**Examples of lipid numbers for lipid transfer analysis**

**0% PS/Chol**

Basal condition (no lipid transfer)

Donor: 500 DOPE, 1500 DOPC

Acceptor: 500 DOPE, 1500 DOPC

1% Donor to acceptor

Donor: 495 DOPE, 1485 DOPC

Acceptor: 505 DOPE, 1115 DOPC, 400 DOPS, 0 Cholesterol

1% Acceptor to donor

Donor: 505 DOPE, 1515 DOPC

Acceptor: 495 DOPE, 1085 DOPC, 400 DOPS, 0 Cholesterol

5% Donor to acceptor

Donor: 475 DOPE, 1425 DOPC

Acceptor: 525 DOPE, 1575 DOPC

5% Acceptor to donor

Donor: 525 DOPE, 1575 DOPC

Acceptor: 475 DOPE, 1425 DOPC, 0 DOPS, 0 Cholesterol

**20% PS/Chol**

Basal condition (no lipid transfer)

Donor: 500 DOPE, 1500 DOPC

Acceptor: 500 DOPE, 700 DOPC, 400 DOPS, 400 Cholesterol

5% Donor to acceptor

Donor: 475 DOPE, 1425 DOPC

Acceptor: 525 DOPE, 775 DOPC, 400 DOPS, 400 Cholesterol

**Author note**

We met some random bugs in the running and we typically solve them in this way:

1. If the generation of input is not successful (due to CHARMM-GUI high demand), we retry it

2. If the run fails to equilibrate, we adjust the lipid to +- 1/2 more or less and retry. These data are highlighted in red. We randomly chose one if both two trials succeed. Also, due to historical reasons, we have 5% run twice. We randomly chose one - a change in a single point should not affect the trend seen in the paper.

**Source data records**

**0% PS, 0% cholesterol in acceptor:**

Basal

4412267980/4412267980: total\_Ave -1716540.6 total\_EstErr 1180.0 total\_RMSD 3563.906

Donor to acceptor 5%, 10%, 15%, 20%, 25%, 30% - looks to have similar changes with acceptor-to-donor

4412268666/4412269640: total\_Ave -1716749.8 total\_EstErr 777.0 total\_RMSD 3104.709

4412270527/4412271561: total\_Ave -1715420.5 total\_EstErr 971.0 total\_RMSD 2922.737

4412272536/4412354929: total\_Ave -1716237.43 total\_EstErr 608.0 total\_RMSD 2732.9840000000004

4430641793/4412354923: total\_Ave -1716257.25 total\_EstErr 630.0 total\_RMSD 2460.215

4412354924/4412359788: total\_Ave -1714771.67 total\_EstErr 781.0 total\_RMSD 2789.252

4412373687/4412385380: total\_Ave -1715220.3199999998 total\_EstErr 777.0 total\_RMSD 2669.227

Acceptor to donor 5%, 10%, 15%

4412385382/4412387016: total\_Ave -1713700.5 total\_EstErr 473.0 total\_RMSD 2524.879

4412387017/4412387015: total\_Ave -1715551.7999999998 total\_EstErr 656.0 total\_RMSD 2554.312

4412387013/4412429634: total\_Ave -1713039.15 total\_EstErr 497.0 total\_RMSD 2468.415

4552210899/4552211398: total\_Ave -1713652.61 total\_EstErr 447.0 total\_RMSD 2257.252

4552211996/4552212720: total\_Ave -1715179.1400000001 total\_EstErr 942.0 total\_RMSD 2963.457

4552348528/4552485990: total\_Ave -1716039.42 total\_EstErr 755.0 total\_RMSD 3071.706

Donor to acceptor 1%, 3%, 5%

4311942768/4325167595: total\_Ave -1716566.6 total\_EstErr 424.0 total\_RMSD 2230.429

4311944239/4325168510: total\_Ave -1715479.2 total\_EstErr 740.0 total\_RMSD 2675.148

4311947424/4325169340: total\_Ave -1715993.1 total\_EstErr 656.0 total\_RMSD 2550.25

Acceptor to donor 1%, 3%, 5%

4312047244/4325170195: total\_Ave -1714323.6 total\_EstErr 637.0 total\_RMSD 2544.659

4312050724/4325170960: total\_Ave -1714895.7999999998 total\_EstErr 641.0 total\_RMSD 2344.282

4312054877/4325172097: total\_Ave -1714700.0 total\_EstErr 619.0 total\_RMSD 2509.883

**20% PS, 20% cholesterol in acceptor:**

Basal

4412267980/4430647936: total\_Ave -1639750.9700000002 total\_EstErr 844.0 total\_RMSD 3111.95

Donor to acceptor 5%, 10%, 15%, 20%, 25%, 30% - looks to be energy favored

4412268666/4412431415: total\_Ave -1642016.4100000001 total\_EstErr 858.0 total\_RMSD 3024.036

4412270527/4412432331: total\_Ave -1642057.83 total\_EstErr 634.0 total\_RMSD 2575.709

4412272536/4412447442: total\_Ave -1643334.02 total\_EstErr 522.0 total\_RMSD 2584.115

