Supporting Information

Authorizing Multiple Chemical Passwords by a Combinatorial Molecular Keypad Lock

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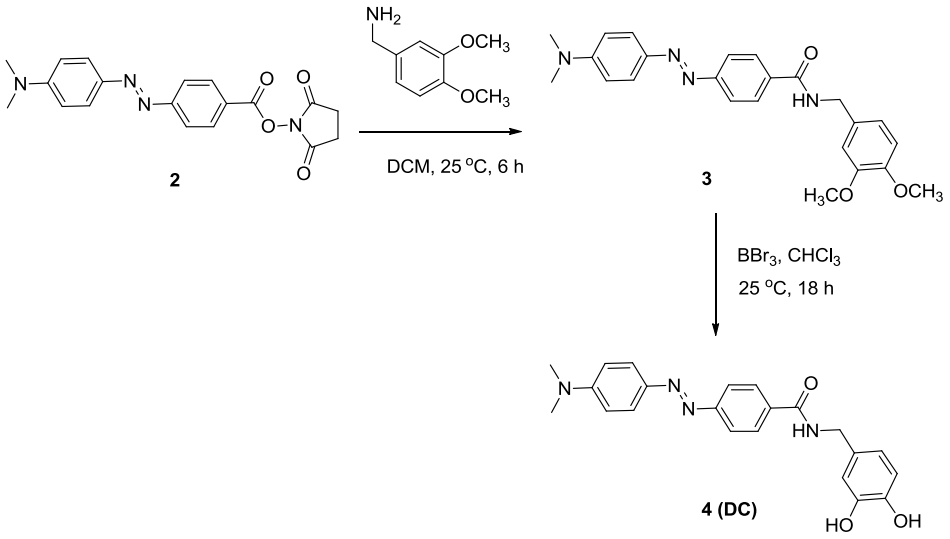
1. Materials and methods

Chemicals, saccharides, anhydrous solvents, and spectroscopic grade solvents were obtained from Sigma Aldrich. The synthesis of the combinatorial fluorescent molecular sensor **1** was previously described.[S13] Anhydrous solvents were transferred using an oven-dried syringe. Flasks were oven-dried under a stream of argon. The Teledyne combiflash was used to purify all the synthetic intermediates. The ^{1}H NMR spectra of all compounds were recorded on a Bruker Avance 300 MHz NMR spectrometer. Mass spectra were recorded on a Waters Micromass LC-Q-TOF micro spectrometer at the Weizmann Institute of Science mass spectrometry facility. Fluorescent measurements were performed on a VarianTechnology International Fluorimeter using quartz cuvettes. Principal Component analysis was performed using XLSTAT version 2013.1.01 (32 bit).

2. Synthetic scheme for the preparation of DC

Specific reaction conditions are provided in the experimental procedure section.



Scheme S1. Synthetic steps for the preparation of DC.

3. Experimental procedures.

Synthesis of compound **3**:

To a stirred solution of DABCYL-NHS **2** (0.25 g, 0.068 mmol) in dry dichloromethane (DCM, 1.5 mL) was added 3,4-dimethoxy benzylamine (0.011g, 0.068 mmol) under argon. The reaction mixture was

stirred at room temperature for 6 h. The solvent was evaporated and the crude reaction mass was subjected to combi-flash column chromatography (silica gel, 1% methanol in DCM) to afford **3** (0.20 g) as a red solid with 70% yield. ^{1}H NMR (300 MHz, $CDCl_3$) 7.87 (6H, s), 6.90 (2H, s), 6.84 (1H, d, J = 9 Hz), 6.75 (2H, d, J = 9 Hz), 6.48 (1H, s, br), 4.59 (2H, d, J = 6 Hz), 3.87 (6H, s), 3.10 (6H, s); MS (ESI+): *m/z* (%) = 419.31 (100) $[M+H]^+$, 441.31 (75) $[M+Na]^+$, 859.52 (60) $[2M+Na]^+$, 1277.80 (25) $[3M+Na]^+$.

Synthesis of compound **4**:

To a stirred solution of **3** (0.20 g, 0.047 mmol) in dry DCM (1.5 mL) was added boron tribromide (0.1g, 0.4 mmol, 400µL of 1M solution of BBr_3) under argon at 0 ^{o}C. The solution was warmed to room temperature and then stirred for 18 h. The reaction was diluted with DCM (25 mL) and washed with a saturated solution of $NaHCO_3$ (2 x 5 mL). The organic layer was washed with brine (5 mL) and dried over anhydrous Na_2CO_3. The solvent was evaporated and the crude reaction mass was subjected to combi-flash column chromatography (silica gel, 4% methanol in DCM) to afford **4** (0.014 g) as a red solid with 76% yield. ^{1}H NMR (300 MHz, $CDCl_3$) 7.94 (2H, d, J = 9 Hz), 7.81-7.85 (4H, m), 6.80 (3H, d, J = 9 Hz), 6.67-6.75 (2H, m), 4.45 (2H, s), 3.10 (6H, s); MS (ESI+): *m/z* (%) = 391.28 (65) $[M+H]^+$, 413.28 (45) $[M+Na]^+$, 803.49 (40) $[2M+Na]^+$.

4. Fluorescence measurements and pattern analysis

Fluorescence measurements were taken in a 3 mm cuvette using an excitation wavelength of 270 nm, an emission filter of 295-1100 nm, and an excitation and emission slit width of 10 nm. The spectra were recorded at a rate of 120 nm per min.

4.1. 2-input chemical passwords

The dependence of the fluorescence emission pattern on the sequence of addition (Figure S1 and Figure 3) was demonstrated by adding 1.5 µL of two different saccharides to a methanol solution of **1** (3 µM, 60 µL) in different orders. The mixture was allowed to equilibrate for 6 min after each saccharide ad-

dition. Aqueous solutions of D-xylose (1 M), D-glucose (100 mM), galactose (1 M), D-fructose (100 mM), and maltitol (1 M) were used for obtaining the various 2-input chemical passwords. For X and G, fluorescence experiments were performed in three replicates and principal component analysis (PCA) was applied to distinguish between the emission patterns generated at seven different wavelengths (304 nm, 326 nm, 397 nm, 421 nm, 449 nm, 496 nm, and 527 nm) in which maximal changes in intensities were observed (Figure 4, main text). The emission of the pure sensor (none) corresponds to the addition of only water.

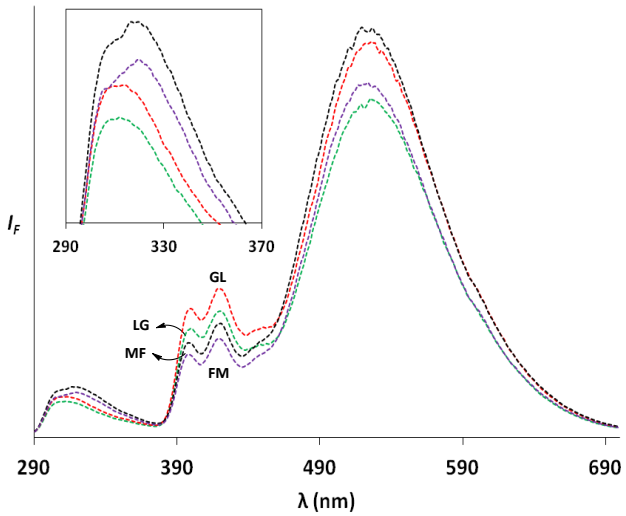


Figure S1. Changes in fluorescence emission spectra of **1** (3μM) upon the addition of galactose (L,) and D-glucose (G) or D-fructose (F) and maltitol (M) in different orders. Excitation wavelength: 270 nm.

