Supporting Information

Controllable synthesis and biological application of Schiff bases from D-glucosamine and terephthalaldehyde

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1. Computational procedures

All the density functional theoretical (DFT) calculations in this work were carried out by using the ωB97XD density functional in conjunction with the 6-311++G(d, p) split valence basis set in the GAUSSIAN 16 software package.[1] The analyses of vibration frequencies have been also implemented at the same theoretical level to make sure all the optimized structures are true minima without any imaginary frequencies on their potential energy surfaces. Based on the optimized structures, the zero-point-corrected Gibbs free energies (*G*) at 298.15 K were calculated at the ωB97XD/6-311++g(d, p) level to obtain $\Delta_r G$ of the considered reactions. The solvation model based on density (SMD)[2] was used to take the effect of solvent into account in all the calculations. Dimensional plots of molecular configurations and orbitals were generated with the GaussView program[3].

References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; et al. *Gaussian 16, Revision A.03*, Gaussian, Inc., Wallingford CT, USA, **2016**.

2. Marenich A. V., Cramer C. J., Truhlar D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. ***J. Phys. Chem. B*** 2009, 113(18), 6378-6396.

3. Dennington, R.; Keith, T.; Millam, J. G. *GaussView*, *Version 6*; Semichem Inc, Shawnee Mission, KS, **2016**.

2. Cartesian coordinates

(1) The optimized structure of Glu without any imaginary frequencies in methanol.

The total energy is -667.366046 au. and free energy is -667.192825 au.

C	-1.56488800	-0.04038300	0.29779400
C	-0.78673400	1.18841700	-0.16719300
C	0.70598000	1.01223800	0.05243300
C	1.17340000	-0.29128200	-0.59872000
C	-0.98365000	-1.28237100	-0.37364100
H	-0.96181300	1.33202800	-1.24470600
H	-1.41732300	-0.15722300	1.37717200
H	1.03712400	-0.21048600	-1.68740300
H	-1.12553000	-1.23634900	-1.46404600
H	0.90245400	0.96801800	1.13081100

O	1.44723500	2.06878000	-0.53813800
H	1.20359600	2.89160200	-0.10403200
O	-1.21350500	2.34451700	0.53614900
H	-2.17846100	2.31325700	0.55339800
O	-1.59737200	-2.41126900	0.15861000
H	-1.43730700	-3.16187900	-0.42170700
C	2.63260500	-0.61435100	-0.33456900
H	2.88018800	-1.55162600	-0.84532500
H	3.25706400	0.17707200	-0.75067100
O	2.94617600	-0.70186600	1.04697800
H	2.45690600	-1.43914000	1.42393300
O	0.40652200	-1.38134600	-0.09737400
N	-2.98160900	0.18440600	0.05154400
H	-3.18017900	0.12822500	-0.94403700
H	-3.53817300	-0.52847700	0.50936900

(2) The optimized structure of TPA without any imaginary frequencies in methanol.

The total energy is -458.873043 au. and free energy is -458.787848 au.

C	-0.69053200	-1.03014600	0.00020900
C	0.69060100	-1.03011400	-0.00007300
C	1.38454800	0.18571100	-0.00023100
C	0.69439700	1.39595900	-0.00014600
C	-0.69444900	1.39592700	0.00004100
C	-1.38453400	0.18564100	0.00024600
H	-1.24176000	-1.96367300	0.00038700
H	1.24188900	-1.96360400	-0.00009900
H	1.24383700	2.33170700	-0.00028000
H	-1.24393900	2.33164600	0.00008200
C	-2.86304300	0.21604800	0.00050800
O	-3.56433800	-0.77447900	-0.00067800
H	-3.31559800	1.22256300	0.00182800
C	2.86305400	0.21607200	-0.00036000
O	3.56429500	-0.77449400	0.00042300
H	3.31566500	1.22256100	-0.00104600

(3) The optimized structure of L_1 without any imaginary frequencies in methanol.

