Electronic Supplementary Material (ESI) for RSC Advances.

A novel series of dipeptide derivatives containing indole-3-carboxylic acid conjugates as potential antimicrobial agents: the design, solid phase peptide synthesis, *in vitro* biological evaluation, and molecular docking study

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Abbreviations

ACN	Acetonitrile
Asn	Asparagine
Asp	Aspartic acid
Boc	tert-Butyloxycarbonyl
CTC	Chlorotrityl Chloride
DCM	Dichloromethane
DMF	N, N-Dimethylformamide
DMSO-d_6	Dimethyl sulfoxide-deuterated
DIPEA	Diisopropylethylamine
ESI	Electron spray ionization
Glu	Glutamic acid
Gly	Glycine
Fmoc	Fluorenylmethyloxycarbony
FTIR	Fourier Transform Infrared Spectroscopy
HBTU	(2-(1*H*-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium
His	Histidine
HOBt.H_2O	N-Hydroxybenzotriazole monohydrate
Ile	Isoleucine
IPA	Isopropyl alcohol
LC-MS	Liquid Chromatography Mass Spectroscopy
Met	Methionine
MHz	Mega Hertz
Mmol	Milli mole
MS	Mass Spectroscopy
MTCC	Microbial Type Culture Collection
ml/gm	Milli litter per gram
nm	nanometre
NMP	1-Methyl-2-pyrrolidone
NMR	Nuclear Magnetic Resonance
TFA	Trifluoroacetic acid
TIS	Triisopropylsilane
Pbf	2,2,4,6,7-Pentamethyldihydrobenzofurane

Phe	Phenylalanine
Ser	Serine
SPPS	Solid-Phase Peptide Synthesis
RT	Room temperature
OtBu	Tert-butoxy
tBu	Tertiary Butyl
Thr	Theanine
Tyr	Tyrosine
TIS	Triisopropyl Silane
v/v	Volume by volume
UV	Ultraviolet-visible spectroscopy

Characterization data:

2-(3-(1H-imidazol-4-yl)-2-(1H-indole-3-carboxamido)propanamido)-3-(4-hydroxyphenyl)propanoic acid (6a): Yield - 90%; mp: 208-210 °C; IR (cm^{-1}): 3210.2, 3145.9, 3080.0, 1730.0. 1645.0, 1537.3, 1514.1, 1206.6, 1138.0, 835.2, 752.2, 723.3; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.79 (s, 1H), 9.31 (s, 1H), 8.95 (s, 1H), 8.20-8.09 (m, 4H), 7.46 (d, *J*=7.7 Hz, 1H), 7.36 (s, 1H), 7.24-7.05 (m, 3H), 7.04 (d, *J*=7.9 Hz, 2H), 6.78-6.63 (m, 1H), 6.58 (d, *J*=7.9 Hz, 2H), 4.91 (td, *J*=8.9, 4.8 Hz, 1H), 4.42 (dd, *J*=8.0, 5.1 Hz, 1H), 3.26-3.18 (m, 1H), 3.14-3.08 (m, 1H), 2.98 (dd, *J*=14.0, 4.9 Hz, 1H), 2.88 (d, *J*=13.8 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 173.24, 171.23, 165.19, 156.49, 136.64, 134.19, 130.63, 130.58, 129.06, 127.69, 126.56, 122.46, 121.34, 121.02, 117.24, 115.53, 112.44, 110.17, 72.57, 54.45, 51.87, 49.18, 36.43, 27.27; LCMS (ESI): *m/z* = 462.28 $[M+1]^{+}$.

2-(2-(1H-indole-3-carboxamido)acetamido)-3-(4-hydroxyphenyl)propanoic acid (6b): Yield - 88%; mp: 185-187 °C; IR (cm^{-1}): 3294.4, 3151.7, 2962.6, 1703.1, 1656.8, 1589.3, 1546.9, 1541.1, 1247.9, 1199.7, 839.0, 777.3, 734.8; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.58 (d, *J*=2.9 Hz, 1H), 9.21 (s, 1H), 8.16-8.10 (m, 2H), 8.07-8.01 (m, 2H), 7.44 (d, *J*=8.0 Hz, 1H), 7.18-7.10 (m, 2H), 7.02-6.99 (m, 2H), 6.60 (d, *J*=8.4 Hz, 2H), 4.39 (dt, *J*=8.1, 4.1 Hz, 1H), 3.96-3.91 (m, 1H), 3.83 (d, *J*=10.7 Hz, 1H), 2.93 (dd, *J*=13.8, 5.1 Hz, 2H), 2.80 (d, *J*=5.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 173.38, 169.97, 165.22, 156.40, 136.58, 130.59, 128.62, 127.78, 126.51, 122.35, 121.39, 120.88, 115.48, 112.32, 110.67, 54.14, 42.20, 36.62; LCMS (ESI): *m/z* = 382.32 $[M+1]^{+}$.

4-((1-carboxy-2-(4-hydroxyphenyl)ethyl)amino)-3-(1H-indole-3-carboxamido)-4-oxobutanoic acid (6c): Yield - 84%; mp: 192-194 °C; IR (cm^{-1}): 3305.9, 3010.0, 2358.9, 1710.9, 1710.8, 1658.8, 1612.5, 1516.0, 1514.2, 1442.7, 1348.2, 1247.9, 1201.6, 837.1, 748.4; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.69 (d, *J*=3.0 Hz, 1H), 9.25 (s, 1H), 8.18-8.06 (m, 3H), 7.92 (d, *J*=7.8 Hz, 1H), 7.47 (d, *J*=7.8 Hz, 1H), 7.43-7.35 (m, 1H), 7.16 (dd, *J*=9.4, 7.4 Hz, 2H), 6.96 (d, *J*=6.1 Hz, 2H), 6.72-6.64 (m, 1H), 6.51 (d, *J*=8.3 Hz, 2H), 4.84 (td, *J*=8.1, 5.3 Hz, 1H), 4.36 (td, *J*=7.7, 4.9 Hz, 1H), 2.93-2.88 (m, 1H), 2.82 (d, *J*=6.5 Hz, 1H), 2.66-2.61 (m, 1H), 2.54 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 173.20, 172.44, 171.93, 165.07, 156.36, 136.62, 130.90, 130.65, 129.09, 127.60, 126.36, 122.40, 121.27, 120.99, 115.75, 115.43, 112.43, 110.52, 54.29, 49.94, 37.39, 36.54; LCMS (ESI): *m/z* = 440.21 $[M+1]^{+}$.

2-(3-hydroxy-2-(1H-indole-3-carboxamido)propanamido)-3-(4-hydroxyphenyl)propanoic acid (6d): Yield - 87%; mp: 189-191 °C; IR (cm^{-1}): 3302.1, 3157.5, 3018.6, 1705.1, 1651.1, 1612.5, 1591.3, 1537.3, 1514.1, 1450.0, 1251.8, 1197.8, 835.2, 767.7, 758.0; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.68 (d, *J*=2.9 Hz, 1H), 9.25 (s, 1H), 8.18-8.10 (m, 2H), 8.00 (d, *J*=7.8 Hz, 1H), 7.82 (d, *J*=8.0 Hz, 1H), 7.46 (d, *J*=7.7 Hz, 1H), 7.19-7.11 (m, 2H), 7.02 (d, *J*=8.2 Hz, 2H), 6.61 (d, *J*=8.1 Hz, 3H), 4.97 (s, 1H), 4.57 (dd, *J*=7.6, 5.5 Hz, 1H), 4.42 (td, *J*=7.5, 5.2 Hz, 1H), 3.70 (t, *J*=5.9 Hz, 2H), 2.95 (dd, *J*=13.8, 5.3 Hz, 1H), 2.89-2.83 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 173.22, 170.97, 165.11, 156.41, 136.59, 130.68, 129.05, 127.65, 126.47, 122.38, 121.29, 120.95, 115.45, 112.40, 110.62, 62.20, 55.50, 54.18, 36.51; LCMS (ESI): *m/z* = 412.24 $[M+1]^{+}$.

2-(2-(1H-indole-3-carboxamido)-3-phenylpropanamido)-3-(4-hydroxyphenyl)propanoic acid (6e): Yield - 90%; mp: 200-202 °C; IR (cm^{-1}): 3250.0, 3062.9, 1703.1, 1684.0, 1598.9, 1540.0, 1514.1, 1438.9, 1230.0, 1210.0, 825.5, 779.2, 748.4; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.59 (d, *J*=2.9 Hz, 1H), 9.23 (s, 1H), 8.25 (d, *J*=7.8 Hz, 1H), 8.08 (d, *J*=2.8 Hz, 1H), 8.00 (dd, *J*=17.0, 8.2 Hz, 2H), 7.43 (d, *J*=8.0 Hz, 1H), 7.36 (d, *J*=7.5 Hz, 2H), 7.24 (t, *J*=7.5 Hz, 2H), 7.22-7.09 (m, 3H), 7.06 (dd, *J*=11.8, 7.7 Hz, 3H), 6.60 (d, *J*=8.2 Hz, 2H), 4.78 (ddd, *J*=10.4, 8.4, 3.9 Hz, 1H), 4.41 (td,

J=7.9, 5.2 Hz, 1H), 3.11 (dd, *J*=13.9, 4.0 Hz, 1H), 2.97 (ddd, *J*=12.2, 9.6, 4.3 Hz, 2H), 2.90-2.83 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 173.39, 172.45, 164.88, 156.41, 139.02, 136.52, 130.61, 129.71, 128.73, 128.48, 127.81, 126.61, 126.46, 122.33, 121.33, 120.86, 115.48, 112.32, 110.54, 54.37, 54.17, 37.58, 36.52.

5-((1-carboxy-2-(4-hydroxyphenyl)ethyl)amino)-4-(1H-indole-3-carboxamido)-5-oxopentanoic acid (6f): Yield - 91%; mp: 194-196 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.67 (d, *J*=3.2 Hz, 1H), 8.27-8.05 (m, 4H), 7.90 (d, *J*=8.0 Hz, 1H), 7.45 (d, *J*=7.8 Hz, 1H), 7.18-7.10 (m, 2H), 7.03 (d, *J*=8.3 Hz, 3H), 6.60 (d, *J*=8.1 Hz, 3H), 4.54 (td, *J*=8.5, 5.2 Hz, 1H), 4.38 (td, *J*=7.9, 5.2 Hz, 1H), 3.00-2.92 (m, 1H), 2.84 (dd, *J*=14.0, 8.1 Hz, 1H), 2.34 (t, *J*=7.9 Hz, 2H), 2.04 (dd, *J*=14.1, 6.5 Hz, 1H), 1.88 (dt, *J*=16.7, 8.7 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 174.26, 172.96, 171.96, 164.70, 156.03, 136.22, 130.20, 128.57, 127.42, 126.23, 121.99, 121.02, 120.55, 115.09, 111.97, 110.05, 72.18, 53.93, 51.71, 48.82, 30.52, 27.29, 26.91.

2-(2-(1H-indole-3-carboxamido)-4-(methylthio)butanamido)-3-(4-hydroxyphenyl)propanoic acid (6g): Yield - 89%; mp: 185-187 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ 11.65 (d, *J*=3.1 Hz, 1H), 8.28-8.19 (m, 1H), 8.18-8.10 (m, 3H), 7.96 (d, *J*=8.1 Hz, 1H), 7.46 (dd, *J*=7.3, 1.8 Hz, 1H), 7.21-7.01 (m, 5H), 6.61 (d, *J*=8.4 Hz, 2H), 4.63 (dt, *J*=8.4, 4.3 Hz, 1H), 4.40 (dt, *J*=8.0, 4.1 Hz, 1H), 2.97 (dd, *J*=14.1, 5.3 Hz, 1H), 2.86 (dd, *J*=14.0, 8.2 Hz, 1H), 2.64-2.53 (m, 2H), 2.06 (s, 3H), 2.04-1.93 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 173.01, 171.96, 164.75, 156.05, 136.24, 130.62, 130.23, 128.61, 127.45, 126.25, 122.03, 121.05, 120.59, 115.55, 115.11, 111.99, 110.10, 53.93, 51.75, 36.04, 31.82, 30.02, 14.82; LCMS (ESI): *m/z* = 456.26 [M+1] $^{+}$.

2-(4-amino-2-(1H-indole-3-carboxamido)-4-oxobutanamido)-3-(4-hydroxyphenyl)propanoic acid (6h): Yield - 85%; mp: 196-199 °C IR (cm^{-1}): 3292.5, 3010.0, 2613.5, 1697.4, 1658.8, 1610.0, 1539.3, 1514.2, 1350.2, 1253.7, 1205.5, 831.3, 769.6, 750.0, 702.1; ^{1}H NMR (400 MHz, DMSO-d6) δ 12.57 (s, 2H), 11.66 (d, *J*=2.9 Hz, 1H), 9.18 (s, 1H), 8.16 (d, *J*=7.9 Hz, 2H), 8.09 (d, *J*=2.9 Hz, 1H), 7.91 (d, *J*=7.9 Hz, 1H), 7.49-7.43 (m, 1H), 7.16 (ddd, *J*=8.8, 7.4, 1.7 Hz, 2H), 6.97 (d, *J*=8.3 Hz, 2H), 6.80-6.62 (m, 1H), 6.52-6.46 (m, 2H), 4.88 (td, *J*=8.2, 5.5 Hz, 1H), 4.37 (td, *J*=7.8, 5.0 Hz, 1H), 2.93-2.88 (m, 1H), 2.85-2.79 (m, 2H), 2.63 (dd, *J*=16.5, 8.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 172.80, 172.17, 171.28, 164.82, 155.97, 136.21, 130.26, 128.64, 127.22, 126.15, 122.06, 121.03, 120.63, 115.05, 112.02, 110.01, 53.91, 49.25, 36.12, 35.91, 17.96; LCMS (ESI): *m/z* = 439.43 [M+1]$^{+}$.

2-(3-hydroxy-2-(1H-indole-3-carboxamido)butanamido)-3-(4-hydroxyphenyl)propanoic acid (6i): Yield - 89%; mp: 193-195 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ 12.75 (s, 1H), 11.68 (s, 1H), 9.23 (s, 1H), 8.20-8.02 (m, 3H), 7.50 (dd, *J*=20.3, 8.1 Hz, 2H), 7.16 (p, *J*=7.1 Hz, 2H), 7.04 (d, *J*=8.0 Hz, 2H), 6.65 (d, *J*=8.0 Hz, 2H), 4.98 (s, 1H), 4.47 (ddd, *J*=20.8, 11.1, 5.8 Hz, 2H), 4.13-4.02 (m, 1H), 2.97-2.85 (m, 2H), 1.12 (d, *J*=6.4 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 173.24, 170.96, 165.00, 156.44, 136.67, 130.65, 129.17, 127.67, 126.28, 122.40, 121.09, 121.00, 115.49, 112.48, 110.73, 67.35, 58.49, 54.15, 36.61, 20.37; LCMS (ESI): *m/z* = 426.42 [M+1]$^{+}$.

2-(2-(1H-indole-3-carboxamido)-3-methylpentanamido)-3-(4-hydroxyphenyl)propanoic acid (6j): Yield - 92%; mp: 180-186 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ 12.55 (s, 1H), 11.64 (d, *J*=3.0 Hz, 1H), 9.19 (s, 1H), 8.29-7.97 (m, 3H), 7.64 (d, *J*=9.0 Hz, 1H), 7.44 (d, *J*=7.7 Hz, 1H), 7.14 (dt, *J*=13.7, 6.8 Hz, 2H), 7.07-7.01 (m, 2H), 6.66 (dd, *J*=50.0, 8.0 Hz, 2H), 4.55-4.29 (m, 2H), 2.94 (dd, *J*=14.0, 5.4 Hz, 1H), 2.84 (dd, *J*=14.0, 8.4 Hz, 1H), 1.87 (td, *J*=12.3, 10.4, 4.9 Hz, 1H), 1.57-1.44 (m, 1H), 1.33-1.15 (m, 1H), 0.97-0.81 (m, 6H); ^{13}C NMR (100 MHz, DMSO-d6) δ

173.40, 172.15, 164.72, 156.37, 136.62, 130.96, 130.52, 128.83, 127.95, 126.57, 122.32, 121.31, 120.88, 115.86, 115.43, 112.34, 110.67, 56.99, 54.27, 36.89, 36.51, 25.02, 15.90, 11.28.

Molecular Docking Studies results

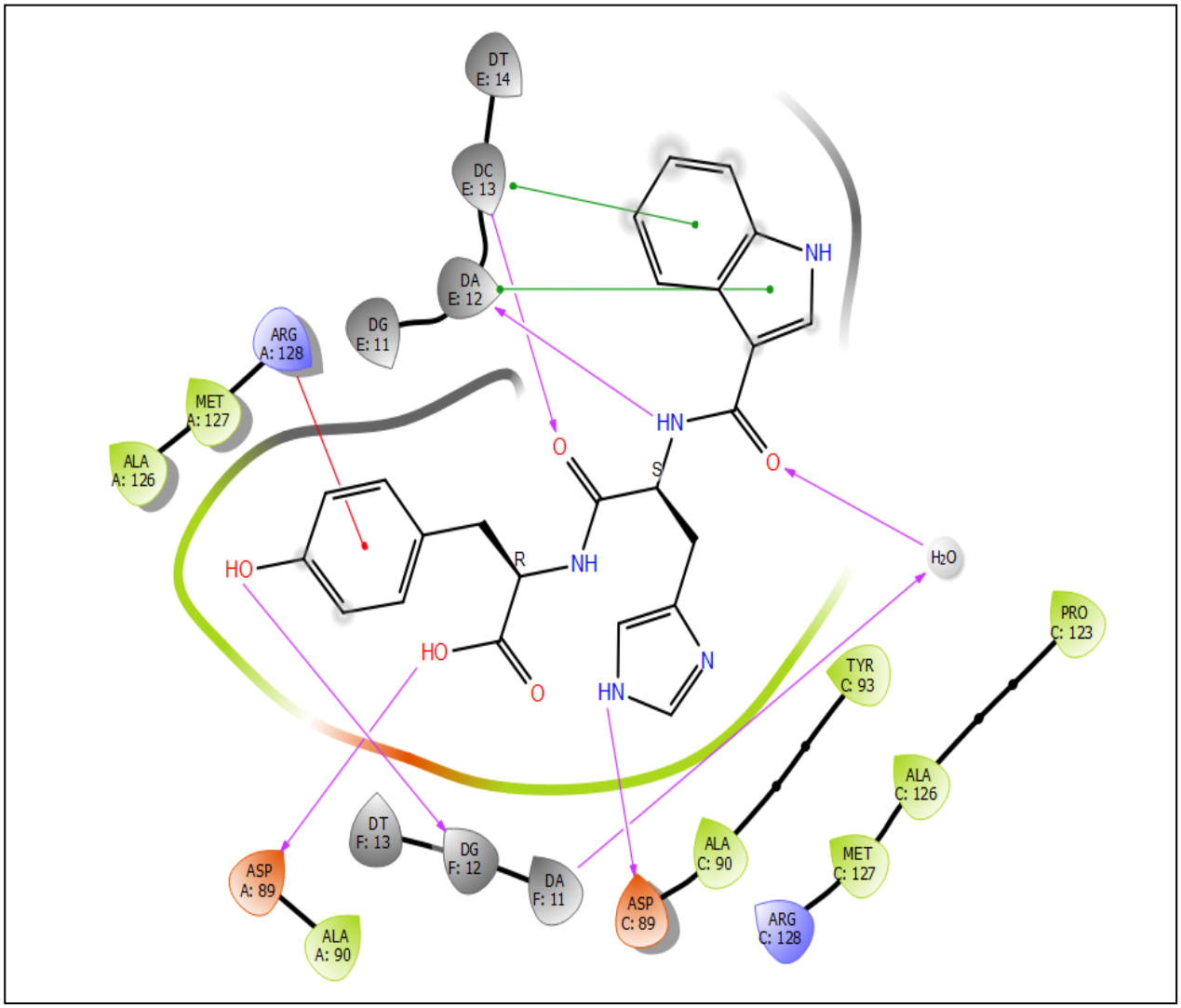


Figure S1. The binding poses and intermolecular interactions of **ID-6a** with lanosterol 14-alpha demethylase.

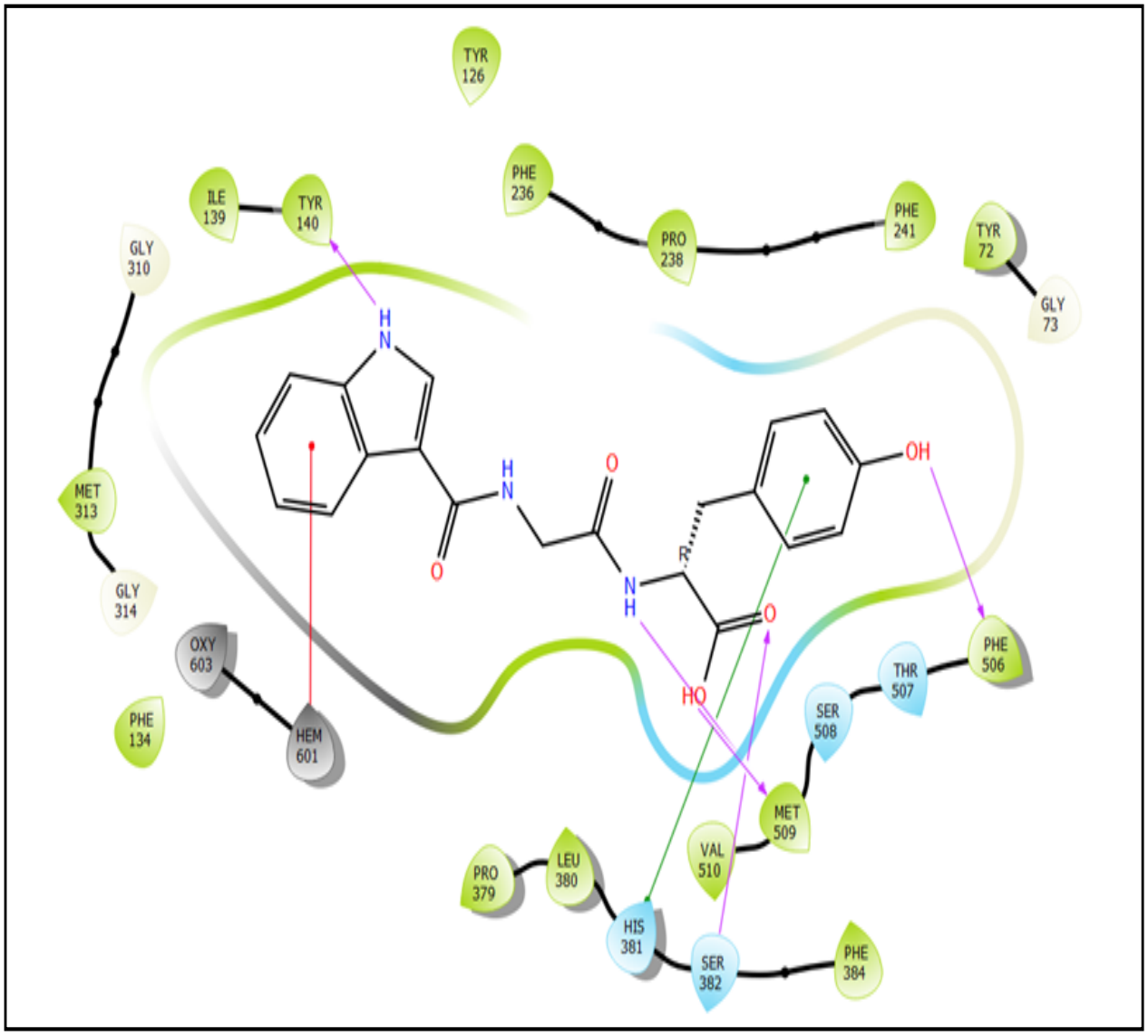


Figure S2. The binding poses and intermolecular interactions of **ID-6b** with lanosterol 14-alpha demethylase.

