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

Exploring the interaction sites in glucose and galactose using phenol as a probe

ELECTRONIC SUPPLEMENTARY INFORMATION

Paúl Pinillos‡, Ander Camiruaga‡, Fernando Torres-Hernández, Francisco J. Basterrechea, Imanol Usabiaga* and José A. Fernández*

[a] Department of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Bº Sarriena s/n, 48940 Spain.
‡ These authors contributed equally to this work.

*Correspondence: i.usabiaga@outlook.es, josea.fernandez@ehu.es

Figure S1. Comparison between the experimental IDIR spectrum of β-PhGlc·PhOH complex and the computational simulations for the five most stable structures at M062x/6-311++G(d,p) level.

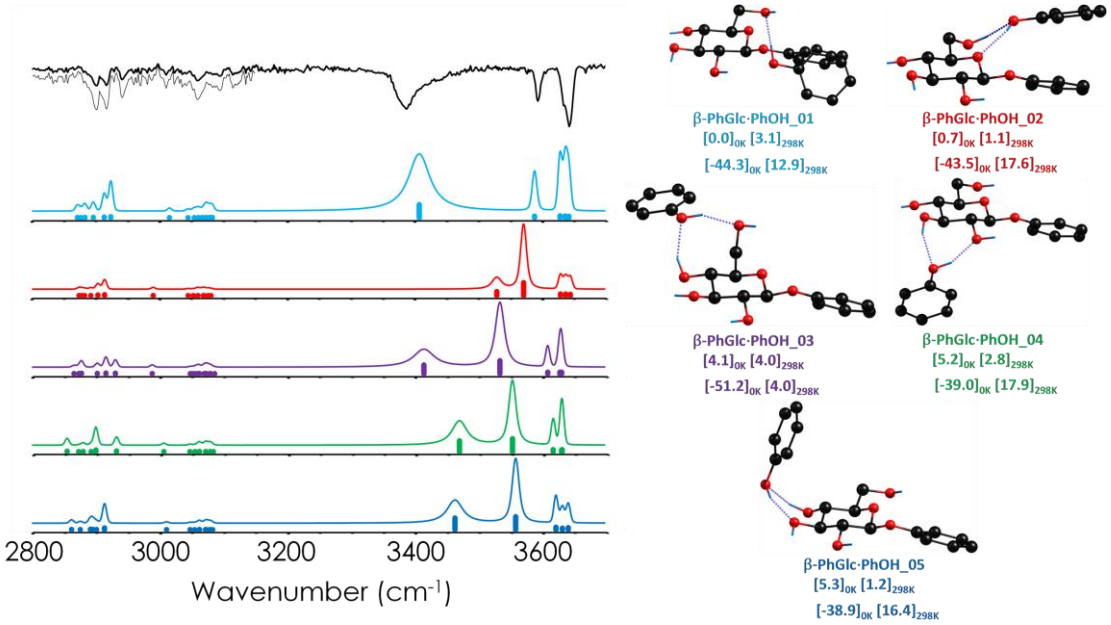

Figure S2. Comparison between the experimental IDIR spectrum of β-PhGlc·PhOH complex and the computational simulations for the five most stable structures at B3LYP(D3)/6-311++G(d,p) level.

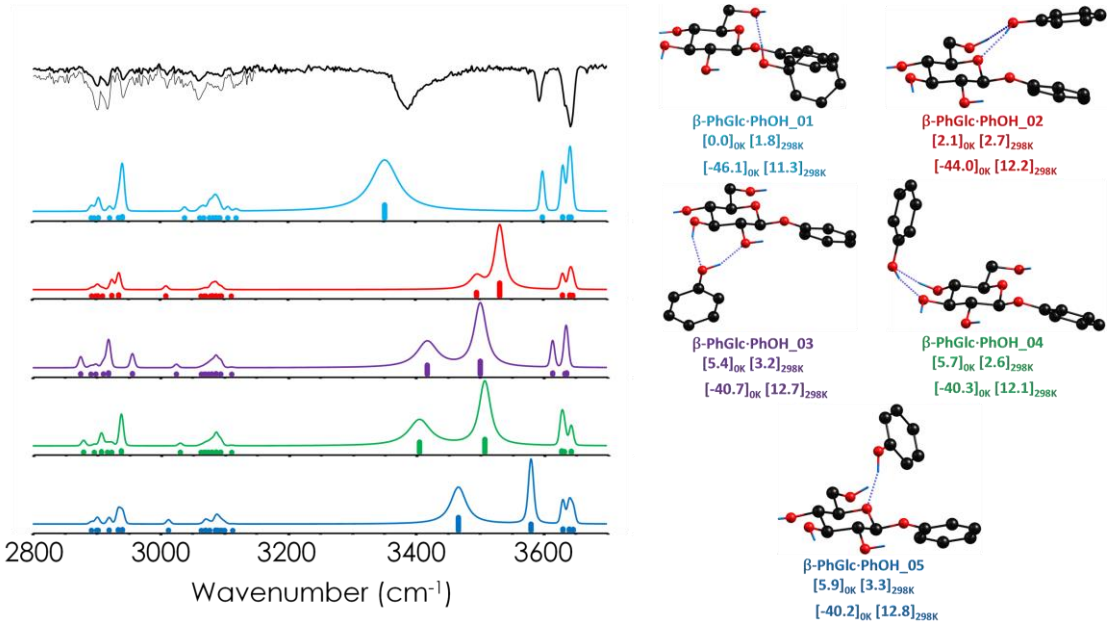

Figure S3. Comparison between the experimental IDIR spectrum for β-PhGal·PhOH complex and the computational simulations for the five most stable structures at M062X/6-311++G(d,p) level.

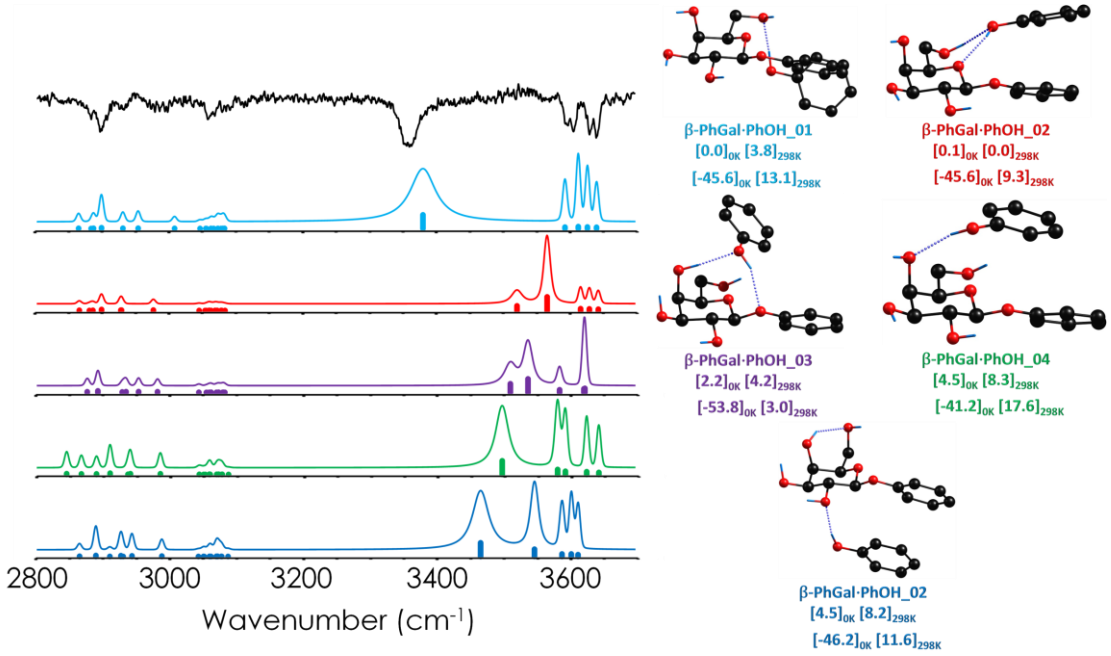

Figure S4. Comparison between the experimental IDIR spectrum for β-PhGal·PhOH complex and the computational simulations for the five most stable structures at B3LYP(D3)/6-311++G(d,p) level.

