

## **Supplementary Information**

# **Dehydration Mechanism of Fructose to 5-Hydroxymethylfurfural Catalyzed by Functionalized Ionic Liquids: A Density Functional Theory Study**

Jiehao Hu<sup>a</sup>, Mengting Yu<sup>a\*</sup>, Yao Li<sup>b</sup>, Xiaoli Shen<sup>a</sup>, Shenyu Cheng<sup>a</sup>, Tianyou Xu<sup>a</sup>, Chengsheng Ge<sup>a</sup>

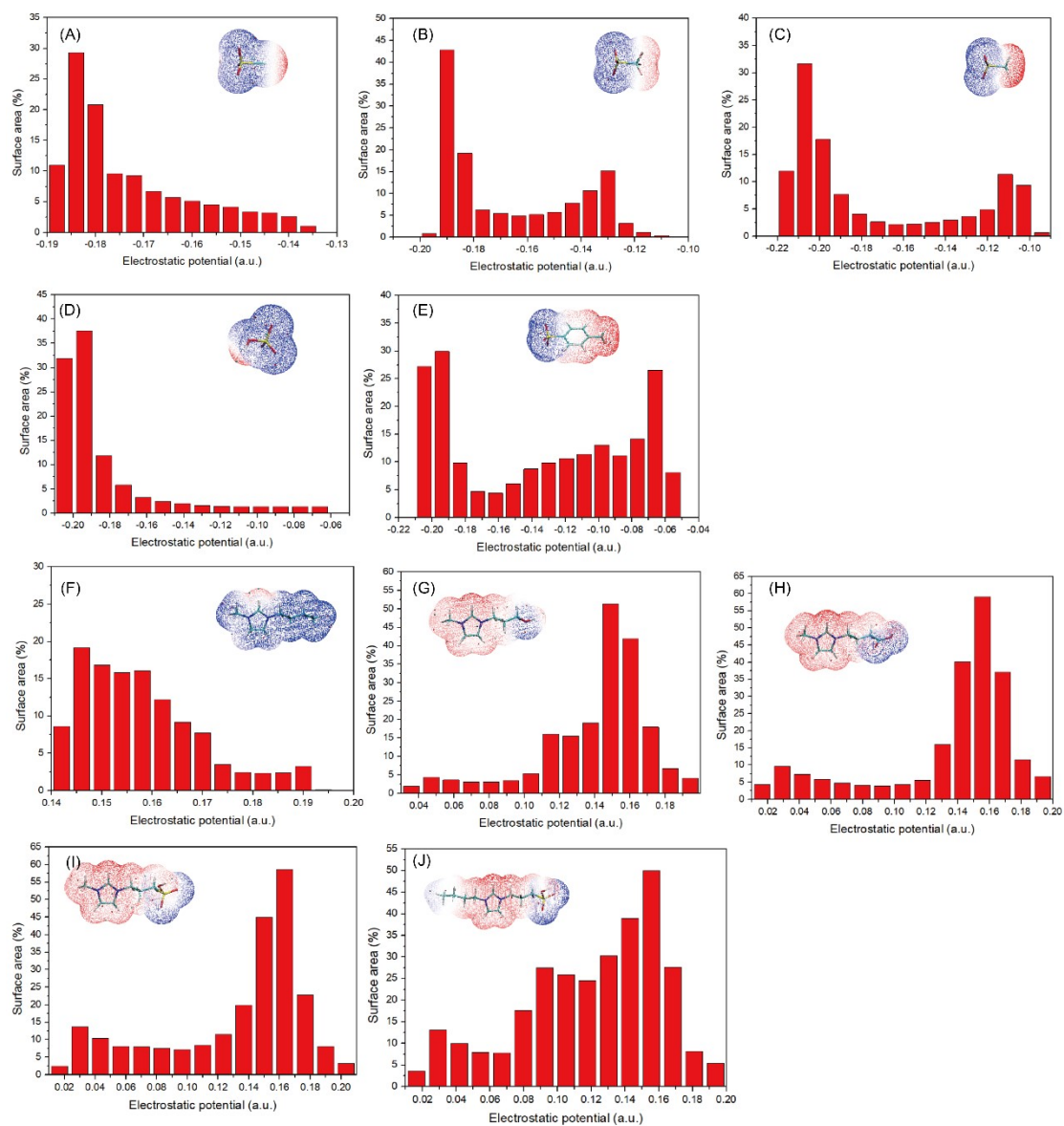
Yihang Yu<sup>a</sup> and Zhaoyang Ju<sup>a\*</sup>

<sup>a</sup>College of Chemical & Material Engineering, Quzhou University, Quzhou, China.

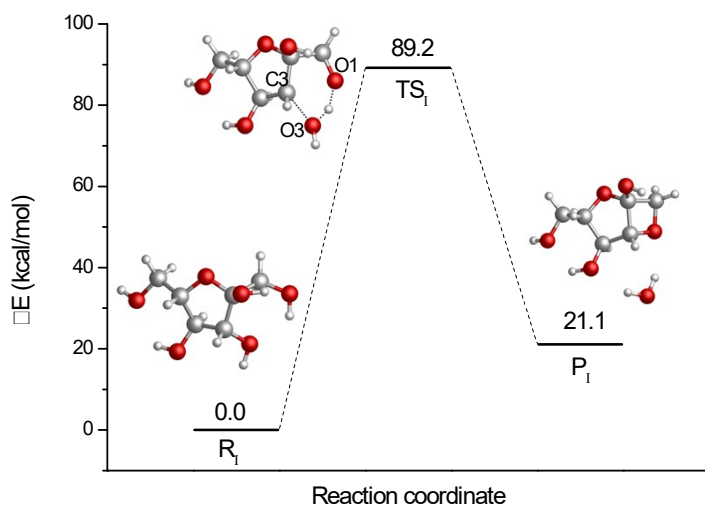
<sup>b</sup>Beijing Key Laboratory of Ionic Liquids Clean Process, State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China.

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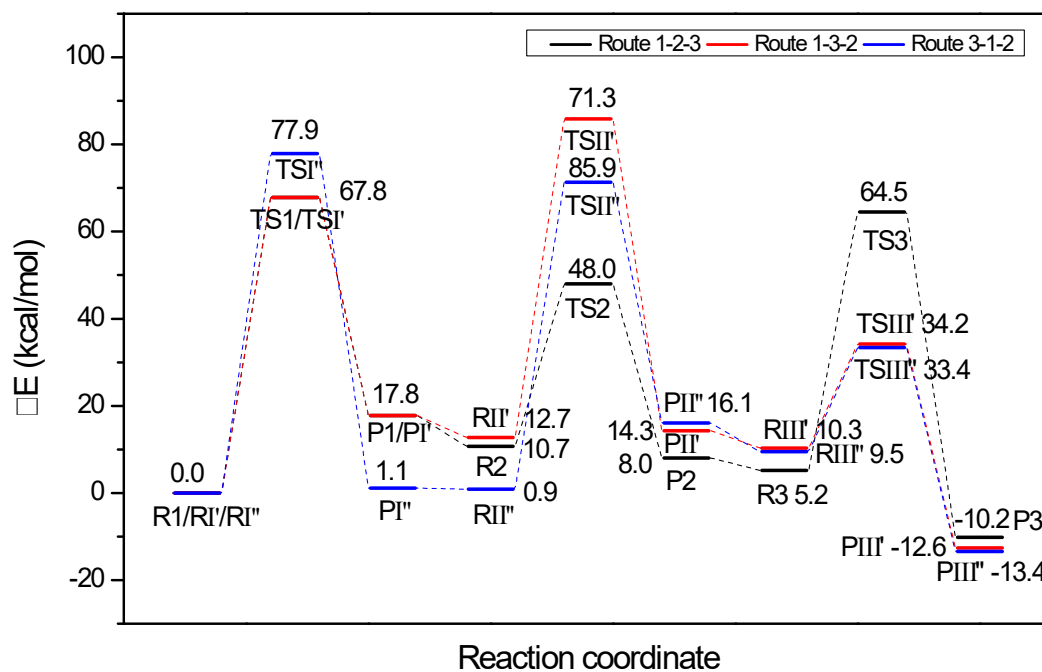
1. ESP mapped molecular vdW surface and area percent of anions and cations.
2. The different dehydration sequences of fructose to HMF.
3. The second and third dehydration catalyzed by  $\text{HSO}_4^-$  through different ways.
4. The energies of second dehydration catalyzed by different anions and cations.
5. The coordinates of reactants, TS and products in the dehydration of fructose to HMF.



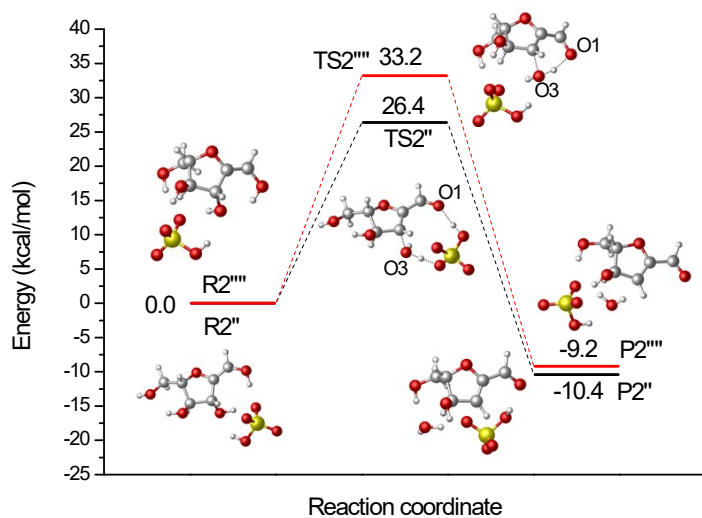
**Figure S1** ESP mapped molecular vdW surface and area percent of anions and cations (A)  $\text{ClSO}_3^-$  (B)  $\text{CF}_3\text{SO}_3^-$  (C)  $\text{CH}_3\text{SO}_3^-$  (D)  $\text{HSO}_4^-$  (E)  $p\text{-CH}_3\text{C}_6\text{H}_4\text{SO}_3^-$  (F)  $\text{Bmim}^+$  (G)  $\text{BmimOH}^+$  (H)  $\text{BmimCOOH}^+$  (I)  $\text{BmimHSO}_3^+$  (J)  $\text{BBimHSO}_3^+$ .



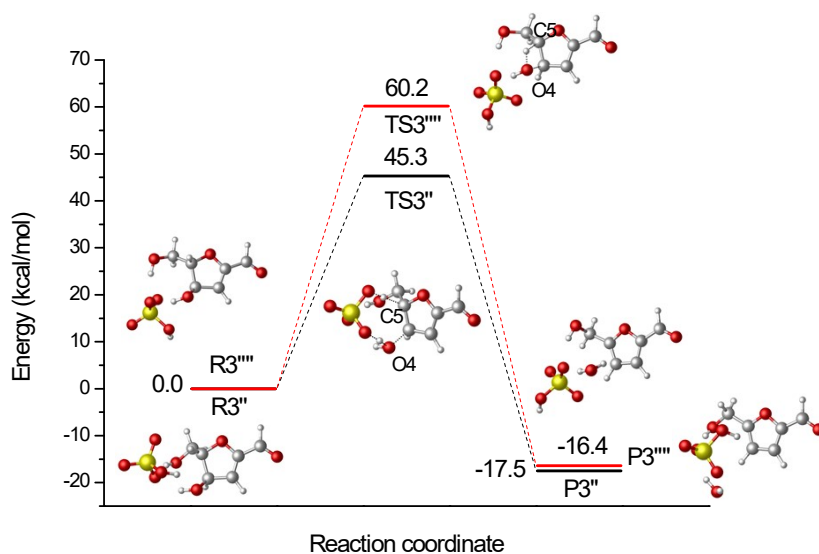
**Figure S2** Computed free energy profiles (energy kcal/mol) and optimized geometries of intermediate and TS for the first dehydration of fructose in route 2-1-3.



