Electronic Supplementary Information (ESI)

Transition-metal-free Synthesis of 1-Pyrroline Derivatives via Cyclization of Terminal Alkynes with 2-Azaallyls

Quanxing Zi, Jielun Cong, Lun Li, Meng Yin, Jingfeng Zhao, Liang Li*,

Xiaodong Yang*

Key Laboratory of Medicinal Chemistry for Natural Resources, Ministry of Education; Yunnan Provincial Center for Research & Development of Natural Products; School of Chemical Science and Technology, Yunnan University, Kunming, 650091, P. R. China. E-mail: xdyang@ynu.edu.cn, liliang5758@sina.com

TABLE OF CONTENT

1. Preparation of ketimines……2

2. Gram scale synthesis of **3ac**……2

3. Mechanistic study……...3

4. X-ray crystal structures of compound **3ac**……..4

5. Supplementary References……..4

6. NMR Spectra……..4

7. HNMR Spectra……..33

Supplementary Methods:

Preparation of ketimines

Ketimines (**2a-2l**) were prepared according to literature procedures.[1]

Procedure and characterization for the cyclization of ketimines and alkynes

Reaction Optimization:

An oven-dried 8 mL reaction vial equipped with a stir bar was charged with ethynylbenzene **1a** (0.2 mmol) and ketimine **2a** (0.1 mmol) under a nitrogen atmosphere in a glove box. A solution of base (0.3 mmol) in 0.5, 1 and 2mL dry solvent was added by a "Titan" brand 1000 μL pipettor to the reaction vial. The reaction mixture turned to a dark purple color. Then the vial was sealed with a cap, removed from the glove box, and stirred for 12 h at 25, 60, 80 and 100 ℃. After the reaction was completed, the reaction mixture was opened to air, quenched with three drops of H_2O, diluted with 3 mL of ethyl acetate, and filtered over a 2 cm pad of $MgSO_4$ and silica. The pad was rinsed with ethyl acetate (3×2 mL), and the combined solutions were concentrated in vacuo. $CDCl_3$ and CH_2Br_2 were then added sequentially to determine the yield of the reaction mixture. CH_2Br_2 was used as an internal standard.

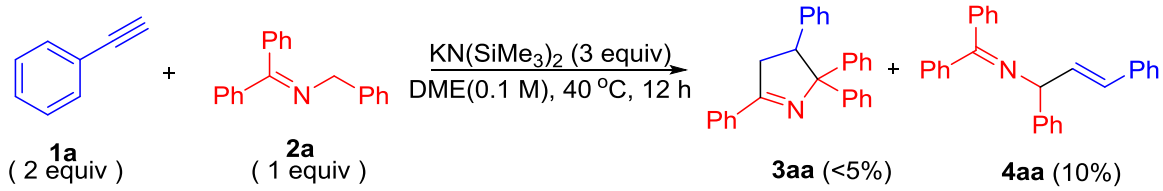
Gram scale synthesis of 3ac

An oven-dried 100 mL Schlenk tube equipped with a stir bar was sealed with a rubber septum and degassed, purged with nitrogen (repeated three times). DCM (10 mL) was added under nitrogen via syringe through the rubber septum. (4-methoxyphenyl)methanamine (411.3 mg, 3.0 mmol) and benzophenone imine (543.3 mg, 3.0 mmol) were added under nitrogen via syringe through the rubber septum. The reaction was stirred at 23 °C for 12 h, the solvent was completely removed in *vacuo* and the tube was filled with nitrogen. A solution (prepared in the glove box) of ethynylbenzene **1a** (606.1 mg, 6.0 mmol) in 10 mL anhydrous DME was added to the Schlenk tube via syringe through the rubber septum. Next, a solution of $KN(SiMe_3)_2$ (1.8 g, 12.0 mmol) in 20 mL anhydrous DME was added by

syringe through the rubber septum. The reaction mixture was stirred for 12 h in total at 100 ℃, opened to air, and quenched with 3 mL of H_2O. The layers were separated and the aqueous layer was extracted with DCM (3 X 5 mL). The combined organic layers were concentrated in *vacuo*. The crude product was separated by flash chromatography on deactivated silica gel hexanes to give the product **3ca** in 86% yield (1.04 g).

Mechanistic study

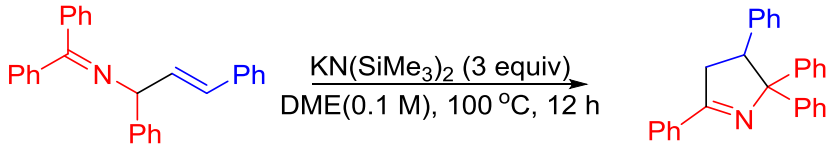
a. Evidence of the mechanism goes through 4aa.



The reaction was performed following the General Procedure with ethynylbenzene **1a** (40.8 mg, 0.4 mmol) and *N*-benzyl-1,1-diphenylmethanimine **2a** (54.2 mg, 0.2 mmol). The crude product was separated by flash chromatography on deactivated silica gel hexanes to give the intermediate **4aa** in 10% yield (7.5 mg).

4aa(major): colorless liquid, R_f = 0.39 (hexanes:ethyl acetate = 30:1); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.61 – 7.55 (m, 5H), 7.48 (dt, *J* = 18.9, 7.4 Hz, 7H), 7.43 – 7.29 (m, 6H), 6.70 (dd, *J* = 16.0, 6.6 Hz, 1H), 6.57 (d, *J* = 15.9 Hz, 1H), 5.33 (d, *J* = 6.5 Hz, 1H) ppm; ^{13}C{^{1}H} NMR (150 MHz, Chloroform-*d*) δ 167.7, 143.6, 140.1, 137.4, 137.0, 132.8, 130.3, 129.6, 128.9, 128.9, 128.7, 128.7, 128.6, 128.5, 128.3, 127.9, 127.6, 127.5, 127.1, 126.6, 68.8 ppm; HRMS (ESI$^+$) $[M+H]^+$ calc'd for $C_{28}H_{24}N^+$: 374.1903, found: 374.1906.

b. 4aa is converted to 3aa.

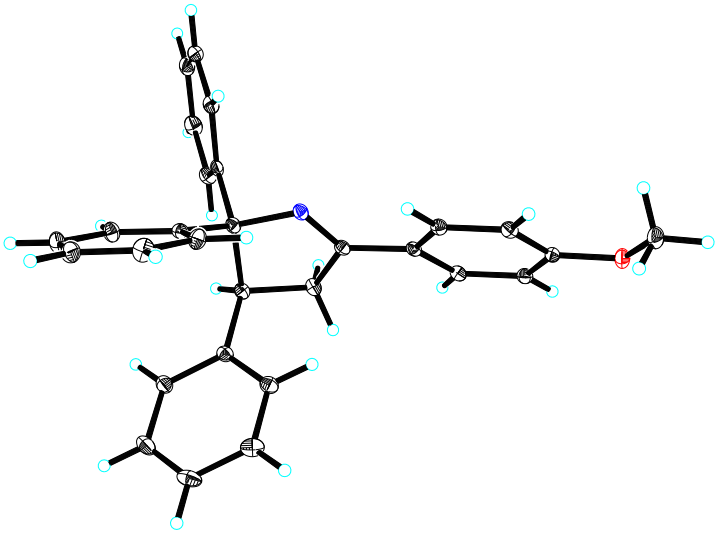


4aa **3aa** (99%)

The reaction was performed following the General Procedure with **4aa**. The crude product was separated by flash chromatography on deactivated silica gel hexanes to give the product **3aa** in 99% yield (7.4 mg).

X-ray crystal structures of compound 3ac.

CCDC 2085476 contains the supplementary crystallographic data for compound **3ac**. The data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.



Supplementary References

(1) Matin, J. O'D.; William, D. B.; Wiiiam, A. B.; Wiiiam, N. J.; Keith, K.; Brigitte, L.; Robin, L. P.; Frederick, G. B.; Susan, R. M., *J. Am. Chem. Soc.* **1998**, *110*, 8520-8525

NMR Spectra

Figure S1. ^{1}H NMR spectra (600 MHz, Chloroform-*d*) of 2,2,3,5-tetraphenyl-3,4-dihydro-2*H*-pyrrole (3aa).

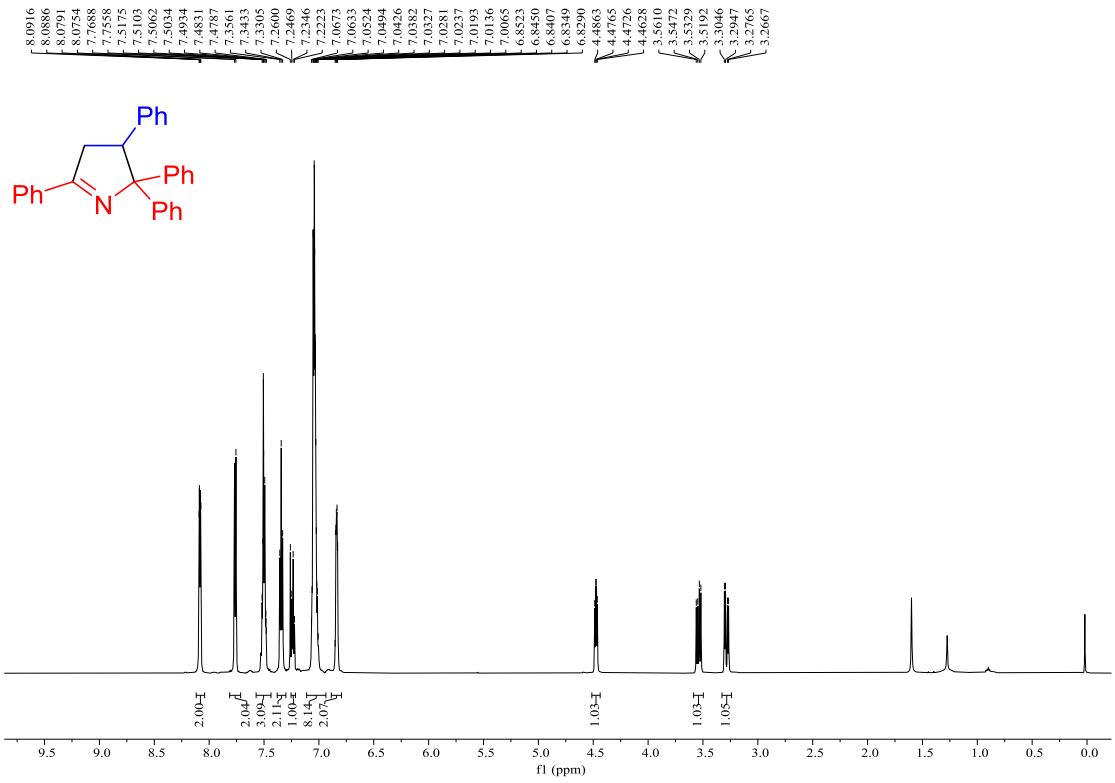


Figure S2. ^{13}C{^{1}H} NMR spectra (150 MHz, Chloroform-*d*) of 2,2,3,5-tetraphenyl-3,4-dihydro-2*H*-pyrrole (3aa).

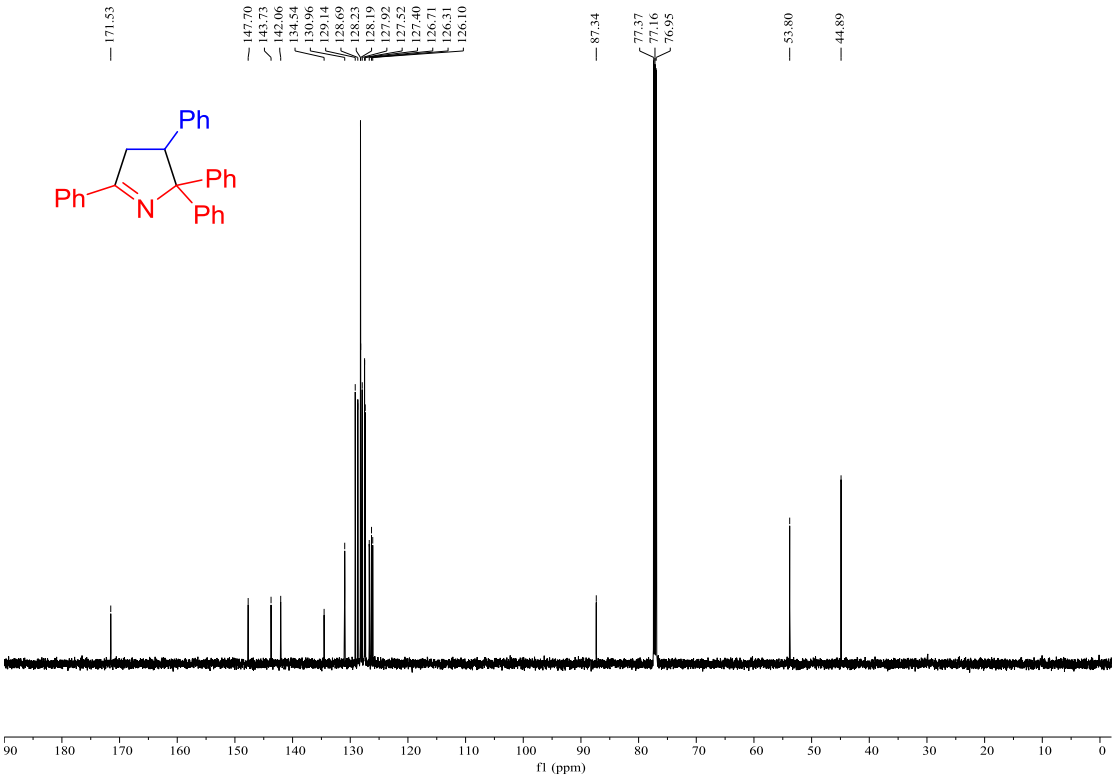


Figure S3. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 2,2,5-triphenyl-3-(p-tolyl)-3,4-dihydro-2*H*-pyrrole (3ba).

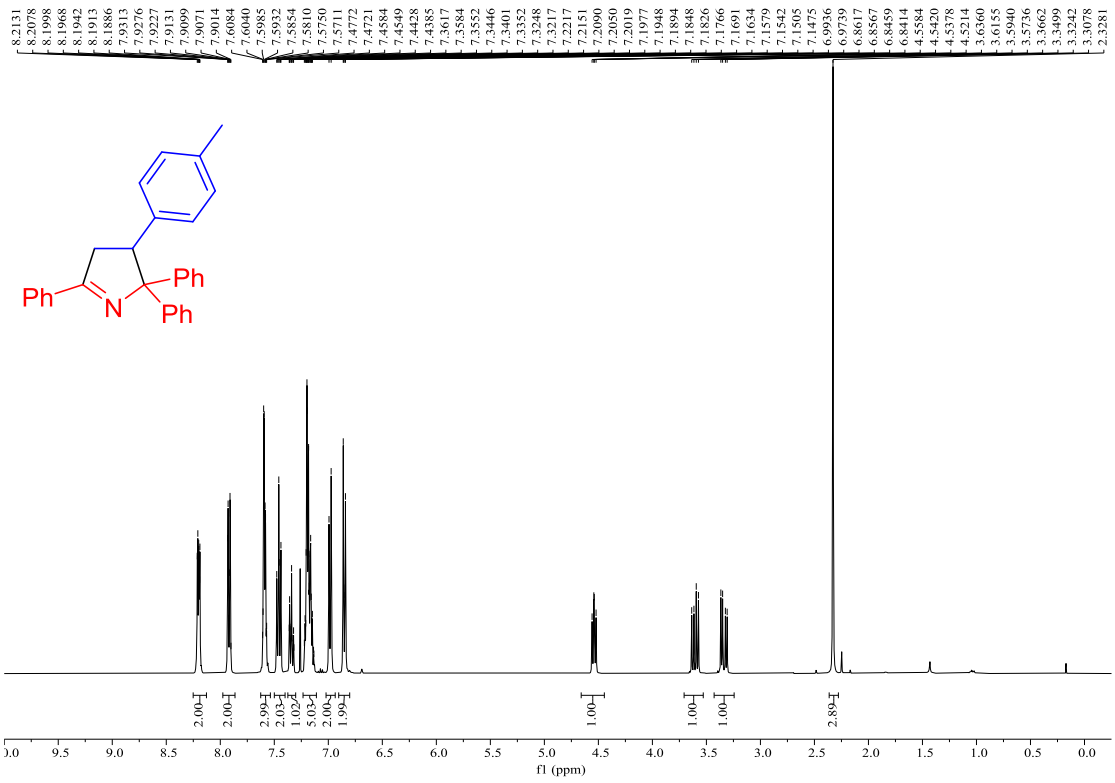


Figure S4. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 2,2,5-triphenyl-3-(p-tolyl)-3,4-dihydro-2*H*-pyrrole (3ba).

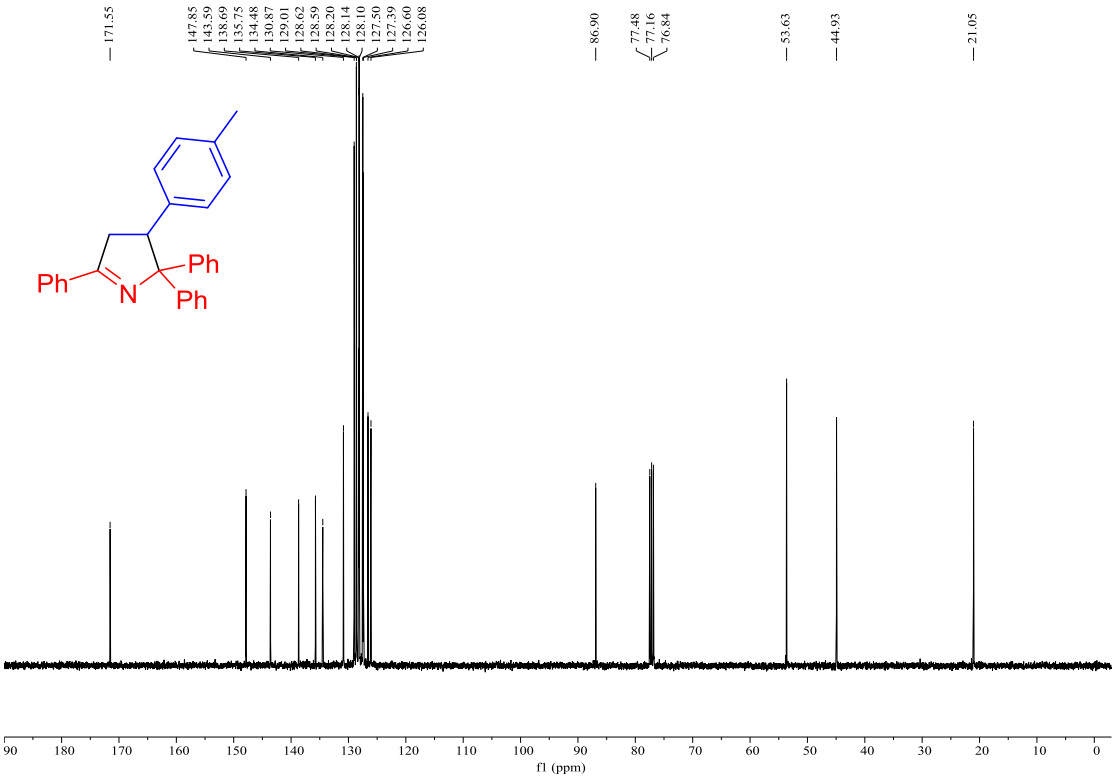


Figure S5. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-(4-(*tert*-butyl)phenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ca).

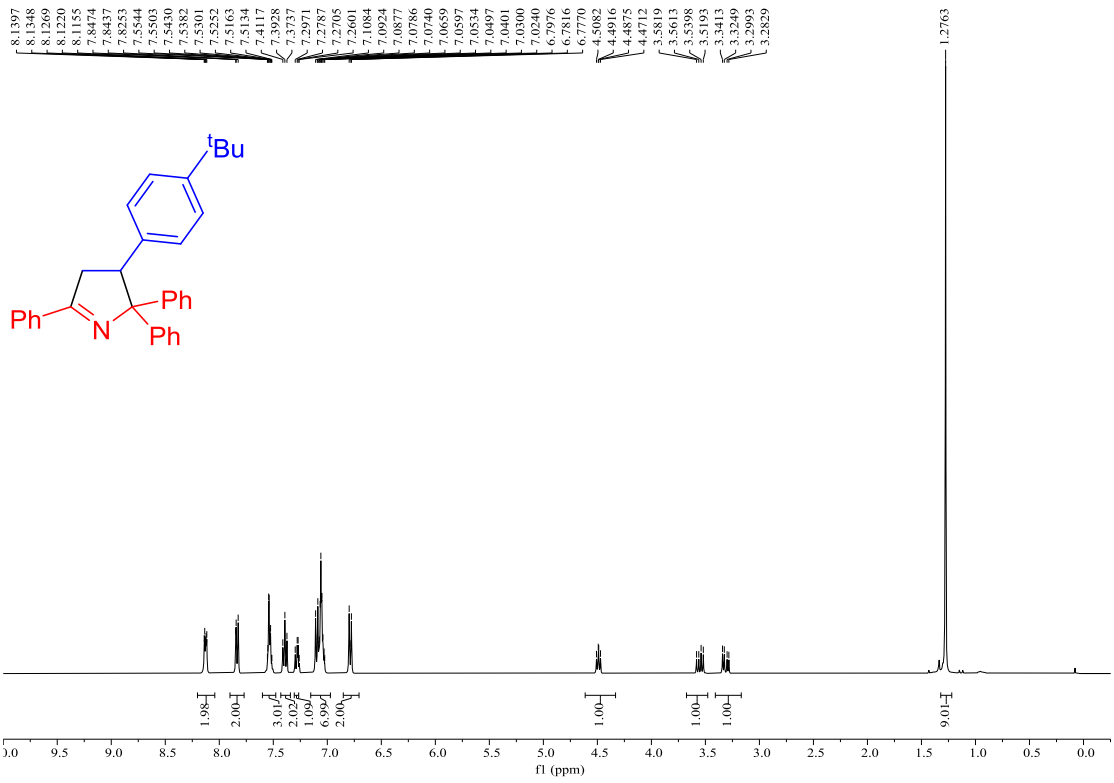


Figure S6. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 3-(4-(*tert*-butyl)phenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ca).

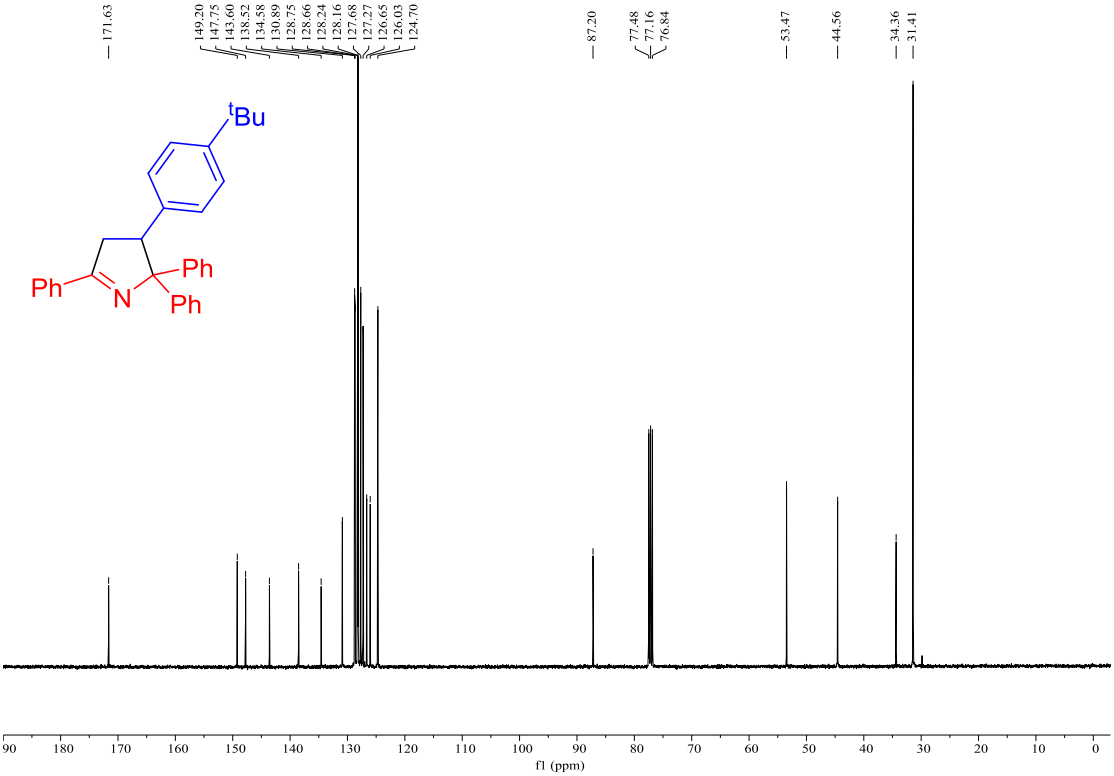


Figure S7. ^{1}H NMR spectra (600 MHz, Chloroform-*d*) of 3-(4-ethoxyphenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3da).

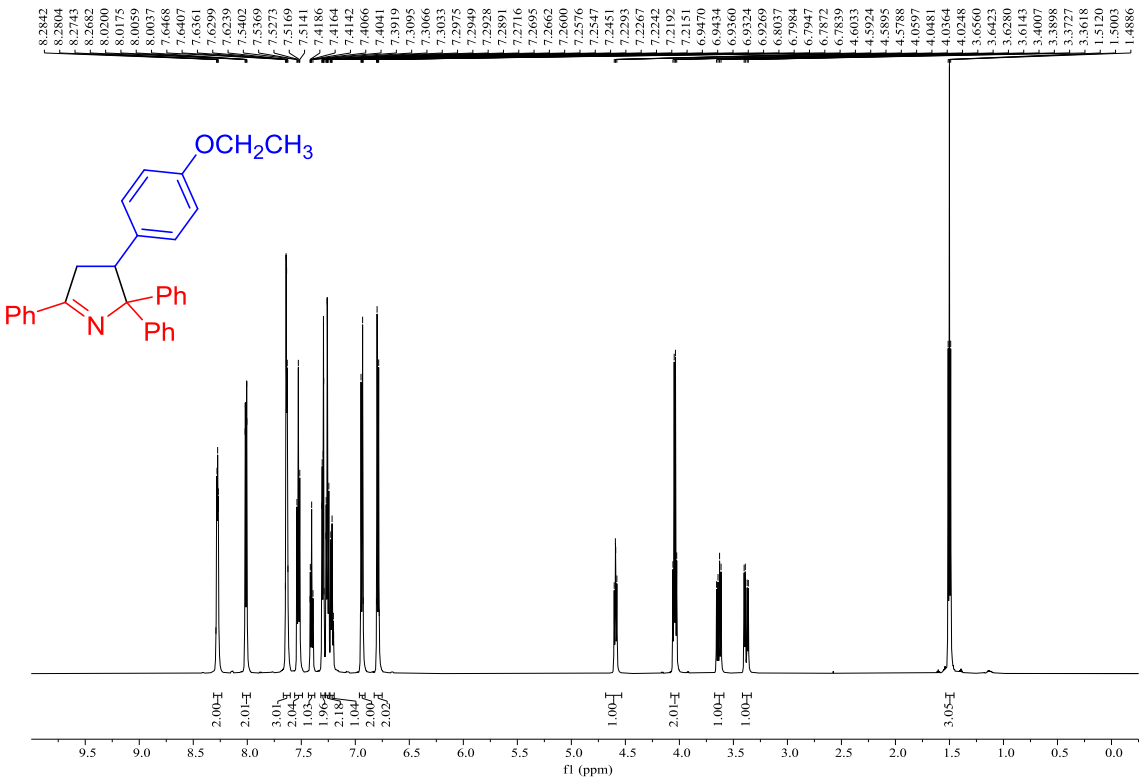


Figure S8. ^{13}C{^{1}H} NMR spectra (150 MHz, Chloroform-*d*) of 3-(4-ethoxyphenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3da).

