Electronic Supplementary Information for the Manuscript:

Insight into the existing form of glycolaldehyde in methanol solution: an experimental and theoretical investigation

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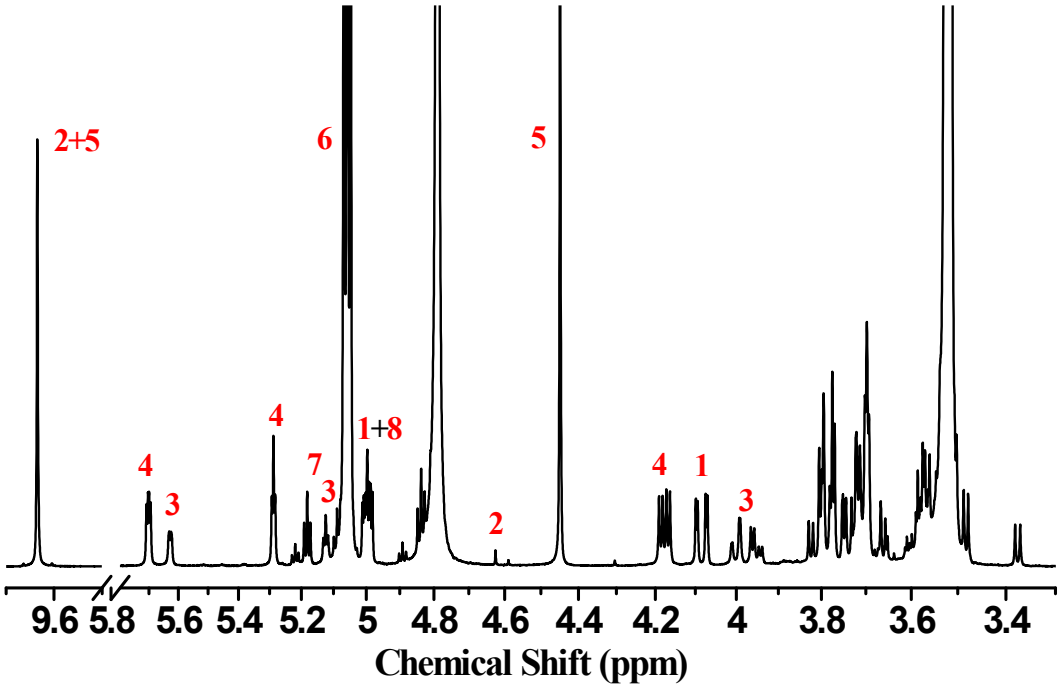

Figure S1. The ^{1}H-NMR spectra of GA in aqueous solution.

