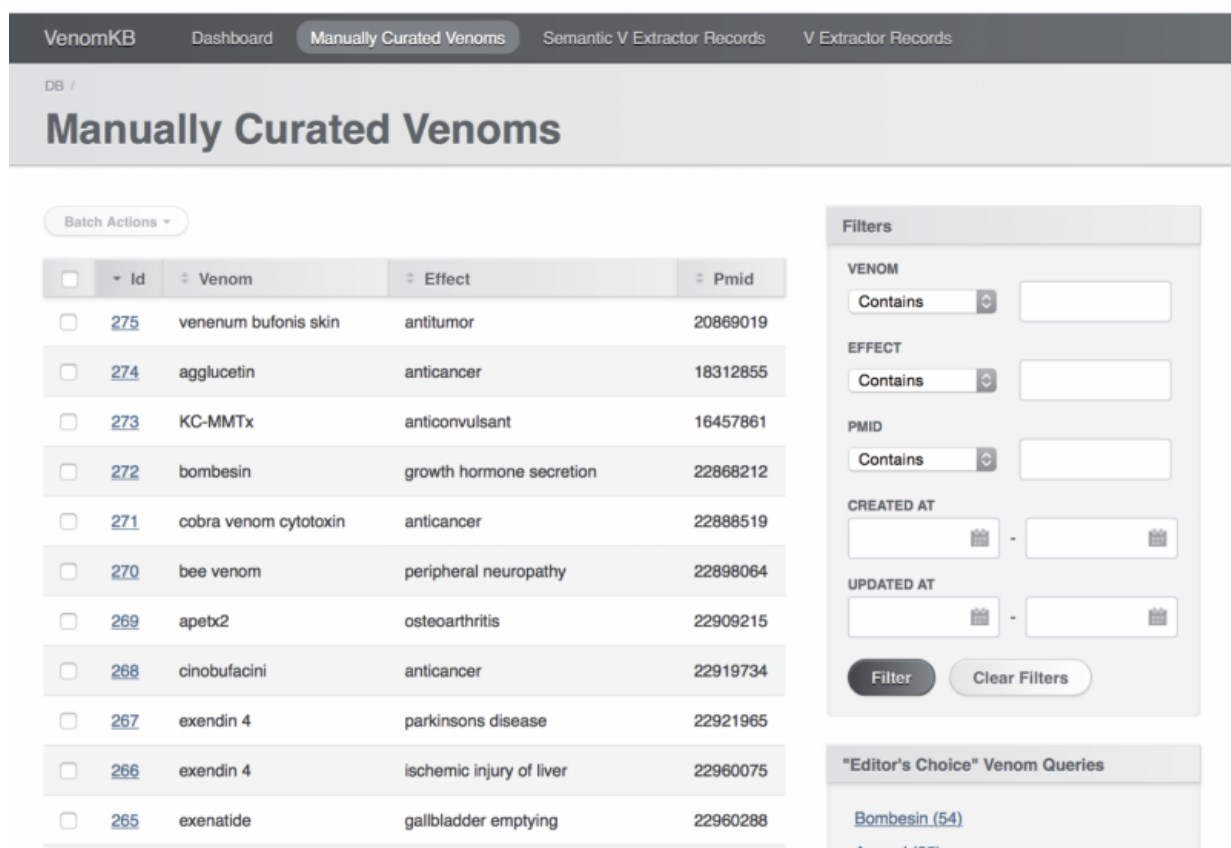


# Data scientists create world's first therapeutic venom database

November 25 2015



The screenshot displays the VenomKB web application interface. At the top, there is a navigation bar with links: VenomKB, Dashboard, **Manually Curated Venoms**, Semantic V Extractor Records, and V Extractor Records. Below the navigation bar, the page title "Manually Curated Venoms" is prominently displayed. A "Batch Actions" dropdown menu is located above a table of venoms. The table has columns for Id, Venom, Effect, and Pmid. The table lists 11 entries, each with a checkbox, a link to the entry, the venom name, the effect, and the PubMed ID (Pmid). To the right of the table is a "Filters" sidebar with sections for VENOM, EFFECT, PMID, CREATED AT, and UPDATED AT. Each section has a "Contains" dropdown menu and a text input field. At the bottom of the filters sidebar are "Filter" and "Clear Filters" buttons. Below the filters sidebar is a section titled "Editor's Choice" Venom Queries, which lists "Bombesin (54)" and "Apoptin (25)".

