Supplementary Information

Identifying Resonant Frequencies of Viruses for Microwave-Based Detection and Inactivation of Pathogenic Viruses

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Supplementary Figures S1-S7 and Tcl script for calculating dipole moments

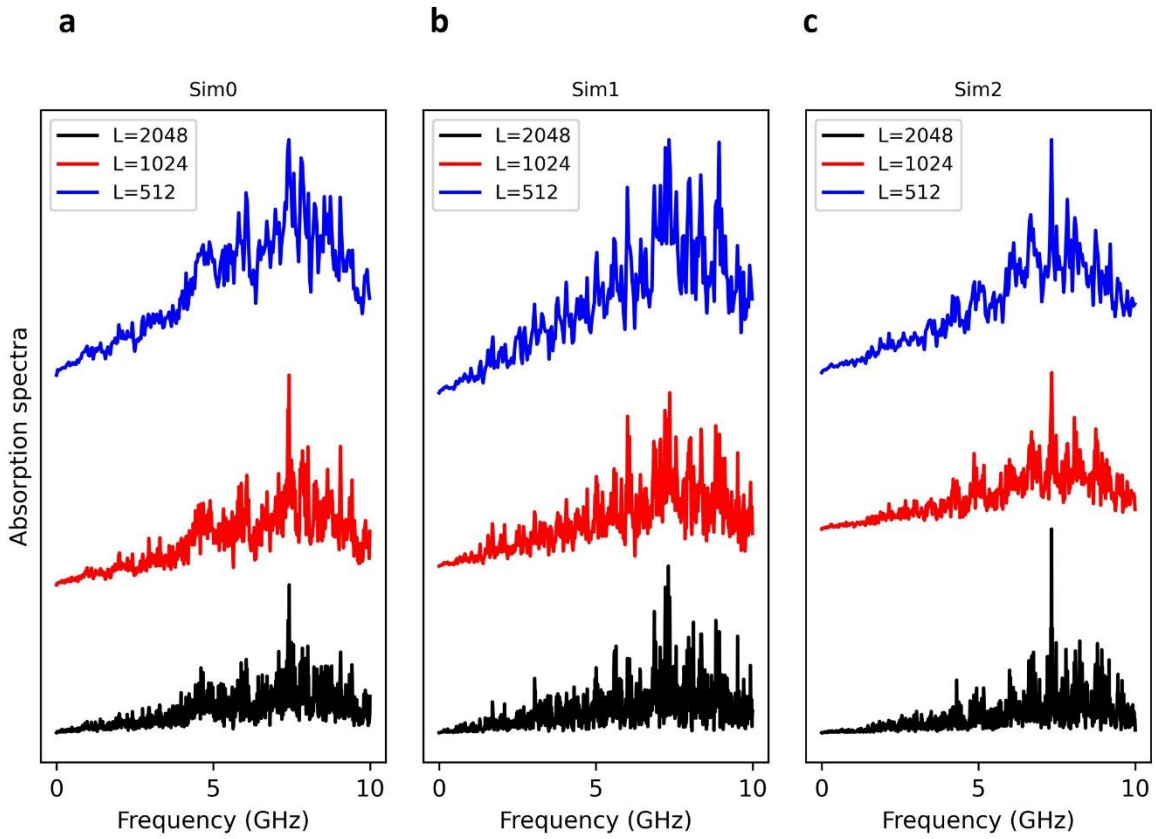

Figure S1. Choice of segment length L. We have calculated the absorption spectra for the segment length composing of 2^9 to 2^{11} sequential samples for Sim0, Sim1, and Sim2, respectively. Although all spectra show a peak around 7.5 GHz, a good balance between resolution and variance is achieved at $L = 2048$. The frequency resolution achieved at $L = 2048$ is 9.765625 MHz.

