Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A trick of the tail: computing the entropic contribution to the energetics of quinone-protein unbindung

Supporting information

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Freiburg, Germany

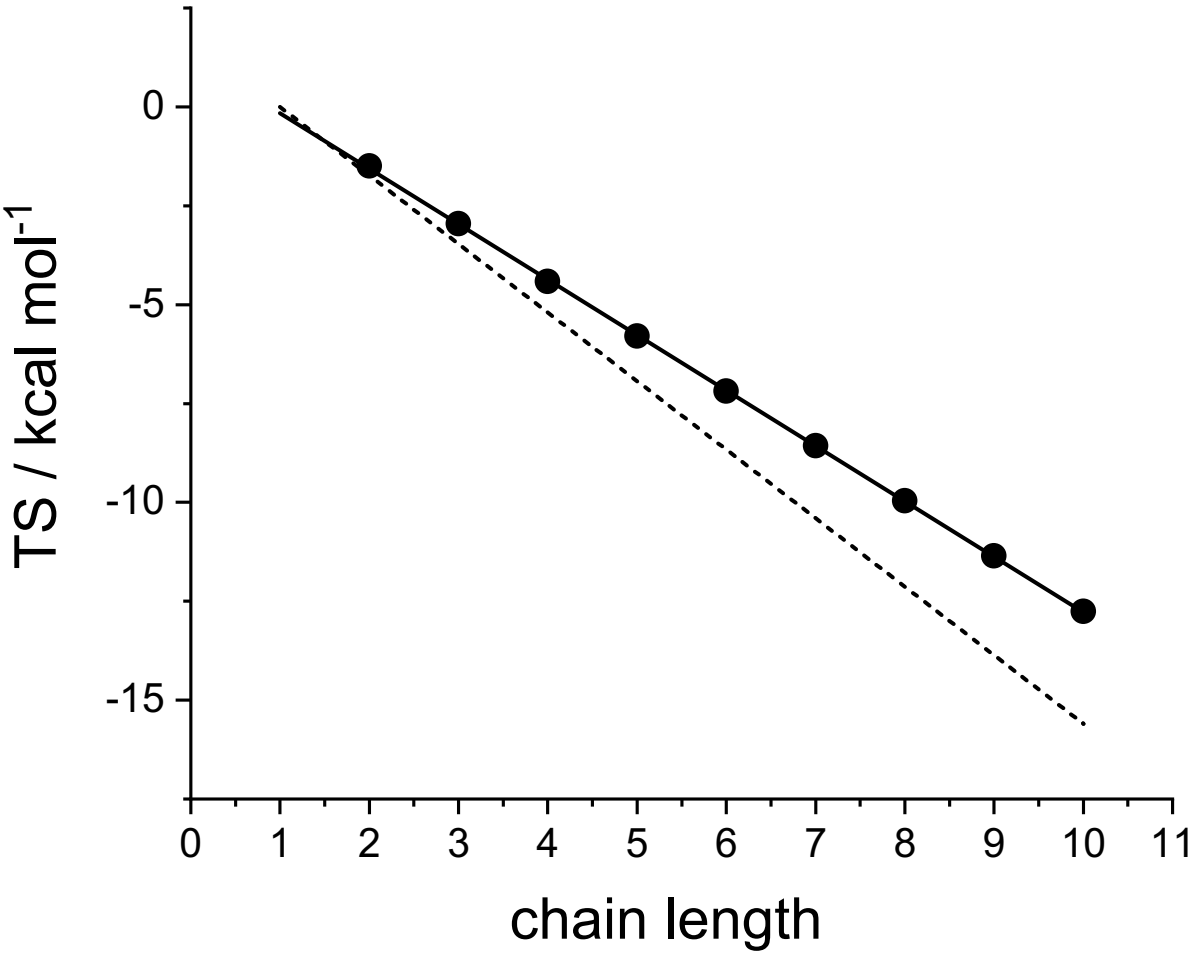


Figure S1. Entropic contributions to the free energy as a function of the isoprenoid side chain length. Linear regression analysis of the data presented in table 1 of the main article. Bullet symbols: computed data, solid line: linear regression line, dashed line: theoretical limit for an acceptance ratio of unity in eq. 1, main article. This corresponds to a fully flexible chain with 18 dihedral angle states per isoprene monomer.

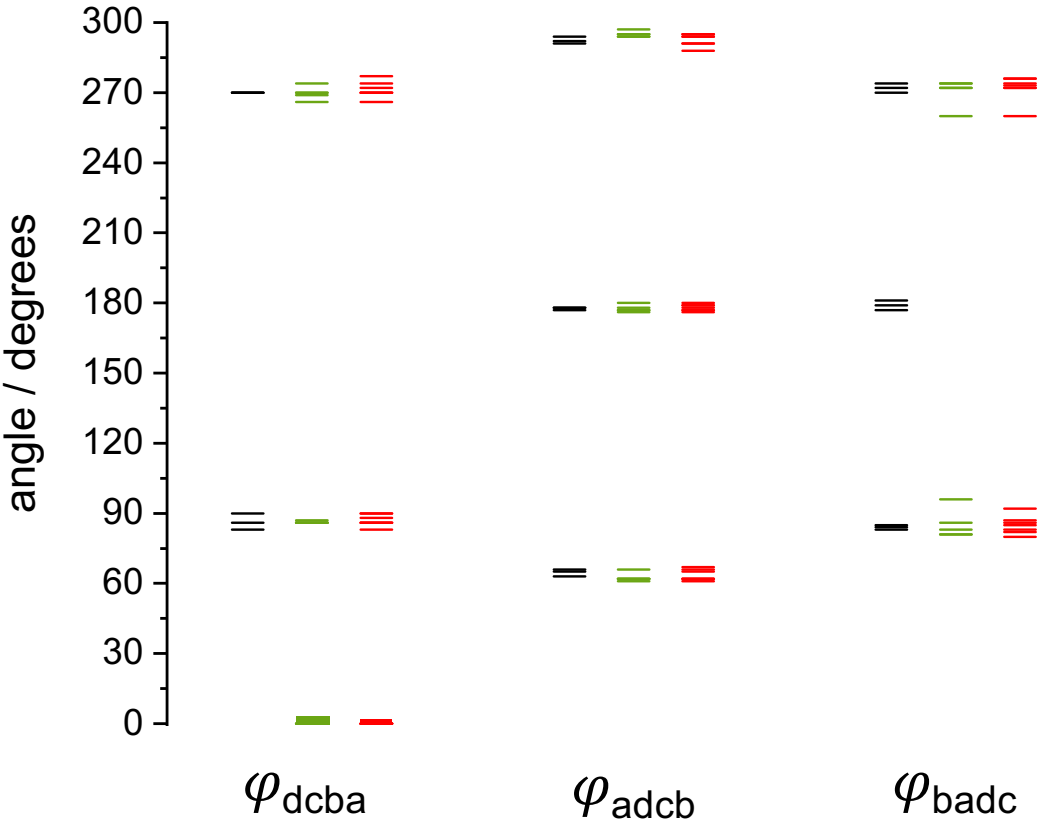


Figure S2. Level plot of the menaquinol dihedral angles, with letters as indicated in figure 1 of the main article. Black: MHK4, green: MHK6, red: MHK8.

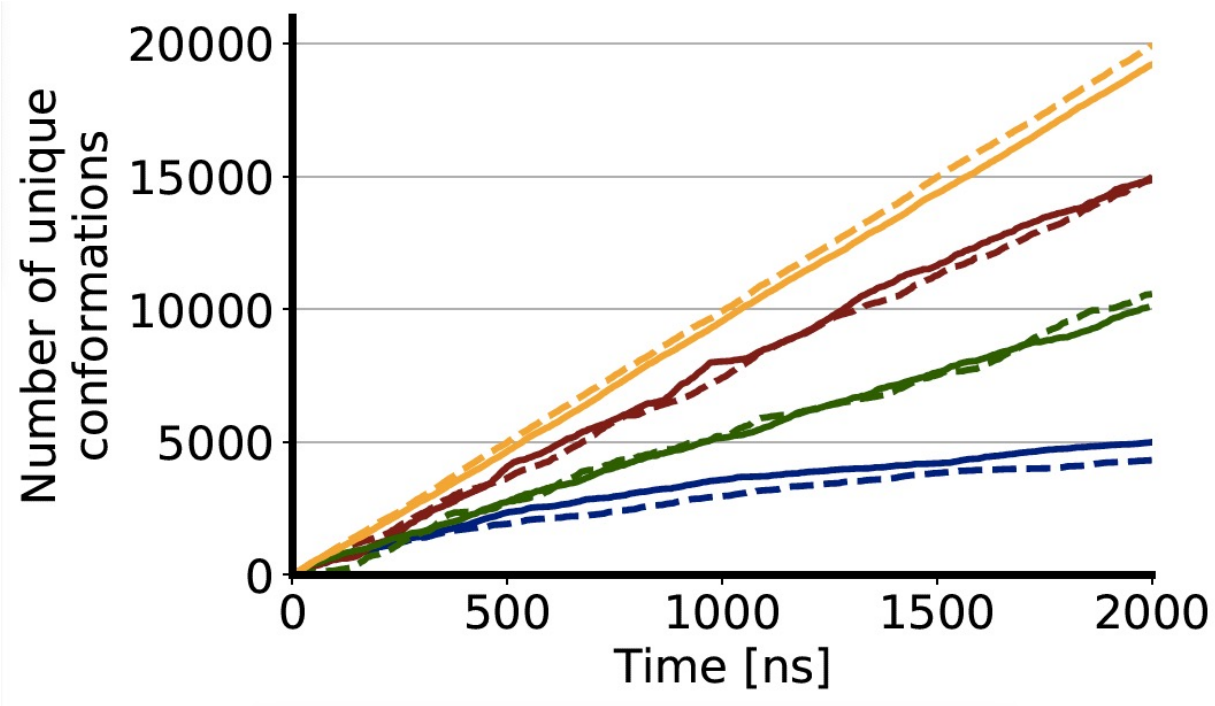


Figure S3. Number of unique conformations found during the MD simulation as a function of time. The lines represent menaquinol-6 (orange dashed line) and menaquinone-6 (full orange line) in n-hexane. In addition, we show menaquinol-8 (red dashed line), menaquinone-8 (full red line), menaquinol-6 (green dashed line) menaquinone-6 (full green line), menaquinol-4 (blue dashed line) menaqinone-4 (full blue line), all embedded in a lipid bilayer membrane.

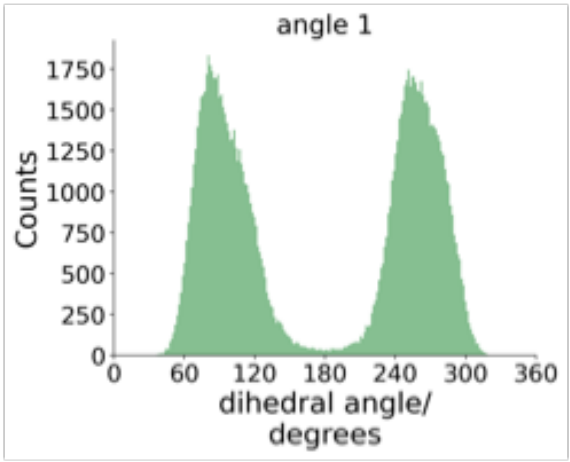
Dihedral angles

Angles are enumerated according to their position in the side chain with reference to the naphtoquinone moiety of the quinone or quinol, cf. figure 1 of the main article.

We have:

- angles 3, 6, 9, … = $\boldsymbol{\varphi}_{badc}$
- angles 4, 7, 10, … = $\boldsymbol{\varphi}_{adcb}$
- angles 5, 8, 11, … = $\boldsymbol{\varphi}_{dcba}$

Figure set S4. Menaquinol-4 (MHK4) in a lipid bilayer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750
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1250
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1750
0
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120
180
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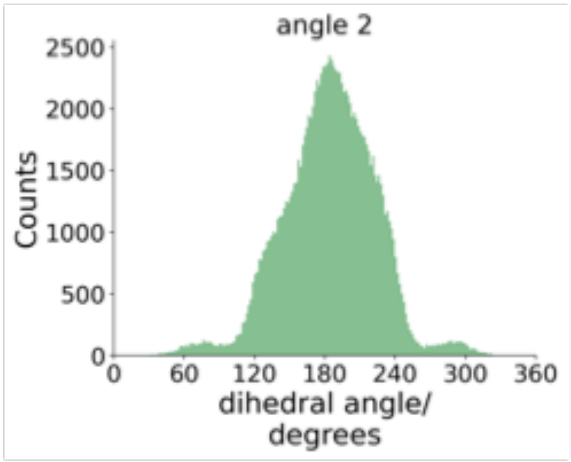
300
360
dihedral angle/
degrees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Counts
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180
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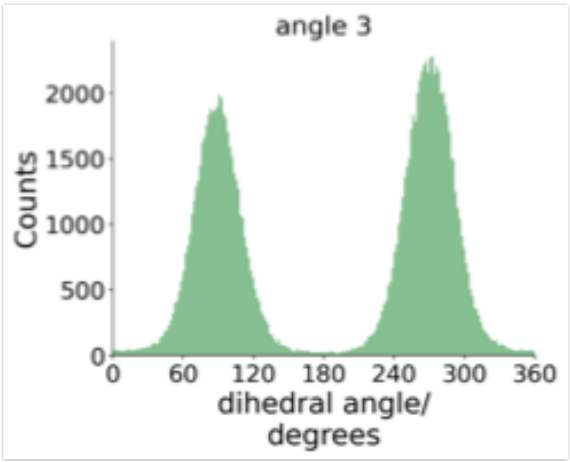
300
360
dihedral angle/
degrees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Counts
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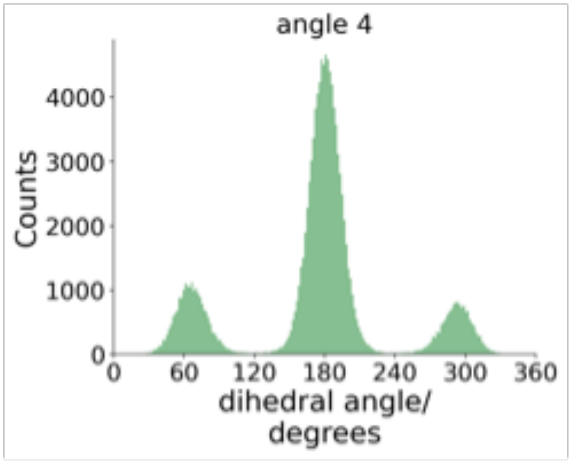
dihedral angle/
degrees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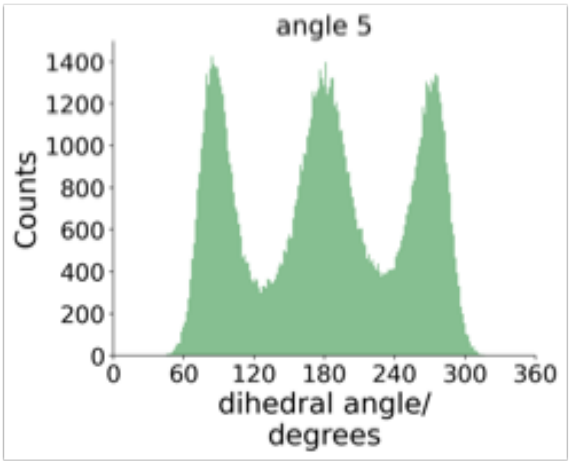
dihedral angle/
degrees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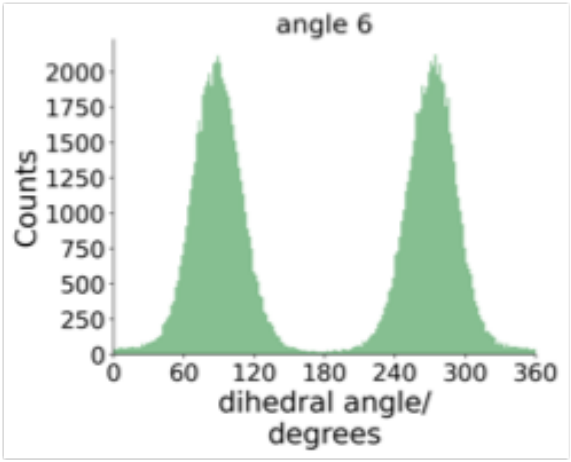
dihedral angle/
degrees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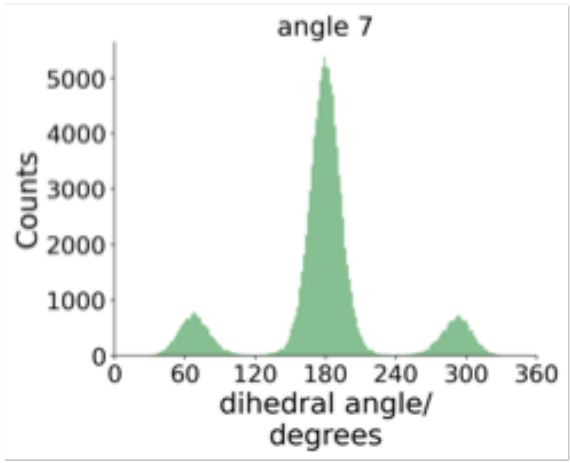
dihedral angle/
degrees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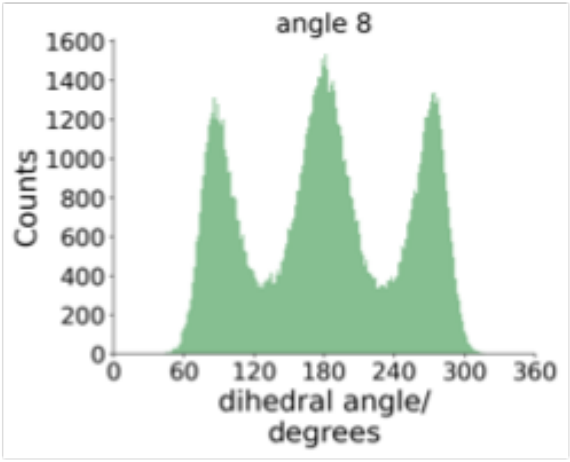
dihedral angle/
degrees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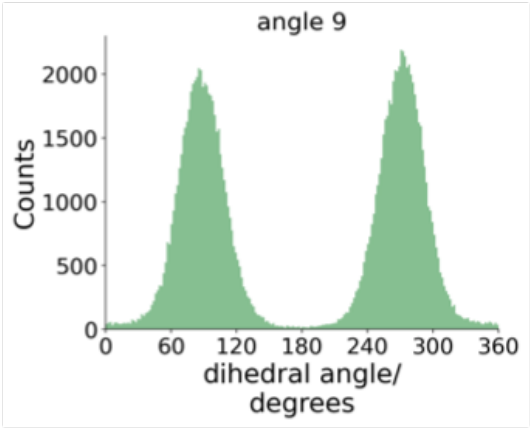
dihedral angle/
degrees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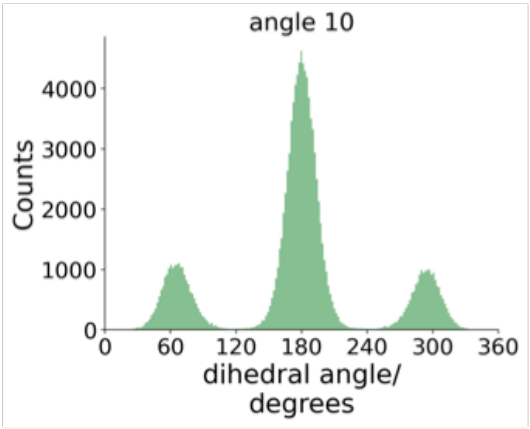
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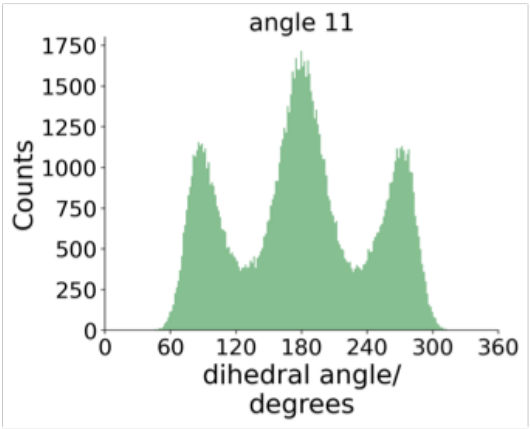
dihedral angle/
degrees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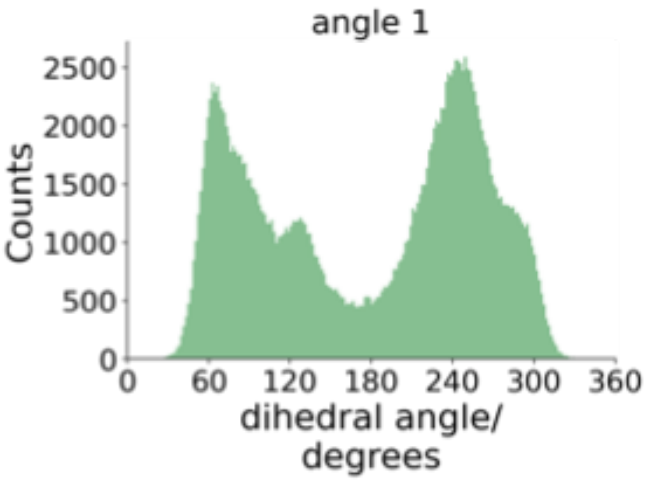
dihedral angle/
degrees

