

A Comparative Study of the Glycating Power of Simple Carbohydrates in the Maillard Reaction by Means of Conceptual DFT Descriptors

Abstract

A large number of density functionals has been assessed for the calculation of the molecular structure and properties of simple carbohydrates that can participate in the nonenzymatic glycation of amino acids and proteins through the Maillard reaction. The chemical reactivity descriptors for these systems have been calculated through Conceptual DFT. A comparison between the descriptors calculated through a Δ SCF procedure and those arising from the "Koopmans in DFT" (KID) procedure have been performed in order to check for the validity of the last procedure and the accuracy of the studied density functionals. The active sites for nucleophilic and electrophilic attacks have been chosen by relating them to the Fukui function indices and the condensed dual descriptor $\Delta f(r)$. Several relationships between the glycating power and the reactivity descriptors have been found that could be useful for the prediction of this behavior for complex carbohydrates.

Keywords: Computational Chemistry, Molecular Modeling, Carbohydrates, Maillard Reaction, Conceptual DFT, Chemical Reactivity Theory

1. Introduction

Protein glycation is initiated by a nucleophilic addition (nonenzymatic glycation or Maillard reaction), reaction between a free amino group from a protein and a carbonyl group from a reducing sugar to form a freely reversible Schiff base. Glycated proteins can undergo further reactions, giving rise to some structures called advanced glycation endproducts (AGEs) [1]. The formation of AGEs could induce oxidative stress, forming a positive feedback loop to augment oxidative damage in the brain. Therefore, AGEs are recognized to play an important role in the development of Alzheimer disease and other neurodegenerative diseases [2]. Also, AGEs play an important role in the development of chronic diabetic complications [3]. Thus, it is of paramount importance to understand how the different carbohydrates react with the amino acids and proteins and to obtain a measure of the extent of this reaction in each case. Indeed, it has been experimentally shown that the ability of different molecules with carbonyl groups to interact with the amino group of a protein, that is, the glycation power, is strongly dependent on their molecular structures and electronic properties.

In a very interesting work, Adrover et al have studied the kinetics of the interaction of pyridoxamine (a potential inhibitor of the formation of AGEs) with hexoses and pentoses [4]. It was found that there is a good correlation between the rate constants for the initial reaction between the carbonyl group of each carbohydrate with the amine group of pyridoxamine, and the net NBO charge over the carbonyl C atom of the corresponding hexose or pentose. These means that the glycation power of a given molecule with a reducing carbonyl can be quantified in terms of the electronic properties of such molecule and paved the way for building a scale for the prediction of the glycation power of more complex carbohydrates.

From an empirical and practical point of view, it is meaningful to follow the procedure of assigning the KS HOMO as equal to and opposite of the vertical ionization potential, $\epsilon_H = -I$ and the KS LUMO as equal to and opposite of

the vertical Electron affinity, $\epsilon_L = -A$. We have coined the acronym KID for this empirical procedure (for "Koopmans in DFT"). This means that how well a given density functional behaves can be estimated by checking how well it follows the "Koopmans in DFT" (KID) procedure and this will be crucial for a good calculation of the Conceptual DFT descriptors that predict and explain the chemical reactivity of molecular systems. Therefore, the objective of this work is twofold: i) to conduct a comparative study of the performance of a large number of density functionals (including the latest Minnesota family of density functionals) for the description of the chemical reactivity of simple hexoses and pentoses which molecular structures are shown in Figure 1; and ii) to build a better glycation power scale by relating the experimental rate constants for the initial reaction (or Maillard) of those carbohydrates with amino groups, with accurately calculated Conceptual DFT descriptors.

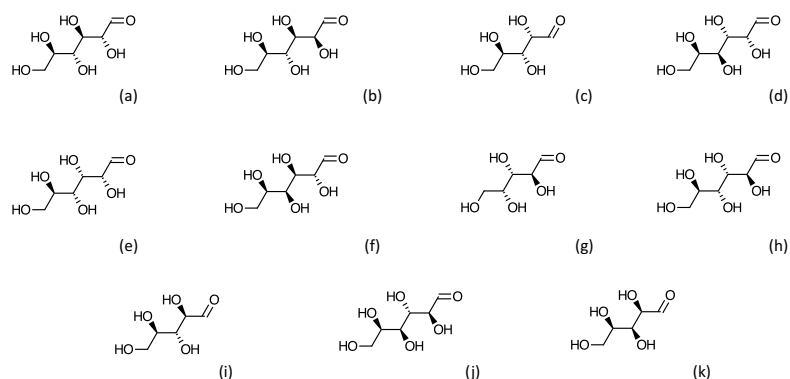


Figure 1: Molecular structures of a) Allose, b) Altrose, c) Arabinose, d) Galactose, e) Glucose, f) Gulose, g) Lyxose, h) Mannose, i) Ribose, j) Talose and k) Xylose

2. Theoretical Background

As this work is part of an ongoing project, the theoretical background is similar to that presented in previous research [5–11] and will be shown here for the sake of completeness. Thus, as has been already described in detail before [5–11], the chemical potential μ is defined within the conceptual framework of DFT [12, 13] as: $\mu = (\partial E / \partial N)_{v(\vec{r})} = -\chi$ where χ is the electronegativity. The global hardness η is: $\eta = (\partial^2 E / \partial N^2)_{v(\vec{r})}$. Using a finite difference approximation and the "Koopmans in DFT" procedure, the former expressions can be written as: $\mu = -\frac{1}{2}(I+A) \approx \frac{1}{2}(\epsilon_L + \epsilon_H) = \chi_K$ and $\eta = (I-A) \approx (\epsilon_L - \epsilon_H) = \eta_K$ where ϵ_H and ϵ_L are the energies of the highest occupied and the lowest unoccupied molecular orbitals, HOMO and LUMO, respectively. The electrophilicity index ω has been defined as [14]: $\omega = \mu^2 / 2\eta = (I+A)^2 / 4(I-A) \approx (\epsilon_L + \epsilon_H)^2 / 4(\epsilon_L - \epsilon_H) = \omega_K$. The electrodonating (ω^-) and electroaccepting (ω^+) powers have been defined as [15]: $\omega^- = (3I+A)^2 / 16(I-A) \approx (3\epsilon_H + \epsilon_L)^2 / 16\eta_K = \omega_K^-$ and $\omega^+ = (I+3A)^2 / 16(I-A) \approx (\epsilon_H + 3\epsilon_L)^2 / 16\eta_K = \omega_K^+$. It follows that a larger ω^+ value corresponds to a better capability of accepting charge, whereas a smaller value of ω^- makes it a better electron donor. In order to compare ω^+ with $-\omega^-$, the following definition of net electrophilicity has been proposed [16]: $\Delta\omega^\pm = \omega^+ - (-\omega^-) = \omega^+ + \omega^- \approx \omega_K^+ - (-\omega_K^-) = \omega_K^+ + \omega_K^- = \Delta\omega_K^\pm$, that is, the electroaccepting power relative to the electrodonating power.

The function $f(\mathbf{r})$ reflects the ability of a molecular site to accept or donate electrons and is defined in terms of the derivative of $\rho(\mathbf{r})$ with respect to N : $f(\mathbf{r}) = (\partial \rho(\mathbf{r}) / \partial N)_{v(\mathbf{r})}$. Since the number of electrons N is a discrete variable [17], right and left derivatives of $\rho(\mathbf{r})$ with respect to N have emerged. By applying a finite difference approximation to the previous equation, two definitions of Fukui functions depending on total electronic densities are obtained: $f^+(\mathbf{r}) = \rho_{N+1}(\mathbf{r}) - \rho_N(\mathbf{r})$ and $f^-(\mathbf{r}) = \rho_N(\mathbf{r}) - \rho_{N-1}(\mathbf{r})$ where $\rho_{N+1}(\mathbf{r})$, $\rho_N(\mathbf{r})$ and $\rho_{N-1}(\mathbf{r})$ are the electronic densities at point $\mathbf{r}$ for the system with $N+1$, N and $N-1$ electrons, respectively. The first one, $f^+(\mathbf{r})$, has been associated

to reactivity for a nucleophilic attack so that it measures the intramolecular
75 reactivity at the site $\mathbf{r}$ towards a nucleophilic reagent. The second one, $f^-(\mathbf{r})$,
has been associated to reactivity for an electrophilic attack so that this func-
tion measures the intramolecular reactivity at the site $\mathbf{r}$ toward an electrophilic
reagent [12].

Morell et al. [18–24] have proposed a local reactivity descriptor (LRD) which
80 is called the dual descriptor (DD) $f^{(2)}(\mathbf{r}) \equiv \Delta f(\mathbf{r})$. Mathematically it is defined
in terms of the derivative of the Fukui function, $f(\mathbf{r})$ [13], with respect to the
number of electrons, N . When $\Delta f_k > 0$ the process is driven by a nucleophilic
attack on atom k and then that atom acts as an electrophilic species; conversely,
when $\Delta f_k < 0$ the process is driven by an electrophilic attack over atom k and
85 therefore atom k acts as a nucleophilic species.

3. Settings and Computational Methods

Following the lines of our previous work and as has been already described in
detail before [5–11], all computational studies were performed with the Gaussian
09 [25] series of programs with density functional methods as implemented in
90 the computational package. The equilibrium geometries of the molecules were
determined by means of the gradient technique. The force constants and vi-
brational frequencies were determined by computing analytical frequencies on
the stationary points obtained after the optimization to check if there were true
minima. The basis set used in this work was Def2SVP for geometry optimiza-
95 tion and frequencies while Def2TZVP was considered for the calculation of the
electronic properties [26, 27].

For the calculation of the molecular structure and properties of the studied
systems, we have chosen several density functionals from the latest Minnesota
density functionals family, which consistently provide satisfactory results for sev-
eral structural and thermodynamic properties [28]: M11, which is a range-
100 separated hybrid meta-GGA[29], M11L, which is a dual-range local meta-GGA
[30], MN12L, which is a nonseparable local meta-NGA [31], MN12SX, which is

a range-separated hybrid nonseparable meta-NGA [32], N12, which is a nonseparable gradient approximation [33], N12SX, which is a range-separated hybrid
 105 nonseparable gradient approximation [32], SOGGA11, which is a GGA density functional [34] and SOGGA11X, which is a hybrid GGA density functional [35]. In these functionals, GGA stands for generalized gradient approximation (in which the density functional depends on the up and down spin densities and their reduced gradient) and NGA stands for nonseparable gradient approx-
 110 imation (in which the density functional depends on the up/down spin densities and their reduced gradient, and also adopts a nonseparable form). Moreover, we have also considered the following density functionals: BLYP [36, 37], B3LYP [37, 38], PBE [39, 40], PBE0 [39–41], CAM-B3LYP [42], LC-wPBE [43–45], HSEh1PBE [46–52], wB97 [53], wB97X [53], wB97XD [54], M05 [55], M052X
 115 [56, 57], M06 [57, 58], M06L [57, 59], M062X [57, 58] and M06HF [57, 60]. All the calculations were performed in the presence of water as a solvent, by doing IEF-PCM computations according to the SMD solvation model [61].

4. Results and Discussion

The molecular structures of Allose, Altrose, Arabinose, Galactose, Glucose,
 120 Gulose, Lyxose, Mannose, Ribose, Talose and Xylose were pre-optimized by starting with the readily available MOL structures, and finding the most stable conformers by means of the Avogadro 1.2.0 program [62, 63] through a random sampling with molecular mechanics techniques and a consideration of all the torsional angles. The structures of the resulting conformers were then reoptimized
 125 with the twenty-four density functionals mentioned in the previous section in conjunction with the Def2SVP basis set and the SMD solvation model, using water as a solvent.

It is worth to calculate the electronegativity χ , the global hardness η and the global electrophilicity ω for the studied systems in order to verify the va-
 130 lidity of the KID procedure. Additionally, we will include in the calculations, the electrodonating (ω^-) and electroaccepting (ω^+) powers as well as the net

electrophilicity $\Delta\omega^\pm$ for further verifications.

The HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η ,
135 global electrophilicity ω , electrodonating power, (ω^-) , electroaccepting power (ω^+) , and net electrophilicity $\Delta\omega^\pm$ of the hexoses and pentoses calculated with the twenty-four density functionals and the Def2TZVP basis set using water as a solvent simulated with the SMD parametrization of the IEF-PCM model are presented in Tables S1A to S24A of the Electronic Supplementary Information
140 (ESI). The upper part of the tables shows the results derived assuming the validity of "Koopmans in DFT" procedure (hence the subscript K) and the lower part shows the results derived from the calculated vertical I and A.

Inspired from previous works on this subject [64, 65], and with the object of analyzing our results in order to verify the fulfillment of the "Koopmans in
145 DFT" procedure, we have designed several descriptors that relate the results obtained through the HOMO and LUMO calculations with those obtained by means of the vertical I and A with a Δ SCF procedure. However, it must be stressed that it is not our intention to perform a gap-fitting by minimizing a descriptor by choosing optimal range-separation parameter γ , but to check if the
150 density functionals considered in this study, in which, some of them contain a fixed range-separation parameter γ , obey the "Koopmans in DFT" procedure. As a matter fact, there is no range-separation parameter γ in our designed descriptors. Moreover, we have considered A as minus the energy of the LUMO of the neutral system instead of considering A as minus the energy of the HOMO
155 of the N+1 electron system, as it was in the mentioned works [64, 65].

The first three descriptors are related to the simplest fulfillment of the "Koopmans in DFT" procedure by relating ϵ_H with -I, ϵ_L with -A, and the behavior of them in the description of the HOMO-LUMO gap: $J_I = |\epsilon_H + E_{gs}(N - 1) - E_{gs}(N)|$, $J_A = |\epsilon_L + E_{gs}(N) - E_{gs}(N + 1)|$ and $J_{HL} = \sqrt{J_I^2 + J_A^2}$, Next,
160 we consider four other descriptors that analyze how well the studied density functionals are useful for the prediction of the electronegativity χ , the global hardness η and the global electrophilicity ω , and for a combination of these

Conceptual DFT descriptors, just considering the energies of the HOMO and LUMO or the vertical I and A: $J_\chi = |\chi - \chi_K|$, $J_\eta = |\eta - \eta_K|$, $J_\omega = |\omega - \omega_K|$ and $J_{D1} = \sqrt{J_\chi^2 + J_\eta^2 + J_\omega^2}$, where D1 stands for the first group of Conceptual DFT descriptors. Finally, we designed other four descriptors to verify the goodness of the studied density functionals for the prediction of the electroaccepting power ω^+ , the electrodonating power ω^- , the net electrophilicity $\Delta\omega^\pm$, and for a combination of these Conceptual DFT descriptors, just considering the energies of the HOMO and LUMO or the vertical I and A: $J_{\omega^+} = |\omega^+ - \omega_K^+|$, $J_{\omega^-} = |\omega^- - \omega_K^-|$, $J_{\Delta\omega^\pm} = |\Delta\omega^\pm - \Delta\omega_K^\pm|$ and $J_{D2} = \sqrt{J_{\omega^-}^2 + J_{\omega^+}^2 + J_{\Delta\omega^\pm}^2}$, where D2 stands for the first group of Conceptual DFT descriptors.

