SUPPORTING INFORMATION

Stabilizing hydroperoxyflavin intermediate formation via peptide appendage: A neutral flavoenzyme model

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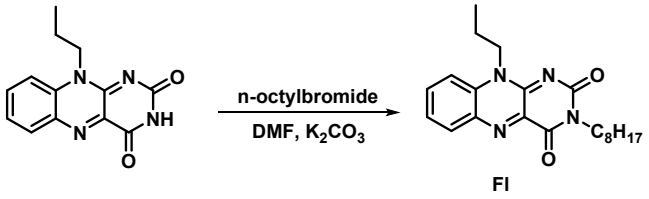
Table of contents

1. Materials and Measurements

All chemicals and reagents are purchased from commercial sources such as Sigma Aldrich, SRL Pvt. Ltd (India), Alfa Aesar and TCI chemicals, and were used without purification. Nuclear magnetic resonance spectra were collected using a Bruker DRX-400 spectrometer. ^{13}C NMR spectra were collected at 100 MHz, and ^{1}H NMR spectra were collected at 400 MHz. Resonances are reported in parts per million (ppm) and coupling constants, *J*, are reported in hertz (Hz). High resolution mass spectra was obtained by Electron Spray Ionization method (ESI) using Agilent QTOF 6538. Yields of catalytic reaction were determined using HPLC (Shimadzu-UFLC) by eluting with Acetonitrile water mixture.

2. Synthetic procedure

Synthesis of Fl. To 10-propylisoalloxazine[1] (0.2 g, 0.78 mmol) taken in 25 ml RB flask, added 4 mL DMF followed by addition of potassium carbonate (0.43 g, 3.12 mmol) and 1-bromooctane (0.67 mL, 3.9 mmol). Reaction was kept at 90 ^{o}C for 1.5 hours. After completion of reaction, monitored by TLC the contents were cooled and added water (10 mL). The precipitate obtained is suction filtrated and washed with 15 mL water and 10 mL diethyl ether. Yellow solid obtained is then dried to give **Fl** with an yield of 78%.



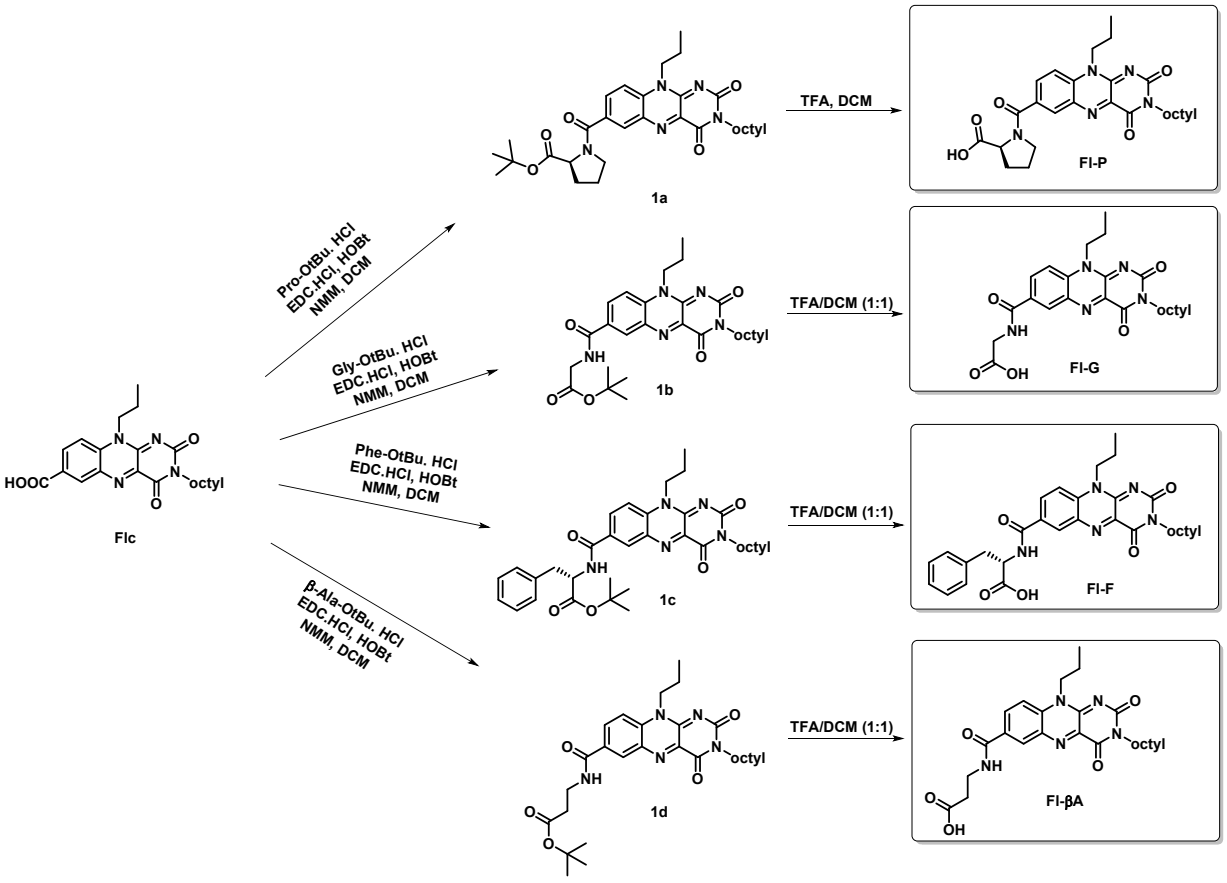
Scheme S1. Synthetic scheme for preparation of Fl

Fl: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.90 (ddd, *J* = 8.7, 7.2, 1.6 Hz, 1H), 7.64-7.6 (m, 2H), 4.67 (t, *J* = 7.9 Hz, 2H), 4.1 (t, *J* = 7.54 Hz, 2H), 1.98-1.88 (m, 2H), 1.76-1.68 (m, 2H), 1.41-1.26 (m, 10H), 1.14 (t, *J* = 7.4 Hz, 3H), 0.87 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.45, 155.56, 148.78, 137.17, 135.90, 135.49, 133.41, 132.62, 126.26, 115.14, 46.13, 42.15, 31.79, 29.30, 29.16, 27.74, 26.95, 22.62, 20.47, 14.06, 11.22. HR-MS (ESI): m/z calcd. for $[C_{21}H_{29}N_4O_2]^+$ $([M+H])^+$: 369.2285; found: 369.2297.

Synthesis of Flavopeptides

Flavopeptides are synthesized by coupling carboxy flavin **Flc** (reported previously by our group) with respective carboxy protected amino acid derivatives.[2]

General procedure for synthesis of protected flavopeptides (**1a-d**). To **Flc** (0.5 mmol) taken in a 50 mL Round bottom flask, added 15 mL dichloromethane. The reaction mixture is cooled to 0 ^{o}C and then added EDC.HCl (0.6 mmol) followed by HOBt (0.5 mmol). Stirring is continued at low temperature under inert atmosphere until the contents becomes clear. Respective amino acid derivatives (0.6 mmol) such as H-Gly-OtBu.HCl, H-β Ala-OtBu.HCl, H-Pro-OtBu.HCl or H-Phe-OtBu.Cl is then added followed by addition of N-methyl morpholine (1.5 mmol) and continued stirring at room temperature under inert atmosphere. After 12 h the reaction is stopped, concentrated to remove DCM and column chromatography is done using gradient elution with chloroform and methanol (up to 10%) to give corresponding flavopeptide (**1a-d**) as a yellow solid.



Scheme S2. Synthetic scheme for preparation of flavopeptide derivatives

Fl-Pro-COOtBu (**1a**). Yield 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 1.9 Hz, 1H), 8.17 (dd, *J* = 8.9, 1.9 Hz, 1H), 7.7 (d, *J* = 9 Hz, 1H), 4.69-4.65 (m, 2H), 4.6-4.57 (m, 1H), 4.11-4.07 (m, 2H), 3.84-3.62 (m, 2H), 2.4-2.31 (m, 1H), 2.11-1.89 (m, 6H), 1.76 – 1.68 (m, 2H), 1.50 (s, 9H), 1.39-1.23 (m, 15H), 1.14 (t, *J* = 7.3 Hz, 3H), 0.87 (dd, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.83, 166.34, 159.18, 155.33, 148.92, 137.91, 135.26, 134.76, 133.85, 133.61, 131.51, 130.46, 115.60, 82.22, 81.55, 61.92, 60.45, 50.10, 47.14, 46.26, 42.20, 31.75, 29.25, 29.12, 27.98, 27.67, 26.92, 25.43, 22.58, 20.46, 14.04, 11.18. HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{31}H_{43}N_5O_5$: 566.3323. Found 566.3323.

Fl-Gly-COOtBu (**1b**). Yield 90%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 2.1 Hz, 1H), 8.44 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.71 (d, *J* = 9.1 Hz, 1H), 7.32 (dd, *J* = 11.1, 6.1 Hz, 1H), 4.66 (t, *J* = 7.76 Hz, 2H), 4.17 (d, *J* = 5.0 Hz, 2H), 4.05 (t, *J* = 7.64 Hz, 2H), 1.99 – 1.86 (m, 2H), 1.74 – 1.64 (m, 2H), 1.50 (s, 9H), 1.44 – 1.19 (m, 10H), 1.14 (t, *J* = 7.4 Hz, 3H), 0.87 (dd, *J* = 9.2, 4.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.86, 164.79, 159.17, 155.38, 148.98, 138.00, 134.98, 134.66, 134.59, 131.54, 131.21, 115.70, 82.74, 46.40, 42.69, 42.24, 31.79, 29.30, 29.18, 28.05, 27.71, 26.96, 22.63, 20.48, 14.10, 11.24. HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{28}H_{39}N_5O_5$: 526.3024. Found 526.3077.

Fl-Phe-COOtBu (**1c**). Yield 83%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.35 (d, *J* = 9.0 Hz, 1H), 7.67 (d, *J* = 9.0 Hz, 1H), 7.3 – 7.18 (m, 5H), 6.96 (s, 1H), 6.96 (s, 1H), 4.98-4.93 (m, 1H), 4.66-4.63 (m, 2H), 4.09-4.06 (m, 2H), 3.27-3.23 (m, 2H), 1.94-1.88 (m, 3H), 1.71-1.69 (m, 2H), 1.45 (s, 9H), 1.39-1.26 (m, 11H), 1.15-1.11 (m, 3H), 0.88-0.85 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.40, 164.17, 159.09, 155.38, 148.97, 138.05, 135.89, 134.97, 134.58, 134.48, 131.71, 131.06, 129.43, 128.54, 127.19, 115.67, 82.96, 54.24, 46.36, 42.26, 37.91, 31.80, 29.31, 29.19, 27.99, 27.72, 26.96, 22.65, 20.48, 14.11, 11.24. HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{35}H_{45}N_5O_5$: 616.3493 Found. 616.3496.

Fl-β ala -COOtBu (**1d**). Yield 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 2.0 Hz, 1H), 8.40 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.67 (d, *J* = 9.1 Hz, 1H), 7.41 (s, 1H), 4.63 (t, *J* = 7.7 Hz, 2H), 4.04 (t, *J* = 7.5 Hz, 2H), 3.71 (q, *J* = 5.9 Hz, 2H), 2.57 (t, *J* = 6.0 Hz, 2H), 2.05 (s, 1H), 1.91-1.85 (m, 2H), 1.7-1.63 (m, 2H), 1.43 (s, 9H), 1.38-1.23 (m, 11H), 1.10 (t, *J* = 7.4 Hz, 3H), 0.83 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.19, 164.61, 159.17, 155.40, 148.96, 137.93, 135.04, 134.74, 134.44, 132.16, 130.84, 115.65, 81.51, 46.39, 42.26, 35.83, 34.68, 31.80, 29.30, 29.18,

28.12, 27.71, 26.96, 22.64, 20.49, 14.10, 11.24. HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{29}H_{41}N_5O_5$: 540.3180 Found 540.3158.

General procedure for synthesis of deprotected flavopeptides. Deprotection of flavopeptides is performed by addition of Trifluoroacetic acid (TFA) and DCM (5 mL, 1:1) to RB flask containing respective flavopeptide **1a-d** (0.5 mmol) and stirred at room temperature for 2 hours. Upon completion of reaction monitored by TLC, the reaction mixture is concentrated under reduced pressure, washed with 10 mL diethyl ether to give corresponding flavopeptides as yellow solids.

Fl-P. Yield 95%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.71 (dd, *J* = 8.6, 5.3 Hz, 1H), 4.65 (s, 2H), 4.1-3.99 (m, 2H), 3.77-3.63 (m, 2H), 2.34-2.05 (m, 3H), 1.92-1.87 (m, 3H), 1.69-1.65 (m, 2H), 1.34-1.26 (m, 10H), 1.11 (t, *J* = 7.4 Hz, 3H), 0.86 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.23, 162.47, 159.22, 155.40, 148.93, 137.94, 135.11, 134.70, 133.80, 133.24, 131.63, 115.91, 50.45, 50.41, 46.37, 46.16, 42.28, 31.79, 29.30, 29.18, 27.71, 26.97, 25.47, 22.63, 20.51, 14.09, 11.22. HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{27}H_{35}N_5O_5$: 510.2711 Found.510.2700.

Fl-G. Yield 96%. ^{1}H NMR (400 MHz, DMSO-d6) δ 9.22 (t, *J* = 5.8 Hz, 1H), 8.65 (d, *J* = 1.8 Hz, 1H), 8.33 (dd, *J* = 9.0, 1.9 Hz, 1H), 8.09 (d, *J* = 9.1 Hz, 1H), 4.55 (t, *J* = 7.8 Hz, 2H), 4.00 (d, *J* = 5.8 Hz, 2H), 3.87 (t, *J* = 7.52 Hz, 2H), 1.77 (dd, *J* = 15.4, 7.6 Hz, 2H), 1.57 (d, *J* = 6.7 Hz, 2H), 1.38 – 1.17 (m, 10H), 1.04 (t, *J* = 7.4 Hz, 3H), 0.85 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d6) δ 171.64, 165.07, 159.51, 155.34, 149.77, 139.24, 134.86, 134.77, 133.60, 130.95, 130.85, 117.17, 46.05, 41.81, 41.46, 31.72, 29.26, 29.10, 27.75, 26.91, 22.57, 20.35, 14.40, 11.43. HRMS (ESI) *m/z*: $(M+K)^+$ calculated for $C_{24}H_{31}N_5O_5$: 508.1957. Found 508.1909.

Fl-F. Yield 94%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.32 (d, *J* = 8.9 Hz, 1H), 7.65 (d, *J* = 9.1 Hz, 1H), 7.58 (s, 1H), 7.17-7.13 (m, 5H), 6.99 (s, 1H), 5.02 (d, *J* = 5.1 Hz, 1H), 4.60 (s, 2H), 4.04 (t, *J* = 6.9 Hz, 2H), 3.34-3.3 (m, 1H), 3.15-3.1 (m, 1H), 1.89-1.83 (m, 2H), 1.68-1.66 (m, 2H), 1.37-1.25 (m, 10H), 1.09 (t, *J* = 7.2 Hz, 3H), 0.86 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.94, 165.10, 159.57, 155.89, 150.96, 148.84, 137.44, 135.99, 135.05, 134.85, 134.76, 131.33, 129.27, 128.60, 127.17, 115.86, 54.27, 46.70, 42.52, 37.33, 31.81, 29.31, 29.22, 27.69, 27.00,

22.65, 20.52, 14.11, 11.16. HRMS (ESI) *m/z*: $[M+H]^+$ calculated for $C_{31}H_{37}N_5O_5$: 560.2867 Found.560.2874.

Fl-βA. Yield 95%. ^{1}H NMR (400 MHz, DMSO-d6) δ 8.87 (t, *J* = 5.3 Hz, 1H), 8.63 (d, *J* = 2.0 Hz, 1H), 8.30 (dd, *J* = 9.0, 2.0 Hz, 1H), 8.05 (d, *J* = 9.2 Hz, 1H), 4.54 (t, *J* = 7.7 Hz, 2H), 3.86 (t, *J* = 7.4 Hz, 2H), 2.57 (t, *J* = 7.0 Hz, 2H), 1.78-1.57 (m, 2H), 1.57 (s, 2H), 1.28-1.24 (m, 10H), 1.03 (t, *J* = 7.4 Hz, 3H), 0.85 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d6) δ 173.35, 164.71, 159.51, 155.35, 149.72, 139.10, 134.83, 134.56, 133.69, 131.44, 130.67, 117.02, 46.04, 41.46, 36.25, 34.02, 31.72, 29.25, 29.10, 27.75, 26.91, 22.57, 20.35, 14.41, 11.43. HRMS (ESI) *m/z*: $[M + H]^+$ calculated for $C_{25}H_{33}N_5O_5$: 484.2554 Found 484.2524.

3. Catalytic studies

Catalytic amount of flavopeptide (10 mol%, 0.016 mmol) was taken in a glass vial, to it added 1.5 mL 2,2,2-Trifluoroethanol, followed by the addition of Caesium carbonate (0.32 mmol, 2 eq.) as base additive. Subsequently, hydrazine hydrate (4 eq.) is added as reducing agent to the reaction mixture. Finally, respective sulphide (0.16 mmol) was added to the glass vial and kept for stirring under oxygen atmosphere for 24 hours in dark. Yield of corresponding sulphoxide is determined by using HPLC.[3]