Figure set S5. Menaquinol-6 (MHK6) in a lipid bilayer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dihedral angle/
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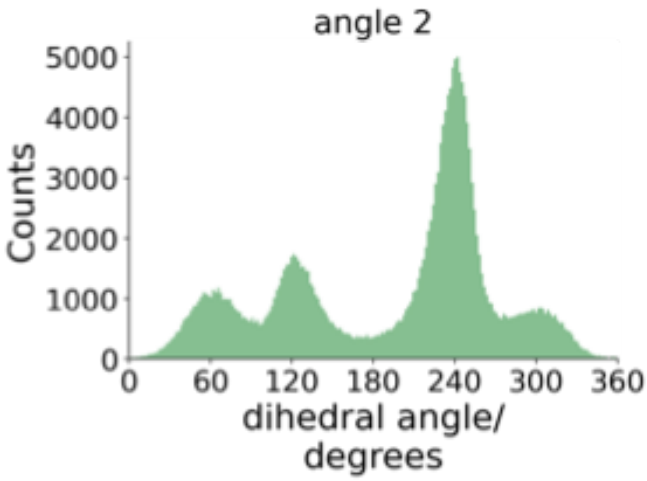
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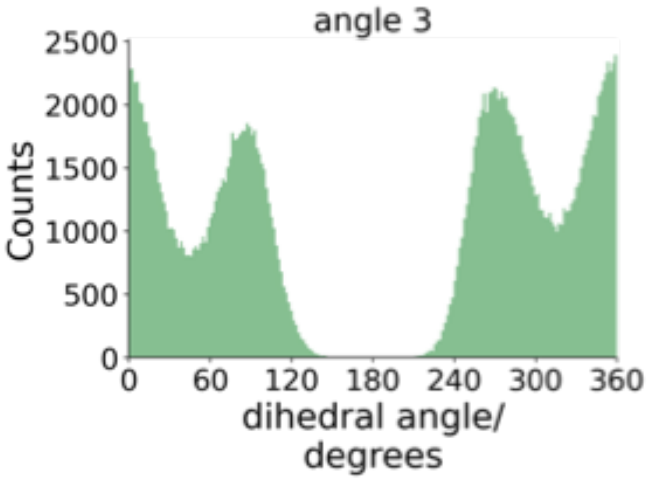
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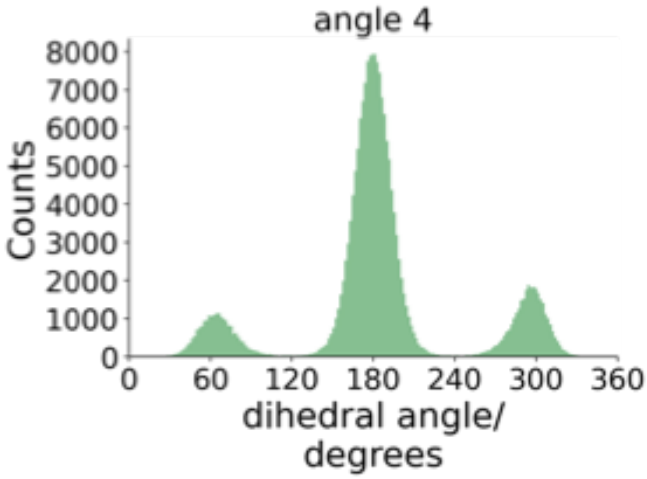
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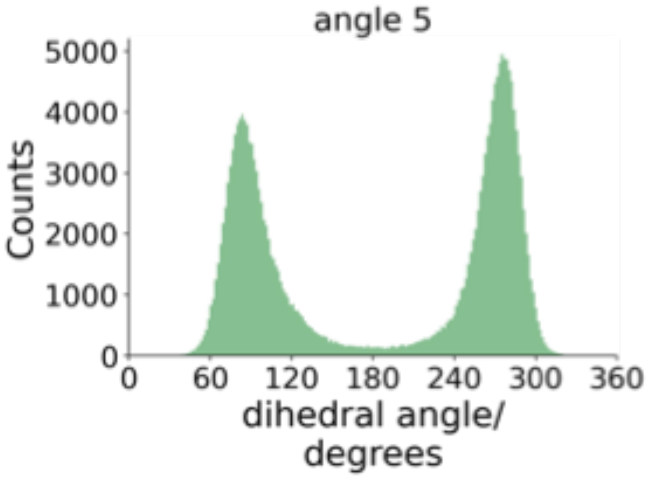
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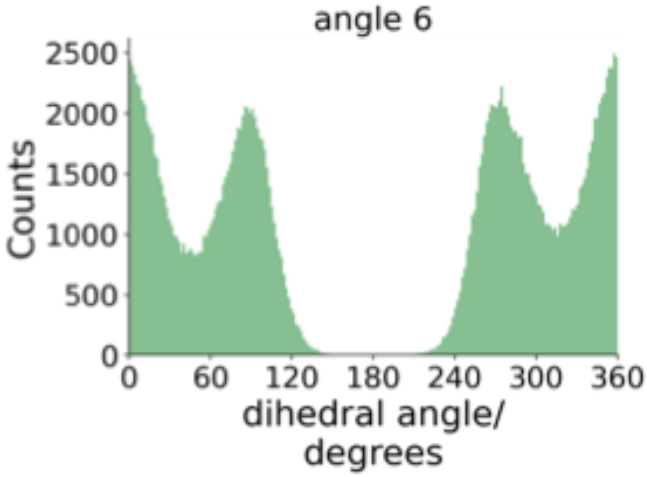
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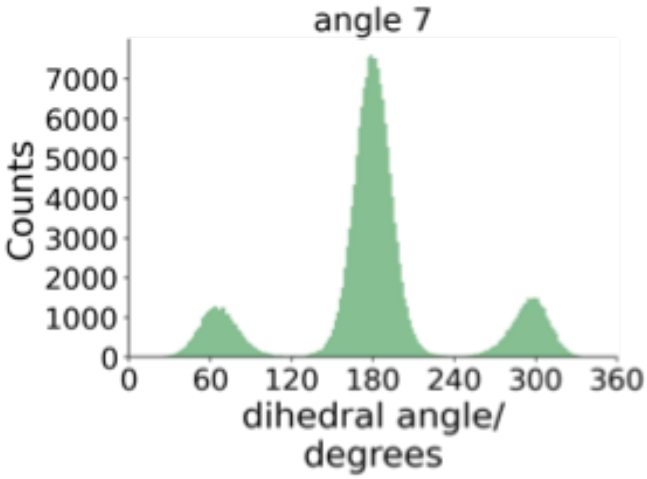
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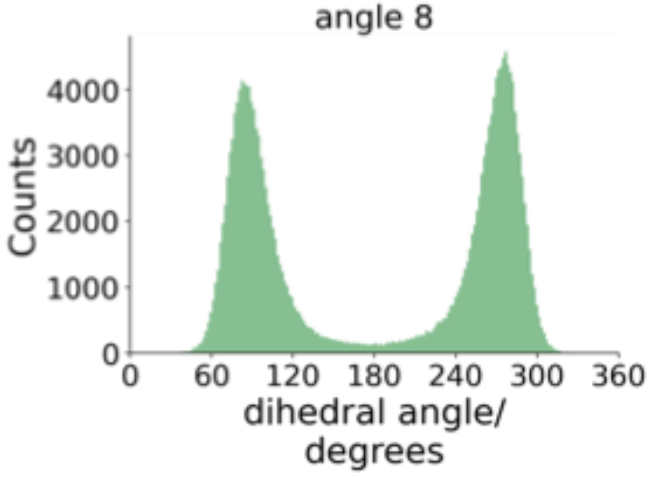
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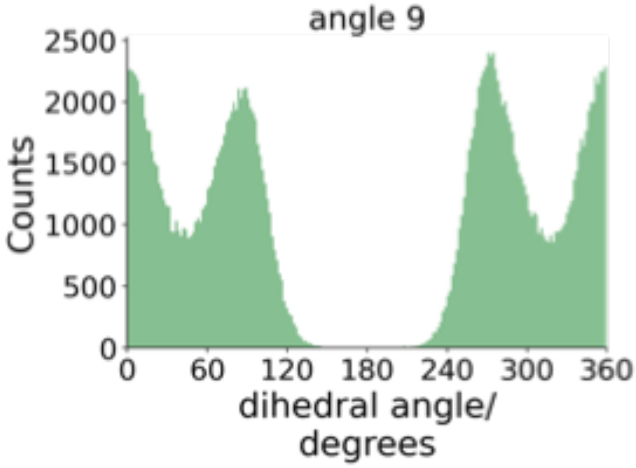
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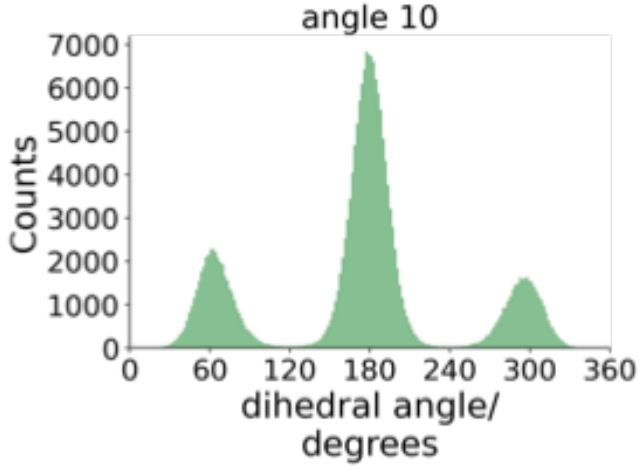
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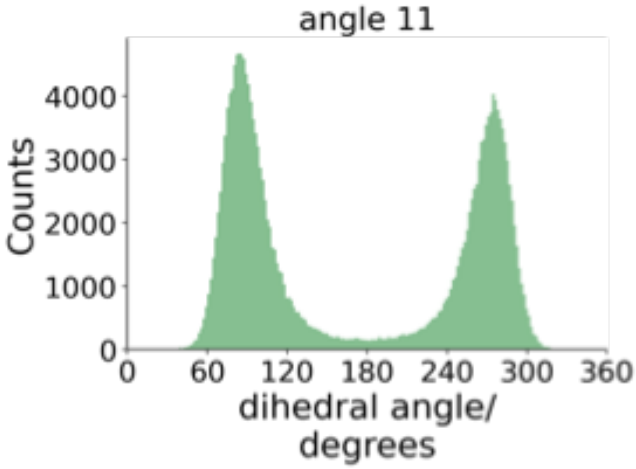
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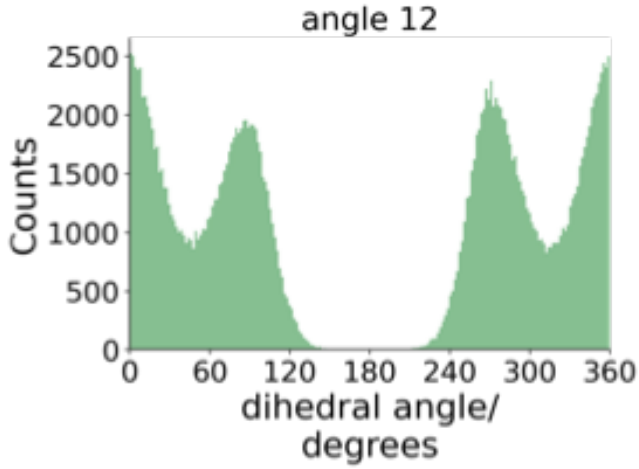
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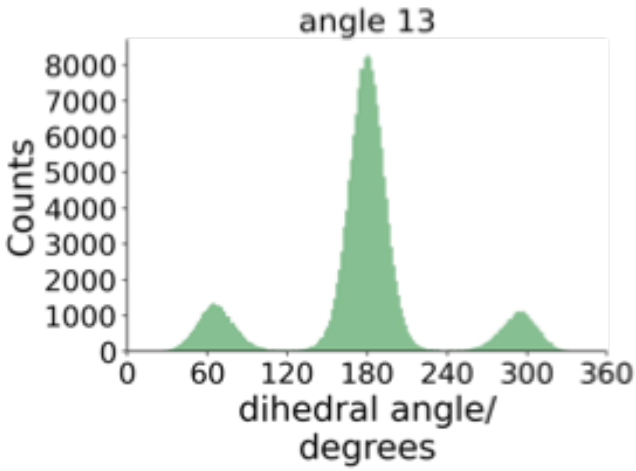
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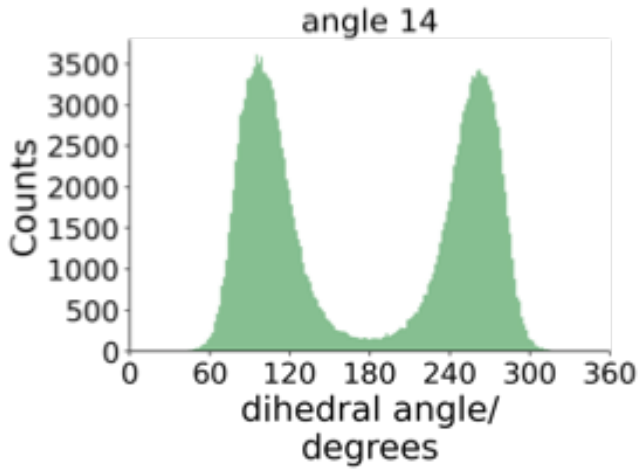
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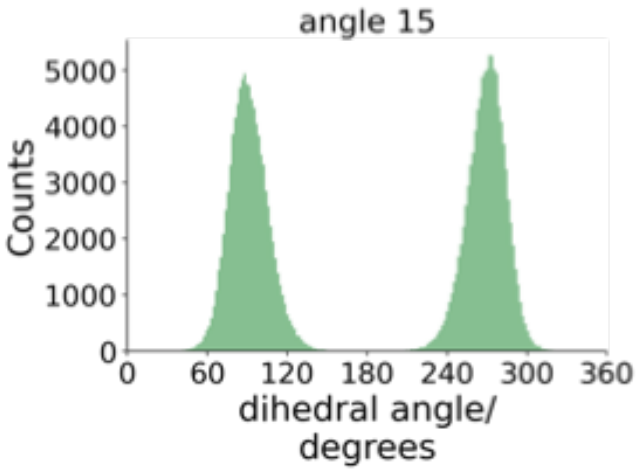
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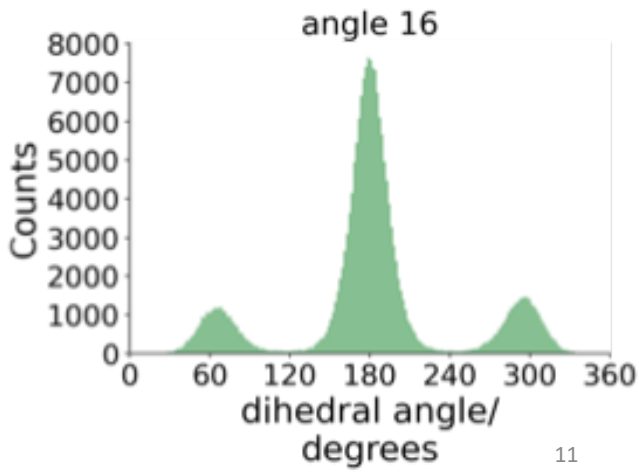