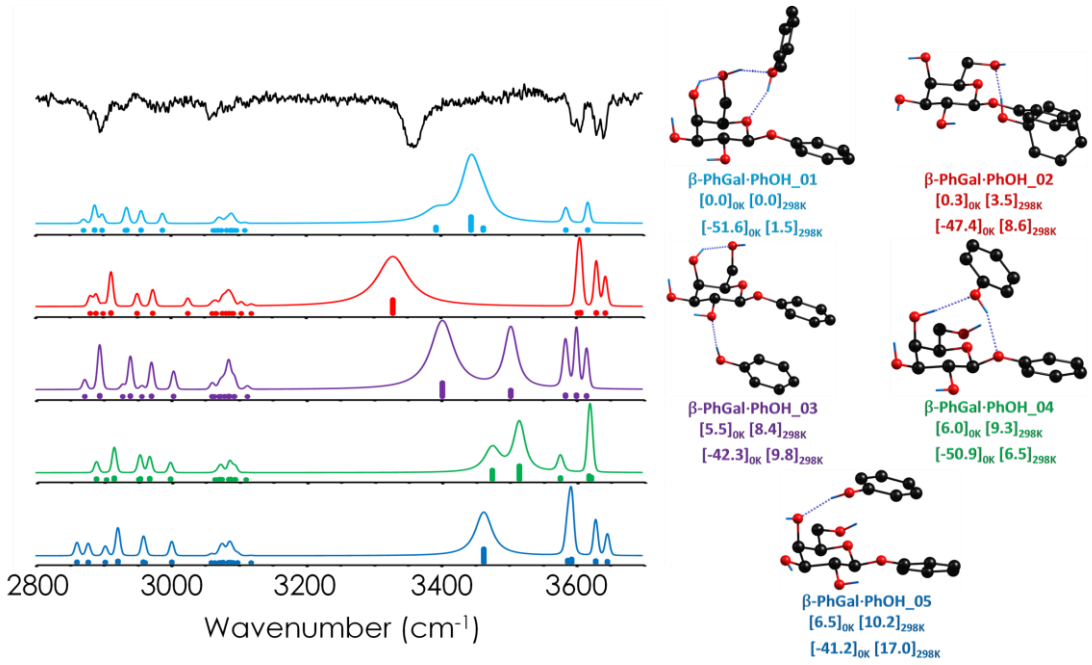

Figure S5. Comparison between the experimental IDIR spectrum for β-MeGlc·PhOH complex and the computational simulations for the five most stable structures at M062X/6-311++G(d,p) level.

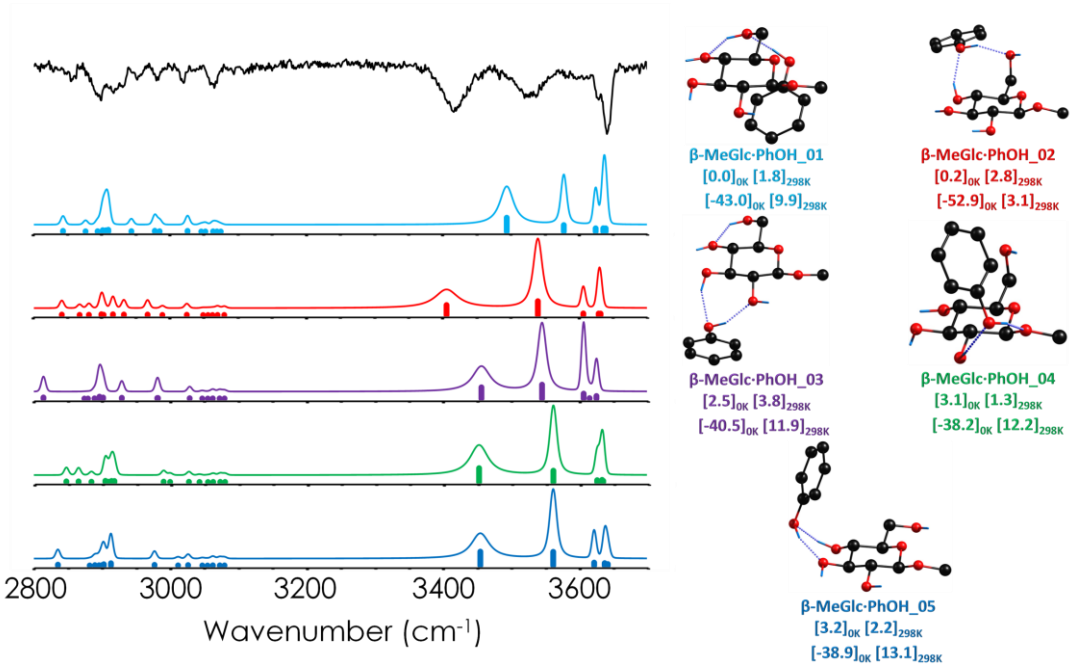

Figure S6. Comparison between the experimental IDIR spectrum for β-MeGlc·PhOH complex and the computational simulations for the five most stable structures at B3LYP(D3)/6-311++G(d,p) level.

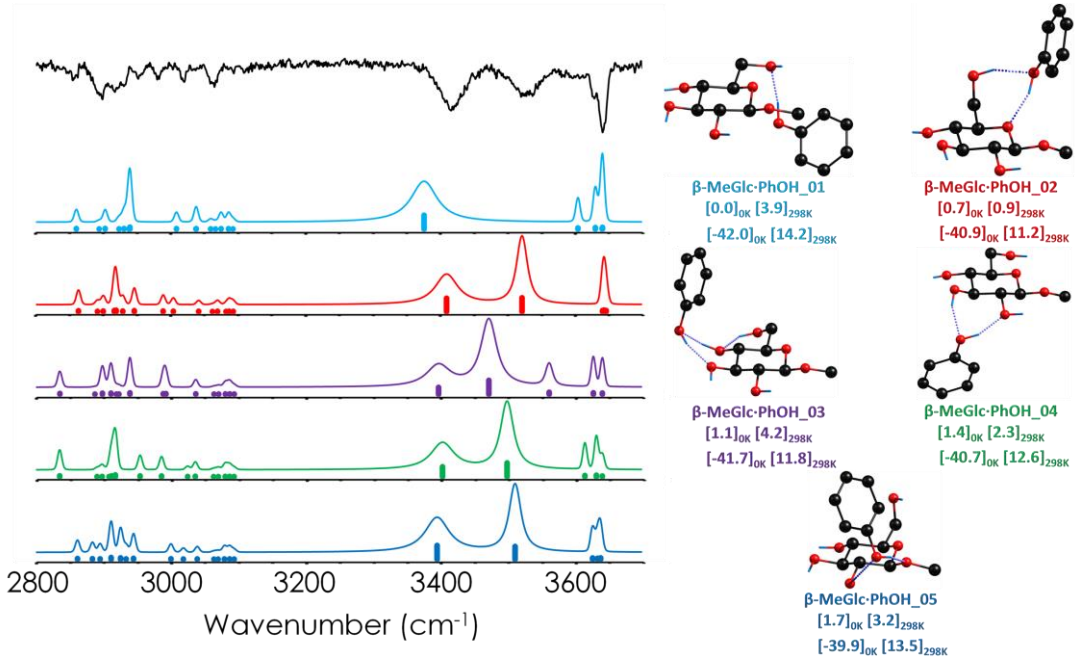

Figure S7. Comparison between the experimental IDIR spectrum for β-MeGal·PhOH complex and the computational simulations for the five most stable structures at M062X/6-311++G(d,p) level.

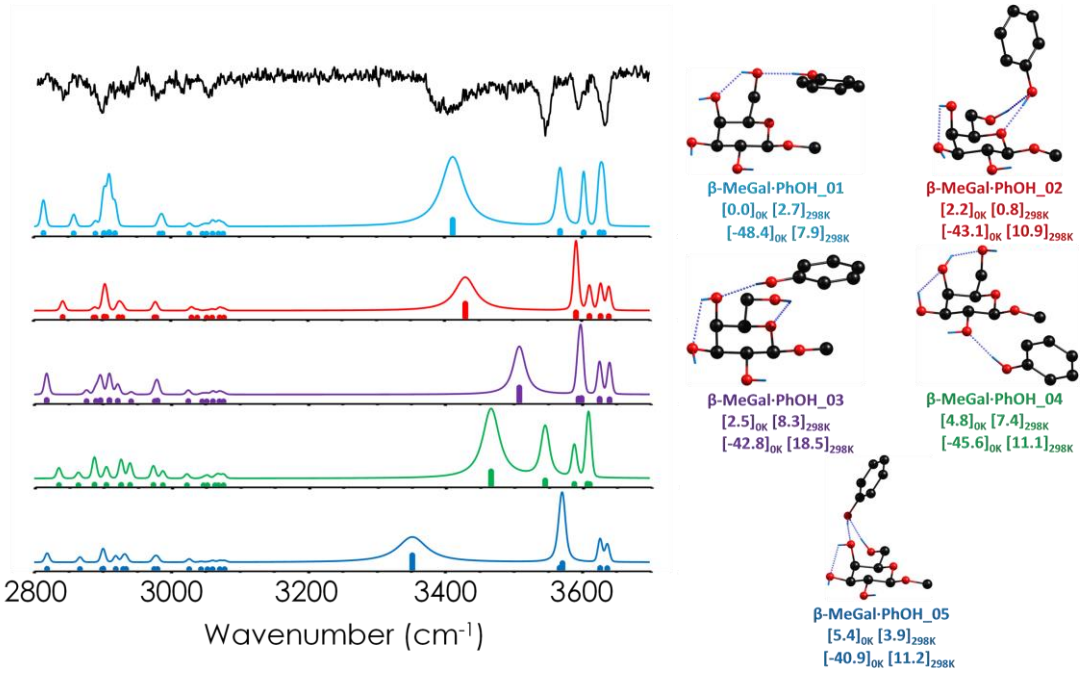

Figure S8. Comparison between the experimental IDIR spectrum for β-MeGal·PhOH complex and the computational simulations for the five most stable structures at B3LYP(D3)/6-311++G(d,p) level.

