

Supporting Information

Discovery and preliminary structure-activity investigation of 3-substituted-1*H*-imidazol-5-yl-1*H*-indoles with *in vitro* activity towards methicillin-resistant *Staphylococcus aureus*

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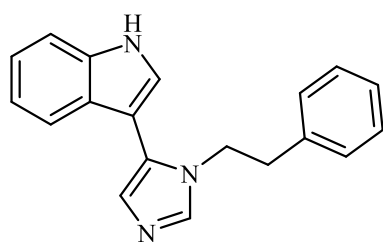
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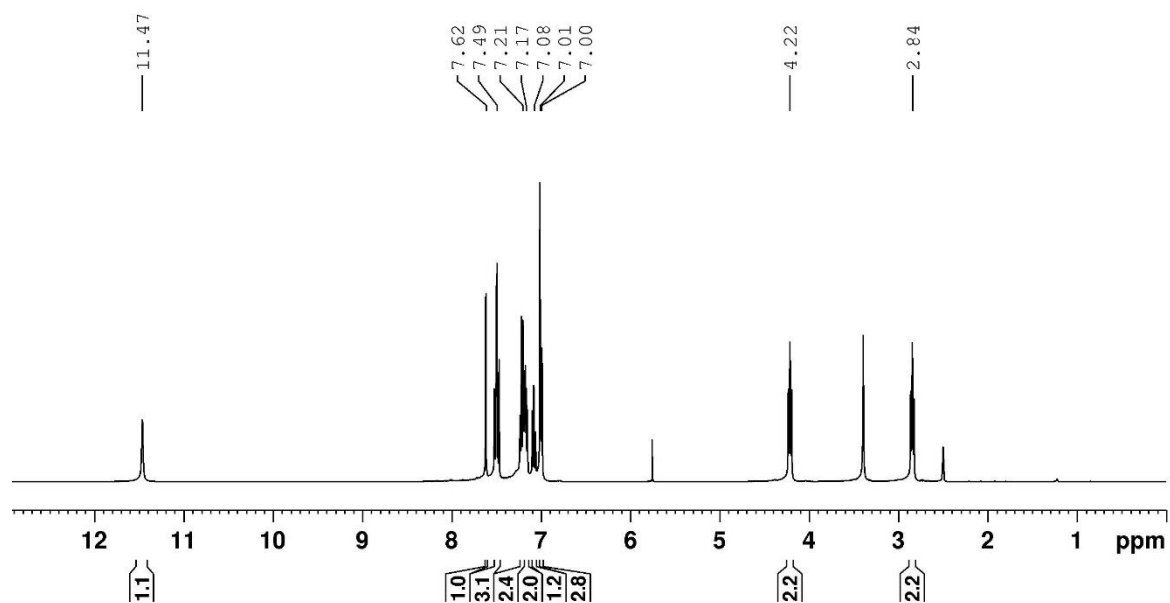
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Figure S1. 3-(1-Phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (1)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

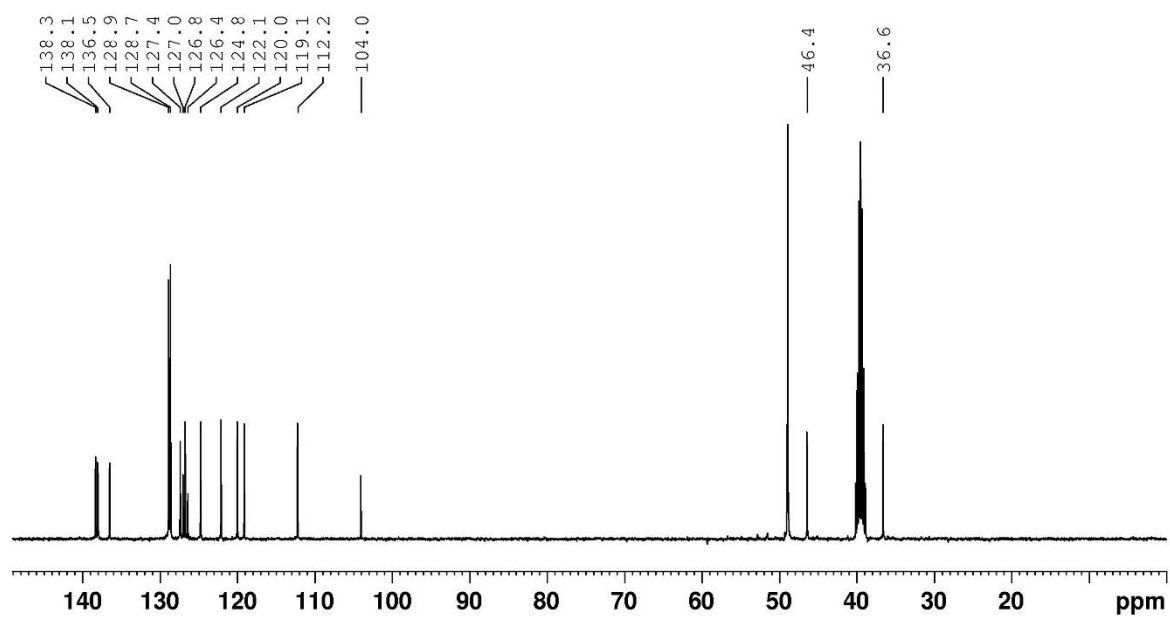
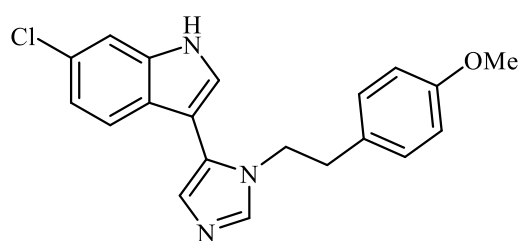
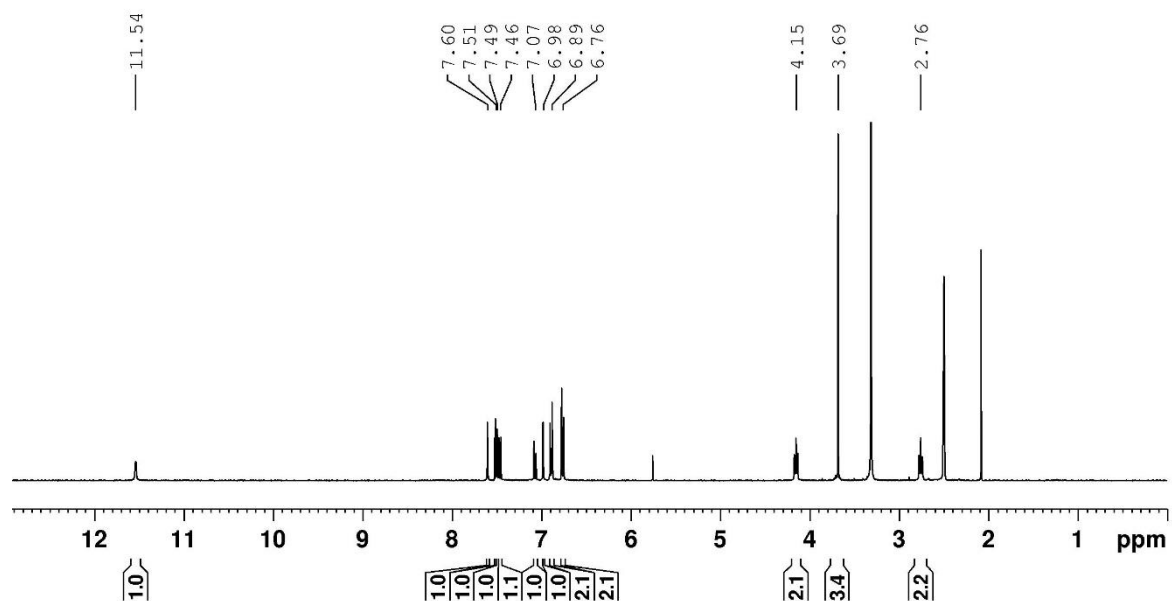


Figure S2. 6-Chloro-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (2)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

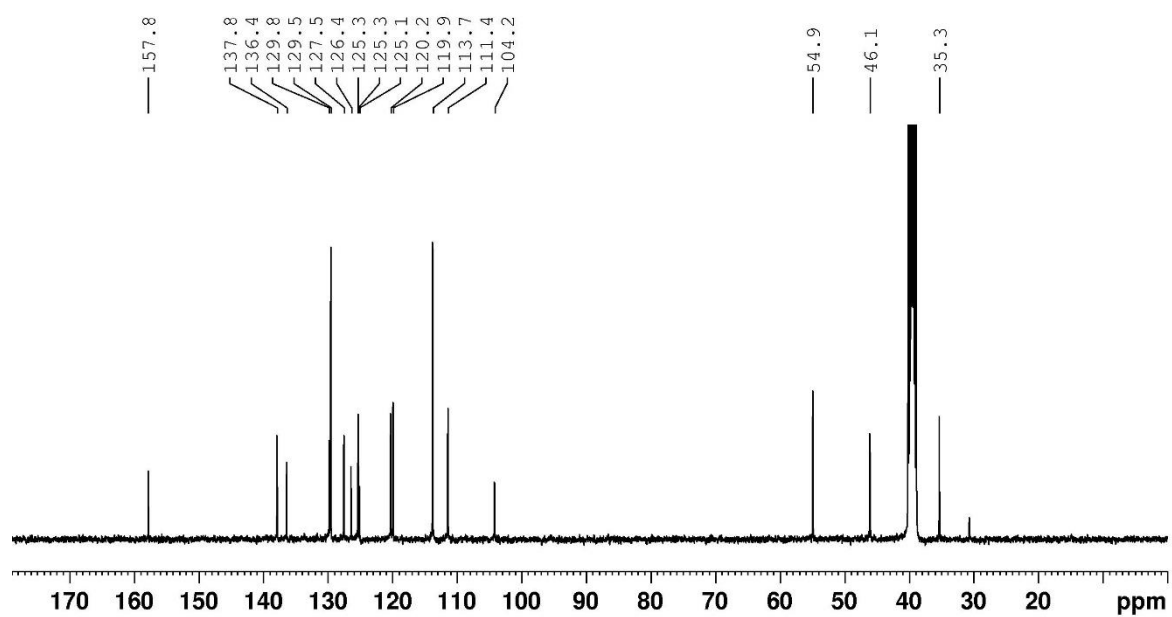
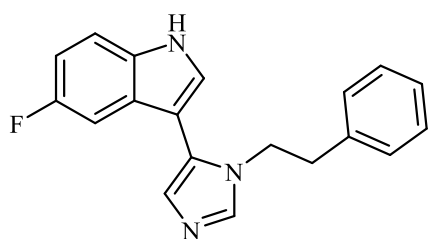
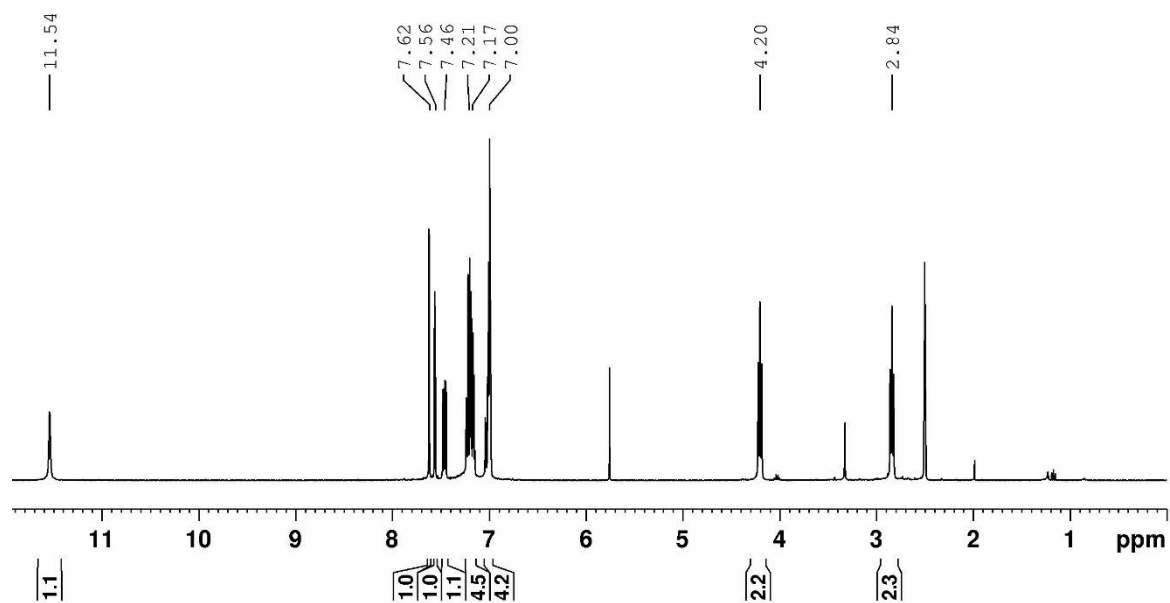


Figure S3. 5-Fluoro-3-(1-phenethyl-1H-imidazol-5-yl)-1H-indole (3)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

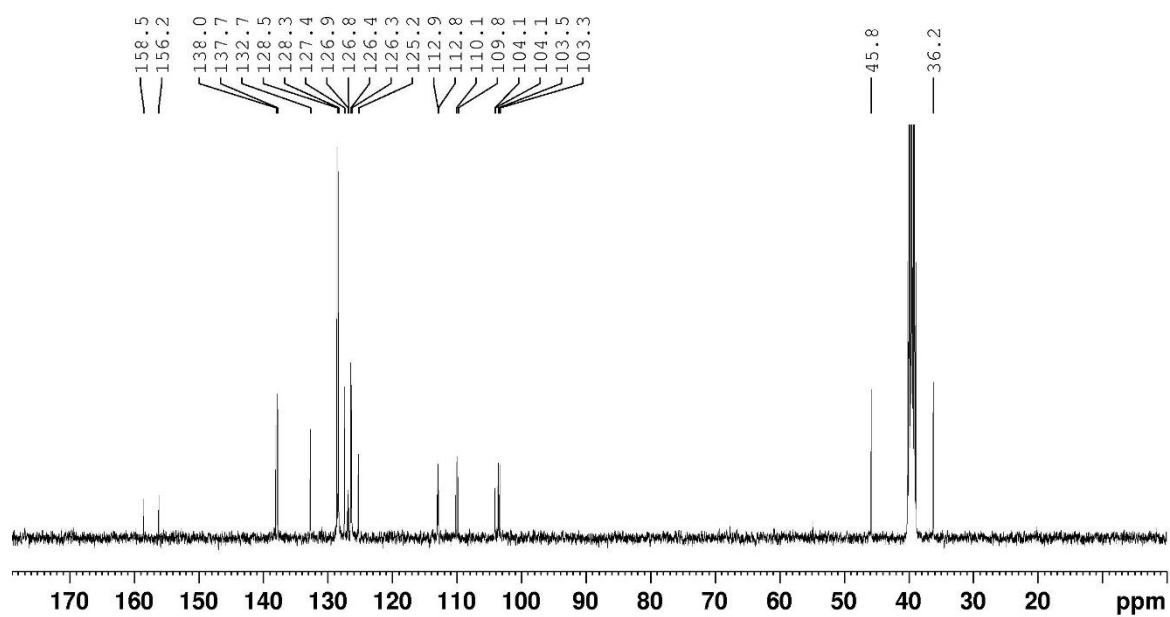
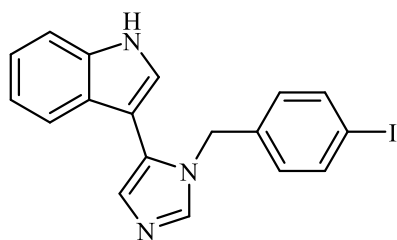
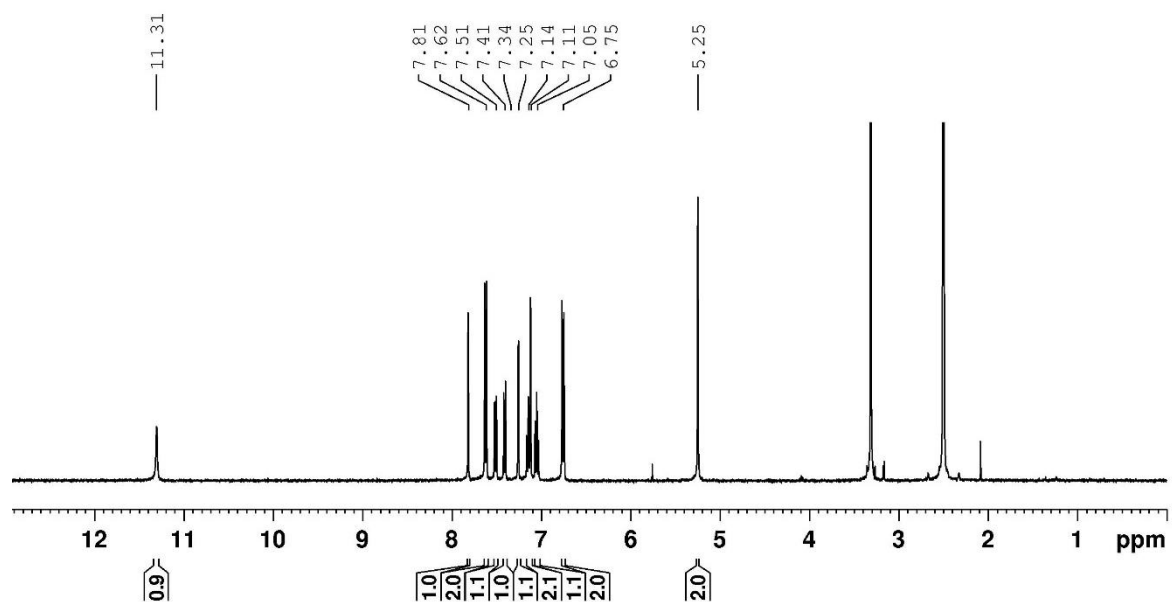


Figure S4. 3-(1-(4-Iodobenzyl)-1H-imidazol-5-yl)-1H-indole (4)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

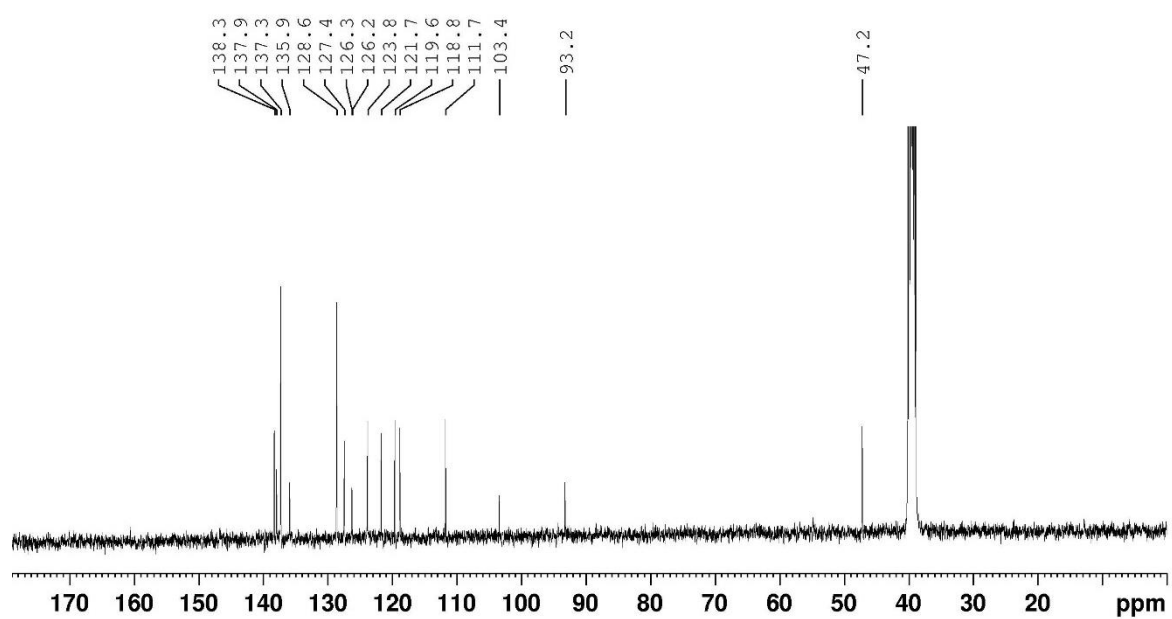
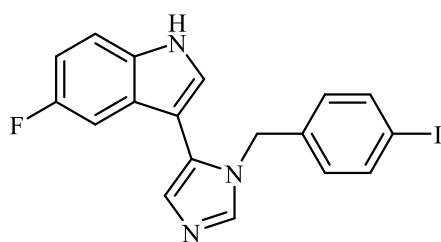
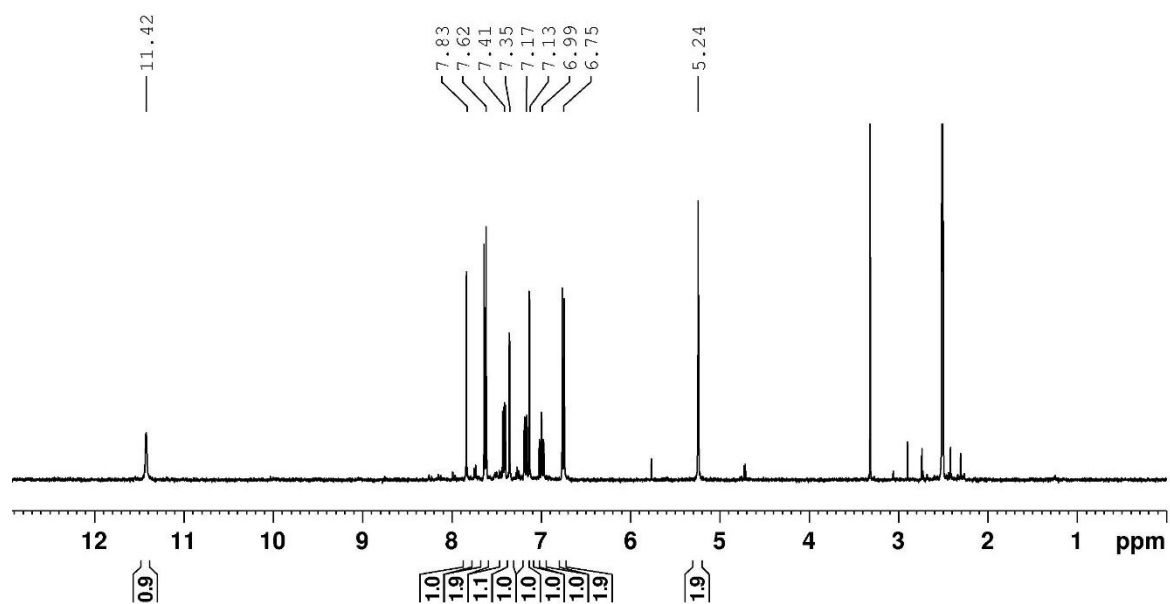


Figure S5. 5-Fluoro-3-(1-(4-iodobenzyl)-1H-imidazol-5-yl)-1H-indole (5)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