4. List of NMR Spectra

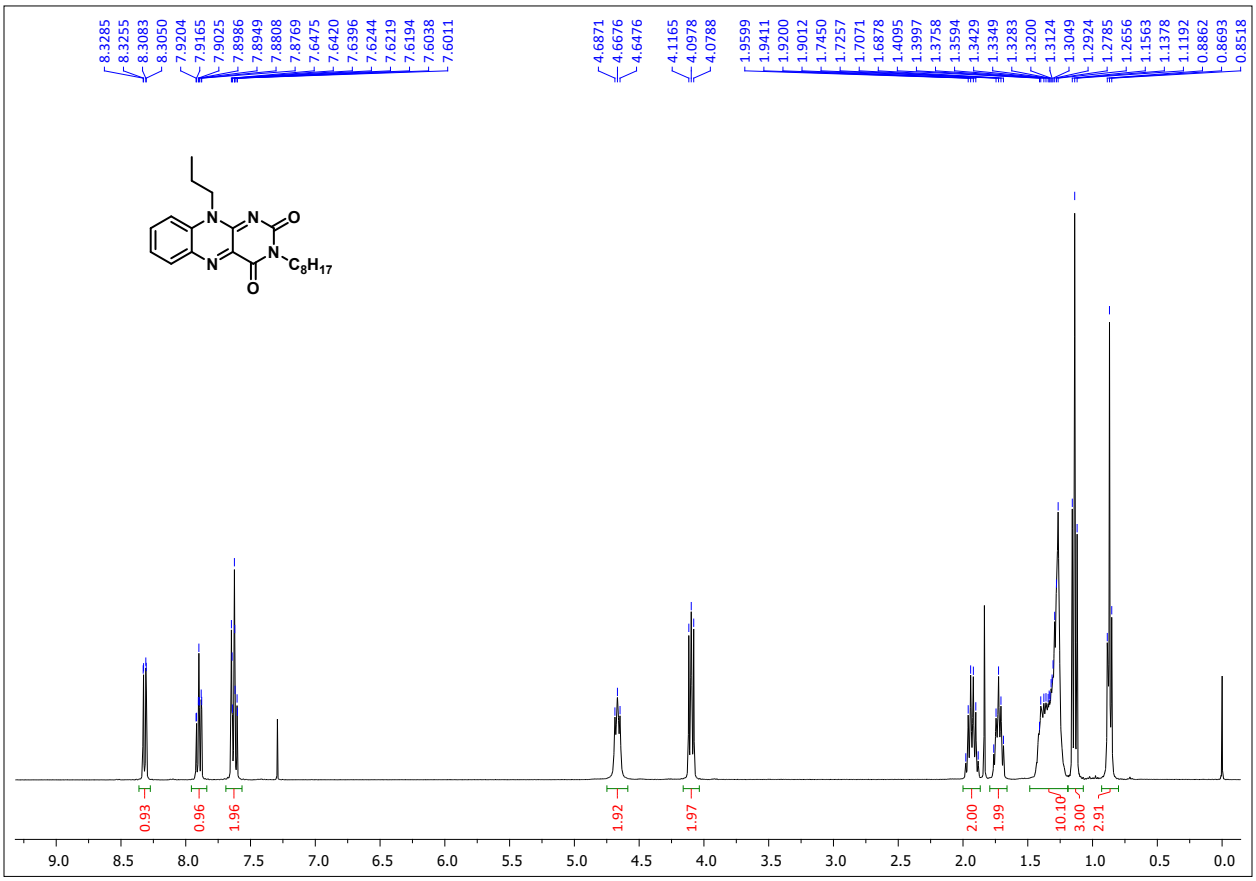


Figure S1. ^{1}H NMR of **Fl** in $CDCl_3$

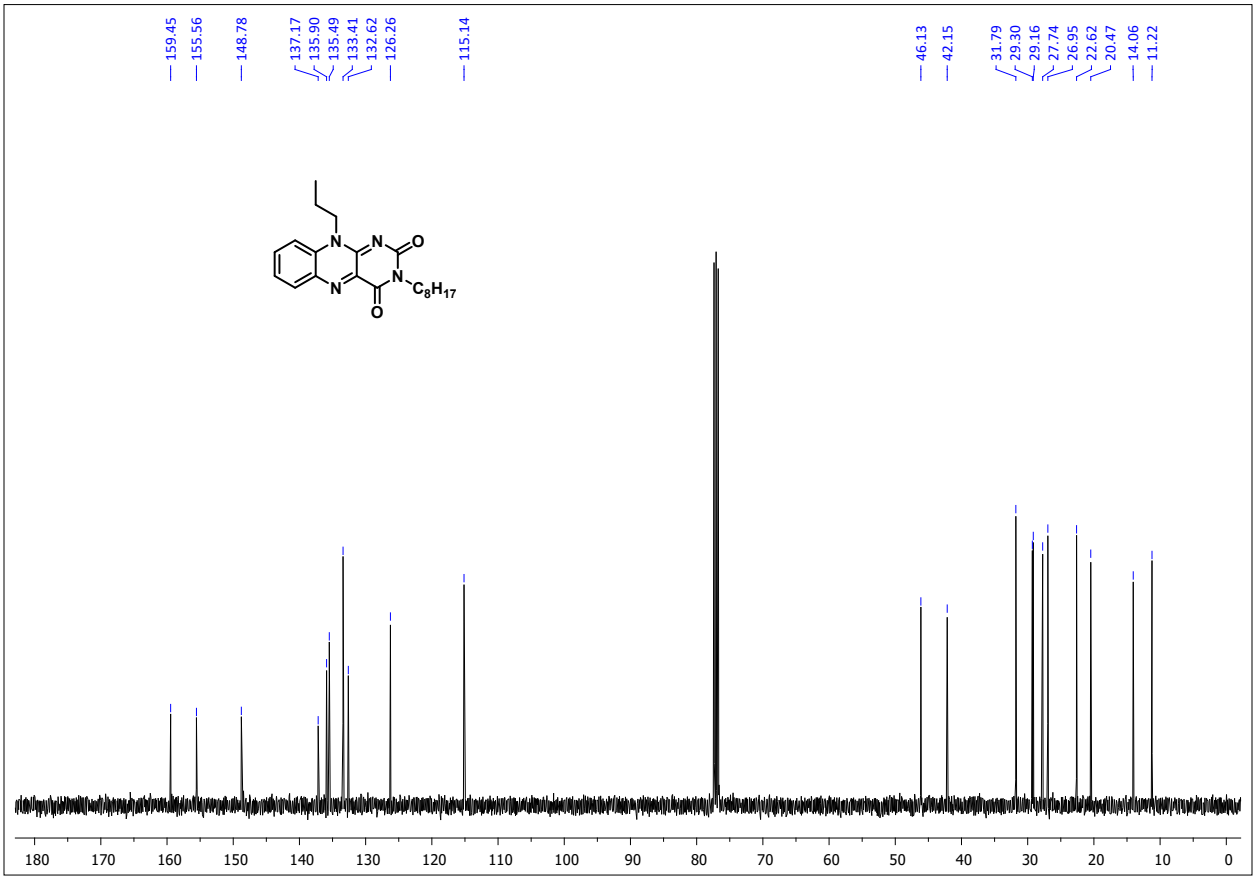


Figure S2. ^{13}C NMR of **Fl** in $CDCl_3$

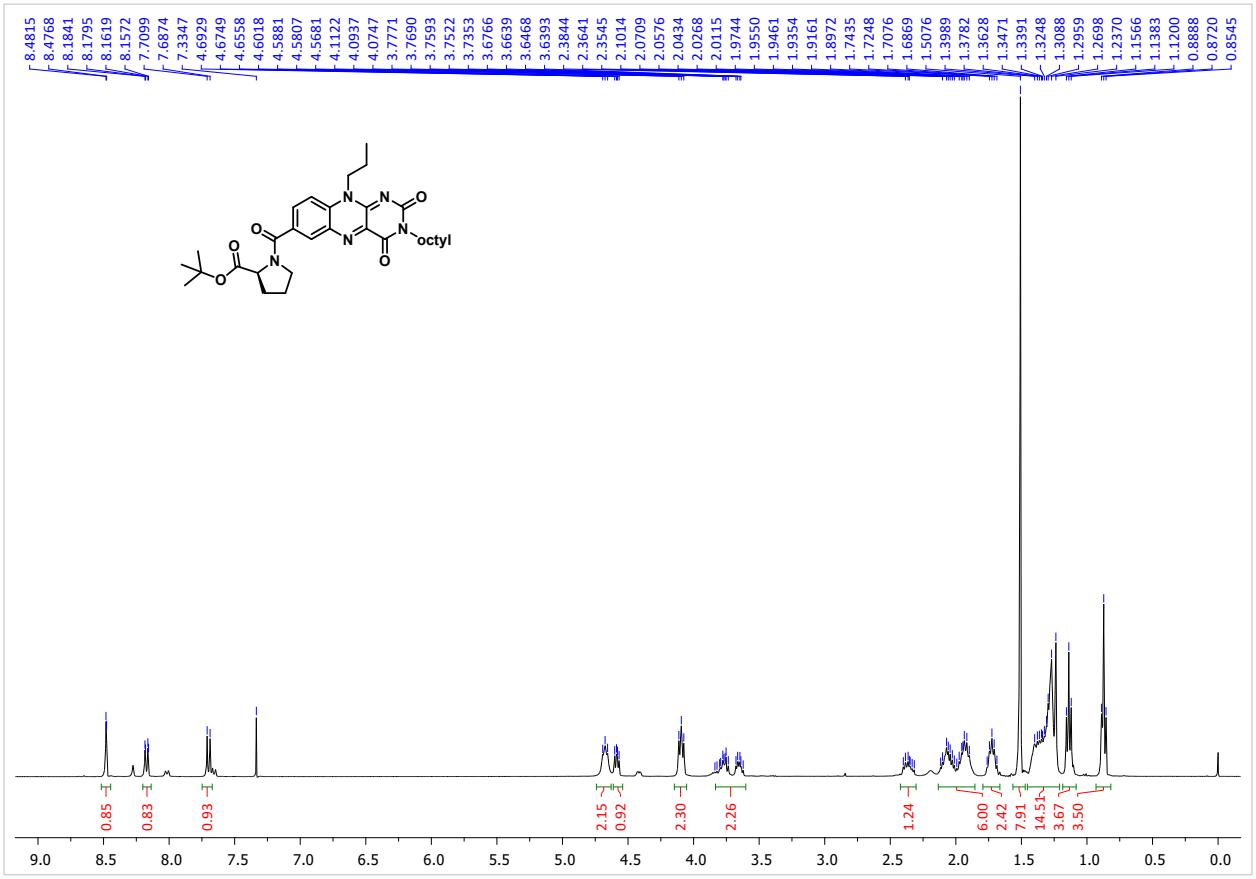


Figure S3. ^{1}H NMR of **1a** in $CDCl_3$

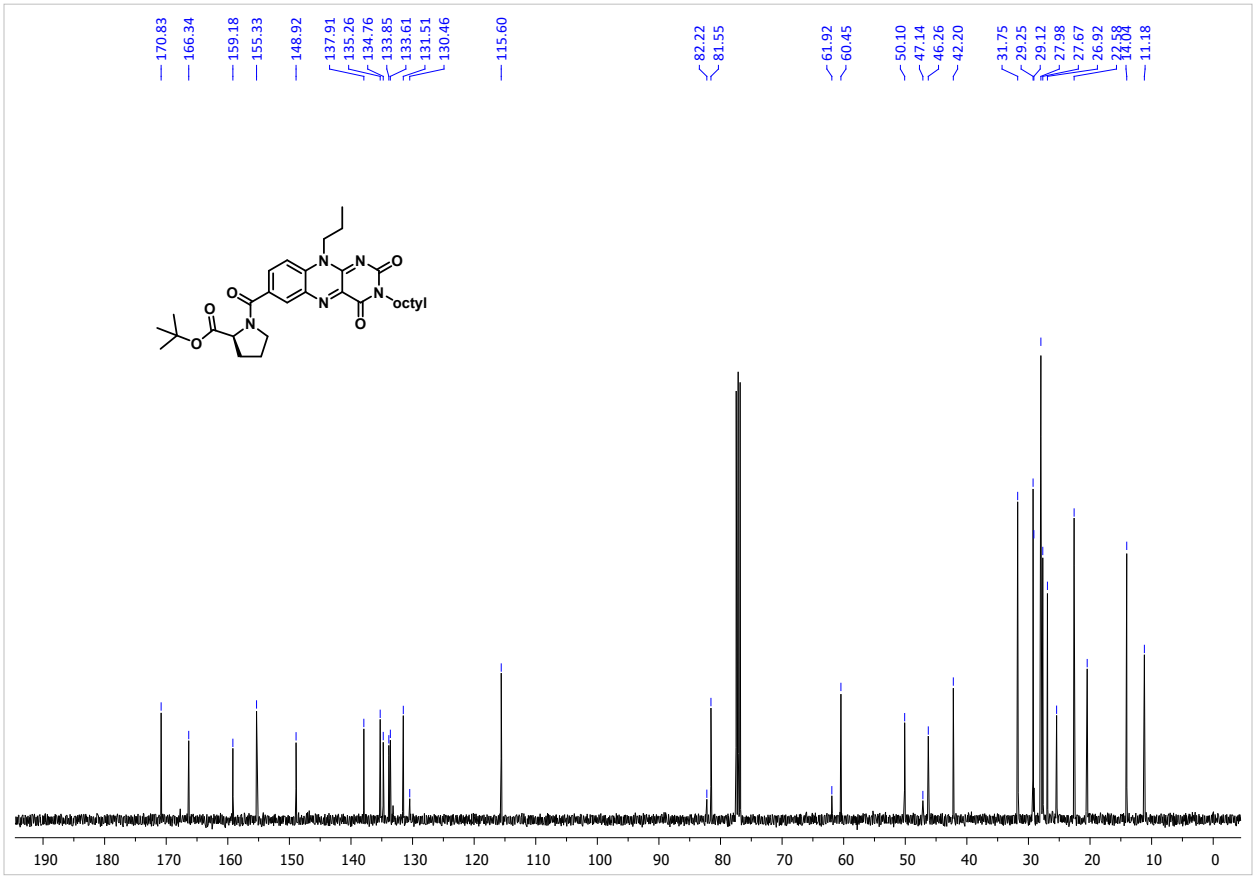


Figure S4. ^{13}C NMR of **1a** in $CDCl_3$.

