

Supporting Information

for

Dipole Moment as Underlying Mechanism for Enhancing Immobilization of Glucose Oxidase by Ferrocene-Chitosan for Superior Specificity Non-invasive Glucose Sensing

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Table S1. The formula for PBS solution in this study and the pH value is 7.4.

Material	Amounts	Molar ratio (M)
NaCl	2 g	0.0685
KCl	50 mg	0.00135
Na ₂ HPO ₄	360 mg	0.005
KH ₂ PO ₄	60 mg	0.0009
DI water	250 ml	n/a

Fourier transform infrared spectroscopy (FTIR) analysis

FTIR spectroscopy was performed to confirm the formation of Fc-Chit (Figure S1). Two characteristic peaks at 1642 and 1550 cm⁻¹ can be attributed to the amide groups and the overlap of amide and amine groups on chitosan, respectively.^[5] In Fc-Chit, the intensity of the peak at 1550 cm⁻¹ for primary amine N-H bending decreases, while a new peak is observed at 823 cm⁻¹, which can be assigned to the cyclopentadiene of ferrocene.^[5b] The result indicates the *N*-alkylation of the glucosamine unit on chitosan with ferrocenecarboxaldehyde occurs, thus forming Fc-Chit.

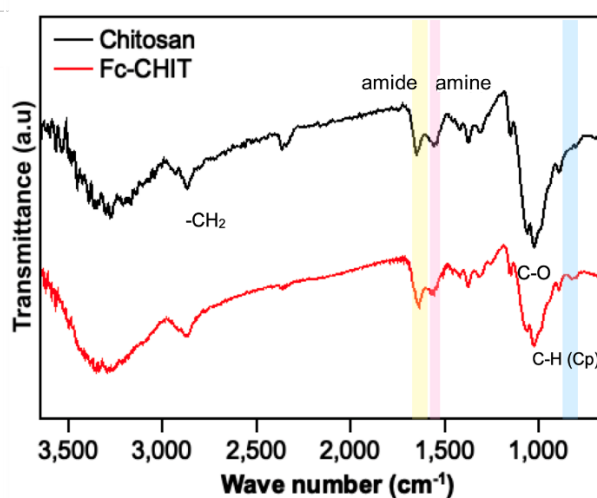


Figure S1. FTIR analysis of pristine chitosan and Fc-Chit.

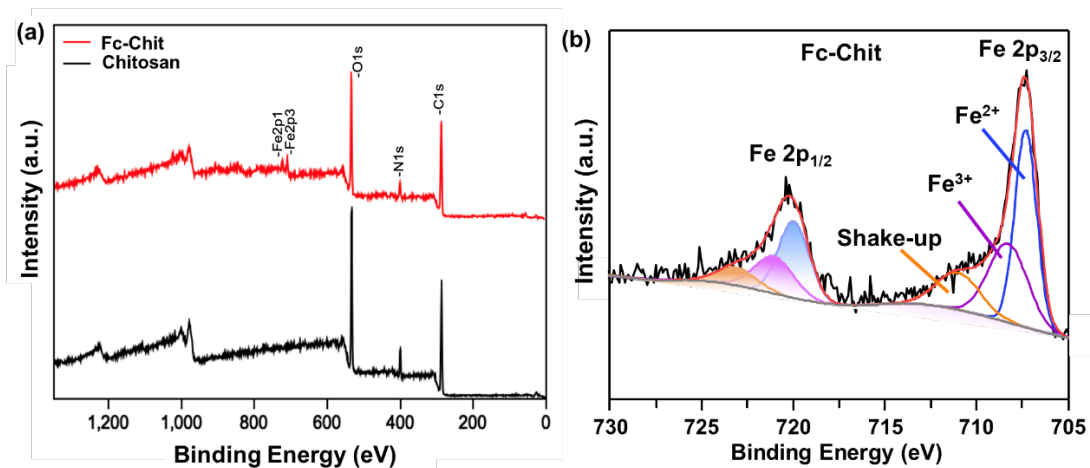


Figure S2. The XPS spectra of chitosan and Fc-Chit. (a) The full scan of XPS spectra. (b) XPS spectrum in the Fe 2p region for Fc-Chitsplit with spin-orbit components of Fe 2p_{1/2} and Fe 2p_{3/2} (energy difference of 13.1 eV).^[3] The peak at around 707.5 eV can be attributed to ferrocene molecules (Fe²⁺) accompanied by a shake-up satellite peak at 711.5 eV. The peak at 708.5 eV representing Fe³⁺ can be assigned to ferrocenium resulting from exposure to X-ray during XPS analysis.^[4] The results confirm the presence of ferrocene in Fc-Chit.

The optimization of drop-casted CNTs layers

The CV measurements were conducted to determine the number of CNTs coating layers, as shown in Figure S3. It shows that the redox peaks increase as the layers of CNTs increase from 5 to 20, but reach saturated as the layers of CNTs increase to 25. Therefore, we chose 20 layers of CNTs to modify the SPE for glucose sensing.

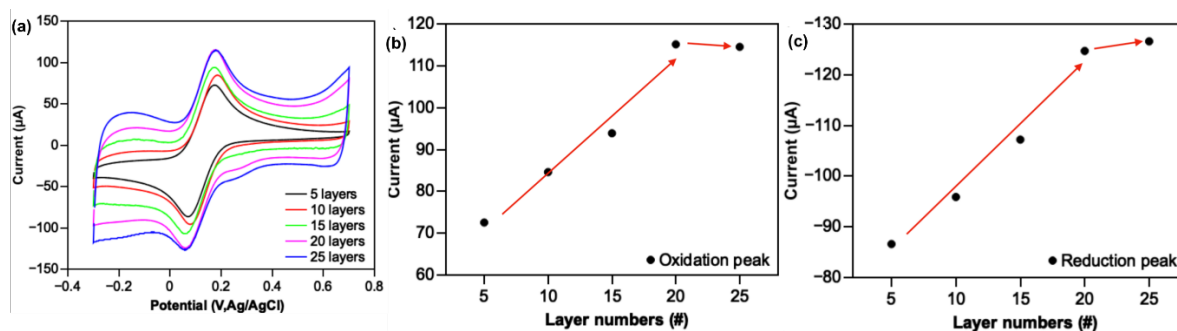


Figure S3. The optimization of CNTs layers on SPE. (a) CV curves of SPE drop-casted different layers of CNTs in electrolyte containing 0.1 M KCl + 5 mM K₃[Fe(CN)₆]. The scan rate is 0.1 V/s. (b) The oxidation peak and (c) reduction peak with different layers of CNTs.

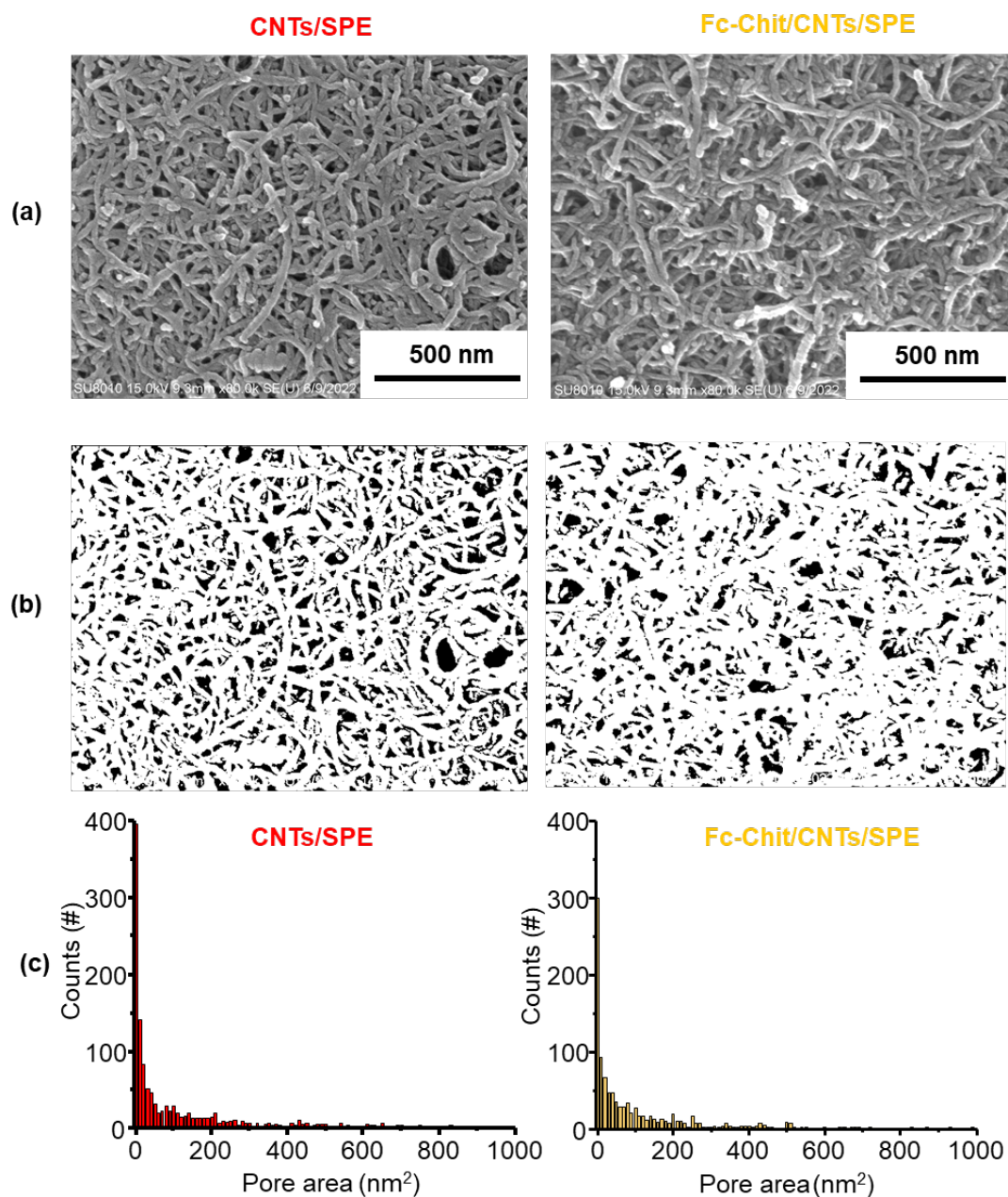


Figure S4. Comparison of the pore size distributions between CNTs/SPE and Fc-Chit/CNTs/SPE. (a) SEM images of CNTs/SPE and Fc-CNTs/SPE. (b) The pore area is identified by the software ImageJ, which is expressed using black-white binary images. (c) The pore area distributions of CNTs/SPE and Fc-Chit/CNTs/SPE clearly show the drop-casting of Fc-Chit film can cover and wrap CNTs, thus decreasing the pore number and size.

