

NPND NIAID Screen

DOWNLOAD NIAID SCREEN DATA (2023)

BACKGROUND

The National Cancer Institute's Program for Natural Product Discovery (NPND) prefractionated natural product library is one of the largest publicly available collections of natural product samples for high throughput screening (HTS). In collaboration with the National Institute of Allergy and Infectious Diseases (NIAID), this prefractionated library has been screened against a panel of four microbial pathogens: *S. aureus* ATCC 29213, efflux competent *E. coli* BW25113 (wild-type), *tolC* efflux deficient *E. coli* JW5503-1, and *C. albicans* ATCC 90028. The results of the HTS are made publicly available for download below.

Screening was carried out in a 384-well plate format at a single point concentration of 10 µg/mL with 2 replicates per well, and results of the HTS on 326,656 NPND fractions is available for [download](#). Furthermore, confirmation of single-point hits was done in eight-point dose-response at a concentration of 0.08 to 10 µg/mL with the results also available for [download](#). Summary of the screening methodology, analysis of the results of the HTS, as well as a small proof-of-concept study that demonstrates the identification of new natural products with selective anti-bacterial and anti-fungal activities can be found in Martínez-Fructuoso *et al.*¹ For further information, please contact the Natural Products Branch at NCINatProdRep@mail.nih.gov.

This project has been funded in whole or in part with Federal funds from the Division of Microbiology and Infectious Diseases, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Department of Health and Human Services, under Contract No. 75N93019D00011 / 75N93019F00210 as well as the National Cancer Institute, National Institutes of Health, under contract HHSN261200800001E and by the National Cancer Institute's Cancer MoonshotSM NCI Program for Natural Products Discovery – Cure (ZIA BC 011854).

1. Martínez-Fructuoso, L., Arends, S. J. R., Freire, V. F., Evans, J. R., DeVries, S., Peyser, B. D., Akee, R. K., Thornburg, C. C., Kumar, R., Ensel, S., Morgan, G. M., McConachie, G. D., Veeder, N., Duncan, L. R., Grkovic, T., & O'Keefe, B. R. (2023). Screen for New Antimicrobial Natural Products from the NCI Program for Natural Product Discovery Prefractionated Extract Library. *ACS Infectious Diseases*. <https://pubs.acs.org/doi/10.1021/acsinfectdis.3c00067>

FILES FOR DOWNLOAD

	DATA FILE SIZE	DOWNLOAD SIZE	LINK
SINGLE-DOSE	25.6 MB	7.3 MB	SINGLE-DOSE.zip
DOSE RESPONSE	970 KB	238 KB	IC50.zip

GENERAL COMMENTS REGARDING THE DOWNLOADABLE FILES

- Downloads are zip-archived comma-separated values (csv) files, containing results from all screened natural product extracts and fractions.

FILE COLUMN HEADERS

10 µg/mL SINGLE-DOSE INHIBITION DATA

1. Sample ID: Sample ID for crude and prefractionated extracts. Digit following the underscore represents polarity of the prefractionation, from 1 (most polar) to 7 (least polar), or 0 for unfractionated crude extract. Initial letter represents sample type: C = marine animal, M = fractionated marine animal, F = microorganism, H = fractionated microorganism, J = marine plant, K = fractionated marine plant, N = non-marine plant, L = fractionated non-marine plant.
2. Parent Extract: Crude extract parent identifier for each prefractionated extract. Initial letter represents sample source (as above).
3. NIH Plate: Plate ID from NCI NPND
4. Well: well identifier within each 384-well plate
5. JMI Plate: Plate number for JMI screening
6. *C. albicans* Replicate 1: percent inhibition values for first replicate of tests for *C. albicans*
7. *C. albicans* Replicate 2: percent inhibition values for second replicate of tests for *C. albicans*
8. *C. albicans* Replicate 3: percent inhibition values for third replicate of tests of some plates for *C. albicans*
9. *C. albicans* Replicate 4: percent inhibition values for fourth replicate of tests of some plates for *C. albicans*
10. *E. coli* (wild-type) Replicate 1: percent inhibition values for first replicate of tests for *E. coli*
11. *E. coli* (wild-type) Replicate 2: percent inhibition values for second replicate of tests for *E. coli*
12. *E. coli* (wild-type) Replicate 3: percent inhibition values for third replicate of tests of some plates for *E. coli*
13. *E. coli* (wild-type) Replicate 4: percent inhibition values for fourth replicate of tests of some plates for *E. coli*
14. *E. coli* (tolC) Replicate 1: percent inhibition values for first replicate of tests for *E. coli* tolC mutant