4.2. 3-input chemical passwords

As a first step toward developing 3-input chemical passwords, solutions of various saccharides were prepared (3 μL, 100 mM) and each solution was added separately to a solution of **1** (3 μM, 60 μL) in methanol. Following a 6 min incubation, fluorescence spectra were recorded in four replicates and PCA was applied to identify chemical inputs that can potentially be used for obtaining 3-digit chemical passwords, namely, the saccharides that induced the most distinguishable changes to the emission patterns

(Figure S2, saccharides **2**-**12**). In addition to maltitol (**9**) and D-xylose (**6**), which were selected from this screening, DC was prepared (Scheme S1) as an additional chemical input.

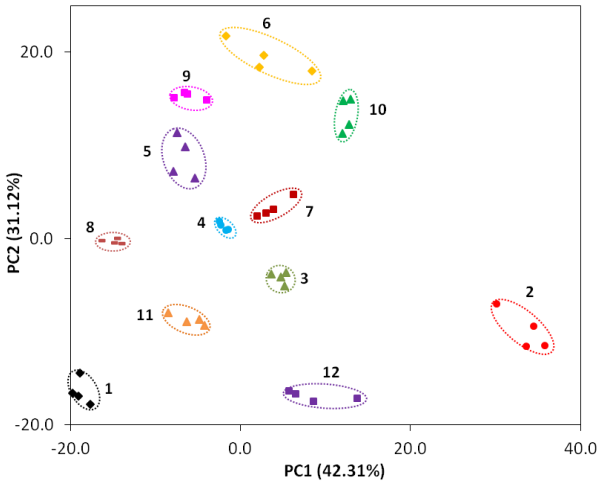


Figure S2. PCA mapping of emission patterns generated by a 5 mM solution of various saccharides. 1) None; 2) D-glucose; 3) L-glucose; 4) D-fructose; 5) L-fructose; 6) D-xylose; 7) L-xylose; 8) mannitol; 9) maltitol; 10) lactulose; 11) D-maltose; 12) maltotriose.

The concentrations of maltitol, D-xylose, and DC were systematically modified to obtain the best differentiation between them (Figure 5b) as well as between the 2-input (Figure 5d) and 3-input passwords (Figure S3, Figure 6 in main text). The final configuration of the molecular keypad lock consisted of a 60 µL solution of **1** (9 µM) in methanol to which a 1 µL solution of each input was added. Following each addition, the mixture was allowed to equilibrate for 6 min. Solutions of maltitol (3 M) and D-glucose (1 M) in water, and DC (7.7 mM) in methanol were used in these measurements, as well as for displacing DC by D-xylose (Figure 5c). Principal component analysis of the patterns generated at eight different wavelengths (305 nm, 325 nm, 395 nm, 420 nm, 445 nm, 520 nm, 530 nm, and 540 nm) was performed using XLSTAT version 2013.1.01 (32 bit). The resulting PCA plot (Figure S3) was applied to differentiate between the unique chemical passwords (i.e., 111, 122, 212, 231, 223, 311, 222, and 333) and the remaining combinations that resulted in overlapping patterns (Figure S3, groups A-D).

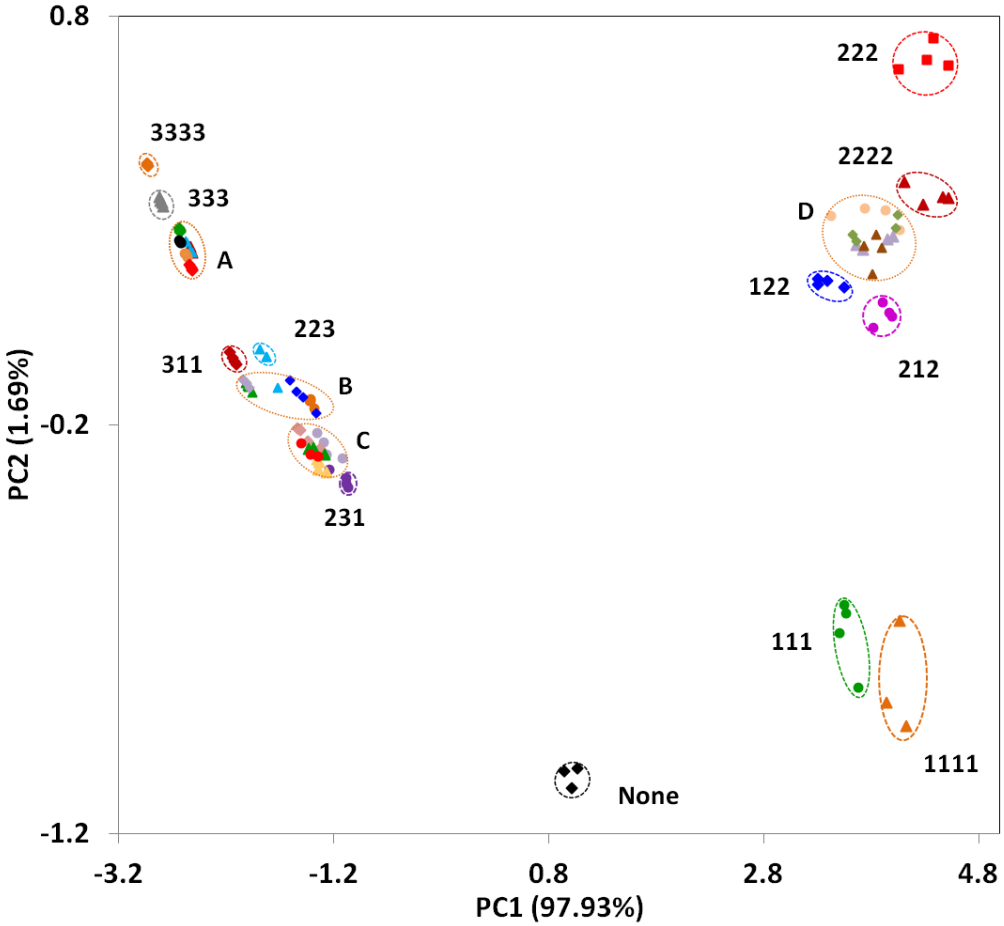


Figure S3. PCA mapping of emission patterns generated by 50 mM maltitol (**1**), 17 mM D-xylose (**2**), and 125 μM DC (**3**) in 27 different combinations. A, B, C, and D are the groups containing passwords that overlap each other. Group A contains 133, 331, 313, 233, 332, and 323; Group B contains 113, 131, 322, and 232; Group C contains 213, 123, 132, 312, and 321; and Group D contains 221, 112, 211, and 121.

