Supporting information for:

Modeling the Tyrosine-Sugar Interactions in Supersonic Expansions: The Glucopyranose-Phenol Clusters

*Imanol Usabiaga, Jorge González, Pedro F. Arnáiz, Iker León, Emilio Cocinero and José A. Fernández**

Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Barrio Sarriena, s/n, 48940 Leioa, Spain

*Corresponding Author:

José A. Fernández, josea.fernandez@ehu.es

pone: +34946015387

fax: +34946013500

web: https://sites.google.com/site/gesemupv/

Figure S1. Gibbs free energy of the 12 most stable conformers (six alpha and six beta anomers) of methyl-D-glucopyranose, relative to the most stable structure. The structure of the 12 species is depicted below, with the structural differences highlighted.

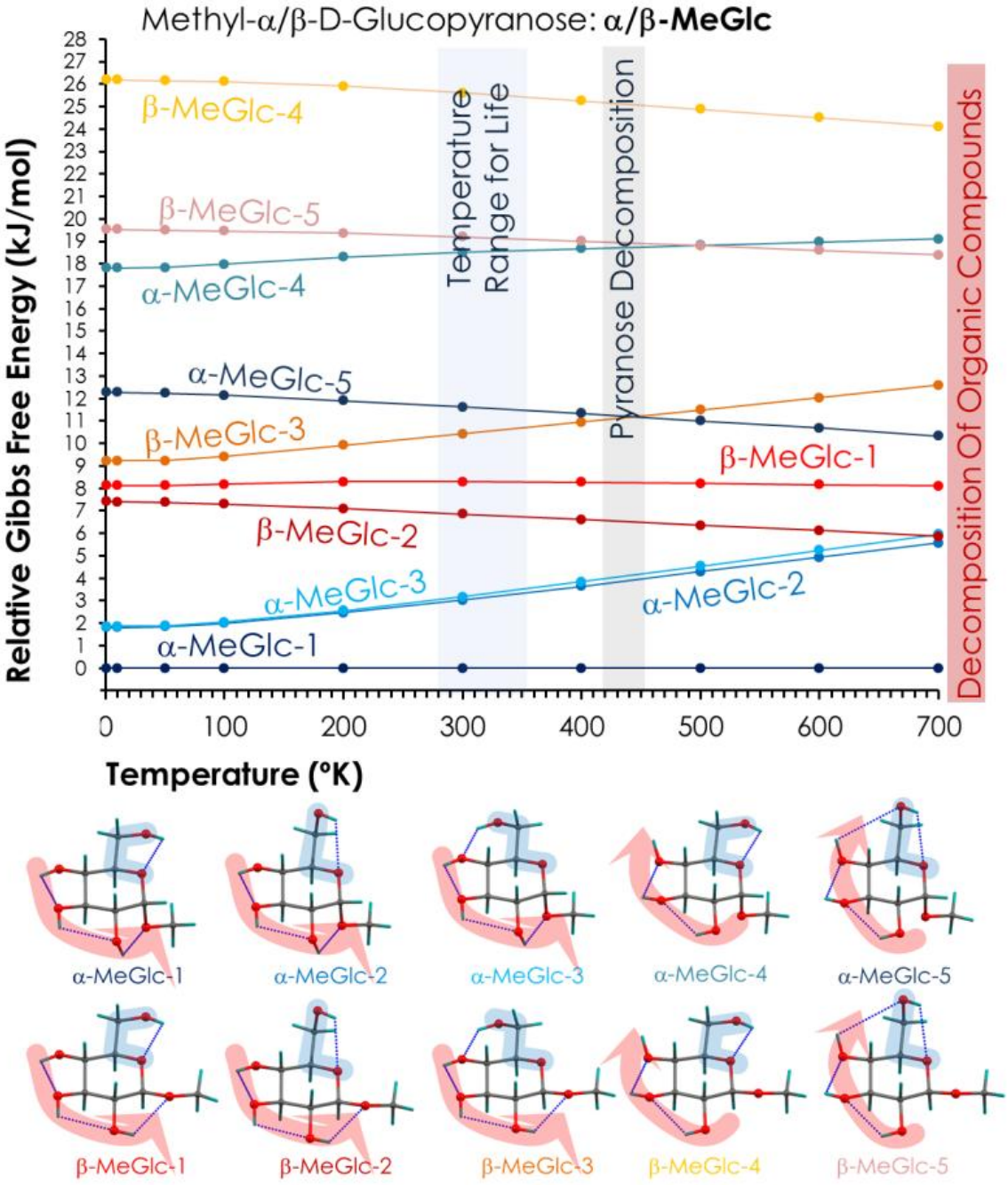


Figure S2. REMPI spectra of phenol, β-phenyl-D-glucopyranose (β-PhGlc), α-methyl-D-glucopyranose···phenol (α-MeGlc·Ph), β-methyl-D-glucopyranose···phenol (β-MeGlc·Ph) and β-phenyl-D-glucopyranose···phenol (β-PhGlc·Ph) in the 36100-37100 region.