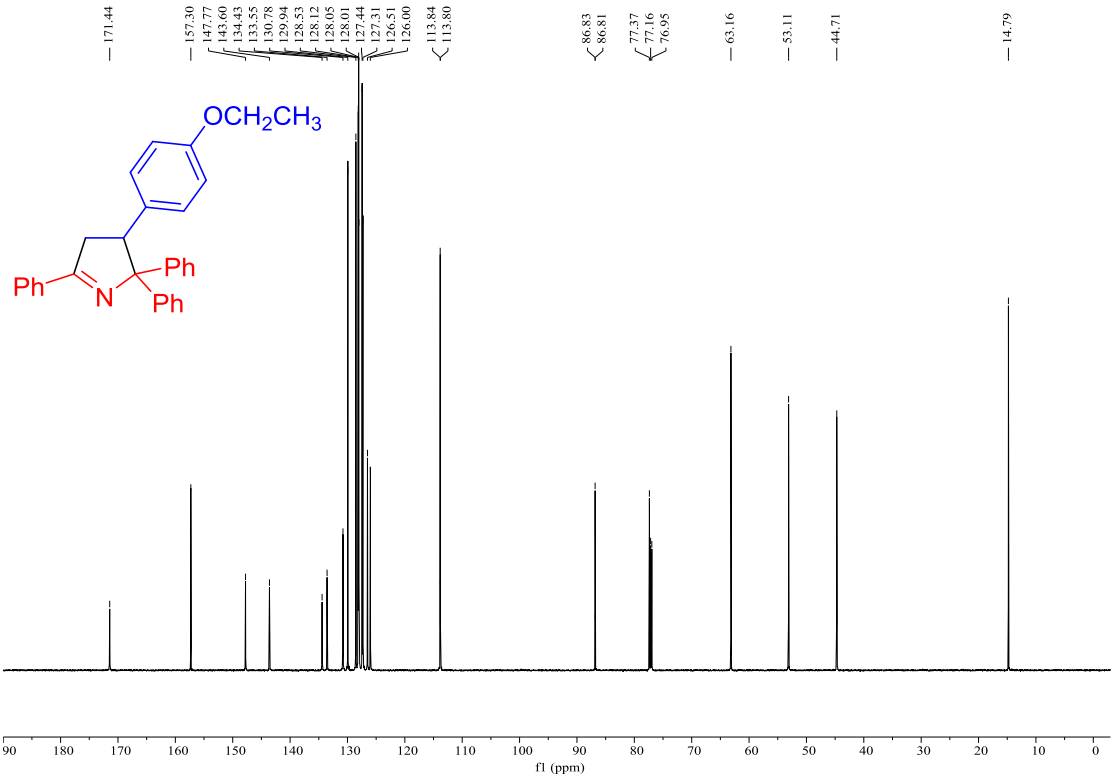


Figure S9. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 2,2,5-triphenyl-3-(4-(trifluoromethoxy)phenyl)-3,4-dihydro-2*H*-pyrrole (3ea).

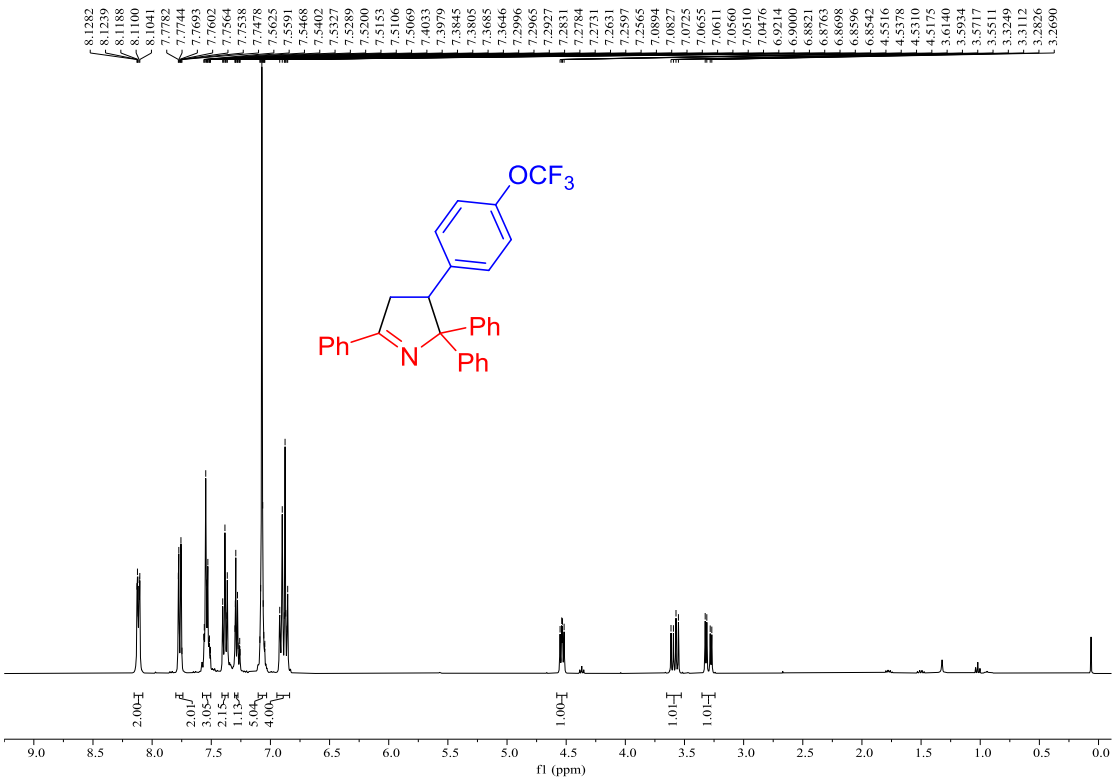


Figure S10. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 2,2,5-triphenyl-3-(4-(trifluoromethoxy)phenyl)-3,4-dihydro-2*H*-pyrrole (3ea).

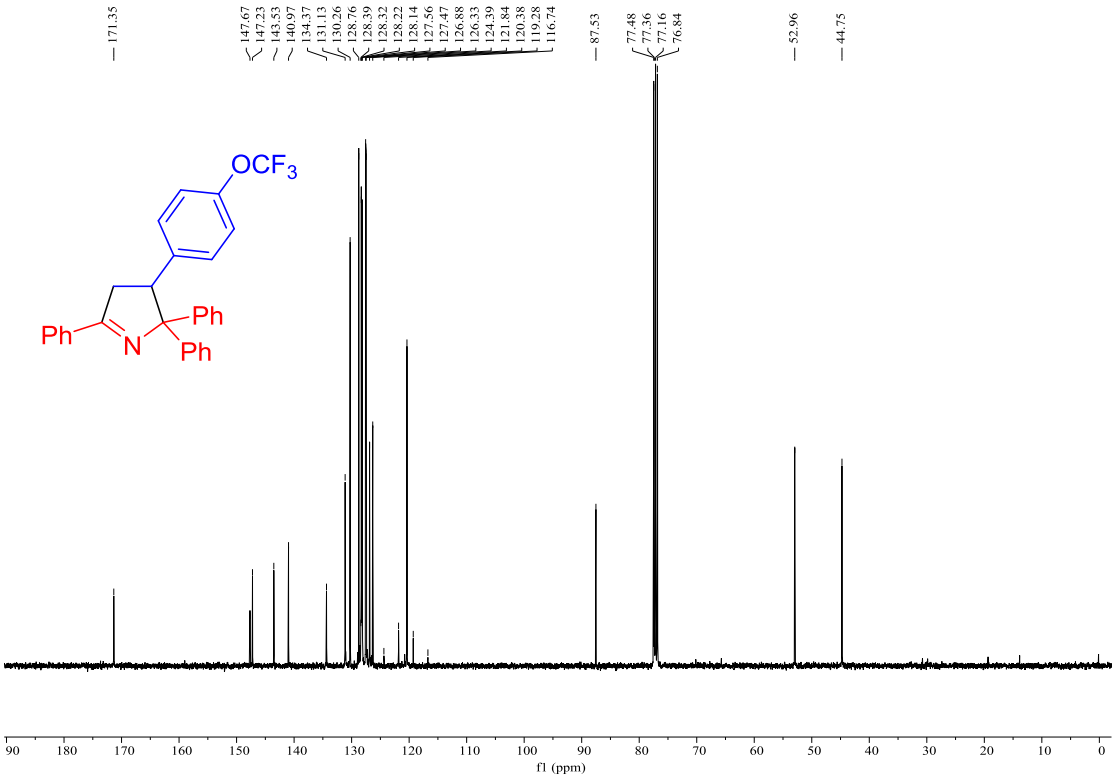


Figure S11. ^{19}F NMR spectra (376 MHz, Chloroform-*d*) of 2,2,5-triphenyl-3-(4-(trifluoromethoxy)phenyl)-3,4-dihydro-2*H*-pyrrole (3ea).

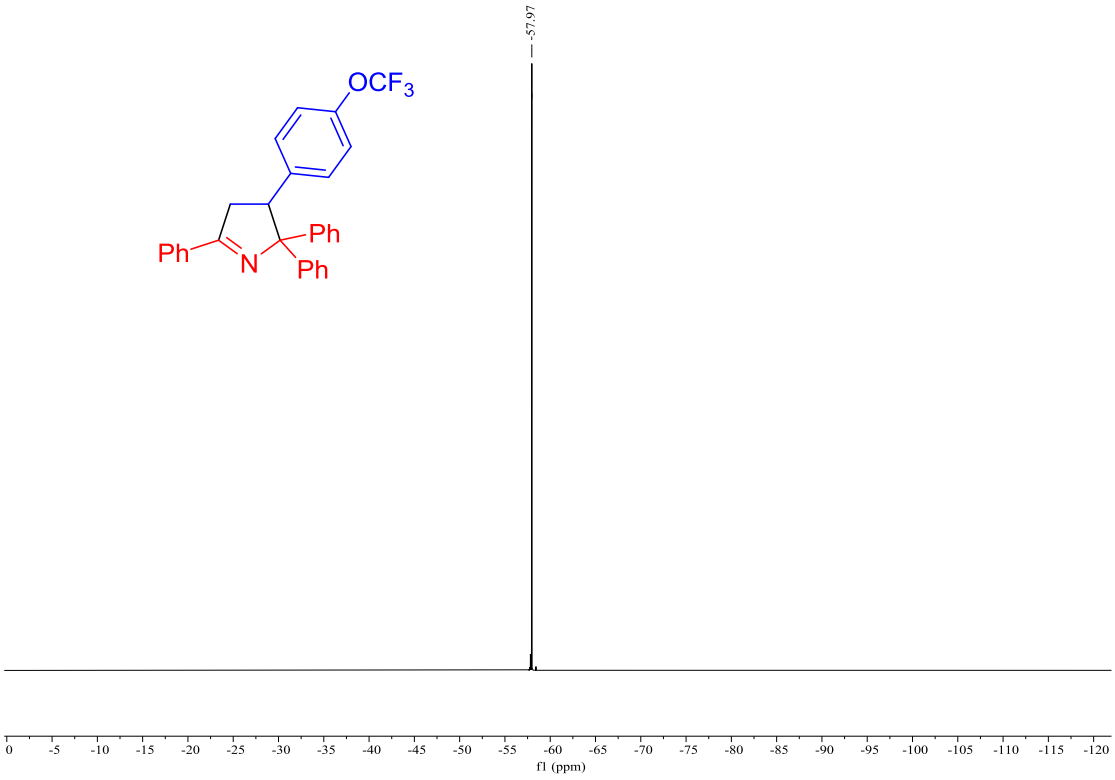


Figure S12. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-([1,1'-biphenyl]-4-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3fa).

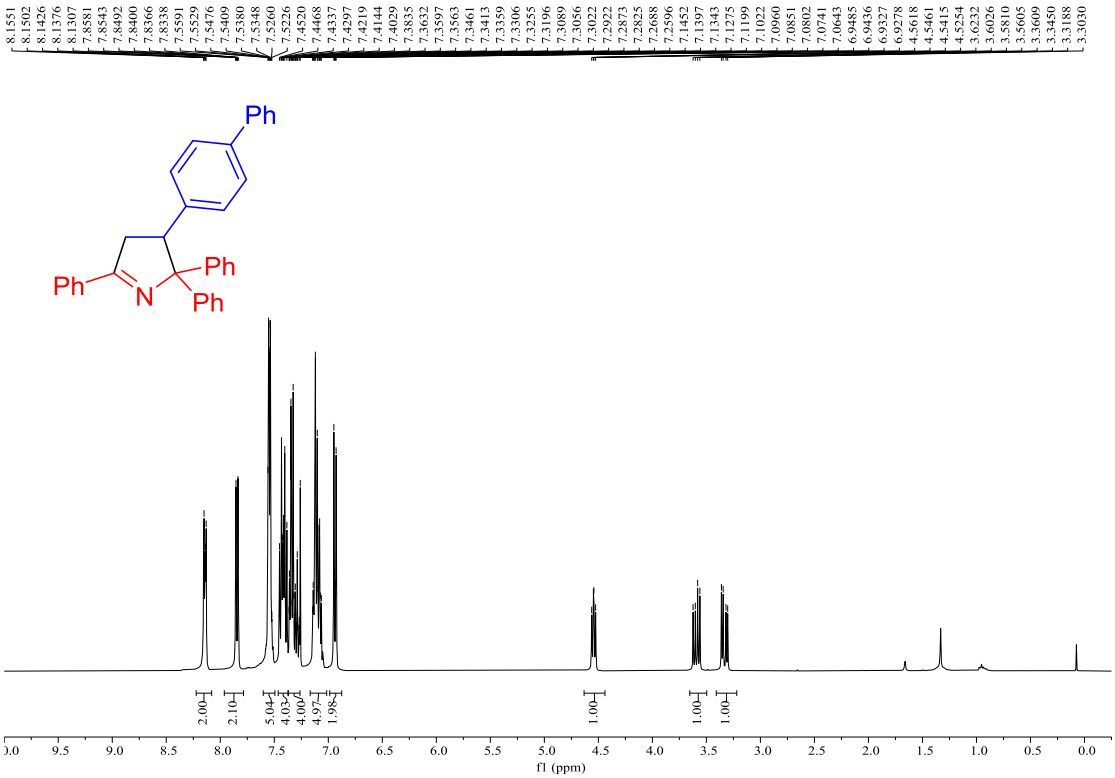


Figure S13. $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 3-([1,1'-biphenyl]-4-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3fa).

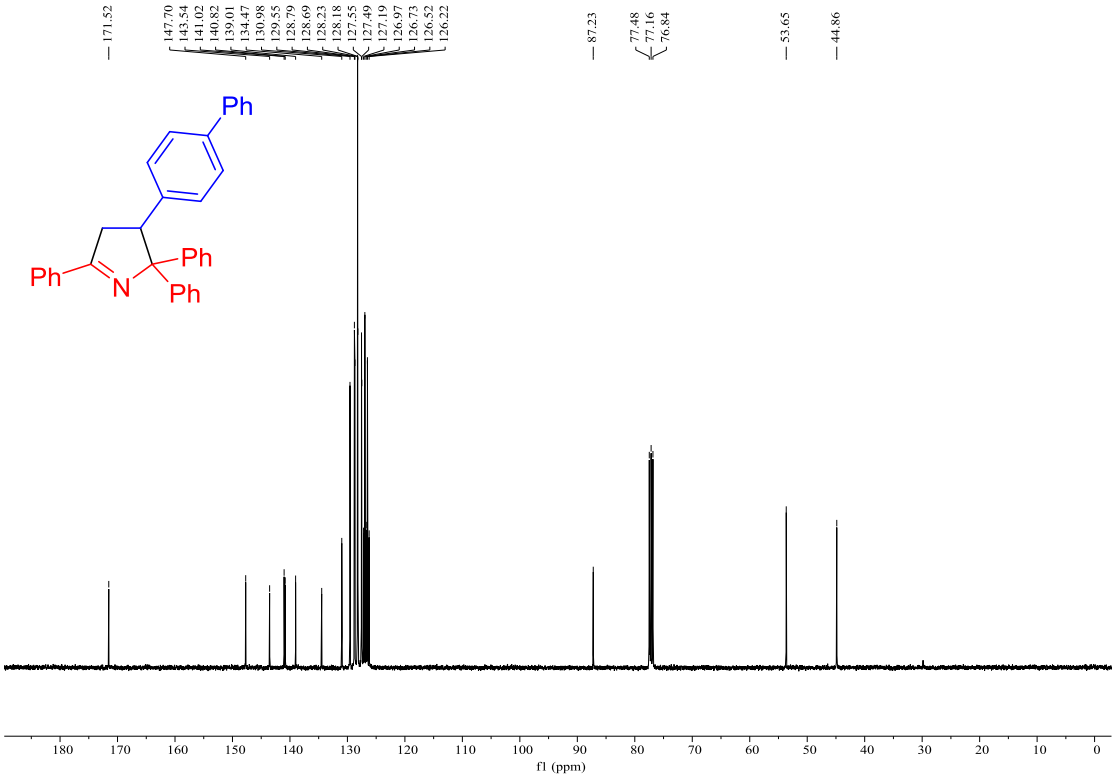


Figure S14. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-(4-fluorophenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ga).

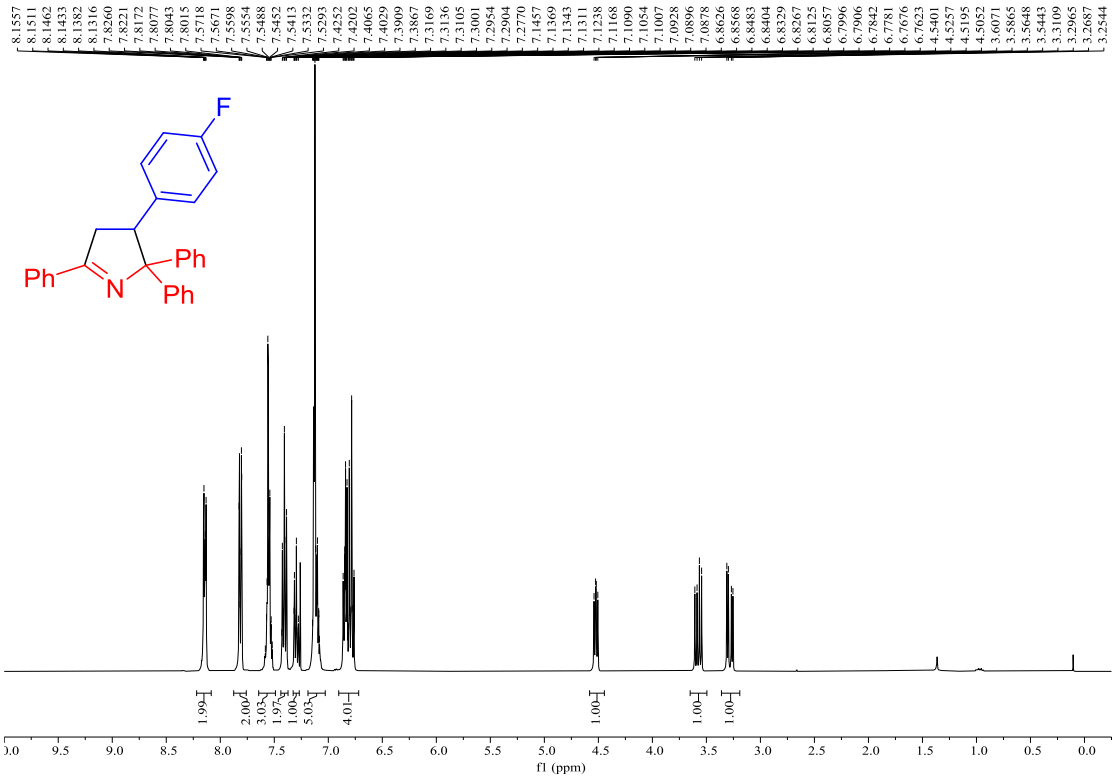


Figure S15. $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 3-(4-fluorophenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ga).

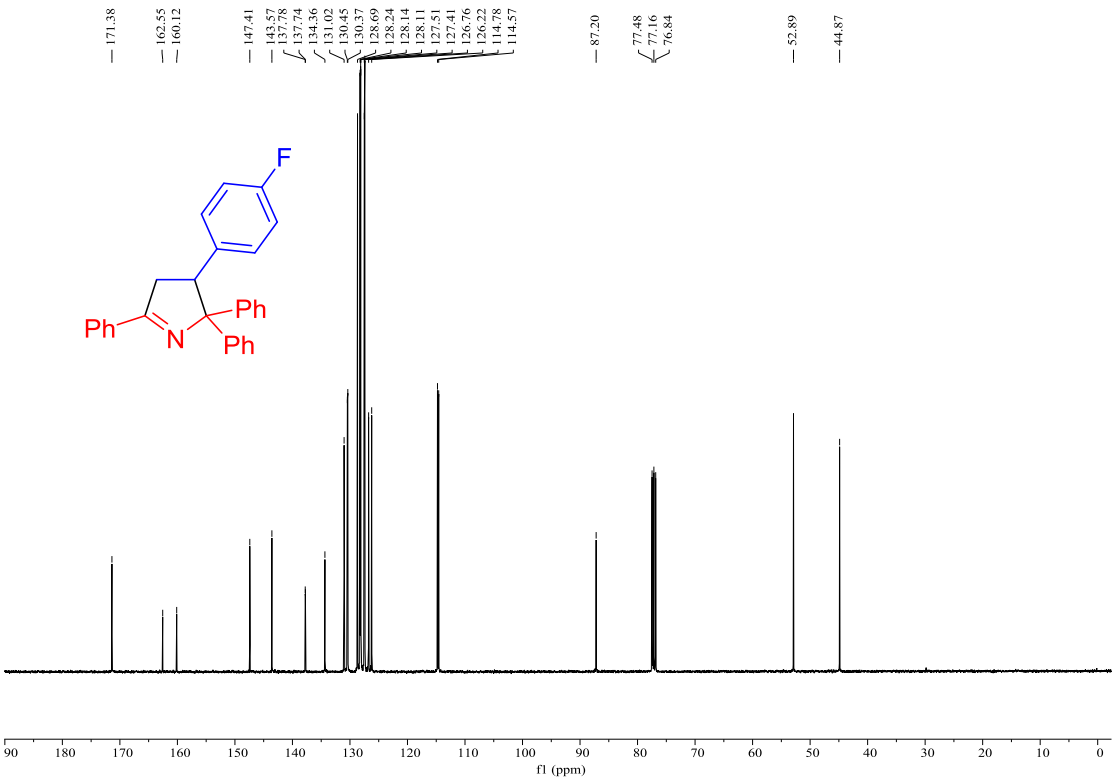


Figure S16. ^{19}F NMR spectra (376 MHz, Chloroform-*d*) of 3-(4-fluorophenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ga).

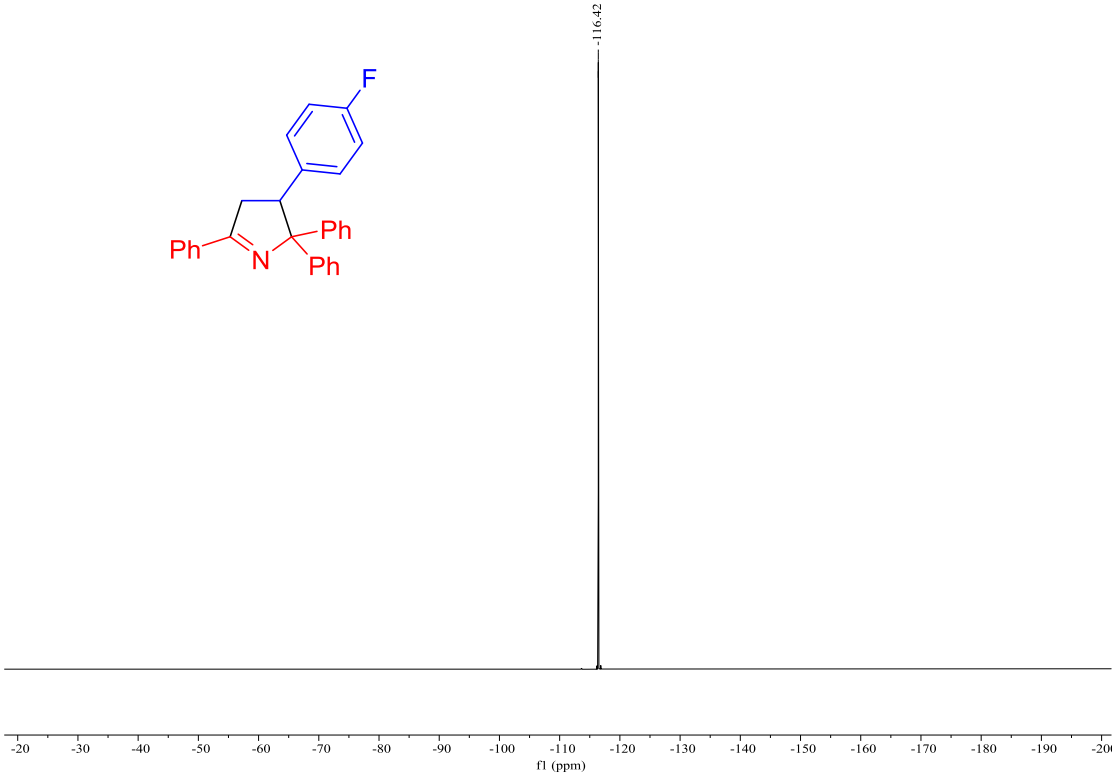


Figure S17. ^{1}H NMR spectra (600 MHz, Chloroform-*d*) of 3-(4-chlorophenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ha).

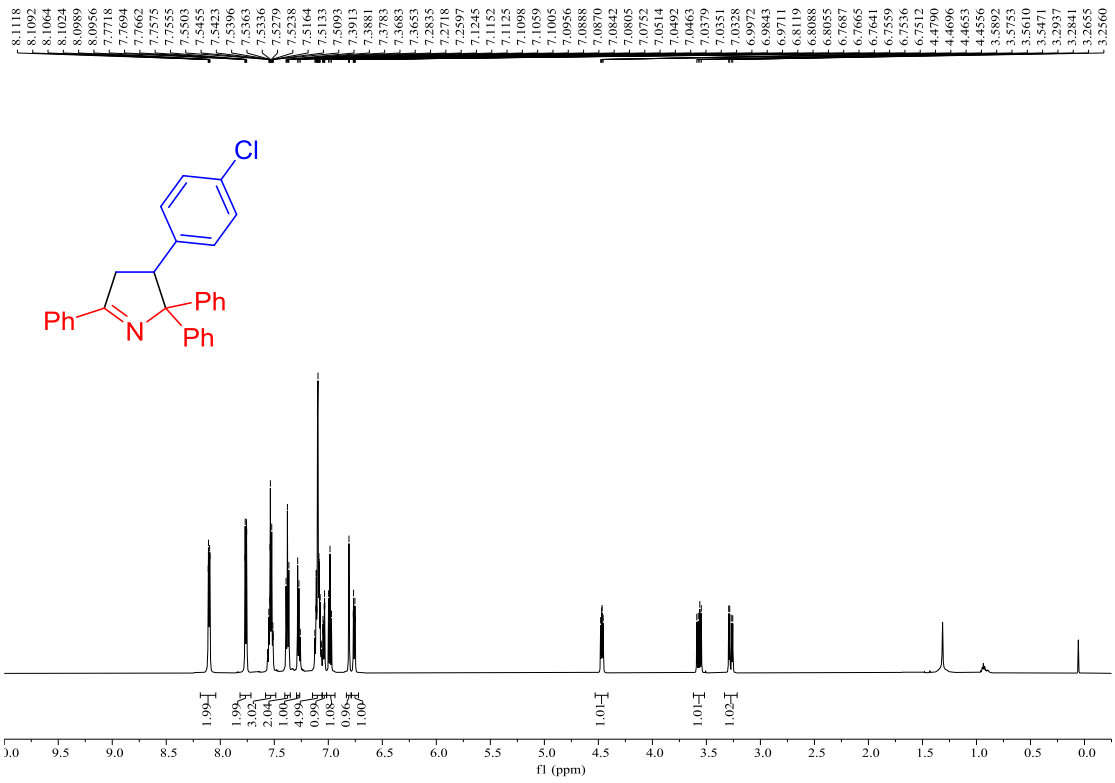


Figure S18. ^{13}C{^{1}H} NMR spectra (150 MHz, Chloroform-*d*) of 3-(4-chlorophenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ha).