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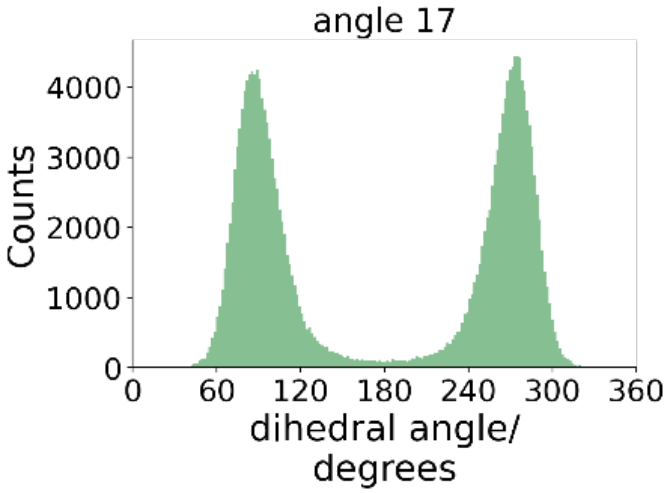
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dihedral angle/
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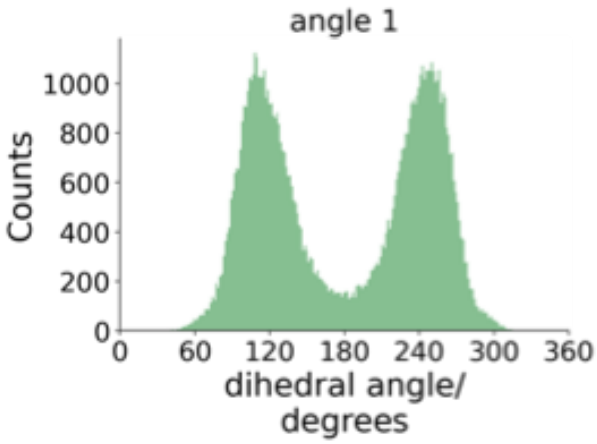
Figure set S6. Menaquinol-6 (MHK6) in n-hexane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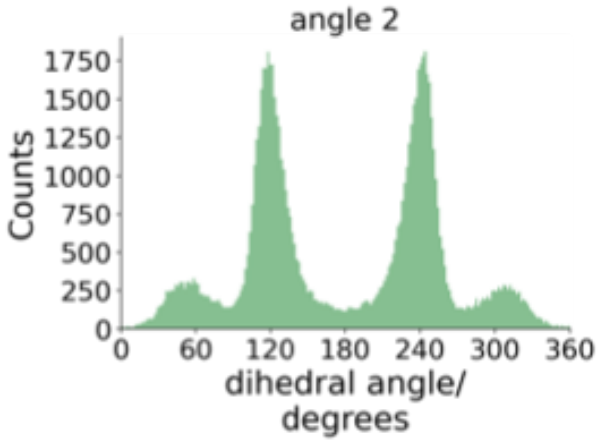
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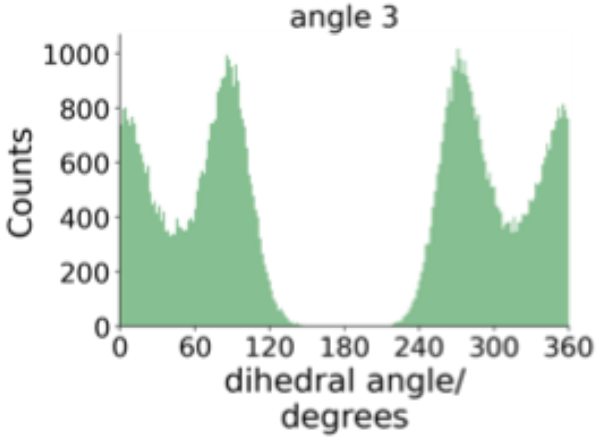
dihedral angle/
degrees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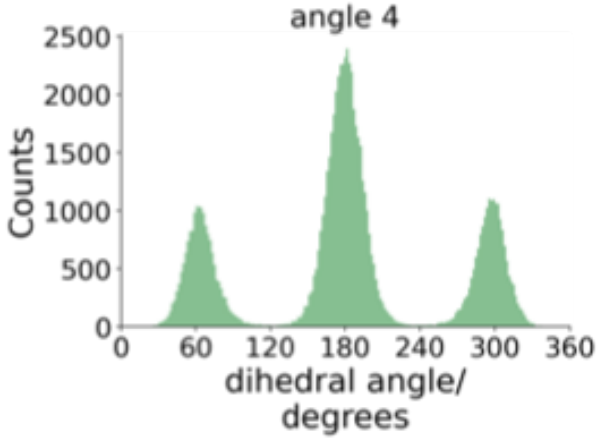
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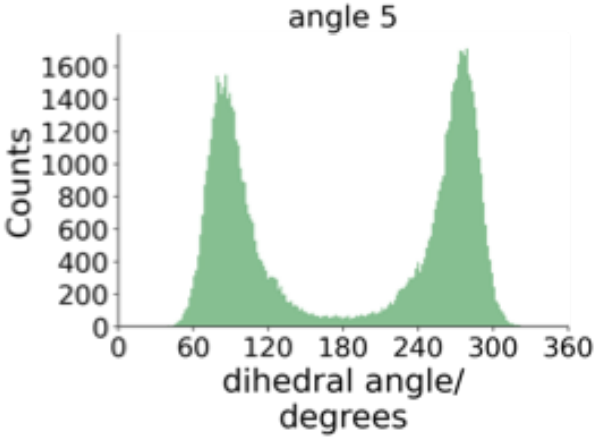
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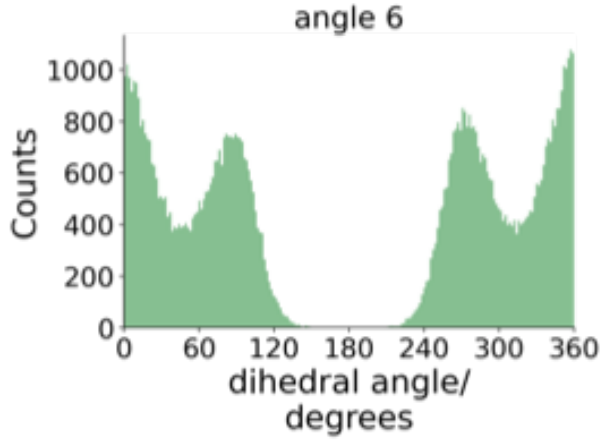
degrees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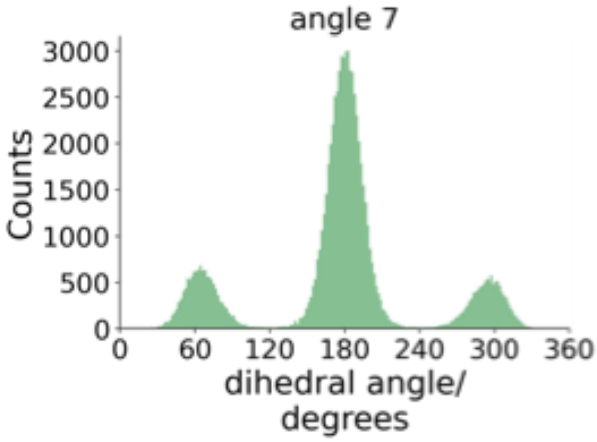
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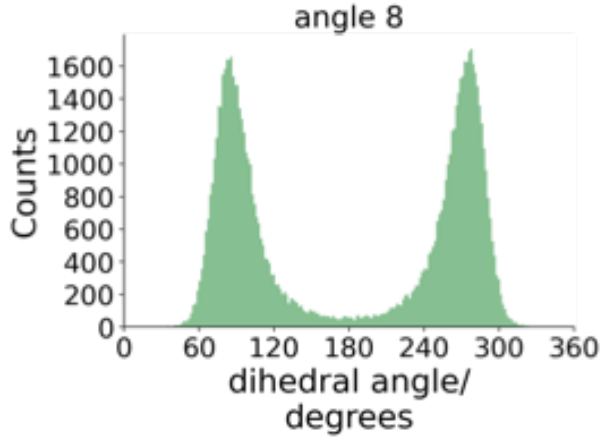
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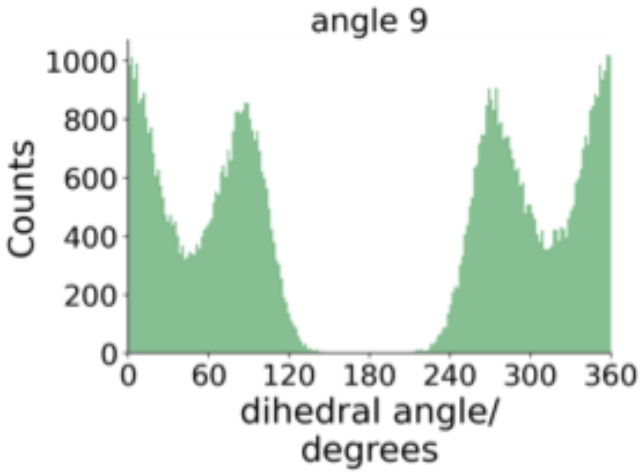
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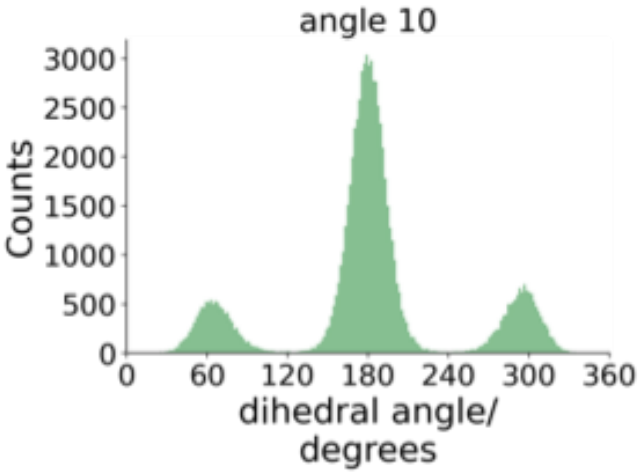
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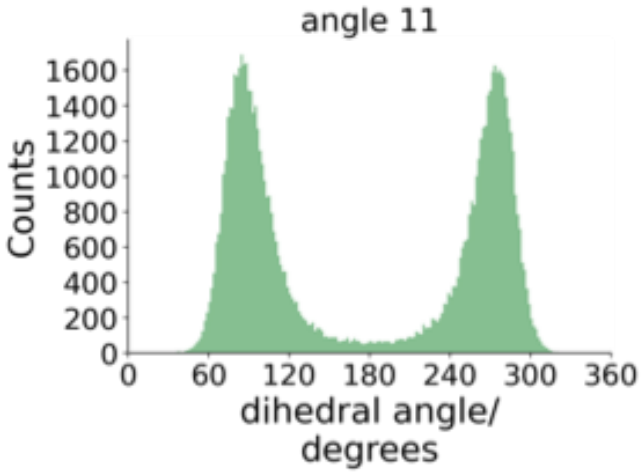
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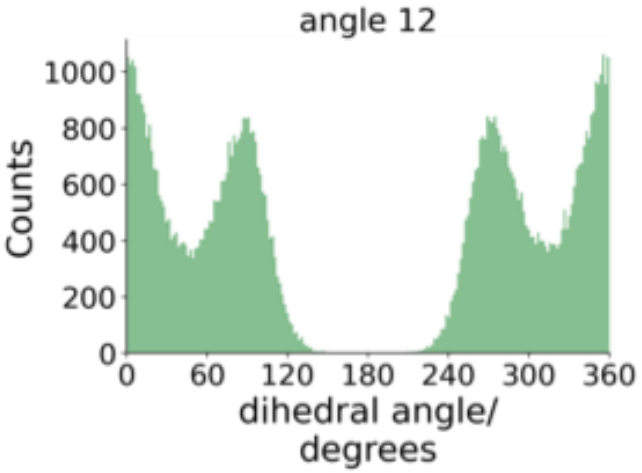
angle 12
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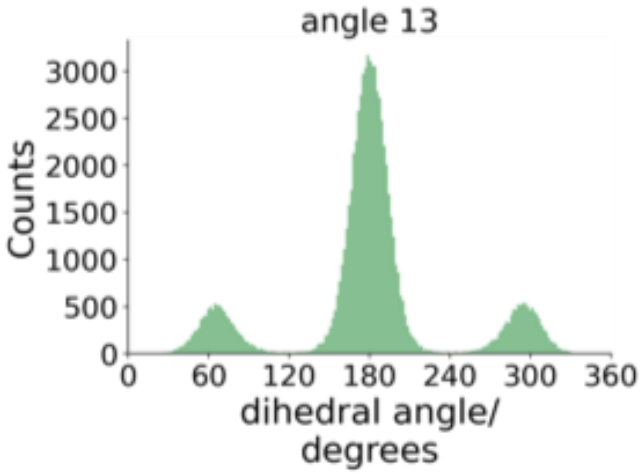
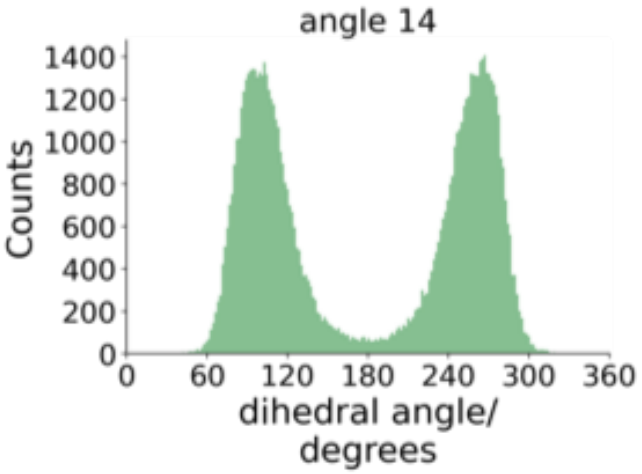
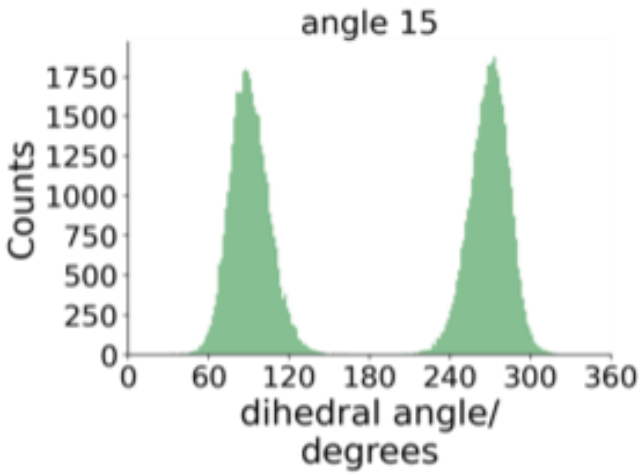
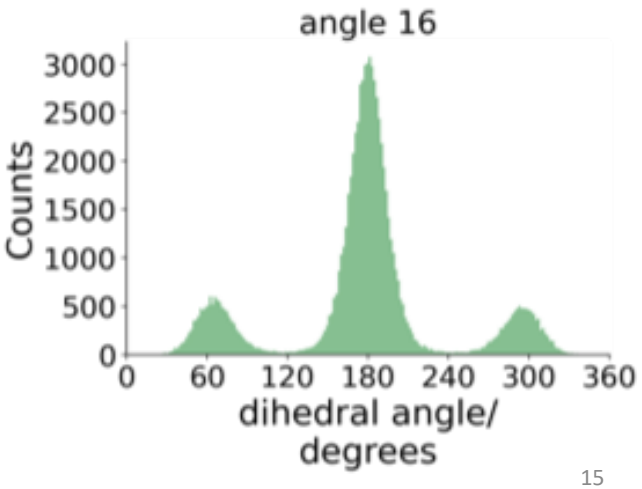