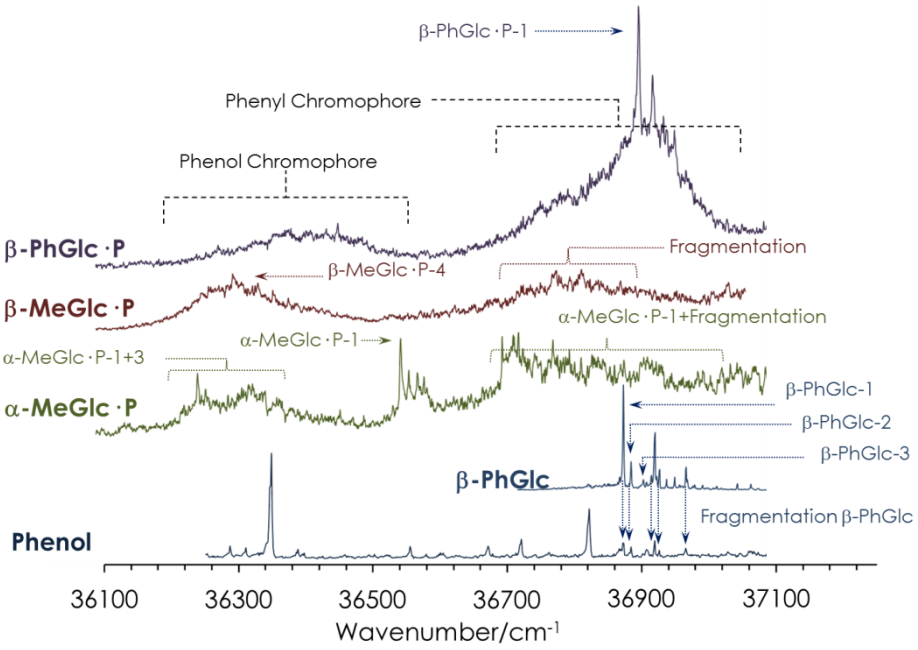


Figure S3. Six most stable structures of β-phenyl-D-glucopyranose, with the values of the dihedral angles for each of the structures

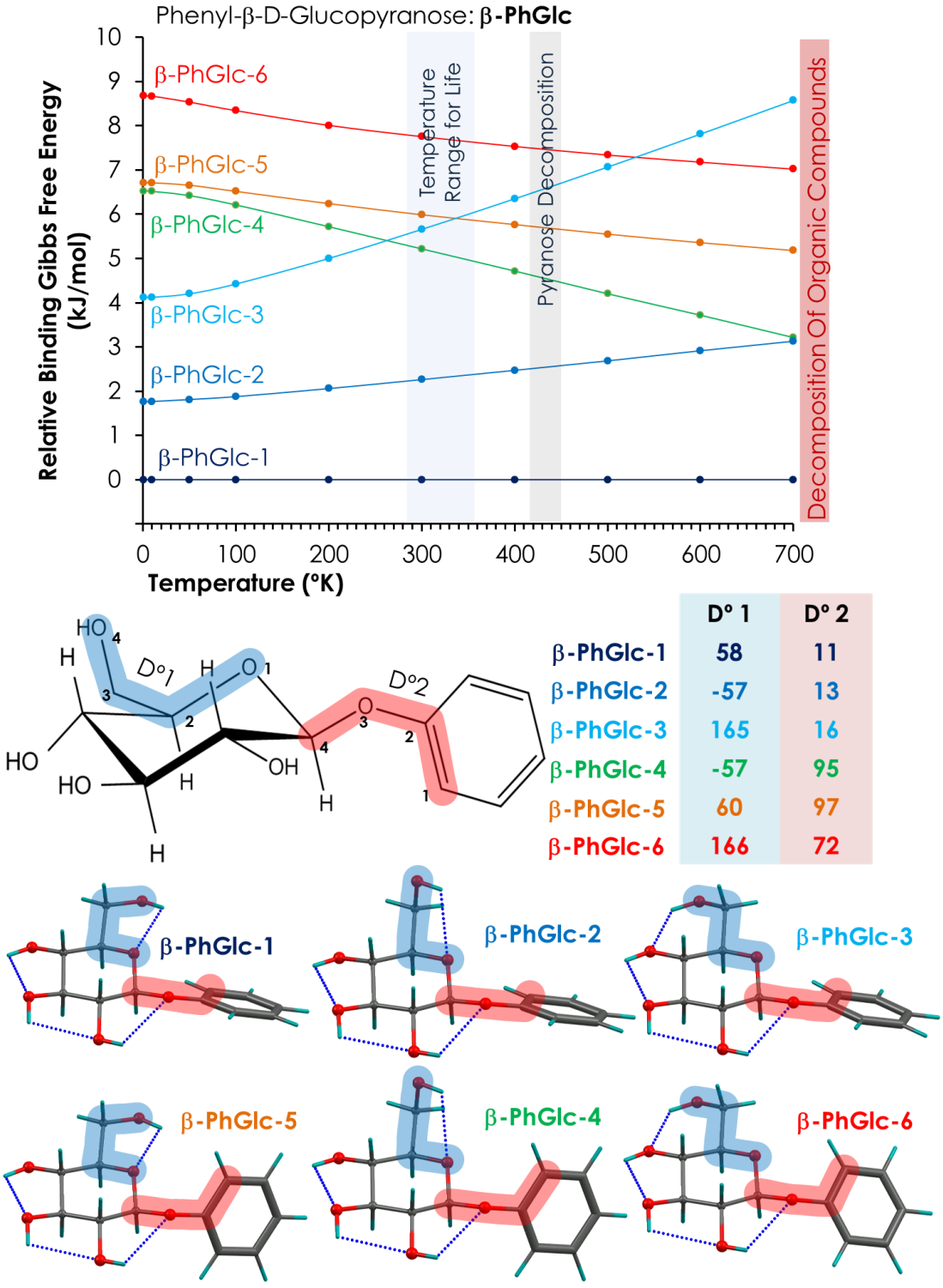


Figure S4. IR/UV spectra of α-MeGlc·Ph obtained probing the REMPI spectrum of the complex at different UV wavelenghts.