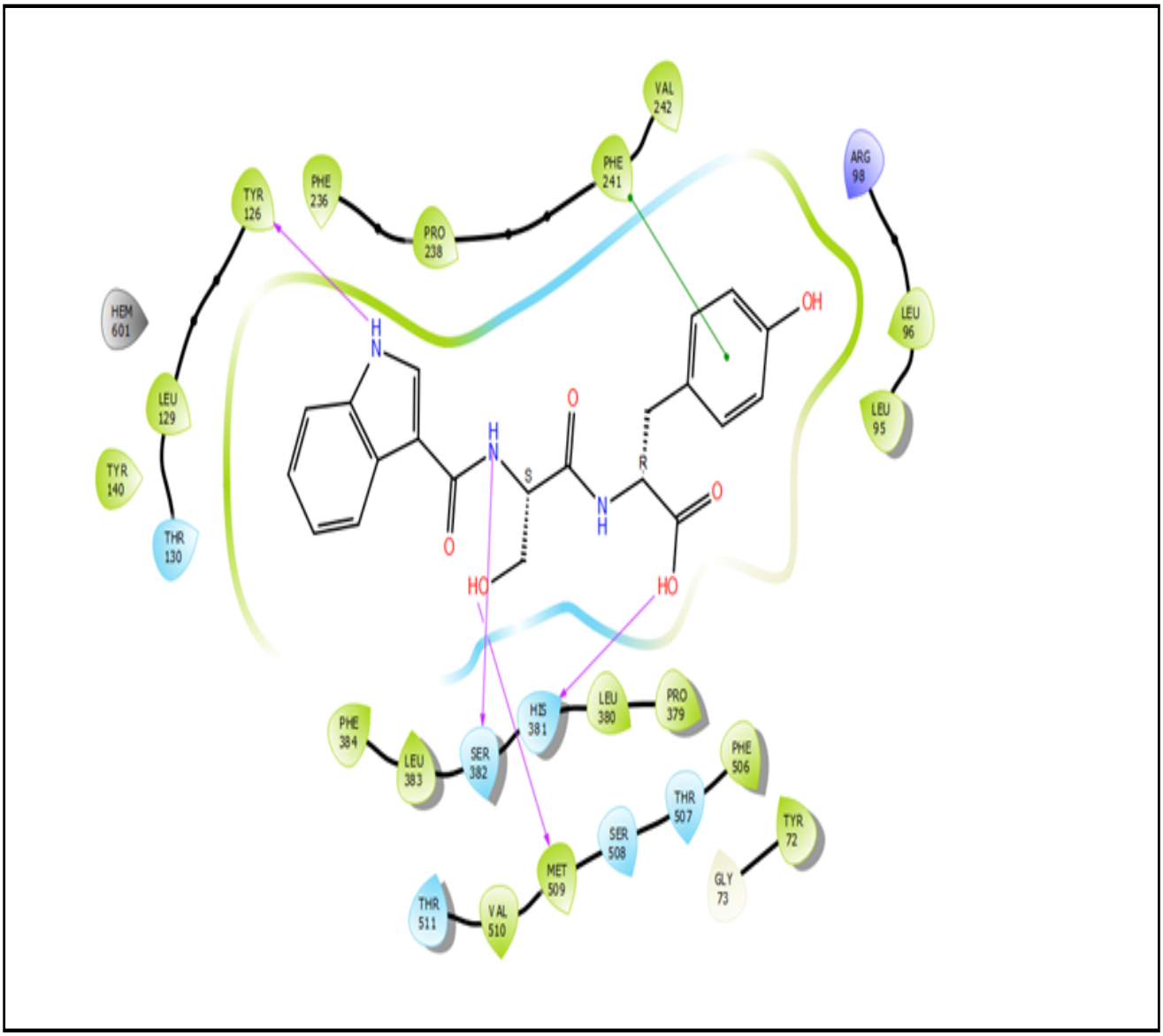


Figure S3. The binding poses and intermolecular interactions of **ID-6d** with lanosterol 14-alpha demethylase.

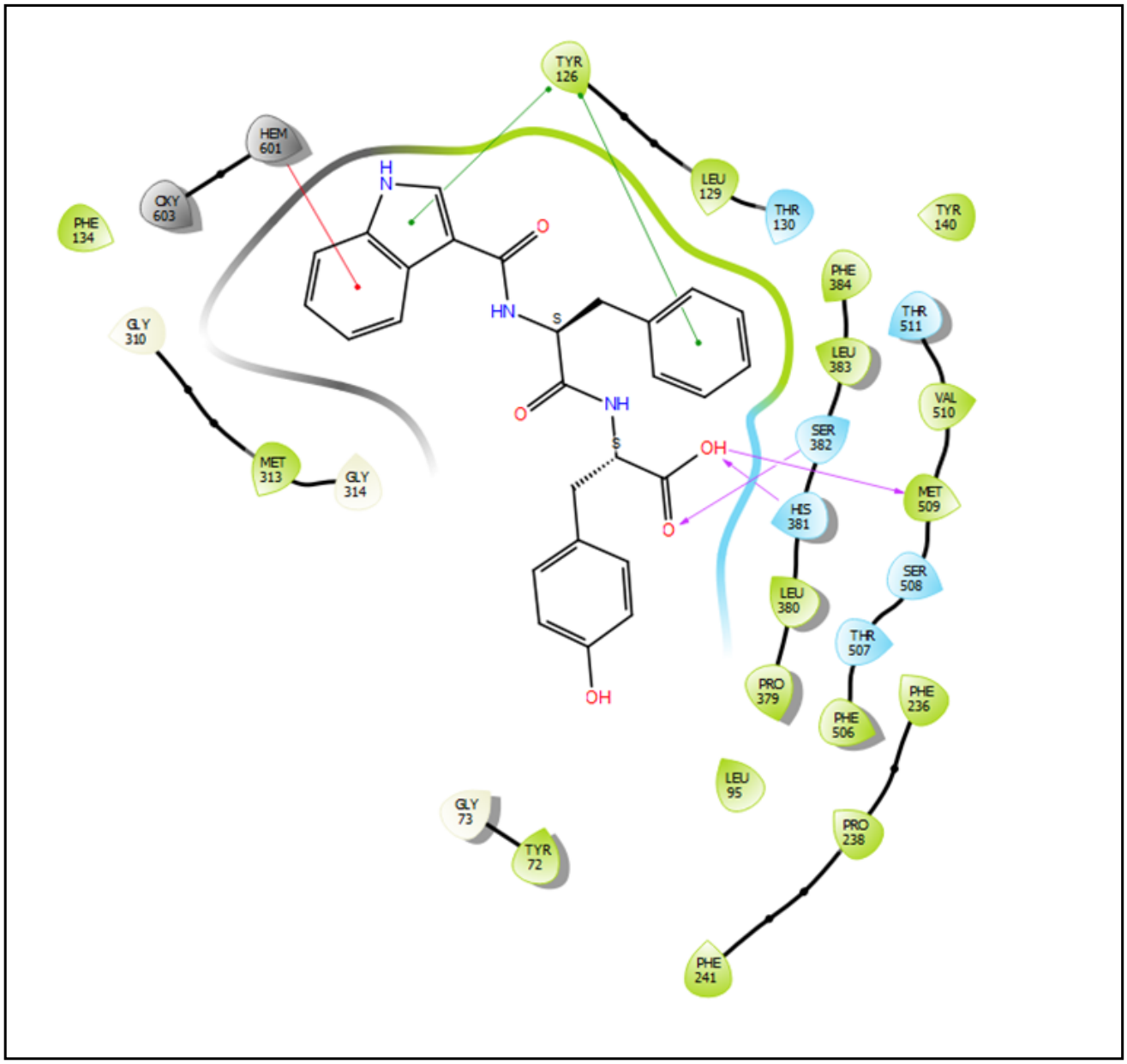


Figure S4. The binding poses and intermolecular interactions of **ID-6e** with lanosterol 14-alpha demethylase.

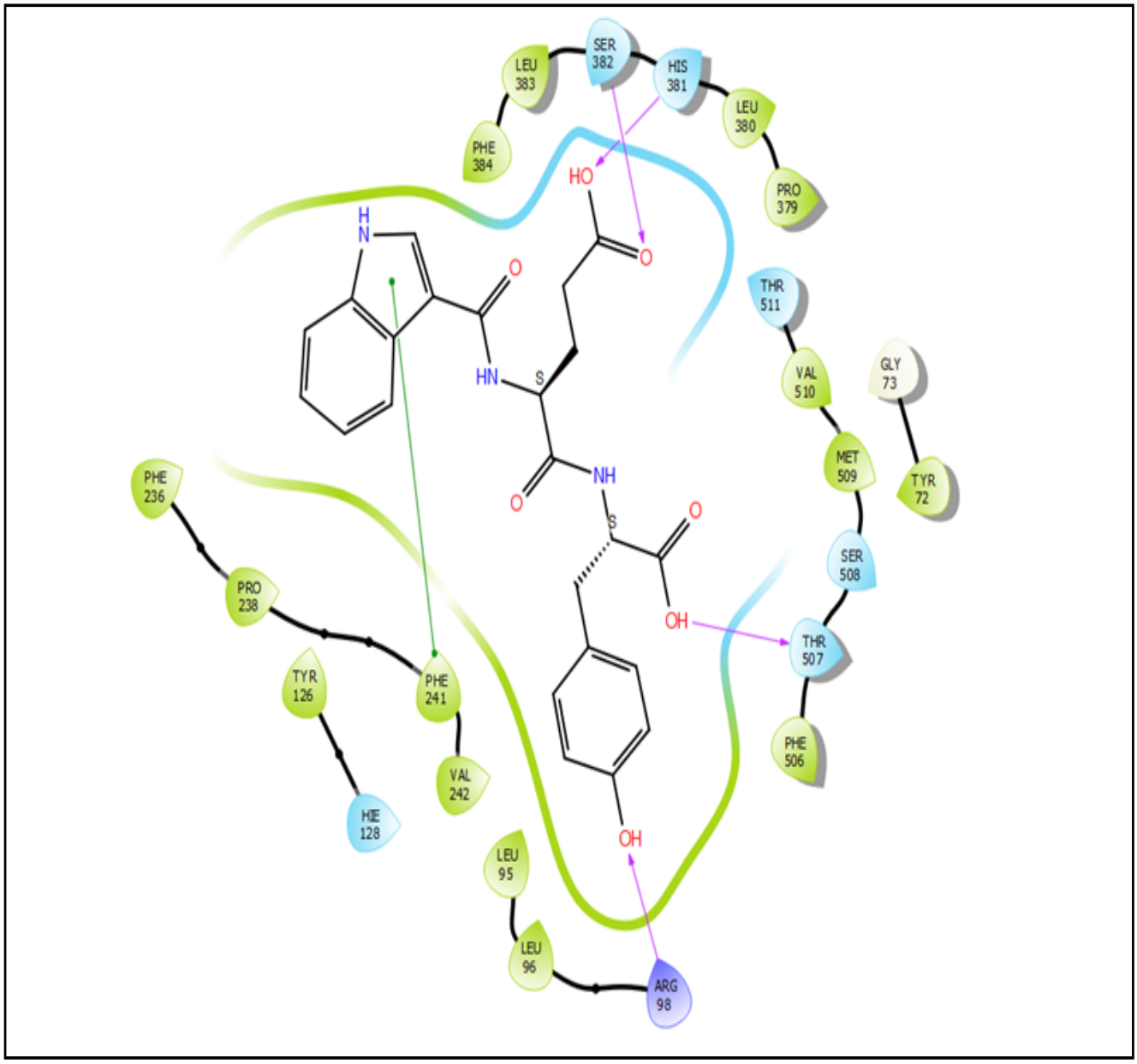


Figure S5. The binding poses and intermolecular interactions of **ID-6f** with lanosterol 14-alpha demethylase.

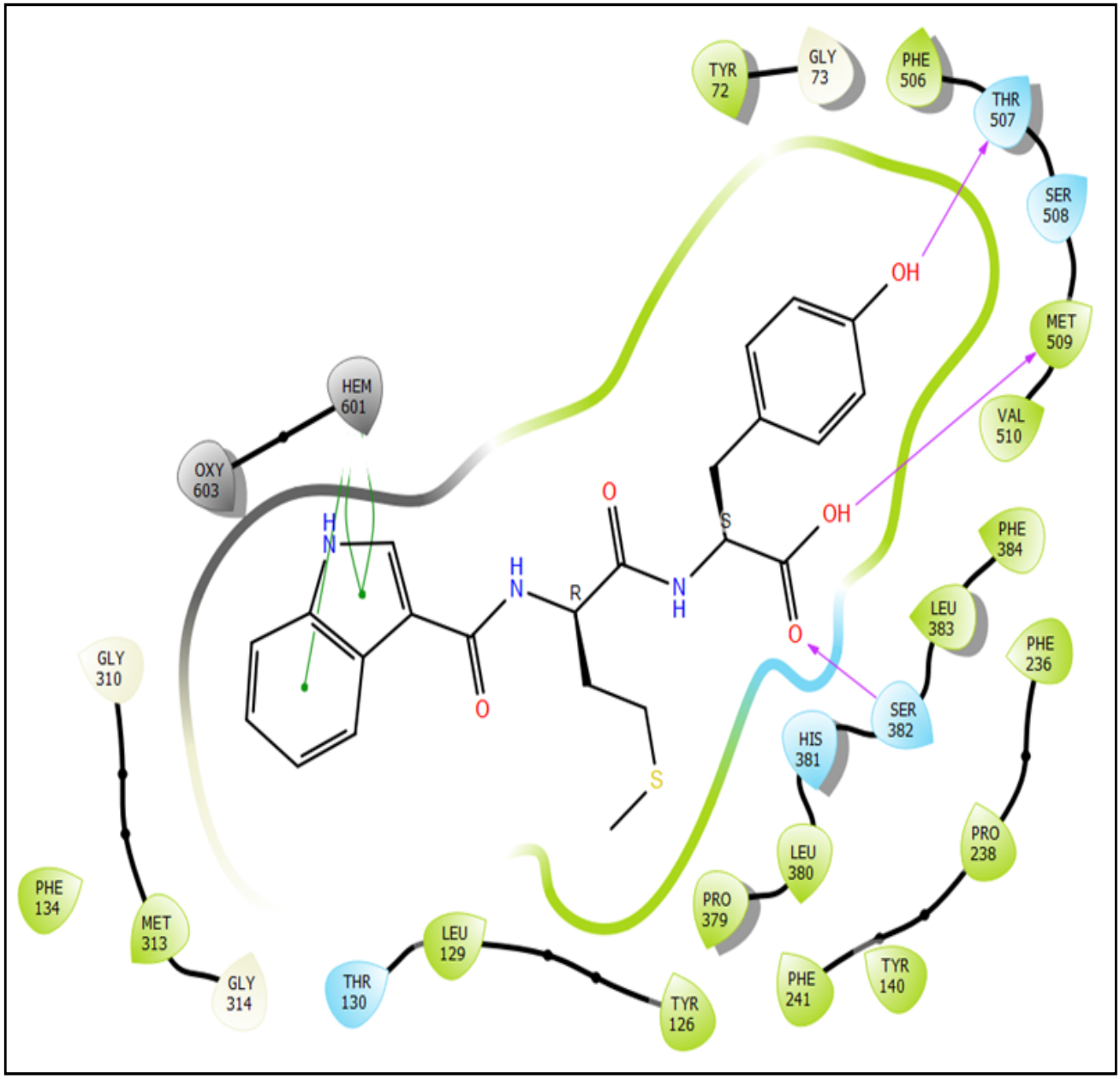


Figure S6. The binding poses and intermolecular interactions of **ID-6g** with lanosterol 14-alpha demethylase.

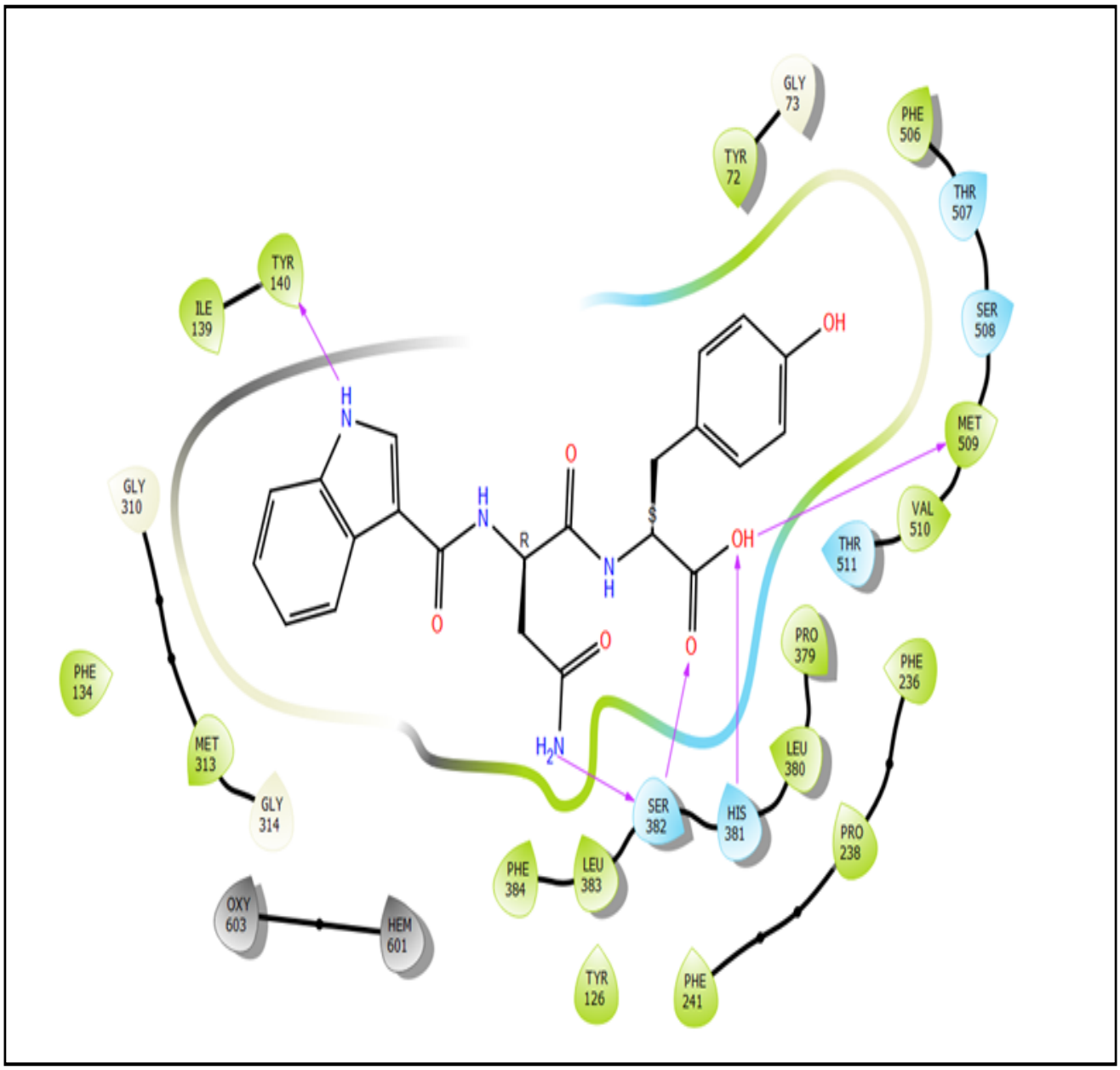


Figure S7. The binding poses and intermolecular interactions of **ID-6h** with lanosterol 14-alpha demethylase.

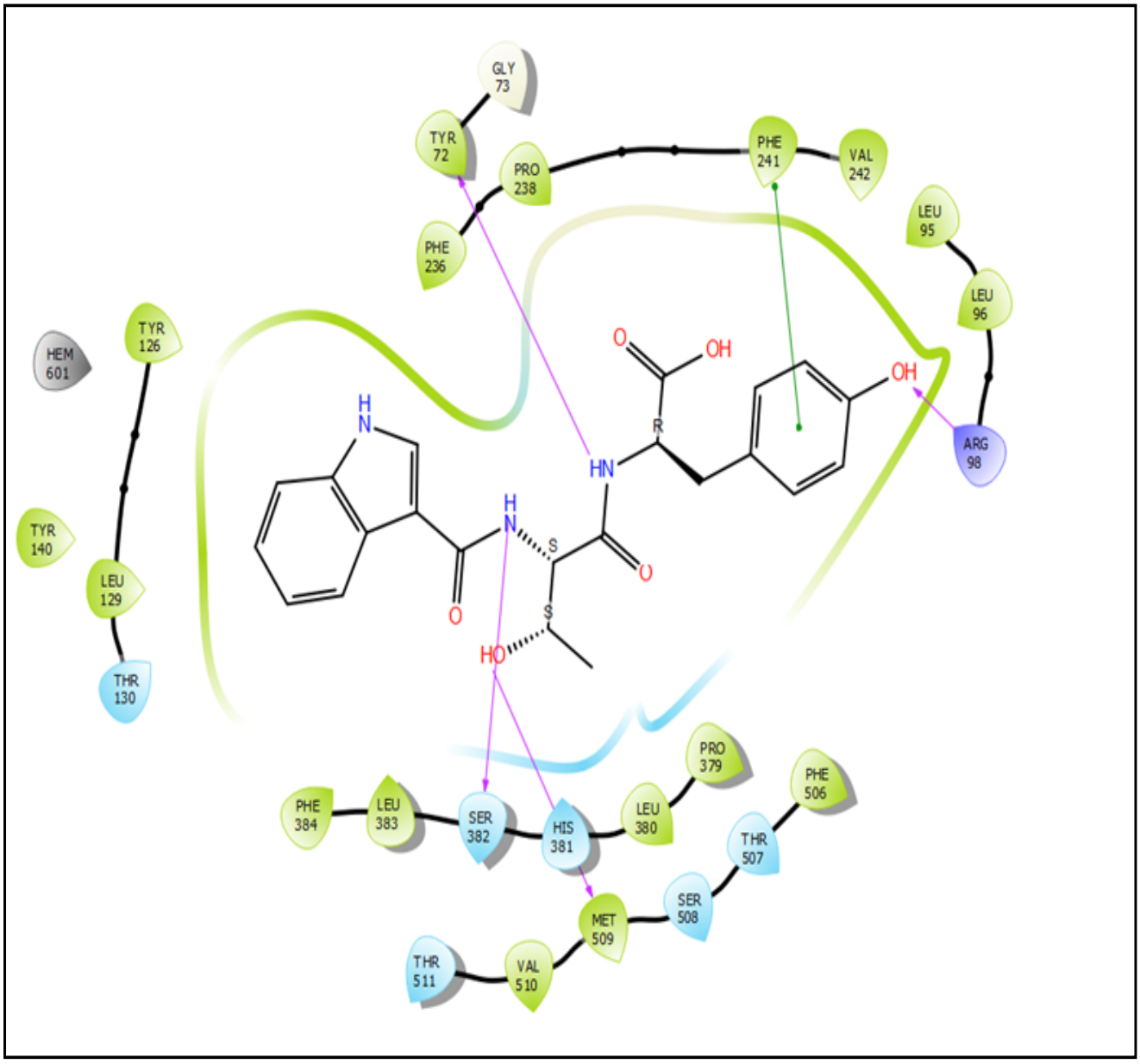


Figure S8. The binding poses and intermolecular interactions of **ID-6i** with lanosterol 14-alpha demethylase.