The results of the calculations of J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the pentoses and hexoses considered in this work are displayed in Tables S1B to S24B of the Electronic Supplementary Information (ESI).

On the basis of the results for the descriptors presented on Tables S1B to S24B of the ESI, we have compiled the average values for for each density functional on the whole group of hexoses and pentoses, and the calculated results are displayed on Table 1.

As can be seen from Table 1, the "Koopman's theorem in DFT" procedure holds with great accuracy for the HSEh1PBE density functional as well as for the MN12SX and N12SX density functionals, which are a range-separated hybrid meta-NGA and a range-separated hybrid NGA density functionals, respectively. Indeed, the values of J_I , J_A and J_{HL} are not exactly zero. However, their values can be favorably compared with the results presented for these quantities in the work of Lima et al [65], where the minima has been obtained by choosing a parameter that enforces that behavior.

It is interesting to see that the same density functionals also fulfill the "Koopmans in DFT" procedure for the other descriptors, namely J_χ , J_η , J_ω , and J_{D1} , as well as for J_{ω^-} , J_{ω^+} , $J_{\Delta\omega^\pm}$, and J_{D2} . These results are very important, because they show that it is not enough to rely only in J_I , J_A and J_{HL} . For example, if we consider only J_χ , for all of the density functionals considered, the values are very close to zero. As for the other descriptors, only the HSEh1PBE,

Table 1: Average descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , $J_{\omega+}$, $J_{\omega-}$, $J_{\Delta\omega\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated with the twenty-four density functionals and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model.

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	$J_{\omega-}$	$J_{\omega+}$	$J_{\Delta\omega\pm}$	J_{D2}
BLYP	0.439	0.697	0.826	0.129	1.136	0.623	1.303	1.240	1.112	2.352	2.882
B3LYP	0.215	0.272	0.349	0.039	0.487	0.159	0.514	0.303	0.274	0.577	0.708
PBE	0.434	0.693	0.820	0.130	1.128	0.662	1.315	1.319	1.189	2.508	3.073
PBE0	0.394	0.547	0.675	0.078	0.941	0.296	0.990	0.571	0.495	1.066	1.306
CAM-B3LYP	1.508	1.812	2.358	0.152	3.320	0.700	3.397	1.268	1.116	2.383	2.921
LC-wPBE	2.618	3.167	4.110	0.275	5.785	0.994	5.877	1.765	1.490	3.255	3.991
HSEh1PBE	0.022	0.157	0.160	0.070	0.177	0.104	0.218	0.233	0.163	0.396	0.358
wB97	2.599	3.114	4.058	0.258	5.713	0.916	5.793	1.604	1.347	2.951	3.619
wB97X	2.425	2.860	3.750	0.217	5.284	0.874	5.361	4.492	0.191	2.837	5.318
wB97XD	2.059	2.376	3.144	0.158	4.435	0.782	4.506	2.868	1.208	2.575	4.042
M05	0.405	0.629	0.749	0.112	1.034	0.311	1.086	0.614	0.502	1.116	1.369
M052X	1.472	1.740	2.280	0.134	3.212	0.668	3.284	1.201	1.068	2.269	2.781
M06	0.384	0.515	0.644	0.071	0.900	0.267	0.941	0.511	0.446	0.957	1.173
M06L	0.362	0.472	0.596	0.055	0.834	0.344	0.904	0.663	0.608	1.271	1.337
M062X	1.401	1.608	2.135	0.106	3.010	2.795	4.110	1.091	0.987	2.078	2.546
M06HF	3.144	3.334	4.584	0.111	6.478	0.955	6.549	1.553	1.458	3.011	3.688
M11	2.462	2.822	3.746	0.180	5.284	0.906	5.365	1.573	1.393	2.965	3.634
M11L	0.503	0.523	0.544	0.556	0.633	0.633	0.711	0.719	0.807	0.992	1.092
MN12L	0.320	0.254	0.411	0.045	0.573	0.141	0.593	0.230	0.263	0.494	0.606
MN12SX	0.051	0.178	0.189	0.067	0.229	0.109	0.305	0.235	0.171	0.405	0.423
N12	0.394	0.690	0.795	0.148	1.084	0.550	1.352	1.105	0.958	2.063	1.993
N12SX	0.009	0.140	0.140	0.066	0.149	0.091	0.215	0.206	0.140	0.346	0.329
SOGGA11	0.451	0.761	0.887	0.155	1.212	0.699	1.510	1.400	1.245	2.645	2.409
SOGGA11X	1.116	1.215	1.652	0.054	2.331	0.506	2.858	0.891	0.842	1.733	3.113

MN12SX and N12SX density functionals show this behavior. That means that
 195 the results for J_χ are due to a fortuitous cancellation of errors.

The usual GGA (SOGGA11) and hybrid-GGA (SOGGA11X) are not good for the fulfillment of the "Koopmans in DFT" procedure, and the same conclusion is valid for the local functionals M11L, MN12L and N12.

An important fact is that although the range-separated hybrid NGA and
 200 range-separated hybrid meta-NGA density functionals can be useful for the calculation of the Conceptual DFT descriptors, it is not the same for the range-separated hybrid GGA (M11) density functional. An inspection of Table S17A of the ESM shows that this is due to the fact that this functional describes inadequately the energy of the LUMO, leading to negative values of A, which
 205 are in contradiction with the Δ SCF results.

As mentioned in the Introduction, the other objective of this work is to find a better description for the glycation power (GP) of the studied carbohydrates in terms of the accurately calculated Conceptual DFT descriptors. To this end, the rate of condensation of monosaccharides with pyridoxamine (k_3), taken from
 210 the work of Adrover et al [4] have been plotted against the different Conceptual DFT descriptors calculated in this study and that are displayed on Tables S1A to S24A of the ESM. After visual inspection of the plots, we have concluded that the best correlations are found between k_3 and the global electrophilicity ω . Thus, we have performed a Linear Regression Analysis of the results according
 215 to the following equation: $GP = a \times \omega + b$, where $GP = k_3$, a is the slope and b is the interception of the linear correlation. The results of this analysis for the twenty-four density functionals are presented in Table 2.

It can be observed from the results on Table 2 that the MCC is high for most of the density functionals with the exception of N12, N12SX, SOGGA11 and
 220 SOGGA11X. The typical error is of the same magnitude for all the density functionals, again with the exception of the N12, N12SX, SOGGA11 and SOGGA11X, which are two or three times greater. However, the MAD for each density functional displays disparate values. Indeed, the best results of the MAD are for M06 and MN12SX, which are below 0.6.

Table 2: Linear regression parameters Slope a, Interception b, Multiple Correlation Coefficient MCC, Typical Error TE and Mean Absolute Deviation MAD for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated with 24 density functionals and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model.

	a	b	MCC	TE	MAD
BLYP	58.5758	-82.4942	0.9498	0.9822	0.7899
B3LYP	65.6780	-102.3943	0.9621	0.8557	0.6722
PBE	45.1506	-65.9714	0.9337	1.1242	0.8727
PBE0	60.7400	-93.1869	0.9491	0.9886	0.8065
CAM-B3LYP	61.1536	-96.6709	0.9489	0.9905	0.8188
LC-wPBE	58.5259	-97.2502	0.9183	1.2429	1.0103
HSEh1PBE	60.2928	-92.7533	0.9507	0.9735	0.7872
wB97	62.6414	-96.7526	0.9328	1.1314	0.9622
wB97X	65.0791	-100.5809	0.9374	1.0933	0.9264
wB97XD	68.1462	-103.7450	0.9536	0.9447	0.7787
M05	64.3986	-91.3532	0.9483	0.9968	0.7813
M052X	72.4292	-117.3654	0.9539	0.9243	0.7444
M06	66.3025	-100.5016	0.9646	0.8283	0.5917
M06L	70.5378	-98.7481	0.9446	1.0303	0.6763
M062X	79.5595	-126.0879	0.9545	0.9362	0.7588
M06HF	79.7895	-137.5252	0.9497	0.9834	0.6850
M11	65.2613	-107.5261	0.9288	1.1637	0.9199
M11L	63.5265	-95.4417	0.9359	1.1059	0.8112
MN12L	82.8255	-109.8228	0.9362	1.1033	0.7651
MN12SX	87.5200	-134.3312	0.9532	0.9496	0.5840
N12	38.4658	-46.5835	0.8808	1.4863	1.2332
N12SX	44.9554	-64.3326	0.6430	2.4044	1.4311
SOGGA11	-4.7053	16.6130	0.1009	3.1233	2.1970
SOGGA11X	-21.8945	46.2125	0.7377	2.1195	1.7211

225 These linear correlations have been obtained by considering a global descriptor. Thus, it would be interesting to check if the inclusion of a local descriptor could lead to a better description of the GP by obtaining a lower MAD.

The condensed Fukui functions can also be employed to determine the reactivity of each atom in the molecule. The corresponding condensed functions are given by $f_k^+ = q_k(N+1) - q_k(N)$ (for nucleophilic attack), $f_k^- =$ 230 $q_k(N) - q_k(N-1)$ (for electrophilic attack), and $f_k^0 = [q_k(N+1) - q_k(N-1)]/2$ (for radical attack), where q_k is the gross charge of atom k in the molecule. The condensed Fukui functions have been calculated using the AOMix molecular analysis program [66, 67] starting from single-point energy calculations.

235 The condensed dual descriptor was calculated as $\Delta f_k = f_k^+ - f_k^-$ [18, 19]. From the interpretation given to the Fukui function, one can note that the sign of the dual descriptor is very important to characterize the reactivity of a site within a molecule toward a nucleophilic or an electrophilic attack. That is, if $\Delta f_k > 0$, then the site is favored for a nucleophilic attack, whereas if $\Delta f_k < 0$, 240 then the site may be favored for an electrophilic attack [18, 19, 68].

The condensed dual descriptor Δf_k over the carbonyl C atoms of the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated with the M06 and MN12SX density functionals and the Def2TZVP basis set using water as solvent simulated with 245 the SMD parametrization of the IEF-PCM model are shown in Table 3.

Table 3: Condensed dual descriptors Δf_k over the carbonyl C atoms of the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated with the M06 and MN12SX density functionals and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model.

	M06	MN12SX
Allose	0.6172	0.6154
Altrose	0.6077	0.5964
Arabinose	0.5558	0.5554
Galactose	0.5691	0.6171
Glucose	0.6140	0.6117
Gulose	0.6278	0.6292
Lyxose	0.5938	0.6027
Mannose	0.6005	0.5957
Ribose	0.5923	0.5835
Talose	0.5960	0.5893
Xylose	0.6099	0.6089

In order to improve the GP prediction, we have performed a new Linear Regression Analysis of the results according to the following equation: $GP = a_1 \times \omega + a_2 \times \Delta f_k + b$, where $GP = k_3$, and a_1 , a_2 and b are the correlation parameters. The results of this analysis for the M06 and MN12SX density functionals are presented in Table 4.

It can be seen from Table 4 that there is indeed an improvement on the MAD, specially for the case of the MN12SX density functional. Thus, it can be concluded that the glycation power GP of simple carbohydrates can be predicted through the following equation: $GP = 94.6491 \times \omega - 29.5963 \times \Delta f_k - 128.2751$, where the global electrophilicity ω and condensed dual descriptor $f^{(2)}(\mathbf{r})$ calculated by means of the MN12SX density functional in connection with the Def2TZVP basis set and the SMD parametrization of the IEF-PCM model using water as a solvent.

Table 4: Linear regression parameters a_1 , a_2 , and b , Multiple Correlation Coefficient MCC, Typical Error TE and Mean Absolute Deviation MAD for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated with the M06 and MN12SX density functionals and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model.

	a_1	a_2	b	MCC	TE	MAD
M06	68.7579	-8.9367	-99.2263	0.9660	0.8613	0.5890
MN12SX	94.6491	-29.5963	-128.2751	0.9706	0.8014	0.5212

5. Conclusions

260 The Minnesota family of density functionals (M11, M11L, MN12L, MN12SX, N12, N12SX, SOGGA11 and SOGGA11X) as well as sixteen other usual density functionals have been tested for the fulfillment of the "Koopmans in DFT" procedure by comparison of the HOMO- and LUMO-derived values with those obtained through a Δ SCF procedure. It has been shown that the range-separated
265 hybrid meta-NGA density functional (MN12SX), the range-separated hybrid NGA density functional (N12SX) and the HSEh1PBE density functional are the best for the accomplishment of this objective. As such, they are a good alternative to those density functionals whose behavior have been tuned through a gap-fitting procedure and a good prospect for their usefulness in the description
270 of the chemical reactivity of molecular systems of large size.

From the whole of the results presented in this work, it can be seen that the sites of interaction of the simple carbohydrates can be predicted by using DFT-based reactivity descriptors such as the electronegativity, global hardness, global electrophilicity, electrodonating and electroaccepting powers, net elec-
275 trophilicity as well as Fukui function, condensed dual descriptor and condensed local hypersoftness calculations. These descriptors were used in the characterization and successfully description of the preferred reactive sites and provide a firm explanation for the reactivity of those molecules.

Moreover, a very good relationship between the glycation power GP of the
280 studied simple carbohydrates and some Conceptual DFT descriptors have been
found. This is based on calculations performed with the MN12SX density func-
tional in connexion with the Def2TZVP basis set and the SMD parametrization
of the IEF-PCM model using water as a solvent. It can be concluded that this
model chemistry (MN12SX/Def2TZVP/SMD(Water)) is the best for fulfilling
285 the "Koopmans in DFT" procedure and for the prediction of the glycation power
GP of simple carbohydrates and could be used for the study of the behavior of
other molecules bearing carbonyl C atoms capable of taking part in the Maillard
reaction, in particular for complex carbohydrates.