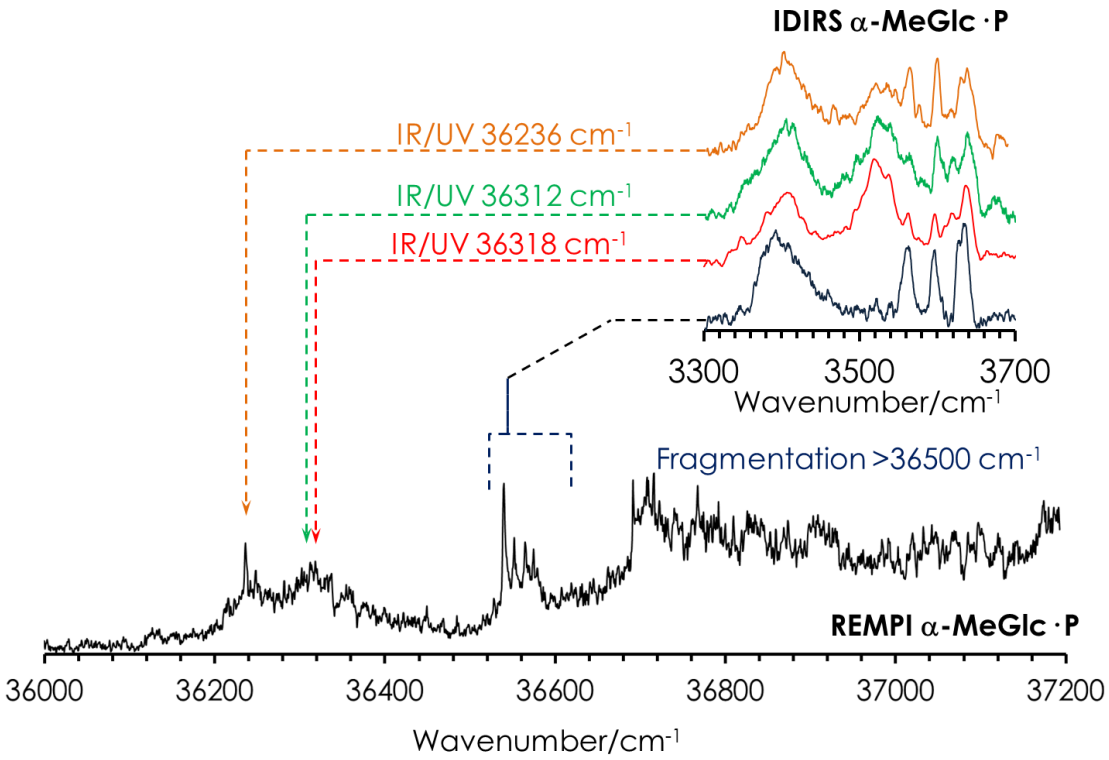


Figure S5. IR/UV hole burning of α-MeGlc·Ph obtained probing two different IR transitions. The REMPI spectra obtained are significantly different, demonstrating the existence of at least two conformers.

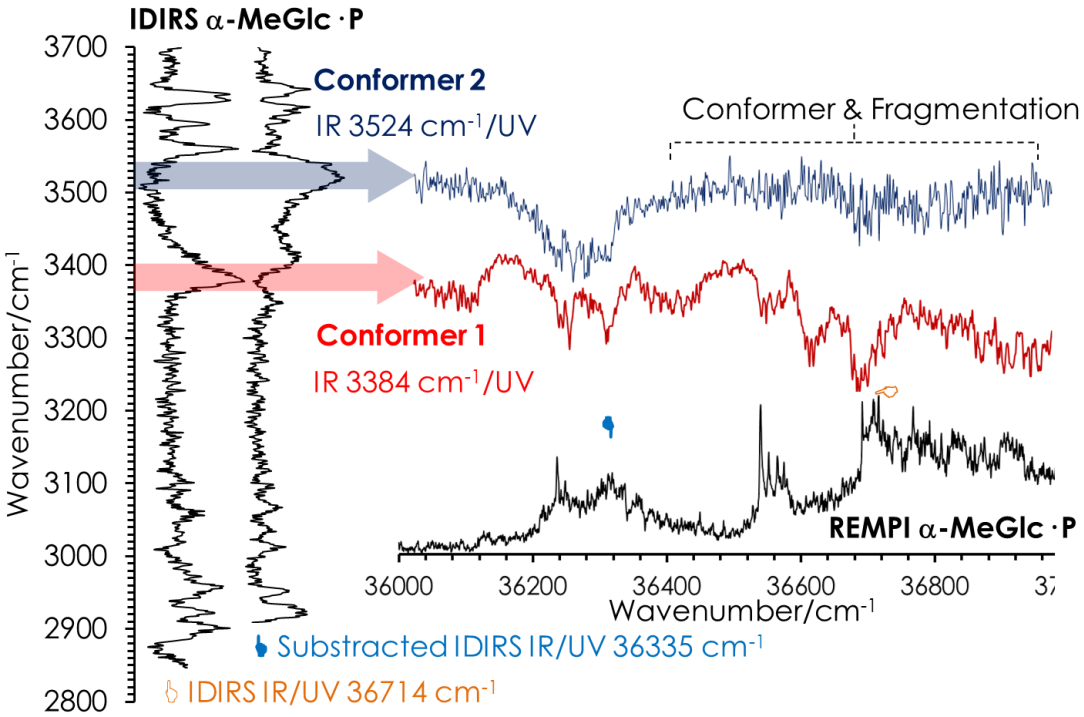


Figure S6. IR/UV hole burning of β-MeGlc·Ph obtained probing two different IR transitions. The differences in the REMPI spectra are mainly due to fragmentation, and therefore it seems that a single isomer is present.