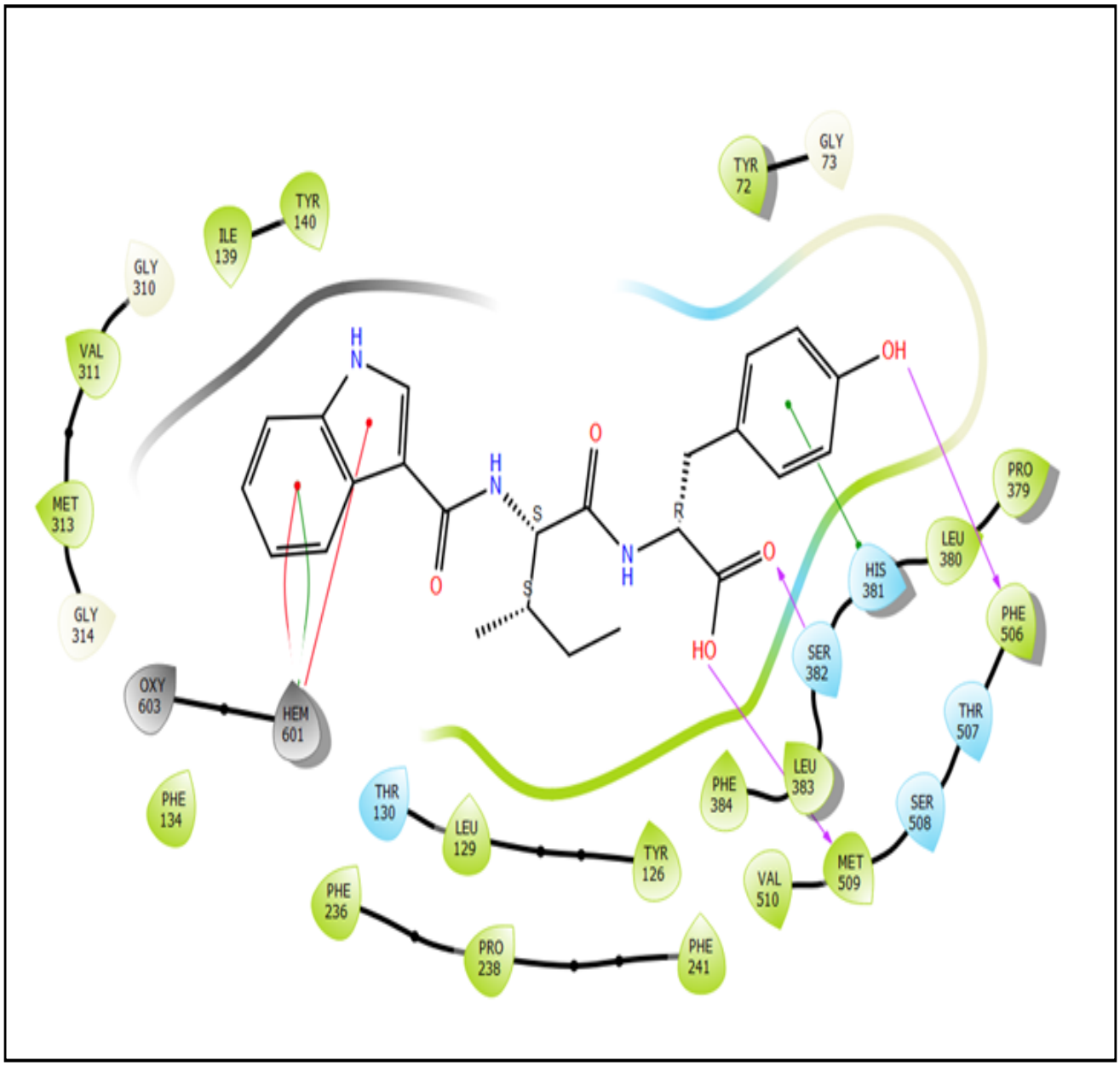


Figure S9. The binding poses and intermolecular interactions of **ID-6j** with lanosterol 14-alpha demethylase.

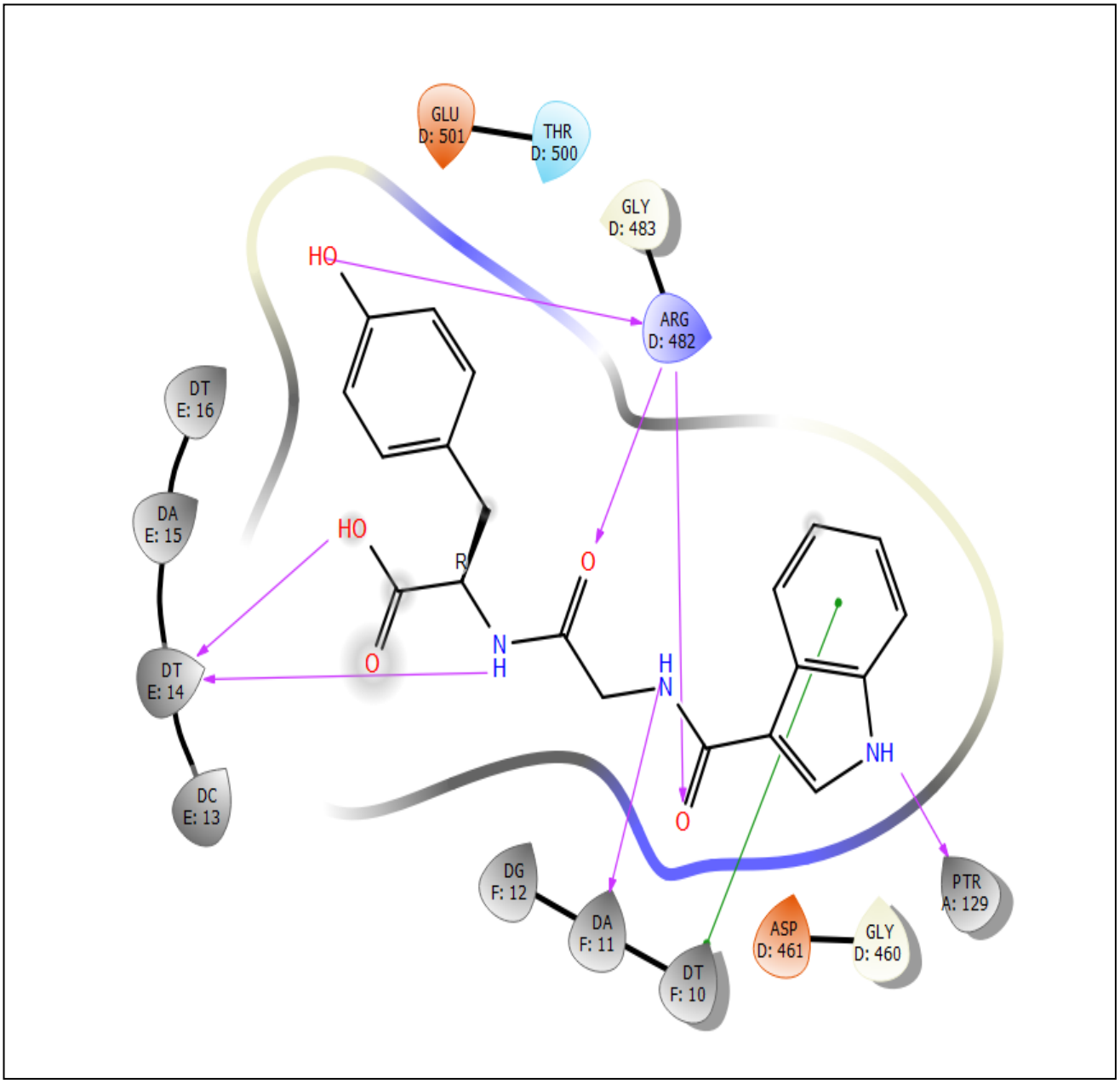


Figure S10. The binding poses of **ID-6b** and its intermolecular interactions with DNA gyrase.

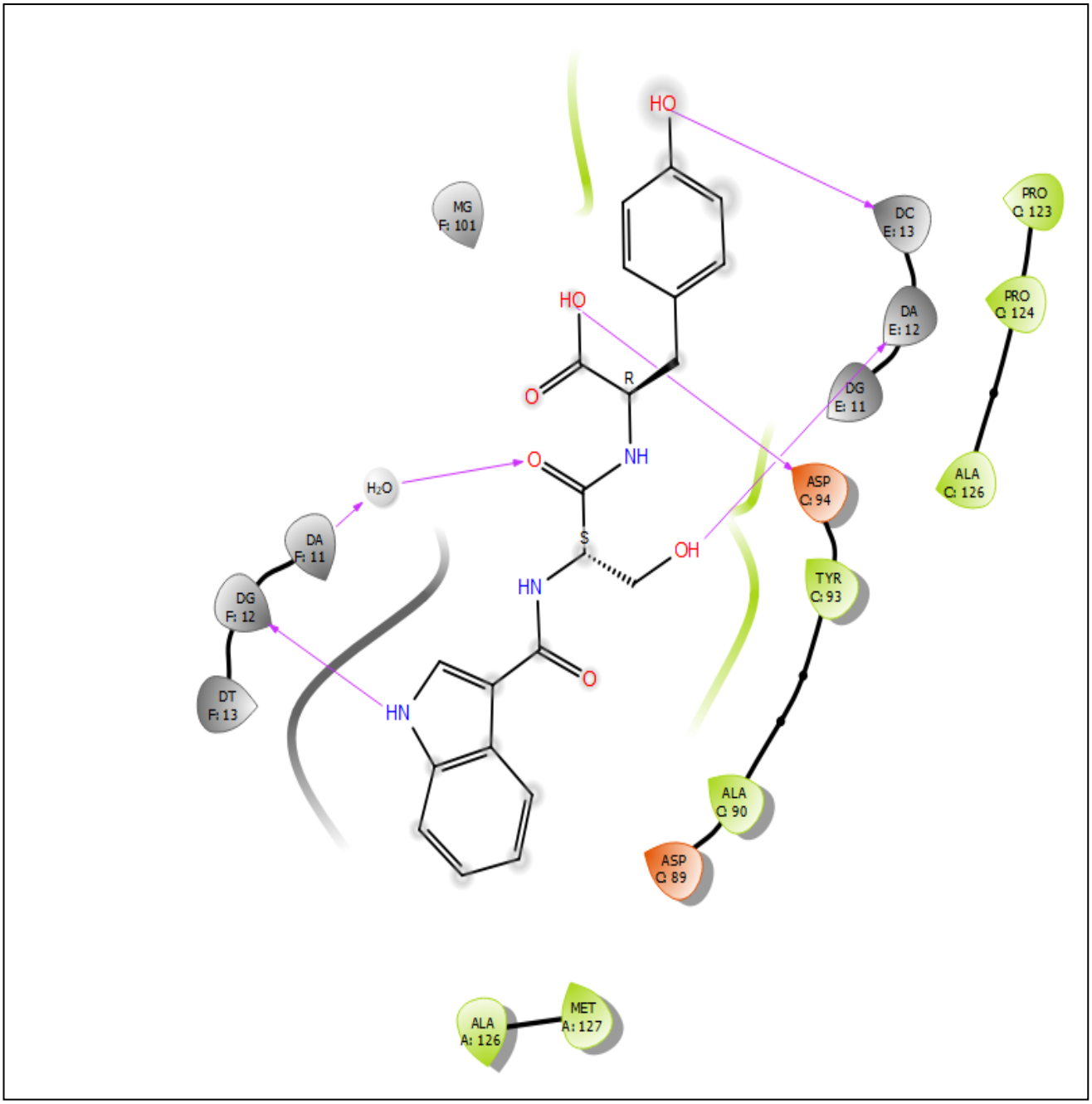


Figure S11. The binding poses of **ID-6d** and its intermolecular interactions with DNA gyrase.

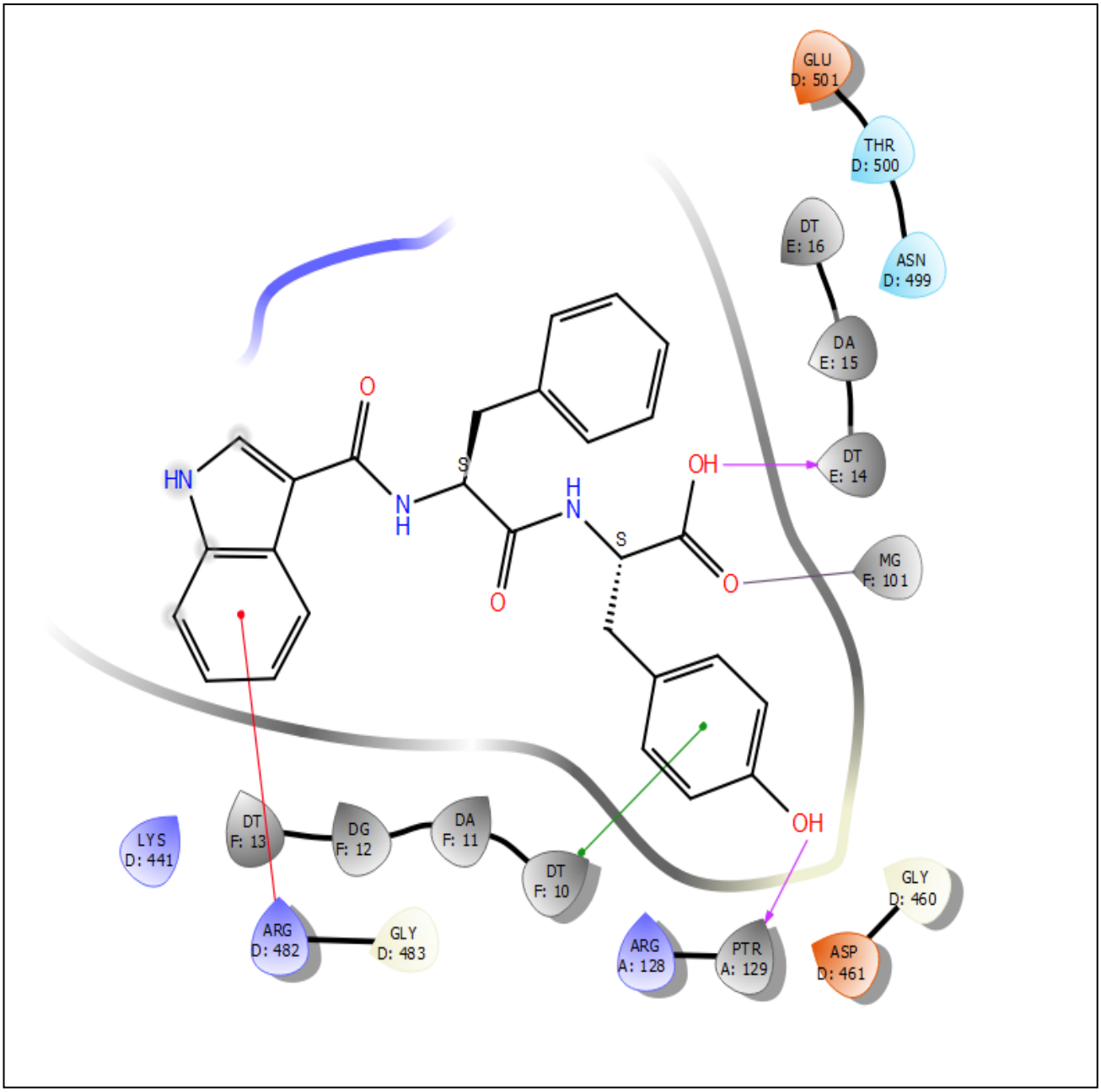


Figure S11. The binding poses of **ID-6e** and its intermolecular interactions with DNA gyrase.

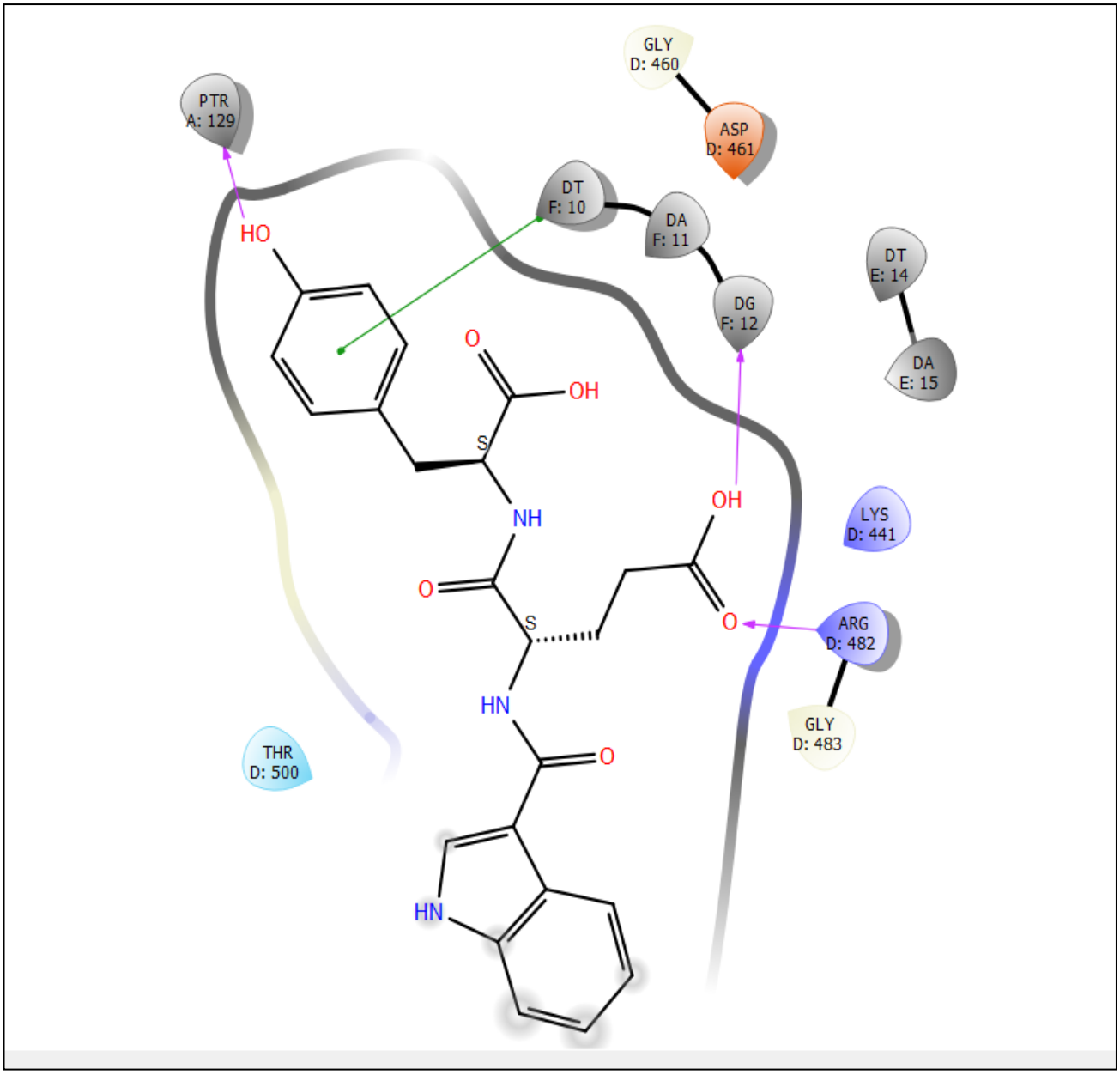


Figure S12. The binding poses of **ID-6f** and its intermolecular interactions with DNA gyrase.

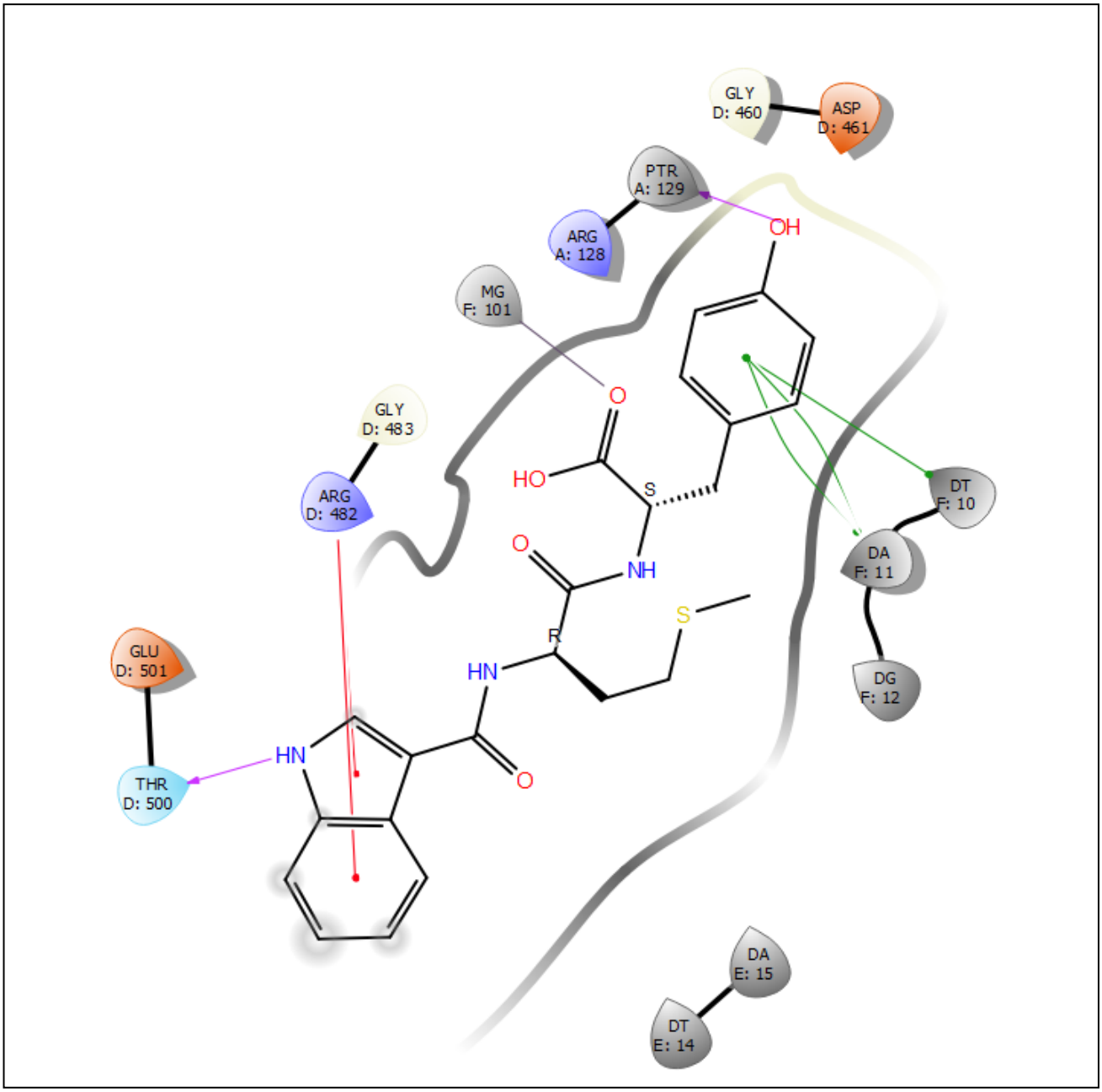


Figure S13. The binding poses of **ID-6g** and its intermolecular interactions with DNA gyrase.