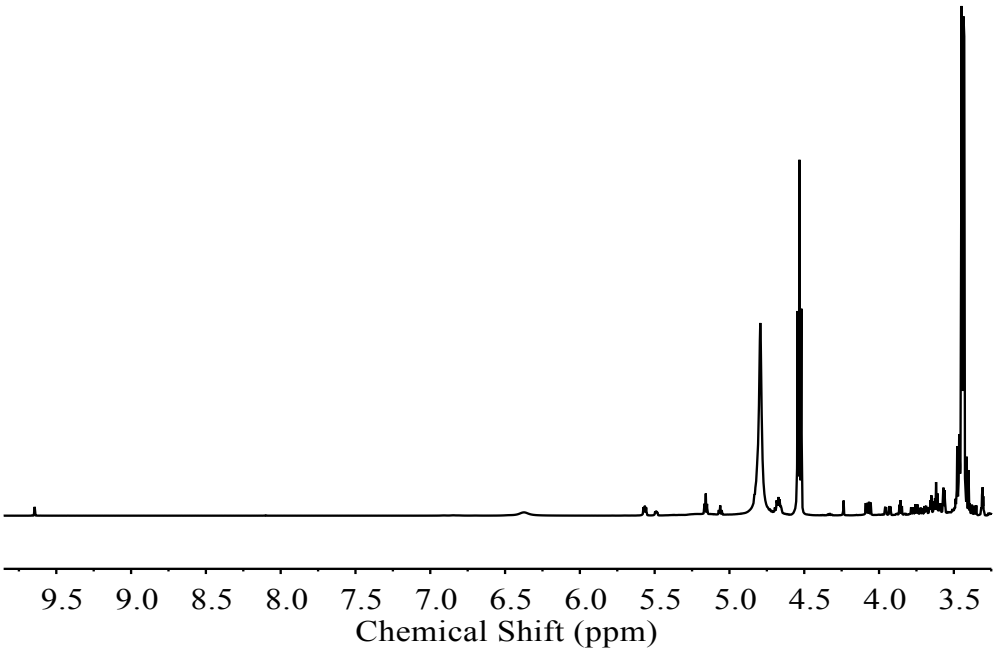

Figure S2. The complete ^{1}H-NMR spectra of GA in CD_3OD solution.

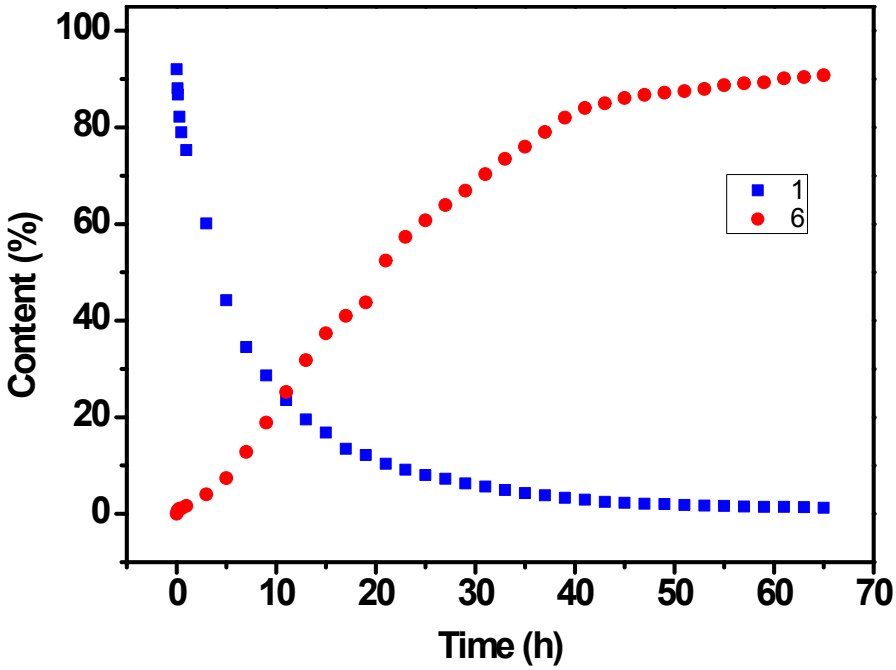

Figure S3. The contents of components 1 and 6 of GA dimer in methanol solution at different times by 1H NMR.