angle 13
Counts
dihedral angle/
degrees


angle 14
Counts
dihedral angle/
degrees


angle 15
Counts
dihedral angle/
degrees


angle 16
Counts
dihedral angle/
degrees

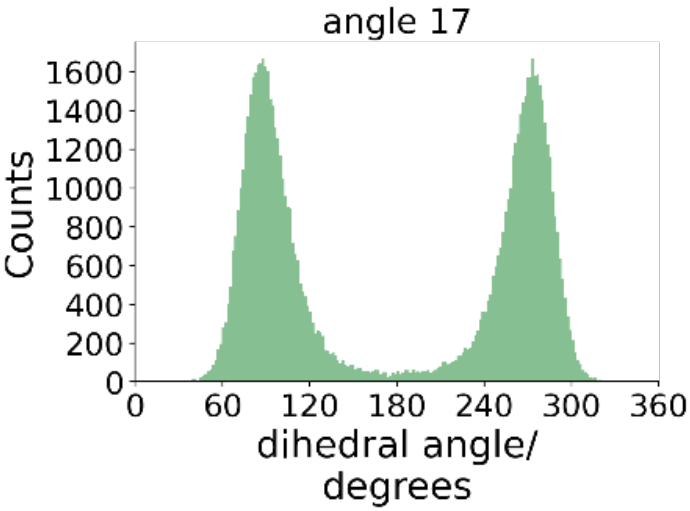
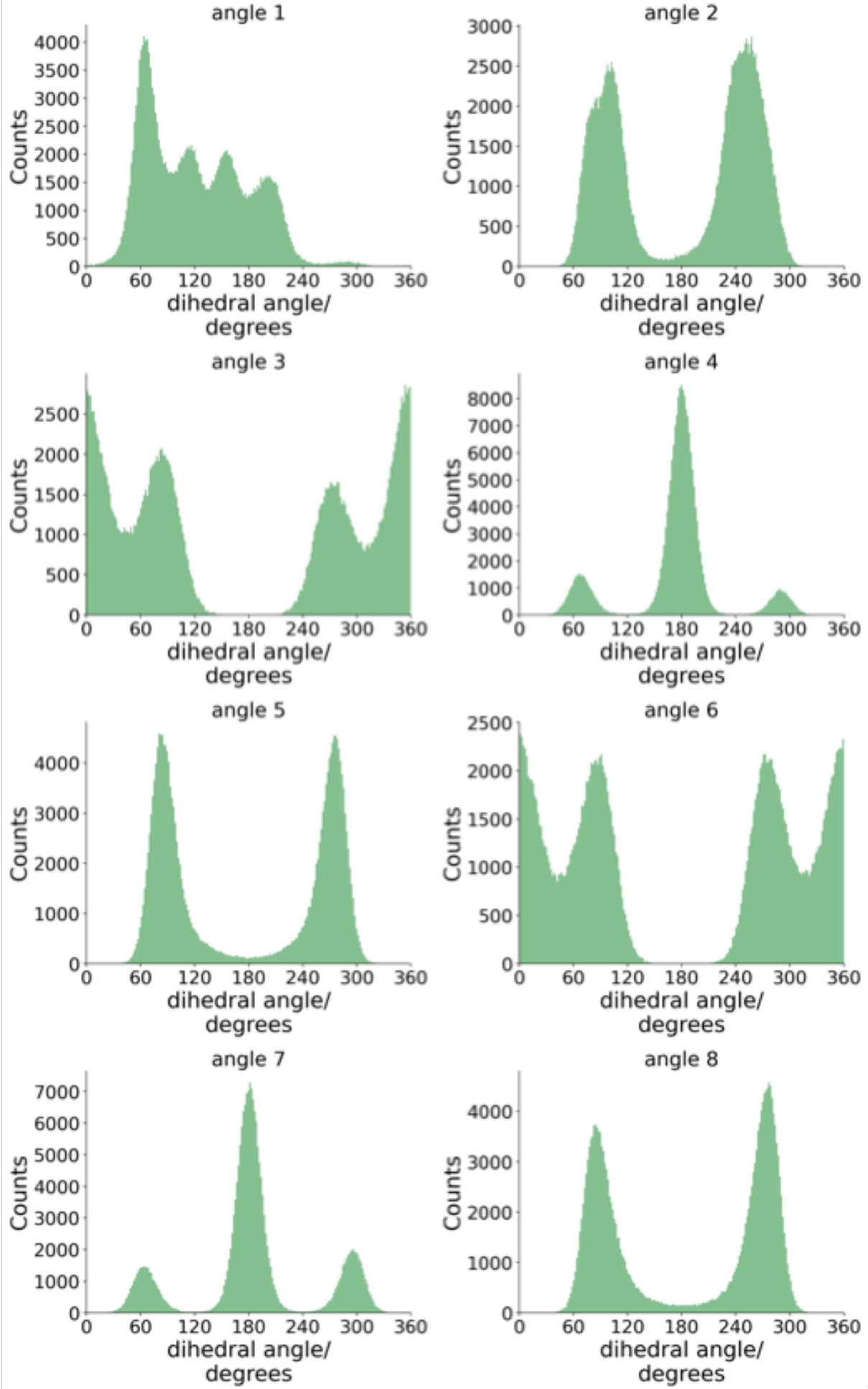
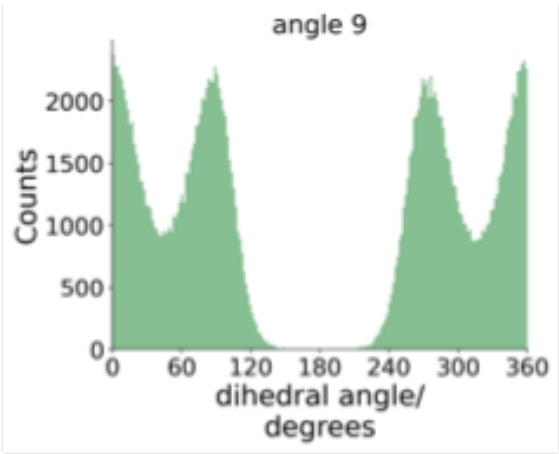
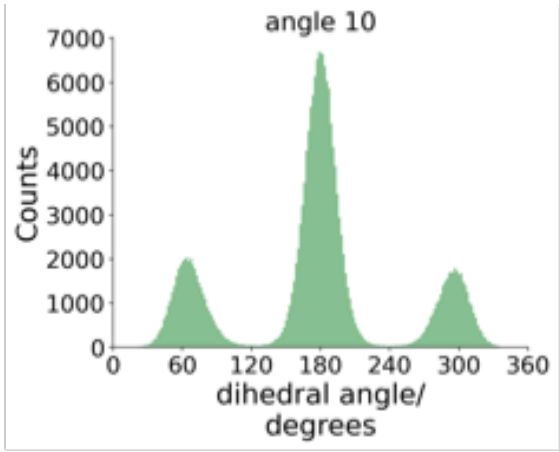
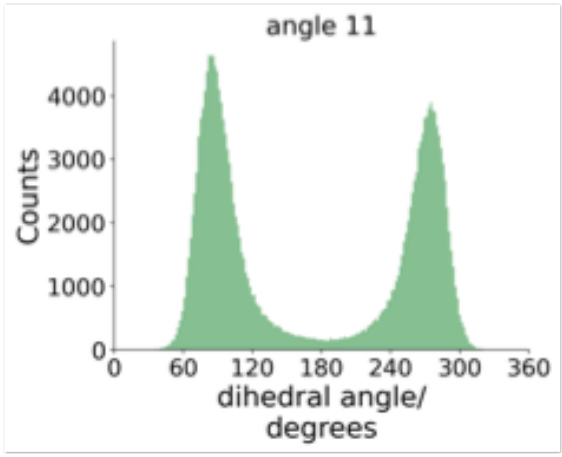

angle 17
Counts
1600
1400
1200
1000
800
600
400
200
0
0
60
120
180
240
300
360
dihedral angle/
degrees

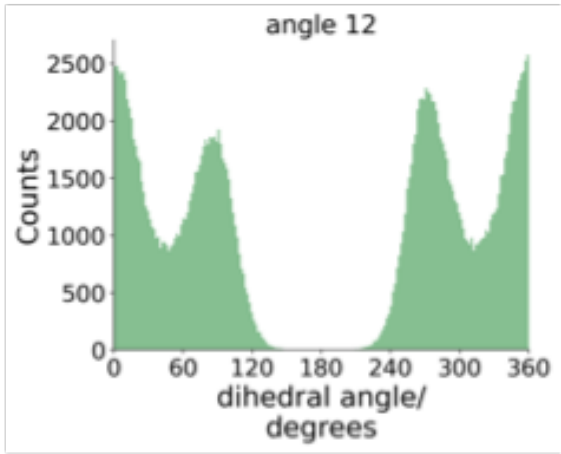
Figure set S7. Menaquinol-8 (MHK8) in a lipid bilayer

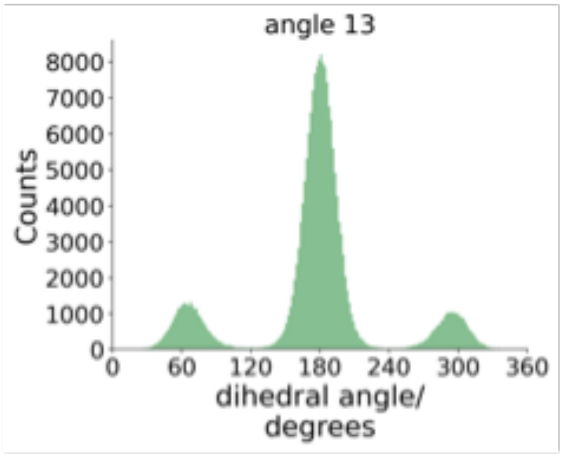

angle 1
Counts
dihedral angle/
degrees
angle 2
Counts
dihedral angle/
degrees
angle 3
Counts
dihedral angle/
degrees
angle 4
Counts
dihedral angle/
degrees
angle 5
Counts
dihedral angle/
degrees
angle 6
Counts
dihedral angle/
degrees
angle 7
Counts
dihedral angle/
degrees
angle 8
Counts
dihedral angle/
degrees

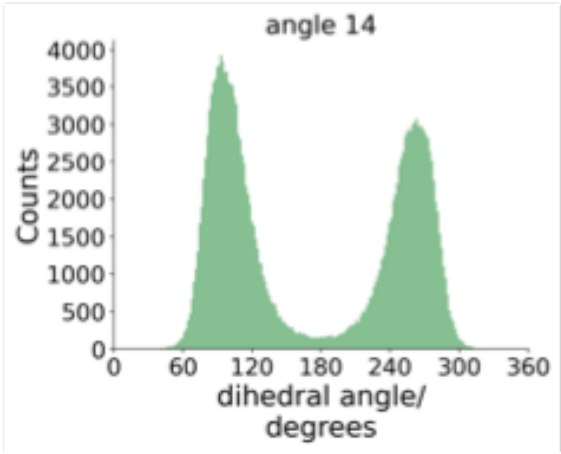

angle 9
Counts
0
500
1000
1500
2000
0
60
120
180
240
300
360
dihedral angle/
degrees

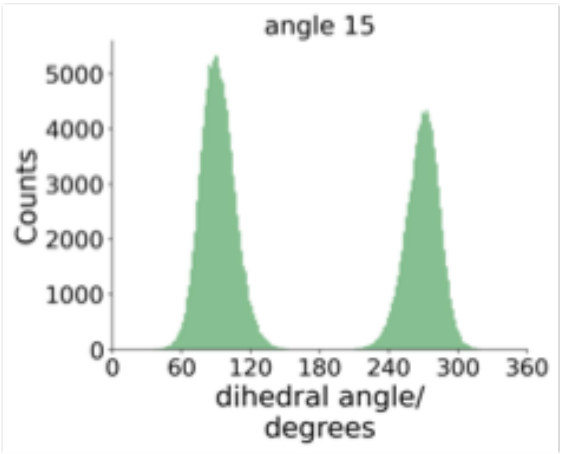

angle 10
Counts
0
1000
2000
3000
4000
5000
6000
7000
0
60
120
180
240
300
360
dihedral angle/
degrees

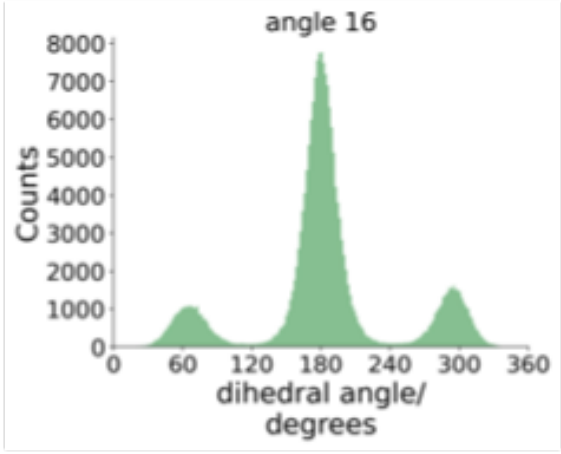

angle 11
Counts
0
1000
2000
3000
4000
0
60
120
180
240
300
360
dihedral angle/
degrees

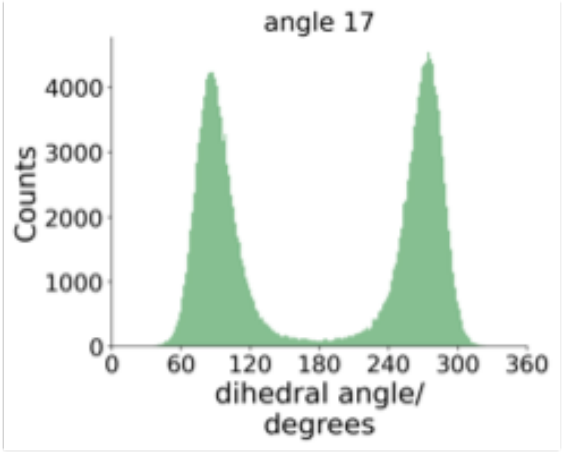

angle 12
Counts
0
500
1000
1500
2000
2500
0
60
120
180
240
300
360
dihedral angle/
degrees

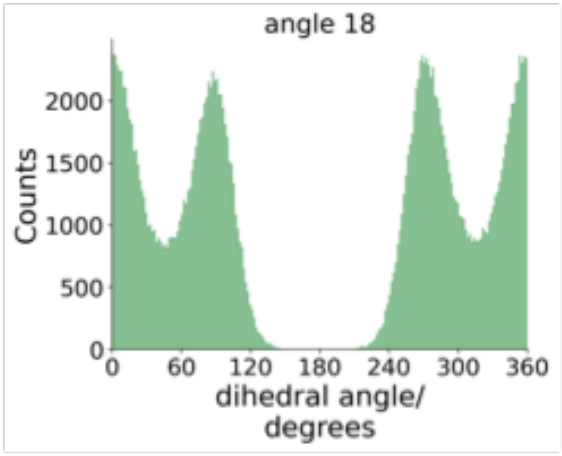

angle 13
Counts
0
1000
2000
3000
4000
5000
6000
7000
8000
0
60
120
180
240
300
360
dihedral angle/
degrees

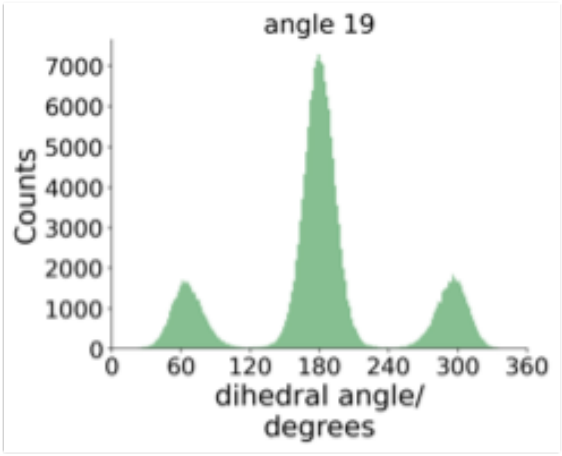

angle 14
Counts
0
500
1000
1500
2000
2500
3000
3500
4000
0
60
120
180
240
300
360
dihedral angle/
degrees

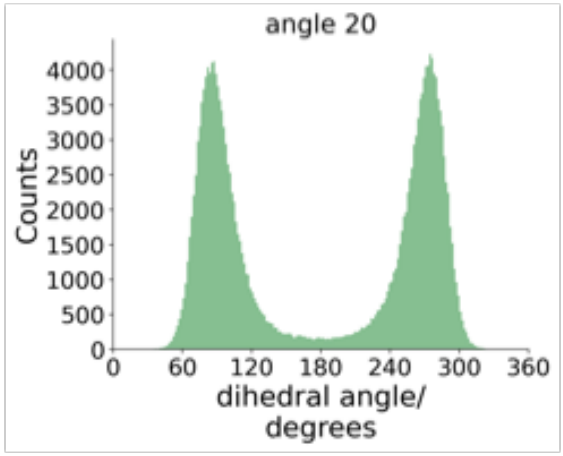

angle 15
Counts
0
1000
2000
3000
4000
5000
0
60
120
180
240
300
360
dihedral angle/
degrees

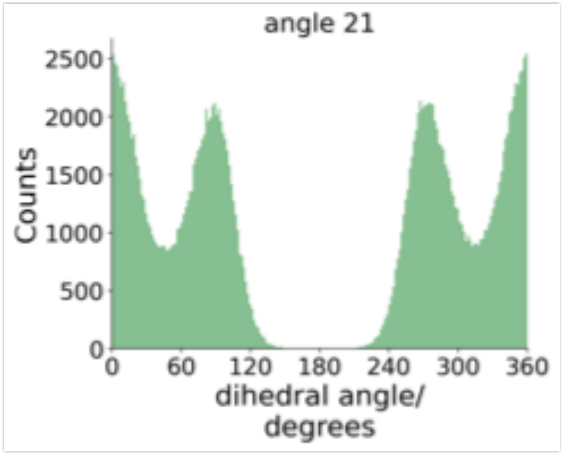

angle 16
Counts
0
1000
2000
3000
4000
5000
6000
7000
8000
0
60
120
180
240
300
360
dihedral angle/
degrees