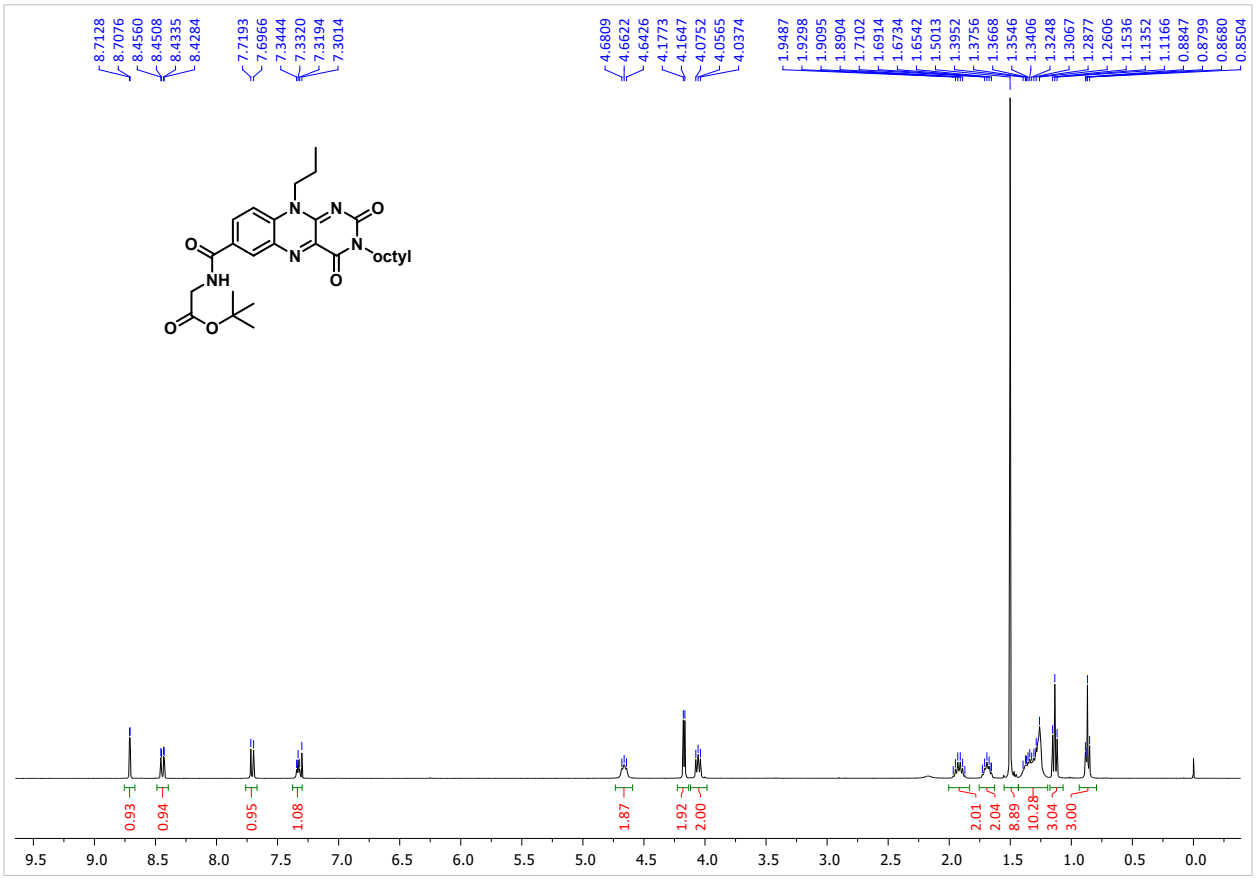


Figure S5. ^{1}H NMR of **1b** in $CDCl_3$

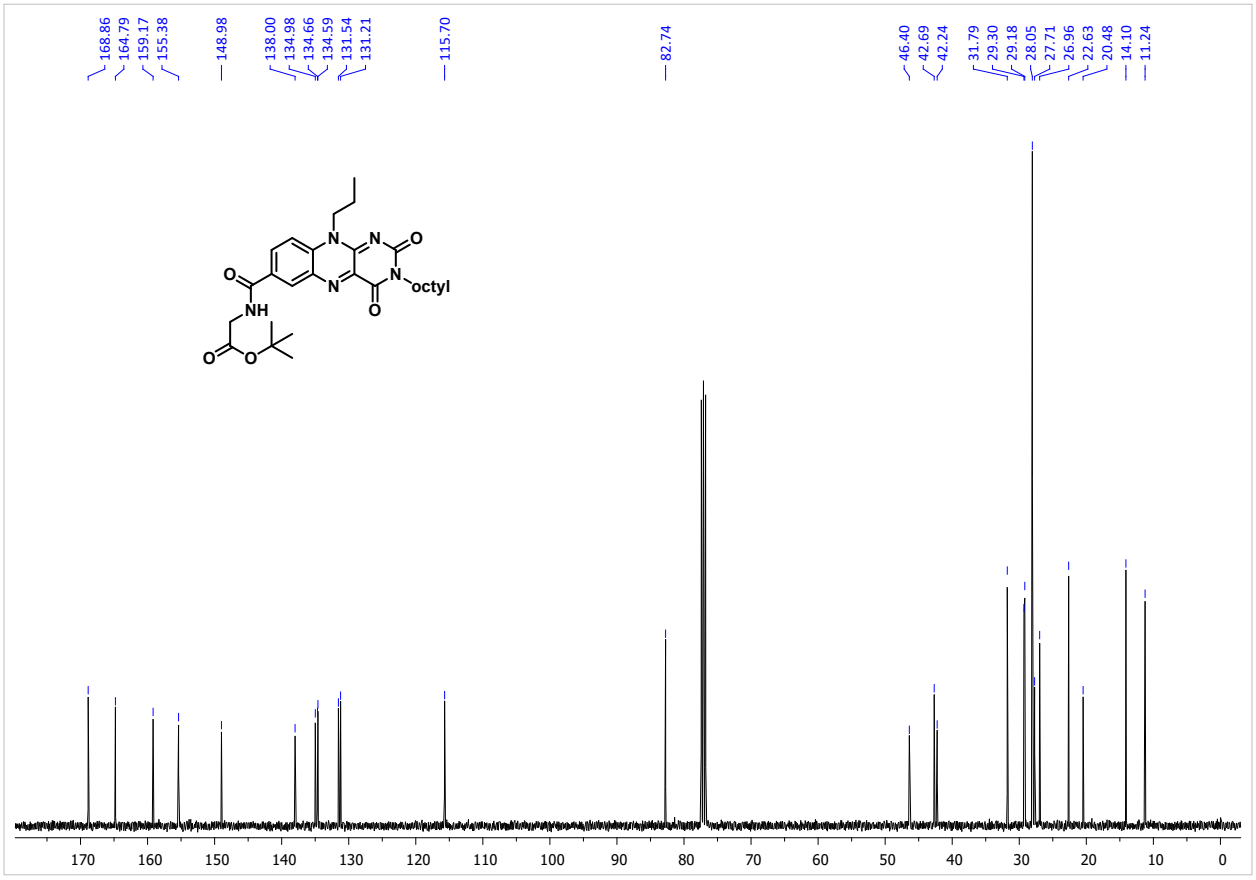


Figure S6. ^{13}C NMR of **1b** in $CDCl_3$

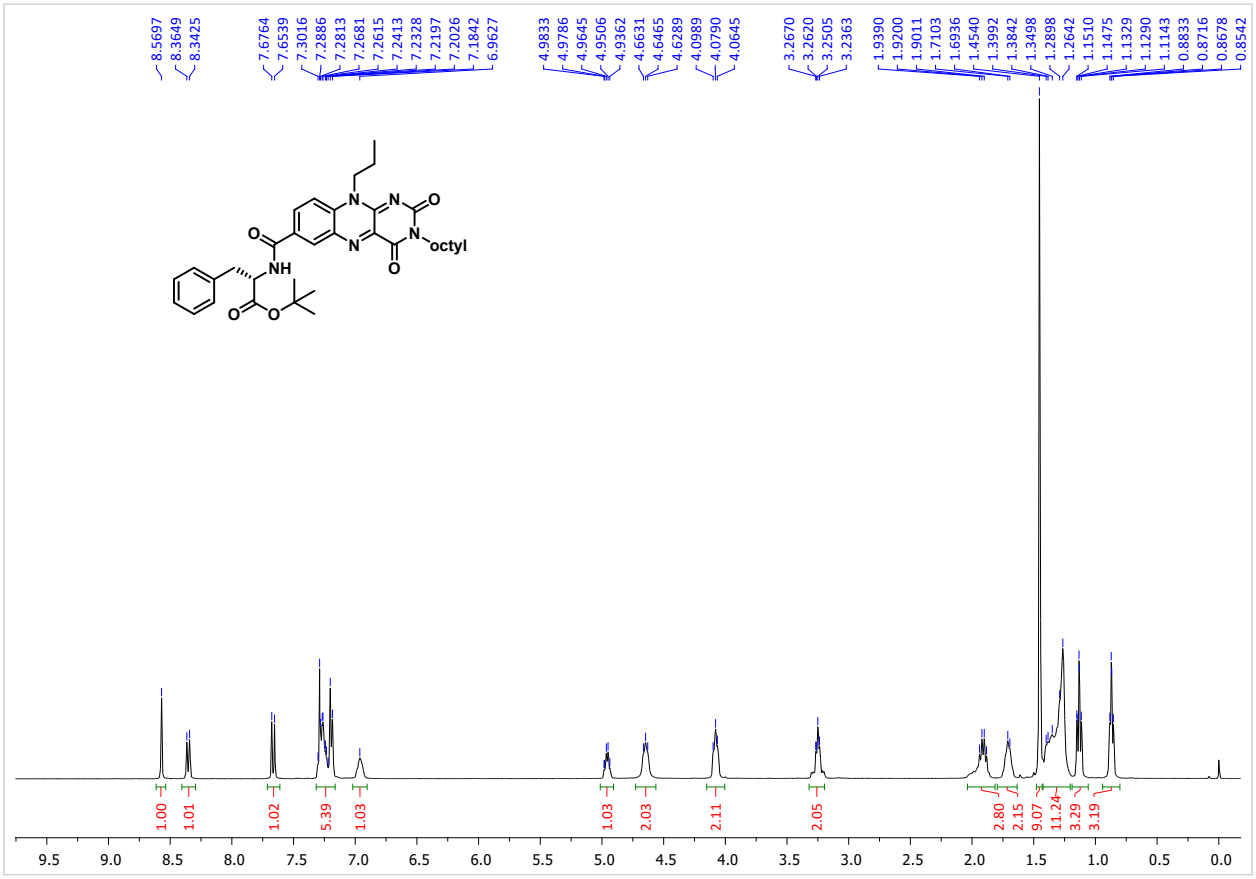


Figure S7. ^{1}H NMR of **1c** in $CDCl_3$

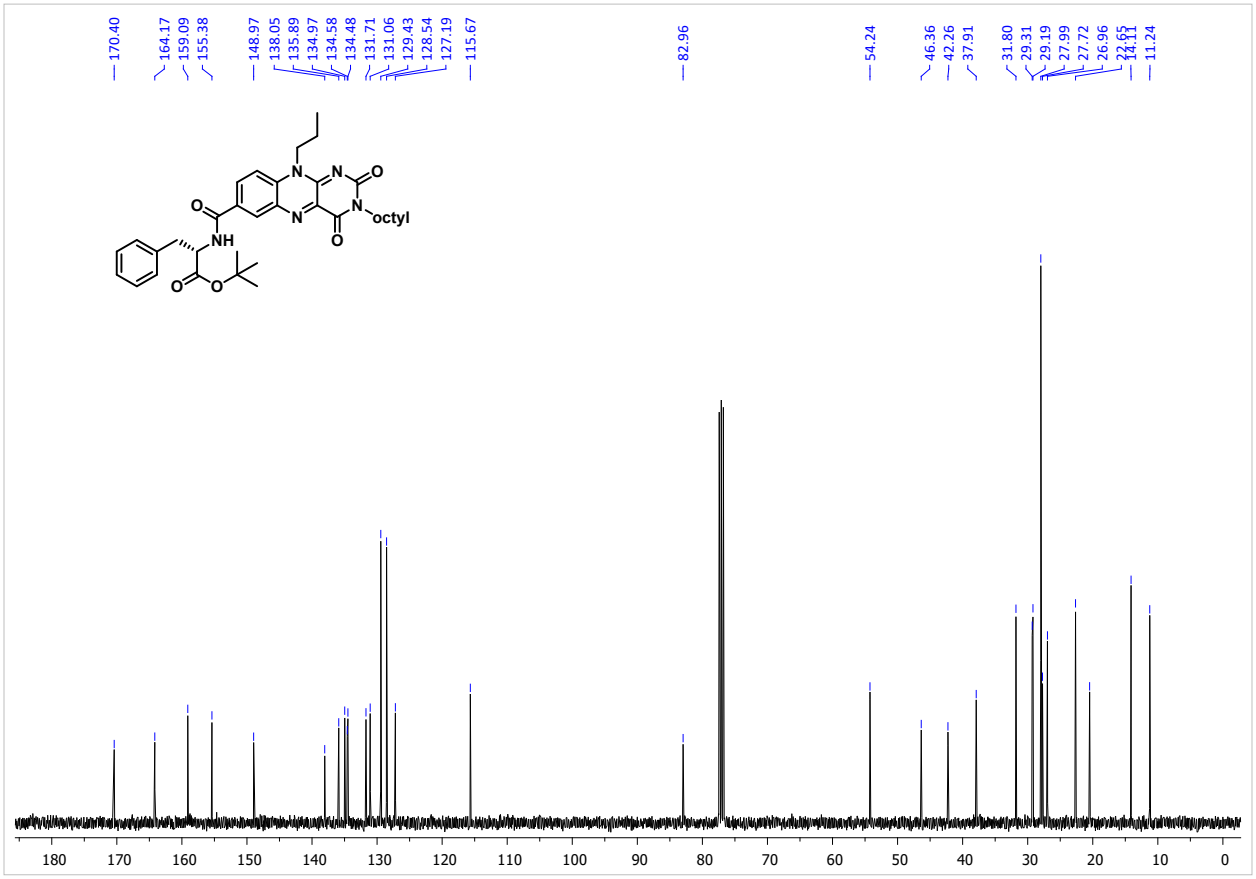


Figure S8. ^{13}C NMR of **1c** in $CDCl_3$

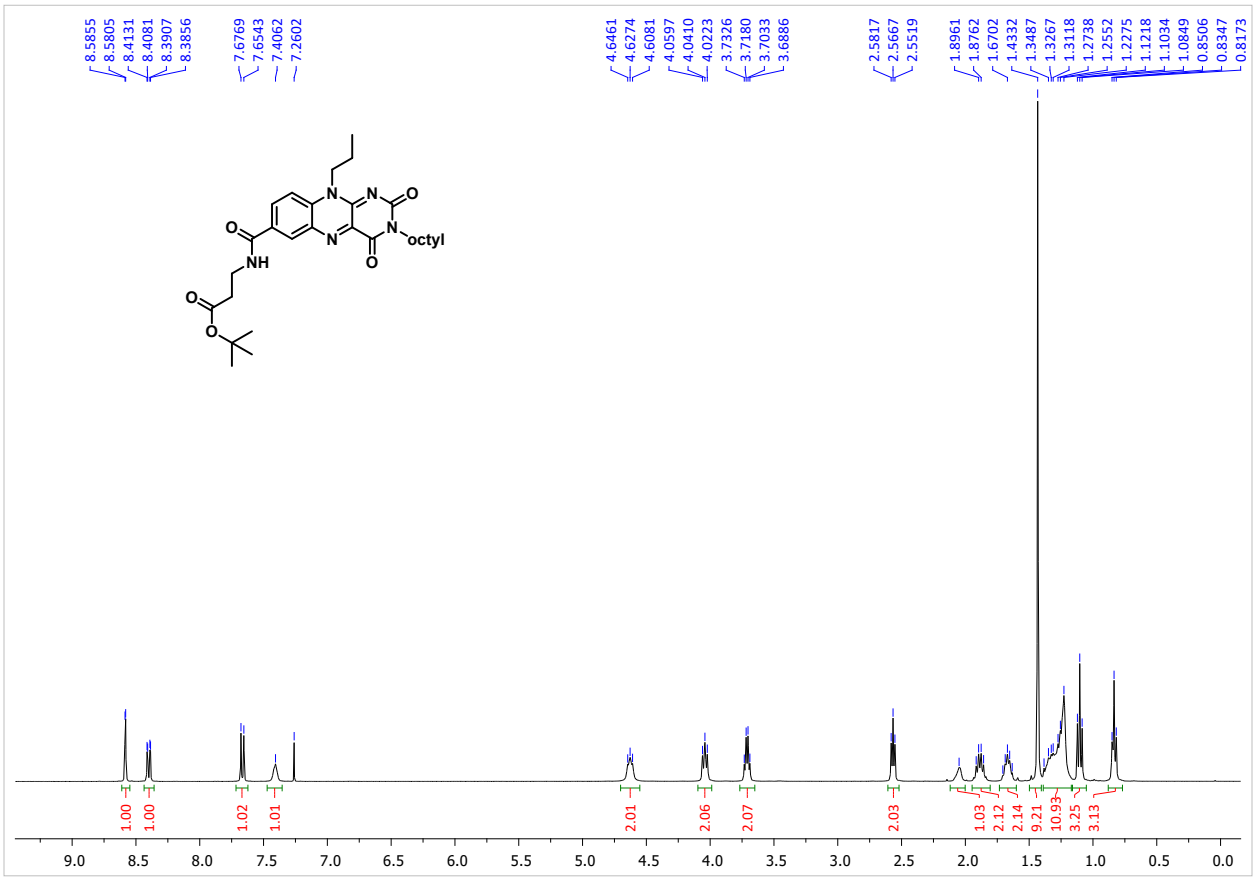


Figure S9. ^{1}H NMR of **1d** in $CDCl_3$

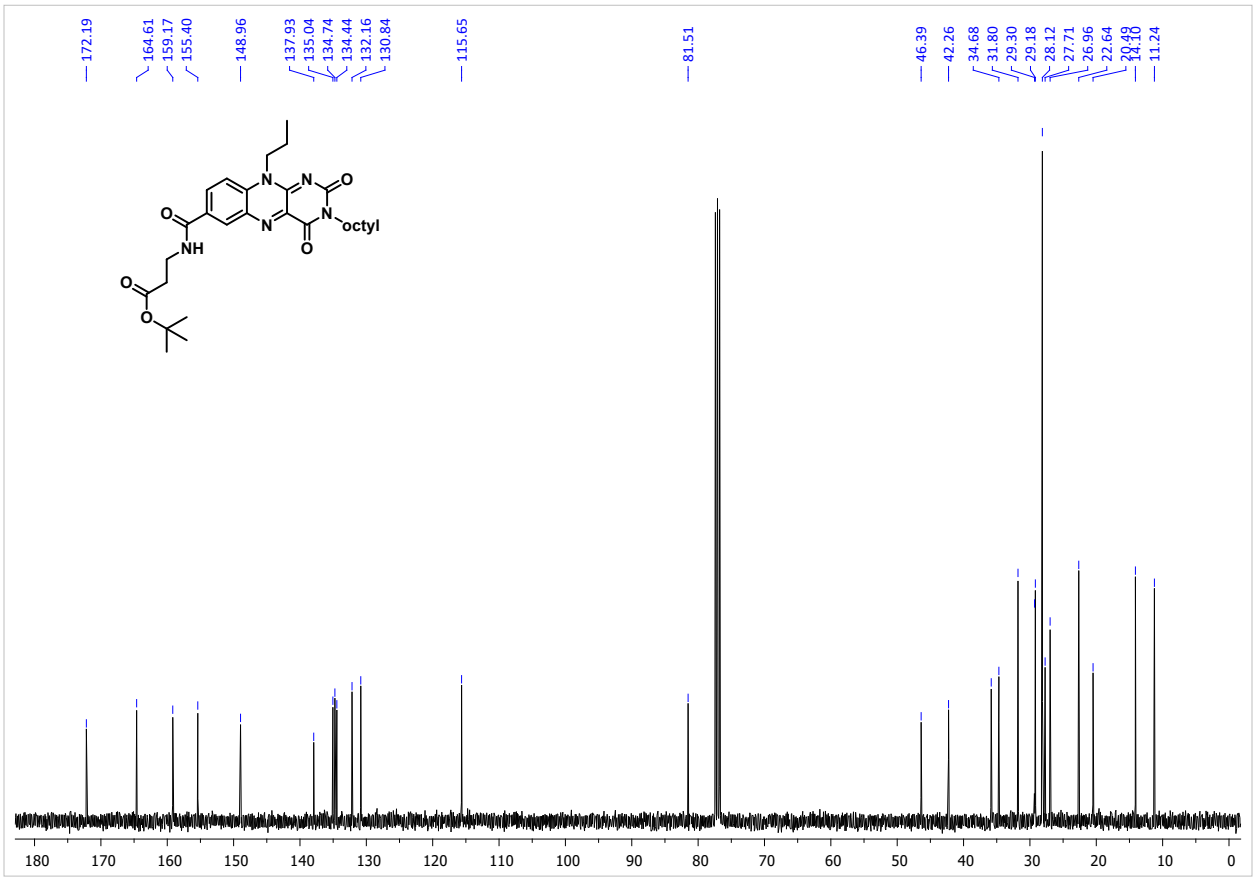


Figure S10. ^{13}C NMR of **1d** in $CDCl_3$

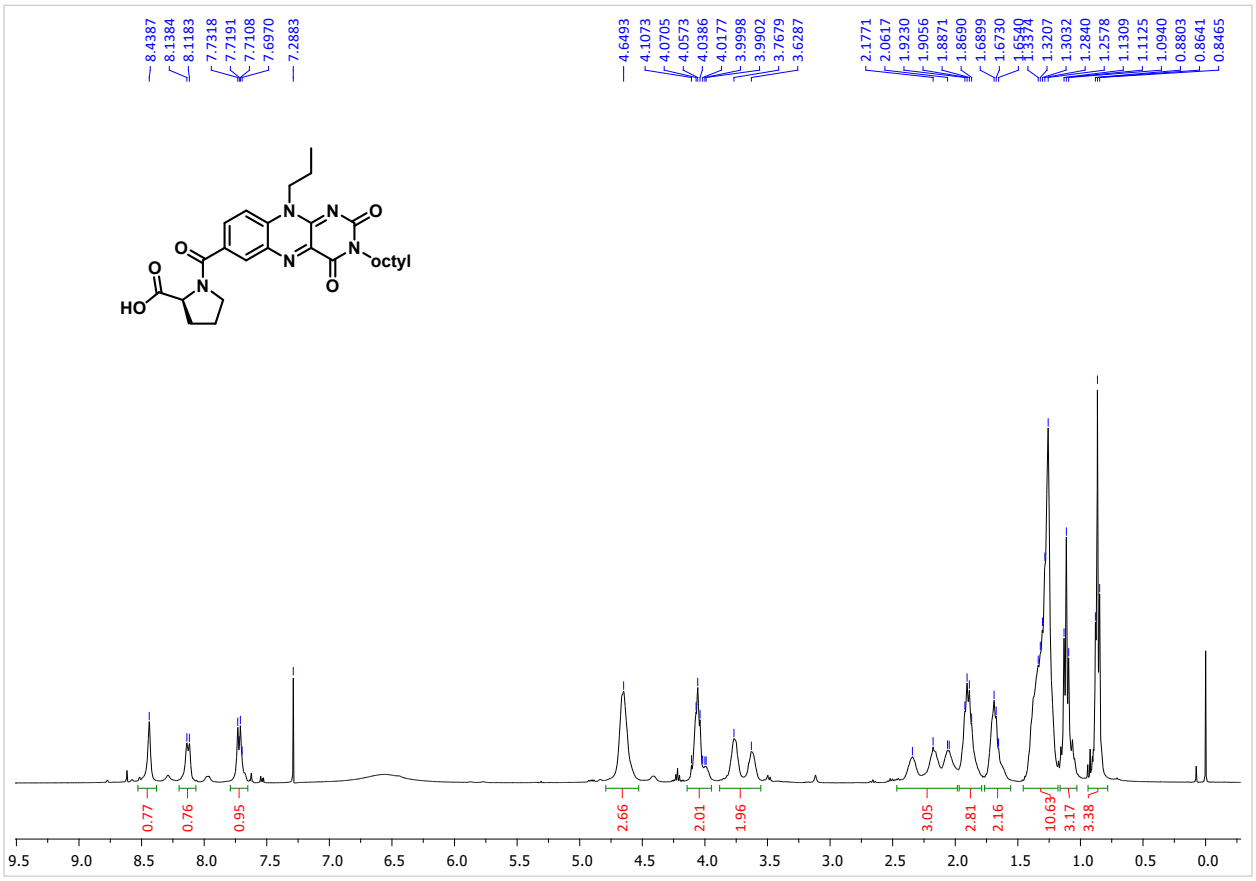


Figure S11. ^{1}H NMR of **Fl-P** in $CDCl_3$

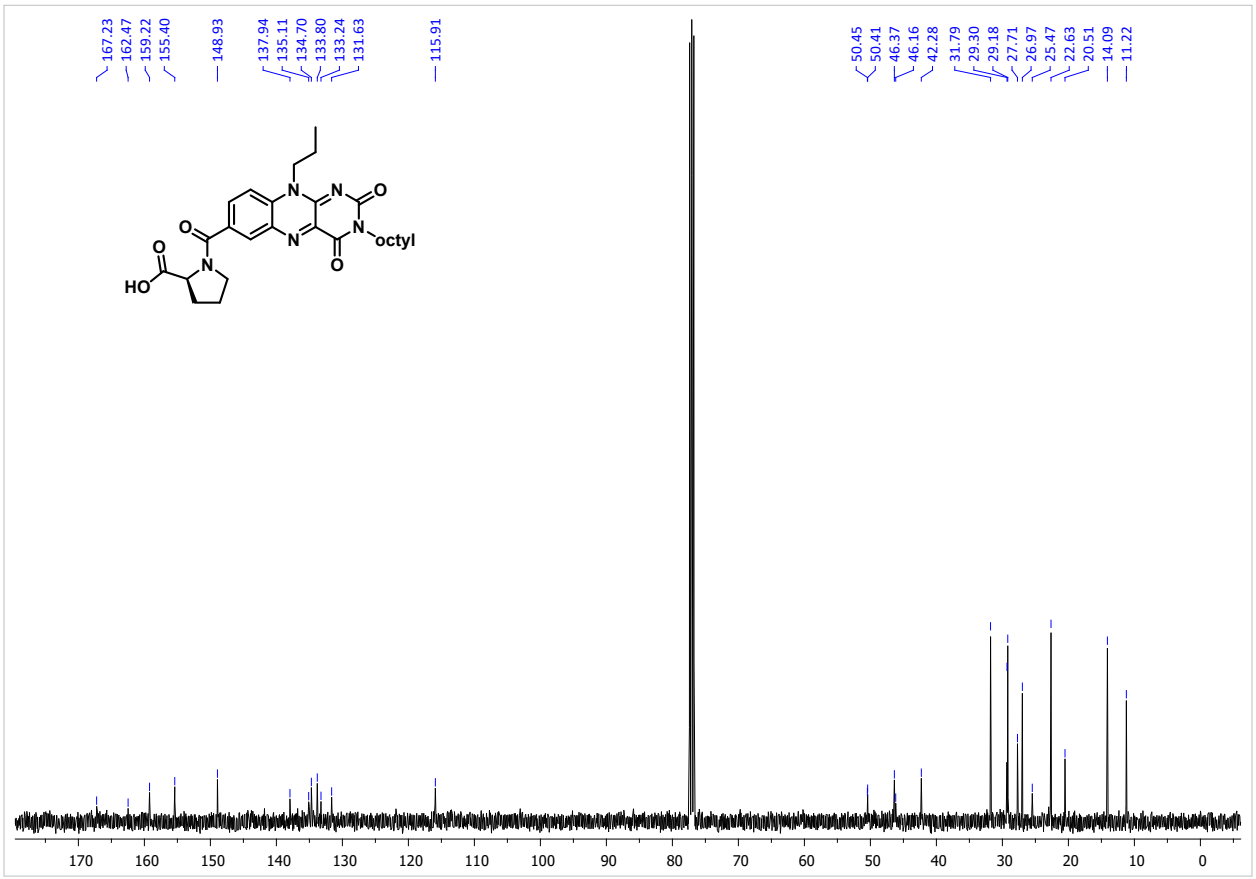


Figure S12. ^{13}C NMR of **Fl-P** in $CDCl_3$

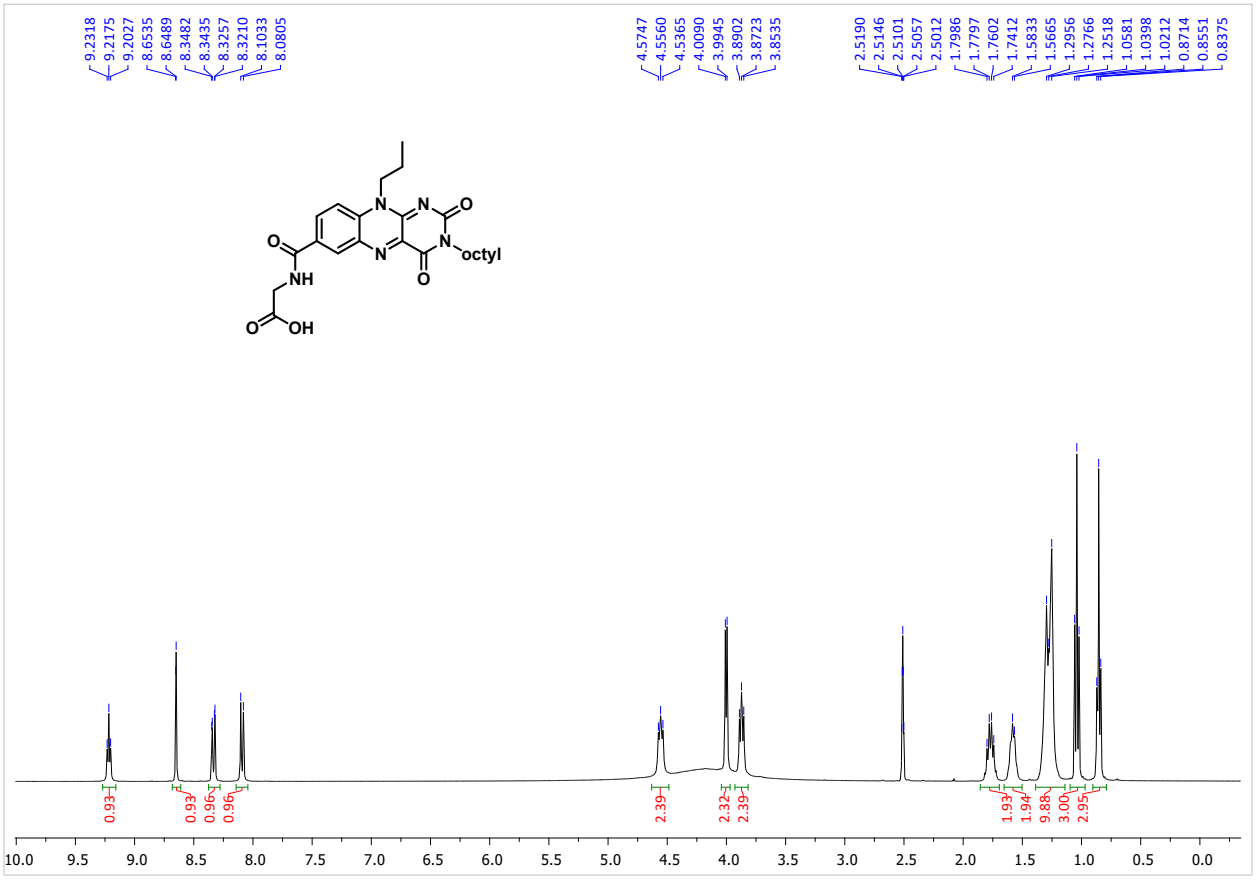


Figure S13. ^{1}H NMR of **Fl-G** in DMSO-d_6

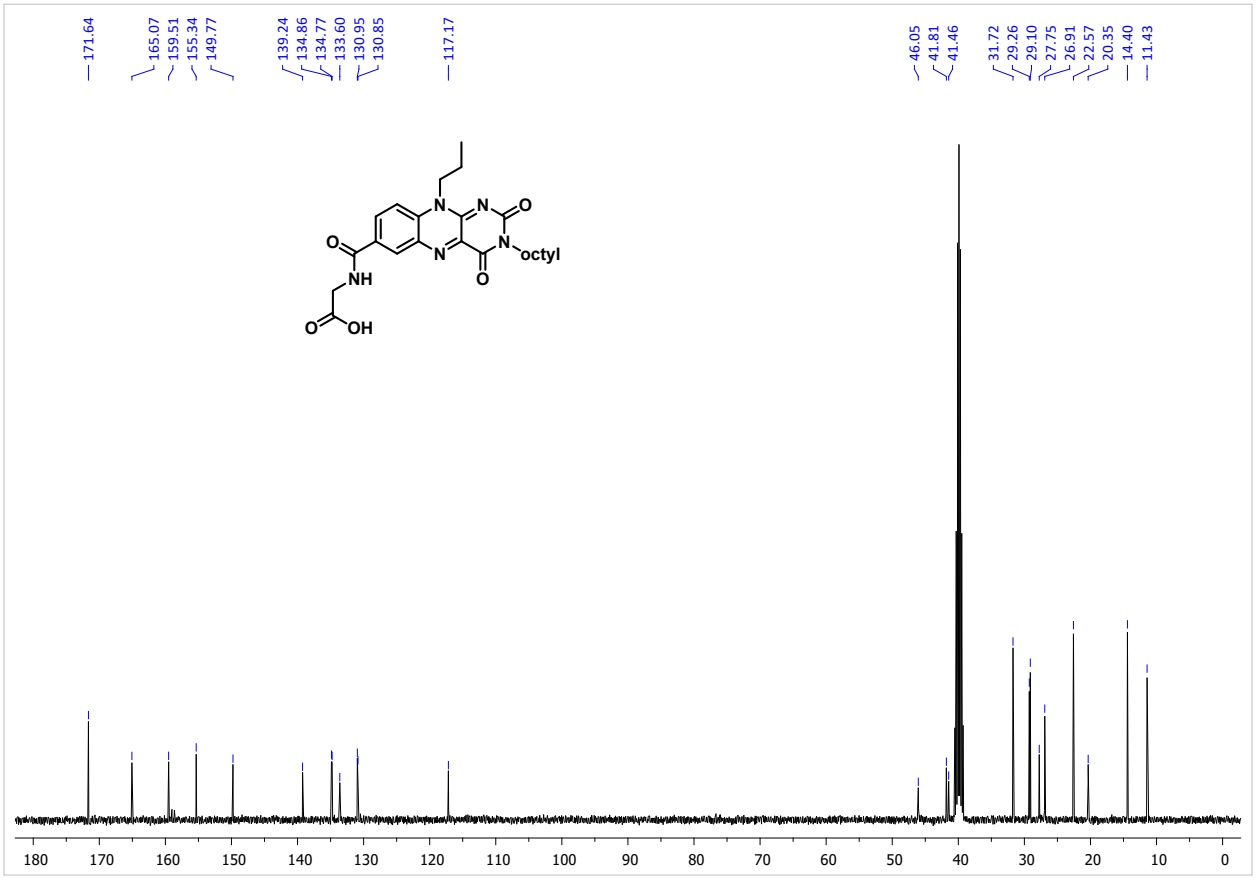


Figure S14. ^{13}C NMR of **Fl-G** in DMSO-d_6

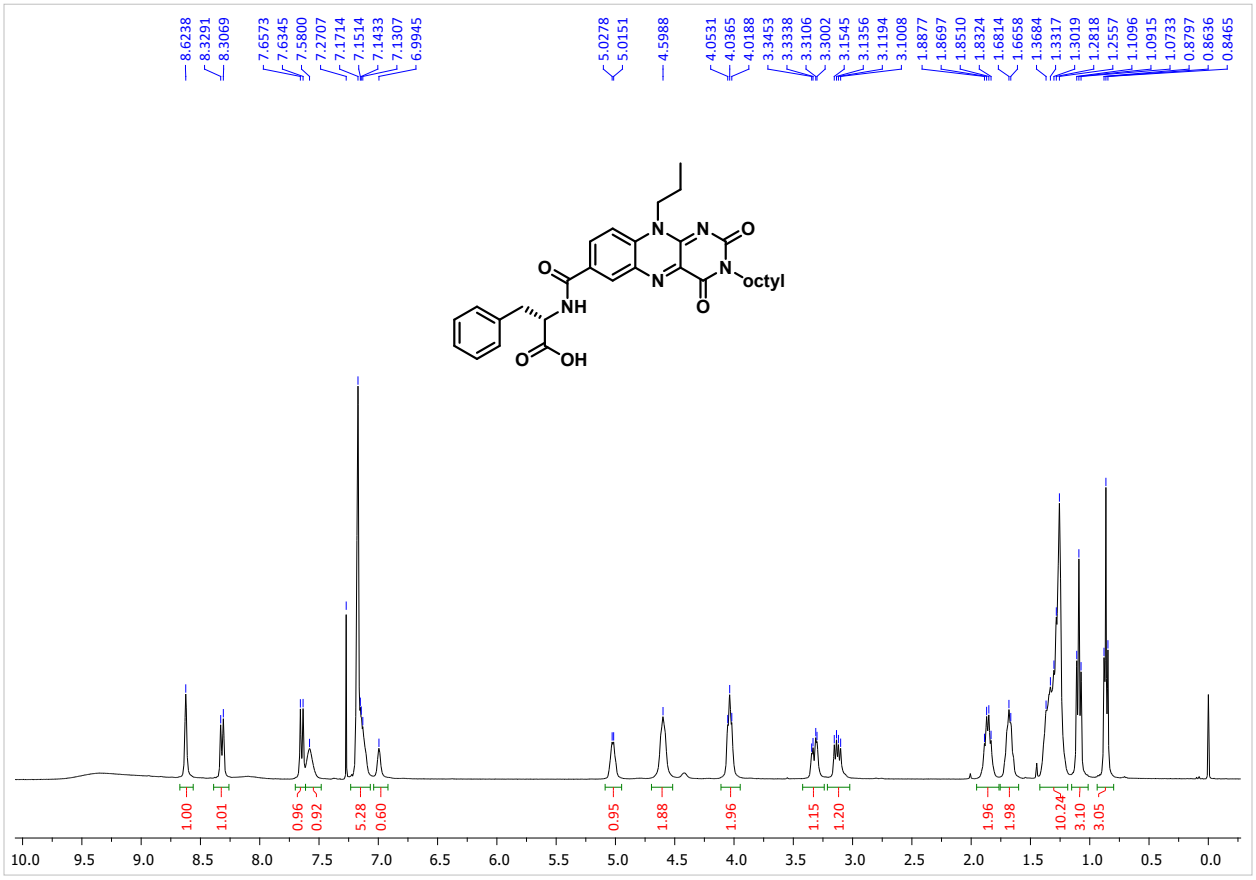


Figure S15. ^{1}H NMR of **Fl-F** in $CDCl_3$

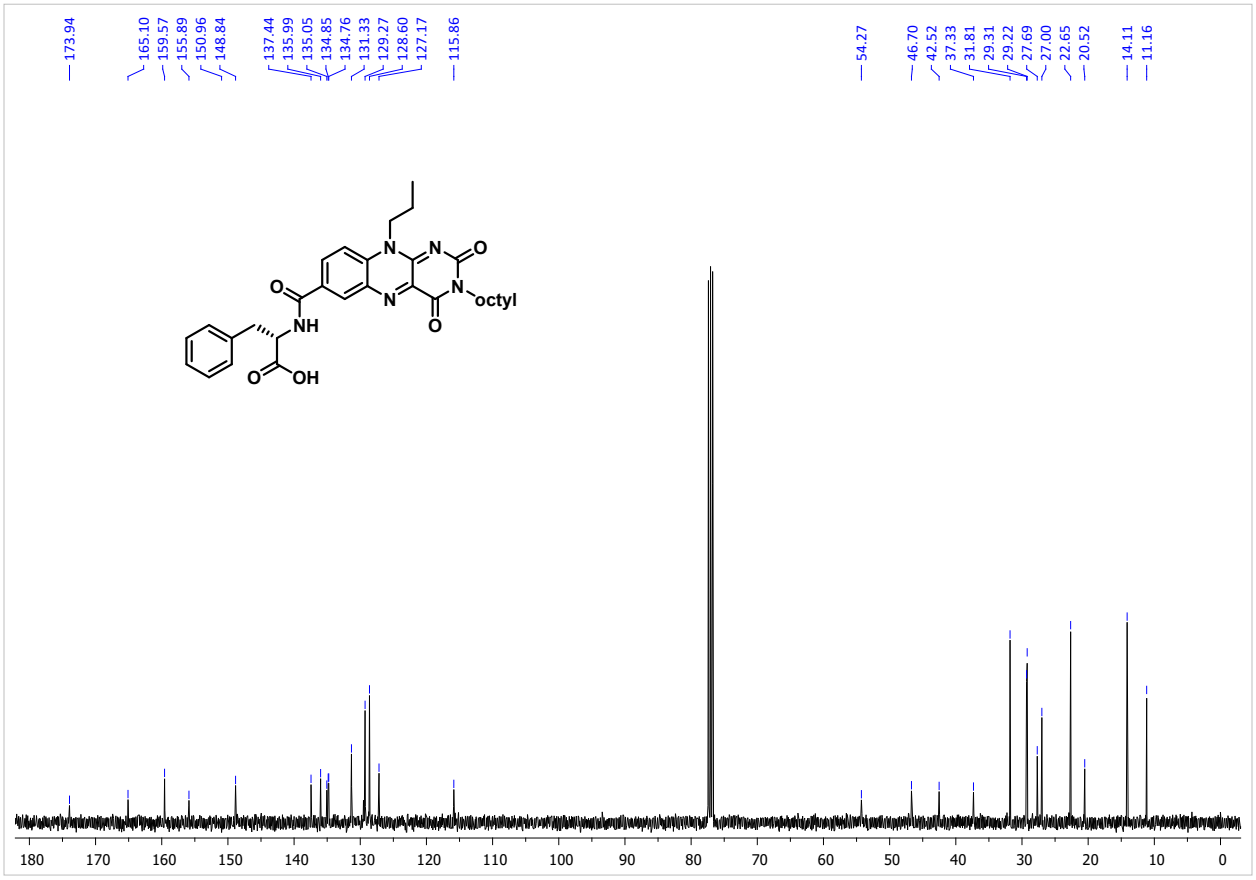


Figure S16. ^{13}C NMR of **Fl-F** in $CDCl_3$

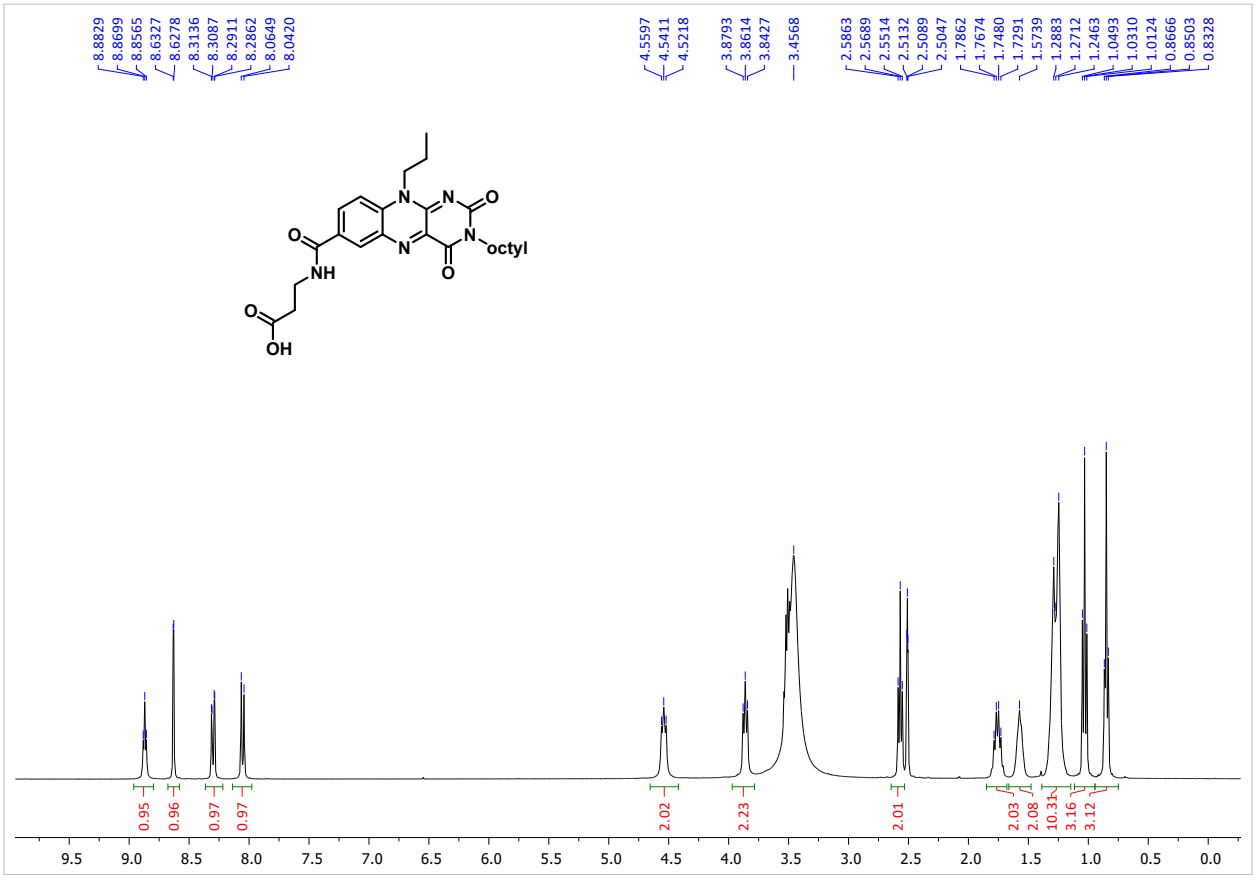


Figure S17. ^{1}H NMR of **Fl-βA** in DMSO-d_6

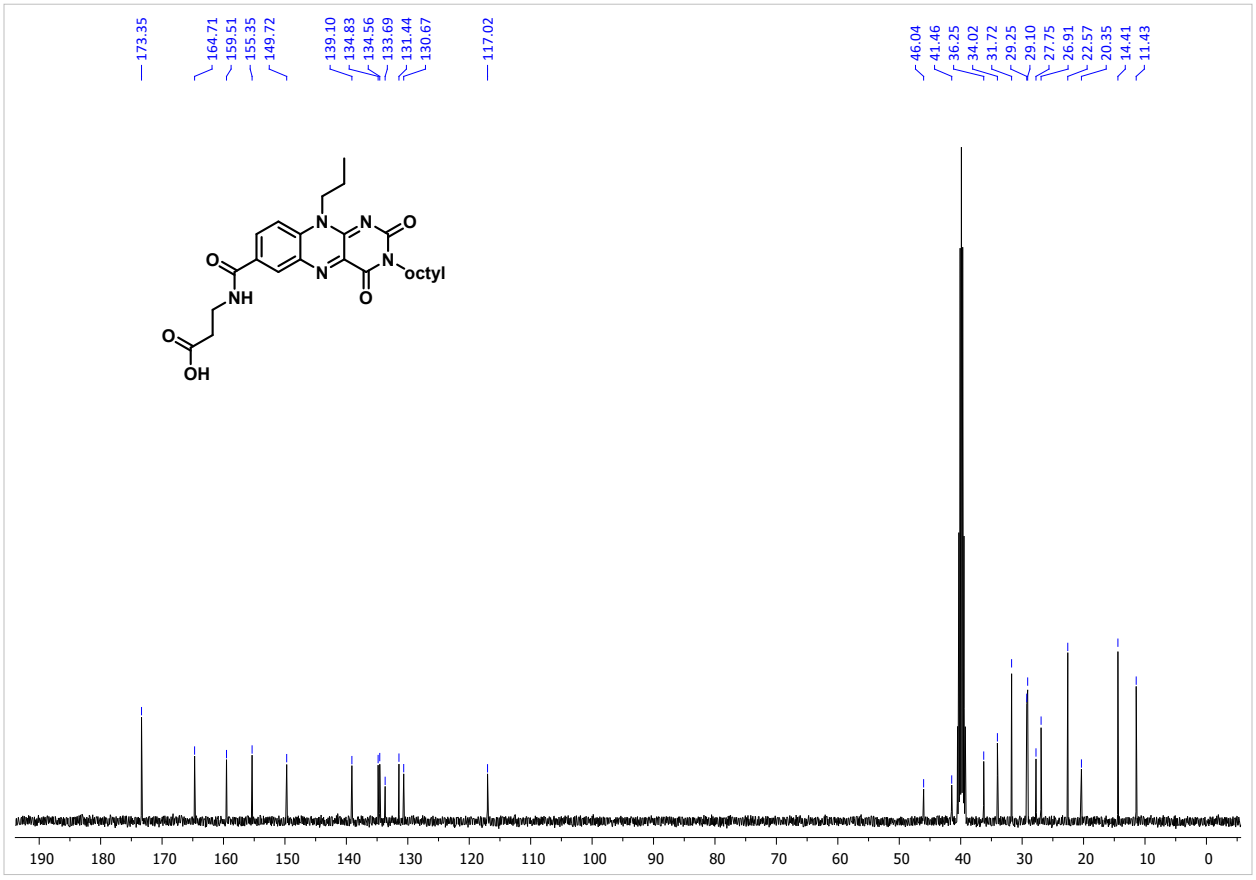


Figure S18. ^{13}C NMR of **Fl-βA** in DMSO-d_6

5. List of HRMS spectra

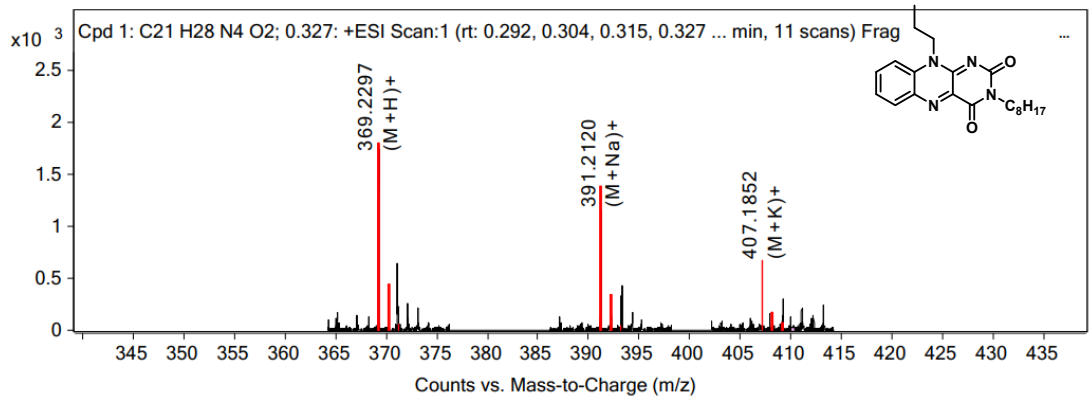


Figure S19. HRMS spectra of **Fl**

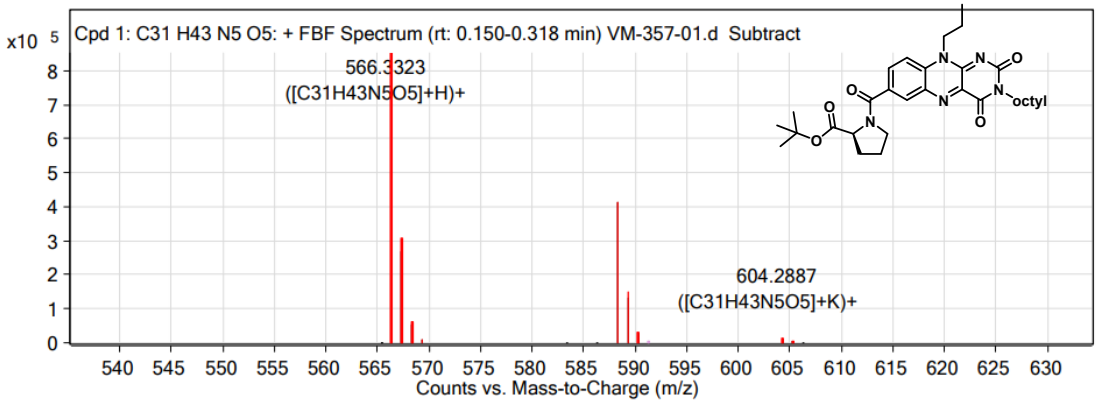


Figure S20. HRMS spectra of **1a**

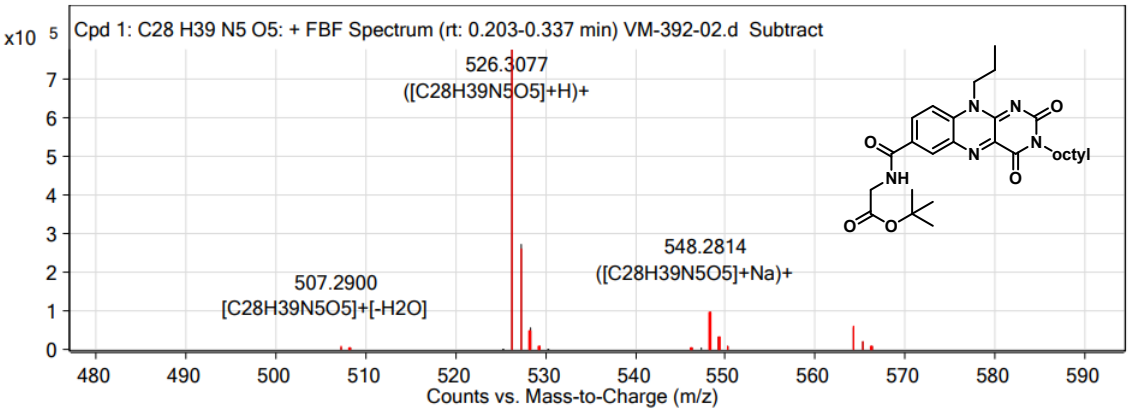


Figure S21. HRMS spectra of **1b**

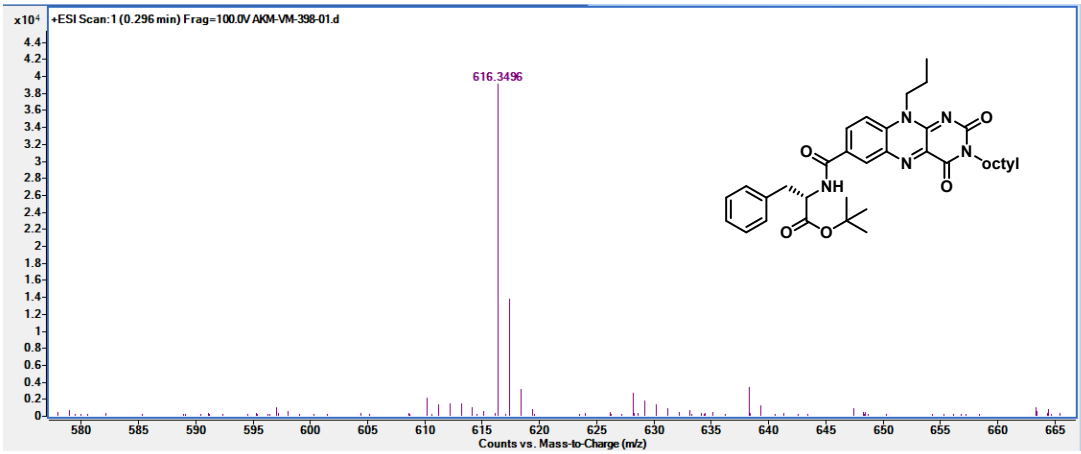


Figure S22. HRMS spectra of **1c**

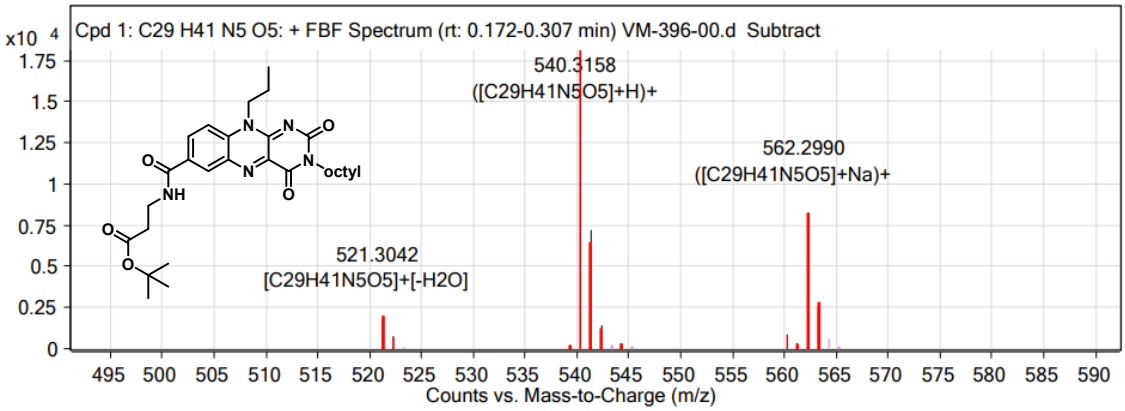


Figure S23. HRMS spectra of **1d**

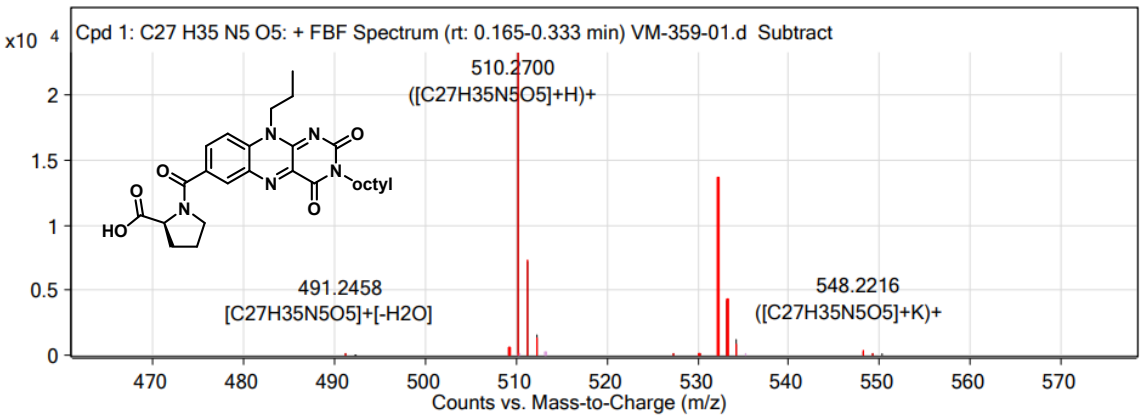


Figure S24. HRMS spectra of **Fl-P**

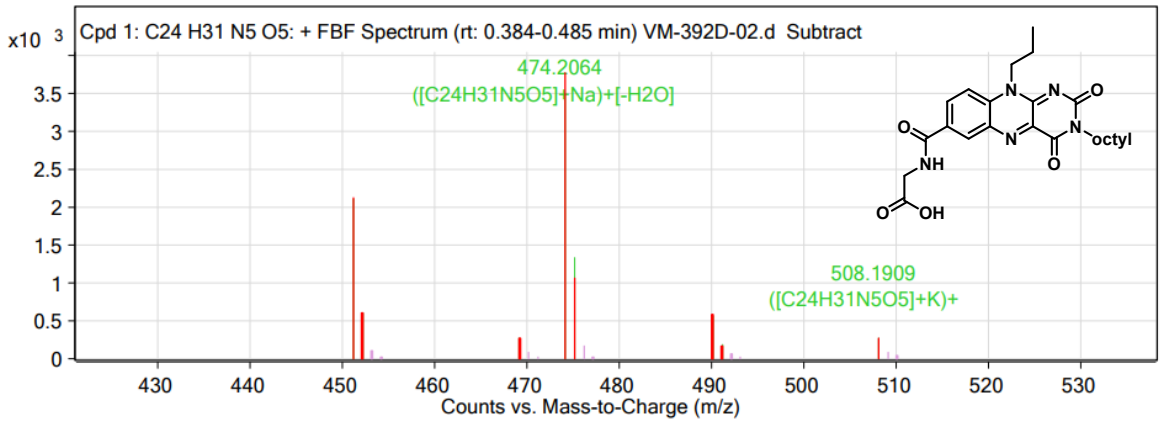


Figure S25. HRMS spectra of **Fl-G**

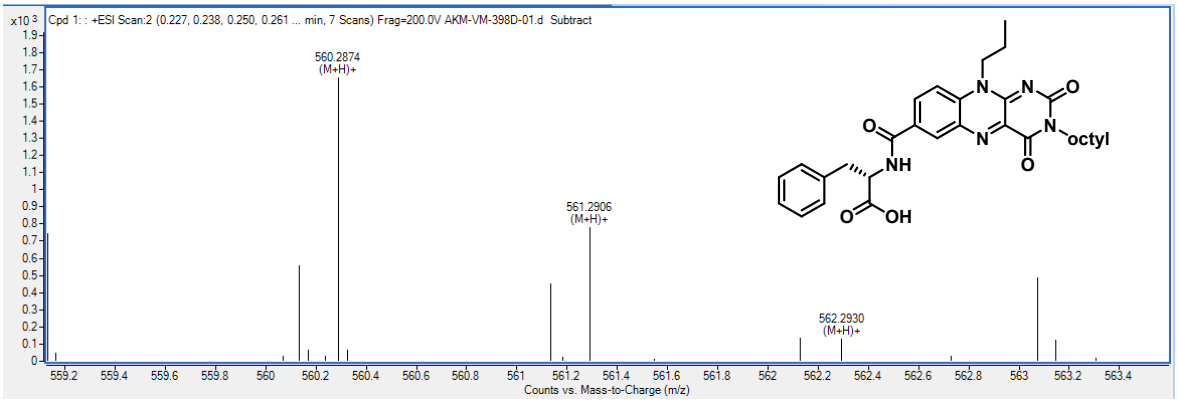


Figure S26. HRMS spectra of **Fl-F**

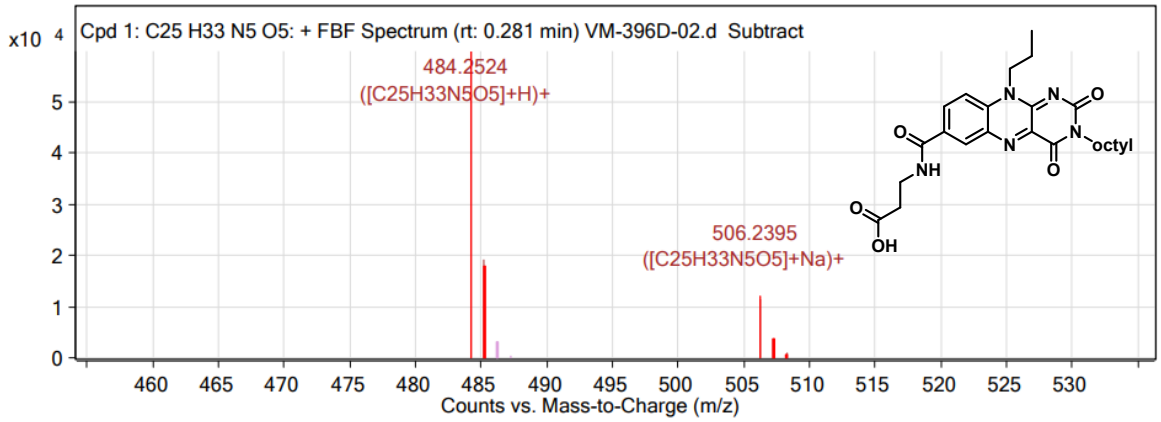


Figure S27. HRMS spectra of **Fl-βA**

6. Computational Methodology