The total energy is -1049.800613 au. and free energy is -1049.544178 au

C	1.21877200	-0.21040800	0.21541300
C	1.87727500	1.08591200	-0.27520900
C	3.37713200	1.06734500	-0.01514700
C	3.99396900	-0.20393000	-0.59762100
C	1.95705800	-1.40759800	-0.37932100
H	1.71464900	1.18466600	-1.35562200
H	1.31747500	-0.26424700	1.30928600

H	3.86984400	-0.19114500	-1.69046200
H	1.85047400	-1.42262600	-1.47311600
H	3.55140000	1.08746200	1.06780300
O	4.01280000	2.17276000	-0.63462700
H	3.63255900	2.97924500	-0.27304400
O	1.34463000	2.21837400	0.39493300
H	0.50168600	2.45545000	-0.00236100
O	1.44439400	-2.56832800	0.18794000
H	1.71839500	-3.32423800	-0.34088500
C	5.47391000	-0.35586800	-0.29881200
H	5.82919100	-1.28461600	-0.75900500
H	6.01658400	0.47690000	-0.74770600
O	5.76973900	-0.33985500	1.08917600
H	5.36423300	-1.11122500	1.49607800
O	3.33408300	-1.34078800	-0.05177600
N	-0.16031300	-0.23292300	-0.21857600
C	-1.05949100	-0.08816500	0.66376300
H	-0.81623600	0.02212700	1.72731600
C	-2.49657300	-0.06003200	0.32633800
C	-3.42462300	0.11364100	1.35825900
C	-2.94266100	-0.20068500	-0.99032100
C	-4.78147700	0.14740700	1.08323200
H	-3.07401700	0.22273300	2.37952700
C	-4.29876900	-0.16876000	-1.26672500
H	-2.22230700	-0.33518300	-1.78821200
C	-5.22346400	0.00616800	-0.23367700
H	-5.50260400	0.28105200	1.88187700
H	-4.65038700	-0.27974400	-2.28788200
C	-6.65932900	0.03640400	-0.56524700
O	-7.54939000	0.19010000	0.24839000
H	-6.89916900	-0.09284000	-1.63540300

(4) The optimized structure of L_2 without any imaginary frequencies in methanol.

The total energy is -1640.723941 au. and free energy is -1640.296617 au

C	-5.09023200	-0.22871300	-0.17515300
C	-5.71331900	1.13383200	0.15546100
C	-7.20777400	1.13143500	-0.13407600
C	-7.87093100	-0.04183100	0.59020300
C	-5.87592200	-1.32707100	0.53868700
H	-5.56722400	1.34653700	1.22200200
H	-5.18010900	-0.40225700	-1.25757100
H	-7.74052700	0.09609200	1.67377700
H	-5.78234900	-1.21948900	1.62849200
H	-7.36098000	1.02235300	-1.21444000
O	-7.81557800	2.32493700	0.32985400

H	-7.39389800	3.06668400	-0.11489900
O	-5.13256600	2.16832500	-0.62393300
H	-4.28229800	2.40993600	-0.24574200
O	-5.39744900	-2.56175600	0.11614200
H	-5.70062300	-3.24142100	0.72625600
C	-9.35445600	-0.16751800	0.32827900
H	-9.72565400	-1.04921900	0.86258100
H	-9.85841000	0.71759400	0.72913000
O	-9.58907300	-0.29423400	-1.06802400
H	-10.53666400	-0.36644400	-1.20799100
O	-7.24625700	-1.25398900	0.18363200
N	-3.71618300	-0.24718700	0.27601800
C	-2.80754700	-0.25265200	-0.60983900
H	-3.04673300	-0.26670800	-1.68038700
C	-1.37173500	-0.24695400	-0.27567100
C	-0.92044700	-0.24955700	1.04607100
C	-0.43847000	-0.24249300	-1.31666500
C	0.43836800	-0.25111200	1.31617500
H	-1.63910100	-0.25349600	1.85714300
C	0.92034500	-0.24131200	-1.04655000
H	-0.78520700	-0.24112100	-2.34540800
C	1.37163500	-0.24736200	0.27518000
H	0.78510700	-0.25664200	2.34490300
H	1.63899500	-0.23880300	-1.85763300
C	5.09013900	-0.22831500	0.17483100
C	5.71373800	1.13439500	-0.15409300
C	7.20820300	1.13116800	0.13535400
C	7.87093300	-0.04159900	-0.59013600
C	5.87546300	-1.32617300	-0.54019400
H	5.56766800	1.34845500	-1.22037100
H	5.17987700	-0.40320800	1.25705000
H	7.74060000	0.09748500	-1.67357000
H	5.78205000	-1.21739800	-1.62989400
H	7.36141200	1.02094800	1.21559600
O	7.81643000	2.32492500	-0.32739000
H	7.39526700	3.06637700	0.11833900
O	5.13337000	2.16810700	0.62662300
H	4.28281100	2.40991800	0.24921300
O	5.39650000	-2.56114400	-0.11903800
H	5.69958800	-3.24026800	-0.72979800
C	9.35440300	-0.16811900	-0.32830600
H	9.72526700	-1.04948900	-0.86338600
H	9.85870600	0.71715600	-0.72835300
O	9.58894500	-0.29616000	1.06788400