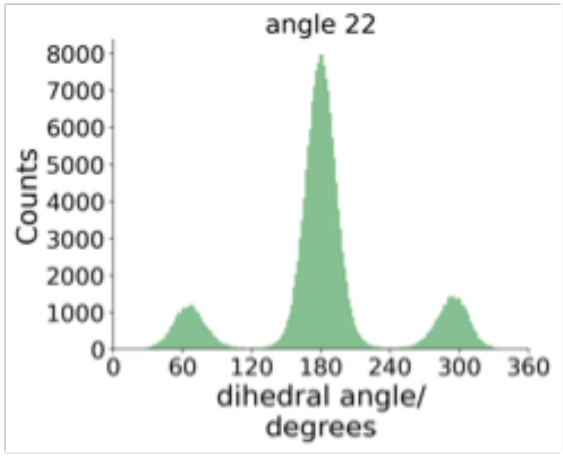

angle 17
Counts
dihedral angle/
degrees


angle 18
Counts
dihedral angle/
degrees


angle 19
Counts
dihedral angle/
degrees


angle 20
Counts
dihedral angle/
degrees


angle 21
Counts
dihedral angle/
degrees


angle 22
Counts
dihedral angle/
degrees

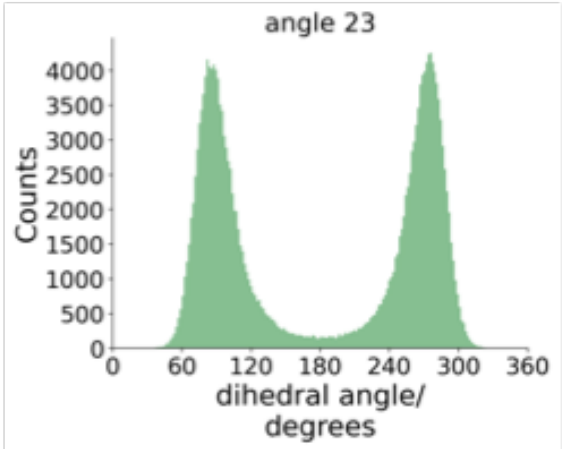
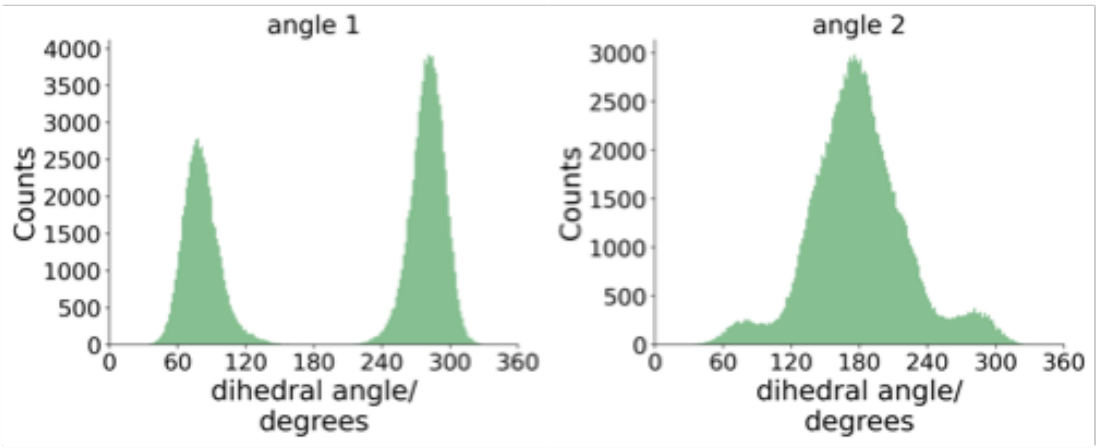
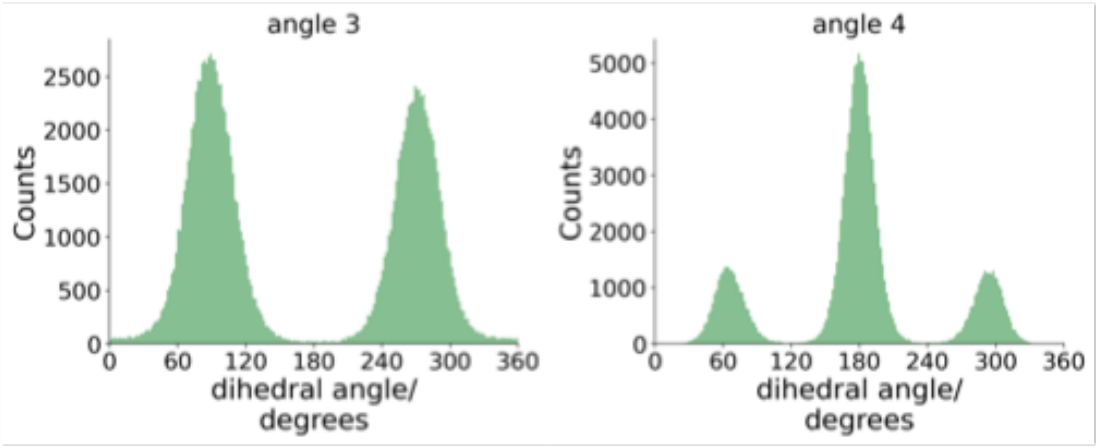

angle 23
Counts
dihedral angle/
degrees

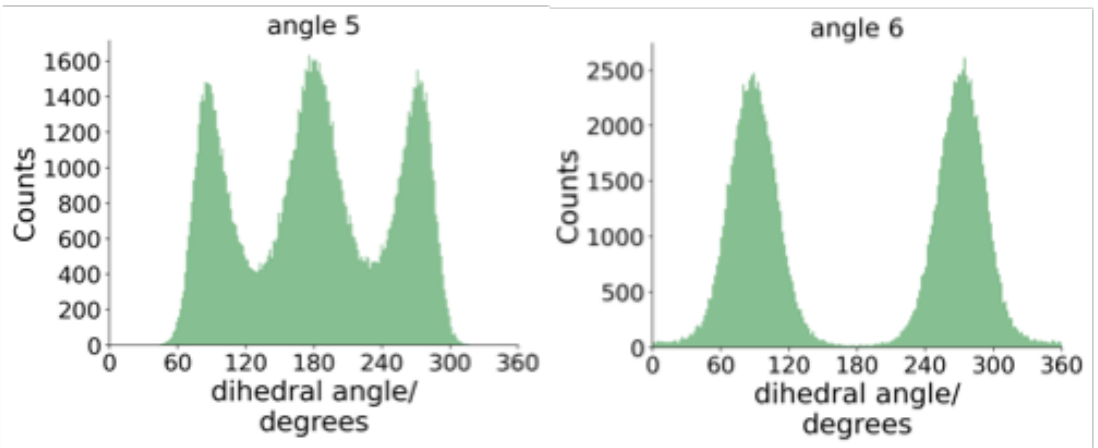
Figure set S8. Menaquinone-4 (MK4) in a lipid bilayer


angle 1
Counts
dihedral angle/
degrees

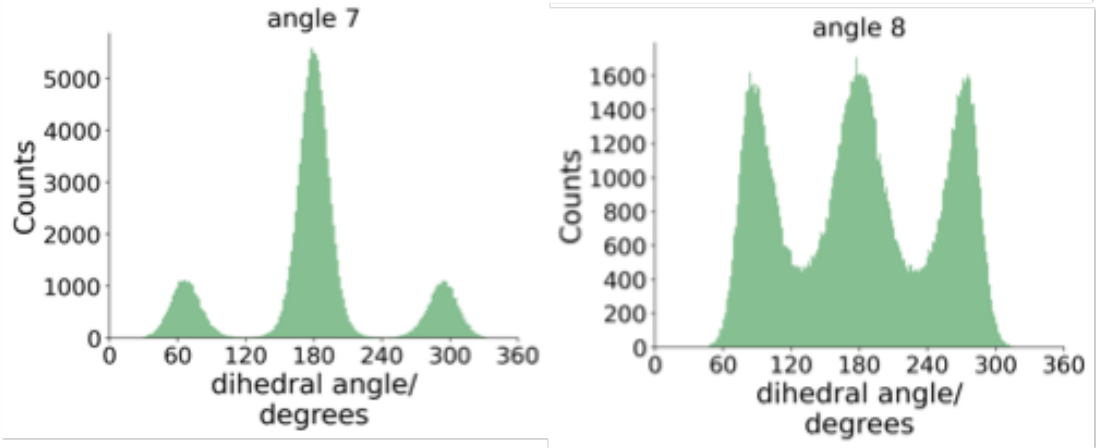
angle 2
Counts
dihedral angle/
degrees


angle 3
Counts
dihedral angle/
degrees

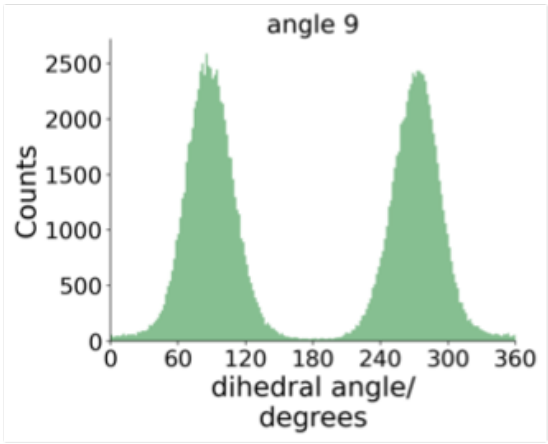
angle 4
Counts
dihedral angle/
degrees

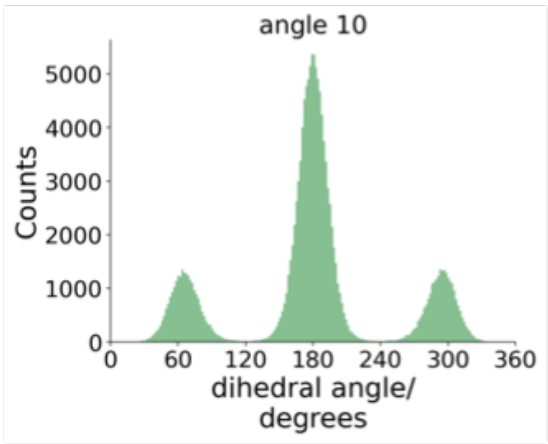

angle 5
Counts
dihedral angle/
degrees

angle 6
Counts
dihedral angle/
degrees


angle 7
Counts
dihedral angle/
degrees

angle 8
Counts
dihedral angle/
degrees


angle 9
Counts
2500
2000
1500
1000
500
0
0
60
120
180
240
300
360
dihedral angle/
degrees


angle 10
Counts
5000
4000
3000
2000
1000
0
0
60
120
180
240
300
360
dihedral angle/
degrees

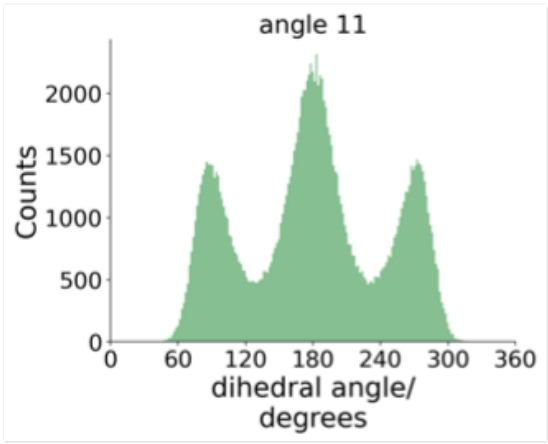
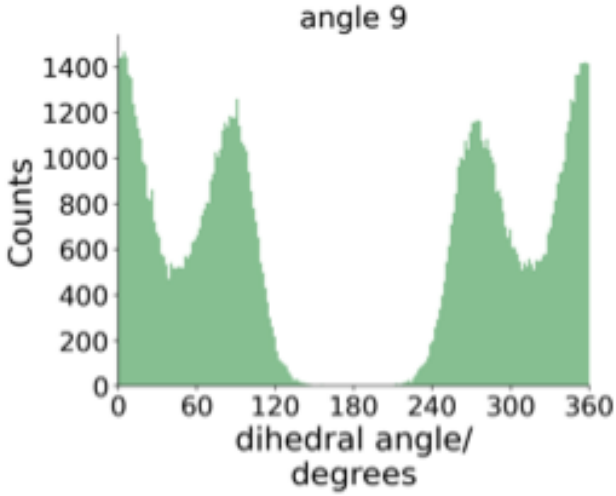
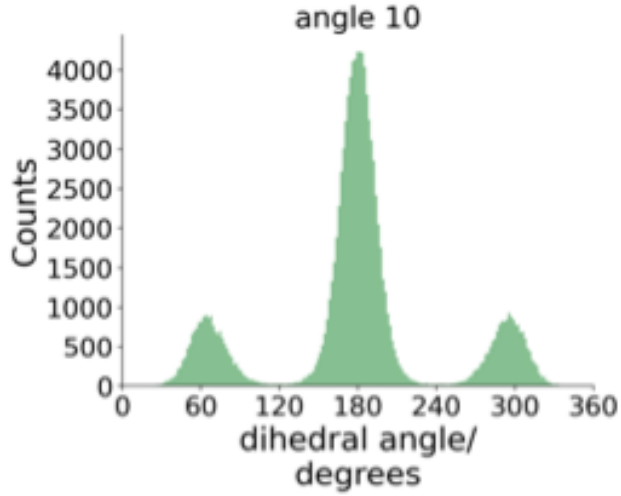
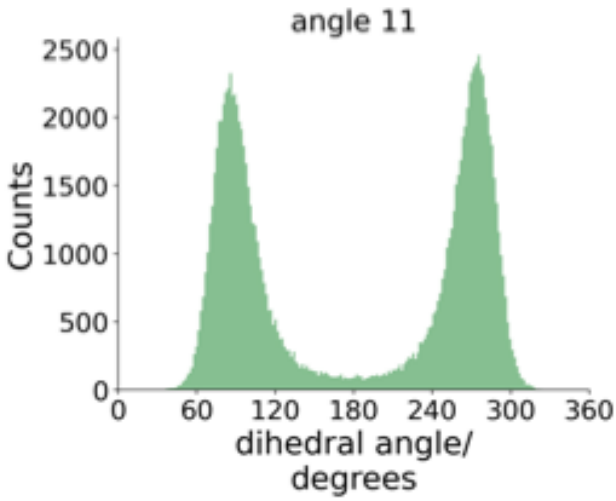
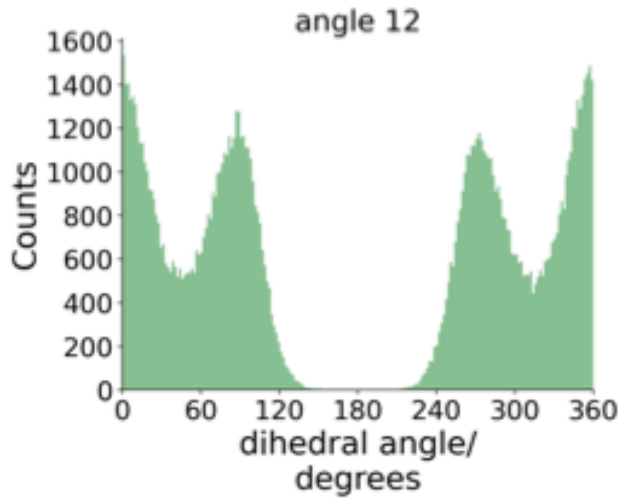

angle 11
Counts
2000
1500
1000
500
0
0
60
120
180
240
300
360
dihedral angle/
degrees

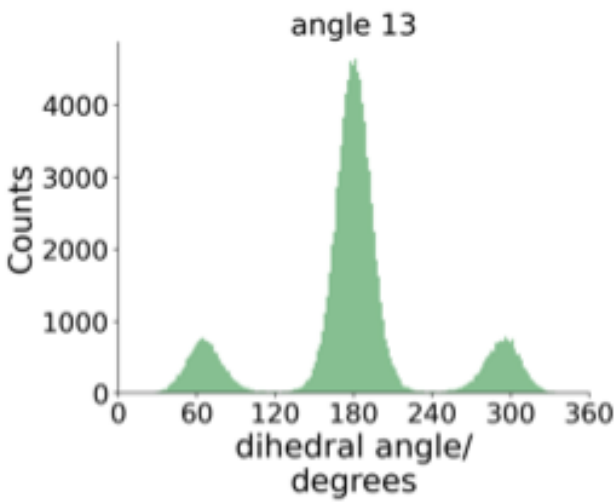
Figure set S9. Menaquinone-6 (MQ6) in n-hexane

