

Supporting Information

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Efficient Acid-Catalyzed $^{18}\text{F}/^{19}\text{F}$ Fluoride Exchange of BODIPY Dyes

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cmdc_201300506_sm_miscellaneous_information.pdf

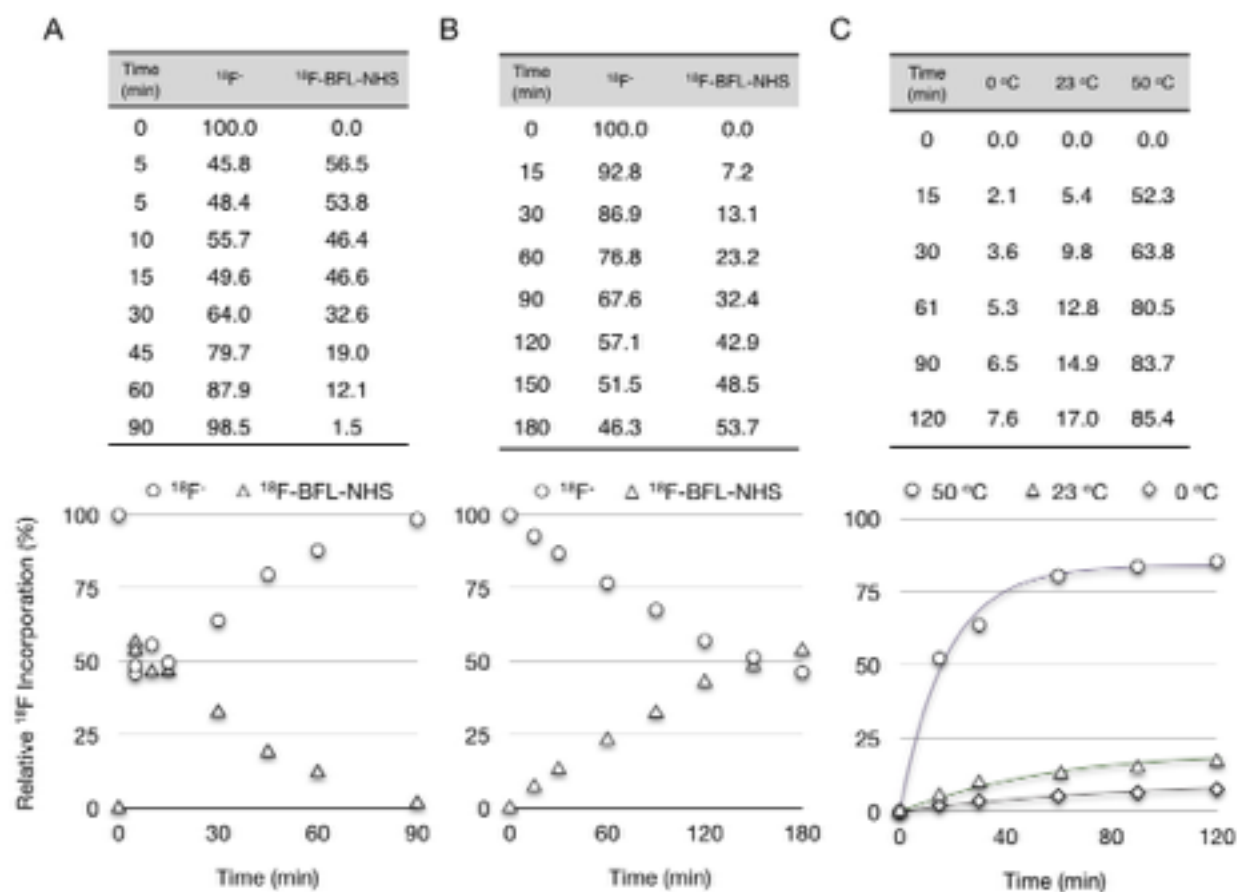
A

| Time (min) | 7 mM | 10 mM | 14 mM | 40 mM |
|------------|------|-------|-------|-------|
| 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 | | 10.6 | | 52.3 |
| 30 | 0.0 | 16.3 | 45.4 | 63.8 |
| 60 | 0.0 | 27.9 | 58.1 | 80.5 |
| 90 | 1.1 | 35.9 | 62.8 | 83.7 |
| 120 | 85.4 | 41.1 | 66.1 | 85.4 |