H	10.53650700	-0.36883500	1.20779300
O	7.24578100	-1.25395200	-0.18487700
N	3.71611200	-0.24556700	-0.27645300
C	2.80744200	-0.25406800	0.60934200
H	3.04659400	-0.27182600	1.67984000

(5) The optimized structure of Glu without any imaginary frequencies in mixed solvent.

The total energy is -667.356301 au. and free energy is -667.182790 au.

C	-1.55391800	-0.07508900	0.29932300
C	-0.80782400	1.17326900	-0.16511500
C	0.68662200	1.03637600	0.06106700
C	1.18892000	-0.24427600	-0.60748100
C	-0.94167400	-1.29666400	-0.38504700
H	-0.98061400	1.30223100	-1.24582200
H	-1.39890500	-0.19522400	1.37721400
H	1.05837900	-0.14936700	-1.69579800
H	-1.08918500	-1.23348700	-1.47598400
H	0.87651400	0.97238500	1.14063600
O	1.39616400	2.12678500	-0.50001100
H	1.01432100	2.93405300	-0.14348300
O	-1.26160100	2.32254000	0.52654000
H	-2.22307100	2.24735500	0.56282800
O	-1.52723100	-2.43998000	0.13317400
H	-1.26948800	-3.19226100	-0.40831600
C	2.64959400	-0.54549600	-0.32299600
H	2.94163700	-1.43086300	-0.90144600
H	3.26378100	0.29560400	-0.64719500
O	2.90447600	-0.74185300	1.05668500
H	2.31108100	-1.43570200	1.35977000
O	0.45125700	-1.35947900	-0.11977600
N	-2.97670300	0.12358700	0.06216600
H	-3.18230900	0.06474700	-0.93195700
H	-3.52006000	-0.59740000	0.52298900

(6) The optimized structure of TPA without any imaginary frequencies in methanol.

The total energy is -458.881392 au. and free energy is -458.795758 au.

C	-0.69098200	-1.02914900	0.00007400
C	0.69098100	-1.02914800	0.00001100
C	1.38666000	0.18566000	-0.00008800
C	0.69474400	1.39525300	-0.00006900
C	-0.69474500	1.39525200	0.00008300
C	-1.38666200	0.18565900	0.00012600
H	-1.24381600	-1.96179100	0.00010700
H	1.24381500	-1.96179000	-0.00000400

H	1.24409500	2.33129100	-0.00014700
H	-1.24409700	2.33128900	0.00012800
C	-2.86989500	0.21336800	0.00028400
O	-3.56986700	-0.77312400	-0.00042500
H	-3.31659000	1.22470300	0.00123900
C	2.86989700	0.21336800	-0.00030000
O	3.56986700	-0.77312400	0.00032400
H	3.31659500	1.22470200	-0.00123300

(7) The optimized structure of L_1 without any imaginary frequencies in methanol.

