

## **Supporting information for**

### **Design, synthesis, and characterization of new 5-fluorocytosine salts**

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**Table S1.** Crystallographic details for all the  $\text{FCH}^+$  and  $\text{FC.FCH}^+$  complexes.

**Table S2.** Hydrogen bond details for all the  $\text{FCH}^+$  and  $\text{FC.FCH}^+$  complexes.

**Table S1.** Crystallographic details for all the  $\text{FCH}^+$  and  $\text{FC.FCH}^+$  complexes.

|                                                            | <b>FCHBr11</b>                                                  | <b>FCHI11</b>                                    | <b>FCHNO<sub>3</sub>11</b>                                   | <b>FCSAC11</b>                                                  | <b>FCHBr21</b>                                                               | <b>FCHI21</b>                                                                                   | <b>FCHNO<sub>3</sub>21</b>                                                 | <b>FCSAC21<br/>(MeOH)</b>                                                         |
|------------------------------------------------------------|-----------------------------------------------------------------|--------------------------------------------------|--------------------------------------------------------------|-----------------------------------------------------------------|------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------|-----------------------------------------------------------------------------------|
| CCDC deposition number                                     | <b>918782</b>                                                   | <b>918789</b>                                    | <b>918785</b>                                                | <b>918787</b>                                                   | <b>918783</b>                                                                | <b>918784</b>                                                                                   | <b>918786</b>                                                              | <b>918788</b>                                                                     |
| Empirical formula                                          | C <sub>4</sub> H <sub>5</sub> Br <sub>1</sub> FN <sub>3</sub> O | C <sub>4</sub> H <sub>5</sub> FIN <sub>3</sub> O | C <sub>4</sub> H <sub>5</sub> FN <sub>4</sub> O <sub>4</sub> | C <sub>11</sub> H <sub>9</sub> FN <sub>4</sub> O <sub>4</sub> S | C <sub>8</sub> H <sub>8</sub> BrF <sub>2</sub> N <sub>6</sub> O <sub>2</sub> | C <sub>16</sub> H <sub>17</sub> F <sub>4</sub> L <sub>4</sub><br>N <sub>12</sub> O <sub>4</sub> | C <sub>8</sub> H <sub>9</sub> F <sub>2</sub> N <sub>7</sub> O <sub>5</sub> | C <sub>16</sub> H <sub>13</sub> F <sub>2</sub> N <sub>7</sub><br>O <sub>6</sub> S |
| Formula wt.                                                | 210.02                                                          | 257.01                                           | 192.12                                                       | 312.28                                                          | 338.11                                                                       | 1025.02                                                                                         | 321.22                                                                     | 469.39                                                                            |
| Crystal system                                             | Monoclinic                                                      | Monoclinic                                       | Monoclinic                                                   | Monoclinic                                                      | Monoclinic                                                                   | Triclinic                                                                                       | Monoclinic                                                                 | Monoclinic                                                                        |
| Space group                                                | C2/c                                                            | P21/c                                            | P21/c                                                        | P21/c                                                           | C2/c                                                                         | P-1                                                                                             | P21/c                                                                      | P21/m                                                                             |
| <i>a</i> [Å]                                               | 16.008(3)                                                       | 5.7117(4)                                        | 12.139(3)                                                    | 8.698(7)                                                        | 15.802(3)                                                                    | 8.2166(14)                                                                                      | 8.8024(18)                                                                 | 8.660(2)                                                                          |
| <i>b</i> [Å]                                               | 11.369(3)                                                       | 10.0899(6)                                       | 13.047(3)                                                    | 10.591(8)                                                       | 5.1171(10)                                                                   | 9.0539(15)                                                                                      | 7.1508(15)                                                                 | 6.4171(16)                                                                        |
| <i>c</i> [Å]                                               | 9.174(2)                                                        | 13.8383(8)                                       | 9.077(2)                                                     | 14.448(9)                                                       | 15.039(3)                                                                    | 10.3624(18)                                                                                     | 19.294(4)                                                                  | 17.198(4)                                                                         |
| $\alpha$ [deg]                                             | 90                                                              | 90                                               | 90                                                           | 90                                                              | 90                                                                           | 76.559(2)                                                                                       | 90                                                                         | 90                                                                                |
| $\beta$ [deg]                                              | 122.953(4)                                                      | 111.922(2)                                       | 98.557(4)                                                    | 107.98(4)                                                       | 94.53(3)                                                                     | 89.110(3)                                                                                       | 91.578(4)                                                                  | 92.918(3)                                                                         |
| $\gamma$ [deg]                                             | 90                                                              | 90                                               | 90                                                           | 90                                                              | 90                                                                           | 79.707(3)                                                                                       | 90                                                                         | 90                                                                                |
| <i>Z</i>                                                   | 8                                                               | 4                                                | 8                                                            | 4                                                               | 4                                                                            | 1                                                                                               | 4                                                                          | 2                                                                                 |
