Supporting Information

Glucose to 5-Hydroxymethylfurfural: Origin of Site-Selectivity Resolved by Machine Learning based Reaction Sampling

Pei-Lin Kang, Cheng Shang and Zhi-Pan Liu**

Collaborative Innovation Center of Chemistry for Energy Material, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Key Laboratory of Computational Physical Science, Department of Chemistry, Fudan University, Shanghai 200433, China

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1. SSW-NN method for dataset generation and NN potential training

Following our recent work, the SSW-NN method[1, 2] is utilized to generate the dataset for organic reactions. Because the vast reaction space of organic molecules, we design an automated procedure for self-learning G-NN potential, not only for general organic molecules containing C, H, O and N four elements but also for glucose pyrolysis reactions. The procedure is elaborated in the following.

Step 1: Building the initial NN potential

The SSW global sampling were performed for 2775 different organic molecular crystals using first principles DFT calculations, each molecular crystal containing two different molecules from the QM9 dataset. The 2775 organic molecular crystals cover the all 63 bonding patterns in QM9 dataset according to the first neighbors of the carbon. By short time SSW global optimization, we select 20 structures from each SSW trajectory and obtain 55500 PES data. Next, by using ECFP4 technique[3] to distinguish the substructure pattern, we screened 22963 structures as the first training dataset to build the first NN potential.

Step 2: Self-learning of G-NN potential

Using the NN potential generated from the first step, we can accelerate greatly the PES sampling of organic molecules, which provide the chance to sample the reaction space of organic molecules. The iterative self-learning procedure is already shown in Figure 2, where the SSW global optimization using G-NN potential is utilized to expand the PES dataset and the G-NN potential is then improved by learning the new dataset from SSW global optimization. For each cycle, a batch of 48 different organic molecular crystals randomly selected from 5476 dataset is explored by SSW, each with 1000 minima. A small additional dataset, 100~200 structures, is thus obtained from the SSW sampling trajectories, containing the structures on PES either randomly selected or exhibiting new atomic environment as exotic structures (explained below).

Step 3: Self-learning of G-NN potential for glucose pyrolysis

To explore the glucose pyrolysis pathways, we have followed the same procedure as Step 2 to improve G-NN potential for predicting the PES of glucose pyrolysis. The only difference between Step 3 and Step 2 is that the 5476 dataset is replaced by typical intermediates/products in glucose pyrolysis, such as glucose, fructose, HAA, HMF and FF.

The exotic structures produced from SSW trajectory are often poorly predicted ones from the NN potentials. They need to be added to the training dataset to improve NN predictability. These structures are found to have either one or all of the following features: (i) the value of the structural descriptor for these structures is out of the boundary defined by existing structures in the train dataset, (ii) the second derivative (frequency) of the structure is either too high or too low, and (iii) the energy (per atom) of the structure is far higher or lower than the structures in the dataset. For example, these structures often have highly unreasonable geometry, such as very high coordination, very short bond distance or a ring structure with too high tension. While these structures are generally not low energy minima, they define the high energy boundary of the PES and thus are essential in practical simulations to be avoided.

2. Dataset analysis according to bonding patterns

To provide an overview of our global dataset (94854 structures) we have performed numerical analysis to classify the functional groups and the bonding patterns in comparison with the standard QM9 organic dataset[4, 5]. Our classification for the functional group follows the convention in organic chemistry where the carbon atom serves as the skeleton of organic compounds (the numerical setup for the definition of neighbor and bond order is detailed in Table S1). According to the octet rule (the maximum bonds for C, N and O is 4, 3 and 2, respectively), the number of possible first neighbor bonding patterns for C is 79 by considering all C, H, O, N four elements and 33 by considering only C, H, O three elements as neighbors. It should be emphasized that these numbers only count the pattern of structural minima of organic molecules where the octet rule is obeyed, but don't include the non-minimum structures on PES, such as radials and the transition states (TS). To be more general, we can name the bonding patterns using a string of letters with each letter representing a neighbor atom and optional superscripts can be included to indicate the multiple bonds (bond order >1). For example, the "OCHH" string represents four single-bond neighbors around the central C atom, as appeared in the carbon atom bonding with OH in ethanol; the "O^2OC" represents a sp^2 hybrid C atom, as appeared in the central carbon atom of carboxyl acid.

Table S1 Bond order definition by pair distance

No	Atom1	Atom2	Distance Range (Å)	Bond Order
1	C	H	<1.19	1
2	C	C	1.44-1.65	1
3	C	C	1.25-1.44	2
4	C	C	<1.25	3
5	C	N	1.40-1.58	1
6	C	N	1.26-1.40	2
7	C	N	<1.26	3
8	C	O	1.3-1.55	1
9	C	O	<1.3	2

Using this nomination of bonding pattern, we can compare the bonding patterns in our dataset with those in the standard QM9 dataset, as shown in Table S2. First, the diversity of bonding pattern for our dataset is larger than that for QM9 dataset. QM9 dataset contains 131,172 minimum structures of organic molecules (in total 836,414 C atoms) with C-H-O-N four elements and up to nine heavy atoms (C, O, N). Among all 79 possible patterns that obey the octet rules, QM9 dataset has 63 of them and the missing ones are rare environments of C, such as "OONC", "ONCH" and "NNCH". For comparison, our dataset contains 488 bonding patterns in all and 78 octet bonding patterns among 656,756 carbon atoms except the "NNNN", although some patterns such as "OOOC", "ONNN" are also rare (less than 10 times) in our database. The larger bonding pattern diversity in our dataset demonstrates the ability of chemical space exploration of SSW method. In addition, we also identify 410 bonding patterns that do not obey the octet rule. They include both too high coordinated carbon atoms (e.g. "CCCCCH" up to six first neighbors and "$N^3N^2NOC^2$" up to 9 bond orders) and too low coordinated atoms (e.g. radials and single atoms). These minority structural patterns are critical for neural network to define the global PES of organic molecules, and thus to predict their reactivity.

Second, the bonding pattern in our dataset is more balanced compared to that in QM9 dataset. In Table S2, we list some common and rare bonding patterns from our dataset and their populations in the two datasets. We can see that the population of the most common patterns is lower in our dataset comparing to QM9. For example, the most common carbon chain patterns, CCHH and CHHH, are 19% and 13% in QM9 dataset, but are only 6% and 4% in our dataset. This fact is due to the data selection in SSW that is biased towards reactive structures and as a result the carbon atoms not obeying the octet rules in our dataset reaches to 239745, 37% in the total set. Furthermore, the initial molecules in SSW data generation are selected randomly from a distinct pool of structure patterns, which also helps to balance the population of different patterns in the dataset.

Table S2 Population for selected bonding patterns in our dataset and in the QM9 dataset

No	Pattern	Representing molecule	Population	
			Train data	QM9 data
1	C^2CH	Alkene	7%	4%
2	OCCH	s-Alcohol	6%	9%
3	CCHH	s-Alkane	5%	19%

4	NCHH	p-Amine	4%	5%
5	OCHH	p-Alcohol	4%	7%
6	CHHH	p-Alkane	4%	13%
7	CCCH	t-Alkane	3%	10%
8	NCCH	s-Amine	2%	5%
9	NHHH	Methylamine	2%	1%
10	OC^2H	Enol	2%	0.4%
58	NNCH		0.05%	-
60	ONCH		0.04%	-
66	NC^3		0.01%	-
74	OONC		0.002%	-
77	NNNH		0.0005%	-
78	OOON		0.0003%	-

We also report the bonding pattern of C atoms (78 in octet rule) for our training dataset in Table S3.

Table S3 The bonding patterns (in octet rule) and the number of C atoms in our dataset

No	Pattern	Representing molecule	Num. of C atoms
1	C^2CH	Alkene	42981
2	OCCH	s-Alcohol	42486
3	CCHH	s-Alkane	34612
4	NCHH	p-Amine	25668
5	OCHH	p-Alcohol	24494
6	CHHH	p-Alkane	23984
7	CCCH	t-Alkane	18743
8	NCCH	s-Amine	15146
9	NHHH	Methylamine	14814
10	OC^2H	Enol	13159
11	O^2CH	Aldehyde	11563
12	OC^2C	Enol	10010
13	C^2HH	Alkene	9174
14	O^2CC	Ketone	7906
15	O^2OC	Acid	7901
16	N^2CH		7895
17	C^2CC	Alkene	7805
18	O^2O^2	Carbon dioxide	7224
19	C^3H	Alkyne	5742
20	NC^2H	Enamine	5430
21	C^2C^2	Allene	5095
22	OCCC	t-Alcohol	4577
23	ON^2H		4407
24	C^3C	Alkyne	4341
25	OOCH		4046
26	N^3C		3653
27	OHHH		3504
28	O^2C^2		3468

29	N^2CC	3436
30	N^3H	2698
31	O^2NH	2410
32	O^2NC	2262
33	NCCC	2072
34	NC^2C	2027
35	OOC^2	2001
36	OON^2	1923
37	CCCC	1922
38	N^2NC	1921
39	O^2HH	1904
40	ON^2C	1843
41	N^2HH	1805
42	N^2NH	1692
43	O^2OH	1679
44	ON^2N	1616
45	O^2N^2	1458
46	N^2C^2	1433
47	O^2ON	1302
48	HHHH	1162
49	OOCC	1162
50	N^2N^2	1136
51	OOHH	1100
52	O^2OO	939
53	O^2NN	628
54	ONC^2	549
55	N^2NN	391
56	ON^3	360
57	OONH	301
58	NNCH	298
59	ONNH	283
60	ONCH	257
61	NNCC	226
62	N^3N	215
63	ONHH	148
64	ONCC	117
65	NNC^2	117
66	NC^3	78
67	NNHH	68
68	OC^3	52
69	ONNC	46
70	OOOH	44
71	OOOC	30
72	OOOO	19

73	NNNC	16
74	OONC	14
75	ONNN	9
76	OONN	9
77	NNNH	3
78	OOON	2
	Other Patterns	239745
	total	656756

3. Benchmark for common molecules and reactions

3.1 Minimum structures

We have examined the accuracy of the NN PES for the representative organic molecular structures and benchmarked them against DFT calculations, as listed in Table S4. These minimum structures were fully optimized using NN until the maximal force component is below 0.05 eV/Å, and then refined using DFT (PBE) for comparison.