The total energy is -1049.797329 au. and free energy is -1049.540796 au

C	1.22426600	-0.17523500	0.22238900
C	1.90100800	1.11195300	-0.26415600
C	3.39817500	1.07451400	-0.00013500
C	3.99959100	-0.18938500	-0.61216600
C	1.94317200	-1.37120500	-0.40514900
H	1.74230700	1.20503000	-1.34681500
H	1.33114900	-0.24913300	1.31420900
H	3.88598900	-0.14280100	-1.70537900
H	1.82363400	-1.34752700	-1.49955000
H	3.56760500	1.05905700	1.08454900
O	4.03918800	2.19264300	-0.58325100
H	3.56689400	2.97664000	-0.28664200
O	1.39427300	2.25995800	0.39746300
H	0.52314600	2.46238100	0.04446400
O	1.41952700	-2.53295000	0.13438000
H	1.75030300	-3.28227300	-0.37074700
C	5.47008500	-0.38388000	-0.28820500
H	5.83185200	-1.26601500	-0.83079100
H	6.03436400	0.48526900	-0.62851700
O	5.70593500	-0.51784900	1.10210200
H	5.15788000	-1.24357100	1.41587100
O	3.32372900	-1.32902300	-0.09516900
N	-0.15695000	-0.16467600	-0.20306000
C	-1.05866100	-0.09251800	0.68525700
H	-0.81908400	-0.05287500	1.75504500
C	-2.49525600	-0.05836600	0.34218800
C	-3.43241400	0.09148400	1.36973000
C	-2.93123700	-0.17704300	-0.98051000
C	-4.78787100	0.12377900	1.08305100
H	-3.09058900	0.18275100	2.39583300
C	-4.28599500	-0.14996300	-1.26708100
H	-2.20239300	-0.29326700	-1.77379700
C	-5.21992300	0.00092200	-0.23873700

H	-5.51810500	0.24049700	1.87593900
H	-4.62902500	-0.24716800	-2.29270200
C	-6.66069200	0.02277400	-0.57664700
O	-7.55208500	0.15084500	0.23260600
H	-6.88731900	-0.09024100	-1.65356100

(8) The optimized structure of L_2 without any imaginary frequencies in methanol.

The total energy is -1640.705876 au. and free energy is -1640.278838 au

C	-5.09009800	-0.12730000	-0.23437900
C	-5.80096700	1.04147200	0.45703700
C	-7.29055200	1.03559800	0.15003600
C	-7.88202600	-0.33009300	0.50157300
C	-5.81103500	-1.42227900	0.14816200
H	-5.67067400	0.93703300	1.54281900
H	-5.17192200	-0.00604800	-1.32474800
H	-7.77165500	-0.48977900	1.58551900
H	-5.72927300	-1.58857700	1.23428900
H	-7.43583500	1.21719800	-0.92209100
O	-7.96081800	2.02174900	0.91263700
H	-7.49383400	2.85140600	0.77435000
O	-5.29748700	2.29806800	0.03070700
H	-4.42508700	2.42759500	0.41383000
O	-5.24530800	-2.46895200	-0.56123300
H	-5.59576100	-3.29551400	-0.21521800
C	-9.35512500	-0.45596300	0.18160200
H	-9.66878400	-1.48202800	0.40911700
H	-9.90652200	0.22741700	0.83643400
O	-9.58725400	-0.14706800	-1.18406500
H	-10.53506600	-0.16357800	-1.33411100
O	-7.17662100	-1.34073000	-0.20462200
N	-3.71741800	-0.17217700	0.21802300
C	-2.79981900	-0.02309600	-0.64513000
H	-3.02552900	0.12079200	-1.70926300
C	-1.36804600	-0.03485300	-0.28999300
C	-0.93833600	-0.16231300	1.03326700
C	-0.41833500	0.09077100	-1.30861300
C	0.41595900	-0.16464100	1.32713000
H	-1.67185800	-0.25524300	1.82572500
C	0.93611200	0.08120500	-1.01556800
H	-0.74883200	0.19585000	-2.33737900
C	1.36585600	-0.04732600	0.30758200
H	0.74640000	-0.26052200	2.35682200
H	1.66888900	0.17673800	-1.80843300
C	5.08941100	-0.09433300	0.23476200

