

A Case Study for Information Integration and Analysis with **Wistract[®]** – A new Platform for Scientific Information

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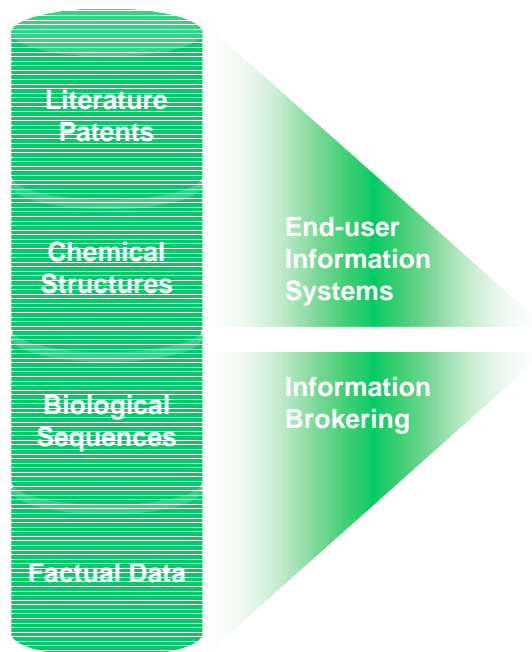
Achim Zielesny

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Institute for Bio- and Chemoinformatics
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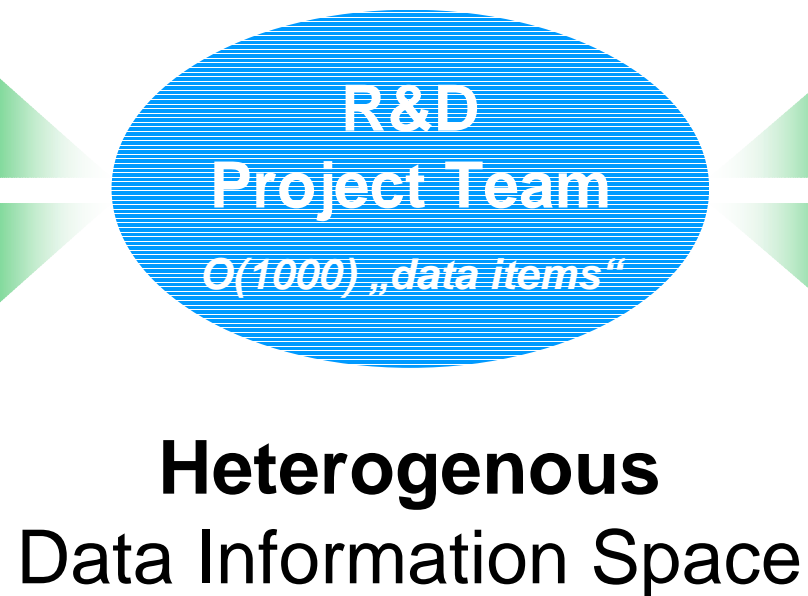
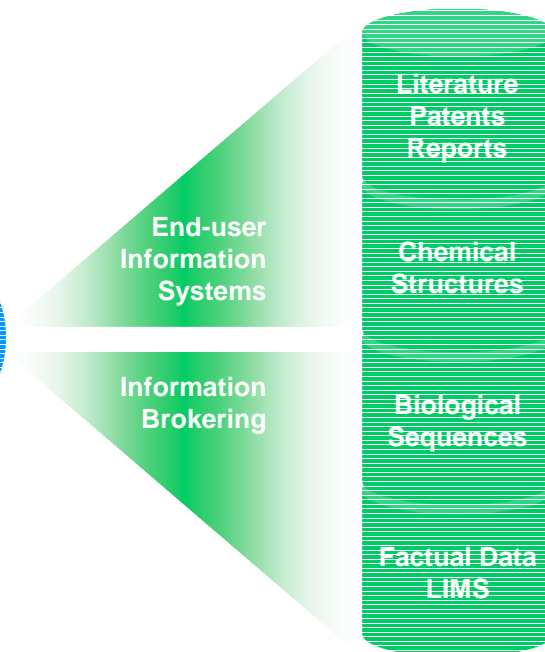