**Figure S3** Computed free energy profiles (energy kcal/mol) for the different dehydration sequences of fructose at M06-2X-D3/6-311+G\*\* level.



**Figure S4** Computed free energy profiles (energy kcal/mol) and optimized geometries of intermediate and TS for the second dehydration catalyzed by  $\text{HSO}_4^-$  through different ways.

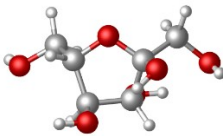
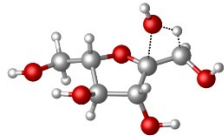


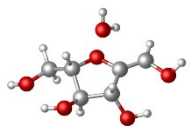
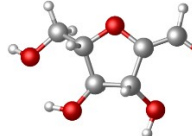
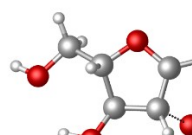
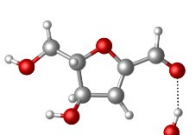
**Figure S5** Computed free energy profiles (energy kcal/mol) and optimized geometries of intermediate and TS for the third dehydration catalyzed by  $\text{HSO}_4^-$  through different ways.

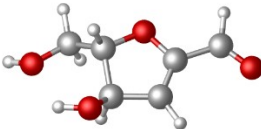
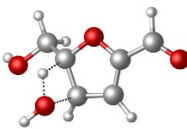
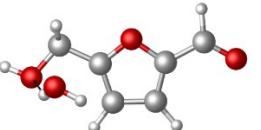
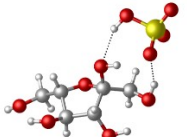
**Table S1** Calculated activation energy (Ga) and reaction energy (Gr) for the second dehydration of fructose catalyzed by different anions and cations at the M06-2X-D3/6-311+G\*\* level.

Anions	Ga	Gr	Cations	Ga	Gr
ClSO <sub>3</sub> <sup>-</sup>	38.3	-6.3	Bmim <sup>+</sup>	37.3	-8.5
CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup>	37.2	-6.6	BmimOH <sup>+</sup>	25.2	0.1
CH <sub>3</sub> SO <sub>3</sub> <sup>-</sup>	33.5	-9.5	BmimCOOH <sup>+</sup>	21.7	-8.2
HSO <sub>4</sub> <sup>-</sup>	33.2	-9.2	BmimHSO <sub>3</sub> <sup>+</sup>	22.7	-4.3
<i>p</i> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> SO <sub>3</sub> <sup>-</sup>	32.9	-7.9	BBimHSO <sub>3</sub> <sup>+</sup>	23.7	-3.7

**Table S2** The coordinates of reactants, TS and products in the dehydration of fructose to HMF.

R1				TS1			
							
O	0.07031800	-0.12042900	1.30227400	O	0.01892400	-1.11369600	-0.68258400
C	-1.03301400	0.14449200	0.46087000	C	-0.99715900	-0.39734100	-0.30841200
C	1.30351800	0.17028500	0.64721800	C	1.18763800	-0.59733600	-0.00890500
H	1.87712300	0.87429600	1.26049200	H	1.19257300	-1.04659500	0.98950600
C	-0.45235800	0.22577500	-0.96938600	C	-0.60426900	0.99425500	0.14124500
H	-1.04481100	0.90195400	-1.59042800	H	-0.98049900	1.19863000	1.14290900
C	0.92865700	0.80762600	-0.69408900	C	0.92311900	0.91039900	0.12004700
H	1.64572200	0.57416900	-1.48357900	H	1.26933900	1.42318600	-0.78709200
O	-0.30691800	-1.04094500	-1.56728700	O	-1.04896200	1.91784600	-0.82816300
H	-1.19565400	-1.37537000	-1.73771600	H	-2.01444600	1.88085300	-0.83262300
O	0.72631200	2.21273900	-0.55780500	O	1.49315600	1.46367800	1.27285500
H	1.55736400	2.62428900	-0.30612700	H	2.44594300	1.33335000	1.20750400
O	-1.67472300	1.34399800	0.80273800	O	-1.29347600	-1.22288000	1.70912500
H	-1.09510400	2.07709000	0.55518700	H	-1.03331000	-1.48056300	2.59872000
C	-2.05531200	-0.96041300	0.64167200	C	-2.33479400	-0.87075300	-0.46395300
H	-2.49409600	-0.87315600	1.63984200	H	-2.21472900	-1.41609600	0.63476100
H	-1.56399900	-1.92764600	0.54941100	H	-2.49592200	-1.58424600	-1.27010900
O	-3.03640200	-0.88831900	-0.37911000	O	-3.28241200	0.17691900	-0.41931000
H	-3.47864800	-0.03704200	-0.29483300	H	-3.78171300	0.09006900	0.39676300
C	2.11139400	-1.10739000	0.49754000	C	2.42316100	-0.93659900	-0.80882000
H	2.19232900	-1.58372300	1.48023300	H	2.60782300	-2.01474500	-0.80341800
H	1.59884300	-1.78453600	-0.19273100	H	2.29139700	-0.59619800	-1.84253700
O	3.38233400	-0.71404800	0.00205500	O	3.46589100	-0.22233100	-0.16025800

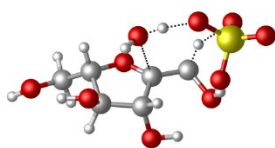
H	3.89625100	-1.49653500	-0.20562400	H	4.30239600	-0.39968200	-0.59491500
P1				R2			
							
O	0.00747100	-0.97072100	-0.91850200	O	-0.02168000	-1.43216800	0.22903100
C	-1.08234700	-0.25925400	-0.50075400	C	-1.15976900	-0.63902000	0.17247800
C	1.14768500	-0.51937000	-0.17868100	C	1.10742100	-0.58877400	0.41901900
H	1.24893200	-1.11609100	0.73380800	H	1.33623200	-0.48806700	1.48846700
C	-0.68301500	0.88519100	0.40967100	C	-0.77952400	0.81091100	0.29823400
H	-0.88599600	0.61610300	1.45439700	H	-0.82504000	1.14296800	1.34539000
C	0.82598100	0.92809300	0.20516800	C	0.68041500	0.77730200	-0.12421500
H	1.02652400	1.59142000	-0.64869100	H	0.72148500	0.76430600	-1.22312900
O	-1.26713800	2.11773200	0.06526400	O	-1.62075700	1.62085100	-0.50369400
H	-2.22113900	1.98723900	0.03057500	H	-1.37997500	2.54134400	-0.36206600
O	1.49390400	1.35947400	1.35916400	O	1.38175000	1.86926900	0.40779600
H	2.43751800	1.26798700	1.18646300	H	2.31690500	1.72637800	0.22032400
O	-0.73526500	-2.08796300	1.80448800	C	-2.37175100	-1.14862200	-0.01310700
H	-0.87954900	-2.88322100	2.32096100	H	-2.53079000	-2.21604700	-0.09428500
C	-2.31620200	-0.56583800	-0.88874100	O	-3.51334000	-0.41139200	-0.11032800
H	-1.26738300	-2.18641200	1.00863100	H	-3.26881900	0.50927400	-0.27534100
H	-2.53795900	-1.36475900	-1.58763200	C	2.29333100	-1.17223700	-0.31768900
O	-3.35526000	0.26959700	-0.50437500	H	2.61745800	-2.10693600	0.14955400
H	-4.07807300	-0.25210900	-0.14826000	H	1.99983200	-1.37170400	-1.35434600
C	2.37210600	-0.64594200	-1.05725500	O	3.30950700	-0.17663500	-0.25143700
H	2.59353900	-1.69808100	-1.26234900	H	4.10812300	-0.49827100	-0.67383500
H	2.18508000	-0.12701200	-2.00444400				
O	3.42568300	-0.02636100	-0.32892500				
H	4.23811000	-0.06641000	-0.83683200				
TS2				P2			
							
O	0.05075500	-1.47921600	0.03960000	O	-0.41343000	-1.42637400	-0.18970300
C	-1.08655000	-0.71208700	0.31522100	C	0.76847000	-0.72808300	-0.12520700
C	1.14632500	-0.63062500	0.34335100	C	-1.44518700	-0.44181700	-0.33551900
H	1.37805800	-0.67690900	1.41685500	H	-1.72187000	-0.38125200	-1.39452300
C	-0.80166900	0.66895200	0.35986300	C	0.64517200	0.59539000	-0.01592500
H	-1.24546700	1.32216100	1.10385400	H	1.45296400	1.31065200	0.07011800
C	0.66067500	0.79968400	0.02499300	C	-0.82238000	0.91191900	0.06914500
H	0.74194900	0.98119700	-1.05696800	H	-1.08395600	1.16642100	1.10750200

O	-1.82361600	1.36144300	-0.99099200	O	3.60684300	1.63146600	0.52942400
H	-2.02434800	2.29073600	-0.82824100	H	4.45509000	2.00336200	0.28367600
O	1.29091900	1.80393400	0.77059400	O	-1.20453400	1.96025800	-0.78772700
H	2.23700000	1.72330900	0.59966100	H	-2.14654300	2.10635300	-0.64714300
C	-2.39713400	-1.13701800	0.21254000	C	1.98318200	-1.56148100	-0.19099200
H	-2.64943800	-2.20156800	0.20217000	H	1.79800700	-2.63606500	-0.36085400
O	-3.31755100	-0.26795600	0.06054600	O	3.10472000	-1.13047800	-0.07609600
H	-2.64779400	0.75997200	-0.60435300	H	3.65987900	0.68717600	0.32988200
C	2.34909800	-1.02971200	-0.48061300	C	-2.64627100	-0.81484300	0.50181800
H	2.72741000	-2.00531700	-0.16206900	H	-3.09290700	-1.74868900	0.14706400
H	2.05642700	-1.08242900	-1.53495000	H	-2.33450800	-0.93972200	1.54552200
O	3.30961300	-0.00084300	-0.26188700	O	-3.53701900	0.28276200	0.35406100
H	4.12078000	-0.20520800	-0.73097900	H	-4.33671400	0.12418400	0.85917300
R3				TS3			
							