C	5.82483900	1.08151400	-0.41501400
C	7.31509200	1.03145100	-0.11806500
C	7.87229800	-0.33355300	-0.52492400
C	5.77747900	-1.39072400	-0.20198200
H	5.68694900	1.01883600	-1.50315000
H	5.17709400	-0.02071500	1.32884900
H	7.75236100	-0.45006500	-1.61331700
H	5.68671500	-1.51358900	-1.29302600
H	7.47102100	1.17035000	0.95881200
O	8.00307200	2.02998800	-0.84855500
H	7.55560300	2.86408800	-0.67654300
O	5.35091700	2.33297400	0.05800900
H	4.47627500	2.48951400	-0.30967300
O	5.19065200	-2.45001600	0.47024800
H	5.51613800	-3.27093600	0.08828000
C	9.34371400	-0.50639300	-0.21909100
H	9.63052200	-1.53187700	-0.48257300
H	9.90808800	0.18451500	-0.85477200
O	9.59186000	-0.24889300	1.15447300
H	10.53969500	-0.29633800	1.29774700
O	7.14640300	-1.35406500	0.14632800
N	3.71472600	-0.08628700	-0.21452600
C	2.79797800	-0.06402800	0.66168000
H	3.02398700	-0.06240900	1.73537800

3. Figures

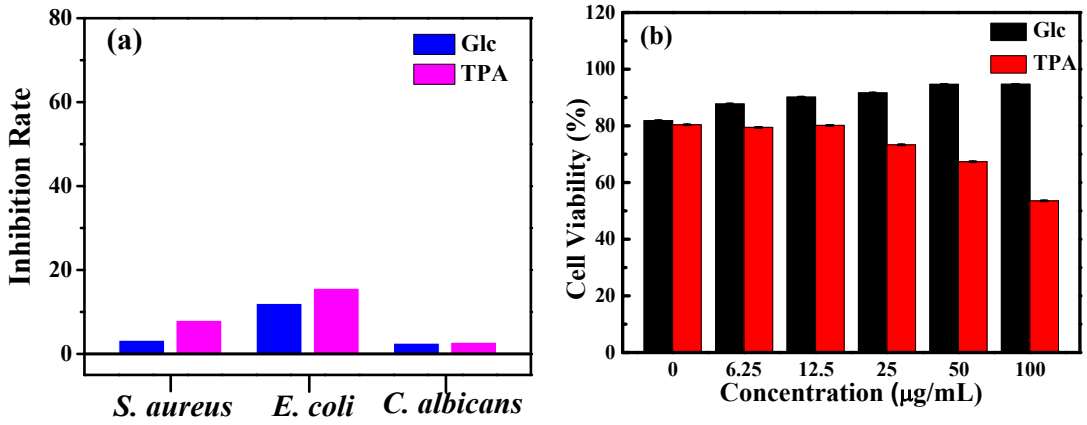
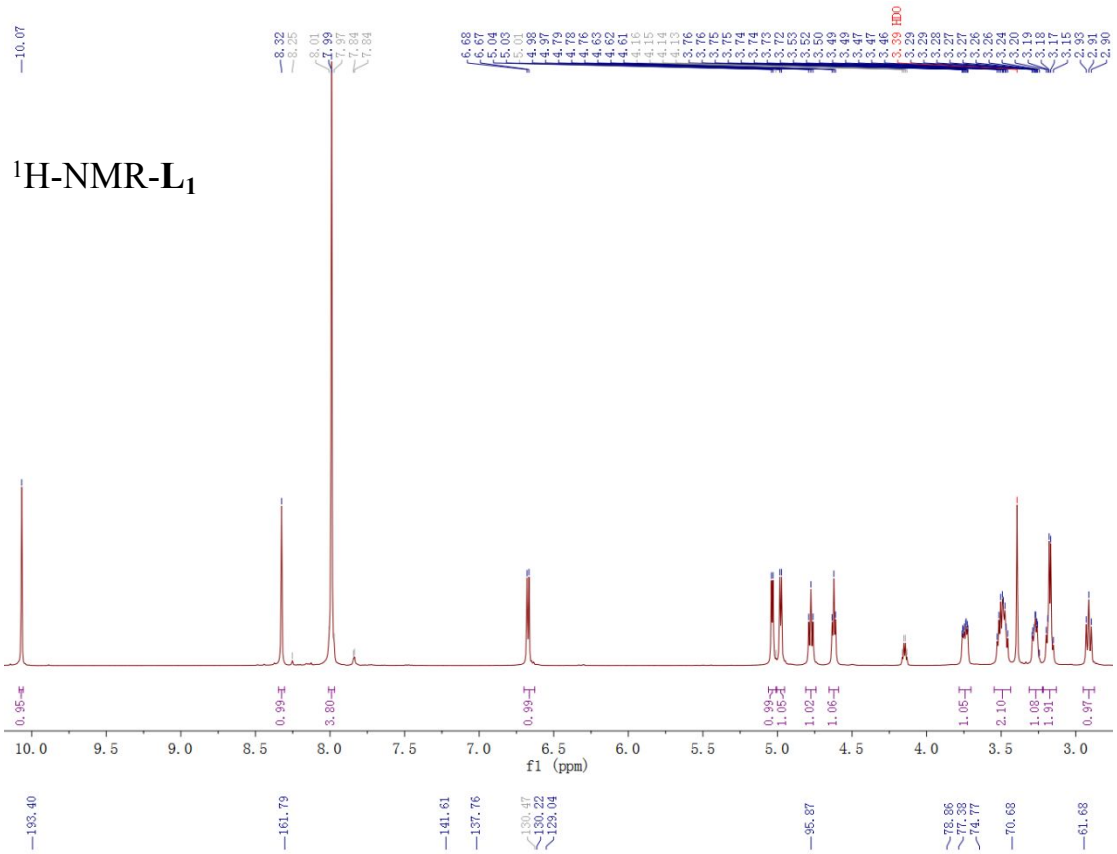
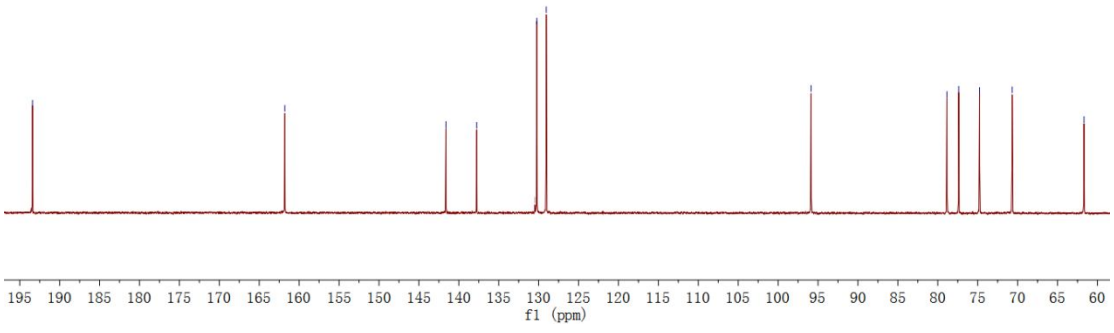