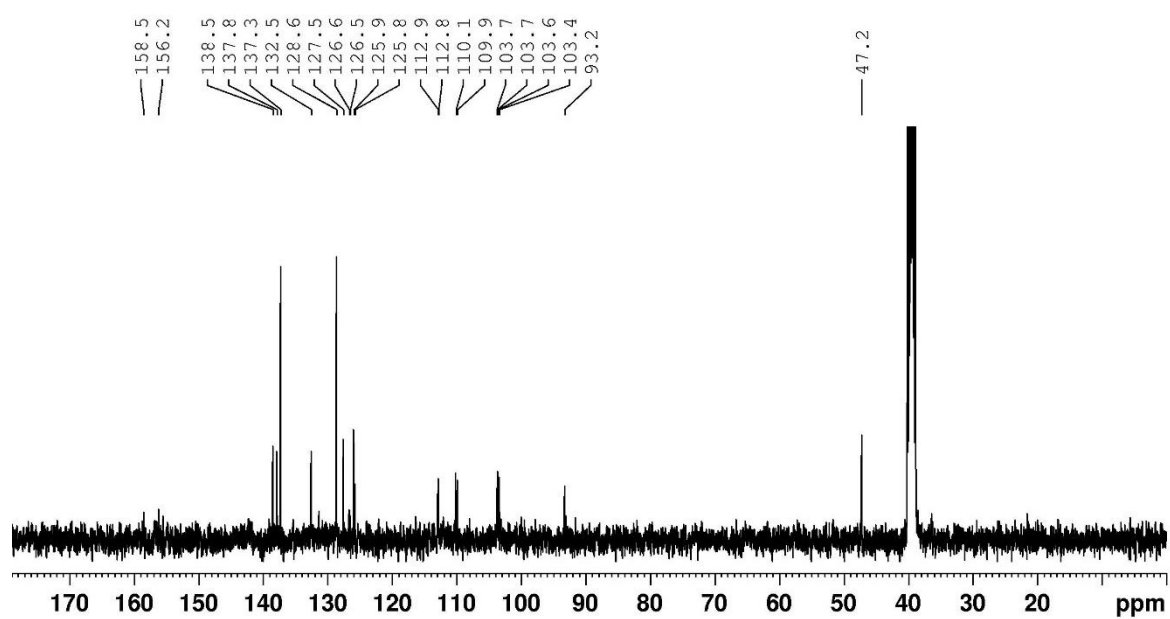
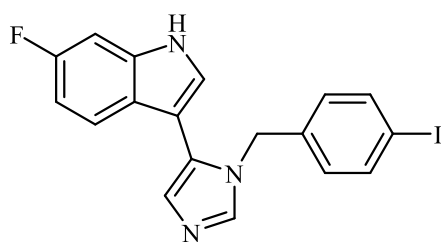
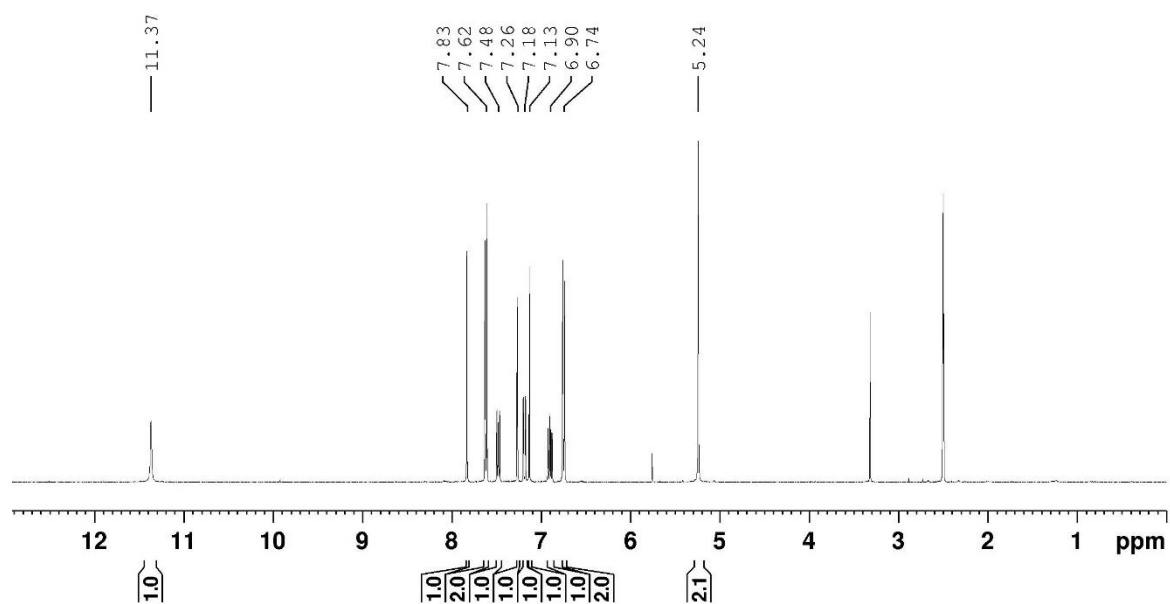


Figure S6. 6-Fluoro-3-(1-(4-iodobenzyl)-1H-imidazol-5-yl)-1H-indole (6)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

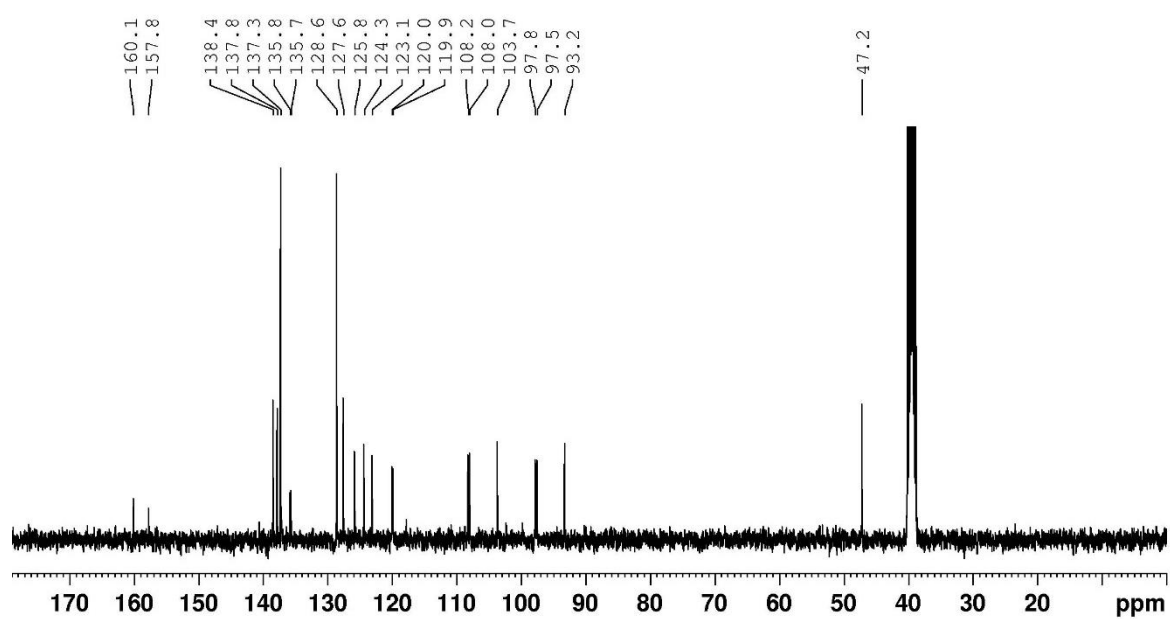
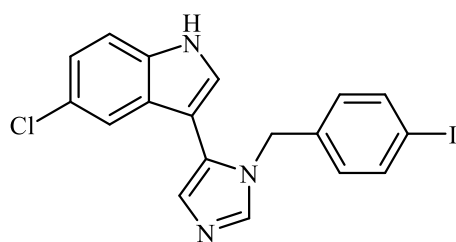
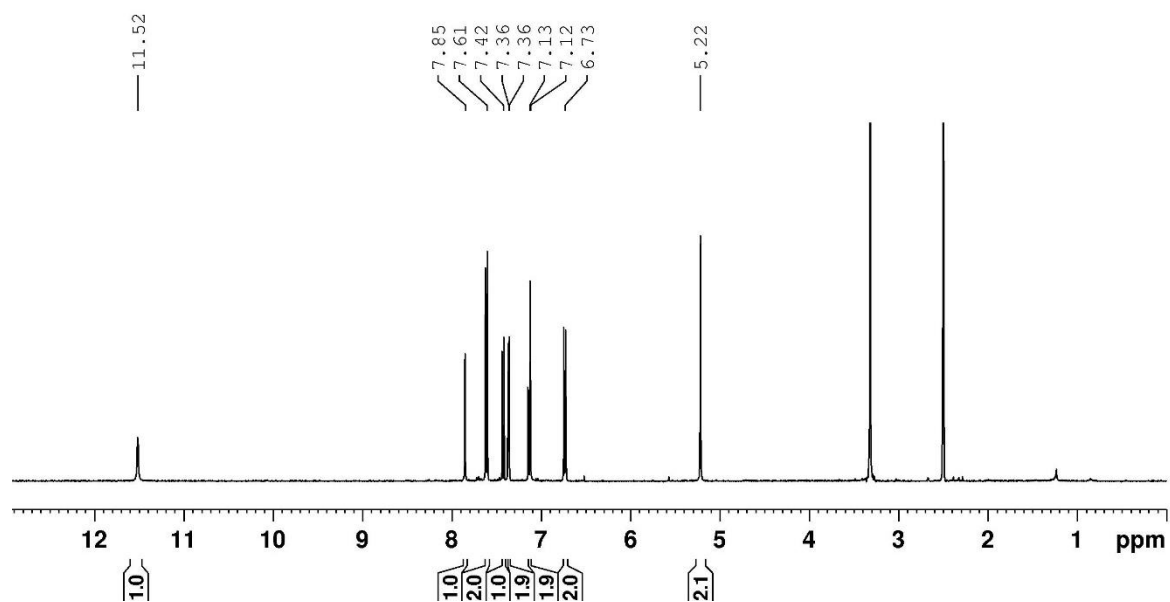


Figure S7. 5-Chloro-3-(1-(4-iodobenzyl)-1H-imidazol-5-yl)-1H-indole (7)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

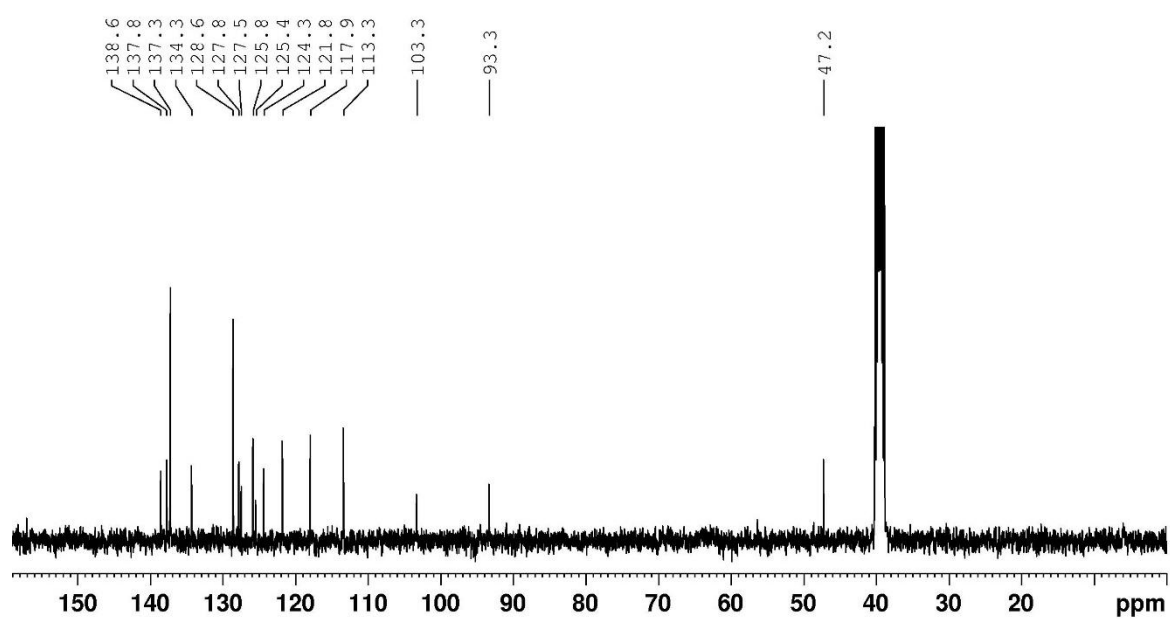
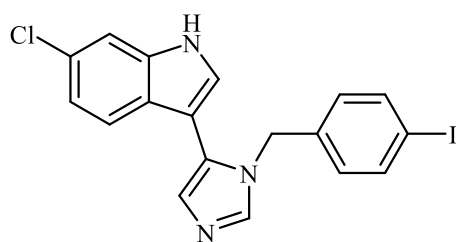
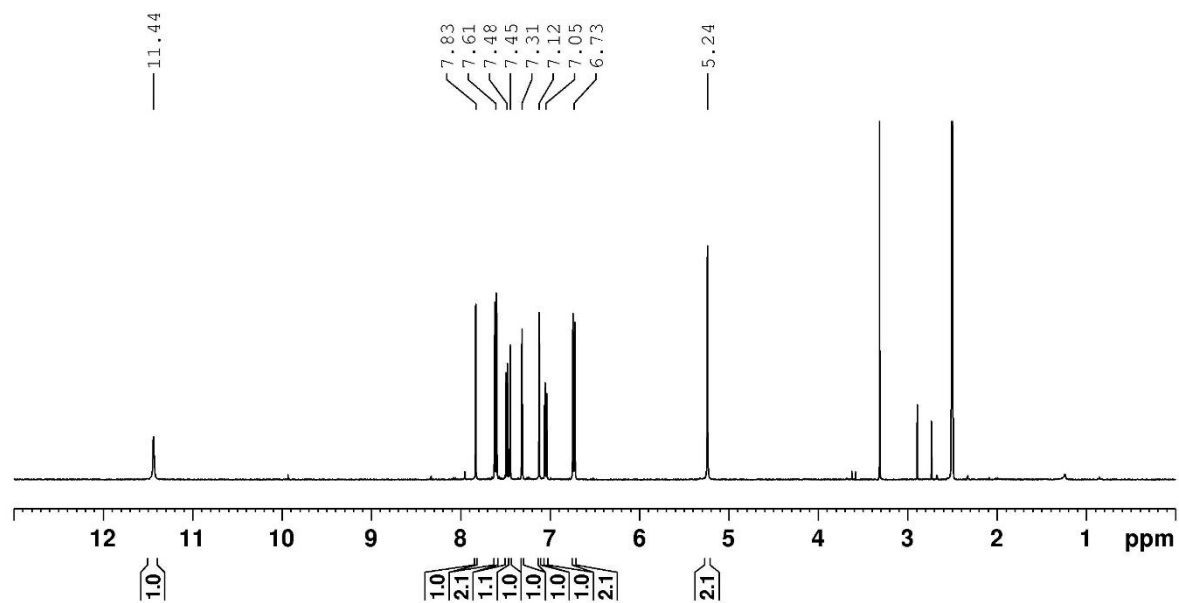


Figure S8. 6-Chloro-3-(1-(4-iodobenzyl)-1H-imidazol-5-yl)-1H-indole (8)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

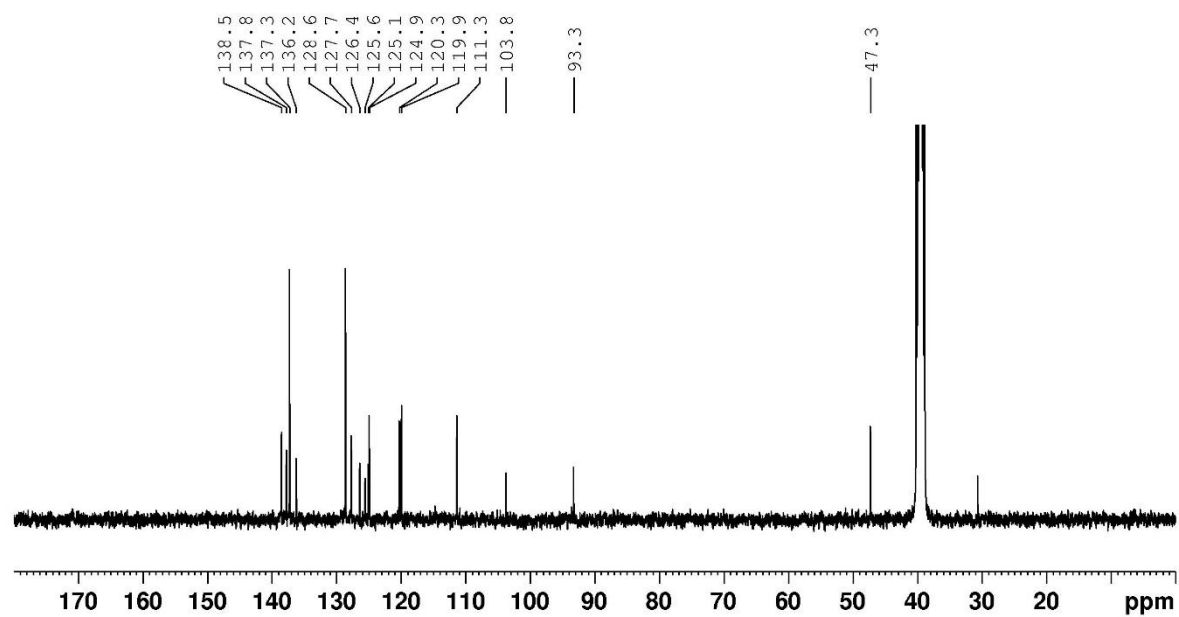
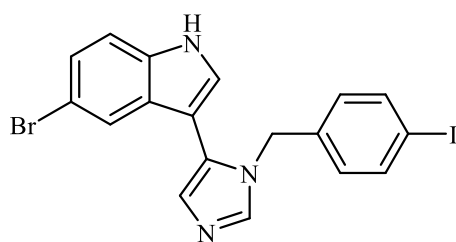
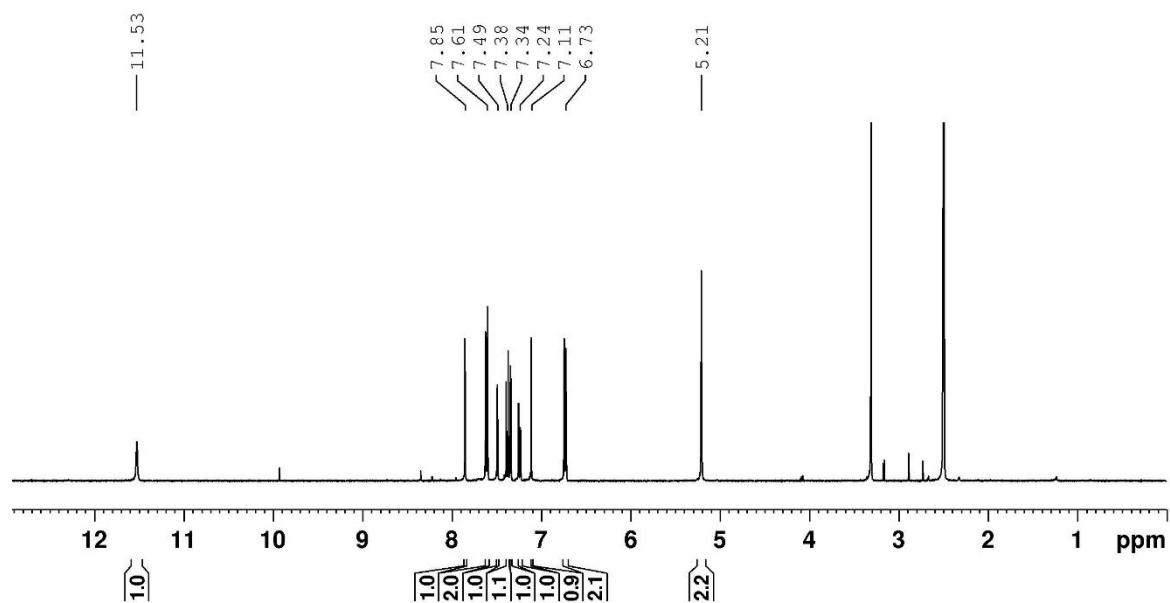


Figure S9. 5-Bromo-3-(1-(4-iodobenzyl)-1H-imidazol-5-yl)-1H-indole (9)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

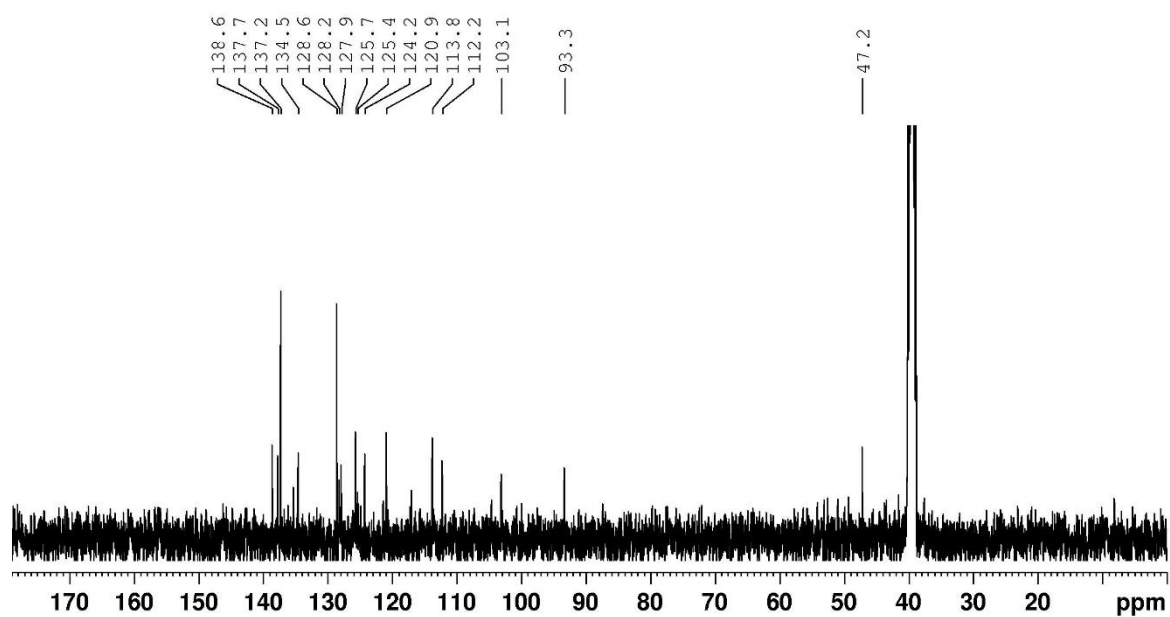
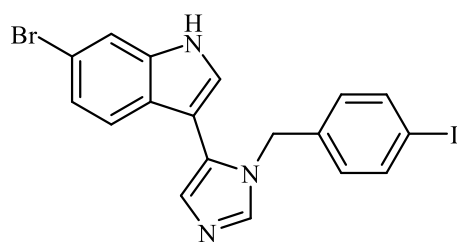
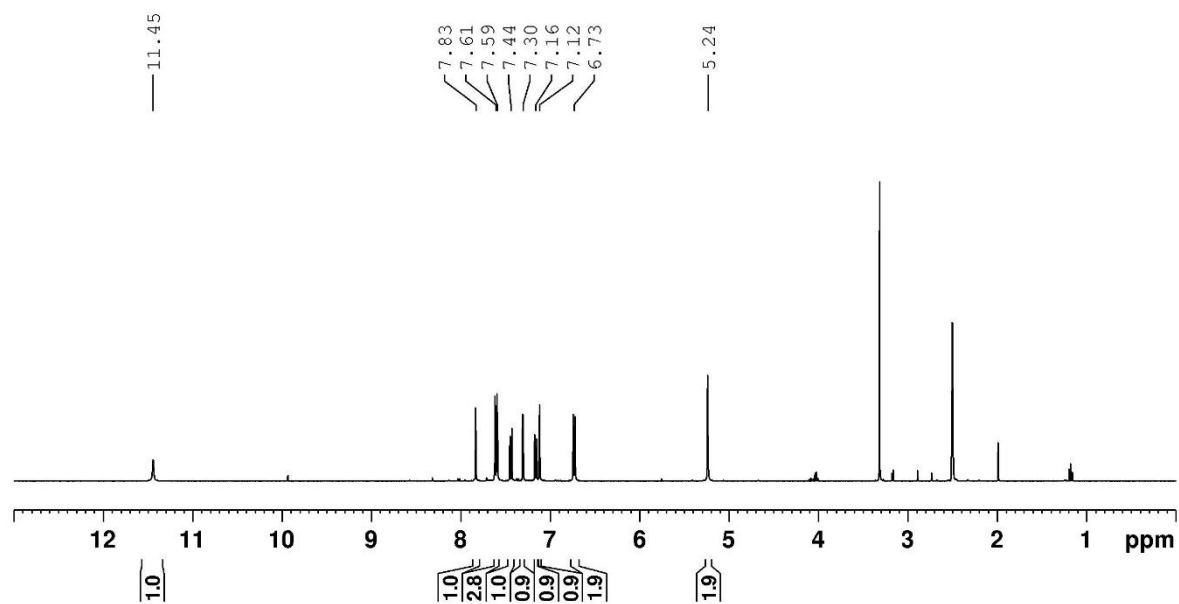