5. Computational methods

All electronic structure calculations were carried out using GAUSSIAN09 REVISION C.01.[S1] Two classes of electronic structure methods were used. Geometries were initially optimized using the semiempirical parameter model 6 (PM6).[S2] PM6 should be sufficient to provide qualitative relative energies. Selected geometries were then reoptimized using density functional theory (DFT). For the geometry optimizations, the Perdew-Burke-Ernzerhof (PBE) functional was used.[S3] Energies were then calculated with Adamo and Barone's hybrid version of this functional (PBE0).[S4] Density fitting basis sets (DFBS), as

implemented in GAUSSIAN09,[S5] were used in order to improve the computational efficiency of the calculation. Because the use of DFBSs precludes the use of a hybrid DFT exchange-correlation functional, they were used in conjunction with the PBE functional for the geometry optimizations. Owing to the rather large size of the system, in order to make the geometry optimizations tractable, the Stuttgart-Dresden effective core potential-basis set was used on all atoms (denoted as SDDall, excluding hydrogen).[S6] The single-point energies employed Pople's 6-31G(d,p) basis set.[S7] Bulk solvation effects were approximated in the single-point energy calculations using Marenich and Truhlar's solvation model-dispersion (SMD),[S8] which is an empirical reparameterization of the polarizable continuum model (PCM),[S9] specifically the integral equation formalism model (IEF-PCM);[S9a,b,S10] methanol was used as the solvent. The accuracy of the DFT methods was improved by adding the empirical dispersion correction as recommended by Grimme.[S11] The older version (DFTD2)[S11a] is available, with analytical gradients and Hessians, in GAUSSIAN09 and was used during geometry optimizations and frequency calculations; our version of GAUSSIAN09 was locally modified to allow for its use for any DFT functional rather than just the limited set included in the commercially available version. The newer, and more accurate, DFTD3 version,[S11b] which includes parameters for most of the periodic table, was used as an *a posteriori* correction to the PBE0 energies obtained from GAUSSIAN09; the code written by Grimme was used.[S12] All DFT-optimized structures were characterized as minima by having zero imaginary frequencies. All energies refer to either relative Gibbs free energy ($\Delta_{rel}G^{298,sol}$) or standard reaction Gibbs free energy ($\Delta_r G^{\circ,sol}$) in methanol solution if not stated otherwise.

6. DFT simulations

The structure of sensor **1** consists of three phenyl boronic acids in the vicinity of the anthracyl (**A**), dansyl (**B**), or naphtyl (**C**) units (Figure S4). Accordingly, for our calculation (Tables S1 and S2) we use a nomenclature that identifies at which sites the sugar is bound (i.e., sites A, B, and/or C) and via which oxygen atoms of the sugar (Scheme S2, oxygens 1-5). A wealth of experimental and theoretical data on boronic acid-based receptors indicate that multivalent receptors such as **1** can interact with different saccharides in various structural modes depending on the type of receptor, saccharide, solvent, and stoichiometry.[S14] According to this data, each of the boronic acids on **1** (Figure S4, sites A, B, or C) could bind to two oxygens on a sugar to form a boronic ester. Alternatively, owing to the chelate effect, individual sugar molecules should also be able to interact with several boronic acids simultaneously, for example, at the **AB**, **AC,** or **BC** sites. What further complicates the modeling of such complexes is that the interaction with such receptors can also dictate the saccharide's isomerization states (e.g., pyranose or furanose) and, as a result, its isomerization dynamics.[S14] Herein, DFT calculations (Table S1 and S2) were applied to demonstrate that similar processes can occur upon the formation of **1**-sacharide complexes and subsequently, provide a proof-of-principle that the order of saccharide binding can affect the system's kinetics.

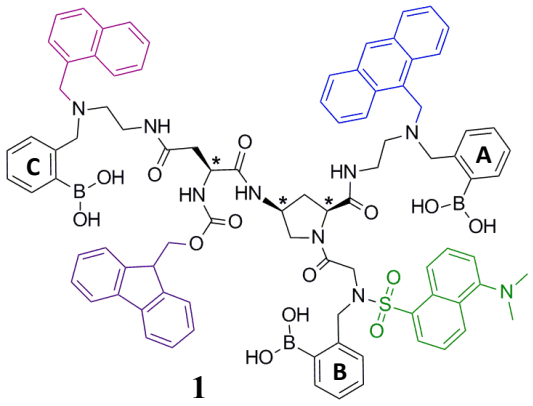
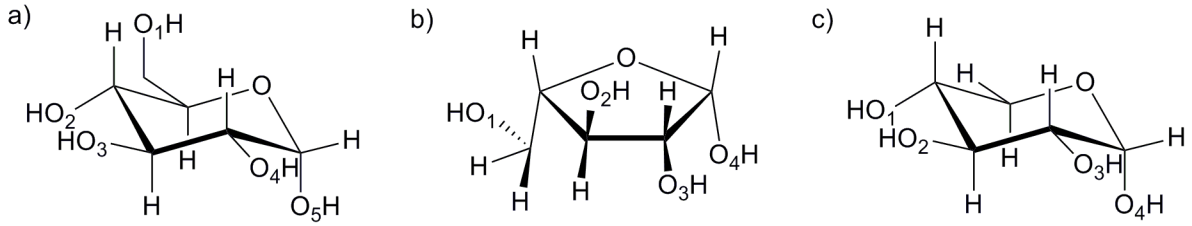


Figure S4. Sensor **1** consists of three sugar bonding sites (A-C) located in the vicinity of anthracyl (A, blue), dansyl (B, green), and naphthyl (C, pink). The fourth chromophore, fluorene, is shown in purple.

We calculated the Gibbs free energy ($\Delta_r G^{298,sol}$) of different complexes that can be formed upon binding of **1** to D-glucose or D-xylose (Tables S1 and S2). The structure of **1** was optimized as previously described.[S13] Due to the numerous possible interaction modes, for simplicity we calculated $\Delta_r G^{298,sol}$ values of complexes containing only a single saccharide or two molecules of the same saccharide. D-glucose was modeled in its pyranose form (Scheme S2a), whereas for D-xylose we considered both the furanose (Scheme S2b) and pyranose isomers (Scheme S2c).



Scheme S2. Schematic representation and numbering of the oxygen atoms of α-pyr-D-glucose (a) and α-D-xylose in its furanose (b) and (c) pyranose forms.

Table S1 lists the energy values ($\Delta_r G^{298,sol}$) obtained for different complexes that can be formed between D-glucose and **1**. Group A contains all possible interaction modes involving a single glucose molecule and each of the boronic acids on **1**, while in group B two boronic acids interact with two glucose molecules via two oxygens on each sugar. Group C contains complexes in which two boronic acids simultaneously bind a single glucose molecule via four oxygens. The most stable complex within each group is highlighted in green. According to these calculations (Table S1), the most stable complex in group A is sensor-G^p-C12 (see Scheme S2a for the numbering of the oxygen atoms of the saccharides) with a $\Delta_r G^{298,sol}$ of -0.5 kJ·mol^{-1}. Formation of sensor-G^p-A12-G^p-C12, which is the most stable complex with two glucose molecules ($\Delta_r G^{298,sol}$ = 3.4 kJ·mol^{-1}), does not result in a thermodynamically more stable product. The most stable structure with $\Delta_r G^{298,sol}$ of -20 kJ·mol^{-1} corresponds to sensor-G^p-A45-B12, in which a glucose molecule bridges two boronic acid centers. This data thus supports the manifestation of the chelate effect, which was expected from various reports involving multivalent boronic acid-sugar complexes. [S14]

Table S1. The reaction energies of the formation of the sensor-glucose complexes.

