Data README Documentation for

Decoding Optical Responses of Contact-Printed Droplets of Liquid-Crystals using Machine Learning for Enabling Surfactant Reporting with Enhanced Sensitivity and Selectivity

Fengrui Wang, [1,¶] Shiyi Qin, [2,¶] Reid C. Van Lehn,[2] Victor M. Zavala,[2,3,*] and David M. Lynn[1,2,*]

[1]*Dept. of Chemistry, Univ. of Wisconsin–Madison, 1101 University Ave., Madison, WI 53706;*
[2]*Dept. of Chemical and Biological Engineering, Univ. of Wisconsin–Madison, 1415 Engineering Dr., Madison, WI 53706;*
[3]*Mathematics and Computer Science Division, Argonne National Laboratory, 9700 S Cass Ave, Lemont, IL, 60439, USA;*
[¶]*Fengrui Wang and Shiyi Qin contributed equally to this work.*
[*]*Email: (D.M.L.) dlynn@engr.wisc.edu, (V.M.Z.) zavalatejeda@wisc.edu*

The zip file contains the images used for training and validating the models reported in the manuscript. The file names are formatted as <trial>_<step>_<stimuli>_<sensor>_<spot>_<light>_<crop>.jpg. A detailed description of each naming segment is provided below.

<trial>

"c100": trials where the liquid-crystal droplets are treated with water (control)

"t100": trials where the liquid-crystal droplets are treated with surfactants

<step>

"step00" is used for control trials where the concentration of stimuli is zero. "step01" through up to "step07" are assigned in the increasing trend that reflects the increasing concentration for a specific stimuli solution used to treat the liquid-crystal droplet.

< stimuli >

Stimuli used to treat the liquid-crystal droplets, including control (water), SDS (sodium dodecyl sulfate), DTAB (dodecyltrimethylammonium bromide), SDS+DTAB, and rhamnolipid.

"step00_control": water treated

"step01_dtab": 0.25 μM DTAB treated

"step02_dtab": 0.25 mM DTAB treated

"step01_sds": 0.05 nM SDS treated

"step02_sds": 5 nM SDS treated

"step03_sds": 25 μM SDS treated

"step04_sds": 01 mM SDS treated

"step05_sds": 0.25 mM SDS treated

"step06_sds": 0.5 mM SDS treated

"step07_sds": 1 mM SDS treated

“step01_sdsdtab”: 6 μM SDS+DTAB treated

“step01_ rhamnolipid”: 5 μg/mL rhamnolipid treated

“step02_ rhamnolipid”: 250 μg/mL rhamnolipid treated

<sensor>

“lc”: liquid-crystal

<spot>

Spot number arbitrarily assigned to different liquid-crystal droplets and the corresponding images taken for each stimuli concentration setting.

<light>

“cp”: cross-polarized

<crop>

“cropL”: the liquid-crystal droplet cropped from the original micrograph by removing the dark peripheral area that does not contain any information