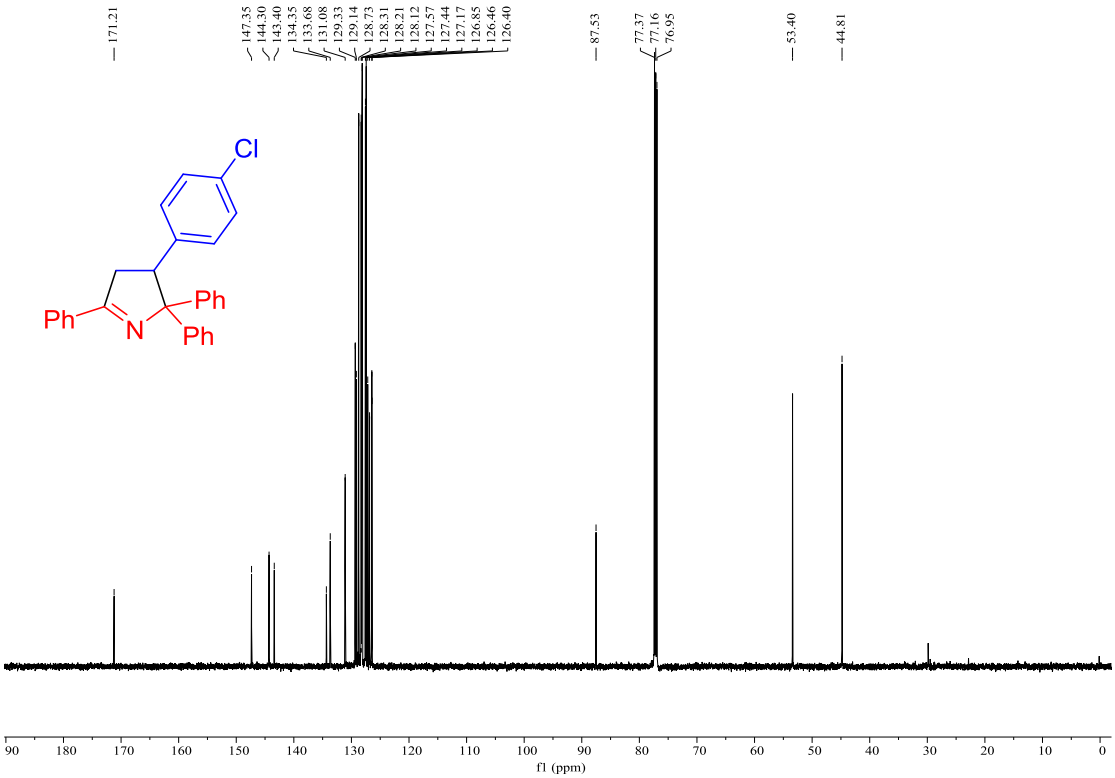


Figure S19. ^{1}H NMR spectra (600 MHz, Chloroform-*d*) of 3-(4-bromophenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ia).

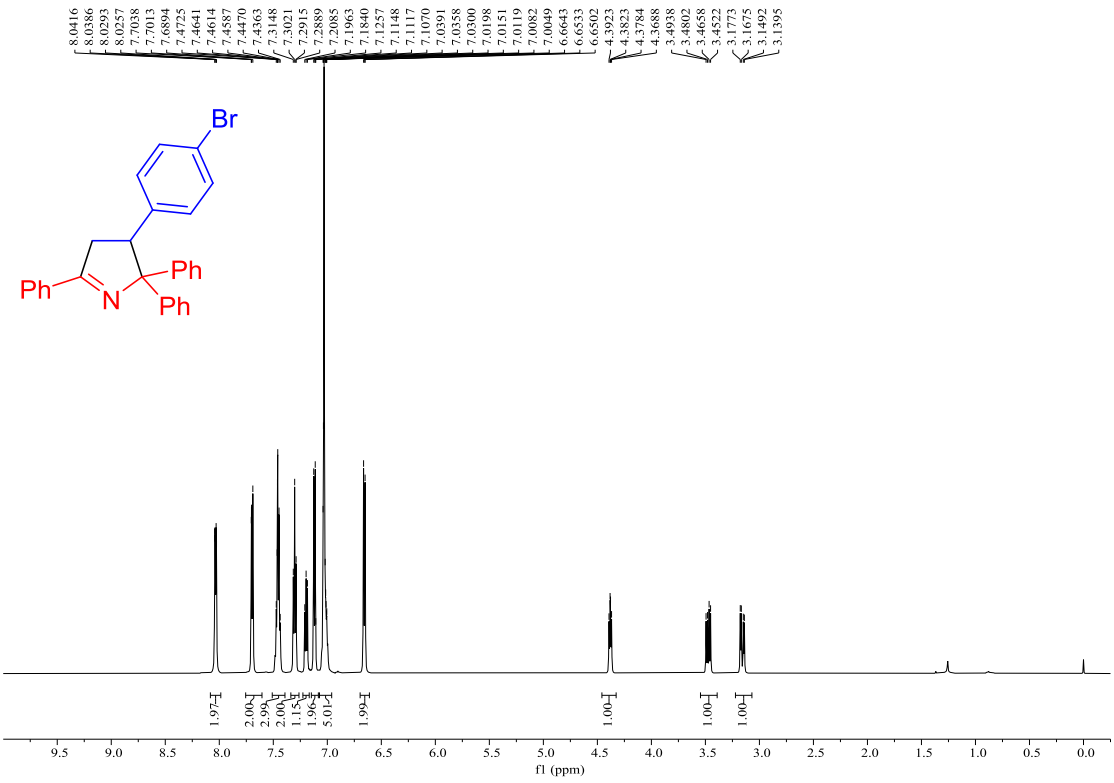


Figure S20. ^{13}C{^{1}H} NMR spectra (150 MHz, Chloroform-*d*) of 3-(4-bromophenyl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ia).

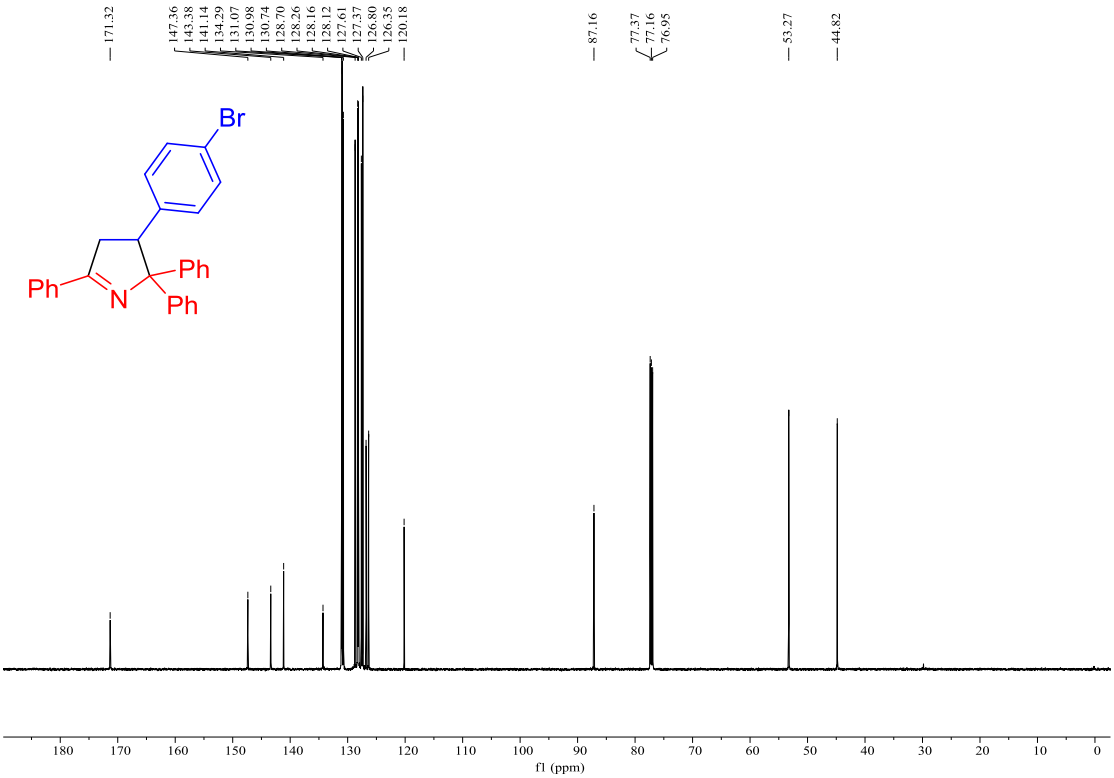


Figure S21. ^{1}H NMR spectra (600 MHz, Chloroform-*d*) of 3-(naphthalen-2-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ja).

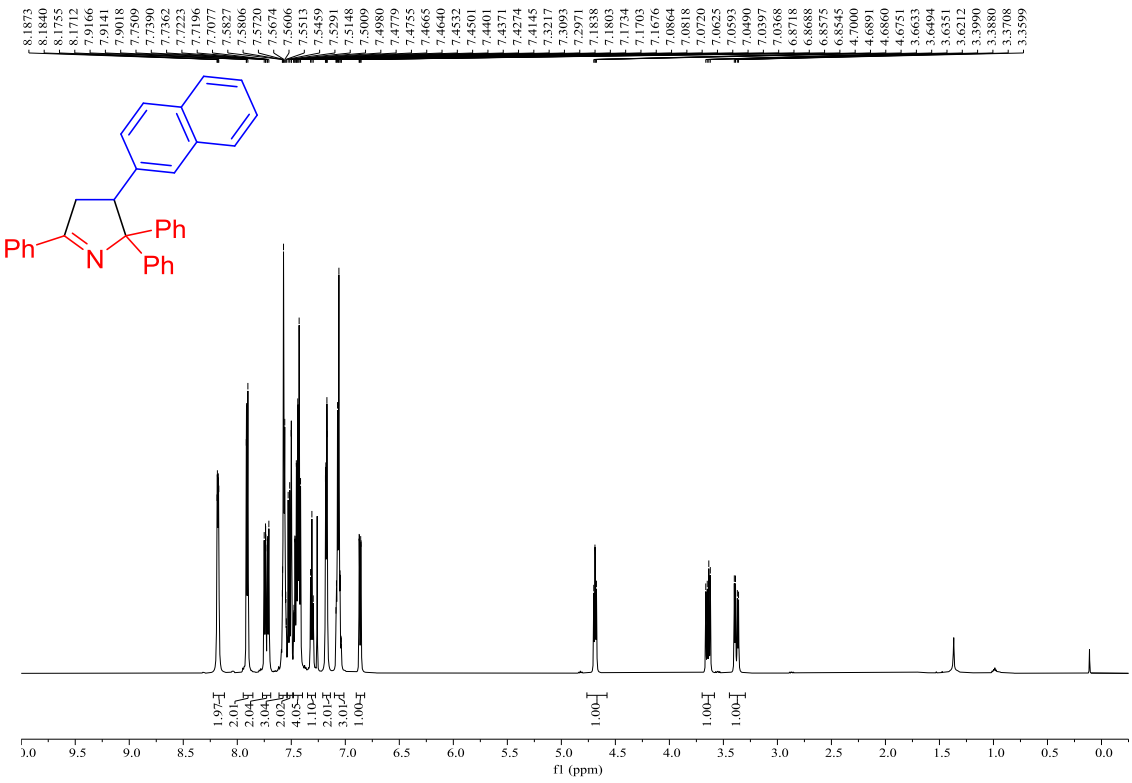


Figure S22. ^{13}C{^{1}H} NMR spectra (150 MHz, Chloroform-*d*) of 3-(naphthalen-2-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ja).

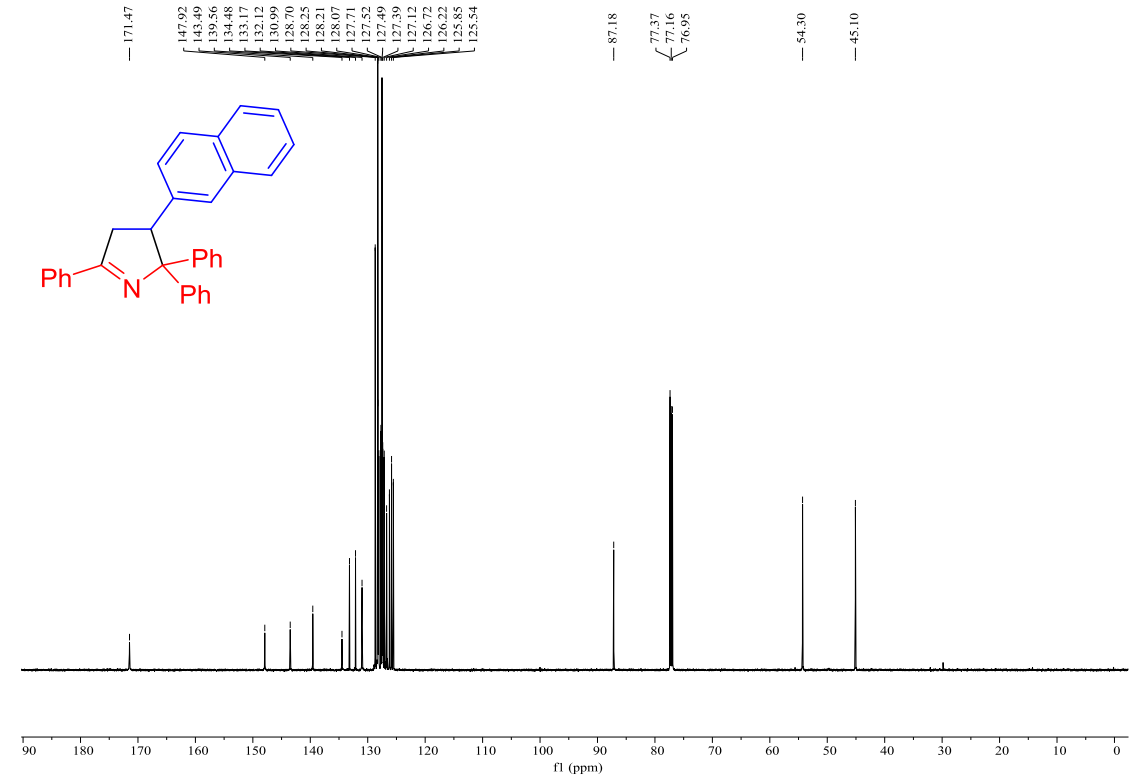


Figure S23. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-(4,4-dimethylthiochroman-6-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ka).

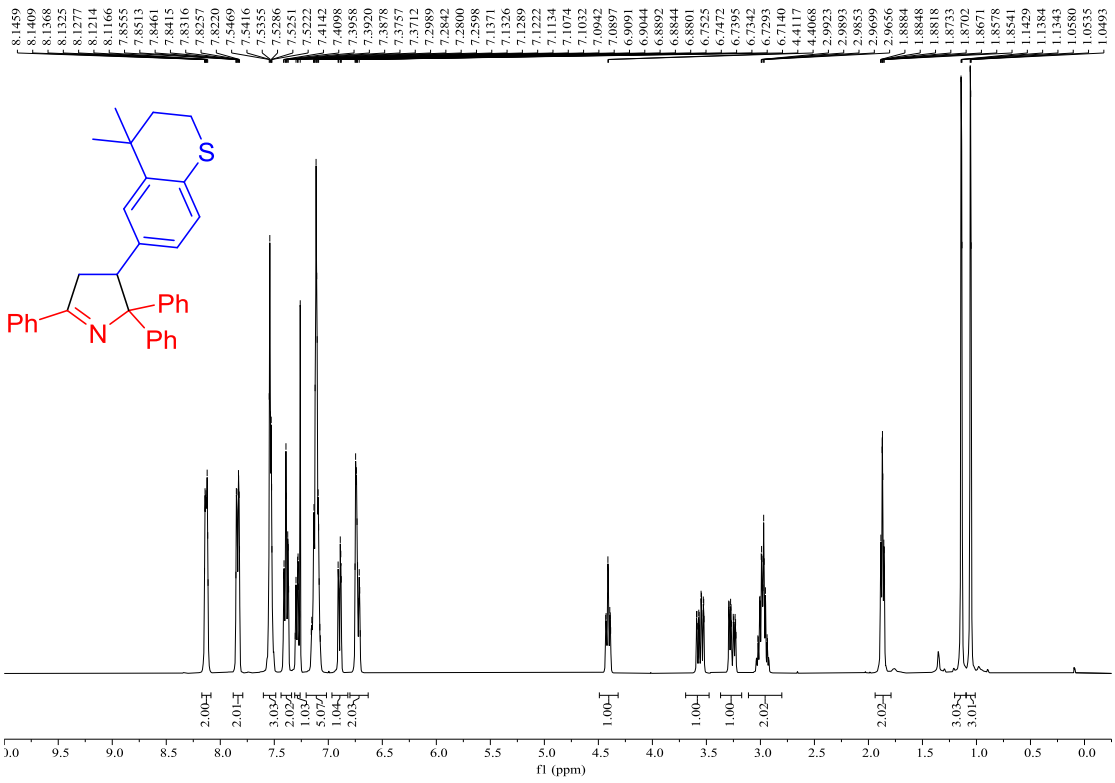


Figure S24. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 3-(4,4-dimethylthiochroman-6-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ka).

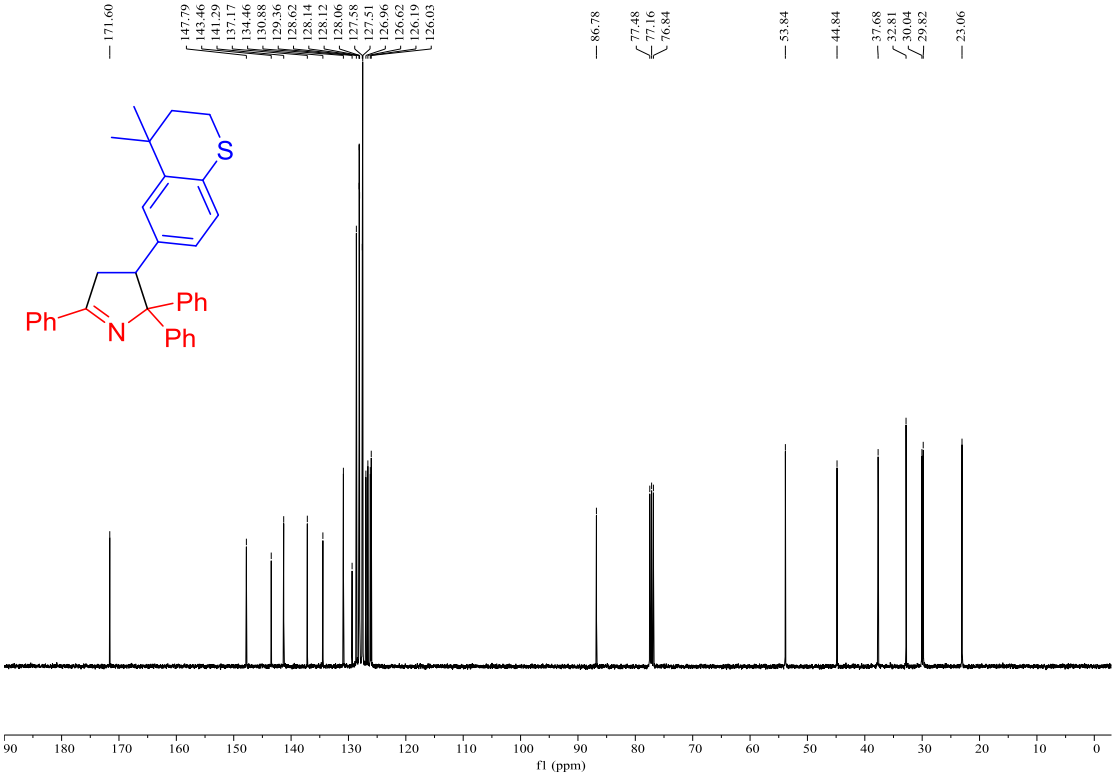


Figure S25. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-(4,4-dimethylthiochroman-6-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3la).

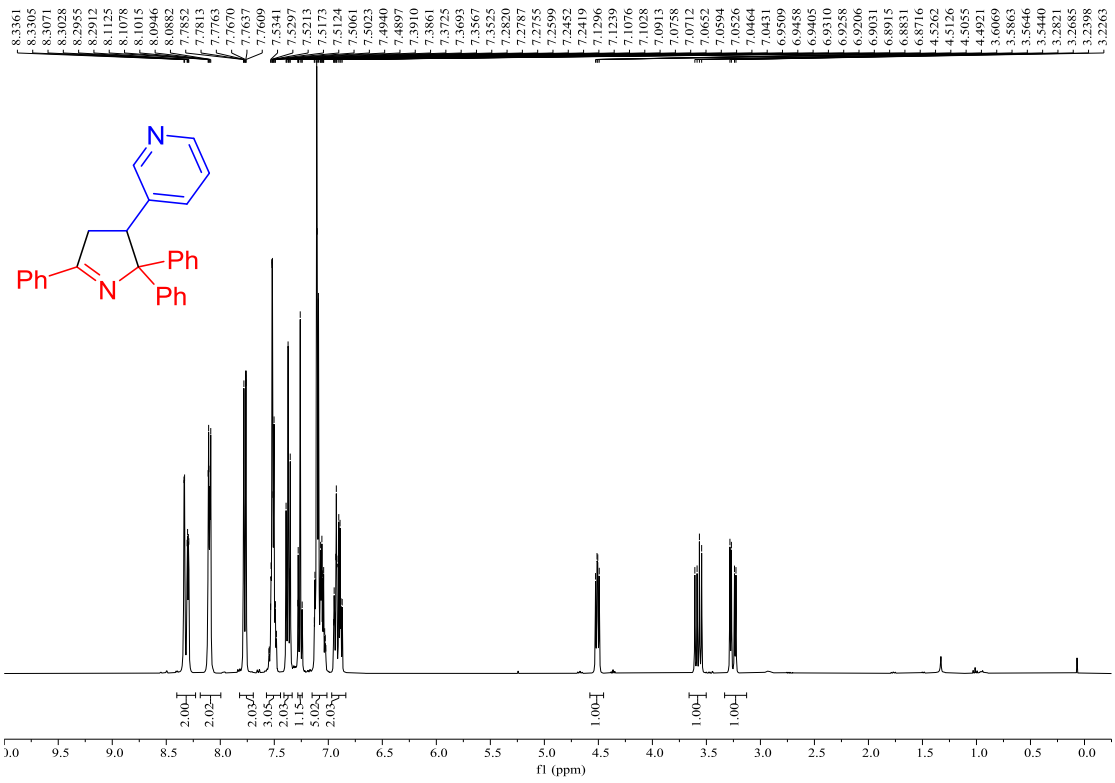


Figure S26. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 3-(4,4-dimethylthiochroman-6-yl)-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3la).

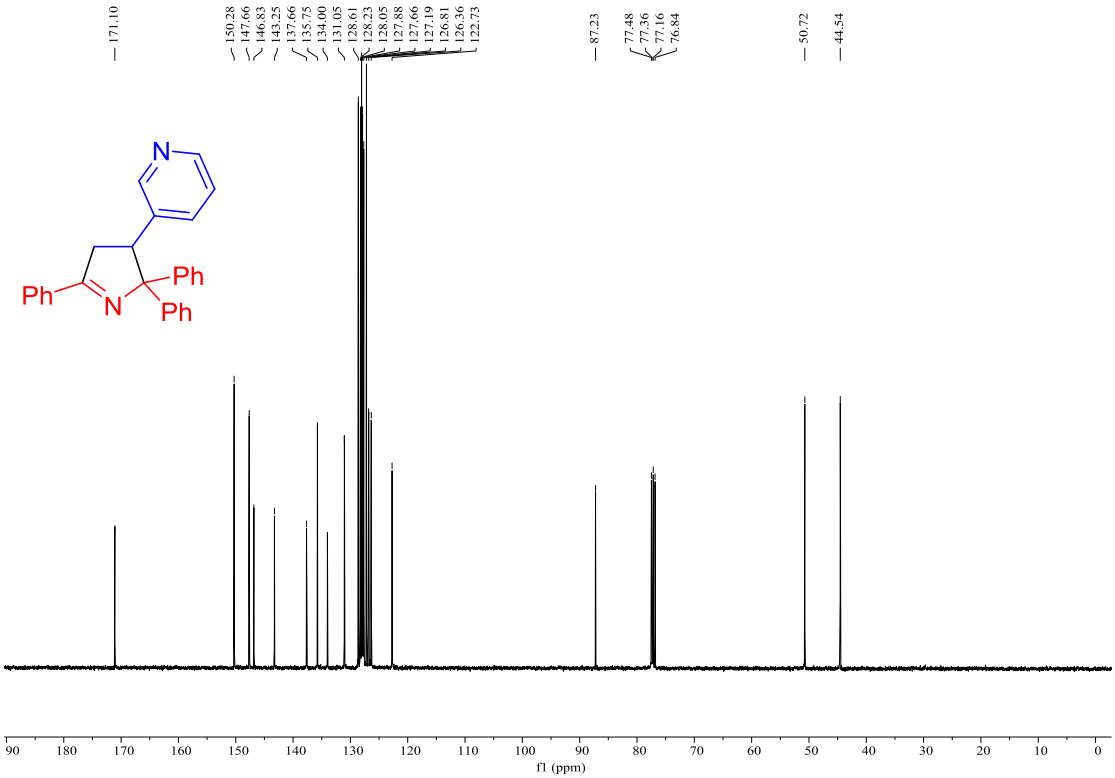


Figure S27. ^{1}H NMR spectra (600 MHz, Chloroform-*d*) of 3-hexyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ma).

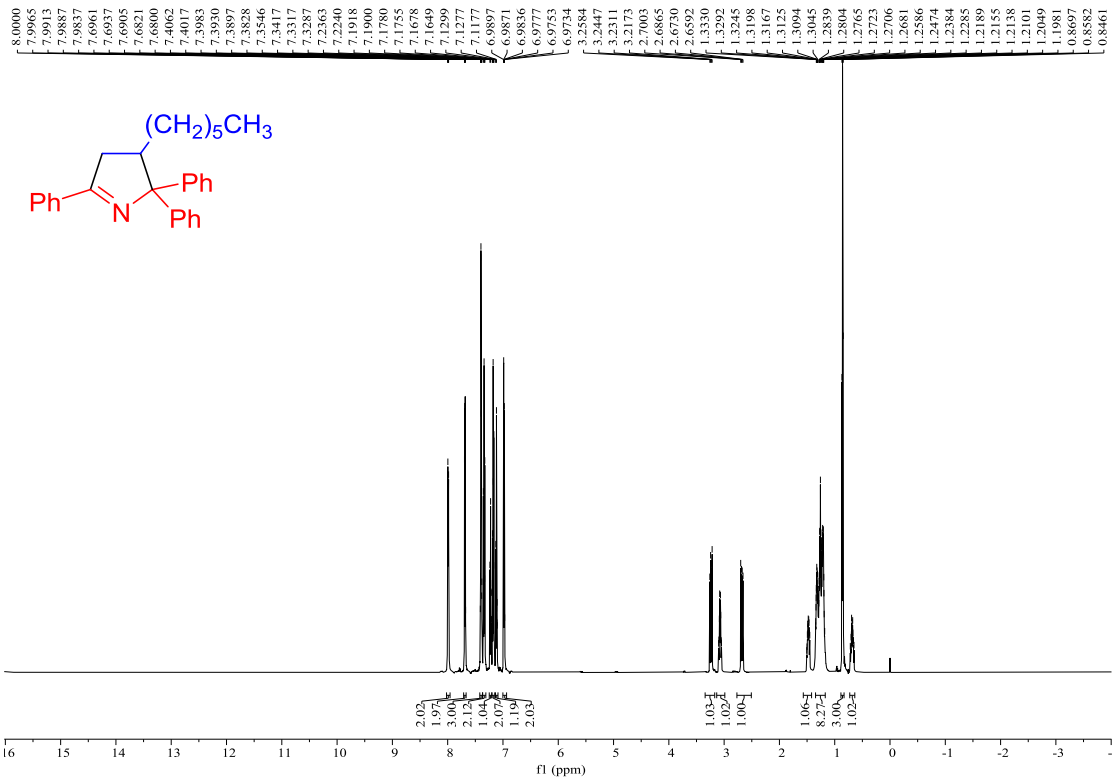


Figure S28. ^{13}C{^{1}H} NMR spectra (150 MHz, Chloroform-*d*) of 3-hexyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3ma).

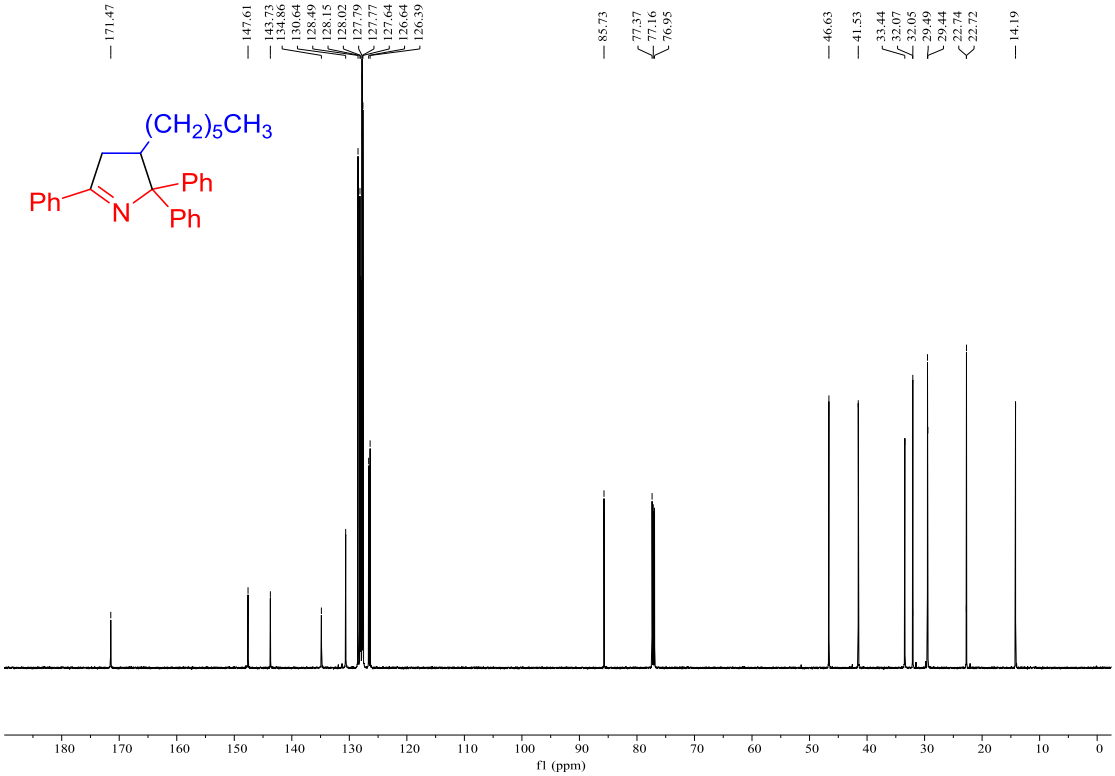


Figure S29. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-cyclopentyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3na).