Supplementary Data

Supplementary data related to this article can be found at the online version of
300 this article.

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A Comparative Study of the Glycating Power of Simple
Carbohydrates in the Maillard Reaction by Means of
Conceptual DFT Descriptors

Electronic Supplementary Information

Table S1A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the BLYP density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-5.916	-2.227	4.071	3.689	2.247	6.759	2.688	9.447
Altrose	-5.867	-2.257	4.062	3.610	2.286	6.828	2.766	9.593
Arabinose	-5.821	-2.041	3.931	3.780	2.044	6.290	2.359	8.649
Galactose	-5.836	-2.059	3.948	3.777	2.063	6.336	2.389	8.725
Glucose	-5.731	-2.202	3.966	3.529	2.229	6.661	2.695	9.356
Gulose	-5.731	-2.202	3.966	3.529	2.229	6.661	2.695	9.356
Lyxose	-5.970	-2.155	4.062	3.815	2.163	6.595	2.533	9.127
Mannose	-5.896	-2.144	4.020	3.752	2.154	6.552	2.532	9.084
Ribose	-5.873	-2.230	4.052	3.643	2.253	6.759	2.708	9.467
Talose	-5.876	-2.228	4.052	3.648	2.251	6.756	2.703	9.459
Xylose	-5.933	-2.201	4.067	3.732	2.217	6.700	2.633	9.332
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	6.288	1.501	3.894	4.788	1.584	5.414	1.520	6.934
Altrose	6.269	1.416	3.842	4.853	1.521	5.267	1.424	6.691
Arabinose	6.289	1.383	3.836	4.905	1.500	5.224	1.388	6.613
Galactose	6.256	1.365	3.811	4.892	1.484	5.180	1.369	6.549
Glucose	6.159	1.510	3.835	4.649	1.581	5.371	1.536	6.907
Gulose	6.332	1.529	3.931	4.804	1.608	5.482	1.551	7.033
Lyxose	6.395	1.479	3.937	4.916	1.577	5.429	1.492	6.922
Mannose	6.270	1.487	3.878	4.783	1.572	5.383	1.504	6.887
Ribose	6.307	1.557	3.932	4.750	1.627	5.518	1.586	7.104
Talose	6.339	1.547	3.943	4.792	1.622	5.515	1.572	7.087
Xylose	6.377	1.512	3.944	4.866	1.599	5.474	1.529	7.003

Table S1B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S1A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.373	0.726	0.816	0.177	1.099	0.663	1.295	1.345	1.168	2.513	3.081
Altrose	0.402	0.842	0.933	0.220	1.243	0.765	1.476	1.561	1.341	2.903	3.558
Arabinose	0.468	0.658	0.807	0.095	1.126	0.544	1.254	1.066	0.971	2.037	2.495
Galactose	0.420	0.695	0.812	0.137	1.115	0.579	1.264	1.157	1.020	2.177	2.667
Glucose	0.428	0.692	0.813	0.132	1.120	0.647	1.300	1.290	1.159	2.449	3.001
Gulose	0.601	0.673	0.903	0.036	1.274	0.621	1.418	1.180	1.144	2.324	2.846
Lyxose	0.426	0.675	0.798	0.125	1.101	0.586	1.253	1.165	1.041	2.206	2.703
Mannose	0.374	0.658	0.756	0.142	1.031	0.582	1.192	1.170	1.028	2.198	2.693
Ribose	0.434	0.673	0.801	0.119	1.107	0.625	1.277	1.241	1.122	2.363	2.896
Talose	0.463	0.682	0.824	0.109	1.145	0.629	1.310	1.241	1.131	2.372	2.906
Xylose	0.444	0.690	0.820	0.123	1.134	0.618	1.297	1.226	1.103	2.329	2.854
Average	0.439	0.697	0.826	0.129	1.136	0.623	1.303	1.240	1.112	2.352	2.882

Table S2A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the B3LYP density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-7.326	-1.339	4.332	5.987	1.567	5.675	1.343	7.018
Altrose	-7.291	-1.387	4.339	5.904	1.594	5.727	1.388	7.115
Arabinose	-7.231	-1.187	4.209	6.045	1.466	5.414	1.204	6.618
Galactose	-7.244	-1.206	4.225	6.038	1.478	5.447	1.222	6.668
Glucose	-7.114	-1.318	4.216	5.796	1.533	5.537	1.321	6.858
Gulose	-7.334	-1.346	4.340	5.987	1.573	5.690	1.350	7.041
Lyxose	-7.371	-1.288	4.330	6.084	1.541	5.626	1.297	6.923
Mannose	-7.277	-1.284	4.280	5.993	1.529	5.572	1.292	6.863
Ribose	-7.268	-1.358	4.313	5.910	1.574	5.674	1.361	7.034
Talose	-7.282	-1.352	4.317	5.929	1.572	5.672	1.355	7.028
Xylose	-7.351	-1.322	4.337	6.030	1.559	5.664	1.327	6.991
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.104	1.590	4.347	5.514	1.714	5.946	1.598	7.544
Altrose	7.067	1.501	4.284	5.566	1.648	5.786	1.503	7.289
Arabinose	7.025	1.490	4.257	5.535	1.637	5.749	1.492	7.241
Galactose	7.021	1.489	4.255	5.532	1.636	5.746	1.491	7.237
Glucose	6.901	1.608	4.254	5.293	1.710	5.877	1.623	7.501
Gulose	7.110	1.632	4.371	5.478	1.744	6.015	1.644	7.660
Lyxose	7.163	1.584	4.373	5.579	1.714	5.964	1.590	7.554
Mannose	7.065	1.582	4.323	5.483	1.704	5.913	1.590	7.503
Ribose	7.060	1.649	4.354	5.411	1.752	6.019	1.665	7.684
Talose	7.079	1.643	4.361	5.436	1.750	6.019	1.658	7.678
Xylose	7.132	1.612	4.372	5.520	1.731	5.993	1.622	7.615

Table S2B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S2A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.222	0.252	0.336	0.015	0.474	0.146	0.496	0.271	0.256	0.526	0.645
Altrose	0.224	0.114	0.251	0.055	0.338	0.054	0.346	0.060	0.115	0.174	0.217
Arabinose	0.207	0.303	0.367	0.048	0.510	0.172	0.540	0.336	0.288	0.623	0.764
Galactose	0.223	0.283	0.360	0.030	0.505	0.158	0.530	0.300	0.270	0.569	0.697
Glucose	0.214	0.290	0.360	0.038	0.504	0.176	0.535	0.340	0.302	0.642	0.787
Gulose	0.224	0.285	0.363	0.031	0.509	0.171	0.538	0.325	0.294	0.619	0.759
Lyxose	0.208	0.296	0.362	0.044	0.504	0.174	0.535	0.338	0.294	0.631	0.774
Mannose	0.212	0.298	0.365	0.043	0.510	0.176	0.541	0.341	0.298	0.639	0.784
Ribose	0.208	0.291	0.357	0.041	0.499	0.178	0.531	0.346	0.304	0.650	0.797
Talose	0.203	0.291	0.355	0.044	0.494	0.178	0.527	0.347	0.303	0.650	0.797
Xylose	0.220	0.290	0.364	0.035	0.510	0.172	0.539	0.329	0.294	0.624	0.764
Average	0.215	0.272	0.349	0.039	0.487	0.159	0.514	0.303	0.274	0.577	0.708

Table S3A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the PBE density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-5.981	-2.361	4.171	3.620	2.403	7.118	2.947	10.065
Altrose	-5.910	-2.389	4.149	3.521	2.445	7.184	3.035	10.219
Arabinose	-5.879	-2.139	4.009	3.740	2.149	6.537	2.527	9.064
Galactose	-5.910	-2.166	4.038	3.744	2.178	6.608	2.570	9.178
Glucose	-5.786	-2.336	4.061	3.450	2.390	7.026	2.965	9.991
Gulose	-5.989	-2.360	4.175	3.629	2.401	7.117	2.942	10.059
Lyxose	-6.057	-2.266	4.161	3.791	2.284	6.886	2.725	9.611
Mannose	-5.982	-2.256	4.119	3.726	2.276	6.845	2.726	9.571
Ribose	-5.949	-2.351	4.150	3.599	2.393	7.085	2.935	10.021
Talose	-5.950	-2.347	4.149	3.603	2.388	7.076	2.927	10.003
Xylose	-6.017	-2.331	4.174	3.685	2.364	7.045	2.871	9.916
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	6.366	1.645	4.006	4.721	1.700	5.697	1.691	7.388
Altrose	6.327	1.493	3.910	4.833	1.582	5.420	1.510	6.930
Arabinose	6.366	1.496	3.931	4.870	1.586	5.443	1.512	6.954
Galactose	6.340	1.482	3.911	4.858	1.574	5.407	1.496	6.903
Glucose	6.220	1.656	3.938	4.564	1.699	5.652	1.714	7.366
Gulose	6.436	1.670	4.053	4.767	1.723	5.771	1.718	7.489
Lyxose	6.492	1.605	4.048	4.887	1.677	5.683	1.635	7.318
Mannose	6.365	1.610	3.987	4.754	1.672	5.635	1.648	7.283
Ribose	6.384	1.690	4.037	4.694	1.736	5.783	1.746	7.529
Talose	6.419	1.677	4.048	4.742	1.728	5.776	1.728	7.504
Xylose	6.474	1.651	4.063	4.822	1.711	5.755	1.693	7.448

Table S3B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S3A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.385	0.716	0.813	0.165	1.101	0.704	1.317	1.421	1.256	2.677	3.280
Altrose	0.417	0.895	0.988	0.239	1.312	0.863	1.589	1.764	1.525	3.288	4.031
Arabinose	0.487	0.644	0.807	0.078	1.130	0.563	1.265	1.094	1.016	2.109	2.584
Galactose	0.430	0.684	0.808	0.127	1.114	0.604	1.274	1.201	1.074	2.275	2.788
Glucose	0.434	0.680	0.807	0.123	1.114	0.691	1.317	1.374	1.251	2.625	3.216
Gulose	0.447	0.690	0.823	0.121	1.138	0.678	1.330	1.346	1.224	2.570	3.149
Lyxose	0.435	0.661	0.792	0.113	1.097	0.608	1.259	1.203	1.090	2.293	2.810
Mannose	0.383	0.645	0.750	0.131	1.028	0.604	1.200	1.210	1.078	2.288	2.804
Ribose	0.434	0.661	0.791	0.113	1.095	0.657	1.282	1.302	1.189	2.491	3.052
Talose	0.469	0.670	0.818	0.101	1.139	0.661	1.320	1.300	1.200	2.500	3.063
Xylose	0.457	0.680	0.819	0.112	1.137	0.653	1.316	1.290	1.179	2.469	3.024
Average	0.434	0.693	0.820	0.130	1.128	0.662	1.315	1.319	1.189	2.508	3.073

Table S4A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the PBE0 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-7.541	-1.052	4.297	6.489	1.423	5.399	1.102	6.501
Altrose	-7.494	-1.099	4.296	6.395	1.443	5.434	1.138	6.571
Arabinose	-7.436	-0.876	4.156	6.560	1.316	5.121	0.965	6.086
Galactose	-7.460	-0.901	4.181	6.559	1.332	5.165	0.984	6.149
Glucose	-7.314	-1.023	4.169	6.291	1.381	5.240	1.071	6.312
Gulose	-7.560	-1.053	4.306	6.508	1.425	5.410	1.103	6.513
Lyxose	-7.595	-0.985	4.290	6.611	1.392	5.342	1.052	6.394
Mannose	-7.486	-0.981	4.234	6.505	1.378	5.279	1.045	6.324
Ribose	-7.488	-1.061	4.274	6.427	1.421	5.382	1.107	6.489
Talose	-7.499	-1.054	4.276	6.445	1.419	5.378	1.102	6.480
Xylose	-7.577	-1.026	4.302	6.551	1.412	5.385	1.083	6.468
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.149	1.579	4.364	5.570	1.710	5.950	1.585	7.535
Altrose	7.087	1.483	4.285	5.604	1.638	5.769	1.484	7.254
Arabinose	7.024	1.454	4.239	5.570	1.613	5.694	1.455	7.150
Galactose	7.061	1.457	4.259	5.604	1.618	5.716	1.457	7.174
Glucose	6.925	1.590	4.257	5.336	1.699	5.859	1.602	7.461
Gulose	7.152	1.615	4.383	5.536	1.735	6.008	1.625	7.633
Lyxose	7.215	1.557	4.386	5.658	1.700	5.946	1.561	7.507
Mannose	7.115	1.553	4.334	5.562	1.688	5.891	1.558	7.449
Ribose	7.102	1.626	4.364	5.476	1.739	6.002	1.638	7.640
Talose	7.113	1.619	4.366	5.494	1.735	5.997	1.630	7.627
Xylose	7.170	1.593	4.381	5.578	1.721	5.981	1.600	7.580

Table S4B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S4A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.392	0.527	0.657	0.067	0.919	0.287	0.965	0.551	0.483	1.034	1.267
Altrose	0.407	0.385	0.560	0.011	0.791	0.195	0.815	0.336	0.347	0.682	0.836
Arabinose	0.412	0.579	0.710	0.083	0.990	0.297	1.037	0.574	0.490	1.064	1.304
Galactose	0.399	0.556	0.684	0.078	0.955	0.286	1.000	0.552	0.473	1.025	1.256
Glucose	0.389	0.566	0.687	0.089	0.955	0.317	1.010	0.619	0.530	1.150	1.409
Gulose	0.409	0.563	0.695	0.077	0.971	0.310	1.023	0.599	0.522	1.121	1.373
Lyxose	0.381	0.572	0.687	0.096	0.953	0.308	1.006	0.604	0.508	1.113	1.365
Mannose	0.371	0.572	0.682	0.100	0.943	0.311	0.998	0.613	0.513	1.125	1.380
Ribose	0.386	0.565	0.684	0.090	0.951	0.317	1.006	0.620	0.531	1.151	1.411
Talose	0.386	0.566	0.685	0.090	0.951	0.316	1.007	0.619	0.528	1.147	1.406
Xylose	0.407	0.566	0.697	0.080	0.973	0.309	1.024	0.596	0.516	1.112	1.364
Average	0.394	0.547	0.675	0.078	0.941	0.296	0.990	0.571	0.495	1.066	1.306

