Supporting Information for

Evaluating Impacts of Bambusuril Pocket Size and Sterics on Anion Binding Trends using ChemFETs

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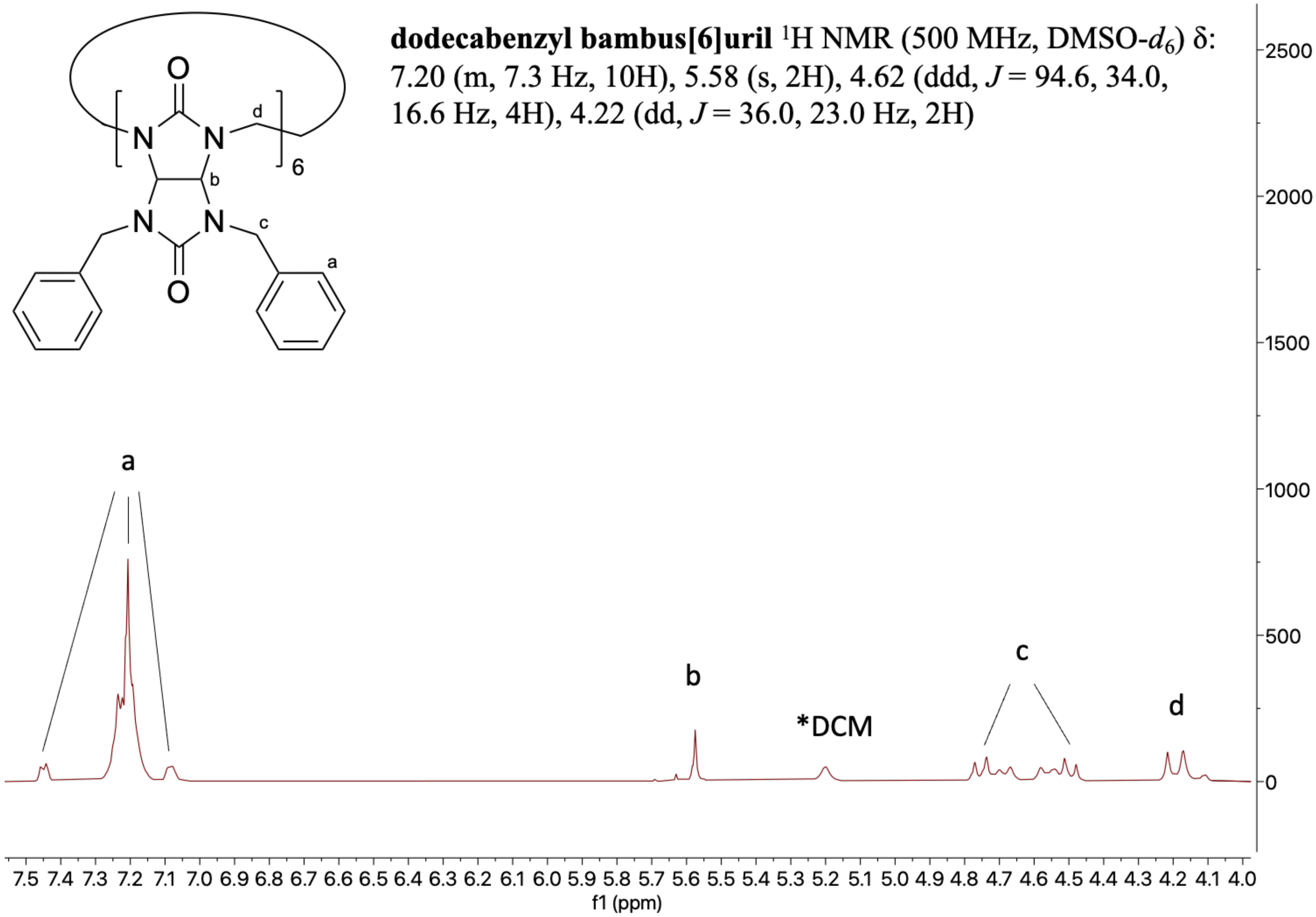

Dodecabenzyl bambus[6]uril ^{1}H NMR. Dodecabenzyl bambus[6]uril was synthesized following literature,[1] with NMR spectra used for confirmation of synthesis product.