The electroactive surface area of GOx/Fc-Chit/CNTs/SPE

The electroactive surface area was calculated to provide more evidence that the preparation of GOx/Fc-Chit/CNTs/SPE through the drop-casting process can improve the active area and electrochemical properties. The cyclic voltammetry curves of the sample electrodes, ranging from -0.3 V to 0.7 V, in 5 mM $\text{K}_3\text{Fe}(\text{CN})_6$ and 0.1 M KCl were examined at different scan rates from 20 to 300 mV/s based on the Randles-Sevcik equation:^[1]

$$I_p = (2.69 \times 10^5) n^{2/3} A D^{1/2} v^{1/2} C \quad (1)$$

where I_p is the peak current (A); n is the number of electrons per molecule in the redox reaction; A represents the electroactive surface area of the electrode surface (cm^2); D is the diffusion coefficient of $[\text{Fe}(\text{CN})_6]^{3-}$ in 0.1 M KCl solution ($6.5 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$);^[2] v is the scan rate (V s^{-1}); and C is the solution concentration in mole mL^{-1} . The electroactive area of GOx/Fc-Chit/CNTs/SPE is calculated to be 0.392 cm^2 , as shown in Figure S5, which is larger than that of bare SPE (0.035 cm^2 , from Zensor R&D Co.).

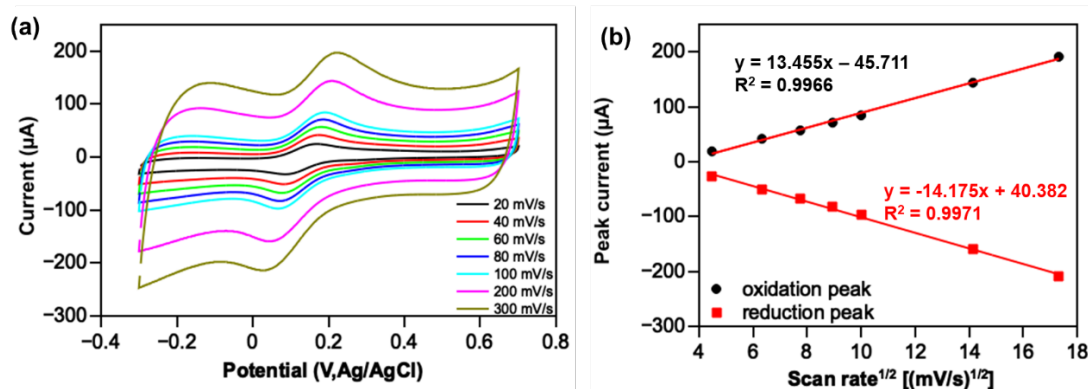


Figure S5. Cyclic voltammograms of (a) GOx/Fc-Chit/CNTs/SPE in 5 mM $\text{K}_3\text{Fe}(\text{CN})_6$ and 0.1 M KCl at different scan rates from 20 to 300 mV/s. (b) Plots of redox peak current versus square root of scan rate.

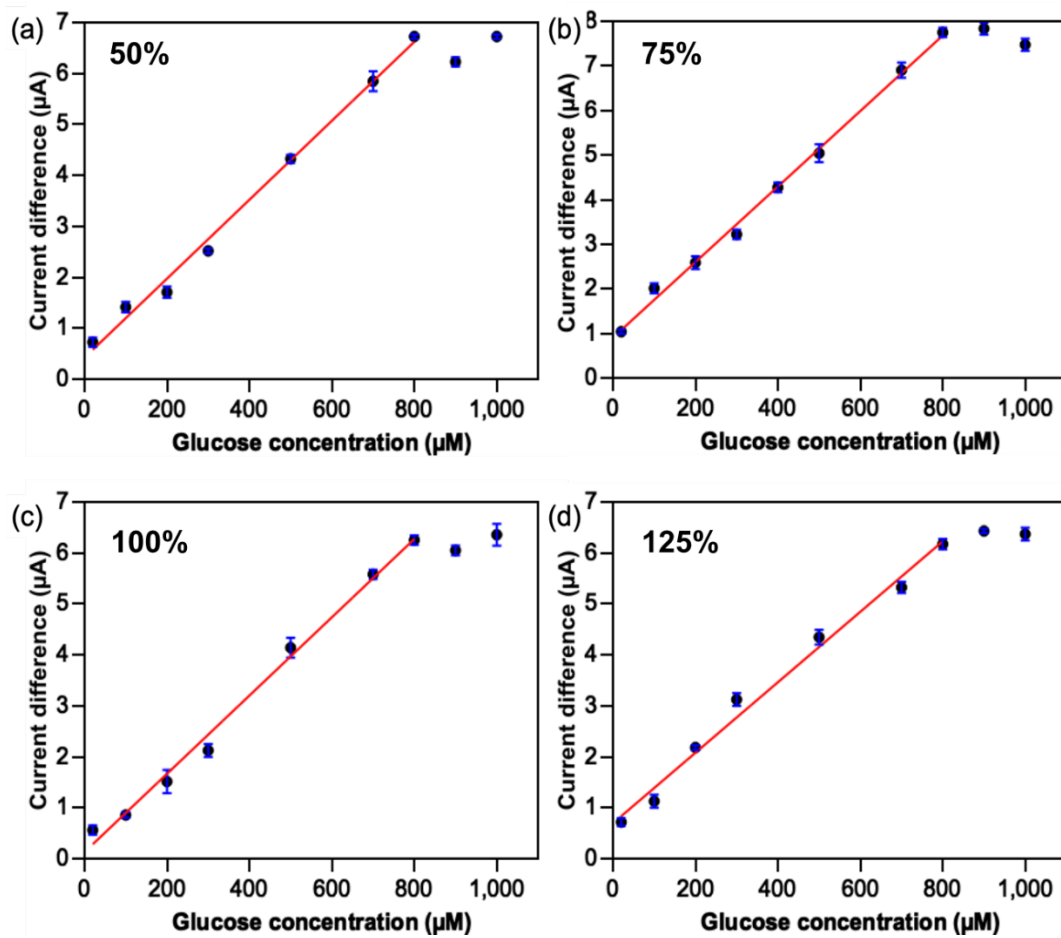


Figure S 6. Calibration curves of the current difference between the glucose concentration and enzyme reduction peak of the GOx/Fc-Chit/CNTs/SPE with ferrocene-to-chitosan w/w branching ratio of (a) 50%, (b) 75%, (c) 100%, and (d) 125%.

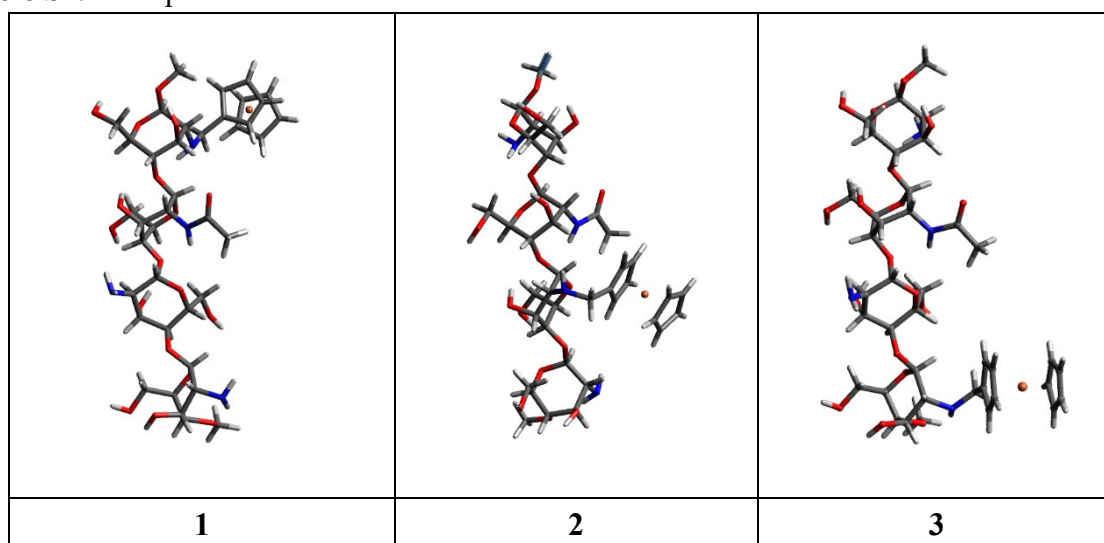
Density Functional Theory (DFT) Calculation Section

