SUPPORTING INFORMATION

A. Input file for APBS

Unless otherwise specified, all APBS computation uses the following set of parameters:

```
mg-auto, dime  513 513 513, cgcent 0 0 0, fgcent 0 0 0, cglen 200 200 200, fglen 100 100 100, mol 1,  lpbe, bcfl mdh, pdie 4.0,  sdie 78.0,  srfm mol, chgm spl2, sdens 10.00, srad 0.0, swin 0.30, temp 298.15, ion charge 1 conc 0.05 radius 0.0, ion charge -1 conc 0.05 radius 0.0.
```

B. Benchmarking – spherical cases:

The grid dimension (`dime`) is varied to `65`, `129`, `257`, and `513` as per Table 2.

Benchmarking – two overlapping spheres:

The coarse grid length (`cglen`) and fine grid length (`fglen`) are varied as per Table A1:

Table A1. APBS parameters for two overlapping spheres benchmarks

Sphere Size [Å]	`cglen`	`fglen`
2	20	10
5	50	20
15	150	60
50	500	200

C. Brome Mosaic Virus

The fine grid length (`fglen`) is set to 120.