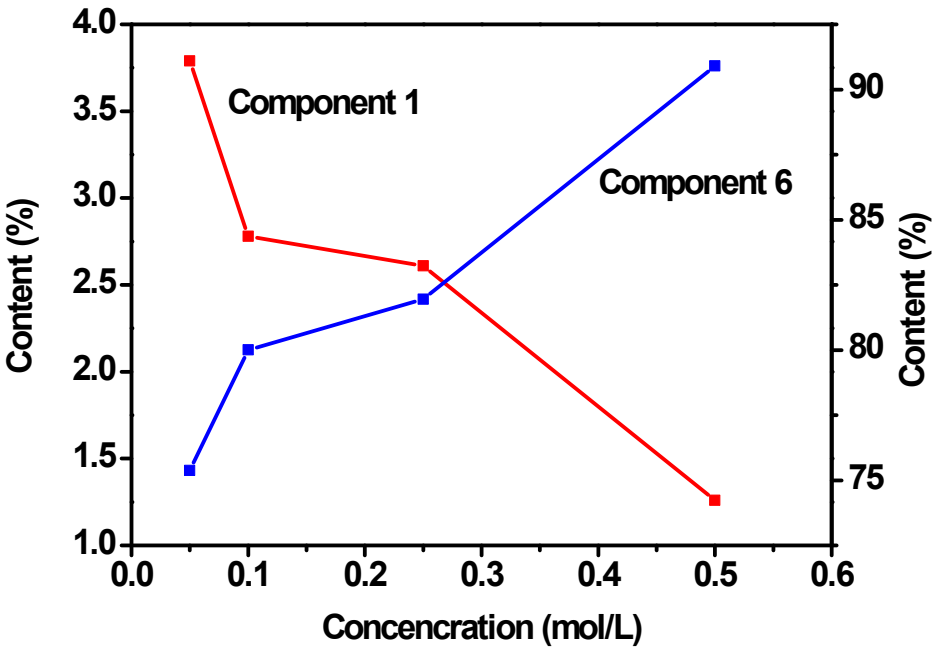

Figure S4. The contents of components 1 and 6 with different concentrations of GA dimer.

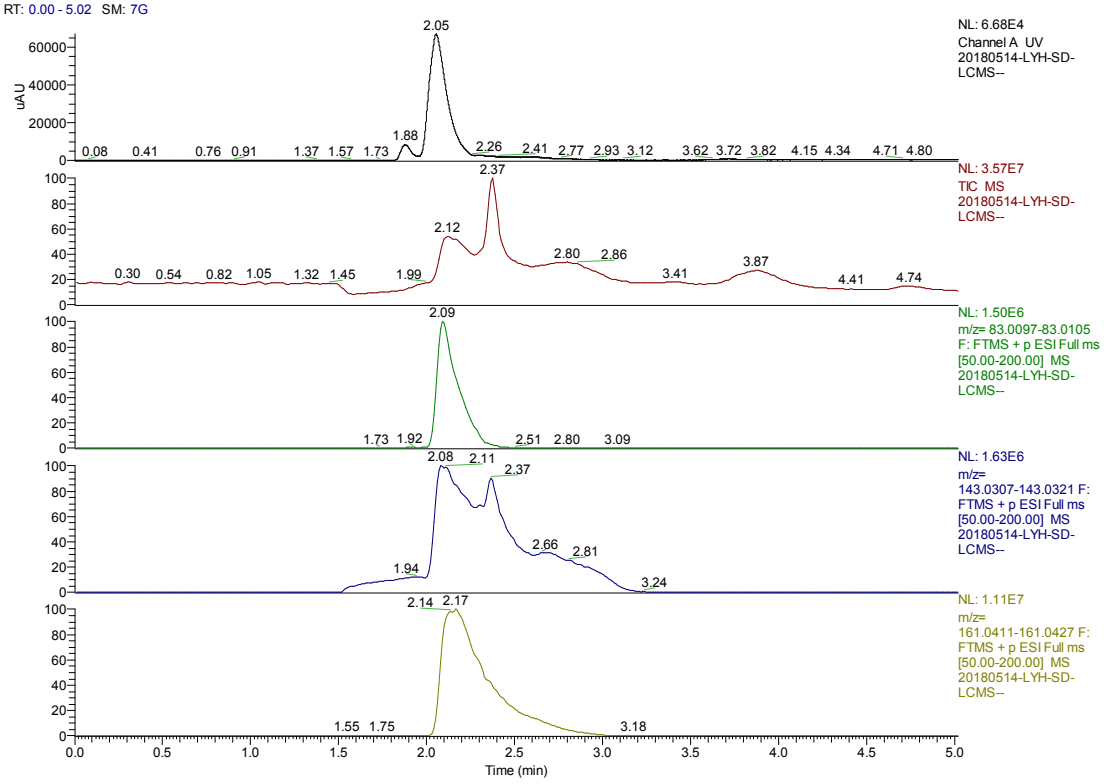

Figure S5. Liquid phase spectrogram of GA in methanol solution.

