

Using The Open Drug Discovery Teams (ODDT) Mobile App To Bring Molecules & SAR From Behind Journal Paywalls

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What is The problem?

Research funded by the tax-payer is locked behind journal paywalls. In most cases many researchers are interested in a few key pieces of information. Drug discovery scientists want to see molecule structures and structure activity relationship data. In the absence of mandates that require the immediate release of tax-payer funded research into the research commons, or the requirement that journals deposit data with such manuscripts into open databases, we now propose a novel approach. As people read scientific papers they can simply tweet molecule related information from the paper like a molecule structure (by using an app to draw it, or retrieve it from a database like ChemSpider) or name, and using mobile apps such as "SAR Table" they can also create SAR tables and tweet these to the appropriate disease community. Data can be freed from behind paywalls.

The Open Drug Discovery Teams (ODDT) project uses a free mobile app as user entry point <http://tinyurl.com/6I9qy4f>. The app has a magazine-like interface, and server-side infrastructure for hosting chemistry-related data as well as value added services. The project is open to participation from anyone and provides the ability for users to make annotations and assertions, thereby contributing to the collective value of the data to the engaged community. The infrastructure for the app is currently based upon the Twitter API and uses Google Alerts RSS feeds as a useful proof of concept for a real time source of publicly generated content.

We now highlight how ODDT can be used to share molecules and SAR data with the research community and general public by tweeting this information as they read a paper with the appropriate hashtag for the disease topic. This could be a valuable asset for the scientific community and release data that is inaccessible to many scientists and patients. In the absence of mandates to free up data it may be possible to use crowdsourcing to deposit such small but important fragments of molecule related information into the public domain.

An example of an article behind a paywall that was funded by the tax-payer

Identification of Drug Modulators Targeting Gene-Dosage Disease CMT1A
Sung-Wook Jung,¹ Camila Lopez-Aranda,¹ Ryan MacArthur,¹ John Svaren,¹ and James Inglese^{1,2}

ABSTRACT: The structural integrity of myelin formed by Schwann cells in the peripheral nervous system (PNS) is required for proper nerve conduction and is dependent on adequate expression of myelin genes including peripheral myelin protein 22 (PMP22). Consequently, severe PMP22 resulting from its genetic amplification and overexpression has been directly associated with the peripheral neuropathy called Charcot-Marie-Tooth disease type 1A (CMT1A), the most prevalent type of CMT. Herein, as an attempt to identify transcriptional inhibitors with therapeutic value toward CMT1A, we developed a consolidating pair of orthogonal reporter assays for luciferase (Luc) and β -galactosidase (Gal), capable of recapitulating PMP22 expression, utilizing the intrinsic regulatory element of the human PMP22 promoter. Each compound from a collection of approximately 1000 approved drugs was tested in a 96-well plate quantitative high-throughput screen (qHTS) format. In conjunction with an independent counter screen for cytotoxicity, the design of an orthogonal screen platform effectively established selection and prioritization of active compounds, among which three drugs (fenretinide, olvanil, and bortezomib) exhibited marked reduction of endogenous PMP22 mRNA and protein. Overall, the findings of this study provide a strategic approach to assay development for gene-dosage diseases such as CMT1A.

abstract -describes 3 active compounds found by HTS screening -structures only in supplemental data

approximately 3,000 approved drugs was tested at multiple titrations in a quantitative high-throughput screen (qHTS) format. In the design of our orthogonal screen platform effectively contributed three drugs (fenretinide, olvanil, and bortezomib) exhibited marked reduction of endogenous PMP22 mRNA and protein. Overall, the findings of this study provide a strategic approach to

SAR from papers can also be created in SAR Table app

Compound	Activity (IC ₅₀)
Compound 1	activity: 115.1 μ M
Compound 2	activity: 2.4 μ M
Compound 3	activity: 52.9 μ M
Compound 4	activity: 1.9 μ M
Compound 11	activity: 1.7 μ M
Compound 12	activity: 2.3 μ M
Compound 13	activity: 15.4 μ M
Compound 14	activity: 15.9 μ M
Compound 15	activity: 2.7 μ M
Compound 16	activity: 23.8 μ M
Compound 17	activity: 3.1 μ M
Compound 18	activity: 15.7 μ M



Tweet each molecule from ChemSpider with a hashtag for disease or other topic

Velcade
ChemSpider ID: 343402
Molecular Formula: C₁₉H₂₅N₄O₄
Average mass: 384.237213 Da
Molecular weight: 384.196899 Da
Systematic name: [(1R)-3-methyl-1-[(2S)-3-phenyl-2-(pyrazin-2-yl)carbamoyl]propanoyl]amino]butylboronic acid

Names and Identifiers
Names and Synonyms: Database IDs
Validated by Experts, Validated by Users, Non-Validated, Removed by Users, Redirected by Users, Redirect Approved by Experts

Properties
Predicted - ACCLabs | Predicted - EPISuite | Predicted - ChemAxon
Predicted data is generated using the ACCLabs' ACDFPhysChem Suite, for more information see their website.

Property	Value
ACCLLogP	2.446
ACCLogD (pH 5.5)	2.45
ACD/BCF (pH 5.5)	42.56
ACD/KOC (pH 5.5)	529.73
#H bond acceptors	8
#H bond donors	4
#Freely Rotating Bonds	11
Bonds	Index of Refraction: 1.564
Molar Volume	316.503 cm ³
# of Rule of 5 Violations	0
ACD/LogD (pH 7.4)	2.44
ACD/BCF (pH 7.4)	42.33
ACD/KOC (pH 7.4)	506.96
Polar Surface Area	124.44 Å ²
Molar Refractivity	102.975 cm ³
Polarizability	40.823 10 ⁻²⁴ cm ³

Disease topic followed in the ODDT app

Sanfilippo Syndrome, Green Chemistry, HIV/AIDS, Tuberculosis, Huntington's Disease, Chagas Disease, Malaria, Leishmaniasis, Giant Axonal Neuropathy

Molecules collected in app

ODDT Incoming
Recent Content
@collabchem: Velcade | C₁₉H₂₅N₄O₄ | ChemSpider: #oddtinfo
@aclarkeyz: @jamesj74: All a-Twitter about chemistry #oddtinfo #ODDT
@oddtinfo: Thanks for sharing! #ODDTinfo RT @teaminspire App Connects Rare Disease Researchers to Data (link) via @GENBio #RareDisease
@aclarkeyz: Open Drug Discovery Teams in press: (link) #oddtinfo #oddt

User can click on link to open in app or click on URL to open in original source

Velcade | C₁₉H₂₅N₄O₄ | ChemSpider: #oddtinfo
<http://www.nature.com/nchem/journal/v...>
@oddtinfo: Thanks for sharing! #ODDTinfo RT @teaminspire App Connects Rare Disease Researchers to Data (link) via @GENBio #RareDisease
@aclarkeyz: Open Drug Discovery Teams in press: (link) #oddtinfo #oddt