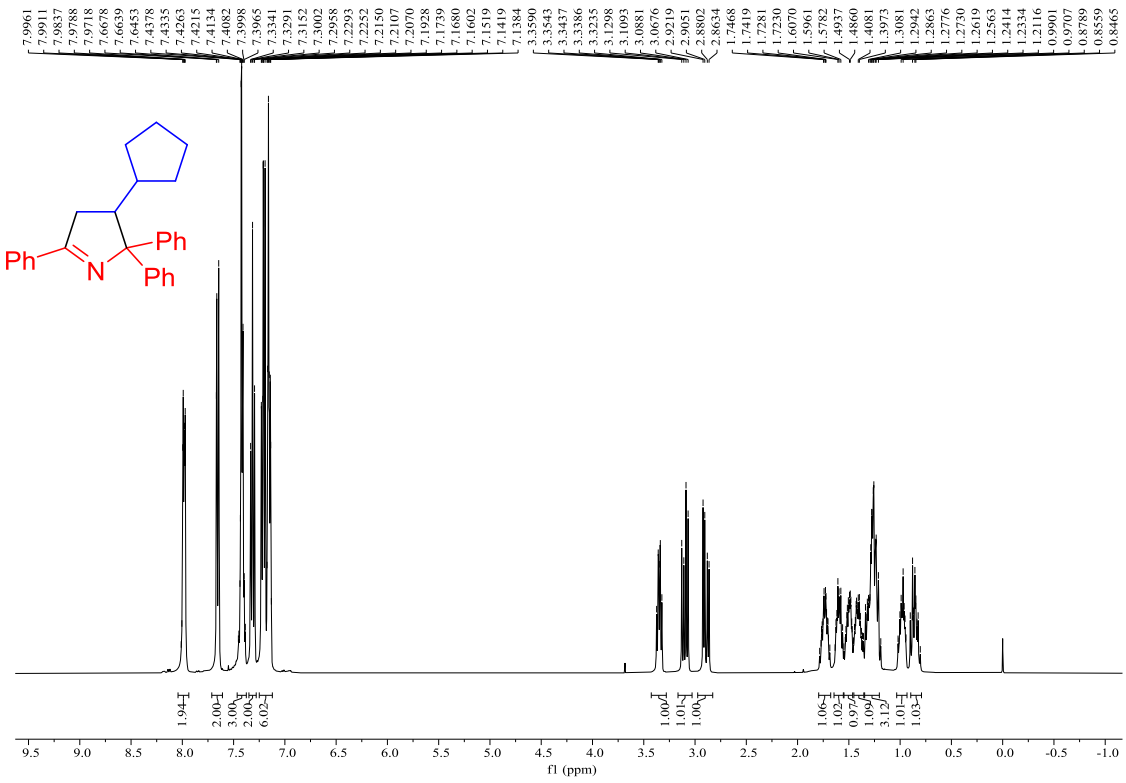


Figure S30. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 3-cyclopentyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3na).

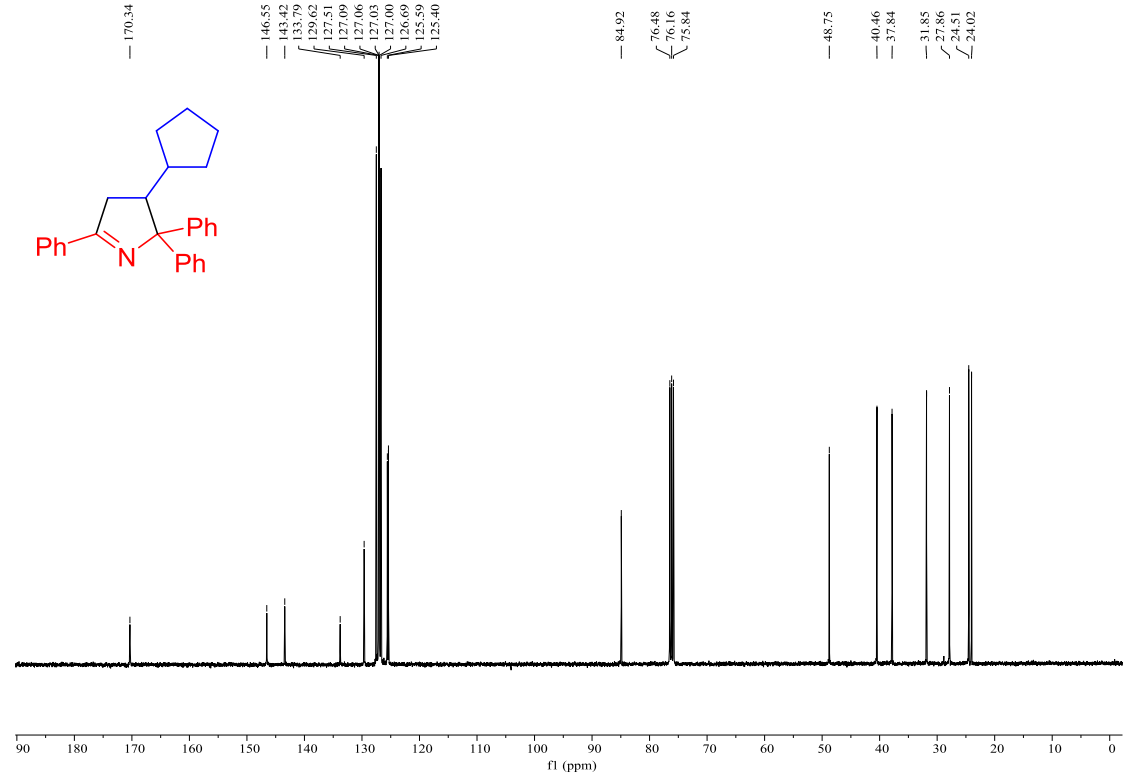


Figure S31. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-cyclohexyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3oa).

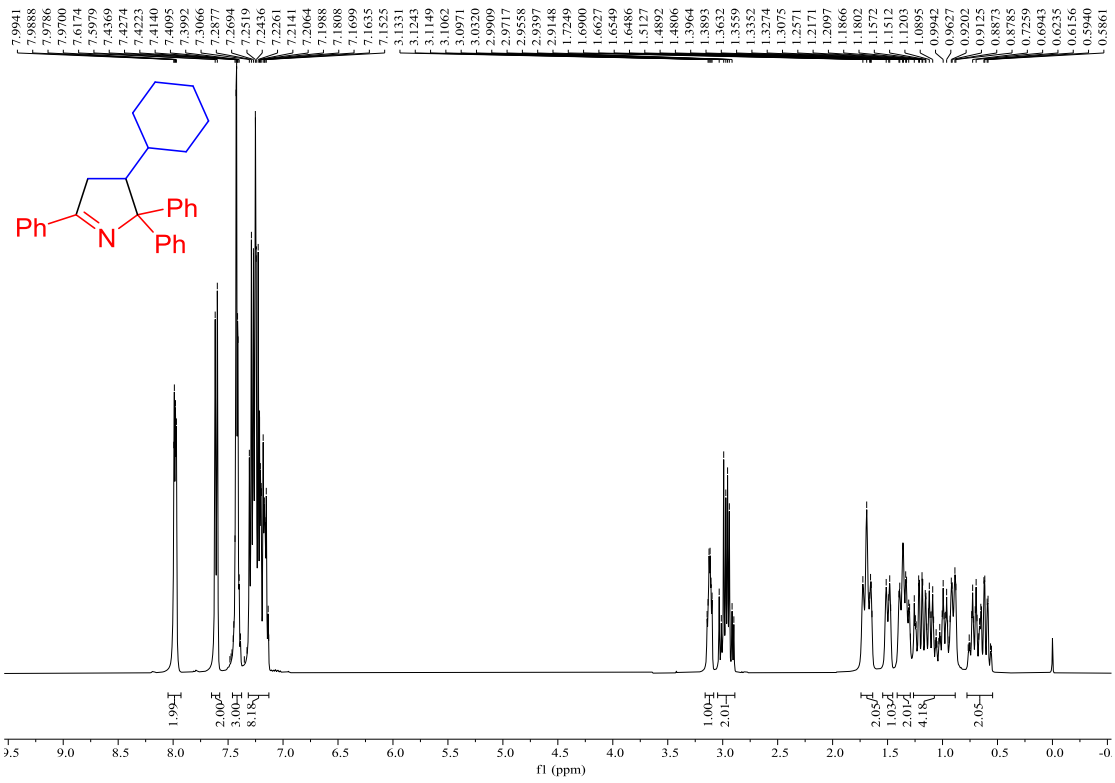


Figure S32. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 3-cyclohexyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3oa).

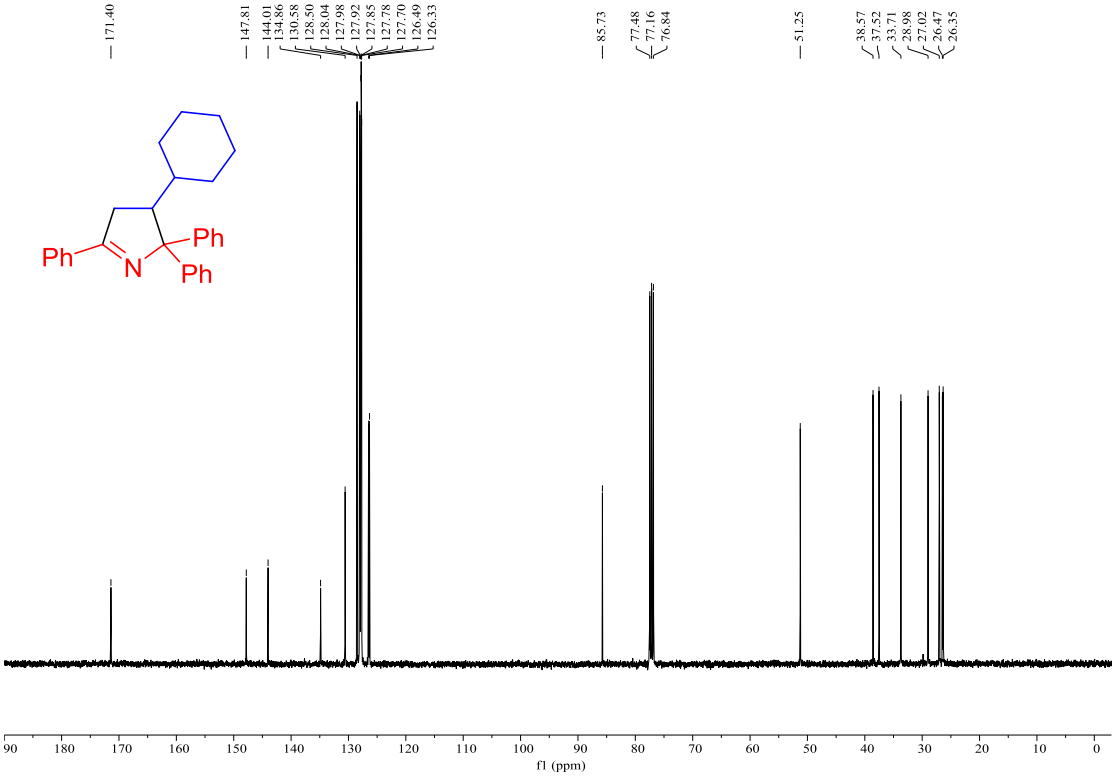


Figure S33. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 2,2,3-triphenyl-5-(m-tolyl)-3,4-dihydro-2*H*-pyrrole (3ab).

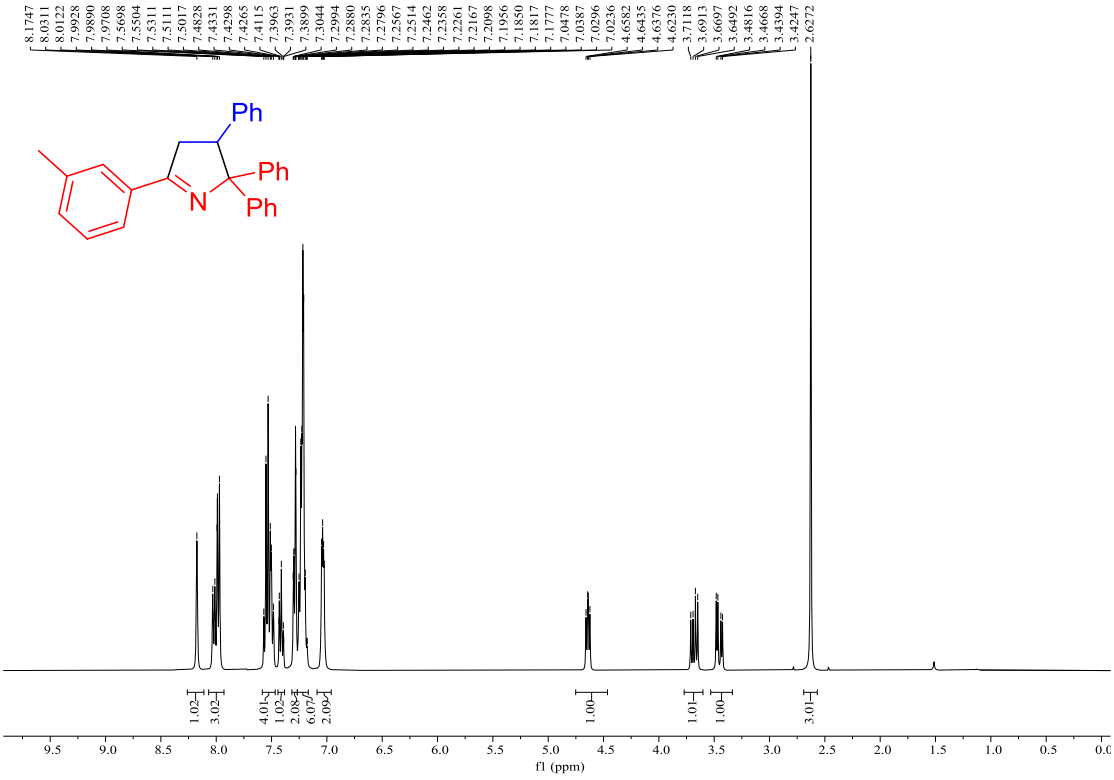


Figure S34. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 2,2,3-triphenyl-5-(m-tolyl)-3,4-dihydro-2*H*-pyrrole (3ab).

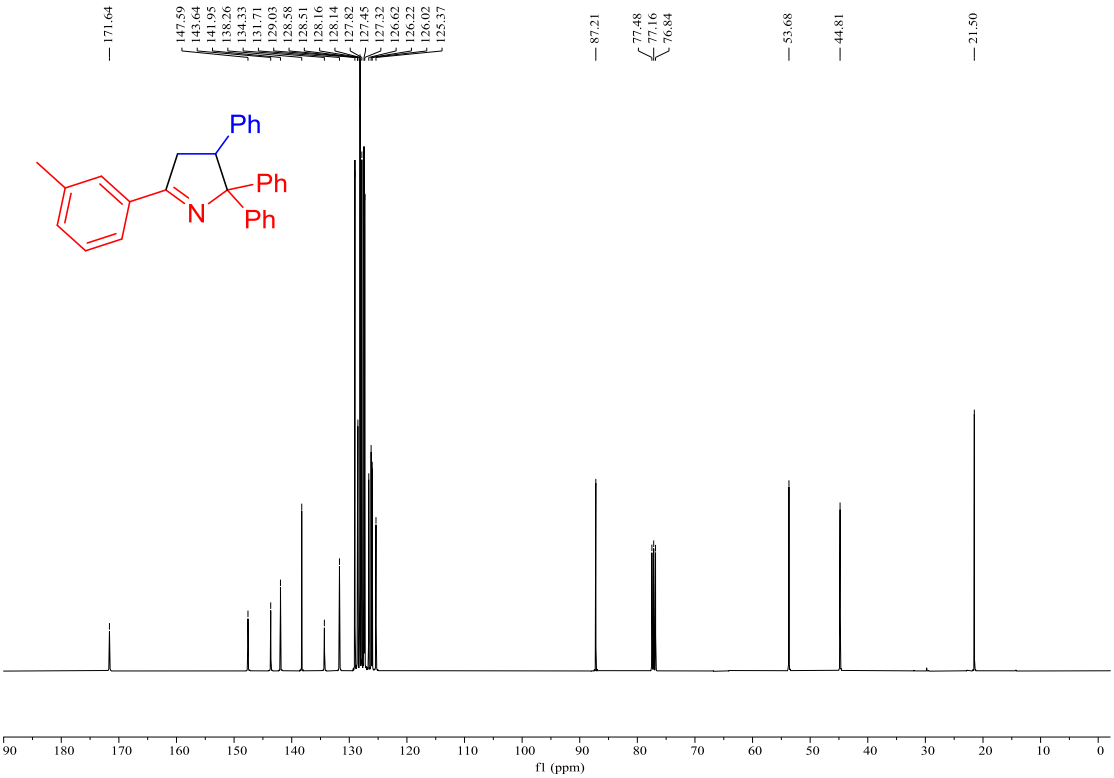


Figure S35. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 5-(4-methoxyphenyl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ac).

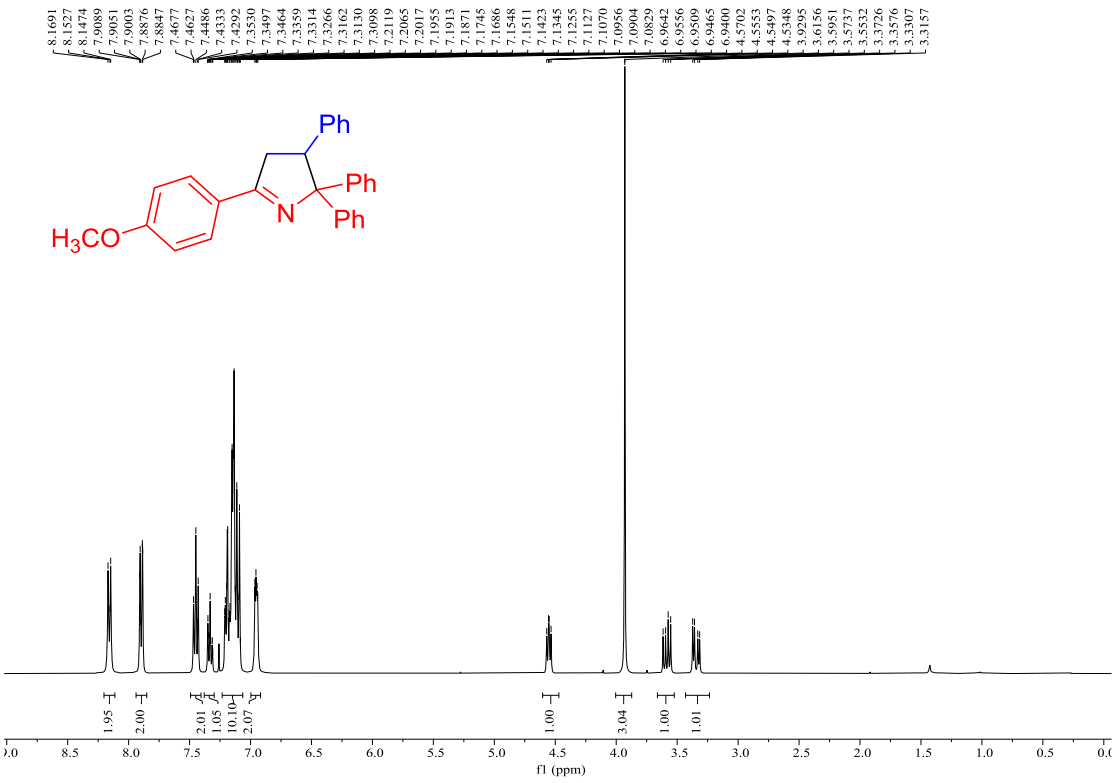


Figure S36. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 5-(4-methoxyphenyl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ac).

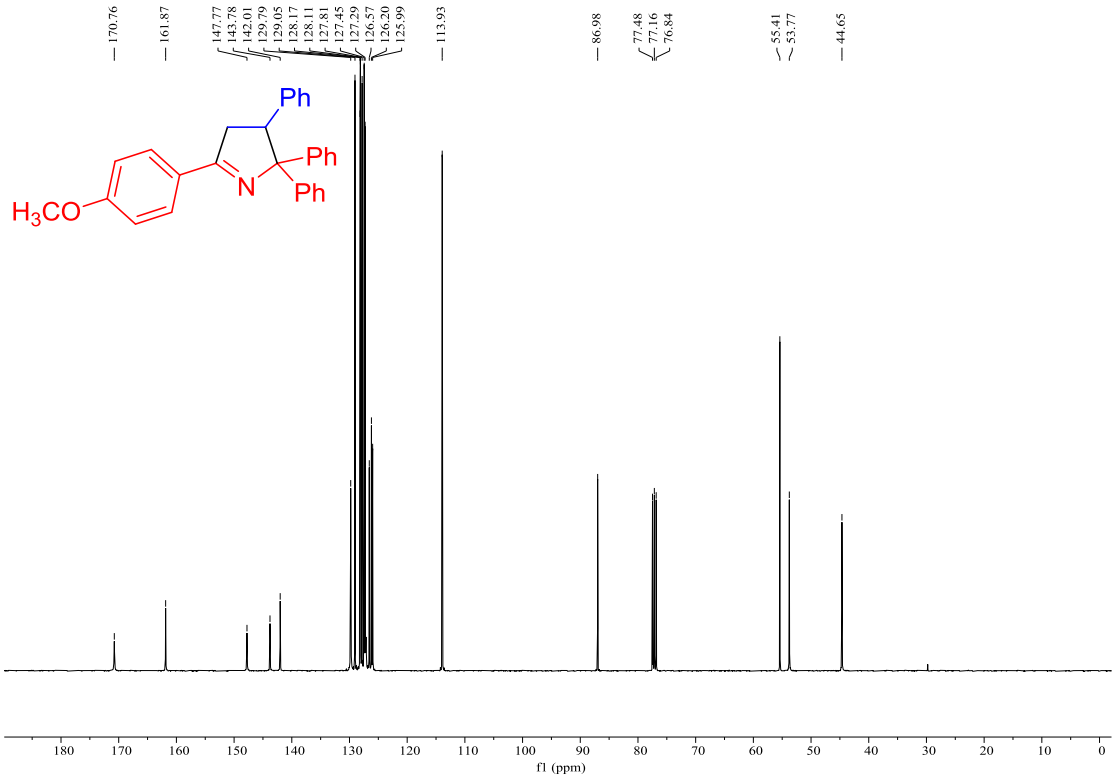


Figure S37. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 5-(benzo[d][1,3]dioxol-5-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ad).

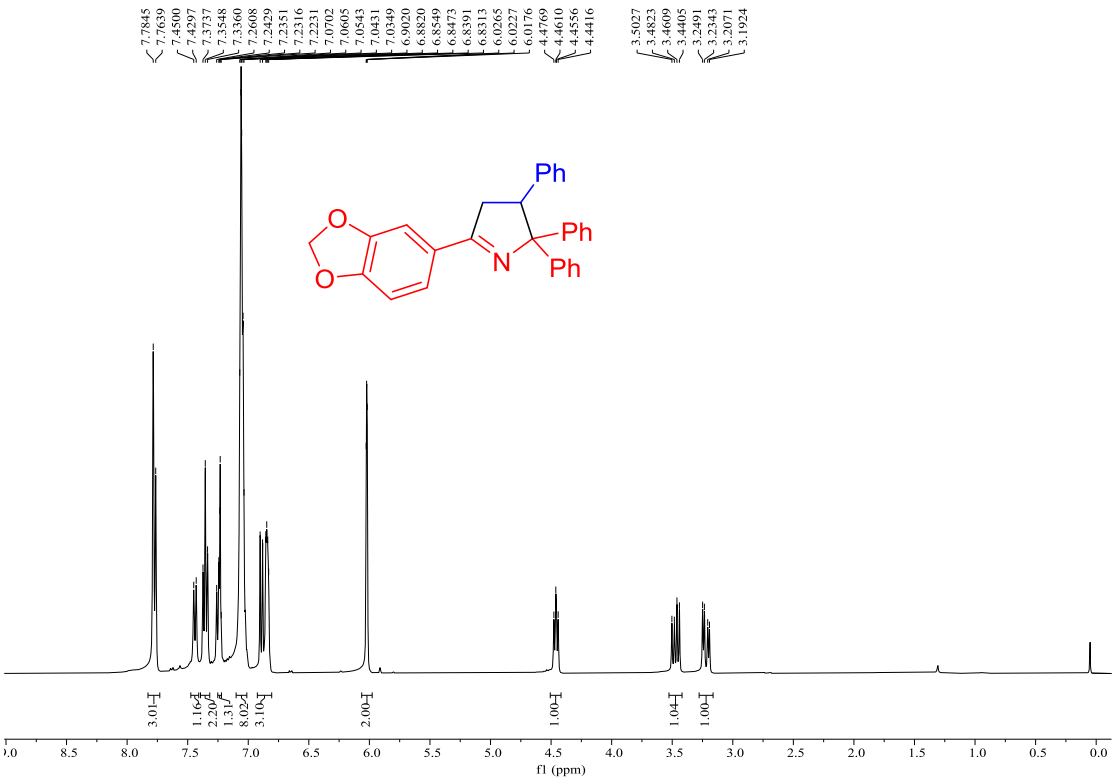


Figure S38. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 5-(benzo[d][1,3]dioxol-5-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ad).

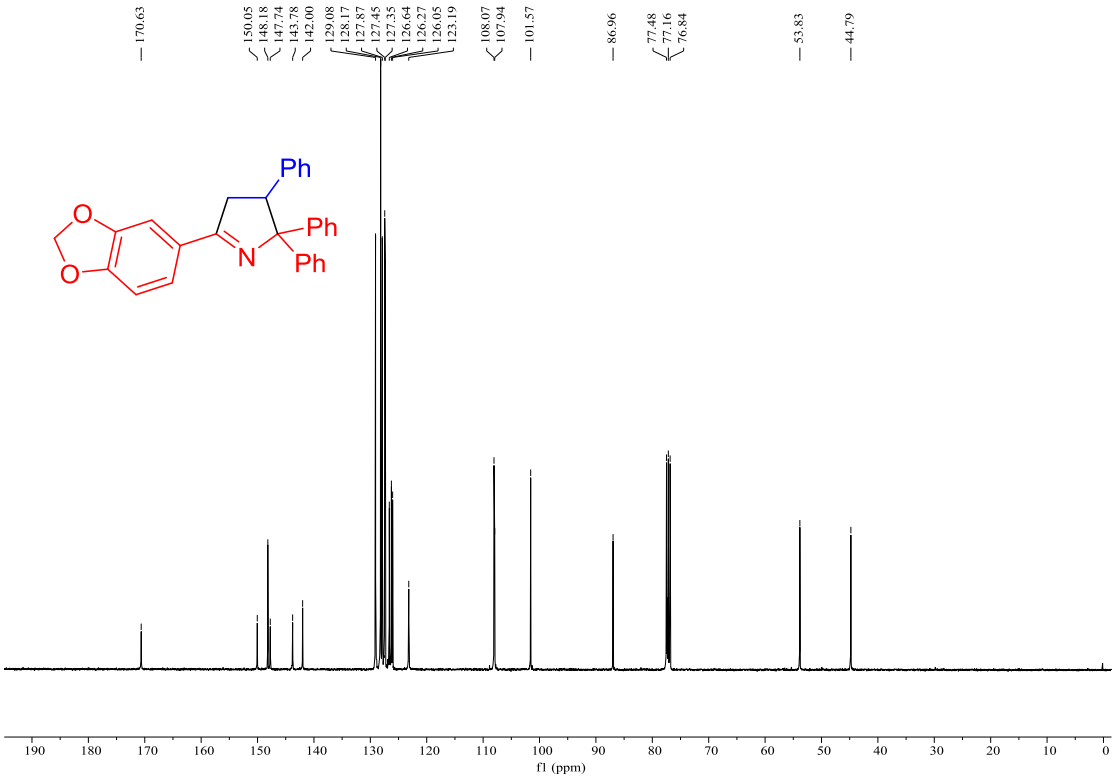


Figure S39. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 5-([1,1'-biphenyl]-4-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ae).