O	0.41293500	-1.11657600	-0.31766100	O	0.35311400	-0.92832600	-0.53176900
C	1.35183100	-0.16300700	-0.01866400	C	1.32138100	-0.18161300	0.00802300
C	-0.83981700	-0.42357900	-0.40156700	C	-0.87401800	-0.29388500	-0.22300500
H	-1.06175600	-0.23456700	-1.45819000	H	-1.19238400	0.77727000	-1.06191300
C	0.86265900	1.03487100	0.29715800	C	0.87120000	0.87922000	0.72541000
H	1.44584500	1.89988700	0.57289500	H	1.48889400	1.58225000	1.25910700
C	-0.63749200	0.94316100	0.28907300	C	-0.56401200	0.86236300	0.61268300
H	-1.02004000	0.91781500	1.32067300	H	-1.23829100	1.26808400	1.35604600
O	-1.24543900	1.99993900	-0.41440400	O	-1.03411100	1.98864300	-0.76118400
H	-2.19709600	1.85543000	-0.36639900	H	-1.83710500	2.51703200	-0.63957000
C	2.76239500	-0.61018600	-0.09022700	C	2.70909800	-0.62642400	-0.25541700
H	2.90187100	-1.65100300	-0.43441600	H	2.79509700	-1.51295800	-0.90847800
O	3.68902900	0.09809900	0.19764400	O	3.66711300	-0.07341500	0.21206200
C	-1.93816100	-1.24839800	0.22703400	C	-1.97258500	-1.26744000	0.09515600
H	-2.08862000	-2.18165600	-0.32401200	H	-2.06616000	-1.98301900	-0.72863400
H	-1.66748000	-1.48367200	1.26310200	H	-1.75275700	-1.82674600	1.01531200
O	-3.08634900	-0.41257900	0.16813800	O	-3.14685400	-0.48739900	0.25192100
H	-3.84262100	-0.87047200	0.53977400	H	-3.85776900	-1.05126400	0.56278000
P3				R1''			
							
O	0.48083900	-0.46091700	-0.80532700	O	1.39554600	-0.58655100	-0.97663900
C	1.53058600	-0.10885700	-0.00553000	C	0.56044600	0.30169400	-0.26311500
C	-0.59785400	-0.57313700	-0.01402800	C	2.48923400	-0.86416000	-0.12584700



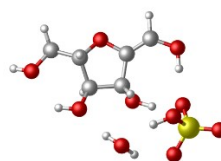
H	-2.68383600	1.33987400	0.16782100	H	2.19104400	-1.53915300	0.68680300
C	1.11169600	0.00314400	1.28640200	C	1.52835600	1.24010800	0.52520300
H	1.73874600	0.27088400	2.12176800	H	1.18805900	1.31547100	1.56230800
C	-0.28030900	-0.30190300	1.28361500	C	2.86445300	0.49809800	0.47003900
H	-0.96463800	-0.32455400	2.11547700	H	3.50455100	1.04045200	-0.23936600
O	-2.39188200	2.10586500	-0.34090600	O	1.68268700	2.51477100	-0.06033600
H	-1.59714600	2.41013200	0.10247400	H	0.79061000	2.88250300	-0.14088900
C	2.82740500	0.07128800	-0.65175600	O	3.48521000	0.40202000	1.73335900
H	2.82790100	-0.10201600	-1.74367500	H	4.24337200	-0.18061500	1.61643300
O	3.82559700	0.38427700	-0.05303500	O	-0.17316300	-0.48055600	0.65122800
C	-1.88100500	-0.94214900	-0.67497100	H	-0.94125900	0.03596800	0.97423100
H	-1.99623300	-0.34018300	-1.58279800	C	-0.33205300	1.03217500	-1.25955600
H	-1.86841500	-2.00356900	-0.94785500	H	-1.06240700	0.33316400	-1.67807500
O	-2.91176200	-0.66939500	0.26117300	H	0.30008500	1.42458200	-2.05768100
H	-3.74183500	-1.01953600	-0.07084800	O	-0.97319600	2.12967200	-0.63403500
				H	-1.75110400	1.78210100	-0.15569100
				C	3.59790700	-1.48446900	-0.94364500
				H	3.29881800	-2.47073000	-1.31217600
				H	3.81486900	-0.83112100	-1.79651000
				O	4.72552700	-1.58108000	-0.07282100
				H	5.47722500	-1.91550600	-0.56397500
				S	-3.49100700	-0.42611800	0.12535900
				O	-2.65595700	0.58593000	0.84931100
				O	-4.81135900	-0.61580600	0.68475700
				O	-3.40437800	-0.23826400	-1.32139700
				O	-2.72909000	-1.83948300	0.44877400
				H	-1.78242300	-1.72512300	0.26277300

TS1''



O	1.59284300	0.53567500	-1.25798900
C	0.62397900	0.82625900	-0.46994900
C	2.53704500	-0.34832600	-0.59984600
H	2.32102600	-1.35282800	-0.96420800
C	0.91870300	0.53490100	0.97784300
H	0.09092400	0.00247400	1.45148500
C	2.22987100	-0.25218100	0.90804500
H	2.99980800	0.34392700	1.40897300
O	1.17513600	1.80500200	1.54952700
H	0.34268500	2.30277800	1.41945300
O	2.11759000	-1.51879200	1.51416800

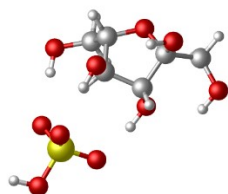
PI''



O	2.60058600	1.56393500	-0.16860900
C	1.20100400	1.58612400	-0.04242300
C	2.93989100	0.21883000	-0.43350400
H	2.75782400	-0.02937100	-1.49007300
C	0.69963200	0.23591500	0.43047300
H	-0.00351700	-0.17684600	-0.30208100
C	1.98154700	-0.59699800	0.43382900
H	2.34973500	-0.62322700	1.46763900
O	0.13300100	0.21477000	1.71851500
H	-0.81811600	0.39245700	1.60180800
O	1.76101500	-1.90734900	-0.05023600

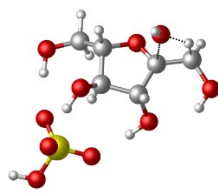
H	2.98409400	-1.93508500	1.48017000	H	2.61872200	-2.34271000	-0.10311000
O	0.04105400	-1.59319600	-0.53000000	O	-0.95595400	-2.67698400	-0.57084100
H	0.33890200	-2.08304300	0.24378500	H	-0.04719900	-2.51781600	-0.28039900
C	-0.50526100	1.64153500	-0.90134600	C	0.53309200	2.68747000	-0.37866000
H	-1.25746200	0.92479400	-1.36061300	H	-1.86315500	-1.29169400	-1.33237600
H	-0.18992300	2.32329000	-1.69912000	H	1.09185500	3.54901100	-0.73041700
O	-1.09064900	2.29964600	0.17883800	O	-0.79163200	2.91050000	-0.31889100
H	-1.74786900	1.56368400	0.57444700	H	-1.31346600	2.12706200	-0.03218000
C	3.93256500	0.10093500	-0.96697400	C	4.39380400	0.00030200	-0.08055600
H	4.08031200	0.04793300	-2.05028200	H	5.04705000	0.56349900	-0.75489400
H	4.08480000	1.13362300	-0.63073400	H	4.55526800	0.34381600	0.94723500
O	4.78781300	-0.79970400	-0.27758400	O	4.62656800	-1.40384700	-0.19574600
H	5.69916500	-0.52688100	-0.39573000	H	5.50943500	-1.60578600	0.11743400
S	-3.08800100	-0.46410600	-0.05032500	S	-3.13211200	-0.20349800	0.02000300
O	-2.26919900	0.32564600	0.99091900	O	-2.23118100	0.83493500	0.60275200
O	-4.48379300	-0.58378600	0.36380300	O	-4.46206200	0.28691800	-0.26732300
O	-2.91617300	0.26649300	-1.35137900	O	-2.48360400	-0.53812700	-1.43235400
O	-2.42568000	-1.81792000	-0.16681400	O	-3.03807400	-1.45789700	0.78256300
H	-0.99138600	-1.69023100	-0.46696800	H	-1.53377800	-2.53709900	0.19776300

R1''''



O	2.49108700	1.13398800	-0.02855600
C	2.49192300	-0.25418700	0.25834300
C	1.20858800	1.70148000	0.25950800
H	1.29071400	2.42890200	1.07223000
C	1.02376700	-0.68598000	0.11524500
H	0.81115800	-1.57233300	0.71985300
C	0.30612100	0.54635600	0.67961700
H	-0.67125300	0.68428500	0.23648500
O	0.73950000	-0.91575900	-1.25026900
H	-0.20651900	-1.14545900	-1.30302300
O	0.19112700	0.45558000	2.09012200
H	-0.67347900	0.04287100	2.24583500
O	2.93861900	-0.49729000	1.56689400
H	2.22663800	-0.25233100	2.17418400
C	3.44030100	-0.93136900	-0.72347900
H	4.46000900	-0.81419400	-0.35353600
H	3.33971800	-0.42149100	-1.68516200
O	3.18753300	-2.31520100	-0.84990700
H	2.30922700	-2.38168500	-1.24405700

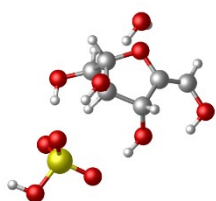
TS1''''



O	2.16288100	0.99118000	-0.84358400
C	2.44125300	-0.17506100	-0.35872400
C	1.09344600	1.60032700	-0.06627000
H	1.57525600	2.18445800	0.72137900
C	1.31387500	-0.76657500	0.44713300
H	1.66370400	-1.08281600	1.42836100
C	0.33766500	0.41794200	0.55090200
H	-0.49544400	0.20326800	-0.11846800
O	0.83546300	-1.86428700	-0.31970800
H	-0.13541000	-1.83495600	-0.40260100
O	-0.09848100	0.70508400	1.84592200
H	-1.00656100	0.37121600	1.93157000
O	3.66314200	0.57283400	1.35802400
H	3.76406800	0.73127000	2.30029700
C	3.64675800	-0.85383100	-0.69511300
H	4.13828900	-0.30057300	0.29465100
H	4.11820800	-0.51368600	-1.61803100
O	3.63564400	-2.24752500	-0.51593700
H	2.74938300	-2.57514400	-0.71322700

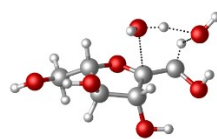
C	0.67341500	2.37772300	-1.00454800	C	0.24897400	2.42112600	-1.03626700
H	1.37608800	3.15356500	-1.31710600	H	0.82699200	3.27724100	-1.39354500
H	0.61426200	1.62572200	-1.79936700	H	0.01305600	1.78293300	-1.89835500
O	-0.57169800	3.00634500	-0.77852500	O	-0.91677600	2.90804800	-0.42551500
H	-1.27717400	2.34266100	-0.75824700	H	-1.59466100	2.21223300	-0.44701000
S	-2.73880600	-0.52394100	-0.02857600	S	-2.82425100	-0.56392000	-0.03195800
O	-2.44263500	-0.55183600	1.41074900	O	-2.66118700	-0.39454900	1.41791700
O	-2.77312800	0.83611900	-0.58489700	O	-2.75314200	0.71323300	-0.75896800
O	-1.96812600	-1.48133100	-0.82351100	O	-2.01552300	-1.63652600	-0.60923200
O	-4.26776700	-1.09009600	-0.17013700	O	-4.34966100	-1.10417000	-0.24405200
H	-4.83928100	-0.47574000	0.30529300	H	-4.93956900	-0.44287000	0.13740400

P1''''

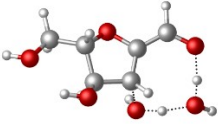
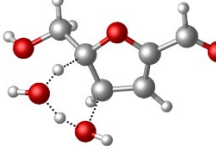
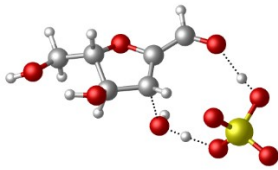
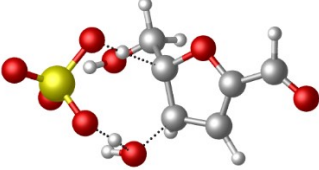