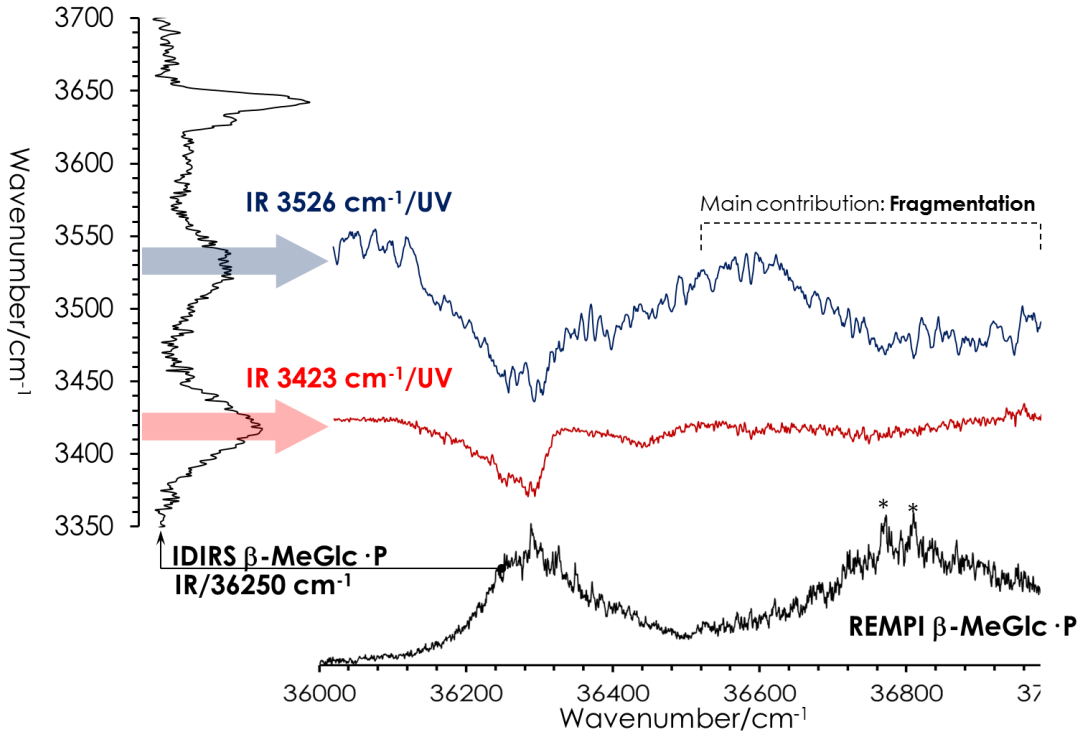


Figure S7. IR/UV spectra of β-PhGlc·Ph obtained probing theREMPI spectrum of the complex at different UV wavelenghts. The fragmentation from β-MeGlc·β-PhGlc appears in the IR trace of the β-MeGlc·P complex, indicating that the IR laser triggers a complex fragmentation mechanism in the β-MeGlc·β-PhGlc complex.

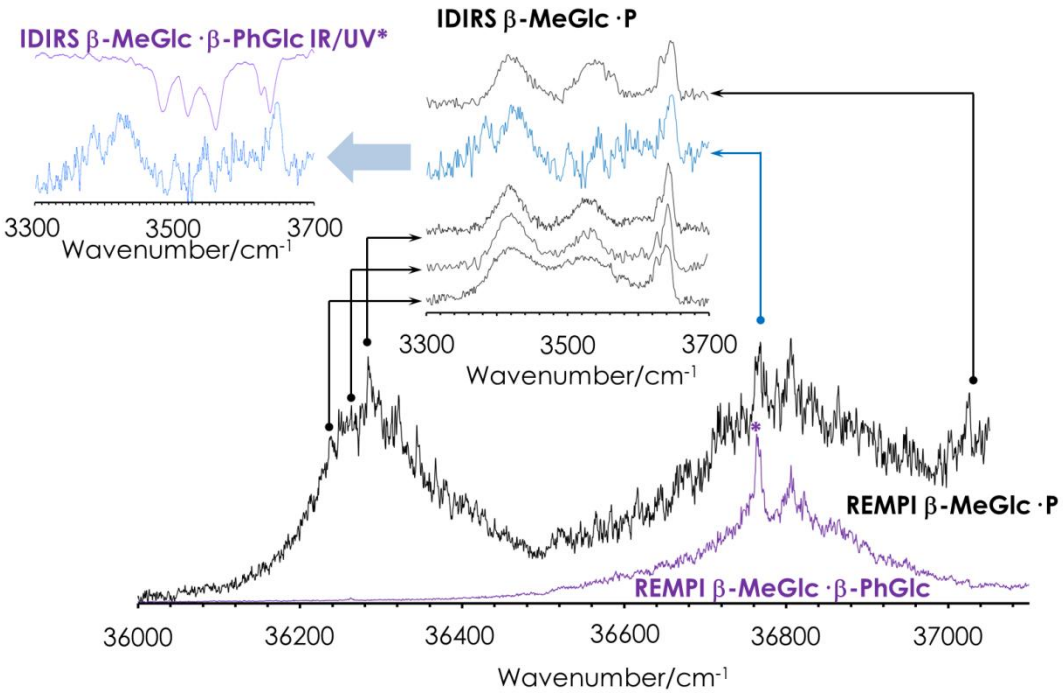


Figure S8. UV/UV hole burning of β-PhGlc·Ph obtained tuning the depopulation laser at 36892 cm^{-1}. The differences with the REMPI spectrum are due to interferences with the bare molecule that produces a very strong signal. The experiment points to the existence of a single isomer.