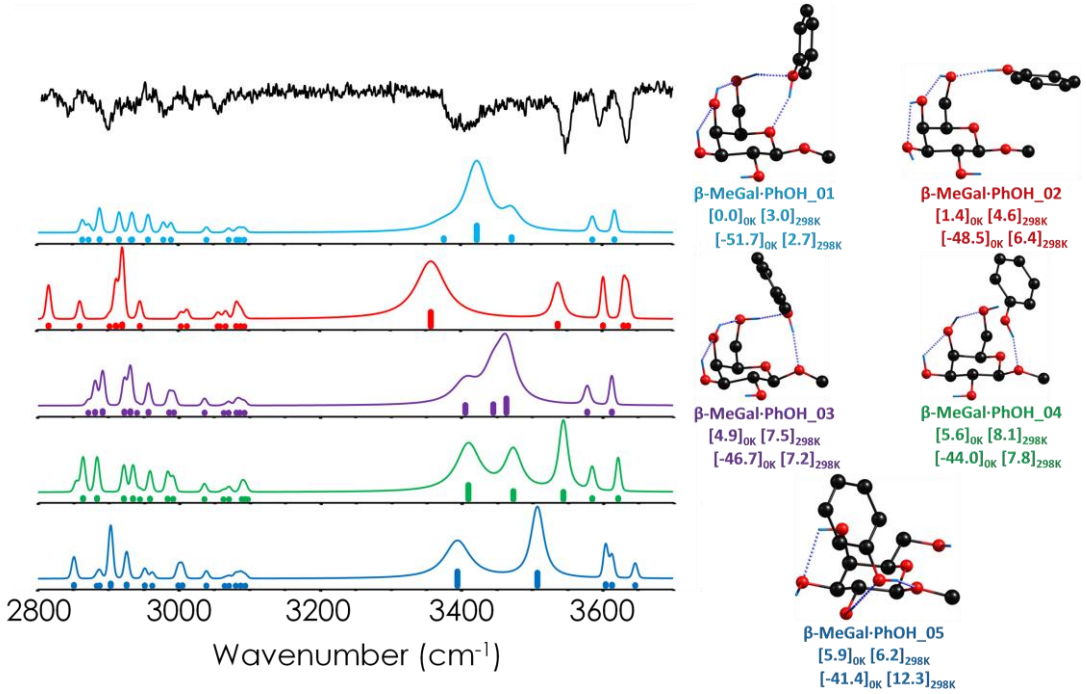

Figure S9. Comparison between the experimental IDIR spectrum for α-MeGlc·PhOH complex and the computational simulations for the five most stable structures at M062X/6-311++G(d,p) level.

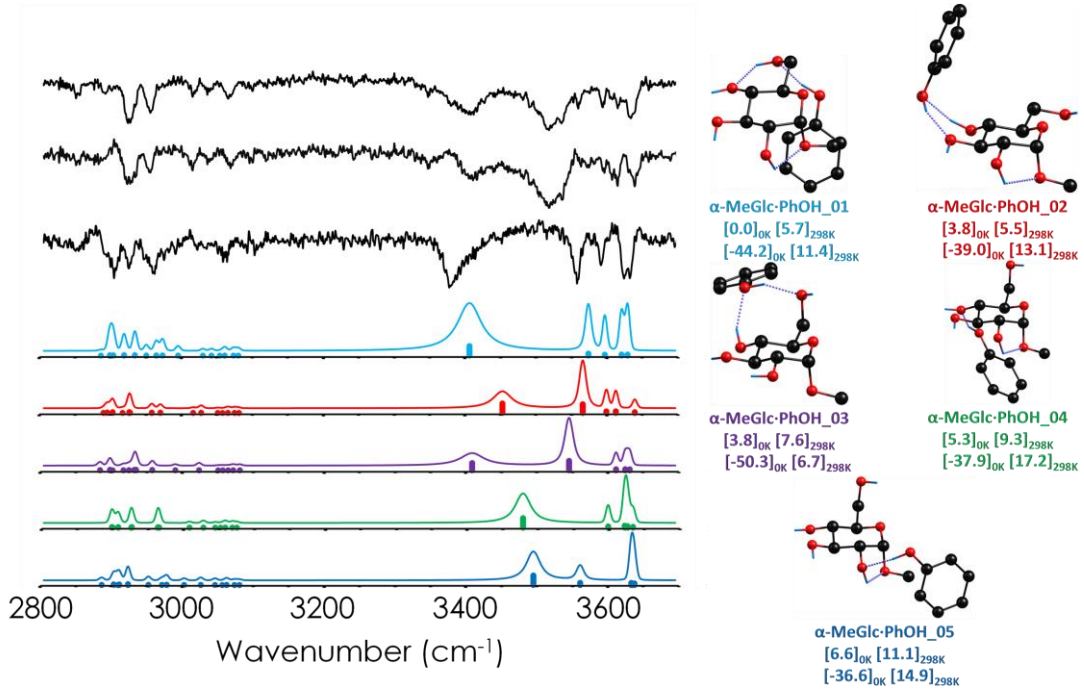

Figure S10. Comparison between the experimental IDIR spectrum for α-MeGlc·PhOH complex and the computational simulations for the five most stable structures at B3LYP(D3)/6-311++G(d,p) level.

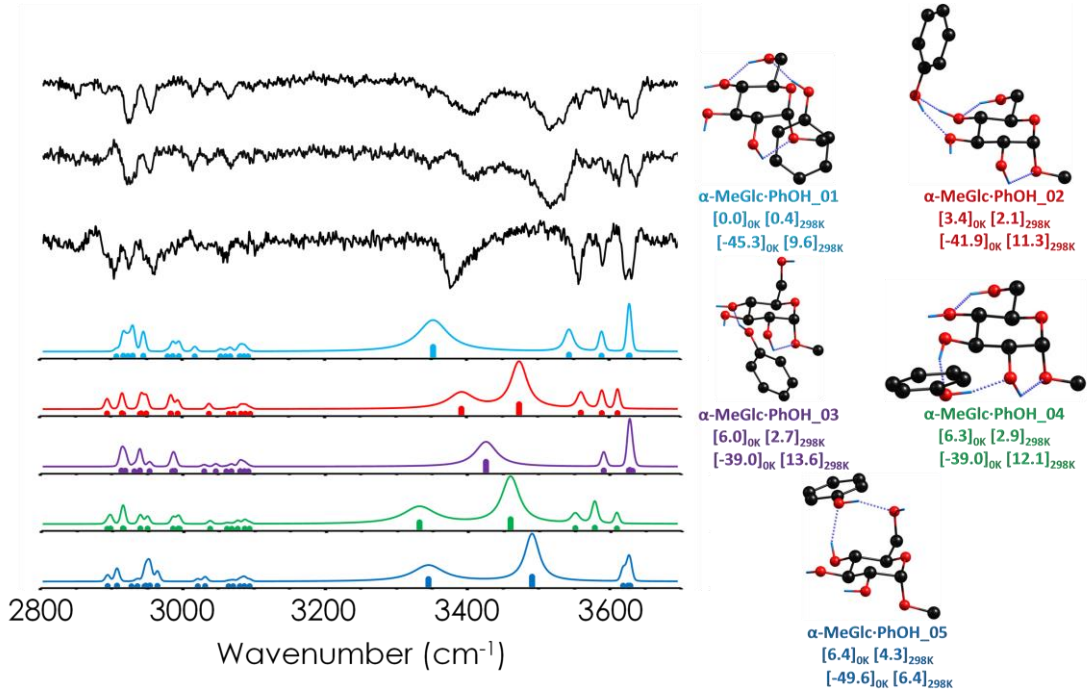

Figure S11. Comparison between the experimental IDIR spectrum for α-MeGal·PhOH complex and the computational simulations for the five most stable structures at M062X/6-311++G(d,p) level.