O	2.67534500	-0.73774000	0.40905200
C	2.47358600	0.57968300	0.04448700
C	1.37279000	-1.29559000	0.67894100
H	1.42241900	-2.36878400	0.49330400
C	1.10512700	0.75928400	-0.56560800
H	1.16727800	0.88884000	-1.65321100
C	0.41574900	-0.59601300	-0.28355200
H	-0.52204500	-0.42448700	0.23221600
O	0.49400800	1.88645900	0.03919400
H	-0.45434800	1.90435000	-0.18981600
O	0.18752400	-1.34603100	-1.45701500
H	-0.76384700	-1.27904300	-1.64654900
O	2.84248400	-2.27331200	-2.11404100
H	1.89204000	-2.09316900	-2.12653100
C	3.34574500	1.55059600	0.28796300
H	3.14206800	-1.80811200	-1.32465500
H	4.30047400	1.37253800	0.76554200
O	3.11795600	2.85551800	-0.05367300
H	2.15664900	2.96885000	-0.11828600
C	0.96845200	-1.00444400	2.12617000
H	1.73093000	-1.40912800	2.79503600
H	0.92882100	0.08356700	2.27087600
O	-0.25445200	-1.62247700	2.45659300
H	-0.99994900	-1.13168800	2.07650800
S	-2.82481800	0.26519300	-0.19084400
O	-2.54908600	-0.73620000	-1.23182700

TS1'

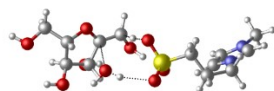


O	-0.31855600	0.31528900	1.32339800
C	0.67520500	0.48880000	0.53656600
C	-1.45603200	-0.22053300	0.58556300
H	-1.43147400	-1.29933800	0.74323000
C	0.29840000	0.50080900	-0.92354100
H	0.90685300	-0.19323100	-1.50230400
C	-1.17543100	0.09339000	-0.89624500
H	-1.76687600	0.95852000	-1.21509200
O	0.42547600	1.83941600	-1.35008800
H	1.37104800	2.04961900	-1.30982900
O	-1.40976600	-1.01304100	-1.72861300
H	-2.35815900	-1.18054900	-1.73217900
O	0.75278700	-2.04111900	0.16882700
H	0.45031000	-2.47736100	-0.63177500
C	2.00593100	0.73971700	1.00435000
H	2.40034100	-0.36240700	1.12168700
H	2.06804100	1.27489400	1.95279900
O	2.83482500	1.22884600	-0.01594100
H	3.32865000	0.41147100	-0.27305600
C	-2.72605800	0.40632800	1.11173600
H	-2.88380300	0.14082000	2.16133700
H	-2.66741000	1.49746500	1.01887800
O	-3.73307600	-0.13403700	0.27223200
H	-4.59099700	0.21224200	0.52610100
O	3.16838200	-1.34782400	0.10459300
H	3.90798100	-1.91186400	0.33516300

O	-2.59749600	-0.24504800	1.16851700	H	1.77283600	-1.95159200	0.09921000
O	-2.23864500	1.57902400	-0.45494200				
O	-4.42916900	0.56002000	-0.28271800				
H	-4.87984900	-0.26962400	-0.08447200				
TS2'				TS3'			
							
O	0.51809500	1.41827100	0.46857200	O	-0.59634400	-0.90064200	0.64757700
C	-0.69158800	0.85571900	0.01021000	C	-1.57127900	-0.22296300	0.04324500
C	1.52202300	0.64088000	-0.15906800	C	0.63716200	-0.47202000	0.06075400
H	1.64298700	0.95039500	-1.20666300	H	1.46582600	0.28305700	1.00206000
C	-0.53231300	-0.53276000	-0.22929200	C	-1.14725800	0.61201200	-0.93563700
H	-1.08936700	-1.01881500	-1.02370400	H	-1.78477900	1.19441500	-1.58213200
C	0.96492600	-0.79578400	-0.15233300	C	0.30721400	0.53450700	-0.94035700
H	1.19962100	-1.27350000	0.80971900	H	0.87729400	0.58319900	-1.86178400
O	-1.21799900	-1.50944300	1.04492300	O	0.91325100	2.11438400	-0.41064900
H	-1.08696600	-0.99271300	1.85071700	H	0.15059200	2.61490500	-0.09792400
O	1.39822000	-1.58540900	-1.22444900	C	-2.94813500	-0.48959300	0.52339100
H	2.36211600	-1.59545900	-1.18859800	H	-3.01603100	-1.20358100	1.36325000
O	-3.42918700	-1.06358400	0.14601800	O	-3.91749700	0.02226000	0.03228900
H	-4.29340000	-1.13671800	0.55431200	C	1.51542800	-1.63887400	-0.31330300
C	-1.78475100	1.65018400	-0.29074100	H	1.40383000	-2.41141900	0.45398800
H	-1.61656200	2.73428200	-0.24160700	H	1.25020600	-2.07586300	-1.28678300
O	-2.93669500	1.23485900	-0.60086400	O	2.85138600	-1.14044600	-0.35790200
H	-3.28622800	-0.08498100	-0.22540200	H	3.41485000	-1.79220000	-0.78047900
C	2.82977200	0.76266100	0.58855600	O	2.10654200	1.16987900	1.39607200
H	3.24542900	1.76837000	0.47981500	H	1.60436800	1.82408100	0.50758800
H	2.65578400	0.55950900	1.65132500	H	3.01634800	0.92151600	1.19454500
O	3.68210400	-0.22017800	0.00903300				
H	4.55170100	-0.17751600	0.41115400				
H	-2.24983900	-1.41438300	0.77907200				
TS2''				TS3''			
							
O	2.36840800	1.46690600	0.27255500	O	-1.73510600	0.34654600	-1.04293800
C	0.98828000	1.30209000	-0.02940400	C	-2.57255900	-0.22373900	-0.17419700
C	2.97931900	0.31589500	-0.27099500	C	-0.65894600	0.90545800	-0.27041700

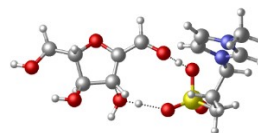
H	3.14267000	0.44457700	-1.35171600	H	0.55199100	0.10221100	-0.93887000
C	0.64057400	-0.05841400	-0.07421900	C	-2.22865500	-0.05537500	1.12310100
H	-0.19265900	-0.41508300	-0.67463600	H	-2.80240300	-0.39141300	1.97192100
C	1.95800800	-0.82283700	-0.08619800	C	-0.97293500	0.70223500	1.13841700
H	2.09743900	-1.30268600	0.89064000	H	-0.88194400	1.55465900	1.81424800
O	-0.06969300	-0.57136500	1.50337100	O	0.16621400	-0.21973500	1.96167000
H	0.02759000	0.23507800	2.02357300	H	0.90825200	0.39208100	2.10222000
O	2.00730600	-1.77713200	-1.11978000	C	-3.71774300	-0.93268300	-0.76697900
H	2.90386900	-2.12830600	-1.11812400	H	-3.69609100	-0.97701000	-1.87188700
C	0.19003900	2.42099700	-0.26784500	O	-4.62071400	-1.41854800	-0.13073300
H	0.74547300	3.37686200	-0.30577500	C	-0.28586200	2.30484200	-0.71089900
O	-1.04467600	2.43487700	-0.42496600	H	-0.05683700	2.30231300	-1.78485200
H	-2.43171000	1.48561900	-0.31332300	H	-1.09593700	3.02989600	-0.54515900
C	4.28924200	0.05050300	0.43351200	O	0.80837300	2.76592900	0.05698800
H	4.99939700	0.86452800	0.25422700	H	1.49783400	2.07913300	0.07162700
H	4.10044600	-0.02999400	1.51001700	S	2.36959500	-0.73749700	-0.21042700
O	4.77743000	-1.18203100	-0.09607500	O	3.54758700	-1.37062200	-0.75100300
H	5.54268600	-1.46338800	0.40763300	O	2.57270100	0.51142200	0.56006200
S	-3.14074400	-0.54245500	-0.06414100	O	1.41391000	-0.35901700	-1.40181100
O	-4.48865900	-1.06558600	-0.06854700	O	1.54295400	-1.69196700	0.64606000
O	-2.23819600	-0.97801100	-1.12933500	H	0.71447400	-1.00840800	1.32708100
O	-3.31219000	1.04050900	-0.20911800				
O	-2.47373400	-0.73714900	1.28463400				
H	-1.16402700	-0.68547000	1.37272300				

TS1''''



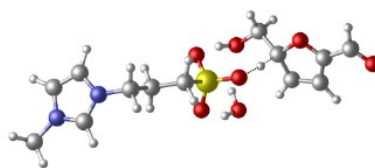
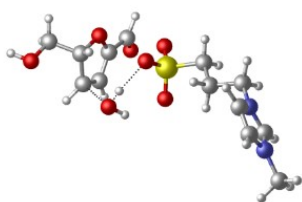
O	-3.45999400	0.67085900	1.34337500
C	-2.59631700	1.03293800	0.43931700
C	-4.59654600	0.01171800	0.72826900
H	-4.44594400	-1.06182800	0.84406300
C	-3.14007500	0.96242000	-0.97106000
H	-2.53444200	0.29962000	-1.59129500
C	-4.54511600	0.39247900	-0.76319400
H	-5.26079100	1.19364600	-0.97288200
O	-3.22468700	2.26822400	-1.48944900
H	-2.32417400	2.61197900	-1.55614200
O	-4.77553800	-0.71464500	-1.60322700
H	-5.70495500	-0.95636800	-1.51896000

TS2''''



O	3.29073100	-1.01729200	-1.44032900
C	2.14936800	-0.49249200	-0.84229100
C	4.04903400	-1.54855100	-0.36031400
H	3.64786200	-2.52832100	-0.06649600
C	2.41684100	-0.05392300	0.46599800
H	1.63673400	-0.01006900	1.21600600
C	3.80642900	-0.56410200	0.80138300
H	4.52844700	0.25912400	0.70830000
O	2.70822600	1.79206300	0.46937700
H	3.16084800	2.07989900	1.27398700
O	3.83457200	-1.13662300	2.07589500
H	4.70350100	-1.54592900	2.17993600

