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ERRATUM

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Erratum to: Implementation of a methodology for determining elastic properties of lipid assemblies from molecular dynamics simulations

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Unfortunately, the original version of this article [1] contained an error. The incorrect version of Scheme 4 was used and Scheme 4 and 6 were also accidentally interchanged during processing. The correct schema and labelling is presented below.

```
import lipid_analysis
from ost import *
p=io.IOProfile(dialect='CHARMM')
eh=io.LoadPDB("aligned.pdb",profile=p)
t=io.LoadCHARMMTraj(eh,"aligned.dcd")

water_name='TIP3'
lipid_names=['DPPC']
head_group_dict={'DPPC':'aname=P,C2'}
tail_dict={'DPPC':'aname=C214,C215,C216,C314,C315,C316'}
distance_dict={'DPPC':'aname=C22,C21,C23,C31,C32,C33'}

for r in eh.Select("cname=M and rname=DPPC").residues:
  r.SetBoolProp("do_tilt",True)
  r.SetBoolProp("do_splay",True)

for r in eh.Select("cname!=M and rname=DPPC").residues:
  r.SetBoolProp("do_tilt",False)
  r.SetBoolProp("do_splay",False)

(tilt_dict,normal_dict,splay_dict,b_eh)=lipid_analysis.AnalyzeLipidTiltAndSplay(
  t,lipid_names,head_group_dict,tail_dict,distance_sele_dict=distance_dict,water_name=water_name,
  tilt_bool_prop="do_tilt",splay_bool_prop="do_splay",outdir="MyOutputDirectory")
```

Scheme 4. Calculating lipid tilts and splays

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```
selections={"upper":"z>0.0","lower":"z<0.0"}
(tilt_dict,normal_dict,splay_dict,b_eh)=lipid_analysis.AnalyzeLipidTiltAndSplay(
  t,lipid_names,head_group_dict,tail_dict,distance_sele_dict=distance_dict,water_name=water_name,
  tilt_bool_prop="do_tilt",splay_bool_prop="do_splay",outdir="MyOutputDirectory",sele_dict=selections)
k_dict=lipid_analysis.ExtractTiltAndSplayModuli(tilt_dict,splay_dict,lipid_area,"MyOutputDirectory")
```

Scheme 6. Calculate tilts and splays for each leaflet of a planar bilayer separately

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Reference

1. Johner N, Harries D, Khelashvili G. Implementation of a methodology for determining elastic properties of lipid assemblies from molecular dynamics simulations. BMC Bioinformatics. 2016;17:161.