Conformational Analysis:

First, we have performed the conformational search analysis using xTB CREST[4] software package. The key procedure implemented in CREST is a conformational search workflow abbreviated as iMTD-GC. The iMTD-GC workflow generates conformer/rotamer ensembles (CREs) by extensive meta-dynamic sampling (MTD) based on an additional genetic z-matrix crossing (GC) step at the end. CRE are the thermally accessible ensemble of minimum-energy structures consisting of conformers as well as rotamers. The energy window was set to 10 kJ/mol, and we have obtained 7 conformers for **Flc**, 10 conformers for **Fl-βA**, 1 conformer for **Fl-G**, 10 conformers for **Fl-P,** and only 3 conformers for **Fl-F**. Interestingly, for the **Fl-G,** we have only one single conformer with a strong hydrogen bond. To further check the other possible structures for **Fl-G** species, we have increased the energy window to 20 kJ/mole, and conformational analysis suggests the formation of only one stable conformer for **Fl-G**. In the next step, we have optimized the geometry using DFT methods to get the precise energy ordering of all the conformers of **Flc, Fl-βA, Fl-G, Fl-P and Fl-F** complexes.

DFT calculations:

All the geometry optimization was carried out using ORCA 4.2.1[5] code. The geometry optimization was carried out using hybrid functional B3LYP[6] and triple-zeta split valence basis set def2-TZVP[7] for all atoms along with Grimme's atom-pairwise correction approach (D3BJ)[8] as implemented in the ORCA code. Solvent effects were incorporated by CPCM model (2,2,2-Trifluoroethanol) during the geometry optimization. Vibrational frequency was calculated at the same level of the theory on all the optimized geometries to characterize them as local minima having no imaginary frequencies. Resolution of identity approximation with chain of the spheres (RIJCOSX) was used for fast calculation. A large integration grid setting (grid6) is used for all atoms. All the thermodynamic parameters were