Table S4 Benchmark between NN and DFT for minimum structures

	Nstr	RMSE(meV/atom)
QM9	200	13.31
Drug	17	7.27

In Table S4, the first row on QM9 is the test of NN potential on 200 structures randomly selected from QM9 data; and the second row on Drug is the transferability test of NN potential on 17 drug molecules selected from drug bank (http://www.drugbank.ca supported by Canadian Institutes of Health Research and other organizations), which contain 10 to 45 heavy atoms and have up to a total of 92 atoms in molecule. As both sets are not contained in our training dataset, it shows that the RMSE of energy for our G-NN potential, i.e. 10.05 meV/atom, are also largely valid for organic molecules in general.

In addition to energetics, we also compared the molecular geometry from G-NN calculations and those from DFT calculations. Figure S1 shows the optimized bond length obtained from NN and from DFT for the 17 drug molecules (Table S4). The correlation for the bond length between two methods is satisfactory with the linear fit R^2=0.999. The overall RMS bond length error is 0.005 Å: the RMS bond length error of C-H, C-C, C-N and C-O bond are 0.003 Å, 0.006 Å, 0.007 Å and 0.006 Å, respectively.

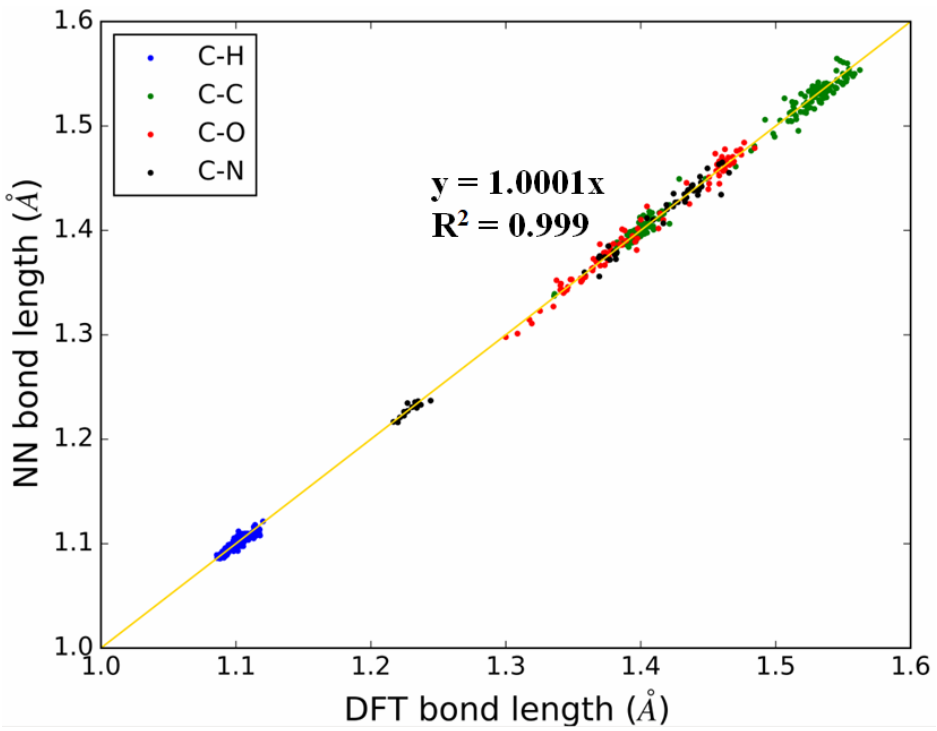

Figure S1 Bond length comparison between NN and DFT calculations for 17 drug molecules. These drug molecules were fully optimized using NN and DFT calculations until the maximal force component is below 0.05 eV/Å.

3.2 Baker Reactions

Table S5 shows our results for ten Baker reactions[6] with C-H-O-N elements, where the NN calculations are utilized to search for the transitions state and evaluate the barrier. The results from DFT calculations are also listed for comparison. Baker reactions are gas phase reactions with common reaction patterns, such as [2+4] reaction, 1,2-H

transfer[6, 7]. The mean error of the NN barrier is 0.13 eV for these reactions. As these reactions are not deliberatively added in our training dataset, the error bar in the calculated barrier should be considered as a guideline for reaction screening.

Table S5 Reaction benchmark between NN and DFT calculations for ten Baker reactions.

No	Reaction	NN energy barrier/eV	DFT energy barrier/eV	ΔE/eV
1	HCCH → CCH_2	2.06	1.98	0.09
2	H_2CO→ H_2+CO	2.93	2.84	0.10
3	H_2CHOH→H_3CCHO	2.28	2.63	-0.36
4	Rotational TS_in_acrolein	0.34	0.28	0.06
5	DA parent	0.67	0.53	0.13
6	Claisen rearrangement	1.69	1.76	-0.07
7	$HCNH_2$→HCN+H_2	2.95	2.76	0.19
8	HCN→HNC	1.36	1.37	-0.01
9	HCONHOH→HCOHNHO	1.43	1.65	-0.22
10	s-tetrazine→2HCN+N_2	2.83	2.77	0.06
	Mean Error			0.13

4. Automated SSW-RS to resolve the reaction network

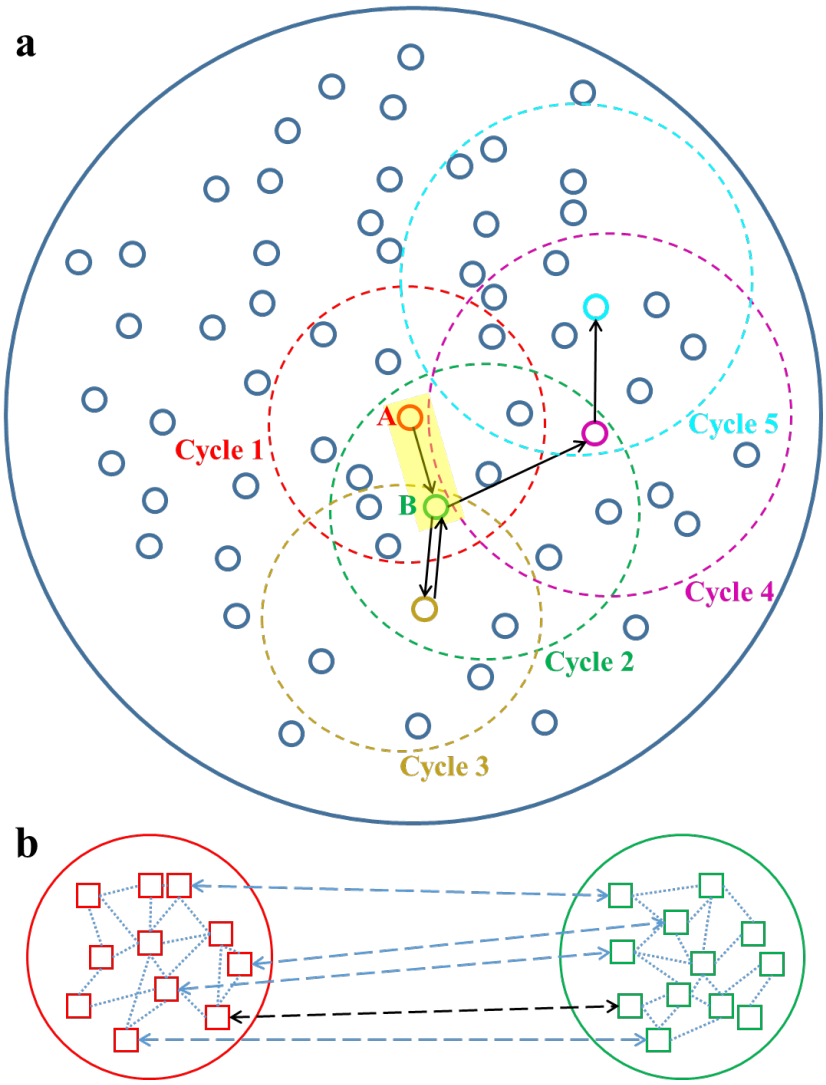

Figure S2 (**a**) Illustration of our reaction network exploration. Each large dashed circle represents a cycle of SSW-RS for one selected intermediate as indicated by the colored small circle. **(b)** The enlarged view for the yellow shaded region in (**a**), where more details on the connection between two intermediates are shown. Each intermediate has a number of possible configurations (small squares) and can have a number of pathways leading to the other intermediate. Only the lowest energy barrier pathway (black dotted line) between the two intermediates will be recorded in the reaction database.