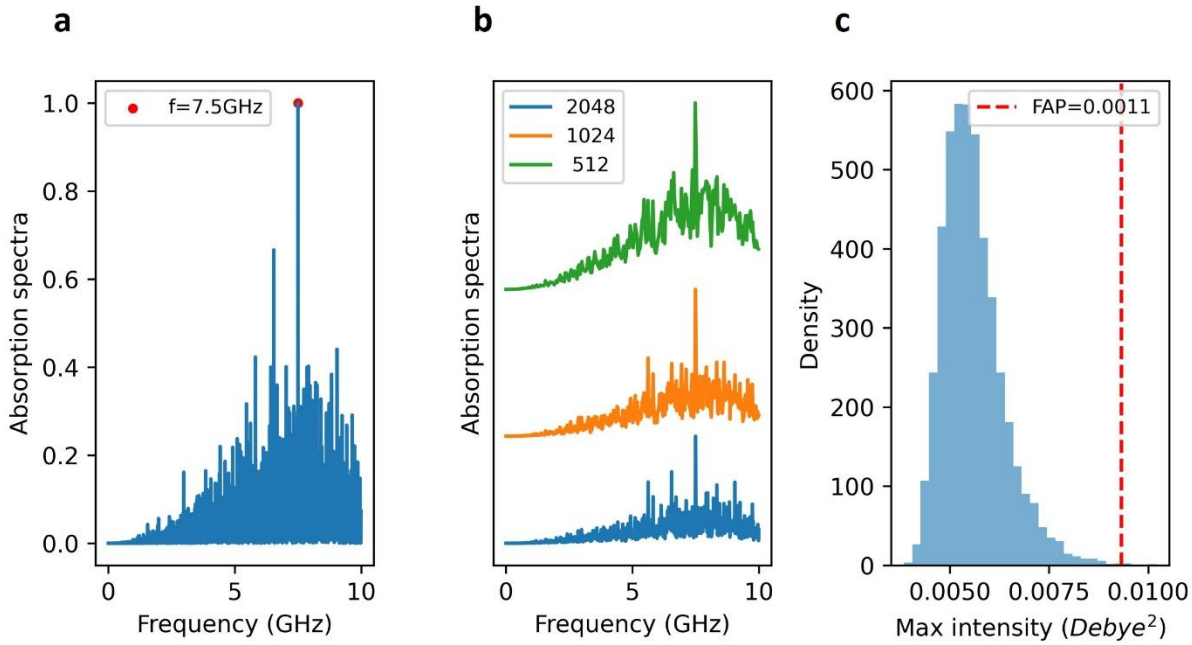

Figure S2. Test of computational methods. Setting random seed using *numpy.random.seed(seed=54321)*, a cosine wave with a frequency at 7.5 GHz is clearly revealed with FAP 0.11% using only 6500 data points.

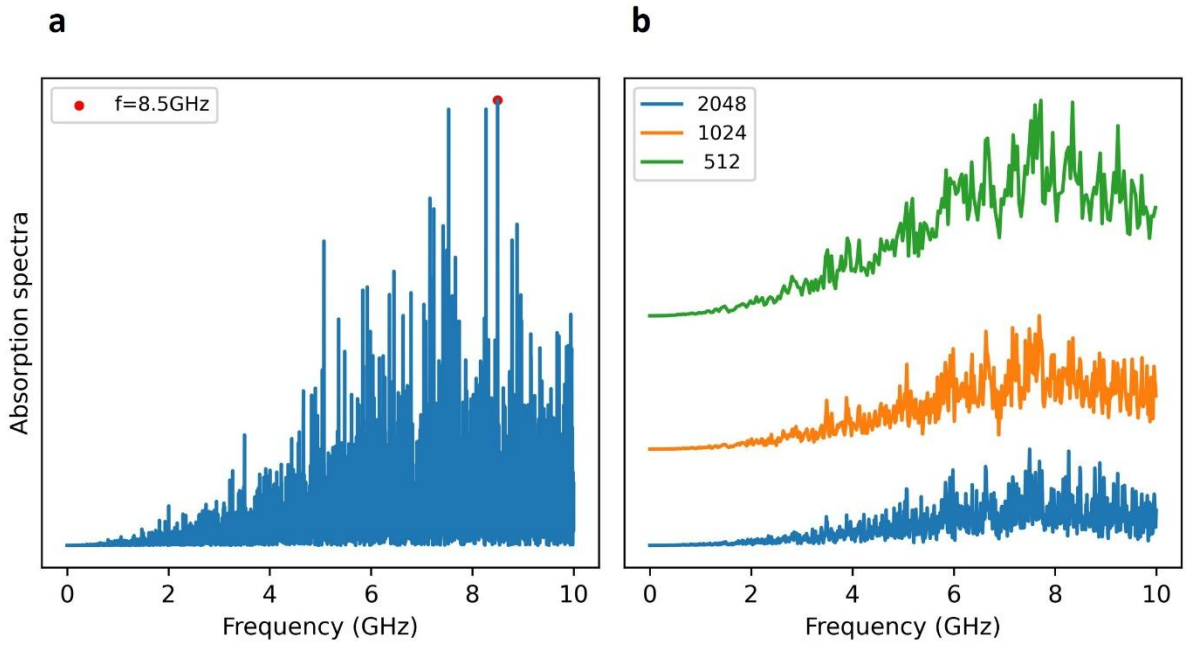

Figure S3. Test of computational methods. Setting random seed using numpy.random.seed(seed=12345), a cosine wave with a frequency at 7.5 GHz is unobservable using only 6500 data points.