Figure S10. 6-Bromo-3-(1-(4-iodobenzyl)-1H-imidazol-5-yl)-1H-indole (**10**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

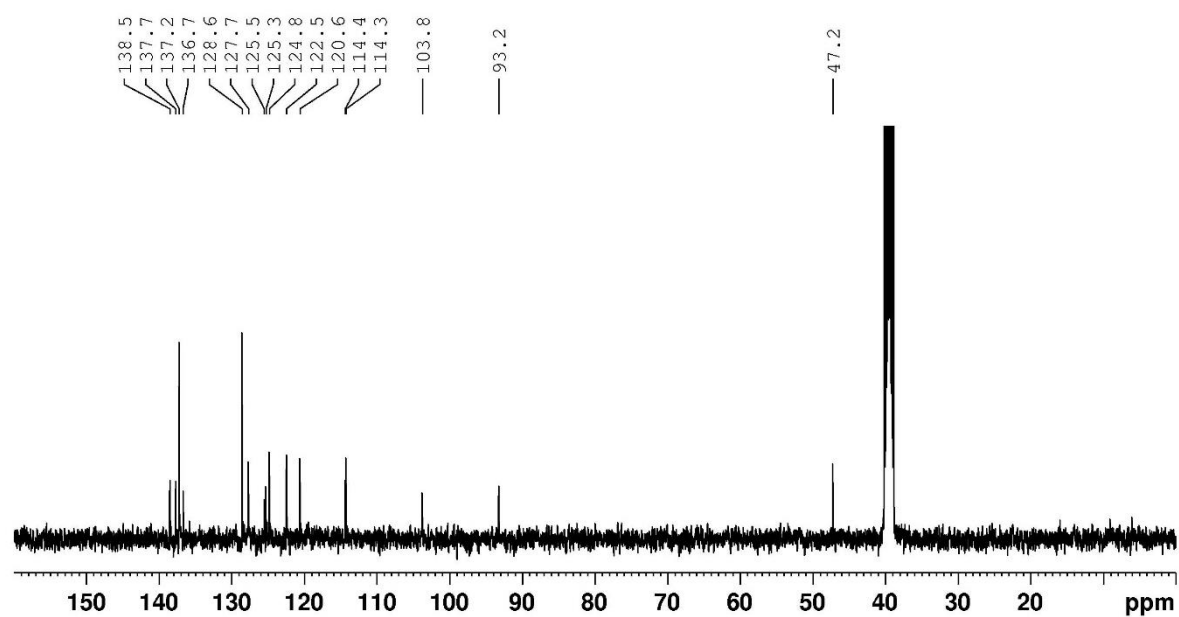
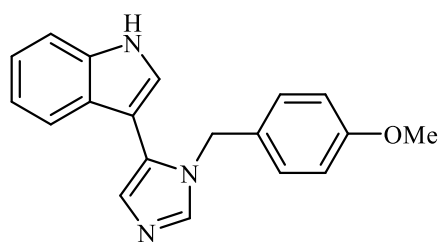
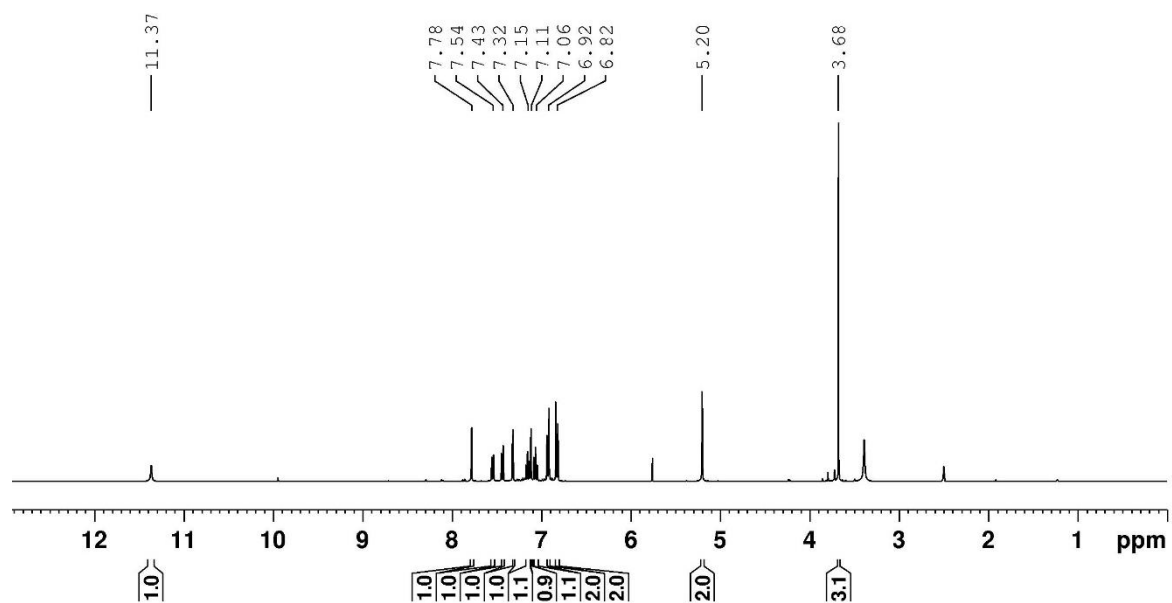


Figure S11. 3-(1-(4-Methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (**11**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

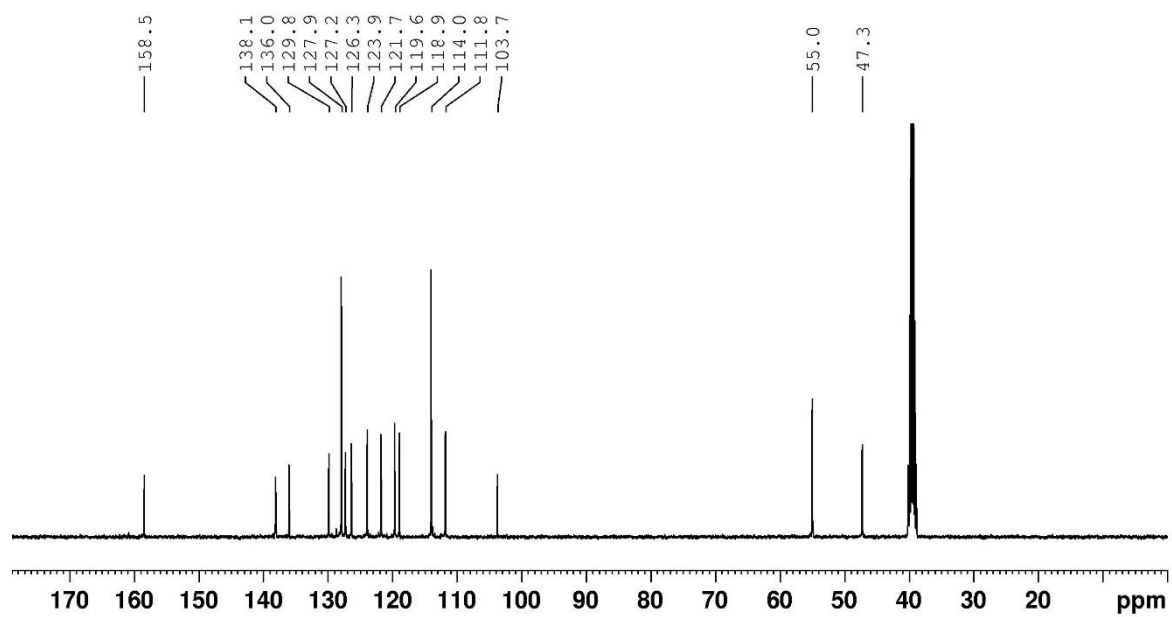
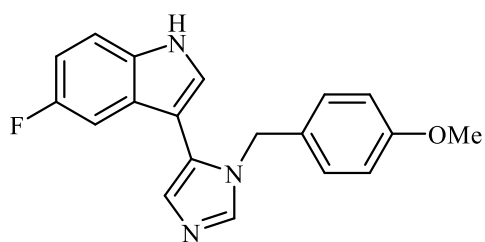
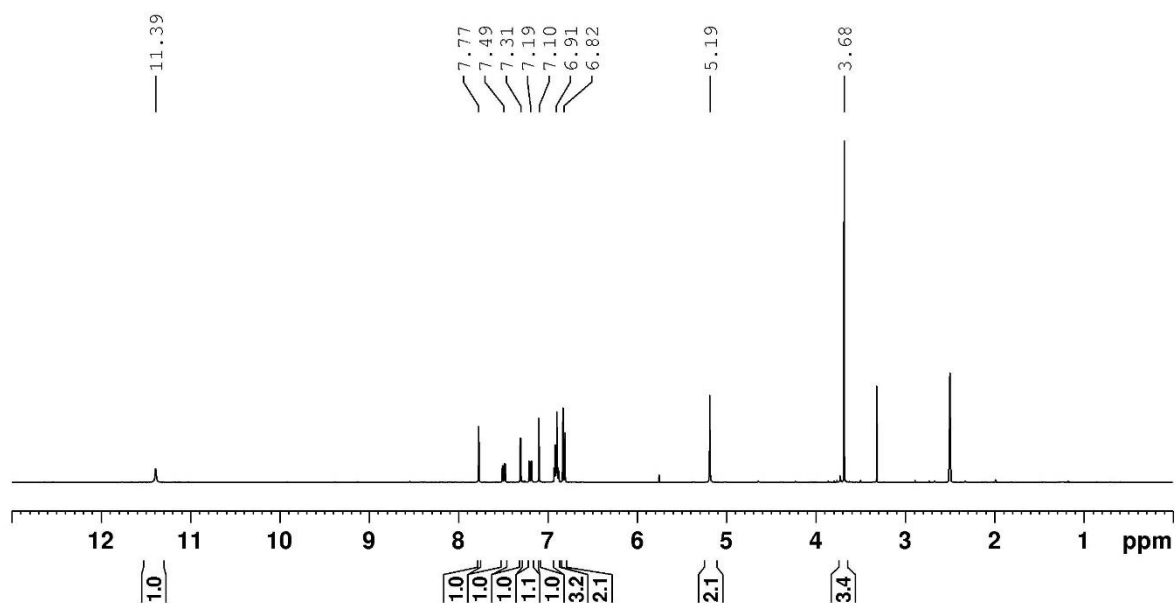


Figure S12. 5-Fluoro-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (12)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

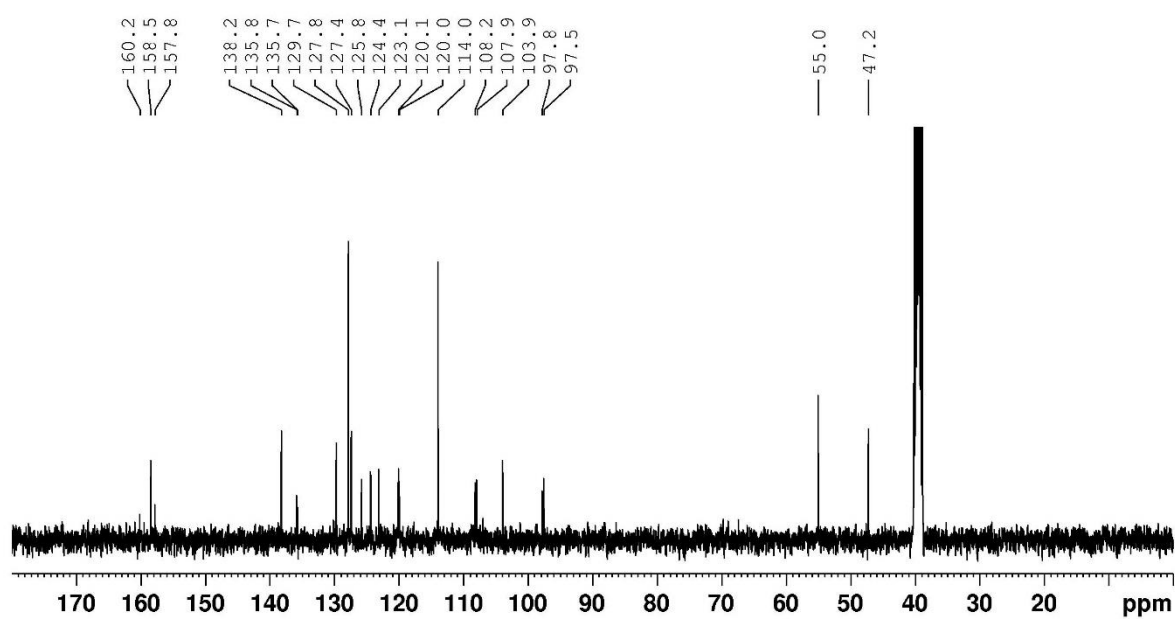
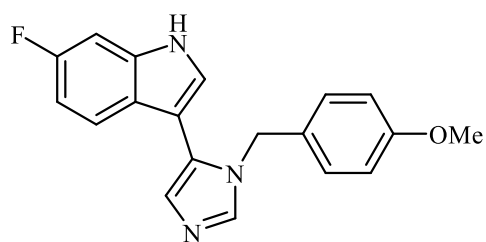
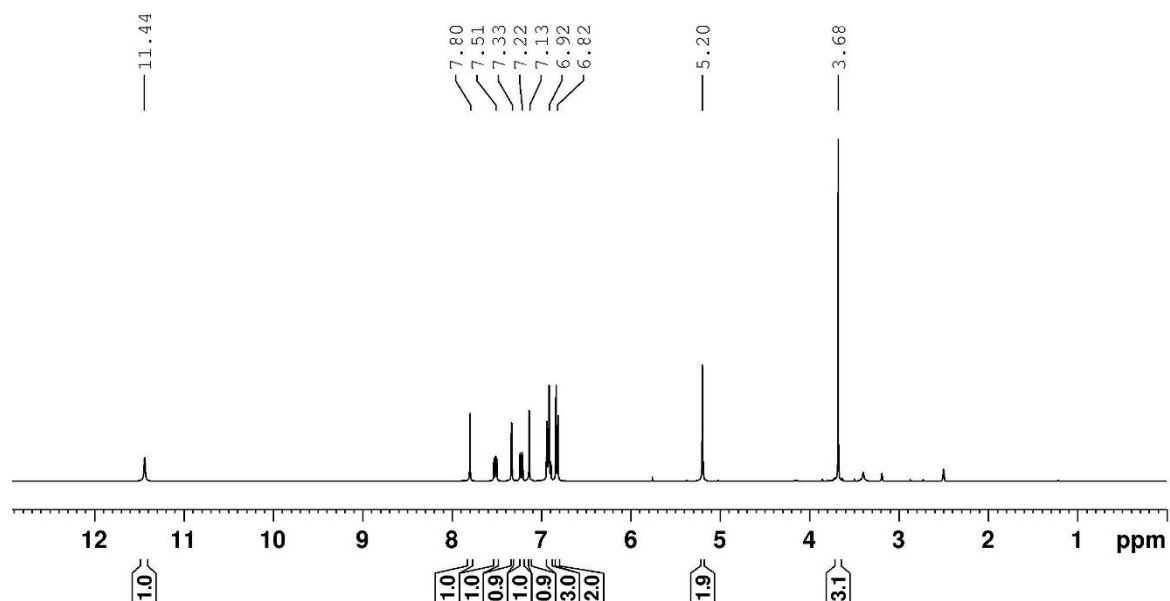


Figure S13. 6-Fluoro-3-(1-(4-methoxybenzyl)-1*H*-imidazol-5-yl)-1*H*-indole (**13**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

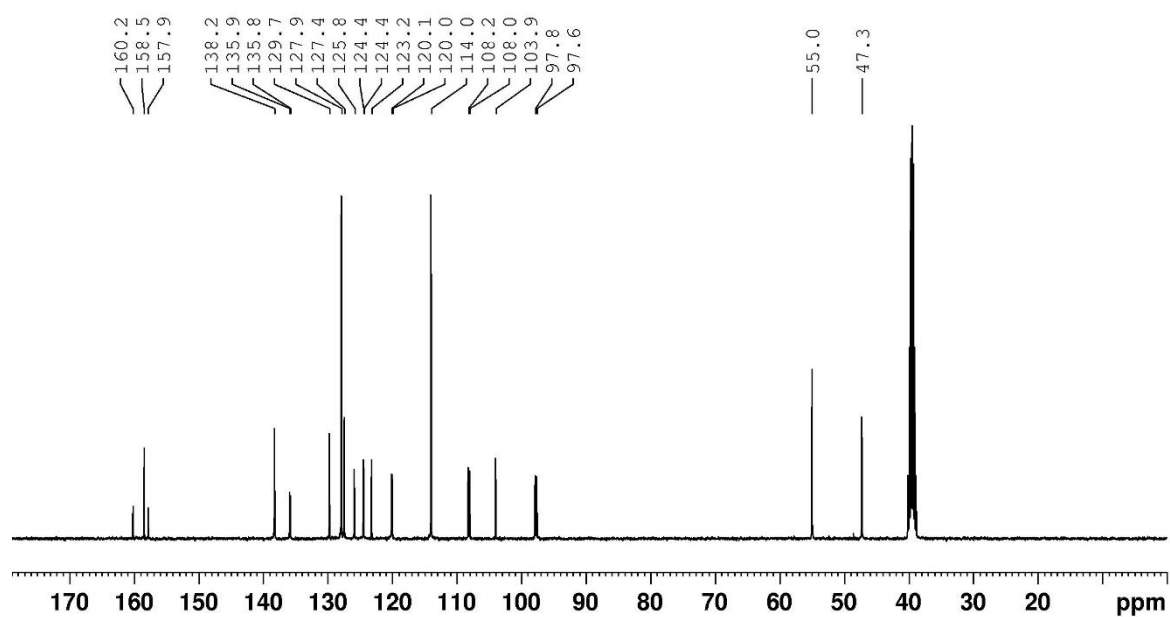
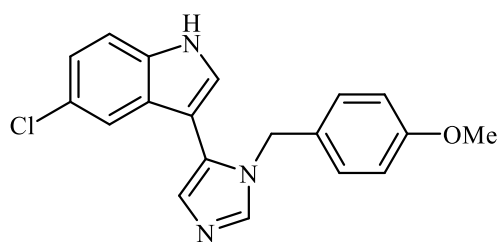
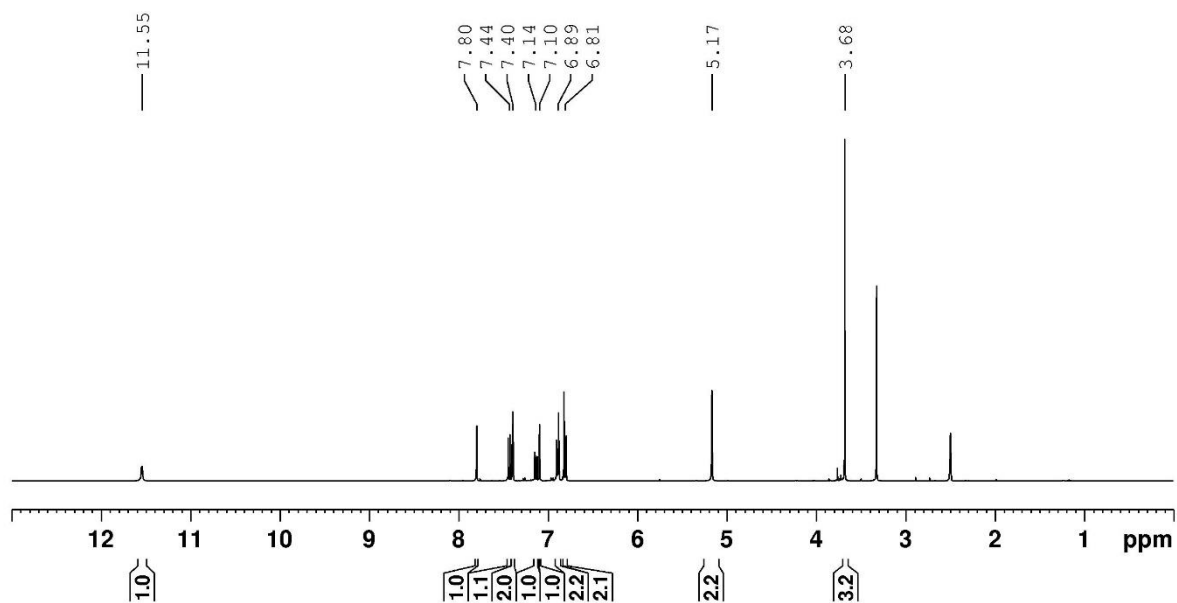


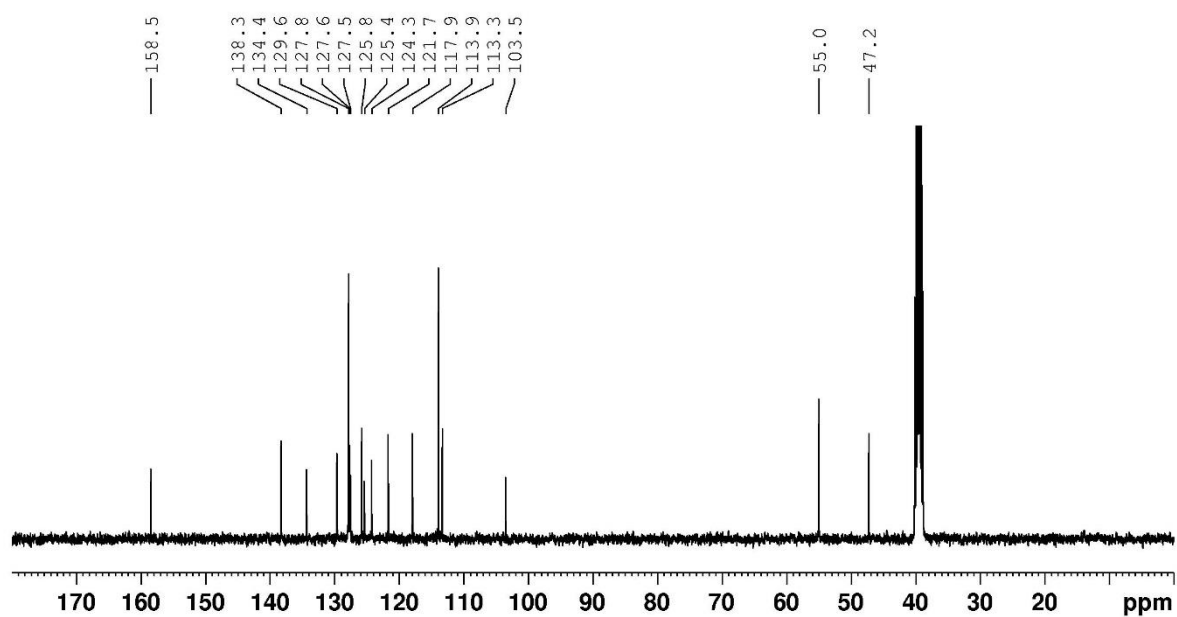
Figure S14. 5-Chloro-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (**14**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