Our reaction sampling can explore a reaction network in an automated way by repeatedly utilizing the SSW-RS simulation to identify the low energy pathways nearby a particular molecule (more details on SSW-RS can be found later). As shown schematically in Figure S2-a, in the Cycle 1 we first start from molecule A (red small circle), the reactant, and utilize SSW-RS to explore its nearby products (red dashed circle). In the SSW-RS, the configurational space of the reactant can be sampled simultaneously in addition to its pathways to other products, as shown in Figure S2-b, where the global minimum of the reactant can be identified. After this cycle of SSW-RS, we obtain the first reaction database by collecting all the reaction pairs and identifying the pathways linking with the reactant A. The reaction database records the initial state (IS), the transition state (TS) and the final state (FS) for each elementary reaction, which can be distinguished by the SMILES name of molecule and the bond matrix

We then select one particular product B (green small circle) that has a low energy barrier from A to B, and thus continue the Cycle 2 SSW-RS simulation, now with B as the reactant. This procedure is repeated and the reaction database is expanded until the whole reaction network is explored, e.g. for glucose, several C1 molecules, e.g. CO_2 and HCOOH, H_2CO molecules appears as the final product in the SSW-RS. It should be mentioned that the selection of the

initial molecule for the next cycle SSW-RS is achieved by sorting the overall barriers of the available reaction pathways. The overall barrier is with respect to the starting molecule, i.e. glucose in our case. The low barrier products will be selected first and the new pathways will always be added to the reaction database to update the reaction network.

In the following, we describe in more detail the SSW-RS method, which can also be found in our previous work[8].

(i) Reaction sampling via extensive SSW global search

The reaction sampling is carried out by using the SSW method, which aims to generate an ensemble of reactant–product pairs for pathway building. The structures of the reactant–product pair are geometrically close on PES thanks to the smooth structure perturbation of the SSW method, and they can be utilized later for TS location and pathway determination using the double-ended TS searching method, e.g. double-ended surface walking method (DESW)[9] in this work.

The SSW reaction sampling starts from one random configuration of the reactant, which is the input structure and may well not be the GM of the reactant. During the simulation, the structures nearby this reactant will be visited, including the conformation isomers of the same reactant (the same phase region) and the likely products with different bonding patterns (the other phase regions). The region of the SSW sampling can be visualized as a large dashed circle as shown in Figure S2. The molecule can be distinguished by the SMILES name and the bond matrix

Different from the Metropolis Monte-Carlo scheme in the global SSW structure search, a special structure selection module (to decide whether a new minimum is accepted or refused) needs to be designed in reaction sampling, which is described as follows. If a new minimum in the other phase regions is identified, we record/output the reactant structure and the product structure of the current SSW step. Then the program will return back to the reactant by rejecting the new minimum to continue the PES exploration; on the other hand, if the new minimum identified is still at the same reactant phase, the simulation will accept the new isomeric structure and continue the structure exploration. The whole procedure will be repeated until a certain number of reactant–product (R–P) pairs are collected, typically a few hundreds of R–P pairs.

(ii) Pathway building and TS determination via DESW

Once enough R–P pairs are collected, we then need to find the reaction pathways connecting these R–P pairs. As shown in Figure S2-b, the reactants and the products obtained from the SSW reaction sampling may be separated by more than one minimum, the highest energy TS along the pathway will be identified first and the extrapolation from the TS to two nearby minima is performed to confirm the reaction. If it is not an elementary reaction, an iterative procedure is invoked to connect each segment and identify the pathway for each elementary reaction using DESW method. If the pathway can be finally established, the barrier is calculated with respect to the GM energy of the reactant, which will be utilized as a quantitative measure to compare different pathways and to select the low energy pathways. The DESW method to identify the highest energy TS for a R–P pair is described briefly below.

The DESW method operates with two structural images starting from the reactant and the product, respectively, to walk step-wisely towards each other. The surface walking involves the repeated bias potential addition and local relaxation with the biased-CBD method to correct the walking direction, in a manner similar to the SSW and BP-CBD method. Since the TS location is the concern, the Gaussian width utilized in the DESW method is generally much smaller, e.g. 0.1–0.2 Å, compared to that (0.6 Å) in the SSW method for PES exploration. The DESW method can fast build a pseudo pathway to connect two minima since the added Gaussian functions effectively smooth the corrugated PES. The TS location is then performed from the highest energy image point at the pseudo pathway using the single-ended CBD TS searching method.

5. Benchmark for glucose pyrolysis reaction network

From the glucose pyrolysis reaction network, 6407 reaction pairs (IS, TS and FS), we have respectively selected 500 lowest energy pathways, 2060 elementary reactions involving 1751 distinct intermediates, that are associated with the glucose to the three key products, i.e. HMF, FF and AA, and benchmarked them with DFT calculations. In Figure S3, we plotted the intermediates from reaction network data using NN energetics (A) and DFT energetics (B), where the x and y axis are the structural parameters obtained from fingerprint similarity metric using RDkit (http://www.rdkit.org. developed by Landrum). As shown, the two maps are largely identical, suggesting the consistency in energetics between two methods. The RMSE in energy between NN and DFT is 10.15 meV/atom for all these data (6180=2060*3).

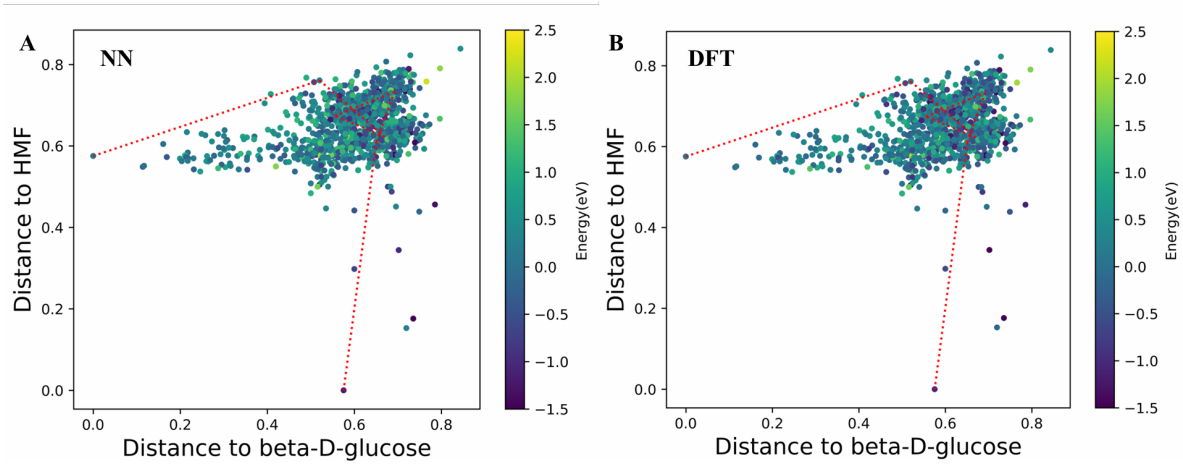

Figure S3 Reaction dataset calculated using NN and DFT. The x and y axis are similarity distances with respect to β-D-glucose and HMF. The similarity distances are calculated using the fingerprint algorithm in RDkit using the Tanimoto similarity. The lowest energy path from β-D-glucose to HMF is marked by red dotted line.

6. Reaction pathways to other products

We have analyzed carefully the pathways in our reaction database to identify the pathways to different products mentioned in experiment, e.g. LG, HAA, different Furan products (HMF, FF, 2-furanmethanol and furan et al.) and formic acid. We found that the LG, HMF, FF and HAA, the major products in most experiments, are indeed the products with lowest energy pathways among these known products. Here we also provided the pathways leading to LG, 2-furanmethanol and formic acid. The reaction pathways and their overall barrier are shown in Figure S4.

As shown, LG product can be produced from glucose in one step and is a major product in glucose pyrolysis. The pathway has been identified in our previous work[8]. The barrier is 1.91 eV, identical to the HMF pathway. The 2-furanmethanol and formic acid share the same pathway with the overall barrier 2.14 eV (with respect to beta-D-glucose). The 2-furanmethanol product has very low yields in experiment, ~0.60 %[10, 11].