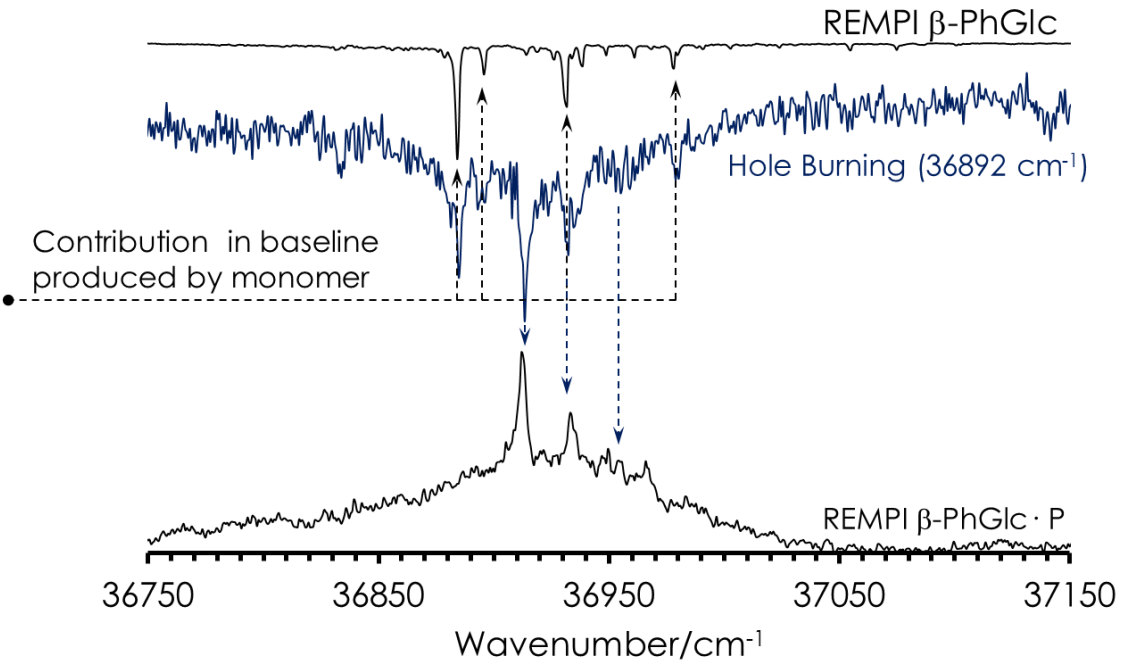


Figure S9. Comparison between the IR/UV spectra of all the species detected with the simulated spectra for the calculated structures to which they have been assigned.

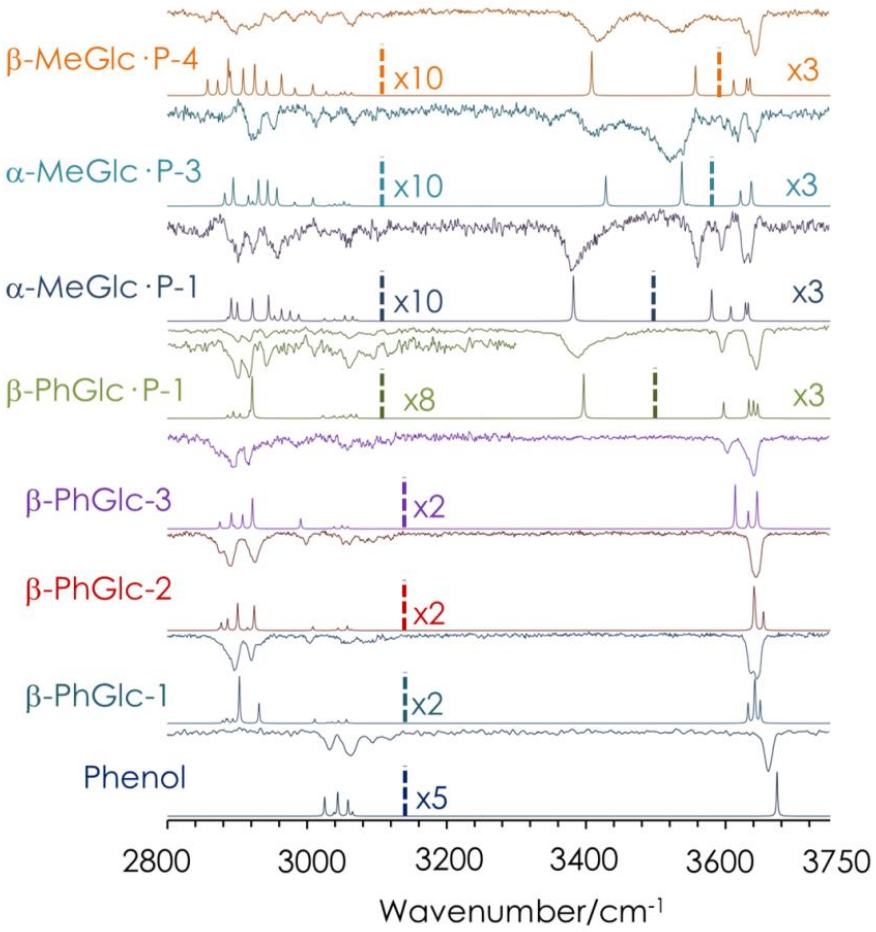
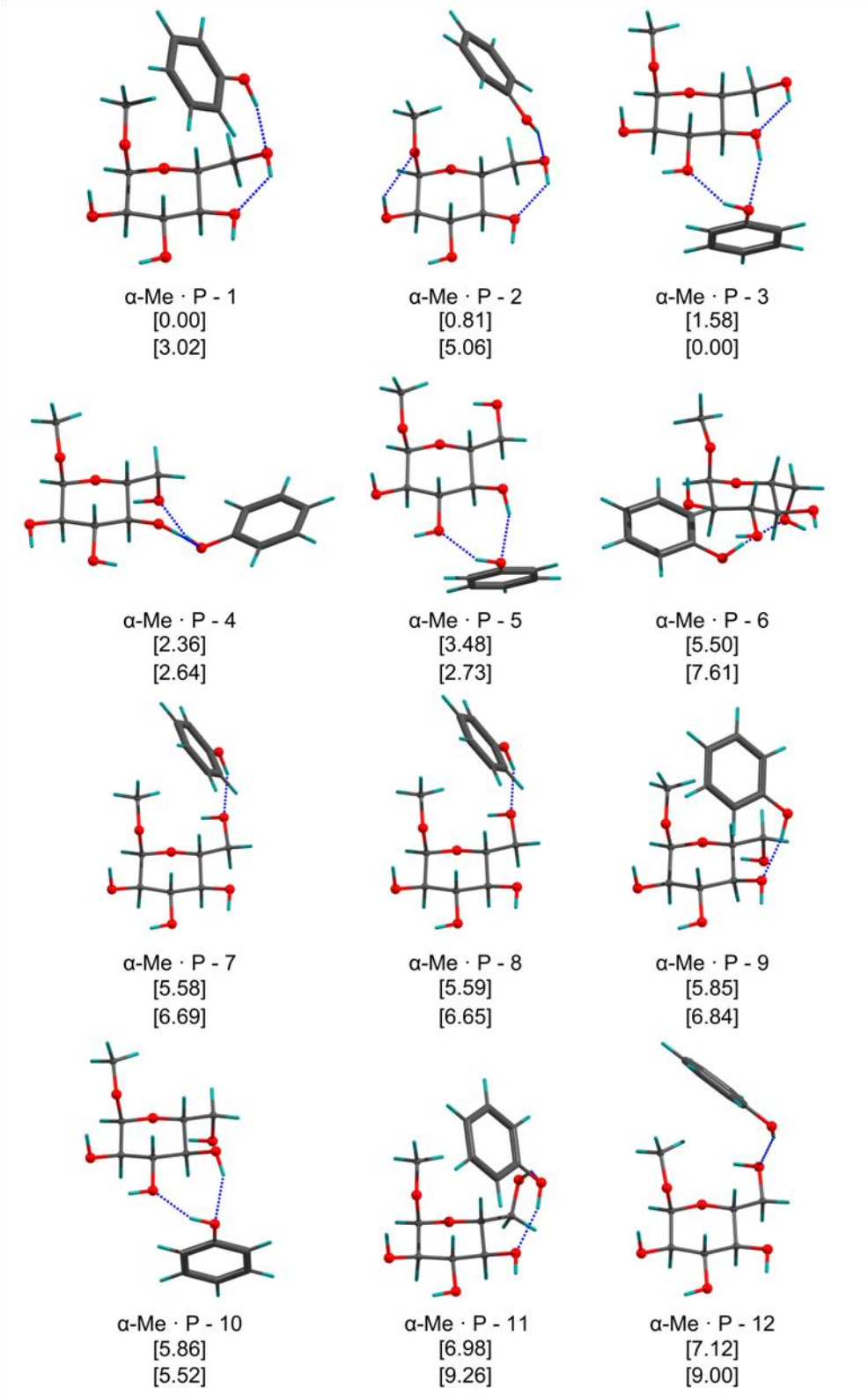
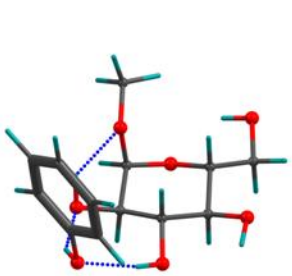
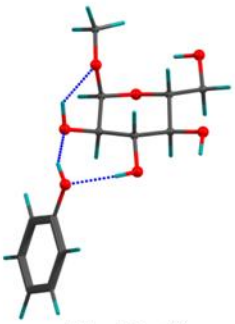