	Complex	$\Delta_r H^{298,sol}$ [kJ·mol^{-1}]	$\Delta_r G^{298,sol}$ [kJ·mol^{-1}]
Group A	sensor-G^p-A12[a]	35.5	20.8
	sensor-G^p-A45	20.6	8.5
	sensor-G^p-B12	29.4	19.9
	sensor-G^p-B45	115.1	69.2
	sensor-G^p-C12	20.6	**-0.5**
	sensor-G^p-C45	78.7	50.7
Group B	sensor-G^p-A12-G^p-B12	90.1	48.6
	sensor-G^p-A12-G^p-B45	82.1	45.8
	sensor-G^p-A12-G^p-C12	58.4	**3.4**
	sensor-G^p-A12-G^p-C45	96.9	55.9
	sensor-G^p-A45-G^p-B12	113.8	43.6
	sensor-G^p-A45-G^p-B45	67.2	3.9
	sensor-G^p-A45-G^p-C12	99.4	44.4
	sensor-G^p-A45-G^p-C45	104.5	66.8
	sensor-G^p-B12-G^p-C12	106.2	52.8
	sensor-G^p-B12-G^p-C45	94.0	48.4
	sensor-G^p-B45-G^p-C12	113.7	56.3
	sensor-G^p-B45-G^p-C45	83.6	45.8
Group C	sensor-G^p-A12-B45	131.0	21.1
	sensor-G^p-A12-C45	227.6	109.1
	sensor-G^p-A45-B12	69.6	**-20.0**
	sensor-G^p-A45-C12	166.8	42.8
	sensor-G^p-B12-B45	205.5	82.7
	sensor-G^p-B45-C12	192.6	73.7

[a] G is glucose and superscript *p* stands for the pyranose form.

Table S2. The reaction energies of the formation of the sensor-xylose complexes.

	Compound	$\Delta_r H^{298,sol}$ [kJ·mol^{-1}]	$\Delta_r G^{298,sol}$ [kJ·mol^{-1}]
Group A	sensor-X^f-A12[a]	103.2	68.0
	sensor-X^f-A34	67.5	32.7
	sensor-X^f-B12	140.4	81.2
	sensor-X^f-B34	107.8	70.4
	sensor-X^f-C12	66.5	40.3
	sensor-X^f-C34	74.4	43.8
	sensor-X^p-A34	48.2	24.0
	sensor-X^p-B34	98.4	67.9
	sensor-X^p-C34	48.4	14.1
Group B	sensor-X^f-A34-X^f-B34	139.9	72.0
	sensor-X^f-A34-X^f-C34	76.3	12.2
	sensor-X^f-B34-X^f-C34	54.1	-2.4
	sensor-X^f-A34-X^p-B34	63.1	1.8
	sensor-X^f-A34-X^p-C34	120.8	52.5
	sensor-X^f-B34-X^p-C34	151.6	74.7
	sensor-X^p-A34-X^f-B34	112.4	54.0
	sensor-X^p-A34-X^f-C34	100.3	42.2
	sensor-X^p-B34-X^f-C34	203.6	125.0
	sensor-X^p-A34-X^p-B34	73.9	30.9
	sensor-X^p-A34-X^p-C34	89.3	37.3
	sensor-X^p-B34-X^p-C34	148.1	73.8
Group C	sensor-X^f-A12-B34	93.2	-7.8
	sensor-X^f-A12-C34	207.2	71.1
	sensor-X^f-A34-B12	139.6	17.2
	sensor-X^f-A34-C12	147.0	32.0
	sensor-X^f-B12-C34	243.5	107.7
	sensor-X^f-B34-C12	204.1	81.4
	sensor-X^p-A12-B34	181.7	60.5
	sensor-X^p-A12-C34	211.0	102.2
	sensor-X^p-A34-B12	142.2	36.3
	sensor-X^p-A34-C12	458.8	354.7
	sensor-X^p-B12-C34	163.8	61.6
	sensor-X^p-B34-C12	278.0	153.9

[a] X is xylose; superscripts *p* and *f* stand for the pyranose and furanose forms, respectively.

Similar calculations for different D-Xylose complexes (Table S2) reveal a similar binding trend in which a single D-xylose molecule preferably interacts with two boronic acids on sites A and B (X^f-A12-B34, $\Delta_r G^{298,sol}$ = -7.8 kJ·mol^{-1}). This interaction is thermodynamically more stable than the binding of D-xylose to a single site (X^p-C34, $\Delta_r G^{298,sol}$ = 14.1 kJ·mol^{-1}), and the binding of two D-xylose molecules at distinct sites (X^f-B34-X^f-C34, $\Delta_r G^{298,sol}$ = -2.4 kJ·mol^{-1}). Interestingly, the favorable isomer within group A involves the pyranose form, whereas in groups B and C it is the furanose isomer that forms the most stable complex, indicating that the receptor-saccharide interaction can also affect the sugar isomerization.

Taken together, these calculations (Table S1 and S2) indicate the feasibility of obtaining kinetically stable complexes upon a sequential addition of saccharides. We can hypothesize, for example, a situation where D-xylose (X) and D-glucose (G) are sequentially added to the solution of **1** to form a password: 1. X, 2. G (Scheme 1, main text). As previously discussed, the thermodynamically favored complex of each of these saccharides involves the binding of the sugar at the AB sites. Moreover, the tetravalent **1**-G complex ($\Delta_r G^{\circ,sol}$ = -20 kJ·mol^{-1}) was found to be more stable than the tetravalent **1**-X complex ($\Delta_r G^{298,sol}$ = -7.8 kJ·mol^{-1}). Although thermodynamically G should displace the sensor-bound X, it would have to overcome a large energetic barrier in order to first bind to sites A or B (Table S1, group 1), which have been occupied by X. Therefore, it is likely that G would initially form a complex with site C to which it has a higher affinity than X ($\Delta_r G^{298,sol}$ = -0.5 kJ·mol^{-1}), and that the conversion to the thermodynamic product will occur over a prolonged reaction time. Naturally, in a complex mixture of two or three saccharides, the displacement rates would largely depend on the saccharide concentration and the metastable complexes that are formed can involve a wide range of different structures.