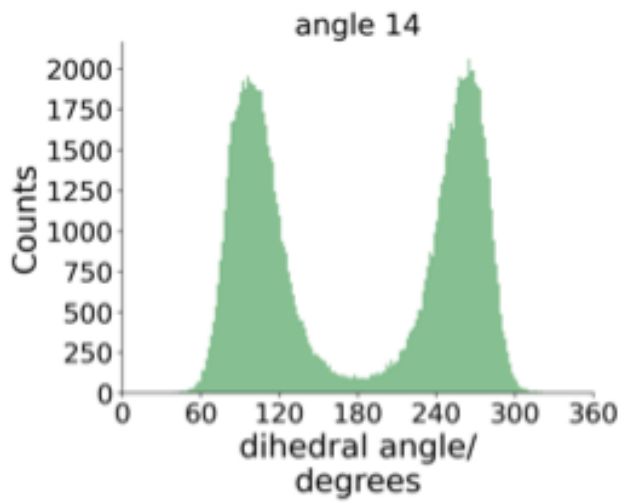

angle 9
Counts
dihedral angle/
degrees

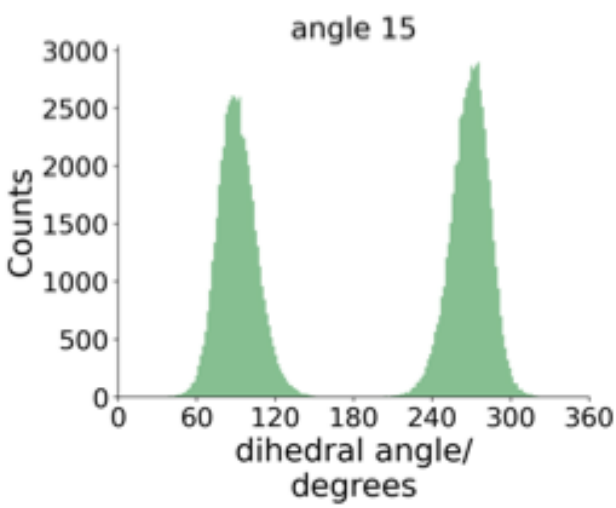

angle 10
Counts
dihedral angle/
degrees

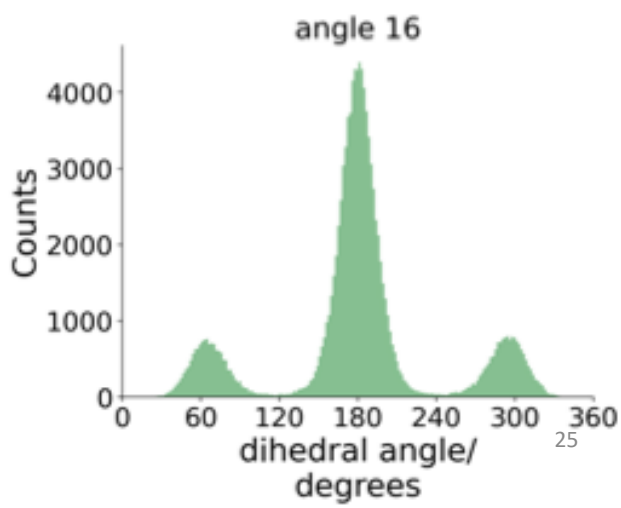

angle 11
Counts
dihedral angle/
degrees

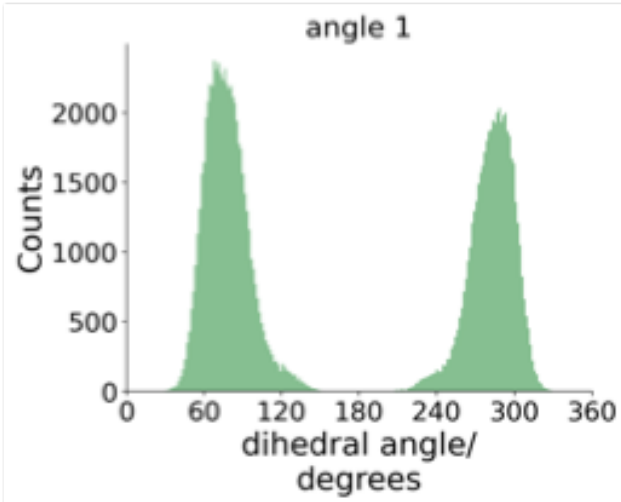

angle 12
Counts
dihedral angle/
degrees

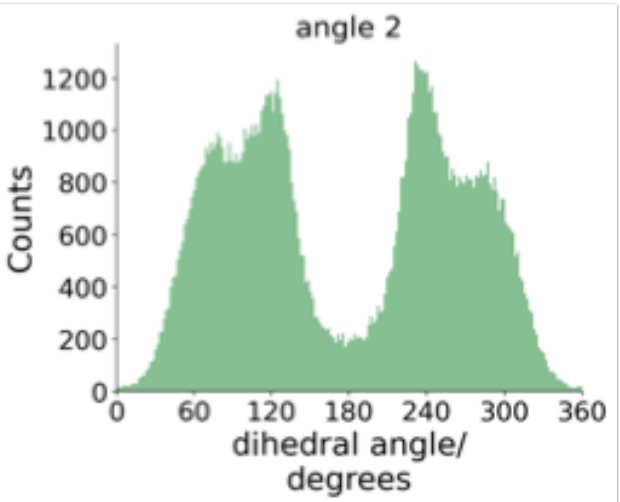

angle 13
Counts
dihedral angle/
degrees

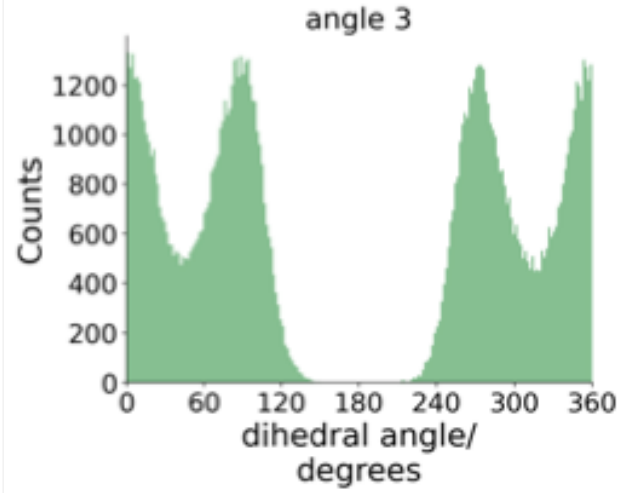

angle 14
Counts
dihedral angle/
degrees

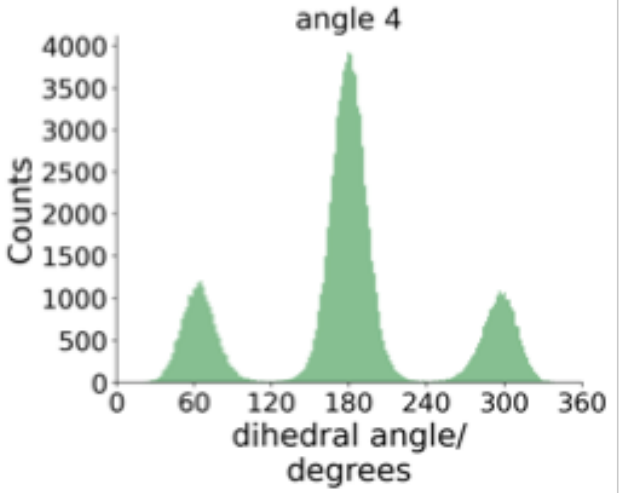

angle 15
Counts
dihedral angle/
degrees

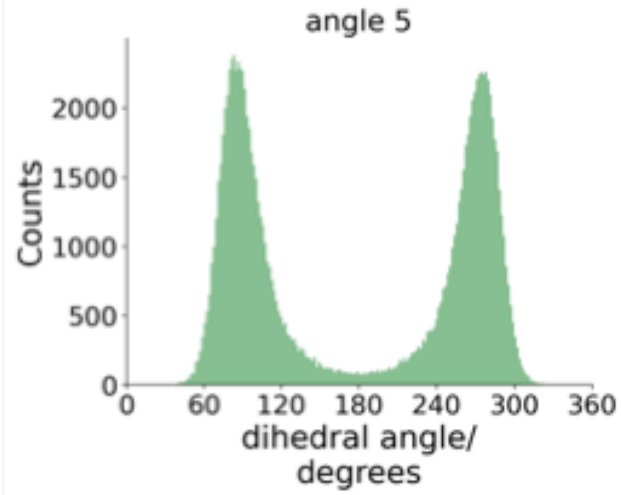

angle 16
Counts
dihedral angle/
degrees

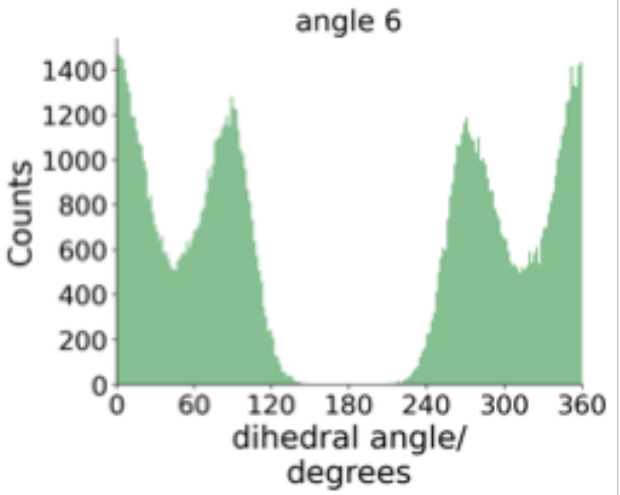

angle 1
Counts
dihedral angle/
degrees

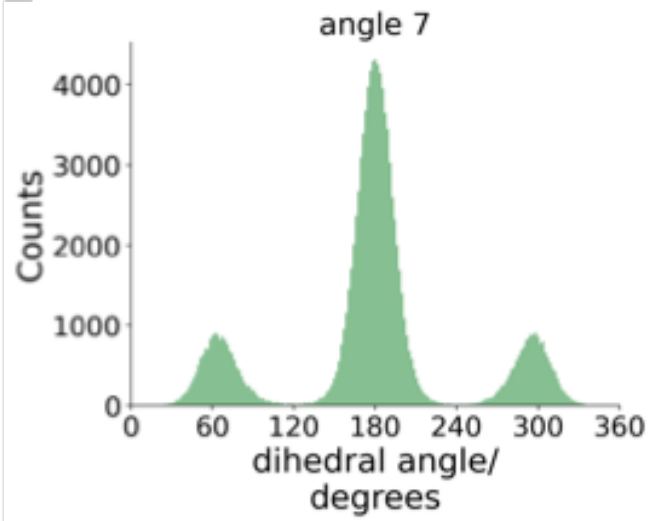

angle 2
Counts
dihedral angle/
degrees

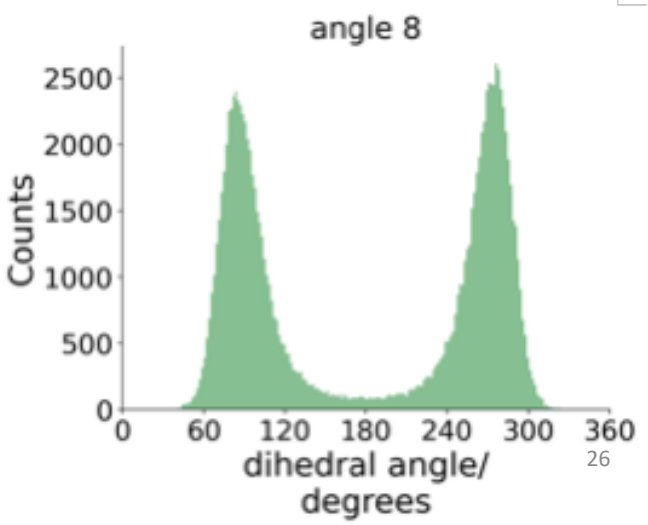

angle 3
Counts
dihedral angle/
degrees


angle 4
Counts
dihedral angle/
degrees


angle 5
Counts
dihedral angle/
degrees


angle 6
Counts
dihedral angle/
degrees


angle 7
Counts
dihedral angle/
degrees


angle 8
Counts
dihedral angle/
degrees

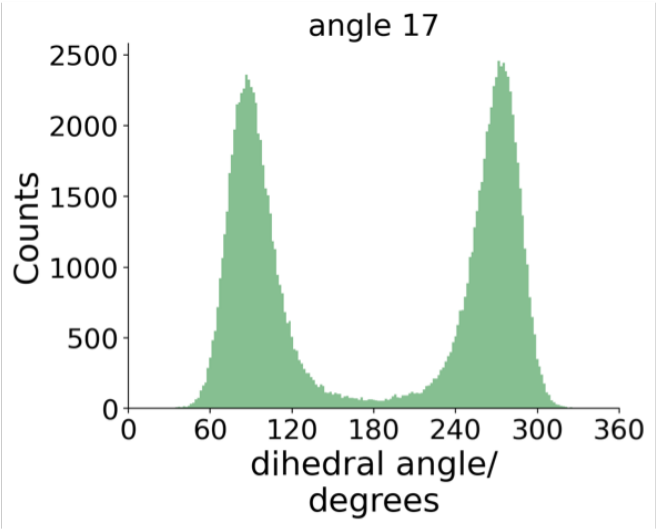
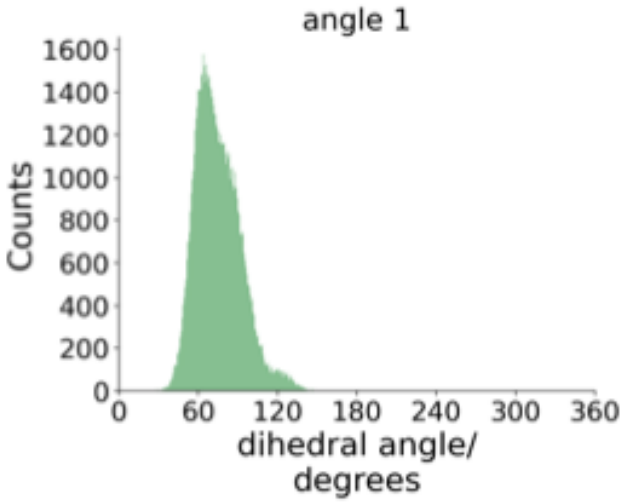
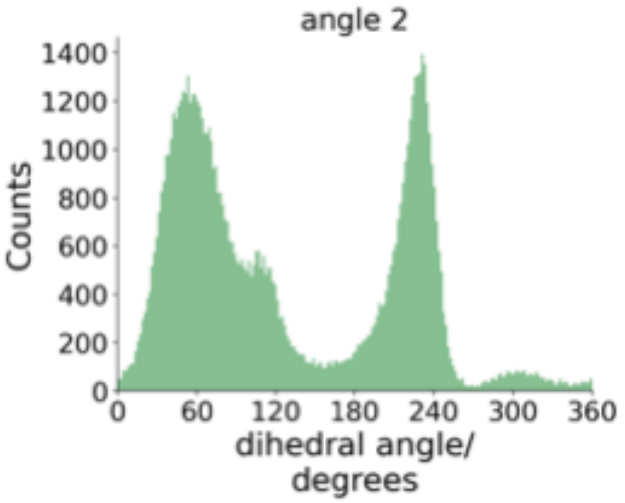
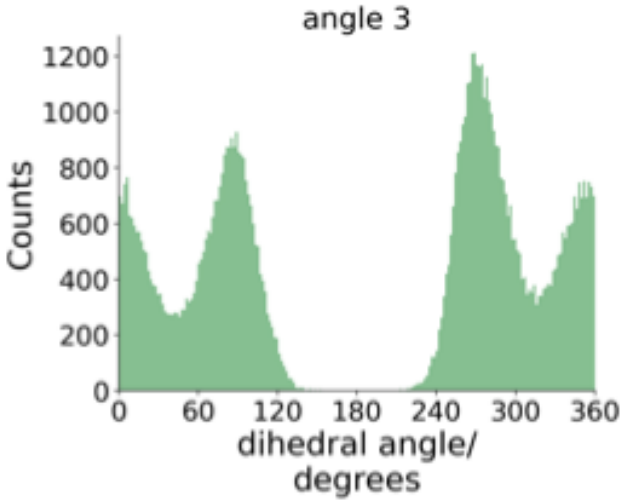
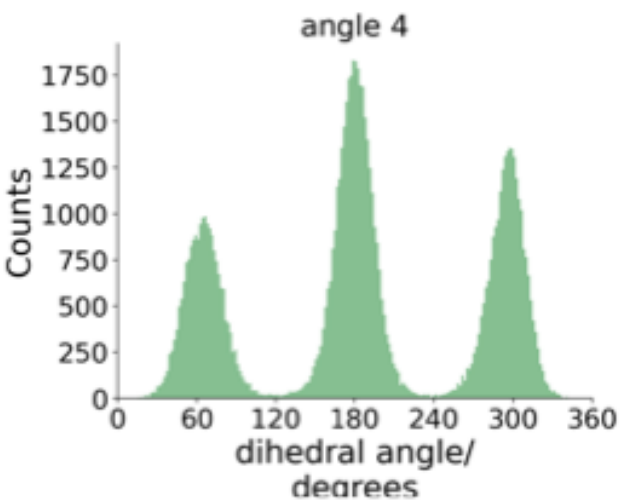

angle 17
2500
2000
1500
1000
500
0
Counts
0
60
120
180
240
300
360
dihedral angle/
degrees

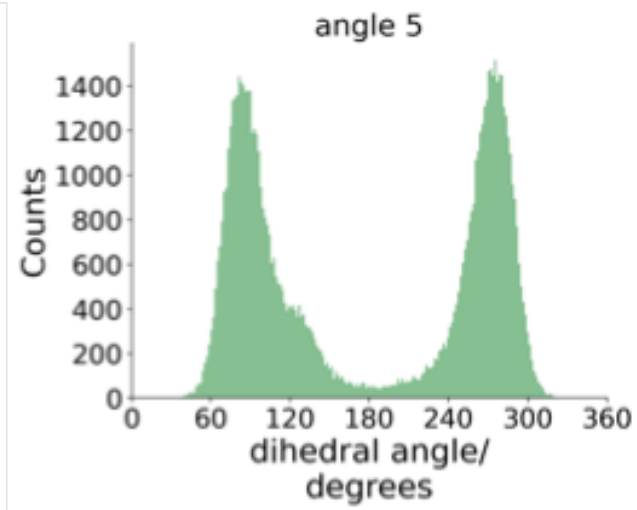
Figure set S10. Menaquinone-6 (MQ6) in a lipid bilayer