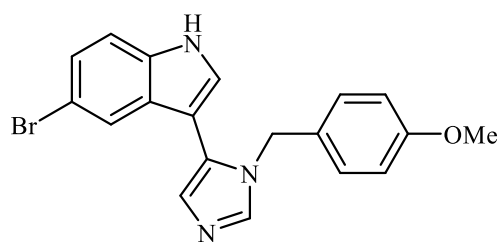


COc1ccc(cc1)CNc2cnc(c2)c3c[nH]c4ccc(Cl)cc34

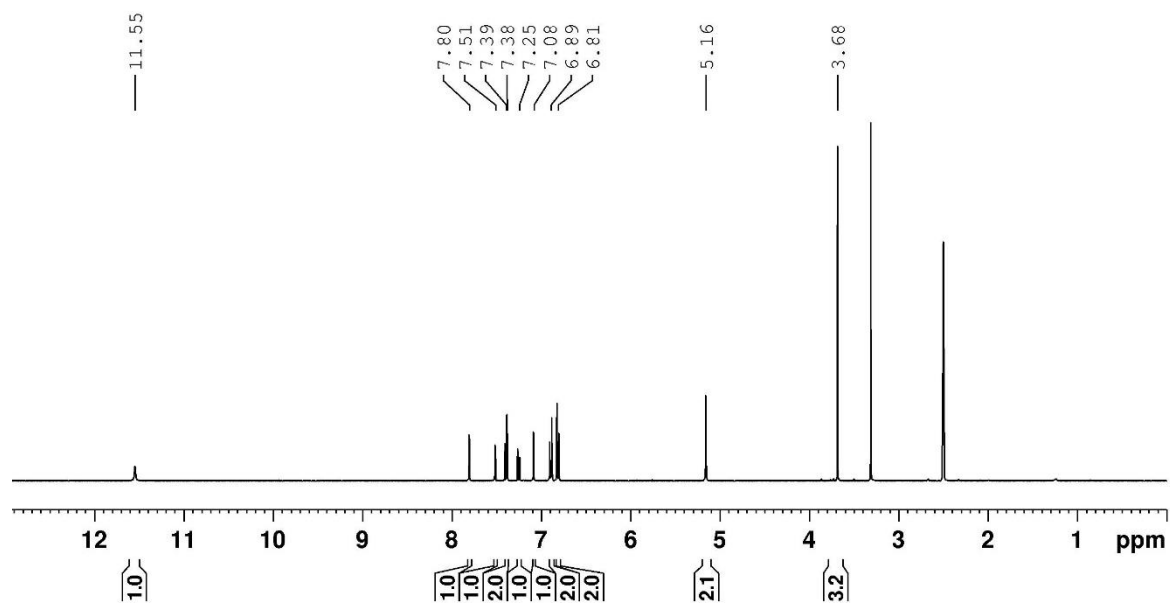
158.5
138.3
136.3
129.7
127.9
127.5
126.4
125.6
125.1
124.9
120.3
119.9
114.0
111.3
104.0
55.0
47.3

ppm

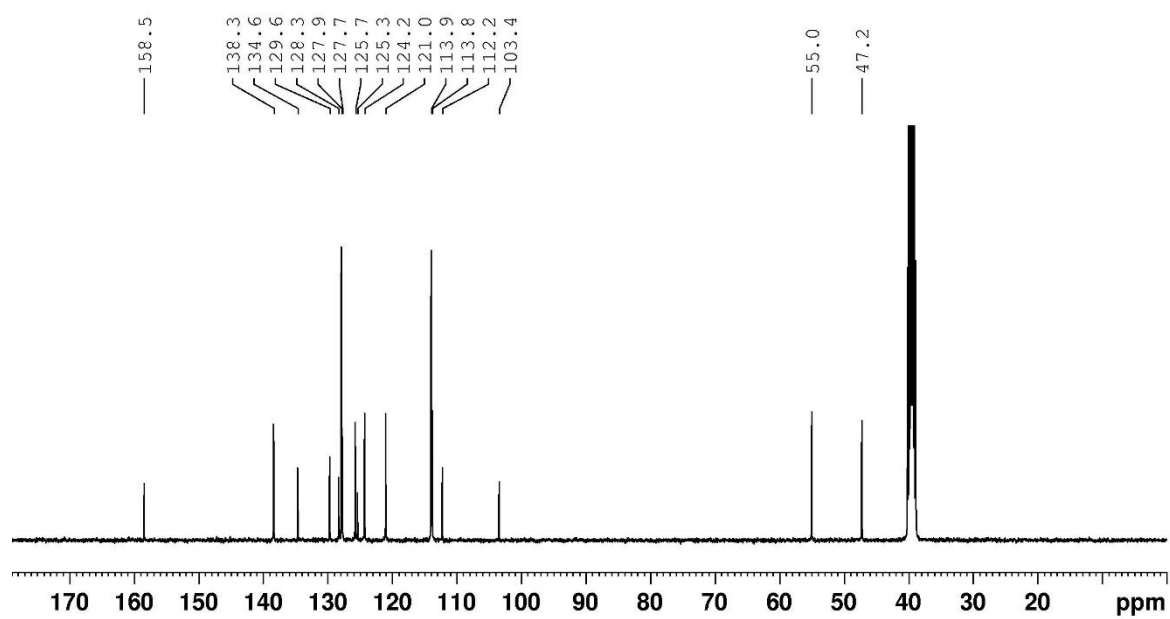
Figure S16. 5-Bromo-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (**16**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

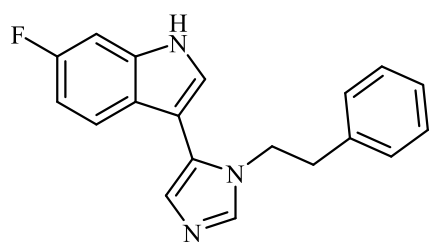


COc1ccc(cc1)CNc2cnc(c2)c3c[nH]c4cc(Br)ccc34

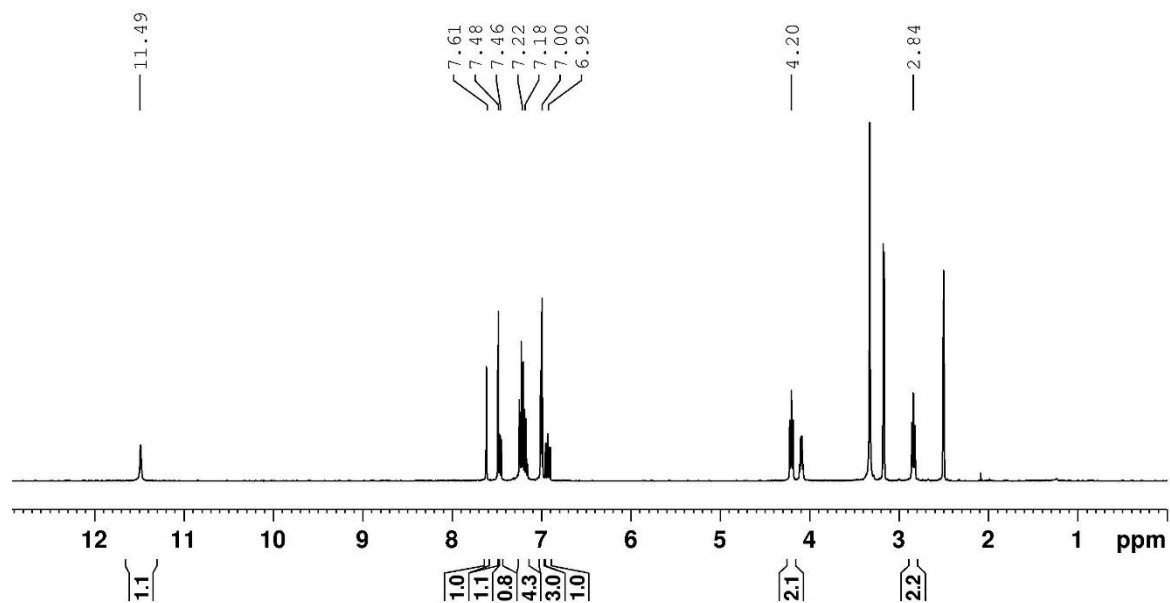
158.4
138.3
136.7
129.6
127.8
127.5
125.5
125.4
124.9
122.4
120.7
114.4
114.3
113.9
104.0
55.0
47.2

ppm

Figure S18. 6-Fluoro-3-(1-phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (**18**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

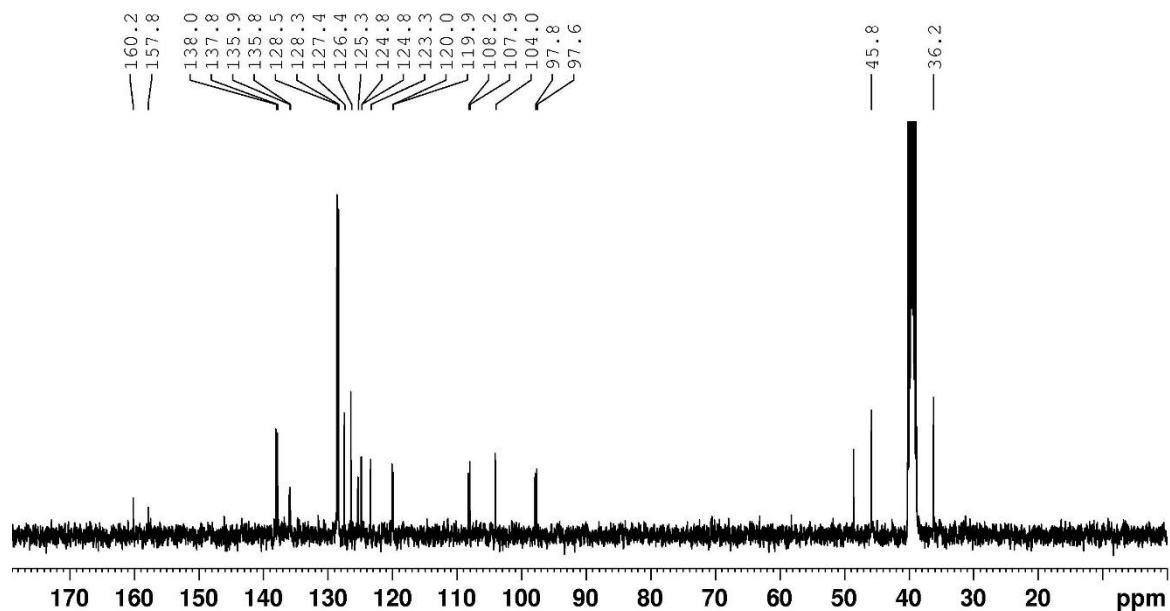
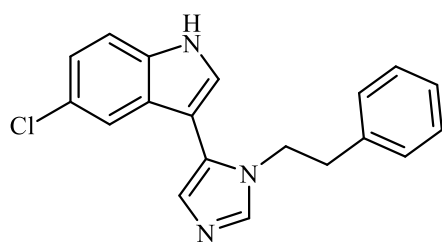
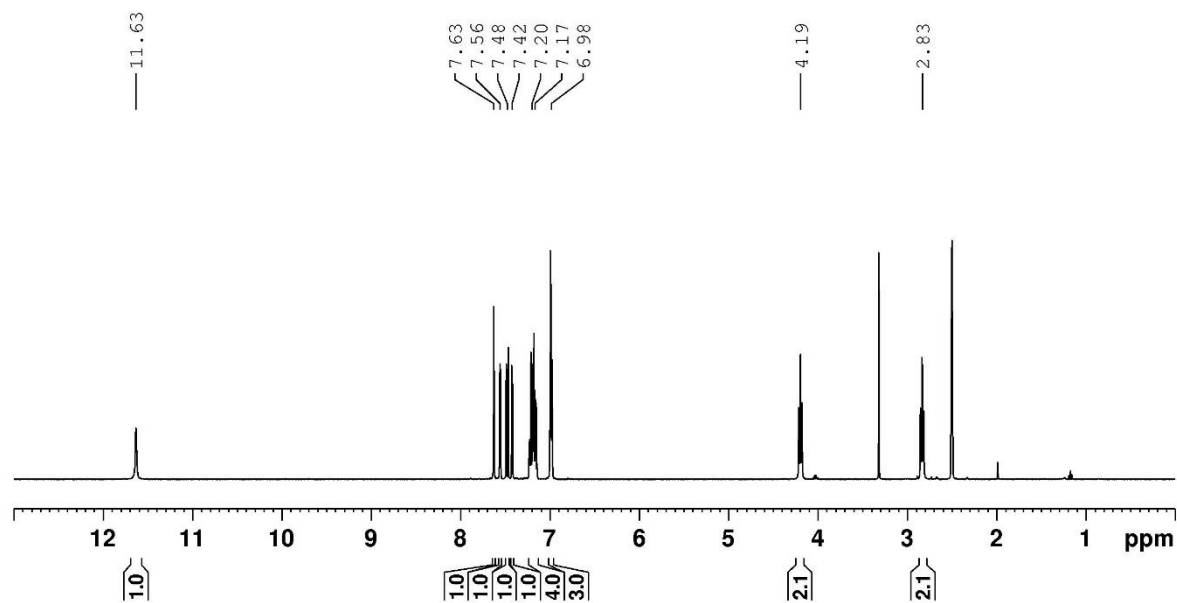


Figure S19. 5-Chloro-3-(1-phenethyl-1H-imidazol-5-yl)-1H-indole (**19**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

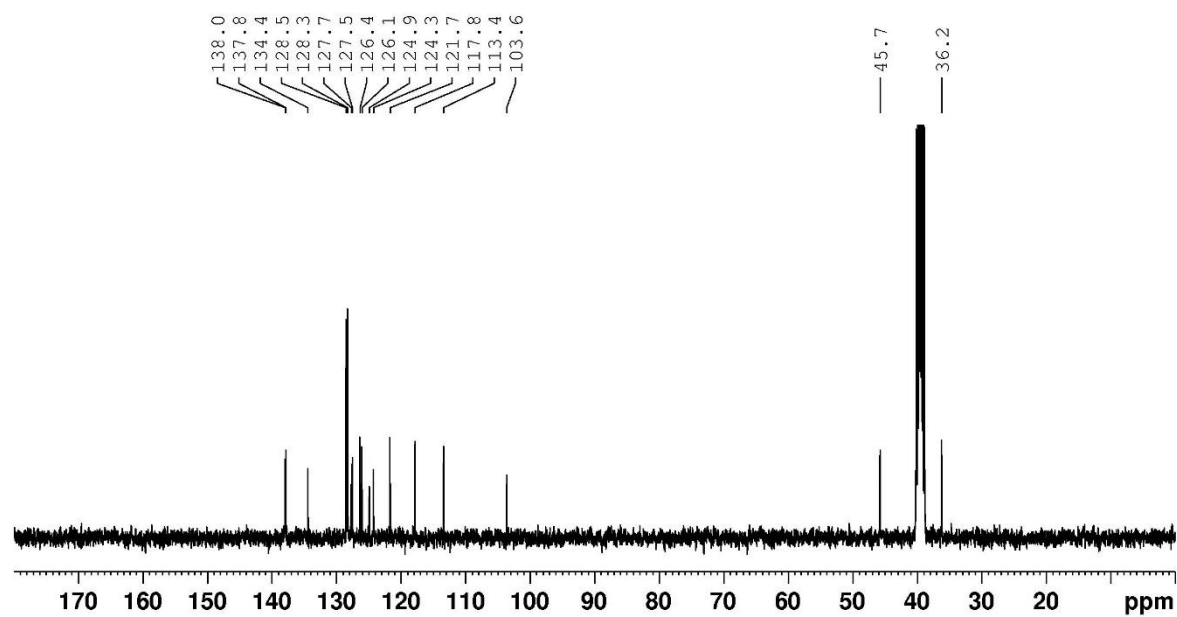
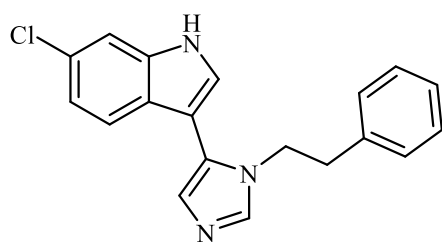
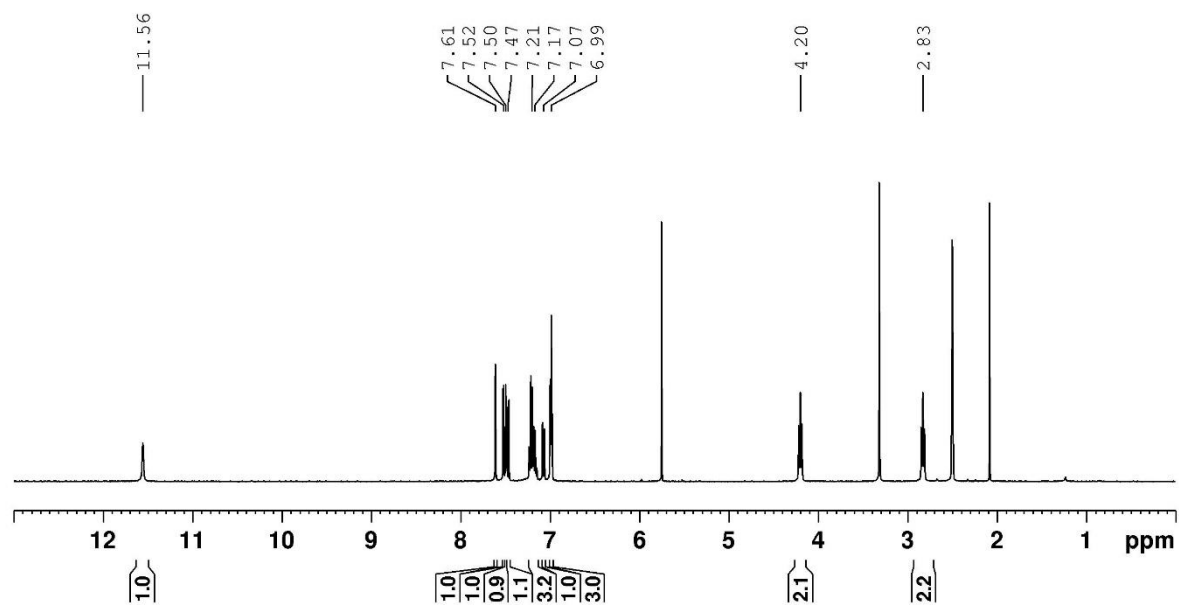


Figure S20. 6-Chloro-3-(1-phenethyl-1H-imidazol-5-yl)-1H-indole (20)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

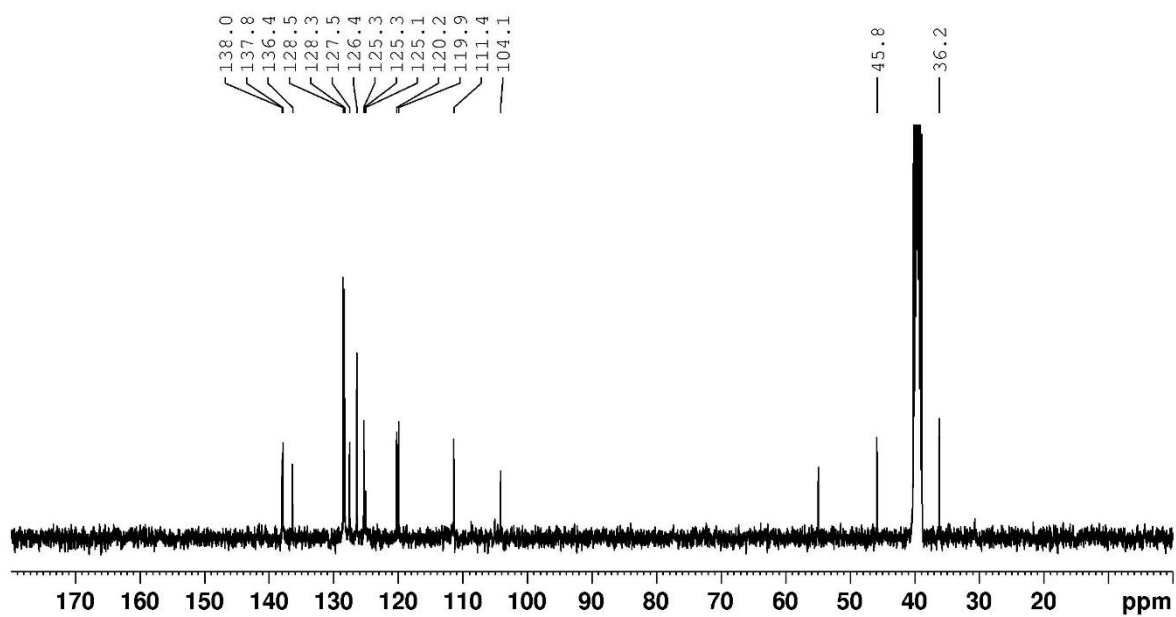
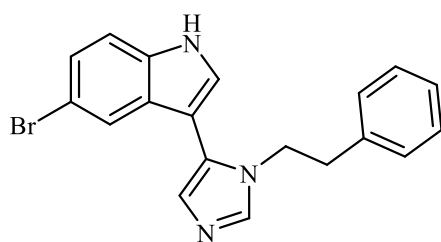
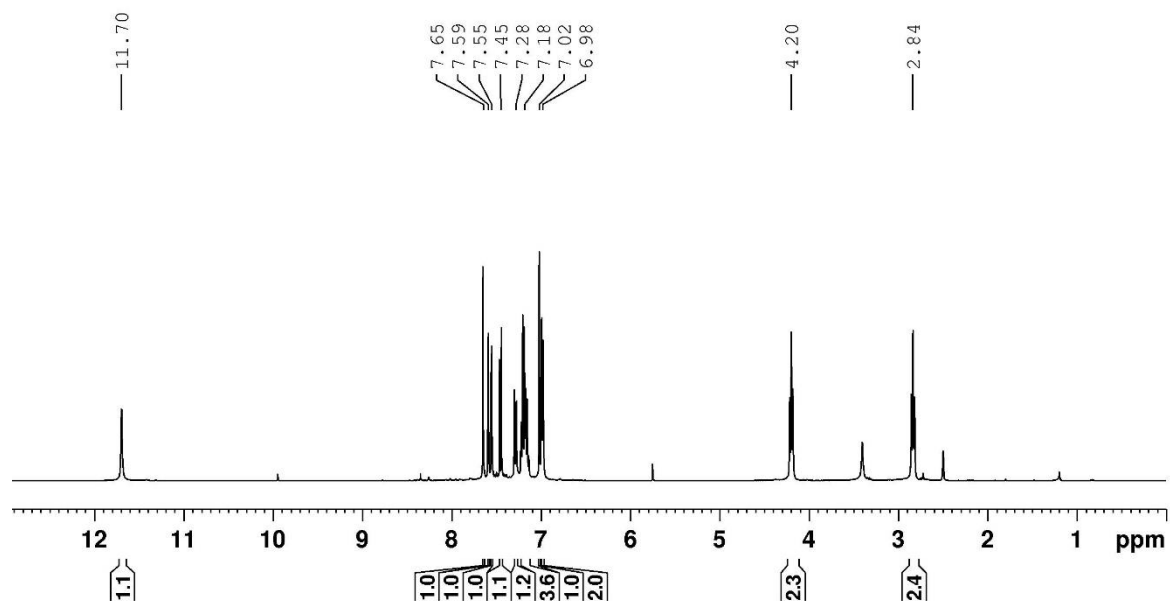


Figure S21. 5-Bromo-3-(1-phenethyl-1H-imidazol-5-yl)-1H-indole (21)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