| Volume [Å <sup>3</sup> ]                                   | 1401.0(5)                                                       | 739.84(8)                                        | 1421.6(6)                                                    | 1266.0(16)                                                      | 1212.3(4)                                                                    | 737.4(2)                                                                                        | 1214.0(4)                                                                  | 954.5(4)                                                                          |
| <i>D</i> <sub>calc</sub> [g/cm <sup>3</sup> ]              | 1.991                                                           | 2.307                                            | 1.795                                                        | 1.638                                                           | 1.853                                                                        | 2.308                                                                                           | 1.758                                                                      | 1.633                                                                             |
| <i>F</i> (000)                                             | 816                                                             | 480                                              | 784                                                          | 640                                                             | 668                                                                          | 477                                                                                             | 656                                                                        | 480                                                                               |
| $\mu$ [mm <sup>-1</sup> ]                                  | 5.820                                                           | 4.283                                            | 0.174                                                        | 0.292                                                           | 3.426                                                                        | 4.297                                                                                           | 0.165                                                                      | 0.243                                                                             |
| 2 $\theta$ <sub>max.</sub>                                 | 2.35 - 25.28                                                    | 2.57 - 27.46                                     | 1.70 to 25.29                                                | 2.43 - 25.36                                                    | 2.59 - 25.30                                                                 | 2.02 - 25.27                                                                                    | 2.11 - 25.27                                                               | 2.35 - 27.68                                                                      |
| Range <i>h</i>                                             | -19<= <i>h</i> <=19                                             | -7<= <i>h</i> <=7                                | -14<= <i>h</i> <=14                                          | -10<= <i>h</i> <=10                                             | -18 ≤ <i>h</i> ≤ 18,                                                         | -9 ≤ <i>h</i> ≤ 9                                                                               | -10<= <i>h</i> <=10                                                        | -11<= <i>h</i> <=11                                                               |
| Range <i>k</i>                                             | -13<= <i>k</i> <=13                                             | -12<= <i>k</i> <=12                              | -15<= <i>k</i> <=15                                          | -12<= <i>k</i> <=11                                             | -6 ≤ <i>k</i> ≤ 6                                                            | -10 ≤ <i>k</i> ≤ 10                                                                             | -8<= <i>k</i> <=8                                                          | -8<= <i>k</i> <=8                                                                 |
| Range <i>l</i>                                             | -10<= <i>l</i> <=11                                             | -17<= <i>l</i> <=17                              | -10<= <i>l</i> <=10                                          | -14<= <i>l</i> <=17                                             | -17 ≤ <i>l</i> ≤ 18                                                          | -12 ≤ <i>l</i> ≤ 12                                                                             | -23<= <i>l</i> <=23                                                        | -22<= <i>l</i> <=22                                                               |
| N-total                                                    | 4962                                                            | 8189                                             | 10156                                                        | 6246                                                            | 5368                                                                         | 7165                                                                                            | 8551                                                                       | 10700                                                                             |
| N-independent                                              | 1270                                                            | 1678                                             | 2576                                                         | 2300                                                            | 1086                                                                         | 2672                                                                                            | 2212                                                                       | 2398                                                                              |
| N-observed                                                 | 911                                                             | 1560                                             | 1627                                                         | 1964                                                            | 1014                                                                         | 2102                                                                                            | 1094                                                                       | 1538                                                                              |
| <i>R</i> <sub>1</sub> [ <i>I</i> >2 $\sigma$ ( <i>I</i> )] | 0.0371                                                          | 0.0221                                           | 0.0379                                                       | 0.0314                                                          | 0.0262                                                                       | 0.0623                                                                                          | 0.0793                                                                     | 0.0668                                                                            |
| <i>wR</i> <sub>2</sub>                                     | 0.0959                                                          | 0.0577                                           | 0.0877                                                       | 0.0891                                                          | 0.0724                                                                       | 0.1599                                                                                          | 0.1904                                                                     | 0.1861                                                                            |
| GOF                                                        | 0.980                                                           | 1.056                                            | 0.885                                                        | 1.077                                                           | 1.225                                                                        | 1.057                                                                                           | 0.853                                                                      | 1.034                                                                             |

