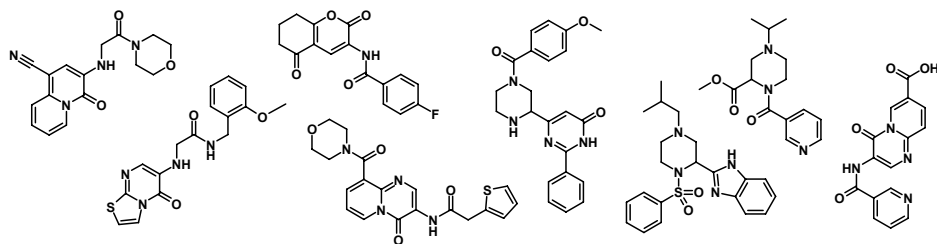


## Example Structures



## Sales and Distributors



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1. Lipinski, C. A.; Lombardo, F.; Dominy, B. W.; Feeney, P. J. *Adv. Drug Delivery Rev.* **1997**, 23, 3.
2. Teague, S.; Davis, A. M.; Leeson, P. D.; Oprea, T. *Angew. Chem. Int. Ed.* **1999**, 38, 3743. Hann, M.M.; Leach, A. R.; Harper, G. *J. Chem. Inf. Comput. Sci.* **2001**, 41, 856.

June 2007

## Introduction

Chemivate Limited is a family owned UK based company formed in June 2004. The company is located in Nottinghamshire, England. Chemivate was founded by Dr Simon Broughton who is the company's Managing Director. Chemivate manufactures and supplies screening compounds to universities, pharmaceutical and biotechnology companies.

Chemivate has considerable expertise in synthetic organic chemistry, parallel synthesis and medicinal chemis-

try. Chemivate owns a variety of synthetic organic chemistry equipment, Radley's parallel synthesis equipment and Merck Hitachi HPLC equipment.

Chemivate is a customer focussed organisation and will be delighted to assist in the further development of compounds and libraries through resynthesis, multigram scale-up, intermediate synthesis, development of virtual libraries and synthesis of new compound libraries on an exclusive or non-exclusive basis.

## Screening Compound Library

Chemivate is continuing to develop a diverse library of novel screening compounds. The compounds are available on a non-exclusive basis either as a complete collection or on a cherry picking basis. Chemivate's screening compounds are drug-like and satisfy the Lipinski Rule of Five.<sup>1</sup> Currently the library consists of 1114 synthetic organic compounds. ISIS database and SDF files are available on CD-ROM or on the website for download.

Chemivate's screening compound collection was manually synthesized using solution phase chemistry and based on the following criteria:

- All compounds must be drug-like and fit the Lipinski criteria to give good ADME profiles<sup>1</sup>
- To include a high proportion of lead-like structures<sup>2</sup>
- To produce only novel compounds
- To maximise diversity
- To include features that will facilitate the binding to GPCR's
- To provide some scope for the identification of early SAR
- Contain no reactive or other unwanted functional groups, such as, alkyl halides, epoxides, acyl halides, etc.

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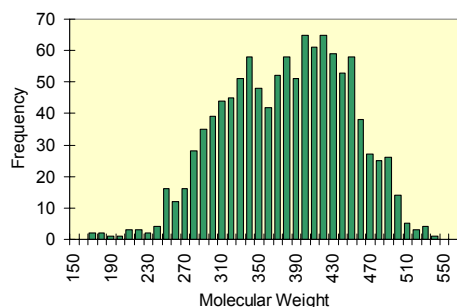
Web: [www.chemivate.com](http://www.chemivate.com)

## Drug-Likeness

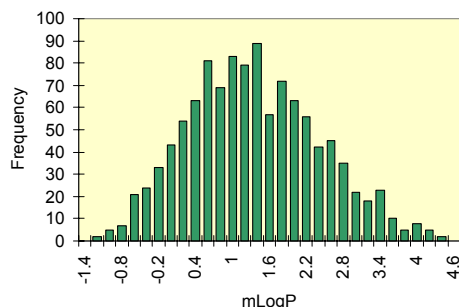
All of the Chemivate screening compound collection is drug-like according to Lipinski's Rule of Five.<sup>1</sup> The table (right) summarises this based upon the entire collection of 1114 compounds. The following distribution plots characterise the compound collection.