O	-2.51827500	-1.75959700	-0.30047600	C	0.92119200	-0.63572200	-1.44500700
H	-3.14865600	-1.94999900	-1.00565600	H	0.91081100	-1.21854000	-2.37405100
C	-1.32101100	1.45987200	0.75079900	O	-0.18642000	-0.16750300	-0.99887500
H	-0.79157000	0.18591500	0.98169200	H	-0.53716200	1.13068900	-1.18691800
H	-1.13551900	1.86378800	1.74568800	C	5.51227000	-1.65546700	-0.72261400
O	-0.61990300	2.05429100	-0.30239800	H	5.67364100	-2.44492000	-1.46124400
H	0.07268600	1.44444700	-0.60544700	H	5.85399200	-0.70015800	-1.13573200
C	-5.87156300	0.46136000	1.40584500	O	6.15574800	-1.94792500	0.51189700
H	-5.89136400	0.13905500	2.45083400	H	7.09145600	-2.10803900	0.37018300
H	-5.95076400	1.55412200	1.36197900	C	-2.68107700	-1.78314300	-0.27117100
O	-6.88472300	-0.16657800	0.63774700	C	-3.29239400	-2.97755500	-0.05406100
H	-7.74951300	0.03948400	0.99933400	C	-4.81052500	-1.39956700	0.15173700
S	0.78643000	-1.24872300	0.05960300	H	-1.66360200	-1.50641100	-0.52198400
O	1.10731700	-0.10450100	-0.82158300	H	-2.90581900	-3.98262000	-0.06888100
O	-0.05475100	-0.77419500	1.23243900	H	-5.75051300	-0.89448200	0.30806200
O	0.24462900	-2.42735800	-0.59675000	N	-3.65174800	-0.81378600	-0.13852900
H	-1.73561800	-2.30116000	-0.46315900	N	-4.62057600	-2.71595000	0.20785800
C	2.34200700	-1.72464900	0.80711200	C	-3.41676400	0.63308500	-0.26842600
H	2.71724400	-0.82200000	1.29389200	H	-2.87025100	0.79295100	-1.19789300
H	2.11620600	-2.47030400	1.56925500	H	-4.39444900	1.11057700	-0.35648100
C	3.27434300	-2.26044000	-0.28759600	C	-2.64631500	1.17018200	0.93744900
H	3.20219800	-3.34728900	-0.33666600	H	-3.23031000	0.99273600	1.84384200
H	2.96468800	-1.90062100	-1.27291900	H	-1.70137800	0.62764400	1.04730900
C	4.73467600	-1.90568300	-0.06109400	C	-5.64813700	-3.72316100	0.48292700
H	5.35547800	-2.35388800	-0.83831300	H	-5.37531200	-4.28115600	1.37697100
H	5.08237000	-2.25594300	0.91261200	H	-6.59934100	-3.22031000	0.64249700
C	4.15759300	0.51988200	-0.67455500	H	-5.72952100	-4.39459900	-0.37015100
C	6.04722000	0.15675400	0.39951900	C	-2.36941500	2.66874900	0.81023900
C	4.79059900	1.71167300	-0.51032300	H	-3.14698600	3.20758100	0.26459700
H	4.49965200	2.70678100	-0.80236900	H	-2.23996800	3.14087900	1.78466200
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H	6.85899000	-0.33893500	0.90835800	H	1.79446600	2.18046700	0.50938300
H	3.19177400	0.29703200	-1.10846100	O	-0.93076500	2.12127800	-1.32647400
C	6.95706900	2.47119000	0.54872700	O	-0.79594300	4.39848800	-0.40862300
H	6.49247800	3.18864300	1.22294000				
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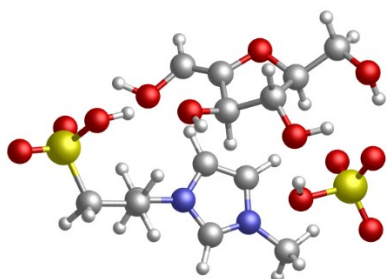


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O	-1.49471200	1.76098400	1.22021700
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C	-3.90130100	-2.30919400	0.09136700
H	-3.82529100	-2.69078200	-0.93502400
O	-4.12791200	-2.97546700	1.05632600
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C	4.96793500	0.99749100	-1.16382300
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C	5.47938900	-0.41481800	0.43988000
H	4.43436500	1.37185900	-2.02167800
H	6.52492400	2.46000600	-0.55924300
H	5.47608000	-1.28030600	1.08373500
N	4.66919500	-0.22032000	-0.59630300
N	6.29433500	0.63253600	0.55202300
C	3.56734100	-1.11214800	-1.00500500
H	3.61260700	-1.20280300	-2.09163000
H	3.77682000	-2.09337200	-0.57550000
C	2.22549800	-0.57092400	-0.52884100
H	2.24383500	-0.44151700	0.55723400
H	2.02962900	0.40729800	-0.97783100
C	7.33802300	0.80560400	1.56715600
H	7.11077100	1.68456300	2.16791700
H	7.35604400	-0.07683800	2.20276000
H	8.30215000	0.92131000	1.07527300
C	1.09913500	-1.52550200	-0.89333800

O	4.51922400	-0.58446500	0.88208700
C	5.38230100	-0.77283200	-0.08276600
C	3.67204800	0.47800600	0.49735700
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C	5.23712900	0.13453100	-1.12164300
H	5.82733600	0.15333100	-2.02369300
C	4.18787900	0.95991600	-0.74169000
H	3.71522200	1.76508700	-1.29814500
O	1.90509600	2.71806000	-1.62524500
H	1.10672400	2.18566500	-1.74636700
C	6.34010100	-1.91416600	0.06200400
H	6.24420900	-2.50538900	0.98680400
O	7.14709500	-2.13690200	-0.79097100
C	3.23511400	1.34220300	1.69617200
H	2.83421300	0.66656600	2.45722600
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O	2.31046900	2.30752900	1.30150900
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C	-6.61677500	0.31903100	0.97155900
C	-5.75613700	-0.72084300	-0.76460500
H	-4.95371600	-0.26998700	2.31817700
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N	-4.93564700	-0.91104400	0.26518100
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C	-3.63256800	-1.59972900	0.21307700
H	-3.56258300	-2.22326900	1.10580200
H	-3.65153900	-2.25677600	-0.65787500
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H	-2.51786000	0.07118800	1.00539100
C	-7.91734300	0.44588900	-1.19357100
H	-7.96464300	1.53324100	-1.20169300
H	-7.76363900	0.08001900	-2.20612300
H	-8.83782500	0.02905100	-0.78894700
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H	-0.90359700	-1.84887400	0.94271200

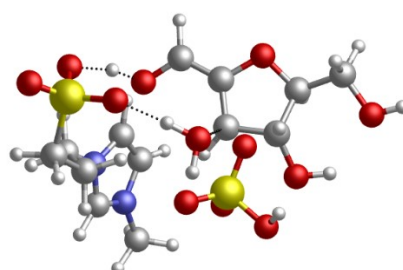
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S	-0.45818500	-0.91310500	-0.23729900	O	-0.21826700	0.77404900	-1.28459400
O	-0.23010600	-0.71711700	1.21039400	H	1.84556400	3.04989900	-0.72259200
H	-1.12282400	1.56487300	0.33156400	O	0.05249900	0.76812100	1.17576000
O	-0.69019800	0.38801300	-0.92773800	O	1.40745100	-0.75505900	-0.20252500
O	-1.45235700	-1.93902500	-0.57000300				

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O	0.98837500	-2.45547800	1.66334100
C	-0.16852800	-1.85634700	1.25112900
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H	2.36565500	-1.16717400	0.79495600
C	-0.09100000	-1.50370500	-0.21402500
H	0.09888800	-0.42722000	-0.34427200
C	1.15600500	-2.26424700	-0.63319000
H	0.89146400	-3.31584700	-0.81410600
O	-1.27208700	-1.87469900	-0.91348100
H	-1.04963500	-1.99371600	-1.84374400
O	1.71683400	-1.68501300	-1.78666600
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C	-1.20063700	-1.59669900	2.04311200
H	-1.24402600	-1.87284800	3.08926200
O	-2.22603300	-0.83882200	1.51164400
H	-3.08565100	-1.01127000	1.91482500
C	3.10257900	-3.20091400	0.71264900
H	3.70942100	-3.05125400	1.61117400
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O	3.87282300	-3.10486100	-0.46775000
H	4.29405400	-2.22722900	-0.49177300
C	-0.27797100	1.60946900	1.64885700
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H	-0.75460200	0.86682300	2.26278700
H	1.89888400	1.73474700	2.11626500
H	-0.38397700	3.77679200	-0.76002400
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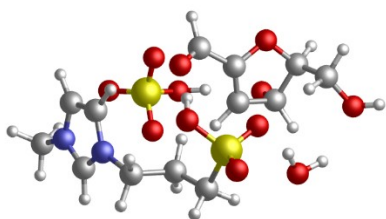


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C	1.28464900	-1.15558800	-0.21365100
H	0.71444600	-0.32882000	-0.61597800
C	2.68487600	-1.54364000	-0.60982200
H	2.59860800	-2.52841800	-1.09024800
O	0.29101800	-2.40144300	-1.47088700
H	0.15238300	-1.98504900	-2.32923800
O	3.33894800	-0.63919000	-1.45807200
H	4.26489400	-0.91737400	-1.48878100
C	-0.04609900	-1.63673400	1.79726800
H	-0.12435800	-2.17986000	2.73975700
O	-1.06535400	-0.93800400	1.37625100
H	-2.01894300	-1.40522100	1.43287600
C	4.47964200	-2.72261300	0.73764500
H	4.98171100	-2.76153900	1.70813900
H	4.10655200	-3.72037300	0.48209900
O	5.34753500	-2.22397400	-0.27682800
H	6.14915200	-2.74940800	-0.31419600
C	-1.39889600	2.15428300	1.53504300
C	-0.72794700	3.33292800	1.46453100
C	-2.05732300	3.20462600	-0.27577700
H	-1.32913600	1.33199000	2.22505900
H	0.06041200	3.73898900	2.07304800
H	-2.56028900	3.43861100	-1.19910000
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N	-1.16586900	3.97718500	0.33126600



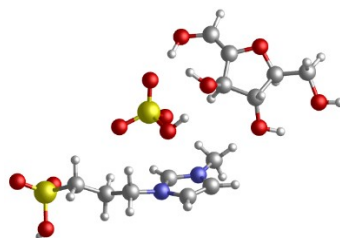
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C	-2.56167600	1.34911900	-0.96114900	C	-2.70706400	0.16450400	-1.05314700
H	-2.08921200	1.91237600	-1.77097400	H	-2.64814700	0.78376400	-1.95258800
H	-2.03381100	0.39467200	-0.88973200	H	-1.69717800	-0.20351500	-0.85558200
C	2.26868900	3.72742600	0.17970600	C	-0.64827300	5.24567500	-0.17820600
H	3.10135300	3.38094300	0.78647000	H	-0.77223700	6.01076300	0.58697700
H	2.49040900	3.48547700	-0.85799900	H	0.40436600	5.10181700	-0.41883800
H	2.10230700	4.79442900	0.32214600	H	-1.21862800	5.51938900	-1.06378100
C	-4.02279000	1.12224900	-1.34154100	C	-3.68491000	-0.98545600	-1.29974100
H	-4.65266000	1.99425300	-1.14708700	H	-4.72430200	-0.69089200	-1.13579400
H	-4.12635000	0.84784400	-2.39174400	H	-3.59950200	-1.37978000	-2.31294100
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O	-3.94614800	-1.47667900	-0.88818600	O	-2.10612300	-2.97809700	-0.66606400
H	-3.03086700	-1.51628600	-0.52056900	H	-0.61553700	-2.62058500	-1.11978000
O	-4.66049000	0.01106600	0.97608400	O	-3.29725100	-1.87109200	1.16038900
O	-6.12293500	-0.41851900	-1.00816100	O	-4.55452700	-3.29287200	-0.42266800
H	2.04995400	0.09206600	-1.53778100	H	3.07114400	1.15631700	-1.61531800
S	3.79926200	0.86129100	-0.51856800	S	1.71923000	2.15757200	-0.33315000
O	3.59643800	0.94398200	0.93543200	O	1.76440700	3.54690200	0.11237300
O	4.26564000	-0.45798700	-0.97257900	O	0.43677500	1.77645000	-0.96883600
O	2.25318400	0.95044800	-1.11834700	O	2.83280000	2.09467100	-1.49978900
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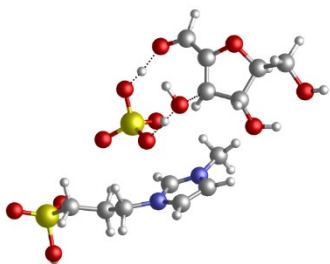
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H	-3.43154500	-3.43004600	0.58278700
C	-1.23047400	-1.20151300	-0.22427600
H	-0.44181600	-0.74608100	-0.80171500
C	-2.18295900	-2.23208600	-0.75473800
H	-2.71012300	-1.92686200	-1.65740600
O	-3.31194600	0.50987500	-2.11829700
H	-4.01717700	-0.14549700	-2.07272100
O	-1.41927900	-3.41886500	-0.99743000
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C	-0.48900300	-0.59847900	2.14335000