<input type="checkbox"/>	Id	Venom	Effect	Pmid
<input type="checkbox"/>	<a href="#">275</a>	venenum bufonis skin	antitumor	20869019
<input type="checkbox"/>	<a href="#">274</a>	agglucetin	anticancer	18312855
<input type="checkbox"/>	<a href="#">273</a>	KC-MMTx	anticonvulsant	16457861
<input type="checkbox"/>	<a href="#">272</a>	bombesin	growth hormone secretion	22868212
<input type="checkbox"/>	<a href="#">271</a>	cobra venom cytotoxin	anticancer	22888519
<input type="checkbox"/>	<a href="#">270</a>	bee venom	peripheral neuropathy	22898064
<input type="checkbox"/>	<a href="#">269</a>	apetx2	osteoarthritis	22909215
<input type="checkbox"/>	<a href="#">268</a>	cinobufacini	anticancer	22919734
<input type="checkbox"/>	<a href="#">267</a>	exendin 4	parkinsons disease	22921965
<input type="checkbox"/>	<a href="#">266</a>	exendin 4	ischemic injury of liver	22960075
<input type="checkbox"/>	<a href="#">265</a>	exenatide	gallbladder emptying	22960288

VenomKB, short for Venom Knowledge Base, summarizes the results of 5,117 studies in the medical literature describing the use of venom toxins as painkillers and as treatments for diseases like cancer, diabetes, obesity, and heart failure. Credit: Tatonetti lab and Columbia University Medical Center/Data Science Institute

What doesn't kill you could cure you. A growing interest in the therapeutic value of animal venom has led a pair of Columbia University data scientists to create the first catalog of known animal toxins and their physiological effects on humans.

VenomKB, short for Venom Knowledge Base, summarizes the results of 5,117 studies in the medical literature describing the use of venom toxins as painkillers and as treatments for diseases like cancer, diabetes, obesity, and heart failure. Drawn from an automated analysis of the literature, VenomKB documents nearly 42,723 effects on the body. Though modern medicine makes use of only a small fraction of the toxins documented thus far, the researchers hope that the catalog will spur the discovery of new compounds and medical treatments.

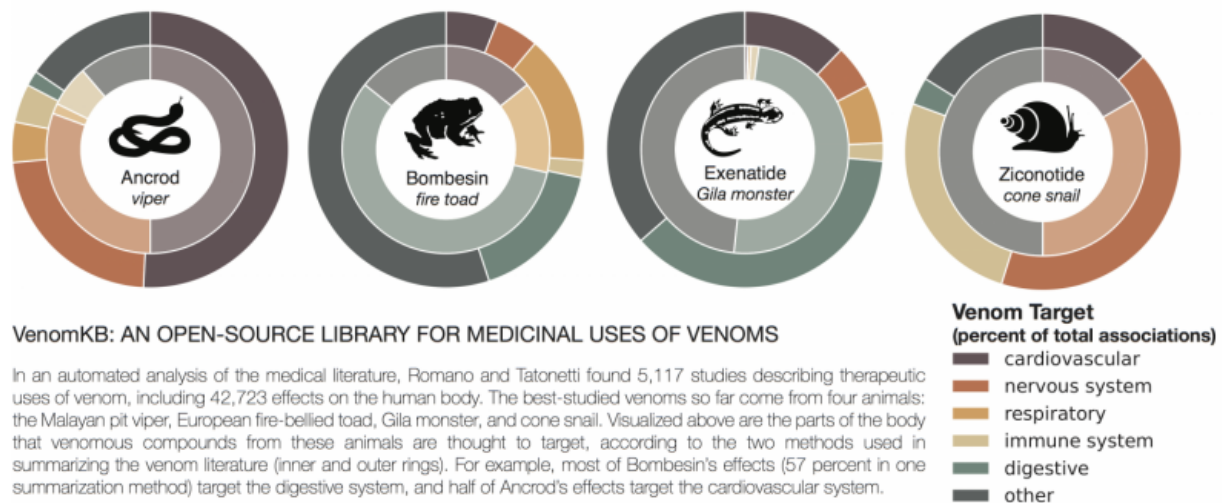
"With this list we can take stock of what we know about venoms and their therapeutic effects" said Nicholas Tatonetti, an assistant professor of biomedical informatics at Columbia University Medical Center and a member of the Data Science Institute. "The questions now is: How can we use this information with other databases to discover new compounds and therapies?"