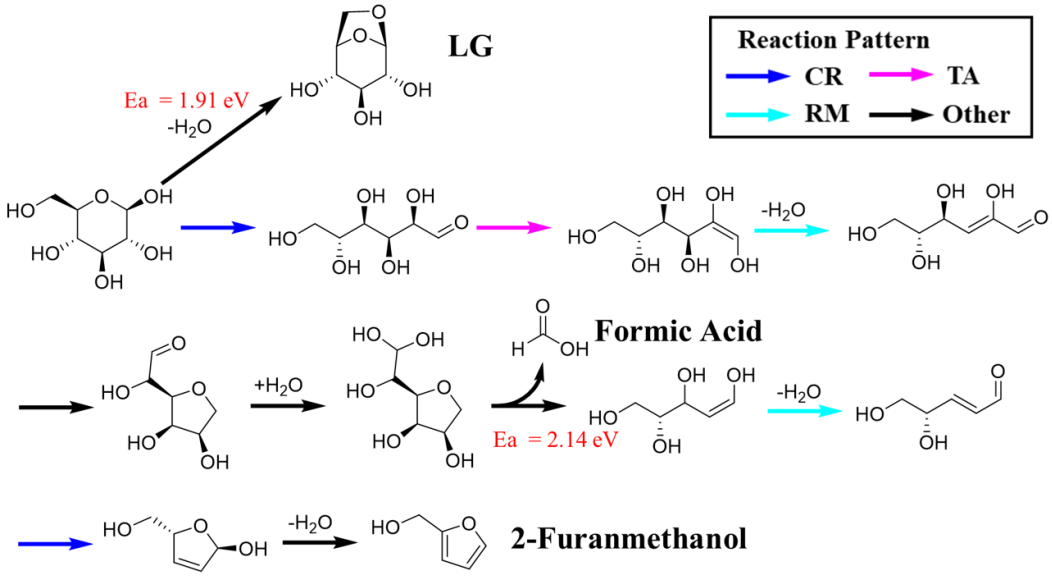

Figure S4 The lowest energy pathways to LG, 2-furanmethanol and formic acid identified from the glucose reaction network. The overall barrier with respect to beta-D-glucose is indicated in the rate-limiting step.

1. Huang, S. D.; Shang, C.; Zhang, X. J.; Liu, Z. P., Material discovery by combining stochastic surface walking global optimization with a neural network. *Chem Sci* **2017,** *8* (9), 6327-6337.
2. Huang, S. D.; Shang, C.; Kang, P. L.; Liu, Z. P., Atomic structure of boron resolved using machine learning and global sampling. *Chem Sci* **2018,** *9* (46), 8644-8655.
3. Rogers, D.; Hahn, M., Extended-connectivity fingerprints. *Journal of chemical information and modeling* **2010,** *50* (5), 742-754.
4. Ramakrishnan, R.; Dral, P. O.; Rupp, M.; von Lilienfeld, O. A., Quantum chemistry structures and properties of 134 kilo molecules. *Sci Data* **2014,** *1*, 140022.
5. Ruddigkeit, L.; van Deursen, R.; Blum, L. C.; Reymond, J. L., Enumeration of 166 billion organic small molecules in the chemical universe database GDB-17. *J Chem Inf Model* **2012,** *52* (11), 2864-75.
6. Baker, J.; Chan, F., The location of transition states: A comparison of Cartesian, Z‐matrix, and natural internal coordinates. *Journal of computational chemistry* **1996,** *17* (7), 888-904.
7. Shang, C.; Liu, Z. P., Constrained Broyden Dimer Method with Bias Potential for Exploring Potential Energy Surface of Multistep Reaction Process. *J Chem Theory Comput* **2012,** *8* (7), 2215-22.
8. Zhang, X. J.; Liu, Z. P., Reaction sampling and reactivity prediction using the stochastic surface walking method. *Phys. Chem. Chem. Phys* **2015,** *17* (4), 2757-69.
9. Zhang, X. J.; Shang, C.; Liu, Z. P., Double-Ended Surface Walking Method for Pathway Building and Transition State Location of Complex Reactions. *J. Chem. Theory Comput* **2013,** *9* (12), 5745-53.
10. Patwardhan, P. R.; Satrio, J. A.; Brown, R. C.; Shanks, B. H., Product distribution from fast pyrolysis of glucose-based carbohydrates. *Journal of Analytical and Applied Pyrolysis* **2009,** *86* (2), 323-330.
11. Mayes, H. B.; Nolte, M. W.; Beckham, G. T.; Shanks, B. H.; Broadbelt, L. J., The Alpha–Bet(a) of Glucose Pyrolysis: Computational and Experimental Investigations of 5-Hydroxymethylfurfural and Levoglucosan Formation Reveal Implications for Cellulose Pyrolysis. *ACS Sustainable Chemistry & Engineering* **2014,** *2* (6), 1461-1473.
12. Frisch, M.; Trucks, G.; Schlegel, H. B.; Scuseria, G.; Robb, M.; Cheeseman, J.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G., Gaussian 09, revision a. 02, gaussian. *Inc., Wallingford, CT* **2009,** *200*, 28.

7. Atomic coordinates for HMF, HAA and FF pathways in Figure 7

For each reaction, only the lowest energy conformation for minimum (IS and FS) and the lowest energy TS are provided. The energy (zero-point-energy corrected) of all structures are calculated using Gaussian 09[12] with UB3LYP/6-311++G(d,p) setup.

14 β-D-glucopyrannose

Energy -18699.8496 eV

H	5.738335861	1.545062383	4.964718513
H	6.709280772	5.123032673	6.207454741
H	5.797800093	6.554454919	3.661943399
H	1.986457911	5.750054467	5.319440534
H	4.416808244	6.383275570	6.379828854
H	8.398988424	4.561960192	4.776805763
H	3.643569968	5.072737873	3.738224135
H	7.289700626	7.721698138	5.004153128
H	4.712269384	3.830848560	6.328891218
H	4.089643783	2.558397534	3.631557038
H	3.052677412	2.410247929	5.068784502
H	3.976402873	8.265579363	5.036327088
C	6.593676258	5.197745028	5.114321654
C	5.813188724	6.466004453	4.755754562
C	4.386446634	6.365187079	5.280528165
C	3.730273309	5.060657883	4.834122133
C	4.612772951	3.870983481	5.234167989
C	4.079983157	2.538621104	4.729723727
O	7.835885726	5.285950421	4.480927245
O	6.393513023	7.625544644	5.345984564
O	3.559922492	7.427352751	4.807580989
O	2.448903796	4.909735213	5.427830861
O	5.914396619	4.043166370	4.642027514
O	4.819101964	1.431701964	5.228901682

1 D-glucose

Energy -18699.7694 eV

H	8.877729097	6.699558914	3.925242318
H	2.575084866	2.078264890	4.409536963
H	3.317806640	3.414438178	6.495334508
H	3.920600536	5.388429837	3.313164357
H	4.949575051	3.273354338	4.819739682
H	8.185015991	4.288734605	5.116813074
H	5.252330108	5.229362968	6.455254913
H	3.697378312	6.599007912	5.424806715
H	6.531571485	5.385025731	3.695425541
H	6.996318638	7.505938622	4.884708784
H	7.451408492	6.604599997	6.348403874
H	1.446983136	5.020231199	5.615576807
C	2.134150979	3.020290343	4.782276781
C	3.054488027	3.942077216	5.562748807
C	4.355957288	4.190616561	4.772813079
C	5.186559456	5.350938713	5.365965154
C	6.606465450	5.366774918	4.793131958
C	7.426050136	6.573162019	5.256645437
O	0.973685213	3.299457979	4.597808850
O	2.375428650	5.148405785	5.874152473
O	4.077208090	4.436979254	3.400315198
O	4.582144265	6.600867994	5.028260284

O	7.232223693	4.159303624	5.217372037
O	8.793836401	6.424178403	4.844502410

2 D-fructose

Energy -18699.8402 eV

H	3.530617902	4.312392615	3.510399016
H	5.397824376	2.898737228	2.573821444
H	6.197321062	4.319120618	1.923166927
H	3.285633606	2.128985134	4.357957076
H	5.536139252	6.140601391	4.299344253
H	7.978338879	2.875136123	3.320060034
H	3.870400790	5.881726139	5.965088436
H	6.464278188	4.940565765	6.361556387
H	3.609212256	3.957113558	7.357982859
H	2.017116023	2.660560810	6.205767102
H	1.884720014	4.289738494	5.520690137
H	5.471380352	2.740803890	6.683711260
C	6.284331465	3.535224307	2.687023565
C	6.236788724	4.200093883	4.044296681
C	5.079143370	5.145796861	4.372302350
C	4.576765819	5.054636815	5.842241245
C	3.845506732	3.773758444	6.301032169
C	2.533315690	3.417772886	5.608833363
O	7.456314756	2.784653410	2.509007026
O	7.167824620	4.042548747	4.820459389
O	4.054673302	5.129882413	3.408514585
O	5.650588726	5.298715168	6.749058964
O	4.662108482	2.608813248	6.178059843
O	2.735025160	2.918317641	4.280868055

10 hex-1-ene-1,2,3,4,5,6-hexaol

Energy -18699.4175 eV

H	4.684944881	2.957511312	5.933703760
H	8.398060697	4.637803374	4.223876725
H	3.529647280	5.178024564	1.964606650
H	9.949018651	5.110018345	5.760316304
H	5.986267551	4.236758451	3.791668741
H	1.940861859	5.460073620	5.999500139
H	5.003493518	6.288136442	4.847059997
H	4.604314148	5.320800870	6.951181766
H	3.123142299	4.088057624	3.922691409
H	2.598137771	7.063471677	4.394580793
H	1.643521499	6.081611040	3.276396086
H	7.372781033	4.771602363	7.541540604
C	8.112666153	4.727398209	5.262603791
C	6.865184893	4.547851896	5.696960377
C	5.675622793	4.232368430	4.836910814
C	4.559428725	5.293475774	4.984556045
C	3.461044908	5.130351224	3.928510856
C	2.249676614	6.041783081	4.186171215
O	9.093948975	5.034696670	6.189028191
O	6.556103725	4.645849360	7.040931802
O	5.174027173	2.922770310	5.101614102
O	3.928308171	5.203459492	6.269929072
O	4.094780079	5.466328664	2.687395198
O	1.395016599	5.559797206	5.208265560