computed at 298.15K. It is important to note here that the amino acid linked flavins were able to form bonds efficiently in the solution optimized structures, while the gas phase optimization led to the detachment of the -COO group. This indicates the importance of the solution phase in stabilizing these intermediates. The conformers obtained from CREST were further optimized on DFT and filtered within the energy window of

10kJ /mol upon which we have obtained 7 conformers for **Flc,** 8 conformers for **Fl-βA,** 1 conformer for **Fl-G**, 5 conformers for **Fl-P,** and 2 conformers for **Fl-F**. NBO analysis was carried out on the lowest energy structure to understand the electronic structure and nature of hydrogen bonding (see Figure S33)

To further probe the nature of hydrogen bonding interactions non-covalent interaction (NCI)[9] analysis has been carried out using Multiwfn code[10] where the Molden file has been take from the converged DFT calculations. Both the NCI scatter plot and reduced density gradient has been generated to analyze the nature of hydrogen bonding interaction in all the lowest energy conformers of **Flc**, **Fl-βA**, **Fl-G**, **Fl-P** and **Fl-F** complexes. on the lowest energy structure of each complex.

QTAIM[11] and ESP[12] analysis were carried out at B3LYP[6] level of theory and all electron TZP basis set for all the atoms using ADF-2021 code[13] (Figure S32 and S29). Various critical points like Bond critical point(BCP), ring critical point (RCP) and atoms critical points are also marked in the Figure S32.

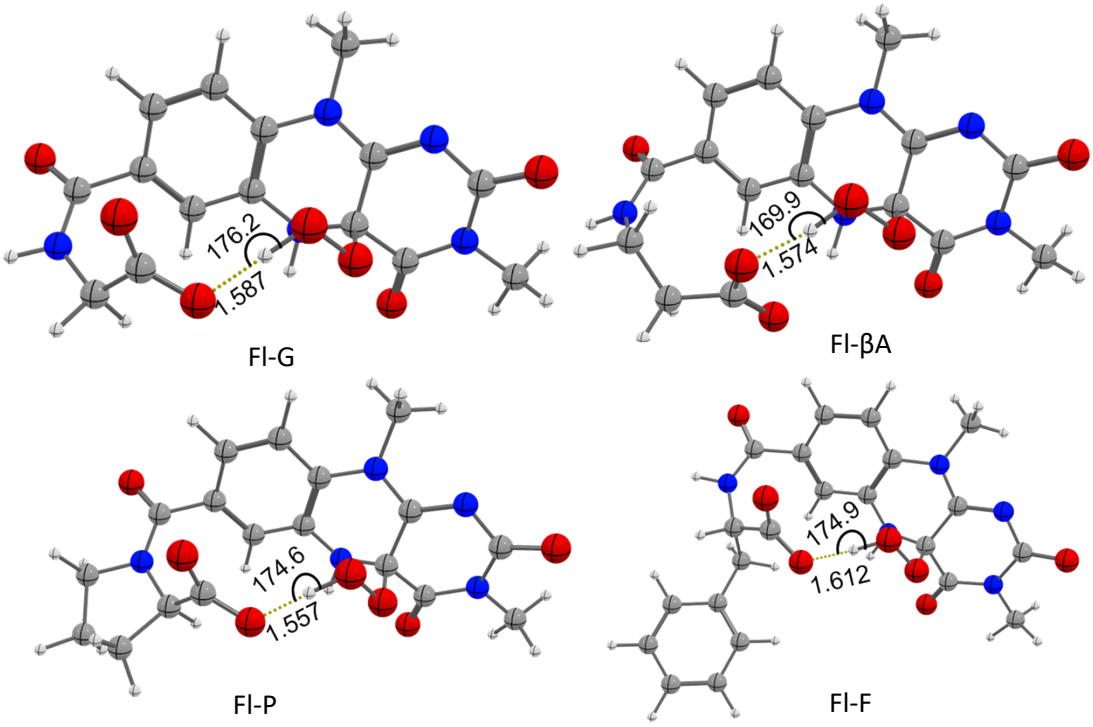


Figure S28: B3LYP/def2-TZVP computed lowest-energy structures with relevant structural parameters for b) Fl-βA c) Fl-G d) Fl-P e) Fl-F (Color code: Red-O; Blue-N; Grey-C; White-H).

Table S1. DFT optimized low-lying conformers along with the absolute SCF electronic energy, enthalpy (H) and Gibbs free energy (G) for the various conformers of amino acid linked flavins. All the values are in kcal/mol (absolute value).