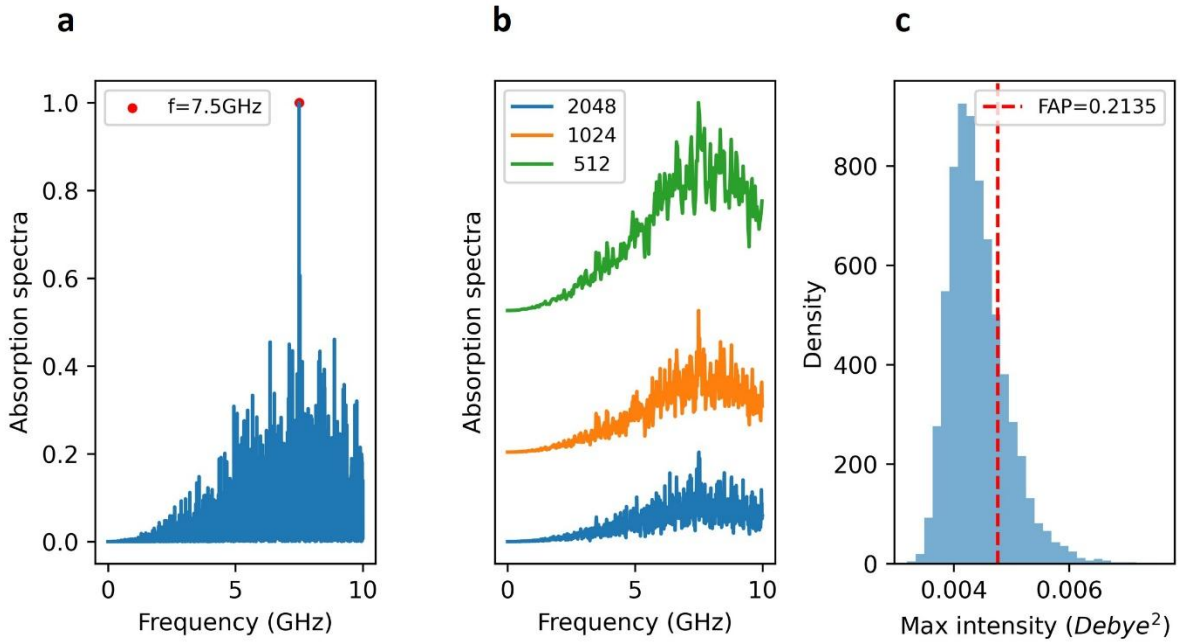

Figure S4. Test of computational methods. Setting random seed using numpy.random.seed(seed=12345), a cosine wave with a frequency at 7.5 GHz is observable with FAP 21.35% using 11000 data points.