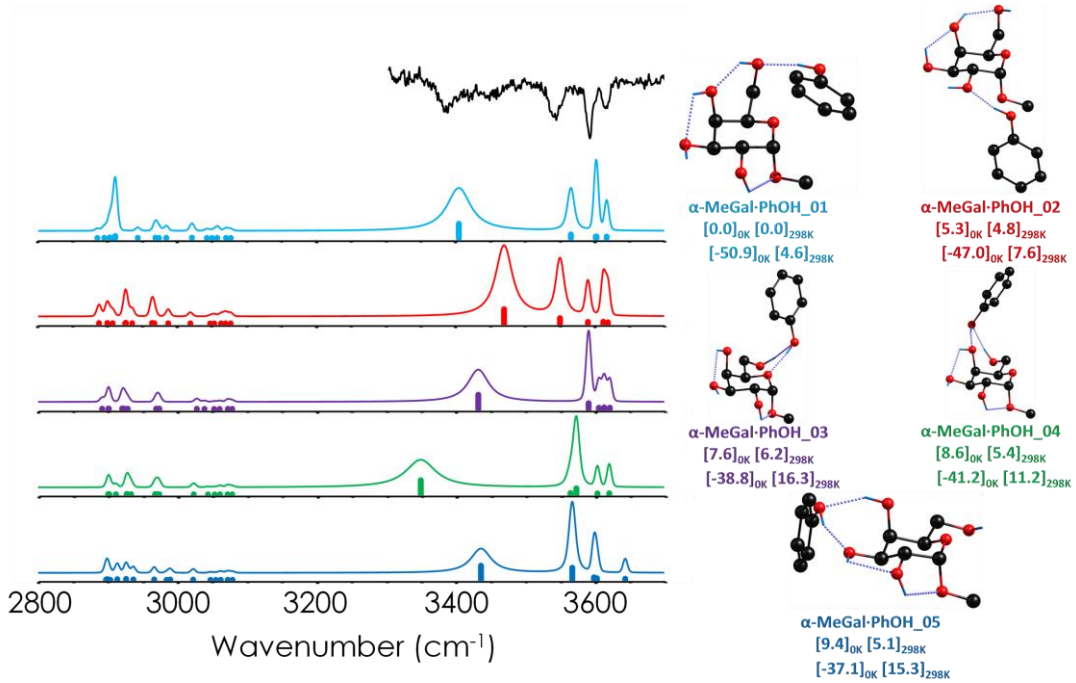

Figure S12. Comparison between the experimental IDIR spectrum for α-MeGal·PhOH complex and the computational simulations for the five most stable structures at B3LYP(D3)/6-311++G(d,p) level.

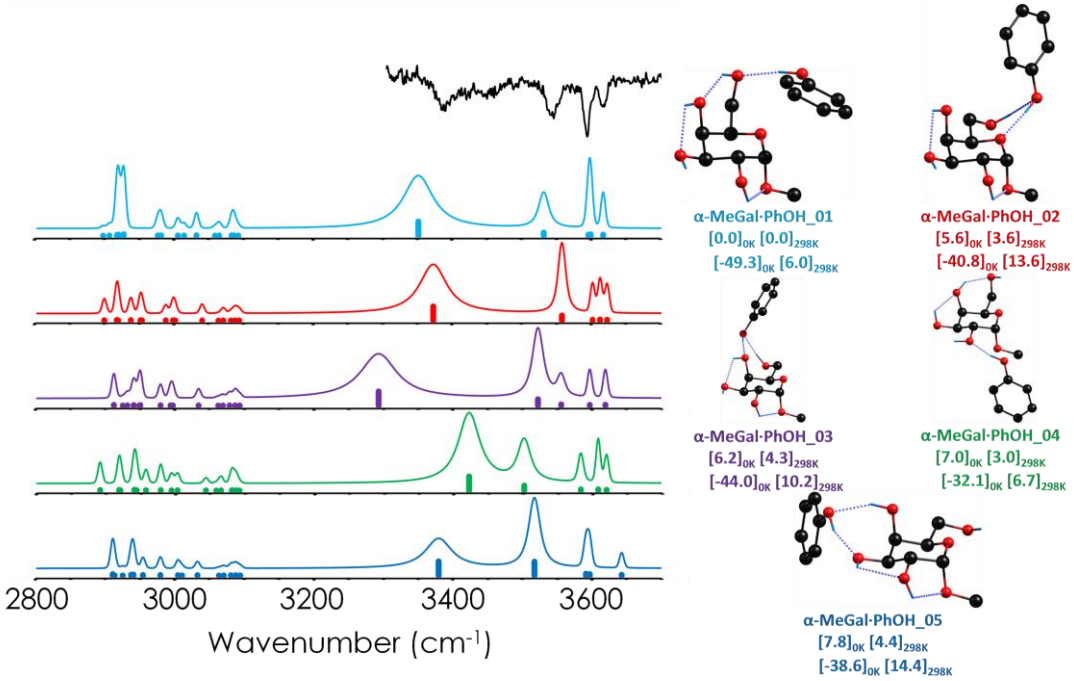

Table S1. Relative Gibbs energies for the most stable conformers of each family of β-PhGlc·PhOH complex. Values include ZPE and BSSE corrections.

LABEL	FAMILY	M062X		B3LYP		RMSD (NO H ATOMS)
		ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	
β-PhGlc·PhOH_01	HO6·HOPh_1	0.0	3.1	0.0	1.8	0.08
β- PhGlc·PhOH_02	O5·HOPh_O6H·OHPh_1	0.7	1.1	2.1	2.7	0.13
β- PhGlc·PhOH_03	O4H·OHPh_HO6·HOPh_1	4.1	4.0	6.0	4.8	0.19
β- PhGlc·PhOH_04	HO2·HOPh_O3H·OHPh_1	5.2	2.8	5.4	3.2	0.17
β- PhGlc·PhOH_05	HO3·HOPh_O4H·OHPh_1	5.3	1.2	5.7	2.6	0.24
β- PhGlc·PhOH_06	O6H·OHPh_1	5.8	1.9	6.0	0.2	0.27
β- PhGlc·PhOH_07	O1·HOPh_1	6.0	4.9	7.8	4.6	0.23
β- PhGlc·PhOH_08	O2H·OHPh_1	6.2	6.7	9.9	7.9	0.16
β- PhGlc·PhOH_09	HO2·HOPh_1	6.3	8.0	7.4	5.2	0.37
β- PhGlc·PhOH_10	HO6·HOPh_1	0.0	3.1	0.0	1.8	0.08

Figure S13. Most stable conformers of β-PhGlc·PhOH complex computed at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level. Energies inside brackets are given in kJ/mol.

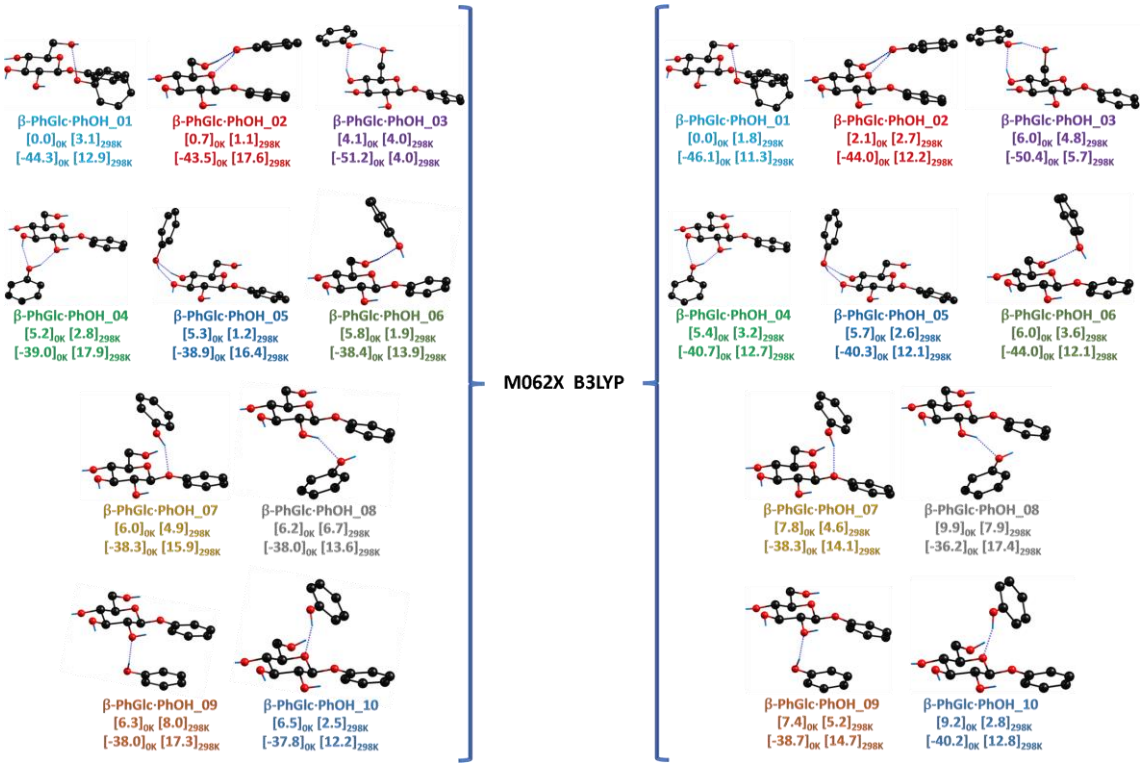

Figure S14. Comparison between the experimental IDIR spectrum for β-PhGlc·PhOH complex and the computational simulations for the ten most stable structures at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level.