R&D Information Space

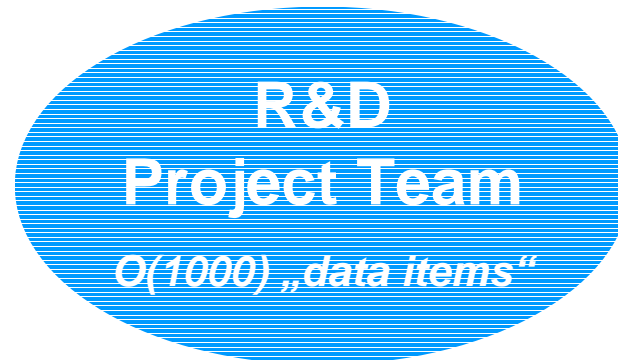
Outside World



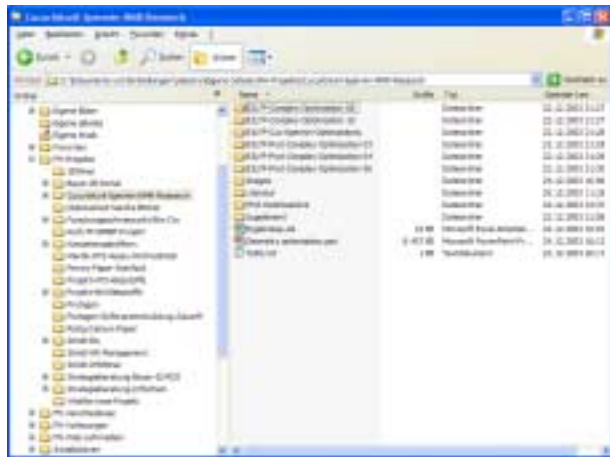
Company



R&D Information Organisation

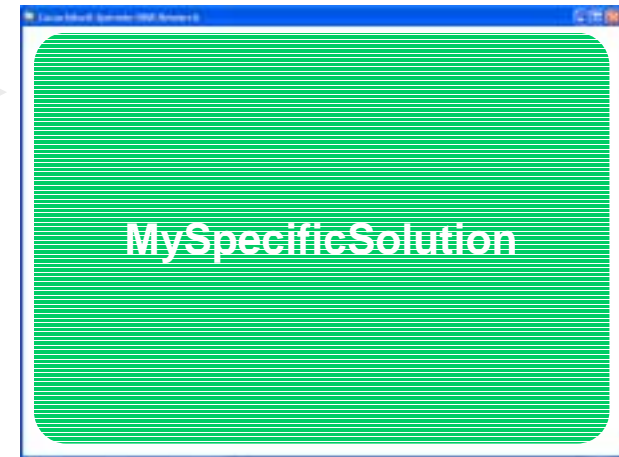


File system (or flat container)