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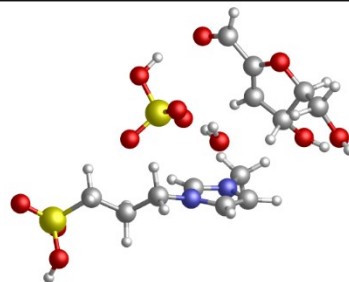


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C	-5.34385000	-0.06805100	0.29090300
H	-5.20565700	-0.28360000	1.36123300
C	-3.14311000	0.64305500	-0.34832600
H	-2.34726500	0.43132000	0.37645000
C	-4.09975600	-0.54591600	-0.46707200
H	-4.34267400	-0.66590400	-1.52978400
O	-2.57072900	0.88193300	-1.64231800
H	-2.17374600	1.76549600	-1.63538800
O	-3.55775500	-1.74585500	0.05632100
H	-4.28909200	-2.37788300	0.05701100
C	-3.75819200	2.93263700	0.67119200

H	-0.23611300	-1.26055600	2.97992900	H	-4.57293400	3.54975200	1.03352600
O	-0.11710500	0.55770500	2.12744100	O	-2.55972800	3.52176500	0.80891800
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C	-4.32367200	-1.44938300	0.37599300	C	-6.61888400	-0.70431200	-0.21377700
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O	-4.98444800	-1.64166100	-0.87218400	O	-6.39399000	-2.11177000	-0.13591700
H	-5.91897000	-1.45067600	-0.77001700	H	-7.16695500	-2.58146000	-0.45467400
C	2.82150500	1.29132400	1.04934500	S	0.32175100	1.27328200	-0.12646100
C	3.91224400	0.48540600	0.98991900	O	1.77212400	1.35372700	-0.25275500
C	3.64412500	1.40343800	-0.98401300	O	-0.13714500	0.81402600	1.19171400
H	2.10422500	1.44941000	1.83806100	O	-0.45608900	2.42489000	-0.61882700
H	4.32921700	-0.19435600	1.71268300	O	-0.04180600	0.06132100	-1.16627100
H	3.76614200	1.64178500	-2.02730600	H	-0.96433600	0.17058200	-1.48926000
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N	4.41817400	0.58377300	-0.28562100	C	-0.43896400	-2.92961400	-0.10888000
C	1.56547600	2.71264900	-0.62000100	C	1.06304900	-1.65293700	0.86217000
H	1.29545300	3.34713500	0.22486600	H	0.80385500	-3.23956500	-1.91849700
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C	0.37919600	1.86029000	-1.06677900	H	1.50762300	-0.95479600	1.54988200
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H	0.18878400	1.10290400	-0.30584800	N	-0.14433800	-2.18507400	1.00979300
C	5.53330300	-0.19960100	-0.81607400	C	2.70503300	-1.42172100	-0.99987600
H	6.41169400	-0.03023000	-0.19507100	H	3.11703200	-2.17486800	-1.67426600
H	5.23265000	-1.24721700	-0.80227800	H	2.28017400	-0.59921800	-1.57913000
H	5.73545200	0.13313300	-1.83235900	C	3.77288300	-0.90053900	-0.04941300
C	-0.86135000	2.71356200	-1.32503600	H	3.32377700	-0.33999000	0.76950100
H	-0.62493100	3.71907300	-1.67926500	H	4.36136000	-1.72545700	0.35935100
H	-1.54062800	2.23592800	-2.03584000	C	-1.03835500	-1.92743600	2.13993700
S	-1.86794100	2.94505300	0.15169500	H	-0.75318000	-0.97123100	2.57367600
O	-2.66584900	1.74125000	0.34844500	H	-2.05208100	-1.85607700	1.74807300
H	-3.21768400	0.82487000	-1.20894500	H	-0.95713500	-2.73531700	2.86698000
O	-0.79435000	2.98318900	1.32718900	C	4.65911300	0.07442200	-0.81237800
O	-2.49811300	4.23598700	0.09588500	H	5.04459600	-0.32246900	-1.75438000
H	0.47895300	-3.20863000	-0.67512300	H	4.12995300	1.01335500	-0.99699700
S	2.13462600	-1.95954400	-0.01769500	S	6.10315000	0.51956900	0.12806200
O	1.55221600	-1.81500700	1.32669100	O	5.77112000	0.71840700	1.52119600
O	3.55784700	-2.28863400	-0.02117600	O	6.87777900	-0.91363200	0.03527500
O	1.45315400	-3.26121100	-0.68430700	O	6.86336600	1.50164200	-0.59653300
O	1.79537500	-0.81501400	-0.89460200	H	7.37381800	-1.04765100	0.85473600
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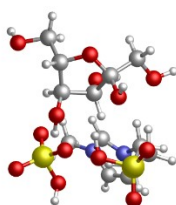
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H	-5.39793900	0.16131000	-1.29985000
C	-3.09596100	-0.50391400	0.16041300
H	-2.16052200	-0.31597200	-0.36017400
C	-4.10011600	0.62398400	0.35035400
H	-4.21881300	0.81301200	1.42337500
O	-2.34682000	-0.59381400	1.80312600
H	-2.43280100	-1.52432200	2.05014100
O	-3.71928100	1.80980400	-0.32010200
H	-4.50217600	2.37641500	-0.31136900
C	-3.45813600	-2.84580400	-0.71511100
H	-4.27571300	-3.48787200	-1.07096000
O	-2.28242400	-3.26344400	-0.85610500
H	-1.18634000	-2.84117800	-0.17336800
C	-6.63472300	0.53021300	0.42922400
H	-7.52727400	0.11876400	-0.05019100
H	-6.64001300	0.26459000	1.49171100
O	-6.55448500	1.94405800	0.25174100
H	-7.33068000	2.36515200	0.62584800
S	0.41724000	-1.30932600	0.08023600
O	1.85727600	-1.50759900	0.19737300
O	-0.04441600	-0.89629500	-1.25527700
O	-0.34284300	-2.61156000	0.46592500
O	-0.02532000	-0.28408800	1.11592300
H	-1.31314600	-0.44510900	1.59277700
C	0.39923300	2.65255300	0.95921300
C	-0.64893600	2.71546600	0.09922500
C	0.98577500	1.62952800	-0.89101200
H	0.49827300	2.98638800	1.97706800
H	-1.64587700	3.10753900	0.20687500
H	1.51275800	1.02534900	-1.60823700
N	1.41747700	1.98093000	0.31748800
N	-0.25474800	2.07406600	-1.05323900
C	2.57005100	1.39403600	1.02055500
H	2.94187900	2.15267000	1.71205800



O	4.52992100	0.97917000	1.25223300
C	3.60159200	1.52981100	0.39598900
C	4.81098100	-0.32159900	0.73018800
H	5.72644400	-0.26839200	0.12659800
C	3.08901400	0.69089300	-0.50332500
H	2.30970400	0.94426700	-1.21140700
C	3.63537700	-0.67417800	-0.19941300
H	2.87815600	-1.24293200	0.35835300
O	1.19545100	-0.79175800	2.08541400
H	1.24362000	-0.40796300	2.96407000
O	4.03957400	-1.40761400	-1.34447500
H	4.53942700	-2.16344300	-1.01162900
C	3.28712800	2.94800500	0.63780600
H	3.88291300	3.42607600	1.43496700
O	2.44950600	3.56353200	0.02612100
H	0.56758500	3.75373100	-0.33682200
C	4.97154500	-1.32298300	1.84972100
H	5.83904700	-1.08441200	2.47180200
H	4.06261600	-1.32083300	2.46056500
O	5.13892100	-2.57132300	1.18017700
H	5.22567000	-3.27590900	1.82502000
S	-0.37227800	1.87436700	-0.53346600
O	-1.79023000	1.51110000	-0.55479600
O	0.33530100	1.54393400	-1.78195500
O	-0.36191300	3.46918500	-0.39180500
O	0.33185600	1.35388800	0.65874200
H	0.93948300	-0.03930800	1.51520400
C	0.24825600	-2.58831700	0.00514300
C	1.08516900	-2.55730500	-1.06275300
C	-0.53666400	-1.11583400	-1.42994700
H	0.31188800	-3.11674600	0.93918700
H	2.00849500	-3.07182000	-1.26264600
H	-1.12964800	-0.33437700	-1.87654400
N	-0.76122900	-1.68445700	-0.24526400
N	0.58131700	-1.62082100	-1.94016400
C	-1.76572200	-1.22448300	0.72766800
H	-1.77226900	-1.95820700	1.53439700

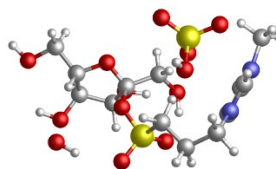
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C	3.67196200	0.93204100	0.07839900	C	-3.14648000	-1.06918500	0.09963100
H	3.25963400	0.36063700	-0.75233800	H	-3.07026800	-0.60739600	-0.88451000
H	4.22965100	1.78675600	-0.31236500	H	-3.63082500	-2.04279600	-0.00636200
C	-1.07719500	1.81737700	-2.23693400	C	1.21794600	-1.16062500	-3.17631500
H	-0.82568800	0.82173800	-2.60036000	H	0.89533200	-0.13421500	-3.34737800
H	-2.12011500	1.84003800	-1.92557100	H	2.29632900	-1.18579500	-3.02039900
H	-0.88809100	2.57827100	-2.99388100	H	0.93442500	-1.80732000	-4.00602900
C	4.58829500	-0.01518500	0.84092700	C	-3.97521400	-0.13915800	0.97431100
H	4.93502600	0.37870200	1.79901200	H	-3.99858300	-0.42980800	2.02719300
H	4.09917600	-0.98148200	0.99185800	H	-3.61884600	0.89068300	0.88118600
S	6.07200700	-0.36680400	-0.07797300	S	-5.67957500	-0.10076100	0.46740600
O	5.78224800	-0.53977800	-1.48417900	O	-5.79394600	-0.07990100	-0.97388900
O	6.78011500	1.09732000	0.06990100	O	-6.08529900	-1.60830200	0.94551900
O	6.86183000	-1.33229600	0.63724100	O	-6.40124800	0.84734900	1.27397500
H	7.26661300	1.28312200	-0.74512300	H	-6.78599500	-1.93607300	0.36485400

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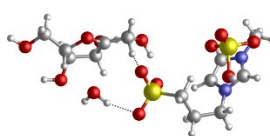
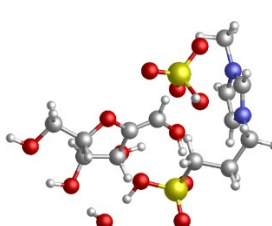


