*Article*

# Effect of the Incorporation of Functionalized Cyclodextrins in the Liposomal Bilayer

**Romina Zappacosta [1], Benedetta Cornelio [2], Serena Pilato [1], Gabriella Siani [1], François Estour [2,*], Massimiliano Aschi [3] and Antonella Fontana [1,*]**

[1] Dipartimento di Farmacia, Università "G. d'Annunzio", Via dei Vestini snc, I-66100 Chieti, Italy; r.zappacosta@unich.it (R.Z.); serena.pilato@unich.it (S.P.); gabriella.siani@unich.it (G.S.)
[2] Normandie Univ, INSA Rouen, UNIROUEN, CNRS, COBRA (UMR 6014 & FR3038), 76000 Rouen, France; benedettacornelio@hotmail.com
[3] Dipartimento di Scienze Fisiche e Chimiche, Università di L'Aquila, Via Vetoio snc, I-67100 L'Aquila, Italy, massimiliano.aschi@univaq.it
* Correspondence: francois.estour@univ-rouen.fr (F.E.); antonella.fontana@unich.it (A.F.); Tel.: +33-(0)2-3552-2921 (F.E.); +39-0871-3554790 (A.F.)

## Supplementary Materials

### S1. Viscosity measurements

### S2. Stability measurements

### S3. Details of Molecular Dynamics Simulations

## S1. Viscosity measurements

### S1.1 Viscosity measurements for pure POPC liposomes

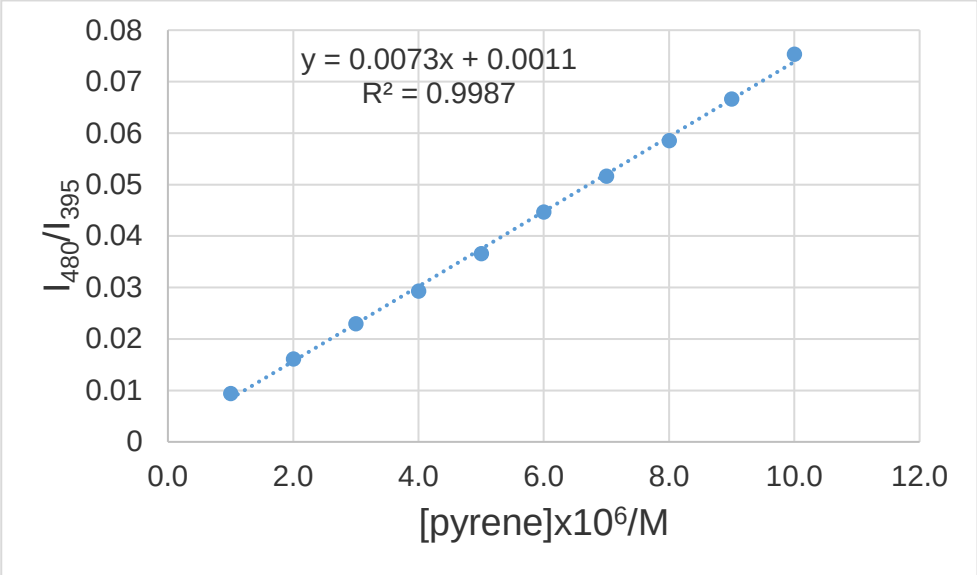


**Figure S1.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for pure POPC liposomes at 25° C.

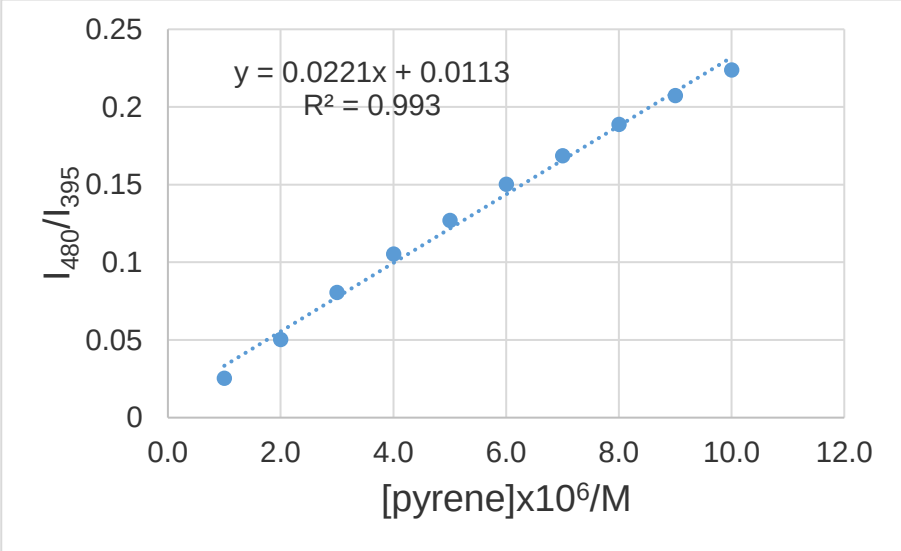


**Figure S2.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for pure POPC liposomes at 37° C.

## S1.2 Viscosity measurements for POPC/β-CD liposomes

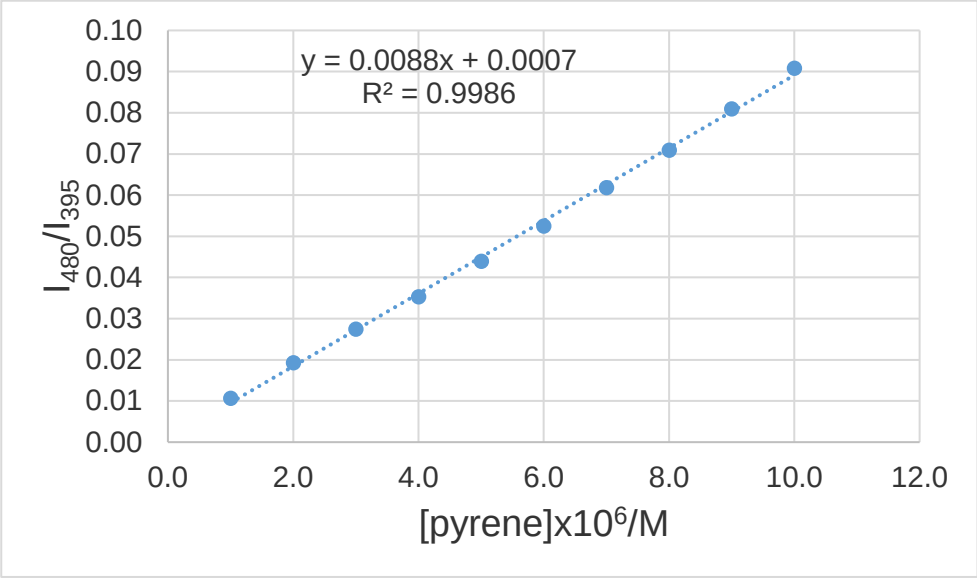