I. Computational methods

All calculations were performed using ORCA 5.0.2 program packages,^[6] molecular graphics and analyses were performed using Avogadro software.^[7] Initial structures of the most stable conformer (with the MMFF94^[8] forcefield) of molecules 1-7 were generated using openbabel.^[9] For geometry optimizations, BP86 functional^{[10],[11]} with the dispersion correction D4^{[12],[13]} were applied. LANL2DZ^{[14],[15],[16]} basis set was applied on iron atoms and 6-31g*^{[17],[18]} basis set was applied on rest of the atoms. The Split-RI-J variant^[19] of the resolution of the identity (RI) approximation was applied to the Coulomb integrals with the def2/J auxiliary basis set.^[20] Analytical frequency calculations were performed on top of the optimized geometries using the same methods. For single-point energy calculations, range-separated hybrid meta-GGA wB97X with the dispersion correction D3 (wB97X-D3)^{[21],[22]} and the basis set def2-TZVPP^[23] for all atoms were used on top of the optimized geometries. The resolution of the identity (RI) approximation was applied to the Coulomb integrals with the def2/J auxiliary basis set^[24] and the chain-of-spheres approximation was applied to the exchange integrals.^[25]

II. Keywords and Energies of Computation

Table S2. The optimized molecular structure of Fc-Chit molecules 1-7.



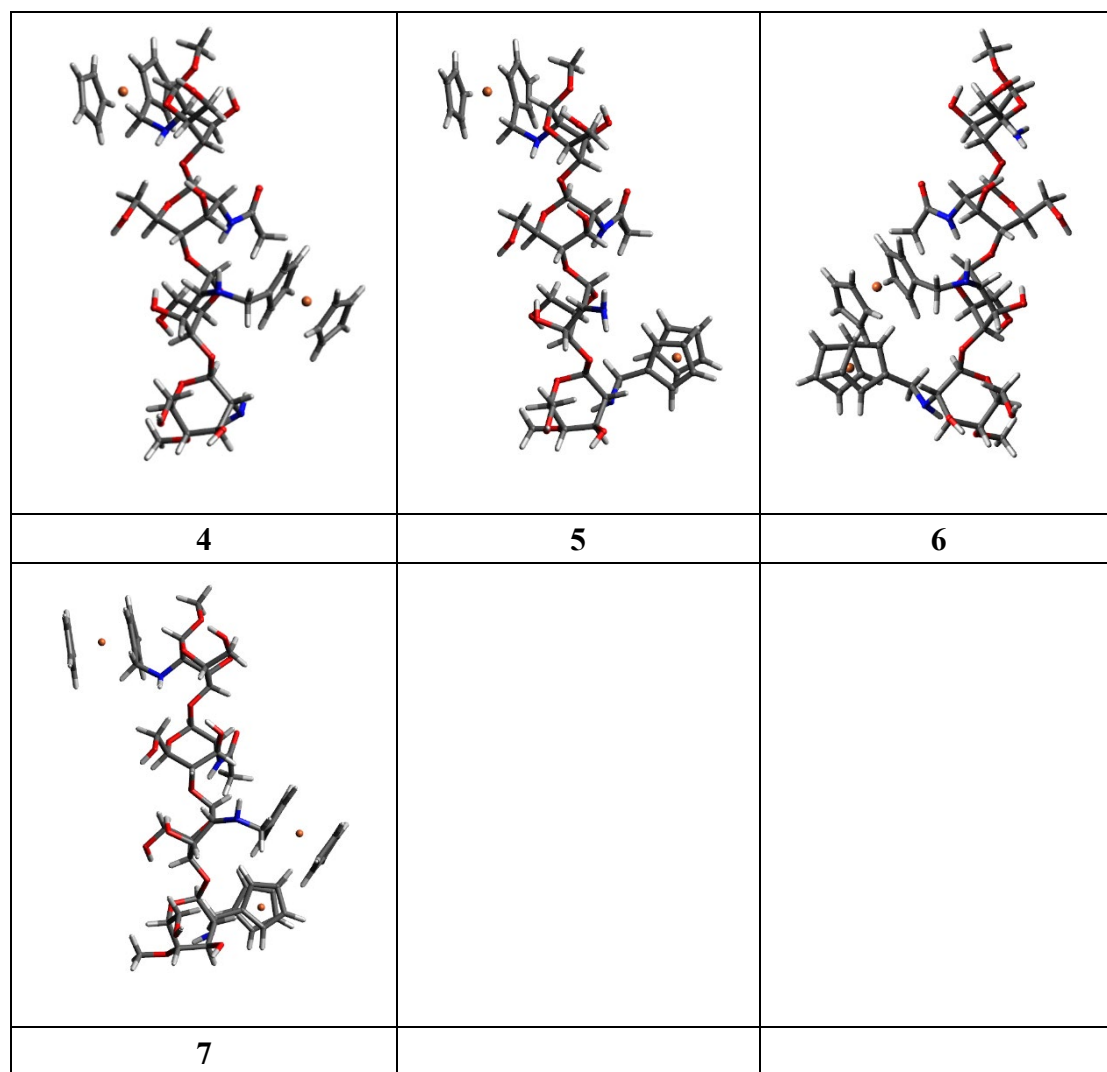


Table S3. Absolute energies (in unit of Eh) of single point energy (**SPE**), zero-point vibrational energy (**ZPVE**), entropy (**S**, at 298.15 K), enthalpy (**H**) and Gibbs free energy (**G**) of Fc-CHIT molecules **1-7**.

MOLECULE	SPE	ZPVE	TS	H^a	G^a
1	-4360.627	1.079	0.149	-4359.548	-4359.697
2	-4360.627	1.079	0.150	-4359.548	-4359.698
3	-4360.634	1.079	0.152	-4359.555	-4359.707
4	-6049.642	1.263	0.168	-6048.389	-6048.557
5	-6049.645	1.263	0.168	-6048.382	-6048.550
6	-6049.644	1.263	0.170	-6048.381	-6048.551
7	-7738.650	1.446	0.190	-7737.204	-7737.394

^aH = SPE+ZPVE. G=H-TS

Table S4. Relative energies (in unit of $\text{kcal}\cdot\text{mol}^{-1}$) of single point energy (ΔE), entropy (ΔS), enthalpy (ΔH), and Gibbs free energies (ΔG) among isomers Fc₁-Chit or Fc₂-Chit.

MOLECULE	ΔE	ΔS	ΔH	ΔG
1	4.30	0.00	4.15	6.03
2	4.17	1.03	4.46	5.31
3	0.00	1.88	0.00	0.00
4	1.87	0.00	0.00	0.00
5	0.00	0.13	4.39	4.39
6	0.67	0.91	5.02	3.77

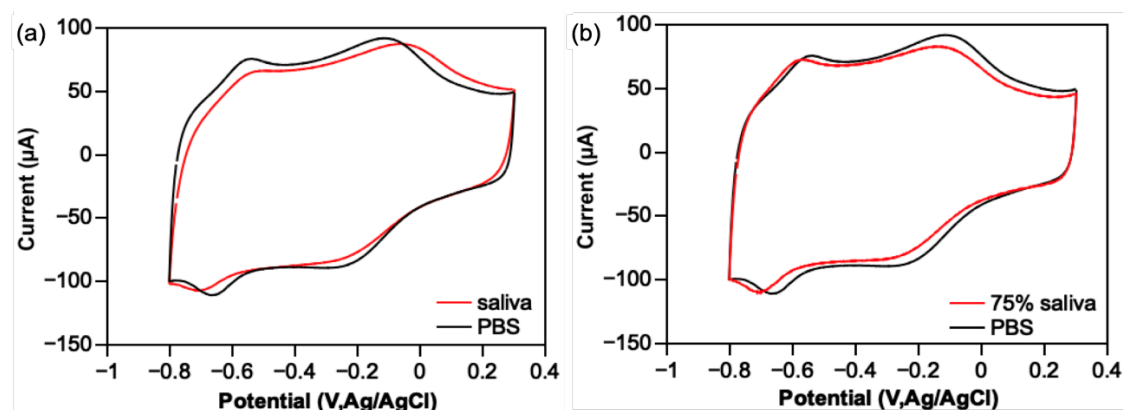


Figure S7. The comparison of CV curves of GOx/Fc-Chit/CNTs/SPE in (a) artificial saliva and PBS; and (b) 75% artificial saliva and PBS.