Species	SCF Electronic Energy (kcal/mol)	H (kcal/mol)	G (kcal/mol)
Flc			
Conformer 1	-735521.73	-735521.13	-735563.76
Conformer 2	-735521.26	-735520.67	-735562.73
Conformer 3	-735522.08	-735521.49	-735562.47
Conformer 4	-735521.27	-735520.68	-735562.99
Conformer 5	-735521.08	-735520.49	-735562.84
Conformer 6	-735521.53	-735520.93	-735563.12
Conformer 7	-735521.40	-735520.81	-735562.60
Fl-βA			
Conformer 1	-890659.00	-890658.41	-890706.58
Conformer 2	-890658.81	-890658.22	-890705.83
Conformer 3	-890657.29	-890656.70	-890704.08
Conformer 4	-890657.82	-890657.23	-890705.01
Conformer 5	-890658.17	-890657.58	-890704.94
Conformer 6	-890658.58	-890657.99	-890704.27
Conformer 7	-890659.58	-890658.98	-890706.46
Conformer 10	-890660.21	-890659.61	-890706.09
Fl-G			
Conformer 1	-866011.25	-866010.65	-866056.42
Fl-P			
Conformer 1	-939204.18	-939203.59	-939252.06
Conformer 2	-939202.30	-939201.71	-939250.41
Conformer 3	-939201.78	-939201.19	-939250.09
Conformer 4	-939202.36	-939201.77	-939250.81
Conformer 5	-939202.71	-939202.12	-939251.03
Fl-F			
Conformer 1	-1035561.97	-1035561.38	-1035613.65
Conformer 2	-1035558.27	-1035557.68	-1035612.87

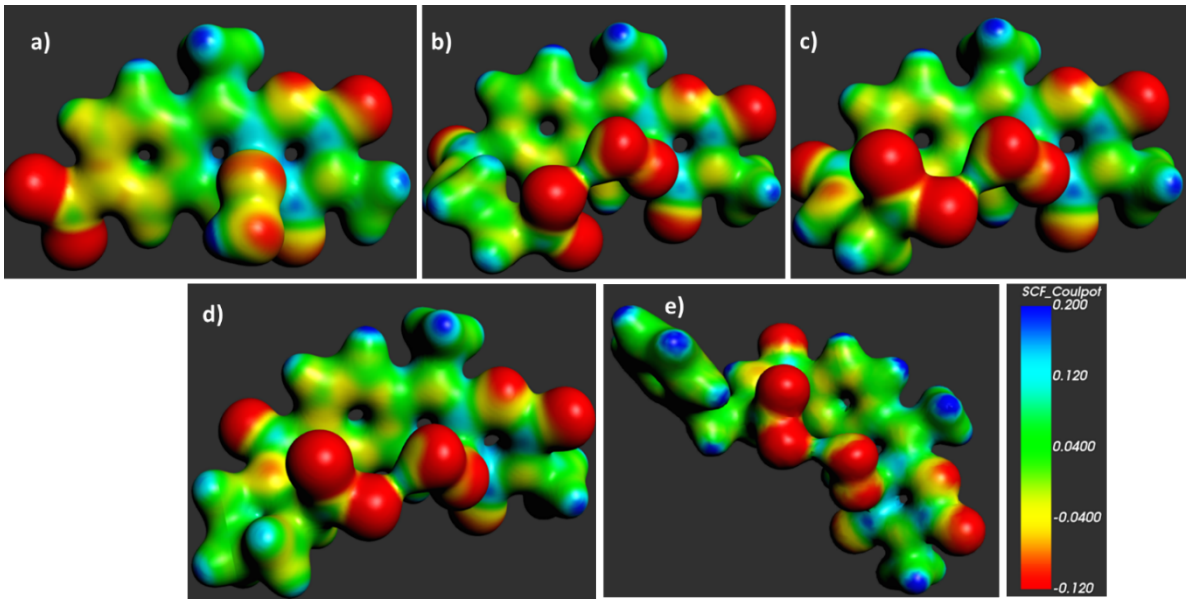


Figure S29. DFT-computed molecular electrostatic potential maps a) Flc b) Fl-βA c) Fl-G d) Fl-P e) Fl-F. The red and blue color represents the most electronegative and electropositive regions, respectively.

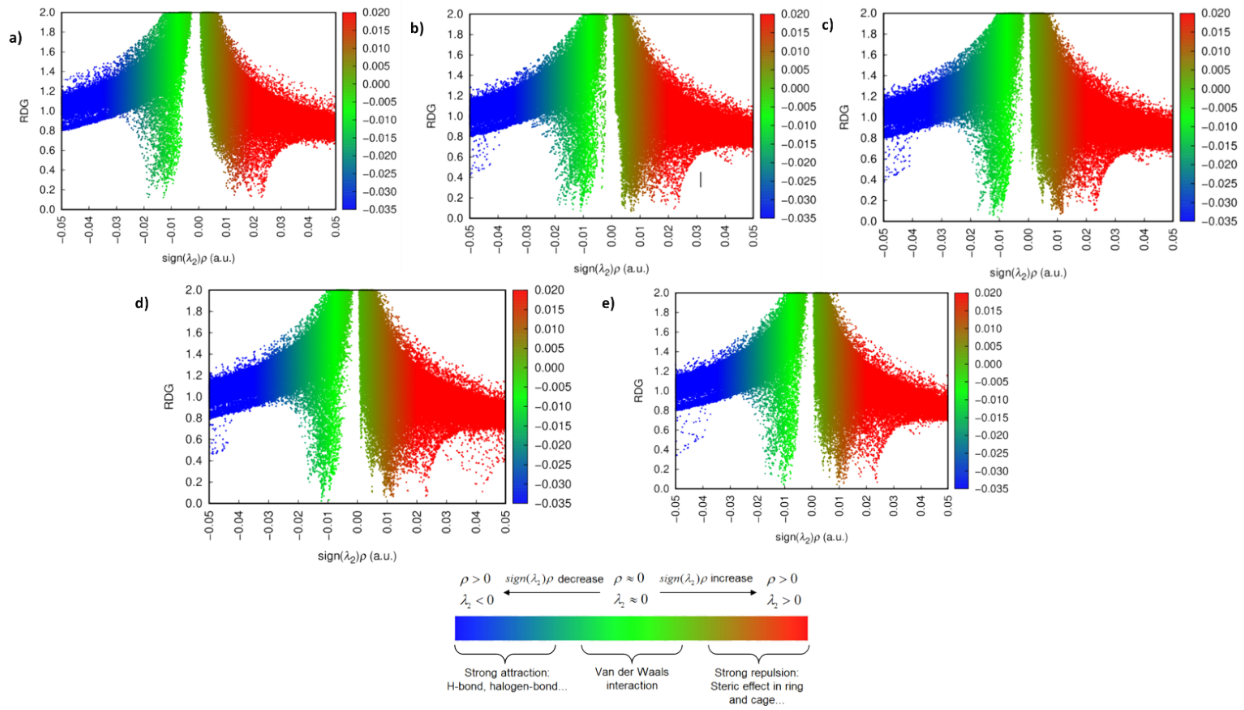


Figure S30. Non-covalent interaction (NCI) scatter diagram for a) Flc b) Fl-βA c) Fl-G d) Fl-P e) Fl-F.

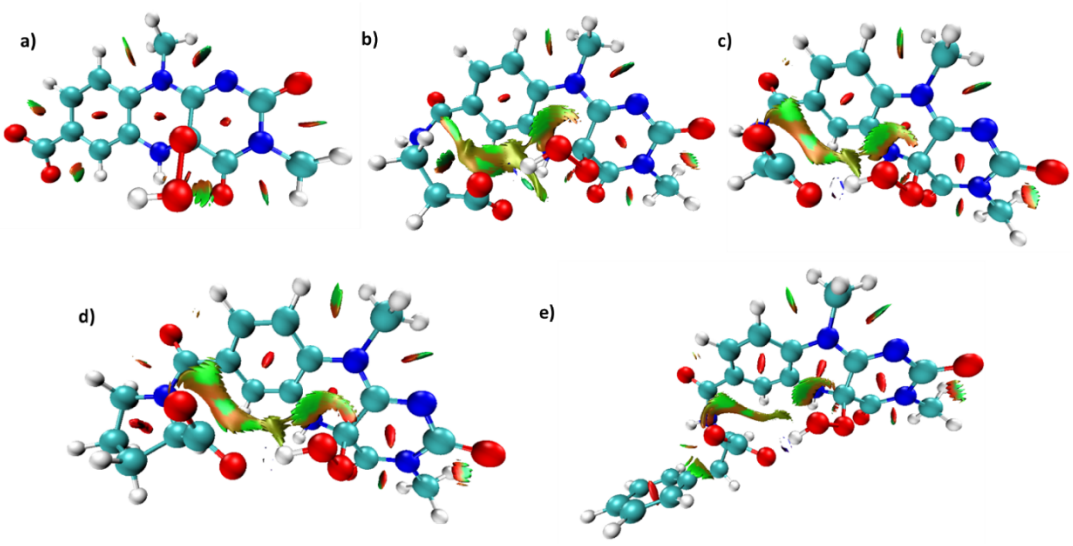


Figure S31. Reduced density gradient (RDG) analysis for a) Flc b) Fl-βA c) Fl-G d) Fl-P e) Fl-F.

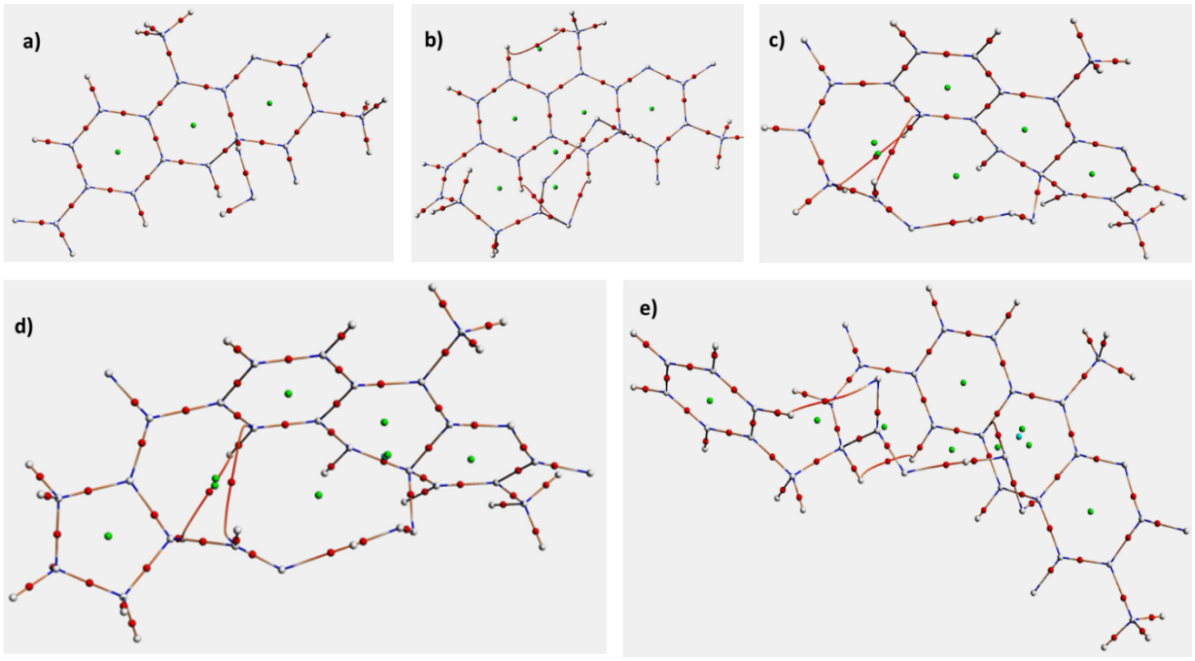


Figure S32. QTAIM topology for a) Flc b) Fl-βA c) Fl-G d) Fl-P e) Fl-F. Here white points represent the atom critical point, green point represents the ring critical point, red point represents the bond critical point.

Table S2. QTAIM Parameters (in a.u.) Corresponding to the H···O bcp, the Electron Density at H···O bcp, ρ_{bcp}, its Laplacian, $\nabla^2\rho_{bcp}$, the Total Electron Energy Density at bcp, H_{bcp}, and the Components of the Latter Value; the Kinetic Electron Energy Density, G_{bcp}, the Potential Electron energy density V_{bcp}

Species	ρbcp	∇^2ρbcp	G_{bcp}	V_{bcp}	H_{bcp}
Fl-βA	0.060	0.135	0.049	-0.065	-0.015
Fl-G	0.062	0.137	0.051	-0.068	-0.017
Fl-P	0.064	0.140	0.053	-0.071	-0.018
Fl-F	0.057	0.131	0.046	-0.060	-0.013

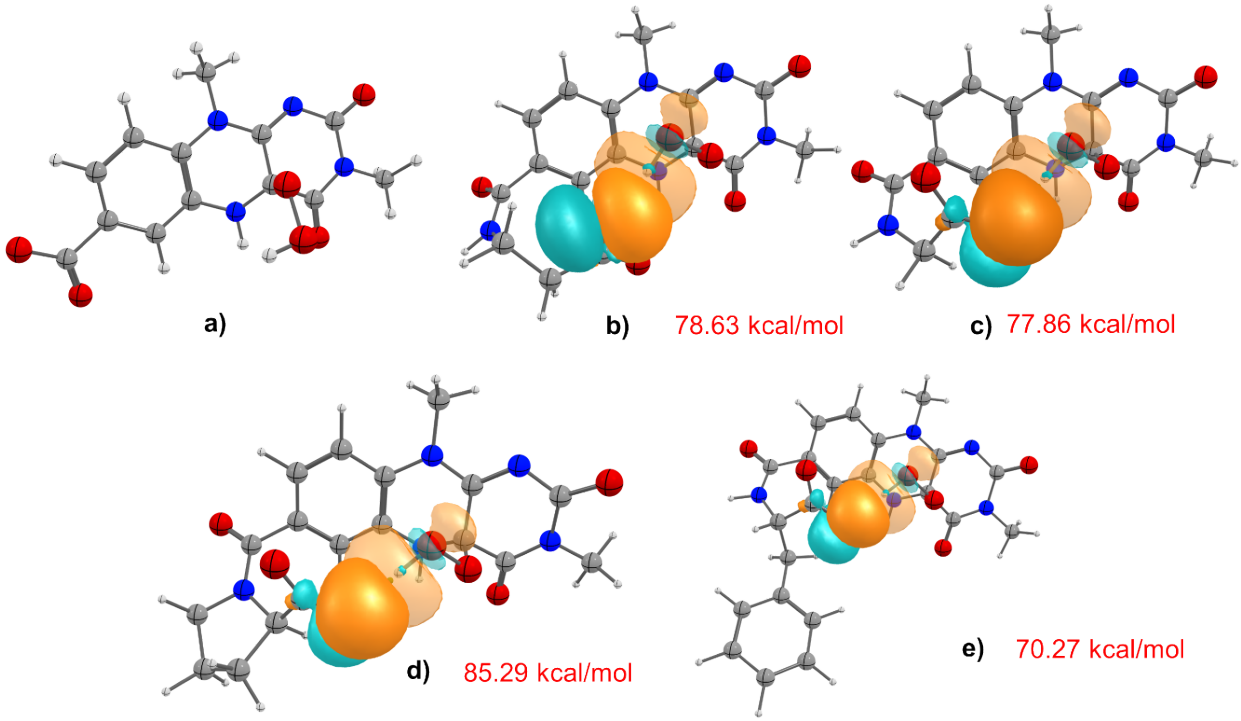


Figure S33. NBO computed Second order perturbation donor acceptor interaction representing the strength of the hydrogen bonds in a) Flc b) Fl-βA c) Fl-G d) Fl-P e) Fl-F. The dark lobes denote the donor orbital (O;2p_z) while the transparent ones represent the acceptor orbital (predominantly H;1s).

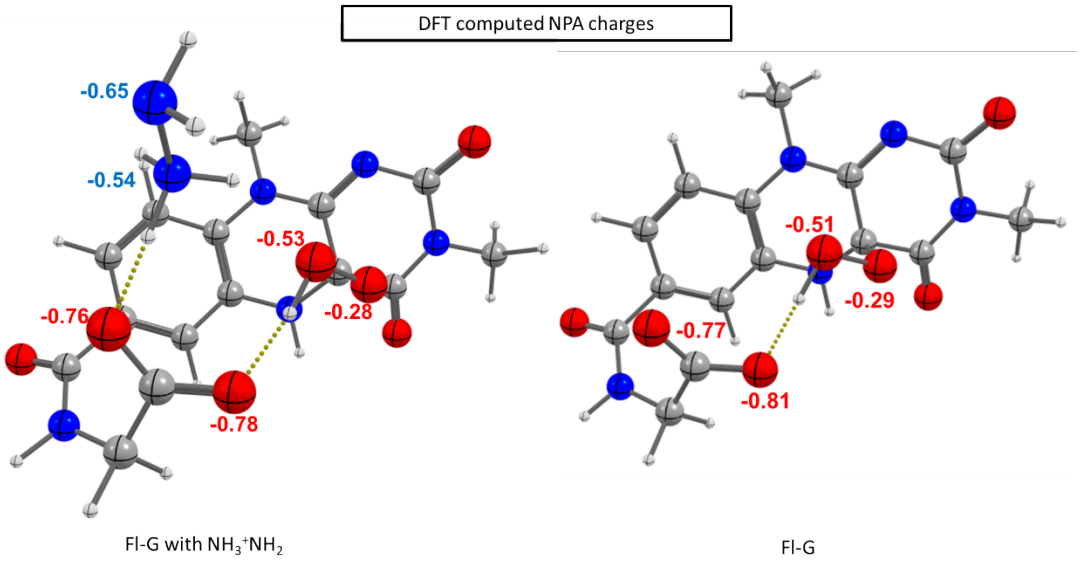


Figure S34. DFT computed NPA charges analysis.

Table S3: DFT optimized structure of low-lying conformers for the flavin linked amino acid complexes. All coordinates are expressed in Å. The lowest lying conformers are marked in bold.

XYZ Coordinates			
Atom	X	Y	Z
Flc			
Conformer 1 G = -1172.213159670 Eh H= -1172.145231740 Eh			
N	-0.22823	1.72531	0.43205
O	-3.53006	-0.70055	0.27222

N	-2.18494	-2.54201	0.25589
N	-1.14488	-0.43753	-0.16228
N	1.18971	-0.23206	0.25889
O	-1.34005	0.98578	0.29728
C	3.59015	-0.02403	0.09938
C	1.0594	1.16582	0.26485
C	2.44925	-0.81323	0.19692
C	2.53949	-1.89113	0.21791
C	-3.64202	0.70499	0.39518
C	-2.33232	-1.33579	0.17067
H	3.45202	1.36523	0.0645
C	4.33351	1.98359	-0.02924
C	2.20221	1.95832	0.15983
C	2.12044	3.03485	0.15024
H	-0.3375	3.15043	0.76123
C	-0.12938	3.75337	-0.12249
H	0.37459	3.39169	1.5461
C	-4.75756	-1.49465	0.36489
H	-5.13414	-1.49678	1.38751
H	-5.50762	-1.06713	-0.29399
C	-4.53106	-2.5105	0.05758
H	4.9597	-0.6755	0.02171
H	5.03979	-1.89127	0.34048
H	5.92092	0.04396	-0.35479
C	0.10103	-1.99624	0.32228
O	-1.14833	-0.24105	-1.63017
O	-1.00439	-1.51418	-2.28369
H	-0.05249	-1.53951	-2.47896
O	-1.34337	3.35337	1.10751
O	-0.22823	1.72531	0.43205

H	-3.53006	-0.70055	0.27222
H	-2.18494	-2.54201	0.25589
Conformer 2 G = -1172.211517990 Eh H= -1172.144491930 Eh			
N	-2.54708	1.4286	0.10765
O	-4.78039	1.12451	-0.083
N	0.02874	-1.05634	0.36825
N	-0.25885	1.64991	0.29086
N	-3.55821	-0.73785	0.38103
O	-2.22114	-2.5416	0.74194
C	-1.17794	-0.57653	-0.15252
C	1.17894	-0.29063	0.24772
C	-1.3541	0.89859	0.10657
C	3.58016	-0.06867	0.09774
C	1.0401	1.10441	0.20445
C	2.44395	-0.8634	0.21094
H	2.54288	-1.93955	0.25973
C	-3.66563	0.65243	0.09728
C	-2.36636	-1.38095	0.40183
C	3.43344	1.31813	0.03076
H	4.31123	1.94045	-0.07127
C	2.17748	1.90325	0.09441
H	2.08772	2.97827	0.04601
C	-0.40221	3.0877	0.54221
H	-0.23743	3.65149	-0.37606
H	0.32421	3.38729	1.29237
C	-4.76458	-1.51828	0.67113
H	-4.71012	-2.46764	0.14307

H	-4.84824	-1.70696	1.74178
H	-5.62429	-0.95432	0.32898
C	4.95371	-0.71288	0.02914
O	5.91225	0.00969	-0.34868
O	5.04048	-1.92719	0.35239
H	0.12564	-2.06222	0.39489
O	-1.3832	-0.83207	-1.58344
O	-0.49667	0.01115	-2.34808
H	0.22774	-0.59871	-2.56712
Conformer 3 G = -1172.211106340 Eh H= -1172.145798520 Eh			
N	-2.53022	1.50195	0.43208
O	-4.76532	1.2129	0.30767
N	0.01901	-0.98486	0.32783
N	-0.22947	1.73114	0.41167
N	-3.53081	-0.6862	0.29949
O	-2.20571	-2.53599	0.17426
C	-1.152	-0.42902	-0.19173
C	1.18165	-0.23145	0.24886
C	-1.34244	0.9962	0.26311
C	3.58466	-0.03224	0.12386
C	1.05701	1.16691	0.2582
C	2.43957	-0.81732	0.20306
H	2.52529	-1.8956	0.223
C	-3.64401	0.72423	0.32486
C	-2.34208	-1.32531	0.13819
C	3.45256	1.35759	0.09015
H	4.33763	1.9727	0.01024
C	2.20415	1.95528	0.17048