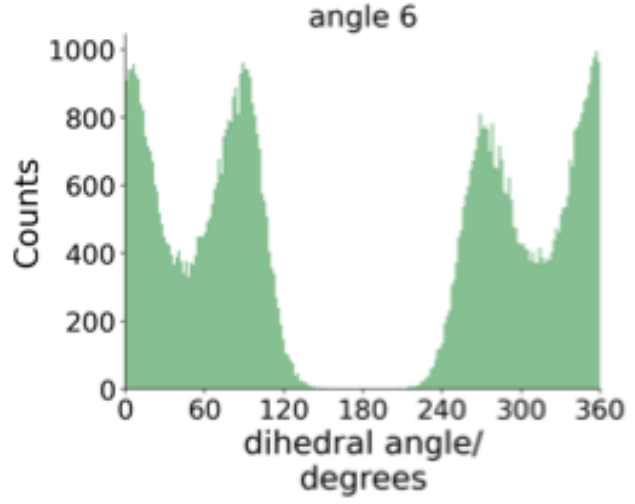

angle 1
Counts
dihedral angle/
degrees

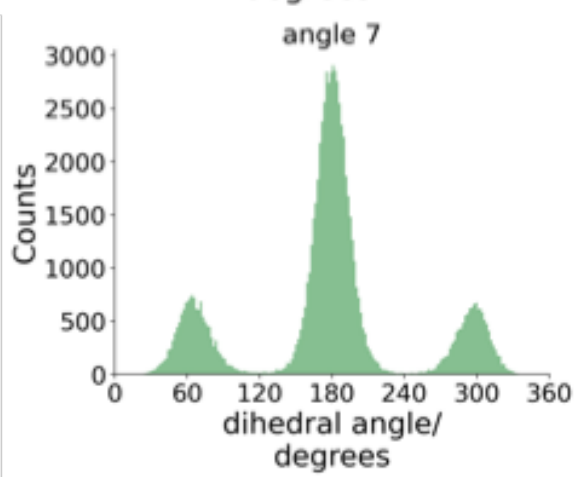

angle 2
Counts
dihedral angle/
degrees

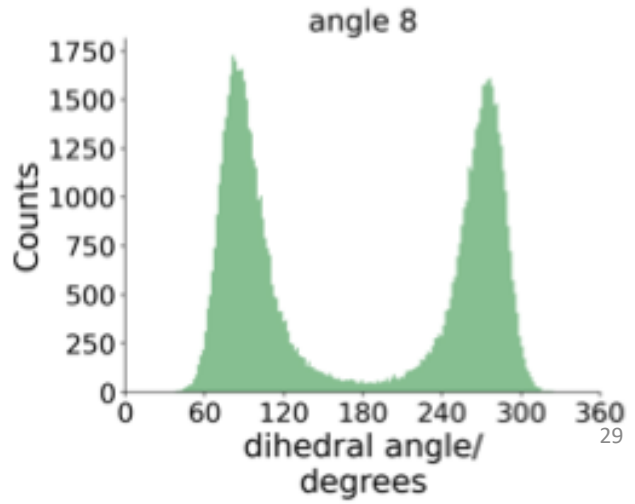

angle 3
Counts
dihedral angle/
degrees

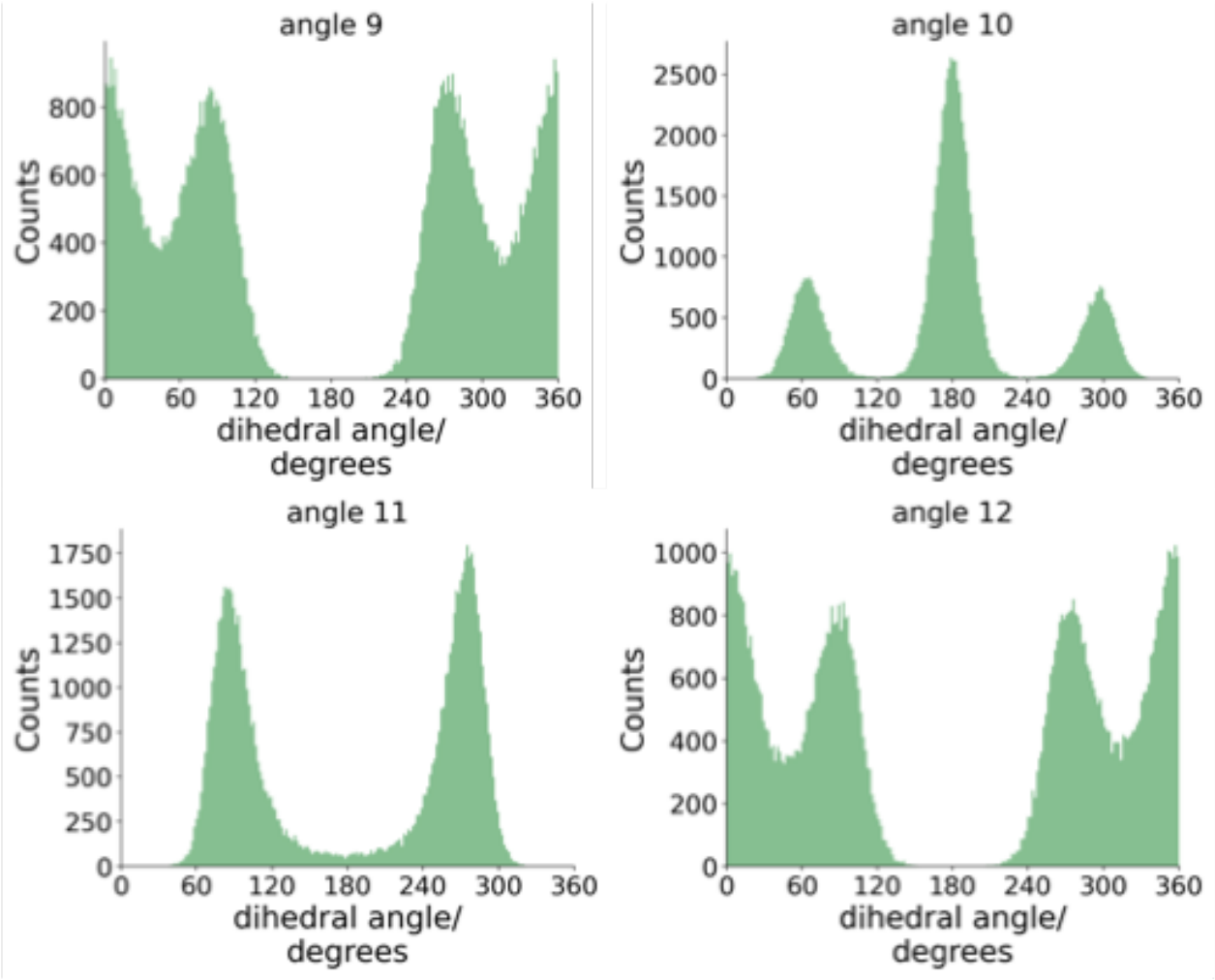

angle 4
Counts
dihedral angle/
degrees


angle 5
Counts
dihedral angle/
degrees


angle 6
Counts
dihedral angle/
degrees


angle 7
Counts
dihedral angle/
degrees


angle 8
Counts
dihedral angle/
degrees


angle 9
Counts
dihedral angle/
degrees
angle 10
Counts
dihedral angle/
degrees
angle 11
Counts
dihedral angle/
degrees
angle 12
Counts
dihedral angle/
degrees

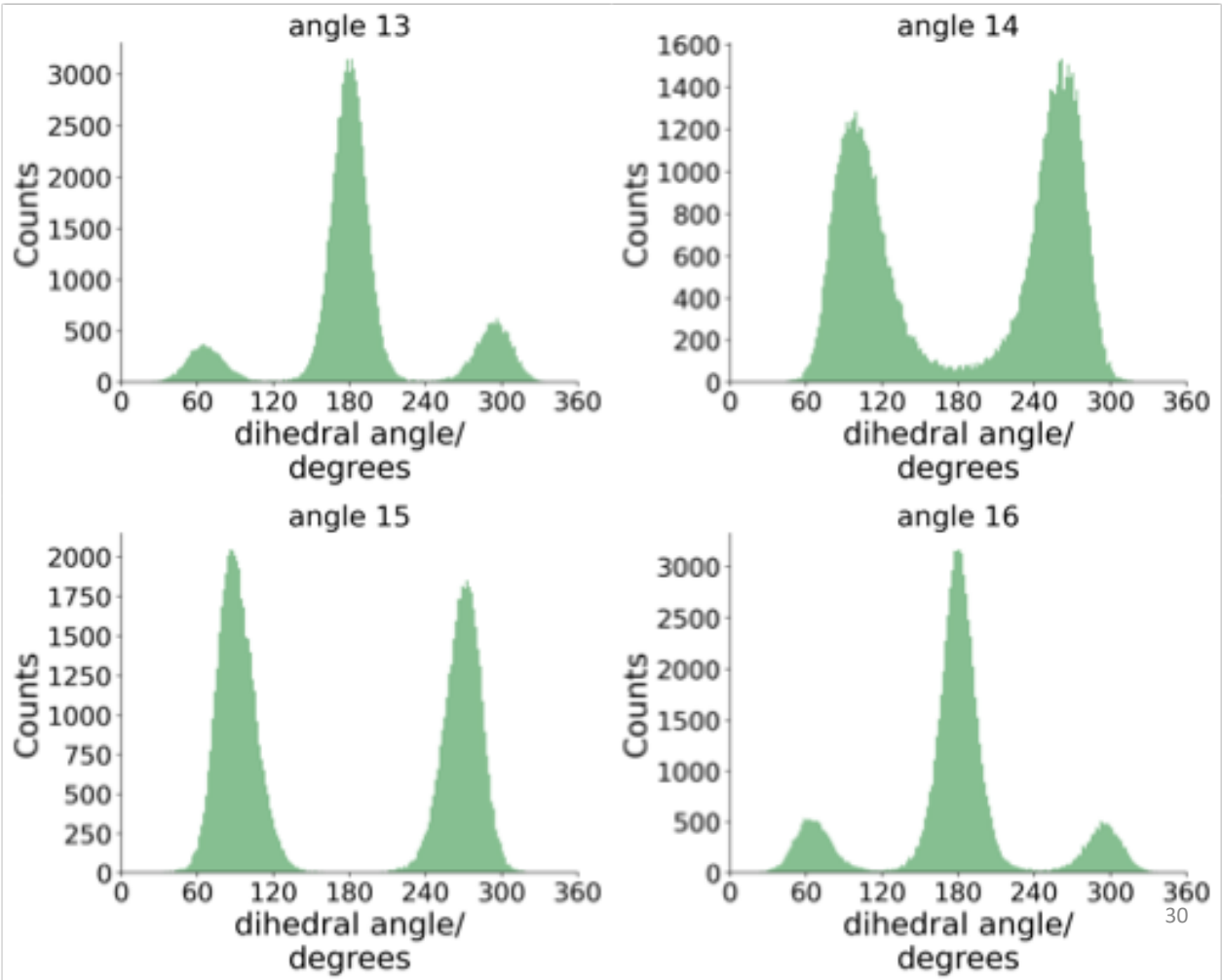
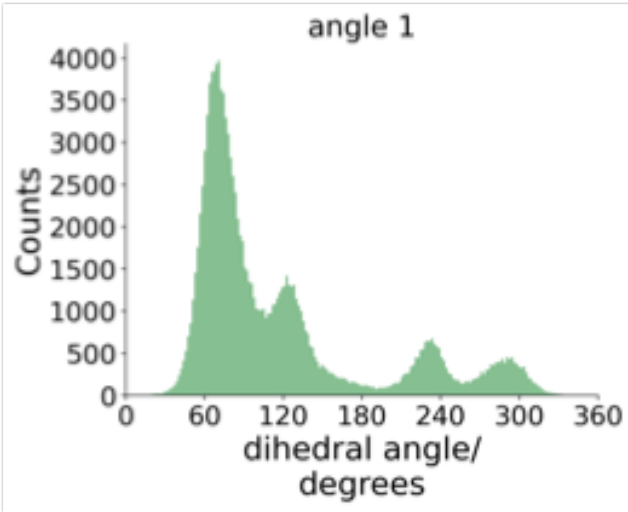
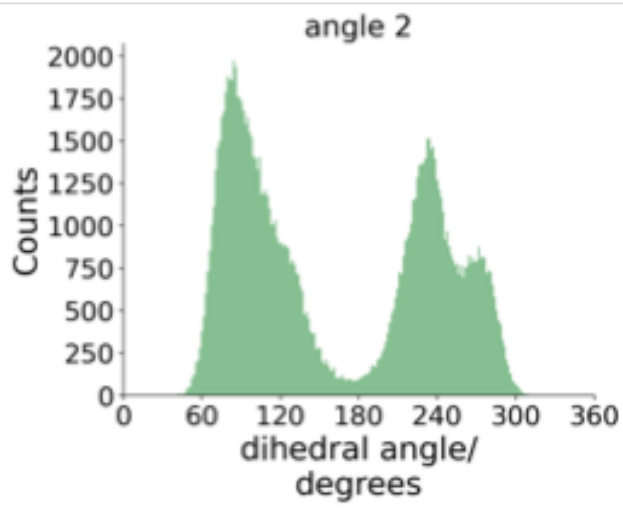
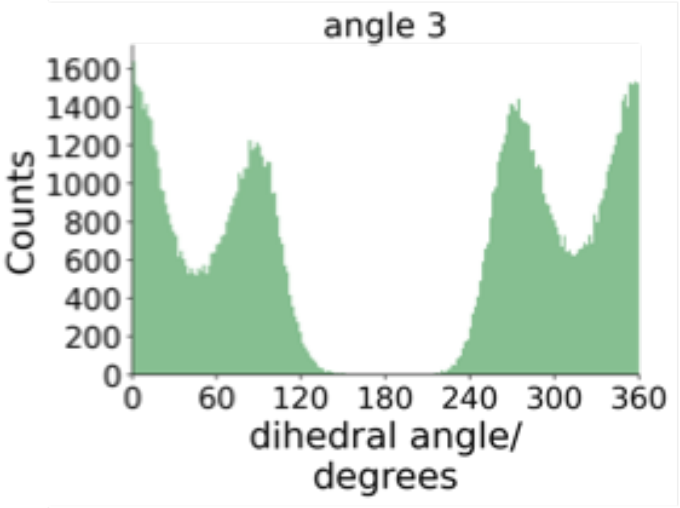
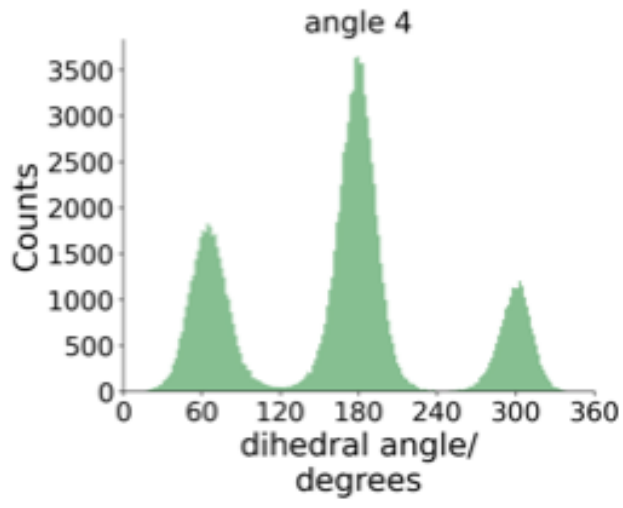

angle 13
Counts
dihedral angle/
degrees
angle 14
Counts
dihedral angle/
degrees
angle 15
Counts
dihedral angle/
degrees
angle 16
Counts
dihedral angle/
degrees

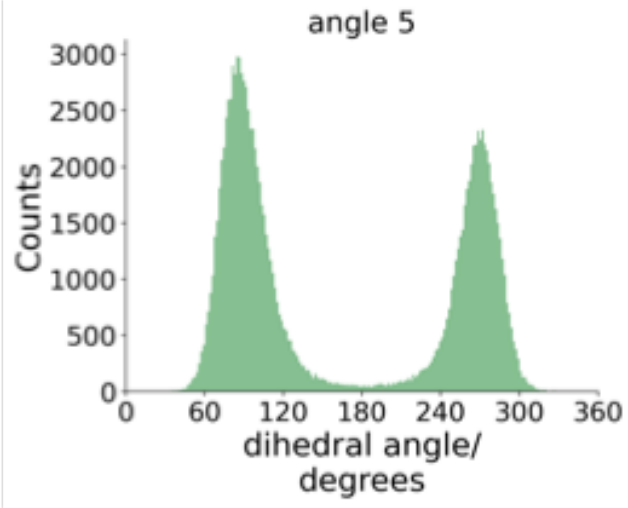
Figure set S11. Menaquinone-8 (MQ8) in a lipid bilayer