7 3-deoxyglucos-2-ene(3-DGE)

Energy -18699.9202 eV

H	1.868787385	4.593349326	8.023845499
H	8.467547940	5.594810676	4.159568609
H	7.598565149	4.934571448	6.277302532
H	3.719180576	2.513173841	3.089720549
H	5.699407375	3.596983262	5.827206805
H	3.926487640	5.964052396	4.985249463
H	5.897772671	5.917296226	3.068269352
H	7.322882627	4.300298649	3.758069199
H	2.245089748	5.520320897	3.379337469
H	6.545395312	7.254830013	5.182432066
H	3.195459551	5.004645198	7.366315854
H	5.381607367	5.932800463	7.306043911
C	7.413097082	5.314326525	4.160519318
C	6.877029455	5.392667681	5.592713181
C	5.524705853	4.675308696	5.834008308
C	4.417092210	5.003087703	4.866488534
C	3.875341963	4.154801730	3.974138631
C	2.669492947	4.519505243	3.202726608
O	6.758503985	6.270537736	3.321318870
O	6.759769166	6.758492189	5.987112571
O	5.090728553	5.017715762	7.160800944
O	2.233288489	5.134008611	7.317811953
O	4.338601267	2.907090484	3.731452591
O	2.174165692	3.725325247	2.427547181

11 5,6-dihydroxy-2-oxohex-3-enal

Energy -18699.8674 eV

H	9.384793764	3.461009321	1.952808746
H	1.744424747	4.390431003	6.149187533
H	0.810738739	5.125379496	2.952363406
H	8.395647242	3.607437649	5.834542854
H	5.456607882	5.096489996	4.851741686
H	9.899211926	3.878813429	5.680738603
H	3.697518625	6.091312334	3.600596723
H	5.510948563	3.887419545	8.400210268
H	2.062080364	6.594745199	5.982660327
H	1.667798919	7.680011418	3.792373921
H	0.211425902	6.861989290	4.391345943
H	9.070919726	3.835573946	3.412958975
C	5.658614589	4.203060614	7.349919165
C	4.359737894	4.652772602	6.659358167
C	4.473152395	5.175005752	5.301426931
C	3.471293386	5.750798373	4.607477470
C	2.044290202	5.978487568	5.071280519
C	1.226129399	6.703149929	4.007032162
O	6.733025687	4.170461080	6.804977120
O	9.058441498	4.178433033	2.502836593
O	3.331575006	4.516186679	7.312853770
O	9.158405895	3.422623000	5.269273495
O	1.367398923	4.749482440	5.331848113
O	1.205818726	5.988926305	2.780187508

15 2,5,6-trihydroxyhexa-2,4-dienal

Energy -18700.6874 eV

H	4.331701605	3.937183409	7.204083379
H	5.985234119	6.403989670	1.335689467
H	7.995488544	5.010138109	5.886660944
H	1.963024193	6.260303103	5.261671321
H	4.535062651	5.531935578	3.022072381
H	5.667417157	4.554596192	9.049134381
H	5.856769784	4.530028091	5.651557380
H	8.465856504	5.597888151	3.445684781
H	6.577861434	4.317196225	7.813861912
H	2.678099707	4.115596833	3.572754109
H	1.743291080	3.935716447	5.067200140
H	8.934306965	4.726630302	7.094073645
C	6.858014427	6.173697403	1.969632377
C	6.594096015	5.568188220	3.259315259
C	5.343020262	5.269050027	3.696471514
C	5.037206992	4.699862259	4.967547417
C	3.784530782	4.388435380	5.399248922
C	2.526812095	4.519117982	4.574234378
O	8.004629552	6.416204158	1.607093065
O	7.720441794	5.312230509	4.006787741
O	5.736842123	4.045852708	8.235833724
O	8.014405135	4.863351867	6.849995135
O	3.522074251	3.944356931	6.637238698
O	2.123812829	5.878450450	4.392157937

16 2-(hydroxymethyl)-5-(hydroxymethylene)-2,5-dihydrofuran-2-ol

Energy -18700.3184 eV

H	6.394389228	6.101956515	3.366142534
H	3.443032399	7.424020383	7.410544906
H	5.813938662	3.109807936	7.196118059
H	5.204786206	2.050934055	5.286926313
H	2.964475393	7.869301236	4.768444631
H	6.718043977	4.304828658	6.890472933
H	3.608294289	6.580310460	2.529503678
H	5.129545161	5.129891185	7.894586094
H	5.683722873	0.910818797	6.229464026
H	3.322346994	3.545822381	4.031152861
H	3.940126740	3.823633583	2.383553986
H	6.008022007	3.047158482	3.340430879
C	4.038455399	6.566960539	7.115224865
C	4.143890448	6.284043996	5.799443525
C	3.560604109	6.971766911	4.678885145
C	3.884291250	6.326740144	3.542349064
C	4.757964207	5.147752832	3.876914745
C	4.209215282	3.782422940	3.444501972
O	4.574606125	5.918881733	8.149106373
O	5.230519184	1.758261330	6.221794819
O	6.055450879	5.202339820	3.292990857
O	6.217038306	3.905487716	7.609408954
O	4.870840087	5.196212320	5.313915709
O	5.153174796	2.731279042	3.662626070

6 HMF

Energy -18700.8928 eV

H	4.867676386	5.372793530	1.818678982
H	2.094077460	5.589703248	7.840959043
H	6.086873051	8.464284758	3.634471766
H	6.852755264	6.299408469	6.466094820
H	1.497662514	3.426921148	6.264905659
H	6.023629207	1.652158079	3.037584474
H	3.018497915	1.838257182	4.630816294
H	5.551863511	6.172891958	2.946582286
H	5.520492538	6.821721491	7.029571908
H	6.163292741	3.583918262	3.934711330
H	6.688114801	2.679198943	5.378774988
H	5.821921882	7.518796357	4.837472923
C	3.146019105	5.534626445	7.506208965
C	3.406336182	4.436413442	6.617012710
C	2.557831508	3.498581627	6.074818185
C	3.338749264	2.675942424	5.226630021
C	4.619008446	3.161789099	5.301364727
C	5.894692212	2.777495180	4.626373525
O	3.960173631	6.366095279	7.886768964
O	6.290487505	7.081149948	6.484940114
O	5.532747767	5.295544108	2.509099768
O	5.593088410	7.682034093	3.895452264
O	4.678717294	4.219766076	6.141948265
O	5.722065410	1.541141852	3.943261022

17 1,2,4,5,6-pentahydroxyhexan-3-one

Energy -18699.7351 eV

H	9.745504947	2.714139759	4.518604332
H	7.814027655	4.204189912	4.026671448
H	6.161564983	2.832144913	5.149078431
H	4.248850637	2.467988547	0.878020811
H	5.608846070	3.774530219	2.797872570
H	7.486168113	0.856654190	4.822715284
H	8.221805464	2.896828463	2.880950143
H	6.251293636	1.116680860	2.253621500
H	3.099066085	1.040421699	2.277092174
H	1.649244232	3.615813973	3.045846621
H	1.012705260	2.412013613	1.916484642
H	1.647952222	1.958293295	4.622765673
C	7.911656460	3.118046739	3.907974755
C	6.566439167	2.453117916	4.204848587
C	5.556040204	2.717437242	3.085057656
C	4.088952986	2.473006939	3.510464531
C	3.081054195	2.134510541	2.397480236
C	1.654391372	2.549941523	2.787541466
O	8.850805850	2.587631081	4.848457130
O	6.714319658	1.034994149	4.269874479
O	5.892888955	1.956181141	1.925435140
O	3.747584152	2.589951647	4.667822342
O	3.391737796	2.797911841	1.180710489
O	1.123950899	1.761120093	3.836804402

18 but-1-ene-1,2,3,4-tetraol + HAA

Energy -18699.1310 eV

H	4.207531891	5.683779751	6.431905770
H	2.824452069	5.882534343	4.255905986

H	2.989038468	4.159297553	2.460413531
H	2.877763396	3.622248557	5.875344108
H	5.632244332	5.171681168	2.550207282
H	7.357640514	7.306608657	6.217489990
H	1.337580282	4.923967372	4.299718093
H	5.501283217	2.791770382	4.109110908
H	5.721984668	4.060306509	6.606867033
H	7.366241725	5.501794143	7.587926626
H	8.103395381	4.589471854	6.249443395
H	5.210005616	6.985538205	4.684295314
C	2.423493521	4.890872484	4.484409577
C	3.003632220	3.880247156	3.529230373
C	5.593952005	5.487362142	3.585603646
C	5.913139453	4.628936159	4.564429138
C	5.990224701	4.962631845	6.040357088
C	7.391498944	5.377587390	6.498383232
O	2.697736868	4.574019896	5.835944391
O	3.401131553	2.793742489	3.900045239
O	5.199939826	6.783170480	3.733259780
O	6.294724374	3.335279808	4.241518153
O	5.108751962	6.046051052	6.394546036
O	7.852613013	6.561100607	5.863645309