8. XYZ coordinates of the discussed complexes

sensor-Xp-C34

220

scf done: -5878.316531

C	1.378372	-2.504542	-1.777830
O	0.977489	-3.704853	-1.669099
C	2.435681	-1.975534	-0.807943
H	2.399921	-0.883611	-0.687576
H	2.250689	-2.444183	0.171804
N	3.760139	-2.344303	-1.361591
C	4.301615	-3.695277	-0.978260
H	3.687271	-4.386156	-1.585824
H	5.345346	-3.747445	-1.324994
C	4.183838	-4.066303	0.492723
C	5.214350	-3.790956	1.438467
C	2.977237	-4.664375	0.921772
C	4.976995	-4.122195	2.796055
C	2.766925	-4.982266	2.275372
H	2.193653	-4.857865	0.177954
C	3.771063	-4.707336	3.217754
H	5.769483	-3.945077	3.533075
H	1.826434	-5.448790	2.586372
H	3.620319	-4.953160	4.273838
B	6.611829	-3.166532	1.075905
O	7.207916	-3.444968	-0.156367
H	8.069332	-2.997432	-0.316538
O	7.430922	-2.528000	2.024231
H	7.007329	-2.178502	2.833847
S	5.013047	-0.925389	-1.030238
O	4.162843	0.452038	-1.428230
O	5.690513	-0.959366	0.496230
C	6.282241	-1.321064	-2.396600
C	7.682791	-1.104456	-2.217833
C	5.708997	-1.724309	-3.591201
C	8.283642	-0.580517	-1.032862
C	8.535387	-1.437858	-3.349410
C	6.547011	-1.940037	-4.713876
H	4.629961	-1.881129	-3.649308
C	9.660307	-0.379992	-0.989670
H	7.663420	-0.343995	-0.167042
C	9.979223	-1.332225	-3.233404
C	7.924330	-1.793478	-4.588206
H	6.098211	-2.209585	-5.673563
C	10.500348	-0.753245	-2.064591
H	10.109143	0.036805	-0.083052
H	8.565373	-1.920014	-5.464060
H	11.581879	-0.638497	-1.955830
N	10.812867	-1.764598	-4.277037
C	10.714762	-3.142842	-4.794057
H	11.512065	-3.776781	-4.350558
H	9.743690	-3.586350	-4.533762
H	10.834111	-3.152758	-5.892187
C	12.163102	-1.199760	-4.383784
H	12.526799	-1.354470	-5.414266
H	12.131248	-0.118259	-4.178557
H	12.884650	-1.679271	-3.686536
N	0.937013	-1.662178	-2.753939
C	-0.098722	-2.089531	-3.735850
H	-0.819541	-2.780739	-3.274042
H	0.382759	-2.581704	-4.600485
C	-0.737848	-0.747961	-4.140302
H	-1.249004	-0.785784	-5.112477
C	0.469520	0.220820	-4.126453
H	0.145259	1.271485	-4.080850
H	1.087092	0.070277	-5.028980
C	1.263032	-0.219800	-2.856520
H	2.352074	-0.072049	-2.956206
C	0.791605	0.554470	-1.601412
O	0.009603	0.009007	-0.744445
N	1.240740	1.812826	-1.465016
H	0.958002	2.340113	-0.628175
C	2.096327	2.576179	-2.387573
C	1.588696	4.028368	-2.378160
H	2.034187	2.158280	-3.403335
H	3.150233	2.513680	-2.063230
H	2.143376	4.630178	-3.132263
H	0.523589	4.025822	-2.668104
N	1.717594	4.589484	-1.018789
C	0.539614	5.374752	-0.553891
H	0.841579	5.931065	0.345686
H	0.205803	6.104102	-1.326322
C	3.049115	5.219363	-0.818510
H	3.796999	4.504810	-1.208649
H	3.157233	6.131183	-1.445954
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C	-2.650102	3.255558	-0.870092
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C	-1.649270	2.811405	1.297604
C	-2.663912	2.567411	0.355519
H	-3.438709	3.075017	-1.608781
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O	0.801134	5.313930	2.483139
H	1.498348	5.446477	3.165276
C	3.366373	5.512663	0.633609
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C	3.889220	3.087168	1.010049
C	4.087788	4.703826	2.882342
C	3.551858	7.073880	2.570019
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C	4.325769	2.076564	1.850133
H	3.624539	2.837973	-0.018365
C	4.522420	3.622756	3.722481
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C	3.416823	8.401627	3.105060
H	2.516020	7.798879	-0.669945
C	2.667413	9.209362	0.934895
C	4.647923	2.343088	3.217743
H	4.434820	1.059800	1.460355
H	4.751264	3.843176	4.771456
H	4.197847	6.202299	4.451861
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H	3.658139	8.559792	4.162323
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H	4.978217	1.519827	3.857961
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N	-5.026744	0.913908	-2.505722
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H	-2.159690	-2.139900	4.099880
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O	-4.498532	-2.082225	1.956582
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O	-7.267776	2.381756	-0.387541
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H	-4.901294	1.041163	3.427270
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H	-4.246479	-5.484260	0.559011
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H	-8.143228	-8.719040	1.544214
H	-9.113340	0.633116	-0.421310
H	-10.072082	-7.932248	2.935572
N	-0.021632	-1.375475	-1.758895
C	1.016258	-1.538719	-0.914039
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H	-1.447799	2.511660	2.896138
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H	1.116082	1.701895	-0.505802
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C	8.110437	-2.021520	0.687671
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C	7.647556	-1.871809	-1.795848
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H	11.401553	-2.880425	2.159858
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B	5.374065	-3.404680	0.972840
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C	3.956708	-4.533709	2.456736
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H	0.858781	-5.300986	1.864291
H	0.150002	-3.431201	3.370244
H	1.232765	-3.501890	4.795923
O	0.591323	-1.592598	4.326897
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B	-0.923876	3.921557	-3.377914
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C	1.095740	5.015554	-2.813347
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C	2.516532	4.449425	-2.917833
H	1.092741	6.112052	-2.861726
O	1.182070	3.154034	-1.353945
H	0.383030	4.985522	-0.633004
C	2.566107	3.278681	-1.889434
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  214
scf done: -5725.587184
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O	1.990862	6.315914	-0.599031
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H	6.256567	1.031043	0.598996
N	5.546230	-0.654892	-0.415136
C	4.665746	-1.080263	-1.530185
C	5.554678	-1.608427	0.723317
H	3.608536	-1.195604	-1.225192
H	4.687753	-0.262867	-2.277048
H	4.527709	-1.791847	1.118968
H	5.918468	-2.576610	0.331776
C	6.413234	-1.125688	1.879013
C	7.849011	-1.087161	1.785783
C	5.793284	-0.654718	3.036929
C	8.553450	-1.595012	0.650610
C	8.611650	-0.532870	2.882632
C	6.548431	-0.118781	4.117379
H	4.699905	-0.695108	3.110388
C	9.942450	-1.547160	0.592955
H	7.981053	-2.028669	-0.170667
C	10.038410	-0.489290	2.789088
C	7.932513	-0.044772	4.041196
H	6.024375	0.243443	5.007777
C	10.691642	-0.983386	1.666383
H	10.468322	-1.948688	-0.280060
H	10.605594	-0.065356	3.626027
H	8.522116	0.378052	4.862378
H	11.784379	-0.949113	1.604368
C	5.161152	-2.358418	-2.201404
C	4.282685	-3.365328	-2.701254
C	6.554941	-2.527888	-2.352955
B	2.724074	-3.267063	-2.724725
C	4.853835	-4.526902	-3.292040
C	7.097225	-3.676631	-2.949446
H	7.197629	-1.724426	-1.983304
O	2.067094	-2.043088	-2.578520
O	2.003003	-4.440179	-3.003056
C	6.240579	-4.692423	-3.413828
H	4.171892	-5.296354	-3.666021
H	8.183043	-3.778283	-3.054498
C	0.595512	-2.037353	-2.527364
C	0.539326	-4.448785	-3.191198
H	6.650512	-5.596707	-3.875757
C	0.041708	-3.045944	-3.537116
C	0.091969	-0.625603	-2.794481
H	0.295970	-2.358478	-1.517986
H	0.078288	-4.783704	-2.247691
H	0.324410	-5.167838	-3.993509
H	0.311008	-2.754369	-4.567469
O	-1.421215	-3.068992	-3.401600
C	-1.439292	-0.606480	-2.951002
H	0.565213	-0.227793	-3.703002
O	0.492696	0.285431	-1.724830
C	-2.043022	-1.802619	-3.741902
H	-1.879106	-0.620086	-1.940452
O	-1.788025	0.608116	-3.671721
H	-0.056099	0.126653	-0.915219
H	-3.099337	-1.944151	-3.470226
O	-1.898666	-1.550308	-5.162720
H	-2.567848	1.107678	-3.261417
H	-1.845882	-0.558326	-5.259608