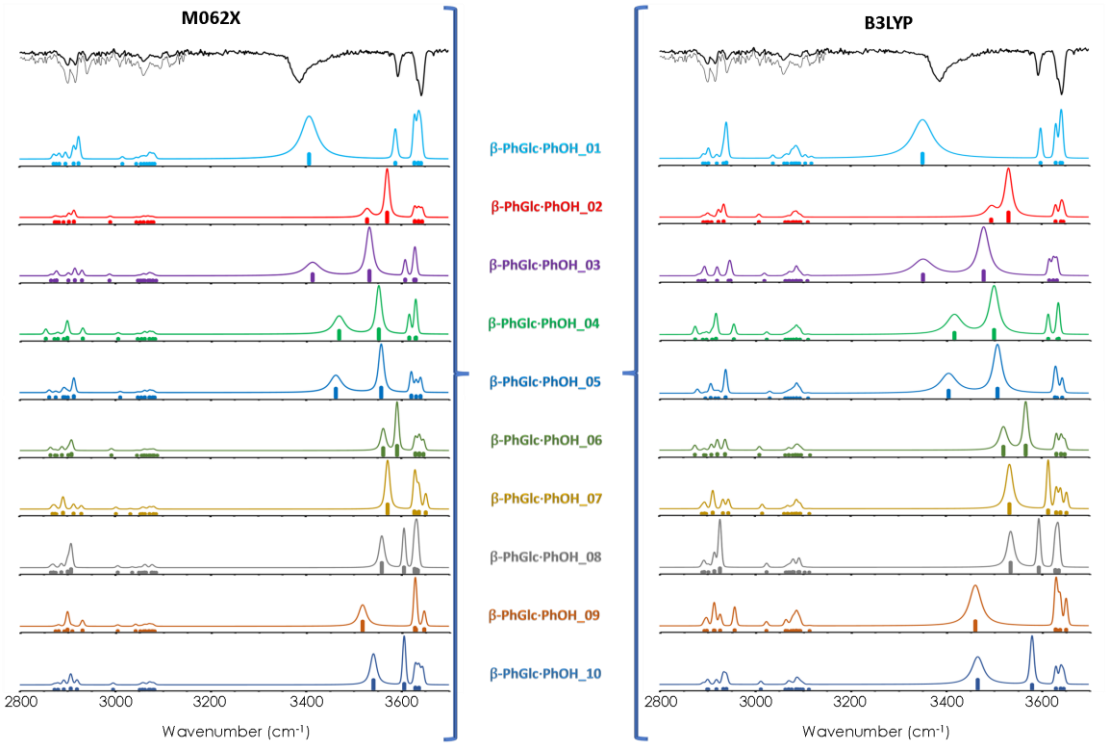

Table S2. Relative Gibbs energies for the most stable conformers of each family of β-PhGal·PhOH complex. Values include ZPE and BSSE corrections.

LABEL	FAMILY	M062X		B3LYP		RMSD (NO H ATOMS)
		ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	
β-PhGal·PhOH_01	HO6·HOPh_1	0.0	3.8	0.3	3.5	0.07
β- PhGal·PhOH_02	O5·HOPh_O6H·OHPh_1	0.1	0.0	1.7	2.9	0.13
β- PhGal·PhOH_03	O4H·OPhH·O1_01	2.2	4.2	6.0	9.3	0.13
β- PhGal·PhOH_04	OPhH·O4_01	4.5	8.3	6.5	10.2	0.09
β- PhGal·PhOH_05	OPhH·O2_01	4.5	8.2	5.5	8.4	0.10
β- PhGal·PhOH_06	O6H·OHPh_1	5.2	6.0	8.3	11.1	0.16
β- PhGal·PhOH_07	O3H·OPhH·O2_01	6.3	3.3	7.4	5.3	0.18
β- PhGal·PhOH_08	O2H·OHPh	7.4	7.9	11.7	10.9	0.17
β- PhGal·PhOH_09	O6H·OPhH·O1	8.6	9.0	7.4	5.2	1.07***
β- PhGal·PhOH_10	OPhH·O1_01	9.2	8.3	10.1	8.5	0.19

Figure S15. Most stable conformers of β-PhGal·PhOH complex computed at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level. Energies inside brackets are given in kJ/mol.

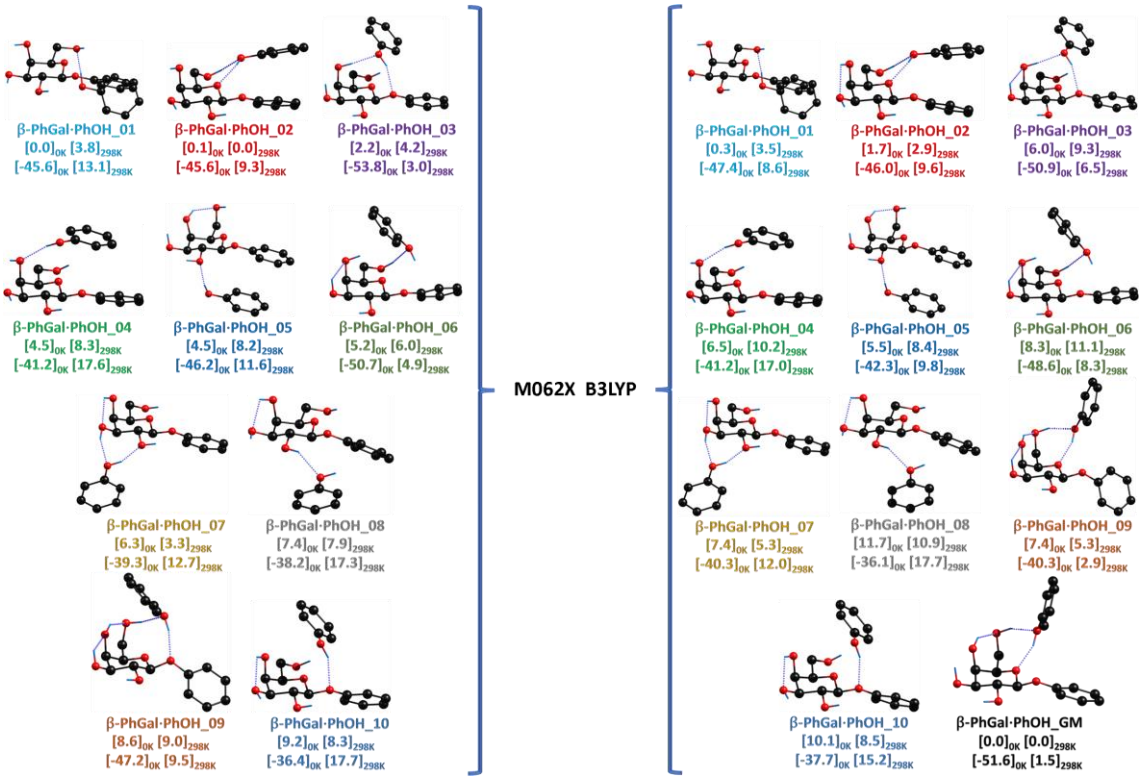

Figure S16. Comparison between the experimental IDIR spectrum for β-PhGal·PhOH complex and the computational simulations for the ten most stable structures at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level.

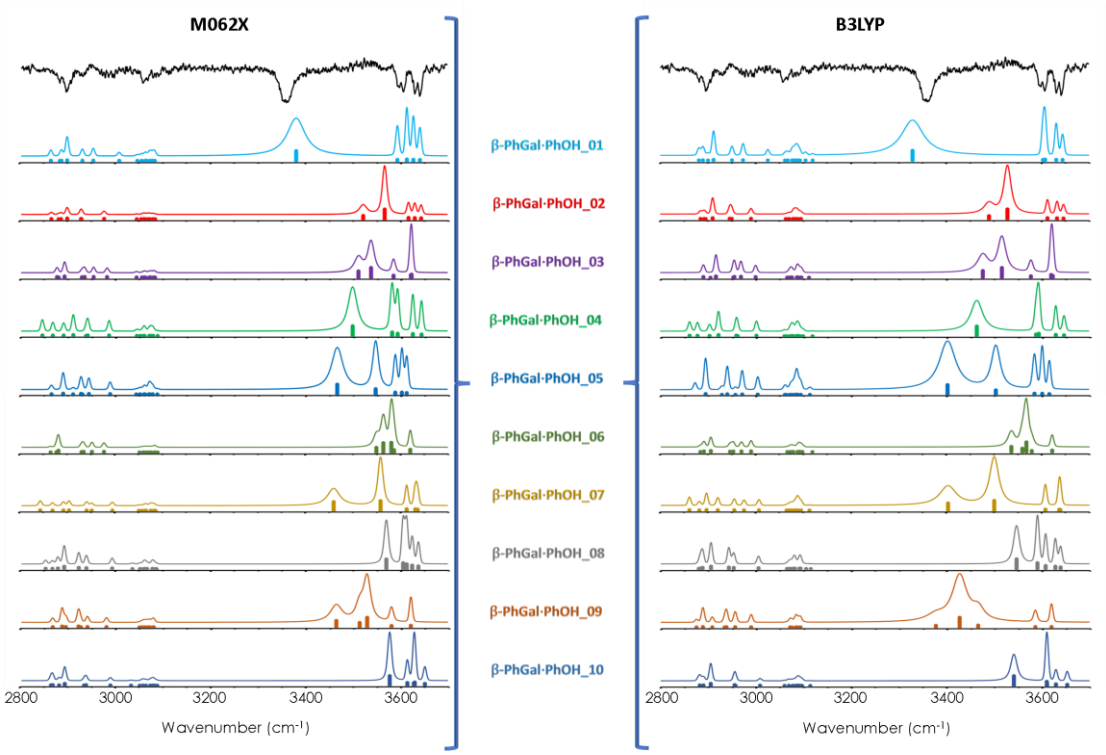

Table S3. Relative Gibbs energies for the most stable conformers of each family of β-MeGlc·PhOH complex. Values include ZPE and BSSE corrections.