19 2,4-dihydroxybut-2-enal + HAA

Energy -18699.3979 eV

H	5.352092997	7.531281811	3.521534563
H	9.565707680	5.454972950	7.375136157
H	9.879781783	3.800400764	5.479993751
H	2.376902025	3.617048924	2.791649880
H	3.343363533	7.492619918	6.213404513
H	2.671937752	3.978956607	5.225762338
H	8.644651355	3.982015343	7.673939892
H	2.130209704	4.668987226	1.702209292
H	5.600990741	5.272478349	3.387139462
H	4.862698570	3.610212950	5.640103552
H	5.015364589	3.086171411	3.963884287
H	7.150263262	5.723969349	6.253453748
C	8.694024453	4.875068224	7.033499690
C	8.975732098	4.422302023	5.624784215
C	3.435432827	6.463022772	5.827110024
C	4.375296037	6.342393858	4.687350150
C	4.865102350	5.195322973	4.184771145
C	4.504962043	3.791928966	4.618289643
O	7.516840400	5.628472456	7.144383184
O	8.260621404	4.720157191	4.696265791
O	2.813582800	5.547077374	6.326769290
O	4.721258984	7.595125420	4.246825427
O	2.124939514	3.720698490	1.857372408
O	3.118243094	3.479314652	4.524367598

20 pent-1-ene-1,2,3,4,5-pentaol +formaldehyde

Energy -18698.9005 eV

H	5.455569590	9.158359605	4.408023003
H	7.061008113	7.863237562	5.274311697
H	7.181052777	5.547841081	4.757001072
H	6.385845674	7.195435026	2.657050950

H	4.255423628	5.752413510	3.921017484
H	5.930936676	4.680843636	2.442429125
H	5.537331717	7.190840238	5.927025470
H	3.675267672	4.710874775	6.922144844
H	5.107701081	2.711074845	6.673646578
H	1.053303811	2.240060338	6.224036502
H	2.752995638	1.708946585	6.824122072
H	5.900182440	2.666701306	3.960425721
C	6.105687325	7.393891844	5.016032079
C	6.380811031	6.097541895	4.254621704
C	5.146938182	5.153987940	4.149797138
C	4.906567843	4.403588946	5.434988781
C	5.277010658	3.138770864	5.691380150
C	1.977157216	2.493562705	6.775351673
O	5.362252460	8.244546206	4.125290915
O	6.856686006	6.396889309	2.938976993
O	5.378874906	4.215121133	3.090694639
O	4.317842290	5.211777303	6.396370898
O	5.868034414	2.249997969	4.840954852
O	2.125518863	3.573695378	7.294305667

21 2,4,5-trihydroxypent-2-enal

Energy -15583.3529 eV

H	3.507176116	3.753034674	1.695051698
H	2.472540557	1.379322852	1.131072808
H	0.811347608	3.108479874	1.502174775
H	4.267202719	2.489683841	5.995573836
H	0.988716170	2.866188825	4.197646007
H	2.761896327	2.814196842	5.883060830
H	1.726746701	1.051166092	2.708423153
H	2.231359936	5.651335215	2.418633284
H	1.178028686	6.197245041	5.677878408
H	3.608567227	1.927417853	3.668016530
C	2.364585826	1.748796219	2.152708362
C	1.716240710	3.145409810	2.120465733
C	1.383158889	3.608030826	3.512359359
C	1.572361244	4.844327602	4.001085580
C	1.364498818	5.134967934	5.438721128
O	3.670107860	1.825223667	2.699123518
O	2.614598880	4.058984879	1.466060503
O	3.468983066	2.261405438	5.509697488
O	1.981351979	5.943437236	3.315228087
O	1.434419756	4.295225005	6.316672263

22 5-hydroxy-2-oxopent-3-enal

Energy -15583.1820 eV

H	3.800819178	4.908292771	7.508037660
H	3.096893827	6.795956273	2.840990965
H	4.528890810	5.441671180	1.562190266
H	3.488310129	6.403313565	7.835336980
H	5.632923543	3.466304666	2.228979888
H	3.933215657	2.834329786	6.875927077
H	2.636360646	5.411969529	3.846051659
H	4.017512520	6.180043972	5.364616675
H	6.621489865	1.994392230	3.791949778
H	4.707425410	2.661330570	8.186864862

C	3.487160668	5.977544581	3.453540146
C	4.337962747	5.083019862	2.571799450
C	4.949602994	3.937397524	2.929580361
C	4.782172318	3.259852441	4.213804547
C	5.821829320	2.160503593	4.541017561
O	4.269240463	6.538500558	4.491841989
O	3.770917403	5.811198323	7.134433746
O	3.926069008	3.082236893	7.816148399
O	3.904494682	3.485292178	5.028127458
O	5.778252814	1.539964620	5.568849682

23 2,5-dihydroxypenta-2,4-dienal

Energy -15584.1043 eV

H	4.313166739	3.922972407	7.213978706
H	5.961145320	6.345006356	1.307258033
H	8.013525394	5.075247933	5.916158461
H	4.503128937	5.463101808	3.024718490
H	5.661021421	4.553010037	9.063513514
H	5.900907469	4.480393148	5.620678983
H	8.443859993	5.638220779	3.446687915
H	6.561319683	4.356625917	7.813559963
H	8.924527756	4.644088874	7.100844913
H	2.934630236	4.552922831	4.802017233
C	6.836170830	6.142961489	1.948006307
C	6.575532026	5.562011333	3.245495284
C	5.332553235	5.244293284	3.691879161
C	5.061916244	4.677968458	4.969515427
C	3.814088994	4.404571841	5.422291600
O	7.979859102	6.395608396	1.583256697
O	7.702676390	5.339546875	4.005660855
O	5.729911452	4.062672358	8.238717315
O	8.024421775	4.893125706	6.872857988
O	3.513373003	3.942256170	6.632313155

24 5-(hydroxymethylene)-2,5-dihydrofuran-2-ol

Energy -15583.5572 eV

H	3.475756762	5.099126754	3.138545294
H	2.538949440	5.040731618	8.132832185
H	6.934741728	7.035664628	3.073127440
H	6.897283315	7.214828790	6.748673153
H	1.953531989	3.065183031	6.291058957
H	3.073182506	2.324384252	3.982662077
H	5.618558570	6.259222807	3.374285677
H	4.740781557	6.691059067	7.275600902
H	6.068259808	7.338475586	5.455912172
H	5.517668554	3.516988008	4.212507981
C	3.358258661	5.314867446	7.478846068
C	3.584631288	4.584229981	6.368806831
C	2.830751328	3.486810922	5.820160659
C	3.387771975	3.110510061	4.653067482
C	4.554751282	4.009950253	4.365940182
O	4.047849007	6.376014928	7.910192033
O	6.034634273	7.488463461	6.423033123
O	4.397538248	4.810452538	3.188353593
O	6.172234607	7.009688923	3.658093461
O	4.658021943	4.843224520	5.522030008

25 FF

Energy -15584.2214 eV

H	5.038448061	5.376054531	1.506912746
H	2.718154106	4.905137634	8.702060752
H	6.616597191	8.057859175	3.452723518
H	6.908045121	6.667025674	6.698424921
H	1.992057541	2.762067580	7.089251852
H	2.719876395	2.055199923	4.536057210
H	5.746258880	5.905840729	2.764463853
H	5.419685573	6.967459618	6.955118577
H	5.952833041	7.367925763	4.670257724
H	4.476725862	4.035848732	3.761372693
C	3.389825345	5.254037480	7.897133102
C	3.360521990	4.431654685	6.717833630
C	2.674460111	3.272993743	6.426921796
C	3.050283599	2.905798107	5.109207180
C	3.934975143	3.861827632	4.683759250
O	4.077247312	6.254737203	8.050681632
O	6.191620475	7.249193085	6.426288239
O	5.510634965	5.080334109	2.290621349
O	5.934872429	7.422382722	3.688540268
O	4.132033694	4.786499447	5.646098992

TS

TS of 14→1

Energy -18698.2539 eV

H	5.200502134	2.300368570	4.899757973
H	4.352049985	5.708010749	2.602261704
H	6.797720914	4.893683625	2.972240759
H	4.249773133	7.269997879	4.954642588
H	7.194837574	3.563589092	5.040220447
H	6.705775375	6.303668261	5.115935591
H	5.662956906	4.059438034	7.010480865
H	4.501575785	3.411664565	2.980699933
H	3.205353595	4.083206464	6.200866829
H	4.973686254	6.452384563	6.849149763
H	3.322476602	6.102182270	7.428441198
H	3.171359668	6.167312058	4.831800571
C	4.920658201	5.691028710	3.544596031
C	5.960797834	4.578798003	3.603523470
C	6.466376404	4.378949279	5.047517741
C	5.318092951	3.920478725	5.980730084
C	4.011933401	4.718526120	5.831984004
C	3.982713933	6.106151127	6.563758950
O	5.280596626	6.839488836	4.045548879
O	5.457611953	3.338032521	3.093634842
O	7.132109290	5.533107607	5.532845491
O	5.064268473	2.527269461	5.830160379
O	3.646859309	5.029146390	4.460243389
O	3.419913699	7.023517018	5.578958524