B

| Time (min) | 0.5 mM | 1.0 mM | 2.0 mM |
|------------|--------|--------|--------|
| 0 | 0.0 | 0.0 | 0.0 |
| 15 | 18.4 | 31.3 | 52.3 |
| 30 | 26.9 | 43.7 | 63.8 |
| 60 | 36.9 | 55.0 | 80.5 |
| 90 | 43.4 | 64.0 | 83.7 |
| 120 | 47.3 | 66.6 | 85.4 |

Supporting information S1. Concentration-versus-time data for the curves in Figure 2 BFL-NHS + $^{18}\text{F}/\text{Tf}_2\text{O}/t\text{BuOH}$. A) Variation of $[\text{Tf}_2\text{O}/t\text{BuOH}]$. B) Variation of $[\text{BFL-NHS}]$.



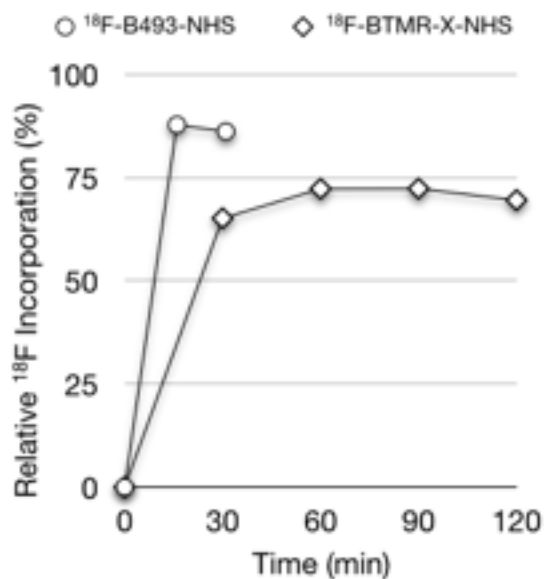
Supporting information S2. A) H^+ induced exchange for BFL-NHS (125 nmol) using TfOH (2.5 μmol) at 50 °C. B) H^+ induced exchange using BFL-NHS (125 nmol) with MsOH (2.5 μmol) at 50 °C. C) Observed temperature dependence for the H^+ induced $^{18}\text{F}/^{19}\text{F}$ exchange for BFL-NHS (125 nmol) and $\text{Tf}_2\text{O}/t\text{BuOH}$ (2.5 μmol) at 0, 23, and 50 °C.