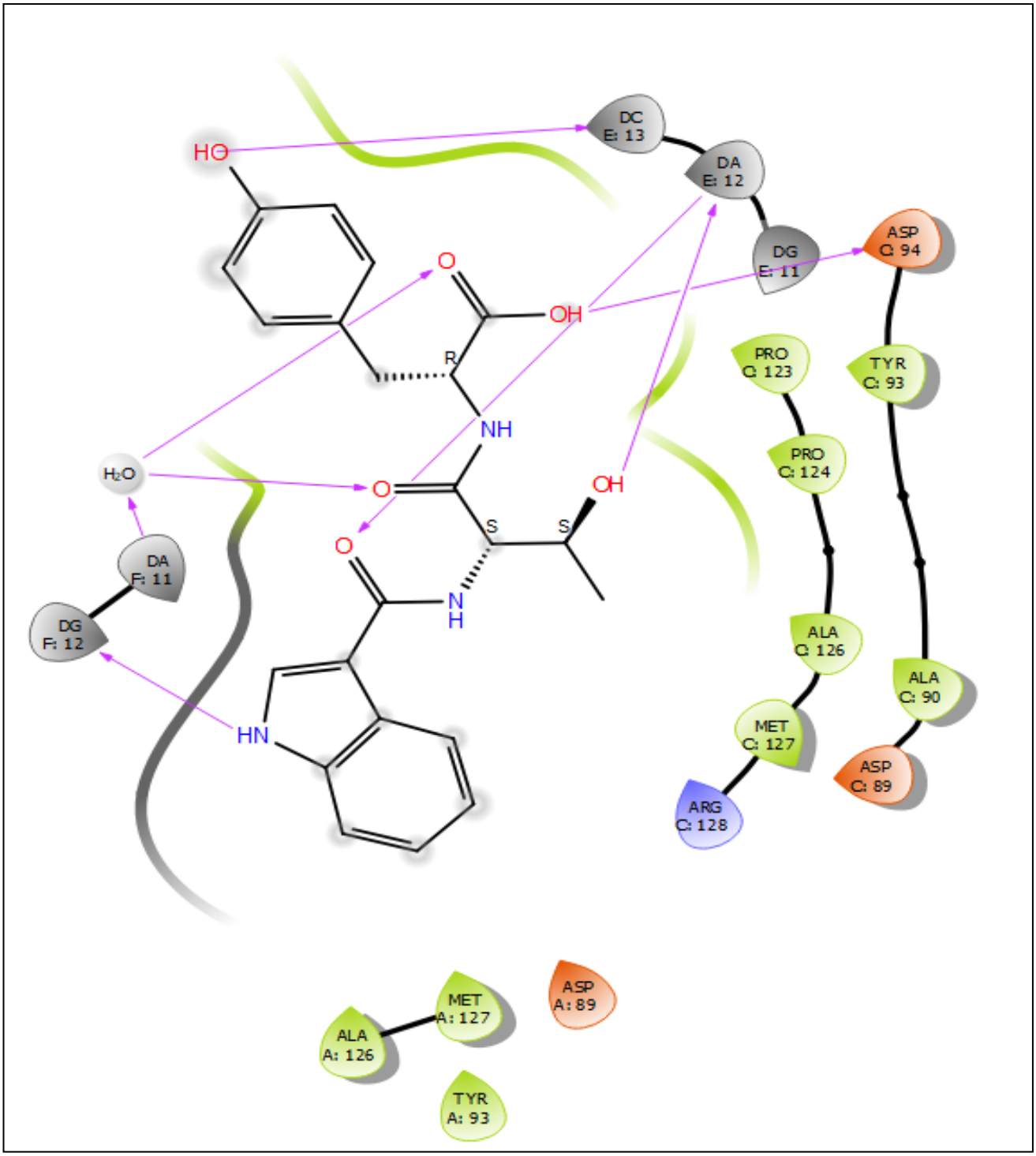


Figure S14. The binding poses of **ID-6i** and its intermolecular interactions with DNA gyrase.

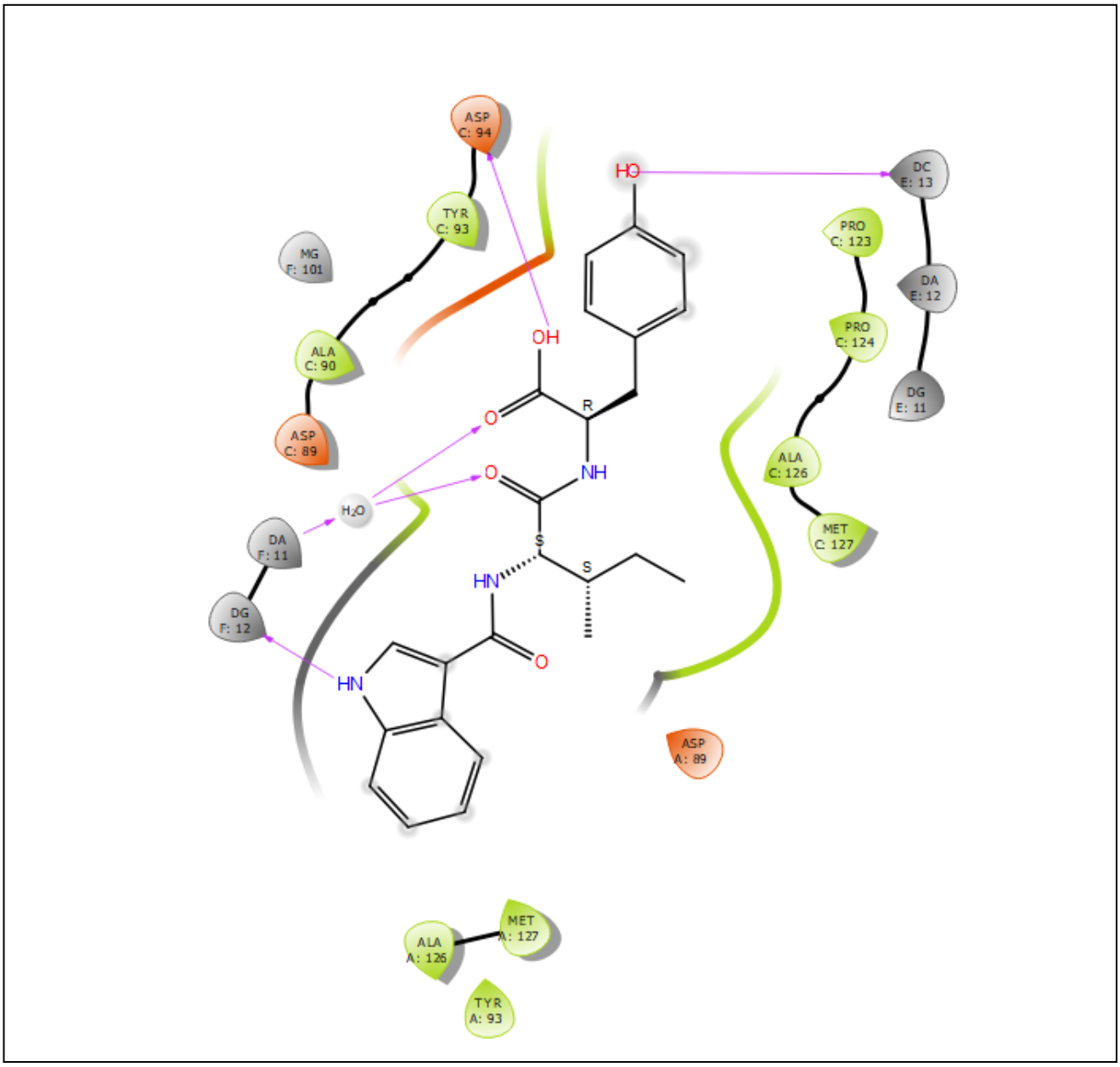


Figure S15. The binding poses of **ID-6j** and its intermolecular interactions with DNA gyrase.

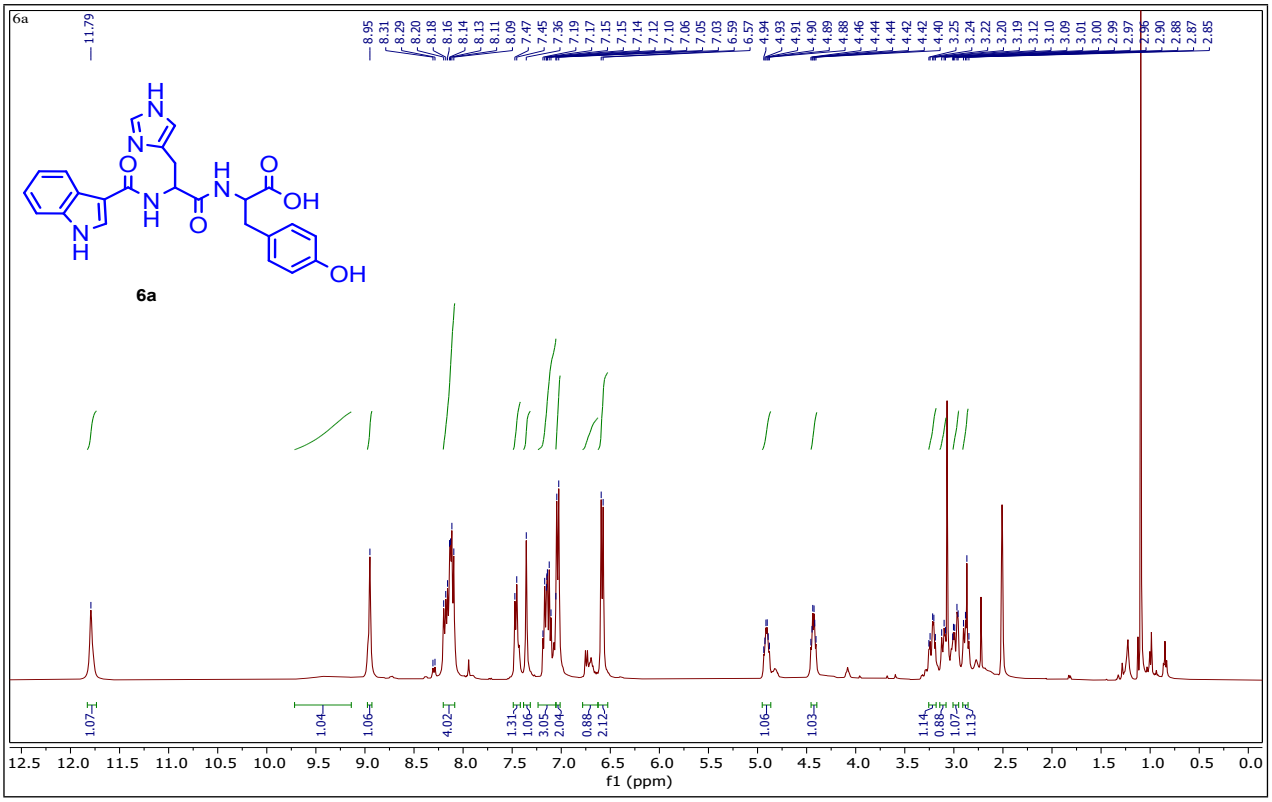


Figure S16. ^{1}H NMR of compound **6a**.

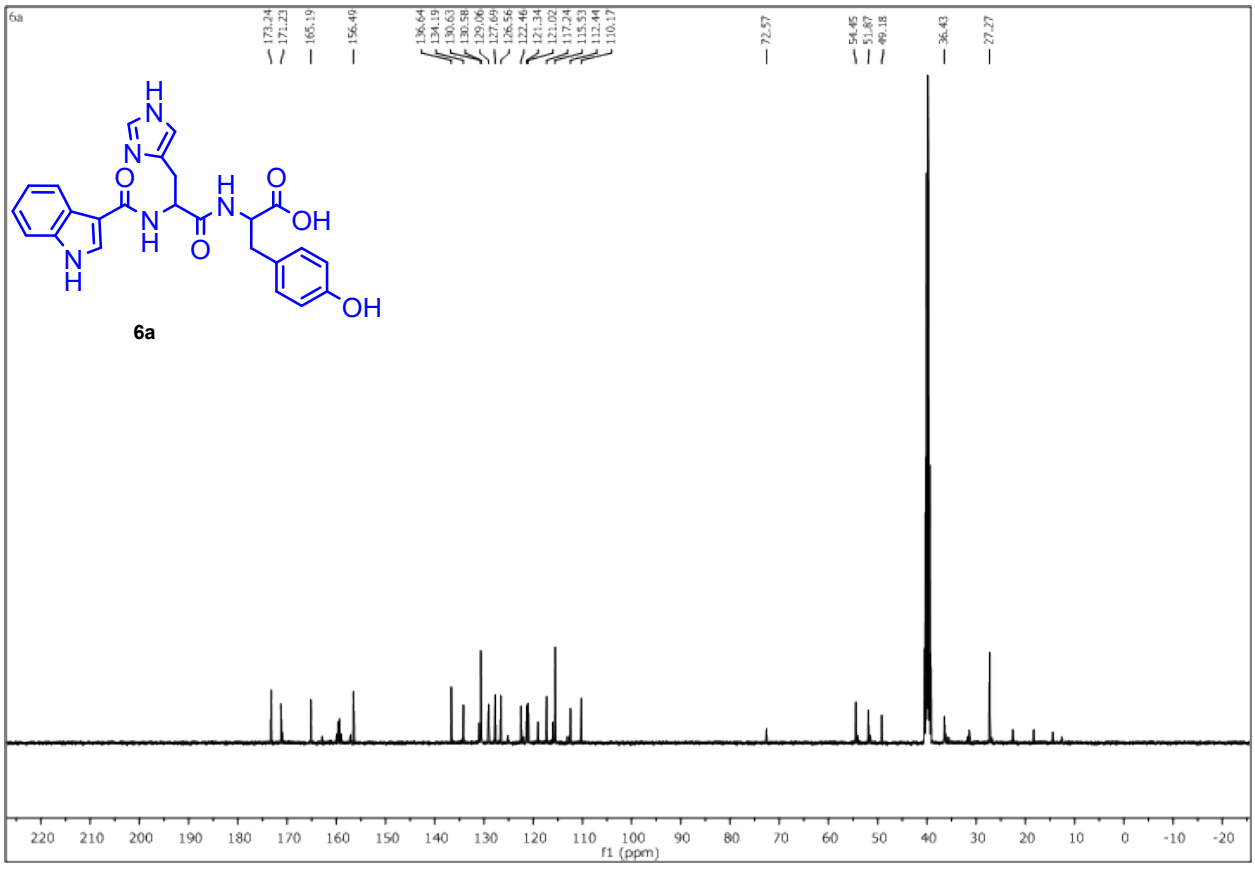


Figure S17. ^{13}C NMR of compound **6a**.

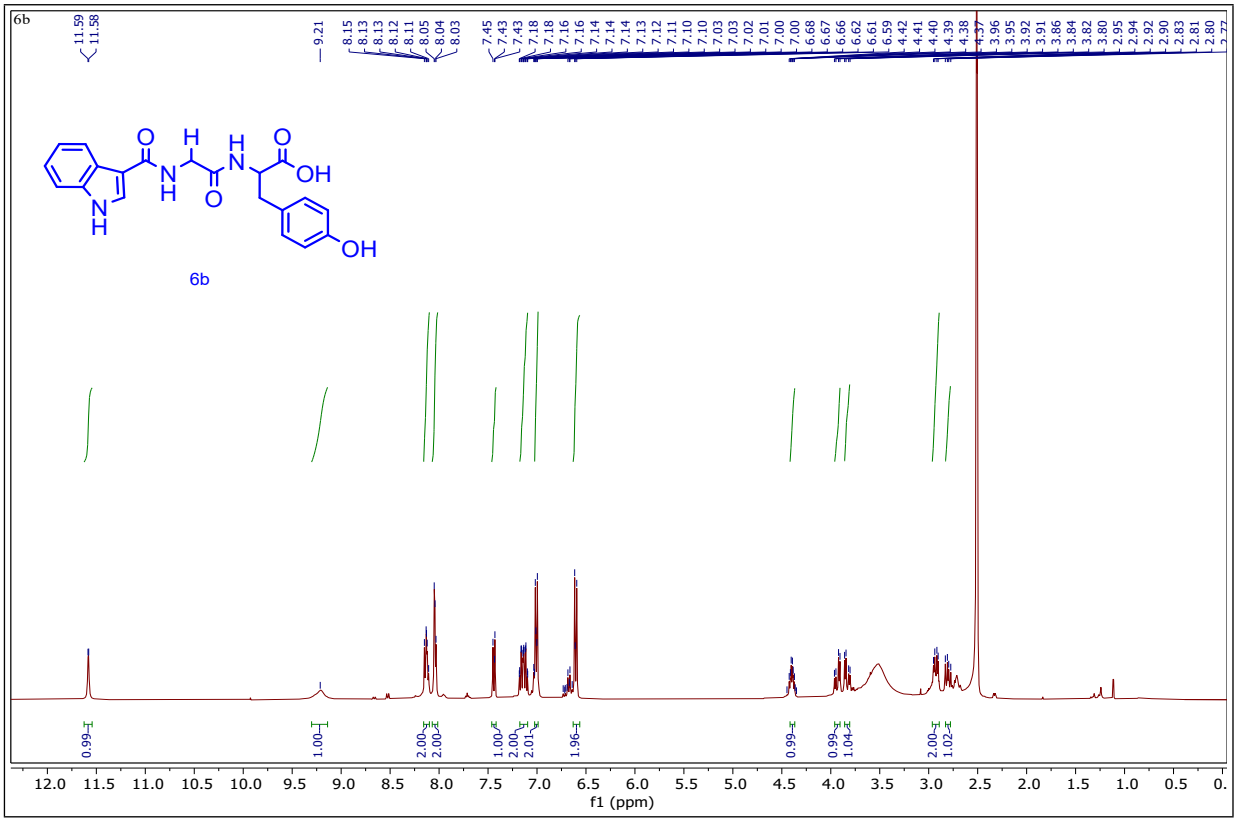


Figure S18. ^{1}H NMR of compound **6b**.

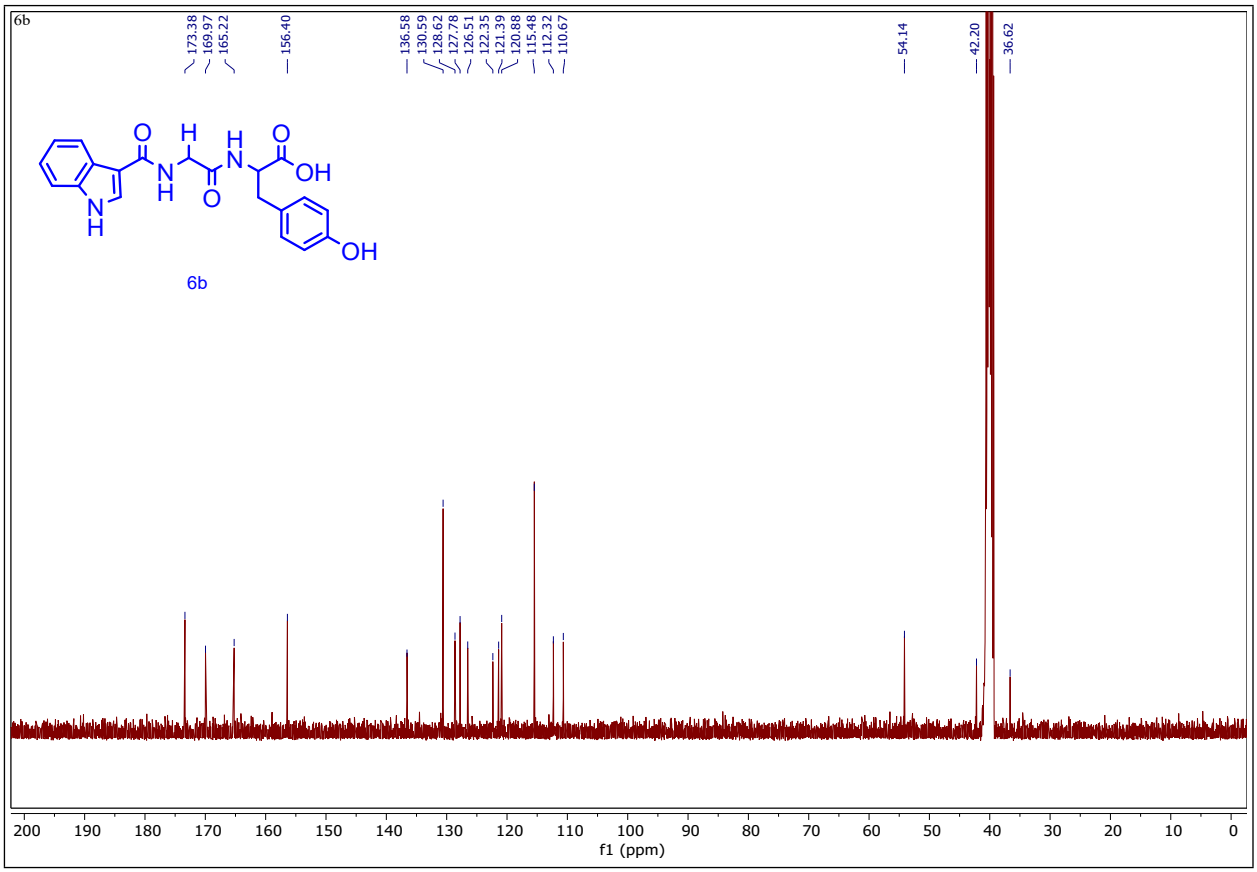


Figure S19. ^{13}C NMR of compound **6b**.