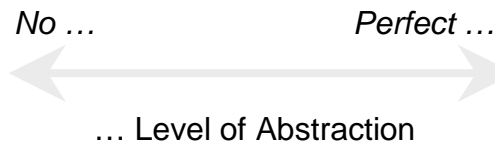


too simple

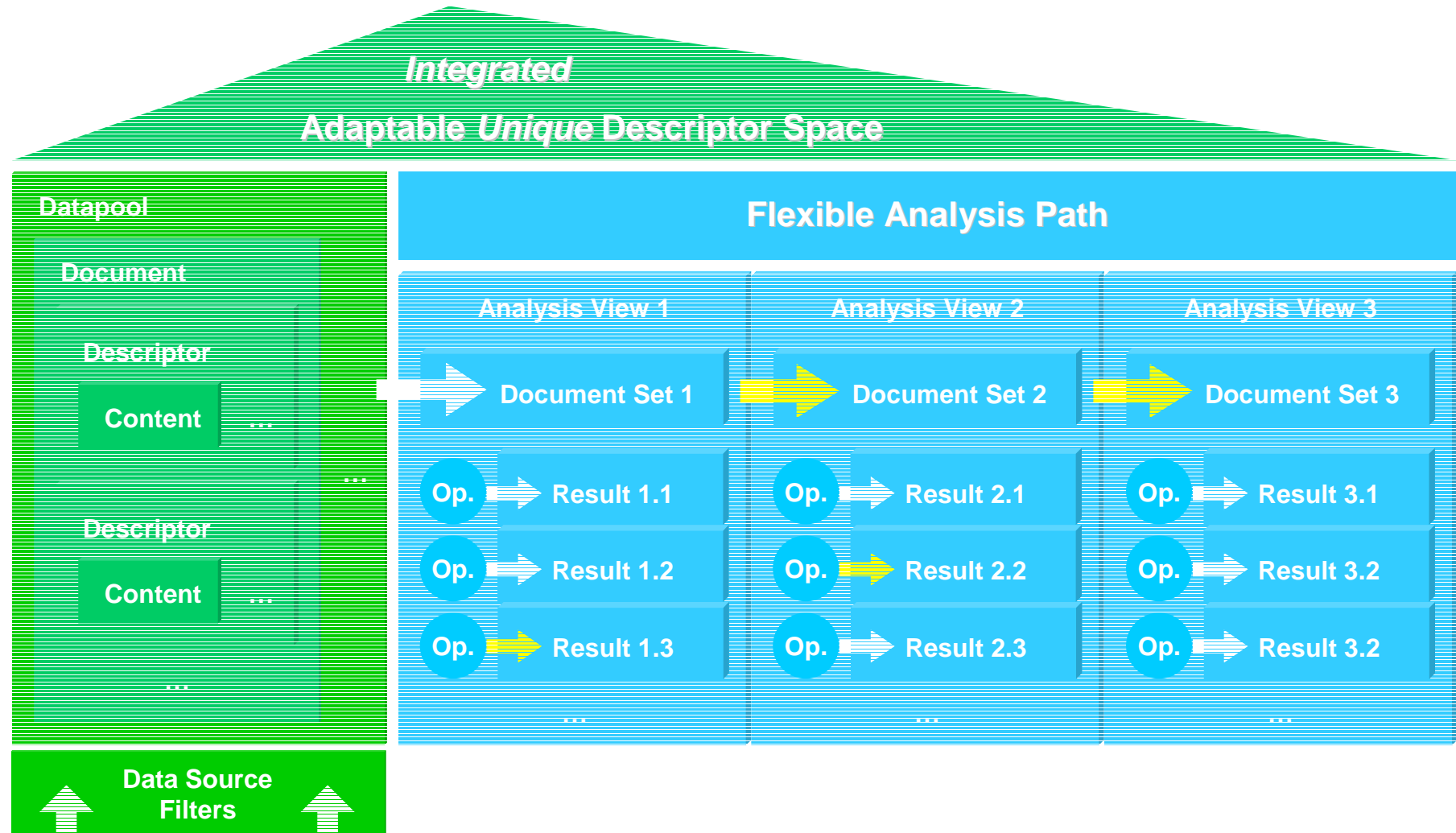
Ideal user specific IT system



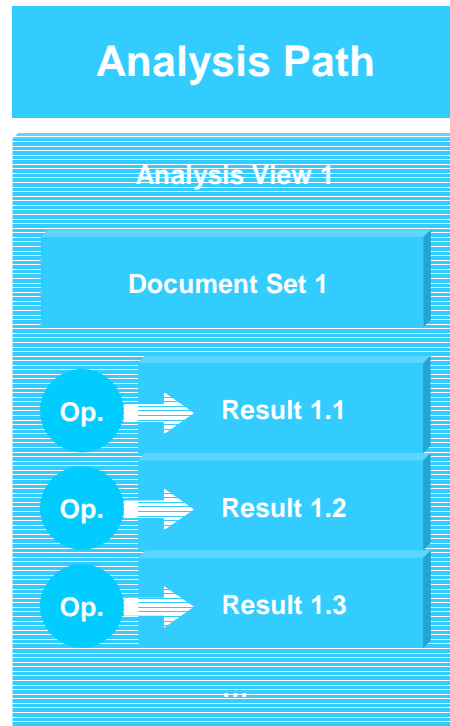
too expensive



Solution Schema



Solution Schema



Op.

Descriptor/content-based analysis operation, e.g.

- **Textual queries**
- **Frequency distributions**
- **Similarity ranking and classification**
- Chemical (sub)structure/similarity search
- Biological sequence alignment
- Rule-based descriptor generation
- Profile scoring ...