**Figure S3.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/β-CD 12 liposomes at 25° C.

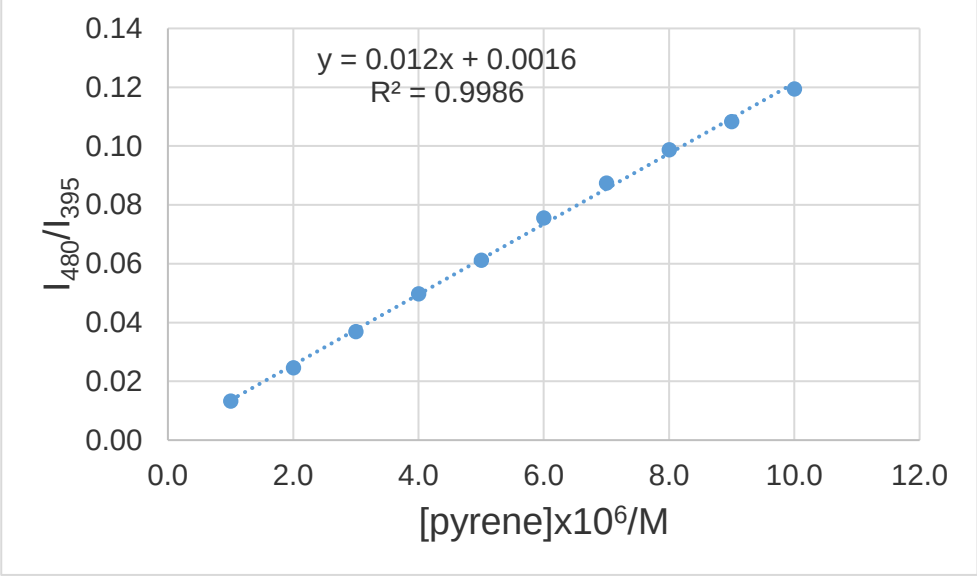


**Figure S4.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/β-CD 12 liposomes at 37° C.

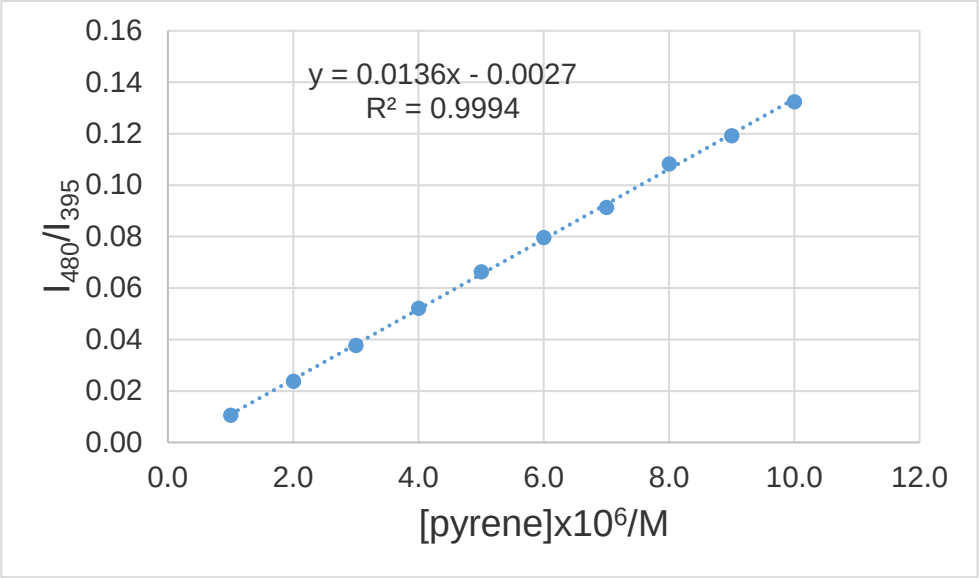


**Figure S5.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/β-CD 5 liposomes at 25° C.

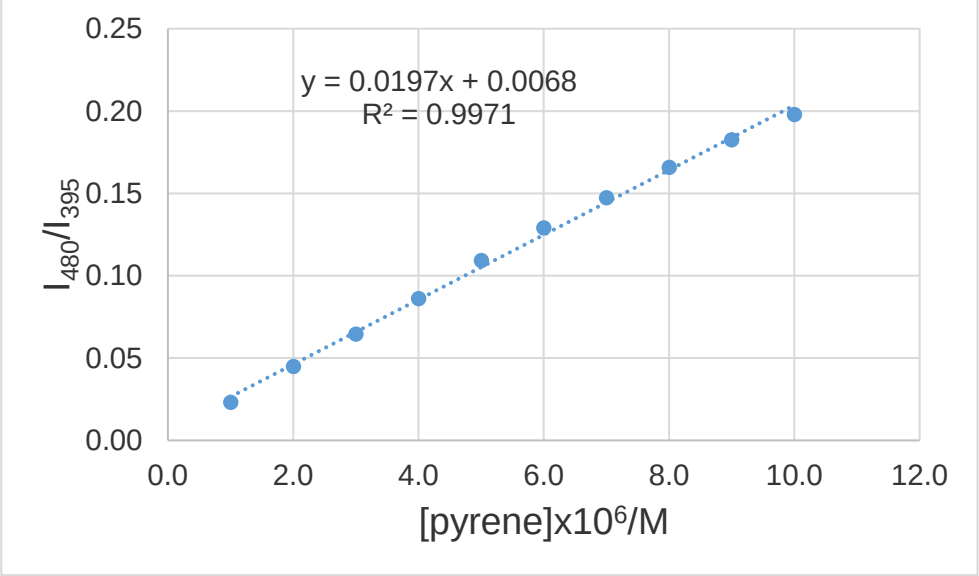


**Figure S6.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/β-CD 5 liposomes at 37° C.

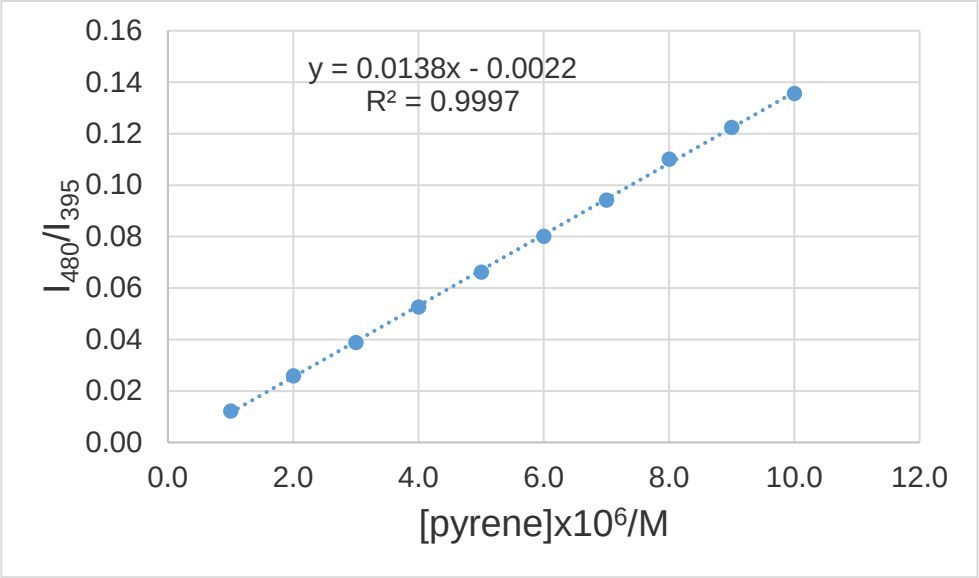


**Figure S7.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/β-CD 2.5 liposomes at 25° C.

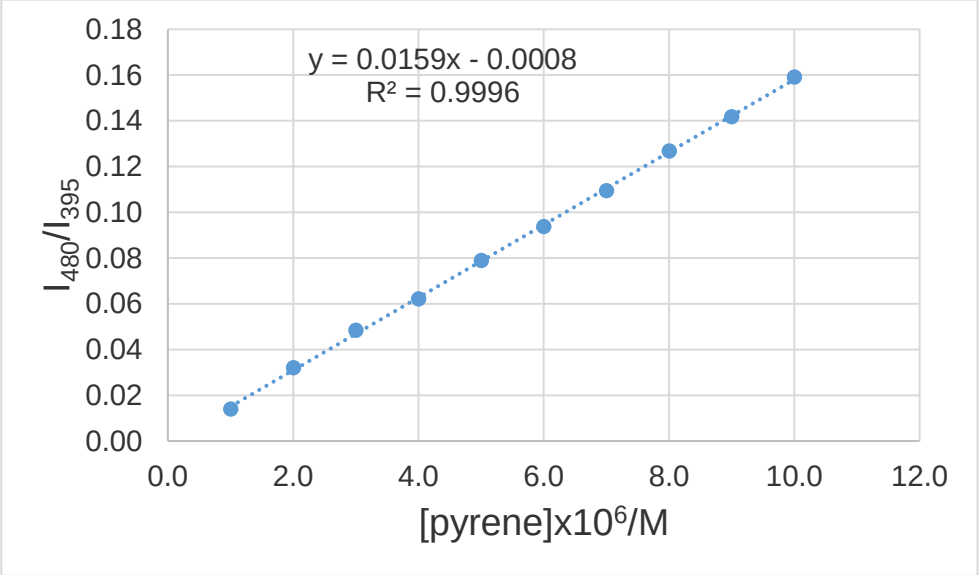


**Figure S8.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/β-CD 2.5 liposomes at 37° C.

**S1.3 Viscosity measurements for POPC/TMCD liposomes**

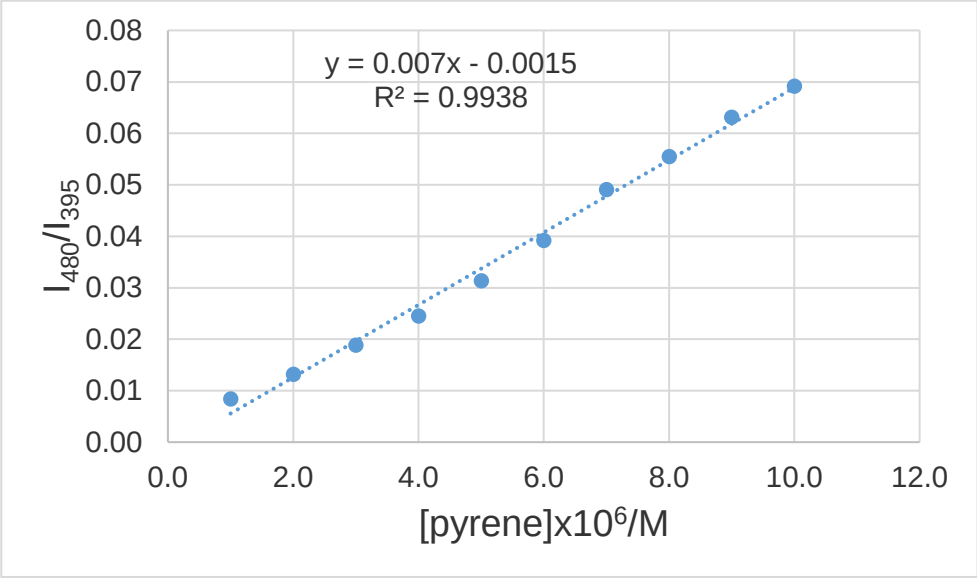


**Figure S9.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/TMCD 12 liposomes at 25° C.

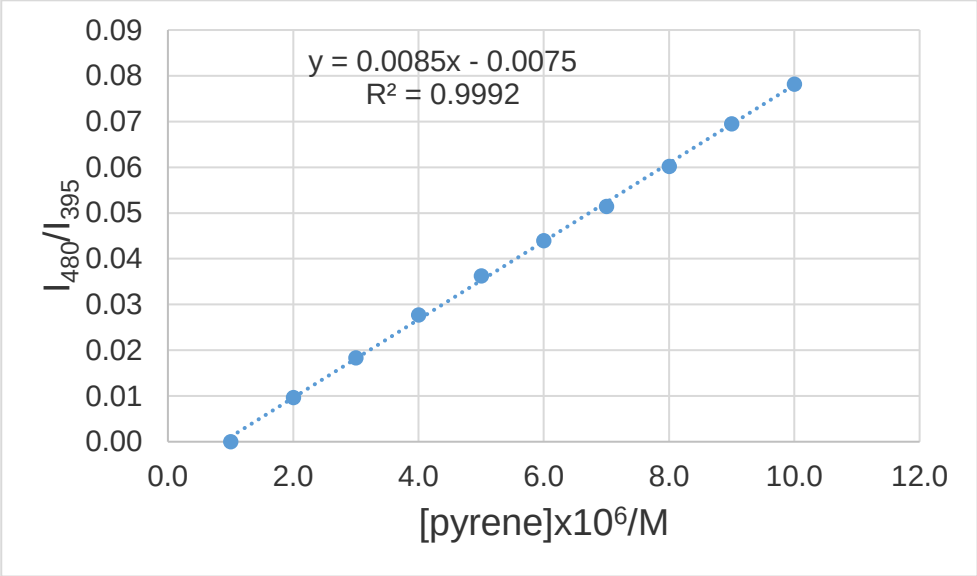


**Figure S10.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/TMCD 12 liposomes at 37° C.

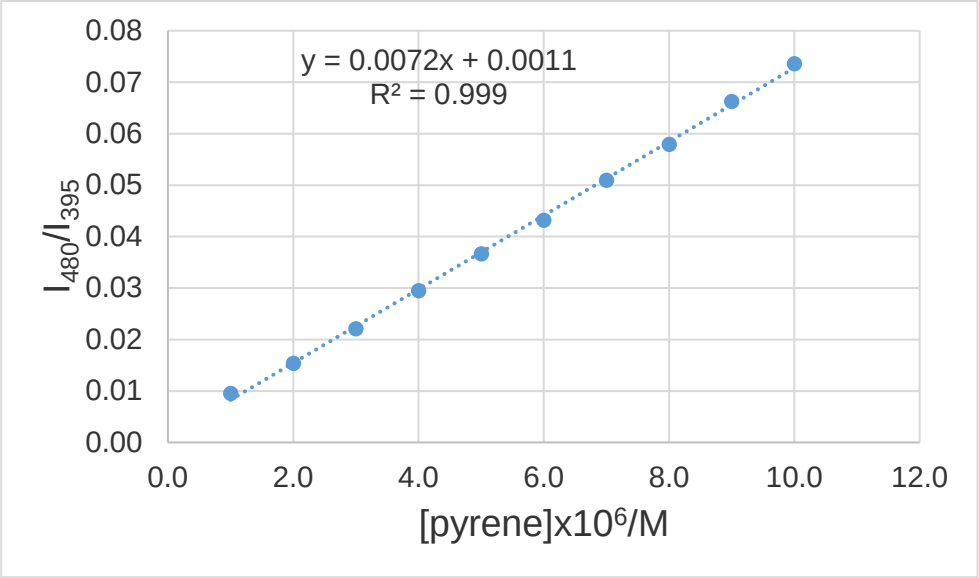


**Figure S11.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/TMCD 5 liposomes at 25° C.

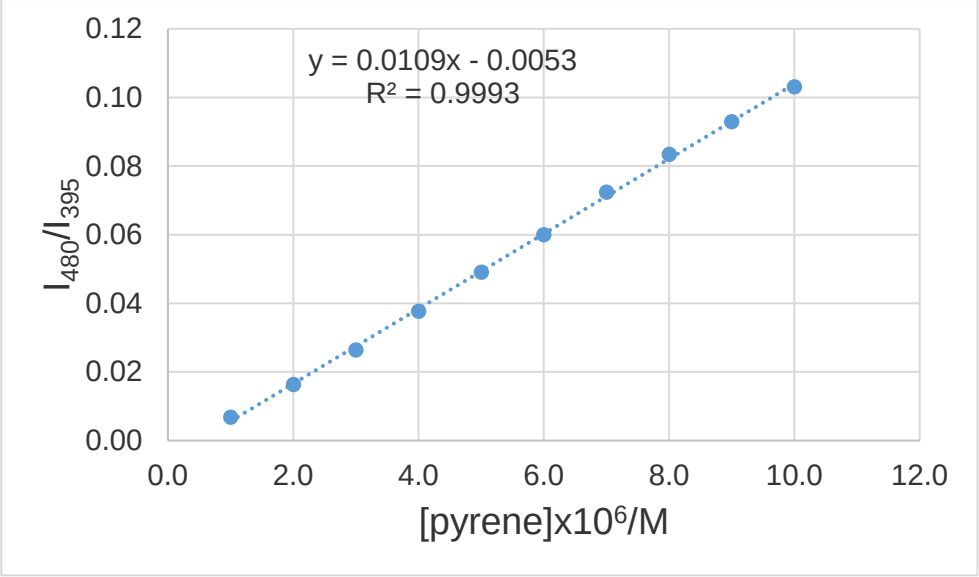


**Figure S12.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/TMCD 5 liposomes at 37° C.

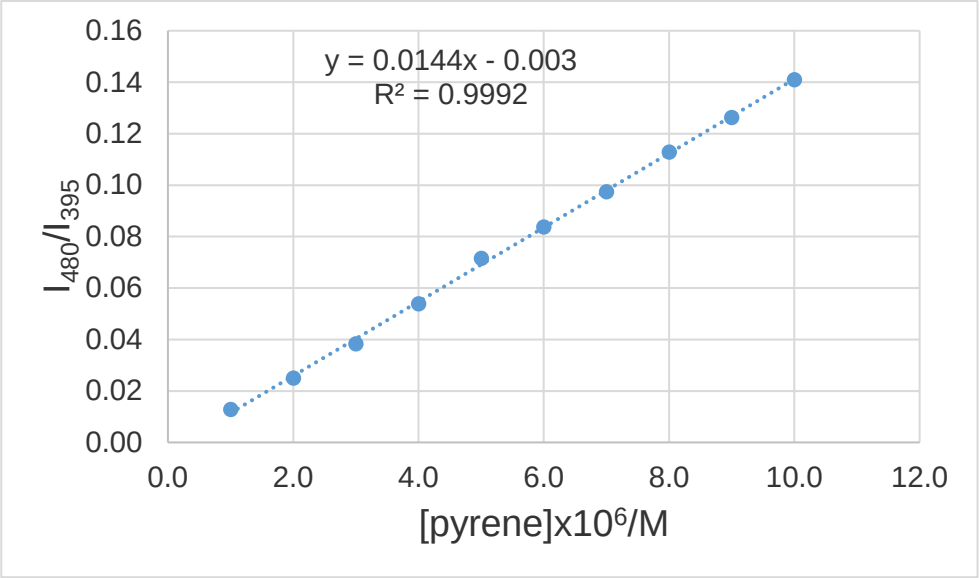


**Figure S13.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/TMCD 2.5 liposomes at 25° C.

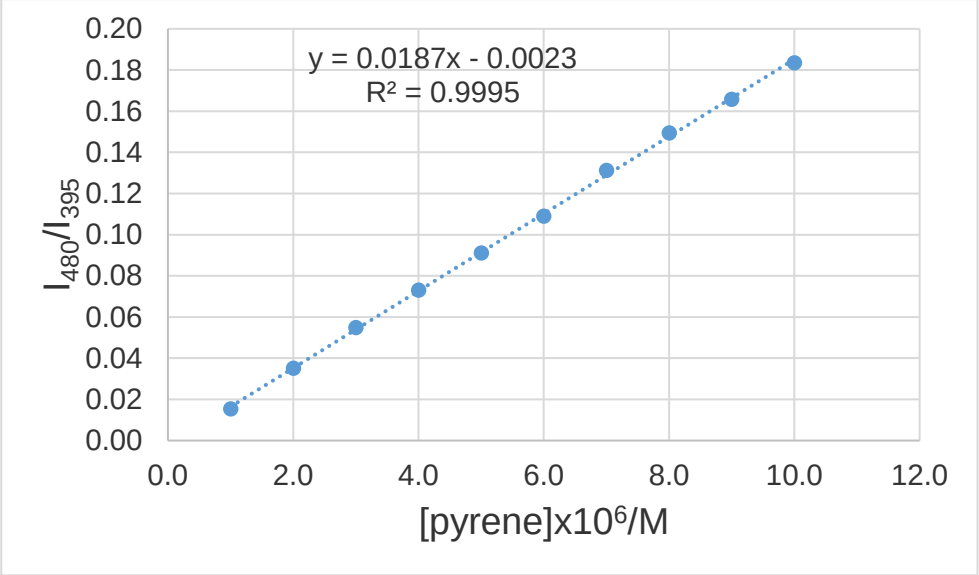