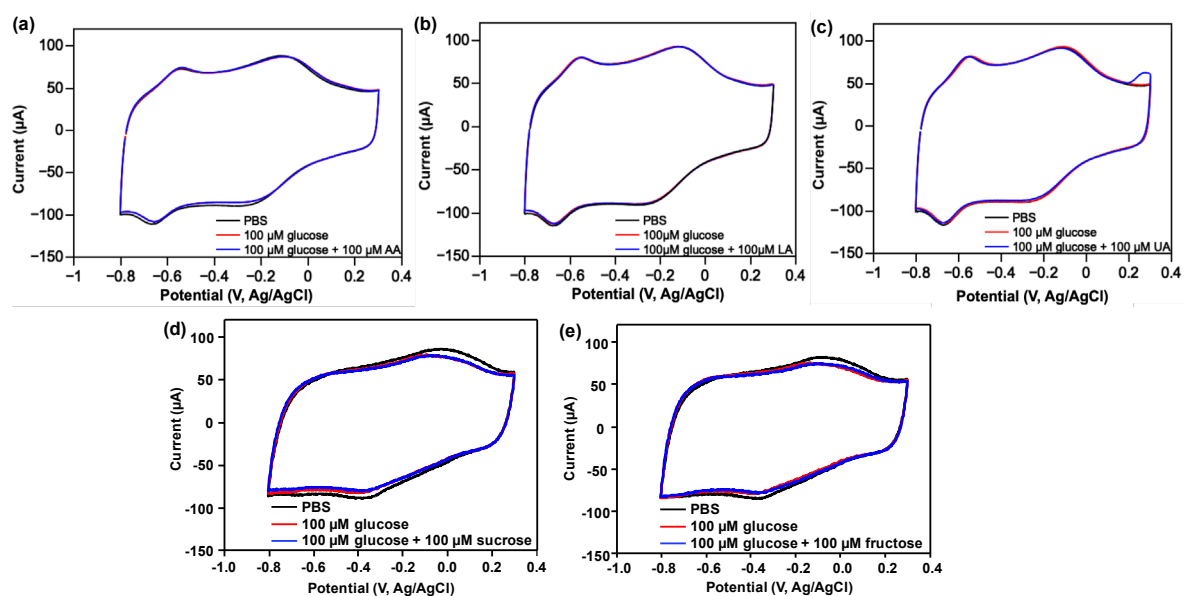


Figure S8. The comparisons of full CV curves of GOx/Fc-Chit/CNTs/SPE for pristine PBS, 100 μM glucose, and glucose solution with additional same concentration of interference: (a) AA, (b) LA, (c) UA, (d) sucrose, and (e) fructose, from -1.0 V to -0.2 V .

Human saliva test

To confirm the feasibility of the practical application of the electrode in real human saliva, we used one healthy people's saliva as a sample and tested it for five days. In Figure S9, fasting saliva glucose concentrations in these five days were all in the normal range, and 2-hour postprandial saliva glucose concentrations showed higher values. The results indicate that the proposed biosensor can detect glucose concentration changes in real human saliva, confirming the practicality of human saliva glucose sensing.

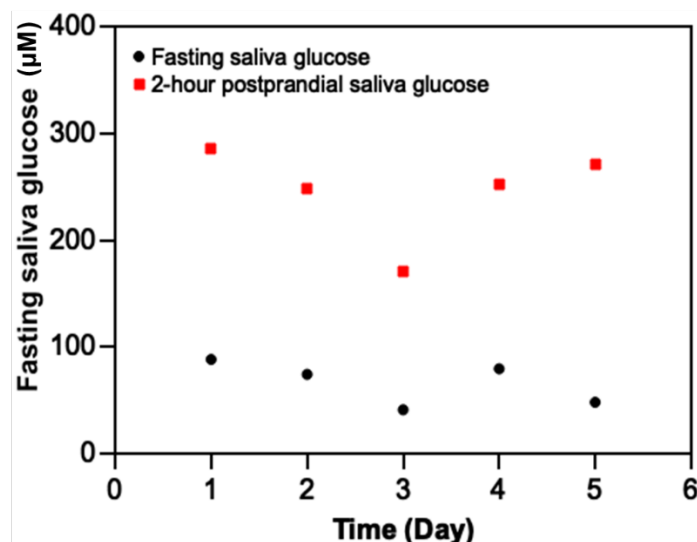


Figure S 9. Human saliva test of fasting saliva glucose and 2-hour postprandial saliva glucose for five different days.

References:

- [1] C. S. Rao Vusa, V. Manju, S. Berchmans, P. Arumugam, *RSC Advances* **2016**, 6, 33409.
- [2] A. Rabti, W. Argoubi, N. Raouafi, *Microchimica Acta* **2016**, 183, 1227.
- [3] L. Li, P. Ma, S. Hussain, L. Jia, D. Lin, X. Yin, Y. Lin, Z. Cheng, L. Wang, *Sustainable Energy & Fuels* **2019**, 3, 1749.
- [4] G. Riveros, S. Meneses, S. Escobar, C. GarÍN, B. Chornik, *Journal of the Chilean Chemical Society* **2010**, 55, 61.
- [5] a)W. Yang, H. Zhou, C. Sun, *Macromolecular Rapid Communications* **2007**, 28, 265;
b)X. Du, H. Jiang, X. Guo, L. Chen, T. Kang, *Reactive and Functional Polymers* **2021**, 169, 105061.
- [6] F. Neese, *WIREs Computational Molecular Science* **2022**, 12, e1606.
- [7] E. Caldeweyher, S. Ehlert, A. Hansen, H. Neugebauer, S. Spicher, C. Bannwarth, S. Grimme, *J. Chem. Phys.* **2019**, 150, 154122.
- [8] A. Najibi, L. Goerigk, *J. Chem. Theory Comput.* **2018**, 14, 5725.
- [9] E. Caldeweyher, C. Bannwarth, S. Grimme, *J. Chem. Phys.* **2017**, 147, 034112.
- [10] N. Mardirossian, M. Head-Gordon, *J. Chem. Phys.* **2016**, 144, 214110.
- [11] M. D. Hanwell, D. E. Curtis, D. C. Lonie, T. Vandermeersch, E. Zurek, G. R. Hutchison,

Journal of Cheminformatics **2012**, 4, 17.

[12] N. M. O'Boyle, M. Banck, C. A. James, C. Morley, T. Vandermeersch, G. R. Hutchison, *Journal of Cheminformatics* **2011**, 3, 33.

[13] F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chemical Physics* **2009**, 356, 98.

[14] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *The Journal of Physical Chemistry B* **2009**, 113, 6378.

[15] F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, 8, 1057.

[16] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, 7, 3297.

[17] F. Neese, *Journal of Computational Chemistry* **2003**, 24, 1740.

[18] T. A. Halgren, *Journal of Computational Chemistry* **1996**, 17, 490.

[19] A. D. Becke, *Phys. Rev. A* **1988**, 38, 3098.

[20] J. P. Perdew, *Phys. Rev. B* **1986**, 33, 8822.

[21] W. R. Wadt, P. J. Hay, *J. Chem. Phys.* **1985**, 82, 284.

[22] P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, 82, 299.

[23] P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, 82, 270.

[24] M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees, J. A. Pople, *J. Chem. Phys.* **1982**, 77, 3654.

[25] W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, 56, 2257.

Coordinates

1				O	-2.72090	-3.96230	-7.43920
O	5.45050	-3.34710	-8.48410	C	-3.65280	-4.99120	-7.04970
C	5.09080	-2.12850	-9.13810	C	-4.05160	-4.82960	-5.57580
C	4.74960	-2.31350	-10.63960	O	-4.77020	-5.97000	-5.09910
O	4.66150	-0.98950	-11.23510	C	-4.79560	-3.49910	-5.37660
C	4.24430	-0.96040	-12.59550	N	-3.95140	-2.31010	-5.48170
C	3.41880	-3.06780	-10.73900	C	-4.30640	-1.13920	-4.82870
C	3.42790	-4.48290	-10.12500	C	-3.36900	0.01970	-5.05170
O	4.51200	-5.24660	-10.64760	O	-5.28780	-1.05740	-4.11910
O	2.40260	-2.19560	-10.23580	C	-5.97710	-3.47810	-6.36760
C	2.49920	-1.93130	-8.83770	O	-6.89730	-4.53690	-6.10840
O	1.91440	-3.03840	-8.08810	C	-7.53220	-4.51880	-4.81670
C	0.58610	-3.39030	-8.60910	C	-8.38060	-3.25740	-4.63580
C	0.15840	-4.83540	-8.24010	O	-8.80050	-3.13610	-3.27320
O	-0.78000	-5.22760	-9.30980	C	-9.55250	-3.24890	-5.65060
C	-0.61210	-5.05480	-6.91390	N	-9.06470	-3.02460	-7.03650
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C	-12.44930	-2.03780	-7.63630	H	-5.17370	-3.49450	-4.35100
C	-10.35800	-4.56290	-5.43390	H	-3.32780	-2.22190	-6.27770
O	-10.99130	-4.59110	-4.14810	H	-2.53750	-0.24300	-5.70850
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O	-9.54620	-5.73590	-5.58940	H	-3.92770	0.84400	-5.50330
C	-8.36790	-5.81260	-4.77640	H	-6.47750	-2.50890	-6.33110
C	-8.64040	-6.32020	-3.35300	H	-6.78380	-4.60030	-4.02500
O	-9.22810	-7.62060	-3.40580	H	-7.77360	-2.36160	-4.79950
O	-5.56250	-3.60890	-7.73560	H	-9.62560	-3.65010	-3.15280
C	-4.81130	-4.78710	-8.04260	H	-10.16520	-2.38500	-5.37950
C	-5.66970	-6.03120	-8.32580	H	-8.43810	-3.79650	-7.29420
O	-4.85700	-7.14090	-8.69420	H	-10.62680	-3.87670	-8.17070
O	-1.00680	-2.56470	-6.92220	H	-9.61370	-2.73940	-9.01930
C	-0.46180	-2.32760	-8.21350	H	-9.73270	-0.00300	-7.78380
C	-1.53690	-1.99120	-9.26940	H	-11.99250	1.29430	-7.31820
O	-0.98640	-1.71380	-10.55070	H	-14.00210	-0.45710	-7.25610
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N	4.20270	0.04030	-8.65810	H	-11.14390	-4.65650	-6.18640
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H	5.99630	-1.50650	-9.07470	H	-12.66950	-3.60750	-4.90110
H	5.54910	-2.86400	-11.14500	H	-11.59180	-2.62960	-3.85100
H	4.24960	0.08090	-12.93110	H	-7.77840	-6.60790	-5.25970
H	3.21630	-1.31930	-12.71170	H	-9.31700	-5.68620	-2.78110
H	4.92640	-1.53940	-13.22180	H	-7.70410	-6.40860	-2.79040
H	3.18460	-3.21640	-11.79580	H	-9.99950	-7.53970	-4.00060
H	2.49010	-4.99510	-10.36070	H	-4.34820	-4.55860	-9.01450
H	3.51050	-4.49080	-9.03630	H	-6.37360	-5.82770	-9.14100
H	4.40350	-6.14730	-10.28900	H	-6.27640	-6.34530	-7.47820
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2

