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### Data Article

# A dataset of small molecules triggering transcriptional and translational cellular responses

Mathilde Koch<sup>a</sup>, Amir Pandi<sup>a</sup>, Baudoin Delépine<sup>a,b,c</sup>,  
Jean-Loup Faulon<sup>a,b,c,d,\*</sup>

<sup>a</sup> Micalis Institute, INRA, AgroParisTech, Université Paris-Saclay, 78350 Jouy-en-Josas, France

<sup>b</sup> UMR 8030 Genomics Metabolics, Systems and Synthetic Biology Lab, CEA, CNRS, University of Evry-val-d'Essonne, University Paris-Saclay, Évry, France

<sup>c</sup> CEA, DRF, IG, Genoscope, Évry 91000, France

<sup>d</sup> SYNBIOCHEM Centre, Manchester Institute of Biotechnology, University of Manchester, 131 Princess Street, Manchester M1 7DN, UK

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### ABSTRACT

The aim of this dataset is to identify and collect compounds that are known for being detectable by a living cell, through the action of a genetically encoded biosensor and is centred on bacterial transcription factors. Such a dataset should open the possibility to consider a wide range of applications in synthetic biology. The reader will find in this dataset the name of the compounds, their InChI (molecular structure), the publication where the detection was reported, the organism in which this was detected or engineered, the type of detection and experiment that was performed as well as the name of the biosensor. A comment field is also provided that explains why the compound was included in the dataset, based on quotes from the reference publication or the database it was extracted from. Manual curation of *ACS Synthetic Biology* abstracts (Volumes 1 to 6 and Volume 7 issue 1) was performed as well as extraction from the following databases: Bionemo v6.0 (Carbajosa et al., 2009) [1], RegTransbase r20120406 (Cipriano et al., 2013) [2], RegulonDB v9.0 (Gama-Castro et al.,

\* Corresponding author at: Micalis Institute, INRA, AgroParisTech, Université Paris-Saclay, 78350 Jouy-en-Josas, France.  
E-mail address: [jean-loup.faulon@inra.fr](mailto:jean-loup.faulon@inra.fr) (J.-L. Faulon).

2016) [3], RegPrecise v4.0 (Novichkov et al., 2013) [4] and Sigmol v20180122 (Rajput et al., 2016) [5].

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## Specifications Table

Subject area	<i>Biology</i>
More specific subject area	<i>Synthetic biology</i>
Type of data	<i>Table</i>
How data was acquired	<i>Database extraction from Bionemo v6.0, RegTransbase r20120406, RegulonDB v9.0, RegPrecise v4.0 and Sigmol v20180122 as well as manual curation ACS Synthetic Biology abstracts (Volumes 1 to 6 and Volume 7 issue 1)</i>
Data format	<i>Analysed</i>
Experimental factors	<i>Not applicable</i>
Experimental features	<i>Not applicable</i>
Data source location	<a href="https://github.com/brsynth/detectable_metabolites">https://github.com/brsynth/detectable_metabolites</a>
Data accessibility	<i>Data is with this article and on GitHub at <a href="https://github.com/brsynth/detectable_metabolites">https://github.com/brsynth/detectable_metabolites</a></i>

## Value of the data

- This dataset provides a basis for the development of new biosensing circuits for synthetic biology and metabolic engineering applications, e.g. the design of whole-cell biosensor, high-throughput screening experiments, dynamic regulation of metabolic pathways, transcription factor engineering or creation of sensing-enabling pathways.
- This dataset provides a unique source of a broad number of compounds that can be detected and acted upon by a cell, increasing the possibility of orthogonal circuit design from the few usual compounds used in those applications.
- The manually curated section provides information on where the biosensor has been first reported and successfully used, enabling the reader to select trustworthy information for his application of choice.
- Detectable compounds can be searched by both by name and chemical similarity.
- This dataset is an update of [10.6084/m9.figshare.3144715.v1].

## 1. Data

The aim of this dataset is to identify and collect compounds that are known for being detectable by a living cell, through the action of a genetically encoded biosensor and is centred on bacterial transcription factors. The dataset should allow the synthetic biology community to consider a wide range of applications. The reader will find in this dataset the name of the compounds, their InChI (molecular structure), the publication where the detection was reported, the organism in which this was detected or engineered, the type of detection and experiment that was performed as well as the name of the biosensor. A comment field is also provided that explains why the compound was included in the dataset, based on quotes from the reference publication or the database it was extracted from. Manual curation of ACS Synthetic Biology abstracts (Volumes 1 to 6 and Volume 7 issue 1) was

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