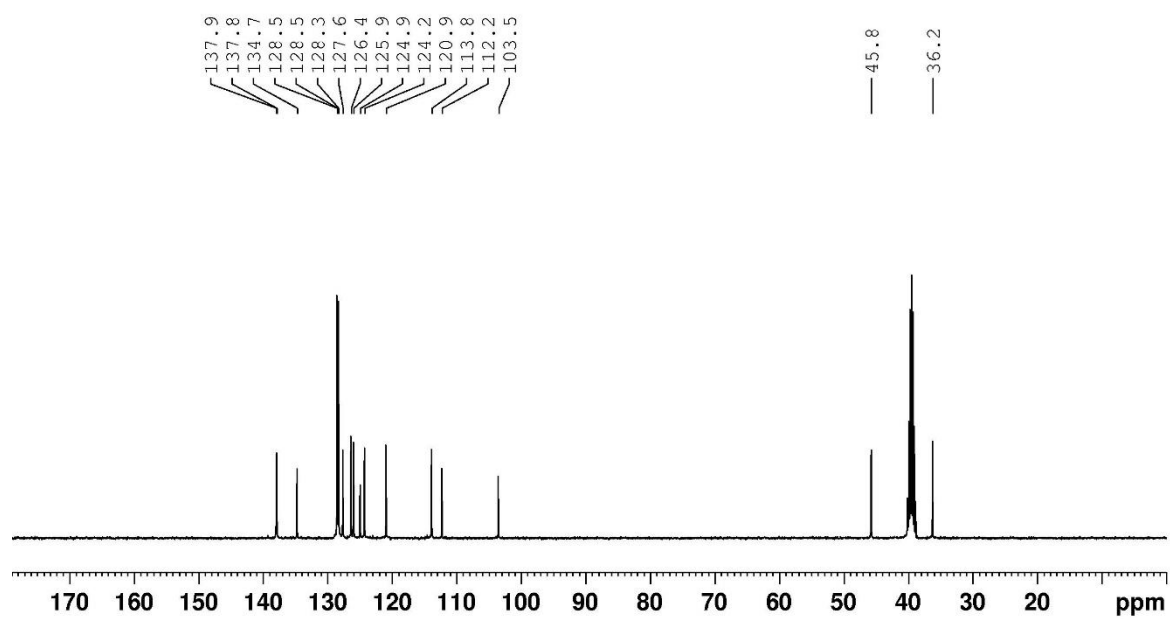
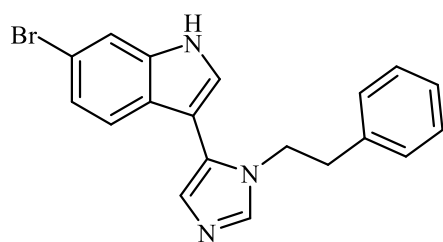
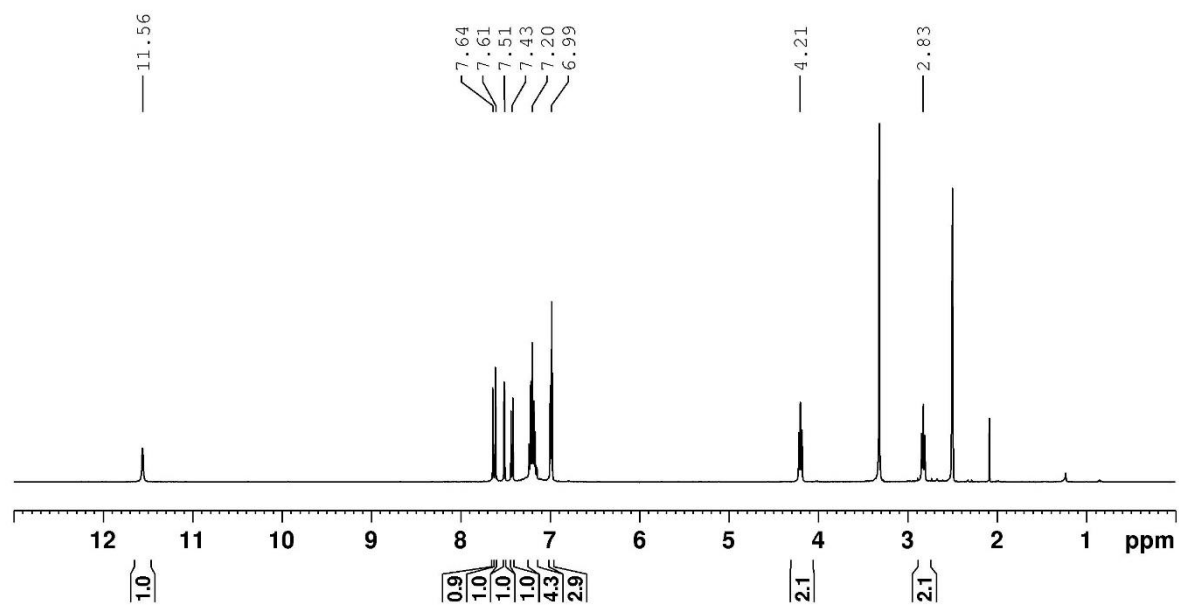


Figure S22. 6-Bromo-3-(1-phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (**22**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

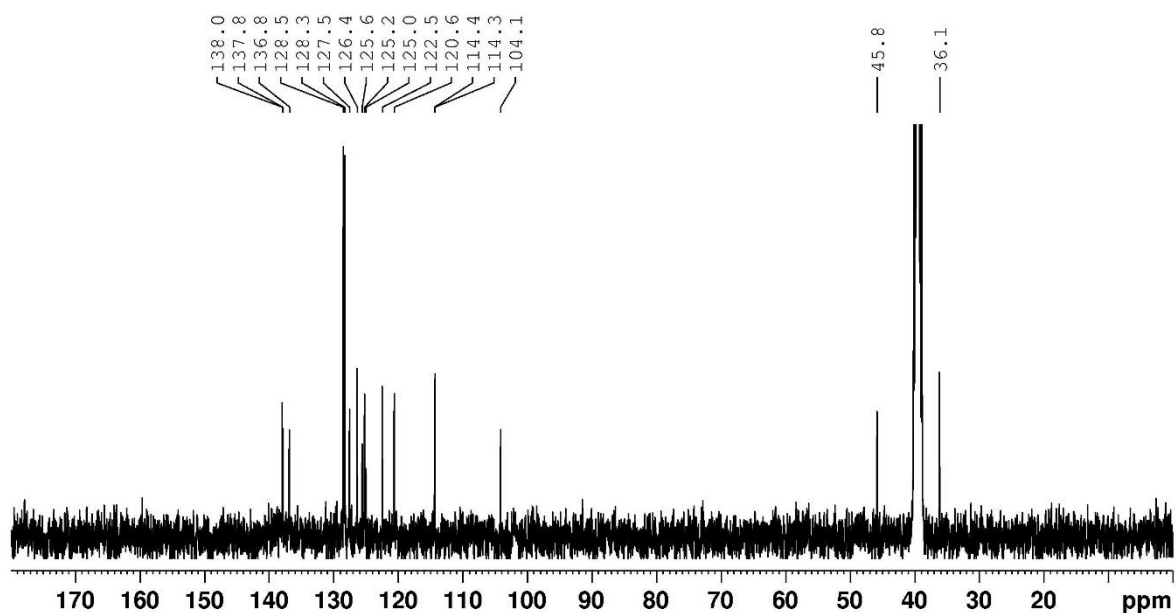
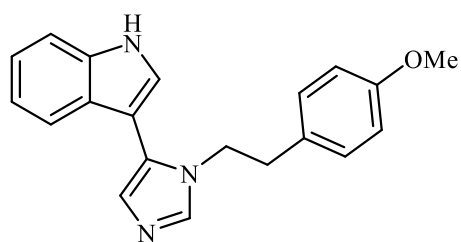
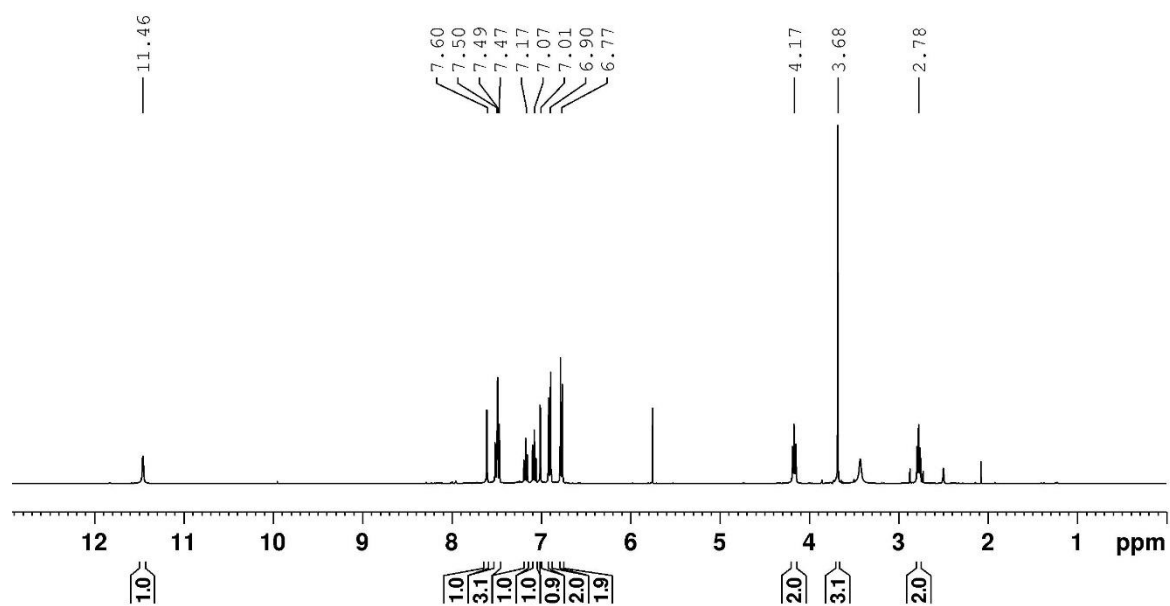


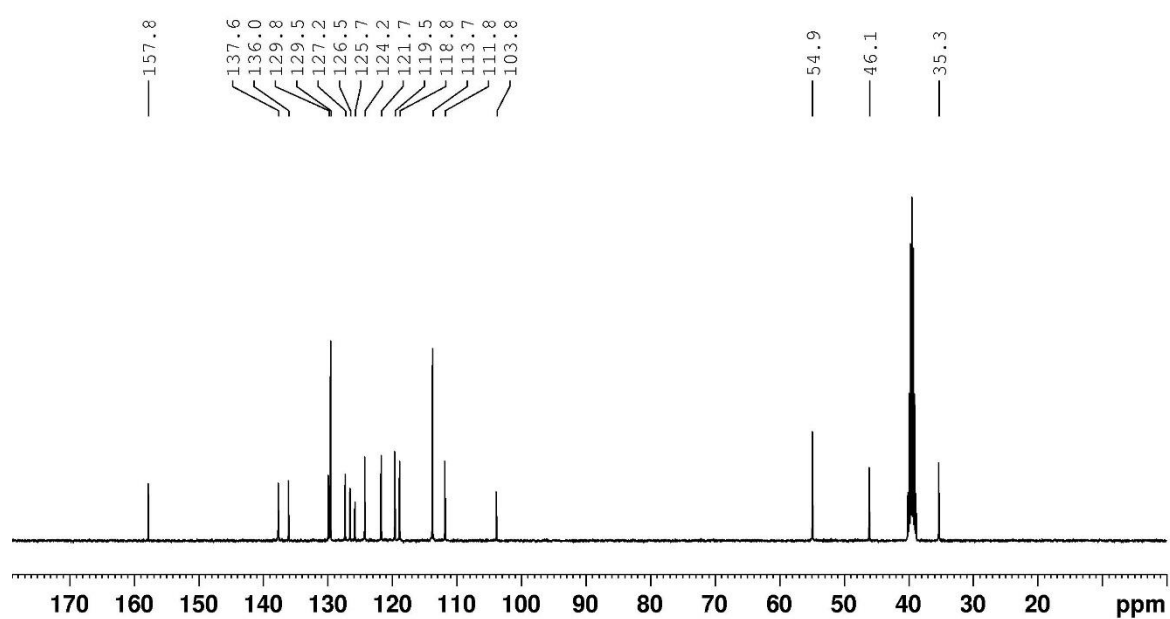
Figure S23. 3-(1-(4-Methoxyphenethyl)-1*H*-imidazol-5-yl)-1*H*-indole (23)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):



COc1ccc(cc1)CCN2C=CN=C2C3C(=N1C=CC=C(C=C1)F)C=C3

Chemical structure of compound **1** is shown above the spectrum. The structure is a substituted benzene ring with a carboxylic acid group, a methoxy group, and a side chain containing a ketone and a terminal methyl group.

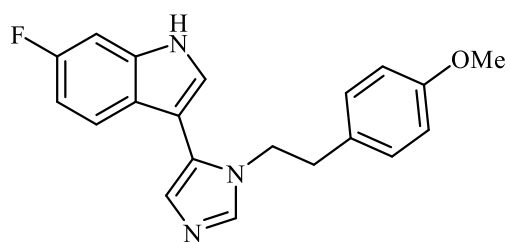
¹H NMR spectrum (CDCl₃) of compound **1**. The x-axis represents chemical shift in ppm, ranging from 1 to 12. The spectrum shows several peaks:

- Singlet at 11.53 ppm (integration 1.1).
- Multiplet between 6.7 and 7.6 ppm (integrations 1.0, 1.0, 1.1, 1.1, 2.0, 2.1, 2.1).
- Singlet at 4.16 ppm (integration 2.1).
- Sharp singlet at 3.69 ppm (integration 3.3).
- Singlet at 2.77 ppm (integration 2.2).
- Small peak at 5.5 ppm.

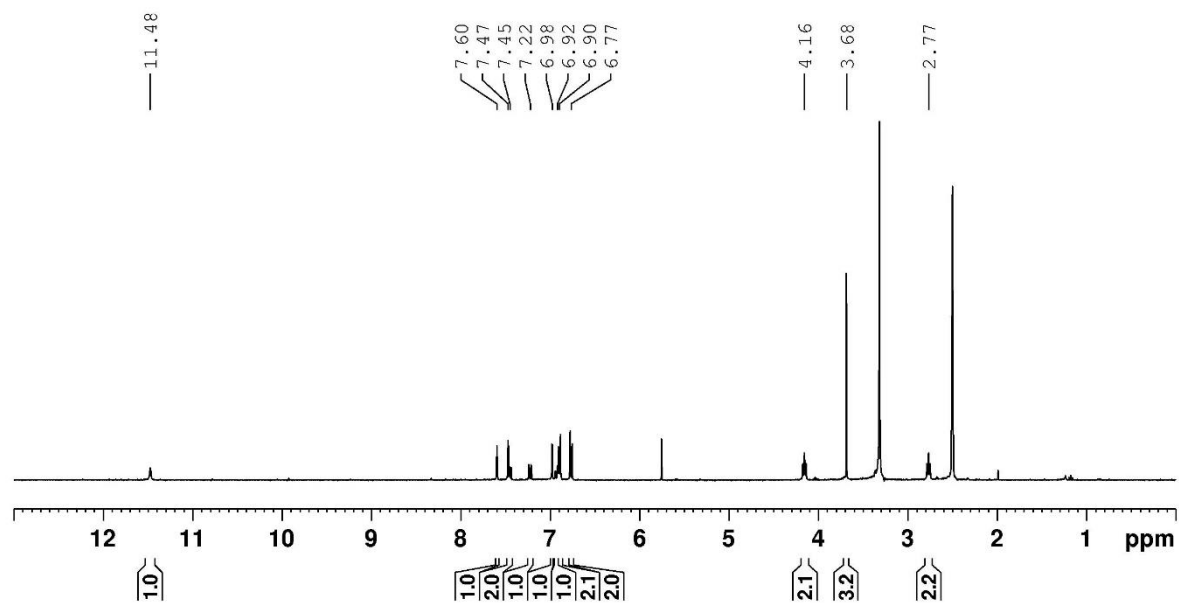
158.5
157.8
156.2
137.7
132.6
129.8
129.5
127.3
126.9
126.8
126.2
125.2
113.7
112.9
112.8
110.1
109.8
104.1
104.1
103.5
103.3
54.9
46.0
35.3

ppm

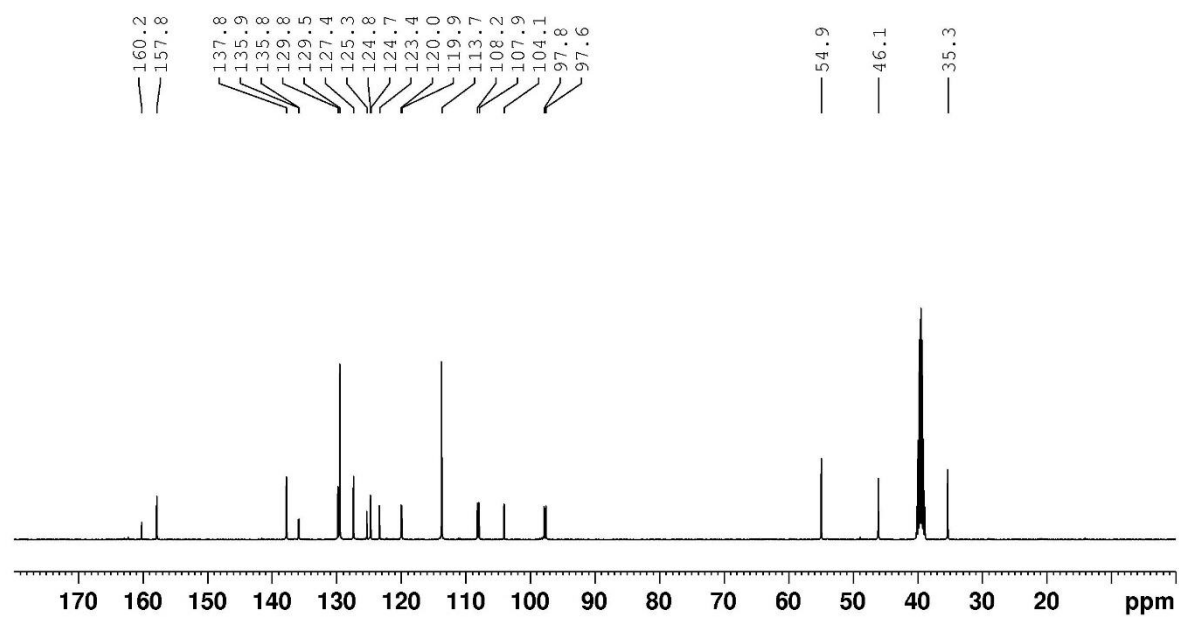
Figure S25. 6-Fluoro-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (**25**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

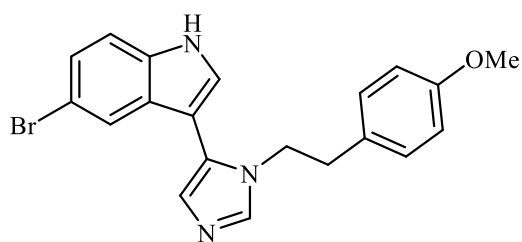


COc1ccc(cc1)CCN2C=CN=C2c3c[nH]c4cc(Cl)ccc34

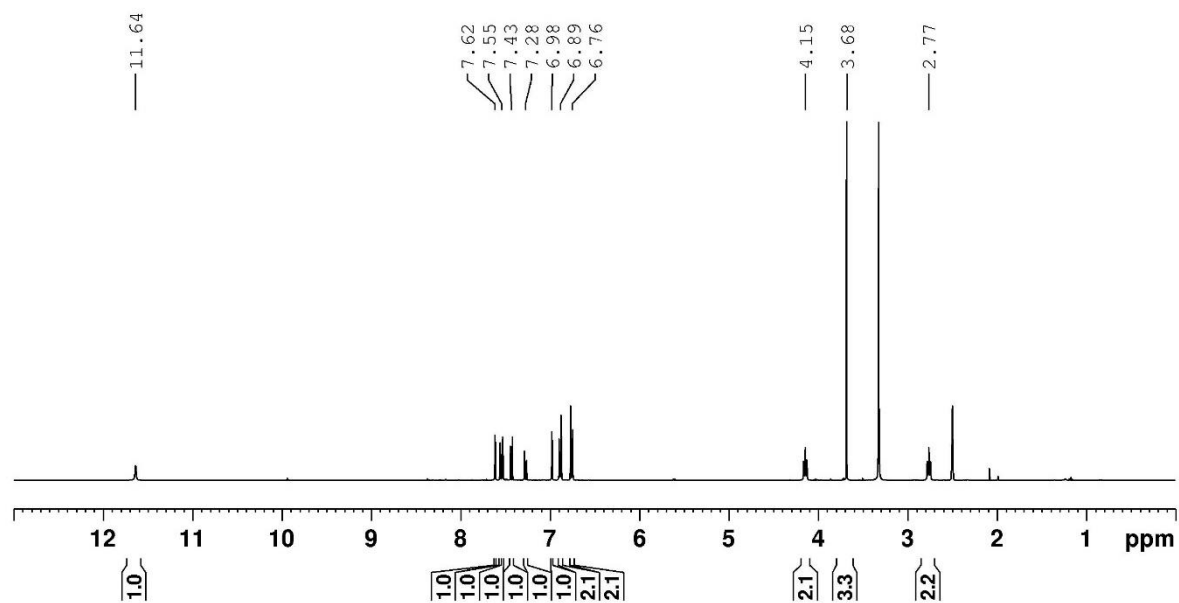
157.8
137.8
134.5
129.8
129.5
127.7
127.5
126.0
125.0
124.3
121.7
117.9
113.7
113.4
103.7
54.9
46.0
35.4

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Figure S27. 5-Bromo-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (27)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

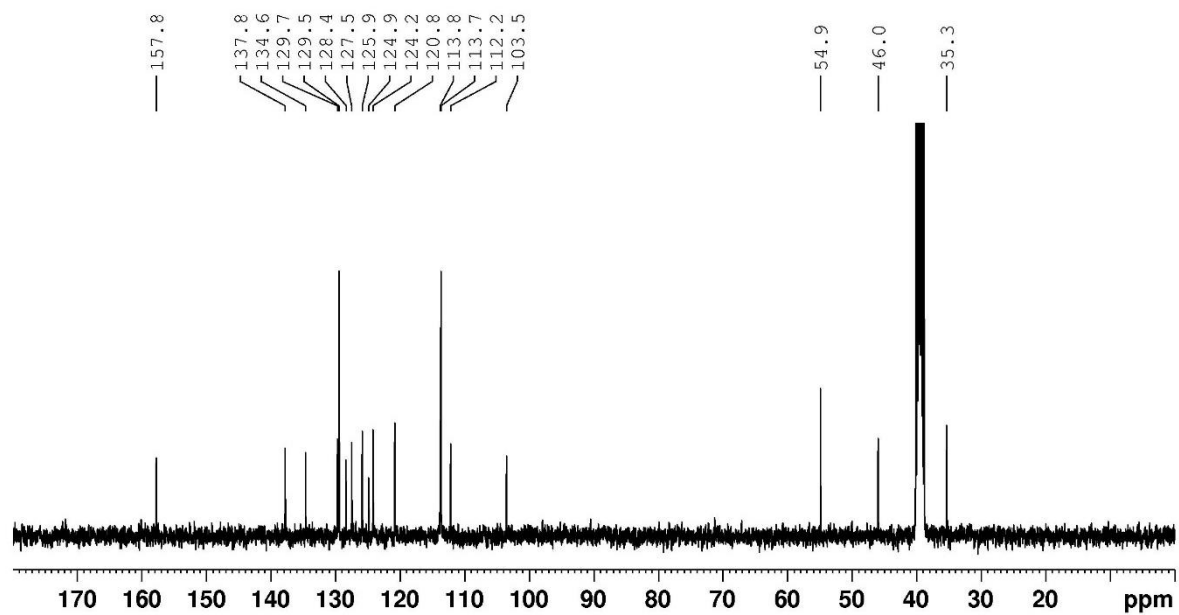
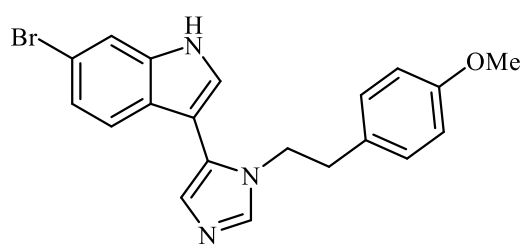
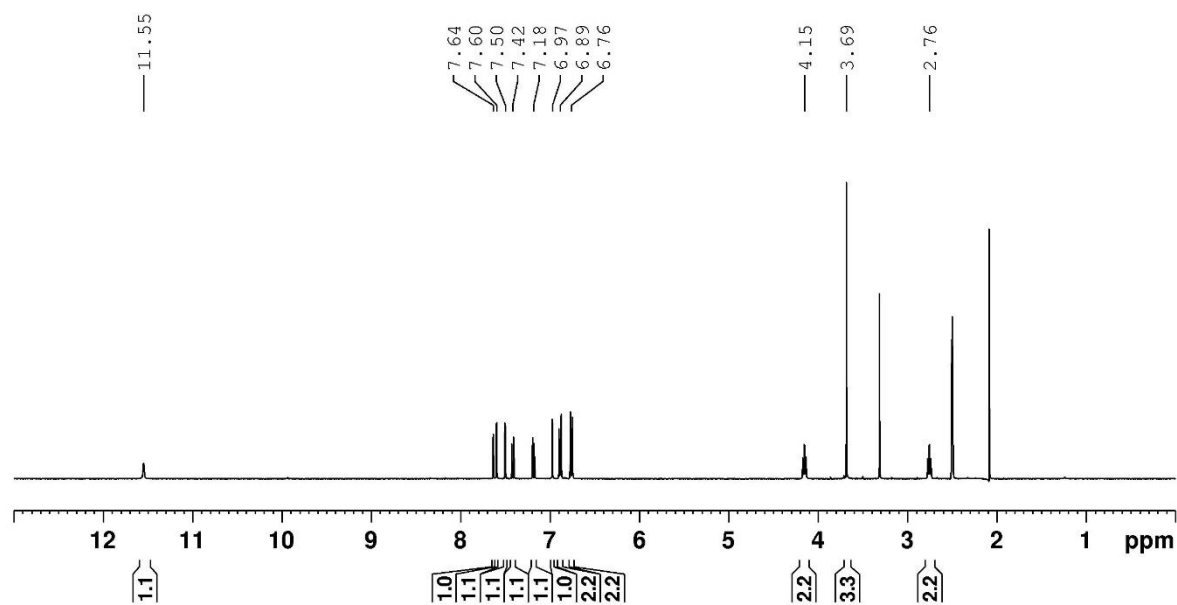