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N 4.20270 0.04030 -8.65810
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H 5.54910 -2.86400 -11.14500
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H 3.21630 -1.31930 -12.71170

H 4.92640 -1.53940 -13.22180
H 3.18460 -3.21640 -11.79580
H 2.49010 -4.99510 -10.36070
H 3.51050 -4.49080 -9.03630
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H 0.99510 -5.53240 -8.31490
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H -1.04520 -6.23610 -5.29750
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H 1.35950 -2.68380 -5.43910
H -0.10650 -0.73360 -4.17110
H -1.54690 -1.99300 -2.31580
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H -1.79090 -3.80270 -5.61710
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H -2.53750 -0.24300 -5.70850
H -2.96350 0.33600 -4.08870
H -3.92770 0.84400 -5.50330
H -6.47750 -2.50890 -6.33110
H -6.78380 -4.60030 -4.02500
H -7.77360 -2.36160 -4.79950
H -9.62560 -3.65010 -3.15280
H -10.16520 -2.38500 -5.37950
H -8.43810 -3.79650 -7.29420
H -11.14390 -4.65650 -6.18640
H -12.61560 -3.87710 -3.14050
H -12.66950 -3.60750 -4.90110
H -11.59180 -2.62960 -3.85100
H -7.77840 -6.60790 -5.25970
H -9.31700 -5.68620 -2.78110

H -7.70410 -6.40860 -2.79040
H -9.99950 -7.53970 -4.00060
H -4.34820 -4.55860 -9.01450
H -6.37360 -5.82770 -9.14100
H -6.27640 -6.34530 -7.47820
H -4.42840 -6.93740 -9.54500
H 0.05100 -1.37330 -8.07850
H -2.09490 -1.10560 -8.94190
H -2.28040 -2.77610 -9.40320
H -0.35380 -0.97830 -10.46980
H 4.03450 -1.58430 -7.30060
H 4.32360 0.15360 -9.67320
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H 1.23290 -2.00290 -0.22190
C 2.48900 -1.73690 -1.90920
H 2.54420 -0.79550 -2.02450
C 3.11940 -2.70670 -2.70670
H 3.67580 -2.53180 -3.45680
C 2.78390 -3.99670 -2.20380
Fe 1.08780 -2.97690 -2.75110
H 3.09730 -5.00190 -2.46490
H 3.32293 0.60554 -8.37235
H -9.88550 -3.03236 -7.74615

3

O 5.45050 -3.34710 -8.48410
C 5.09080 -2.12850 -9.13810
C 4.74960 -2.31350 -10.63960
O 4.66150 -0.98950 -11.23510
C 4.24430 -0.96040 -12.59550
C 3.41880 -3.06780 -10.73900
C 3.42790 -4.48290 -10.12500
O 4.51200 -5.24660 -10.64760
O 2.40260 -2.19560 -10.23580
C 2.49920 -1.93130 -8.83770
O 1.91440 -3.03840 -8.08810

C	0.58610	-3.39030	-8.60910	N	4.20270	0.04030	-8.65810
C	0.15840	-4.83540	-8.24010	C	3.28890	1.05280	-8.16140
O	-0.78000	-5.22760	-9.30980	C	3.33020	1.21530	-6.68990
C	-0.61210	-5.05480	-6.91390	C	4.51310	1.51590	-5.92030
N	-0.20160	-5.87090	-5.74580	C	4.12850	1.54270	-4.63870
C	-1.53340	-3.84830	-6.66890	C	2.69780	1.27970	-4.56290
O	-2.72090	-3.96230	-7.43920	C	2.20720	1.09430	-5.79550
C	-3.65280	-4.99120	-7.04970	H	5.96600	-3.88130	-9.11720
C	-4.05160	-4.82960	-5.57580	H	5.99630	-1.50650	-9.07470
O	-4.77020	-5.97000	-5.09910	H	5.54910	-2.86400	-11.14500
C	-4.79560	-3.49910	-5.37660	H	4.24960	0.08090	-12.93110
N	-3.95140	-2.31010	-5.48170	H	3.21630	-1.31930	-12.71170
C	-4.30640	-1.13920	-4.82870	H	4.92640	-1.53940	-13.22180
C	-3.36900	0.01970	-5.05170	H	3.18460	-3.21640	-11.79580
O	-5.28780	-1.05740	-4.11910	H	2.49010	-4.99510	-10.36070
C	-5.97710	-3.47810	-6.36760	H	3.51050	-4.49080	-9.03630
O	-6.89730	-4.53690	-6.10840	H	4.40350	-6.14730	-10.28900
C	-7.53220	-4.51880	-4.81670	H	1.83150	-1.09560	-8.65640
C	-8.38060	-3.25740	-4.63580	H	0.65710	-3.39960	-9.70020
O	-8.80050	-3.13610	-3.27320	H	0.99510	-5.53240	-8.31490
C	-9.55250	-3.24890	-5.65060	H	-1.61760	-4.75560	-9.16830
N	-9.06470	-3.02460	-7.03650	H	-1.29130	-5.83540	-7.26810
C	-10.35800	-4.56290	-5.43390	H	-1.04520	-6.23610	-5.29750
O	-10.99130	-4.59110	-4.14810	H	-1.79090	-3.80270	-5.61710
C	-12.01910	-3.62240	-4.02140	H	-3.22300	-5.98060	-7.21760
O	-9.54620	-5.73590	-5.58940	H	-3.18020	-4.82540	-4.92150
C	-8.36790	-5.81260	-4.77640	H	-5.58510	-6.06960	-5.62140
C	-8.64040	-6.32020	-3.35300	H	-5.17370	-3.49450	-4.35100
O	-9.22810	-7.62060	-3.40580	H	-3.32780	-2.22190	-6.27770
O	-5.56250	-3.60890	-7.73560	H	-2.53750	-0.24300	-5.70850
C	-4.81130	-4.78710	-8.04260	H	-2.96350	0.33600	-4.08870
C	-5.66970	-6.03120	-8.32580	H	-3.92770	0.84400	-5.50330
O	-4.85700	-7.14090	-8.69420	H	-6.47750	-2.50890	-6.33110
O	-1.00680	-2.56470	-6.92220	H	-6.78380	-4.60030	-4.02500
C	-0.46180	-2.32760	-8.21350	H	-7.77360	-2.36160	-4.79950
C	-1.53690	-1.99120	-9.26940	H	-9.62560	-3.65010	-3.15280
O	-0.98640	-1.71380	-10.55070	H	-10.16520	-2.38500	-5.37950
C	3.92810	-1.40530	-8.37730	H	-8.43810	-3.79650	-7.29420

H	-11.14390	-4.65650	-6.18640	4			
H	-12.61560	-3.87710	-3.14050	O	5.45050	-3.34710	-8.48410
H	-12.66950	-3.60750	-4.90110	C	5.09080	-2.12850	-9.13810
H	-11.59180	-2.62960	-3.85100	C	4.74960	-2.31350	-10.63960
H	-7.77840	-6.60790	-5.25970	O	4.66150	-0.98950	-11.23510
H	-9.31700	-5.68620	-2.78110	C	4.24430	-0.96040	-12.59550
H	-7.70410	-6.40860	-2.79040	C	3.41880	-3.06780	-10.73900
H	-9.99950	-7.53970	-4.00060	C	3.42790	-4.48290	-10.12500
H	-4.34820	-4.55860	-9.01450	O	4.51200	-5.24660	-10.64760
H	-6.37360	-5.82770	-9.14100	O	2.40260	-2.19560	-10.23580
H	-6.27640	-6.34530	-7.47820	C	2.49920	-1.93130	-8.83770
H	-4.42840	-6.93740	-9.54500	O	1.91440	-3.03840	-8.08810
H	0.05100	-1.37330	-8.07850	C	0.58610	-3.39030	-8.60910
H	-2.09490	-1.10560	-8.94190	C	0.15840	-4.83540	-8.24010
H	-2.28040	-2.77610	-9.40320	O	-0.78000	-5.22760	-9.30980
H	-0.35380	-0.97830	-10.46980	C	-0.61210	-5.05480	-6.91390
H	4.03450	-1.58430	-7.30060	N	-0.20160	-5.87090	-5.74580
H	4.32360	0.15360	-9.67320	C	0.65530	-5.38160	-4.67170
H	2.26920	0.90100	-8.52710	C	0.31750	-4.08680	-4.02830
H	3.60180	2.00860	-8.60270	C	0.68500	-2.81820	-4.60780
H	5.50430	1.66860	-6.32270	C	-0.09630	-1.89860	-4.02180
H	4.76190	1.71690	-3.78360	C	-0.88650	-2.53220	-2.97520
H	2.13950	1.25100	-3.63550	C	-0.50160	-3.79520	-3.10340
H	1.18630	0.88960	-6.07600	C	-1.53340	-3.84830	-6.66890
C	3.93420	4.78050	-6.38630	O	-2.72090	-3.96230	-7.43920
H	4.76370	4.90350	-6.83310	C	-3.65280	-4.99120	-7.04970
C	3.71420	4.88610	-4.98850	C	-4.05160	-4.82960	-5.57580
H	4.37260	5.09010	-4.33500	O	-4.77020	-5.97000	-5.09910
C	2.34100	4.63480	-4.73610	C	-4.79560	-3.49910	-5.37660
H	1.91820	4.64250	-3.88540	N	-3.95140	-2.31010	-5.48170
C	1.71760	4.37360	-5.96780	C	-4.30640	-1.13920	-4.82870
H	0.79710	4.17340	-6.09220	C	-3.36900	0.01970	-5.05170
C	2.69650	4.45750	-6.99940	O	-5.28780	-1.05740	-4.11910
Fe	3.21250	3.01040	-5.63710	C	-5.97710	-3.47810	-6.36760
H	2.64450	4.39750	-8.08140	O	-6.89730	-4.53690	-6.10840
H	-9.90068	-3.29122	-7.79757	C	-7.53220	-4.51880	-4.81670
H	0.50090	-5.70534	-4.93042	C	-8.38060	-3.25740	-4.63580
				O	-8.80050	-3.13610	-3.27320