Table S5A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the CAM-B3LYP density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-9.021	0.211	4.405	9.232	1.051	4.881	0.476	5.358
Altrose	-8.976	0.145	4.415	9.121	1.069	4.915	0.500	5.415
Arabinose	-8.923	0.360	4.282	9.284	0.987	4.696	0.414	5.110
Galactose	-8.938	0.342	4.298	9.281	0.995	4.720	0.422	5.141
Glucose	-8.790	0.224	4.283	9.014	1.018	4.740	0.457	5.197
Gulose	-9.043	0.196	4.423	9.240	1.059	4.907	0.483	5.390
Lyxose	-9.063	0.257	4.403	9.320	1.040	4.864	0.461	5.326
Mannose	-8.953	0.253	4.350	9.206	1.028	4.806	0.456	5.262
Ribose	-8.959	0.180	4.389	9.140	1.054	4.874	0.485	5.359
Talose	-8.969	0.191	4.389	9.161	1.051	4.870	0.481	5.351
Xylose	-9.052	0.223	4.414	9.276	1.050	4.888	0.473	5.361
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.478	1.586	4.532	5.892	1.743	6.120	1.588	7.708
Altrose	7.424	1.486	4.455	5.939	1.671	5.941	1.486	7.426
Arabinose	7.306	1.479	4.393	5.827	1.656	5.872	1.479	7.352
Galactose	7.512	1.485	4.499	6.027	1.679	5.984	1.485	7.470
Glucose	7.308	1.613	4.460	5.695	1.747	6.080	1.619	7.699
Gulose	7.462	1.640	4.551	5.823	1.779	6.196	1.645	7.842
Lyxose	7.606	1.582	4.594	6.024	1.752	6.177	1.583	7.759
Mannose	7.527	1.578	4.552	5.949	1.742	6.131	1.579	7.710
Ribose	7.495	1.646	4.571	5.849	1.786	6.222	1.652	7.874
Talose	7.479	1.639	4.559	5.840	1.780	6.204	1.645	7.849
Xylose	7.502	1.615	4.559	5.887	1.765	6.177	1.618	7.795

Table S5B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S5A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	1.543	1.797	2.368	0.127	3.339	0.692	3.413	1.239	1.112	2.350	2.880
Altrose	1.552	1.631	2.251	0.039	3.183	0.602	3.239	1.025	0.986	2.011	2.463
Arabinose	1.617	1.840	2.449	0.111	3.457	0.669	3.523	1.177	1.065	2.242	2.747
Galactose	1.426	1.827	2.318	0.201	3.253	0.684	3.331	1.264	1.064	2.328	2.855
Glucose	1.482	1.837	2.360	0.178	3.319	0.729	3.402	1.340	1.162	2.502	3.067
Gulose	1.581	1.836	2.423	0.128	3.417	0.720	3.494	1.290	1.162	2.452	3.004
Lyxose	1.457	1.839	2.346	0.191	3.296	0.711	3.377	1.312	1.122	2.434	2.984
Mannose	1.426	1.830	2.320	0.202	3.257	0.714	3.340	1.325	1.123	2.448	3.002
Ribose	1.464	1.826	2.341	0.181	3.290	0.732	3.376	1.348	1.167	2.516	3.084
Talose	1.490	1.831	2.360	0.170	3.321	0.728	3.404	1.334	1.164	2.498	3.062
Xylose	1.550	1.838	2.404	0.144	3.388	0.714	3.466	1.289	1.145	2.434	2.983
Average	1.508	1.812	2.358	0.152	3.320	0.700	3.397	1.268	1.116	2.383	2.921

Table S6A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the LC-wPBE density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-10.343	1.482	4.431	11.825	0.830	4.615	0.184	4.799
Altrose	-10.306	1.407	4.450	11.713	0.845	4.648	0.198	4.845
Arabinose	-10.230	1.639	4.296	11.869	0.777	4.444	0.149	4.593
Galactose	-10.249	1.608	4.320	11.858	0.787	4.476	0.155	4.631
Glucose	-10.092	1.494	4.299	11.586	0.797	4.469	0.170	4.639
Gulose	-10.373	1.467	4.453	11.840	0.837	4.641	0.188	4.830
Lyxose	-10.369	1.531	4.419	11.810	0.821	4.594	0.175	4.770
Mannose	-10.252	1.526	4.363	11.778	0.808	4.534	0.171	4.705
Ribose	-10.261	1.453	4.404	11.714	0.828	4.590	0.186	4.776
Talose	-10.279	1.464	4.408	11.743	0.827	4.592	0.185	4.777
Xylose	-10.374	1.494	4.440	11.868	0.831	4.623	0.183	4.806
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.641	1.669	4.655	5.972	1.814	6.329	1.674	8.004
Altrose	7.597	1.592	4.594	6.005	1.758	6.188	1.593	7.781
Arabinose	7.412	1.554	4.483	5.857	1.716	6.039	1.556	7.595
Galactose	7.817	1.569	4.693	6.248	1.763	6.262	1.569	7.832
Glucose	7.550	1.697	4.623	5.852	1.826	6.330	1.707	8.037
Gulose	7.617	1.727	4.672	5.890	1.853	6.410	1.738	8.148
Lyxose	7.838	1.663	4.751	6.175	1.828	6.416	1.666	8.082
Mannose	7.772	1.658	4.715	6.114	1.818	6.375	1.660	8.035
Ribose	7.682	1.725	4.703	5.958	1.857	6.437	1.734	8.171
Talose	7.698	1.719	4.709	5.978	1.854	6.436	1.723	8.164
Xylose	7.713	1.701	4.707	6.012	1.842	6.414	1.707	8.120

Table S6B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S6A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	2.702	3.151	4.151	0.224	5.853	0.984	5.939	1.715	1.490	3.205	3.929
Altrose	2.710	2.998	4.041	0.144	5.708	0.912	5.782	1.540	1.395	2.935	3.597
Arabinose	2.818	3.193	4.259	0.188	6.012	0.938	6.087	1.595	1.407	3.002	3.679
Galactose	2.432	3.177	4.001	0.373	5.609	0.976	5.706	1.787	1.414	3.201	3.929
Glucose	2.543	3.192	4.081	0.324	5.734	1.029	5.835	1.861	1.537	3.398	4.168
Gulose	2.756	3.194	4.219	0.219	5.950	1.016	6.040	1.769	1.550	3.319	4.067
Lyxose	2.531	3.194	4.075	0.332	5.725	1.007	5.822	1.822	1.490	3.312	4.064
Mannose	2.481	3.184	4.036	0.352	5.664	1.010	5.764	1.841	1.490	3.331	4.087
Ribose	2.579	3.177	4.092	0.299	5.756	1.029	5.855	1.847	1.548	3.395	4.164
Talose	2.582	3.183	4.098	0.301	5.765	1.027	5.863	1.844	1.543	3.388	4.154
Xylose	2.661	3.194	4.158	0.267	5.856	1.012	5.948	1.791	1.524	3.315	4.064
Average	2.618	3.167	4.110	0.275	5.785	0.994	5.877	1.765	1.490	3.255	3.991

Table S7A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the wB97 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-10.263	1.597	4.333	11.860	0.792	4.491	0.158	4.649
Altrose	-10.236	1.521	4.358	11.757	0.807	4.529	0.171	4.700
Arabinose	-10.152	1.728	4.212	11.880	0.747	4.342	0.130	4.472
Galactose	-10.163	1.704	4.230	11.867	0.754	4.364	0.134	4.498
Glucose	-10.018	1.613	4.202	11.631	0.759	4.346	0.144	4.490
Gulose	-10.309	1.582	4.364	11.890	0.801	4.526	0.163	4.689
Lyxose	-10.272	1.641	4.315	11.913	0.782	4.465	0.150	4.615
Mannose	-10.167	1.635	4.266	11.802	0.771	4.413	0.147	4.559
Ribose	-10.171	1.569	4.301	11.740	0.788	4.460	0.159	4.619
Talose	-10.206	1.577	4.315	11.783	0.790	4.474	0.159	4.633
Xylose	-10.293	1.616	4.338	11.909	0.790	4.494	0.156	4.649
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.587	1.506	4.547	6.081	1.700	6.053	1.506	7.559
Altrose	7.543	1.399	4.471	6.144	1.627	5.873	1.402	7.275
Arabinose	7.363	1.410	4.387	5.953	1.616	5.798	1.411	7.209
Galactose	7.639	1.425	4.532	6.214	1.653	5.960	1.428	7.388
Glucose	7.484	1.529	4.506	5.955	1.705	6.035	1.529	7.564
Gulose	7.567	1.562	4.564	6.005	1.734	6.126	1.562	7.689
Lyxose	7.766	1.502	4.634	6.264	1.714	6.137	1.503	7.639
Mannose	7.710	1.499	4.605	6.210	1.707	6.105	1.500	7.604
Ribose	7.684	1.557	4.621	6.127	1.742	6.178	1.557	7.735
Talose	7.659	1.556	4.607	6.103	1.739	6.163	1.556	7.719
Xylose	7.657	1.529	4.593	6.128	1.721	6.121	1.529	7.650

Table S7B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S7A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	2.676	3.102	4.097	0.213	5.779	0.908	5.854	1.561	1.348	2.909	3.566
Altrose	2.693	2.920	3.972	0.114	5.613	0.819	5.673	1.344	1.231	2.575	3.155
Arabinose	2.789	3.138	4.198	0.175	5.927	0.870	5.993	1.456	1.281	2.737	3.355
Galactose	2.524	3.129	4.020	0.303	5.654	0.899	5.733	1.596	1.294	2.890	3.546
Glucose	2.534	3.142	4.036	0.304	5.676	0.946	5.762	1.689	1.385	3.074	3.771
Gulose	2.742	3.143	4.171	0.201	5.885	0.934	5.962	1.600	1.399	3.000	3.676
Lyxose	2.506	3.143	4.020	0.319	5.649	0.933	5.734	1.671	1.353	3.024	3.711
Mannose	2.457	3.134	3.983	0.339	5.592	0.936	5.680	1.692	1.353	3.045	3.737
Ribose	2.487	3.126	3.995	0.320	5.614	0.955	5.703	1.718	1.398	3.117	3.824
Talose	2.547	3.133	4.037	0.293	5.680	0.949	5.766	1.690	1.397	3.086	3.786
Xylose	2.636	3.145	4.104	0.254	5.781	0.931	5.861	1.627	1.373	3.000	3.679
Average	2.599	3.114	4.058	0.258	5.713	0.916	5.793	1.604	1.347	2.951	3.619

Table S8A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the wB97X density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-10.016	1.337	4.339	11.353	0.829	4.538	0.198	4.736
Altrose	-9.988	1.268	4.360	11.256	0.844	4.572	0.212	4.785
Arabinose	-9.912	1.475	4.219	11.387	0.782	4.384	0.165	4.549
Galactose	-9.921	1.450	4.235	11.371	0.789	4.406	0.171	4.576
Glucose	-9.778	1.354	4.212	11.132	0.797	4.395	0.183	4.578
Gulose	-10.046	1.322	4.362	11.369	0.837	4.565	0.203	4.768
Lyxose	-10.036	1.382	4.327	11.418	0.820	4.517	0.190	4.707
Mannose	-9.927	1.379	4.274	11.306	0.808	4.459	0.185	4.645
Ribose	-9.934	1.311	4.311	11.245	0.826	4.511	0.200	4.711
Talose	-9.964	1.318	4.323	11.282	0.828	4.523	0.200	4.724
Xylose	-10.043	1.354	4.345	11.397	0.828	4.541	0.196	4.737
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.528	1.508	4.518	6.020	1.695	6.026	1.508	7.534
Altrose	7.484	1.407	4.445	6.077	1.626	5.854	1.409	7.263
Arabinose	7.324	1.411	4.368	5.913	1.613	5.779	1.412	7.191
Galactose	7.626	1.424	4.525	6.202	1.651	5.951	1.427	7.378
Glucose	7.395	1.531	4.463	5.864	1.698	5.995	1.532	7.527
Gulose	7.511	1.563	4.537	5.948	1.731	6.101	1.564	7.666
Lyxose	7.682	1.505	4.594	6.177	1.708	6.099	1.505	7.604
Mannose	7.619	1.501	4.560	6.118	1.699	6.061	1.501	7.562
Ribose	7.588	1.561	4.574	6.027	1.736	6.136	1.562	7.697
Talose	7.573	1.560	4.566	6.014	1.734	6.127	1.560	7.687
Xylose	7.564	1.534	4.549	6.030	1.716	6.082	1.534	7.616

Table S8B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S8A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	2.488	2.845	3.780	0.179	5.333	0.866	5.406	4.538	0.198	2.798	5.335
Altrose	2.505	2.675	3.664	0.085	5.179	0.781	5.239	4.572	0.212	2.478	5.205
Arabinose	2.588	2.886	3.876	0.149	5.473	0.831	5.538	4.384	0.165	2.642	5.121
Galactose	2.295	2.874	3.678	0.290	5.170	0.862	5.249	4.406	0.171	2.802	5.224
Glucose	2.382	2.885	3.742	0.251	5.268	0.902	5.350	4.395	0.183	2.948	5.296
Gulose	2.535	2.886	3.841	0.175	5.421	0.894	5.497	4.565	0.203	2.897	5.411
Lyxose	2.354	2.887	3.725	0.266	5.241	0.888	5.322	4.517	0.190	2.897	5.370
Mannose	2.308	2.880	3.691	0.286	5.188	0.891	5.272	4.459	0.185	2.917	5.332
Ribose	2.346	2.872	3.709	0.263	5.218	0.910	5.304	4.511	0.200	2.986	5.414
Talose	2.391	2.877	3.741	0.243	5.269	0.905	5.351	4.523	0.200	2.963	5.411
Xylose	2.480	2.887	3.806	0.204	5.367	0.887	5.444	4.541	0.196	2.879	5.380
Average	2.425	2.860	3.750	0.217	5.284	0.874	5.361	4.492	0.191	2.837	5.318