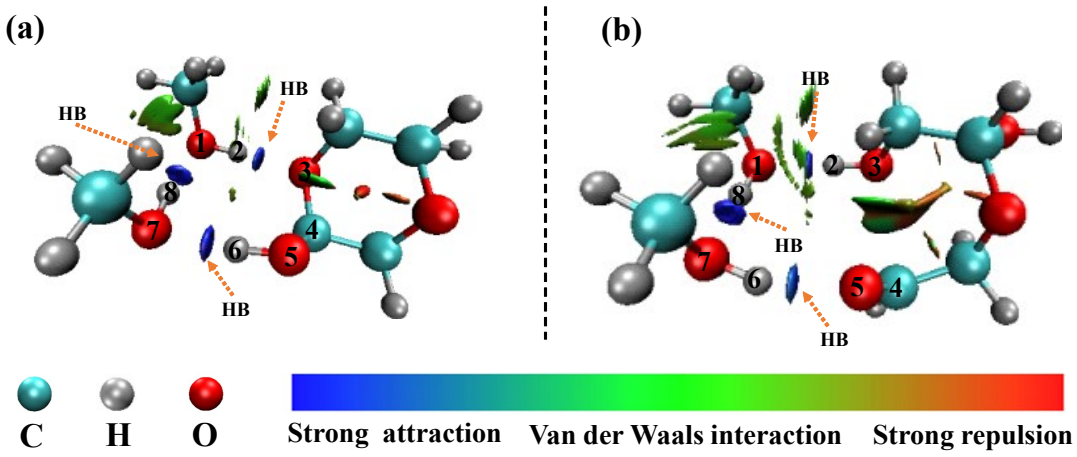

Figure S6. The reaction path of **1→2** reactant and product of GA in methanol solution, (a) reactant, (b) product.

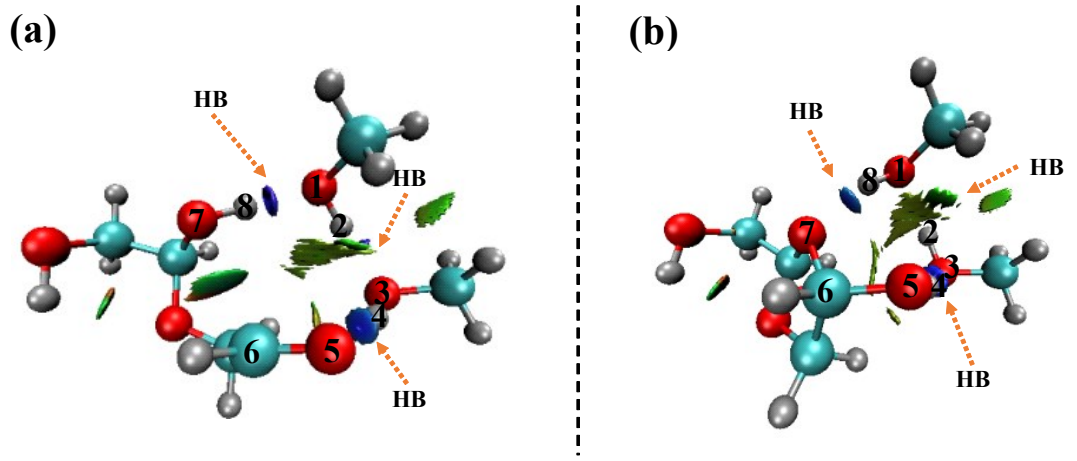

Figure S7. The reaction path of **2→3** reactant and product of GA in methanol solution, (a) reactant, (b) product.