TS of 1→2

Energy -18698.2309 eV

H	6.255494397	5.918326545	3.615378578
H	3.207894588	6.869037154	7.391380484
H	4.645623406	5.471169042	6.913180601
H	5.762217410	7.736081216	6.645088633
H	2.758709362	5.121221579	5.522874484
H	5.060666717	3.138509775	6.569800633
H	3.568231901	3.205942264	4.265057725
H	6.647057362	4.847133813	5.481248295
H	5.792354987	2.415699802	4.333740588
H	7.101275964	3.727900849	2.817336720
H	5.423090876	3.565455660	2.270624515
H	4.237294884	5.814758917	3.215188546
C	4.155920732	6.959693150	6.875167251
C	4.643470049	6.103961507	5.832197526
C	3.710031038	5.208042474	4.988803274
C	4.257645329	3.756097534	4.913311621
C	5.702018362	3.505328853	4.405826505
C	6.068820102	4.035069578	3.017557835
O	5.002876274	7.847160123	7.298806692
O	5.840776000	6.438832933	5.415572214
O	3.414796244	5.792255723	3.748541336
O	4.155742765	3.208133674	6.230692833
O	6.654567795	3.869742559	5.406900535
O	5.933423493	5.444445422	2.825722816

TS of 2→10

Energy -18697.9366 eV

H	3.990611141	6.042365325	2.871205095
H	4.357792866	2.802259119	3.783156438
H	5.354936216	3.817871312	1.978649648
H	4.489466784	2.083455083	5.227485101
H	5.579977228	6.231098270	4.317390333
H	7.391679833	2.400819312	3.330499375
H	3.718630946	5.882348789	5.941487693
H	6.363331000	5.120720898	6.483037514
H	3.508829335	3.933966863	7.251801689
H	2.244399726	2.526425059	5.777646276
H	2.457619939	3.897383361	4.635683952
H	5.861008811	3.115482441	5.991930710
C	5.932929388	3.491916532	2.830709653
C	5.980398275	4.135976648	4.029952380
C	5.038327863	5.280460858	4.371757983
C	4.546106096	5.172677536	5.841326162
C	3.979949523	3.793157150	6.277102362
C	2.956698474	3.180598878	5.278848136
O	6.794961399	2.451624212	2.565845848
O	6.786539054	3.745430127	5.001970097
O	3.892274304	5.322057882	3.499276649
O	5.555169101	5.598596471	6.736129950
O	4.975634240	2.761793897	6.413047172
O	3.768098036	2.267209515	4.445301940

TS of 10→7

Energy -18698.0261 eV

H	8.155041618	5.898436626	2.913889420
H	3.188130630	5.806382632	6.909466054

H	2.324000195	3.350673914	5.293145972
H	4.859455593	4.260214342	2.970164975
H	4.704868764	3.232258477	5.359817014
H	5.399262889	5.430854518	6.166794292
H	4.866547243	6.531950024	3.583610530
H	1.717597653	4.864787909	7.133488376
H	3.459539042	6.418605398	4.387857576
H	7.998960430	5.618941145	5.709925865
H	3.032719543	3.172889681	7.897028948
H	2.130393021	4.904918919	3.678390982
C	2.766955505	4.801934429	6.828300730
C	2.845116269	4.311438146	5.383178398
C	4.274814027	4.095996269	4.829612038
C	5.264521111	5.217665373	5.110345519
C	6.410026886	5.370972750	4.236844567
C	7.671152174	5.619415902	4.679936581
O	3.527251054	3.975992295	7.704799347
O	2.152408817	5.279677368	4.571827824
O	4.120909186	3.804777311	3.453982335
O	4.413586847	6.662777027	4.482757846
O	6.087603462	5.486944893	2.945839424
O	8.629138222	5.881494742	3.768995571

TS of 7→11

Energy -18698.4379 eV

H	2.710382866	5.917667102	4.389569331
H	3.355914575	1.093343658	3.818868936
H	7.118800782	4.933171426	2.162742520
H	4.174423327	2.279473786	4.331717847
H	7.162874418	6.443944371	3.804758553
H	6.951982558	6.044960787	7.649742932
H	6.564912515	7.620252004	5.789794415
H	4.458047014	4.719405777	5.524079132
H	4.677094969	7.220196162	7.189045985
H	3.721264667	8.393827790	5.292588369
H	2.597635062	7.359954825	6.182640262
H	5.611172595	5.178378435	6.931913255
C	5.706891294	4.917092976	3.876295229
C	6.292213579	4.341151664	2.605129367
C	6.303341240	6.073792178	4.350569278
C	6.000961716	6.711471154	5.596317100
C	4.605230206	6.676477918	6.237306457
C	3.449600312	7.352067806	5.489957668
O	4.742909205	4.255819277	4.415082443
O	5.911922053	3.313674368	2.108196548
O	3.729108280	1.469271291	4.621171315
O	6.687227875	5.593045478	6.835653235
O	4.372605898	5.301217114	6.550454386
O	3.093482948	6.790342717	4.246405441

TS of 11→15

Energy -18698.8805 eV

H	5.025538027	3.709187584	2.135684691
H	3.136869431	8.119420798	5.039031383
H	4.050917601	5.343171681	3.769680379
H	6.110547338	1.648183597	1.156929528

H	7.454432890	5.429150183	6.762948253
H	5.684337147	1.350071186	2.605713130
H	6.165174748	5.874890032	4.699807764
H	7.624095086	4.180897558	8.716730250
H	4.082564249	4.937934114	6.591903536
H	4.002115804	7.049291941	7.496669087
H	2.474661821	6.610089541	6.702061248
H	4.210203932	4.863682613	1.512073119
C	6.558277809	3.867298341	8.698048245
C	5.708349013	4.693808745	7.775368422
C	6.371676586	5.442877430	6.786562498
C	5.646144864	5.827247750	5.657282841
C	4.225655444	5.903548186	5.660108037
C	3.504220511	6.947240362	6.536492360
O	6.150386688	2.974441582	9.396904981
O	4.767093149	4.639858130	2.264404104
O	4.437128983	4.578667430	7.808724997
O	5.528695124	1.944209030	1.864302673
O	3.553965939	5.843115862	4.447704611
O	3.526947664	8.221716230	5.914863806

TSs of 15→16

Energy -18699.1677 eV

H	6.182256807	2.226840534	2.475956715
H	7.445834657	7.325960204	4.703430567
H	6.821926687	2.956207623	5.614144370
H	7.977679983	4.561690878	5.291701875
H	5.258459465	7.855842151	3.866950836
H	5.461384712	4.005989269	3.232750640
H	2.911879397	7.030208191	3.506329062
H	2.016550381	5.548884231	5.126603825
H	7.440689192	1.423555307	2.052939649
H	3.418097504	2.868727902	3.687910070
H	2.867950147	3.783656434	2.274540371
H	7.665284076	2.475056058	4.439326056
C	7.169752517	6.292477117	4.881648013
C	5.886347344	5.883293419	4.595488989
C	4.987632881	6.815885425	4.003517669
C	3.730968318	6.351442769	3.728843912
C	3.376682739	4.971284224	3.941385570
C	3.626171338	3.749737933	3.067011940
O	8.175112409	5.541769413	5.298958423
O	6.955713368	1.744758249	2.818989096
O	2.263101407	4.745248643	4.645789772
O	7.738703377	2.906044254	5.312287974
O	5.418417934	4.648523575	4.742468116
O	4.898014292	3.696776868	2.478513682

TS of 16→6

Energy -18699.6361 eV

H	4.197576835	4.671293497	2.620510470
H	2.232910502	5.770529733	7.586616128
H	5.915714652	7.433142147	3.313528914
H	6.841997305	6.611884228	6.602282313
H	1.657817900	3.631058093	5.944293448
H	5.755337529	2.942969701	2.848378560
H	3.223352988	2.100651257	4.340375893

H	5.331131900	5.876963698	3.540258064
H	4.990906498	6.800192130	7.104746336
H	6.900206671	3.594078900	4.709394063
H	6.394452603	2.048244766	5.419521906
H	5.884994439	7.048594344	5.377726713
C	3.261310549	5.720975993	7.227454460
C	3.559470479	4.667957365	6.389062828
C	2.724164296	3.705267746	5.789597301
C	3.512432897	2.922244088	4.974343929
C	4.824477971	3.426680924	5.081753439
C	6.131071957	2.812772764	4.678225527
O	4.040589957	6.648447519	7.648946319
O	6.068706490	7.148009348	6.401836584
O	5.046978957	4.624442148	3.071963646
O	5.534313593	6.856242738	3.979373962
O	4.859200486	4.431713763	5.960192871
O	6.037656540	2.196276208	3.424119314

TS of 1→17

Energy -18697.8932 eV

H	4.159410982	2.306293342	5.437897832
H	2.428316394	6.479776695	3.988390999
H	4.151230697	7.039710536	6.409460793
H	3.035116614	4.876104176	6.275039130
H	5.686627245	6.127199430	3.957152688
H	6.319722674	5.806433787	6.688476751
H	3.689898469	5.006345487	4.332138485
H	7.674426804	4.828154737	4.654724507
H	5.228051259	3.551111171	3.193948401
H	6.859115624	3.055515338	5.731273799
H	7.014893990	2.130964613	4.231096865
H	5.116670258	8.566804007	4.885357335
C	2.949652133	6.139064381	4.886364036
C	4.217693406	6.896785099	5.322735471
C	5.369697699	5.931412402	4.984980380
C	4.689997856	4.546276314	5.050676722
C	5.269930200	3.357053967	4.269564205
C	6.754769514	3.107979524	4.640322346
O	2.256390993	5.543326293	5.801264389
O	4.287459061	8.136707130	4.647437454
O	6.530126687	6.083965088	5.787807110
O	4.168295818	4.221440579	6.216390321
O	4.500561381	2.203542719	4.535040649
O	7.641944071	4.058033188	4.072459447