Table S9A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the wB97XD density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-9.454	0.865	4.295	10.318	0.894	4.580	0.285	4.865
Altrose	-9.429	0.803	4.313	10.232	0.909	4.614	0.301	4.915
Arabinose	-9.359	1.014	4.172	10.373	0.839	4.412	0.240	4.653
Galactose	-9.376	0.985	4.196	10.361	0.849	4.444	0.249	4.693
Glucose	-9.225	0.889	4.168	10.114	0.859	4.434	0.266	4.700
Gulose	-9.487	0.855	4.316	10.343	0.901	4.606	0.290	4.895
Lyxose	-9.473	0.915	4.279	10.389	0.881	4.551	0.272	4.823
Mannose	-9.376	0.916	4.230	10.292	0.869	4.497	0.267	4.763
Ribose	-9.373	0.847	4.263	10.220	0.889	4.548	0.285	4.834
Talose	-9.407	0.852	4.277	10.259	0.892	4.563	0.286	4.849
Xylose	-9.484	0.885	4.299	10.369	0.891	4.580	0.281	4.862
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.380	1.494	4.437	5.887	1.672	5.931	1.494	7.424
Altrose	7.329	1.393	4.361	5.936	1.602	5.756	1.395	7.150
Arabinose	7.209	1.392	4.300	5.817	1.590	5.693	1.393	7.085
Galactose	7.378	1.402	4.390	5.976	1.613	5.794	1.404	7.198
Glucose	7.182	1.510	4.346	5.672	1.665	5.858	1.512	7.369
Gulose	7.373	1.542	4.458	5.830	1.704	6.001	1.544	7.545
Lyxose	7.454	1.487	4.470	5.966	1.675	5.958	1.487	7.445
Mannose	7.395	1.482	4.439	5.913	1.666	5.921	1.482	7.403
Ribose	7.352	1.544	4.448	5.808	1.703	5.994	1.546	7.540
Talose	7.369	1.543	4.456	5.826	1.704	6.001	1.544	7.545
Xylose	7.374	1.515	4.445	5.860	1.686	5.960	1.515	7.475

Table S9B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S9A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	2.074	2.358	3.140	0.142	4.432	0.778	4.502	2.908	1.209	2.559	4.058
Altrose	2.100	2.197	3.039	0.048	4.297	0.693	4.353	3.012	1.094	2.236	3.907
Arabinose	2.150	2.406	3.227	0.128	4.556	0.751	4.619	2.823	1.152	2.433	3.901
Galactose	1.998	2.388	3.113	0.195	4.386	0.763	4.456	2.832	1.155	2.505	3.953
Glucose	2.043	2.399	3.151	0.178	4.442	0.806	4.518	2.769	1.246	2.670	4.043
Gulose	2.115	2.398	3.197	0.141	4.512	0.803	4.586	2.901	1.254	2.650	4.125
Lyxose	2.020	2.403	3.139	0.191	4.422	0.794	4.497	2.876	1.215	2.622	4.077
Mannose	1.981	2.399	3.111	0.209	4.380	0.797	4.456	2.831	1.216	2.640	4.057
Ribose	2.021	2.391	3.131	0.185	4.412	0.814	4.490	2.845	1.260	2.706	4.124
Talose	2.038	2.395	3.145	0.179	4.433	0.812	4.510	2.859	1.259	2.696	4.126
Xylose	2.110	2.400	3.195	0.145	4.510	0.794	4.581	2.895	1.234	2.614	4.091
Average	2.059	2.376	3.144	0.158	4.435	0.782	4.506	2.868	1.208	2.575	4.042

Table S10A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the HSEh1PBE density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-7.149	-1.455	4.302	5.694	1.625	5.758	1.455	7.213
Altrose	-7.098	-1.502	4.300	5.596	1.652	5.804	1.504	7.307
Arabinose	-7.045	-1.278	4.161	5.767	1.501	5.443	1.282	6.726
Galactose	-7.069	-1.303	4.186	5.766	1.520	5.493	1.307	6.800
Glucose	-6.924	-1.426	4.175	5.498	1.585	5.601	1.426	7.028
Gulose	-7.169	-1.456	4.312	5.713	1.628	5.768	1.456	7.224
Lyxose	-7.205	-1.385	4.295	5.819	1.585	5.681	1.386	7.067
Mannose	-7.097	-1.382	4.239	5.715	1.572	5.622	1.382	7.004
Ribose	-7.097	-1.463	4.280	5.635	1.625	5.743	1.463	7.206
Talose	-7.108	-1.455	4.281	5.653	1.621	5.737	1.455	7.192
Xylose	-7.184	-1.428	4.306	5.756	1.611	5.734	1.428	7.162
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.124	1.590	4.357	5.534	1.715	5.954	1.597	7.551
Altrose	7.066	1.493	4.280	5.573	1.643	5.774	1.495	7.269
Arabinose	7.011	1.464	4.237	5.547	1.619	5.702	1.465	7.167
Galactose	7.043	1.467	4.255	5.577	1.623	5.722	1.467	7.190
Glucose	6.907	1.600	4.253	5.307	1.704	5.867	1.614	7.481
Gulose	7.137	1.626	4.381	5.511	1.742	6.018	1.637	7.655
Lyxose	7.191	1.566	4.379	5.625	1.704	5.950	1.571	7.521
Mannose	7.086	1.563	4.324	5.523	1.693	5.893	1.569	7.462
Ribose	7.083	1.637	4.360	5.447	1.745	6.010	1.650	7.661
Talose	7.095	1.630	4.362	5.465	1.741	6.005	1.642	7.647
Xylose	7.155	1.602	4.379	5.553	1.726	5.989	1.611	7.600

Table S10B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S10A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.025	0.134	0.137	0.054	0.160	0.090	0.191	0.196	0.142	0.338	0.309
Altrose	0.032	0.009	0.033	0.020	0.023	0.009	0.032	0.029	0.009	0.038	0.044
Arabinose	0.034	0.186	0.189	0.076	0.220	0.117	0.261	0.259	0.183	0.442	0.411
Galactose	0.026	0.163	0.165	0.068	0.189	0.103	0.226	0.229	0.161	0.390	0.360
Glucose	0.017	0.174	0.175	0.078	0.191	0.119	0.239	0.266	0.187	0.453	0.403
Gulose	0.032	0.170	0.173	0.069	0.202	0.114	0.242	0.250	0.181	0.431	0.392
Lyxose	0.013	0.181	0.181	0.084	0.194	0.119	0.243	0.269	0.185	0.453	0.407
Mannose	0.011	0.181	0.181	0.085	0.192	0.120	0.242	0.271	0.187	0.458	0.409
Ribose	0.014	0.174	0.175	0.080	0.188	0.120	0.237	0.267	0.187	0.455	0.403
Talose	0.013	0.175	0.175	0.081	0.187	0.120	0.237	0.268	0.187	0.455	0.404
Xylose	0.029	0.174	0.177	0.073	0.203	0.116	0.245	0.255	0.183	0.438	0.398
Average	0.022	0.157	0.160	0.070	0.177	0.104	0.218	0.233	0.163	0.396	0.358

Table S11A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M05 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-7.491	-0.775	4.133	6.716	1.272	5.030	0.897	5.926
Altrose	-7.467	-0.822	4.144	6.646	1.292	5.072	0.928	6.000
Arabinose	-7.369	-0.639	4.004	6.730	1.191	4.805	0.801	5.605
Galactose	-7.377	-0.647	4.012	6.730	1.196	4.818	0.806	5.624
Glucose	-7.277	-0.756	4.016	6.522	1.237	4.889	0.873	5.762
Gulose	-7.506	-0.787	4.146	6.719	1.279	5.052	0.905	5.957
Lyxose	-7.560	-0.738	4.149	6.821	1.262	5.024	0.875	5.900
Mannose	-7.443	-0.737	4.090	6.707	1.247	4.958	0.868	5.827
Ribose	-7.434	-0.803	4.119	6.631	1.279	5.032	0.913	5.945
Talose	-7.444	-0.798	4.121	6.646	1.278	5.031	0.910	5.942
Xylose	-7.528	-0.764	4.146	6.765	1.270	5.037	0.891	5.927
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.082	1.397	4.239	5.684	1.581	5.637	1.397	7.034
Altrose	7.054	1.269	4.162	5.786	1.497	5.436	1.274	6.710
Arabinose	6.968	1.289	4.129	5.679	1.501	5.421	1.292	6.714
Galactose	6.968	1.301	4.134	5.667	1.508	5.438	1.303	6.741
Glucose	6.866	1.408	4.137	5.458	1.568	5.546	1.409	6.955
Gulose	7.094	1.437	4.265	5.658	1.608	5.702	1.437	7.139
Lyxose	7.162	1.387	4.274	5.775	1.582	5.662	1.387	7.049
Mannose	7.041	1.384	4.213	5.657	1.569	5.597	1.385	6.982
Ribose	7.042	1.448	4.245	5.594	1.610	5.693	1.448	7.141
Talose	7.048	1.443	4.246	5.605	1.608	5.690	1.444	7.133
Xylose	7.113	1.415	4.264	5.698	1.595	5.678	1.415	7.093

Table S11B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S11A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.410	0.622	0.745	0.106	1.032	0.309	1.082	0.607	0.501	1.107	1.358
Altrose	0.413	0.447	0.609	0.017	0.860	0.204	0.884	0.364	0.347	0.710	0.870
Arabinose	0.401	0.650	0.764	0.125	1.051	0.310	1.103	0.617	0.492	1.108	1.360
Galactose	0.409	0.654	0.771	0.123	1.063	0.313	1.115	0.620	0.497	1.117	1.371
Glucose	0.411	0.653	0.771	0.121	1.064	0.331	1.121	0.656	0.536	1.192	1.463
Gulose	0.412	0.650	0.769	0.119	1.061	0.329	1.117	0.650	0.531	1.182	1.450
Lyxose	0.398	0.649	0.761	0.125	1.046	0.320	1.101	0.637	0.512	1.149	1.410
Mannose	0.402	0.648	0.762	0.123	1.050	0.322	1.105	0.639	0.516	1.155	1.417
Ribose	0.392	0.644	0.754	0.126	1.036	0.331	1.095	0.661	0.535	1.196	1.467
Talose	0.396	0.645	0.757	0.125	1.041	0.330	1.100	0.658	0.533	1.192	1.462
Xylose	0.415	0.651	0.772	0.118	1.066	0.325	1.121	0.642	0.524	1.166	1.430
Average	0.405	0.629	0.749	0.112	1.034	0.311	1.086	0.614	0.502	1.116	1.369

Table S12A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M052X density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-9.233	0.148	4.543	9.381	1.100	5.057	0.515	5.572
Altrose	-9.219	0.071	4.574	9.290	1.126	5.120	0.546	5.666
Arabinose	-9.116	0.278	4.419	9.393	1.039	4.876	0.456	5.332
Galactose	-9.138	0.239	4.449	9.377	1.056	4.922	0.473	5.394
Glucose	-8.993	0.172	4.410	9.165	1.061	4.900	0.490	5.390
Gulose	-9.276	0.135	4.571	9.412	1.110	5.093	0.523	5.616
Lyxose	-9.215	0.202	4.506	9.417	1.078	4.998	0.492	5.489
Mannose	-9.104	0.199	4.453	9.303	1.066	4.939	0.486	5.426
Ribose	-9.140	0.130	4.505	9.270	1.095	5.021	0.516	5.538
Talose	-9.179	0.136	4.521	9.315	1.097	5.037	0.516	5.553
Xylose	-9.260	0.169	4.546	9.429	1.096	5.054	0.508	5.562
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.731	1.574	4.653	6.156	1.758	6.227	1.575	7.802
Altrose	7.684	1.489	4.587	6.195	1.698	6.076	1.490	7.566
Arabinose	7.490	1.489	4.489	6.001	1.679	5.978	1.489	7.467
Galactose	7.726	1.505	4.615	6.221	1.712	6.121	1.505	7.626
Glucose	7.559	1.590	4.574	5.969	1.753	6.165	1.591	7.757
Gulose	7.716	1.628	4.672	6.088	1.793	6.302	1.630	7.932
Lyxose	7.809	1.568	4.688	6.241	1.761	6.256	1.568	7.823
Mannose	7.748	1.566	4.657	6.182	1.754	6.223	1.566	7.789
Ribose	7.724	1.626	4.675	6.098	1.792	6.303	1.628	7.931
Talose	7.742	1.625	4.684	6.117	1.793	6.310	1.627	7.937
Xylose	7.750	1.596	4.673	6.154	1.775	6.270	1.597	7.867

Table S12B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S12A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	1.502	1.722	2.286	0.110	3.225	0.658	3.293	1.170	1.060	2.230	2.732
Altrose	1.535	1.560	2.189	0.012	3.095	0.572	3.147	0.956	0.944	1.900	2.327
Arabinose	1.626	1.767	2.401	0.070	3.392	0.640	3.453	1.103	1.033	2.135	2.616
Galactose	1.412	1.744	2.244	0.166	3.156	0.657	3.228	1.199	1.033	2.232	2.736
Glucose	1.435	1.762	2.272	0.164	3.197	0.691	3.275	1.265	1.101	2.366	2.900
Gulose	1.560	1.763	2.355	0.102	3.324	0.683	3.395	1.209	1.107	2.317	2.838
Lyxose	1.406	1.770	2.260	0.182	3.176	0.683	3.253	1.258	1.076	2.334	2.861
Mannose	1.356	1.764	2.226	0.204	3.121	0.688	3.202	1.284	1.080	2.363	2.898
Ribose	1.416	1.756	2.256	0.170	3.172	0.697	3.253	1.282	1.112	2.393	2.933
Talose	1.436	1.761	2.273	0.163	3.198	0.696	3.277	1.273	1.111	2.384	2.922
Xylose	1.510	1.765	2.323	0.128	3.275	0.679	3.347	1.217	1.089	2.306	2.825
Average	1.472	1.740	2.280	0.134	3.212	0.668	3.284	1.201	1.068	2.269	2.781