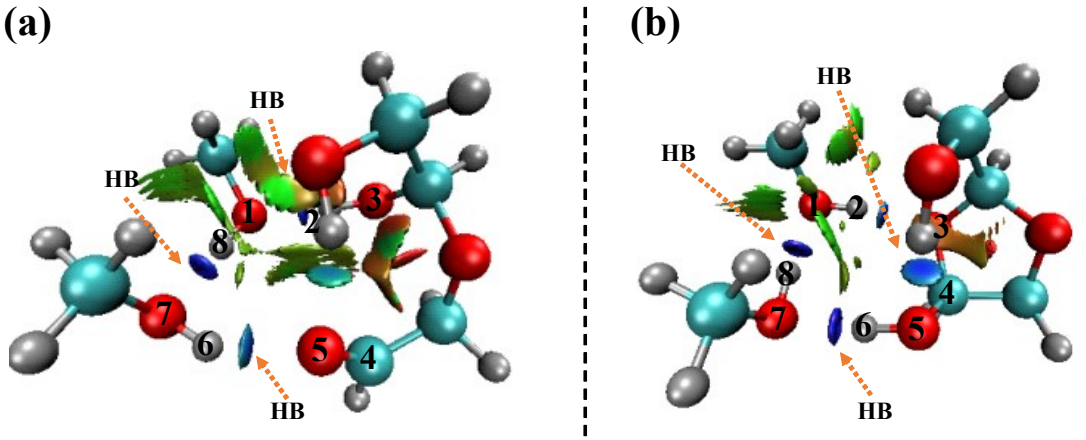

Figure S8. The reaction path of **2→4** reactant and product of GA in methanol solution, (a) reactant, (b) product.

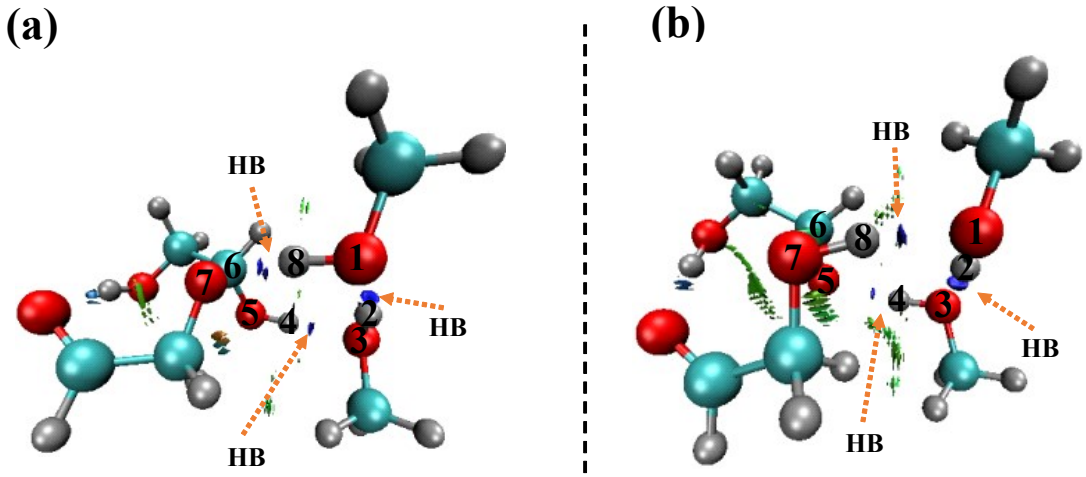

Figure S9. The reaction path of **2→5** reactant and product of GA in methanol solution, (a) reactant, (b) product.