4430641793/4412486423: total\_Ave -1642056.15 total\_EstErr 627.0 total\_RMSD 2371.6710000000003

4412354924/4412447446: total\_Ave -1640822.4700000002 total\_EstErr 713.0 total\_RMSD 2458.5190000000002

~~4412373687/4430656543 failed~~

Add

Donor: 349 DOPE, 1047 DOPC (ID: 4606498400)

Acceptor: 651 DOPE, 1153 DOPC, 400 DOPS, 400 Cholesterol (ID: 4606498540)

Donor: 348 DOPE, 1044 DOPC (ID: 4606498678)

Acceptor: 652 DOPE, 1156 DOPC, 400 DOPS, 400 Cholesterol (ID: 4606498844)

4606498400/4606498540: total\_Ave -1641928.06 total\_EstErr 437.0 total\_RMSD 2323.1319999999996

4606498678/4606498844: total\_Ave -1642110.95 total\_EstErr 508.0 total\_RMSD 2448.5429999999997

Accceptor to donor 5%, 10%, 15%, 20%, 25%, 30% - looks to be not energy favored

4412269640/4412487276: total\_Ave -1640834.83 total\_EstErr 987.0 total\_RMSD 3222.515

~~4412271561/4412488039~~

Add

Donor: 549 DOPE, 1647 DOPC (ID: 4606499014)

Acceptor: 451 DOPE, 553 DOPC, 400 DOPS, 400 Cholesterol (ID: 4606499180)

Donor: 548 DOPE, 1644 DOPC (ID: 4606499333)

Acceptor: 452 DOPE, 556 DOPC, 400 DOPS, 400 Cholesterol (ID: 4606499468)

4606499333/4606499468: total\_Ave -1640776.6 total\_EstErr 892.0 total\_RMSD 2944.7619999999997

4412354929/4412488904: total\_Ave -1636698.4 total\_EstErr 544.0 total\_RMSD 2620.107

4412354923/4412533051: total\_Ave -1637325.5899999999 total\_EstErr 573.0 total\_RMSD 2504.505

4412359788/4412534033: total\_Ave -1637155.74 total\_EstErr 528.0 total\_RMSD 2697.8199999999997

4412385380/4412534032: total\_Ave -1636282.39 total\_EstErr 801.0 total\_RMSD 2690.5609999999997

1%, 3%, 5% donor to acceptor

4311942768/4312298733: total\_Ave -1640624.3199999998 total\_EstErr 554.0 total\_RMSD 2312.398

4311944239/4312299508: total\_Ave -1639597.15 total\_EstErr 957.0 total\_RMSD 3007.367

4311947424/4382352315: total\_Ave -1641450.42 total\_EstErr 696.0 total\_RMSD 2578.13

1%, 3%, 5% acceptor to donor

4312047244/4382353057: total\_Ave -1640150.77 total\_EstErr 634.0 total\_RMSD 2895.656

4312050724/4312920487: total\_Ave -1638624.45 total\_EstErr 615.0 total\_RMSD 2508.193

4312054877/4388072778: total\_Ave -1638102.02 total\_EstErr 478.0 total\_RMSD 2564.148

**10% PS, 10% cholesterol in acceptor:**

Basal

4282160273/4325292322: total\_Ave -1680720.1 total\_EstErr 708.0 total\_RMSD 2900.5060000000003

1% 3% 5% donor to acceptor

4311942768/4325292922: total\_Ave -1680957.8 total\_EstErr 661.0 total\_RMSD 2699.79

4311944239/4325293833: total\_Ave -1681161.0 total\_EstErr 802.0 total\_RMSD 3015.19

4311947424/4325294853: total\_Ave -1681308.8 total\_EstErr 852.0 total\_RMSD 2935.307

1% 3% 5% reverse

4312047244/4325295659: total\_Ave -1680490.5 total\_EstErr 1099.5 total\_RMSD 3385.0649999999996

4312050724/4325296716: total\_Ave -1680014.12 total\_EstErr 718.0 total\_RMSD 2688.746

4312054877/4325297440: total\_Ave -1680132.56 total\_EstErr 569.0 total\_RMSD 2504.665

Basal

4552639276/4552639960: total\_Ave -1680271.2999999998 total\_EstErr 613.0 total\_RMSD 2680.8239999999996

Forward transfer 10%, 20%, 30%

4552640521/4552885328: total\_Ave -1680947.1 total\_EstErr 487.0 total\_RMSD 2485.505

4552886153/4552886967: total\_Ave -1680146.85 total\_EstErr 758.0 total\_RMSD 2883.0170000000003

4553223774/4553224189: total\_Ave -1680986.1099999999 total\_EstErr 410.0 total\_RMSD 2270.5016

Reverse transfer 10%, 20%, 30%

4553224440/4553363883: total\_Ave -1680019.24 total\_EstErr 639.0 total\_RMSD 2741.309

4553468789/4553501094: total\_Ave -1679499.35 total\_EstErr 777.0 total\_RMSD 2918.5969999999998

4553574075/4555169491: total\_Ave -1678925.41 total\_EstErr 648.0 total\_RMSD 2805.473