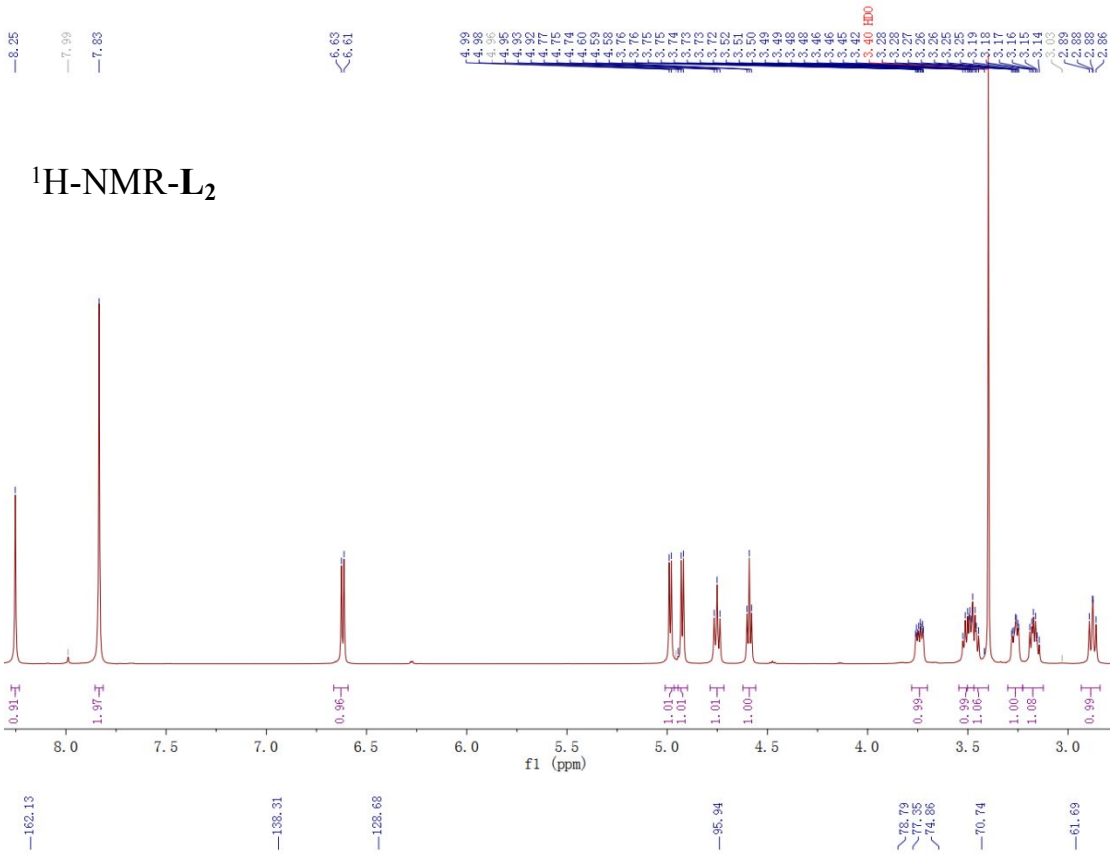
Figure S1. (a) Anti-bacterial against *S. aureus*, *E. coli* and *C. albicans*, and (b) cytotoxicity on HepG2 cells for Glc and TPA.

^{1}H-NMR-**L_1**

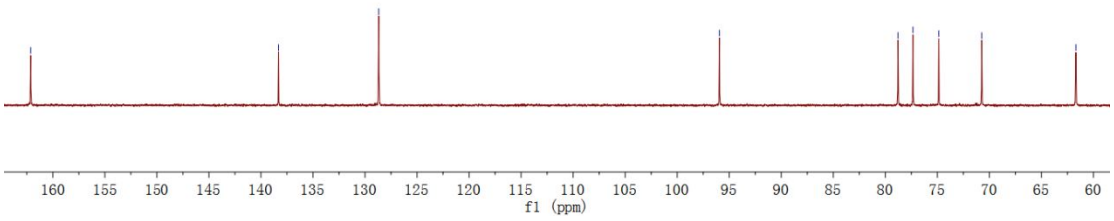


^{13}C-NMR-**L_1**





^{1}H-NMR-$\mathbf{L_2}$



^{13}C-NMR-$\mathbf{L_2}$

Figure S2. ^{1}H-NMR and ^{13}C-NMR spectra of compounds $\mathbf{L_1}$ and $\mathbf{L_2}$