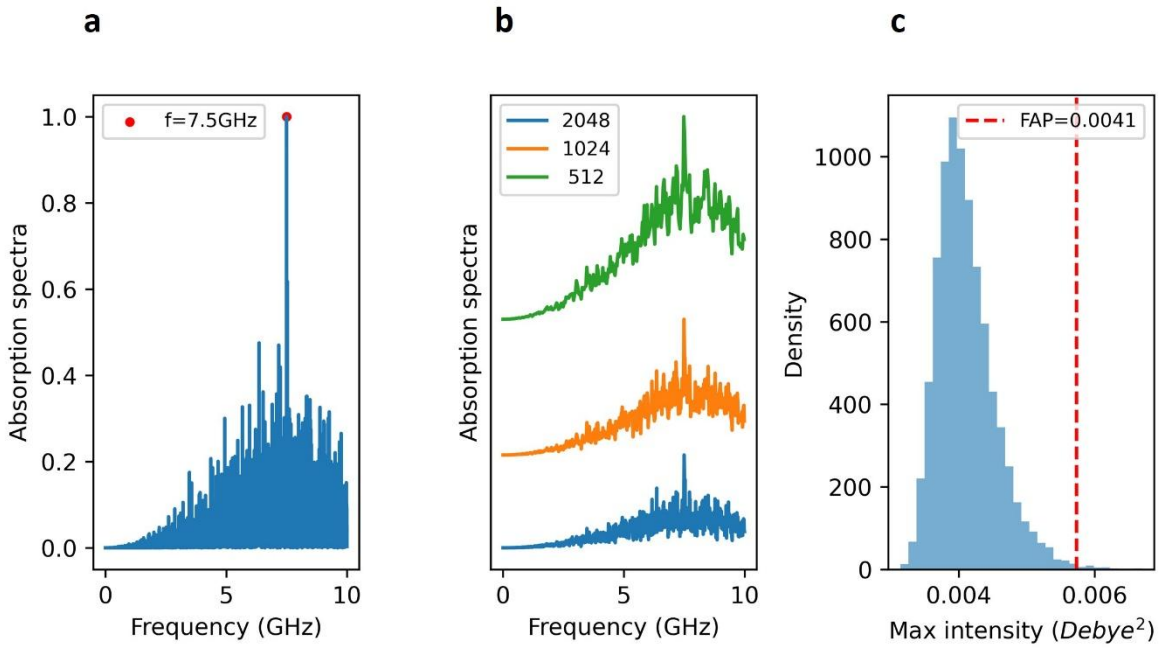

Figure S5. Test of computational methods. Setting random seed using numpy.random.seed(seed=12345), a cosine wave with a frequency at 7.5 GHz is observable with FAP 0.41% using 13000 data points.

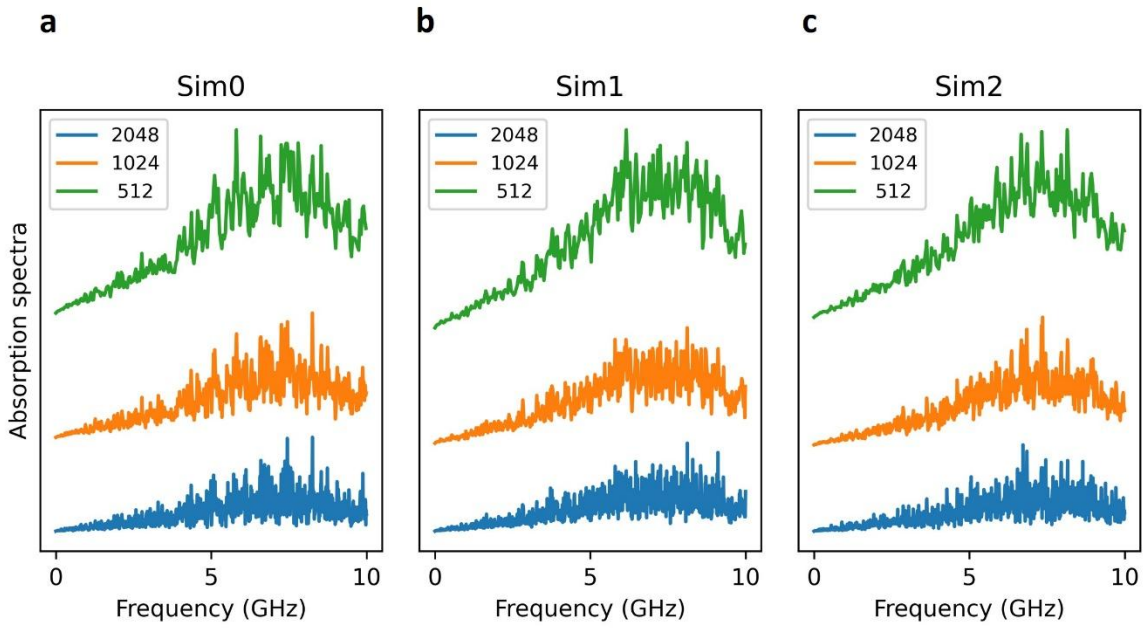

Figure S6. Localized dipole moment analysis for the S1 domain. We have recalculated the absorption spectra after selecting the S1 subunit of S protein. No significant peaks are observed in the S1 domain.