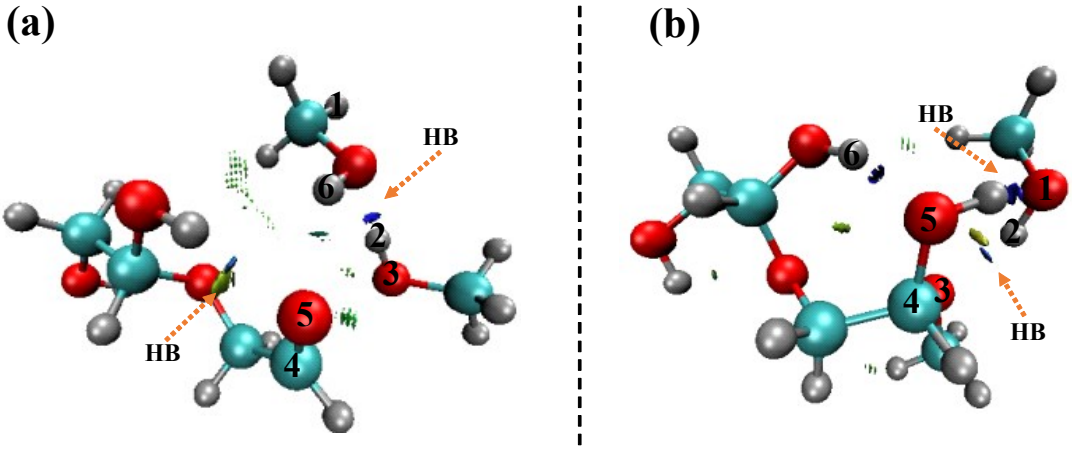

Figure S10. The reaction path of **2→7** reactant and product of GA in methanol solution, (a) reactant, (b) product.

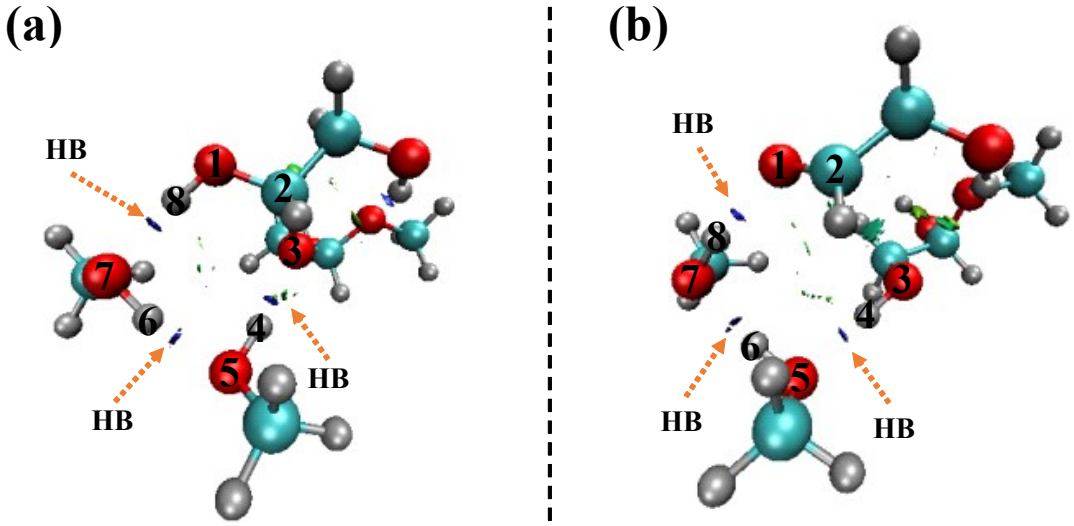

Figure S11. The reaction path of **7→5** reactant and product of GA in methanol solution, (a) reactant, (b) product.

Table S1. The content of components of with different concentrations of GA dimer in methanol solution via ^{1}H NMR spectra.