Figure S10. The 20 most stable structures of α-MeGlc · Ph calculated at M06-2X/6-31+G(d) level together with their relative stability (kJ/ mol) and Gibbs relative energies (kJ/ mol) in brackets. ZPE correction was applied to all energy values.

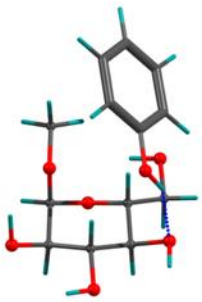




α-Me · P - 13
[7.30]
[5.43]



α-Me · P - 14
[7.85]
[7.83]

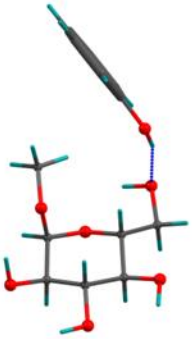


α-Me · P - 15
[7.97]
[12.26]

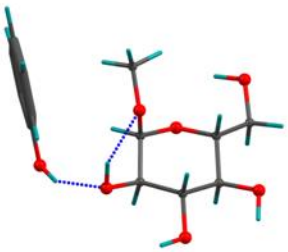
α-Me · P - 16
[7.97]
[8.87]

α-Me · P - 17
[8.01]
[8.94]

α-Me · P - 18
[8.34]
[7.54]