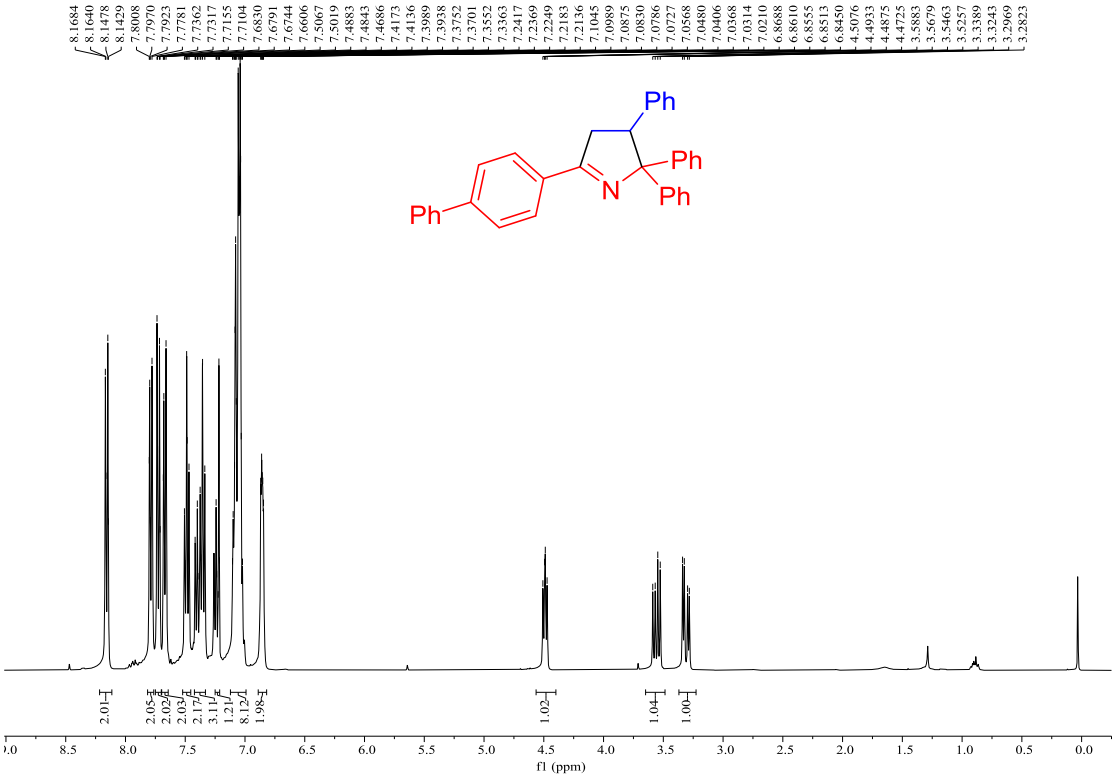


Figure S40. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 5-([1,1'-biphenyl]-4-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ae).

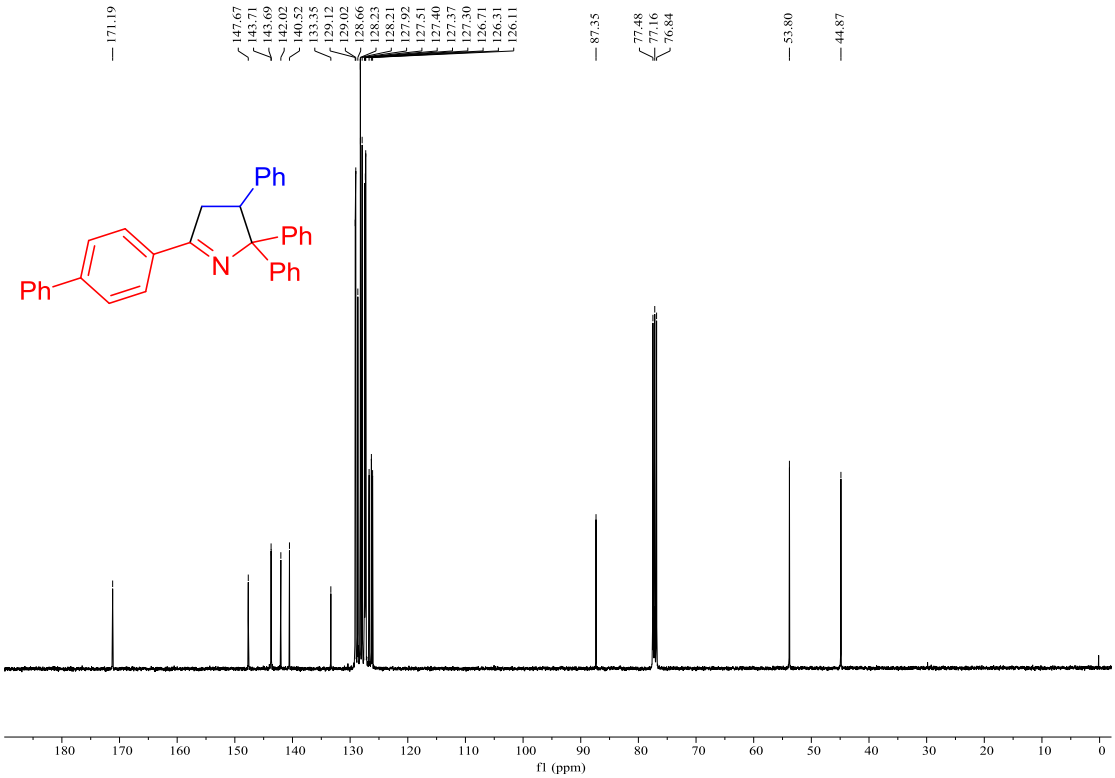


Figure S41. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 3-cyclohexyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3af).

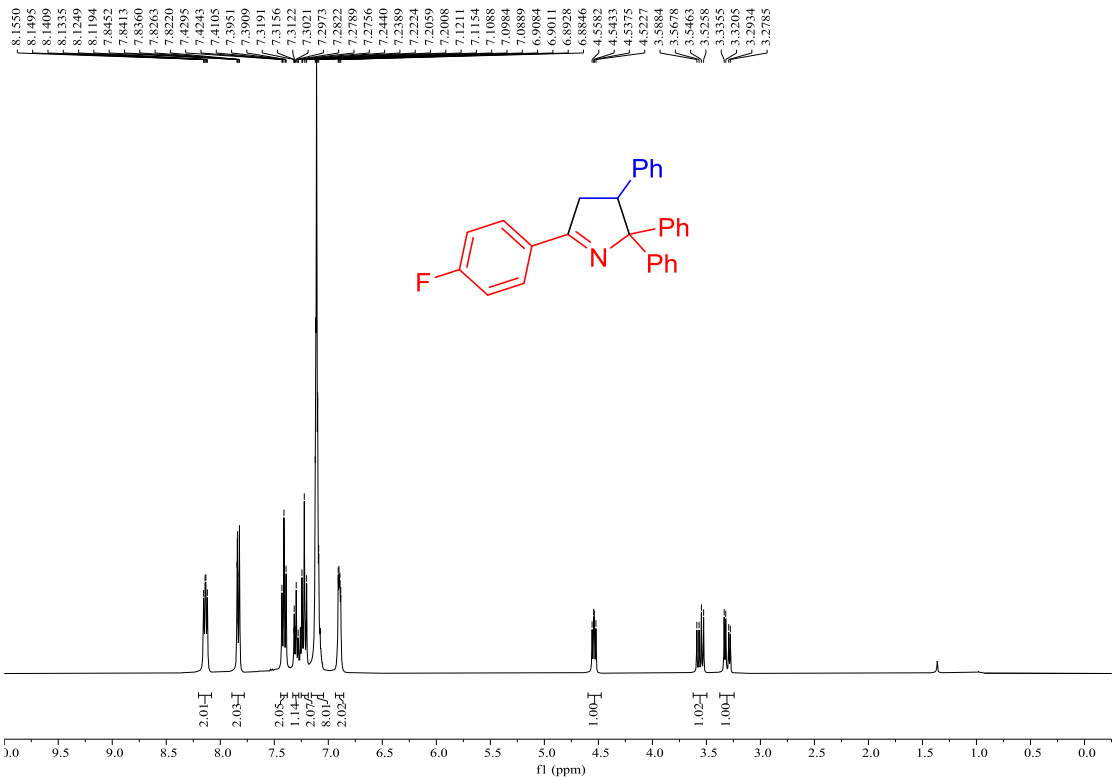


Figure S42. ^{13}C{^{1}H} NMR spectra (100 MHz, Chloroform-*d*) of 3-cyclohexyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3af).

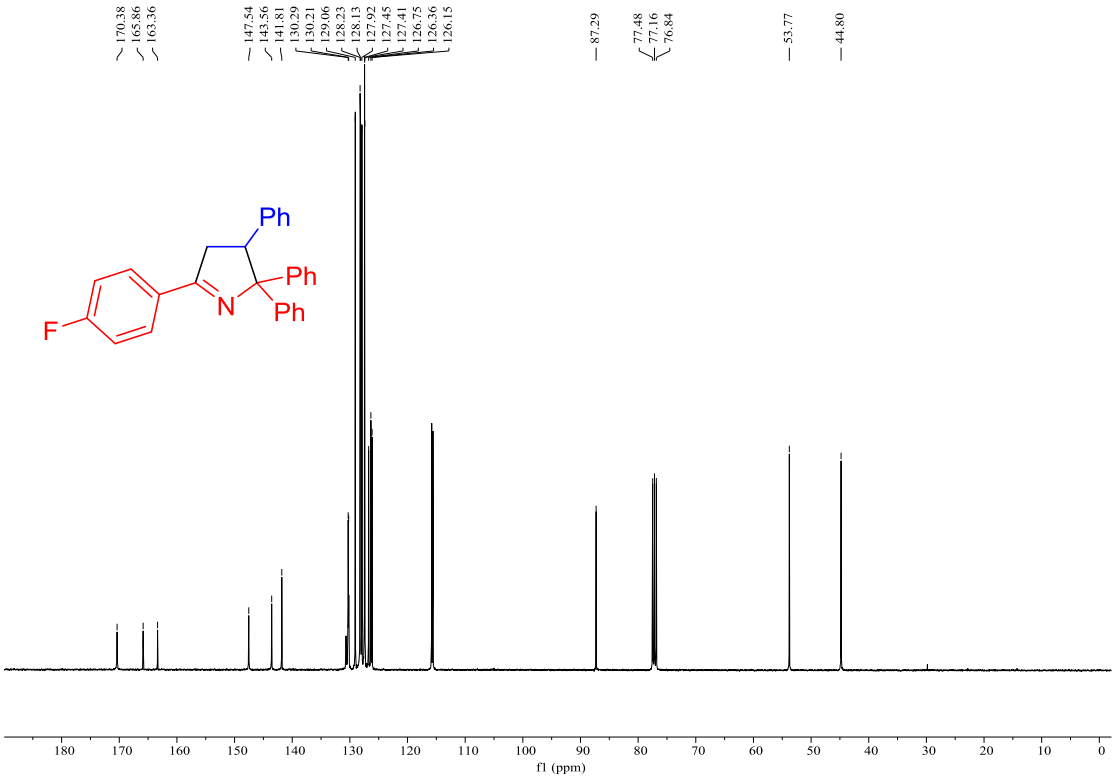


Figure S43. ^{19}F NMR spectra (376 MHz, Chloroform-*d*) of 3-cyclohexyl-2,2,5-triphenyl-3,4-dihydro-2*H*-pyrrole (3af).

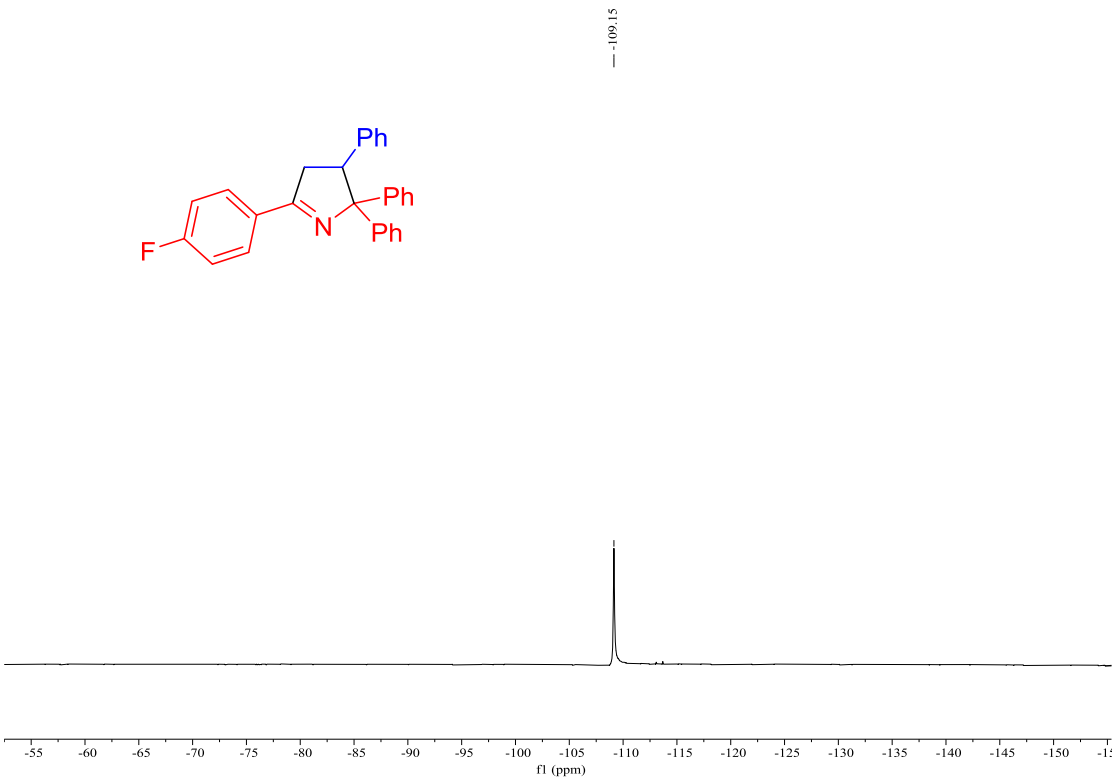


Figure S44. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 5-(4-chlorophenyl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ag).

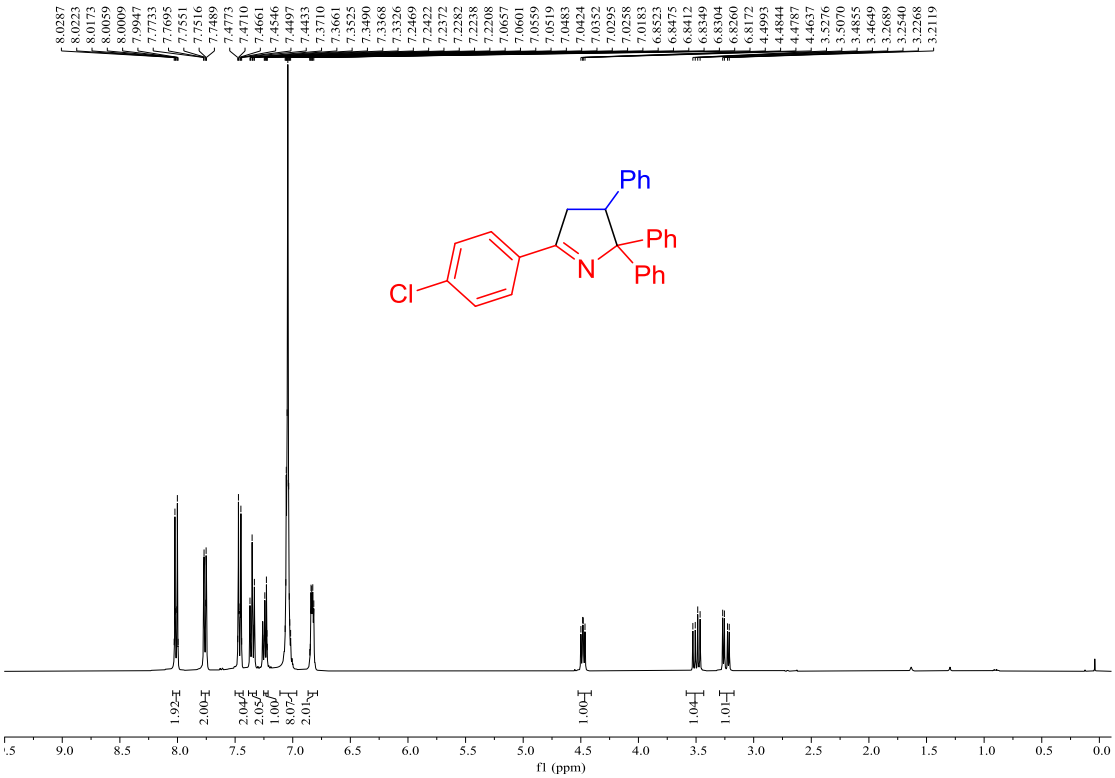


Figure S45. $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 5-(4-chlorophenyl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ag).

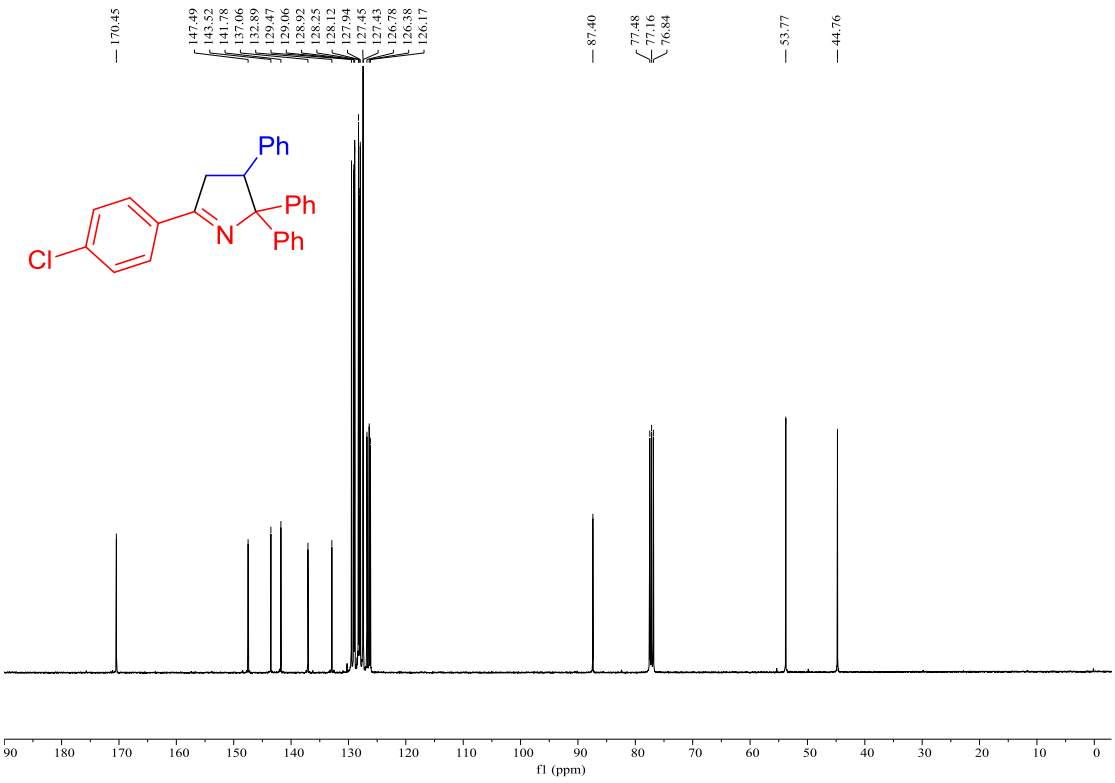


Figure S46. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 2,2,3-triphenyl-5-(*o*-tolyl)-3,4-dihydro-2*H*-pyrrole (3ah).

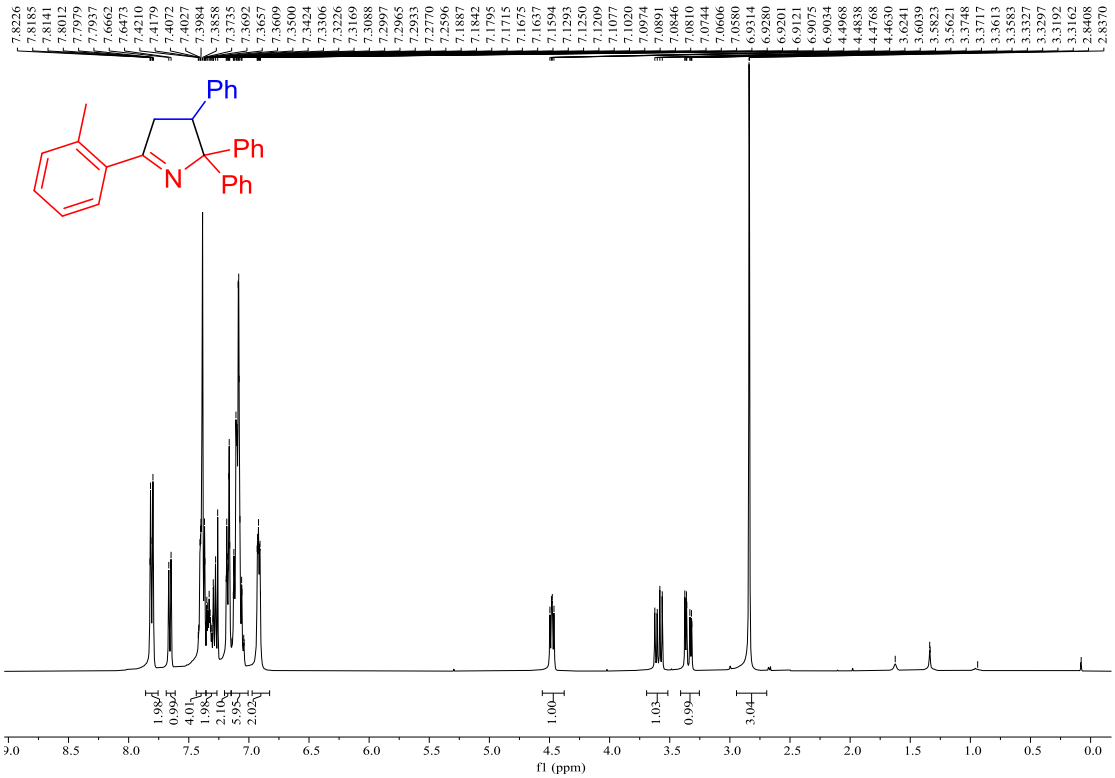


Figure S47. $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 2,2,3-triphenyl-5-(*o*-tolyl)-3,4-dihydro-2*H*-pyrrole (3ah).

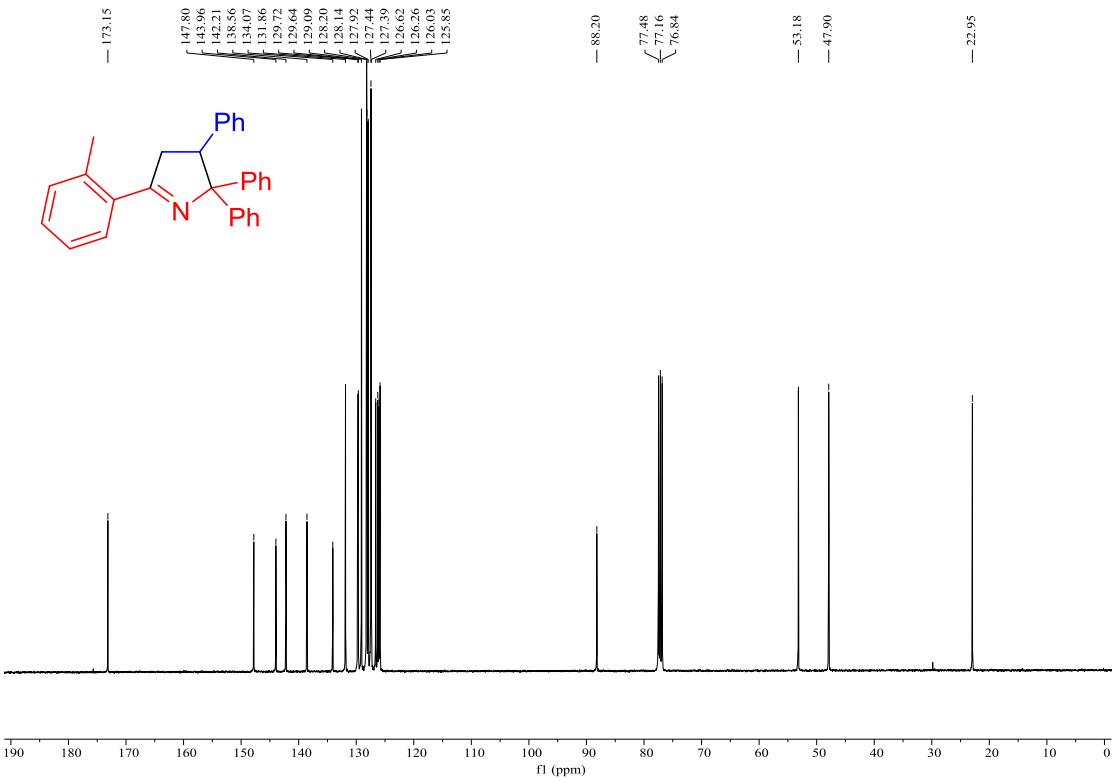


Figure S48. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 5-(naphthalen-2-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ai).

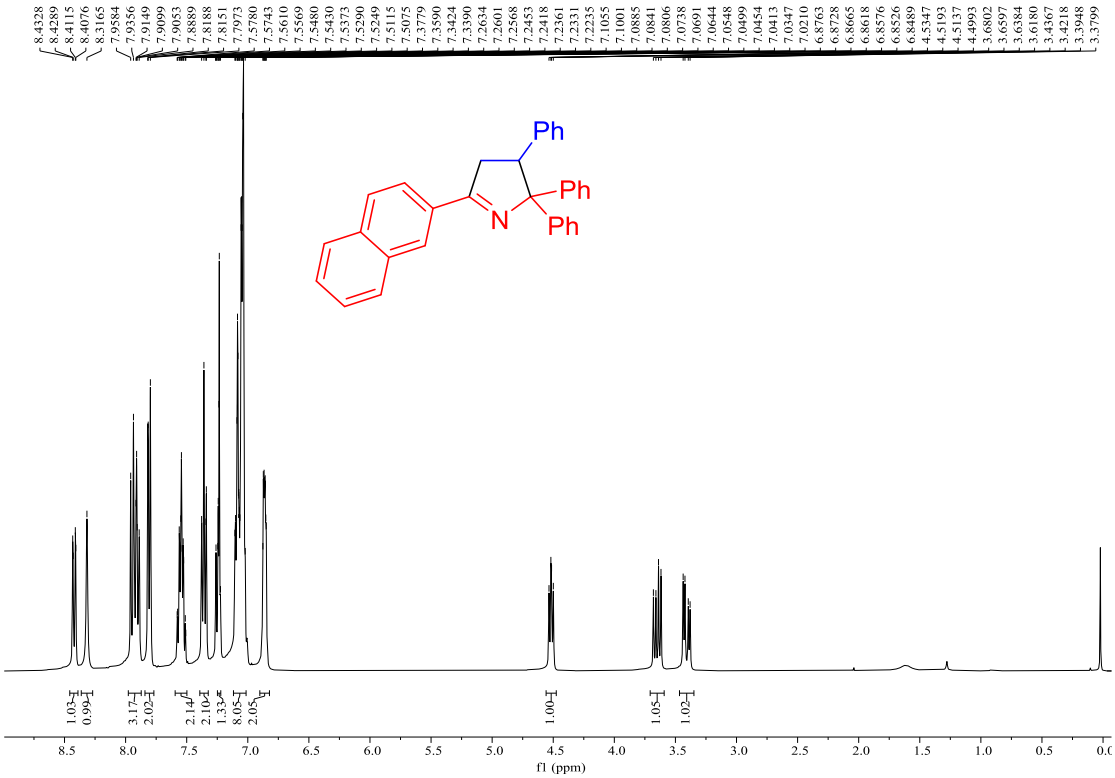


Figure S49. $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 5-(naphthalen-2-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3ai).