LABEL	FAMILY	M062X		B3LYP		RMSD (NO H ATOMS)
		ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	
β-MeGlc·PhOH_01	HO6·HOPh_1	0.0	1.8	2.4	1.8	0.28
β-MeGlc·PhOH_02	O4H·OHPh_HO6·HOPh	0.2	2.8	2.2	4.8	0.16
β-MeGlc·PhOH_03	HO2·HOPh_O3H·OHPh	2.5	3.8	1.5	4.7	0.19
β-MeGlc·PhOH_04	O1·HOPh_O2H·OHPh	3.1	1.3	1.7	3.2	0.14
β-MeGlc·PhOH_05	HO3·HOPh_O4H·OHPh	3.2	2.2	1.6	2.0	0.21
β-MeGlc·PhOH_06	O5·HOPh_O6H·OHPh	4.2	4.6	1.9	0.0	0.42
β-MeGlc·PhOH_07	O1·HOPh	4.6	6.5	7.5	8.1	0.12
β-MeGlc·PhOH_08	HO2·HOPh	4.6	5.2	5.3	6.6	0.18
β-MeGlc·PhOH_09	HO4·HOPh	6.6	5.5	5.7	3.6	0.08
β-MeGlc·PhOH_10	HO3·HOPh	6.6	7.6	5.1	5.6	0.28

Figure S17. Most stable conformers of β-MeGlc·PhOH complex computed at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level. Energies inside brackets are given in kJ/mol. The global minimum at B3LYP(D3)/6-311++G(d,p) level corresponds to an isomer with different relative orientations of the two molecules than the global minimum obtained using M062X/6-311++G(d,p)

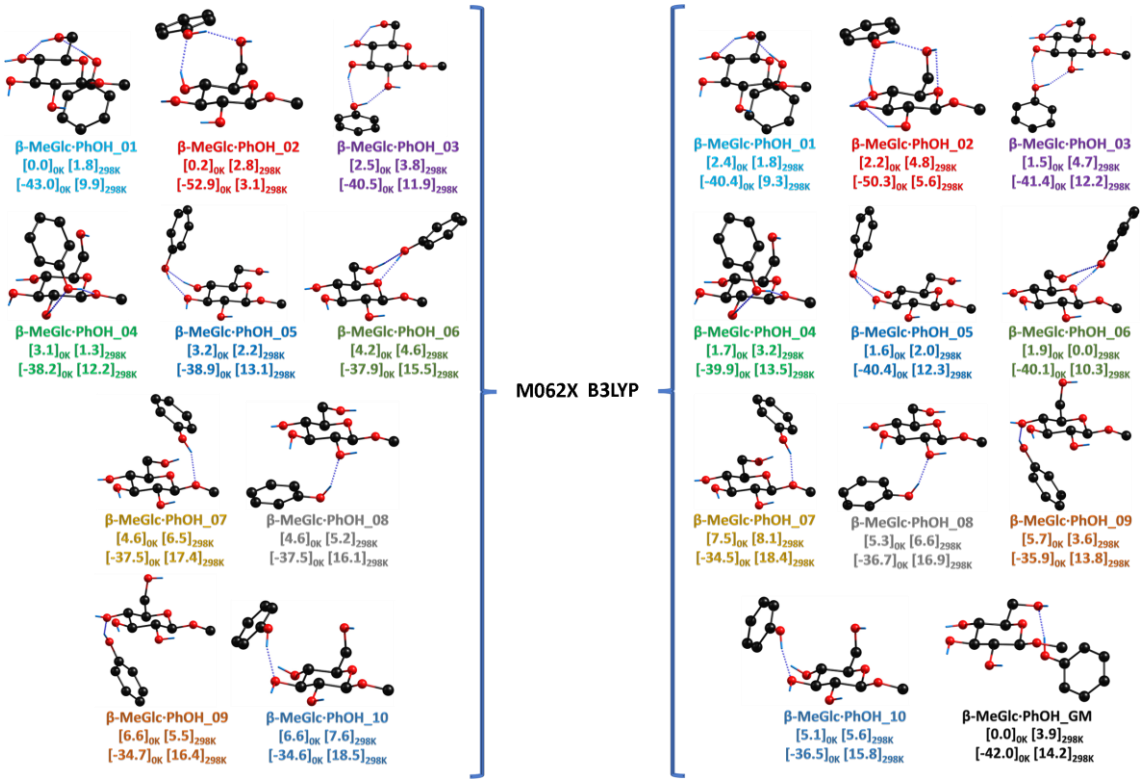

Figure S18. Comparison between the experimental IDIR spectrum for β-MeGlc·PhOH complex and the computational simulations for the ten most stable structures at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level.

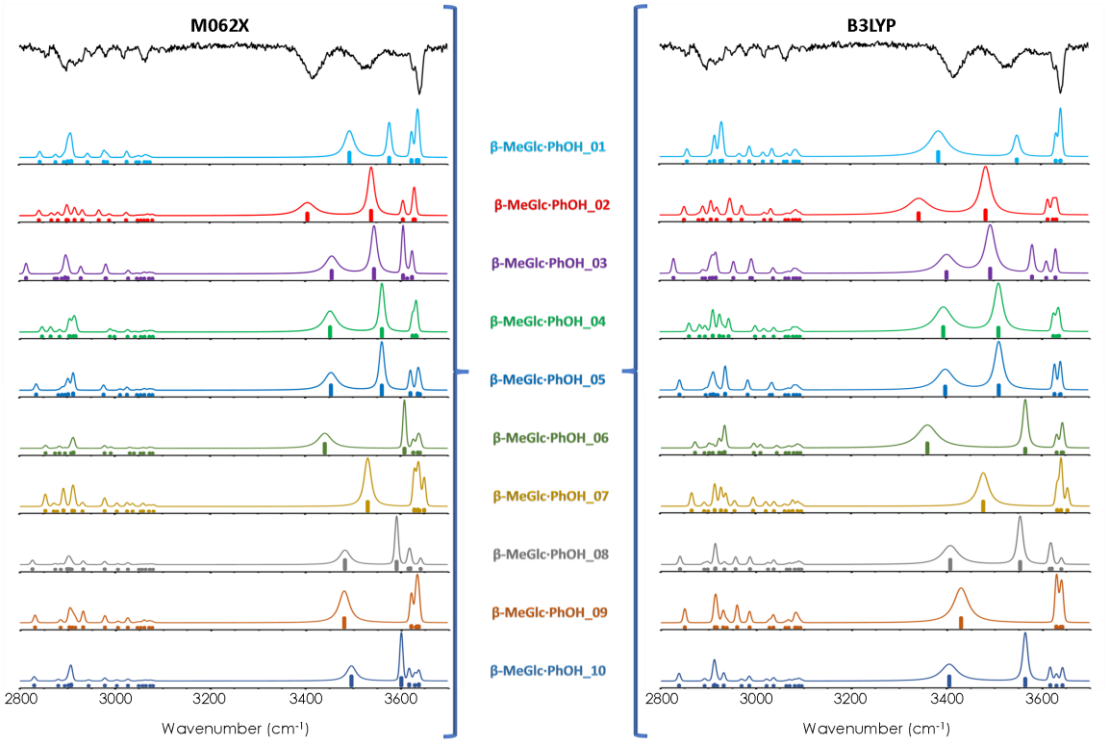

Table S4. Relative Gibbs energies for the most stable conformers of each family of β-MeGal·PhOH complex. Values include ZPE and BSSE corrections.