**Table S2.** Hydrogen bond details for all the **FCH<sup>+</sup>** and **FC.FCH<sup>+</sup>** complexes.

| FCHBr11               |           |           |          |           | FCHBr21                       |         |         |          |           |
|-----------------------|-----------|-----------|----------|-----------|-------------------------------|---------|---------|----------|-----------|
| D - H...A             | D - H     | H...A     | D...A    | D - H...A | D - H...A                     | D - H   | H...A   | D...A    | D - H...A |
| N(11)-H(11)...O(12)   | 0.86      | 2.24      | 2.893(6) | 133       | N(11)-H(11A)...O(12)          | 0.86    | 1.94    | 2.792(3) | 171       |
| N(13)-H(13)...Br(1)   | 0.86      | 2.41      | 3.229(4) | 160       | N(14)-H(141)...O(12)          | 0.86(3) | 1.95(3) | 2.810(3) | 177(3)    |
| N(14)-H(141)...Br(1)  | 0.86      | 2.63      | 3.396(4) | 148       | N(14)-H(142)...Br(1)          | 0.81(3) | 2.56(3) | 3.343(2) | 162(3)    |
| N(14)-H(141)...F(15)  | 0.86      | 2.28      | 2.800(5) | 119       | C(16)-H(16)...Br(1)           | 0.96(2) | 2.83(2) | 3.787(2) | 179(2)    |
| N(14)-H(142)...F(15)  | 0.86      | 2.43      | 2.727(6) | 101       |                               |         |         |          |           |
| N(14)-H(142)...Br(1)  | 0.86      | 2.61      | 3.440(4) | 162       |                               |         |         |          |           |
| C(16)-H(16)...Br(1)   | 0.93      | 2.87      | 3.684(5) | 146       |                               |         |         |          |           |
| C(16)-H(16)...O(12)   | 0.93      | 2.56      | 3.059(6) | 114       |                               |         |         |          |           |
| FCHI11                |           |           |          |           | FCHI21                        |         |         |          |           |
| N(11)-H(11)...I(1)    | 0.78(3)   | 2.72(3)   | 3.464(2) | 160(3)    | N(11)-H(11A)...O(22)          | 0.86    | 1.99    | 2.762(6) | 149       |
| N(13)-H(13)...I(1)    | 0.84(3)   | 2.65(3)   | 3.465(2) | 163(2)    | N(13)-H(13)...N(13)           | 1.40    | 1.40    | 2.808(7) | 180       |
| N(14)-H(141)...I(1)   | 0.86(3)   | 2.99(3)   | 3.732(2) | 147(2)    | N(21)-H(21)...O(22)           | 0.86    | 1.93    | 2.784(5) | 170       |
| N(14)-H(141)...O(12)  | 0.92(3)   | 1.92(3)   | 2.822(3) | 167(3)    | N(14)-H(141)...O(12)          | 0.87(8) | 1.97(8) | 2.836(7) | 176(9)    |
|                       |           |           |          |           | N(14)-H(142)...F(15)          | 0.79(7) | 2.50(7) | 2.744(7) | 100(5)    |
|                       |           |           |          |           | N(14)-H(142)...O(22)          | 0.79(7) | 2.18(7) | 2.957(7) | 167(8)    |
|                       |           |           |          |           | N(24)-H(241)...N(23)          | 0.96(8) | 2.07(8) | 3.029(7) | 172(7)    |
|                       |           |           |          |           | N(24)-H(242)...F(25)          | 0.83(9) | 2.46(8) | 2.743(7) | 101(6)    |
|                       |           |           |          |           | N(24)-H(242)...O(12)          | 0.83(9) | 2.26(8) | 3.008(8) | 150(7)    |
| FCHNO <sub>3</sub> 11 |           |           |          |           | FCHNO <sub>3</sub> 21         |         |         |          |           |
| N(11)-H(11)...O(51)   | 0.90(3)   | 2.21(2)   | 2.875(3) | 131(2)    | N(11)-H(11)...O(312)          | 1.01(6) | 2.11(6) | 3.109(5) | 171(4)    |
| N(11)-H(11)...O(53)   | 0.90(3)   | 2.13(3)   | 3.030(3) | 171(2)    | N(11)-H(11)...O(313)          | 1.01(6) | 2.20(5) | 2.903(5) | 125(4)    |
| N(13)-H(13)...O(51)   | 0.98(2)   | 1.71(2)   | 2.670(3) | 167.6(19) | N(13)-H(13)...N(13)           | 1.39    | 1.39    | 2.786(4) | 180       |