H	2.12673	3.03215	0.16338
C	-0.33777	3.15715	0.73687
H	-0.11032	3.75772	-0.14373
H	0.36066	3.39649	1.53459
C	-4.75576	-1.48227	0.41521
H	-5.23782	-1.577	-0.55797
H	-4.49202	-2.46719	0.78753
H	-5.43271	-0.99273	1.10749
C	4.95289	-0.68736	0.06589
O	5.02556	-1.90381	0.38416
O	5.92087	0.03093	-0.29501
H	0.08659	-1.9927	0.29289
O	-1.15398	-0.23243	-1.66198
O	-0.98989	-1.50203	-2.31666
H	-0.03743	-1.51213	-2.51051
H	-1.34886	3.36574	1.06397
Conformer 4 G = -1172.21194091 Eh H= -1172.14450523 Eh			
N	-2.54875	1.43017	0.04035
O	-4.78204	1.08251	-0.14686
N	0.02693	-1.06319	0.28504
N	-0.25986	1.64971	0.23313
N	-3.54241	-0.71991	0.44393
O	-2.20376	-2.55063	0.6981
C	-1.18931	-0.57791	-0.20175
C	1.17494	-0.29418	0.18823
C	-1.35557	0.8997	0.05061
C	3.57843	-0.07083	0.12983
C	1.03837	1.10164	0.16956

C	2.43961	-0.86801	0.1582
H	2.53624	-1.94558	0.16081
C	-3.65886	0.64481	0.06641
C	-2.36247	-1.38337	0.38848
C	3.43638	1.31763	0.11512
H	4.31915	1.94032	0.08862
C	2.17962	1.90155	0.12181
H	2.09292	2.97705	0.08816
C	-0.40036	3.08916	0.47616
H	-1.4168	3.29528	0.78809
H	-0.1781	3.6484	-0.43269
C	-4.76655	-1.45249	0.77626
H	-5.29529	-1.73926	-0.13255
H	-4.49203	-2.34246	1.33336
H	-5.40716	-0.81972	1.38298
C	4.95516	-0.70445	0.10455
O	5.02732	-1.92995	-0.17698
O	5.93098	0.04514	0.36669
H	0.12237	-2.06912	0.30952
O	-1.43376	-0.8389	-1.62642
O	-0.54686	-0.01728	-2.41365
H	0.16201	-0.64206	-2.64174
H	0.28815	3.38268	1.26413
Conformer 5 G = -1172.211698580 Eh H= -1172.144206860 Eh			
N	-2.54472	1.52429	0.40142
O	-4.77965	1.23163	0.32053
N	-4.85E-4	-0.9434	0.54709
N	-0.24793	1.75901	0.41918

N	-3.5472	-0.66473	0.22204
O	-2.2227	-2.52114	0.23894
C	-1.13648	-0.43254	-0.0915
C	1.16626	-0.20242	0.37419
C	-1.35388	1.01392	0.27259
C	3.55764	-0.01644	0.10995
C	1.03984	1.19212	0.29045
C	2.41849	-0.79373	0.29499
H	2.5047	-1.87002	0.36131
C	-3.65765	0.7447	0.30212
C	-2.35122	-1.30959	0.17654
C	3.42388	1.37025	0.01519
H	4.30376	1.97781	-0.14217
C	2.17948	1.97447	0.11426
H	2.09755	3.04864	0.03845
C	-0.36778	3.19302	0.70071
H	-1.35756	3.39107	1.09463
H	-0.21994	3.77009	-0.21213
C	-4.78323	-1.45134	0.25844
H	-5.18719	-1.48078	1.27023
H	-5.51152	-0.99672	-0.40632
H	-4.55798	-2.45975	-0.07329
C	4.91687	-0.68338	-0.01762
O	4.99151	-1.90427	0.28301
O	5.87509	0.02644	-0.41914
H	0.082	-1.95094	0.51813
O	-1.01481	-0.35242	-1.57093
O	-0.51725	-1.6056	-2.06447
H	-1.32797	-2.05731	-2.35528
H	0.37951	3.47272	1.4379

Conformer 6 G = -1172.212148260 Eh H= -1172.144913910 Eh			
N	-2.46719	1.44265	0.30139
O	-4.69771	1.12646	0.4494
N	0.06697	-1.02606	0.29979
N	-0.17641	1.69697	0.14098
N	-3.44152	-0.76129	0.36416
O	-2.17068	-2.60313	-0.02205
C	-1.08843	-0.50605	-0.29551
C	1.23246	-0.27134	0.22198
C	-1.28448	0.93944	0.08728
C	3.63876	-0.07608	0.26307
C	1.1117	1.1205	0.09291
C	2.48809	-0.85438	0.32356
H	2.56915	-1.92487	0.4577
C	-3.5736	0.65282	0.35398
C	-2.28512	-1.38953	0.04691
C	3.51425	1.3021	0.07879
H	4.40526	1.90952	0.00953
C	2.26569	1.89871	5.69E-4
H	2.19306	2.96849	-0.12565
C	-0.28556	3.14433	0.34668
H	0.01301	3.66929	-0.56039
H	0.35958	3.44273	1.16984
C	-4.62264	-1.59113	0.61693
H	-5.35358	-0.99666	1.15218
H	-5.05203	-1.94353	-0.32158
H	-4.3244	-2.4462	1.21747
C	5.00655	-0.71837	0.41556

O	5.04482	-1.94328	0.70701
O	6.0095	0.02288	0.25028
H	0.14915	-2.03434	0.27919
O	-0.89101	-0.58322	-1.75093
O	-2.06196	-0.05272	-2.419
H	-2.45236	-0.85739	-2.79974
H	-1.31342	3.3876	0.58478
Conformer 7 G = -1172.211315000 Eh H= -1172.144716830 Eh			
N	-2.46476	1.41344	0.3612
O	-4.69543	1.08221	0.48416
N	0.09036	-1.03135	0.39945
N	-0.17595	1.68169	0.20462
N	-3.44564	-0.79474	0.32072
O	-2.10844	-2.63536	0.13771
C	-1.06831	-0.53193	-0.20563
C	1.25057	-0.27289	0.28359
C	-1.27825	0.91638	0.15403
C	3.65347	-0.06155	0.22803
C	1.11596	1.11597	0.13845
C	2.51243	-0.84701	0.3479
H	2.60632	-1.91545	0.49002
C	-3.5682	0.61791	0.37434
C	-2.26035	-1.42416	0.12848
C	3.51308	1.3135	0.03487
H	4.39753	1.92337	-0.08011
C	2.25924	1.90198	-7.57E-4
H	2.17396	2.96942	-0.13835
C	-0.29605	3.12973	0.39879

H	-1.31408	3.36116	0.68634
H	-0.05166	3.64923	-0.52761
C	-4.66836	-1.58526	0.48074
H	-4.43727	-2.62106	0.25546
H	-5.03686	-1.50227	1.50265
H	-5.42697	-1.21719	-0.20419
C	5.03077	-0.69336	0.30569
O	6.01174	0.043	0.02621
O	5.09959	-1.90427	0.64513
H	0.17603	-2.03948	0.40689
O	-0.86163	-0.63099	-1.662
O	-2.00689	-0.07744	-2.35372
H	-2.42021	-0.87645	-2.72183
H	0.38536	3.44528	1.18494
Fl-ßA			
Conformer 1 G = -1419.45272034 Eh H= -1419.37595372 Eh			
N	4.83971	0.35349	-0.21302
N	-3.28058	-1.3736	0.4062
O	5.07333	-1.49284	-1.4925
O	-5.42263	-0.64811	0.46696
N	-0.38447	0.39011	-0.80944
N	-1.08872	-2.05367	0.23622
N	-3.96052	0.69238	-0.62616
O	-2.38122	2.08369	-1.51025
C	-1.59624	0.3268	-0.09519
C	0.61303	-0.52531	-0.52968
C	-2.02537	-1.09563	0.17605
C	2.94536	-1.14231	-0.48317

C	0.27493	-1.77021	0.01658
C	1.94503	-0.23486	-0.79867
H	2.18748	0.71322	-1.25361
C	-4.25716	-0.46556	0.13655
C	-2.68752	1.11363	-0.84236
C	4.36851	-0.78187	-0.75863
C	2.61053	-2.38075	0.06098
H	3.38421	-3.09314	0.31304
C	1.28051	-2.68986	0.30777
H	1.03427	-3.64312	0.7493
C	-1.4854	-3.42625	0.57059
H	-0.88694	-4.12083	-0.0103
H	-2.53221	-3.55724	0.32409
C	-5.08387	1.47029	-1.15397
H	-5.77281	0.8062	-1.67076
H	-5.60675	1.97749	-0.34418
H	-4.6906	2.20469	-1.84884
H	5.78528	0.58453	-0.48778
C	4.28713	1.1114	0.9122
H	3.6461	0.45878	1.50025
H	5.13872	1.37103	1.53874
C	1.99722	2.29941	0.74953
O	1.23572	2.81267	-0.10307
O	1.61328	1.72417	1.81368
H	-0.06617	1.33853	-0.99261
O	-1.59697	1.06572	1.16125
O	-0.6354	0.475	2.05823
H	0.19655	1.04602	1.90969
C	3.51027	2.38514	0.53139
H	3.71835	2.67099	-0.49964

H	3.85244	3.21074	1.16169
H	-1.33753	-3.61225	1.63535
Conformer 2 G = -1419.45152635 Eh H= -1419.37565138 Eh			
N	5.02759	0.04771	0.01726
N	-3.28811	-1.46231	0.43191
O	4.6599	-0.50331	-2.14161
O	-5.45141	-0.82108	0.56432
N	-0.59721	0.14794	-1.26829
N	-1.04907	-2.00717	0.31959
N	-4.09059	0.57935	-0.57674
O	-2.67113	1.79583	-1.88609
C	-1.68507	0.22532	-0.37622
C	0.5105	-0.55394	-0.81577
C	-2.05933	-1.14497	0.13543
C	2.88031	-0.88917	-0.61508
C	0.2878	-1.64027	0.04149
C	1.80545	-0.21218	-1.17432
H	1.96923	0.62728	-1.83649
C	-4.3094	-0.59077	0.18481
C	-2.86092	0.93112	-1.05019
C	4.25665	-0.4342	-0.97082
C	2.66314	-1.94004	0.27338
H	3.49933	-2.45649	0.72433
C	1.36953	-2.33042	0.5809
H	1.20861	-3.15298	1.26129
C	-1.32718	-3.35222	0.83282
H	-0.62499	-4.04853	0.38441

H	-2.33852	-3.6284	0.55603
C	-5.26384	1.37594	-0.94356
H	-5.7759	1.70315	-0.04095
H	-4.92543	2.23901	-1.50698
H	-5.94623	0.78521	-1.55187
H	5.92764	0.38869	-0.2957
C	4.60077	0.50337	1.34287
H	4.03751	-0.2785	1.84694
H	5.52041	0.65595	1.90401
C	2.25603	1.60547	1.37633
O	1.79799	0.75667	2.16319
O	1.55773	2.38383	0.6458
H	-0.42779	0.9943	-1.79477
O	-1.41143	0.93766	0.87035
O	-0.99282	2.28188	0.56814
H	0.03483	2.23461	0.65429
C	3.7762	1.79752	1.32065
H	4.05069	2.41078	0.46241
H	4.02408	2.37569	2.21625
H	-1.22987	-3.37663	1.91903
Conformer 3 G = -1419.44874027 Eh H= -1419.37322375 Eh			
N	4.98672	0.09128	-0.0286
N	-3.28926	-1.30201	0.58198
O	4.61142	-0.47609	-2.18029
O	-5.46244	-0.67788	0.64289
N	-0.61945	0.18622	-1.26639
N	-1.07906	-1.91012	0.38763
N	-4.12707	0.56195	-0.69772

O	-2.69066	1.80539	-1.96576
C	-1.70997	0.32047	-0.37796
C	0.47982	-0.52924	-0.81962
C	-2.0666	-1.02004	0.22033
C	2.84701	-0.87995	-0.64007
C	0.25722	-1.58847	0.07015
C	1.77149	-0.21724	-1.21277
H	1.934	0.60416	-1.8961
C	-4.32332	-0.49055	0.23162
C	-2.89656	0.95474	-1.11749
C	4.2153	-0.41123	-1.00668
C	2.63274	-1.90115	0.28373
H	3.47032	-2.40576	0.74531
C	1.3391	-2.27261	0.61712
H	1.17966	-3.06953	1.32775
C	-1.37963	-3.22605	0.95924
H	-2.38996	-3.50585	0.68175
H	-1.29853	-3.20036	2.04702
C	-5.32093	1.24893	-1.19781
H	-6.0027	0.52621	-1.64053
H	-5.82086	1.76355	-0.37883
H	-5.01172	1.96895	-1.94726
H	5.8766	0.44838	-0.35356
C	4.58372	0.52617	1.30941
H	3.93157	-0.21582	1.7619
H	5.49847	0.5592	1.89898
C	2.39876	1.8721	1.04177
O	1.94403	2.56632	0.10961
O	1.70242	1.13947	1.81281
H	-0.42987	1.01682	-1.81221

O	-1.52398	1.30443	0.67809
O	-0.79539	0.72742	1.7827
H	0.18827	0.9976	1.63727
C	3.90362	1.8989	1.33455
H	4.40442	2.57766	0.64332
H	4.02068	2.30791	2.34231
H	-0.6788	-3.94909	0.55359
Conformer 4 G = -1419.45022067 Eh H= -1419.37407268 Eh			
N	5.03425	0.20588	-0.27759
N	-3.28017	-1.29665	0.54728
O	4.75032	-1.19593	-2.02072
O	-5.4555	-0.67233	0.53043
N	-0.50677	0.31073	-1.06721
N	-1.05814	-1.88854	0.44242
N	-4.07987	0.52695	-0.80941
O	-2.58582	1.77765	-2.00508
C	-1.69094	0.35867	-0.30649
C	0.55619	-0.45893	-0.6367
C	-2.04302	-1.0029	0.24282
C	2.91001	-0.95619	-0.53769
C	0.29042	-1.57356	0.16794
C	1.86589	-0.17006	-1.00331
H	2.05671	0.68822	-1.6334
C	-4.30447	-0.49723	0.14785
C	-2.83471	0.94214	-1.15388
C	4.30593	-0.65728	-0.9943
C	2.65204	-2.03373	0.30652
H	3.46562	-2.63225	0.69358

C	1.34451	-2.34302	0.65156
H	1.15315	-3.18103	1.30441
C	-1.38001	-3.22851	0.94614
H	-0.72018	-3.94718	0.46919
H	-2.40867	-3.45845	0.69355
C	-5.25444	1.17418	-1.39889
H	-5.79568	1.72807	-0.63337
H	-4.9161	1.85545	-2.17189
H	-5.90939	0.42157	-1.8321
H	5.95049	0.40457	-0.65663
C	4.68692	0.85008	0.99056
H	4.28361	0.10913	1.67848
H	5.63224	1.19371	1.40454
C	2.30631	1.71839	1.43524
O	1.31937	2.31665	0.89416
O	2.20828	0.94718	2.41073
H	-0.29644	1.15543	-1.58123
O	-1.70244	1.33367	0.77371
O	-0.71241	0.97286	1.76007
H	0.0909	1.53172	1.45603
C	3.69768	2.01951	0.87774
H	3.62473	2.36943	-0.15182
H	4.07128	2.86198	1.46728
H	-1.25276	-3.2722	2.02847
Conformer 5 G = -1419.45010572 Eh H= -1419.37463205 Eh			
N	4.70023	0.75098	-0.91971
N	-3.30119	-1.2842	0.50933

O	5.0726	-1.4341	-1.28755
O	-5.4752	-0.65781	0.54478
N	-0.56841	0.32249	-1.15291
N	-1.08236	-1.88144	0.35104
N	-4.11408	0.60838	-0.74549
O	-2.63966	1.86672	-1.95599
C	-1.71256	0.38245	-0.33314
C	0.50916	-0.43579	-0.73462
C	-2.06925	-0.98712	0.19179
C	2.87464	-0.86328	-0.6155
C	0.26008	-1.55707	0.06513
C	1.80998	-0.11148	-1.09103
H	1.97061	0.74457	-1.72867
C	-4.32852	-0.46281	0.15977
C	-2.87368	1.0129	-1.11885
C	4.28573	-0.52964	-0.96032
C	2.62755	-1.97148	0.19794
H	3.45494	-2.552	0.58111
C	1.32966	-2.31588	0.53587
H	1.15461	-3.16356	1.18088
C	-1.39931	-3.22475	0.84883
H	-0.7256	-3.93736	0.38295
H	-2.42169	-3.46432	0.57893
C	-5.29453	1.30002	-1.27005
H	-4.96196	2.05008	-1.97926
H	-5.9501	0.58857	-1.7677
H	-5.83257	1.77986	-0.45435
H	5.67743	0.84931	-1.15928
C	4.08014	1.94801	-0.33926
H	4.76959	2.7534	-0.58296

H	3.14105	2.18466	-0.83329
C	2.47528	1.47019	1.649
O	2.38597	0.64352	2.57998
O	1.48202	2.03877	1.08945
H	-0.36997	1.17348	-1.66175
O	-1.63879	1.323	0.77458
O	-0.70104	0.84304	1.76509
H	0.16761	1.332	1.50939
C	3.86885	1.89417	1.17828
H	4.0184	2.9039	1.57293
H	4.61891	1.25402	1.64203
H	-1.29165	-3.26701	1.93343
Conformer 6 G = -1419.44904109 Eh H= -1419.37527800 Eh			
N	4.69616	0.7059	-0.92699
N	-3.31032	-1.26192	0.51996
O	5.10554	-1.49583	-1.08614
O	-5.47837	-0.613	0.52627
N	-0.55972	0.26071	-1.18615
N	-1.09565	-1.87968	0.39569
N	-4.10119	0.58968	-0.80713
O	-2.60938	1.82701	-2.01838
C	-1.70313	0.36486	-0.36698
C	0.51336	-0.482	-0.72486
C	-2.0748	-0.98383	0.20111
C	2.87715	-0.90171	-0.54431
C	0.25111	-1.56852	0.11761
C	1.81987	-0.17478	-1.07479
H	1.99104	0.64922	-1.75054

C	-4.32923	-0.44493	0.1367
C	-2.85559	0.98496	-1.17256
C	4.29577	-0.57965	-0.86762
C	2.6153	-1.97201	0.31399
H	3.43649	-2.53381	0.73618
C	1.31167	-2.30494	0.64092
H	1.12424	-3.12487	1.31777
C	-1.42492	-3.20988	0.92009
H	-2.44475	-3.45145	0.64202
H	-1.33199	-3.22912	2.00664
C	-5.27358	1.26801	-1.36622
H	-5.78806	1.82401	-0.58393
H	-4.93609	1.95147	-2.13758
H	-5.95211	0.53428	-1.79501
H	5.68075	0.7895	-1.14107
C	4.06875	1.93109	-0.41848
H	4.75263	2.72531	-0.70979
H	3.12742	2.13227	-0.92317
C	2.46621	1.57383	1.60021
O	1.47358	2.09683	0.99809
O	2.37395	0.82556	2.59567
H	-0.35004	1.09438	-1.71916
O	-1.62089	1.34362	0.70536
O	-0.68876	0.89341	1.71501
H	0.17511	1.38562	1.44979
C	3.86153	1.9585	1.10071
H	4.02236	2.98506	1.44431
H	4.6073	1.33552	1.59392
H	-0.74786	-3.93494	0.47858

Conformer 7 G = -1419.45252937 Eh H= -1419.37686669 Eh			
N	4.81939	0.28467	-0.09123
N	-3.29301	-1.52096	0.26122
O	5.11355	-1.52149	-1.41456
O	-5.41361	-0.77211	0.49283
N	-0.39228	0.31035	-0.81991
N	-1.09474	-2.18493	0.08389
N	-3.94829	0.69251	-0.42073
O	-2.37723	2.08618	-1.31203
C	-1.57886	0.20216	-0.06774
C	0.6161	-0.60119	-0.55252
C	-2.03762	-1.23041	0.07336
C	2.94807	-1.21234	-0.47643
C	0.27266	-1.87269	-0.07127
C	1.95188	-0.29513	-0.77627
H	2.20078	0.66967	-1.18992
C	-4.25485	-0.55864	0.1583
C	-2.66864	1.08271	-0.68932
C	4.3765	-0.83515	-0.68904
C	2.60805	-2.47522	0.00415
H	3.38049	-3.19393	0.24205
C	1.27523	-2.80226	0.20217
H	1.02234	-3.77734	0.58911
C	-1.48865	-3.58097	0.29925
H	-1.37296	-3.84901	1.35039
H	-0.8656	-4.2239	-0.31445
C	-5.06831	1.56456	-0.78232
H	-5.5807	1.90764	0.11489