LABEL	FAMILY	M062X		B3LYP		RMSD (NO H ATOMS)
		ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	
β-MeGal·PhOH_01	HO6·HOPh	0.0	2.7	1.4	4.6	0.16
β-MeGal·PhOH_02	O5·HOPh_O6H·OHPh	2.2	0.8	3.5	4.8	0.06
β-MeGal·PhOH_03	HO4·HOPh	2.5	8.3	8.2	11.4	0.12
β-MeGal·PhOH_04	HO2·HOPh	4.8	7.4	8.1	6.9	0.29
β-MeGal·PhOH_05	HO4·HOPh_O6H·OHPh	5.4	3.9	6.1	7.9	0.09
β-MeGal·PhOH_06	O1·HOPh	5.4	6.2	5.6	8.1	0.17
β-MeGal·PhOH_07	O1·HOPh_O6H·OHPh	5.4	6.5	4.9	7.5	0.24
β-MeGal·PhOH_08	HO2·HOPh_O3H·OHPh	5.7	1.8	7.2	6.1	0.19
β-MeGal·PhOH_09	O1·HOPh_O4H·OHPh	5.9	8.0	11.5	15.4	0.13
β-MeGal·PhOH_10	HO6·HOPh	0.0	2.7	1.4	4.6	0.16

Figure S19. Most stable conformers of β-MeGal·PhOH complex computed at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level. Energies inside brackets are given in kJ/mol. The global minimum at B3LYP(D3)/6-311++G(d,p) level corresponds to an isomer with different relative orientations of the two molecules than the global minimum obtained using M062X/6-311++G(d,p)

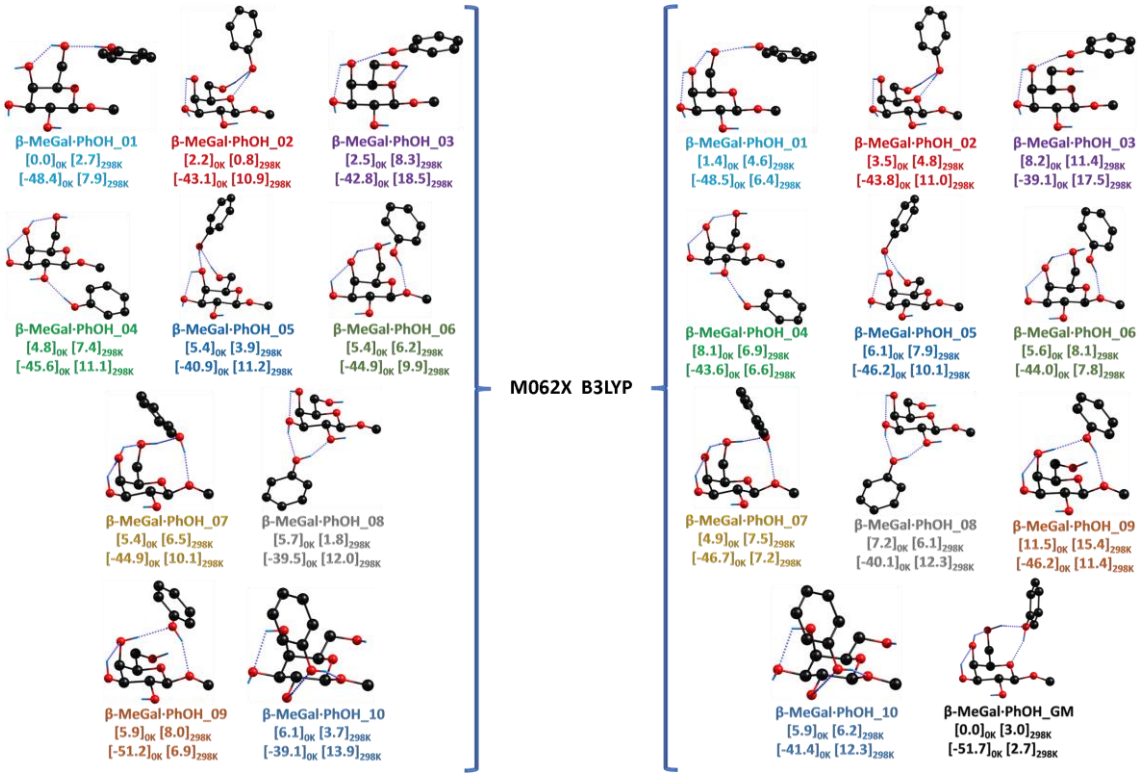

Figure S20. Comparison between the experimental IDIR spectrum for β-MeGal·PhOH complex and the computational simulations for the ten most stable structures at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level.

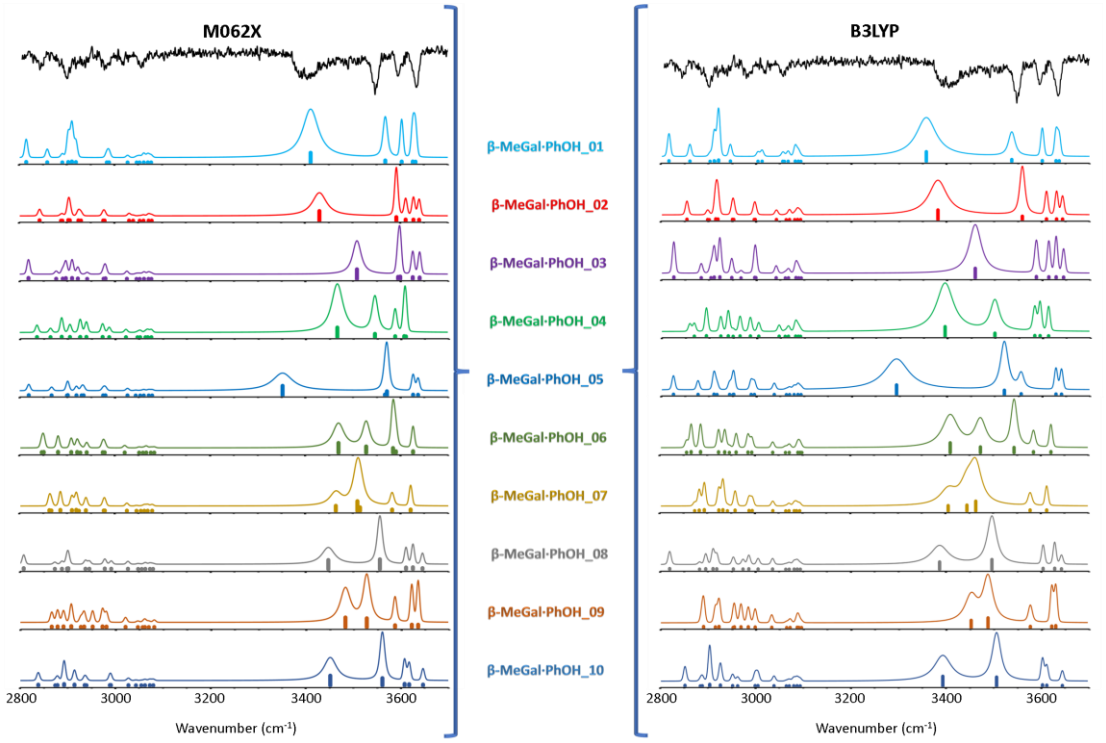

Table S5. Relative Gibbs energies for the most stable conformers of each family of α-MeGlc·PhOH complex. Values include ZPE and BSSE corrections.

LABEL	FAMILY	M062X		B3LYP		RMSD (NO H ATOMS)
		ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	
α-MeGlc·PhOH_01	HO6·HOPh	0.0	5.7	0.0	0.4	0.12
α-MeGlc·PhOH_02	HO3·HOPh_O4H·OHPh	3.8	5.5	4.0	0.8	0.21
α-MeGlc·PhOH_03	O4H·OHPh_HO6·HOPh	3.8	7.6	6.4	4.3	0.17
α-MeGlc·PhOH_04	HO4·HOPh	5.3	9.3	6.0	2.7	0.12
α-MeGlc·PhOH_05	HO2·HOPh	6.6	11.1	10.4	7.6	0.08
α-MeGlc·PhOH_06	HO2·HOPh_O3H·OHPh	0.0	5.7	0.0	0.4	0.12
α-MeGlc·PhOH_07	HO3·HOPh	3.8	5.5	4.0	0.8	0.21
α-MeGlc·PhOH_08	O5·HOPh_O6H·OHPh	3.8	7.6	6.4	4.3	0.17
α-MeGlc·PhOH_09	O1·HOPh_O2H·OHPh	5.3	9.3	6.0	2.7	0.12
α-MeGlc·PhOH_10	HO4·HOPh_O6H·OHPh	6.6	11.1	10.4	7.6	0.08

Figure S21. Most stable conformers of α-MeGlc·PhOH complex computed at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level. Energies inside brackets are given in kJ/mol.