Table S13A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M06 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-7.658	-1.004	4.331	6.655	1.409	5.400	1.069	6.469
Altrose	-7.617	-1.065	4.341	6.552	1.438	5.456	1.115	6.571
Arabinose	-7.544	-0.865	4.204	6.679	1.323	5.166	0.962	6.128
Galactose	-7.572	-0.884	4.228	6.689	1.336	5.205	0.977	6.181
Glucose	-7.470	-0.984	4.227	6.486	1.378	5.274	1.047	6.321
Gulose	-7.676	-1.024	4.350	6.652	1.422	5.436	1.086	6.521
Lyxose	-7.741	-0.948	4.344	6.794	1.389	5.375	1.031	6.405
Mannose	-7.611	-0.944	4.277	6.667	1.372	5.299	1.022	6.321
Ribose	-7.618	-1.026	4.322	6.591	1.417	5.407	1.085	6.491
Talose	-7.634	-1.021	4.327	6.612	1.416	5.409	1.082	6.491
Xylose	-7.707	-0.992	4.350	6.716	1.409	5.412	1.062	6.474
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.273	1.504	4.389	5.769	1.669	5.894	1.505	7.399
Altrose	7.223	1.396	4.310	5.828	1.593	5.706	1.396	7.102
Arabinose	7.154	1.412	4.283	5.743	1.597	5.695	1.412	7.107
Galactose	7.181	1.415	4.298	5.766	1.602	5.713	1.415	7.128
Glucose	7.085	1.518	4.301	5.567	1.662	5.822	1.521	7.343
Gulose	7.283	1.555	4.419	5.728	1.705	5.977	1.558	7.535
Lyxose	7.373	1.491	4.432	5.882	1.670	5.923	1.491	7.414
Mannose	7.234	1.487	4.361	5.747	1.654	5.849	1.488	7.336
Ribose	7.242	1.562	4.402	5.681	1.705	5.967	1.565	7.532
Talose	7.258	1.558	4.408	5.700	1.704	5.969	1.561	7.530
Xylose	7.314	1.526	4.420	5.788	1.688	5.947	1.527	7.474

Table S13B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S13A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.385	0.501	0.632	0.058	0.886	0.260	0.925	0.494	0.436	0.930	1.139
Altrose	0.394	0.331	0.514	0.031	0.725	0.155	0.742	0.250	0.281	0.531	0.651
Arabinose	0.390	0.547	0.672	0.079	0.937	0.274	0.979	0.529	0.450	0.979	1.200
Galactose	0.392	0.531	0.660	0.070	0.923	0.266	0.963	0.508	0.438	0.947	1.161
Glucose	0.386	0.534	0.658	0.074	0.919	0.284	0.965	0.548	0.474	1.022	1.253
Gulose	0.393	0.531	0.660	0.069	0.924	0.282	0.968	0.541	0.472	1.013	1.242
Lyxose	0.368	0.543	0.656	0.088	0.911	0.281	0.958	0.548	0.460	1.009	1.237
Mannose	0.377	0.544	0.661	0.083	0.920	0.282	0.966	0.549	0.466	1.015	1.244
Ribose	0.375	0.535	0.654	0.080	0.911	0.289	0.959	0.560	0.480	1.040	1.276
Talose	0.375	0.537	0.655	0.081	0.912	0.288	0.960	0.560	0.479	1.040	1.275
Xylose	0.394	0.534	0.663	0.070	0.928	0.279	0.971	0.535	0.465	1.000	1.226
Average	0.384	0.515	0.644	0.071	0.900	0.267	0.941	0.511	0.446	0.957	1.173

Table S14A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M06L density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-6.274	-1.927	4.100	4.347	1.934	6.189	2.089	8.278
Altrose	-6.228	-1.949	4.089	4.278	1.954	6.219	2.130	8.349
Arabinose	-6.173	-1.747	3.960	4.427	1.772	5.800	1.840	7.639
Galactose	-6.189	-1.781	3.985	4.407	1.802	5.871	1.886	7.757
Glucose	-6.081	-1.878	3.979	4.203	1.884	6.020	2.041	8.061
Gulose	-6.274	-1.921	4.098	4.353	1.929	6.179	2.081	8.260
Lyxose	-6.370	-1.824	4.097	4.546	1.846	6.024	1.928	7.952
Mannose	-6.255	-1.825	4.040	4.430	1.842	5.980	1.941	7.921
Ribose	-6.214	-1.895	4.055	4.318	1.903	6.104	2.049	8.153
Talose	-6.244	-1.896	4.070	4.348	1.905	6.117	2.047	8.163
Xylose	-6.294	-1.882	4.088	4.412	1.894	6.107	2.019	8.127
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	6.604	1.432	4.018	5.173	1.560	5.453	1.435	6.889
Altrose	6.569	1.321	3.945	5.248	1.483	5.267	1.321	6.588
Arabinose	6.555	1.318	3.936	5.237	1.479	5.254	1.318	6.571
Galactose	6.541	1.309	3.925	5.232	1.473	5.235	1.309	6.544
Glucose	6.457	1.417	3.937	5.040	1.538	5.359	1.422	6.780
Gulose	6.646	1.454	4.050	5.192	1.580	5.509	1.459	6.967
Lyxose	6.736	1.381	4.058	5.355	1.538	5.440	1.381	6.821
Mannose	6.568	1.385	3.977	5.183	1.525	5.363	1.387	6.750
Ribose	6.593	1.450	4.021	5.142	1.572	5.477	1.455	6.932
Talose	6.629	1.447	4.038	5.182	1.573	5.489	1.451	6.940
Xylose	6.680	1.420	4.050	5.260	1.559	5.473	1.422	6.895

Table S14B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S14A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.331	0.495	0.595	0.082	0.826	0.373	0.910	0.736	0.654	1.389	1.470
Altrose	0.341	0.628	0.715	0.144	0.969	0.471	1.087	0.953	0.809	1.761	1.923
Arabinose	0.381	0.429	0.574	0.024	0.810	0.292	0.862	0.546	0.522	1.068	1.105
Galactose	0.352	0.472	0.589	0.060	0.824	0.329	0.889	0.636	0.577	1.213	1.267
Glucose	0.376	0.461	0.595	0.043	0.837	0.346	0.907	0.661	0.619	1.280	1.344
Gulose	0.371	0.467	0.597	0.048	0.839	0.349	0.910	0.670	0.622	1.292	1.358
Lyxose	0.366	0.443	0.575	0.038	0.809	0.308	0.866	0.584	0.546	1.131	1.175
Mannose	0.313	0.439	0.540	0.063	0.753	0.316	0.819	0.617	0.554	1.171	1.220
Ribose	0.379	0.445	0.585	0.033	0.824	0.331	0.889	0.627	0.594	1.221	1.277
Talose	0.385	0.449	0.592	0.032	0.834	0.332	0.898	0.628	0.595	1.223	1.279
Xylose	0.386	0.462	0.602	0.038	0.848	0.334	0.912	0.635	0.597	1.232	1.289
Average	0.362	0.472	0.596	0.055	0.834	0.344	0.904	0.663	0.608	1.271	1.337

Table S15A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M062X density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-9.077	0.068	4.504	9.146	1.109	5.042	0.538	5.580
Altrose	-9.060	0.008	4.526	9.068	1.129	5.089	0.563	5.651
Arabinose	-8.976	0.199	4.388	9.175	1.049	4.866	0.478	5.344
Galactose	-8.980	0.160	4.410	9.140	1.064	4.904	0.494	5.398
Glucose	-8.846	0.106	4.370	8.952	1.067	4.878	0.508	5.386
Gulose	-9.129	0.067	4.531	9.196	1.116	5.073	0.542	5.614
Lyxose	-9.074	0.132	4.471	9.206	1.086	4.982	0.511	5.494
Mannose	-8.962	0.124	4.419	9.086	1.074	4.926	0.507	5.434
Ribose	-8.989	0.064	4.462	9.053	1.100	4.997	0.534	5.531
Talose	-9.027	0.069	4.479	9.096	1.103	5.013	0.534	5.548
Xylose	-9.119	0.108	4.505	9.227	1.100	5.029	0.524	5.553
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.646	1.521	4.583	6.125	1.715	6.104	1.521	7.625
Altrose	7.599	1.426	4.513	6.173	1.650	5.941	1.429	7.370
Arabinose	7.439	1.440	4.440	5.999	1.643	5.880	1.441	7.321
Galactose	7.624	1.453	4.538	6.171	1.669	5.992	1.454	7.446
Glucose	7.480	1.524	4.502	5.956	1.702	6.027	1.524	7.551
Gulose	7.637	1.564	4.601	6.073	1.742	6.165	1.564	7.729
Lyxose	7.736	1.506	4.621	6.230	1.714	6.128	1.507	7.634
Mannose	7.676	1.507	4.592	6.168	1.709	6.099	1.508	7.607
Ribose	7.640	1.560	4.600	6.079	1.740	6.160	1.560	7.721
Talose	7.661	1.561	4.611	6.101	1.743	6.172	1.561	7.733
Xylose	7.687	1.524	4.605	6.163	1.721	6.130	1.524	7.654

Table S15B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S15A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	1.431	1.589	2.139	0.079	3.020	2.824	4.136	1.062	0.983	2.045	2.505
Altrose	1.461	1.435	2.047	0.013	2.895	2.779	4.013	0.853	0.866	1.719	2.105
Arabinose	1.537	1.640	2.247	0.051	3.176	2.692	4.164	1.014	0.963	1.976	2.421
Galactose	1.356	1.612	2.107	0.128	2.969	2.733	4.037	1.088	0.960	2.048	2.510
Glucose	1.366	1.630	2.127	0.132	2.996	2.768	4.081	1.148	1.016	2.165	2.653
Gulose	1.492	1.631	2.211	0.070	3.123	2.859	4.235	1.092	1.023	2.115	2.591
Lyxose	1.338	1.638	2.115	0.150	2.976	2.800	4.089	1.145	0.995	2.141	2.624
Mannose	1.286	1.632	2.078	0.173	2.918	2.783	4.036	1.173	1.000	2.173	2.664
Ribose	1.349	1.624	2.111	0.137	2.973	2.840	4.114	1.164	1.026	2.190	2.684
Talose	1.365	1.630	2.126	0.132	2.995	2.845	4.133	1.159	1.027	2.185	2.678
Xylose	1.432	1.632	2.172	0.100	3.065	2.821	4.166	1.100	1.000	2.101	2.574
Average	1.401	1.608	2.135	0.106	3.010	2.795	4.110	1.091	0.987	2.078	2.546

Table S16A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M06HF density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-11.369	1.676	4.847	13.046	0.900	5.039	0.193	5.232
Altrose	-11.392	1.574	4.909	12.966	0.929	5.124	0.214	5.338
Arabinose	-11.264	1.779	4.743	13.043	0.862	4.911	0.168	5.080
Galactose	-11.299	1.775	4.762	13.074	0.867	4.932	0.171	5.103
Glucose	-11.049	1.711	4.669	12.760	0.854	4.841	0.172	5.012
Gulose	-11.467	1.678	4.895	13.145	0.911	5.091	0.197	5.288
Lyxose	-11.297	1.720	4.788	13.017	0.881	4.969	0.181	5.150
Mannose	-11.134	1.697	4.718	12.832	0.867	4.896	0.178	5.074
Ribose	-11.268	1.626	4.821	12.894	0.901	5.019	0.198	5.216
Talose	-11.280	1.638	4.821	12.918	0.899	5.017	0.196	5.213
Xylose	-11.368	1.719	4.824	13.086	0.889	5.009	0.184	5.193
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	8.230	1.654	4.942	6.576	1.857	6.596	1.654	8.250
Altrose	8.205	1.567	4.886	6.638	1.798	6.455	1.568	8.023
Arabinose	7.757	1.596	4.676	6.160	1.775	6.273	1.597	7.870
Galactose	8.254	1.587	4.921	6.666	1.816	6.509	1.588	8.097
Glucose	7.963	1.656	4.809	6.307	1.834	6.466	1.657	8.123
Gulose	8.225	1.694	4.960	6.531	1.883	6.655	1.695	8.350
Lyxose	8.205	1.641	4.923	6.564	1.846	6.563	1.641	8.204
Mannose	8.161	1.636	4.899	6.525	1.839	6.535	1.636	8.171
Ribose	8.178	1.698	4.938	6.480	1.882	6.638	1.699	8.337
Talose	8.204	1.696	4.950	6.508	1.883	6.647	1.697	8.344
Xylose	8.223	1.655	4.939	6.567	1.857	6.594	1.655	8.249

Table S16B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S16A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	3.139	3.330	4.577	0.095	6.470	0.957	6.541	1.557	1.461	3.018	3.697
Altrose	3.187	3.141	4.474	0.023	6.328	0.869	6.387	1.331	1.354	2.685	3.288
Arabinose	3.507	3.375	4.867	0.066	6.882	0.913	6.943	1.362	1.428	2.790	3.418
Galactose	3.045	3.362	4.536	0.159	6.407	0.949	6.479	1.576	1.418	2.994	3.669
Glucose	3.086	3.366	4.567	0.140	6.453	0.979	6.528	1.625	1.485	3.111	3.811
Gulose	3.242	3.373	4.678	0.065	6.615	0.972	6.686	1.563	1.498	3.062	3.750
Lyxose	3.092	3.361	4.567	0.134	6.453	0.965	6.526	1.594	1.460	3.054	3.741
Mannose	2.973	3.334	4.467	0.180	6.307	0.971	6.384	1.639	1.458	3.097	3.795
Ribose	3.090	3.325	4.539	0.118	6.414	0.981	6.490	1.619	1.501	3.120	3.822
Talose	3.076	3.335	4.537	0.129	6.411	0.983	6.487	1.630	1.501	3.132	3.836
Xylose	3.145	3.374	4.612	0.114	6.519	0.968	6.591	1.585	1.471	3.056	3.744
Average	3.144	3.334	4.584	0.111	6.478	0.955	6.549	1.553	1.458	3.011	3.688