H	-4.67359	2.41572	-1.32668
H	-5.76834	1.01872	-1.41129
H	5.77591	0.52481	-0.31739
C	4.2088	1.03425	1.00782
H	3.45533	0.41478	1.48763
H	5.00069	1.19351	1.73854
C	2.06968	2.41687	0.54163
O	1.4623	1.96175	1.56144
O	1.50413	2.88742	-0.47198
H	-0.10028	1.26344	-1.01813
O	-1.44833	0.59633	1.33685
O	-1.10553	1.99521	1.40315
H	-0.0799	1.97992	1.44391
C	3.59782	2.38991	0.60088
H	4.00843	2.71926	-0.35311
H	3.88172	3.13579	1.34781
H	-2.52619	-3.70021	0.01075
Conformer 8 G = -1419.45193211 Eh H= -1419.37787011 Eh			
N	4.79554	0.23793	-0.17356
N	-3.31338	-1.54236	0.27047
O	5.07919	-1.5736	-1.49157
O	-5.43215	-0.7893	0.50738
N	-0.42002	0.27139	-0.86225
N	-1.12014	-2.215	0.06699
N	-3.97177	0.66405	-0.43127
O	-2.4075	2.03998	-1.36136
C	-1.5996	0.1729	-0.09809

C	0.58851	-0.64072	-0.59743
C	-2.05969	-1.25713	0.06366
C	2.91954	-1.25765	-0.5415
C	0.24631	-1.90891	-0.10708
C	1.92297	-0.33865	-0.83423
H	2.17009	0.62473	-1.25197
C	-4.27517	-0.58029	0.1638
C	-2.69437	1.04693	-0.72029
C	4.34711	-0.8835	-0.76457
C	2.58051	-2.519	-0.05616
H	3.353	-3.23991	0.17473
C	1.24882	-2.84121	0.1569
H	0.99696	-3.81474	0.54838
C	-1.51745	-3.60909	0.28892
H	-1.39401	-3.87566	1.3395
H	-0.90211	-4.25542	-0.32895
C	-5.09355	1.53504	-0.79
H	-5.60349	1.87695	0.10897
H	-4.70104	2.38691	-1.33488
H	-5.79518	0.98936	-1.41746
H	5.75181	0.47376	-0.40532
C	4.1949	0.99205	0.92785
H	3.44122	0.37699	1.41303
H	4.99176	1.14801	1.65389
C	2.06143	2.38323	0.46637
O	1.49482	2.83441	-0.55506
O	1.45491	1.95053	1.49646
H	-0.12591	1.22167	-1.07099
O	-1.45563	0.58239	1.30084
O	-1.11313	1.98225	1.34946

H	-0.08739	1.96758	1.38512
C	3.58946	2.35143	0.52357
H	4.00052	2.67952	-0.43061
H	3.87821	3.09386	1.27182
H	-2.55781	-3.72485	0.00902
Fl-G			
Conformer 1 G = -1380.16960011 Eh H= -1380.09665871 Eh			
N	4.62304	0.77547	-0.69657
N	-3.18077	-1.13968	0.76781
O	5.1537	-1.30521	-1.37418
O	-5.24807	-0.32633	1.19278
N	-0.56551	0.36261	-1.17921
N	-1.0533	-1.87122	0.28872
N	-4.04446	0.80346	-0.36007
O	-2.6804	1.98308	-1.76184
C	-1.62417	0.45346	-0.25189
C	0.51235	-0.44812	-0.85999
C	-1.98907	-0.91072	0.28816
C	2.87262	-0.91666	-0.8239
C	0.27271	-1.60202	-0.10472
C	1.80856	-0.12631	-1.23682
H	1.97066	0.77689	-1.80579
C	-4.18234	-0.23402	0.59821
C	-2.8437	1.14165	-0.89708
C	4.29013	-0.49278	-1.00401
C	2.62868	-2.08714	-0.10509
H	3.45742	-2.69855	0.22349
C	1.33522	-2.42823	0.25245

H	1.16478	-3.31187	0.84801
C	-1.39471	-3.20915	0.78355
H	-1.20452	-3.28126	1.85554
H	-0.79434	-3.94096	0.25251
C	-5.24838	1.55347	-0.72757
H	-5.56582	2.18241	0.10326
H	-5.01514	2.174	-1.58632
H	-6.04531	0.85846	-0.9793
H	5.60497	0.97906	-0.82178
C	3.79522	1.86641	-0.19556
H	4.48147	2.60891	0.2162
H	3.24579	2.35098	-1.00201
C	2.81529	1.50986	0.93728
O	1.72079	2.15532	0.91307
O	3.16072	0.6795	1.7948
H	-0.36032	1.22775	-1.66157
O	-1.40048	1.37938	0.8469
O	-0.38226	0.85477	1.7279
H	0.44615	1.37558	1.4478
H	-2.44531	-3.3957	0.59073
Fl-P			
Conformer 1 G = -1496.81602462 Eh H= -1496.73879014 Eh			
N	-4.13788	-0.16865	-0.46283
N	3.87338	0.92782	0.56783
O	-4.50368	1.96743	-1.08223
O	5.8092	-0.18638	0.94875
N	1.01924	-0.23931	-1.26068
N	1.82658	1.91537	0.17488

N	4.43937	-1.0904	-0.61347
O	2.8658	-2.1154	-1.91579
C	2.09553	-0.45596	-0.37764
C	0.04951	0.67027	-0.86812
C	2.64496	0.85298	0.1359
C	-2.24617	1.35589	-0.65884
C	0.45577	1.78939	-0.13298
C	-1.29347	0.47434	-1.14942
H	-1.58052	-0.40757	-1.70269
C	4.73691	-0.10606	0.36552
C	3.1801	-1.29073	-1.07553
C	-3.70634	1.06851	-0.75912
C	-1.83893	2.49276	0.04027
H	-2.57936	3.17694	0.43053
C	-0.49573	2.7099	0.30074
H	-0.19978	3.56938	0.88273
C	2.33379	3.19888	0.66822
H	1.79599	4.00008	0.17111
H	3.38967	3.27207	0.43138
C	5.52304	-1.97138	-1.0495
H	6.41708	-1.3789	-1.22394
H	5.72932	-2.72462	-0.28949
H	5.21831	-2.4587	-1.97013
C	-3.36745	-1.31021	0.06975
C	-2.35224	-0.97327	1.17465
O	-1.28995	-1.6703	1.14563
O	-2.64913	-0.11825	2.02655
H	0.69824	-1.07465	-1.73257
O	1.81294	-1.33056	0.74723
O	0.99366	-0.62631	1.70847

H	0.0718	-1.02636	1.5394
C	-4.46421	-2.23705	0.61434
C	-5.57774	-0.47094	-0.5393
C	-5.64085	-1.97665	-0.32106
H	-6.10884	0.07445	0.2454
H	-5.97881	-0.15203	-1.49989
H	-5.4918	-2.5001	-1.26801
H	-6.59532	-2.28997	0.10098
H	-4.13312	-3.2744	0.62753
H	-4.72087	-1.93464	1.63239
H	-2.8406	-1.8124	-0.74066
H	2.19871	3.27517	1.74838
Conformer 2 G = -1496.81340043 Eh H= -1496.73578503 Eh			
N	-4.06567	-0.44424	-0.78487
N	3.90036	1.14945	0.44448
O	-4.35092	1.40949	-2.04492
O	5.98716	0.37743	0.85197
N	1.15485	-0.62919	-0.99121
N	1.78085	1.88002	-0.10017
N	4.56363	-1.10171	-0.10245
O	3.01651	-2.60114	-0.85508
C	2.17802	-0.53244	-0.0303
C	0.15804	0.32952	-0.99195
C	2.66734	0.89152	0.09727
C	-2.14252	0.97133	-1.29172
C	0.46779	1.61846	-0.54075
C	-1.13621	0.02197	-1.38748

H	-1.34537	-0.98593	-1.71195
C	4.84779	0.17602	0.44821
C	3.30414	-1.51107	-0.39123
C	-3.59377	0.64165	-1.42589
C	-1.81845	2.27555	-0.91406
H	-2.59525	3.02496	-0.85551
C	-0.52313	2.5983	-0.54561
H	-0.30179	3.6025	-0.21928
C	2.15461	3.27163	0.17614
H	3.19479	3.30342	0.47349
H	1.53616	3.65875	0.98457
C	5.68471	-2.02066	-0.31158
H	6.04957	-2.39948	0.64233
H	5.33661	-2.84726	-0.92202
H	6.48762	-1.49686	-0.8235
C	-3.30273	-1.4252	0.01108
C	-2.3899	-0.82411	1.1001
O	-2.70828	0.23748	1.66138
O	-1.36442	-1.52946	1.36212
H	0.89095	-1.57564	-1.23237
O	1.83504	-1.04558	1.29106
O	0.82134	-0.21574	1.89931
H	-0.03502	-0.73595	1.72345
C	-4.40356	-2.31062	0.63644
C	-5.51793	-0.65303	-0.66384
C	-5.64492	-1.41924	0.64706
H	-6.02756	0.30764	-0.66936
H	-5.88913	-1.24005	-1.5092
H	-6.57266	-1.98679	0.7121
H	-5.60522	-0.72054	1.48526

H	-4.57161	-3.17647	-0.0065
H	-4.11695	-2.67599	1.62206
H	-2.67954	-2.0333	-0.63761
H	2.00733	3.87303	-0.71887
Conformer 3 G = -1496.81438514 Eh H= -1496.73644846 Eh			
N	-3.98537	-0.63725	-0.70287
N	3.89356	1.31552	0.1783
O	-4.35342	0.88246	-2.33808
O	5.95696	0.62048	0.77933
N	1.23545	-0.64481	-1.12231
N	1.75336	1.94236	-0.43762
N	4.5245	-1.01705	0.15994
O	3.01859	-2.59818	-0.51128
C	2.17132	-0.41782	-0.10332
C	0.17973	0.25411	-1.16181
C	2.66857	1.00605	-0.13516
C	-2.15104	0.76231	-1.44014
C	0.43861	1.58549	-0.80973
C	-1.10537	-0.14667	-1.48693
H	-1.27917	-1.18691	-1.72464
C	4.82392	0.34412	0.40682
C	3.28467	-1.451	-0.19551
C	-3.57684	0.32783	-1.54346
C	-1.88533	2.10344	-1.16553
H	-2.69615	2.81831	-1.14312
C	-0.59878	2.51495	-0.85487
H	-0.41824	3.55004	-0.60906

C	2.09274	3.3645	-0.33709
H	1.48804	3.83078	0.43905
H	1.90253	3.85166	-1.29183
C	5.6241	-1.98007	0.25753
H	5.9511	-2.06886	1.29252
H	5.2659	-2.94029	-0.09788
H	6.45801	-1.64743	-0.35571
C	-3.18111	-1.25675	0.37038
C	-2.59758	-0.23923	1.37112
O	-3.26136	0.78059	1.6357
O	-1.48862	-0.55005	1.90306
H	1.01419	-1.62107	-1.26876
O	1.62826	-0.49622	1.26625
O	0.82709	-1.6875	1.40136
H	-0.09454	-1.29458	1.50279
C	-4.19567	-2.19139	1.05705
C	-5.42009	-0.94866	-0.57742
C	-5.54265	-1.50264	0.83733
H	-6.00555	-0.04705	-0.74708
H	-5.71111	-1.68745	-1.32871
H	-6.38651	-2.18314	0.94365
H	-5.66839	-0.68359	1.5468
H	-4.18111	-3.15906	0.55139
H	-3.95216	-2.35207	2.10683
H	-2.36393	-1.83823	-0.04178
H	3.14007	3.45635	-0.07753
Conformer 4 G = -1496.81404620 Eh H= -1496.73588981 Eh			
N	-4.11803	-0.16004	-0.60221

N	3.84924	0.90314	0.63994
O	-4.47696	1.98654	-1.21954
O	5.78359	-0.21774	1.00707
N	1.05567	-0.15914	-1.32423
N	1.81413	1.912	0.24395
N	4.42328	-1.0923	-0.57876
O	2.86536	-2.09726	-1.91375
C	2.07891	-0.43482	-0.39346
C	0.07064	0.72791	-0.91497
C	2.62928	0.84812	0.18272
C	-2.2348	1.38093	-0.72336
C	0.4509	1.80046	-0.10133
C	-1.26089	0.54542	-1.2489
H	-1.52284	-0.29094	-1.87886
C	4.71455	-0.12544	0.41953
C	3.17146	-1.27772	-1.06498
C	-3.69071	1.08493	-0.88143
C	-1.85492	2.46965	0.06331
H	-2.60983	3.11959	0.48353
C	-0.51914	2.68248	0.3684
H	-0.24488	3.5043	1.01273
C	2.31516	3.17646	0.78969
H	2.18379	3.20814	1.8725
H	1.77089	3.99396	0.32728
C	5.50812	-1.97182	-1.01525
H	5.20417	-2.45675	-1.93731
H	6.4022	-1.37842	-1.18711
H	5.71345	-2.7266	-0.25674
C	-3.30926	-1.28916	-0.10579
C	-2.47919	-0.96965	1.15136

O	-1.4255	-1.67234	1.27013
O	-2.88295	-0.11313	1.95616
H	0.75171	-0.9672	-1.85189
O	1.71688	-1.33563	0.68901
O	0.91521	-0.62531	1.66104
H	-0.00636	-1.02138	1.52251
C	-4.35655	-2.38879	0.17253
C	-5.55941	-0.45757	-0.56774
C	-5.65899	-1.62335	0.40564
H	-6.10857	0.4255	-0.24802
H	-5.90824	-0.73782	-1.56609
H	-6.54333	-2.23328	0.22481
H	-5.70189	-1.24562	1.42934
H	-4.44402	-3.02711	-0.7077
H	-4.06642	-3.01705	1.01366
H	-2.62161	-1.63666	-0.86943
H	3.37011	3.26614	0.55264
Conformer 5 G = -1496.81288490 Eh H= -1496.73495786 Eh			
N	-4.08687	-0.76724	0.1966
N	3.80722	1.0995	-0.97738
O	-4.41531	-1.14417	-1.9995
O	5.7735	1.5532	0.04899
N	1.15022	-1.00819	0.17039
N	1.76969	0.60556	-1.92
N	4.50686	-0.05531	1.01567
O	3.06925	-1.49547	2.0512
C	2.13195	-0.02531	0.41954
C	0.13402	-0.68097	-0.71648

C	2.61245	0.58509	-0.87769
C	-2.18787	-0.65911	-1.34725
C	0.43673	0.16887	-1.78411
C	-1.16499	-1.13102	-0.53658
H	-1.36241	-1.79774	0.28722
C	4.72105	0.92909	0.01687
C	3.2947	-0.6283	1.2264
C	-3.63371	-0.90294	-1.06305
C	-1.88168	0.18325	-2.41917
H	-2.67484	0.5566	-3.05136
C	-0.57526	0.58438	-2.64494
H	-0.35756	1.26066	-3.45786
C	2.21811	1.14355	-3.20823
H	3.27808	0.9415	-3.32174
H	2.04731	2.21985	-3.25907
C	5.62552	-0.38227	1.90074
H	6.51492	-0.57176	1.30536
H	5.81595	0.44554	2.5831
H	5.36462	-1.26941	2.46802
C	-3.31431	-0.50701	1.42445
C	-2.4037	0.73384	1.36009
O	-2.76898	1.73518	0.72059
O	-1.32349	0.62918	2.02455
H	0.88491	-1.543	0.98739
O	1.74675	1.02196	1.35585
O	0.65405	1.79613	0.81358
H	-0.14123	1.39981	1.31081
C	-4.40239	-0.36131	2.51299
C	-5.53664	-0.76911	0.44231
C	-5.67764	-0.00355	1.74911

H	-6.04927	-0.29908	-0.3943
H	-5.90262	-1.79627	0.53195
H	-6.58125	-0.28447	2.28902
H	-5.7144	1.0684	1.54572
H	-4.5223	-1.31884	3.02112
H	-4.12819	0.38206	3.26042
H	-2.6889	-1.36093	1.66551
H	1.66831	0.64497	-4.00048
Fl-F			
Conformer 1 G = -1650.38031110 Eh H= -1650.29701992 Eh			
N	3.45322	-1.56939	-0.19717
N	-4.71045	-0.76253	0.60266
O	3.22914	-3.74377	-0.70692
O	-6.49156	0.62403	0.74924
N	-1.52238	-0.13596	-0.9089
N	-2.89596	-2.13957	0.31143
N	-4.71001	1.4294	-0.39146
O	-2.8396	2.18029	-1.45948
C	-2.57498	0.26053	-0.06003
C	-0.83031	-1.29287	-0.58515
C	-3.4508	-0.92003	0.29611
C	1.21122	-2.54809	-0.38791
C	-1.52391	-2.32437	0.05684
C	0.52519	-1.43133	-0.84213
H	1.03751	-0.6343	-1.35434
C	-5.34346	0.41897	0.37514
C	-3.39571	1.38066	-0.72911
C	2.6923	-2.65098	-0.45358

C	0.51362	-3.58736	0.23007
H	1.04922	-4.45807	0.58041
C	-0.85006	-3.48169	0.43927
H	-1.37733	-4.27708	0.9434
C	-3.72761	-3.30869	0.61466
H	-4.75275	-3.0875	0.34114
H	-3.68007	-3.5496	1.67717
C	-5.53741	2.54963	-0.84757
H	-5.93941	3.08416	0.01087
H	-4.91573	3.21422	-1.43806
H	-6.35865	2.17585	-1.45614
H	4.44048	-1.77005	-0.28671
C	3.15935	-0.21008	0.28051
H	4.02164	0.03533	0.90378
C	1.96945	-0.14115	1.28353
O	1.10618	0.76353	1.10005
O	1.98997	-0.9533	2.22794
H	-0.98512	0.62935	-1.29518
O	-2.15321	0.95627	1.15066
O	-1.29192	0.10034	1.93809
H	-0.36098	0.39355	1.65486
C	3.05159	3.308	-0.39676
C	3.78331	2.12951	-0.53795
C	3.69273	4.51921	-0.14736
C	5.17351	2.18707	-0.39611
C	5.07722	4.56573	-0.02393
C	5.81739	3.39218	-0.14407
H	3.10903	5.42664	-0.05118
H	5.57772	5.50756	0.16455
H	6.89612	3.41738	-0.0464

C	3.11236	0.82004	-0.86861
H	3.62205	0.37813	-1.72694
H	2.08173	1.01167	-1.15917
H	5.76024	1.28129	-0.50359
H	1.97285	3.279	-0.49219
H	-3.36971	-4.15066	0.02993
Conformer 2 G = -1650.37908250 Eh H= -1650.29111740 Eh			
N	3.54296	-1.77981	-0.4846
N	-4.88401	-0.73897	0.4321
O	2.86246	-3.85243	-0.97703
O	-6.69721	0.61321	0.46651
N	-1.51332	0.11772	-0.48711
N	-2.97267	-2.02171	0.39007
N	-4.85303	1.45965	-0.5417
O	-2.88849	2.2588	-1.39693
C	-2.74954	0.40115	0.10431
C	-0.84013	-1.05549	-0.21321
C	-3.58978	-0.83541	0.30299
C	1.16068	-2.4098	-0.22022
C	-1.57618	-2.14573	0.27387
C	0.52215	-1.19792	-0.46925
H	1.04894	-0.36359	-0.90892
C	-5.52297	0.43406	0.17389
C	-3.5077	1.46225	-0.71624
C	2.58037	-2.70665	-0.57918
C	0.42889	-3.47093	0.31906
H	0.92483	-4.40705	0.52895
C	-0.92414	-3.34081	0.56588

H	-1.47167	-4.17517	0.9756
C	-3.77106	-3.23632	0.59061
H	-4.80023	-3.02209	0.33125
H	-3.71684	-3.55755	1.63104
C	-5.66671	2.55117	-1.08092
H	-5.01565	3.21956	-1.63481
H	-6.43019	2.1472	-1.7427
H	-6.14441	3.09165	-0.26566
H	4.4663	-2.13369	-0.70981
C	3.58227	-0.44804	0.09802
H	2.65014	-0.23639	0.61244
C	4.72807	-0.37584	1.13358
O	4.57958	0.43813	2.07379
O	5.72585	-1.11106	0.92822
H	-1.00949	0.90334	-0.87405
O	-2.66998	1.11305	1.38545
O	-2.15615	0.2099	2.38591
H	-1.22429	0.48042	2.44526
C	3.04279	2.89752	-0.49874
C	4.08843	1.98533	-0.63883
C	3.29376	4.2188	-0.14412
C	5.39354	2.42368	-0.4065
C	4.59937	4.64579	0.07929
C	5.64969	3.74118	-0.0472
H	2.47062	4.91616	-0.04763
H	4.79732	5.67528	0.35136
H	6.66855	4.06544	0.1276
C	3.82628	0.56379	-1.04957
H	4.68106	0.19161	-1.61894
H	2.96123	0.52333	-1.71529

H	6.21556	1.72477	-0.51055
H	2.02407	2.5744	-0.68045
H	-3.38774	-4.01991	-0.05661

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