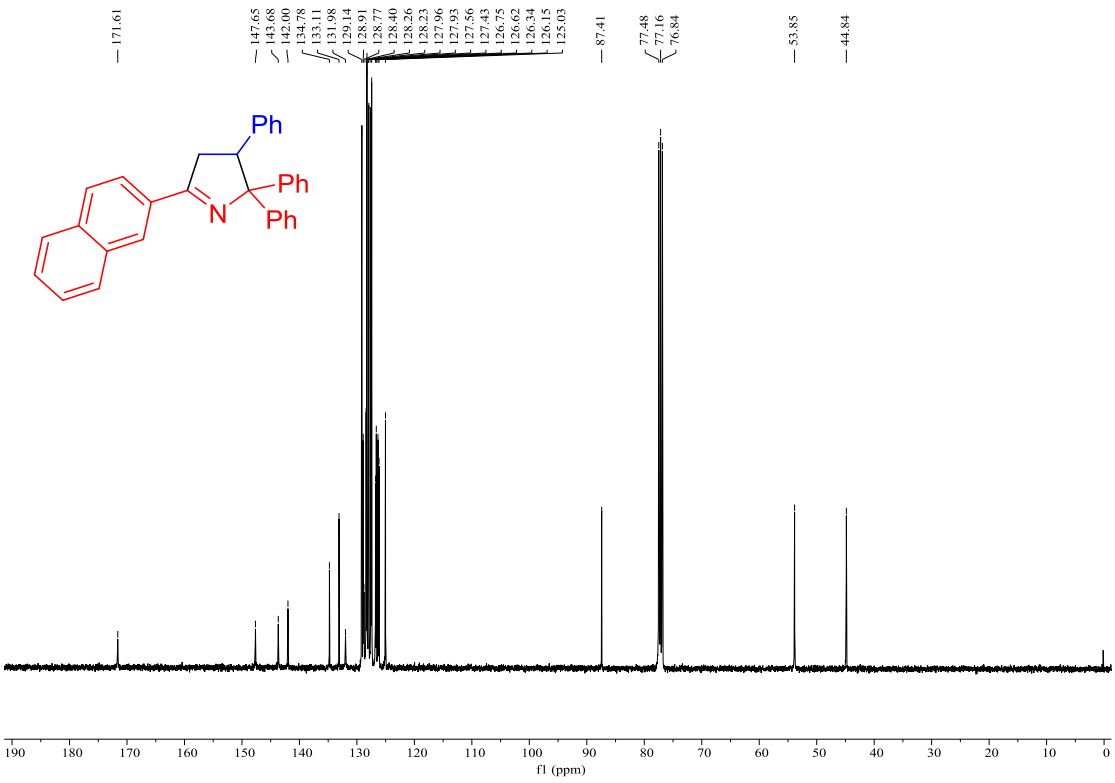


Figure S50. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 2-(2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrol-5-yl)pyridine (3aj).

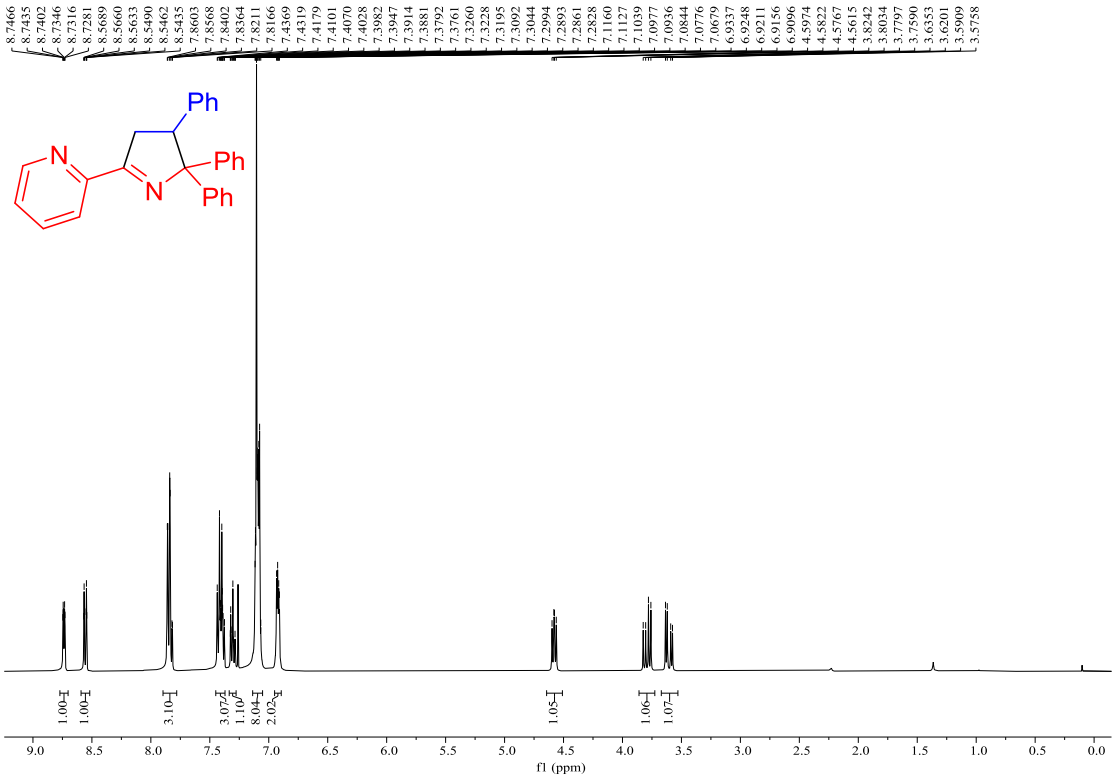


Figure S51 $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 2-(2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrol-5-yl)pyridine (3aj).

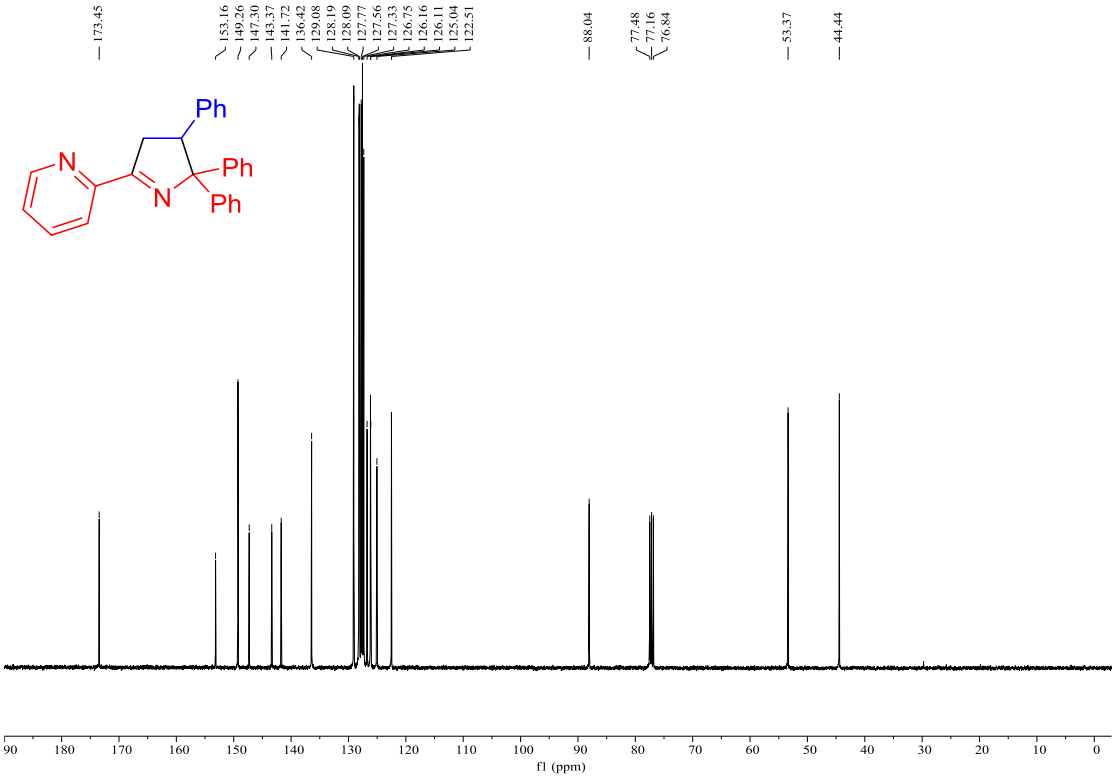


Figure S52. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 4-(2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrol-5-yl)pyridine (3ak).

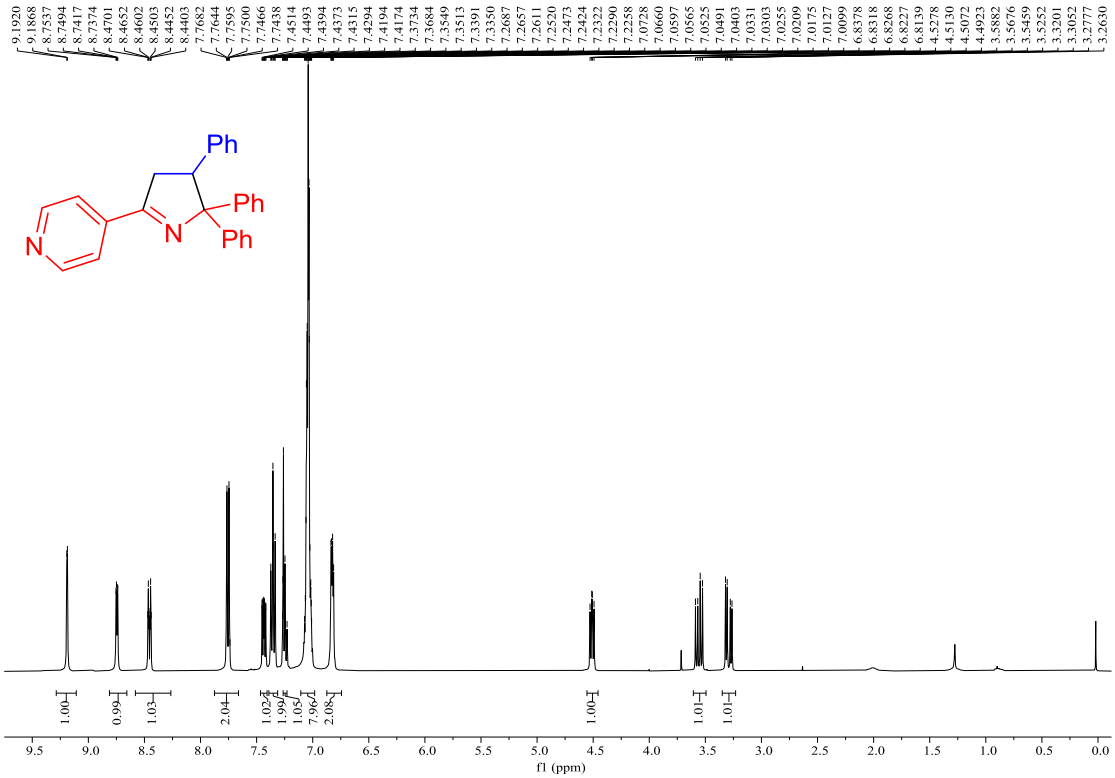


Figure S53. $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 4-(2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrol-5-yl)pyridine (3ak).

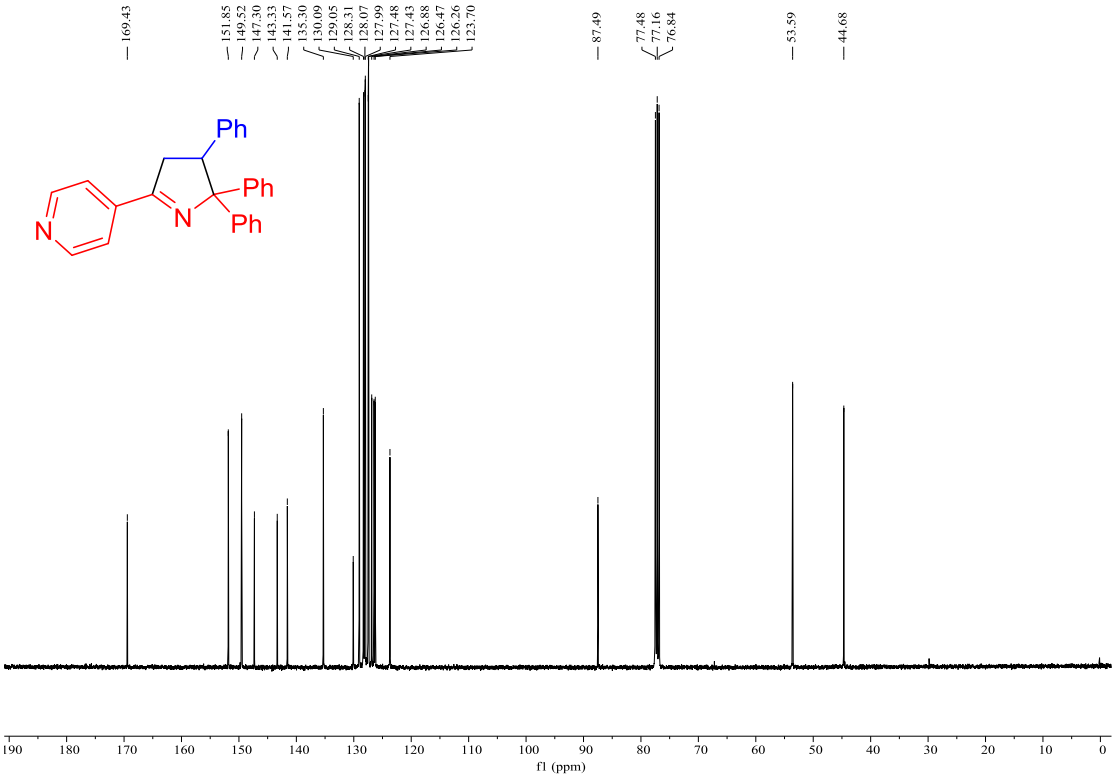


Figure S54. ^{1}H NMR spectra (400 MHz, Chloroform-*d*) of 5-(furan-2-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3al).

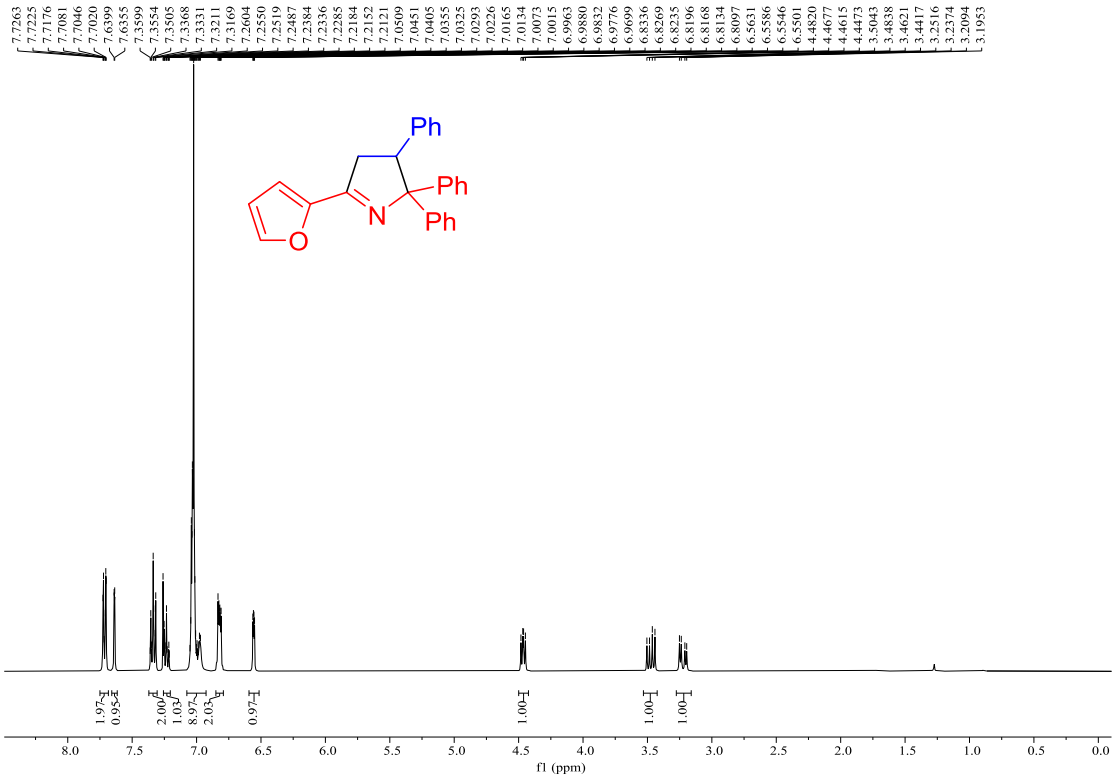


Figure S55. $^{13}C\{^{1}H\}$ NMR spectra (100 MHz, Chloroform-*d*) of 5-(furan-2-yl)-2,2,3-triphenyl-3,4-dihydro-2*H*-pyrrole (3al).

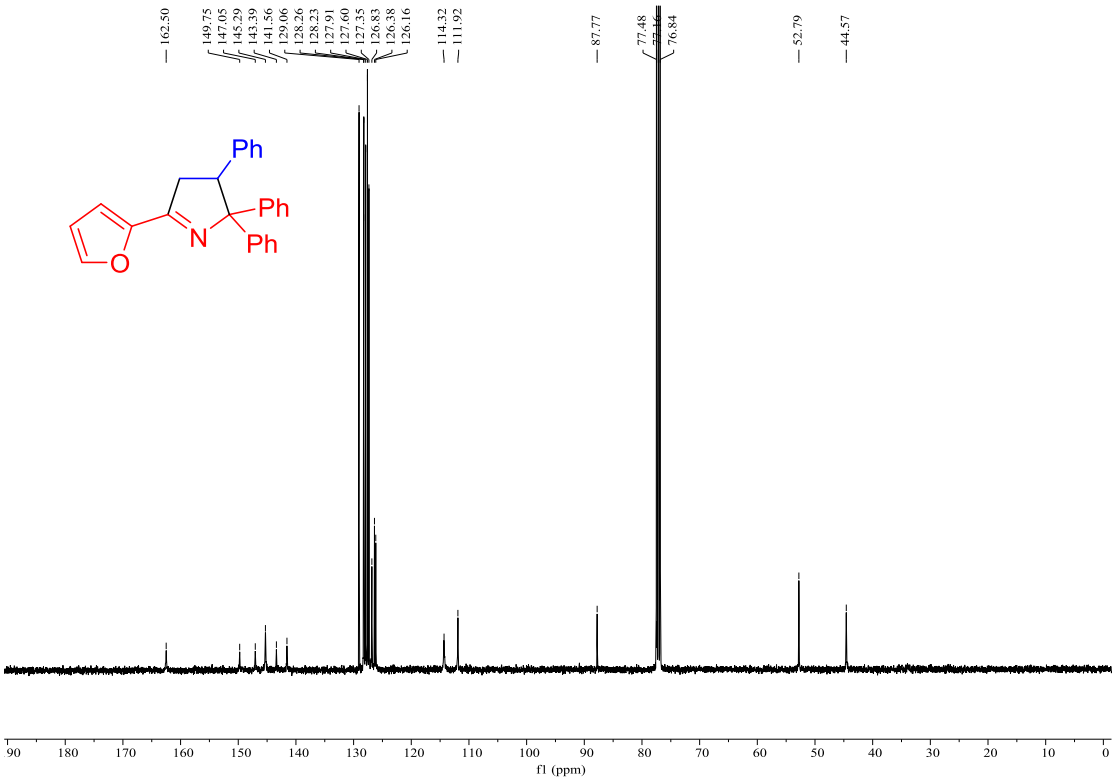


Figure S56. ^{1}H NMR spectra (600 MHz, Chloroform-*d*) of (E)-*N*-(1,3-diphenylallyl)-1,1-diphenylmethanimine (4aa).

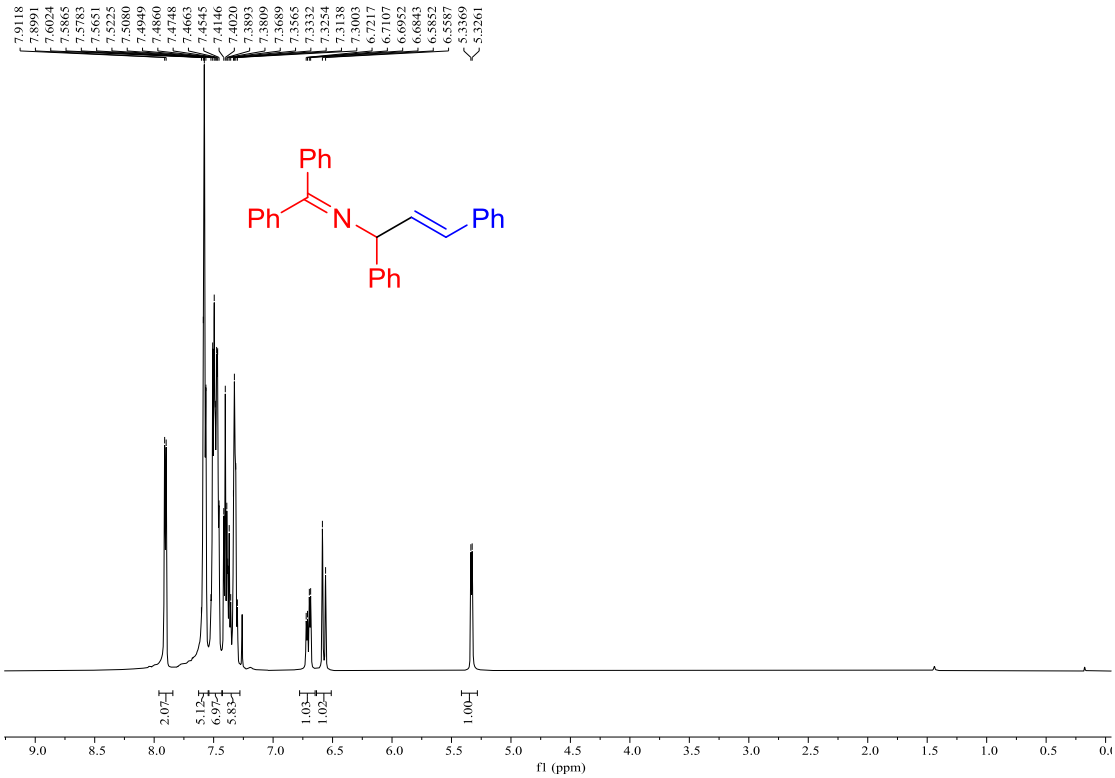
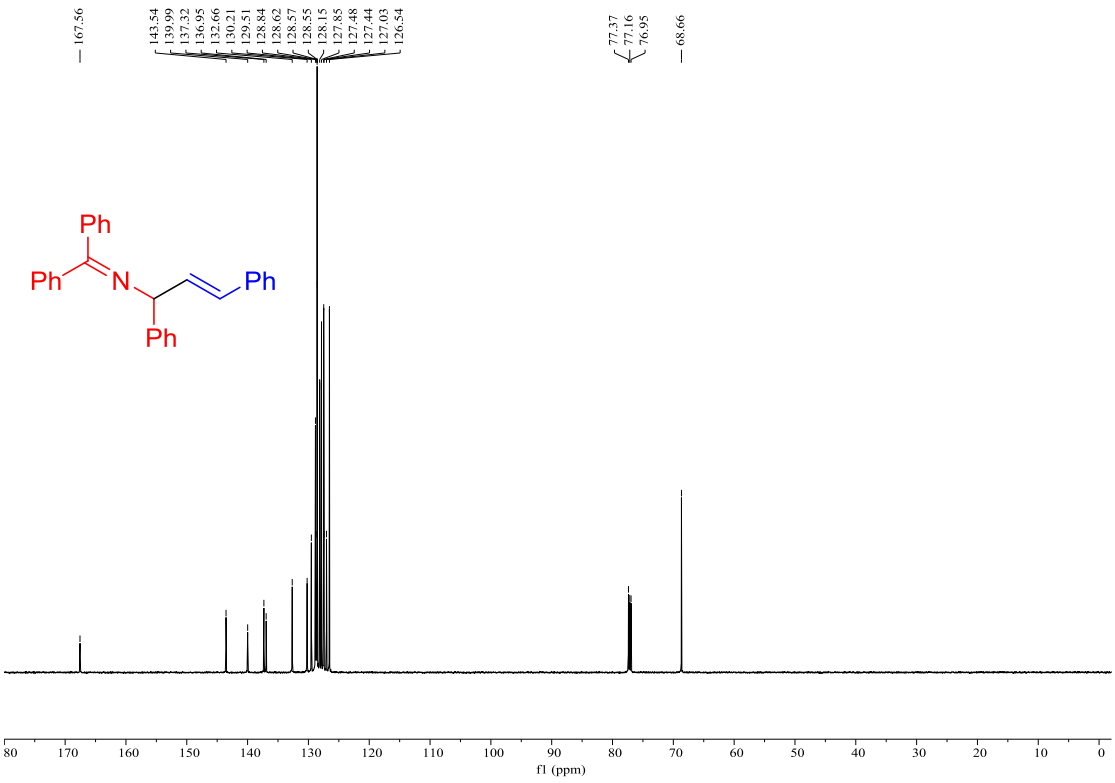
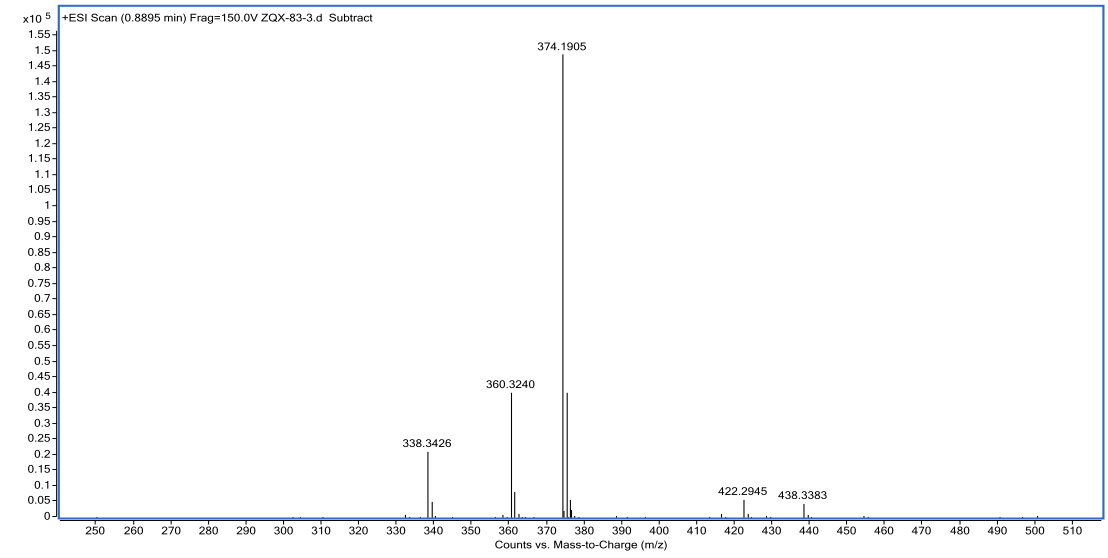


Figure S57. $^{13}C\{^{1}H\}$ NMR spectra (150 MHz, Chloroform-*d*) of (E)-*N*-(1,3-diphenylallyl)-1,1-diphenylmethanimine (4aa).