	0.05M	0.1M	0.25M	0.5M
1	3.77	2.78	2.61	1.26
2	0.41	0.38	0.26	0.06
3	6.41	5.67	4.66	2.31
4	13.50	10.36	10.19	4.97
5	0.51	0.65	0.32	0.54
6	75.38	80.01	81.95	90.87
7	0.03	0.06	0.04	0.05

Table S2. The mass spectra of different components in methanol solution, experimental and theoretical values.

components No.	m/z (experimental)	m/z (theoretical)	Composition
1	143.0135	143.0135	$C_4H_8O_4Na$
2			
3			
4			
5	83.0102	83.0104	C_2H_402Na
6	115.0365	115.0366	$C_3H_8O_3Na$
7	175.0578	175.0577	$C_5H_{12}O_5Na$

Table S3. The bond length and angle of 1→2 reactant and product of GA in methanol solution.

Parameters		Reactant	product
Bond length (Å)	O1-H2	0.98	1.71
	H2-O3	1.75	0.99
	O3-C4	1.44	2.72
	C4-O5	1.40	1.22
	O5-H6	1.22	1.80
	H6-O7	1.73	0.98
	O7-H8	0.99	1.73
Bond angle (°)	H2-O3-C4	113.6	96.4
	C4-O5-H6	108.4	117.4
	O5-H6-O7	172.3	162.8
	O7-H8-O1	167.7	103.9

Table S4. The bond length and angle of 2→3 reactant and product of GA in methanol solution.

Parameters		Reactant	product
Bond length (Å)	O1-H2	0.98	1.75
	H2-O3	1.74	0.98
	O3-H4	0.98	1.72
	H4-O5	1.81	0.99
	O5-C6	1.22	1.38
	C6-O7	2.60	1.46
	O7-H8	0.99	1.79
Bond angle (°)	H2-O3-H4	95.8	91.2
	O3-H4-O5	163.5	171.4
	O5-C6-O7	113.7	110.9
	C6-O7-H8	90.6	115.7

Table S5. The bond length and angle of 2→4 reactant and product of GA in methanol solution.

Parameters		Reactant	product
Bond length (Å)	O1-H2	1.73	0.98
	H2-O3	0.99	1.82
	O3-C4	3.09	1.44
	C4-O5	1.22	1.40
	O5-H6	1.86	0.99
	H6-O7	0.97	1.69
	O7-H8	1.75	0.99
Bond angle (°)	H2-O3-C4	79.2	117.8
	O3-C4-O5	88.8	111.5
	C4-O5-H6	130.5	109.6
	H6-O7-H8	96.4	96.3

Table S6. The bond length and angle of 2→5 reactant and product of GA in methanol solution.

Parameters		Reactant	product
Bond length (Å)	O1-H2	1.74	0.99
	H2-O3	0.99	1.72
	O3-H4	1.70	0.98
	H4-O5	0.99	1.79
	O5-C6	1.39	1.22
	C6-O7	1.47	2.76
	O7-H8	1.78	0.99
Bond angle (°)	H2-O3-H4	99.5	100.8
	O3-H4-O5	171.6	166.8
	O5-C6-O7	112.1	95.2
	C6-O7-H8	104.9	85.9

Table S7. The bond length and angle of 2→7 reactant and product of GA in methanol solution.

Parameters		Reactant	product
Bond length (Å)	O1-H2	1.72	0.98
	H2-O3	0.99	1.90
	O3-C4	2.34	1.46
	C4-O5	1.26	1.44
	O5-H6	1.97	0.99
Bond angle (°)	O1-H2-O3	162.4	141.4
	H2-O3-C4	95.7	109.6
	O3-C4-O5	101.1	107.1
	C4-O5-H6	117.8	110.8

Table S8. The bond length and angle of 7→5 reactant and product of GA in methanol solution.

Parameters		Reactant	product
Bond length (Å)	O1-C2	1.39	1.22
	C2-O3	1.45	2.58
	O3-H4	1.75	0.99
	H4-O5	0.98	1.68
	O5-H6	1.74	0.99
	H6-O7	0.99	1.72
	O7-H8	1.72	0.98
Bond angle (°)	O1-C2-O3	112.4	104.3
	C2-O3-H4	109.8	94.9
	O7-H8-O1	170.8	163.9
	H8-O1-C2	108.7	115.9