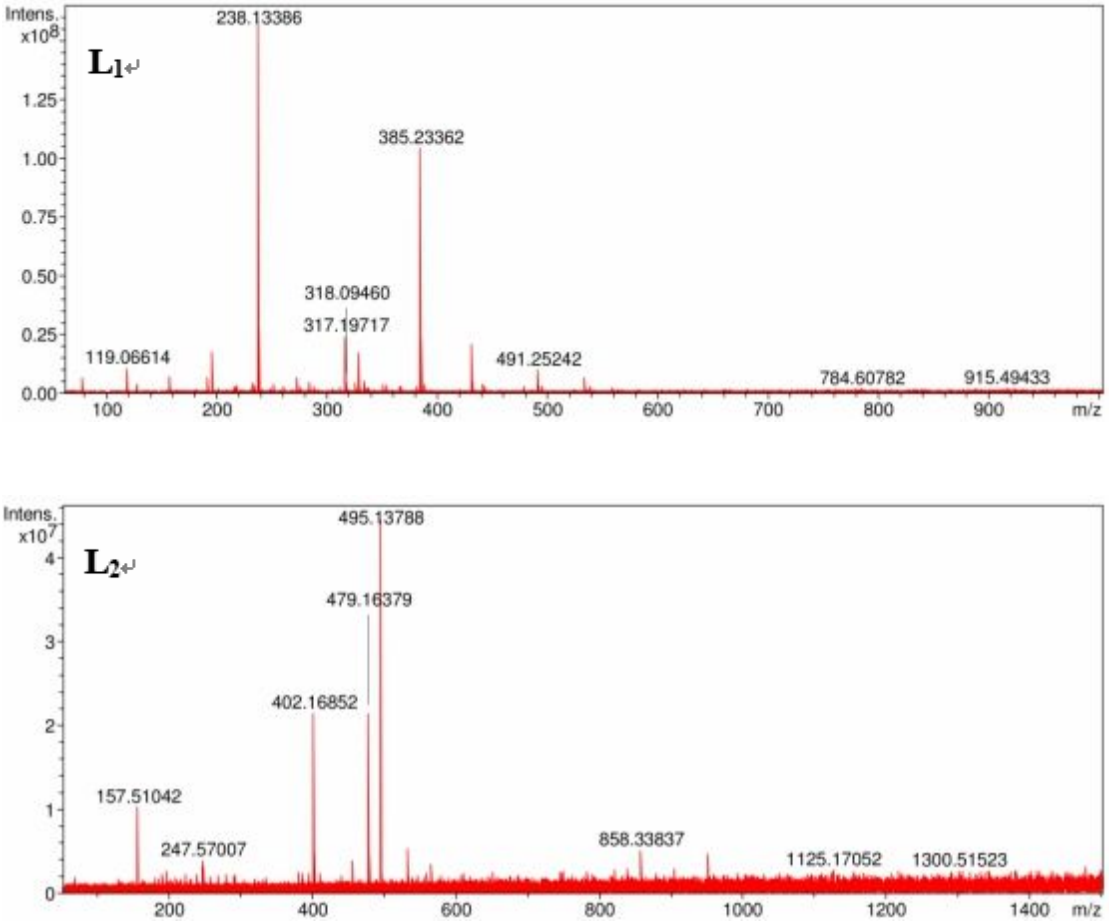


Figure S3. Mass spectra of compounds $\mathbf{L_1}$ and $\mathbf{L_2}$

Table S1. FT-IR data of the compound $\mathbf{L_1}$ and $\mathbf{L_2}$.

	ν_{O-H}	ν_{C-H} (Glc)	$\nu_{C=N}$	$\nu_{C=C}$ (Ar)	ν_{C-C} (Glc)	ν_{C-OH} (Glc)	$\nu_{(-O-)}$	Glc	-CHO
L_1	3481	2936 2882	1640	1572 1439 1410	1374	1268 1219 1165 1151	1087	603 573 549	1689
L_2	3514	2925 2906	1640	1475 1422	1370	1255 1216 1191	1083	589 574 530	

* Units are cm^{-1}