O	3.35484300	-1.84974000	0.54902300
C	2.64734500	-0.72288400	0.96832300
C	2.57799400	-2.63176600	-0.38243500
H	3.13833500	-2.74318500	-1.31223600
C	1.16978000	-0.95250600	0.60203400
H	0.68405200	-0.01684800	0.32209500
C	1.29578900	-1.84339600	-0.64091100
H	0.42753500	-2.50185400	-0.73397300
O	0.44627200	-1.62284300	1.62139500
H	0.56563500	-1.12261300	2.43736800
O	1.48097800	-1.04556400	-1.78618800
H	0.60682500	-0.67542400	-2.00124500
O	3.03786100	0.42942800	0.25067000
H	3.99921400	0.46377400	0.18241000
C	2.91316500	-0.54511300	2.45702000
H	3.93437100	-0.18033700	2.59846900
H	2.80316900	-1.51119400	2.95656000
O	1.95264900	0.39166000	2.94854000
H	2.25870600	0.75915900	3.78068400
C	2.33399500	-3.99229000	0.24695000
H	3.29045100	-4.39106400	0.60348100

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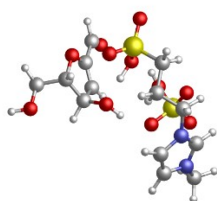
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C	-1.80991900	-0.28711200	0.80242900
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H	-3.45299600	-0.85684100	-1.22725900
C	-3.04595600	0.39940900	1.43171200
H	-3.04719600	1.47829900	1.24431000
C	-4.21310300	-0.29420000	0.71579300
H	-4.78453100	-0.82198800	1.48574000
O	-3.14075500	0.09408400	2.80064600
H	-2.33472000	0.41437500	3.22853500
O	-5.03943000	0.62189000	0.02999400
H	-5.76129400	0.10695200	-0.35202300
O	-3.84359600	1.30243300	-2.52600400
H	-4.24089200	1.30489700	-1.64629000
C	-0.58810200	-0.48764000	1.69775400
H	0.30845300	-0.61364700	1.08361400
H	-0.76068500	-1.42192300	2.23106700
O	-0.43648300	0.52431300	2.68158800
H	-0.29312100	1.35927300	2.21478100
C	-4.26871000	-2.62048700	-0.29161800
H	-3.82017600	-3.27924800	-1.04029400

H	1.65478800	-3.87573400	1.09978000	H	-4.22879400	-3.10571900	0.69053600
O	1.77379000	-4.80934800	-0.76194300	O	-5.60249100	-2.26401900	-0.63694500
H	1.38233600	-5.58844400	-0.36392700	H	-6.12226900	-3.05525800	-0.78874300
C	-3.45746700	1.96409800	1.52829100	S	-0.69914300	1.82466500	-0.61696500
C	-4.46546700	1.06229800	1.42306200	O	-0.39275800	2.37180500	0.70743300
C	-2.56766000	-0.05024500	1.41913600	O	-1.49024600	0.47035800	-0.46495800
H	-3.46910100	3.03791700	1.60138900	O	-1.42288900	2.67618500	-1.53324600
H	-5.53199800	1.19587700	1.37159000	H	-3.08346100	1.88654200	-2.44342800
H	-1.84079600	-0.84970900	1.33309100	C	0.83057800	1.29909600	-1.36619200
N	-2.28261100	1.24706000	1.53889600	H	1.20291000	0.47834600	-0.74555800
N	-3.88993000	-0.18477600	1.37282900	H	0.56831600	0.88572500	-2.33985900
C	-0.93608500	1.81584300	1.65880300	C	1.78842600	2.49771900	-1.44929800
H	-0.96673600	2.54970700	2.46831000	H	1.74010600	2.95200700	-2.43948300
H	-0.27680200	1.00675200	1.97628200	H	1.48742300	3.27764600	-0.74427200
C	-0.44214500	2.42986000	0.35231700	C	3.24159600	2.11864700	-1.17705800
H	-0.54922200	1.68503100	-0.44193300	H	3.86759600	3.01264400	-1.18381900
H	-1.04305300	3.29993100	0.07722600	H	3.60189000	1.40812900	-1.91966200
C	-4.62703800	-1.43080500	1.15878300	C	2.63068900	1.66816800	1.26054200
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H	-3.95933600	-2.26741400	1.33937300	C	3.01188800	0.73706500	2.17101500
H	-5.47207100	-1.44931000	1.84610200	H	2.64496300	0.53879200	3.16367300
C	1.02055100	2.82943400	0.52897800	N	3.38535400	1.44773900	0.12493000
H	1.14008200	3.77697900	1.05988200	N	4.00114700	-0.02070700	1.58883900
H	1.60363700	2.06199000	1.04062900	H	4.83491900	-0.05892000	-0.37692700
S	1.84802700	3.09175000	-1.03643700	H	1.87394400	2.43231600	1.31533000
O	1.57041700	1.73155700	-1.81474700	C	4.53601400	-1.26822000	2.13344400
H	2.08512800	0.97089800	-1.46647400	H	3.77210600	-2.03709900	2.02538800
O	3.26387200	3.23350100	-0.77321900	H	5.40501400	-1.56107400	1.55119900
O	1.12611300	4.10820200	-1.76155600	H	4.80188900	-1.10818900	3.17700100
H	-3.53556100	0.74627300	-2.17498200	S	2.78469200	-2.04245500	-1.03135000
S	-2.28864200	-0.95342300	-1.68738900	O	4.16600200	-2.31277700	-0.62305200
O	-2.63693100	-1.99654900	-0.72586800	O	2.02464600	-1.32555600	0.00565900
O	-2.38192000	-1.27758600	-3.09385200	O	2.09863100	-3.10857900	-1.72449100
O	-3.49211300	0.16408800	-1.40616000	O	2.94043600	-0.81697300	-2.17521700
O	-1.05838300	-0.22673300	-1.30139400	H	3.09578000	-1.24161300	-3.02823700
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O	4.00342000	1.43835600	-0.69952200	O	-1.88112900	-1.73544300	0.28671000
C	3.23492000	1.07704900	0.27234600	C	-1.68572800	-0.71589700	1.18114600

C	5.24200500	0.67481100	-0.68551300	C	-3.14096800	-1.54058900	-0.33036200
H	5.12697100	-0.12350100	-1.41797500	H	-3.03583900	-0.89005600	-1.20788800
C	3.91713500	0.18971500	1.28690900	C	-2.97614300	0.02677900	1.46581500
H	3.42476200	-0.78476300	1.32605500	H	-2.94179100	1.03095900	1.02289100
C	5.33770900	0.08013800	0.73103600	C	-3.99474700	-0.83131900	0.72697700
H	5.98237000	0.70744600	1.35677500	H	-4.40056800	-1.55858900	1.43933300
O	3.92849600	0.85282400	2.52811700	O	-3.28964100	0.10652700	2.83753700
H	3.00332200	0.97640800	2.78611000	H	-2.48593900	0.38875700	3.29155300
O	5.79145100	-1.25083600	0.72359900	O	-5.04849700	-0.06944500	0.15643700
H	6.70697400	-1.23938100	0.42263400	H	-5.59455800	-0.69434700	-0.34056500
O	3.49915200	-1.60649400	-0.95469800	O	-4.00613100	1.88235700	-1.37992900
H	4.10015800	-2.20466900	-0.49919600	H	-4.52108800	1.28118700	-0.79780600
C	1.88939000	1.45861900	0.36381300	C	-0.51045000	-0.45079600	1.73463000
H	1.45127100	0.64582600	-0.50191900	H	-2.54705700	1.52759800	-1.35487900
H	1.60330300	2.40808700	-0.09050300	H	0.38715500	-1.00985200	1.49963900
O	1.30306500	1.17450500	1.60045600	O	-0.40946200	0.59614900	2.64771600
H	0.76195500	0.36573700	1.48699600	H	-0.51547000	1.41463300	2.13287700
C	6.39440900	1.59159300	-1.02666500	C	-3.71411300	-2.87771600	-0.74369100
H	6.31244700	1.95139500	-2.05622800	H	-3.13403700	-3.31060900	-1.56281000
H	6.40516600	2.44881200	-0.34287000	H	-3.69079800	-3.55593400	0.11614400
O	7.53560400	0.76756100	-0.84331300	O	-5.05581100	-2.59869200	-1.14200000
H	8.33003700	1.24753300	-1.08625500	H	-5.46829900	-3.39577500	-1.47984500
S	0.20249700	-1.42497000	-0.61163500	S	-0.62079700	2.34572500	-0.79477500
O	0.23512200	-1.20515200	0.86103800	O	-0.67066900	2.50510300	0.66285000
O	0.74101900	-0.21605500	-1.32724100	O	-1.58252600	1.19098700	-1.24785400
O	0.86072600	-2.66343900	-1.04016300	O	-0.87631500	3.54218700	-1.57279500
H	2.69373700	-2.11350900	-1.14799100	H	-4.24944400	2.78972200	-1.17805500
C	-1.51882500	-1.51545700	-1.05891600	C	0.95863800	1.64635200	-1.21473200
H	-1.94896500	-0.56099000	-0.74005400	H	1.05770100	0.72916100	-0.62261000
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C	-2.16579300	-2.73540400	-0.39386000	C	2.02514900	2.71135600	-0.92866400
H	-2.16579500	-3.58560700	-1.07688900	H	2.12775500	3.37477800	-1.78849600
H	-1.58139100	-3.05118600	0.47487300	H	1.71325300	3.34817000	-0.09550400
C	-3.60403800	-2.47317800	0.03375000	C	3.39421300	2.12029400	-0.61966200
H	-4.02804800	-3.36059200	0.50774200	H	4.10717600	2.91931200	-0.40793100
H	-4.21459900	-2.17926300	-0.81974900	H	3.75006900	1.51266800	-1.45067700
C	-2.71486600	-0.96864500	1.89540400	C	2.45903900	1.30651600	1.60878800
C	-4.68412600	-0.48021900	1.03979300	C	4.03166600	0.09575900	0.65969900
C	-3.17864200	0.15137100	2.50406000	C	2.66580800	0.20656600	2.37475700
H	-2.72513500	0.78864600	3.24290000	H	2.15783400	-0.12197100	3.26555400
N	-3.68017400	-1.35303600	0.98674300	N	3.33139500	1.22134500	0.54266000
N	-4.41412800	0.42887300	1.96751500	N	3.66295100	-0.52563800	1.77288400
H	-5.53691400	-0.45839800	0.38019600	H	4.71863100	-0.30054700	-0.07121900
H	-1.76416900	-1.46813600	1.98464900	H	1.74415700	2.10366500	1.71823300

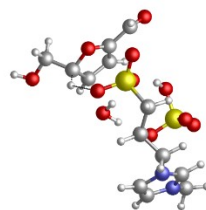
C	-5.16676800	1.66203000	2.18636000	C	4.03615500	-1.89331100	2.12983500
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H	-6.14870500	1.55810300	1.73387600	H	4.90389200	-2.18220300	1.54367000
H	-5.24666500	1.83799800	3.25823800	H	4.25048900	-1.93422200	3.19655500
S	-4.10068700	1.45327200	-1.36133700	S	2.60041700	-1.89968300	-1.30997200
O	-5.39645800	1.69574200	-0.71547600	O	3.88601300	-2.39602100	-0.80675300
O	-3.00332500	1.31161700	-0.39874100	O	1.77655000	-1.29431900	-0.25651000
O	-3.83724200	2.22455100	-2.55865600	O	1.92560100	-2.74253900	-2.27400800
O	-4.23618100	-0.13460100	-1.91456700	O	3.02675000	-0.52360800	-2.18503500
H	-4.60283300	-0.08984700	-2.80582200	H	3.25774400	-0.81747300	-3.07477700