Dodeca-n-butyl Bambus[6]uril Characterization

All characterization of dodeca-n-butyl bambus[6]uril was reported in the electronic supplementary information (ESI) of a previous publication: DOI 10.1039/D3SC03616B

ChemFET Sensor and Construction

Silicon nitride-gated field effect transistors (FETs) were purchased from Winsense (http://www.winsense.co.th, WIPS-C) and cleaned with ethanol and soaked in H_2O_2 for 10 minutes prior to functionalization. Polyvinyl chloride (PVC), 2-nitrophenyl octyl ether (NPOE), and Tetraoctylammonium Nitrate (TOAN) were obtained from Fisher Scientific and TCI Chemicals. All receptor-containing sensors contained 65 weight percent PVC, 32 weight percent NPOE, 2 weight percent TOAN, and 1 weight percent bambusuril receptor. Control sensors membrane composition was 66 weight percent PVC, 32 weight percent NPOE, and 2 weight percent TOAN. Chemically selective membranes were deposited onto the FET surface by manual drop-casting. Four aliquots of 1.6 µL were applied at 30-minute increments before being placed in an oven at 60 °C overnight, yielding an approximate film thickness of 50 µm. ChemFETs in this report were made in-house following previously-reported procedures.[2,3]

ChemFET Reference Electrode (RE) Construction

Ag/AgCl REs were used in all potentiometric experiments. All REs in this report were made in-house following previously-reported procedures.[2,3]

ChemFET Sensor and Reference Electrode (RE) Operation

The ChemFETs were driven by a benchtop power source. In operation, the drain voltage (V_{ds}) is held at 617.5 mV and the drain current (I_{ds}) at 100 mA. The external RE is held at ground, and the voltage between ground and the source (V_{gs}) terminal changes to maintain the values of V_{ds} and I_{ds}. V_{gs} is recorded as the measurement signal. NI-DAQ 6009 at a rate of 1 kHz was used for data acquisition paired with a custom Labview program for collection. All potentiometric tests were recorded for 300 seconds, and comprised of four identically-constructed ChemFETs. The four ChemFET sensors were run through a series of 0.100 M, 50.0 mM, 10.0 mM, 5.00 mM, 1.00 mM, 500 µM, 100 µM, 50.0 µM, 10.0 µM, 5.00 µM, 1.00 µM, and 0.500 µM analyte, each with constant 50.0 mM PIPES.

Each data point consisted of four identically-constructed ChemFET sensors run through 12 solutions, in triplicate, of alternating order (low to high concentration, then high to low concentration, then low to high concentration).

ChemFET Data Analysis

Detection limits for all analytes were calculated by determining the analyte concentration at which background slope intercepts Nernstian slope when plotting response vs activity. Detection limits were calculated for each sensor, with results averaged. Then detection limits were then calculated for the average readings at each concentration. These were averaged to provide the reported detection limit. The results of these two methods were averaged to provide the reported detection limit. This data is summarized in the attached spreadsheet.

All sensor data analysis was accomplished following previously-reported procedures.[2–4]

References:

1 V. Havel, J. Svec, M. Wimmerova, M. Dusek, M. Pojarova and V. Sindelar, *Org. Lett.*, 2011, **13**, 4000–4003.

2 T. J. Sherbow, G. M. Kuhl, G. A. Lindquist, J. D. Levine, M. D. Pluth, D. W. Johnson and S. A. Fontenot, *Sensing and Bio-Sensing Research*, 2021, **31**, 100394.

3 G. M. Kuhl, D. H. Banning, H. A. Fargher, W. A. Davis, M. M. Howell, L. Zakharov, M. D. Pluth and D. W. Johnson, *Chem. Sci.*, 2023, **14**, 10273–10279.

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