

## Supporting Information for

### Key Factors Governing Initial Stages of Lipid Droplet Formation

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#### Coarse-grained model attraction parameters ( $B$ in eq. 1 of the main text)

$k_B T / \text{\AA}$	H	PGL	TGL	T
H	0.0	0.0	0.0	0.0
PGL	0.0	1.0	0.0	0.0
TGL	0.0	0.0	1.1	1.0
T	0.0	0.0	1.0	1.0

## PLUMED script for biasing simulations

```
MOLINFO STRUCTURE=molinfo.pdb
```

```
lq:      COORDINATIONNUMBER  SPECIES={@mda:{name TGI}}  SWITCH={CUBIC D_0=1.95 D_MAX=2.0}  LOWMEM
cm:      CONTACT_MATRIX      ATOMS=lq                        SWITCH={CUBIC D_0=1.95 D_MAX=2.0}
dfs:     DFSCUSTERING        MATRIX=cm                          LOWMEM
clust1:  CLUSTER_PROPERTIES  CLUSTERS=dfs    CLUSTER=1    SUM
```

```
METAD ...
label=m
ARG=clust1.sum
HEIGHT=2.0
SIGMA=10
PACE=500
GRID_MIN=0
GRID_MAX=3000
GRID_WSTRIDE=500000
GRID_WFILE=grid.dat
TEMP=310
BIASFACTOR=50
CALC_RCT
... METAD
```

```
ss: CLUSTER_NATOMS CLUSTERS=dfs CLUSTER=1
PRINT ARG=clust1.sum,ss,m.bias,m.rbias STRIDE=500 FILE=colvar
```