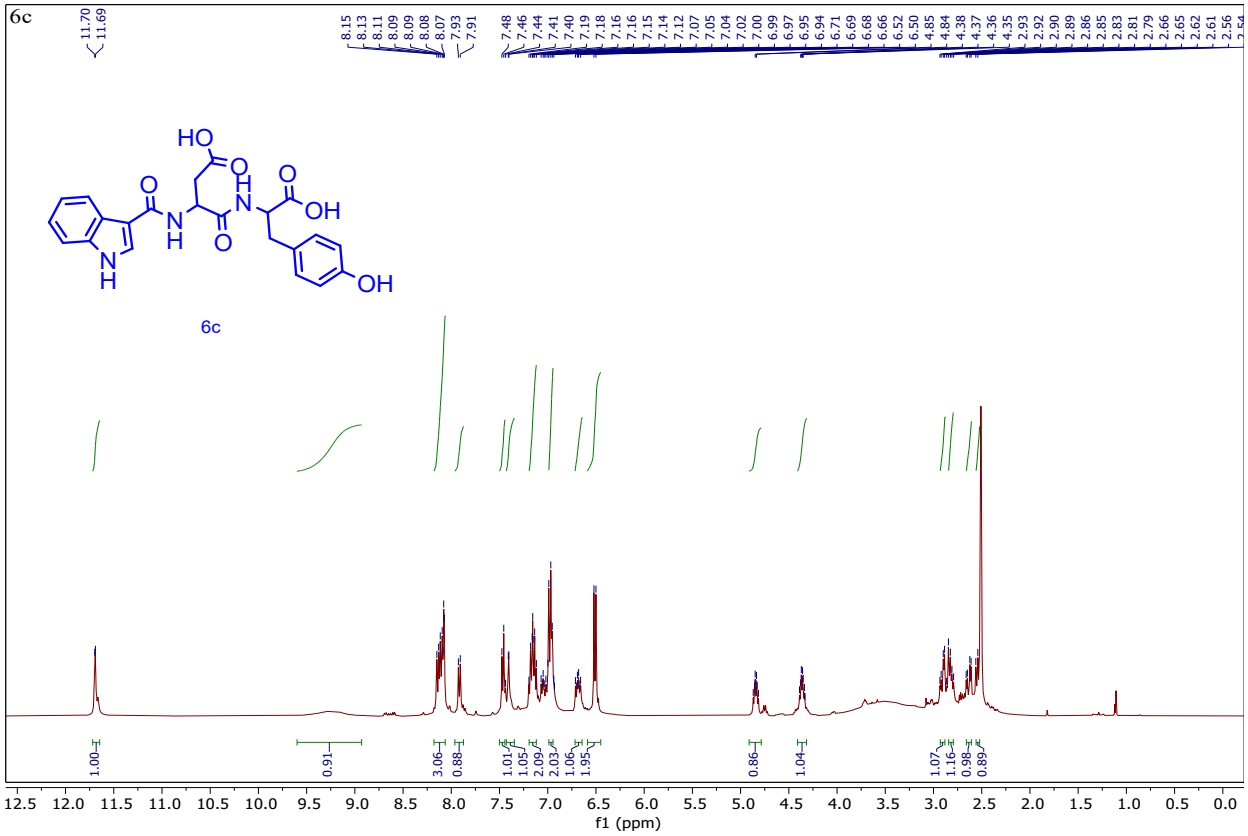


Figure S20. ^{1}H NMR of compound **6c**.

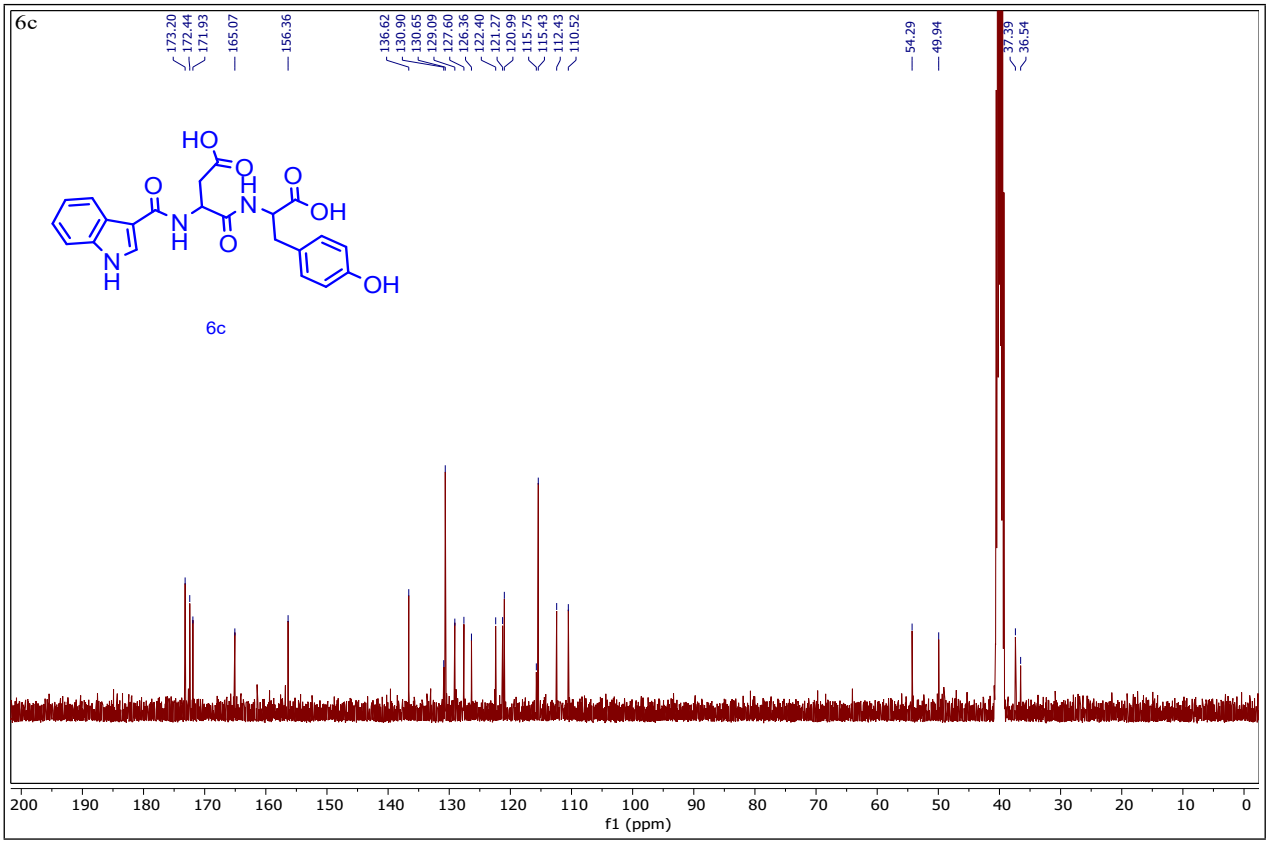


Figure S21. ^{13}C NMR of compound **6c**.

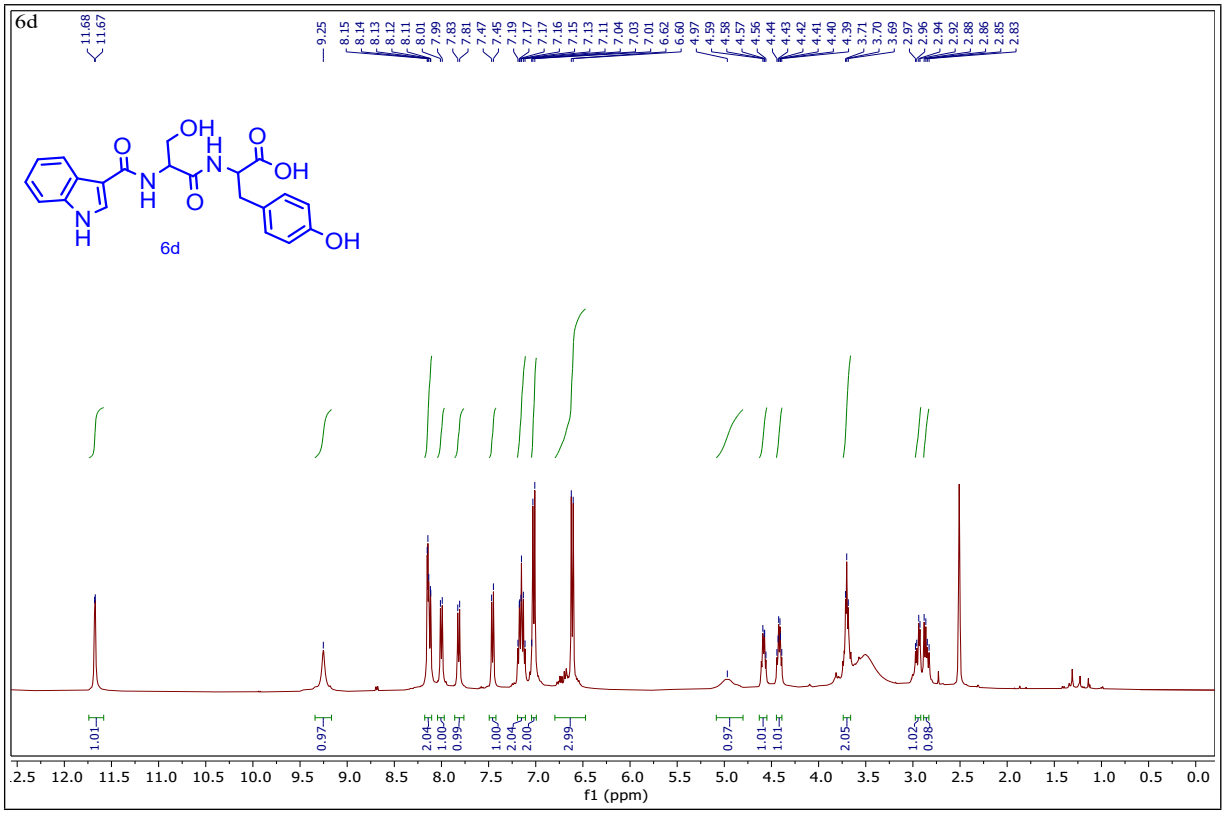


Figure S22. ^{1}H NMR of compound **6d**.

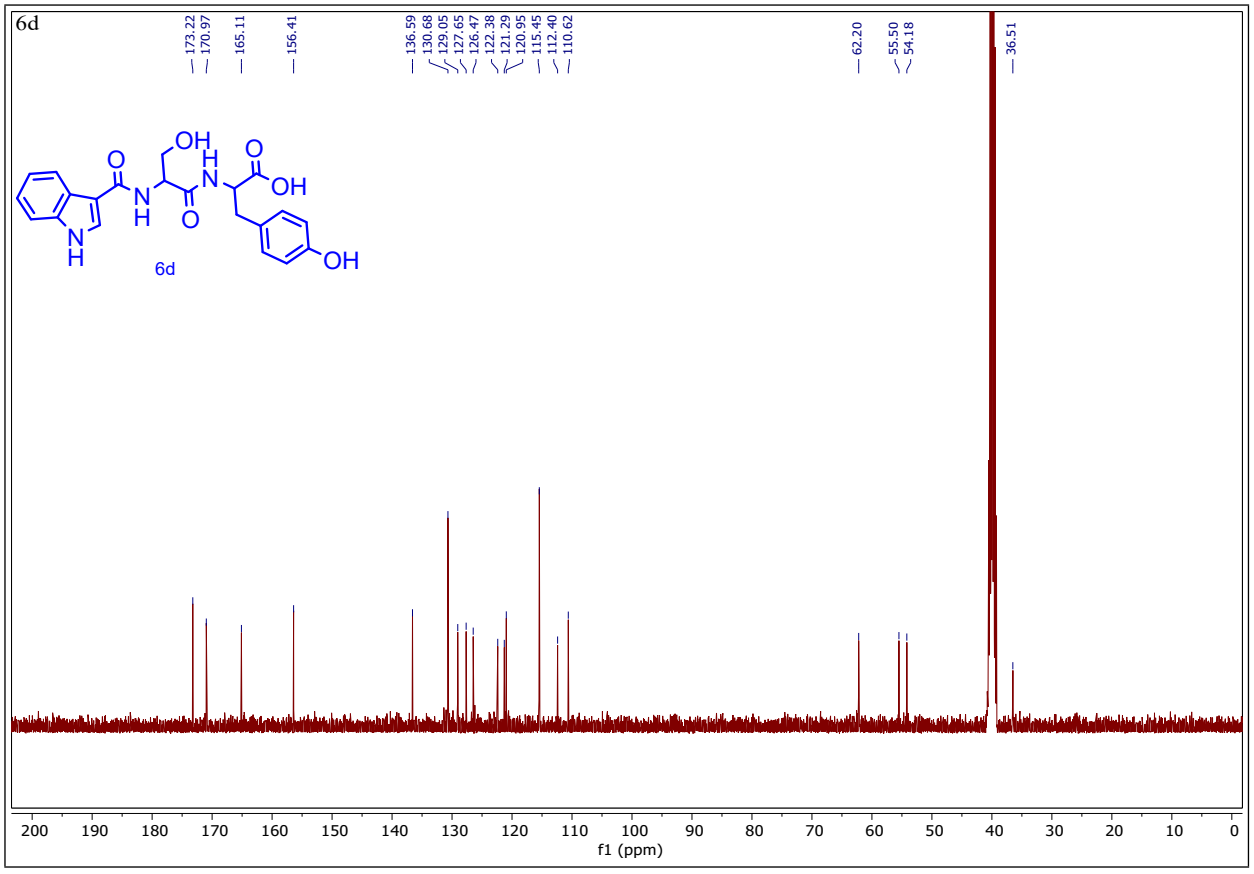


Figure S23. ^{13}C NMR of compound **6d**.

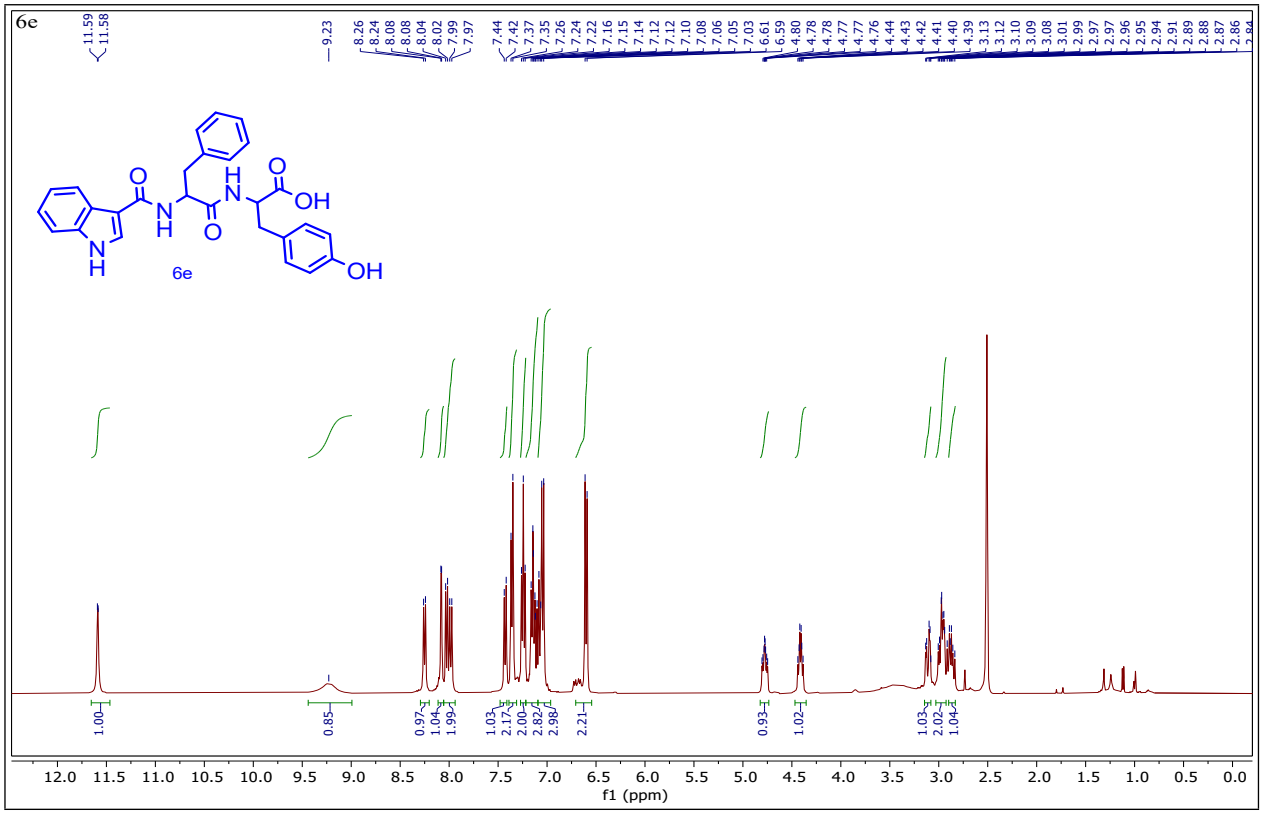


Figure S24. ^{1}H NMR of compound **6e**.

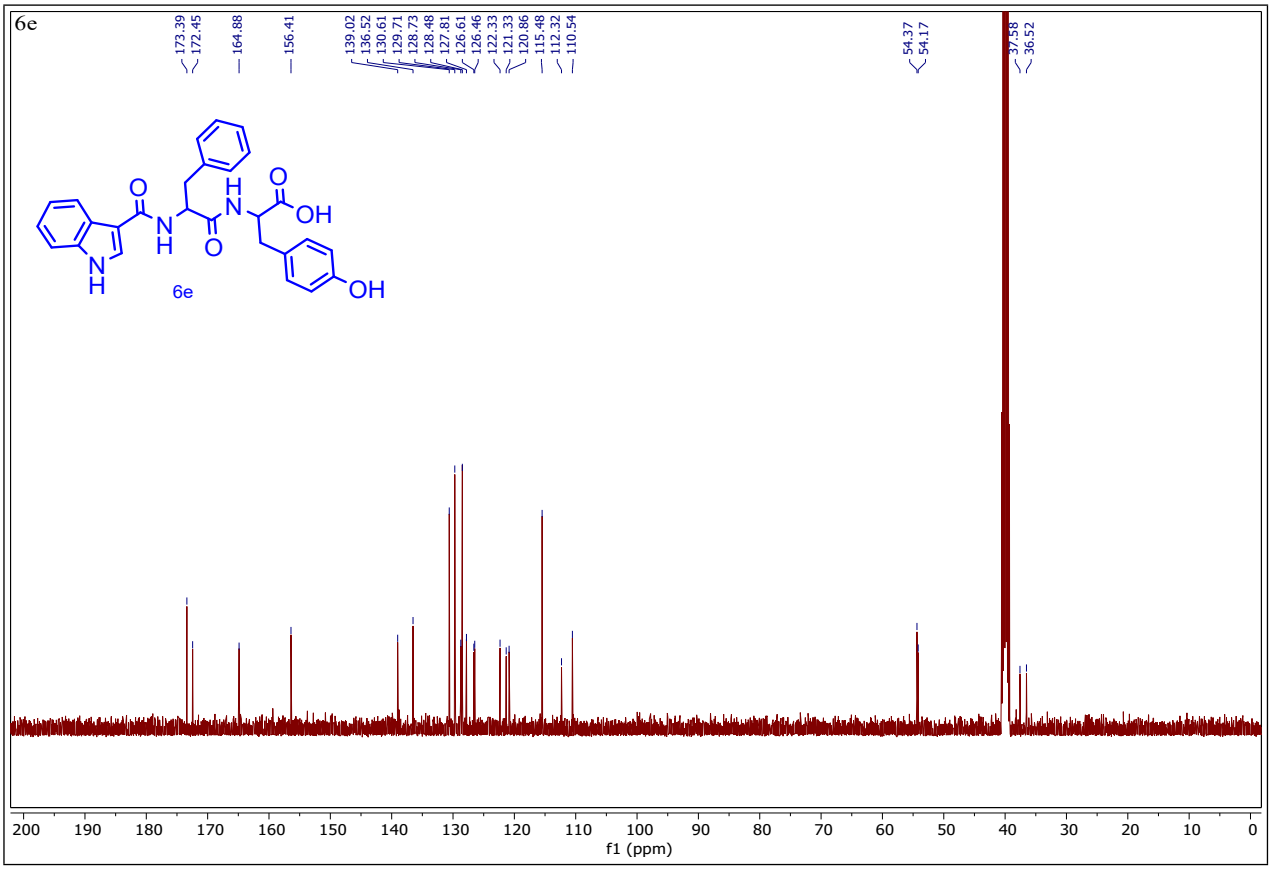


Figure S25. ^{13}C NMR of compound **6e**.

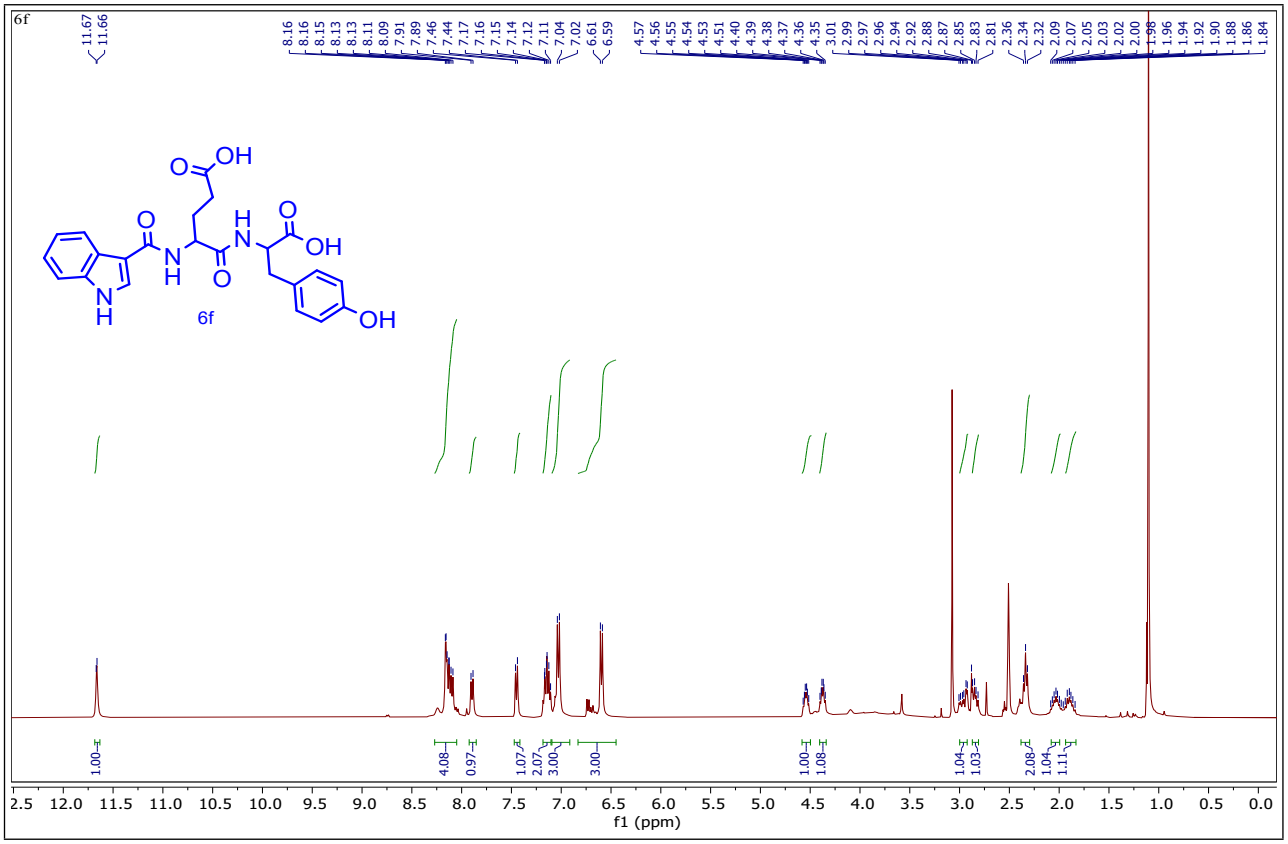


Figure S26. ^{1}H NMR of compound **6f**.