Table S17A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M11 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-10.223	1.175	4.524	11.398	0.898	4.770	0.246	5.016
Altrose	-10.192	1.095	4.548	11.287	0.916	4.813	0.264	5.077
Arabinose	-10.113	1.305	4.404	11.419	0.849	4.614	0.210	4.825
Galactose	-10.120	1.252	4.434	11.372	0.864	4.657	0.223	4.879
Glucose	-9.984	1.190	4.397	11.175	0.865	4.627	0.230	4.857
Gulose	-10.285	1.152	4.566	11.436	0.912	4.821	0.255	5.076
Lyxose	-10.232	1.226	4.503	11.459	0.885	4.737	0.234	4.972
Mannose	-10.116	1.217	4.449	11.333	0.873	4.680	0.230	4.910
Ribose	-10.159	1.154	4.502	11.313	0.896	4.750	0.248	4.998
Talose	-10.181	1.162	4.510	11.343	0.896	4.756	0.247	5.003
Xylose	-10.268	1.192	4.538	11.460	0.898	4.782	0.244	5.026
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.718	1.635	4.676	6.083	1.797	6.313	1.637	7.950
Altrose	7.668	1.521	4.595	6.147	1.717	6.116	1.521	7.638
Arabinose	7.528	1.551	4.540	5.978	1.724	6.091	1.551	7.642
Galactose	7.696	1.582	4.639	6.113	1.760	6.222	1.583	7.805
Glucose	7.570	1.659	4.614	5.911	1.801	6.279	1.664	7.943
Gulose	7.710	1.698	4.704	6.011	1.841	6.409	1.705	8.114
Lyxose	7.841	1.626	4.733	6.215	1.802	6.360	1.626	7.986
Mannose	7.782	1.626	4.704	6.156	1.797	6.331	1.627	7.958
Ribose	7.767	1.683	4.725	6.084	1.835	6.413	1.687	8.100
Talose	7.743	1.681	4.712	6.062	1.832	6.398	1.686	8.084
Xylose	7.767	1.660	4.713	6.107	1.819	6.376	1.663	8.039

Table S17B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S17A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	2.505	2.809	3.764	0.152	5.315	0.899	5.392	1.543	1.391	2.933	3.594
Altrose	2.524	2.617	3.635	0.046	5.140	0.801	5.203	1.304	1.257	2.561	3.137
Arabinose	2.585	2.856	3.852	0.135	5.441	0.874	5.513	1.477	1.341	2.818	3.452
Galactose	2.424	2.834	3.730	0.205	5.259	0.896	5.339	1.565	1.360	2.926	3.586
Glucose	2.415	2.849	3.735	0.217	5.264	0.936	5.351	1.651	1.434	3.086	3.782
Gulose	2.575	2.850	3.841	0.138	5.425	0.929	5.506	1.588	1.450	3.038	3.722
Lyxose	2.392	2.852	3.722	0.230	5.243	0.917	5.328	1.622	1.392	3.014	3.695
Mannose	2.334	2.843	3.678	0.255	5.177	0.924	5.265	1.652	1.397	3.048	3.738
Ribose	2.392	2.837	3.711	0.223	5.229	0.939	5.317	1.663	1.440	3.102	3.803
Talose	2.437	2.843	3.745	0.203	5.281	0.935	5.367	1.642	1.439	3.081	3.776
Xylose	2.501	2.852	3.794	0.176	5.354	0.921	5.435	1.594	1.419	3.013	3.692
Average	2.462	2.822	3.746	0.180	5.284	0.906	5.365	1.573	1.393	2.965	3.634

Table S18A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the M11L density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-6.596	-1.901	4.248	4.695	1.922	6.261	2.013	8.275
Altrose	-6.420	-1.654	4.037	4.766	1.709	5.735	1.698	7.434
Arabinose	-6.432	-1.724	4.078	4.708	1.766	5.866	1.788	7.654
Galactose	-6.484	-1.760	4.122	4.724	1.799	5.954	1.831	7.785
Glucose	-6.392	-1.860	4.126	4.532	1.878	6.102	1.977	8.079
Gulose	-6.612	-1.891	4.251	4.721	1.914	6.249	1.998	8.247
Lyxose	-6.667	-1.809	4.238	4.858	1.849	6.120	1.882	8.003
Mannose	-6.547	-1.805	4.176	4.742	1.839	6.061	1.885	7.947
Ribose	-6.530	-1.875	4.202	4.656	1.897	6.186	1.983	8.169
Talose	-6.549	-1.865	4.207	4.684	1.889	6.175	1.968	8.143
Xylose	-6.664	-1.870	4.267	4.794	1.899	6.231	1.964	8.195
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	6.894	1.566	4.230	5.328	1.679	5.807	1.577	7.383
Altrose	6.740	1.465	4.103	5.275	1.595	5.572	1.469	7.041
Arabinose	6.366	1.496	3.931	4.870	1.586	5.443	1.512	6.954
Galactose	6.818	1.434	4.126	5.384	1.581	5.562	1.436	6.998
Glucose	6.737	1.561	4.149	5.176	1.663	5.724	1.575	7.299
Gulose	6.941	1.588	4.264	5.353	1.699	5.864	1.600	7.464
Lyxose	7.020	1.524	4.272	5.496	1.660	5.800	1.528	7.328
Mannose	6.858	1.528	4.193	5.330	1.649	5.727	1.535	7.262
Ribose	6.880	1.587	4.233	5.292	1.693	5.834	1.600	7.434
Talose	6.923	1.575	4.249	5.347	1.688	5.835	1.586	7.421
Xylose	7.028	1.546	4.287	5.481	1.677	5.839	1.552	7.391

Table S18B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S18A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.298	0.334	0.448	0.018	0.633	0.243	0.678	0.455	0.437	0.892	1.092
Altrose	0.320	0.188	0.372	0.066	0.509	0.114	0.526	0.163	0.229	0.393	0.483
Arabinose	0.066	0.228	0.238	0.147	0.163	0.180	0.284	0.423	0.276	0.699	0.863
Galactose	0.334	0.326	0.467	0.004	0.660	0.217	0.695	0.391	0.396	0.787	0.964
Glucose	0.345	0.299	0.457	0.023	0.644	0.215	0.679	0.378	0.402	0.780	0.955
Gulose	0.329	0.303	0.447	0.013	0.632	0.216	0.668	0.385	0.398	0.783	0.959
Lyxose	0.353	0.285	0.454	0.034	0.638	0.189	0.666	0.320	0.354	0.674	0.826
Mannose	0.311	0.277	0.416	0.017	0.588	0.190	0.618	0.334	0.351	0.685	0.839
Ribose	0.349	0.287	0.452	0.031	0.637	0.203	0.669	0.352	0.383	0.734	0.900
Talose	0.374	0.290	0.473	0.042	0.663	0.201	0.694	0.340	0.382	0.722	0.885
Xylose	0.364	0.324	0.487	0.020	0.687	0.222	0.722	0.392	0.412	0.804	0.984
Average	0.503	0.523	0.544	0.556	0.633	0.633	0.711	0.719	0.807	0.992	1.092

Table S19A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the MN12L density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-6.440	-1.533	3.986	4.908	1.619	5.538	1.552	7.090
Altrose	-6.418	-1.578	3.998	4.840	1.651	5.603	1.606	7.209
Arabinose	-6.366	-1.391	3.878	4.975	1.512	5.274	1.395	6.669
Galactose	-6.325	-1.437	3.881	4.888	1.540	5.327	1.446	6.772
Glucose	-6.253	-1.492	3.872	4.761	1.575	5.383	1.511	6.894
Gulose	-6.468	-1.536	4.002	4.932	1.623	5.556	1.554	7.110
Lyxose	-6.519	-1.436	3.977	5.083	1.556	5.418	1.441	6.859
Mannose	-6.393	-1.426	3.909	4.967	1.539	5.343	1.433	6.776
Ribose	-6.396	-1.503	3.949	4.894	1.594	5.468	1.519	6.987
Talose	-6.431	-1.502	3.966	4.929	1.596	5.482	1.516	6.999
Xylose	-6.494	-1.498	3.996	4.996	1.598	5.507	1.511	7.018
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	6.734	1.248	3.991	5.486	1.452	5.242	1.251	6.492
Altrose	6.707	1.156	3.931	5.551	1.392	5.097	1.166	6.262
Arabinose	6.686	1.173	3.930	5.513	1.401	5.111	1.181	6.292
Galactose	6.666	1.172	3.919	5.493	1.398	5.099	1.180	6.278
Glucose	6.590	1.251	3.921	5.339	1.439	5.173	1.252	6.425
Gulose	6.784	1.294	4.039	5.490	1.486	5.334	1.295	6.629
Lyxose	6.834	1.216	4.025	5.618	1.442	5.247	1.222	6.469
Mannose	6.676	1.209	3.942	5.467	1.421	5.156	1.213	6.369
Ribose	6.732	1.280	4.006	5.452	1.472	5.288	1.281	6.569
Talose	6.777	1.278	4.027	5.499	1.475	5.307	1.280	6.587
Xylose	6.833	1.262	4.047	5.571	1.470	5.312	1.265	6.577

Table S19B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S19A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.294	0.285	0.409	0.004	0.578	0.167	0.602	0.296	0.301	0.597	0.732
Altrose	0.289	0.422	0.511	0.066	0.711	0.259	0.759	0.506	0.440	0.947	1.160
Arabinose	0.320	0.218	0.387	0.051	0.538	0.111	0.552	0.163	0.215	0.378	0.464
Galactose	0.341	0.264	0.431	0.038	0.605	0.142	0.623	0.228	0.266	0.494	0.606
Glucose	0.337	0.241	0.414	0.048	0.578	0.135	0.595	0.210	0.259	0.469	0.575
Gulose	0.316	0.242	0.398	0.037	0.558	0.138	0.576	0.222	0.259	0.481	0.589
Lyxose	0.315	0.220	0.384	0.048	0.535	0.114	0.549	0.171	0.219	0.390	0.479
Mannose	0.283	0.217	0.357	0.033	0.501	0.117	0.515	0.187	0.220	0.406	0.498
Ribose	0.336	0.223	0.403	0.057	0.559	0.122	0.574	0.180	0.237	0.418	0.513
Talose	0.346	0.223	0.412	0.061	0.570	0.121	0.585	0.175	0.236	0.411	0.506
Xylose	0.339	0.236	0.413	0.051	0.575	0.128	0.592	0.194	0.246	0.440	0.540
Average	0.320	0.254	0.411	0.045	0.573	0.141	0.593	0.230	0.263	0.494	0.606

Table S20A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the MN12SX density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-7.341	-1.324	4.333	6.018	1.560	5.662	1.329	6.991
Altrose	-7.330	-1.374	4.352	5.957	1.590	5.728	1.376	7.104
Arabinose	-7.252	-1.195	4.223	6.056	1.473	5.435	1.212	6.647
Galactose	-7.231	-1.222	4.227	6.010	1.486	5.462	1.235	6.696
Glucose	-7.137	-1.287	4.212	5.850	1.516	5.504	1.292	6.796
Gulose	-7.365	-1.325	4.345	6.040	1.563	5.675	1.330	7.006
Lyxose	-7.400	-1.261	4.330	6.139	1.527	5.603	1.273	6.876
Mannose	-7.267	-1.268	4.267	5.998	1.518	5.545	1.277	6.822
Ribose	-7.279	-1.325	4.302	5.954	1.554	5.631	1.329	6.960
Talose	-7.310	-1.320	4.315	5.990	1.554	5.640	1.325	6.966
Xylose	-7.384	-1.290	4.337	6.094	1.543	5.635	1.299	6.934
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.287	1.489	4.388	5.799	1.660	5.877	1.489	7.367
Altrose	7.257	1.410	4.333	5.847	1.606	5.744	1.410	7.154
Arabinose	7.175	1.397	4.286	5.777	1.590	5.684	1.398	7.082
Galactose	7.199	1.409	4.304	5.790	1.600	5.714	1.410	7.124
Glucose	7.094	1.485	4.290	5.609	1.640	5.776	1.487	7.263
Gulose	7.295	1.522	4.408	5.773	1.683	5.932	1.523	7.455
Lyxose	7.359	1.458	4.408	5.901	1.647	5.866	1.458	7.324
Mannose	7.242	1.460	4.351	5.782	1.637	5.811	1.460	7.271
Ribose	7.234	1.517	4.375	5.717	1.674	5.894	1.518	7.412
Talose	7.270	1.514	4.392	5.756	1.676	5.907	1.515	7.422
Xylose	7.322	1.489	4.406	5.832	1.664	5.895	1.490	7.385

Table S20B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S20A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.054	0.165	0.174	0.056	0.219	0.101	0.285	0.215	0.160	0.375	0.391
Altrose	0.073	0.036	0.082	0.018	0.109	0.016	0.138	0.016	0.034	0.050	0.143
Arabinose	0.077	0.202	0.216	0.063	0.279	0.117	0.359	0.249	0.186	0.435	0.474
Galactose	0.032	0.188	0.190	0.078	0.220	0.114	0.301	0.252	0.175	0.427	0.430
Glucose	0.042	0.199	0.203	0.078	0.241	0.124	0.325	0.272	0.194	0.467	0.466
Gulose	0.070	0.197	0.210	0.064	0.268	0.121	0.346	0.256	0.193	0.449	0.472
Lyxose	0.041	0.197	0.201	0.078	0.238	0.119	0.322	0.263	0.185	0.448	0.455
Mannose	0.025	0.192	0.193	0.083	0.217	0.119	0.302	0.266	0.183	0.449	0.442
Ribose	0.045	0.192	0.197	0.074	0.237	0.120	0.317	0.263	0.189	0.452	0.453
Talose	0.040	0.194	0.198	0.077	0.234	0.122	0.316	0.267	0.190	0.457	0.455
Xylose	0.062	0.200	0.209	0.069	0.262	0.121	0.342	0.260	0.191	0.450	0.470
Average	0.051	0.178	0.189	0.067	0.229	0.109	0.305	0.235	0.171	0.405	0.423

Table S21A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the N12 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-5.975	-2.094	4.035	3.881	2.097	6.454	2.419	8.873
Altrose	-5.844	-1.813	3.829	4.031	1.818	5.803	1.974	7.777
Arabinose	-5.874	-1.873	3.873	4.001	1.875	5.936	2.063	7.999
Galactose	-5.903	-1.904	3.904	4.000	1.905	6.011	2.108	8.119
Glucose	-5.763	-2.066	3.914	3.697	2.072	6.332	2.418	8.750
Gulose	-5.985	-2.091	4.038	3.895	2.093	6.449	2.411	8.860
Lyxose	-6.051	-1.999	4.025	4.052	1.999	6.264	2.239	8.504
Mannose	-5.971	-1.991	3.981	3.980	1.991	6.221	2.240	8.462
Ribose	-5.947	-2.085	4.016	3.861	2.089	6.427	2.410	8.837
Talose	-5.933	-2.077	4.005	3.856	2.080	6.404	2.399	8.803
Xylose	-6.009	-2.064	4.036	3.945	2.065	6.394	2.358	8.752
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	6.324	1.389	3.857	4.935	1.507	5.251	1.394	6.645
Altrose	6.185	1.119	3.652	5.066	1.317	4.776	1.124	5.899
Arabinose	6.315	1.201	3.758	5.114	1.381	4.960	1.202	6.162
Galactose	6.293	1.204	3.749	5.089	1.381	4.953	1.205	6.158
Glucose	6.159	1.369	3.764	4.790	1.479	5.139	1.375	6.514
Gulose	6.401	1.384	3.893	5.016	1.510	5.280	1.388	6.668
Lyxose	6.440	1.316	3.878	5.124	1.467	5.194	1.316	6.510
Mannose	6.307	1.326	3.816	4.981	1.462	5.143	1.327	6.470
Ribose	6.352	1.407	3.880	4.944	1.522	5.293	1.413	6.706
Talose	6.380	1.390	3.885	4.990	1.512	5.279	1.394	6.673
Xylose	6.434	1.366	3.900	5.068	1.500	5.268	1.368	6.635