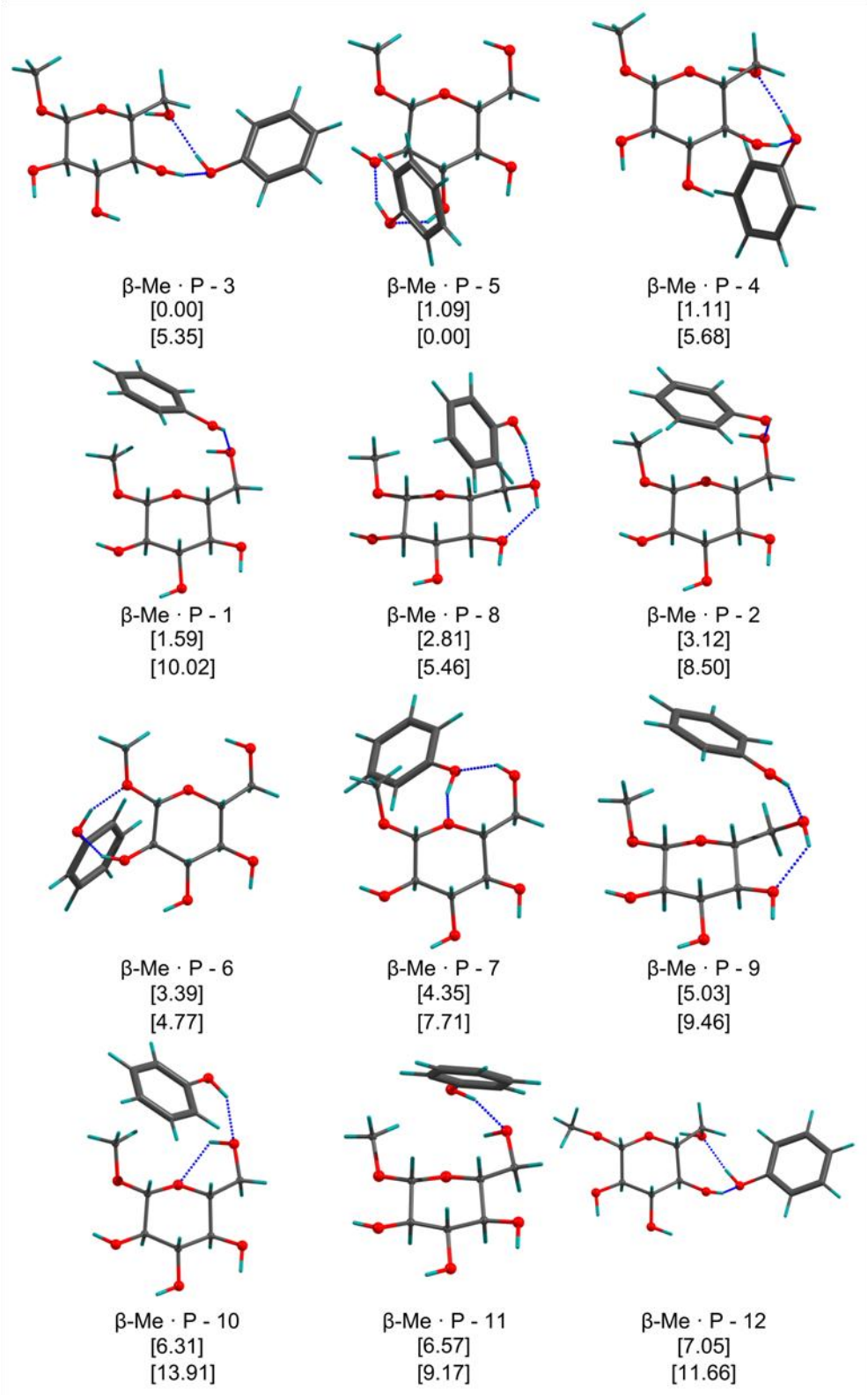


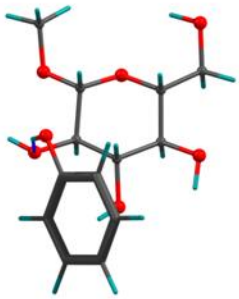
α-Me · P - 19
[8.39]
[5.36]



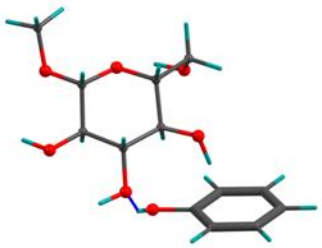
α-Me · P - 20
[8.55]
[11.36]

Figure S11. The 20 most stable structures of β-MeGlc · Ph calculated at M06-2X/6-31+G(d) level together with their relative stability (kJ/mol) and Gibbs relative energies (kJ/mol) in brackets. ZPE correction was applied to the energy values.

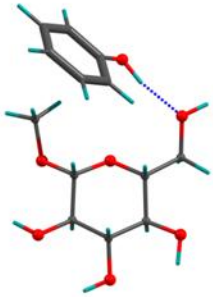




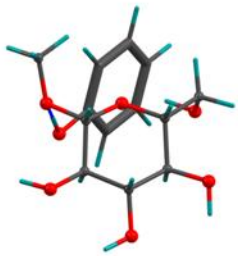
β-Me · P - 13
[7.41]
[11.69]



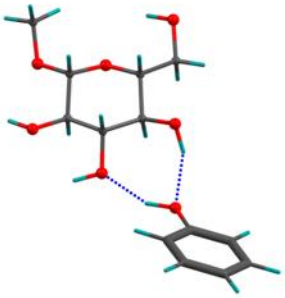
β-Me · P - 14
[7.51]
[13.03]



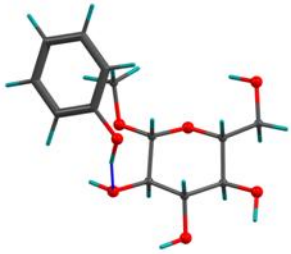
β-Me · P - 15
[8.00]
[17.37]



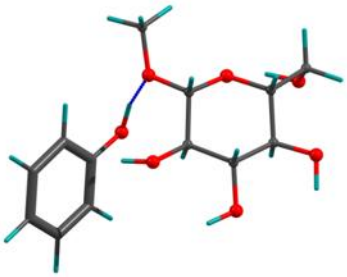
β-Me · P - 16
[8.30]
[14.29]



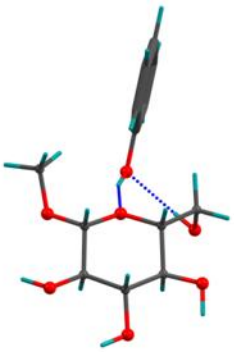
β-Me · P - 17
[8.99]
[7.95]



β-Me · P - 18
[9.09]
[16.66]