IMf



O	-3.82373500	-0.13292200	0.14140500
C	-3.35616200	-1.06352800	-0.73207400
C	-3.20921200	-0.41313000	1.41367400
H	-2.84939300	0.52779300	1.83438300
C	-2.39352300	-1.85882700	-0.26053700
H	-1.88191900	-2.62642100	-0.82152300
C	-2.03836300	-1.36117500	1.11763700
H	-1.94029500	-2.13083500	1.88465200
O	-0.83856300	-0.57357400	1.09222600
H	-0.98891300	0.41994600	0.00229900
C	-3.94790900	-1.01394600	-2.09410500
H	-4.60123700	-0.14448000	-2.28449600
O	-3.72785400	-1.84989800	-2.92711100
C	-4.27217800	-1.04453800	2.29537500
H	-5.09614300	-0.33328100	2.40577700
H	-4.65146400	-1.95192700	1.80735400
O	-3.66149700	-1.34153100	3.53748200
H	-4.33218100	-1.63930100	4.15482500
C	3.17557100	0.17408800	2.25045900
C	3.66619600	-1.08407600	2.11918700
C	4.05919700	-0.00694900	0.24770000
H	2.65064400	0.64649800	3.06298700
H	3.65177700	-1.92237200	2.79349300
H	4.31356800	0.19894700	-0.77983600
N	3.43876200	0.83389000	1.07037600
N	4.22455800	-1.17151900	0.86419000
C	2.88382400	2.13744500	0.67069100

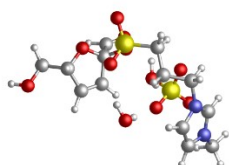
TSf-g



O	3.69354000	-0.00540900	0.10529400
C	3.19258200	0.42966900	-1.01956300
C	3.32918000	0.93632900	1.13159000
H	2.73962500	0.38002300	1.86738200
C	2.57845700	1.66775700	-0.94649400
H	2.11178900	2.17723400	-1.77410000
C	2.52471200	1.96903000	0.40889900
H	2.29618300	2.91898400	0.86653800
O	0.66543900	1.31193900	1.10128800
H	0.76228900	0.41520000	0.71340800
C	3.32015600	-0.48584300	-2.21053700
H	3.41081500	-1.55567300	-1.96441700
O	3.29091100	-0.03182200	-3.31711300
C	4.61344000	1.48898100	1.74270800
H	5.13917000	0.66383500	2.23107700
H	5.24573700	1.89445000	0.94380400
O	4.21355700	2.48812300	2.65321000
H	4.95289400	2.72346700	3.21757100
C	-3.36473600	0.03986600	2.25926500
C	-3.97099500	1.19627400	1.89081500
C	-4.15322500	-0.22346700	0.22739800
H	-2.83620700	-0.22461700	3.15868000
H	-4.07428400	2.13554700	2.40521000
H	-4.32307200	-0.62933200	-0.75665900
N	-3.49563600	-0.83766400	1.20534400
N	-4.46914000	1.00496400	0.62188100
C	-2.76700800	-2.10877600	1.04637400

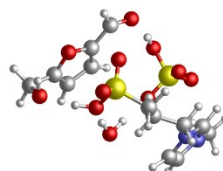
H	3.33826100	2.91056500	1.29241300	H	-3.16363000	-2.82856500	1.76440900
H	3.18505200	2.28251100	-0.36556100	H	-2.98007500	-2.44732100	0.03365100
C	1.35335600	2.10655000	0.78677800	C	-1.26491100	-1.85621100	1.21812500
H	1.04826000	1.06583600	0.67321700	H	-1.08024700	-0.83173600	0.89069400
H	1.02188700	2.44811700	1.76949300	H	-0.96767800	-1.93262300	2.26644400
C	4.65136200	-2.40859200	0.20903100	C	-4.94583400	2.06101500	-0.27135200
H	3.76103700	-2.95603400	-0.10002400	H	-4.07736500	2.56990400	-0.69181100
H	5.22646600	-2.15350100	-0.67788600	H	-5.51495100	1.60638400	-1.07941300
H	5.26214400	-2.98221100	0.90378400	H	-5.58017700	2.74016300	0.29516700
C	0.69046700	2.93306100	-0.30810600	C	-0.41750300	-2.79530900	0.36783600
H	0.74520800	4.01065200	-0.14137400	H	-0.34093600	-3.80633900	0.77114700
H	1.08914800	2.67760700	-1.29108600	H	-0.77477000	-2.81920000	-0.66352300
S	-1.06051300	2.56311800	-0.40479300	S	1.26256400	-2.15819600	0.27191300
O	-1.04707700	1.03006400	-0.83046900	O	1.08959800	-0.84512700	-0.47518100
H	-0.05680000	-1.07139600	0.75214600	H	-0.15741400	1.60978200	0.65382400
O	-1.62194400	2.64676500	0.93103900	O	1.69235700	-1.87394500	1.64779900
O	-1.62968000	3.31641500	-1.49217100	O	2.07024400	-3.10293500	-0.49148200
H	-0.26604700	-0.32246800	-2.10541600	H	0.24721300	0.01997800	-1.73382800
S	1.68711700	-0.88673000	-1.47710000	S	-1.76002000	0.64548600	-1.56199100
O	1.40730800	-1.22535100	-0.05048900	O	-1.67877100	1.24053700	-0.19557300
O	2.63714800	-1.80744900	-2.07525100	O	-2.61203300	1.41979600	-2.44819700
O	0.29955700	-1.10051600	-2.26261800	O	-0.27328900	0.73462800	-2.16666000
O	2.02212200	0.53907900	-1.62598500	O	-2.07256200	-0.79368200	-1.49275400

IMg



O	-3.55472200	0.18425300	0.28894600
C	-2.32007000	0.78420200	0.50504700
C	-3.77135700	-0.04222400	-1.11303900
H	-3.77412800	-1.11851300	-1.31055500
C	-1.77728900	1.11852200	-0.86028900
H	-0.82945600	1.62330000	-0.98983500
C	-2.60582400	0.62720700	-1.77255300
H	-2.47824500	0.64830900	-2.84608100
O	0.26503900	-1.09927700	-2.42799000
H	-0.51355600	-1.36816000	-1.92466400
C	-2.54946100	2.01985800	1.38474700
H	-3.47450200	2.56040600	1.11043600
O	-1.82070900	2.38824700	2.25686600
C	-5.11943000	0.55850500	-1.47605100

IMh



O	-3.32305600	-1.50321400	0.21262200
C	-2.10312900	-1.99200100	-0.14442200
C	-3.27504500	-1.24898700	1.53550900
H	-3.15335300	1.29814600	0.86383000
C	-1.28722800	-2.07389300	0.94530100
H	-0.26016900	-2.40927500	0.95568200
C	-2.05658200	-1.58404600	2.04356100
H	-1.72891000	-1.45917200	3.06328200
O	0.16762600	0.62572000	2.33847700
H	-0.66931000	0.62337500	1.86130600
C	-1.92687200	-2.28880400	-1.56332500
H	-2.81090400	-2.10108900	-2.18964400
O	-0.89789300	-2.71622700	-2.03576100
C	-4.46805100	-0.56058100	2.09721600



H	-5.89716900	0.07557000	-0.87509900	H	-5.37485400	-1.14995100	1.94351700
H	-5.10471200	1.63121600	-1.24619200	H	-4.32754900	-0.40306900	3.16550100
O	-5.29790300	0.32222100	-2.85867900	O	-4.62707100	0.73439500	1.49287900
H	-6.17185100	0.61622000	-3.12183000	H	-5.24168700	0.67702400	0.75413200
C	3.15236300	-1.63154000	-1.50864900	C	2.65896300	2.05302700	1.33220200
C	3.88007700	-0.64382100	-2.08651200	C	3.71513300	1.37155400	1.83949500
C	4.05876300	-0.42252700	0.09084400	C	3.72252200	1.09335200	-0.33859800
H	2.49523500	-2.36293100	-1.94725900	H	1.87000300	2.58634800	1.83188600
H	4.01560400	-0.38313400	-3.12145300	H	4.03455700	1.22344800	2.85600500
H	4.26371000	-0.00149000	1.06204500	H	3.95211200	0.71126600	-1.31987100
N	3.28856900	-1.48197700	-0.14491600	N	2.68610500	1.87202600	-0.03452400
N	4.44303600	0.09514200	-1.06952400	N	4.37037700	0.78767800	0.77865900
C	2.48976100	-2.17611100	0.87771300	C	1.67361300	2.33824100	-0.99166700
H	2.82521100	-3.21308300	0.93791100	H	1.74378500	3.42755700	-1.05466000
H	2.69403800	-1.66766300	1.81872700	H	1.92829900	1.89559200	-1.95470400
C	1.01271700	-2.05210600	0.50448300	C	0.29127400	1.87874100	-0.54713500
H	0.88430300	-1.08370300	0.02505200	H	0.26444300	0.78909600	-0.62978500
H	0.72675000	-2.81996800	-0.21664300	H	0.12764300	2.14707900	0.49506000
C	5.15165000	1.36321700	-1.23349800	C	5.46779400	-0.17217400	0.88730500
H	4.44012700	2.11102500	-1.57981700	H	5.07942500	-1.08928000	1.32598900
H	5.52709100	1.67878400	-0.26380500	H	5.82432800	-0.40490200	-0.11202500
H	5.96987800	1.22455200	-1.93856600	H	6.26077800	0.26708600	1.49096900
C	0.09134300	-2.09043800	1.70987800	C	-0.80751400	2.51133200	-1.39162000
H	-0.01111900	-3.07078600	2.17934300	H	-0.97879100	3.56312000	-1.15810800
H	0.36381300	-1.33294500	2.44781300	H	-0.63905700	2.39294900	-2.46480500
S	-1.57118500	-1.67183700	1.18136900	S	-2.36669700	1.67457400	-1.11996400
O	-1.41620300	-0.06004900	1.25405800	O	-2.32246500	0.39515400	-1.79390500
H	0.58728700	-0.31102000	-1.96535000	H	0.72856200	0.00982400	1.83270300
O	-1.75549500	-2.05309200	-0.21127600	O	-2.25478300	1.45276600	0.46625400
O	-2.51809900	-2.11780700	2.16983800	O	-3.48582100	2.55699800	-1.37455200
H	0.11930300	2.28816500	1.69997300	H	0.68827000	-2.82112200	-1.29327600
S	1.78994300	1.53833100	0.57073600	S	2.22993200	-1.51774500	-0.54516900
O	1.46154800	0.95518600	-0.74656200	O	1.81419000	-1.04280000	0.79615800
O	3.00822600	2.34048700	0.53731500	O	3.66290300	-1.79812600	-0.61028500
O	0.56452300	2.54849600	0.87656100	O	1.50402000	-2.93204500	-0.75731900
O	1.75899000	0.54674900	1.66098800	O	1.74309700	-0.62959700	-1.61616200