C	-9.55250	-3.24890	-5.65060	H	-1.61760	-4.75560	-9.16830
N	-9.06470	-3.02460	-7.03650	H	-1.29130	-5.83540	-7.26810
C	-10.10540	-2.91960	-8.05510	H	-1.04520	-6.23610	-5.29750
C	-11.07050	-1.81340	-7.82110	H	1.69860	-5.38960	-5.00540
C	-10.72360	-0.41700	-7.70610	H	0.35260	-5.98610	-4.11780
C	-11.87640	0.23200	-7.46620	H	1.35950	-2.68380	-5.43910
C	-12.97070	-0.72710	-7.42670	H	-0.10650	-0.73360	-4.17110
C	-12.44930	-2.03780	-7.63630	H	-1.54690	-1.99300	-2.31580
C	-10.35800	-4.56290	-5.43390	H	-1.00920	-4.57170	-2.25400
O	-10.99130	-4.59110	-4.14810	H	-1.79090	-3.80270	-5.61710
C	-12.01910	-3.62240	-4.02140	H	-3.22300	-5.98060	-7.21760
O	-9.54620	-5.73590	-5.58940	H	-3.18020	-4.82540	-4.92150
C	-8.36790	-5.81260	-4.77640	H	-5.58510	-6.06960	-5.62140
C	-8.64040	-6.32020	-3.35300	H	-5.17370	-3.49450	-4.35100
O	-9.22810	-7.62060	-3.40580	H	-3.32780	-2.22190	-6.27770
O	-5.56250	-3.60890	-7.73560	H	-2.53750	-0.24300	-5.70850
C	-4.81130	-4.78710	-8.04260	H	-2.96350	0.33600	-4.08870
C	-5.66970	-6.03120	-8.32580	H	-3.92770	0.84400	-5.50330
O	-4.85700	-7.14090	-8.69420	H	-6.47750	-2.50890	-6.33110
O	-1.00680	-2.56470	-6.92220	H	-6.78380	-4.60030	-4.02500
C	-0.46180	-2.32760	-8.21350	H	-7.77360	-2.36160	-4.79950
C	-1.53690	-1.99120	-9.26940	H	-9.62560	-3.65010	-3.15280
O	-0.98640	-1.71380	-10.55070	H	-10.16520	-2.38500	-5.37950
C	3.92810	-1.40530	-8.37730	H	-8.43810	-3.79650	-7.29420
N	4.20270	0.04030	-8.65810	H	-10.62680	-3.87670	-8.17070
H	5.96600	-3.88130	-9.11720	H	-9.61370	-2.73940	-9.01930
H	5.99630	-1.50650	-9.07470	H	-9.73270	-0.00300	-7.78380
H	5.54910	-2.86400	-11.14500	H	-11.99250	1.29430	-7.31820
H	4.24960	0.08090	-12.93110	H	-14.00210	-0.45710	-7.25610
H	3.21630	-1.31930	-12.71170	H	-13.05100	-2.88390	-7.67760
H	4.92640	-1.53940	-13.22180	H	-11.14390	-4.65650	-6.18640
H	3.18460	-3.21640	-11.79580	H	-12.61560	-3.87710	-3.14050
H	2.49010	-4.99510	-10.36070	H	-12.66950	-3.60750	-4.90110
H	3.51050	-4.49080	-9.03630	H	-11.59180	-2.62960	-3.85100
H	4.40350	-6.14730	-10.28900	H	-7.77840	-6.60790	-5.25970
H	1.83150	-1.09560	-8.65640	H	-9.31700	-5.68620	-2.78110
H	0.65710	-3.39960	-9.70020	H	-7.70410	-6.40860	-2.79040
H	0.99510	-5.53240	-8.31490	H	-9.99950	-7.53970	-4.00060

H	-4.34820	-4.55860	-9.01450	O	4.66150	-0.98950	-11.23510
H	-6.37360	-5.82770	-9.14100	C	4.24430	-0.96040	-12.59550
H	-6.27640	-6.34530	-7.47820	C	3.41880	-3.06780	-10.73900
H	-4.42840	-6.93740	-9.54500	C	3.42790	-4.48290	-10.12500
H	0.05100	-1.37330	-8.07850	O	4.51200	-5.24660	-10.64760
H	-2.09490	-1.10560	-8.94190	O	2.40260	-2.19560	-10.23580
H	-2.28040	-2.77610	-9.40320	C	2.49920	-1.93130	-8.83770
H	-0.35380	-0.97830	-10.46980	O	1.91440	-3.03840	-8.08810
H	4.03450	-1.58430	-7.30060	C	0.58610	-3.39030	-8.60910
H	4.32360	0.15360	-9.67320	C	0.15840	-4.83540	-8.24010
C	-11.25830	-0.51590	-11.13730	O	-0.78000	-5.22760	-9.30980
H	-10.35040	-0.28760	-11.29960	C	-0.61210	-5.05480	-6.91390
C	-12.31550	0.39450	-10.87870	N	-0.20160	-5.87090	-5.74580
H	-12.23790	1.34010	-10.83490	C	-1.53340	-3.84830	-6.66890
C	-13.50820	-0.35200	-10.69700	O	-2.72090	-3.96230	-7.43920
H	-14.36890	0.00530	-10.51220	C	-3.65280	-4.99120	-7.04970
C	-13.19040	-1.71300	-10.84010	C	-4.05160	-4.82960	-5.57580
H	-13.80240	-2.43610	-10.76790	O	-4.77020	-5.97000	-5.09910
C	-11.79630	-1.82820	-11.11000	C	-4.79560	-3.49910	-5.37660
Fe	-12.10280	-0.89800	-9.30530	N	-3.95140	-2.31010	-5.48170
H	-11.15180	-2.66670	-11.35180	C	-4.30640	-1.13920	-4.82870
C	1.94050	-3.80870	-1.07890	C	-3.36900	0.01970	-5.05170
H	1.56520	-4.49610	-0.54100	O	-5.28780	-1.05740	-4.11910
C	1.75620	-2.41320	-0.90010	C	-5.97710	-3.47810	-6.36760
H	1.23290	-2.00290	-0.22190	O	-6.89730	-4.53690	-6.10840
C	2.48900	-1.73690	-1.90920	C	-7.53220	-4.51880	-4.81670
H	2.54420	-0.79550	-2.02450	C	-8.38060	-3.25740	-4.63580
C	3.11940	-2.70670	-2.70670	O	-8.80050	-3.13610	-3.27320
H	3.67580	-2.53180	-3.45680	C	-9.55250	-3.24890	-5.65060
C	2.78390	-3.99670	-2.20380	N	-9.06470	-3.02460	-7.03650
Fe	1.08780	-2.97690	-2.75110	C	-10.10540	-2.91960	-8.05510
H	3.09730	-5.00190	-2.46490	C	-11.07050	-1.81340	-7.82110
H	3.32293	0.60554	-8.37235	C	-10.72360	-0.41700	-7.70610
5				C	-11.87640	0.23200	-7.46620
O	5.45050	-3.34710	-8.48410	C	-12.97070	-0.72710	-7.42670
C	5.09080	-2.12850	-9.13810	C	-12.44930	-2.03780	-7.63630
C	4.74960	-2.31350	-10.63960	C	-10.35800	-4.56290	-5.43390
				O	-10.99130	-4.59110	-4.14810