**Figure S14.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/TMCD 2.5 liposomes at 37° C.

**S1.4 Viscosity measurements for POPC/DACD liposomes**

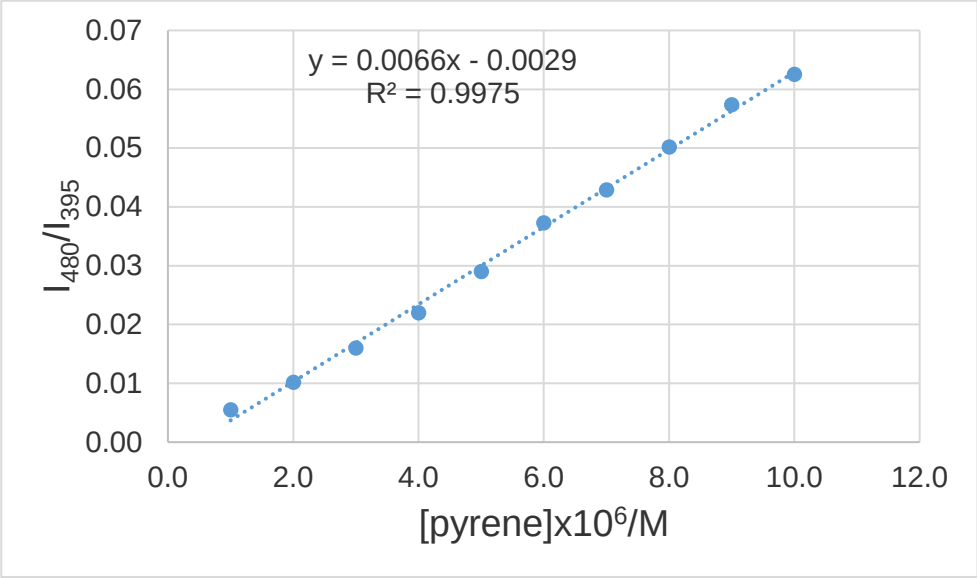


**Figure S15.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/DACD 12 liposomes at 25° C.

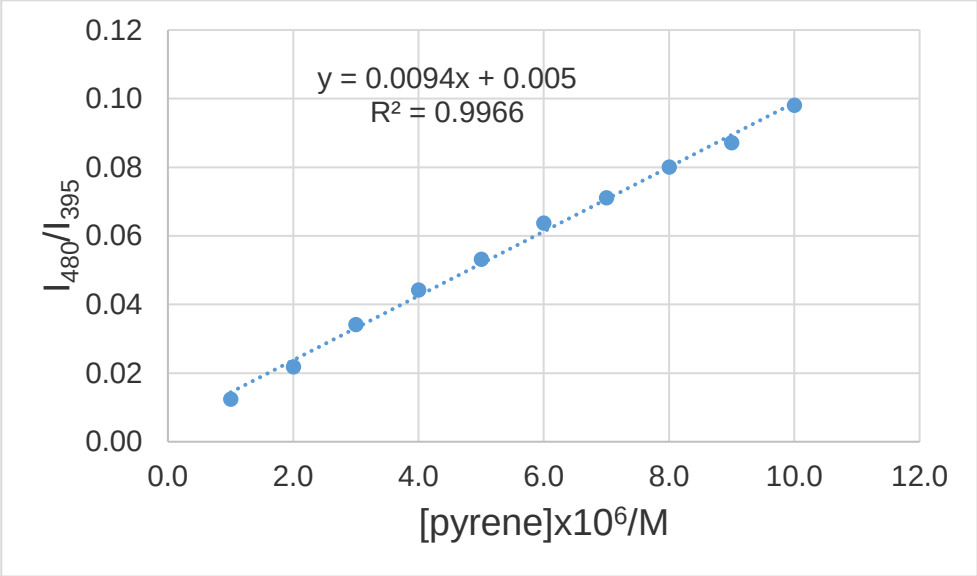


**Figure S16.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/DACD 12 liposomes at 37° C.

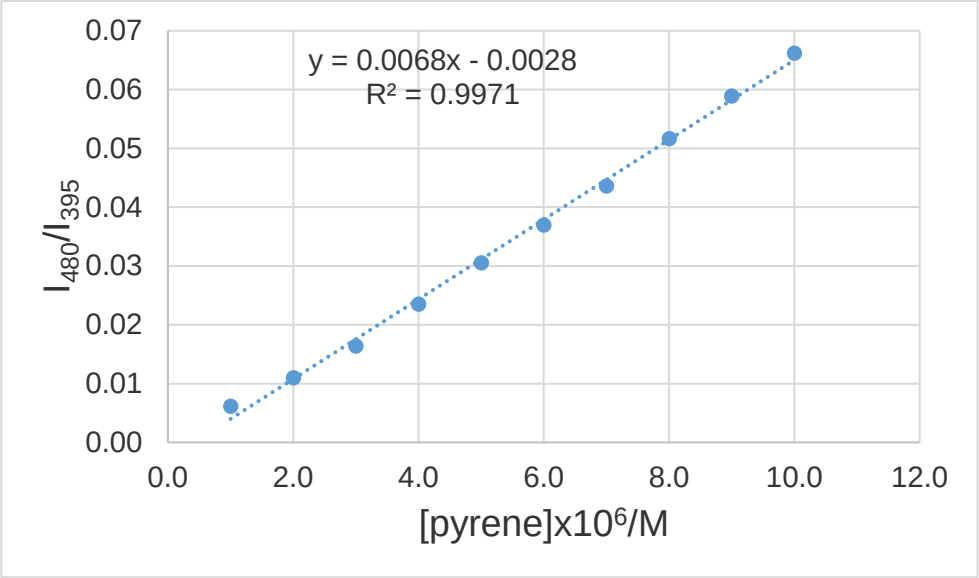


**Figure S17.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/DACD 5 liposomes at 25° C.

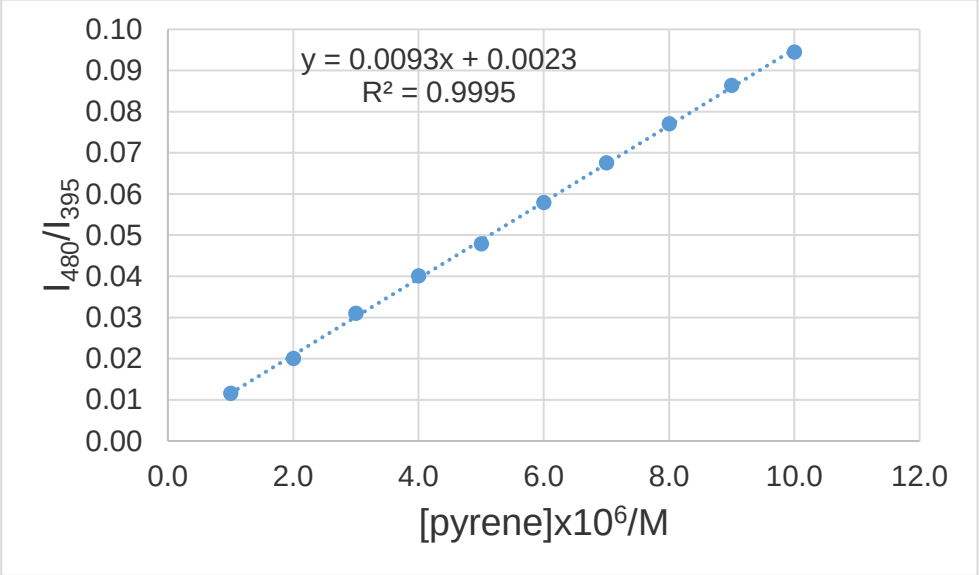


**Figure S18.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/DACD 5 liposomes at 37° C.

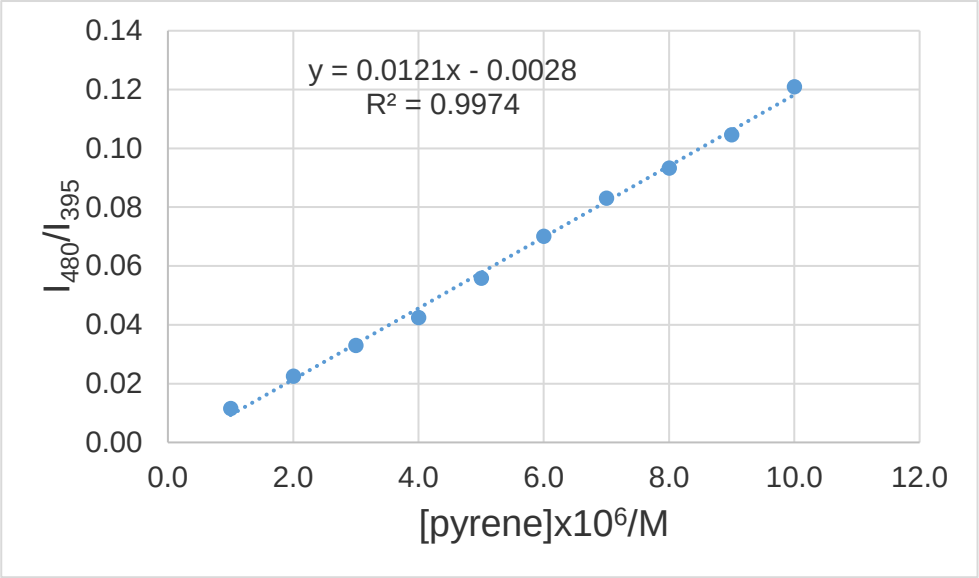


**Figure S19.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/DACD 2.5 liposomes at 25° C.

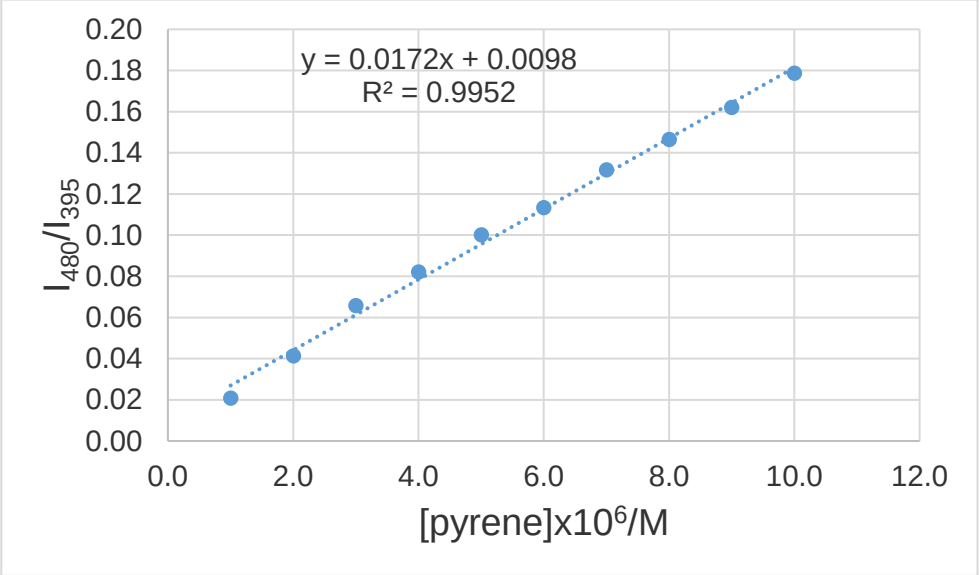


**Figure S20.** Representative plot of $I_E/I_M$ *vs.* pyrene concentration for POPC/DACD 2.5 liposomes at 37° C.

## S2. Stability measurements

### S2.1 Stability measurements for pure POPC liposomes

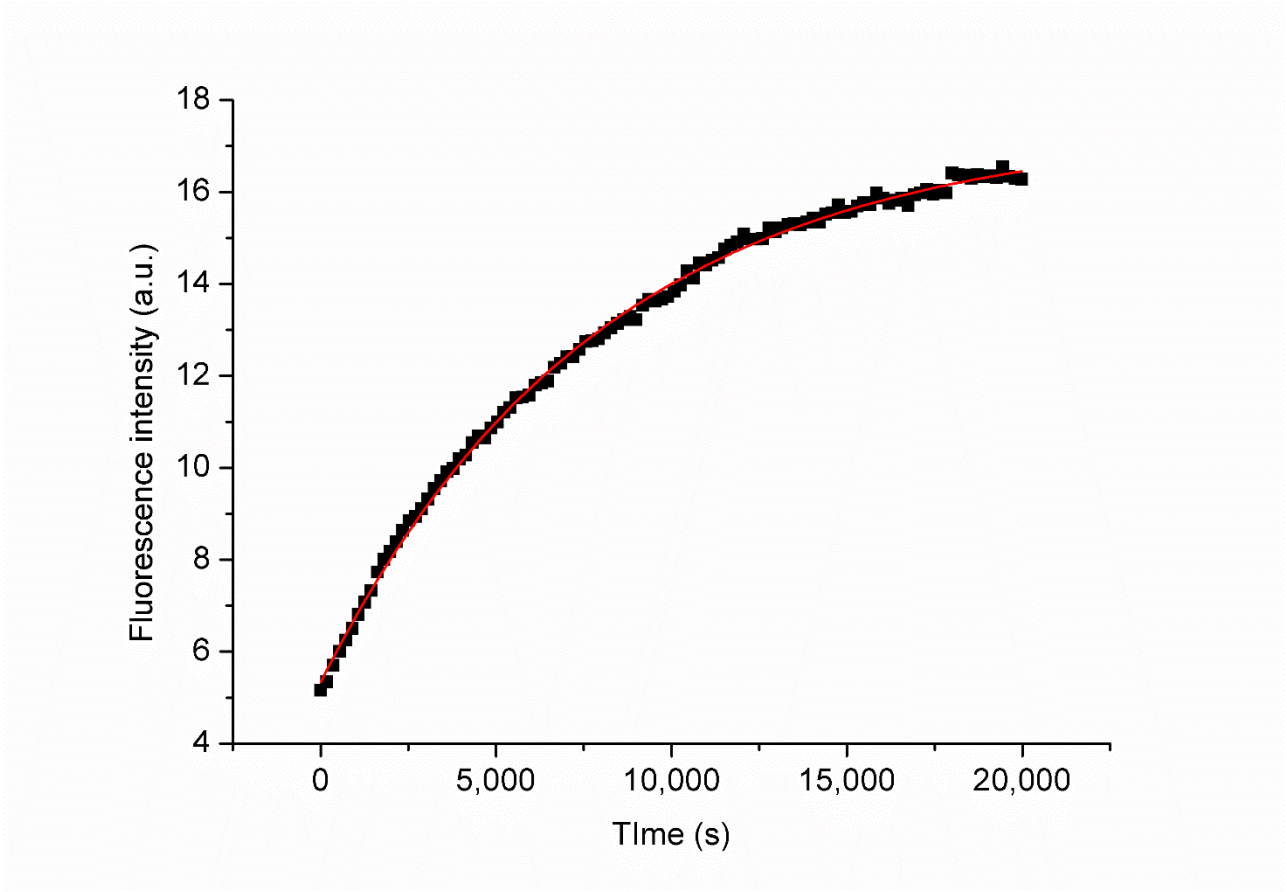


**Figure S21.** Representative kinetic profile of the release of $CF^{3-}$ from pure POPC liposomes at 25° C.

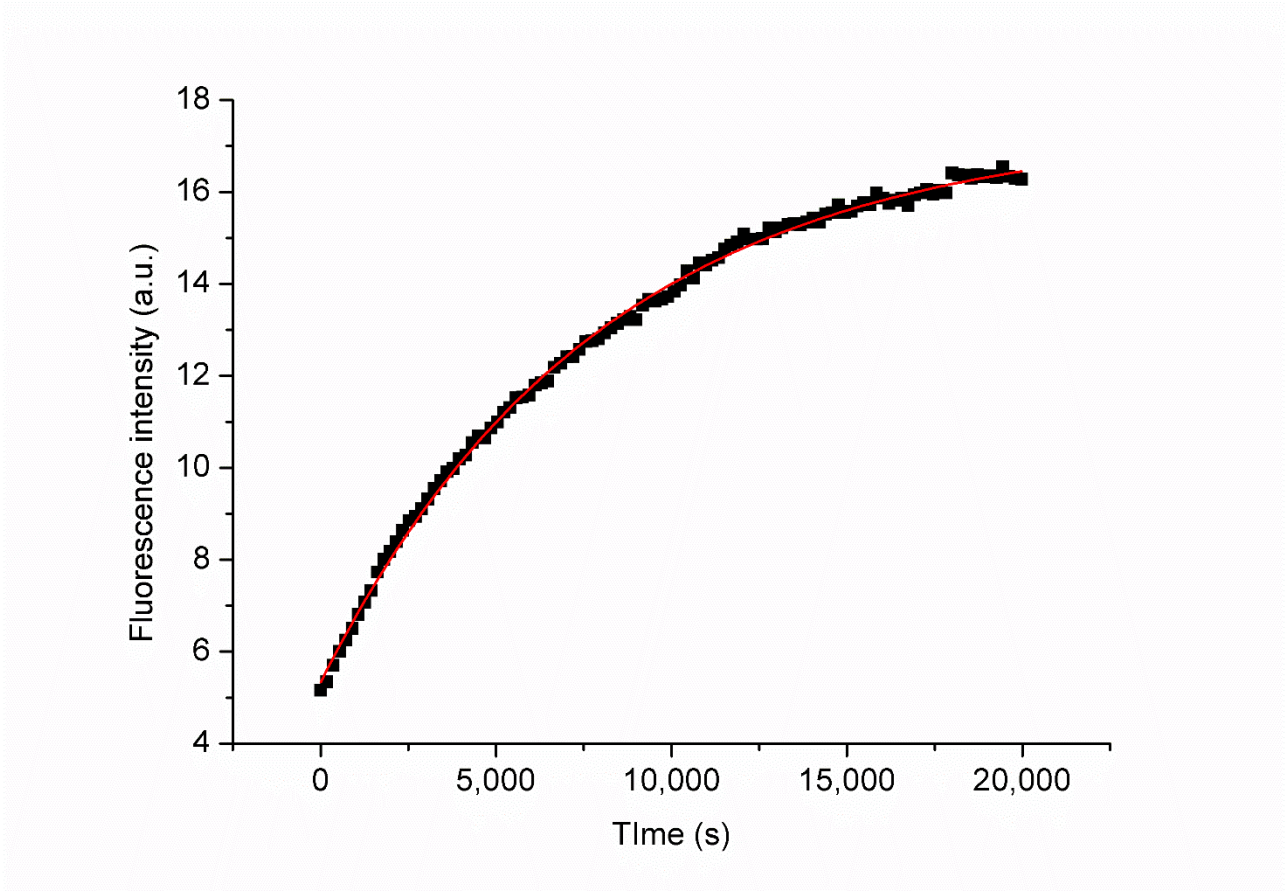


**Figure S22.** Representative kinetic profile of the release of $CF^{3-}$ from pure POPC liposomes at 37° C.

**S2.2 Stability measurements for POPC/β-CD liposomes**

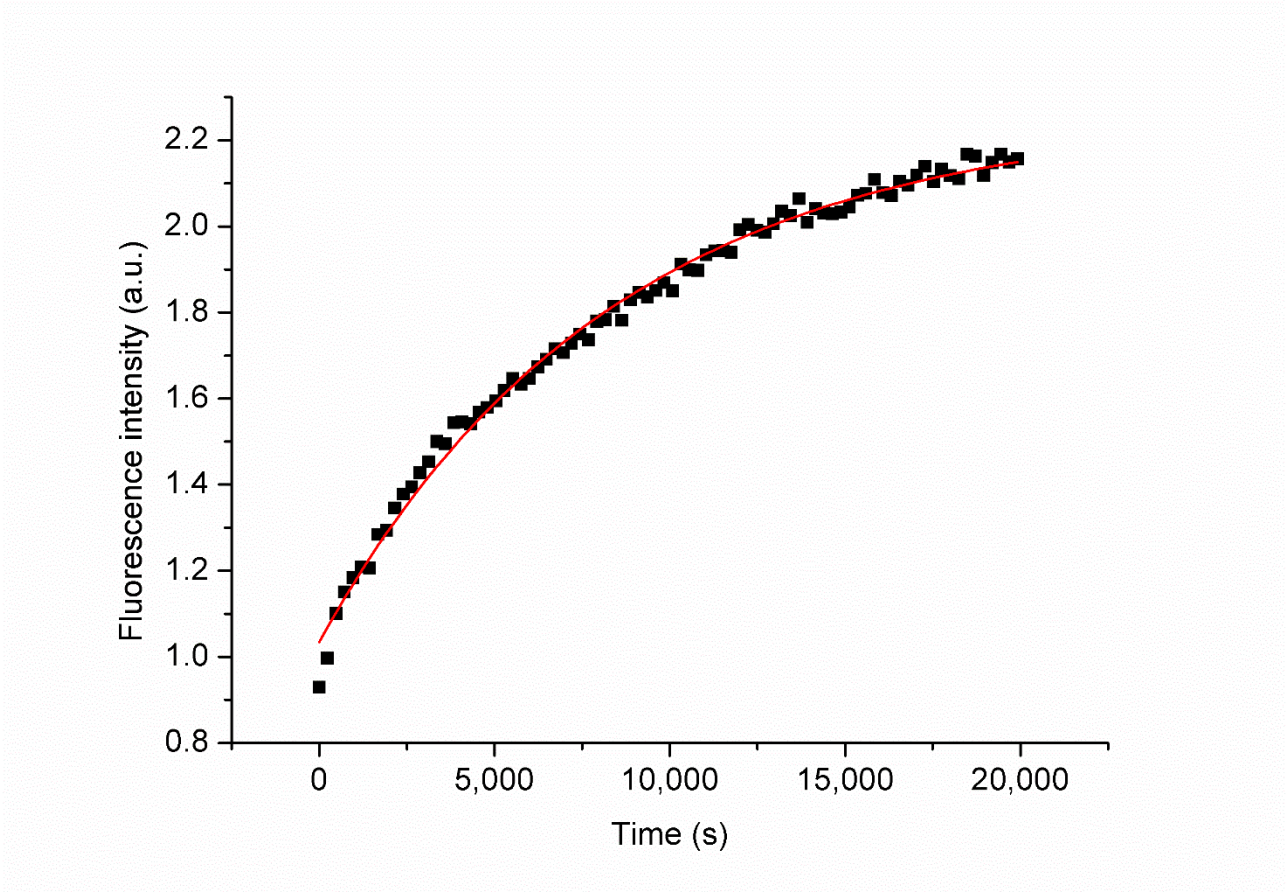