Figure S28. 6-Bromo-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (**28**)



^1H NMR ($\text{DMSO}-d_6$, 400 MHz):



^{13}C NMR ($\text{DMSO}-d_6$, 100 MHz):

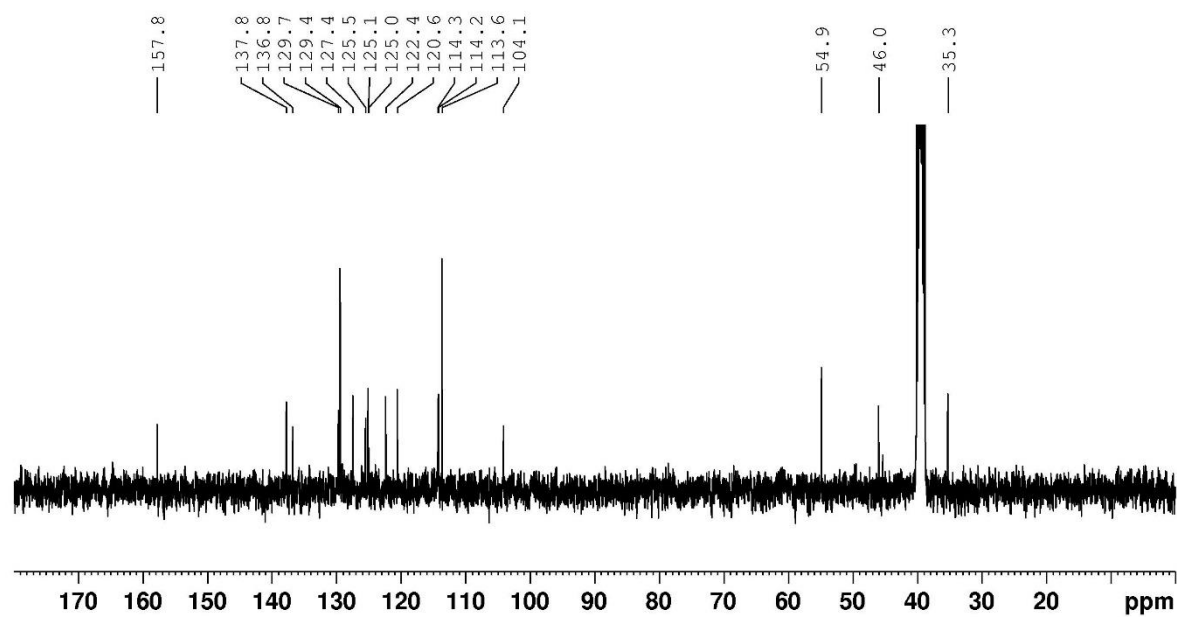
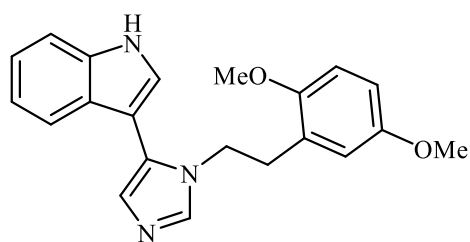
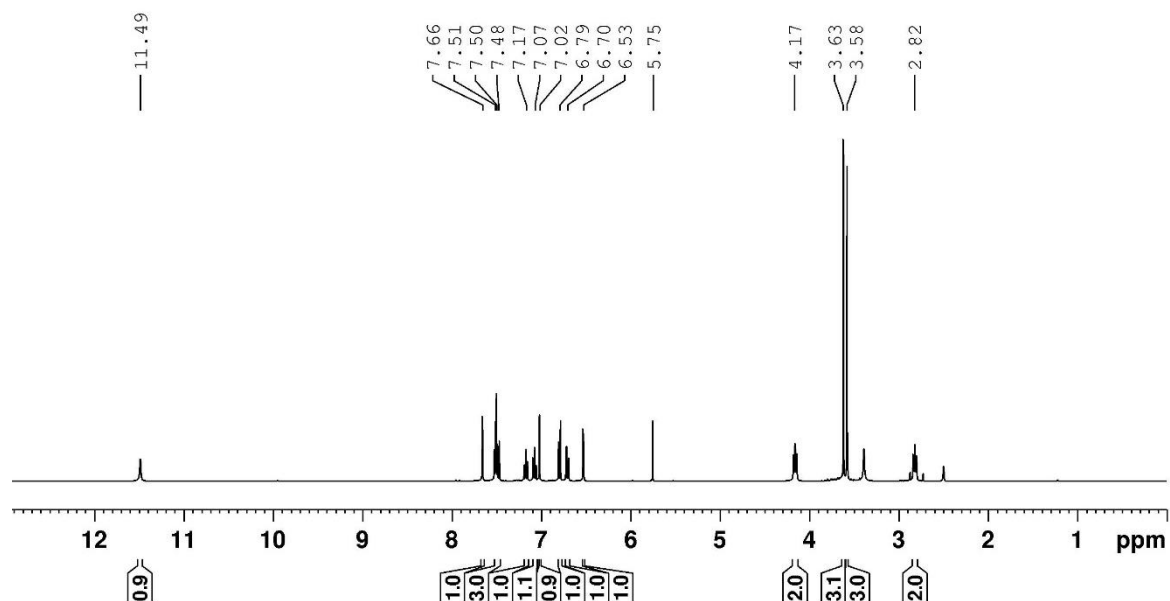


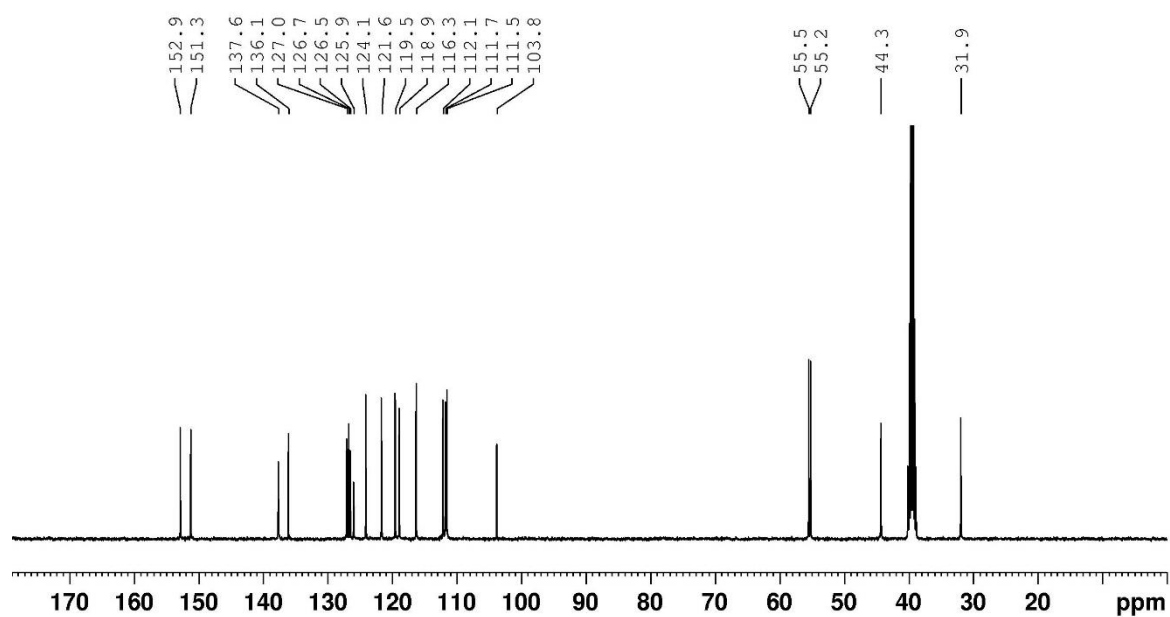
Figure S29. 3-(1-(2,5-Dimethoxyphenethyl)-1*H*-imidazol-5-yl)-1*H*-indole (**29**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

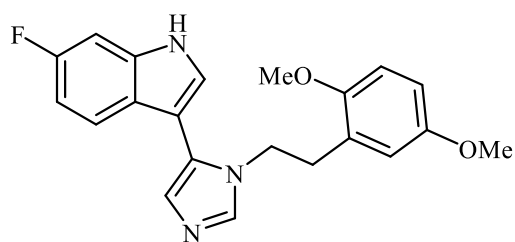


COc1ccc(OC)cc1CCN2C=CN=C2C3=C(C=C4C(=C(C=C4)F)N=C5C=CC=CC=C35)N6

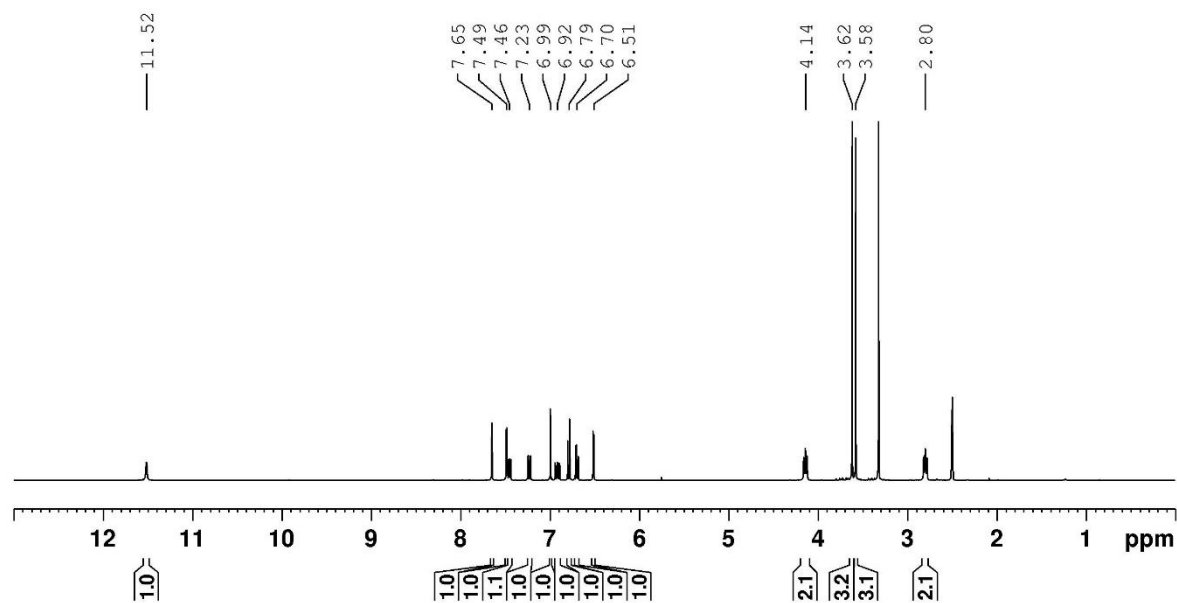
158.5
156.2
152.9
151.2
137.7
132.7
127.1
126.8
126.7
126.6
126.1
125.4
116.3
112.8
112.7
112.1
111.5
110.0
109.7
104.1
104.0
103.6
103.4
55.5
55.2
44.2
32.0

ppm

Figure S31. 3-(1-(2,5-Dimethoxyphenethyl)-1H-imidazol-5-yl)-6-fluoro-1H-indole (**31**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

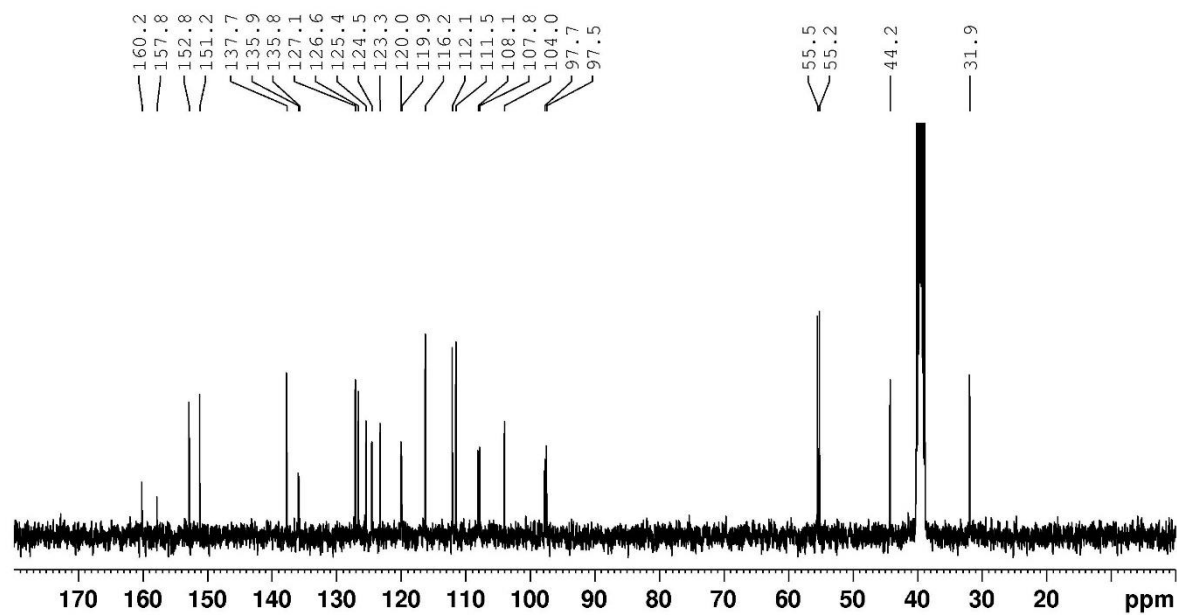
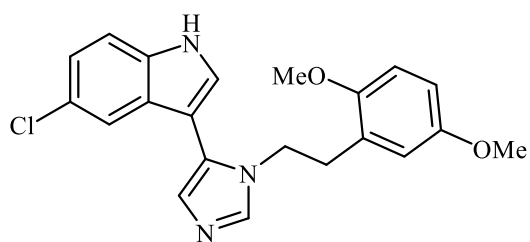
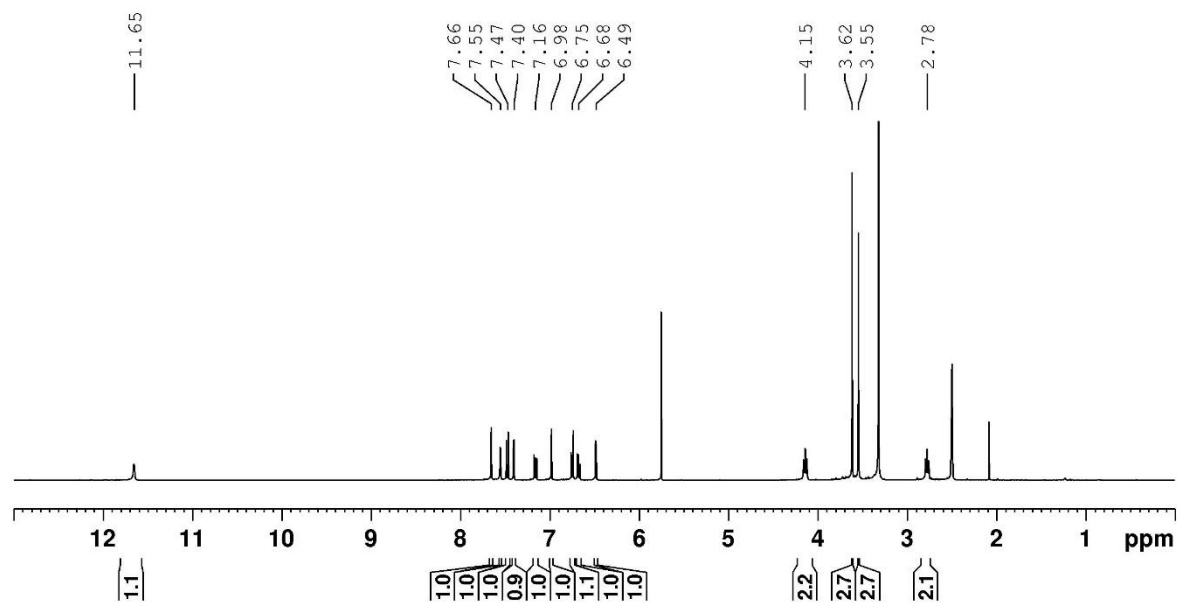


Figure S32. 5-Chloro-3-(1-(2,5-dimethoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (32)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

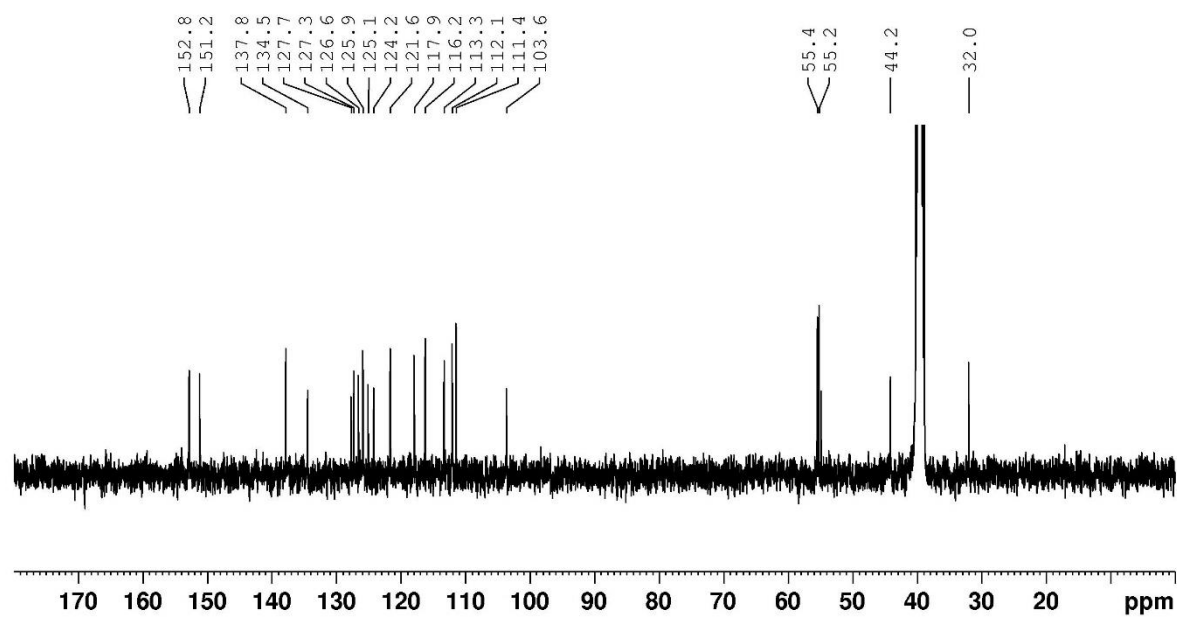
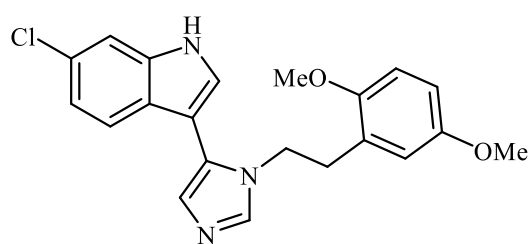
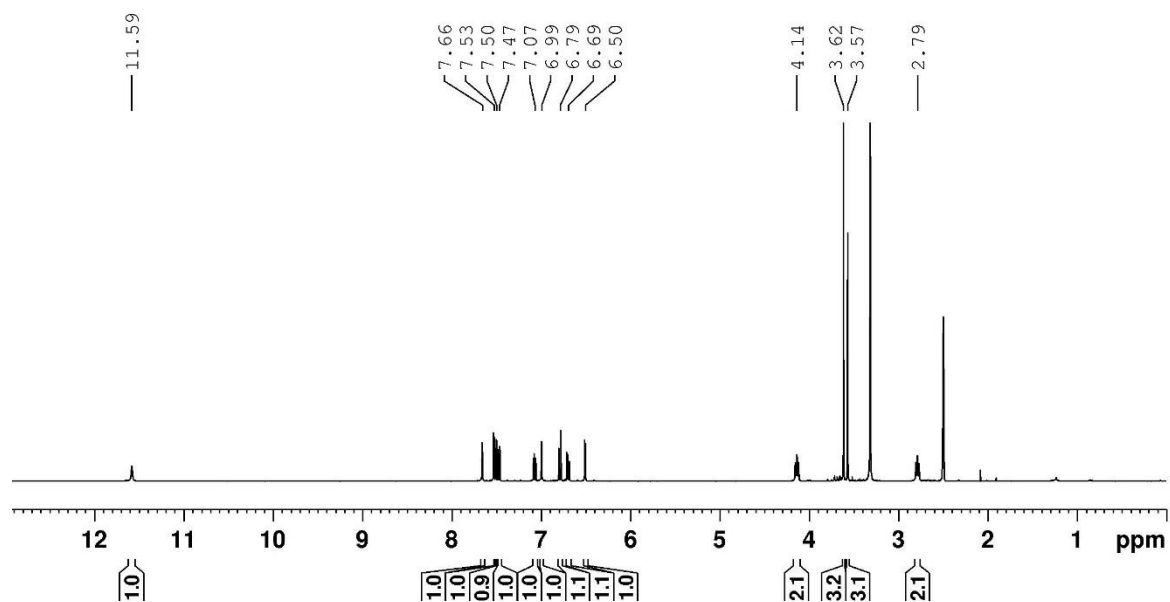


Figure S33. 6-Chloro-3-(1-(2,5-dimethoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (33)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