C	-12.01910	-3.62240	-4.02140	H	-3.22300	-5.98060	-7.21760
O	-9.54620	-5.73590	-5.58940	H	-3.18020	-4.82540	-4.92150
C	-8.36790	-5.81260	-4.77640	H	-5.58510	-6.06960	-5.62140
C	-8.64040	-6.32020	-3.35300	H	-5.17370	-3.49450	-4.35100
O	-9.22810	-7.62060	-3.40580	H	-3.32780	-2.22190	-6.27770
O	-5.56250	-3.60890	-7.73560	H	-2.53750	-0.24300	-5.70850
C	-4.81130	-4.78710	-8.04260	H	-2.96350	0.33600	-4.08870
C	-5.66970	-6.03120	-8.32580	H	-3.92770	0.84400	-5.50330
O	-4.85700	-7.14090	-8.69420	H	-6.47750	-2.50890	-6.33110
O	-1.00680	-2.56470	-6.92220	H	-6.78380	-4.60030	-4.02500
C	-0.46180	-2.32760	-8.21350	H	-7.77360	-2.36160	-4.79950
C	-1.53690	-1.99120	-9.26940	H	-9.62560	-3.65010	-3.15280
O	-0.98640	-1.71380	-10.55070	H	-10.16520	-2.38500	-5.37950
C	3.92810	-1.40530	-8.37730	H	-8.43810	-3.79650	-7.29420
N	4.20270	0.04030	-8.65810	H	-10.62680	-3.87670	-8.17070
C	3.28890	1.05280	-8.16140	H	-9.61370	-2.73940	-9.01930
C	3.33020	1.21530	-6.68990	H	-9.73270	-0.00300	-7.78380
C	4.51310	1.51590	-5.92030	H	-11.99250	1.29430	-7.31820
C	4.12850	1.54270	-4.63870	H	-14.00210	-0.45710	-7.25610
C	2.69780	1.27970	-4.56290	H	-13.05100	-2.88390	-7.67760
C	2.20720	1.09430	-5.79550	H	-11.14390	-4.65650	-6.18640
H	5.96600	-3.88130	-9.11720	H	-12.61560	-3.87710	-3.14050
H	5.99630	-1.50650	-9.07470	H	-12.66950	-3.60750	-4.90110
H	5.54910	-2.86400	-11.14500	H	-11.59180	-2.62960	-3.85100
H	4.24960	0.08090	-12.93110	H	-7.77840	-6.60790	-5.25970
H	3.21630	-1.31930	-12.71170	H	-9.31700	-5.68620	-2.78110
H	4.92640	-1.53940	-13.22180	H	-7.70410	-6.40860	-2.79040
H	3.18460	-3.21640	-11.79580	H	-9.99950	-7.53970	-4.00060
H	2.49010	-4.99510	-10.36070	H	-4.34820	-4.55860	-9.01450
H	3.51050	-4.49080	-9.03630	H	-6.37360	-5.82770	-9.14100
H	4.40350	-6.14730	-10.28900	H	-6.27640	-6.34530	-7.47820
H	1.83150	-1.09560	-8.65640	H	-4.42840	-6.93740	-9.54500
H	0.65710	-3.39960	-9.70020	H	0.05100	-1.37330	-8.07850
H	0.99510	-5.53240	-8.31490	H	-2.09490	-1.10560	-8.94190
H	-1.61760	-4.75560	-9.16830	H	-2.28040	-2.77610	-9.40320
H	-1.29130	-5.83540	-7.26810	H	-0.35380	-0.97830	-10.46980
H	-1.04520	-6.23610	-5.29750	H	4.03450	-1.58430	-7.30060
H	-1.79090	-3.80270	-5.61710	H	4.32360	0.15360	-9.67320

H	2.26920	0.90100	-8.52710	O	4.51200	-5.24660	-10.64760
H	3.60180	2.00860	-8.60270	O	2.40260	-2.19560	-10.23580
H	5.50430	1.66860	-6.32270	C	2.49920	-1.93130	-8.83770
H	4.76190	1.71690	-3.78360	O	1.91440	-3.03840	-8.08810
H	2.13950	1.25100	-3.63550	C	0.58610	-3.39030	-8.60910
H	1.18630	0.88960	-6.07600	C	0.15840	-4.83540	-8.24010
C	3.93420	4.78050	-6.38630	O	-0.78000	-5.22760	-9.30980
H	4.76370	4.90350	-6.83310	C	-0.61210	-5.05480	-6.91390
C	3.71420	4.88610	-4.98850	N	-0.20160	-5.87090	-5.74580
H	4.37260	5.09010	-4.33500	C	0.65530	-5.38160	-4.67170
C	2.34100	4.63480	-4.73610	C	0.31750	-4.08680	-4.02830
H	1.91820	4.64250	-3.88540	C	0.68500	-2.81820	-4.60780
C	1.71760	4.37360	-5.96780	C	-0.09630	-1.89860	-4.02180
H	0.79710	4.17340	-6.09220	C	-0.88650	-2.53220	-2.97520
C	2.69650	4.45750	-6.99940	C	-0.50160	-3.79520	-3.10340
Fe	3.21250	3.01040	-5.63710	C	-1.53340	-3.84830	-6.66890
H	2.64450	4.39750	-8.08140	O	-2.72090	-3.96230	-7.43920
C	-11.25830	-0.51590	-11.13730	C	-3.65280	-4.99120	-7.04970
H	-10.35040	-0.28760	-11.29960	C	-4.05160	-4.82960	-5.57580
C	-12.31550	0.39450	-10.87870	O	-4.77020	-5.97000	-5.09910
H	-12.23790	1.34010	-10.83490	C	-4.79560	-3.49910	-5.37660
C	-13.50820	-0.35200	-10.69700	N	-3.95140	-2.31010	-5.48170
H	-14.36890	0.00530	-10.51220	C	-4.30640	-1.13920	-4.82870
C	-13.19040	-1.71300	-10.84010	C	-3.36900	0.01970	-5.05170
H	-13.80240	-2.43610	-10.76790	O	-5.28780	-1.05740	-4.11910
C	-11.79630	-1.82820	-11.11000	C	-5.97710	-3.47810	-6.36760
Fe	-12.10280	-0.89800	-9.30530	O	-6.89730	-4.53690	-6.10840
H	-11.15180	-2.66670	-11.35180	C	-7.53220	-4.51880	-4.81670
H	0.74093	-6.51714	-5.72867	C	-8.38060	-3.25740	-4.63580
				O	-8.80050	-3.13610	-3.27320
6				C	-9.55250	-3.24890	-5.65060
O	5.45050	-3.34710	-8.48410	N	-9.06470	-3.02460	-7.03650
C	5.09080	-2.12850	-9.13810	C	-10.35800	-4.56290	-5.43390
C	4.74960	-2.31350	-10.63960	O	-10.99130	-4.59110	-4.14810
O	4.66150	-0.98950	-11.23510	C	-12.01910	-3.62240	-4.02140
C	4.24430	-0.96040	-12.59550	O	-9.54620	-5.73590	-5.58940
C	3.41880	-3.06780	-10.73900	C	-8.36790	-5.81260	-4.77640
C	3.42790	-4.48290	-10.12500	C	-8.64040	-6.32020	-3.35300

O	-9.22810	-7.62060	-3.40580	H	-1.00920	-4.57170	-2.25400
O	-5.56250	-3.60890	-7.73560	H	-1.79090	-3.80270	-5.61710
C	-4.81130	-4.78710	-8.04260	H	-3.22300	-5.98060	-7.21760
C	-5.66970	-6.03120	-8.32580	H	-3.18020	-4.82540	-4.92150
O	-4.85700	-7.14090	-8.69420	H	-5.58510	-6.06960	-5.62140
O	-1.00680	-2.56470	-6.92220	H	-5.17370	-3.49450	-4.35100
C	-0.46180	-2.32760	-8.21350	H	-3.32780	-2.22190	-6.27770
C	-1.53690	-1.99120	-9.26940	H	-2.53750	-0.24300	-5.70850
O	-0.98640	-1.71380	-10.55070	H	-2.96350	0.33600	-4.08870
C	3.92810	-1.40530	-8.37730	H	-3.92770	0.84400	-5.50330
N	4.20270	0.04030	-8.65810	H	-6.47750	-2.50890	-6.33110
C	3.28890	1.05280	-8.16140	H	-6.78380	-4.60030	-4.02500
C	3.33020	1.21530	-6.68990	H	-7.77360	-2.36160	-4.79950
C	4.51310	1.51590	-5.92030	H	-9.62560	-3.65010	-3.15280
C	4.12850	1.54270	-4.63870	H	-10.16520	-2.38500	-5.37950
C	2.69780	1.27970	-4.56290	H	-8.43810	-3.79650	-7.29420
C	2.20720	1.09430	-5.79550	H	-11.14390	-4.65650	-6.18640
H	5.96600	-3.88130	-9.11720	H	-12.61560	-3.87710	-3.14050
H	5.99630	-1.50650	-9.07470	H	-12.66950	-3.60750	-4.90110
H	5.54910	-2.86400	-11.14500	H	-11.59180	-2.62960	-3.85100
H	4.24960	0.08090	-12.93110	H	-7.77840	-6.60790	-5.25970
H	3.21630	-1.31930	-12.71170	H	-9.31700	-5.68620	-2.78110
H	4.92640	-1.53940	-13.22180	H	-7.70410	-6.40860	-2.79040
H	3.18460	-3.21640	-11.79580	H	-9.99950	-7.53970	-4.00060
H	2.49010	-4.99510	-10.36070	H	-4.34820	-4.55860	-9.01450
H	3.51050	-4.49080	-9.03630	H	-6.37360	-5.82770	-9.14100
H	4.40350	-6.14730	-10.28900	H	-6.27640	-6.34530	-7.47820
H	1.83150	-1.09560	-8.65640	H	-4.42840	-6.93740	-9.54500
H	0.65710	-3.39960	-9.70020	H	0.05100	-1.37330	-8.07850
H	0.99510	-5.53240	-8.31490	H	-2.09490	-1.10560	-8.94190
H	-1.61760	-4.75560	-9.16830	H	-2.28040	-2.77610	-9.40320
H	-1.29130	-5.83540	-7.26810	H	-0.35380	-0.97830	-10.46980
H	-1.04520	-6.23610	-5.29750	H	4.03450	-1.58430	-7.30060
H	1.69860	-5.38960	-5.00540	H	4.32360	0.15360	-9.67320
H	0.35260	-5.98610	-4.11780	H	2.26920	0.90100	-8.52710
H	1.35950	-2.68380	-5.43910	H	3.60180	2.00860	-8.60270
H	-0.10650	-0.73360	-4.17110	H	5.50430	1.66860	-6.32270
H	-1.54690	-1.99300	-2.31580	H	4.76190	1.71690	-3.78360