**Figure S23.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/β-CD 12 liposomes at 25° C.

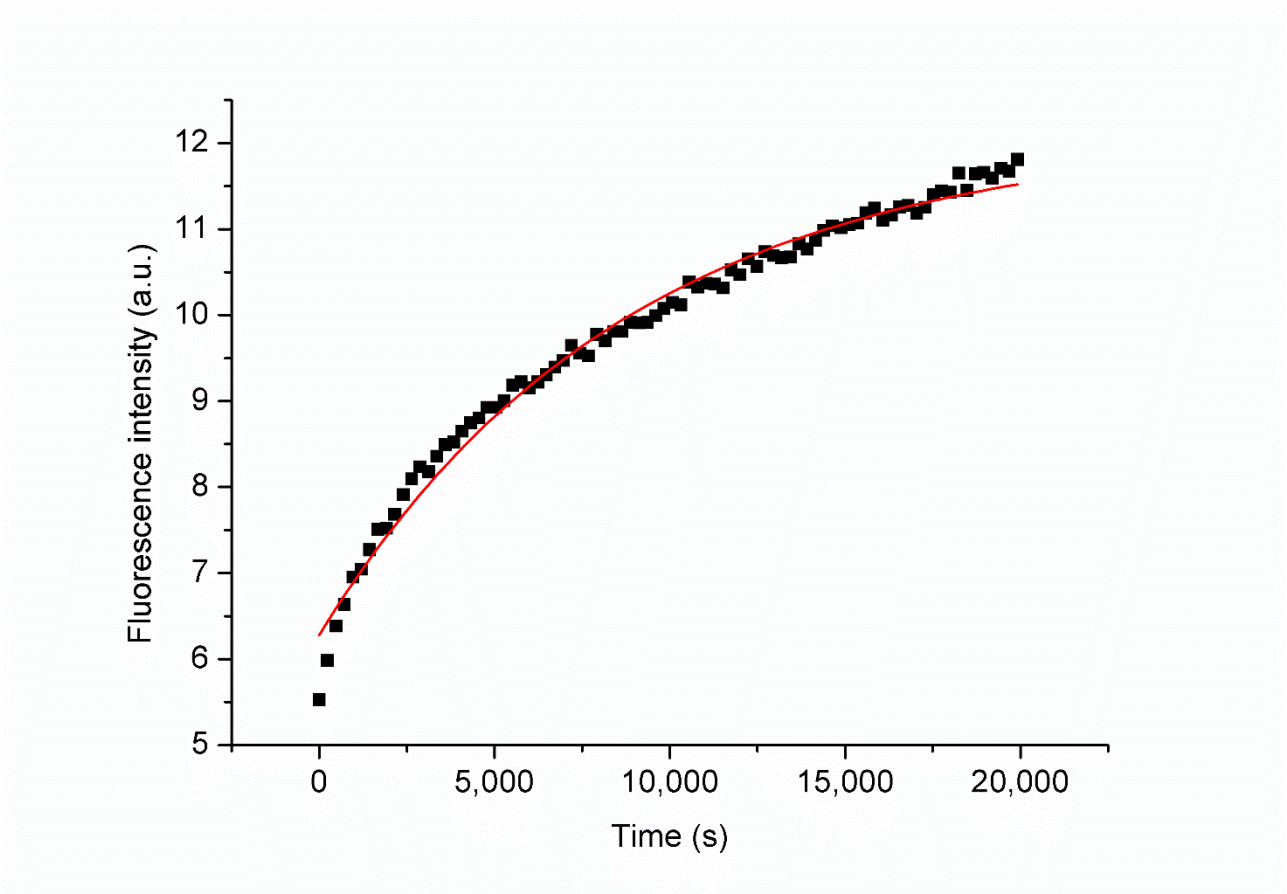


**Figure S24.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/β-CD 12 liposomes at 37° C.

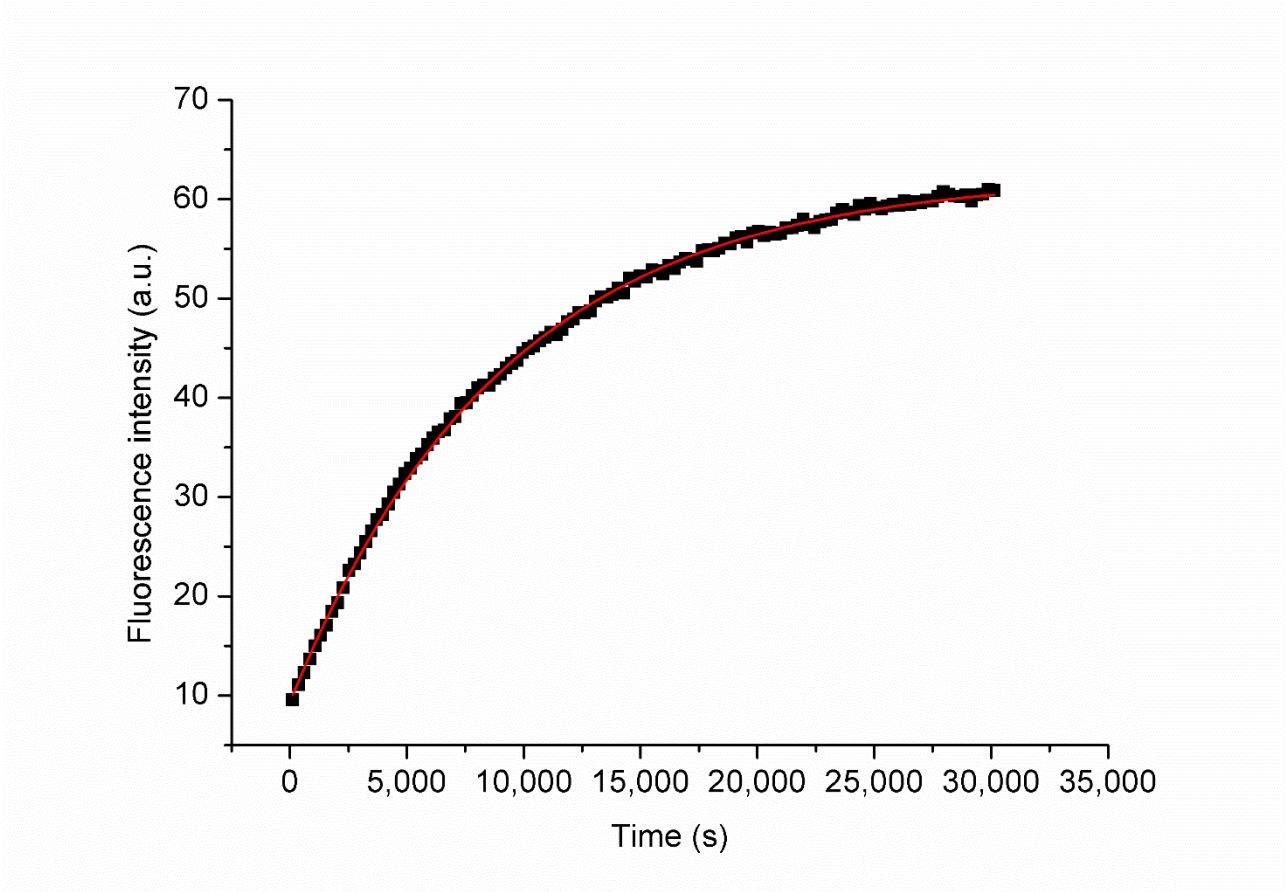


**Figure S25.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/β-CD 5 liposomes at 25° C.

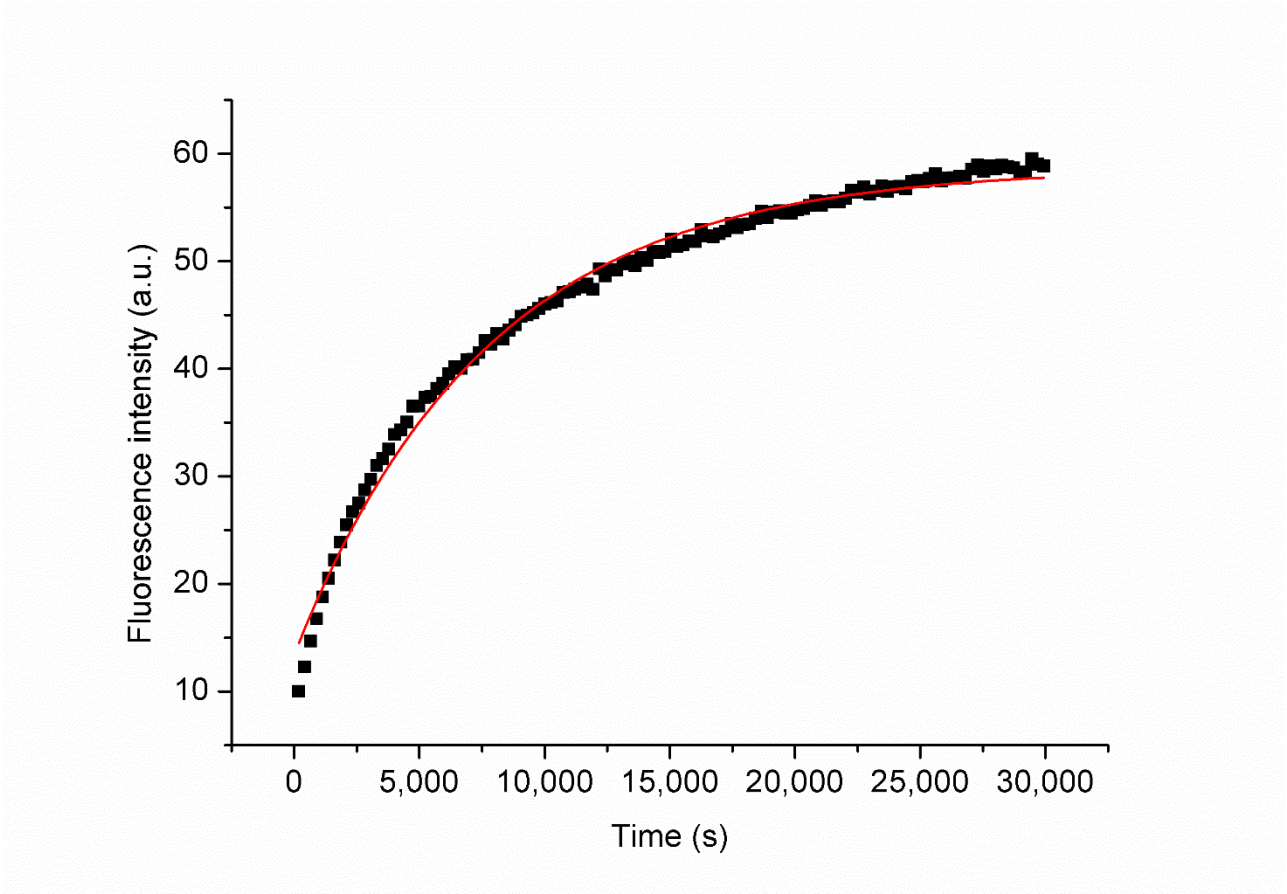


**Figure S26.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/β-CD 5 liposomes at 37° C.

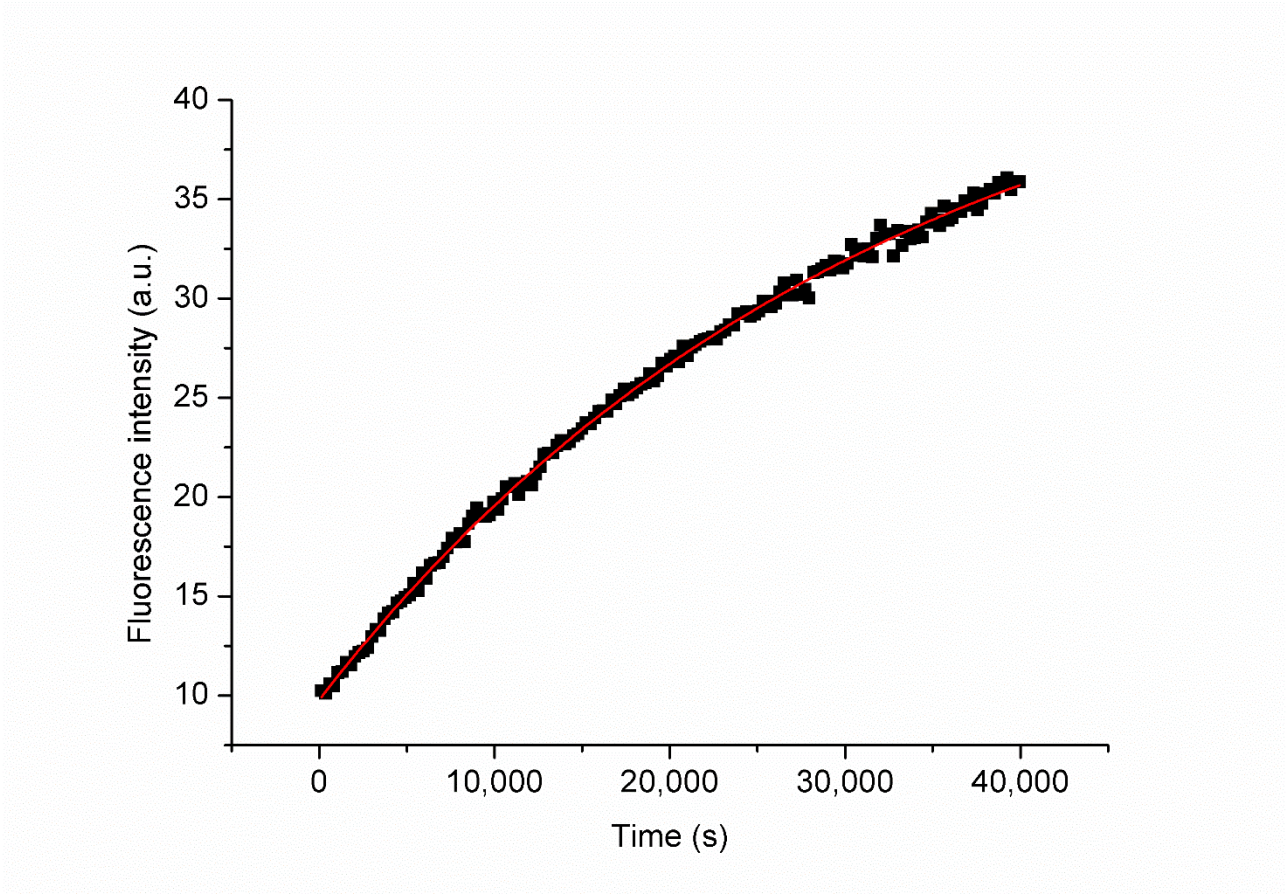


**Figure S27.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/β-CD 2.5 liposomes at 25° C.

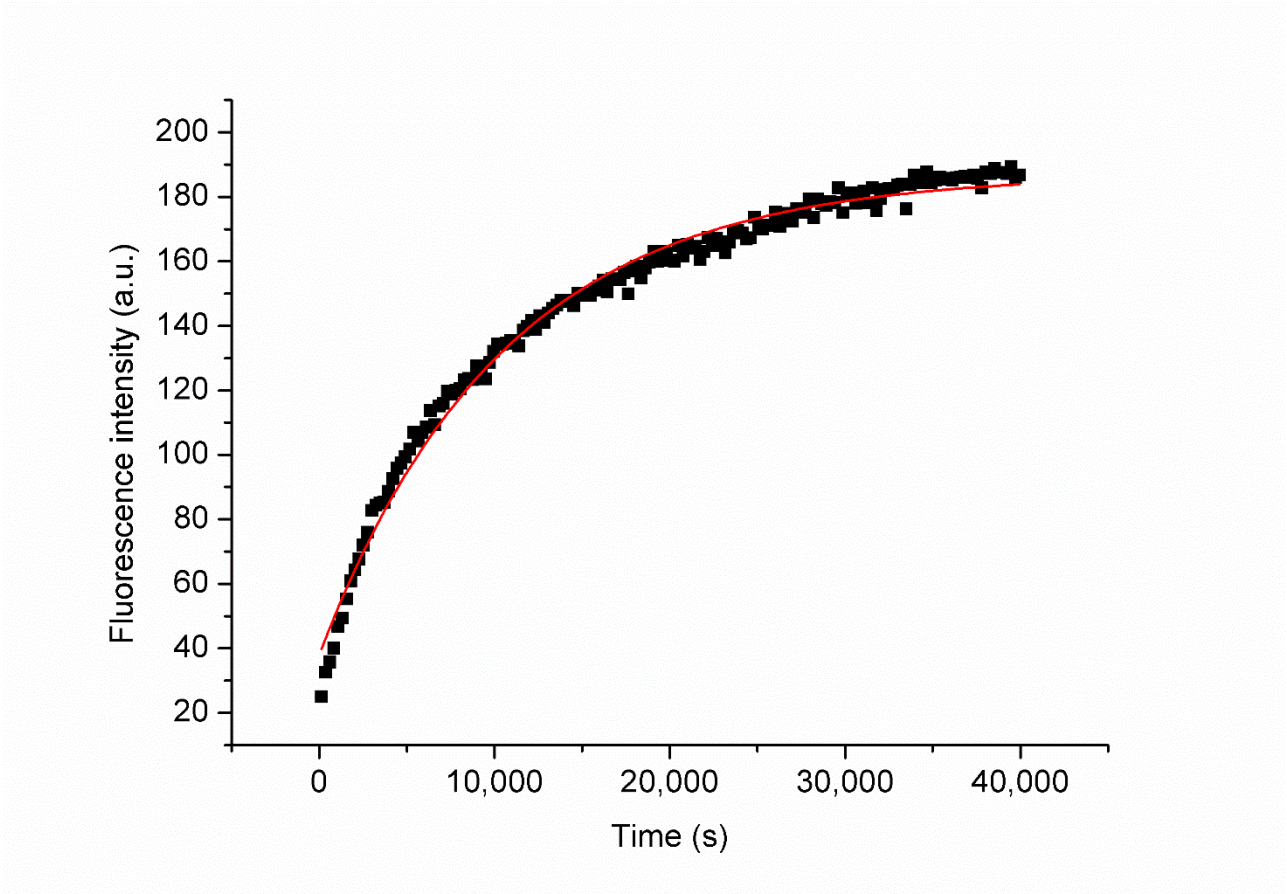


**Figure S28.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/β-CD 2.5 liposomes at 37° C.

**S2.3 Stability measurements for POPC/TMCD liposomes**

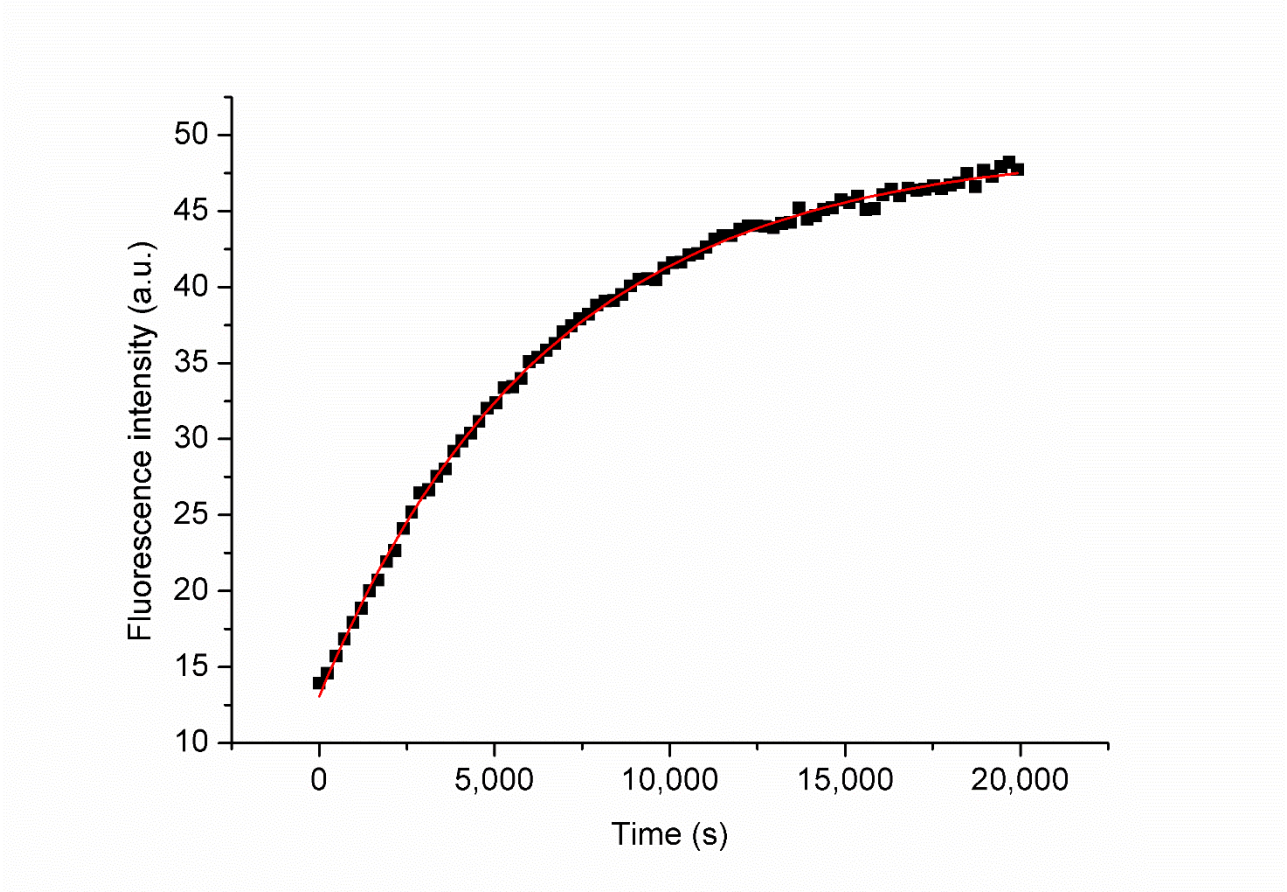


**Figure S29.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/TMCD 12 liposomes at 25° C.

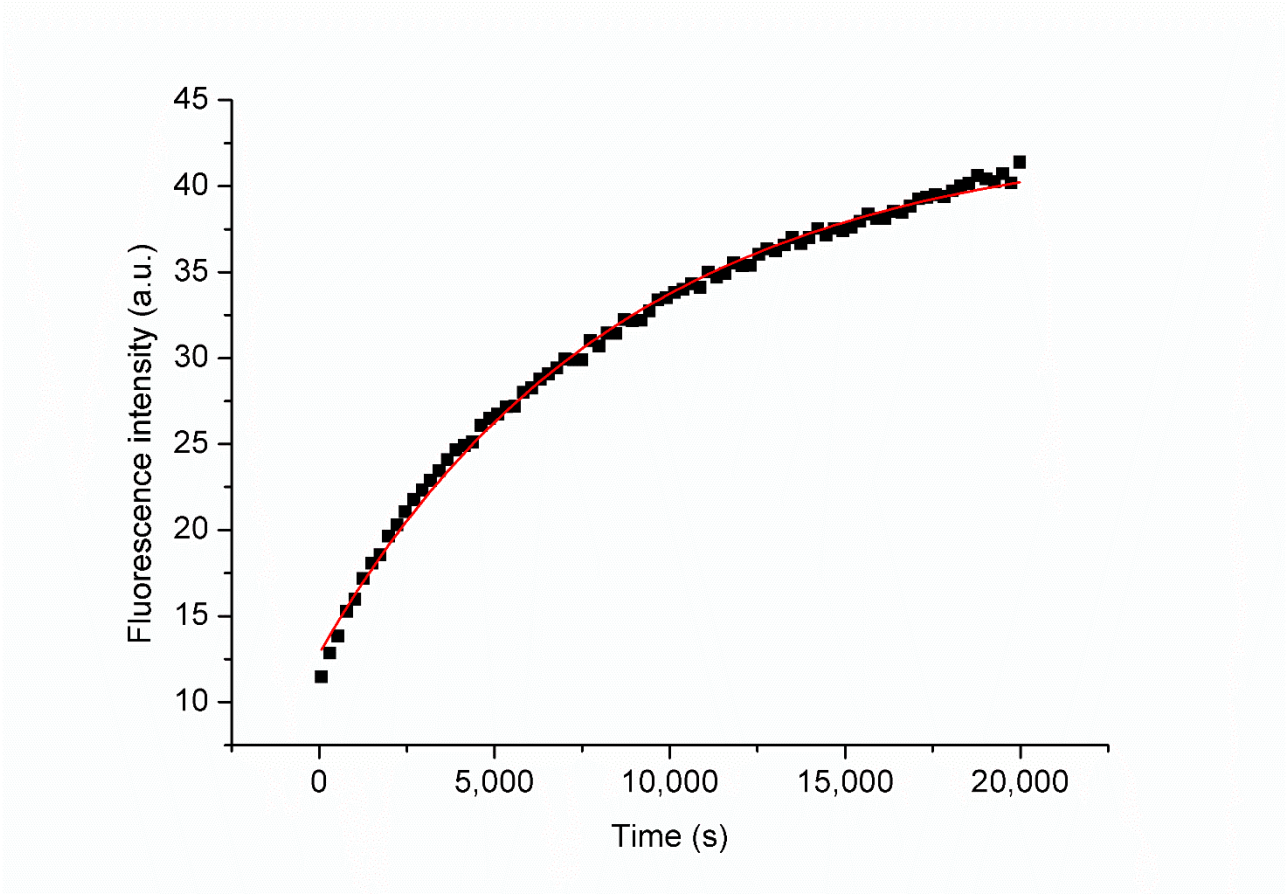


**Figure S30.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/TMCD 12 liposomes at 37° C.

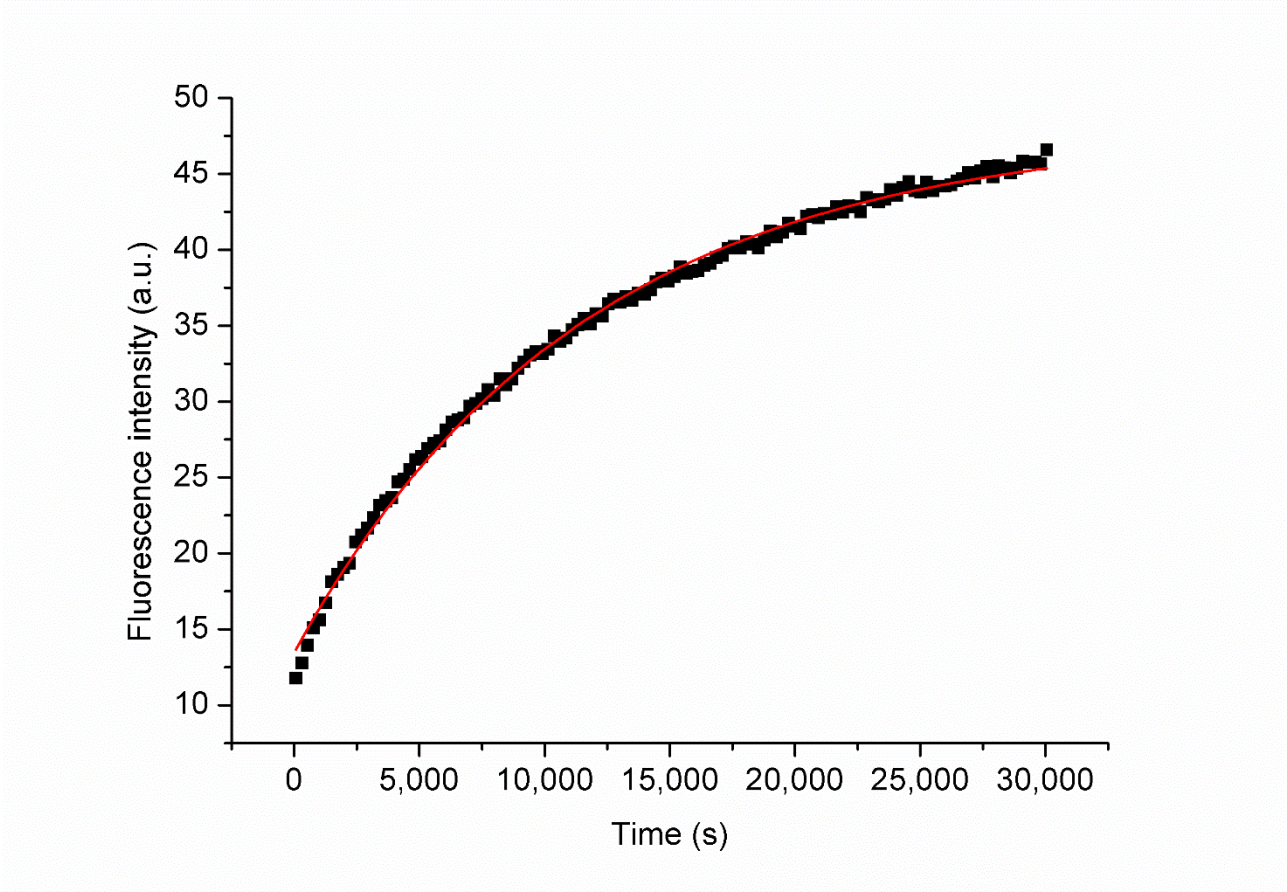


**Figure S31.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/TMCD 5 liposomes at 25° C.

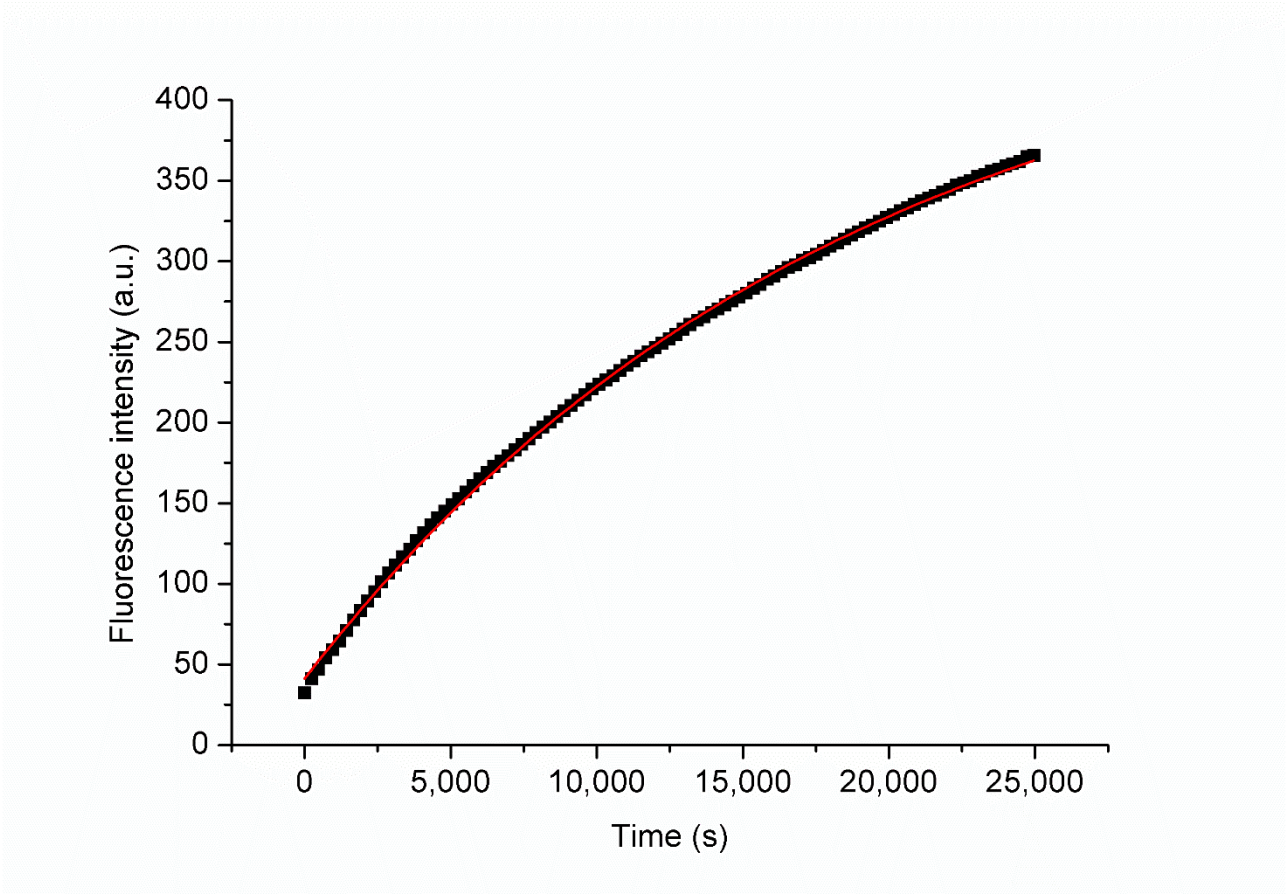


**Figure S32.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/TMCD 5 liposomes at 37° C.

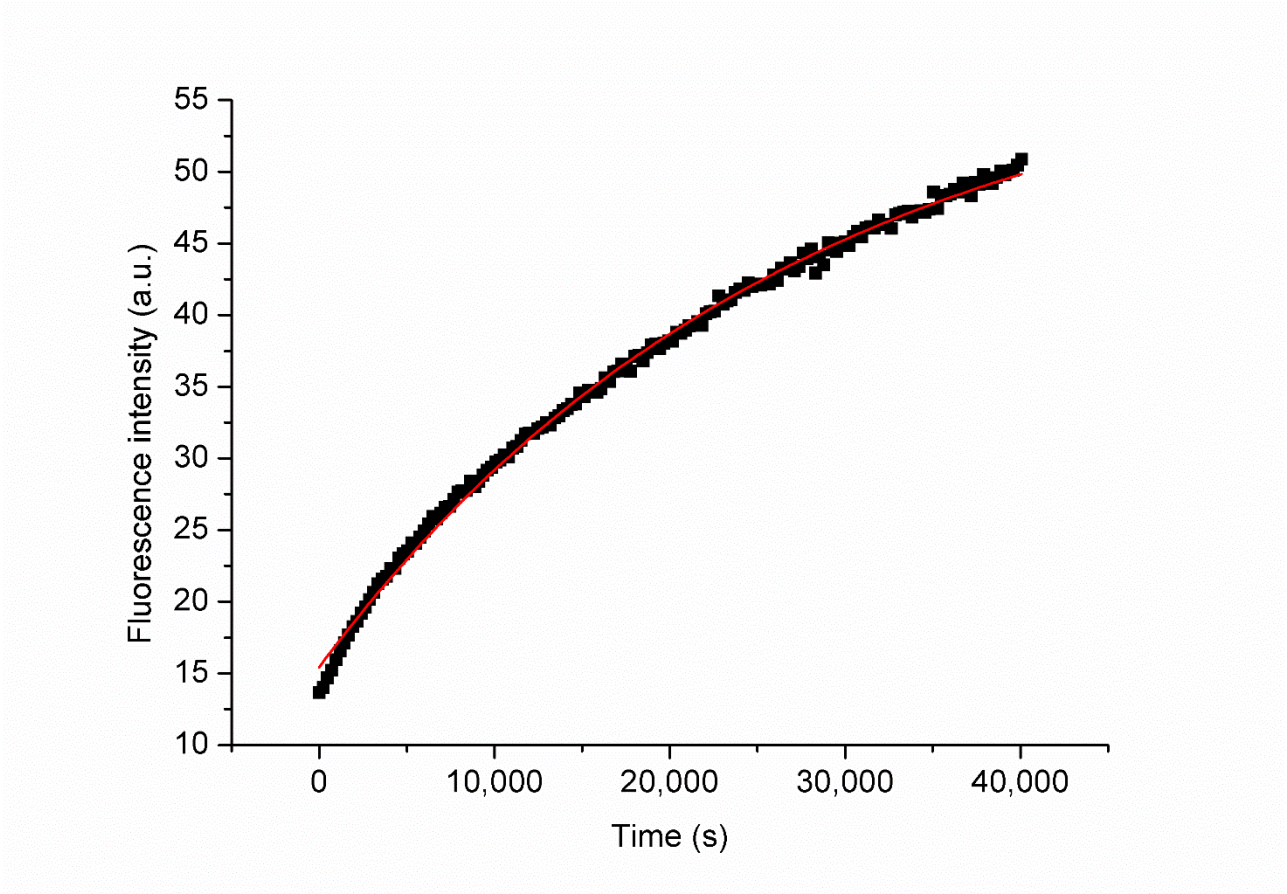


**Figure S33.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/TMCD 2.5 liposomes at 25° C.

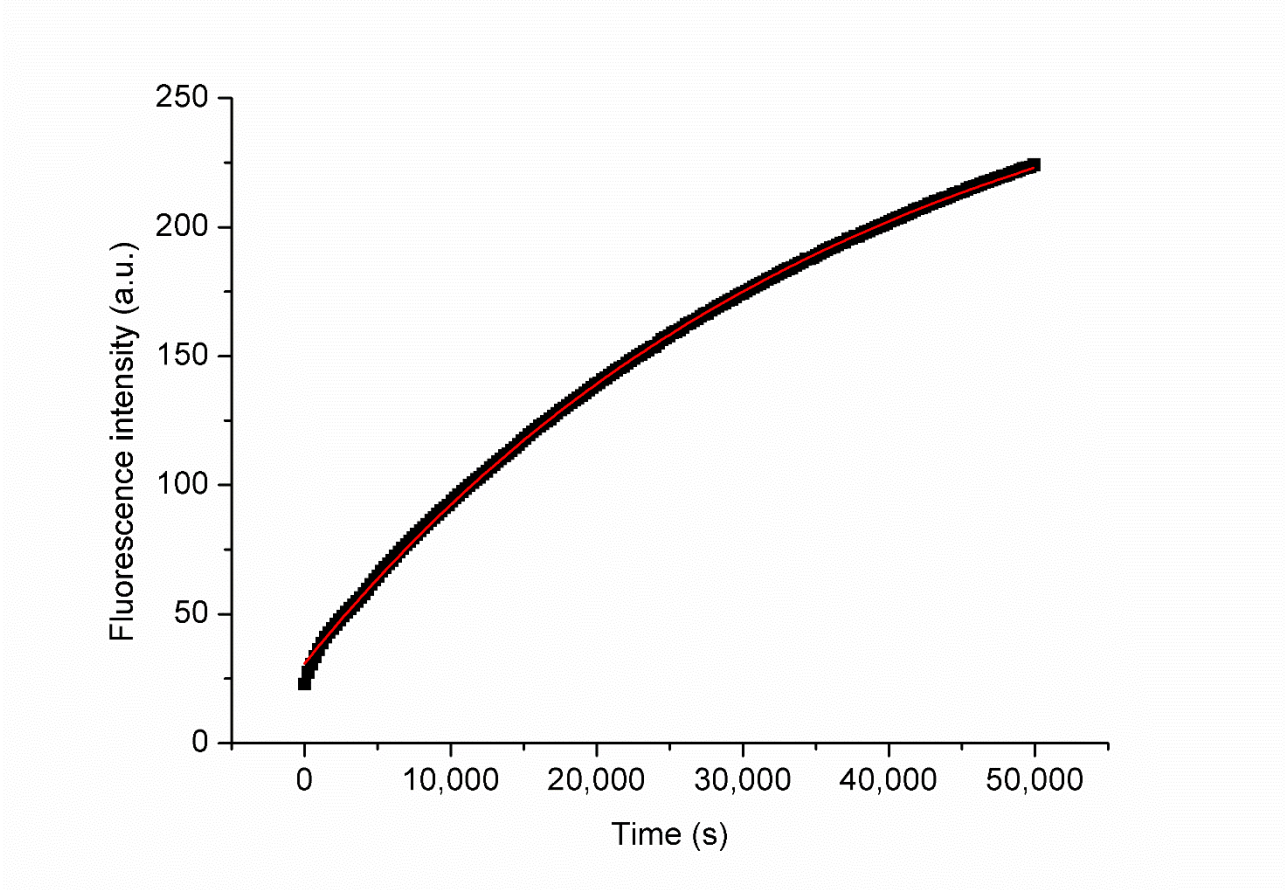