HRMS Spectra

3aa

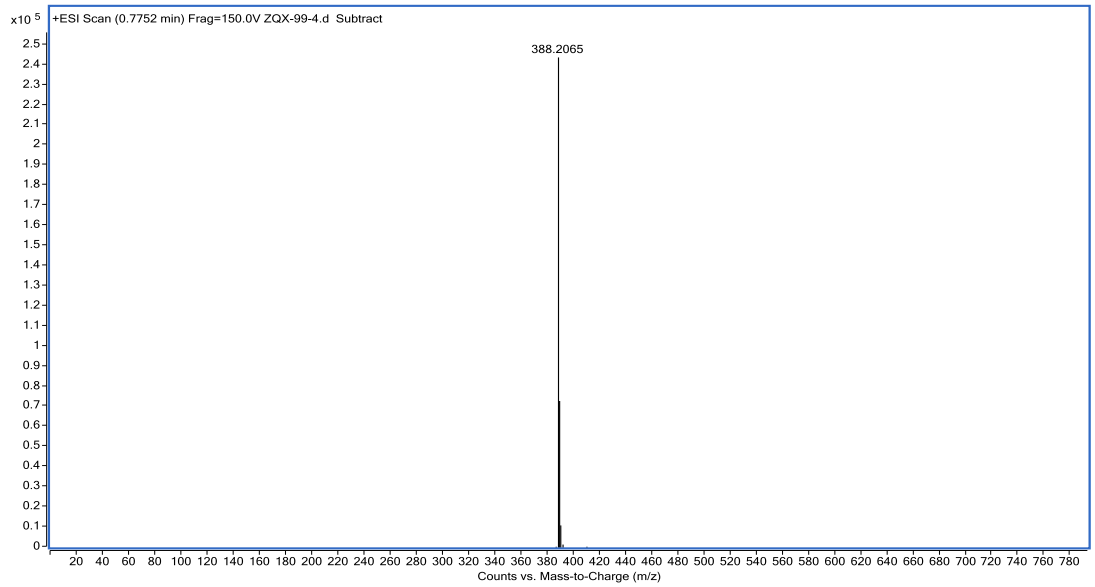


MS Formula Results: + Scan (0.8895 min) Sub (ZQX-83-3.d)

m/z	Ion	Formula	Abundance
374.1905	(M+H)+	C28 H24 N	148848.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H23 N	C28 H24 N	97.06		374.1903	-0.55	99.75	91.82	98

3ba

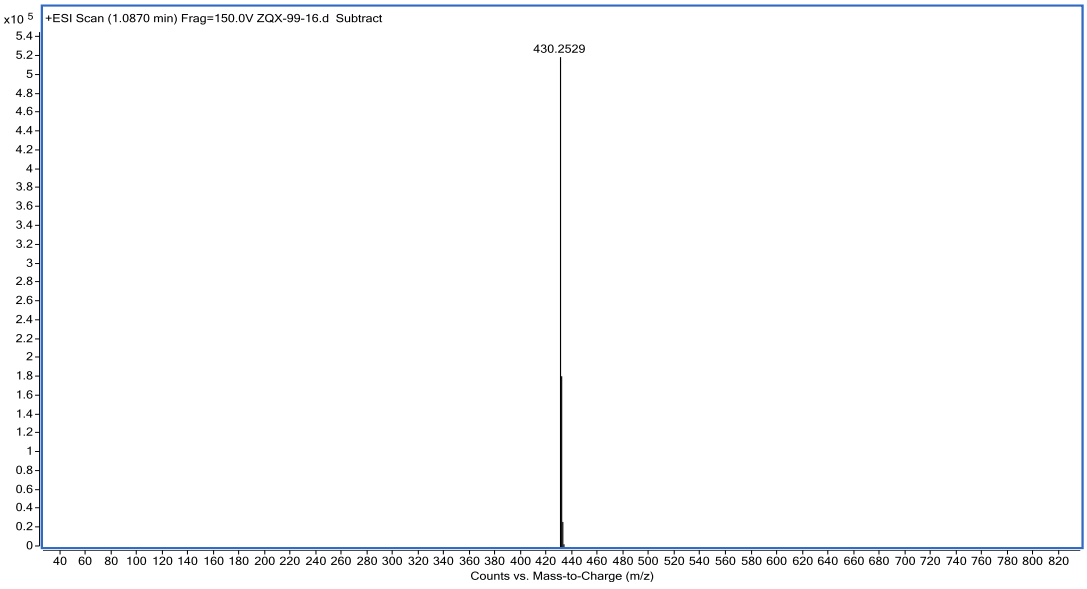


MS Formula Results: + Scan (0.7752 min) Sub (ZQX-99-4.d)

m/z	Ion	Formula	Abundance
388.2065	(M+H)+	C29 H26 N	243512.4

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C29 H25 N	C29 H26 N	98.3		388.206	-1.37	98.4	97.79	98.71

3ca

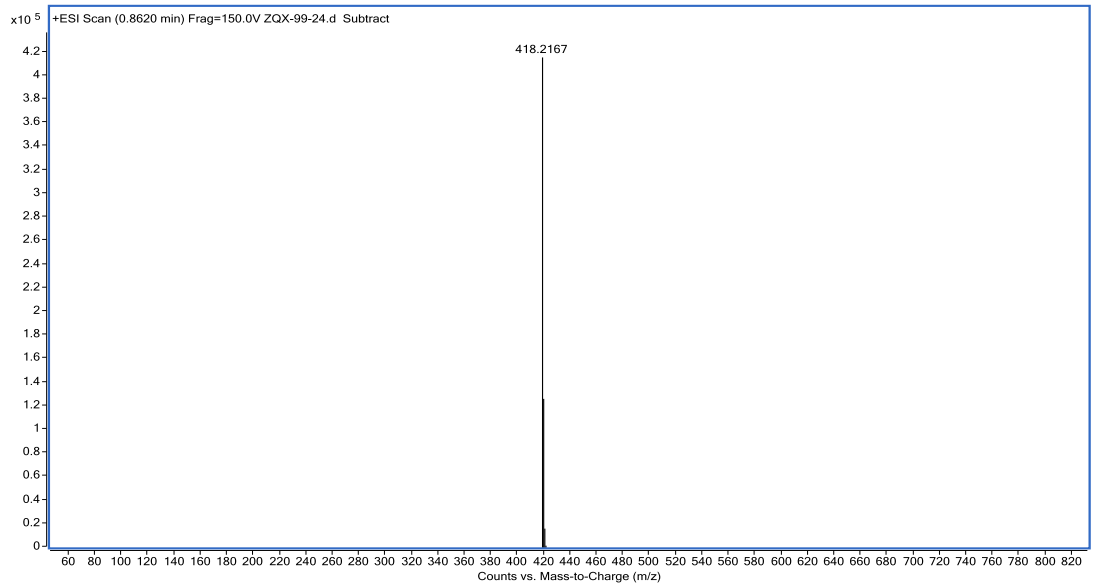


MS Formula Results: + Scan (1.0870 min) Sub (ZQX-99-16.d)

m/z	Ion	Formula	Abundance
430.2529	(M+H)+	C32 H32 N	518959.7

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C32 H31 N	C32 H32 N	99.54		430.2529	-0.01	100	99.4	98.78

3da

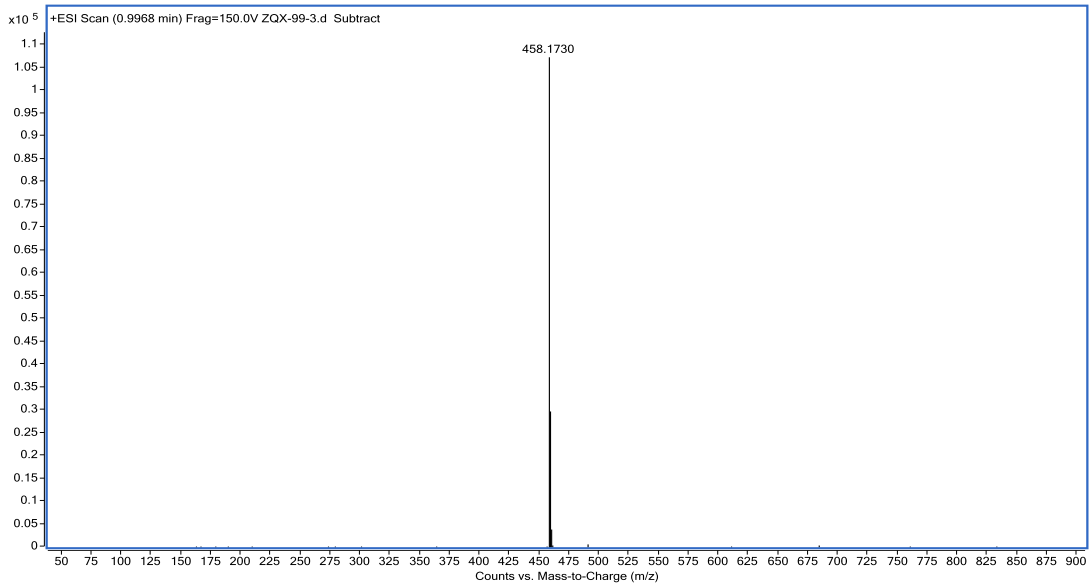


MS Formula Results: + Scan (0.8620 min) Sub (ZQX-99-24.d)

m/z	Ion	Formula	Abundance
418.2167	(M+H)+	C30 H28 N O	415132.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C30 H27 N O	C30 H28 N O	97.86		418.2165	-0.48	99.79	94.95	97.5

3ea

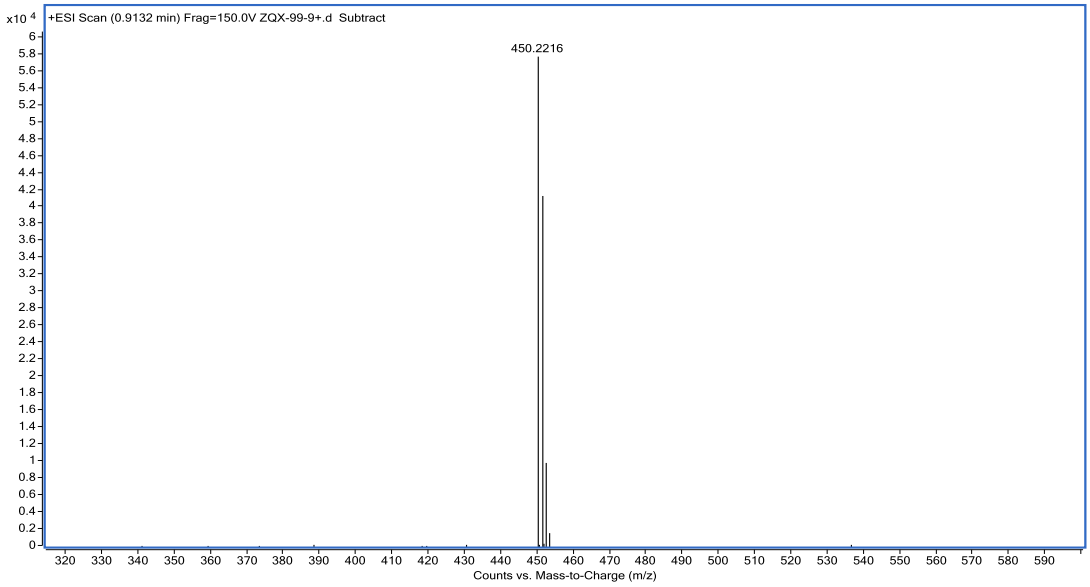


MS Formula Results: + Scan (0.9968 min) Sub (ZQX-99-3.d)

m/z	Ion	Formula	Abundance
458.173	(M+H)+	C29 H23 F3 N O	107270.9

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C29 H22 F3 N O	C29 H23 F3 N O	95.74		458.1726	-0.92	99.15	90.81	94.82

3fa

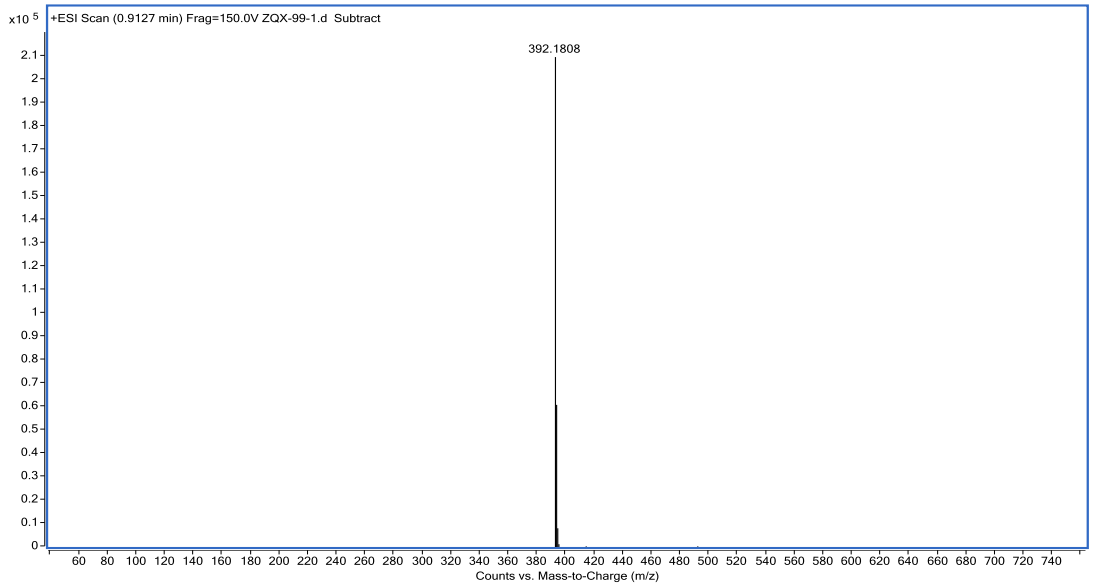


MS Formula Results: + Scan (0.9132 min) Sub (ZQX-99-9+.d)

m/z	Ion	Formula	Abundance
450.2216	(M+H)+	C34 H28 N	57708.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C34 H27 N	C34 H28 N	47.61		450.2216	0.16	99.97	0	0

3ga

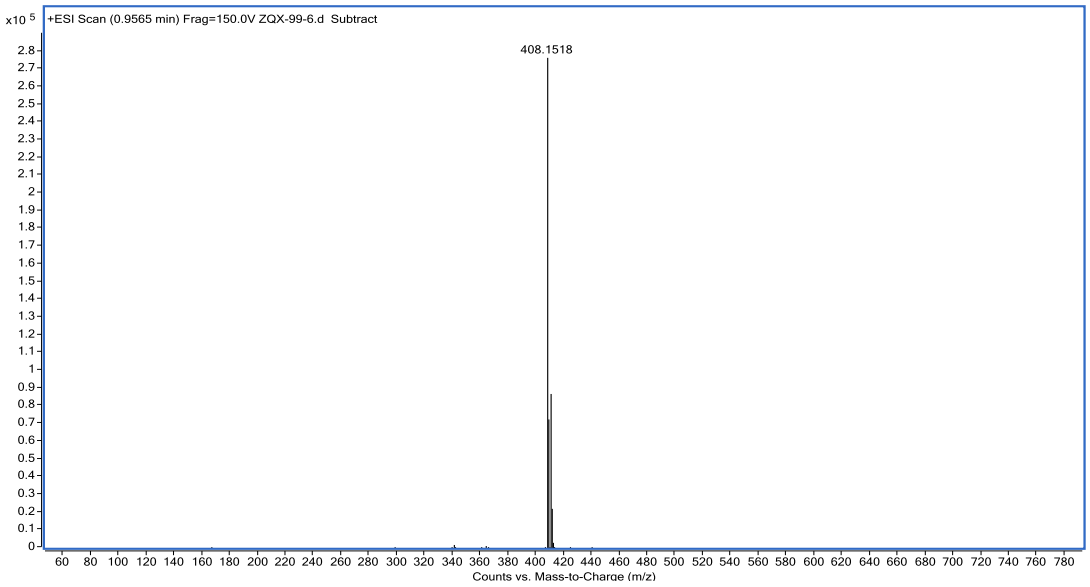


MS Formula Results: + Scan (0.9127 min) Sub (ZQX-99-1.d)

m/z	Ion	Formula	Abundance
392.1808	(M+H)+	C28 H23 F N	209452.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H22 F N	C28 H23 F N	99.03		392.1809	0.12	99.99	98.11	98.2

3ha

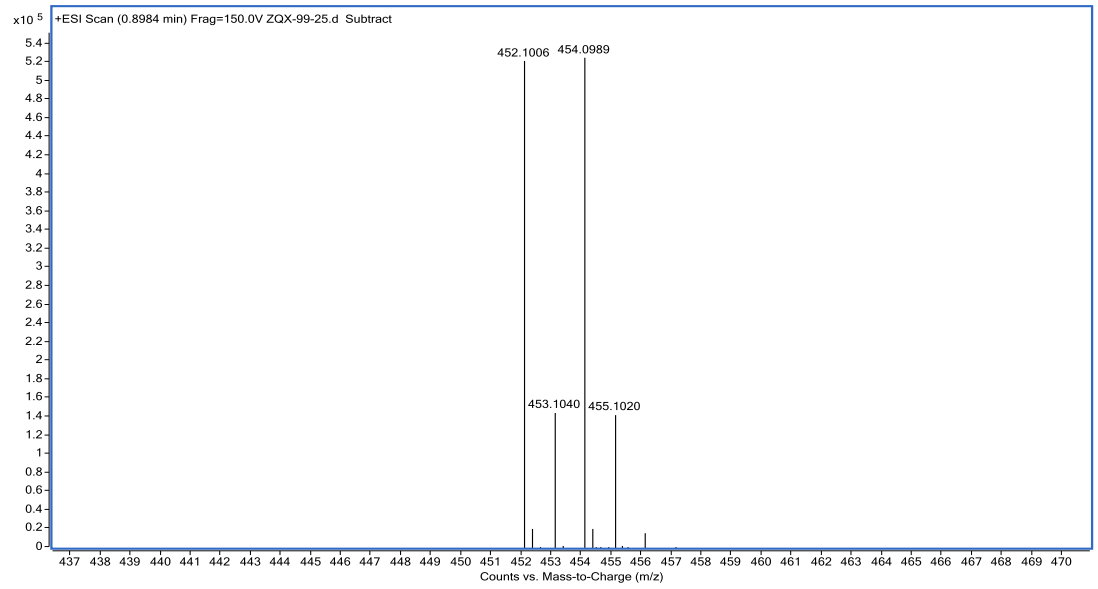


MS Formula Results: + Scan (0.9565 min) Sub (ZQX-99-6.d)

m/z	Ion	Formula	Abundance
408.1518	(M+H)+	C28 H23 Cl N	276104.8

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H22 Cl N	C28 H23 Cl N	96.12		408.1514	-1.26	98.57	90.5	97.98

3ia

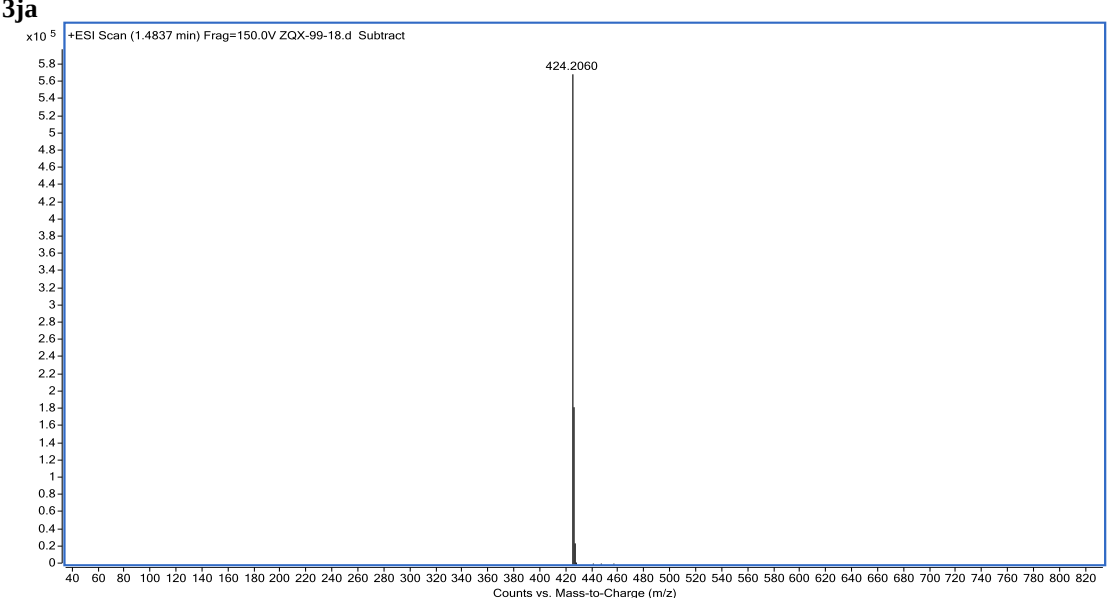


MS Formula Results: + Scan (0.8984 min) Sub (ZQX-99-25.d)

m/z	Ion	Formula	Abundance
452.1006	(M+H)+	C28 H23 Br N	521714.3

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H22 Br N	C28 H23 Br N	98.05		452.1008	0.63	99.61	93.94	99.87

3ja

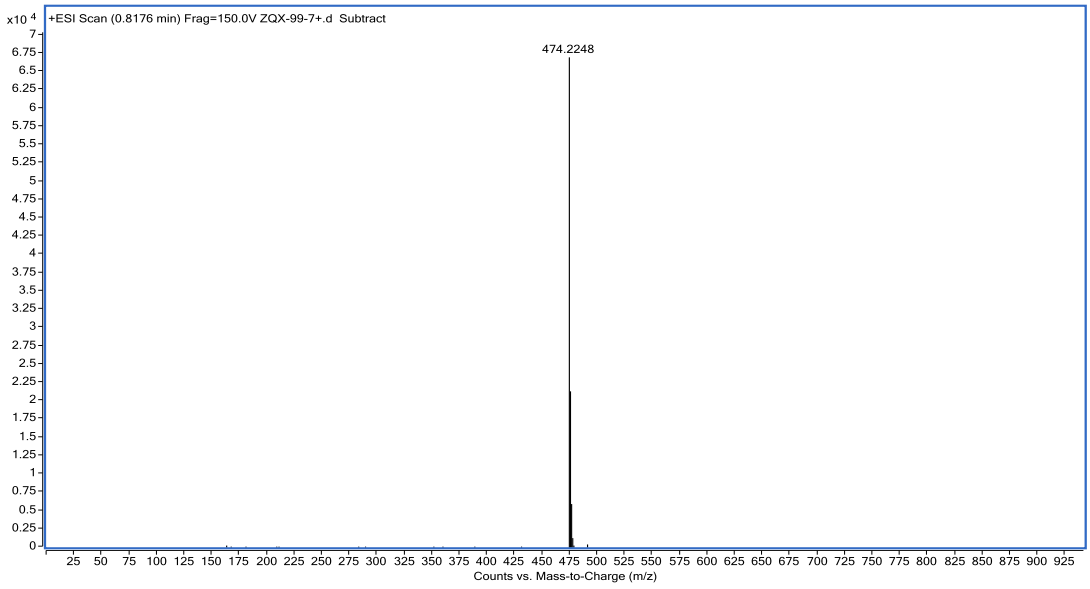


MS Formula Results: + Scan (1.4837 min) Sub (ZQX-99-18.d)

m/z	Ion	Formula	Abundance
424.206	(M+H)+	C32 H26 N	568757.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C32 H25 N	C32 H26 N	98.42		424.206	-0.02	100	94.51	99.95

3ka

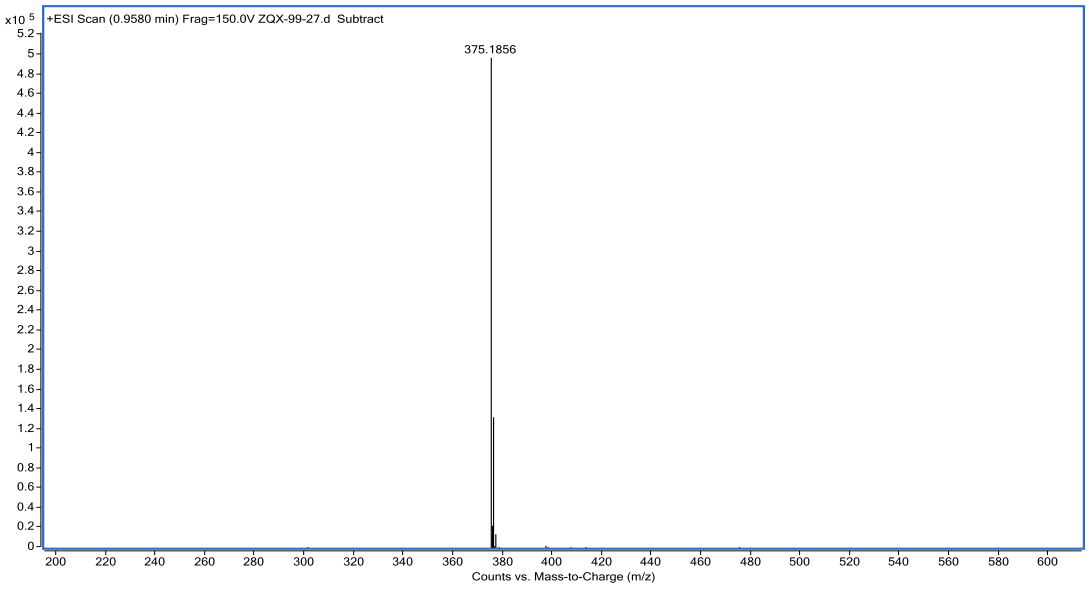


MS Formula Results: + Scan (0.8176 min) Sub (ZQX-99-7+.d)

m/z	Ion	Formula	Abundance
474.2248	(M+H)+	C33 H32 N S	66904.7

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C33 H31 N S	C33 H32 N S	96.55		474.225	0.43	99.81	88.5	99.7

3la

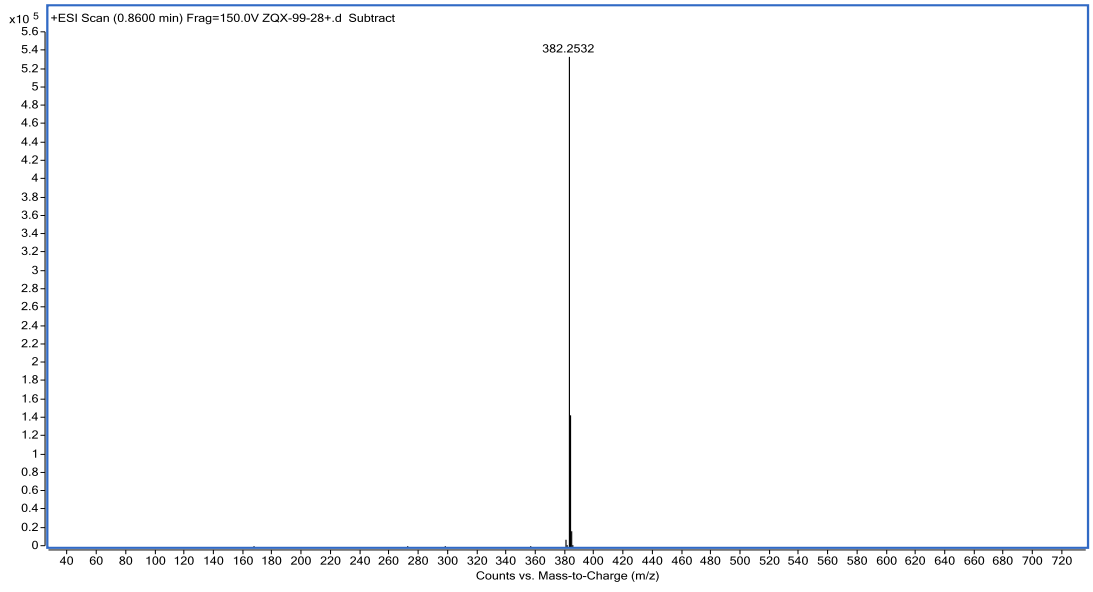


MS Formula Results: + Scan (0.9580 min) Sub (ZQX-99-27.d)

m/z	Ion	Formula	Abundance
375.1856	(M+H)+	C27 H23 N2	496650.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C27 H22 N2	C27 H23 N2	97.84		375.1856	-0.19	99.97	92.51	99.96

3ma

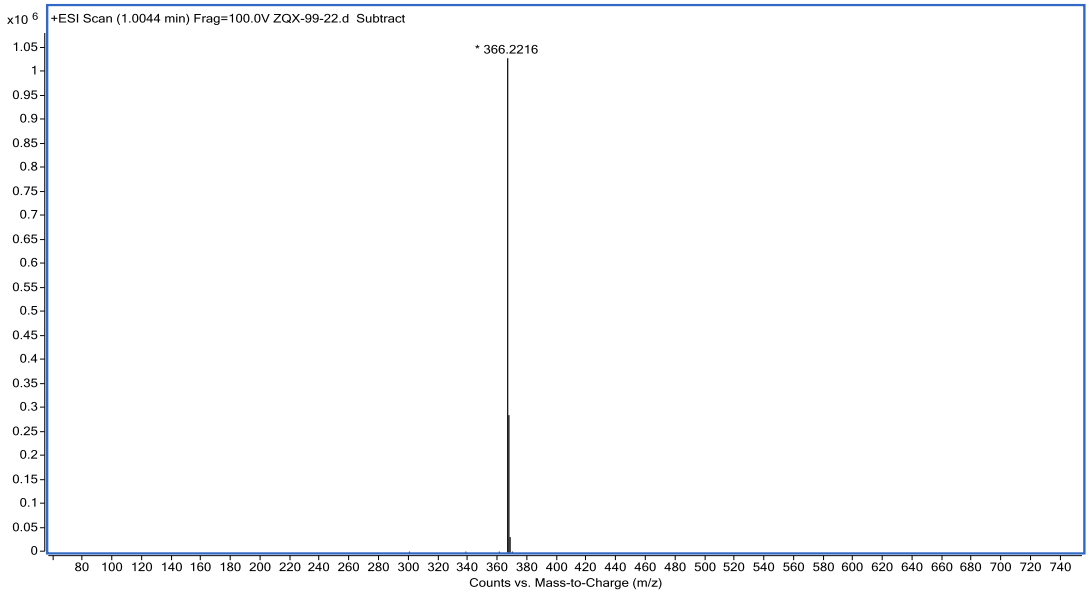


MS Formula Results: + Scan (0.8600 min) Sub (ZQX-99-28+.d)

m/z	Ion	Formula	Abundance
382.2532	(M+H)+	C28 H32 N	533341.3

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H31 N	C28 H32 N	97.15		382.2529	-0.62	99.68	90.84	99.67