TS of 17→18

Energy -18698.6330 eV

H	4.210755130	5.678604142	6.473788736
H	2.693635379	6.003123262	4.382342012
H	3.377152559	4.490465321	2.476184113
H	2.909791708	3.603991189	5.854494509
H	5.531286726	4.997324962	2.607559085
H	7.323273318	7.309044522	6.122159848
H	1.539126647	4.675389868	4.191034646
H	5.003075294	2.873038117	4.036509896
H	5.744217875	4.094385429	6.718167114

H	7.455294081	5.525183967	7.536466614
H	8.104183832	4.599085324	6.167351418
H	5.013469697	6.858975217	4.668849247
C	2.572192606	4.922964148	4.473501510
C	3.496827596	4.188968588	3.524106454
C	5.296743355	5.296761899	3.620777539
C	5.819705464	4.510261051	4.652893872
C	5.980157035	4.966855046	6.097111851
C	7.409570237	5.392687309	6.448315517
O	2.808893625	4.567030269	5.833509433
O	3.761058272	2.950270045	3.777117717
O	5.012549093	6.627607241	3.722867691
O	6.004003782	3.244270154	4.426767710
O	5.107967772	6.058141633	6.417203626
O	7.825068879	6.565571291	5.770919829

TS of 18→19

Energy -18697.9615 eV

H	5.446080403	7.424002295	3.602630063
H	9.383444405	5.485411394	7.304471804
H	9.733197201	3.856487947	5.406418943
H	2.821897057	3.832249865	3.591691456
H	3.301858368	7.232414032	6.047480961
H	2.808121218	4.239935279	5.471341095
H	8.464392003	4.008112569	7.581672763
H	2.730818851	5.220218474	2.402645784
H	5.368419338	5.045505878	3.062733139
H	4.945508803	3.712750690	5.526136211
H	4.920358285	2.844690688	3.968389273
H	6.989576883	5.780214045	6.155400515
C	8.515847869	4.906708593	6.948224995
C	8.817179787	4.464048746	5.541661149
C	3.422644322	6.242265196	5.599686700
C	4.214659379	6.174607279	4.454833493
C	4.568813233	4.972529166	3.792649545
C	4.467921094	3.650288444	4.546585965
O	7.333285153	5.650607793	7.051631453
O	8.107758854	4.755048864	4.606135366
O	2.809851915	5.271572176	6.172733606
O	4.516742904	7.406031700	3.851746830
O	3.246552868	4.432074180	2.612833609
O	3.065069734	3.392224746	4.700265214

TS of 17→20

Energy -18698.4305 eV

H	5.399812033	9.074423166	4.464073507
H	7.092106460	7.723442659	5.275477271
H	7.027429396	5.382998921	4.839319501
H	6.397090270	7.029961942	2.693254628
H	4.117201302	5.805354096	4.004556165
H	5.710789868	4.545679008	2.557763787
H	5.527810791	7.183050964	5.956074355
H	3.327203647	4.671063792	6.951216286
H	5.141931699	2.879764213	6.900437995
H	2.494095545	2.771234696	5.276470664
H	3.159424954	1.816231724	6.705574730

H	5.349068076	2.584146519	4.097289135
C	6.103026277	7.317161735	5.036718443
C	6.273636089	5.980670560	4.320340350
C	4.956125697	5.139719601	4.238975959
C	4.708928974	4.479709648	5.581505443
C	4.925037616	3.130533662	5.870353931
C	2.889300306	2.796525151	6.299805111
O	5.419665208	8.178922474	4.115054881
O	6.765877496	6.187018511	2.997324621
O	5.102995275	4.159408645	3.210182195
O	4.212796176	5.249270261	6.511555692
O	5.383963804	2.193713047	4.989421407
O	2.514683111	3.719995052	7.107253941

TS of 20→21

Energy -15581.6492 eV

H	3.690722752	3.628178105	1.753579455
H	2.405438315	1.381881160	1.107626125
H	0.939205382	3.167768184	1.796580891
H	3.871382438	3.145944754	5.068448375
H	1.027648152	2.829687972	4.285232637
H	2.173511902	3.331671121	5.906605663
H	1.725836033	0.968483382	2.696288261
H	2.262058763	5.584430490	2.494617889
H	1.248434337	6.061065013	5.904580717
H	3.688393733	1.676480498	3.595008731
C	2.408653434	1.645357034	2.167421906
C	1.910635579	3.093738778	2.309148840
C	1.655605416	3.513021690	3.728334354
C	1.639747537	4.855555558	4.143435487
C	1.441065441	5.070325267	5.500058809
O	3.737694654	1.526301389	2.626286129
O	2.798408922	3.988387480	1.634209650
O	3.063152147	2.616313340	5.016677286
O	1.882196105	5.928323569	3.322403378
O	1.554097794	4.090964949	6.353108421

TS of 21→22

Energy -15582.2766 eV

H	5.293489514	7.310449444	6.181915434
H	6.755358553	7.339235618	4.256902538
H	5.736697455	5.774230968	2.739501813
H	4.636168960	8.827971371	5.889917804
H	4.782528339	3.651807012	3.280092007
H	4.232249319	7.293835250	4.861259243
H	7.550707400	5.776014138	4.455648384
H	6.172572262	5.349254306	6.314769925
H	4.695381544	1.715118712	4.287550980
H	3.470512828	5.959404465	4.032077801
C	6.614557288	6.319147356	4.627229389
C	5.538352644	5.618952766	3.799444497
C	5.196524071	4.231821214	4.097525897
C	5.451959389	3.559411274	5.289269407
C	5.123455420	2.072047542	5.249279261
O	6.334291390	6.383664006	6.017551154
O	4.213109245	6.573582289	3.938812376
O	4.423663541	7.889928243	5.941182249

O	5.951175640	4.012672955	6.367826444
O	5.318789169	1.314566212	6.162332540

TS of 22→23

Energy -15582.2754 eV

H	4.953140986	3.773402512	2.153076177
H	3.962553415	5.344150539	3.837263774
H	6.255272369	1.794456117	1.248290039
H	7.499635971	5.336333314	6.715944946
H	5.669924687	1.420399210	2.623070151
H	6.138055533	5.817905175	4.713263755
H	7.717454741	4.131659200	8.717013004
H	4.089821462	4.873514915	6.672765553
H	3.971169454	4.820292664	1.580797124
H	3.778995449	6.479225943	6.451537206
C	6.642185096	3.854339330	8.749741446
C	5.781040487	4.676378785	7.831763321
C	6.419895667	5.366905874	6.786704213
C	5.652007574	5.745830839	5.685706123
C	4.230656296	5.799100621	5.723529849
O	6.235082891	2.997572196	9.493995803
O	4.614725465	4.677410295	2.281987234
O	4.510877220	4.613280294	7.920781478
O	5.595574493	2.051602626	1.899351927
O	3.495135994	5.805165086	4.562807023

TS of 23→24

Energy -15582.4237 eV

H	2.088438862	7.404221530	4.207350303
H	6.367633817	3.321122303	6.708665900
H	5.348680473	8.729110543	7.059442278
H	7.579897636	5.723960817	5.684978655
H	3.995028135	3.142077439	6.597610670
H	7.084480737	7.051165452	4.191648898
H	1.838013611	4.373545358	5.961208804
H	5.223440303	7.610079786	5.971946639
H	7.263827313	7.846159608	5.465751764
H	3.395122552	5.766308497	3.772333122
C	6.360226580	4.307861816	6.258971606
C	5.165793381	4.814707736	5.791816379
C	3.978484459	4.057726156	6.019277578
C	2.818165805	4.647000287	5.590597125
C	2.939434438	5.791635399	4.752712037
O	7.566539748	4.842174087	6.152503084
O	5.608517957	8.492380422	6.164495404
O	2.057074482	6.777622404	4.941659730
O	7.726420802	7.201232783	4.897044069
O	5.006938931	5.962296545	5.133849908

TS of 24→25

Energy -15582.7520 eV

H	3.819839603	5.101925507	2.887278294
H	2.499414977	5.361291479	7.950820997
H	6.361671450	7.401768774	3.457425018
H	6.855351778	6.868101424	6.680826981

H	1.774809734	3.431246562	6.103932274
H	3.054917296	2.363985199	3.984439547
H	5.242999294	6.075562134	3.606869697
H	5.217756651	6.819926179	7.020014017
H	5.880929761	7.138862837	5.246471429
H	5.608371073	3.313233307	4.218978658
C	3.450423881	5.467579314	7.415464235
C	3.640258484	4.574973176	6.375700132
C	2.774504919	3.653344070	5.759966650
C	3.418777421	3.111372070	4.670944109
C	4.697541960	3.761508554	4.587362253
O	4.246585482	6.377666222	7.808290740
O	6.025008540	7.267963075	6.403245816
O	4.729052093	4.965978634	3.180686720
O	5.685241871	7.028957999	4.028792288
O	4.861700466	4.534631084	5.686219960