**Figure S34.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/TMCD 2.5 liposomes at 37° C.

**S2.4 Stability measurements for POPC/DACD liposomes**

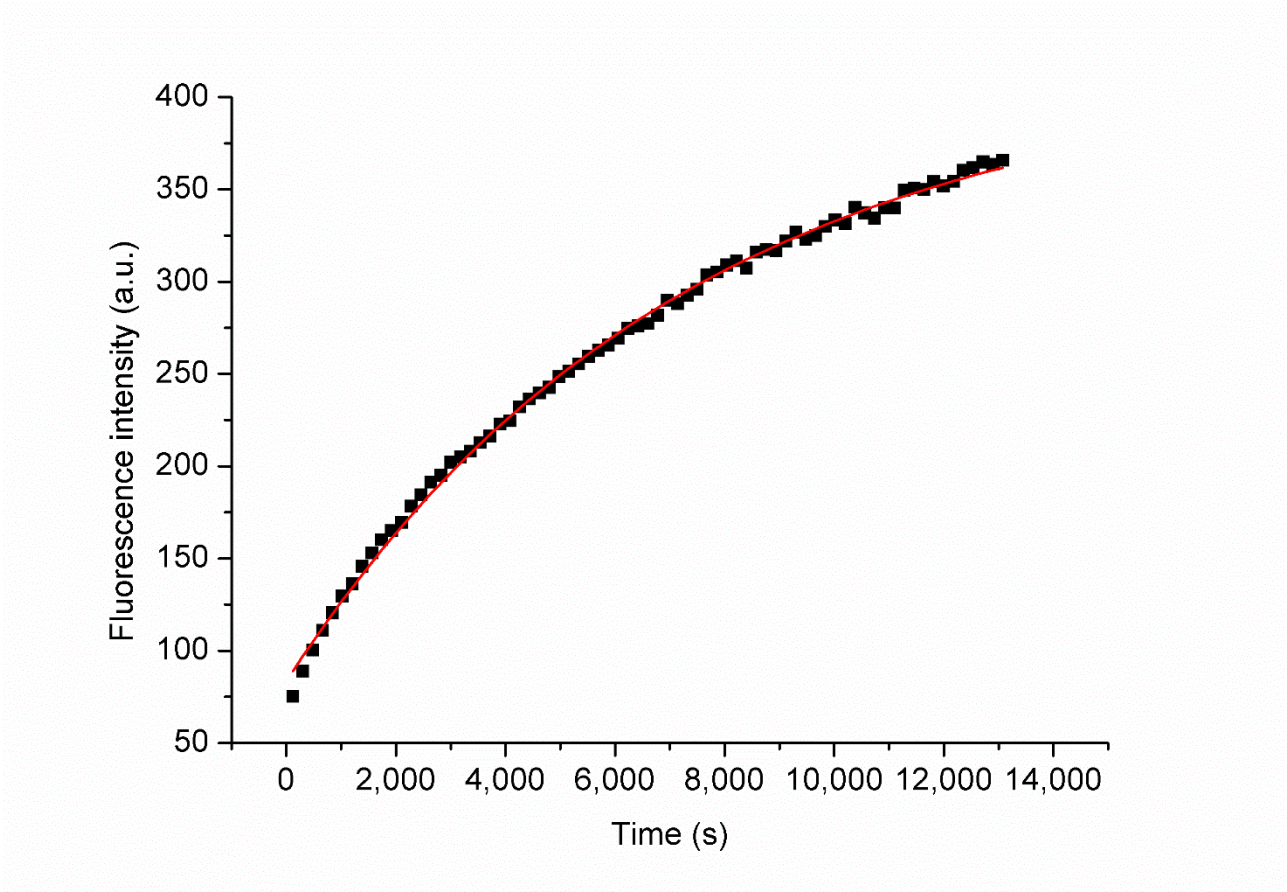


**Figure S35.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/DACD 12 liposomes at 25° C.

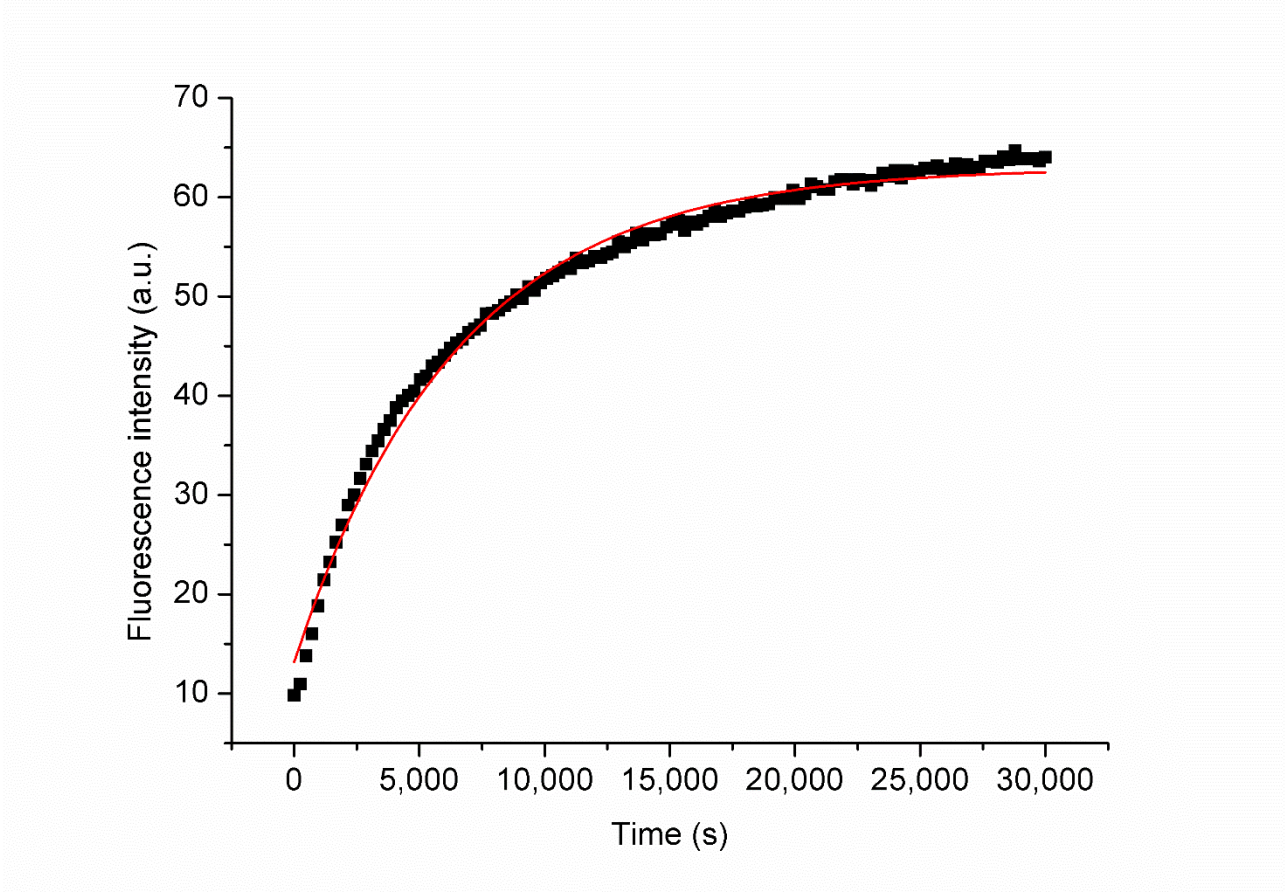


**Figure S36.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/DACD 12 liposomes at 37° C.

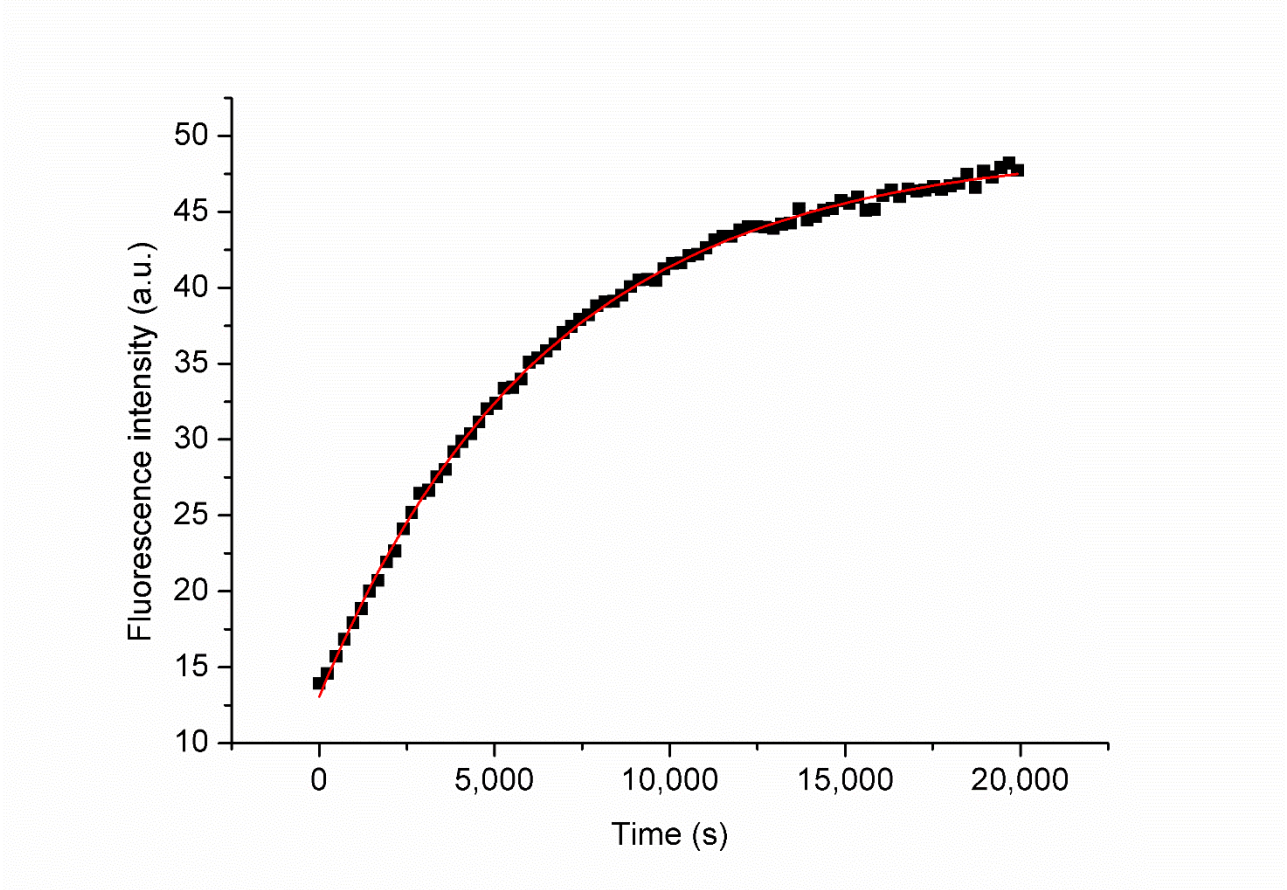


**Figure S37.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/DACD 5 liposomes at 25° C.

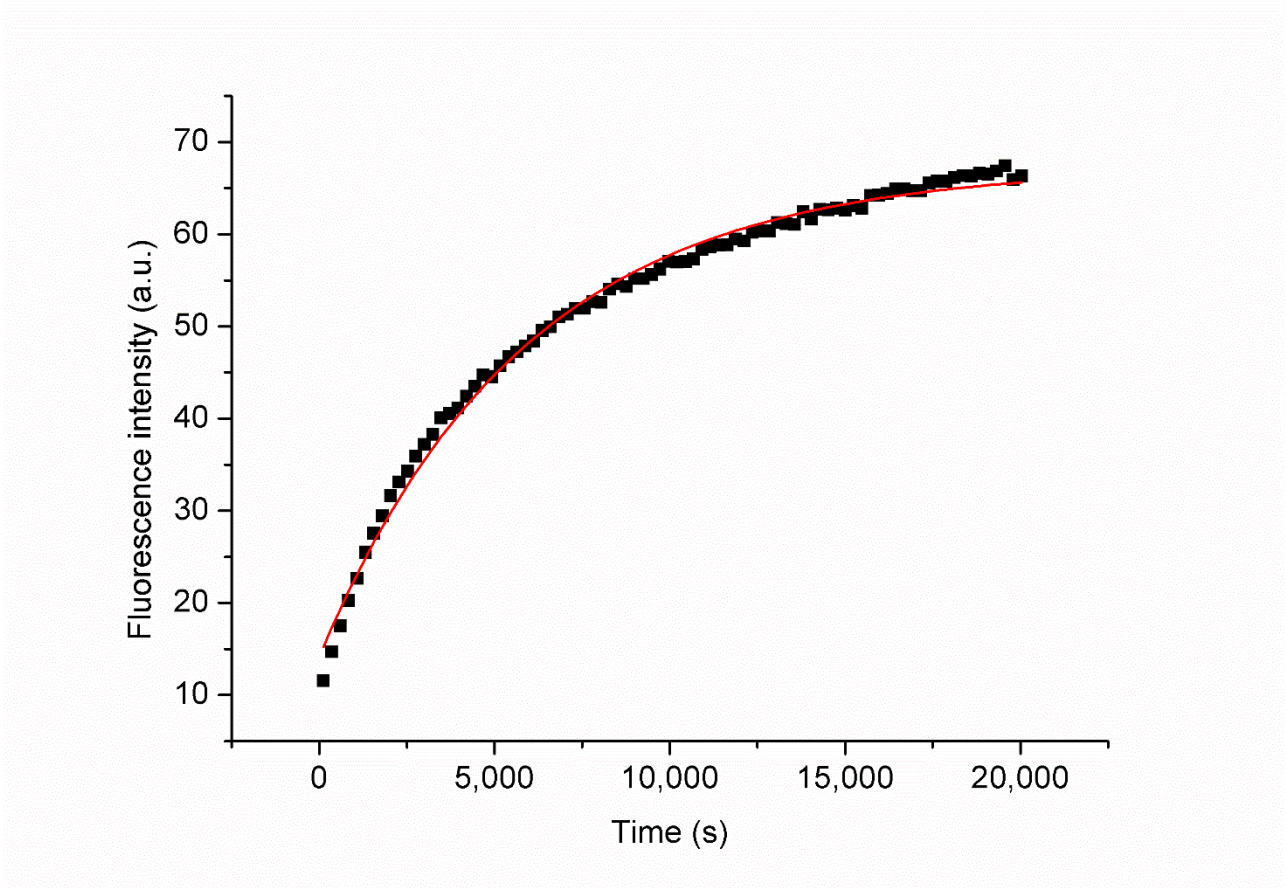


**Figure S38.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/DACD 5 liposomes at 37° C.

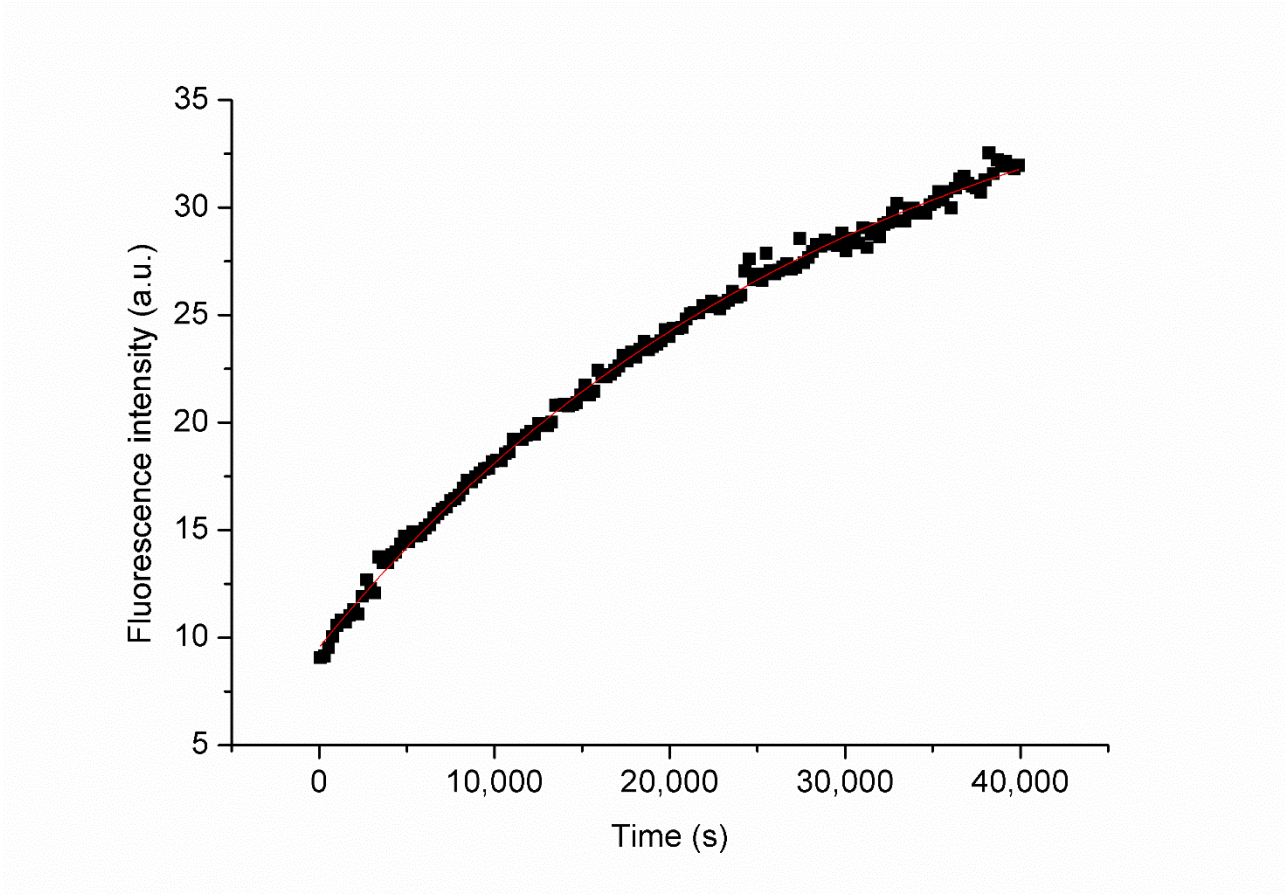


**Figure S39.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/DACD 2.5 liposomes at 25° C.

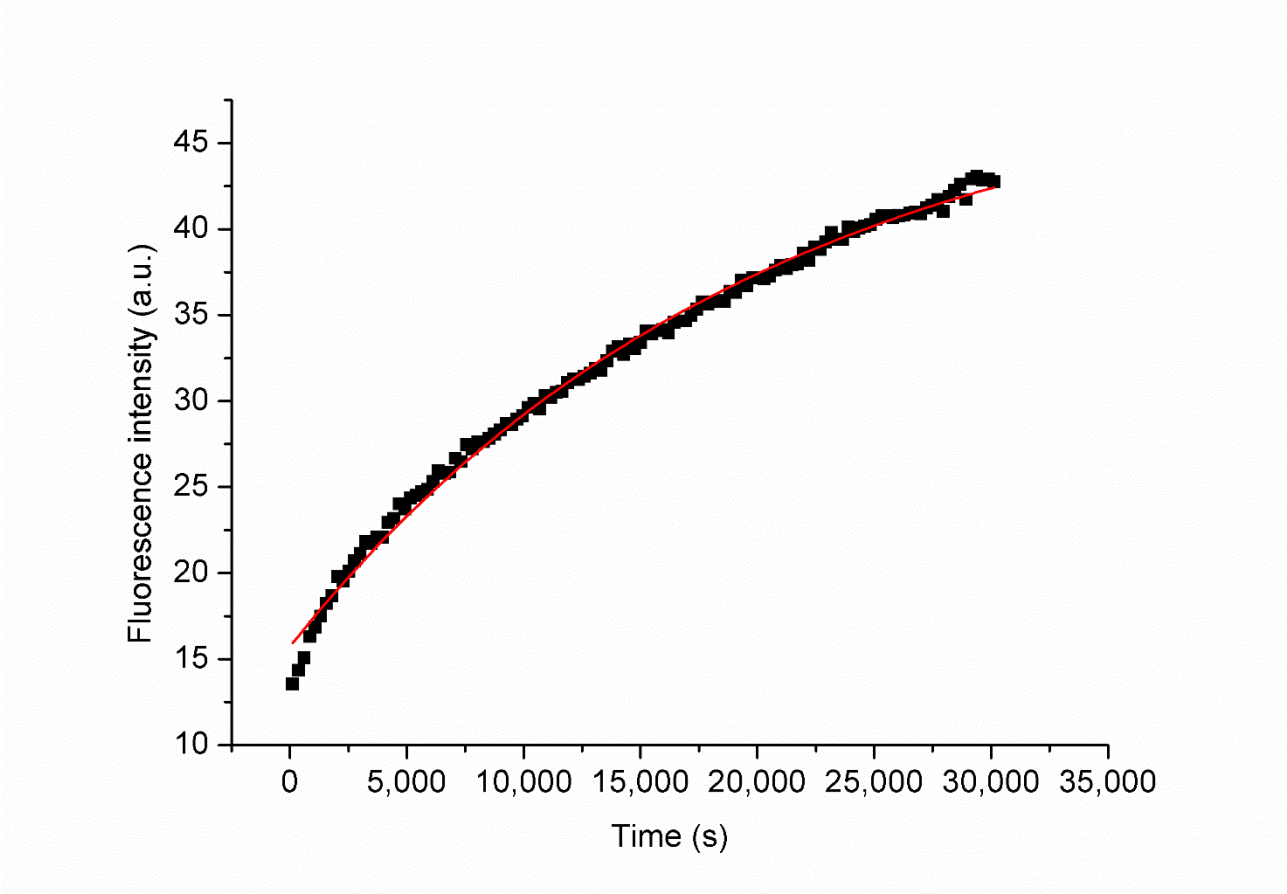


**Figure S40.** Representative kinetic profile of the release of $CF^{3-}$ from POPC/DACD 2.5 liposomes at 37° C.

## S3. Details of Molecular Dynamics Simulations

### S3.1 Cartesian coordinates of β-CD (Angstrom).

| | | | |
|---|---|---|---|
| O | 23.520000 | 21.980000 | 47.910000 |
| H | 24.450000 | 22.340000 | 47.970000 |
| C | 22.840000 | 21.890000 | 49.170000 |
| C | 23.680000 | 21.270000 | 50.280000 |
| O | 24.850000 | 22.080000 | 50.480000 |
| H | 25.390000 | 21.680000 | 51.220000 |
| C | 23.020000 | 21.080000 | 51.630000 |
| O | 23.950000 | 20.330000 | 52.440000 |
| C | 21.720000 | 20.360000 | 51.310000 |