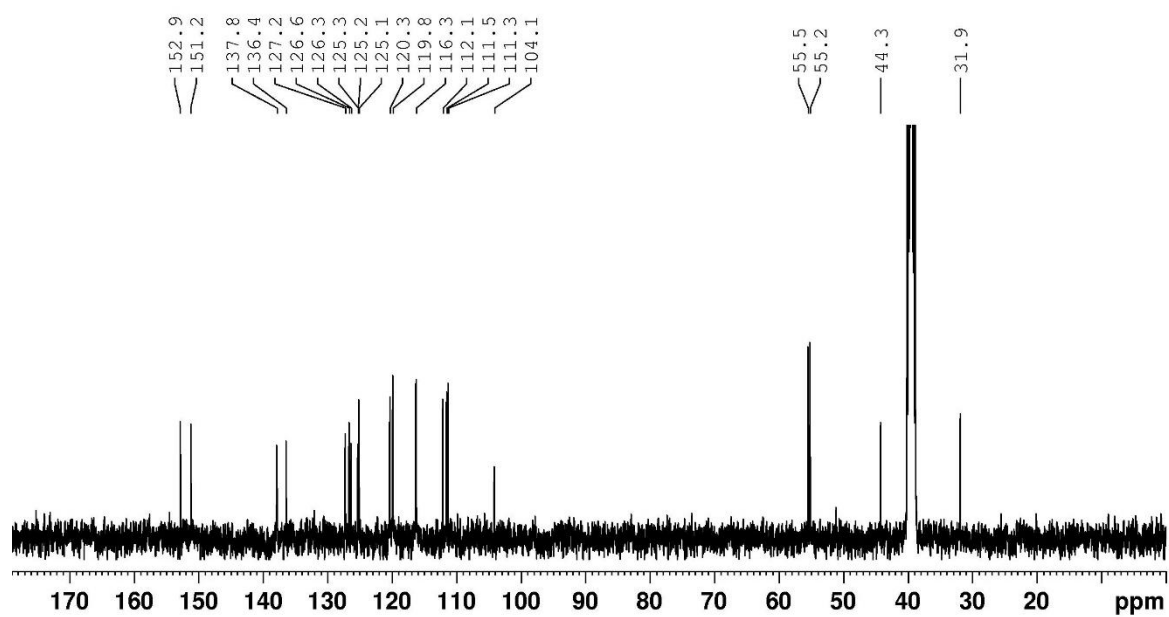
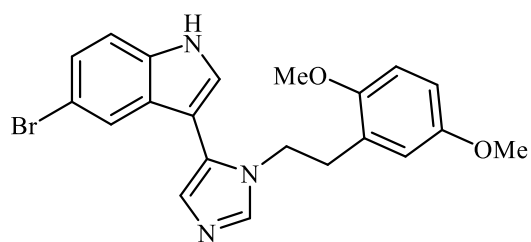
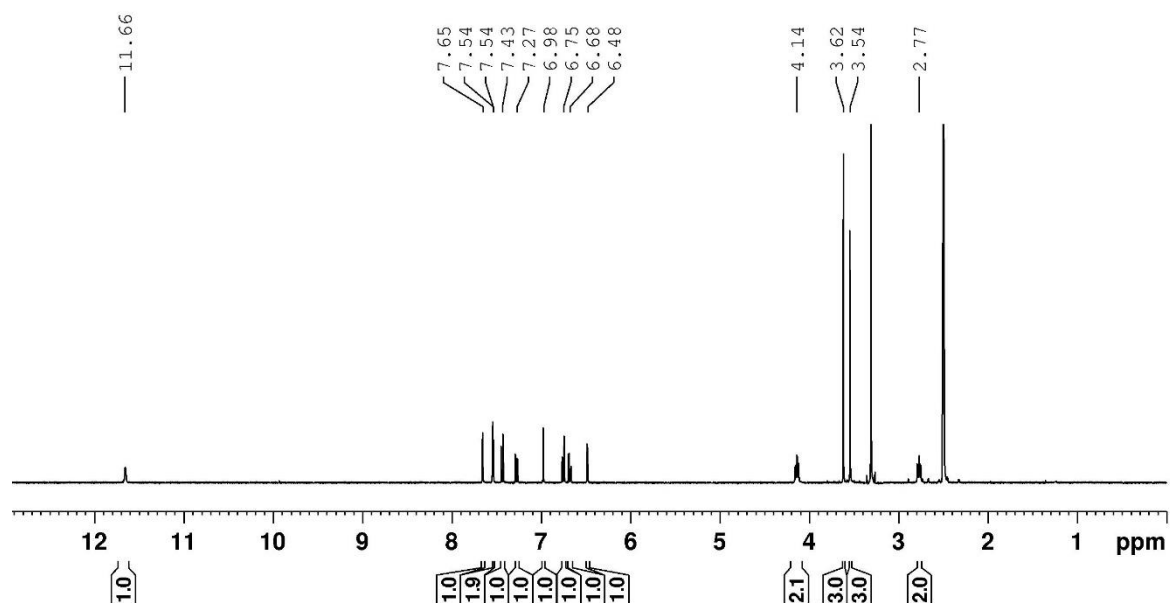


Figure S34. 5-Bromo-3-(1-(2,5-dimethoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (34)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

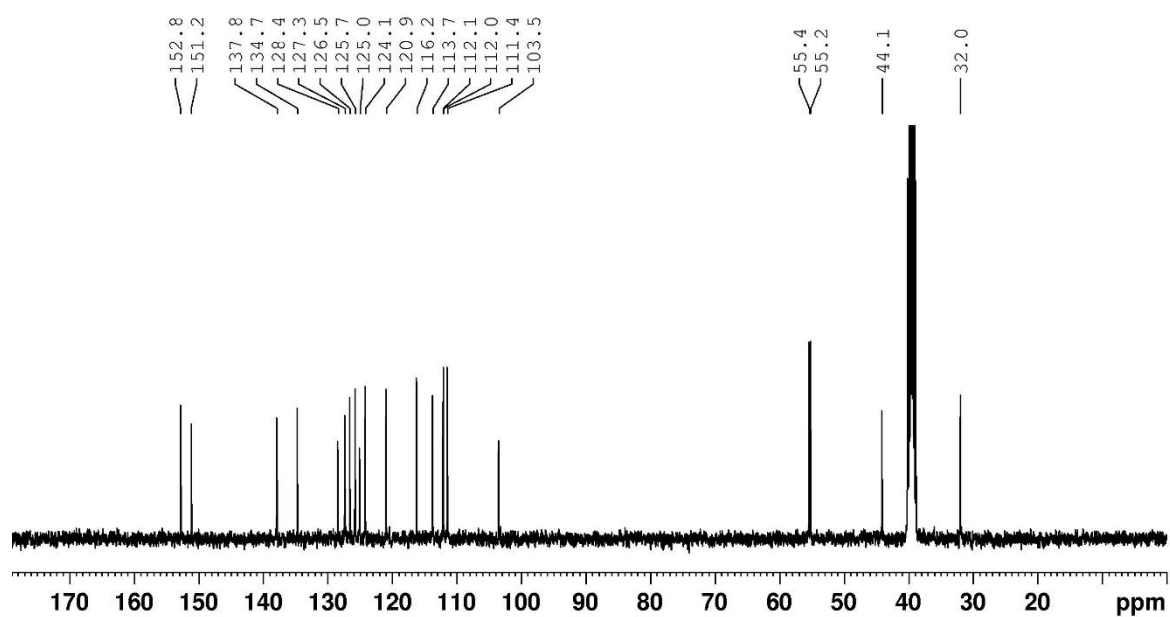
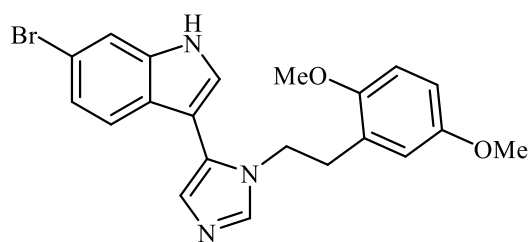
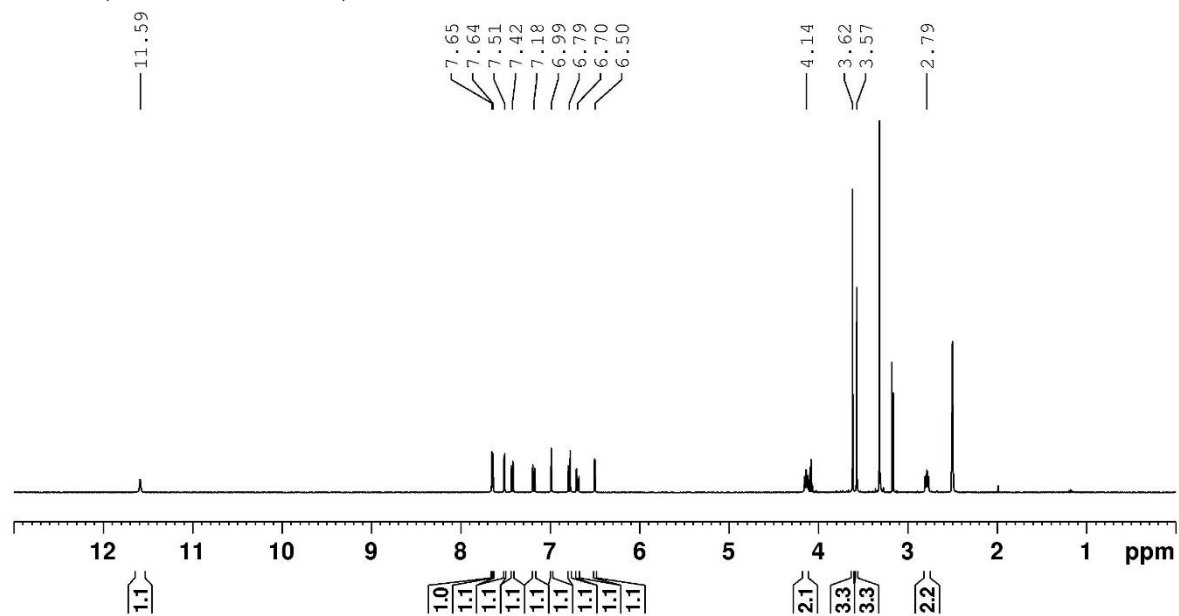


Figure S35. 6-Bromo-3-(1-(2,5-dimethoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (35)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

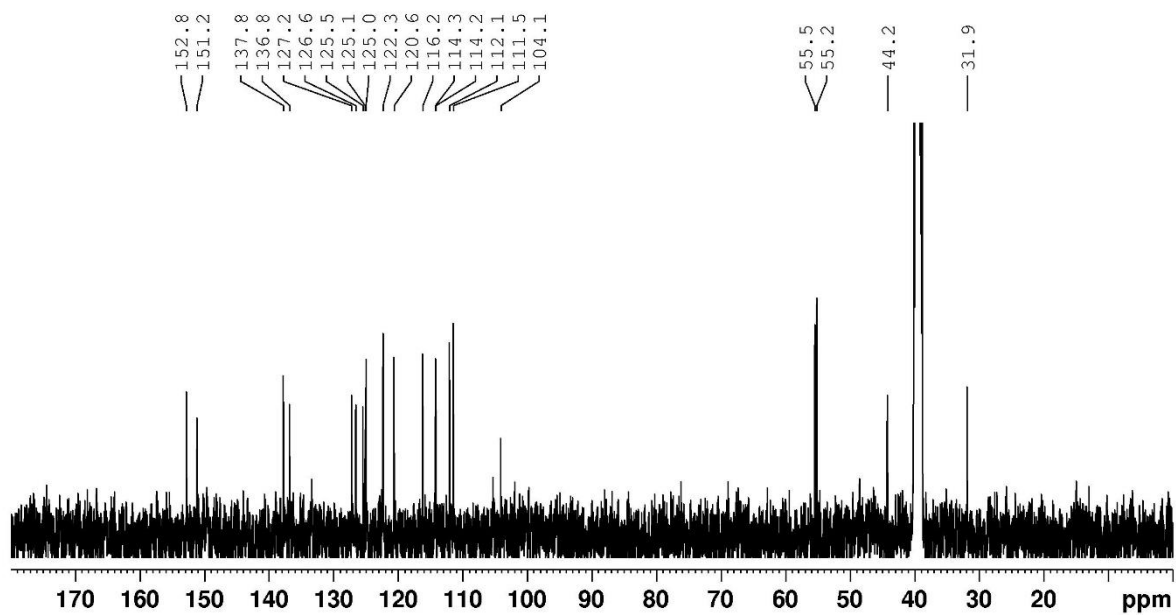
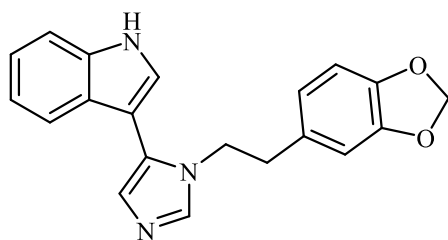
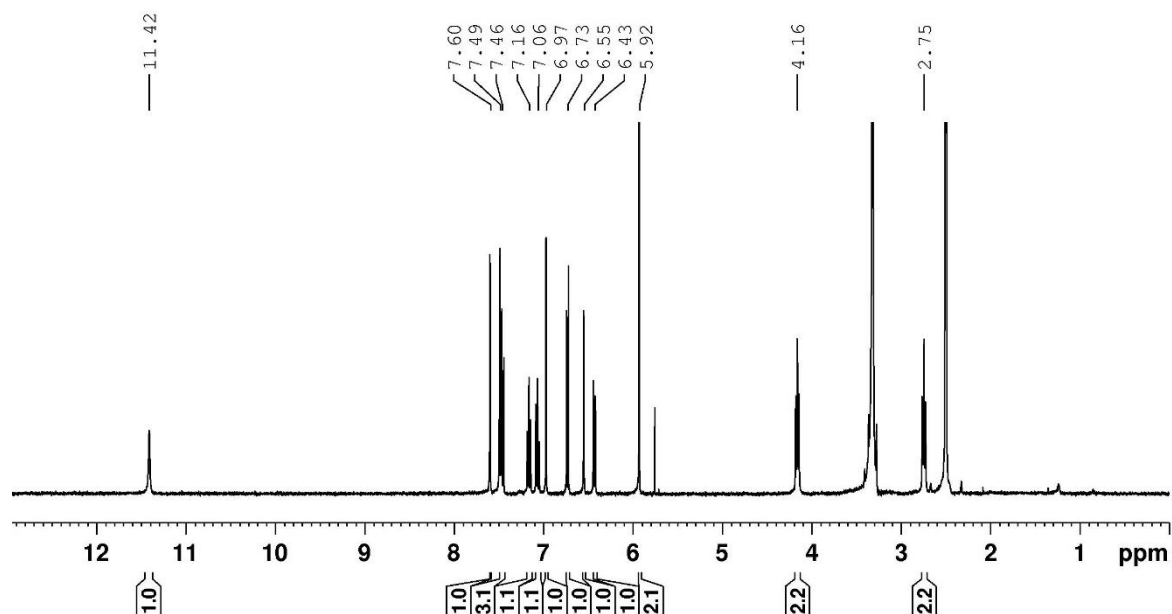


Figure S36. 3-(1-(2-(Benzo[d][1,3]dioxol-5-yl)ethyl)-1H-imidazol-5-yl)-1H-indole (36)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

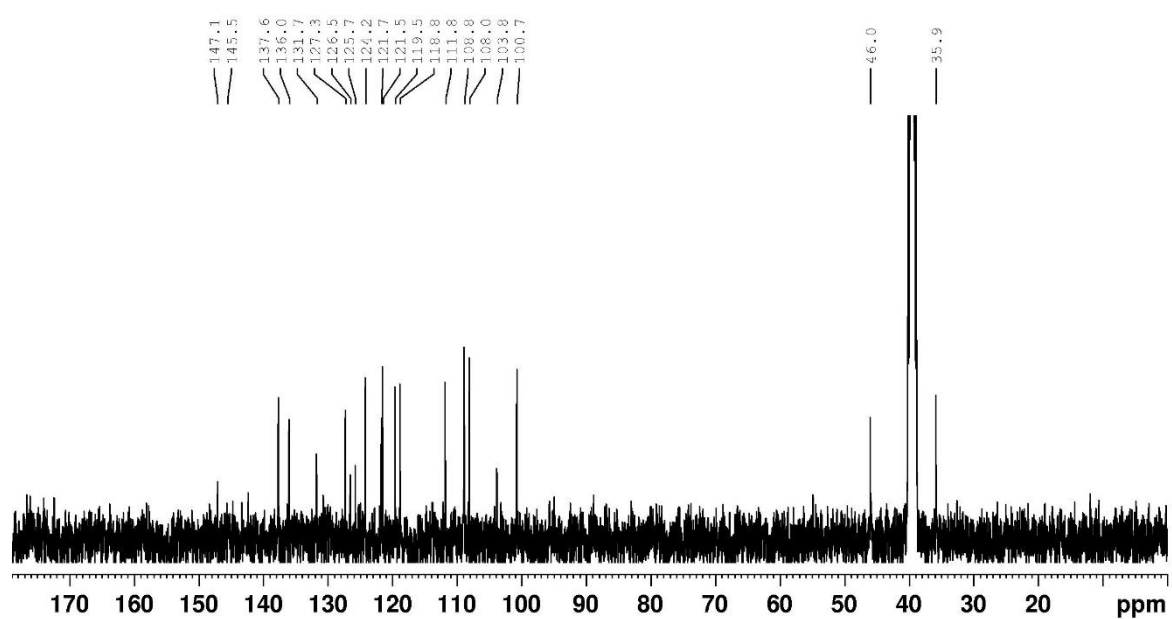
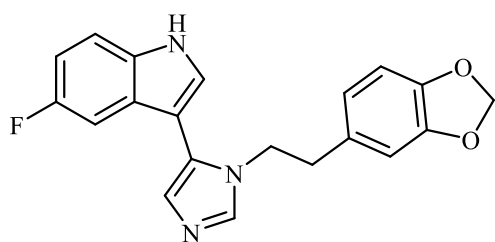
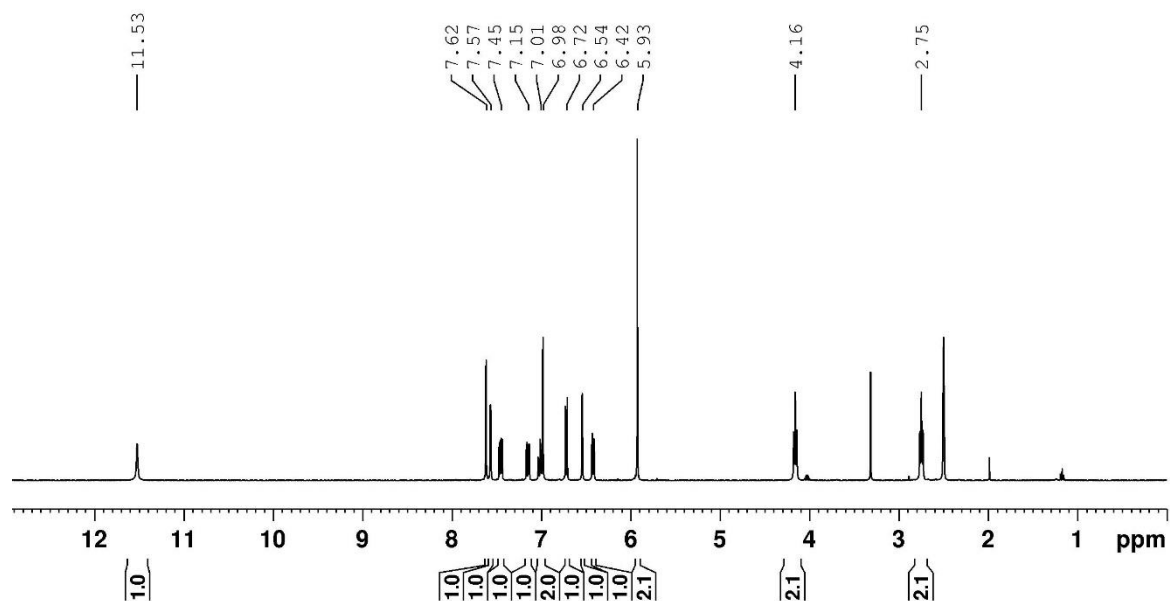


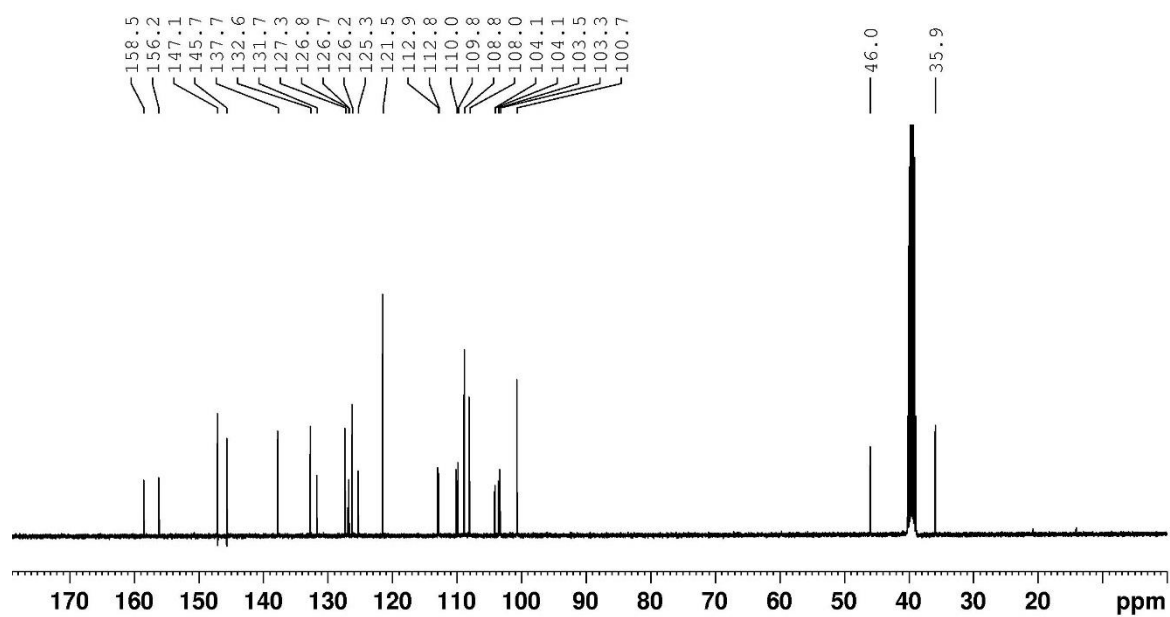
Figure S37. 3-(1-(2-(Benzo[d][1,3]dioxol-5-yl)ethyl)-1H-imidazol-5-yl)-5-fluoro-1H-indole (37)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

