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TECHNICAL DATA SHEET Second edition: January 2017
Chemical library of new nucleoside analogues for tests of antiviral activity

Product code
DIS-BIO-VIR

Product type
Chemical library of new nucleoside analogues with potential antiviral activity.

Description
The nucleosides are involved in many biochemical processes of the nature, mainly in the storage and transference of the genetic information. Nucleoside analogues (NA) are structural related molecules with natural nucleosides whose mechanism of action is developed through their incorporation and change of DNA or RNA chains, the interference with different enzymes involved in the nucleic acid synthesis or through modifications in the metabolism of the natural nucleosides. For this reason, they are cytotoxic agents with a special importance as anticancer and antiviral agents.

Most of the antiviral granted (like Sofosbuvir, Zidovudina (AZT), didanosine or 2',3'-didesoxiinosine (ddI) that are used to treat hepatitis, Acquired Immune Deficiency Syndrome (AIDS) produced by HIV virus and other viral infections, like herpes and the flu) are natural nucleoside analogues, that act interfering the viral nucleic acid synthesis, due to its similarity with the pathogenic ones.

To get these products through the conventional chemical synthesis methods is complex and lead to low yields.

Through the HTB platform, IUCT owns a powerful technological tool to construct libraries of new nucleoside analogues through the synergy of coupling biotechnologic and organic synthesis tools.
Our compounds belong to a much wider collection as a result of a diversity study with more than 77,000 molecules. A subgroup containing about 500 molecules is diverse enough and representative of the global collection.

The molecules of the collection exhibit *drug-like* properties, have defined structure and known purity.

Available information:

- Structural characterization (MS)
- Purity (HPLC)
- Complete technical data sheet of every molecule in ChemFinder database: chemical structure, molecular weight, IUPAC name, purity, physical estate, etc.
- Product concentration in the sample.

All the compounds can be delivered:

- Individually,
- As subsets (according to the customer's needs),
- As library or global collection.

Format: the molecules are available as dry powder, neat oils or in solution, for instance, in DMSO (dimethylsulfoxide) solution in 96-well plates to the required concentration (according to the product stock and customer needs).

Moreover, we can prepare focused molecules based on structural requirements of the customer.

We additionally offer the technical support of the *Drug Discovery* platform scientists.

Development phase

The synthetic methodology of this kind of compounds is fully developed through a biotechnological "one-pot" process, in only one step, with low cost commercial nucleosides as starting point, in water as reaction medium and using biocatalysts developed by IUCT.
Compounds available for an immediate delivery: please, inquire.

Compounds of the collection prepared under contract: according to the number of compounds and *building blocks* availability, please inquire the delivery time.

Moreover, we offer our expertise in structure optimization (*hit optimization, lead optimization*) of the selected candidate structures.

Intelectual property status

THERMOSTABLE BIOCATALYST COMBINATION FOR NUCLEOSIDE SYNTHESIS.
US 8759034 (B2)
EP 2516637 (B1)
JP 5819315 (B2)

DEAMINATION OF ORGANOPHOSPHORUS-NUCLEOSIDES
WO2016146808 (A1)

Uses

- Identification of new products (Drug discovery) in companies interested in new antiviral drugs.
- *Screening* of new pharmacological activities.

Advantages

- Structural novelty for the majority of the molecules in the collection.
- Compounds fulfilling drug requirements (drug-like structures).
- Possibility of identifying *hits* o *lead compounds* in the R&D of new antiviral drugs.
- Possibility of identifying *hits* in the R&D of new pharmacological activities.
- Delivery and scale-up: it is possible to re-synthesize or to scale the products up to 1-2 g.

Publications

(1) Parker,W. *Chem. Rev.* **2009**, *109*, 2880.
(2) Gates, K. S. *Chem. Res. Toxicol.* **2010**, 23, 99.
(3) Galmarini, C. M.; Mackey, J. R.; Dumontet, C. *The Lancet Oncology*. **2002**, 3, 415.
(4) Mathé, C.; Gosselin, G. *Antiviral Res.* **2006**, 71, 276.