| C | 20.740000 | 20.190000 | 52.470000 |
| O | 20.840000 | 18.930000 | 53.140000 |
| H | 20.230000 | 18.910000 | 53.930000 |
| O | 20.860000 | 20.910000 | 50.290000 |
| C | 21.630000 | 20.970000 | 49.070000 |
| O | 21.970000 | 19.610000 | 48.740000 |
| C | 21.320000 | 19.100000 | 47.560000 |
| C | 20.330000 | 18.000000 | 47.920000 |
| O | 21.090000 | 17.000000 | 48.630000 |
| C | 19.400000 | 17.580000 | 46.780000 |
| O | 18.400000 | 18.570000 | 46.530000 |
| H | 17.740000 | 18.120000 | 45.940000 |
| C | 22.440000 | 18.540000 | 46.710000 |
| O | 22.150000 | 18.250000 | 45.330000 |
| H | 22.940000 | 18.630000 | 44.840000 |
| C | 23.190000 | 17.410000 | 47.390000 |
| O | 24.080000 | 17.990000 | 48.360000 |
| H | 23.530000 | 18.490000 | 49.040000 |
| C | 22.120000 | 16.410000 | 47.810000 |
| O | 22.540000 | 15.280000 | 48.600000 |
| C | 23.130000 | 14.140000 | 47.960000 |
| C | 22.360000 | 12.820000 | 48.010000 |
| O | 23.100000 | 11.800000 | 47.310000 |
| C | 20.950000 | 12.810000 | 47.420000 |
| O | 21.000000 | 13.130000 | 46.030000 |
| H | 20.320000 | 12.570000 | 45.560000 |
| C | 24.510000 | 13.860000 | 48.530000 |
| O | 25.380000 | 15.000000 | 48.550000 |
| H | 24.740000 | 15.760000 | 48.640000 |
| C | 25.260000 | 12.720000 | 47.850000 |
| O | 26.550000 | 12.380000 | 48.380000 |
| H | 27.210000 | 13.020000 | 47.980000 |
| C | 24.380000 | 11.480000 | 47.880000 |
| O | 24.130000 | 11.020000 | 49.220000 |
| C | 24.080000 | 9.630000 | 49.600000 |
| C | 23.590000 | 9.460000 | 51.030000 |
| O | 24.560000 | 8.770000 | 51.850000 |