Table S21B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S21A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.349	0.705	0.786	0.178	1.054	0.590	1.327	1.203	1.025	2.228	2.063
Altrose	0.341	0.694	0.773	0.176	1.035	0.502	1.304	1.027	0.850	1.877	1.865
Arabinose	0.441	0.672	0.803	0.116	1.112	0.494	1.377	0.976	0.861	1.837	1.895
Galactose	0.390	0.700	0.801	0.155	1.090	0.524	1.361	1.058	0.903	1.961	1.946
Glucose	0.396	0.697	0.801	0.150	1.093	0.593	1.363	1.193	1.043	2.236	2.090
Gulose	0.416	0.706	0.820	0.145	1.122	0.583	1.397	1.169	1.023	2.192	2.089
Lyxose	0.389	0.683	0.786	0.147	1.072	0.532	1.338	1.071	0.923	1.994	1.946
Mannose	0.336	0.665	0.745	0.165	1.001	0.529	1.259	1.078	0.914	1.992	1.893
Ribose	0.405	0.678	0.790	0.137	1.083	0.567	1.347	1.134	0.997	2.131	2.024
Talose	0.447	0.687	0.820	0.120	1.134	0.568	1.405	1.125	1.005	2.130	2.061
Xylose	0.425	0.698	0.817	0.136	1.123	0.564	1.395	1.127	0.990	2.117	2.049
Average	0.394	0.690	0.795	0.148	1.084	0.550	1.352	1.105	0.958	2.063	1.993

Table S22A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the N12SX density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-7.133	-1.383	4.258	5.750	1.577	5.642	1.384	7.026
Altrose	-7.084	-1.430	4.257	5.654	1.603	5.687	1.430	7.117
Arabinose	-7.044	-1.222	4.133	5.822	1.467	5.365	1.232	6.597
Galactose	-7.065	-1.252	4.159	5.813	1.488	5.418	1.259	6.677
Glucose	-6.913	-1.361	4.137	5.552	1.541	5.497	1.361	6.858
Gulose	-7.150	-1.391	4.271	5.759	1.584	5.663	1.392	7.054
Lyxose	-7.194	-1.324	4.259	5.870	1.545	5.586	1.327	6.913
Mannose	-7.084	-1.320	4.202	5.764	1.532	5.525	1.323	6.848
Ribose	-7.093	-1.398	4.245	5.695	1.582	5.643	1.398	7.041
Talose	-7.093	-1.391	4.242	5.701	1.578	5.634	1.392	7.025
Xylose	-7.168	-1.363	4.265	5.805	1.567	5.630	1.364	6.994
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.120	1.517	4.318	5.603	1.664	5.838	1.519	7.357
Altrose	7.067	1.560	4.313	5.507	1.689	5.879	1.566	7.445
Arabinose	7.034	1.371	4.202	5.663	1.559	5.573	1.371	6.944
Galactose	7.055	1.388	4.221	5.666	1.573	5.610	1.388	6.998
Glucose	6.905	1.503	4.204	5.402	1.636	5.712	1.507	7.219
Gulose	7.134	1.531	4.332	5.603	1.675	5.866	1.534	7.400
Lyxose	7.191	1.468	4.330	5.724	1.638	5.798	1.468	7.266
Mannose	7.081	1.465	4.273	5.616	1.626	5.739	1.466	7.205
Ribose	7.092	1.537	4.315	5.555	1.676	5.856	1.541	7.398
Talose	7.095	1.531	4.313	5.564	1.672	5.848	1.535	7.383
Xylose	7.153	1.505	4.329	5.648	1.659	5.836	1.507	7.343

Table S22B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S22A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.013	0.134	0.134	0.060	0.147	0.087	0.208	0.196	0.135	0.331	0.316
Altrose	0.017	0.130	0.131	0.056	0.147	0.087	0.205	0.192	0.136	0.328	0.312
Arabinose	0.010	0.148	0.149	0.069	0.159	0.092	0.228	0.208	0.139	0.348	0.339
Galactose	0.011	0.136	0.136	0.063	0.147	0.085	0.210	0.192	0.129	0.321	0.312
Glucose	0.007	0.143	0.143	0.068	0.150	0.095	0.218	0.214	0.147	0.361	0.339
Gulose	0.016	0.140	0.140	0.062	0.156	0.091	0.219	0.204	0.142	0.346	0.331
Lyxose	0.003	0.144	0.144	0.071	0.147	0.093	0.218	0.212	0.141	0.353	0.335
Mannose	0.003	0.145	0.145	0.071	0.148	0.094	0.219	0.214	0.143	0.357	0.338
Ribose	0.000	0.140	0.140	0.070	0.140	0.094	0.210	0.213	0.144	0.357	0.332
Talose	0.002	0.140	0.140	0.071	0.137	0.094	0.209	0.214	0.143	0.358	0.332
Xylose	0.015	0.142	0.143	0.064	0.157	0.092	0.222	0.206	0.143	0.349	0.335
Average	0.009	0.140	0.140	0.066	0.149	0.091	0.215	0.206	0.140	0.346	0.329

Table S23A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the SOGGA11 density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-5.756	-2.212	3.984	3.543	2.239	6.692	2.708	9.400
Altrose	-5.910	-2.337	4.123	3.573	2.379	7.044	2.920	9.964
Arabinose	-5.873	-2.164	4.019	3.709	2.177	6.595	2.577	9.172
Galactose	-5.809	-2.169	3.989	3.640	2.186	6.594	2.604	9.198
Glucose	-5.890	-2.333	4.111	3.557	2.376	7.031	2.919	9.950
Gulose	-5.930	-2.299	4.114	3.631	2.331	6.945	2.831	9.777
Lyxose	-5.890	-2.307	4.098	3.583	2.344	6.961	2.862	9.823
Mannose	-5.993	-2.336	4.165	3.657	2.371	7.054	2.889	9.942
Ribose	-5.790	-2.135	3.963	3.655	2.148	6.506	2.544	9.050
Talose	-5.798	-2.135	3.967	3.663	2.148	6.508	2.541	9.049
Xylose	-5.915	-2.312	4.114	3.603	2.349	6.979	2.866	9.845
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	6.266	1.476	3.871	4.790	1.564	5.364	1.493	6.856
Altrose	6.303	1.592	3.948	4.710	1.654	5.577	1.629	7.206
Arabinose	6.289	1.390	3.839	4.899	1.504	5.234	1.395	6.629
Galactose	6.170	1.408	3.789	4.762	1.507	5.207	1.418	6.625
Glucose	6.277	1.519	3.898	4.758	1.596	5.439	1.541	6.981
Gulose	6.345	1.551	3.948	4.793	1.626	5.526	1.578	7.103
Lyxose	6.418	1.515	3.966	4.903	1.604	5.498	1.532	7.030
Mannose	6.359	1.587	3.973	4.772	1.654	5.593	1.620	7.213
Ribose	6.321	1.375	3.848	4.946	1.497	5.226	1.379	6.605
Talose	6.371	1.369	3.870	5.002	1.497	5.242	1.372	6.615
Xylose	6.392	1.584	3.988	4.808	1.654	5.603	1.615	7.218

Table S23B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S23A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	0.511	0.736	0.896	0.113	1.246	0.675	1.539	1.328	1.216	2.544	2.369
Altrose	0.393	0.744	0.842	0.176	1.137	0.725	1.426	1.467	1.291	2.758	2.419
Arabinose	0.416	0.775	0.879	0.179	1.190	0.673	1.491	1.361	1.182	2.542	2.339
Galactose	0.361	0.761	0.842	0.200	1.122	0.678	1.417	1.387	1.187	2.573	2.311
Glucose	0.387	0.814	0.902	0.214	1.202	0.780	1.518	1.591	1.378	2.969	2.595
Gulose	0.415	0.747	0.854	0.166	1.162	0.705	1.452	1.420	1.254	2.674	2.386
Lyxose	0.528	0.792	0.952	0.132	1.320	0.739	1.633	1.463	1.330	2.793	2.564
Mannose	0.366	0.749	0.834	0.191	1.115	0.717	1.405	1.461	1.269	2.730	2.391
Ribose	0.531	0.760	0.927	0.115	1.291	0.652	1.594	1.280	1.165	2.445	2.353
Talose	0.573	0.766	0.957	0.096	1.339	0.651	1.649	1.266	1.169	2.435	2.385
Xylose	0.477	0.728	0.871	0.126	1.205	0.695	1.492	1.377	1.251	2.628	2.385
Average	0.451	0.761	0.887	0.155	1.212	0.699	1.510	1.400	1.245	2.645	2.409

Table S24A: HOMO and LUMO orbital energies (in eV), ionization potentials I and electron affinities A (in eV), and global electronegativity χ , total hardness η , global electrophilicity ω , electrodonating power (ω^-), electroaccepting power (ω^+), and net electrophilicity $\Delta\omega^\pm$ of Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose calculated with the SOGGA11X density functional and the Def2TZVP basis set using water as solvent simulated with the SMD parametrization of the IEF-PCM model. The upper part of the table shows the results derived assuming the validity of "Koopmans in DFT" procedure and the lower part shows the results derived from the calculated vertical I and A.

Property	HOMO	LUMO	χ_K	η_K	ω_K	ω_K^-	ω_K^+	$\Delta\omega_K^\pm$
Allose	-8.322	-0.202	4.262	8.120	1.119	4.876	0.614	5.489
Altrose	-8.432	-0.285	4.358	8.147	1.166	5.020	0.662	5.682
Arabinose	-8.694	-0.419	4.557	8.275	1.255	5.305	0.748	6.053
Galactose	-8.584	-0.410	4.497	8.174	1.237	5.234	0.737	5.971
Glucose	-8.291	-0.395	4.343	7.896	1.195	5.054	0.711	5.765
Gulose	-8.266	-0.203	4.235	8.064	1.112	4.845	0.610	5.455
Lyxose	-8.442	-0.368	4.405	8.075	1.202	5.110	0.705	5.815
Mannose	-8.474	-0.251	4.362	8.223	1.157	5.010	0.647	5.657
Ribose	-8.304	-0.085	4.194	8.219	1.070	4.751	0.557	5.308
Talose	-8.329	-0.131	4.230	8.199	1.091	4.810	0.580	5.390
Xylose	-8.741	-0.452	4.596	8.289	1.274	5.365	0.769	6.133
Property	I	A	χ	η	ω	ω^-	ω^+	$\Delta\omega^\pm$
Allose	7.183	1.388	4.286	5.795	1.585	5.675	1.389	7.064
Altrose	7.337	1.528	4.432	5.809	1.691	5.961	1.529	7.490
Arabinose	7.467	1.625	4.546	5.843	1.768	6.175	1.629	7.804
Galactose	7.440	1.619	4.530	5.821	1.762	6.154	1.624	7.777
Glucose	7.352	1.646	4.499	5.705	1.774	6.154	1.655	7.809
Gulose	7.153	1.406	4.279	5.747	1.593	5.686	1.406	7.092
Lyxose	7.301	1.594	4.447	5.708	1.733	6.046	1.598	7.644
Mannose	7.574	1.484	4.529	6.090	1.684	6.013	1.484	7.497
Ribose	7.133	1.285	4.209	5.848	1.514	5.499	1.290	6.789
Talose	7.159	1.332	4.246	5.827	1.547	5.581	1.335	6.916
Xylose	7.500	1.656	4.578	5.844	1.793	6.240	1.662	7.903

Table S24B: Descriptors J_I , J_A , J_{HL} , J_χ , J_η , J_ω , J_{D1} , J_{ω^+} , J_{ω^-} , $J_{\Delta\omega^\pm}$ and J_{D2} for the Allose, Altrose, Arabinose, Galactose, Glucose, Gulose, Lyxose, Mannose, Ribose, Talose and Xylose molecules calculated from the results of Table S24A

	J_I	J_A	J_{HL}	J_χ	J_η	J_ω	J_{D1}	J_{ω^-}	J_{ω^+}	$J_{\Delta\omega^\pm}$	J_{D2}
Allose	1.139	1.186	1.644	0.024	2.325	0.466	2.848	0.799	0.775	1.575	3.058
Altrose	1.095	1.243	1.656	0.074	2.337	0.525	2.866	0.941	0.867	1.808	3.138
Arabinose	1.226	1.205	1.719	0.011	2.432	0.514	2.978	0.870	0.881	1.751	3.225
Galactose	1.144	1.209	1.664	0.032	2.353	0.525	2.882	0.920	0.887	1.807	3.153
Glucose	0.940	1.251	1.565	0.156	2.191	0.579	2.696	1.099	0.944	2.043	3.061
Gulose	1.114	1.203	1.639	0.045	2.317	0.481	2.839	0.841	0.796	1.636	3.065
Lyxose	1.141	1.226	1.675	0.042	2.367	0.531	2.900	0.936	0.893	1.829	3.175
Mannose	0.900	1.233	1.526	0.166	2.132	0.527	2.628	1.003	0.837	1.840	2.934
Ribose	1.171	1.200	1.677	0.014	2.371	0.444	2.904	0.747	0.733	1.480	3.087
Talose	1.170	1.202	1.677	0.016	2.372	0.456	2.905	0.771	0.755	1.526	3.099
Xylose	1.241	1.204	1.729	0.018	2.445	0.519	2.994	0.876	0.894	1.769	3.245
Average	1.116	1.215	1.652	0.054	2.331	0.506	2.858	0.891	0.842	1.733	3.113