A

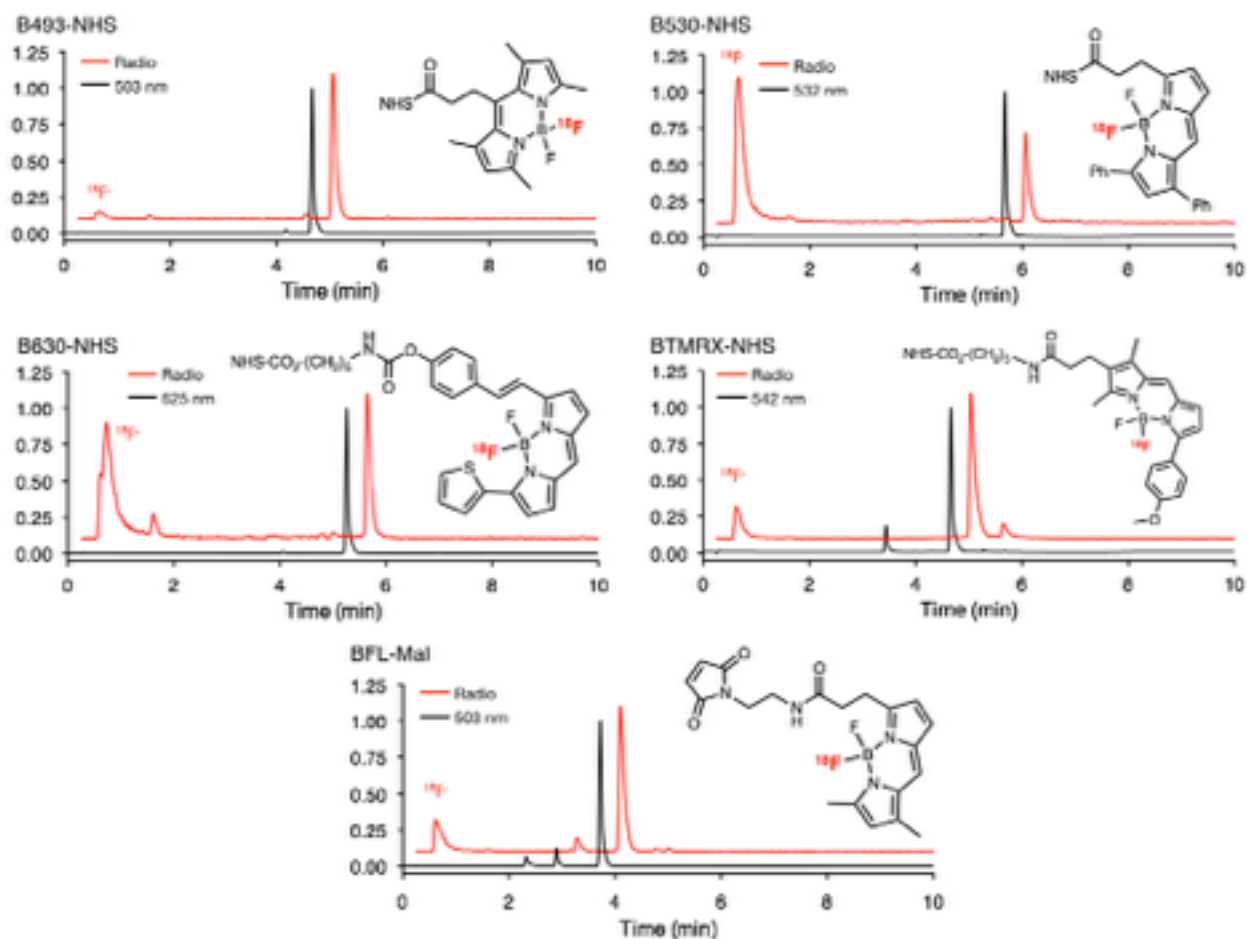
| Time (min) | ¹⁸ F-B493-NHS | ¹⁸ F-BTMR-X-NHS |
|------------|--------------------------|----------------------------|
| 0 | 0.0 | 0.0 |
| 16 | 87.8 | |
| 31 | 86.2 | 65.1 |
| 60 | | 72.3 |
| 90 | | 72.3 |
| 120 | | 69.5 |

B

| Time (min) | BFL-NHS | BFL-Mal | B630-X-NHS | B530-NHS |
|------------|---------|---------|------------|----------|
| 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 | 52.3 | 46.1 | | 10.2 |
| 30 | 63.8 | 60.5 | 24.3 | 16.2 |
| 60 | 80.5 | 74.4 | 35.0 | 25.6 |
| 90 | 83.7 | 74.8 | 46.1 | 34.8 |
| 120 | 85.4 | 72.7 | 49.0 | 43.2 |



Supplementary information S3. Concentration-versus-time data for H⁺ induced ¹⁸F/¹⁹F exchange Bodipys (125 nmol) and Tf₂O/tBuOH (2.5 μmol). A) B493-NHS (**1**) and BTMR-X-NHS (**4**). B) BFL-NHS (**2**), BFL-Mal (**6**), B630-X-NHS (**5**) and B530-NHS (**3**).



Supplementary information S4. Representative HPLC chromatograms (Red: radio; Black: UV) for B493-NHS (**1**) at 30 min reaction time, B530-NHS(**3**) at 60 min, B630-X-NHS at 60 min(**5**) at 60 min, BTMR-X-NHS (**4**) at 60 min, and BFL-Mal (**6**) at 60 min.