

Data README Documentation for
**Decoding Optical Responses of Contact-Printed Arrays of Thermotropic Liquid Crystals
Using Machine Learning: Detection and Reporting of Aqueous Amphiphiles with
Enhanced Sensitivity and Selectivity**

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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 μ M 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 μ M 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 μ M SDS+DTAB treated

“step01_rhamnolipid”: 5 μ g/mL rhamnolipid treated

“step02_rhamnolipid”: 250 μ g/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