| | | | |
|---|---|---|---|
| C | 22.270000 | 8.700000 | 51.000000 |
| O | 21.330000 | 9.150000 | 50.010000 |
| H | 20.730000 | 9.810000 | 50.470000 |
| C | 25.340000 | 8.850000 | 49.270000 |
| O | 25.050000 | 7.440000 | 49.150000 |
| H | 25.670000 | 7.000000 | 48.500000 |
| C | 26.410000 | 9.080000 | 50.320000 |
| O | 27.250000 | 10.210000 | 50.020000 |
| H | 27.070000 | 10.490000 | 49.080000 |
| C | 25.960000 | 9.100000 | 51.770000 |
| O | 25.960000 | 10.340000 | 52.500000 |
| C | 26.940000 | 10.560000 | 53.540000 |
| C | 26.310000 | 11.000000 | 54.850000 |
| O | 27.330000 | 11.360000 | 55.800000 |
| C | 25.250000 | 10.070000 | 55.440000 |
| O | 24.040000 | 10.120000 | 54.680000 |
| H | 24.290000 | 9.790000 | 53.770000 |
| C | 27.840000 | 11.680000 | 53.060000 |
| O | 28.550000 | 11.480000 | 51.820000 |
| H | 27.890000 | 10.980000 | 51.260000 |
| C | 28.890000 | 12.070000 | 54.100000 |
| O | 29.870000 | 12.990000 | 53.580000 |
| H | 29.940000 | 12.760000 | 52.610000 |
| C | 28.280000 | 12.390000 | 55.450000 |
| O | 27.460000 | 13.580000 | 55.490000 |
| C | 27.710000 | 14.790000 | 56.240000 |
| C | 26.390000 | 15.340000 | 56.760000 |
| O | 26.570000 | 16.660000 | 57.300000 |
| C | 25.720000 | 14.470000 | 57.820000 |
| O | 25.350000 | 13.160000 | 57.360000 |
| H | 26.210000 | 12.770000 | 57.050000 |
| C | 28.450000 | 15.810000 | 55.390000 |
| O | 29.780000 | 15.480000 | 54.940000 |
| H | 29.700000 | 14.670000 | 54.360000 |
| C | 28.560000 | 17.170000 | 56.050000 |
| O | 29.240000 | 18.140000 | 55.230000 |
| H | 30.020000 | 17.650000 | 54.860000 |
| C | 27.210000 | 17.690000 | 56.520000 |
| O | 26.360000 | 17.850000 | 55.360000 |
| C | 25.760000 | 19.140000 | 55.150000 |
| C | 26.400000 | 19.790000 | 53.940000 |
| O | 27.810000 | 19.990000 | 54.130000 |
| H | 28.220000 | 19.250000 | 54.660000 |
| C | 25.860000 | 21.200000 | 53.760000 |
| O | 26.510000 | 21.960000 | 52.720000 |
| H | 27.490000 | 21.930000 | 52.920000 |
| C | 24.350000 | 21.110000 | 53.570000 |
| O | 23.760000 | 20.460000 | 54.710000 |
| C | 24.260000 | 19.120000 | 54.900000 |
| C | 23.530000 | 18.420000 | 56.050000 |
| O | 22.250000 | 17.900000 | 55.680000 |
| H | 22.340000 | 16.980000 | 55.290000 |

## S3.2 Cartesian coordinates of TMCD (Angstrom).

| | | | |
|---|---|---|---|
| O | 29.310000 | 29.210000 | 3.770000 |
| C | 29.210000 | 29.570000 | 2.420000 |
| C | 28.330000 | 29.920000 | 4.560000 |
| C | 28.800000 | 30.160000 | 5.980000 |
| O | 29.930000 | 31.050000 | 5.940000 |
| C | 31.140000 | 30.360000 | 6.140000 |
| C | 27.770000 | 30.760000 | 6.920000 |
| O | 28.210000 | 30.390000 | 8.240000 |
| C | 26.400000 | 30.160000 | 6.700000 |
| C | 25.300000 | 31.030000 | 7.330000 |
| O | 24.030000 | 30.380000 | 7.300000 |
| C | 23.820000 | 29.680000 | 8.490000 |
| O | 26.070000 | 30.010000 | 5.300000 |
| C | 26.990000 | 29.200000 | 4.550000 |
| O | 27.010000 | 27.860000 | 5.080000 |
| C | 26.350000 | 26.820000 | 4.330000 |
| C | 25.070000 | 26.330000 | 5.000000 |
| O | 24.500000 | 25.170000 | 4.380000 |
| C | 23.950000 | 27.370000 | 5.110000 |
| O | 23.590000 | 27.940000 | 3.840000 |
| C | 22.570000 | 28.880000 | 4.060000 |
| C | 27.300000 | 25.640000 | 4.160000 |
| O | 28.360000 | 26.040000 | 3.270000 |
| C | 29.610000 | 25.980000 | 3.900000 |
| C | 26.620000 | 24.420000 | 3.560000 |
| O | 27.480000 | 23.300000 | 3.280000 |
| C | 28.270000 | 22.770000 | 4.310000 |
| C | 25.370000 | 24.020000 | 4.330000 |
| O | 25.580000 | 23.500000 | 5.660000 |
| C | 24.670000 | 22.500000 | 6.160000 |
| C | 24.310000 | 22.820000 | 7.600000 |
| O | 23.720000 | 21.740000 | 8.340000 |
| C | 23.410000 | 24.050000 | 7.690000 |
| O | 22.210000 | 23.860000 | 6.930000 |
| C | 21.470000 | 25.050000 | 6.910000 |
| C | 25.270000 | 21.100000 | 6.040000 |
| O | 25.350000 | 20.660000 | 4.670000 |
| C | 24.150000 | 20.360000 | 4.020000 |
| C | 24.590000 | 20.060000 | 6.900000 |
| O | 25.100000 | 18.720000 | 6.790000 |
| C | 26.490000 | 18.520000 | 6.800000 |
| C | 24.480000 | 20.520000 | 8.350000 |
| O | 25.750000 | 20.770000 | 8.980000 |
| C | 26.100000 | 20.230000 | 10.270000 |
| C | 25.490000 | 20.980000 | 11.440000 |
| O | 26.450000 | 21.350000 | 12.450000 |
| C | 24.370000 | 20.150000 | 12.070000 |

| | | | |
|---|---|---|---|
| O | 23.710000 | 20.850000 | 13.120000 |
| C | 22.560000 | 21.470000 | 12.630000 |
| C | 27.620000 | 20.240000 | 10.340000 |
| O | 28.130000 | 19.260000 | 11.270000 |
| C | 28.460000 | 18.080000 | 10.590000 |
| C | 28.160000 | 21.620000 | 10.670000 |
| O | 27.960000 | 22.550000 | 9.590000 |
| C | 28.990000 | 22.490000 | 8.640000 |
| C | 27.580000 | 22.120000 | 11.980000 |
| O | 27.250000 | 23.520000 | 12.050000 |
| C | 27.780000 | 24.190000 | 13.210000 |
| C | 26.730000 | 25.010000 | 13.940000 |
| O | 27.300000 | 25.600000 | 15.120000 |
| C | 25.510000 | 24.190000 | 14.360000 |
| O | 24.490000 | 25.020000 | 14.900000 |
| C | 23.490000 | 24.220000 | 15.470000 |
| C | 28.900000 | 25.150000 | 12.840000 |
| O | 29.950000 | 24.500000 | 12.090000 |
| C | 30.170000 | 25.200000 | 10.900000 |
| C | 29.500000 | 25.780000 | 14.090000 |
| O | 30.530000 | 26.720000 | 13.750000 |
| C | 31.740000 | 26.380000 | 14.380000 |
| C | 28.420000 | 26.480000 | 14.890000 |
| O | 27.950000 | 27.710000 | 14.310000 |
| C | 27.610000 | 28.710000 | 15.290000 |
| C | 26.610000 | 29.690000 | 14.700000 |
| O | 27.020000 | 31.070000 | 14.720000 |
| C | 25.240000 | 29.500000 | 15.360000 |
| O | 25.270000 | 29.740000 | 16.770000 |
| C | 24.050000 | 29.350000 | 17.330000 |
| C | 28.810000 | 29.430000 | 15.870000 |
| O | 28.530000 | 29.960000 | 17.180000 |
| C | 29.150000 | 29.170000 | 18.150000 |
| C | 29.390000 | 30.520000 | 14.980000 |
| O | 30.430000 | 29.960000 | 14.160000 |
| C | 31.690000 | 30.230000 | 14.710000 |
| C | 28.350000 | 31.300000 | 14.200000 |
| O | 28.330000 | 31.030000 | 12.780000 |
| C | 28.630000 | 32.200000 | 12.000000 |
| C | 29.890000 | 31.970000 | 11.190000 |
| O | 30.500000 | 33.180000 | 10.720000 |
| C | 31.600000 | 33.520000 | 11.520000 |
| C | 29.730000 | 30.990000 | 10.040000 |
| O | 29.610000 | 29.630000 | 10.510000 |
| C | 30.870000 | 29.020000 | 10.540000 |
| C | 28.540000 | 31.410000 | 9.200000 |
| O | 27.360000 | 31.570000 | 10.010000 |
| C | 27.450000 | 32.520000 | 11.090000 |
| C | 27.430000 | 33.980000 | 10.640000 |
| O | 26.250000 | 34.300000 | 9.910000 |
| C | 26.220000 | 35.670000 | 9.640000 |

## S3.3 Cartesian coordinates of DACD (Angstrom).

| | | | |
|---|---|---|---|
| O | 39.010000 | 39.650000 | 13.940000 |
| C | 37.680000 | 40.090000 | 13.930000 |
| C | 39.600000 | 39.640000 | 15.260000 |
| C | 41.040000 | 40.120000 | 15.370000 |
| O | 41.200000 | 41.350000 | 14.640000 |
| C | 42.010000 | 41.110000 | 13.530000 |
| C | 41.520000 | 40.330000 | 16.800000 |
| O | 42.940000 | 40.570000 | 16.690000 |
| C | 41.360000 | 39.000000 | 17.530000 |
| C | 41.890000 | 38.950000 | 18.960000 |
| O | 41.910000 | 37.690000 | 19.650000 |
| H | 40.980000 | 37.330000 | 19.720000 |
| O | 40.050000 | 38.430000 | 17.330000 |
| C | 39.750000 | 38.290000 | 15.930000 |
| O | 40.750000 | 37.490000 | 15.270000 |
| C | 40.500000 | 36.100000 | 14.990000 |
| C | 40.630000 | 35.090000 | 16.120000 |
| O | 41.990000 | 34.820000 | 16.520000 |
| C | 39.850000 | 33.780000 | 15.980000 |
| O | 39.960000 | 32.950000 | 17.130000 |
| H | 39.170000 | 32.320000 | 17.110000 |
| C | 41.330000 | 35.550000 | 13.840000 |
| O | 40.730000 | 34.440000 | 13.130000 |
| C | 40.650000 | 34.760000 | 11.770000 |
| C | 42.780000 | 35.260000 | 14.200000 |
| O | 43.510000 | 36.450000 | 14.570000 |
| C | 44.840000 | 36.500000 | 14.150000 |
| C | 42.660000 | 34.290000 | 15.360000 |
| O | 43.950000 | 33.810000 | 15.760000 |
| C | 44.110000 | 32.690000 | 16.640000 |
| C | 45.220000 | 33.000000 | 17.640000 |
| O | 45.730000 | 31.900000 | 18.410000 |
| C | 44.850000 | 34.020000 | 18.720000 |
| O | 44.390000 | 35.300000 | 18.290000 |
| H | 43.480000 | 35.250000 | 17.880000 |
| C | 44.450000 | 31.370000 | 15.980000 |
| O | 43.470000 | 31.000000 | 14.990000 |
| C | 43.900000 | 30.970000 | 13.660000 |
| C | 44.860000 | 30.230000 | 16.900000 |
| O | 45.010000 | 28.920000 | 16.320000 |
| C | 43.910000 | 28.060000 | 16.230000 |
| C | 46.080000 | 30.740000 | 17.630000 |
| O | 47.290000 | 31.050000 | 16.900000 |
| C | 48.530000 | 30.620000 | 17.490000 |
| C | 48.970000 | 31.480000 | 18.670000 |
| O | 49.220000 | 32.830000 | 18.250000 |
| C | 50.130000 | 30.910000 | 19.500000 |
| O | 50.760000 | 31.770000 | 20.460000 |
| H | 50.290000 | 32.050000 | 21.290000 |

| | | | |
|---|---|---|---|
| C | 49.470000 | 30.720000 | 16.310000 |
| O | 50.750000 | 30.050000 | 16.300000 |
| C | 50.640000 | 28.740000 | 15.810000 |
| C | 49.650000 | 32.180000 | 15.910000 |
| O | 48.550000 | 32.860000 | 15.270000 |
| C | 48.860000 | 33.490000 | 14.060000 |
| C | 50.080000 | 33.000000 | 17.120000 |
| O | 50.220000 | 34.420000 | 16.890000 |
| C | 50.900000 | 35.190000 | 17.890000 |
| C | 50.090000 | 36.370000 | 18.420000 |
| O | 50.830000 | 37.100000 | 19.420000 |
| C | 48.700000 | 36.000000 | 18.930000 |
| O | 48.720000 | 34.920000 | 19.870000 |
| H | 48.940000 | 34.150000 | 19.270000 |
| C | 52.180000 | 35.820000 | 17.370000 |
| O | 53.070000 | 34.810000 | 16.860000 |
| C | 53.580000 | 35.150000 | 15.610000 |
| C | 52.890000 | 36.650000 | 18.420000 |
| O | 54.100000 | 37.260000 | 17.940000 |
| C | 55.250000 | 36.650000 | 18.460000 |
| C | 51.910000 | 37.770000 | 18.760000 |
| O | 51.490000 | 38.750000 | 17.790000 |
| C | 51.510000 | 40.110000 | 18.250000 |
| C | 50.460000 | 40.460000 | 19.300000 |
| O | 49.090000 | 40.440000 | 18.850000 |
| C | 50.910000 | 41.660000 | 20.130000 |
| O | 51.970000 | 41.260000 | 21.010000 |
| H | 51.650000 | 40.810000 | 21.850000 |
| C | 51.220000 | 40.840000 | 16.950000 |
| O | 51.460000 | 42.250000 | 17.180000 |
| C | 52.250000 | 42.800000 | 16.170000 |
| C | 49.820000 | 40.530000 | 16.450000 |
| O | 49.590000 | 39.250000 | 15.840000 |
| C | 50.090000 | 39.280000 | 14.540000 |
| C | 48.830000 | 40.940000 | 17.520000 |
| O | 47.500000 | 40.410000 | 17.330000 |
| C | 46.400000 | 41.290000 | 17.610000 |
| C | 45.760000 | 41.880000 | 16.370000 |
| O | 46.640000 | 42.690000 | 15.570000 |
| C | 46.630000 | 42.230000 | 14.240000 |
| C | 44.470000 | 42.570000 | 16.770000 |
| O | 43.840000 | 43.410000 | 15.780000 |
| C | 43.550000 | 44.670000 | 16.330000 |
| C | 43.460000 | 41.670000 | 17.460000 |
| O | 44.120000 | 41.160000 | 18.630000 |
| C | 45.380000 | 40.500000 | 18.420000 |
| C | 45.920000 | 40.070000 | 19.780000 |
| O | 46.980000 | 39.130000 | 19.690000 |
| H | 47.720000 | 39.500000 | 19.120000 |
| O | 36.880000 | 39.210000 | 14.040000 |
| C | 37.190000 | 41.400000 | 13.780000 |
| O | 42.210000 | 40.090000 | 12.930000 |

| | | | |
|---|---|---|---|
| C | 42.330000 | 42.290000 | 12.850000 |
| O | 40.730000 | 35.880000 | 11.350000 |
| C | 40.380000 | 33.760000 | 10.830000 |
| O | 45.170000 | 36.100000 | 13.070000 |
| C | 45.760000 | 37.160000 | 14.970000 |
| O | 44.920000 | 30.410000 | 13.380000 |
| C | 42.890000 | 31.320000 | 12.750000 |
| O | 42.920000 | 28.130000 | 16.920000 |
| C | 44.100000 | 26.960000 | 15.390000 |
| O | 49.750000 | 28.440000 | 15.070000 |
| C | 51.620000 | 27.810000 | 16.160000 |
| O | 49.520000 | 32.890000 | 13.260000 |
| C | 48.460000 | 34.800000 | 13.770000 |
| O | 53.320000 | 36.190000 | 15.070000 |
| C | 54.210000 | 34.150000 | 14.850000 |
| O | 55.270000 | 36.440000 | 19.640000 |
| C | 56.370000 | 36.710000 | 17.630000 |
| O | 52.220000 | 42.310000 | 15.070000 |
| C | 52.860000 | 44.050000 | 16.370000 |
| O | 50.030000 | 40.260000 | 13.840000 |
| C | 50.520000 | 38.130000 | 13.870000 |
| O | 45.600000 | 41.900000 | 13.730000 |
| C | 47.740000 | 42.390000 | 13.400000 |
| O | 44.380000 | 45.320000 | 16.910000 |
| C | 42.310000 | 45.310000 | 16.380000 |

## S3.4 Atom-types and charges for topology of β-CD (see S3.1).

[ atoms ]

| ; nr | type | resnr | resid | atom | cgnr | charge | mass |
|---|---|---|---|---|---|---|---|
| 1 | OA | 1 | 2 | OBX | 1 | -0.60 | 15.9994 |
| 2 | H | 1 | 2 | HBX | 1 | 0.42 | 1.0080 |
| 3 | CH1 | 1 | 2 | CBS | 1 | 0.1 | 13.0190 |
| 4 | CH1 | 1 | 2 | CBR | 1 | 0.45 | 13.0190 |
| 5 | OA | 1 | 2 | OBY | 1 | -0.60 | 15.9994 |
| 6 | H | 1 | 2 | HBY | 1 | 0.43 | 1.0080 |
| 7 | CH1 | 1 | 2 | CBQ | 1 | 0.10 | 13.0190 |
| 8 | OA | 1 | 2 | OBP | 2 | -0.64 | 15.9994 |
| 9 | CH1 | 1 | 2 | CBV | 2 | 0.38 | 13.0190 |
| 10 | CH2 | 1 | 2 | CBZ | 2 | 0.16 | 14.0270 |
| 11 | OA | 1 | 2 | OCA | 2 | -0.64 | 15.9994 |

```
12      H    1   2    HCA    2    0.43 1.0080
13      OA   1   2    OBU    2   -0.50 15.9994
14      CH1  1   2    CBT    2    0.45 13.0190
15      OA   1   2    O4     2   -0.58 15.9994
16      CH1  1   2    C4     3    0.10  13.0190
17      CH1  1   2    C5     3    0.38 13.0190
18      OA   1   2    O5     3   -0.50 15.9994
19      CH2  1   2    C6     3    0.16 14.0270
20      OA   1   2    O6     3   -0.64 15.9994
21      H    1   2    H63    3    0.43  1.0080
22      CH1  1   2    C3     3    0.45 13.0190
23      OA   1   2    O3     3   -0.60  15.9994
24      H    1   2    H32    3    0.43  1.0080
25      CH1  1   2    C2     4    0.10 13.0190
26      OA   1   2    O2     4   -0.60 15.9994
27      H    1   2    H22    4    0.43 1.0080
28      CH1  1   2    C1     4    0.45 13.0190
29      OA   1   2    O1     4   -0.58  15.9994
30      CH1  1   2    CAH    4    0.10 13.0190
31      CH1  1   2    CAM    4    0.38 13.0190
32      OA   1   2    OAL    4   -0.50 15.9994
33      CH2  1   2    CCT    5    0.16 14.0270
34      OA   1   2    OCU    5   -0.64 15.9994
35      H    1   2    HCU    5    0.43 1.0080
36      CH1  1   2    CAI    6    0.45 13.0190
37      OA   1   2    OCS    6   -0.60 15.9994
38      H    1   2    HCS    6    0.43  1.0080
39      CH1  1   2    CAJ    7    0.10  13.0190
40      OA   1   2    OCR    7   -0.60 15.9994
41      H    1   2    HCR    7    0.43  1.0080
42      CH1  1   2    CAK    7    0.45 13.0190
43      OA   1   2    OAN    7   -0.58 15.9994
44      CH1  1   2    CAO    7    0.10 13.0190
```