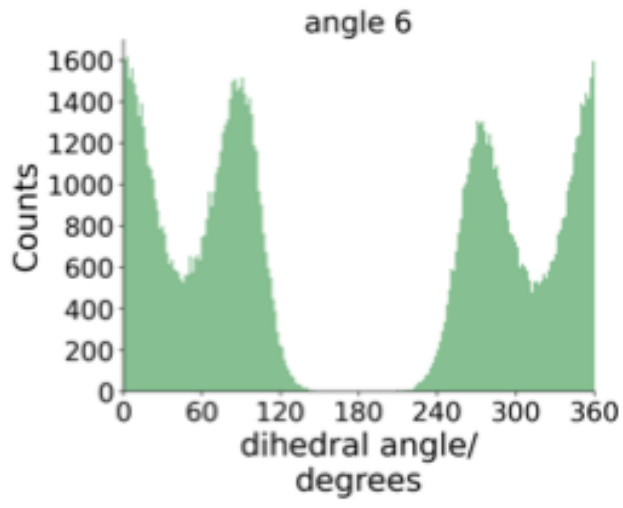

angle 1
Counts
dihedral angle/
degrees

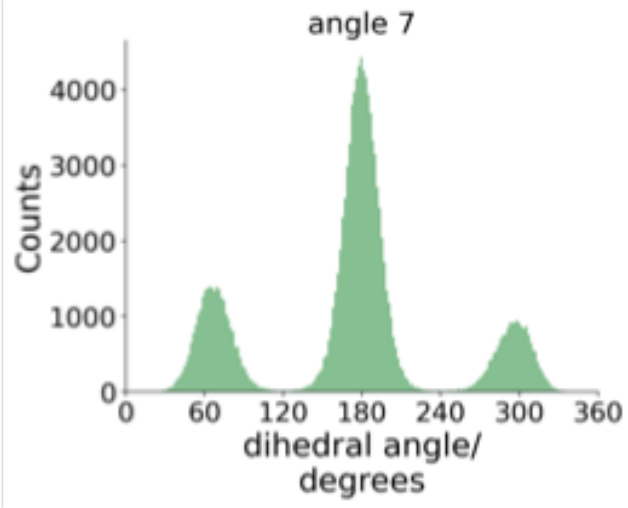

angle 2
Counts
dihedral angle/
degrees

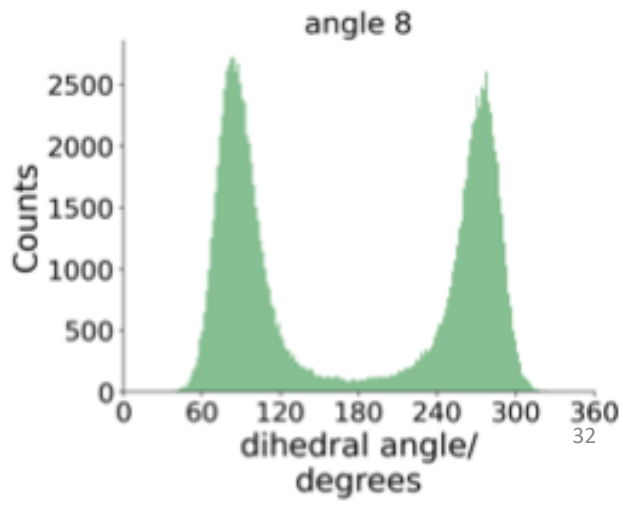

angle 3
Counts
dihedral angle/
degrees

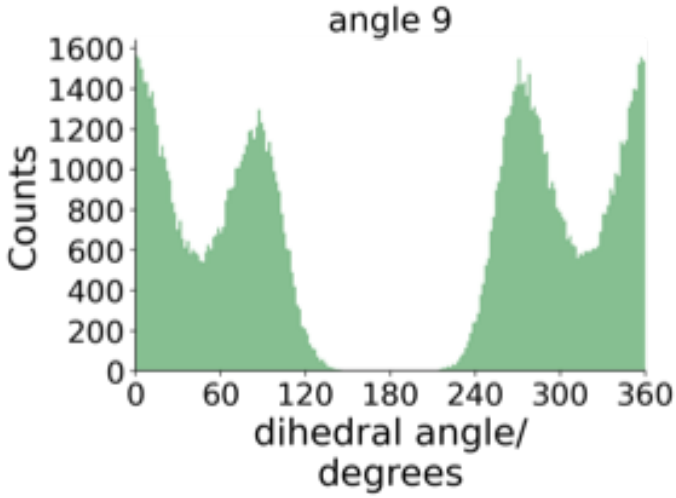

angle 4
Counts
dihedral angle/
degrees

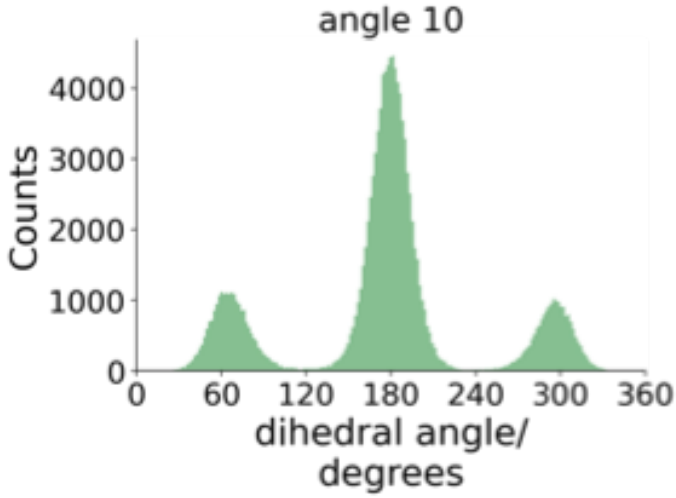

angle 5
Counts
dihedral angle/
degrees

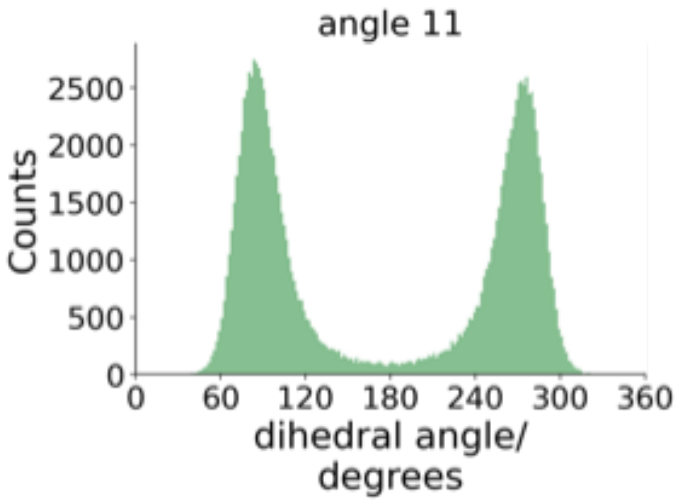

angle 6
Counts
dihedral angle/
degrees

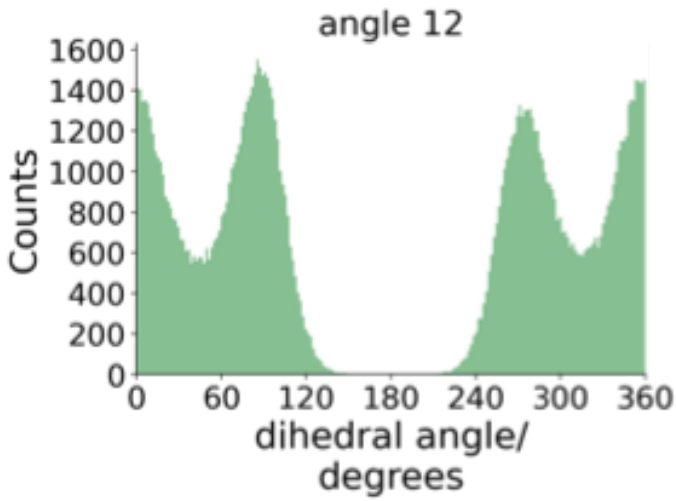

angle 7
Counts
dihedral angle/
degrees

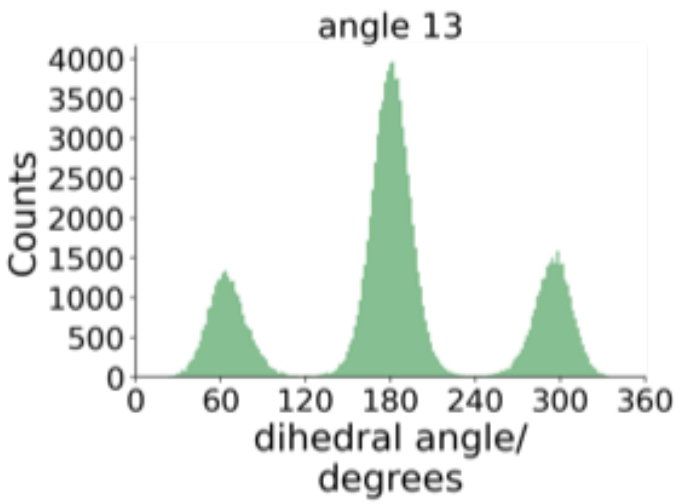

angle 8
Counts
dihedral angle/
degrees

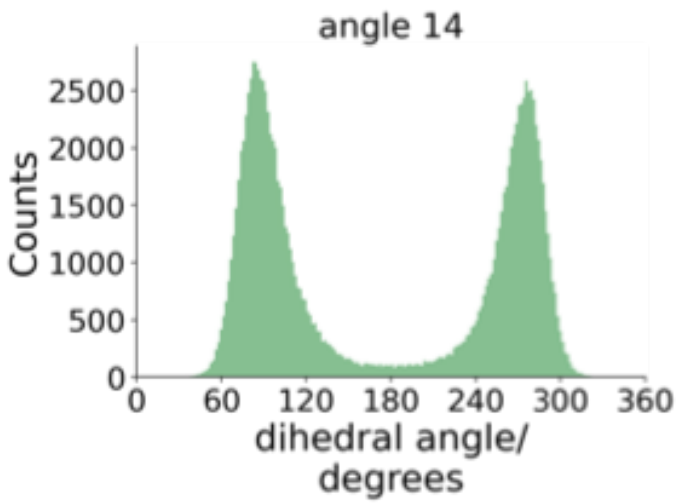

angle 9
Counts
dihedral angle/
degrees

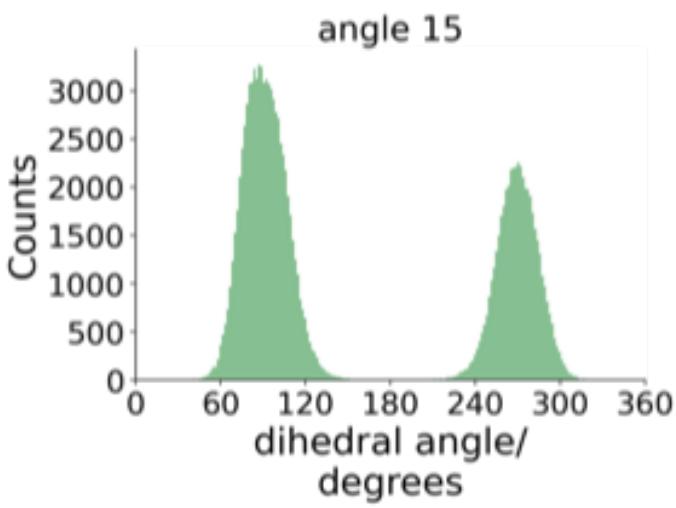

angle 10
Counts
dihedral angle/
degrees

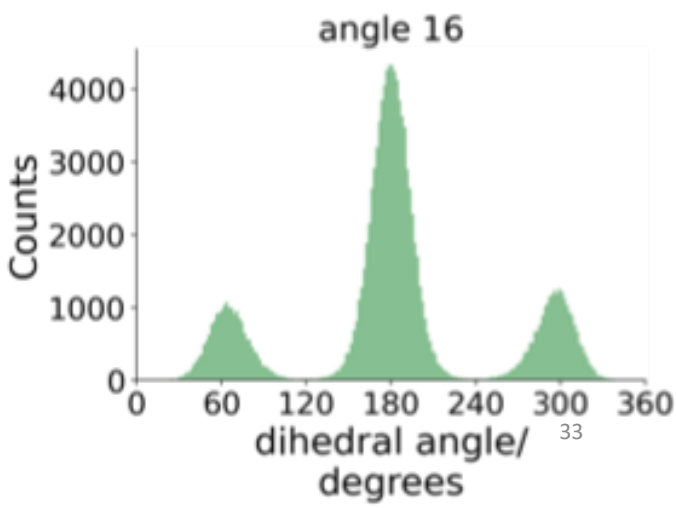

angle 11
Counts
dihedral angle/
degrees

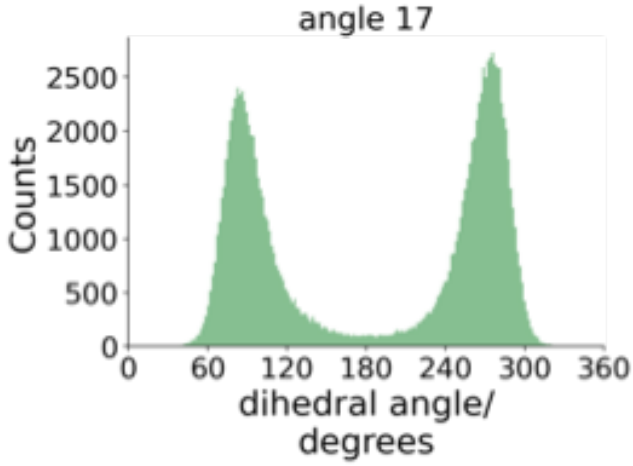

angle 12
Counts
dihedral angle/
degrees


angle 13
Counts
dihedral angle/
degrees


angle 14
Counts
dihedral angle/
degrees


angle 15
Counts
dihedral angle/
degrees


angle 16
Counts
dihedral angle/
degrees


angle 17
Counts
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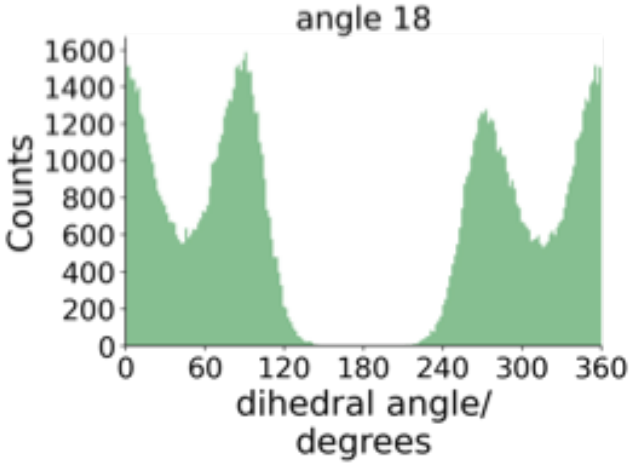
2000
1500
1000
500
0
0 60 120 180 240 300 360
dihedral angle/
degrees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Counts
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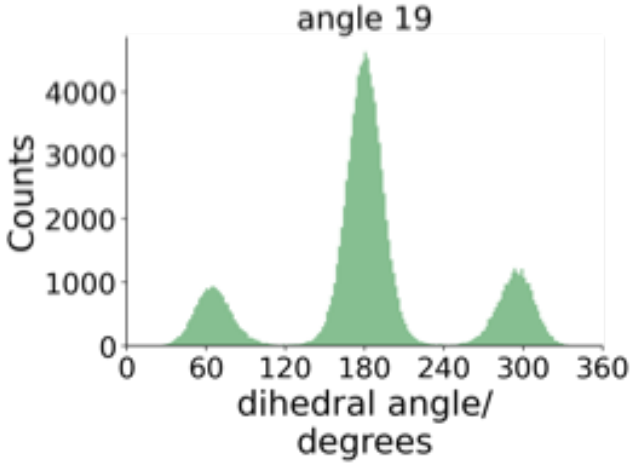
1400
1200
1000
800
600
400
200
0
0 60 120 180 240 300 360
dihedral angle/
degrees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Counts
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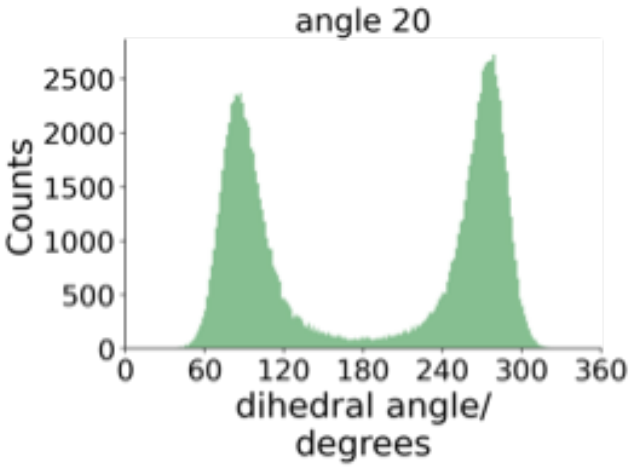
3000
2000
1000
0
0 60 120 180 240 300 360
dihedral angle/
degrees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1500
1000
500
0
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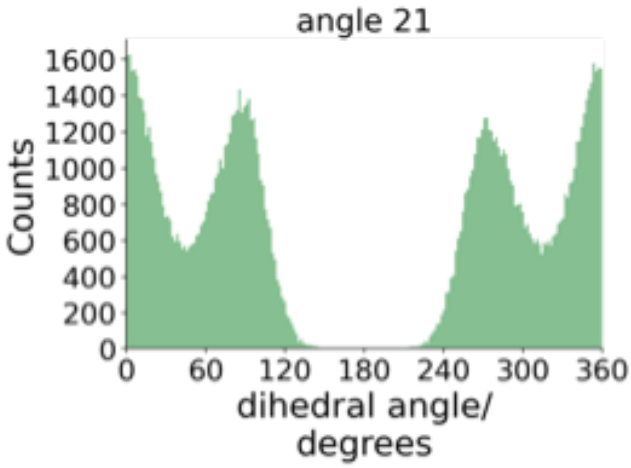
dihedral angle/
degrees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Counts
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200
0
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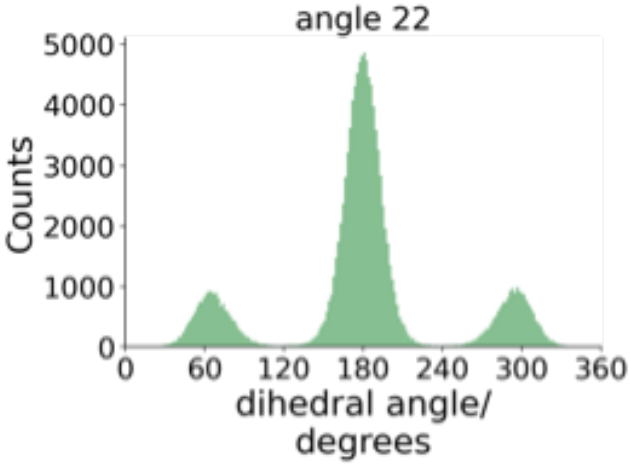
dihedral angle/
degrees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4000
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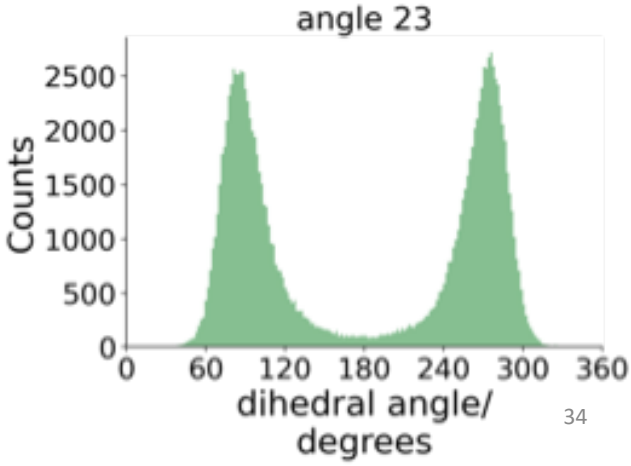
dihedral angle/
degrees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1000
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0
0 60 120 180 240 300 360
dihedral angle/
degrees