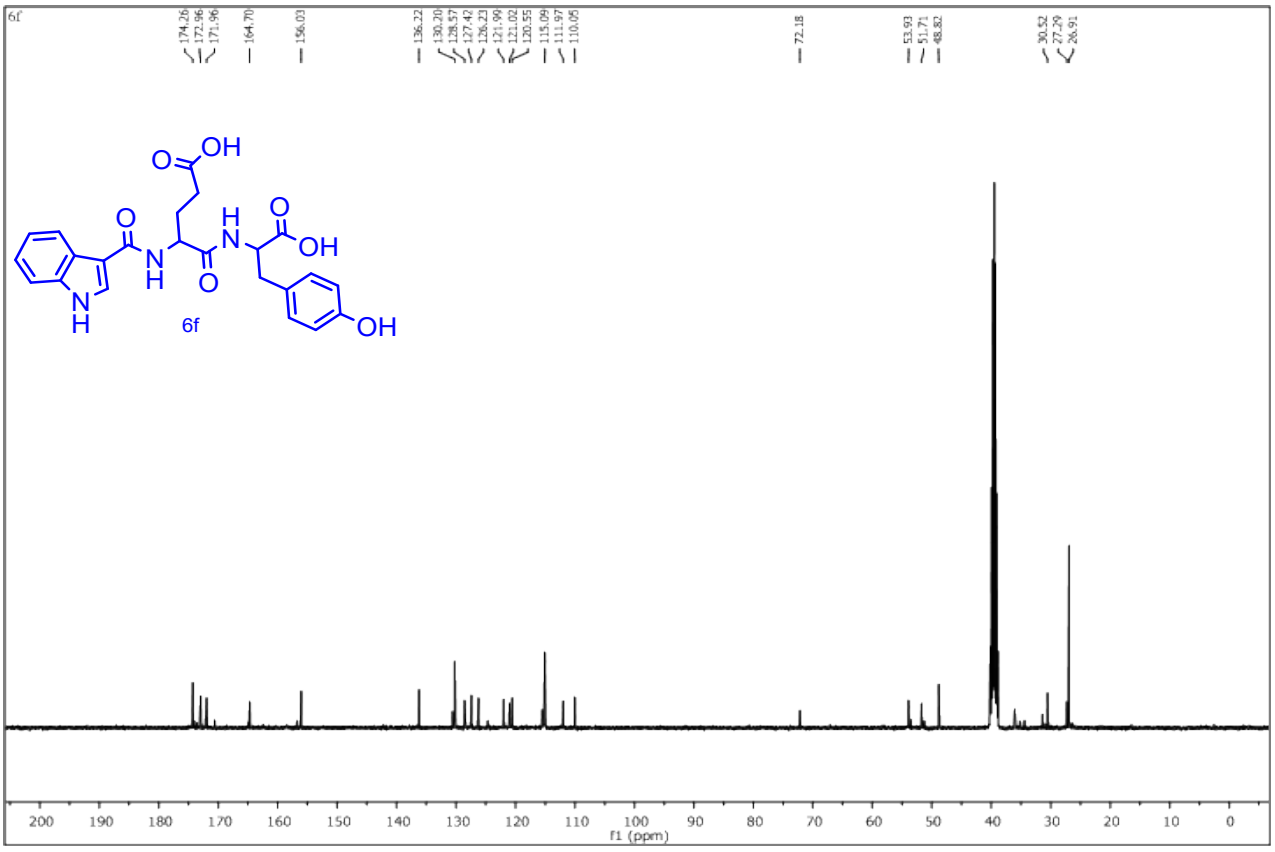


Figure S27. ^{13}C NMR of compound **6f**.

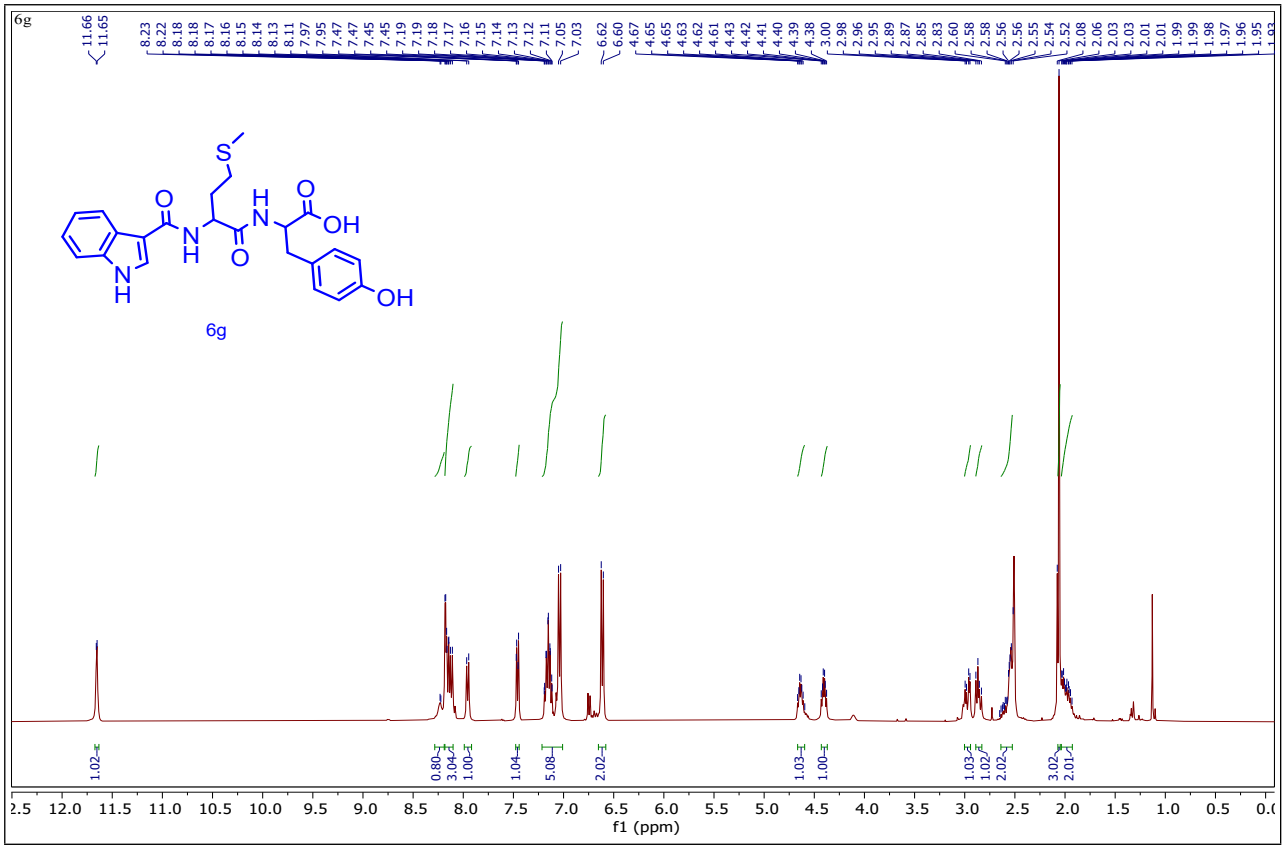


Figure S28. ^{1}H NMR of compound **6g**.

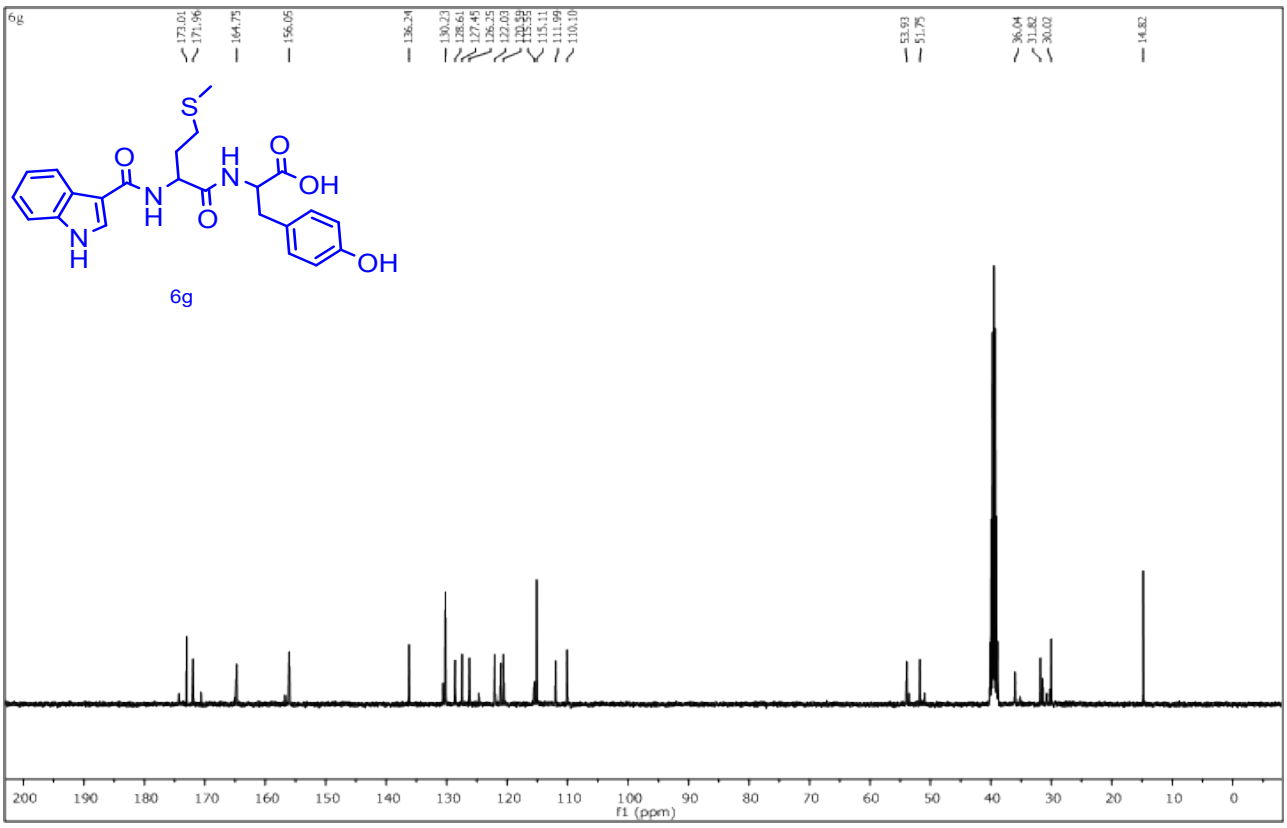


Figure S29. ^{13}C NMR of compound **6g**.

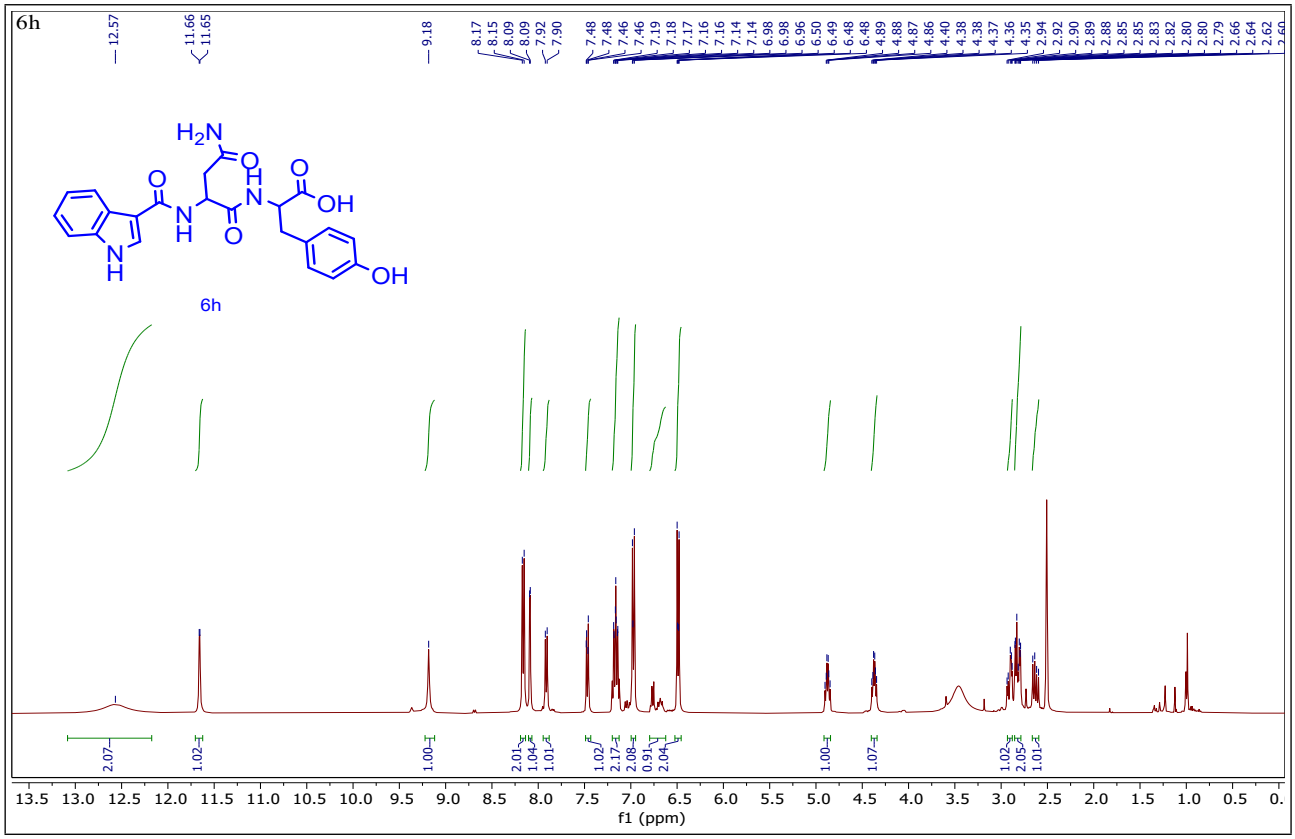


Figure S30. ^{1}H NMR of compound **6h**.

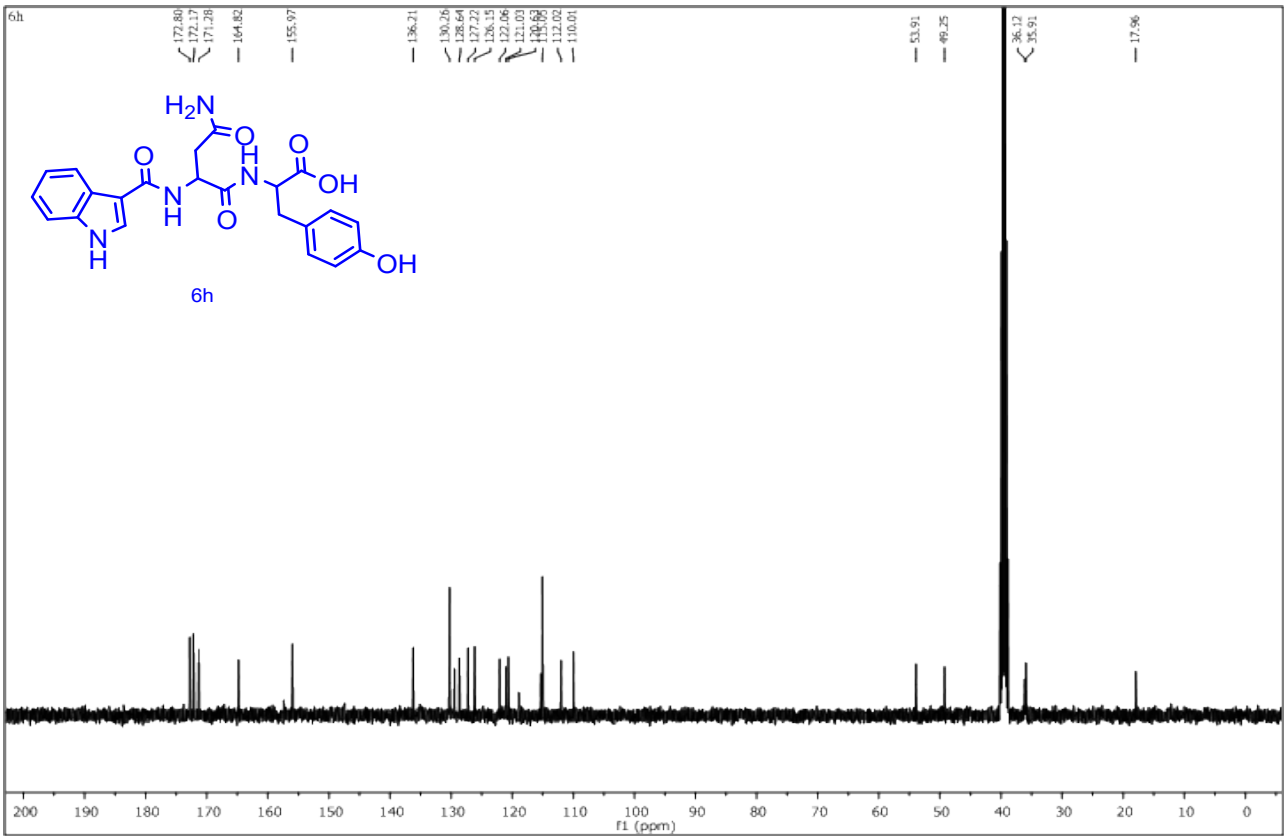


Figure S31. ^{13}C NMR of compound **6h**.

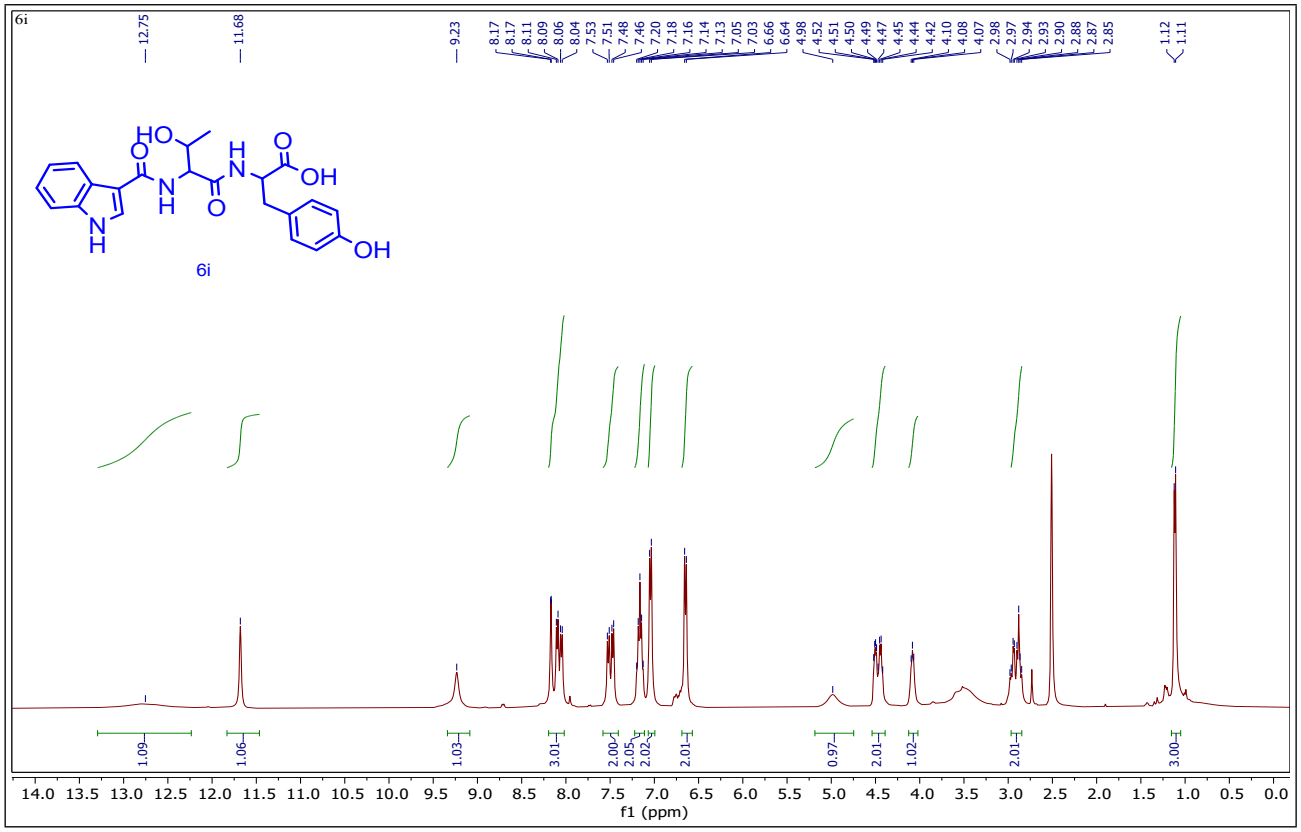


Figure S32. ^{1}H NMR of compound **6i**.

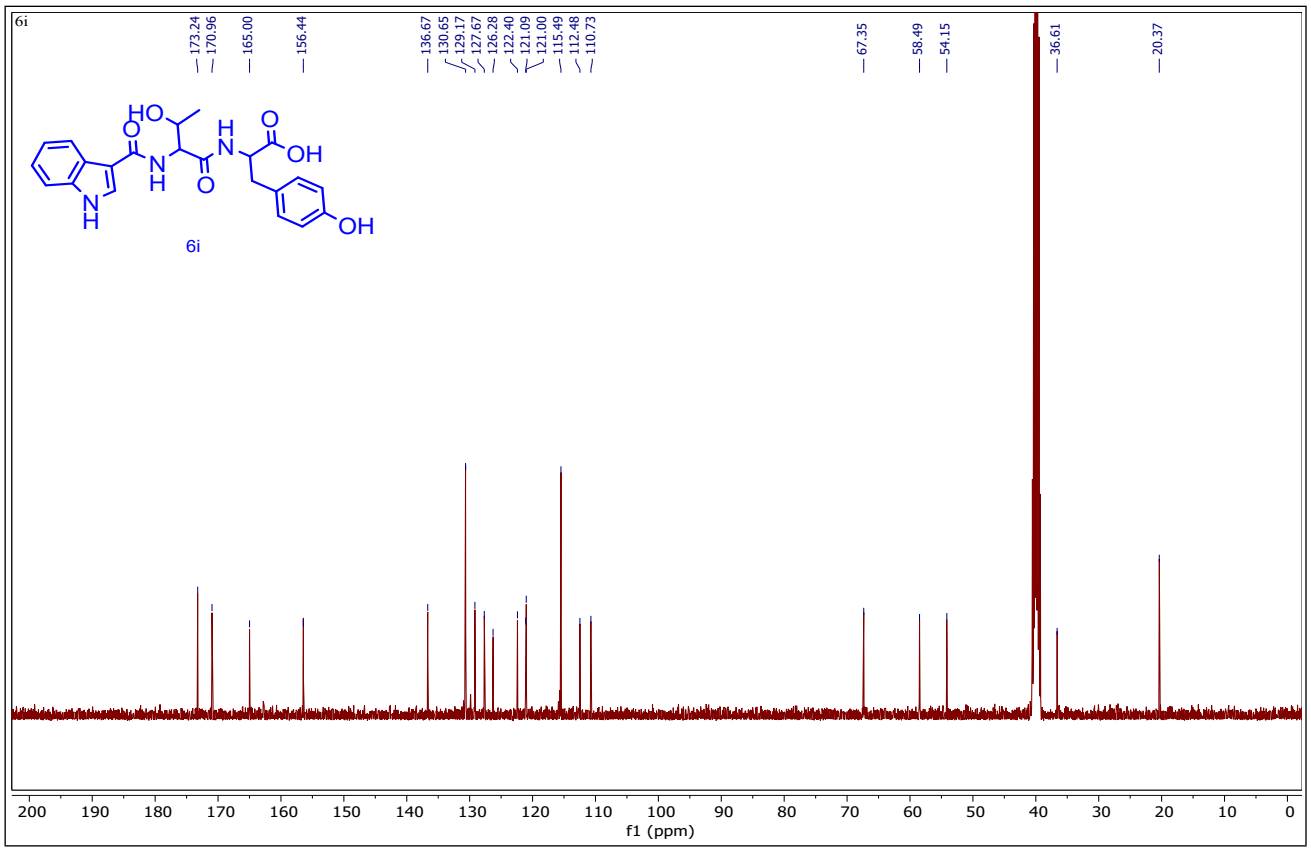


Figure S33. ^{13}C NMR of compound **6i**.

