## **SPRINGER NATURE**

## Deposit of chemical structure data from publications to public databases Steffen Pauly

23 August 2019

ADVANCING **DISCOVERY** 

### **Our research business brands and imprints**



### **How Springer Nature Advances Discovery**



### **Chemical Entity Recognition and Annotation**



### **PubChem**



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#### 10.5 Springer Nature References

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		SORT BY	Relevance	$\sim$
Thumbnail	Title	Publication Name	Publication Date	PMID
Amino Acids	Aromatic amino acid biosynthesis and production of related compounds from p-hydroxyphenylpyruvic acid by rumen bacteria, protozoa and their mixture	Amino Acids	2002	12395184
	Tyrosinaemia type III: Immunochemical studies on 4- hydroxyphenylpyruvic acid dioxygenase and molecular cloning of cDNA for the enzyme	Journal of Inherited Metabolic Disease	1991	
	The reduction of aromatic alpha-keto acids by cytoplasmic malate dehydrogenase and lactate dehydrogenase	Biochemical Genetic	5 1987	



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### ChemSpider



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### **Initial Deposit to PubChem October 2017**

	Count	Comment
Input documents	7,133,996	Selected SpringerLink subject collections, 6 Nature journals
Documents containing significant chemistry	3,981,327	Containing at least one compound with relevance value > 0.1
Documents having a PMID	858,934	Also available via PubMed
Documents Open/free access	294,380	
Unique chemical compounds	604,506	
Compound -> DOI links	26,839,100	

### **Continuous Deposit to PubChem since February 2018**



New Springer Nature Compounds in PubChem



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# Thank you

#### **Steffen Pauly**

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#### The story behind the image



#### Alfred Nobel (1833-1896)

Alfred Nobel was a Swedish chemist, engineer and inventor of dynamite. Dynamite made him very wealthy but partly in response to concerns about its negative uses, he decided to give the vast majority of his estate to establish the four Nobel Prizes with a fifth awarded in his memory, to people or organisations who promote peace around the world.

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