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C	4.060728	1.171265	1.238973
O	3.926854	0.050418	0.638606
C	4.993029	2.206821	0.637992
H	4.515144	2.678706	-0.244355
H	5.251084	3.000242	1.357680
N	6.273990	1.614497	0.183633
C	6.808165	0.386900	0.872416
H	6.275889	-0.526382	0.555980
H	7.860255	0.302308	0.546375

C	6.717522	0.545901	2.380872
C	6.207819	-0.504806	3.197146
C	7.166105	1.749129	2.969894
C	6.167084	-0.286920	4.602832
C	7.091255	1.949647	4.357472
H	7.569733	2.531924	2.316780
C	6.581490	0.925970	5.178175
H	5.781575	-1.083846	5.249692
H	7.437767	2.890613	4.796687
H	6.521375	1.066658	6.262470
B	5.656171	-1.918200	2.705553
O	4.621608	-2.129597	1.832996
H	4.236218	-1.362900	1.295875
O	6.152491	-3.076988	3.327462
H	6.920026	-2.977247	3.926702
S	6.190841	1.197351	-1.710088
O	6.180834	-0.447086	-1.979264
O	4.985274	2.144264	-2.348013
C	7.933675	1.764554	-2.207208
C	8.322171	3.126013	-2.029884
C	8.757054	0.779382	-2.721222
C	7.439778	4.175449	-1.641273
C	9.710519	3.441884	-2.321291
C	10.074719	1.133177	-3.110937
H	8.378240	-0.238889	-2.839728
C	7.917109	5.478166	-1.553538
H	6.385125	3.958656	-1.465615
C	10.213503	4.785740	-2.098407
C	10.531193	2.432027	-2.908311
H	10.715330	0.381812	-3.579796
C	9.282563	5.783313	-1.763956
H	7.229424	6.286641	-1.286261
H	11.534013	2.710360	-3.242075
H	9.623112	6.811678	-1.618615
N	11.576470	5.075622	-2.262792
C	11.980842	6.455441	-2.552660
H	11.278091	6.905657	-3.271089
H	12.022973	7.091033	-1.641057
H	12.987141	6.438228	-3.005835
C	12.605802	4.299337	-1.547667
H	12.974141	4.869744	-0.668346
H	12.190773	3.347878	-1.186983
H	13.465309	4.090383	-2.209580
N	3.491296	1.422348	2.437339
C	3.409780	2.741001	3.117932
H	3.191281	3.542575	2.396917
H	4.356459	2.954267	3.649090
C	2.246217	2.540443	4.120760
H	2.326265	3.215790	4.985526
C	2.398828	1.044879	4.505288
H	1.474931	0.634698	4.940097
H	3.226873	0.927541	5.226746
C	2.782846	0.352606	3.168513
H	3.472457	-0.493111	3.329256
C	1.562398	-0.128243	2.364164
O	0.972543	0.649592	1.555734
N	1.165336	-1.382585	2.667070
H	1.790805	-1.973242	3.215382
C	-0.056033	-2.006501	2.146481
C	0.290478	-3.111245	1.134934
H	-0.676772	-1.204903	1.722303
H	-0.614918	-2.458799	2.984584
H	0.918572	-2.705804	0.314305
H	0.909347	-3.854958	1.658335
N	-0.943189	-3.757474	0.676471
C	-0.894823	-5.242175	0.521573
H	-1.922990	-5.555626	0.268435
H	-0.221289	-5.557530	-0.295683
C	-1.713715	-3.012672	-0.353484
H	-2.736536	-3.421833	-0.351021
H	-1.845287	-1.974923	-0.006342
C	-1.134275	-3.019046	-1.771497
C	-1.553630	-4.003367	-2.725303
C	-0.157791	-2.045307	-2.164687
C	-2.579089	-4.975472	-2.438917
C	-0.963659	-4.024375	-4.058843
C	0.420150	-2.089383	-3.501730
C	0.286933	-0.996104	-1.282809
C	-2.983565	-5.895929	-3.396342
H	-3.061942	-4.990684	-1.460388
C	-1.396760	-5.010882	-5.012131
C	0.017648	-3.080180	-4.416814
C	1.420977	-1.123354	-3.872099
H	-0.151709	-0.876601	-0.292500
C	1.286440	-0.117279	-1.664309
C	-2.383891	-5.924667	-4.694996
H	-3.760333	-6.626677	-3.145729
H	-0.926802	-5.011840	-6.002316
H	0.468641	-3.111621	-5.415392
C	1.868125	-0.176768	-2.967037
H	1.826825	-1.169727	-4.890097
H	1.635342	0.626707	-0.942666
H	-2.708807	-6.671098	-5.426327
H	2.667642	0.523622	-3.232090
N	0.940857	2.782476	3.499628
C	0.012494	3.616093	4.054574
H	0.673822	2.158609	2.720074
O	0.231490	4.351320	5.060316
C	-1.365829	3.569237	3.349048
H	-1.223727	3.169413	2.331203
N	-2.275577	2.667090	4.070158
C	-2.230457	1.320773	3.884901
O	-1.398272	0.713167	3.160933
O	-3.254187	0.690253	4.591171
C	-3.597887	-0.690928	4.150255
H	-2.669292	-1.277341	4.060913
H	-4.228802	-1.066672	4.965537
C	-4.353019	-0.658407	2.810913
C	-5.683629	0.098204	2.845296
H	-3.682914	-0.228525	2.041149
C	-4.790058	-2.052057	2.348479
C	-5.939570	1.433340	3.183441
C	-6.746781	-0.752613	2.434305
C	-4.007516	-3.181127	2.072661
C	-6.196310	-2.082638	2.133546
C	-7.263048	1.915150	3.100083
H	-5.138192	2.103177	3.503784
C	-8.063196	-0.268472	2.334712
C	-4.649628	-4.338441	1.578178
H	-2.914182	-3.178609	2.172826
C	-6.833217	-3.240518	1.657130
C	-8.312733	1.075358	2.672495
H	-7.467455	2.958606	3.361884
H	-8.872195	-0.920645	1.990645
C	-6.046085	-4.372035	1.380595
H	-4.053021	-5.220365	1.323846
H	-7.910443	-3.244818	1.468088
H	-9.330418	1.473556	2.597653
H	-6.515335	-5.281541	0.991188
H	-3.075397	3.088563	4.555307
C	-1.966158	4.994475	3.280890
H	-1.386099	5.571567	2.541233
C	-3.461456	5.037334	2.985415
H	-1.807107	5.465868	4.268481
O	-4.301811	4.542838	3.807121
N	-3.839264	5.651613	1.829275
H	-3.115439	5.961951	1.183368
C	-5.237916	5.896301	1.440684
C	-5.541885	5.413213	-0.005160
H	-5.439707	6.982398	1.522066
H	-5.874316	5.374273	2.173202
H	-6.375089	6.013431	-0.414055
H	-4.660424	5.613555	-0.649649
N	-5.911758	4.007419	-0.125536
C	-7.340437	3.685826	0.048889
C	-4.942008	3.018316	0.331878
H	-7.426258	2.597757	0.186946
H	-7.766273	4.166131	0.960710
H	-4.692091	3.129352	1.410171
H	-5.443720	2.040241	0.237937
C	-3.624122	2.936368	-0.443669
C	-3.452149	3.200309	-1.852404
C	-2.554727	2.386068	0.275506
C	-4.491270	3.729358	-2.685381
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C	-1.311921	2.067291	-0.337976