45 CH1 1 2 CAT 7 0.38 13.0190

46 OA 1 2 OAS 7 -0.50 15.9994

47 CH2 1 2 CCP 8 0.16 14.0270

48 OA 1 2 OCQ 8 -0.64 15.9994

49 H 1 2 HCQ 8 0.43 1.0080

50 CH1 1 2 CAP 9 0.45 13.0190

51 OA 1 2 OCO 9 -0.60 15.9994

52 H 1 2 HCO 9 0.43 1.0080

53 CH1 1 2 CAQ 10 0.10 13.0190

54 OA 1 2 OCN 10 -0.60 15.9994

55 H 1 2 HCN 10 0.43 1.0080

56 CH1 1 2 CAR 10 0.45 13.0190

57 OA 1 2 OAU 10 -0.58 15.9994

58 CH1 1 2 CAV 10 0.10 13.0190

59 CH1 1 2 CBA 10 0.38 13.0190

60 OA 1 2 OAZ 10 -0.50 15.9994

61 CH2 1 2 CCL 11 0.16 14.0270

62 OA 1 2 OCM 11 -0.64 15.9994

63 H 1 2 HCM 11 0.43 1.0080

64 CH1 1 2 CAW 12 0.45 13.0190

65 OA 1 2 OCK 12 -0.60 15.9994

66 H 1 2 HCK 12 0.43 1.0080

67 CH1 1 2 CAX 13 0.10 13.0190

68 OA 1 2 OCJ 13 -0.60 15.9994

69 H 1 2 HCJ 13 0.43 1.0080

70 CH1 1 2 CAY 13 0.45 13.0190

71 OA 1 2 OBB 13 -0.58 15.9994

72 CH1 1 2 CBC 13 0.10 13.0190

73 CH1 1 2 CBH 13 0.38 13.0190

74 OA 1 2 OBG 13 -0.50 15.9994

75 CH2 1 2 CCH 14 0.16 14.0270

76 OA 1 2 OCI 14 -0.64 15.9994

77 H 1 2 HCI 14 0.43 1.0080

```
   78      CH1    1   2    CBD    14    0.45 13.0190
   79       OA    1   2    OCG    14    -0.60 15.9994
   80        H    1   2    HCG    14    0.43  1.0080
   81      CH1    1   2    CBE    14    0.10 13.0190
   82       OA    1   2    OCF    14    -0.60 15.9994
   83        H    1   2    HCF    14    0.43  1.0080
   84      CH1    1   2    CBF    14    0.45 13.0190
   85       OA    1   2    OBI    15    -0.58 15.9994
   86      CH1    1   2    CBJ    15    0.10 13.0190
   87      CH1    1   2    CBK    15    0.45 13.0190
   88       OA    1   2    OCC    15    -0.60 15.9994
   89        H    1   2    HCC    15    0.43 1.0080
   90      CH1    1   2    CBL    16    0.10 13.0190
   91       OA    1   2    OCB    16    -0.60 15.9994
   92        H    1   2    HCB    16    0.43 1.0080
   93      CH1    1   2    CBM    16    0.45 13.0190
   94       OA    1   2    OBN    16    -0.50 15.9994
   95      CH1    1   2    CBO    16    0.38 13.0190
   96      CH2    1   2    CCD    16    0.16 14.0270
   97       OA    1   2    OCE    16    -0.64 15.9994
   98        H    1   2    HCE    16    0.43 1.0080
```

## S3.5 Atom-types and charges for topology of TMCD (see S3.1).

```
 [ atoms ]
;  nr     type  resnr resid  atom  cgnr   charge     mass
    1       OA    1   _2    OBX    1   -0.18  15.9994
    2      CH3    1   _2      C    1    0.05  15.000
    3      CH1    1   _2    CBS    1    0.1 13.0190
    4      CH1    1   _2    CBR    1    0.30 13.0190
    5       OA    1   _2    OBY    1    -0.20 15.9994
    6      CH3    1   _2    HBX    1    0.05  15.000
    7      CH1    1   _2    CBQ    1    0.10 13.0190
```

8 OA 1 _2 OBP 2 -0.20 15.9994

9 CH1 1 _2 CBV 2 0.22 13.0190

10 CH2 1 _2 CBZ 2 0.16 14.0270

11 OA 1 _2 OCA 2 -0.20 15.9994

12 CH3 1 _2 HBX 2 0.05 15.000

13 OA 1 _2 OBU 2 -0.40 15.9994

14 CH1 1 _2 CBT 2 0.30 13.0190

15 OA 1 _2 O4 2 -0.35 15.9994

16 CH1 1 _2 C4 3 0.10 13.0190

17 CH1 1 _2 C5 3 0.22 13.0190

18 OA 1 _2 O5 3 -0.40 15.9994

19 CH2 1 _2 C6 3 0.16 14.0270

20 OA 1 _2 O6 3 -0.20 15.9994

21 CH3 1 _2 HBX 3 0.05 15.000

22 CH1 1 _2 C3 3 0.30 13.0190

23 OA 1 _2 O3 3 -0.20 15.9994

24 CH3 1 _2 HBX 3 0.05 15.000

25 CH1 1 _2 C2 4 0.10 13.0190

26 OA 1 _2 O2 4 -0.20 15.9994

27 CH3 1 _2 HBX 4 0.05 15.000

28 CH1 1 _2 C1 4 0.30 13.0190

29 OA 1 _2 O1 4 -0.35 15.9994

30 CH1 1 _2 CAH 4 0.10 13.0190

31 CH1 1 _2 CAM 4 0.22 13.0190

32 OA 1 _2 OAL 4 -0.40 15.9994

33 CH2 1 _2 CCT 5 0.16 14.0270

34 OA 1 _2 OCU 5 -0.20 15.9994

35 CH3 1 _2 HBX 5 0.05 15.000

36 CH1 1 _2 CAI 6 0.30 13.0190

37 OA 1 _2 OCS 6 -0.20 15.9994

38 CH3 1 _2 HBX 6 0.05 15.000

39 CH1 1 _2 CAJ 7 0.10 13.0190

40 OA 1 _2 OCR 7 -0.20 15.9994

41 CH3 1 _2 HBX 7 0.05 15.000

42 CH1 1 _2 CAK 7 0.30 13.0190

43 OA 1 _2 OAN 7 -0.35 15.9994

44 CH1 1 _2 CAO 7 0.10 13.0190

45 CH1 1 _2 CAT 7 0.22 13.0190

46 OA 1 _2 OAS 7 -0.40 15.9994

47 CH2 1 _2 CCP 8 0.16 14.0270

48 OA 1 _2 OCQ 8 -0.20 15.9994

49 CH3 1 _2 HBX 8 0.05 15.000

50 CH1 1 _2 CAP 9 0.30 13.0190

51 OA 1 _2 OCO 9 -0.20 15.9994

52 CH3 1 _2 HBX 9 0.05 15.000

53 CH1 1 _2 CAQ 10 0.10 13.0190

54 OA 1 _2 OCN 10 -0.20 15.9994

55 CH3 1 _2 HBX 10 0.05 15.000

56 CH1 1 _2 CAR 10 0.30 13.0190

57 OA 1 _2 OAU 10 -0.35 15.9994

58 CH1 1 _2 CAV 10 0.10 13.0190

59 CH1 1 _2 CBA 10 0.22 13.0190

60 OA 1 _2 OAZ 10 -0.40 15.9994

61 CH2 1 _2 CCL 11 0.16 14.0270

62 OA 1 _2 OCM 11 -0.20 15.9994

63 CH3 1 _2 HBX 11 0.05 15.000

64 CH1 1 _2 CAW 12 0.30 13.0190

65 OA 1 _2 OCK 12 -0.20 15.9994

66 CH3 1 _2 HBX 12 0.05 15.000

67 CH1 1 _2 CAX 13 0.10 13.0190

68 OA 1 _2 OCJ 13 -0.20 15.9994

69 CH3 1 _2 HBX 13 0.04 15.000

70 CH1 1 _2 CAY 13 0.30 13.0190

71 OA 1 _2 OBB 13 -0.35 15.9994

72 CH1 1 _2 CBC 13 0.10 13.0190

73 CH1 1 _2 CBH 13 0.22 13.0190

74 OA 1 _2 OBG 13 -0.40 15.9994

75 CH2 1 _2 CCH 14 0.16 14.0270

76 OA 1 _2 OCI 14 -0.20 15.9994

77 CH3 1 _2 HBX 14 0.05 15.000

78 CH1 1 _2 CBD 14 0.30 13.0190

79 OA 1 _2 OCG 14 -0.20 15.9994

80 CH3 1 _2 HBX 14 0.04 15.000

81 CH1 1 _2 CBE 14 0.10 13.0190

82 OA 1 _2 OCF 14 -0.20 15.9994

83 CH3 1 _2 HBX 14 0.05 15.000

84 CH1 1 _2 CBF 14 0.30 13.0190

85 OA 1 _2 OBI 15 -0.35 15.9994

86 CH1 1 _2 CBJ 15 0.10 13.0190

87 CH1 1 _2 CBK 15 0.30 13.0190

88 OA 1 _2 OCC 15 -0.20 15.9994

89 CH3 1 _2 HBX 15 0.05 15.000

90 CH1 1 _2 CBL 16 0.10 13.0190

91 OA 1 _2 OCB 16 -0.20 15.9994

92 CH3 1 _2 HBX 16 0.05 15.000

93 CH1 1 _2 CBM 16 0.30 13.0190

94 OA 1 _2 OBN 16 -0.40 15.9994

95 CH1 1 _2 CBO 16 0.22 13.0190

96 CH2 1 _2 CCD 16 0.16 14.0270

97 OA 1 _2 OCE 16 -0.20 15.9994

98 CH3 1 _2 HBX 16 0.04 15.000

## S3.6 Atom-types and charges for topology of DACD (see S3.1).

[ atoms ]

; nr type resnr resid atom cgnr charge mass

1 OA 1 _2 OBX 1 -0.50 15.9994

2 C 1 _2 C 1 0.70 12.0080

3 CH1 1 _2 CBS 1 0.1074 13.0190

4 CH1 1 _2 CBR 1 0.45 13.0190

5 OA 1 _2 OBY 1 -0.50 15.9994

6 C 1 _2 C 1 0.70 12.0080

7 CH1 1 _2 CBQ 1 0.10 13.0190

8 OA 1 _2 OBP 2 -0.50 15.9994

9 CH1 1 _2 CBV 2 0.38 13.0190

10 CH2 1 _2 CBZ 2 0.16 14.0270

11 OA 1 _2 OCA 2 -0.50 15.9994

12 H 1 _2 HCA 2 0.43 1.0080

13 OA 1 _2 OBU 2 -0.50 15.9994

14 CH1 1 _2 CBT 2 0.45 13.0190

15 OA 1 _2 O4 2 -0.55 15.9994

16 CH1 1 _2 C4 3 0.10 13.0190

17 CH1 1 _2 C5 3 0.38 13.0190

18 OA 1 _2 O5 3 -0.50 15.9994

19 CH2 1 _2 C6 3 0.16 14.0270

20 OA 1 _2 O6 3 -0.50 15.9994

21 H 1 _2 H63 3 0.43 1.0080

22 CH1 1 _2 C3 3 0.45 13.0190

23 OA 1 _2 O3 3 -0.50 15.9994

24 C 1 _2 C 3 0.70 12.0080

25 CH1 1 _2 C2 4 0.10 13.0190

26 OA 1 _2 O2 4 -0.50 15.9994

27 C 1 _2 C 4 0.70 12.080

28 CH1 1 _2 C1 4 0.45 13.0190

29 OA 1 _2 O1 4 -0.55 15.9994

30 CH1 1 _2 CAH 4 0.10 13.0190

31 CH1 1 _2 CAM 4 0.38 13.0190

32 OA 1 _2 OAL 4 -0.50 15.9994

33 CH2 1 _2 CCT 5 0.16 14.0270

34 OA 1 _2 OCU 5 -0.50 15.9994

35 H 1 _2 HCU 5 0.43 1.0080

36 CH1 1 _2 CAI 6 0.45 13.0190

37 OA 1 _2 OCS 6 -0.50 15.9994

38 C 1 _2 C 6 0.70 12.080

39 CH1 1 _2 CAJ 7 0.10 13.0190

40 OA 1 _2 OCR 7 -0.50 15.9994

41 C 1 _2 C 7 0.70 12.080

42 CH1 1 _2 CAK 7 0.45 13.0190

43 OA 1 _2 OAN 7 -0.55 15.9994

44 CH1 1 _2 CAO 7 0.10 13.0190

45 CH1 1 _2 CAT 7 0.38 13.0190

46 OA 1 _2 OAS 7 -0.50 15.9994

47 CH2 1 _2 CCP 8 0.16 14.0270

48 OA 1 _2 OCQ 8 -0.50 15.9994

49 H 1 _2 HCQ 8 0.43 1.0080

50 CH1 1 _2 CAP 9 0.45 13.0190

51 OA 1 _2 OCO 9 -0.50 15.9994

52 C 1 _2 C 9 0.70 12.080

53 CH1 1 _2 CAQ 10 0.10 13.0190

54 OA 1 _2 OCN 10 -0.50 15.9994

55 C 1 _2 C 10 0.70 12.080

56 CH1 1 _2 CAR 10 0.45 13.0190

57 OA 1 _2 OAU 10 -0.55 15.9994

58 CH1 1 _2 CAV 10 0.10 13.0190

59 CH1 1 _2 CBA 10 0.38 13.0190

60 OA 1 _2 OAZ 10 -0.50 15.9994

61 CH2 1 _2 CCL 11 0.16 14.0270

62 OA 1 _2 OCM 11 -0.50 15.9994

63 H 1 _2 HCM 11 0.43 1.0080

64 CH1 1 _2 CAW 12 0.45 13.0190

65 OA 1 _2 OCK 12 -0.50 15.9994

66 C 1 _2 C 12 0.70 12.080

67 CH1 1 _2 CAX 13 0.10 13.0190

68 OA 1 _2 OCJ 13 -0.50 15.9994

69 C 1 _2 C 13 0.70 12.080

70 CH1 1 _2 CAY 13 0.45 13.0190

71 OA 1 _2 OBB 13 -0.55 15.9994

72 CH1 1 _2 CBC 13 0.10 13.0190

73 CH1 1 _2 CBH 13 0.38 13.0190

74 OA 1 _2 OBG 13 -0.50 15.9994

75 CH2 1 _2 CCH 14 0.16 14.0270

76 OA 1 _2 OCI 14 -0.50 15.9994

77 H 1 _2 HCI 14 0.43 1.0080

78 CH1 1 _2 CBD 14 0.45 13.0190

79 OA 1 _2 OCG 14 -0.50 15.9994

80 C 1 _2 C 14 0.70 12.0080

81 CH1 1 _2 CBE 14 0.10 13.0190

82 OA 1 _2 OCF 14 -0.50 15.9994

83 C 1 _2 C 14 0.70 12.0080

84 CH1 1 _2 CBF 14 0.45 13.0190

85 OA 1 _2 OBI 15 -0.55 15.9994

86 CH1 1 _2 CBJ 15 0.10 13.0190

87 CH1 1 _2 CBK 15 0.45 13.0190

88 OA 1 _2 OCC 15 -0.50 15.9994

89 C 1 _2 C 15 0.70 12.080

90 CH1 1 _2 CBL 16 0.10 13.0190

91 OA 1 _2 OCB 16 -0.50 15.9994

92 C 1 _2 C 16 0.70 12.080

93 CH1 1 _2 CBM 16 0.45 13.0190

94 OA 1 _2 OBN 16 -0.50 15.9994

95 CH1 1 _2 CBO 16 0.38 13.0190

96 CH2 1 _2 CCD 16 0.16 14.0270

97 OA 1 _2 OCE 16 -0.50 15.9994

98 H 1 _2 HCE 16 0.43 1.0080

99 O 1 _2 O 17 -0.56 16.00

100 CH3 1 _2 C 18 0.0959 15.

101 O 1 _2 O 19 -0.56 16.00

102 CH3 1 _2 C 20 0.0959 15.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 103 | O | 1 | _2 | O | 21 | -0.56 | 16.00 |
| 104 | CH3 | 1 | _2 | C | 22 | 0.0959 | 15. |
| 105 | O | 1 | _2 | O | 23 | -0.56 | 16.00 |
| 106 | CH3 | 1 | _2 | C | 24 | 0.0959 | 15. |
| 107 | O | 1 | _2 | O | 25 | -0.56 | 16.00 |
| 108 | CH3 | 1 | _2 | C | 26 | 0.0959 | 15. |
| 109 | O | 1 | _2 | O | 27 | -0.56 | 16.00 |
| 110 | CH3 | 1 | _2 | C | 28 | 0.0959 | 15. |
| 111 | O | 1 | _2 | O | 29 | -0.56 | 16.00 |
| 112 | CH3 | 1 | _2 | C | 30 | 0.0959 | 15. |
| 113 | O | 1 | _2 | O | 31 | -0.56 | 16.00 |
| 114 | CH3 | 1 | _2 | C | 32 | 0.0959 | 15. |
| 115 | O | 1 | _2 | O | 33 | -0.56 | 16.00 |
| 116 | CH3 | 1 | _2 | C | 34 | 0.0959 | 15. |
| 117 | O | 1 | _2 | O | 35 | -0.56 | 16.00 |
| 118 | CH3 | 1 | _2 | C | 36 | 0.0959 | 15. |
| 119 | O | 1 | _2 | O | 37 | -0.56 | 16.00 |
| 120 | CH3 | 1 | _2 | C | 38 | 0.0959 | 15. |
| 121 | O | 1 | _2 | O | 39 | -0.56 | 16.00 |
| 122 | CH3 | 1 | _2 | C | 40 | 0.0959 | 15. |
| 123 | O | 1 | _2 | O | 41 | -0.56 | 16.00 |
| 124 | CH3 | 1 | _2 | C | 42 | 0.0959 | 15. |
| 125 | O | 1 | _2 | O | 43 | -0.56 | 16.00 |
| 126 | CH3 | 1 | _2 | C | 44 | 0.0959 | 15. |