS.* (SENSOR)