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H    -2.706542     2.134597     1.331668
C    -4.301092     3.878747    -4.054193
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C    -2.015503     3.054348    -3.880287
C    -1.123375     2.309810    -1.691640
H    -0.525451     1.597629     0.260751
C    -3.057962     3.537909    -4.660837
H    -5.125988     4.250642    -4.670753
H    -1.053100     2.783881    -4.329439
H    -0.187028     2.031293    -2.185485
H    -2.929047     3.658758    -5.741674
C    -0.500317    -5.911983     1.835808
C     0.847133    -6.244645     2.171691
C    -1.517311    -6.136424     2.790320
C     1.110280    -6.797117     3.453756
C    -1.239413    -6.704797     4.044031
H    -2.545938    -5.855794     2.544108
C     0.085403    -7.040053     4.379608
H     2.149933    -7.023050     3.708446
H    -2.053168    -6.879453     4.756120
H     0.316381    -7.480039     5.355688
B     2.082531    -5.959080     1.252986
C    -8.157879     4.113635    -1.164137
C    -8.063176     3.449563    -2.427227
C    -9.011445     5.228960    -1.032804
B    -7.160991     2.202587    -2.724320
C    -8.830613     3.954025    -3.508378
C    -9.767365     5.709281    -2.118009
H    -9.083387     5.721102    -0.054504
O    -6.550440     1.464469    -1.700049
O    -7.013003     1.813852    -4.066220
C    -9.673754     5.068897    -3.364860
H    -8.750047     3.444324    -4.472888
H   -10.422573     6.577299    -1.988210
C    -5.565003     0.436144    -2.076033
C    -6.178534     0.664560    -4.479444
H   -10.254900     5.432473    -4.218902
C    -6.068512    -0.314762    -3.314579
C    -5.284300    -0.496235    -0.883081
H    -4.632400     0.959140    -2.356661
H    -5.181056     1.048013    -4.753201
H    -6.667526     0.214430    -5.354004
H    -7.036505    -0.792040    -3.096482
O    -5.056331    -1.332708    -3.642965
C    -5.492313    -1.968532    -1.241666
H    -5.955684    -0.238205    -0.046711
O    -3.875984    -0.429037    -0.460875
C    -4.853088    -2.340117    -2.593798
H    -5.030584    -2.594771    -0.459570
O    -6.937398    -2.197857    -1.280504
H    -3.546951     0.503922    -0.436421
H    -3.762155    -2.441129    -2.508340
O    -5.458747    -3.603784    -2.961563
H    -7.080942    -3.087857    -1.688124
H    -4.846305    -4.143216    -3.515189
O     1.929047    -5.775769    -0.123123
C     3.108832    -5.471615    -0.950987
C     4.068238    -4.608141    -0.115692
C     2.671838    -4.723086    -2.198700
H     3.583068    -6.427197    -1.234792
C     4.529421    -5.351350     1.132584
H     3.558125    -3.673457     0.174180
O     5.256140    -4.270237    -0.916230
C     3.918872    -4.265912    -2.986942
H     2.079038    -3.837954    -1.903392
O     1.871095    -5.625009    -3.015154
O     3.334241    -5.833422     1.869873
H     5.143352    -6.227151     0.863542
C     4.893602    -3.472287    -2.100664
H     4.421979    -5.151554    -3.399546
O     3.517137    -3.462293    -4.137616
H     1.443810    -5.102440    -3.734693
H     5.854393    -3.286505    -2.603432
O     4.223481    -2.255844    -1.757697
H     3.220770    -2.579341    -3.790913
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scf done: -5840.011445