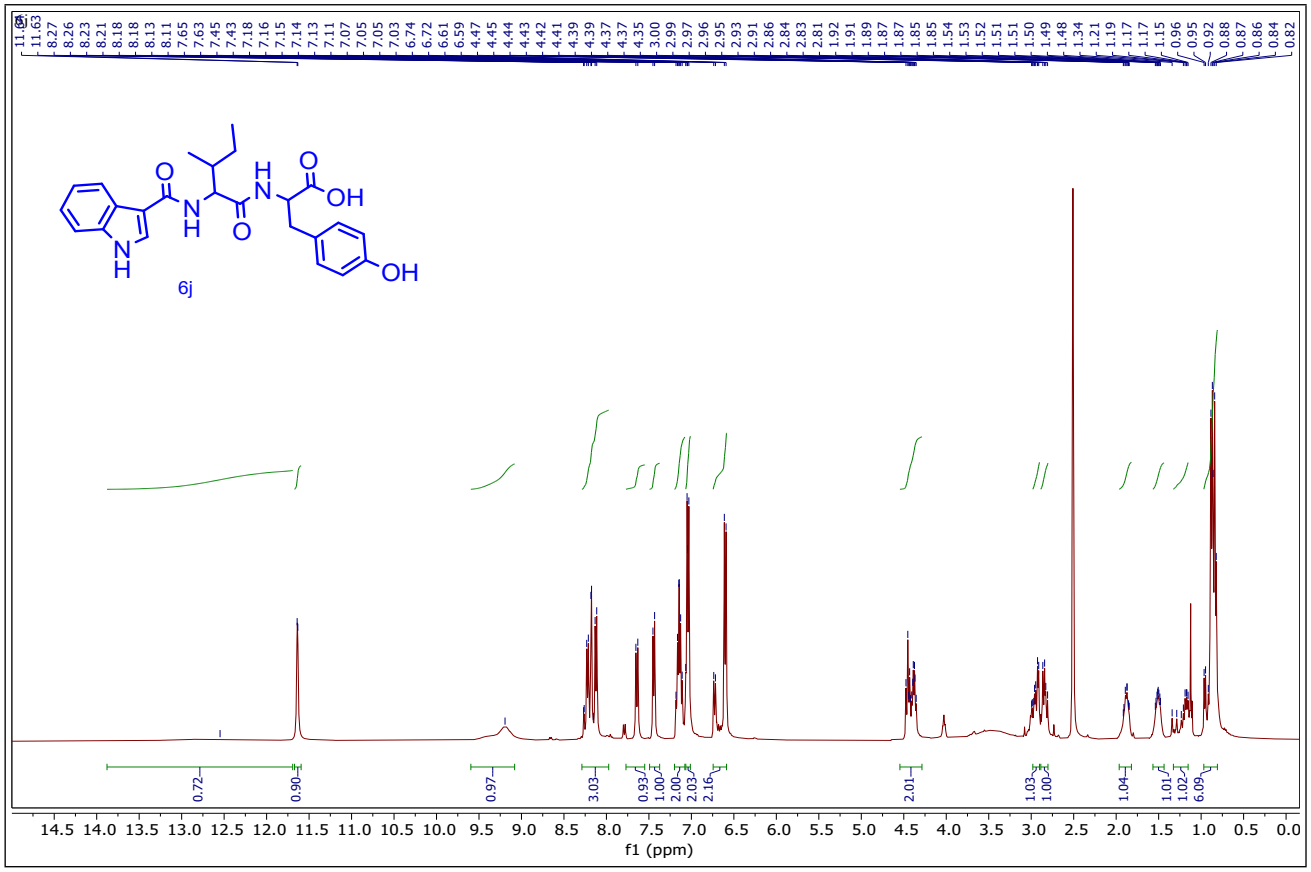


Figure S34. ^{1}H NMR of compound **6j**.

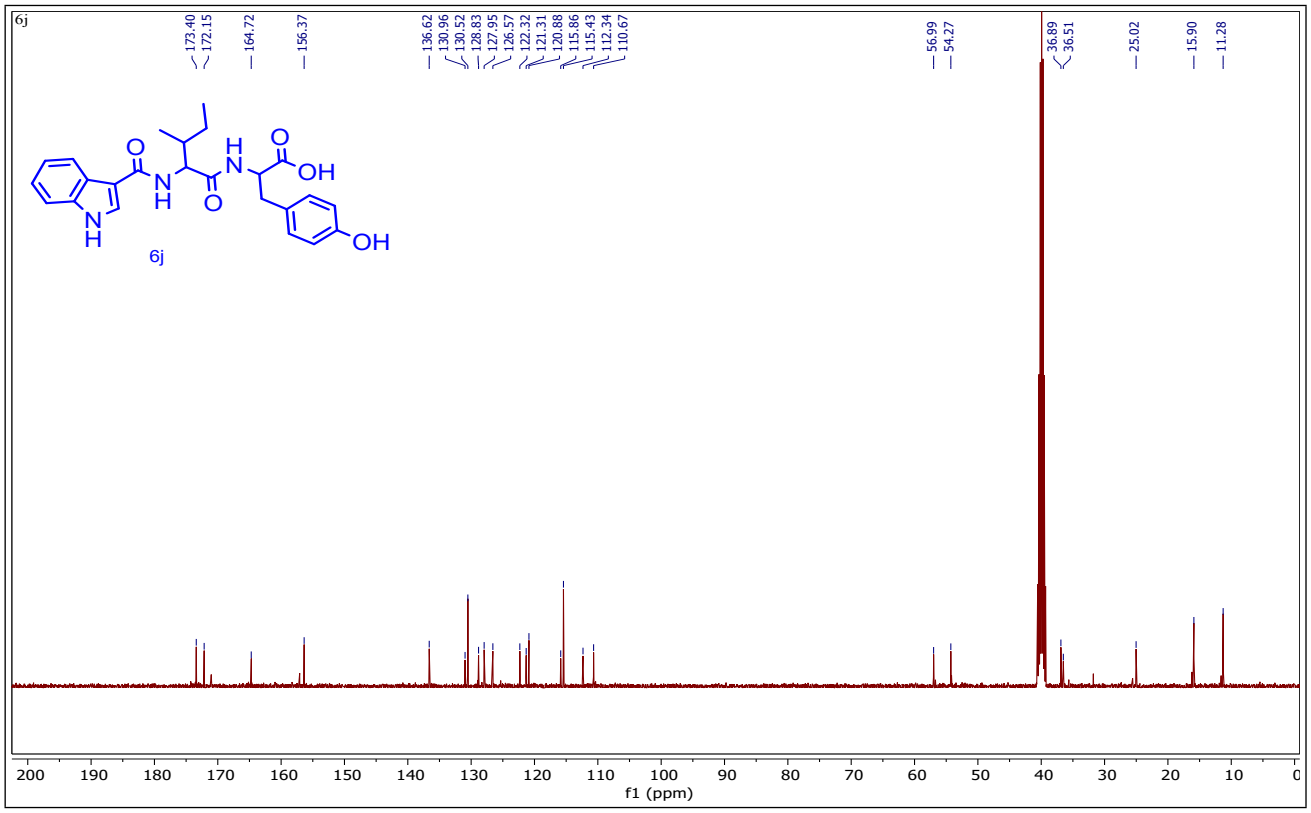
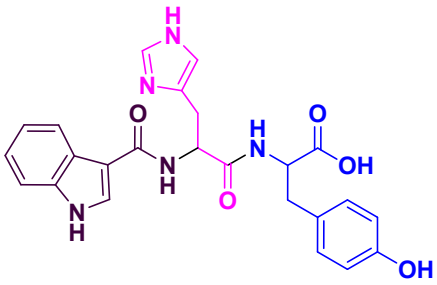


Figure S35. ^{13}C NMR of compound **6j**.



6a

Exact Mass: 461.17

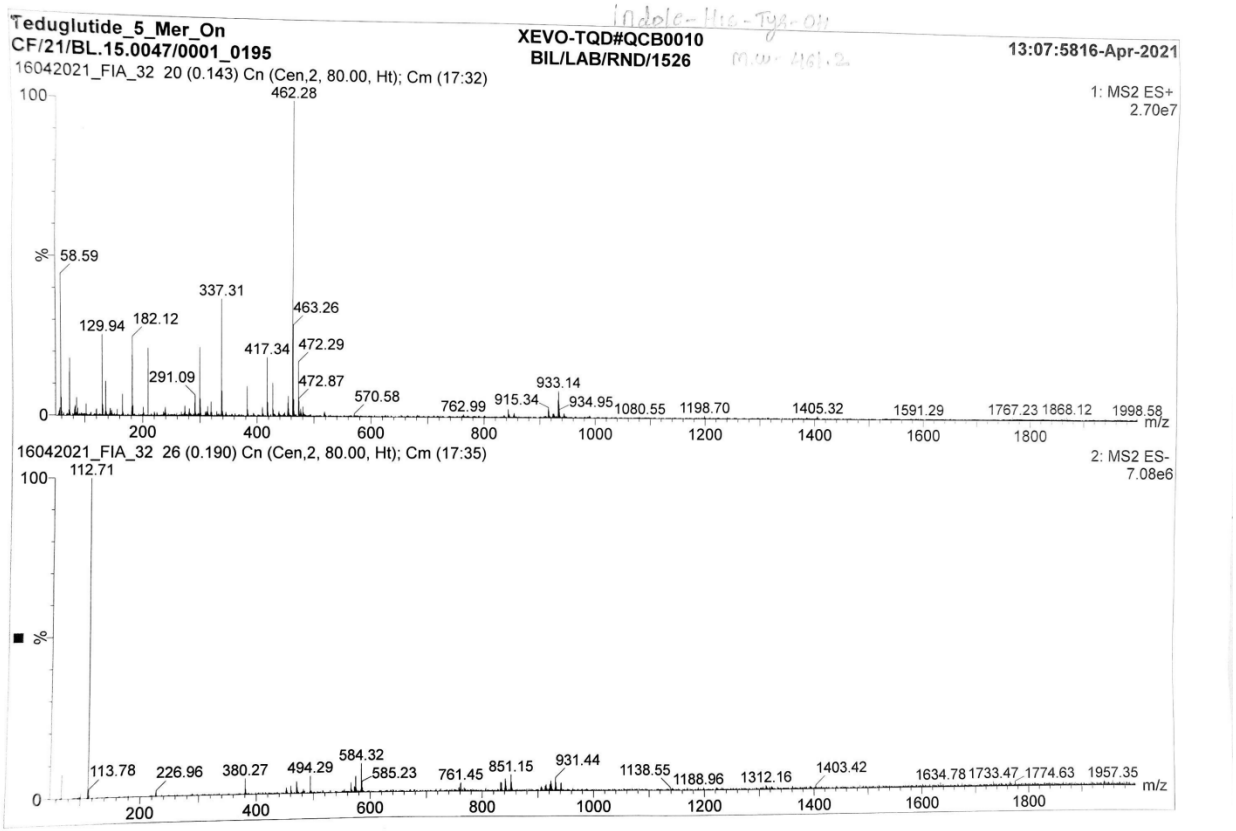
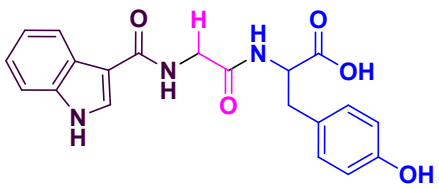


Figure S36. Mass spectrum data of (1H-indole-3-carbonyl)-L-histidyl-L-tyrosine **6a**.



6b

Exact Mass: 381.13

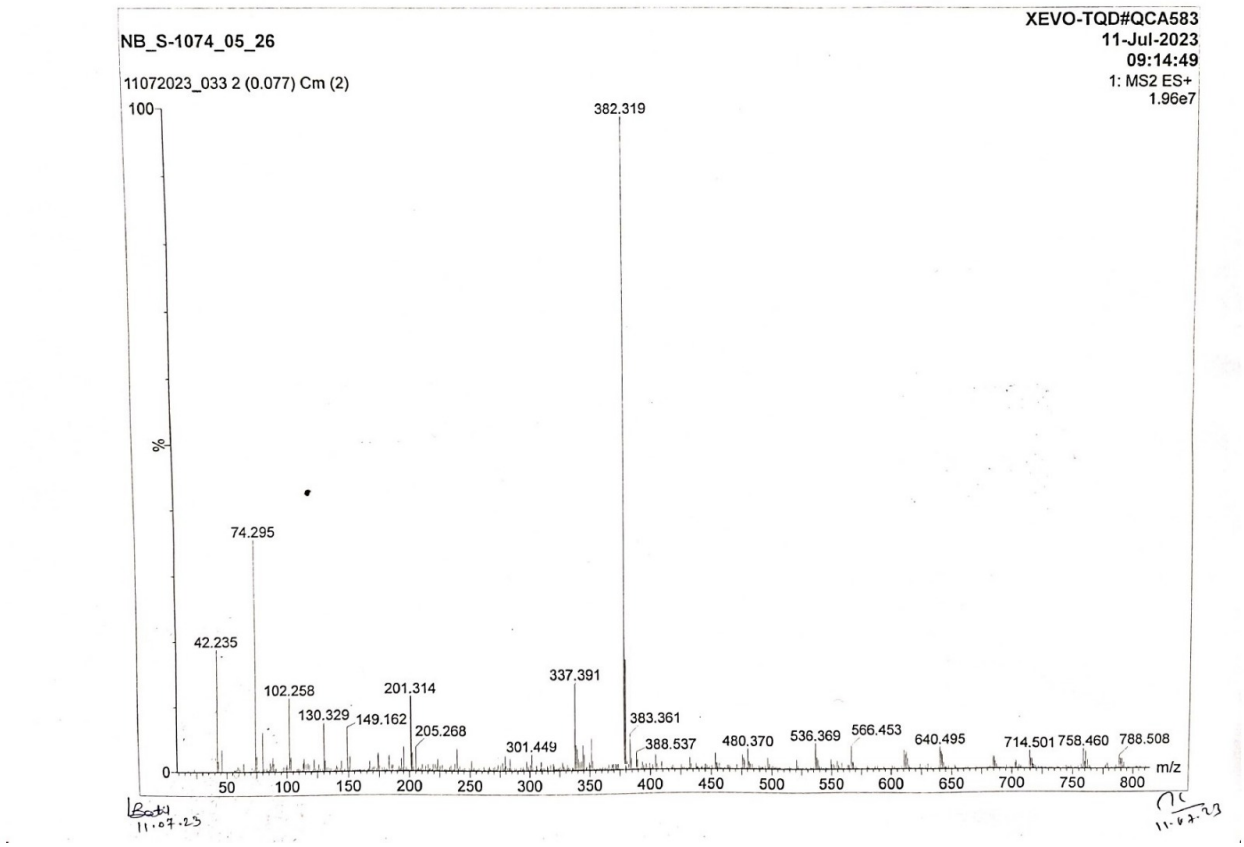
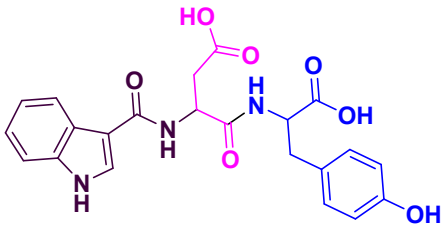


Figure S37. Mass spectrum data of (1H-indole-3-carbonyl)glycyltyrosine **6b**.



6c

Exact Mass: 439.14

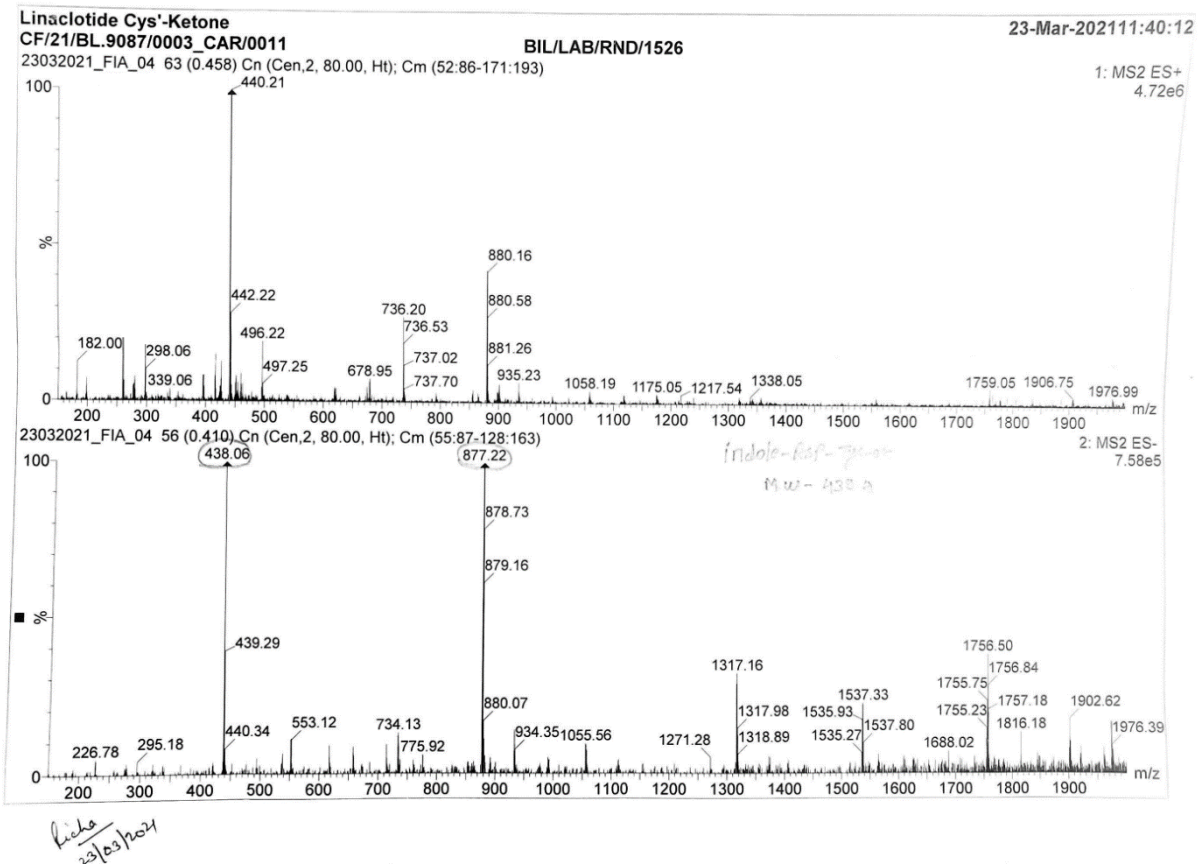
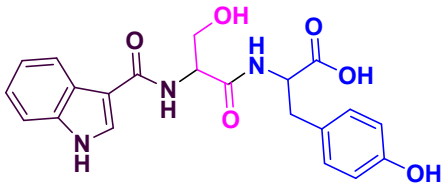


Figure S38. Mass spectrum data of 4-((1-carboxy-2-(4-hydroxyphenyl)ethyl)amino)-3-(1H-indole-3-carboxamido)-4-oxobutanoic acid **6c**.



6d

Exact Mass: 411.14

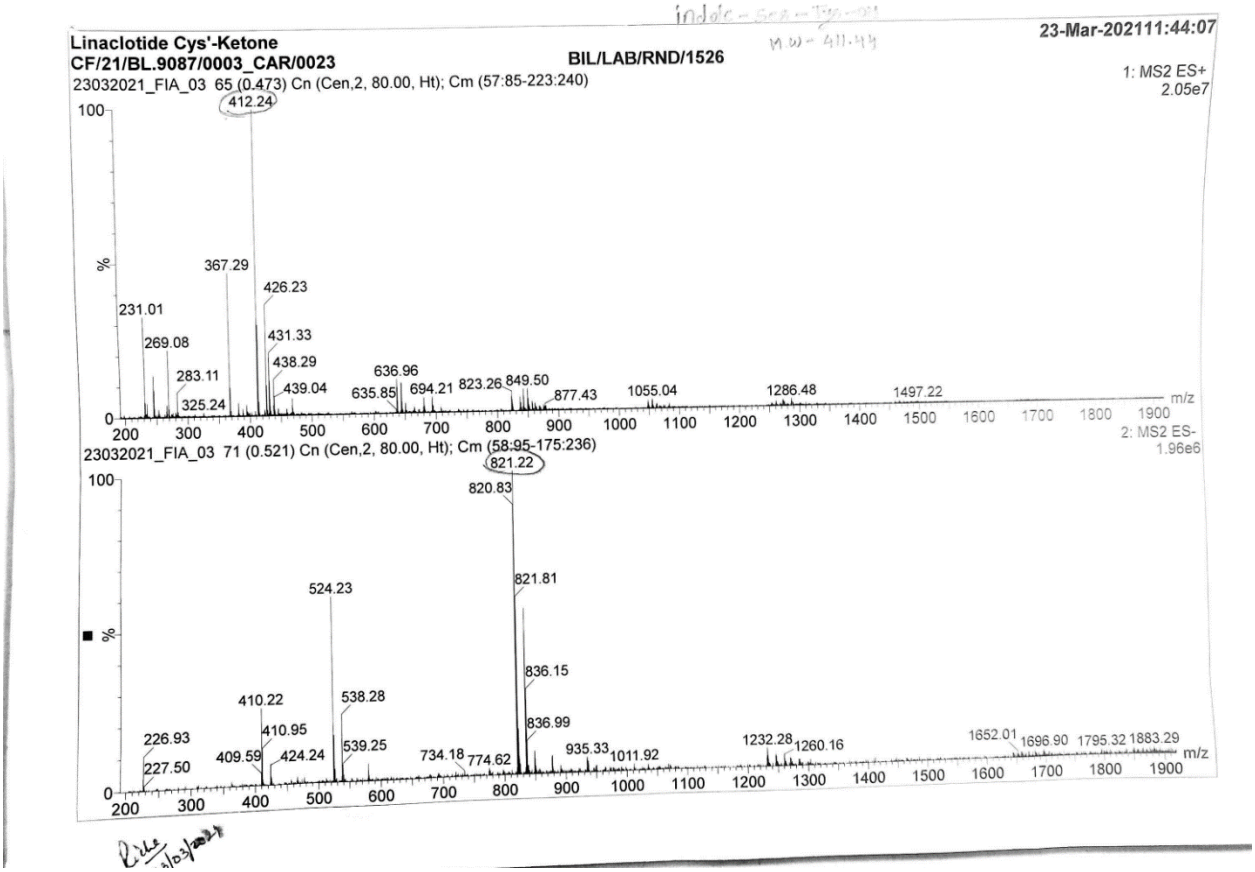
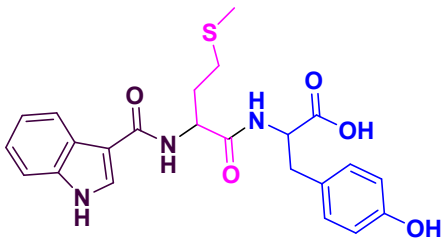


Figure S39. Mass spectrum data of (1H-indole-3-carbonyl)seryltyrosine **6d**.