15. *E. coli* (tolC) Replicate 2: percent inhibition values for second replicate of tests for *E. coli* tolC mutant
16. *E. coli* (tolC) Replicate 3: percent inhibition values for third replicate of tests of some plates for *E. coli* tolC mutant
17. *E. coli* (tolC) Replicate 4: percent inhibition values for fourth replicate of tests of some plates for *E. coli* tolC mutant
18. *S. aureus* Replicate 1: percent inhibition values for first replicate of tests for *S. aureus*
19. *S. aureus* Replicate 2: percent inhibition values for second replicate of tests for *S. aureus*
20. *S. aureus* Replicate 3: percent inhibition values for third replicate of tests of some plates for *S. aureus*

CONCENTRATION/RESPONSE IC₅₀ DATA

1. Sample ID: Sample ID for crude and prefractionated extracts. Digit following the underscore represents polarity of the prefractionation, from 1 (most polar) to 7 (least polar), or 0 for unfractionated crude extract. Initial letter represents sample type: C = marine animal, M = fractionated marine animal, F = microorganism, H = fractionated microorganism, J = marine plant, K = fractionated marine plant, N = non-marine plant, L = fractionated non-marine plant.
2. Parent Extract: Crude extract parent identifier for each prefractionated extract. Initial letter represents sample source (as above).
3. NIH Plate: Plate ID from NCI NPND
4. Well: well identifier within each 384-well plate
5. JMI Plate: Plate number for JMI screening
6. IC50 *C. albicans* Replicate 1: IC₅₀ values for the first replicate of tests for *C. albicans*
7. R2 *C. albicans* Replicate 1: R² values for the first replicate of tests indicating a goodness-of-fit value of the nonlinear Hill plot for *C. albicans*. Missing R² values indicate that the IC₅₀ value is greater than or less than the indicated number.
8. IC50 *C. albicans* Replicate 2: IC₅₀ values for the second replicate of tests for *C. albicans*
9. R2 *C. albicans* Replicate 2: R² values for the second replicate of tests for *C. albicans*.
10. IC50 *C. albicans* Replicate 3: IC₅₀ values for the third replicate of tests for *C. albicans*
11. R2 *C. albicans* Replicate 3: R² values for the third replicate of tests for *C. albicans*.
12. IC50 *E. coli* wild type Replicate 1: IC₅₀ values for the first replicate of tests for *E. coli* (wild type).
13. R2 *E. coli* wild type Replicate 1: R² values for the first replicate of tests for *E. coli* (wild type).
14. IC50 *E. coli* wild type Replicate 2: IC₅₀ values for the second replicate of tests for *E. coli* (wild type).
15. R2 *E. coli* wild type Replicate 2: R² values for the second replicate of tests for *E. coli* (wild type).
16. IC50 *E. coli* tolC Replicate 1: IC₅₀ values for the first replicate of tests for *E. coli* (tolC mutant).
17. R2 *E. coli* tolC Replicate 1: R² values for the first replicate of tests for *E. coli* (tolC mutant).
18. IC50 *E. coli* tolC Replicate 2: IC₅₀ values for the second replicate of tests for *E. coli* (tolC mutant).
19. R2 *E. coli* tolC Replicate 2: R² values for the second replicate of tests for *E. coli* (tolC mutant).
20. IC50 *S. aureus* Replicate 1: IC₅₀ values for the first replicate of tests for *S. aureus*.
21. R2 *S. aureus* Replicate 1: R² values for the first replicate of tests for *S. aureus*.
22. IC50 *S. aureus* Replicate 2: IC₅₀ values for the second replicate of tests for *S. aureus*.
23. R2 *S. aureus* Replicate 2: R² values for the second replicate of tests for *S. aureus*.