Flexible analysis operation step = **Every** useful operation on one ore more descriptors

Wistract[®] – Platform for Scientific Information

Word Classification

Word	Count
Class 1	100
Class 2	80
Class 3	60
Class 4	40
Class 5	20
Class 6	10
Class 7	5
Class 8	3
Class 9	2
Class 10	1
Class 11	1
Class 12	1

Studies on constituents from Chamocyparh giffens and antibacterial activity of diterpenes

Shin, Da; Eberhard, Michael; Bost, Tobias; Mitter, Benedikt; Eickens, Matthias; Mierisch, Matthias; Mieschke, Daniela; Exner, Karoline; Nöcker, Sabine

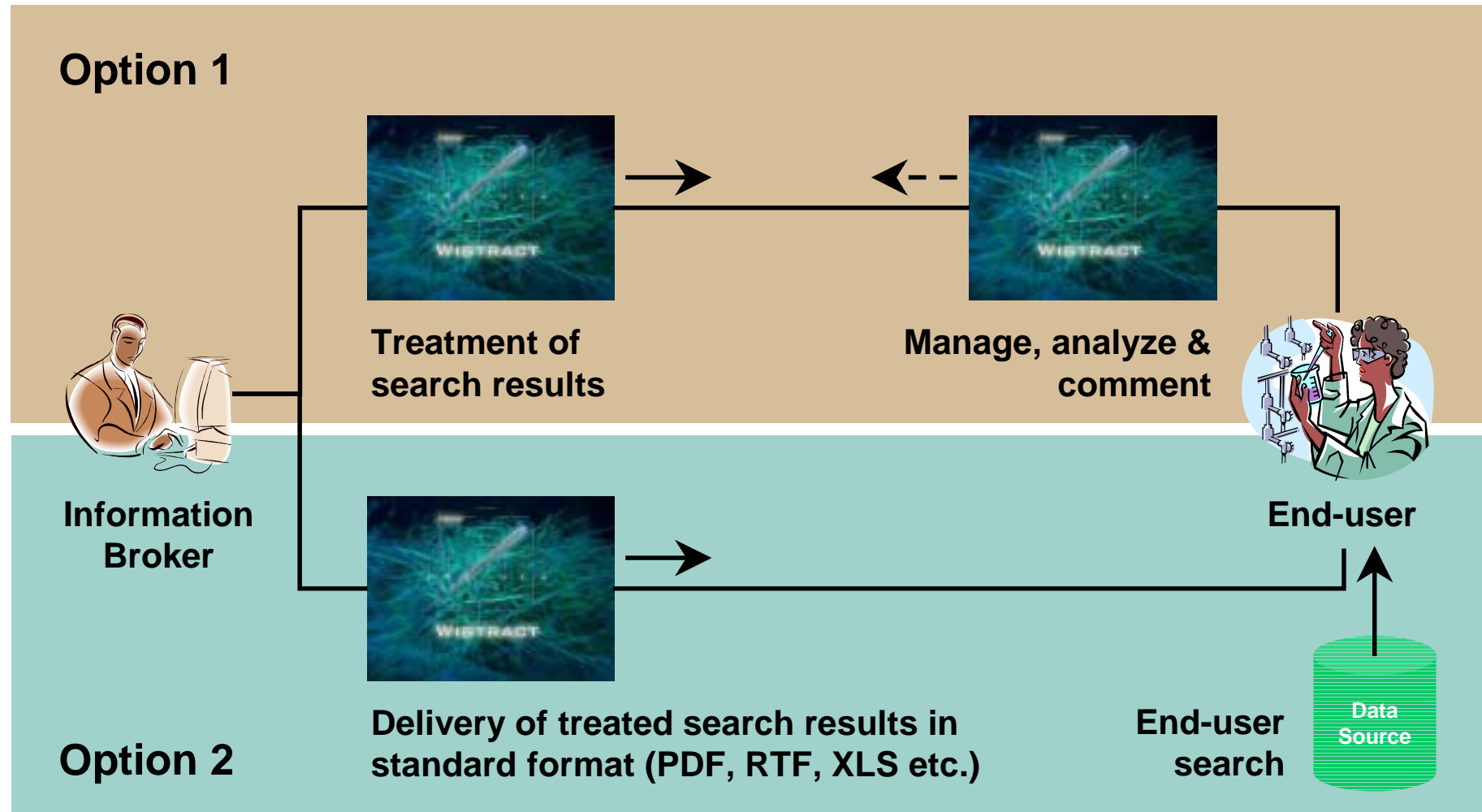
College of Pharmacy and Botany, Bielefeld University, P.O. Box 100131, Post Box, Clara Zetkin and Pharmaceutical School (201), 48119, 32113