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C     0.696825    -5.787199     1.191259
H    -0.162363    -6.467696     1.349097
H     1.603697    -6.225553     1.643084
N     0.332534    -4.479230     1.737511
C     1.240548    -3.330207     1.699705
H     1.691675    -3.352934     0.685619
H     0.642294    -2.406193     1.723806
S    -1.002125    -4.528998     3.041831
O    -2.169599    -5.482264     2.343710
O    -0.449095    -4.971267     4.544936
C    -1.567350    -2.700404     2.964295
C    -0.935217    -1.684545     3.741646
C    -2.535008    -2.456378     2.008475
C     0.111469    -1.924343     4.681199
C    -1.373224    -0.319076     3.508766
C    -2.894541    -1.109421     1.739353
H    -3.000543    -3.267233     1.443171
C     0.705038    -0.858353     5.338446
H     0.434859    -2.946356     4.881310
C    -0.825032     0.756750     4.300289
C    -2.309927    -0.074369     2.457871
H    -3.604932    -0.921555     0.931349
C     0.234896     0.467839     5.166006
H     1.531005    -1.047225     6.030146
H    -2.534042     0.960915     2.183926
H     0.687637     1.262382     5.762840
N    -1.367765     2.079383     4.173149
C    -2.818509     2.222996     4.505453
H    -3.403891     1.389523     4.096427
H    -2.955025     2.242496     5.606070
H    -3.166621     3.172650     4.070123
C    -0.606035     3.154751     4.848257
H    -1.076194     4.107148     4.563249
H    -0.630419     3.041340     5.952529
H     0.437540     3.138921     4.500063
N     0.029194    -5.100986    -1.102190
C    -1.360085    -4.717200    -0.715535
H    -1.347425    -3.860198    -0.028466
H    -1.855358    -5.554269    -0.197433
C    -2.047631    -4.364197    -2.065165
H    -3.083373    -4.737347    -2.073597
C    -1.150234    -5.025999    -3.141412
H    -1.235319    -4.522048    -4.114946
H    -1.425875    -6.087042    -3.259845
C     0.271779    -4.933942    -2.561942
H     0.934428    -5.750098    -2.895814
C     0.979264    -3.578051    -2.818511
O     0.425569    -2.630714    -3.467563
N     2.210332    -3.478403    -2.260593
H     2.592417    -4.307409    -1.783257
C     3.034305    -2.262212    -2.344494
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H     3.678870    -2.223357    -1.454249
H     2.370341    -1.381318    -2.354883
H     4.297279    -3.270800    -3.809528
H     3.226710    -2.025301    -4.481193
N     4.984797    -1.274273    -3.556289
C     5.061264    -0.143951    -4.517104
H     5.553513     0.694692    -3.991668
H     5.689204    -0.410388    -5.400081
C     6.296601    -1.796478    -3.119930
H     6.459534    -2.811471    -3.540057
H     7.082105    -1.170258    -3.574545
C     6.478179    -1.826932    -1.603018
C     6.067955    -2.966859    -0.842728
C     7.039697    -0.702800    -0.921681
C     5.567885    -4.170089    -1.459794
C     6.120596    -2.923861     0.612451
C     7.184289    -0.730645     0.528266
C     7.484372     0.479400    -1.617554
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H     5.566135    -4.264607    -2.546714
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C	5.584846	-4.023425	1.370122
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H	7.316792	0.573877	-2.692011
C	8.096346	1.520621	-0.938483
C	5.058490	-5.131760	0.737064
H	4.670030	-6.104675	-1.171942
H	5.583868	-3.947895	2.461942
H	6.727235	-1.800751	2.363240
C	8.295074	1.461526	0.479620
H	7.952218	0.312627	2.282616
H	8.437336	2.403243	-1.489405
H	4.619060	-5.950427	1.313795
H	8.824834	2.275165	0.987924
N	-2.087220	-2.918661	-2.319314
C	-2.992020	-2.094347	-1.735386
H	-1.360286	-2.552020	-2.955655
O	-3.834283	-2.477650	-0.869466
C	-2.864382	-0.629204	-2.207947
H	-2.630888	-0.619115	-3.288074
N	-4.104882	0.100405	-1.979390
C	-5.260262	-0.293302	-2.584985
O	-5.397992	-1.267815	-3.358844
O	-6.304805	0.558827	-2.197250
C	-7.677709	0.076616	-2.430790
H	-8.293953	0.962862	-2.229395
H	-7.778598	-0.243659	-3.479978
C	-8.063064	-1.085824	-1.478935
C	-9.585732	-1.222459	-1.485627
H	-7.540086	-1.998901	-1.813892
C	-7.780039	-0.779730	-0.010892
C	-10.437090	-1.543968	-2.549311
C	-10.118365	-0.902786	-0.204622
C	-6.544190	-0.669348	0.638272
C	-8.995747	-0.627280	0.710845
C	-11.831244	-1.554771	-2.326347
H	-10.031215	-1.792930	-3.536256
C	-11.506804	-0.911849	0.016633
C	-6.531002	-0.357311	2.014770
H	-5.614769	-0.870253	0.094637
C	-8.981342	-0.313939	2.082317
C	-12.358271	-1.240603	-1.056242
H	-12.509891	-1.813591	-3.145660
H	-11.917398	-0.672413	1.003358
C	-7.736416	-0.169413	2.724938
H	-5.572813	-0.284831	2.542304
H	-9.916487	-0.200071	2.641264
H	-13.442645	-1.256715	-0.902977
H	-7.702918	0.067871	3.793833
H	-4.116413	0.944058	-1.406138
C	-1.705299	0.072424	-1.471462
H	-0.798815	-0.549531	-1.593252
C	-1.435310	1.440297	-2.089490
H	-1.923486	0.147382	-0.391309
O	-1.388386	1.594671	-3.350497
N	-1.246825	2.467923	-1.224010
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C	-0.918658	3.786770	-1.765188
C	-0.325208	4.715808	-0.717354
H	-1.802039	4.214688	-2.273895
H	-0.141143	3.646766	-2.537176
H	0.409432	4.162856	-0.117059
H	0.185478	5.531820	-1.257705
N	-1.275021	5.385966	0.264153
C	-2.449797	6.028554	-0.474215
C	-0.485894	6.496999	0.982621
H	-2.761024	6.911062	0.113366
H	-2.114949	6.373800	-1.469101
C	-3.543470	4.981343	-0.513875
H	-0.417855	7.342295	0.275925
H	-1.119123	6.790777	1.833614
C	0.879817	6.064909	1.475723
C	-3.394653	4.023232	0.509365
C	-4.599404	4.907625	-1.439268
C	2.094299	6.284288	0.725531
C	0.948023	5.390837	2.693771
C	-4.345078	2.987675	0.623584
B	-2.061467	4.245340	1.366963
C	-5.532906	3.859657	-1.323618
H	-4.689104	5.637976	-2.252222
C	2.134891	7.005815	-0.511433
C	3.333562	5.730319	1.231806
C	2.171767	4.874230	3.196255
H	0.013759	5.240096	3.238522
C	-5.416473	2.908918	-0.285994
H	-4.244244	2.235374	1.416370
O	-2.273114	4.955429	2.664653
O	-1.204254	3.078023	1.535406
H	-6.342021	3.763023	-2.053576
C	3.324707	7.143766	-1.220516
H	1.223221	7.459311	-0.910623
C	4.536009	5.884947	0.473254
C	3.344025	5.017635	2.468541
H	2.183901	4.349583	4.157332
H	-6.142935	2.093605	-0.218440
H	-3.169787	5.341761	2.758108
H	-1.193878	2.696381	2.471686
C	4.534989	6.572795	-0.733800
H	3.331134	7.697703	-2.165049
H	5.445025	5.410522	0.855800
H	4.287988	4.578283	2.806067
H	5.458378	6.682555	-1.311548
C	3.700359	0.293932	-5.020139
C	2.833014	1.128205	-4.256315
C	3.259529	-0.203481	-6.264101
C	1.527596	1.388770	-4.753472
C	1.964875	0.069562	-6.741529
H	3.939574	-0.832835	-6.850550
C	1.087432	0.852699	-5.972842
H	0.838445	1.995634	-4.161023
H	1.640433	-0.342248	-7.702806
H	0.063410	1.044519	-6.306311
C	3.098339	-2.023154	2.843204
C	4.142808	-1.950432	3.797626
C	2.349668	-3.232391	2.742641
C	4.426795	-3.023660	4.658897
H	4.719962	-1.023010	3.861551
C	2.642519	-4.303357	3.606548
C	3.666814	-4.203238	4.565473
H	5.225972	-2.938183	5.402811
H	2.026719	-5.206376	3.572015
H	3.857028	-5.041746	5.242668
B	2.769454	-0.713103	2.062376
O	3.799480	0.209364	1.827476
O	1.454073	-0.438488	1.661771
C	3.505065	1.491933	1.161575
C	1.066340	0.872769	1.109294
C	2.241033	1.399646	0.302278
C	4.708785	1.922127	0.317974
H	3.327416	2.246268	1.945386
H	0.816776	1.558431	1.932591
H	0.177424	0.710097	0.489449
H	2.402595	0.761070	-0.586854
O	1.970351	2.784331	-0.103216
C	4.317935	2.633603	-1.001208
H	5.279061	1.023577	0.034148
O	5.544301	2.816917	1.128191
C	2.894853	3.269336	-1.092826
H	5.087285	3.385532	-1.228646
O	4.328339	1.622150	-2.102599
H	6.462158	2.449891	1.158230
H	2.870390	4.359127	-1.018621
O	2.407076	2.885149	-2.425076
B	3.213817	1.837032	-2.937863

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