Tatonetti and Joseph Romano, a graduate student, searched on the term "venoms/therapeutic use" in a database of 22 million medical research papers. This produced a list of 5,117 venom-related studies whose results they summarized using a pair of computer algorithms. After cross-referencing toxins and drugs listed under multiple names and correcting other irregularities in the data, they found 42,723 unique mentions of venoms having a specific effect on the body. Their results are published in a companion study to Venom KB in the journal *Scientific Data*.

Venom's capacity to heal is paradoxically linked to its fast-acting, lethal

effects in the wild. Found in more than 173,000 species, venoms evolved over millions of years to target molecules that are often involved in disease. The toxic proteins and amino acids known as peptides that make up venom act on cell receptors and ion channels, controlling how cells behave.

By mimicking or altering how these toxins act on specific human cells, researchers can develop drugs that inhibit pain or treat diseases, often with fewer side effects than those of drugs already on the market.



In an automated analysis of the medical literature, Romano and Tatonetti found 5,117 studies describing therapeutic uses of venom, including 42,723 effects on

the human body. The best-studied venoms so far come from four animals: the Malayan pit viper, European fire-bellied toad, Gila monster, and cone snail. Visualized above are the parts of the body that venomous compounds from these animals are thought to target, according to the two methods used in summarizing the venom literature (inner and outer rings). For example, most of Bombesin's effects (57 percent in one summarization method) target the digestive system, and half of Ancrod's effects target the cardiovascular system. Credit: Tatonetti lab and Columbia University Medical Center/Data Science Institute

About a dozen major drugs have emerged from this strategy so far, National Geographic magazine reported in 2013. One of the first, an anticoagulant called Arvin, gained favor in the late 1960s after a doctor discovered that ancrod, a protein found in the venom of the Malayan pit viper, could treat blood clots in the legs.

The widely used type 2 diabetes drug Byetta, is made from the toxin exenatide, found in the saliva of the venomous Gila monster, a lizard native to the United States and Mexico.

Another drug, bombesin, uses a toxin found in the skin of the venomous European fire-bellied toad to treat gastrointestinal disorders. Bombesin's ability to bind to neuronal tumors has led to interest in developing a fluorescent version that could guide surgeons around the edges of a tumor.

Five compounds produced by the venomous cone snail have made it to clinical trials, including ziconotide, the generic term for an analgesic similar to morphine.

The Malayan pit viper, Gila monster, European fire-bellied toad, and cone snail account for about 18 percent of the 5,117 venom-related studies now catalogued in Venom KB. Yet there are 10 million or more venomous species that have yet to be studied. Zoltan Takacs, a

toxinologist who earned his PhD in evolutionary studies at Columbia, estimates there are 20 million venom toxins waiting to be screened.

Venom KB got its start after Romano approached Tatonetti, his thesis adviser, about studying medicinal uses of venom. Tatonetti suggested that Romano start looking through the venom database. To their surprise there was neither a database nor a list. Still modest in size, VenomKB is expected to grow more useful as researchers contribute more data. "With a large enough library we can screen for more effective, safer compounds," said Romano.

Databases of compounds and their biological effects have been used in recent years to discover and develop new drugs as well as uncover problems with drugs already in use. Tatonetti and his colleagues mined a federal database of documented drug side effects, the FDA Adverse Event Reporting System (FAERS), and discovered that the interaction of the anti-depressant paroxetine, sold under the brand name Paxil, and the statin pravastatin, sold as Pravachol, could raise blood glucose levels in diabetic patients.

With VenomKB up and running, Tatonetti and Romano plan to contribute data of their own. Starting with samples of dried venom from the black mamba, they will perform experiments and explore new treatments for chronic pain, diabetes and heart disease.

The paper is titled, "VenomKB, a new knowledge base for facilitating the validation of putative [venom](#) therapies."

Provided by Columbia University Medical Center

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