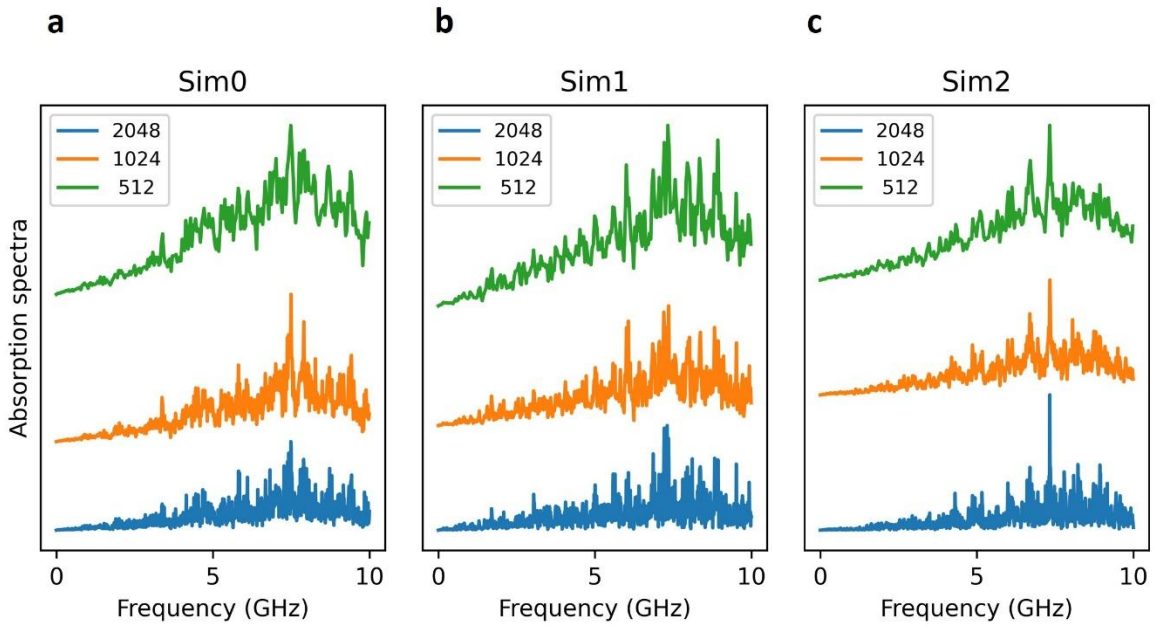

Figure S7. Localized dipole moment analysis for the S2 domain. We have recalculated the absorption spectra after selecting the S2 subunit of S protein. A peak around 7.5 GHz is clearly seen in all three simulations Sim0, Sim1, and Sim2. This implies that S2 makes dominant contribution to the global dipole moment fluctuations, which is in agreement with experimentally observed flexibility of the S2 domain.

 # Tcl script for calculating dipole moments

```
## load trajectory and packages
cd /p/work1/kuangz/SARS_charmgui/ps50_npt_0
mol new com.psf type psf waitfor all
mol addfile ps50.dcd type dcd waitfor all
package require pbctools
pbc readxst prod1.restart.xsc
## open output files for dipole moments and radius of gyration
### full S protein
set DipoleS pbcDipoleS.dat
set DipoleSID [open $DipoleS w]
set RgyrS pbcRgyrS.dat
set RgyrSID [open $RgyrS w]
### S1 subunit
set DipoleS1 pbcDipoleS1.dat
set DipoleS1ID [open $DipoleS1 w]
set RgyrS1 pbcRgyrS1.dat
set RgyrS1ID [open $RgyrS1 w]
### S2 subunit
set DipoleS2 pbcDipoleS2.dat
set DipoleS2ID [open $DipoleS2 w]
set RgyrS2 pbcRgyrS2.dat
set RgyrS2ID [open $RgyrS2 w]
## loop all trajectory
set n [molinfo top get numframes]
for { set i 0 } { $i < $n } { incr i } {
```

```
    ### update snapshot and wrap protein back to COM
    animate goto $i
    display update ui
    pbc wrap -now -centersel "not (water or ions or segname MEMB)" -center com -compound residue
    pbc wrap -now -centersel "not (water or ions or segname MEMB)" -center com -compound residue
    pbc wrap -now -centersel "not (water or ions or segname MEMB)" -center com -compound residue
    ### select atoms
    set prt [atomselect top "not (water or ions or segname MEMB)" frame $i]
    set S1 [atomselect top "(same segname as (within 1.6 of ((resid 1 to 685) and protein))) and (not (water or ions or segname MEMB or (protein and resid 686 to 1273) ))"]
    set S2 [atomselect top "(same segname as (within 1.6 of ((resid 686 to 1273) and protein))) and (not (water or ions or segname MEMB or (protein and resid 1 to 685) ))"]
    ### calcuate dipole moments and radius of gyration
    puts $DipoleSID "[measure dipole $prt -debye -masscenter]"
    puts $RgyrSID "[measure rgyr $prt weight mass]"
    puts $DipoleS1ID "[measure dipole $S1 -debye -masscenter]"
    puts $RgyrS1ID "[measure rgyr $S1 weight mass]"
    puts $DipoleS2ID "[measure dipole $S2 -debye -masscenter]"
    puts $RgyrS2ID "[measure rgyr $S2 weight mass]"
}
## close files
close $DipoleSID
close $RgyrSID
close $DipoleS1ID
```

```
close $RgyrS1ID

close $DipoleS2ID

close $RgyrS2ID

exit
```