H	2.13950	1.25100	-3.63550	C	0.58611	-3.39030	-8.60912
H	1.18630	0.88960	-6.07600	C	0.15842	-4.83545	-8.24015
C	3.93420	4.78050	-6.38630	O	-0.78004	-5.22761	-9.30977
H	4.76370	4.90350	-6.83310	C	-0.61206	-5.05478	-6.91387
C	3.71420	4.88610	-4.98850	N	-0.20162	-5.87089	-5.74579
H	4.37260	5.09010	-4.33500	C	0.65532	-5.38165	-4.67166
C	2.34100	4.63480	-4.73610	C	0.31755	-4.08679	-4.02827
H	1.91820	4.64250	-3.88540	C	0.68499	-2.81822	-4.60784
C	1.71760	4.37360	-5.96780	C	-0.09626	-1.89860	-4.02181
H	0.79710	4.17340	-6.09220	C	-0.88655	-2.53225	-2.97519
C	2.69650	4.45750	-6.99940	C	-0.50156	-3.79520	-3.10338
Fe	3.21250	3.01040	-5.63710	C	-1.53344	-3.84831	-6.66888
H	2.64450	4.39750	-8.08140	O	-2.72094	-3.96227	-7.43924
C	1.94050	-3.80870	-1.07890	C	-3.65281	-4.99117	-7.04972
H	1.56520	-4.49610	-0.54100	C	-4.05157	-4.82963	-5.57575
C	1.75620	-2.41320	-0.90010	O	-4.77018	-5.97000	-5.09908
H	1.23290	-2.00290	-0.22190	C	-4.79564	-3.49906	-5.37656
C	2.48900	-1.73690	-1.90920	N	-3.95137	-2.31014	-5.48168
H	2.54420	-0.79550	-2.02450	C	-4.30635	-1.13917	-4.82868
C	3.11940	-2.70670	-2.70670	C	-3.36896	0.01974	-5.05171
H	3.67580	-2.53180	-3.45680	O	-5.28784	-1.05744	-4.11914
C	2.78390	-3.99670	-2.20380	C	-5.97707	-3.47805	-6.36758
Fe	1.08780	-2.97690	-2.75110	O	-6.89733	-4.53689	-6.10842
H	3.09730	-5.00190	-2.46490	C	-7.53219	-4.51879	-4.81669
H	-9.69478	-2.69045	-7.62231	C	-8.38057	-3.25738	-4.63580
				O	-8.80047	-3.13613	-3.27323
7				C	-9.55254	-3.24886	-5.65058
O	5.45055	-3.34714	-8.48409	N	-9.06469	-3.02460	-7.03647
C	5.09082	-2.12847	-9.13814	C	-10.10545	-2.91963	-8.05515
C	4.74964	-2.31346	-10.63963	C	-11.07051	-1.81339	-7.82108
O	4.66153	-0.98946	-11.23510	C	-10.72359	-0.41701	-7.70610
C	4.24435	-0.96044	-12.59553	C	-11.87639	0.23204	-7.46619
C	3.41880	-3.06781	-10.73903	C	-12.97073	-0.72714	-7.42668
C	3.42791	-4.48293	-10.12497	C	-12.44928	-2.03777	-7.63629
O	4.51199	-5.24662	-10.64764	C	-10.35800	-4.56294	-5.43387
O	2.40265	-2.19562	-10.23585	O	-10.99130	-4.59108	-4.14813
C	2.49921	-1.93130	-8.83766	C	-12.01912	-3.62238	-4.02143
O	1.91441	-3.03842	-8.08805	O	-9.54620	-5.73594	-5.58940

C	-8.36791	-5.81257	-4.77643	H	-0.10650	-0.73358	-4.17111
C	-8.64044	-6.32020	-3.35300	H	-1.54689	-1.99300	-2.31584
O	-9.22812	-7.62064	-3.40581	H	-1.00916	-4.57169	-2.25405
O	-5.56253	-3.60891	-7.73561	H	-1.79094	-3.80273	-5.61712
C	-4.81128	-4.78709	-8.04264	H	-3.22304	-5.98063	-7.21758
C	-5.66973	-6.03123	-8.32579	H	-3.18018	-4.82541	-4.92155
O	-4.85703	-7.14085	-8.69422	H	-5.58515	-6.06958	-5.62143
O	-1.00677	-2.56467	-6.92217	H	-5.17366	-3.49453	-4.35102
C	-0.46178	-2.32755	-8.21348	H	-3.32782	-2.22190	-6.27765
C	-1.53691	-1.99124	-9.26939	H	-2.53749	-0.24303	-5.70847
O	-0.98638	-1.71376	-10.55067	H	-2.96350	0.33603	-4.08868
C	3.92809	-1.40526	-8.37730	H	-3.92770	0.84396	-5.50334
N	4.20273	0.04026	-8.65812	H	-6.47745	-2.50889	-6.33111
C	3.28885	1.05277	-8.16141	H	-6.78384	-4.60028	-4.02503
C	3.33019	1.21532	-6.68989	H	-7.77361	-2.36161	-4.79951
C	4.51307	1.51594	-5.92030	H	-9.62562	-3.65007	-3.15285
C	4.12846	1.54266	-4.63871	H	-10.16517	-2.38497	-5.37947
C	2.69776	1.27972	-4.56286	H	-8.43811	-3.79654	-7.29422
C	2.20720	1.09429	-5.79550	H	-10.62681	-3.87675	-8.17074
H	5.96603	-3.88135	-9.11724	H	-9.61368	-2.73944	-9.01934
H	5.99632	-1.50647	-9.07475	H	-9.73273	-0.00297	-7.78383
H	5.54911	-2.86396	-11.14502	H	-11.99250	1.29428	-7.31816
H	4.24955	0.08085	-12.93108	H	-14.00212	-0.45705	-7.25608
H	3.21625	-1.31934	-12.71172	H	-13.05100	-2.88393	-7.67761
H	4.92640	-1.53942	-13.22178	H	-11.14390	-4.65649	-6.18636
H	3.18460	-3.21636	-11.79581	H	-12.61560	-3.87712	-3.14051
H	2.49015	-4.99506	-10.36069	H	-12.66948	-3.60750	-4.90111
H	3.51050	-4.49081	-9.03633	H	-11.59178	-2.62960	-3.85101
H	4.40348	-6.14727	-10.28904	H	-7.77839	-6.60789	-5.25971
H	1.83154	-1.09562	-8.65645	H	-9.31700	-5.68620	-2.78108
H	0.65710	-3.39963	-9.70017	H	-7.70407	-6.40860	-2.79040
H	0.99512	-5.53239	-8.31493	H	-9.99953	-7.53973	-4.00057
H	-1.61757	-4.75559	-9.16828	H	-4.34817	-4.55859	-9.01455
H	-1.29135	-5.83536	-7.26812	H	-6.37357	-5.82769	-9.14105
H	-1.04515	-6.23611	-5.29750	H	-6.27636	-6.34534	-7.47817
H	1.69862	-5.38965	-5.00540	H	-4.42836	-6.93740	-9.54502
H	0.35260	-5.98609	-4.11778	H	0.05096	-1.37325	-8.07851
H	1.35951	-2.68378	-5.43908	H	-2.09492	-1.10562	-8.94194

H	-2.28037	-2.77608	-9.40319	H	-10.35040	-0.28764	-11.29958
H	-0.35383	-0.97832	-10.46982	C	-12.31551	0.39446	-10.87865
H	4.03446	-1.58435	-7.30063	H	-12.23794	1.34006	-10.83487
H	4.32360	0.15363	-9.67325	C	-13.50824	-0.35196	-10.69701
H	2.26919	0.90097	-8.52707	H	-14.36891	0.00526	-10.51225
H	3.60176	2.00856	-8.60265	C	-13.19035	-1.71303	-10.84011
H	5.50435	1.66865	-6.32269	H	-13.80243	-2.43614	-10.76789
H	4.76194	1.71690	-3.78356	C	-11.79628	-1.82816	-11.11002
H	2.13952	1.25103	-3.63551	Fe	-12.10283	-0.89797	-9.30532
H	1.18627	0.88961	-6.07602	H	-11.15180	-2.66670	-11.35178
C	3.93421	4.78047	-6.38629	C	1.94050	-3.80869	-1.07885
H	4.76365	4.90353	-6.83311	H	1.56515	-4.49613	-0.54097
C	3.71423	4.88613	-4.98853	C	1.75624	-2.41320	-0.90007
H	4.37259	5.09007	-4.33502	H	1.23290	-2.00295	-0.22191
C	2.34098	4.63476	-4.73606	C	2.48903	-1.73685	-1.90919
H	1.91815	4.64246	-3.88538	H	2.54418	-0.79549	-2.02452
C	1.71757	4.37363	-5.96782	C	3.11944	-2.70671	-2.70669
H	0.79713	4.17345	-6.09220	H	3.67576	-2.53181	-3.45680
C	2.69651	4.45749	-6.99941	C	2.78387	-3.99668	-2.20379
Fe	3.21247	3.01037	-5.63714	Fe	1.08779	-2.97692	-2.75111
H	2.64454	4.39745	-8.08137	H	3.09734	-5.00192	-2.46490
C	-11.25833	-0.51592	-11.13733				