| N(13)-H(13)...O(52)   | 0.98(2)   | 2.60(2)   | 3.390(2) | 138.0(15) | N(21)-H(21)...O(313)          | 0.83(4) | 1.99(4) | 2.799(6) | 165(4)    |
| N(21)-H(21)...O(61)   | 0.87(3)   | 1.98(3)   | 2.849(3) | 179(2)    | N(23)-H(23)...N(23)           | 1.40    | 1.40    | 2.810(5) | 180       |
| N(23)-H(23)...O(63)   | 0.840(19) | 1.93(2)   | 2.763(2) | 171.3(19) | N(14)-H(141)...O(12)          | 0.86    | 1.96    | 2.816(5) | 171       |
| N(14)-H(141)...O(52)  | 0.88(2)   | 2.17(2)   | 2.999(3) | 159.0(19) | N(14)-H(142)...F(15)          | 0.86    | 2.42    | 2.723(5) | 102       |
| N(14)-H(141)...O(22)  | 0.88(2)   | 2.497(19) | 2.986(3) | 116.0(15) | N(14)-H(142)...O(312)         | 0.86    | 2.31    | 3.072(5) | 148       |
| N(14)-H(142)...F(15)  | 0.87(2)   | 2.40(2)   | 2.718(3) | 102.2(15) | N(24)-H(241)...O(22)          | 1.03(6) | 1.83(6) | 2.844(5) | 170(4)    |
| N(14)-H(142)...O(63)  | 0.87(2)   | 2.10(2)   | 2.936(3) | 162.2(19) | N(24)-H(242)...F(25)          | 0.88(4) | 2.41(4) | 2.736(5) | 102(3)    |
| N(24)-H(241)...O(62)  | 0.89(3)   | 2.24(3)   | 3.089(3) | 160(2)    | N(24)-H(242)...O(311)         | 0.88(4) | 2.29(4) | 3.155(6) | 165(4)    |
| N(24)-H(241)...O(52)  | 0.89(3)   | 2.51(3)   | 2.963(3) | 112.2(19) | N(24)-H(242)...F(15)          | 0.88(4) | 2.47(4) | 2.821(5) | 105(3)    |
| N(24)-H(242)...F(25)  | 0.90(2)   | 2.42(3)   | 2.728(2) | 100.2(19) | C(16)-H(16)...O(22)           | 0.84(4) | 2.48(4) | 3.237(6) | 150(3)    |
| N(24)-H(242)...O(12)  | 0.90(2)   | 2.10(2)   | 2.994(3) | 172(2)    | C(16)-H(16)...O(313)          | 0.84(4) | 2.49(4) | 2.990(7) | 119(3)    |
| C(16)-H(16)...O(12)   | 0.90(2)   | 2.52(2)   | 3.372(3) | 159.5(16) | C(26)-H(26)...O(12)           | 0.87(4) | 2.34(4) | 3.181(6) | 165(3)    |
| C(16)-H(16)...O(51)   | 0.90(2)   | 2.480(19) | 3.030(3) | 119.9(15) |                               |         |         |          |           |
| C(26)-H(26)...O(62)   | 0.979(19) | 2.586(19) | 3.290(3) | 128.9(15) |                               |         |         |          |           |
| C(26)-H(26)...O(53)   | 0.979(19) | 2.58(2)   | 3.477(3) | 152.3(16) |                               |         |         |          |           |
| FCSAC11               |           |           |          |           | FCSAC21- monomethanol solvate |         |         |          |           |
| N(11)-H(11)...O(27)   | 0.86(2)   | 1.90(2)   | 2.749(3) | 170(2)    | N(11)-H(11A)...O(22)          | 0.88    | 1.97    | 2.846(4) | 177       |
| N(13)-H(13)...O(27)   | 0.876(19) | 1.861(19) | 2.726(3) | 168.9(17) | N(13)-H(13)...N(23)           | 1.03(5) | 1.85(5) | 2.883(5) | 178(5)    |
| N(14)-H(141)...N(28)  | 0.88(2)   | 1.99(2)   | 2.876(3) | 176(2)    | N(14)-H(14A)...O(22)          | 0.88    | 1.94    | 2.817(5) | 176       |
| N(14)-H(142)...F(15)  | 0.862(19) | 2.440(19) | 2.745(3) | 101.5(15) | N(14)-H(14B)...O(41)          | 0.88    | 1.82    | 2.689(6) | 167       |
| N(14)-H(142)...O(12)  | 0.862(19) | 2.016(19) | 2.852(3) | 163.2(18) | N(21)-H(21A)...O(12)          | 0.88    | 1.94    | 2.822(4) | 178       |
| C(16)-H(16)...O(292)  | 0.941(18) | 2.301(18) | 2.992(3) | 129.9(14) | N(24)-H(24A)...O(12)          | 0.88    | 2.13    | 3.011(5) | 175       |
|                       |           |           |          |           | N(24)-H(24B)...N(36)          | 0.88    | 2.16    | 3.042(5) | 176       |
|                       |           |           |          |           | C(26)-H(26A)...O(38)          | 0.95    | 2.03    | 2.963(6) | 168       |
|                       |           |           |          |           | C(32)-H(32A)...F(25)          | 0.95    | 2.51    | 3.455(6) | 171       |

D = donor; H = hydrogen and A = acceptor