Rule	Freq	%	Ave
Mol. weight < 500	1100	98.7	375
LogP < 5	1114	100	1.25
H-Bond (D) ≤ 5	1114	100	2
H-Bond (A) ≤ 10	1111	99.7	7
Lipinski compliance	1114	100	

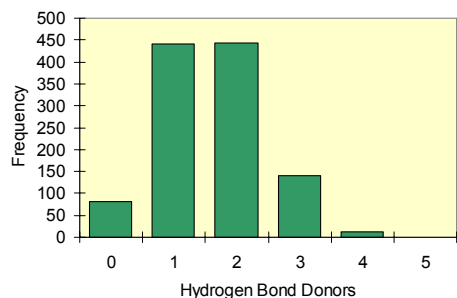
Distribution of Molecular Weight



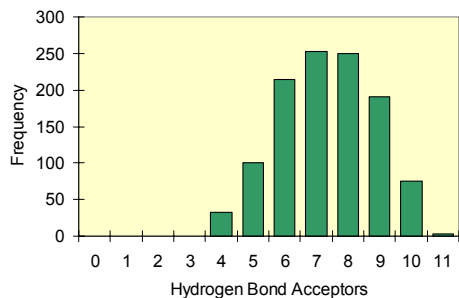
Distribution of mLogP



Distribution of H-Bond Donors



H-Bond Acceptors



## Lead-Likeness

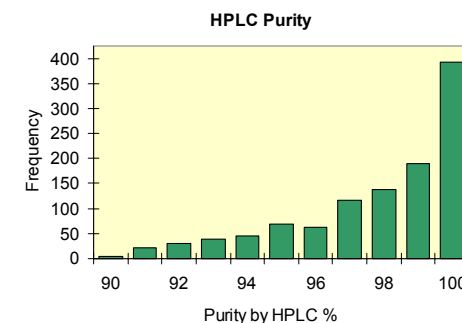
The Chemivate screening compound collection includes a high proportion of lead-like compounds.<sup>2</sup> These compounds satisfy the Lipinski requirements for drug-likeness but have lower molecular weight (< 350) and lower lipophilicity (< 3). They are included in the main screening compounds database. There

are 406 lead-like compounds available.

Lead-like compounds offer a good starting point in lead optimisation because it is generally easier to increase molecular weight and logP to achieve increased potency and demonstrate structure activity relationships

## Purity and Quality Control

Chemivate aims to produce screening compounds with a minimum purity of 90% by HPLC. Most compounds have a purity of 98% or greater. A sample of compounds was also verified by <sup>1</sup>H NMR. HPLC and NMR spectra along with method details are available on CD-ROM with the dispatch of screening compounds. The distribution plot (right) shows the purity of the Chemivate screening compound collection.



## Supply Formats and Delivery

Chemivate will endeavor to accommodate customers' supply format requirements. We will supply in vials or well-plates available from major suppliers such as VWR and Fisher Scientific. Alternatively, we can use a customer's own labeled or bar-coded vials.

We will endeavor to deliver as quickly as possible from receipt of your purchase order. Please allow up to 28 days for delivery. An accurate delivery schedule will be given upon quotation.

## Pricing and Availability

The majority of the Chemivate screening compound collection is in stock with 100+ mg available. Regular database updates will be issued to customers and out of stock compounds will be deleted. However, some of the most difficult compounds to make are only

available in small quantities and may go out of stock quickly. Chemivate's general pricing structure is given in the table (below left). The prices do not include shipping and taxes.

Qty	Price of Compounds (GBP)				
	2mg	5mg	10mg	25mg	50mg
1	18	20	25	40	80
10	16	18	20	35	70
50	14	16	18	30	60
100+	12	14	15	26	52

Stock Levels