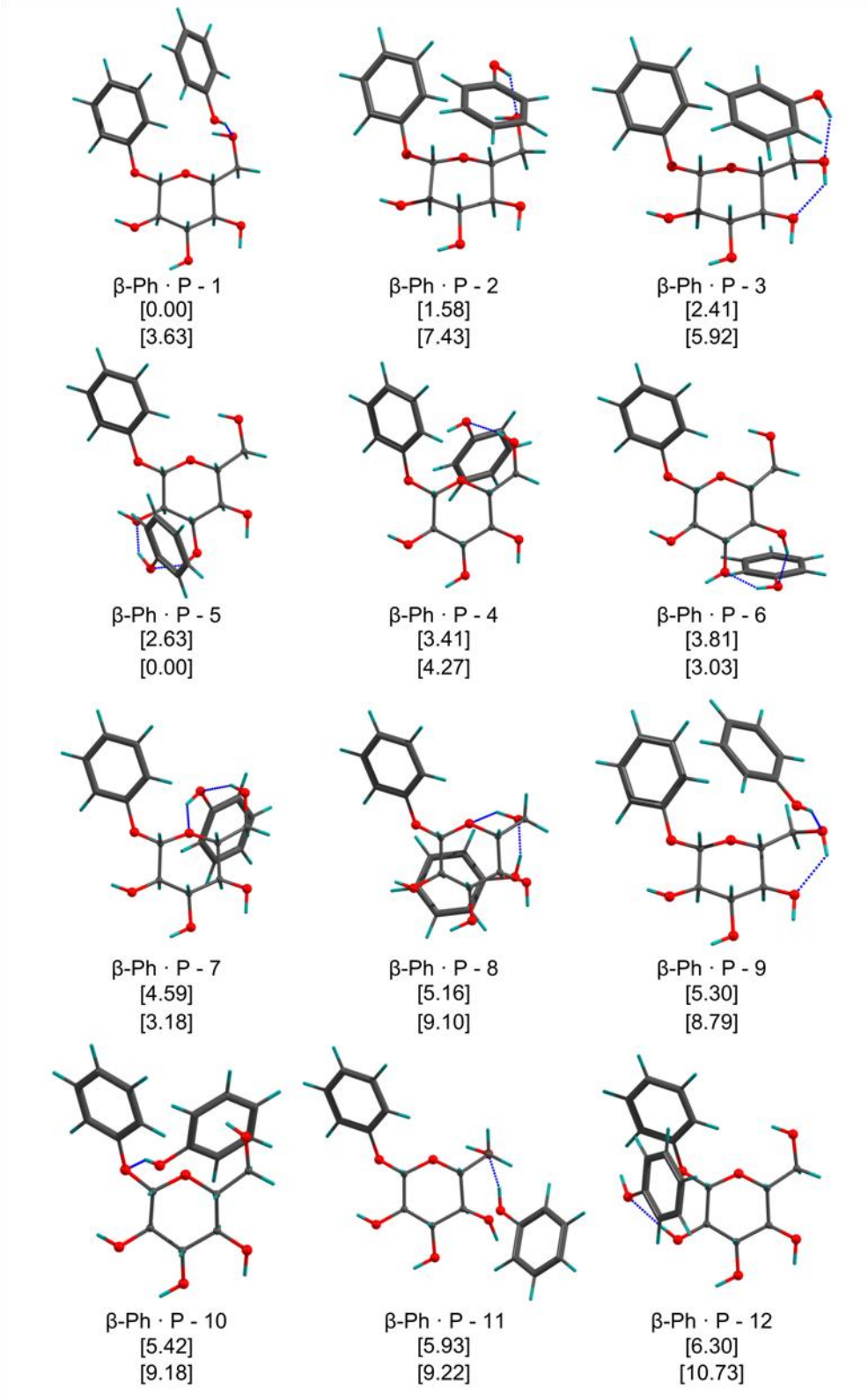


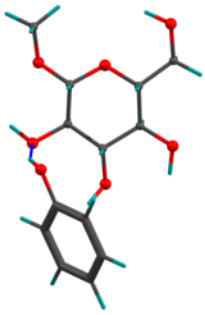
β-Me · P - 19
[9.29]
[13.06]



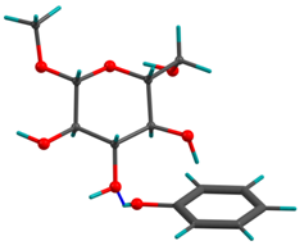
β-Me · P - 20
[9.44]
[15.47]

Figure S12. The 20 most stable structures of β-PhGlc · Ph calculated at M06-2X/6-31+G(d) level together with their relative stability (kJ/mol) and Gibbs relative energies (kJ/mol) in brackets. ZPE correction was applied to the energy values.

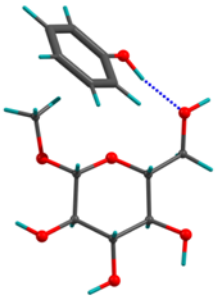




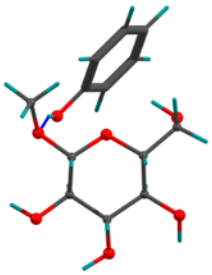
β-Ph· P - 13
[6.68]
[5.38]



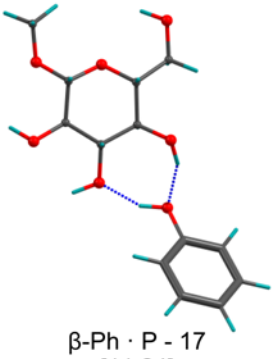
β-Ph · P - 14
[6.96]
[6.03]



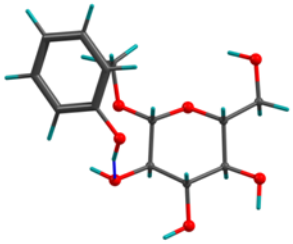
β-Phe · P - 15
[7.11]
[5.49]



β-Ph · P - 16
[9.39]
[15.83]



β-Ph · P - 17
[11.24]
[16.30]



β-Ph · P - 18
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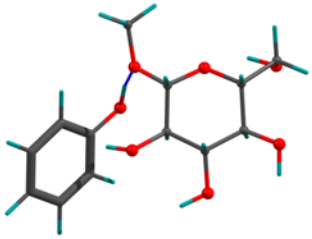
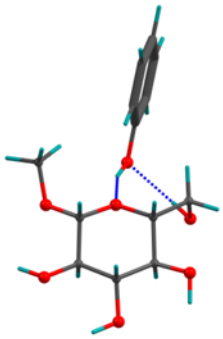
[9.28]



β-Ph · P - 19
[12.40]
[16.12]



β-Ph · P - 20
[12.44]
[13.35]