6g

Exact Mass: 455.15

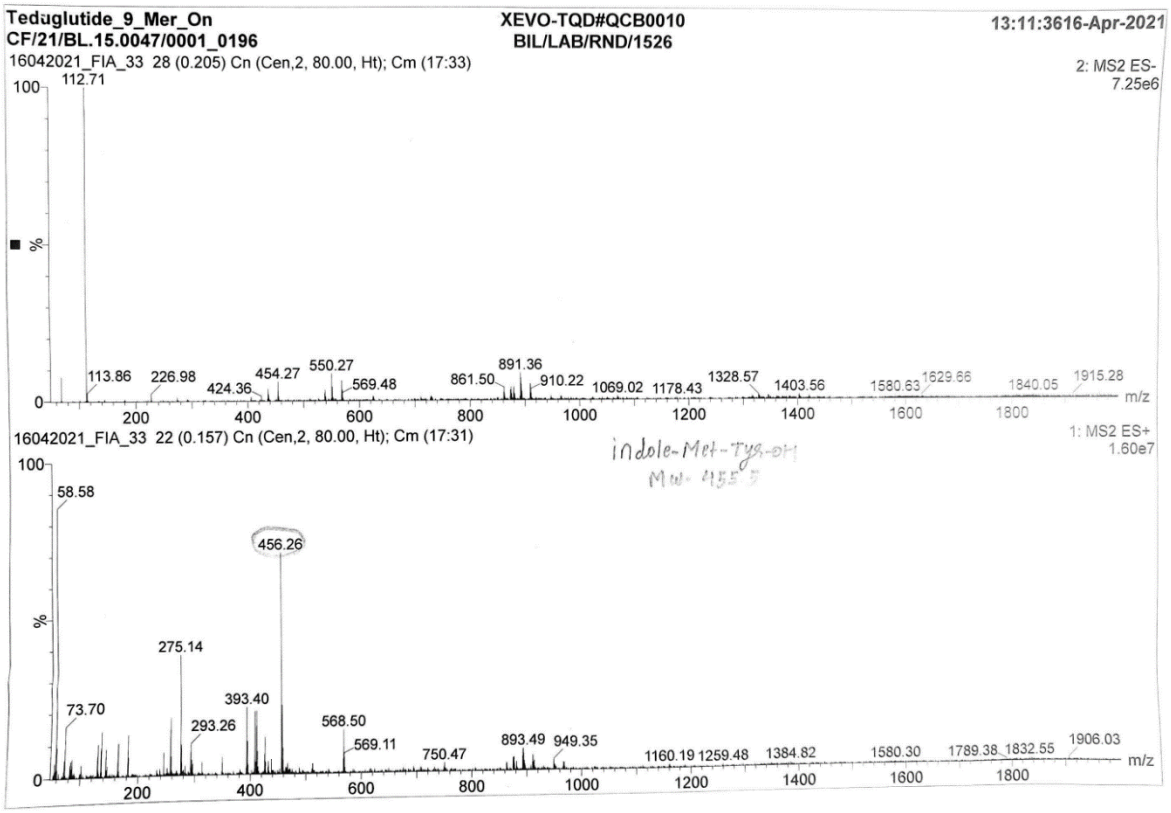
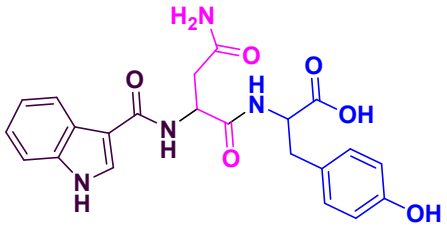


Figure S40. Mass spectrum data of (1H-indole-3-carbonyl)-L-methionyl-L-tyrosine **6g**.



6h

Exact Mass: 438.15

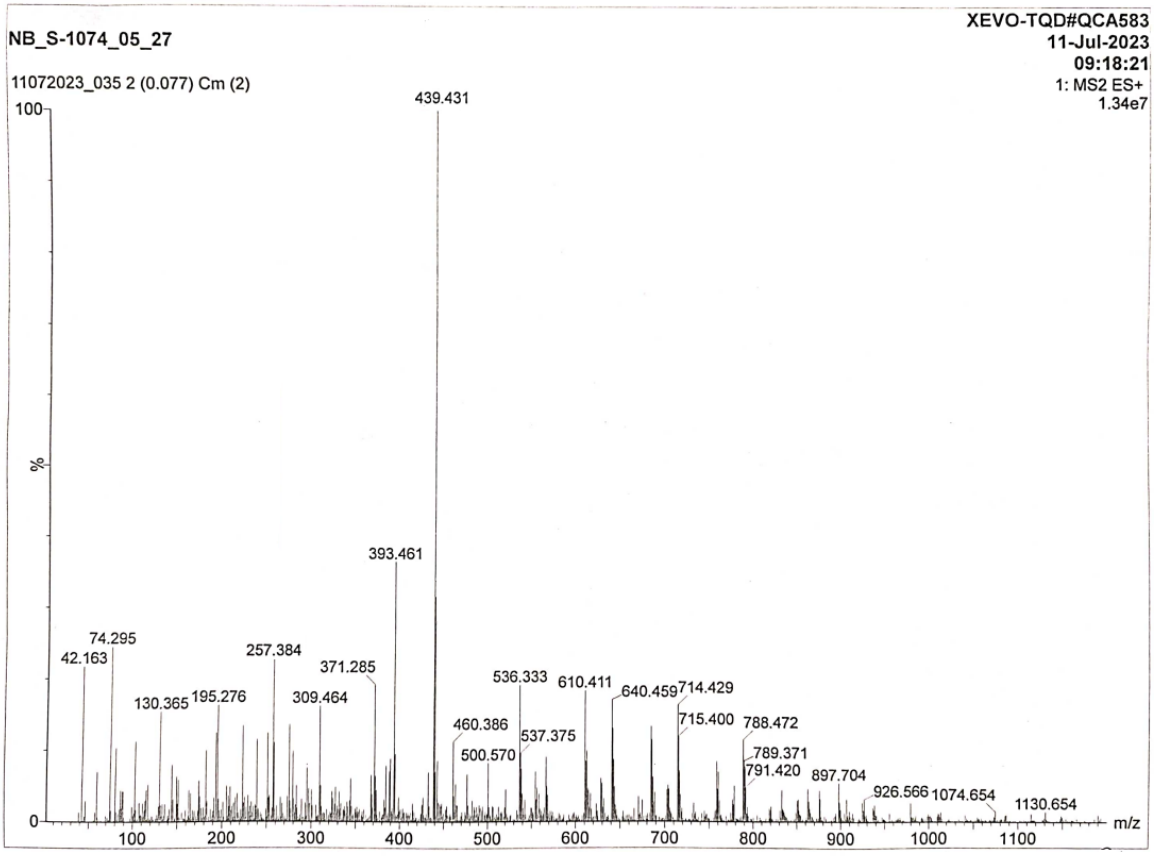
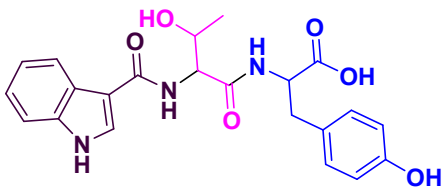


Figure S41. Mass spectrum data of (1H-indole-3-carbonyl)asparaginyltyrosine **6h**.



6i

Exact Mass: 425.16

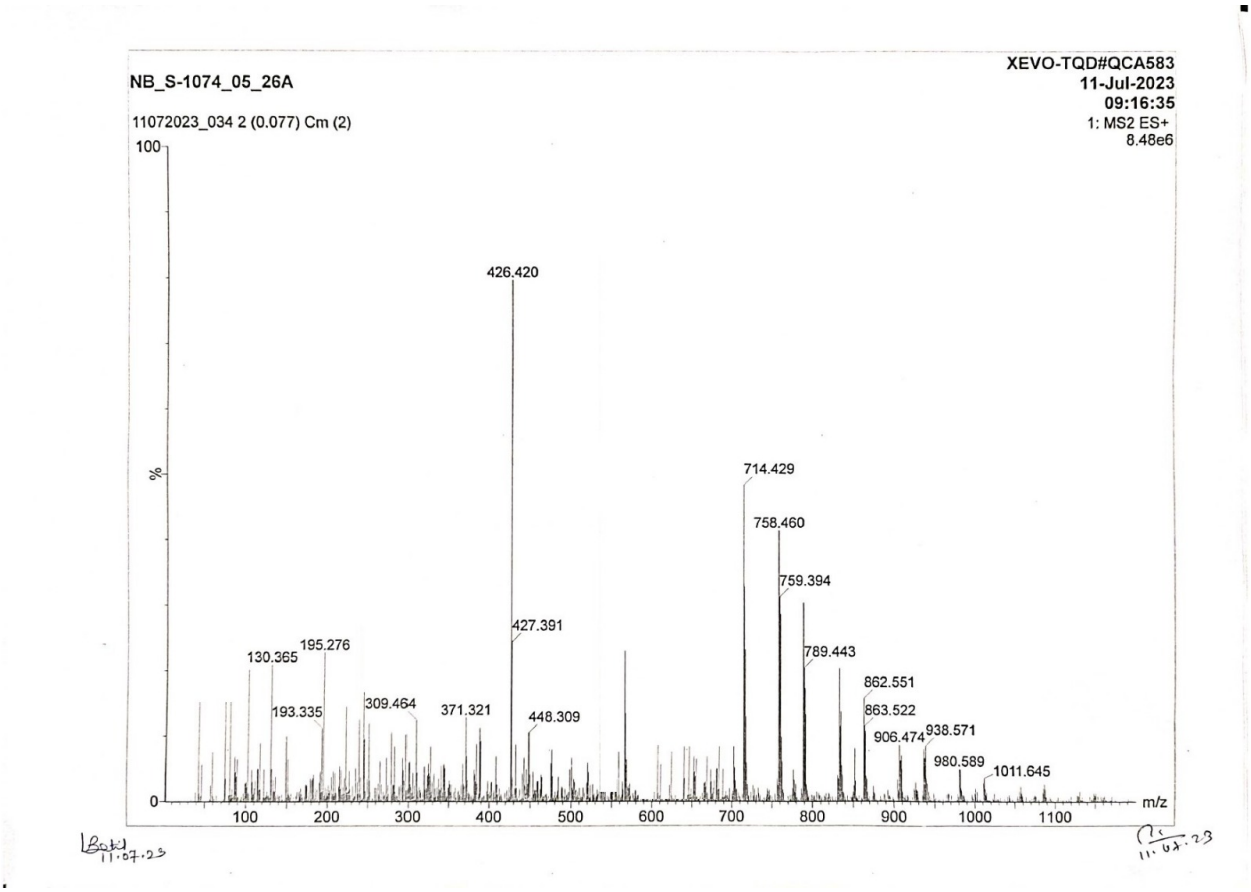


Figure S42. Mass spectrum data of (1H-indole-3-carbonyl)threonyltyrosine **6i**.

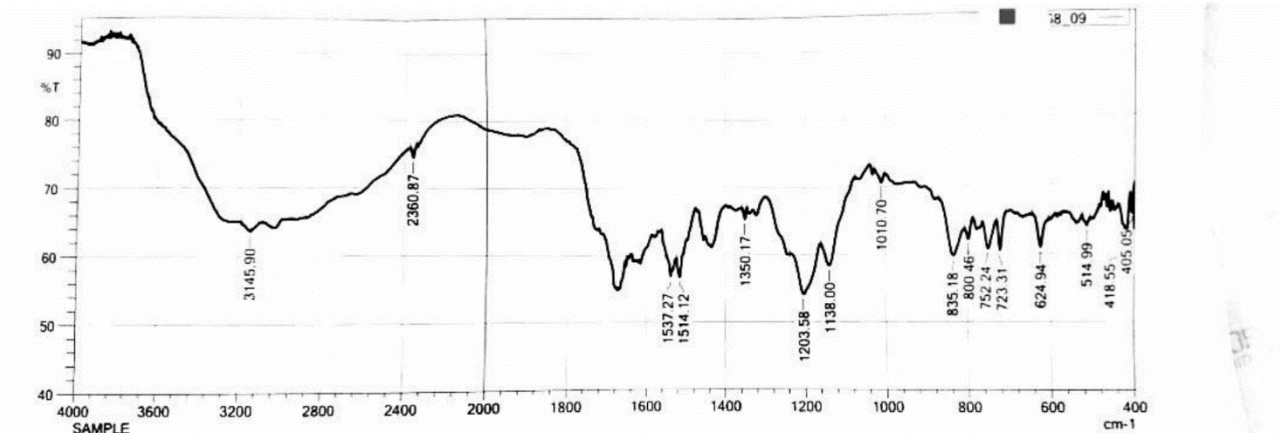


Figure S43. IR spectrum data of (1H-indole-3-carbonyl)histidyltyrosine **6a**.

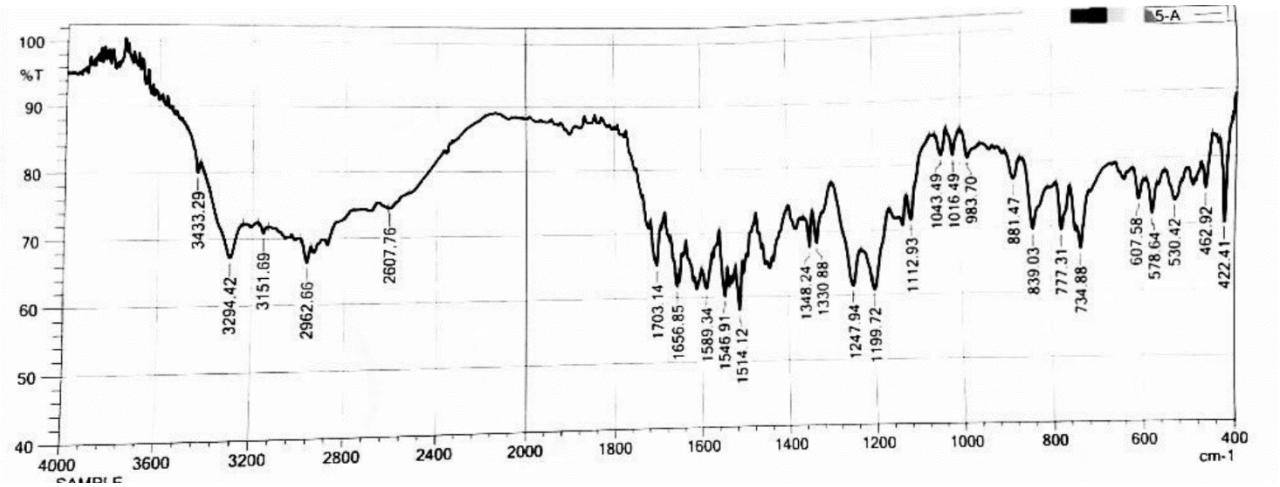


Figure S44. IR spectrum data of (1H-indole-3-carbonyl)glycyltyrosine **6b**.

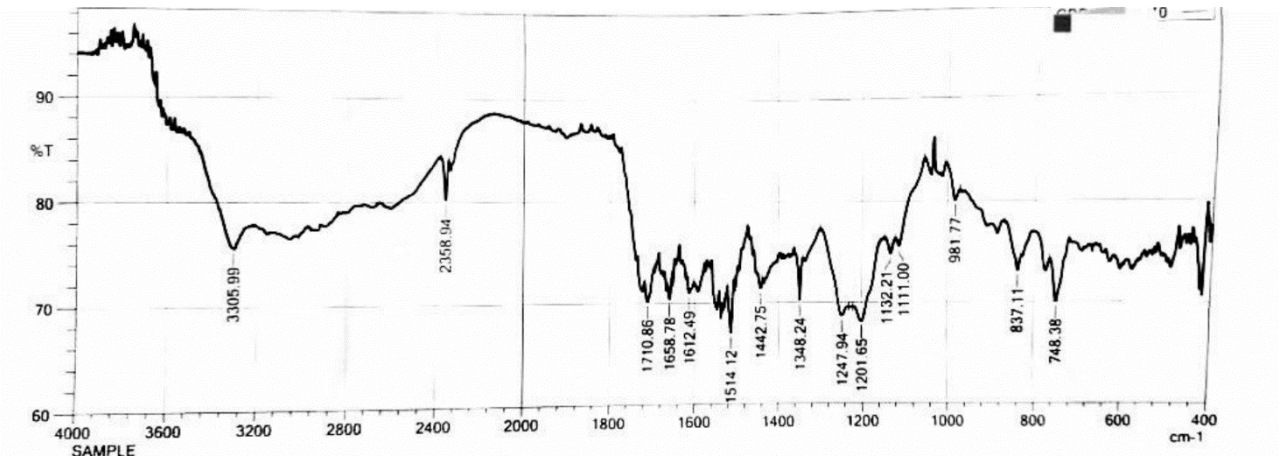


Figure S45. IR spectrum data of 4-((1-carboxy-2-(4-hydroxyphenyl)ethyl)amino)-3-(1H-indole-3-carboxamido)-4-oxobutanoic acid **6c**.

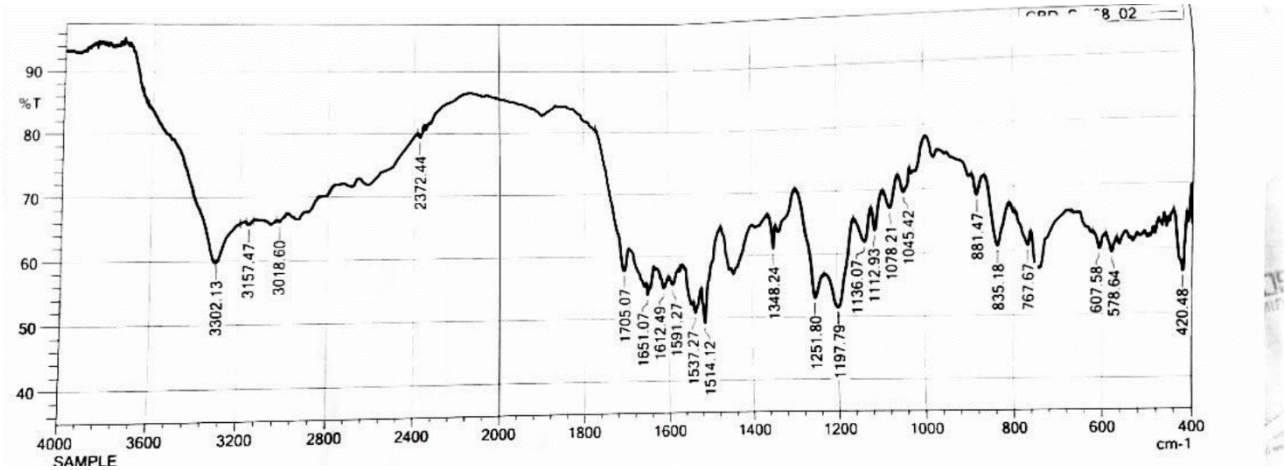


Figure S46. IR spectrum data of (1H-indole-3-carbonyl)seryltyrosine **6d**.

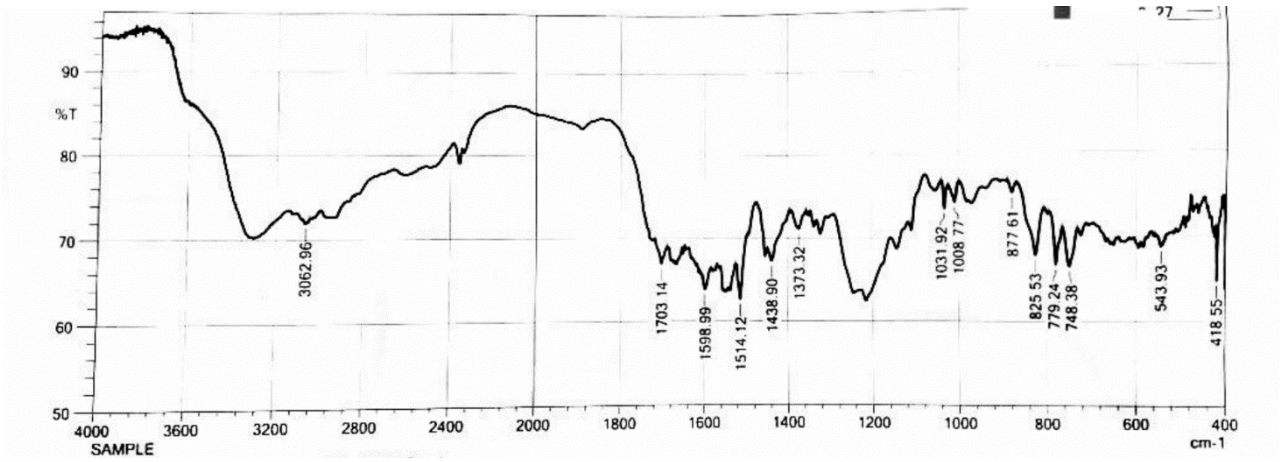


Figure S47. IR spectrum data of (1H-indole-3-carbonyl)phenylalanyltyrosine **6e**.

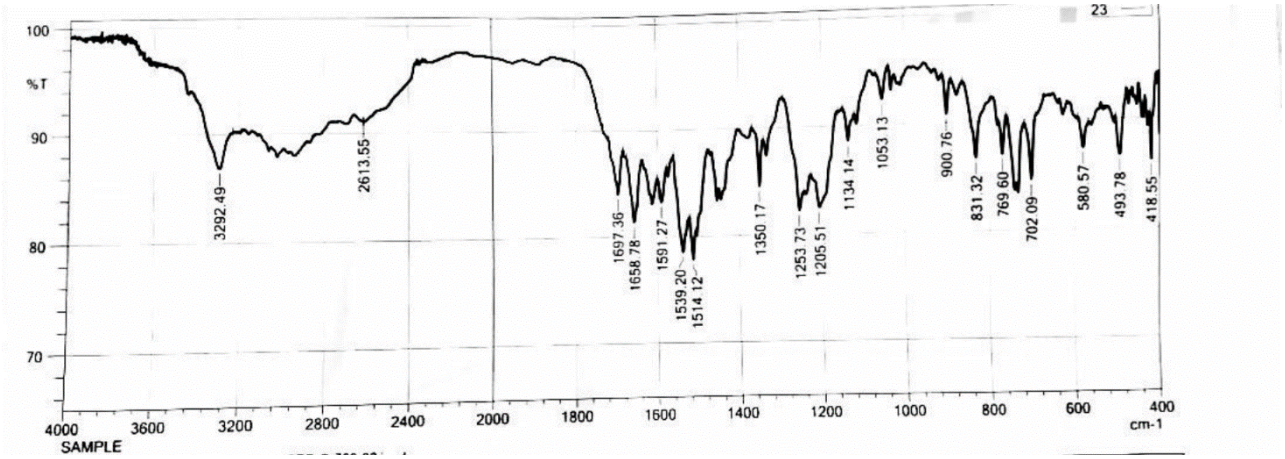


Figure S48. IR spectrum data of (1H-indole-3-carbonyl)asparaginyltyrosine **6h**.