3na

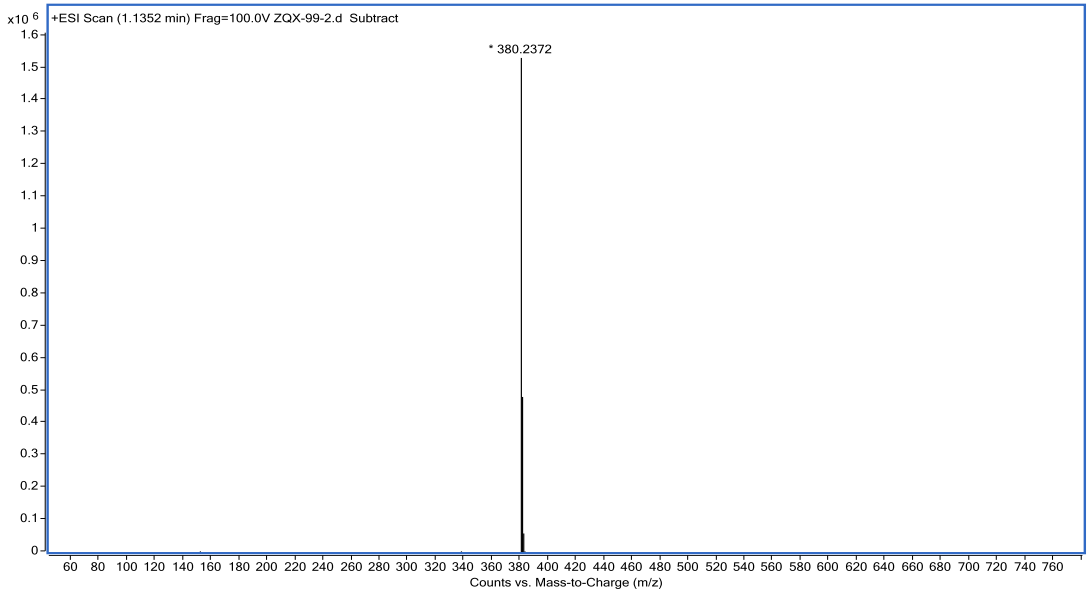


MS Formula Results: + Scan (1.0044 min) Sub (ZQX-99-22.d)

m/z	Ion	Formula	Abundance
366.2216	(M+H)+	C27 H28 N	1028606.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C27 H27 N	C27 H28 N	98.74		366.2216	0.16	99.98	97.16	98.15

3oa

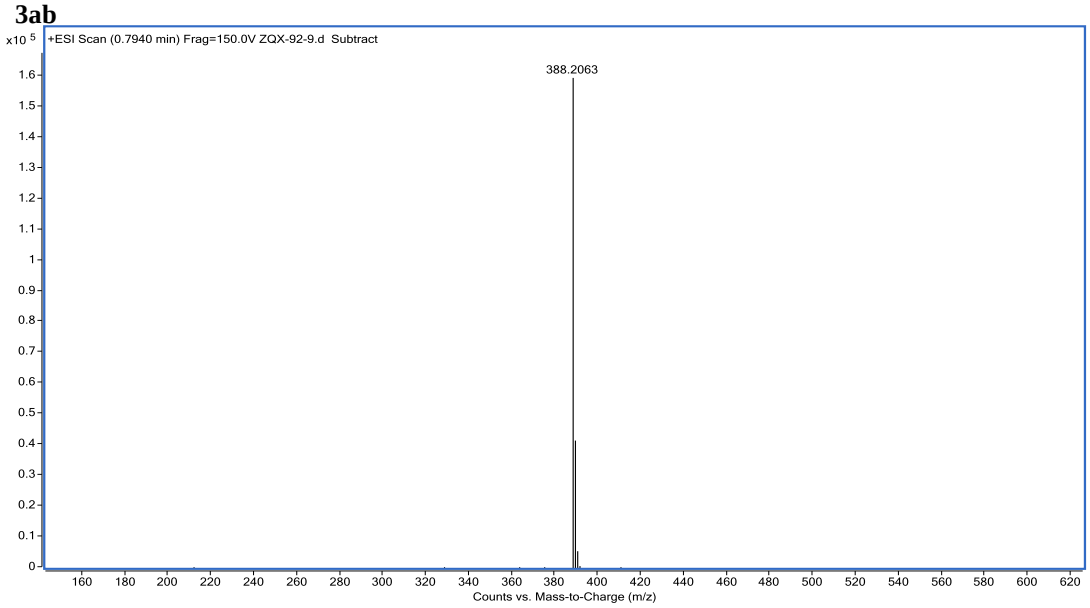


MS Formula Results: + Scan (1.1352 min) Sub (ZQX-99-2.d)

m/z	Ion	Formula	Abundance
380.2372	(M+H)+	C28 H30 N	1529291.6

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H29 N	C28 H30 N	98.39		380.2373	0.33	99.91	98.96	94.67

3ab

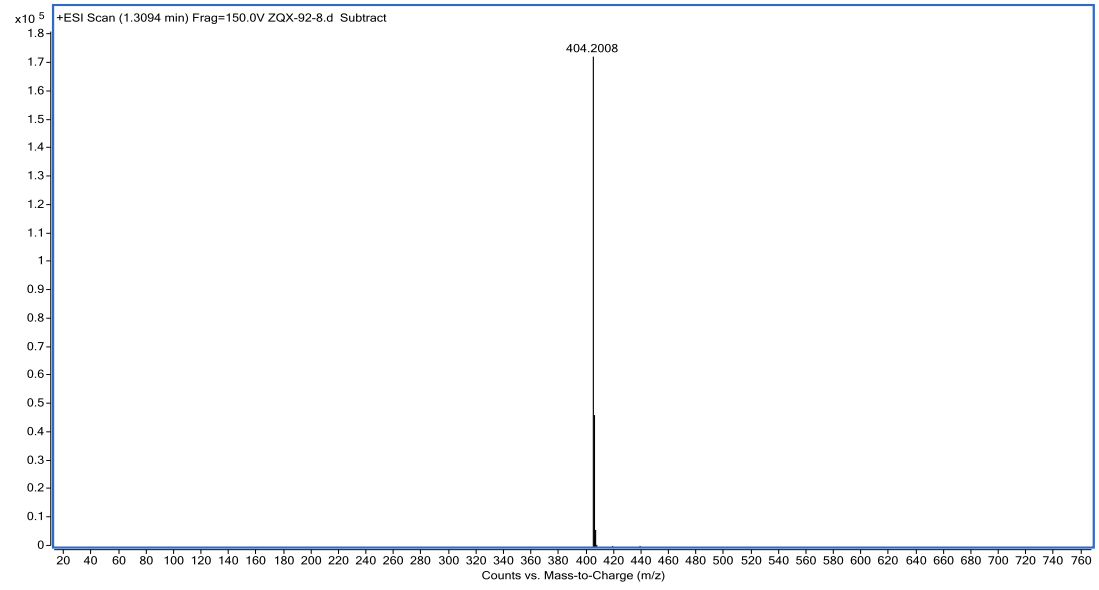


MS Formula Results: + Scan (0.7940 min) Sub (ZQX-92-9.d)

m/z	Ion	Formula	Abundance
388.2063	(M+H)+	C29 H26 N	159290

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C29 H25 N	C29 H26 N	94.25		388.206	-0.91	99.29	81.47	99.53

3ac

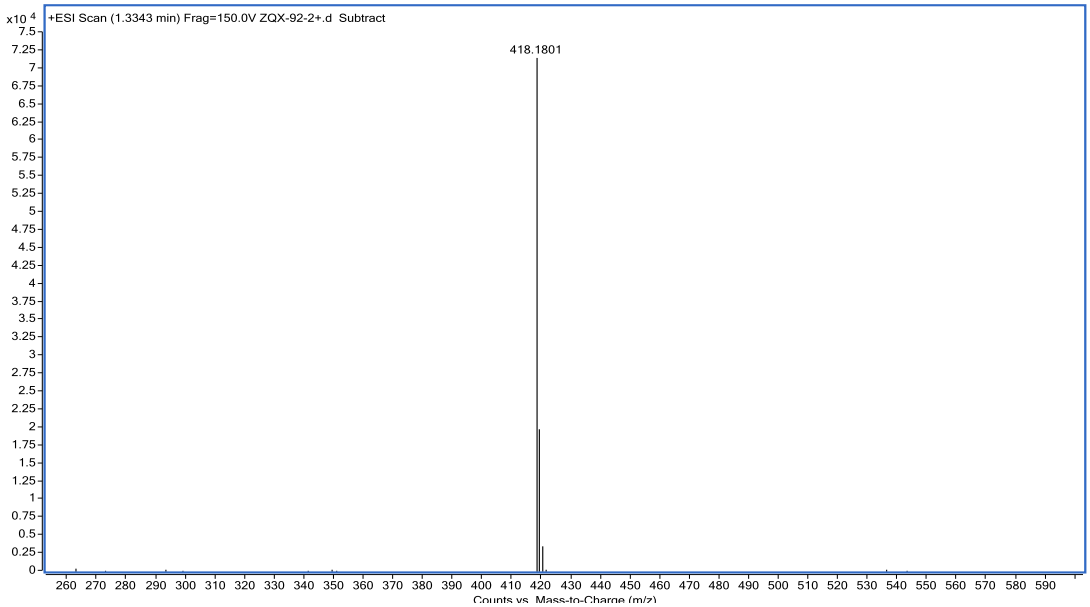


MS Formula Results: + Scan (1.3094 min) Sub (ZQX-92-8.d)

m/z	Ion	Formula	Abundance
404.2008	(M+H)+	C29 H26 N O	172314.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C29 H25 N O	C29 H26 N O	95.83		404.2009	0.17	99.97	86.52	98.7

3ad

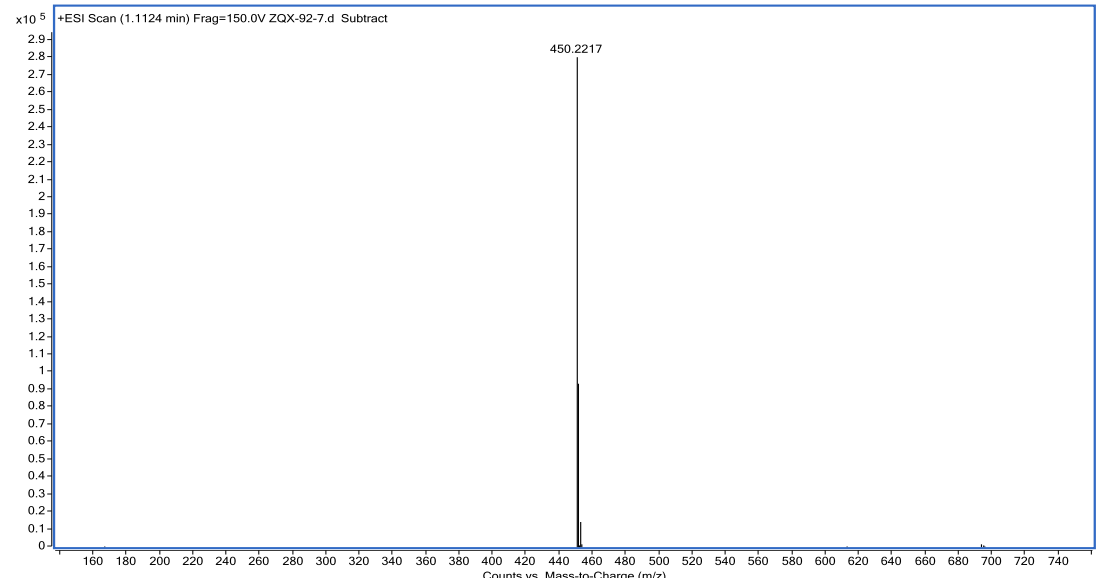


MS Formula Results: + Scan (1.3343 min) Sub (ZQX-92-2+.d)

m/z	Ion	Formula	Abundance
418.1801	(M+H)+	C29 H24 N O2	71435.7

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C29 H23 N O2	C29 H24 N O2	96.98		418.1802	0.07	100	90.34	98.93

3ae

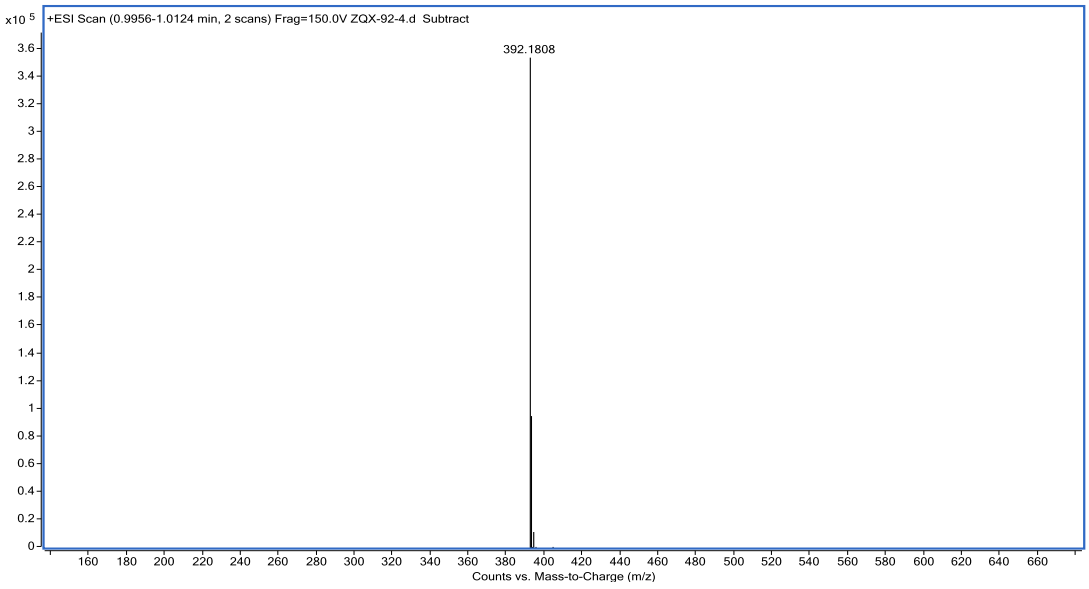


MS Formula Results: + Scan (1.1124 min) Sub (ZQX-92-7.d)

m/z	Ion	Formula	Abundance
450.2217	(M+H)+	C34 H28 N	280195.3

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C34 H27 N	C34 H28 N	97.66		450.2216	-0.15	99.98	92.4	99.33

3af

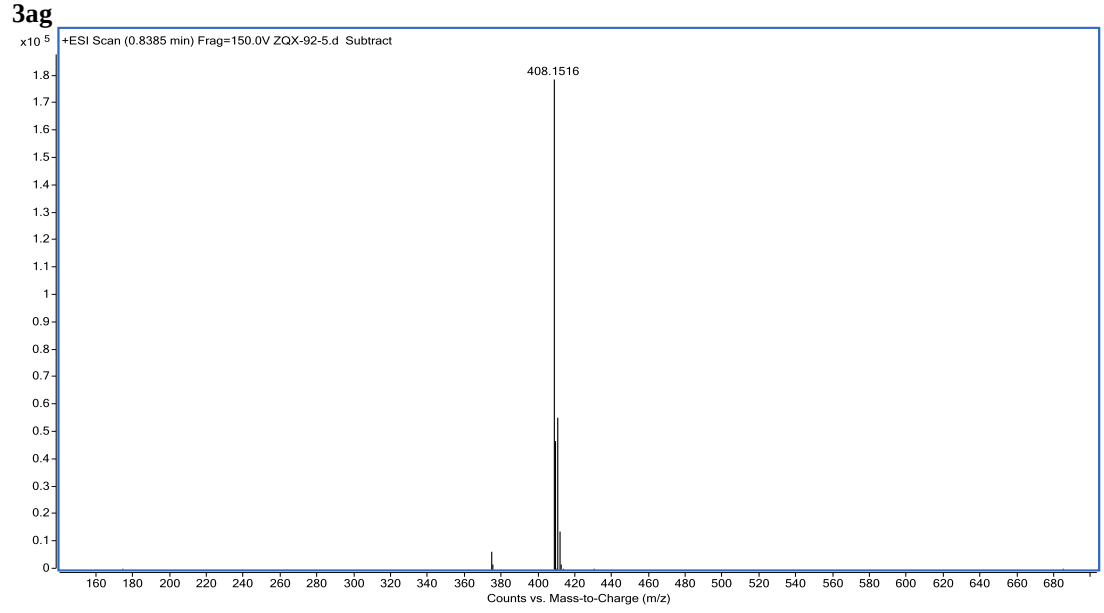


MS Formula Results: + Scan (0.9956-1.0124 min) Sub (ZQX-92-4.d)

m/z	Ion	Formula	Abundance
392.1808	(M+H)+	C28 H23 F N	353691.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H22 F N	C28 H23 F N	97.33		392.1809	0.15	99.98	91.08	99.54

3ag

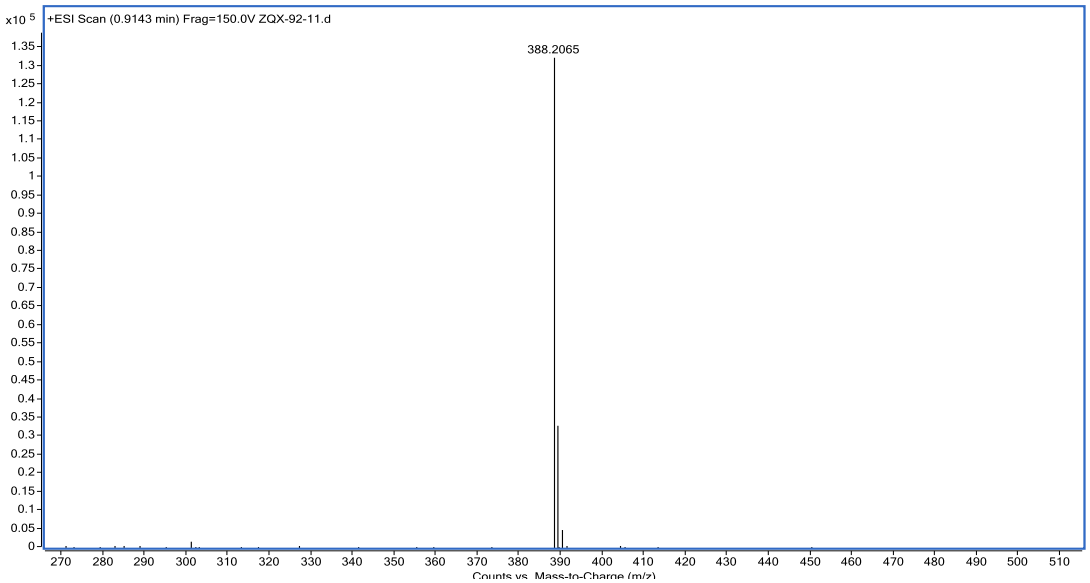


MS Formula Results: + Scan (0.8385 min) Sub (ZQX-92-5.d)

m/z	Ion	Formula	Abundance
408.1516	(M+H)+	C28 H23 Cl N	178678.3

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C28 H22 Cl N	C28 H23 Cl N	95.93		408.1514	-0.78	99.46	89.55	96.5

3ah

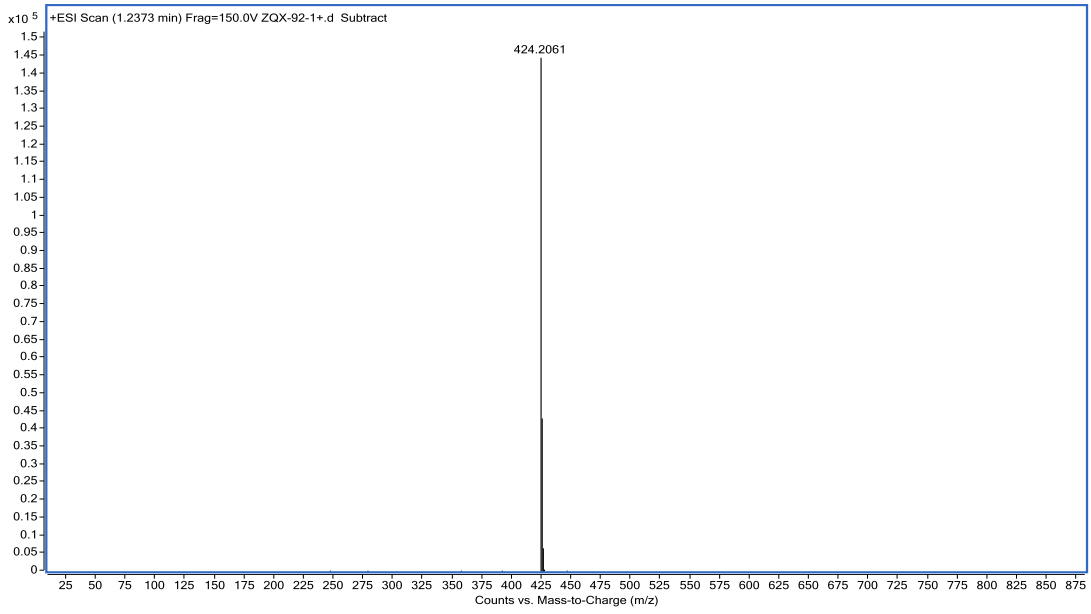


MS Formula Results: + Scan (0.9143 min) (ZQX-92-11.d)

m/z	Ion	Formula	Abundance
388.2065	(M+H)+	C29 H26 N	132194.3

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C29 H25 N	C29 H26 N	91.77		388.206	-1.33	98.49	75.05	98.37

3ai

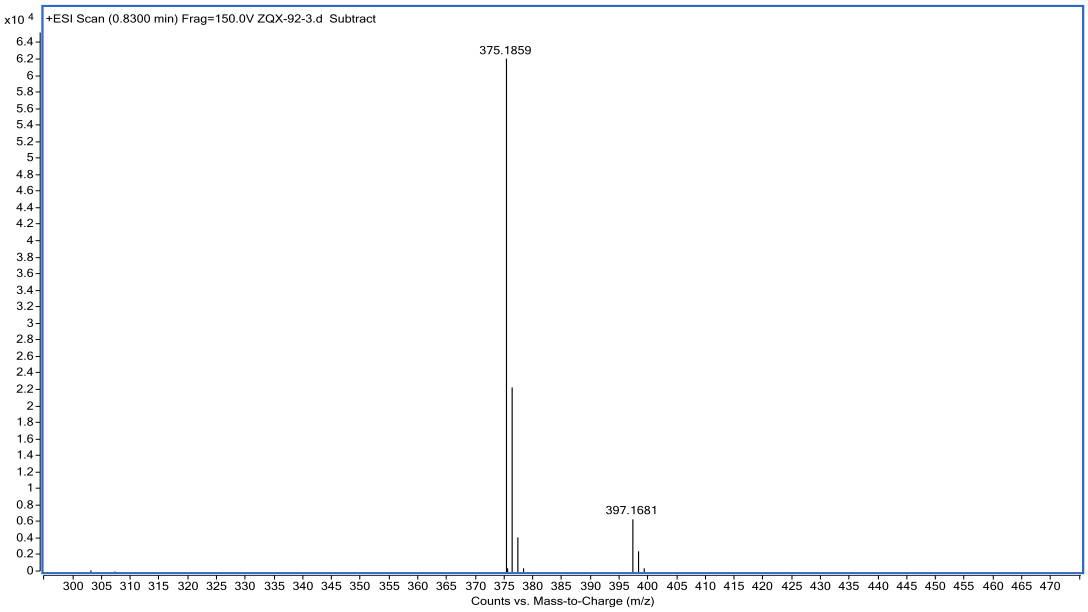


MS Formula Results: + Scan (1.2373 min) Sub (ZQX-92-1+.d)

m/z	Ion	Formula	Abundance
424.2061	(M+H)+	C32 H26 N	144377.8

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C32 H25 N	C32 H26 N	95.33		424.206	-0.4	99.85	86.18	97.28

3aj

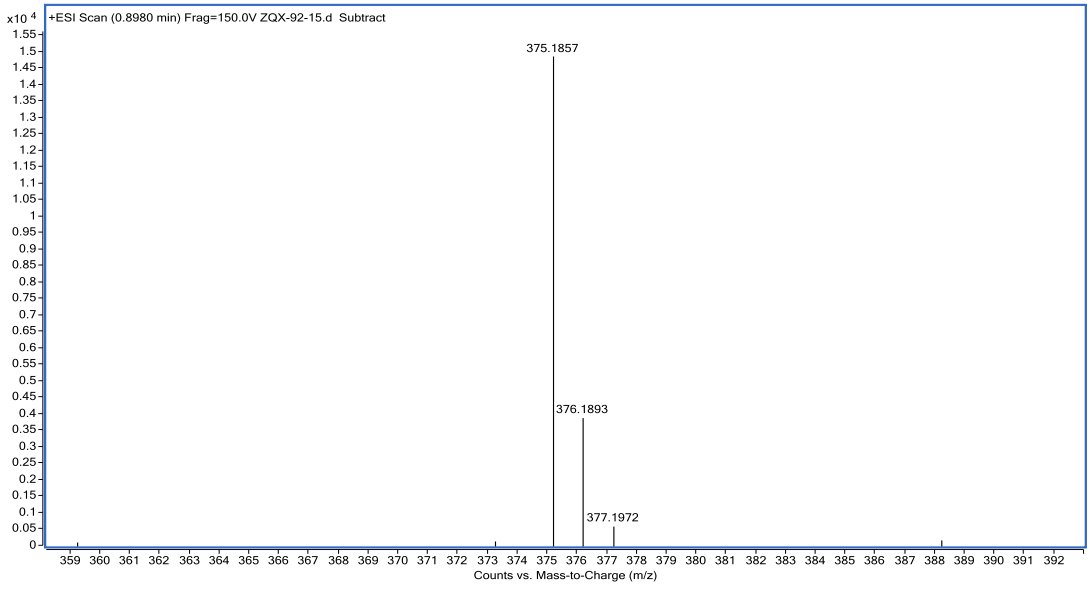


MS Formula Results: + Scan (0.8300 min) Sub (ZQX-92-3.d)

m/z	Ion	Formula	Abundance
375.1859	(M+H)+	C27 H23 N2	62110.9

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C27 H22 N2	C27 H23 N2	92.25		375.1856	-0.98	99.2	84.16	88.06

3ak

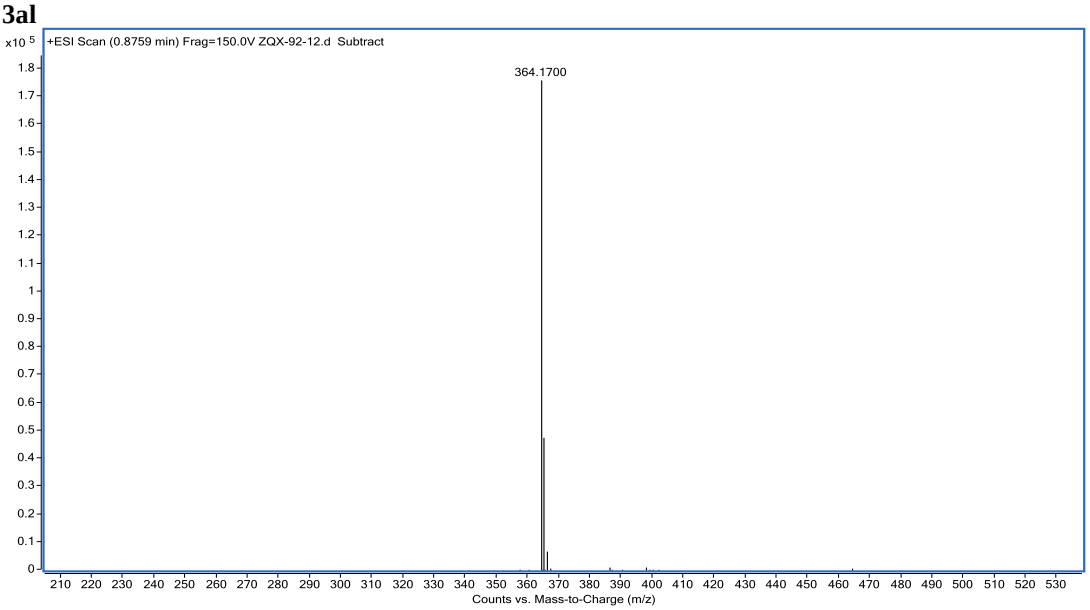


MS Formula Results: + Scan (0.8980 min) Sub (ZQX-92-15.d)

m/z	Ion	Formula	Abundance
375.1857	(M+H)+	C27 H23 N2	14858

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C27 H22 N2	C27 H23 N2	95.32		375.1856	-0.35	99.9	91.38	90.91

3al



MS Formula Results: + Scan (0.8759 min) Sub (ZQX-92-12.d)

m/z	Ion	Formula	Abundance
364.17	(M+H)+	C26 H22 N O	175784.5

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C26 H21 N O	C26 H22 N O	98.79		364.1696	-1.24	98.76	98.59	99.11