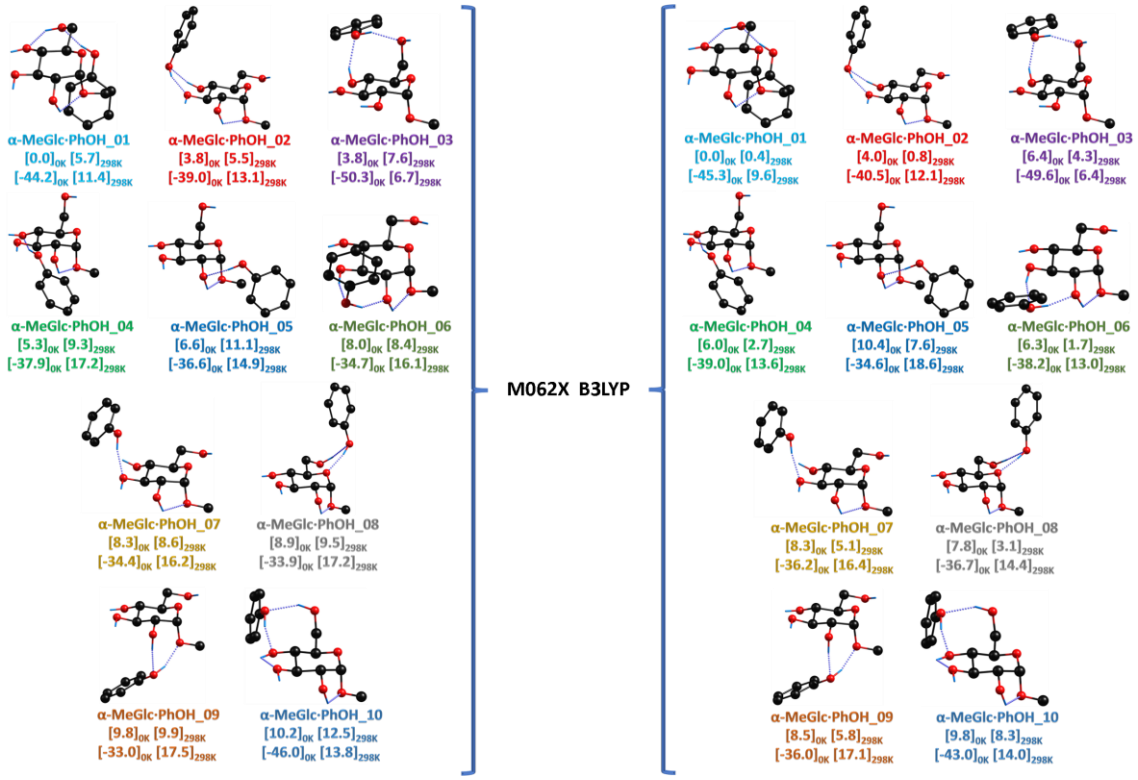

Figure S22. Comparison between the experimental IDIR spectrum for α-MeGlc·PhOH complex and the computational simulations for the ten most stable structures at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level.

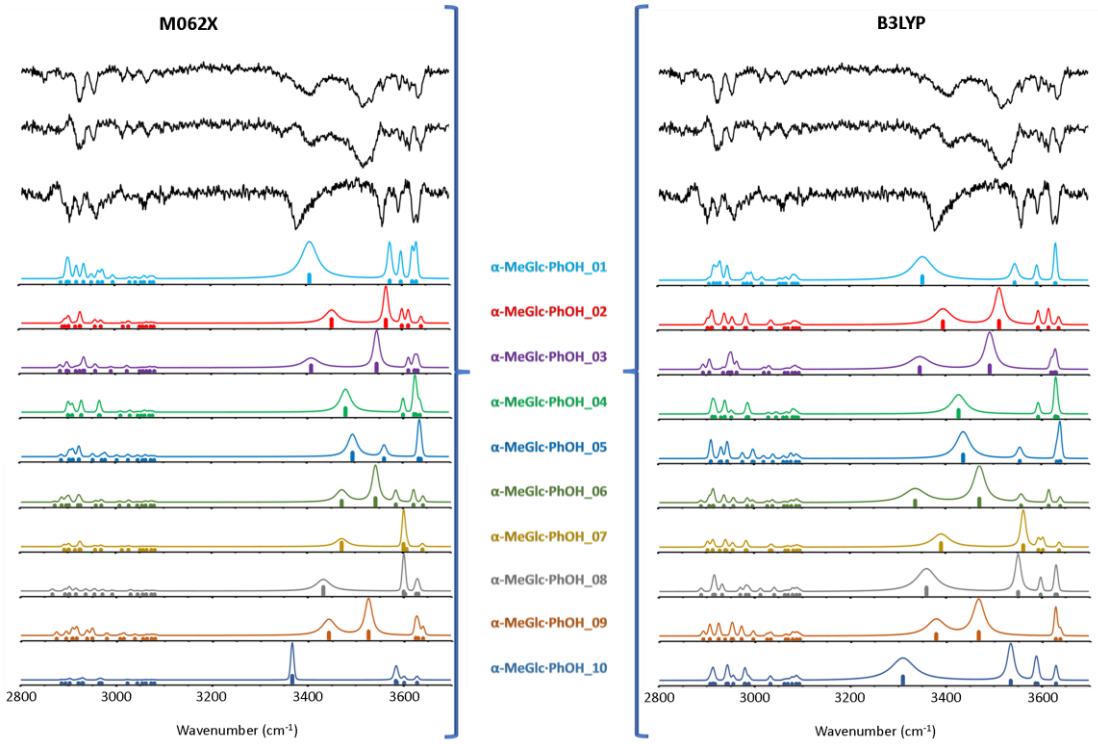

Table S6. Relative Gibbs energies for the most stable conformers of each family of α-MeGal·PhOH complex. Values include ZPE and BSSE corrections.

LABEL	FAMILY	M062X		B3LYP		RMSD (NO H ATOMS)
		ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	ΔG (0K) (kJ/mol)	ΔG (298K) (kJ/mol)	
α-MeGal·PhOH_01	HO6·HOPh	0.0	0.0	0.0	0.0	0.11
α-MeGal·PhOH_02	HO2·HOPh	5.3	4.8	7.0	3.0	0.14
α-MeGal·PhOH_03	O5·HOPh_O6H·OHPh	7.6	6.2	5.6	3.6	0.09
α-MeGal·PhOH_04	HO4·HOPh_O6H·OHPh	8.6	5.4	6.2	4.3	0.10
α-MeGal·PhOH_05	HO3·HOPh_O4H·OHPh	9.4	5.1	7.8	4.4	0.15
α-MeGal·PhOH_06	HO4·HOPh	9.7	8.4	9.0	6.2	0.12
α-MeGal·PhOH_07	HO2·HOPh_O3H·OHPh	11.0	6.4	7.9	1.6	0.39
α-MeGal·PhOH_08	HO3·HOPh	12.4	8.8	11.9	7.0	0.11
α-MeGal·PhOH_09	O2H·OHPh_HO3·HOPh	12.4	9.0	12.5	9.3	0.14
α-MeGal·PhOH_10	O5·HOPh	12.7	3.3	9.9	4.5	0.14

Figure S23. Most stable conformers of α-MeGal·PhOH complex computed at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level. Energies inside brackets are given in kJ/mol.

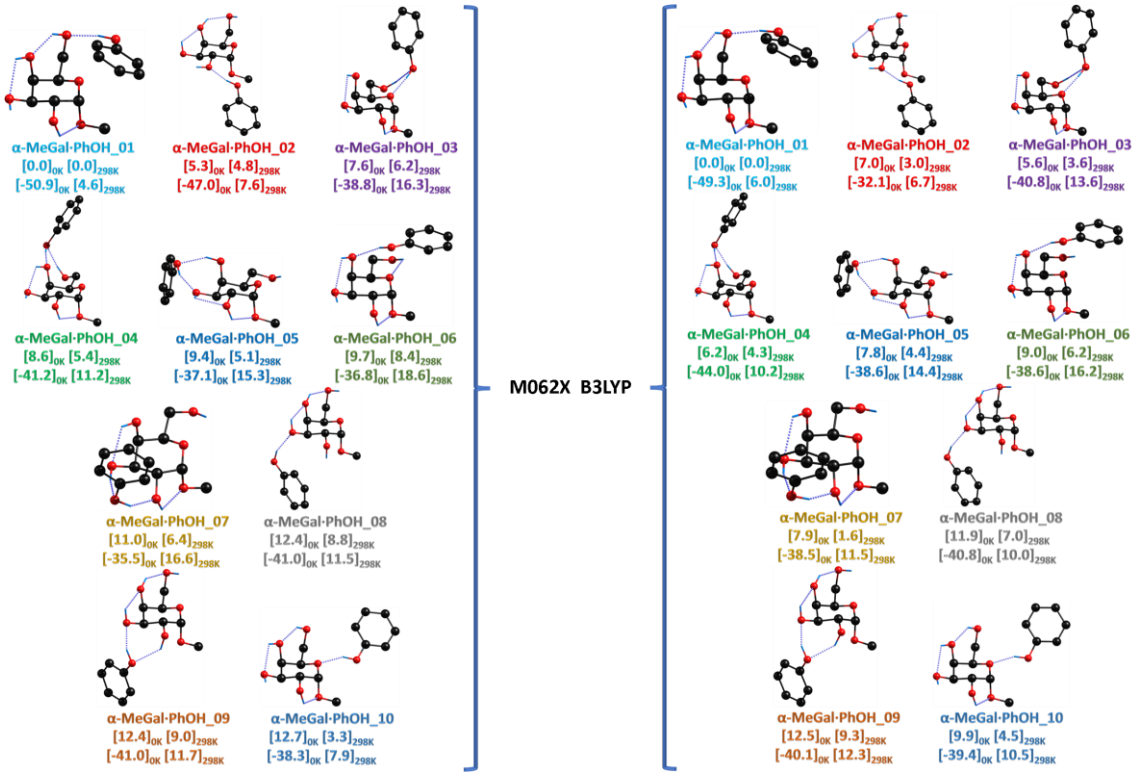

Figure S24. Comparison between the experimental IDIR spectrum for α-MeGal·PhOH complex and the computational simulations for the ten most stable structures at B3LYP(D3)/6-311++G(d,p) and M062X/6-311++G(d,p) level.