Language: English
Publication Year: 2011
DOI: 10.1002/ps.2001

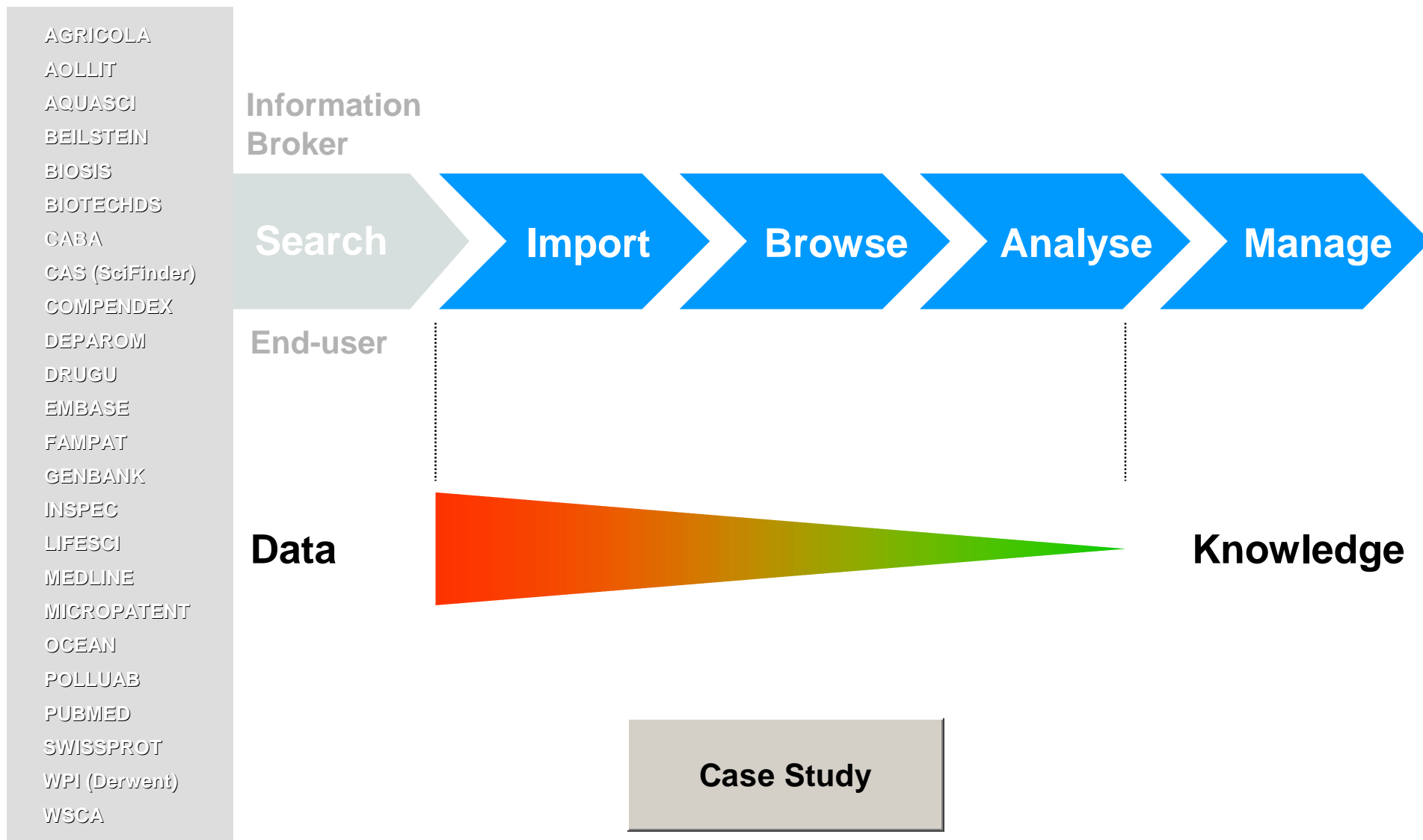
In the course of our investigations that explore constituents from medicinal plants, a diterpenoid (1) and an abietane-type (2) were isolated along with several diterpenes from Chamocyparh giffens. Structures of the new compounds were identified as 1,7-diterpenes (1) and 2,6-diterpenes (2) by means of spectral methods including two-dimensional 13C-NMR spectra. Some of these abietane-type compounds isolated from the plant showed antibacterial activity against the gram-positive bacteria Staphylococcus aureus and Bacillus subtilis.

Substance Information
EINECS: 201-107-7
CAS: 1400-04-7
Molecular Weight: 284.44

Wistract[®] – Use Cases



Wistract[®] – Case Study



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www.wistract.com

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