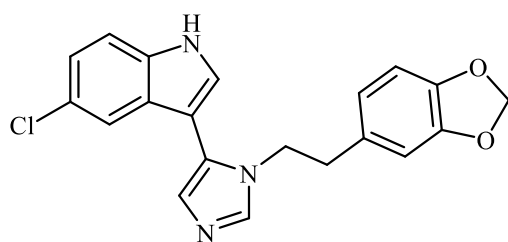


Fc1ccc2c(c1)c(c[nH]2)C3=CN=CN=C3NCCc4ccc5c(c4)OCO5

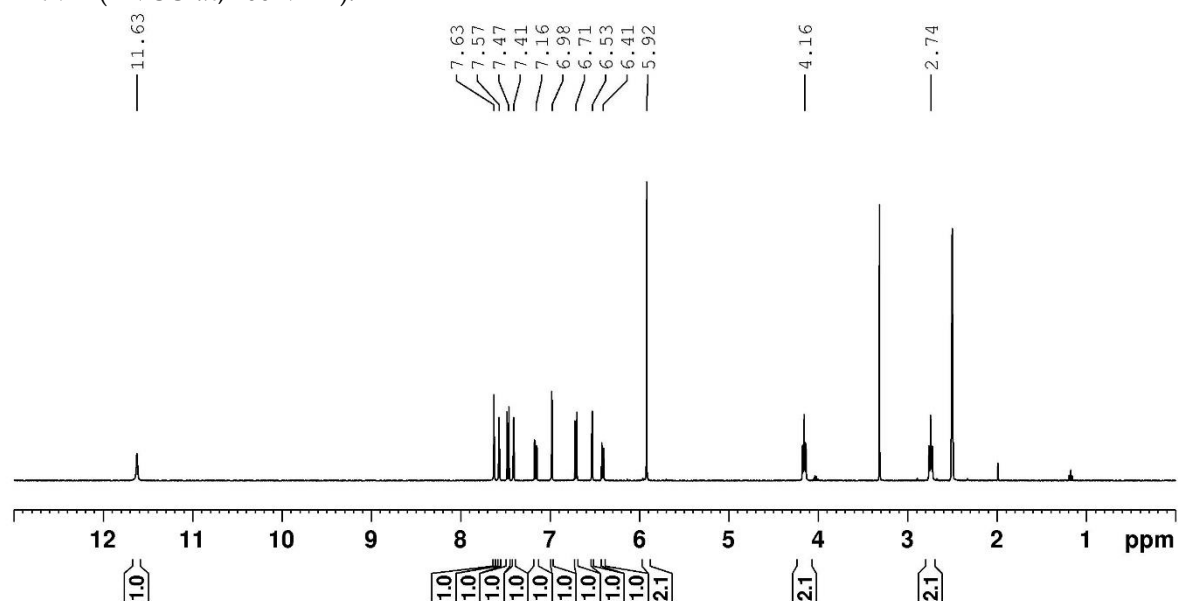
Chemical shifts (ppm) labeled above the spectrum:

- 160.2
- 157.9
- 147.1
- 145.7
- 137.8
- 135.8
- 131.7
- 127.4
- 125.3
- 124.7
- 123.3
- 121.5
- 120.0
- 119.9
- 108.8
- 108.2
- 108.0
- 104.1
- 100.7
- 97.8
- 97.6
- 46.0
- 35.9

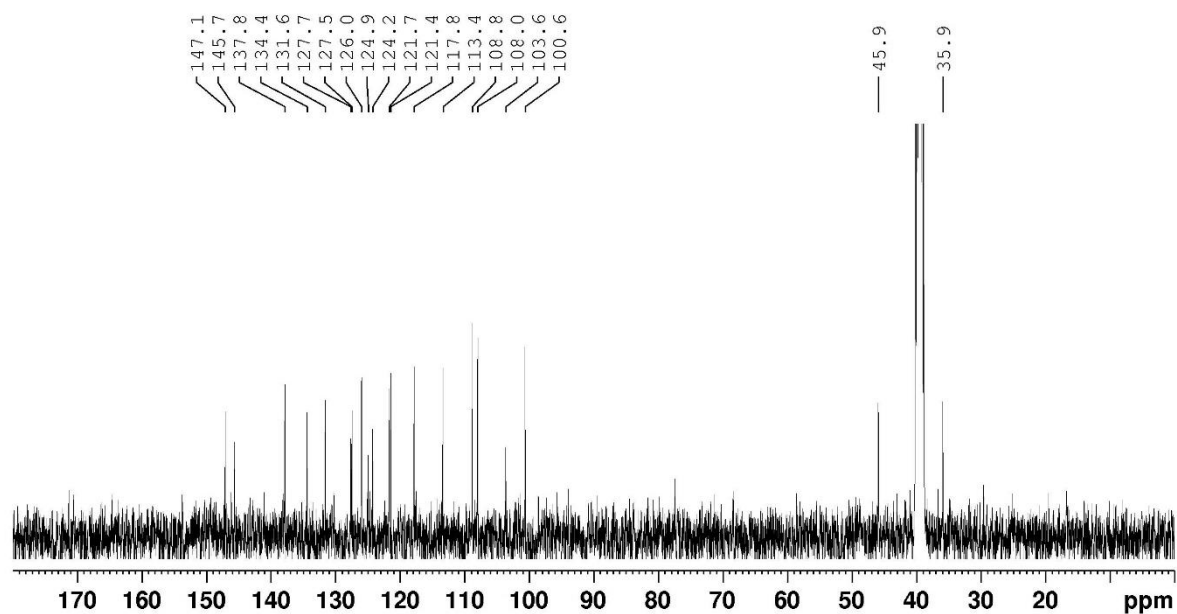
Figure S39. 3-(1-(2-(Benzo[d][1,3]dioxol-5-yl)ethyl)-1H-imidazol-5-yl)-5-chloro-1H-indole (39)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):



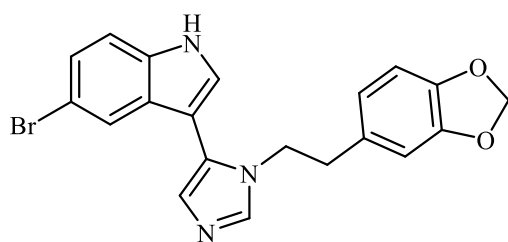
Clc1ccc2c(c1)c(c[nH]2)c3c[nH]cnc3CCc4ccc5c(c4)OCO5[illegible]

147.1
145.7
137.8
136.3
131.6
127.5
126.4
125.3
125.2
125.1
121.5
120.2
119.9
111.3
108.8
108.0
104.1
100.7

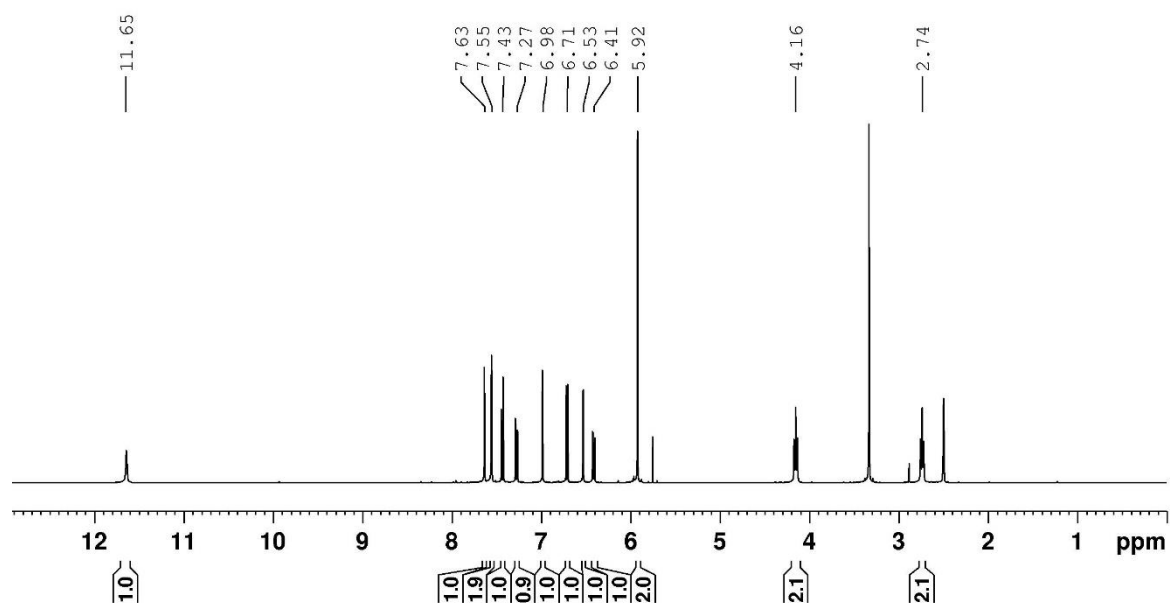
— 46.0
— 35.9

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Figure S41. 3-(1-(2-(Benzo[d][1,3]dioxol-5-yl)ethyl)-1H-imidazol-5-yl)-5-bromo-1H-indole (41)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

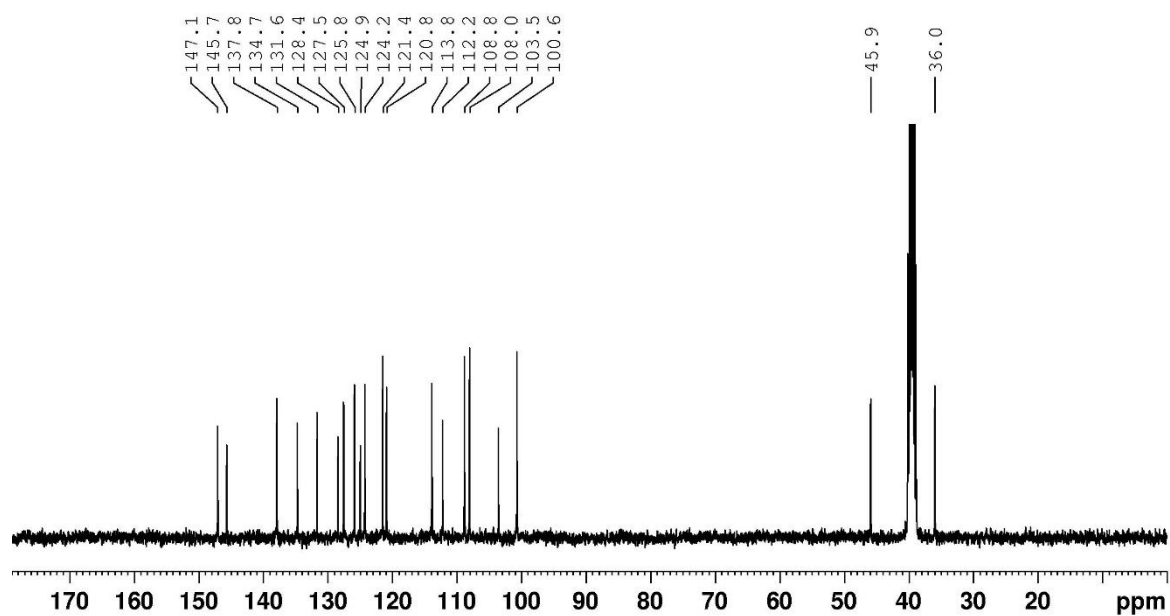
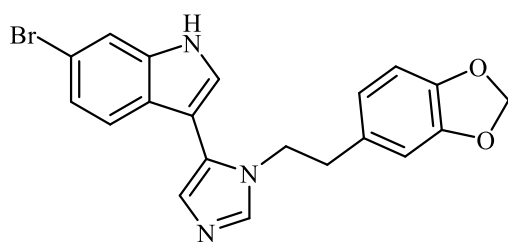
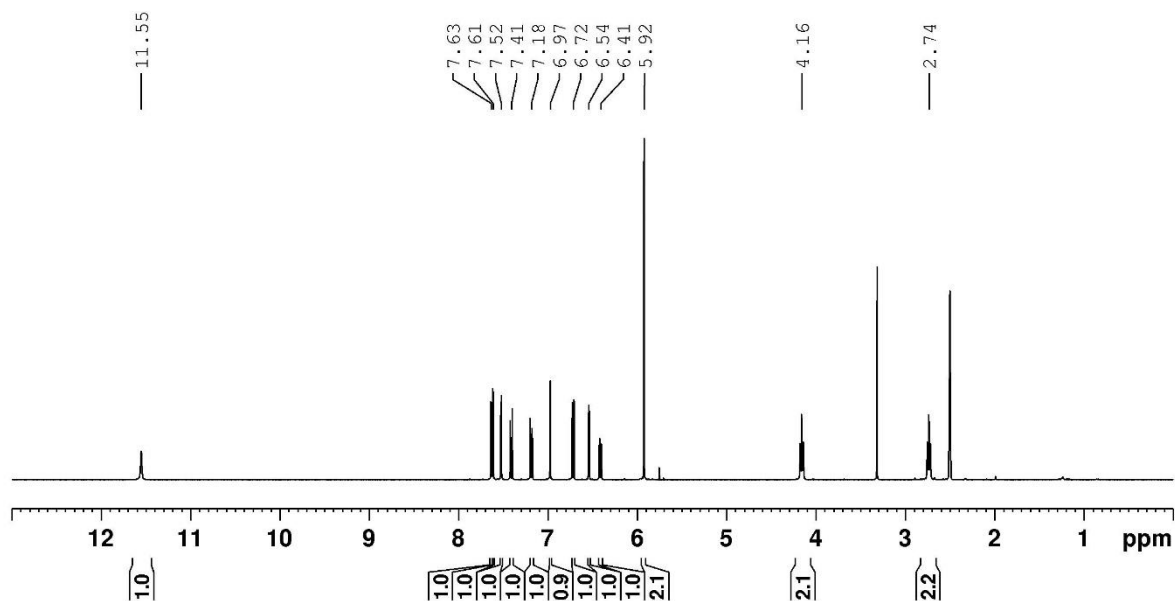


Figure S42. 3-(1-(2-(Benzo[d][1,3]dioxol-5-yl)ethyl)-1H-imidazol-5-yl)-6-bromo-1H-indole (**42**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

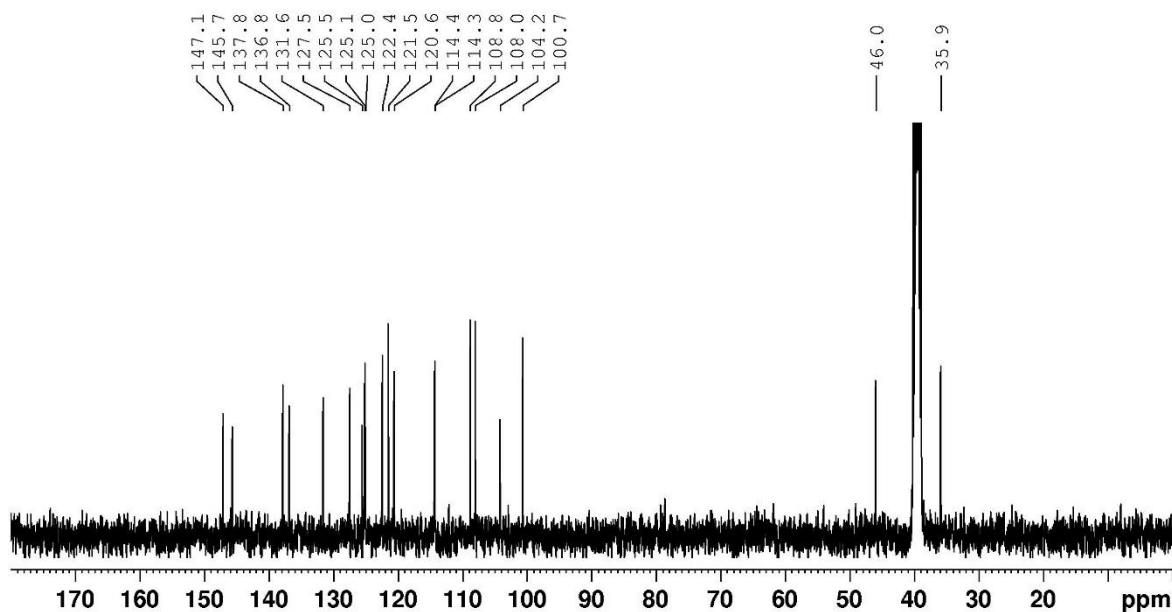
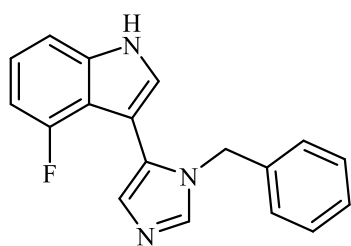
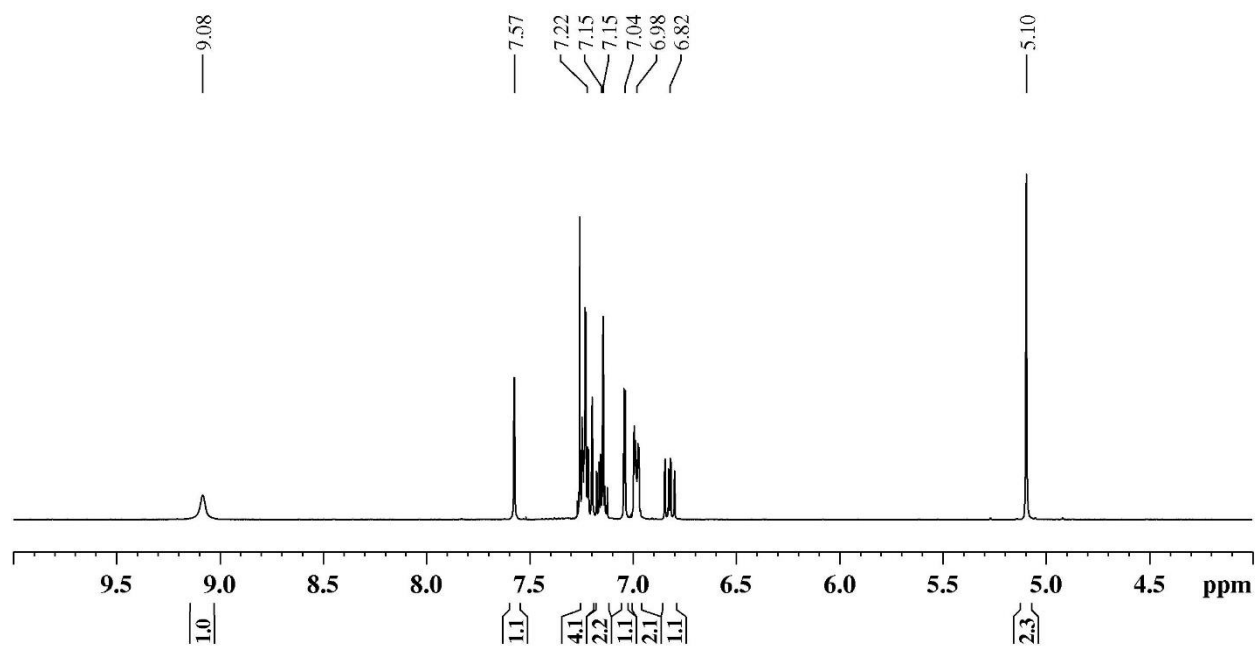


Figure S43. 3-(1-Benzyl-1H-imidazol-5-yl)-4-fluoro-1H-indole (43)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

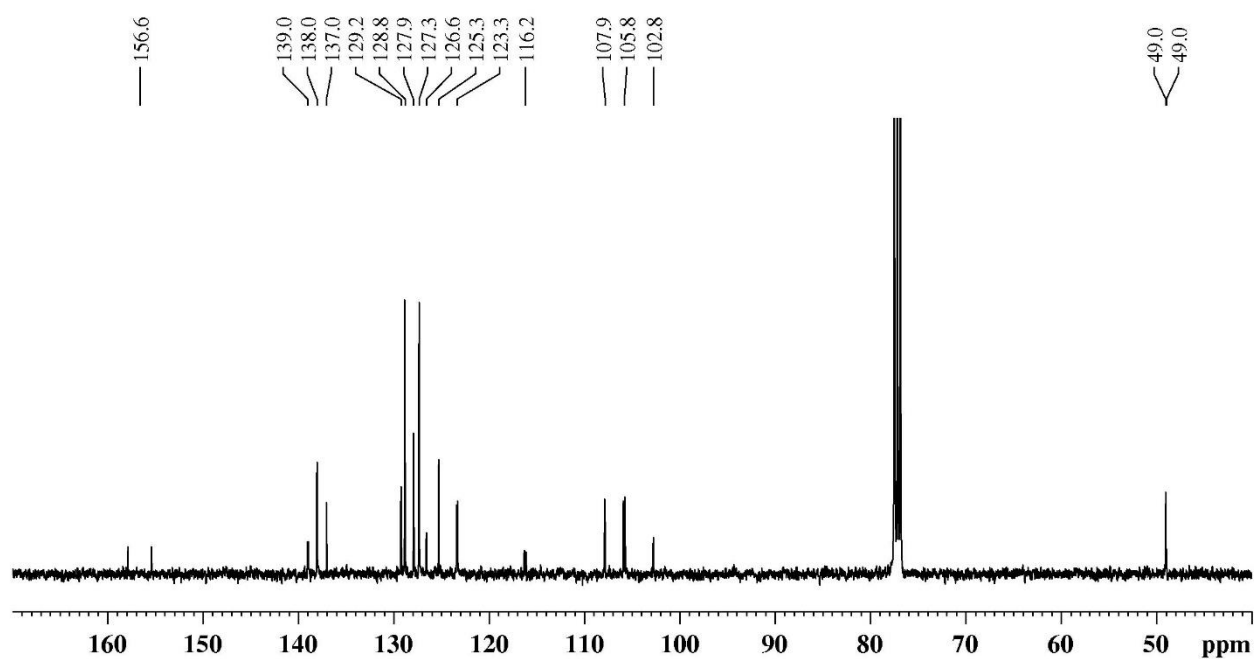
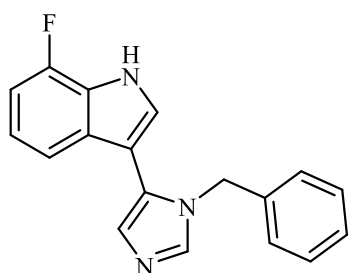
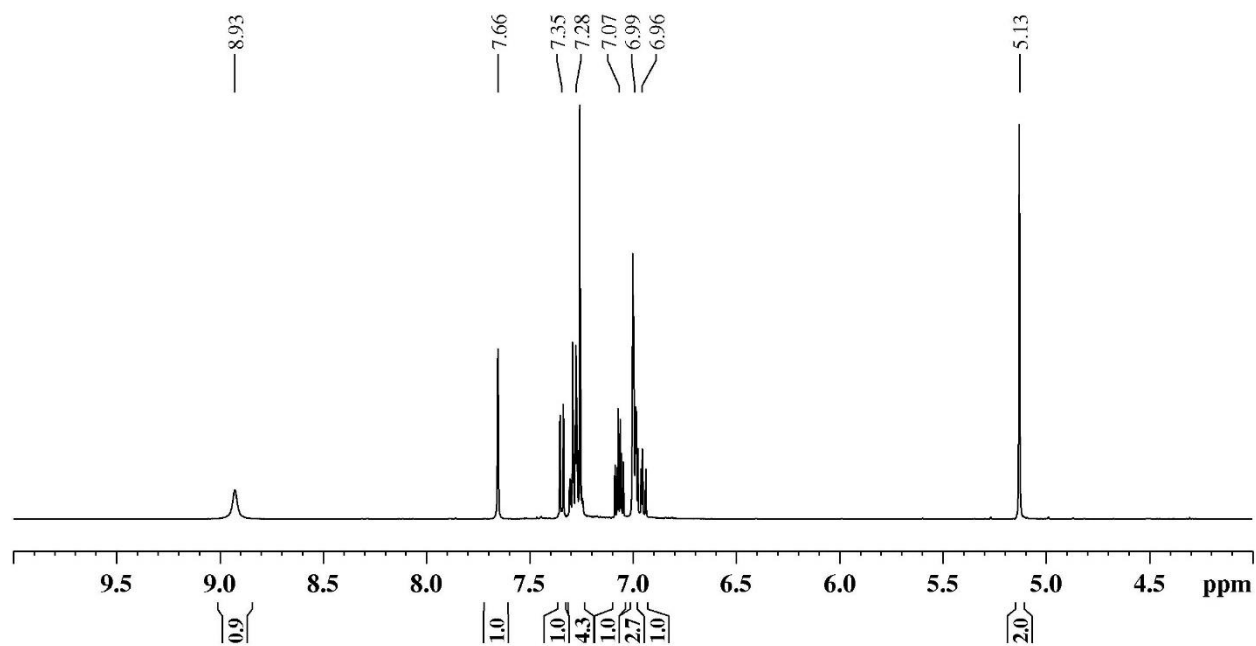


Figure S44. 3-(1-Benzyl-1H-imidazol-5-yl)-7-fluoro-1H-indole (**44**)



^1H NMR (CDCl_3 , 500 MHz):



^{13}C NMR (CDCl_3 , 125 MHz):

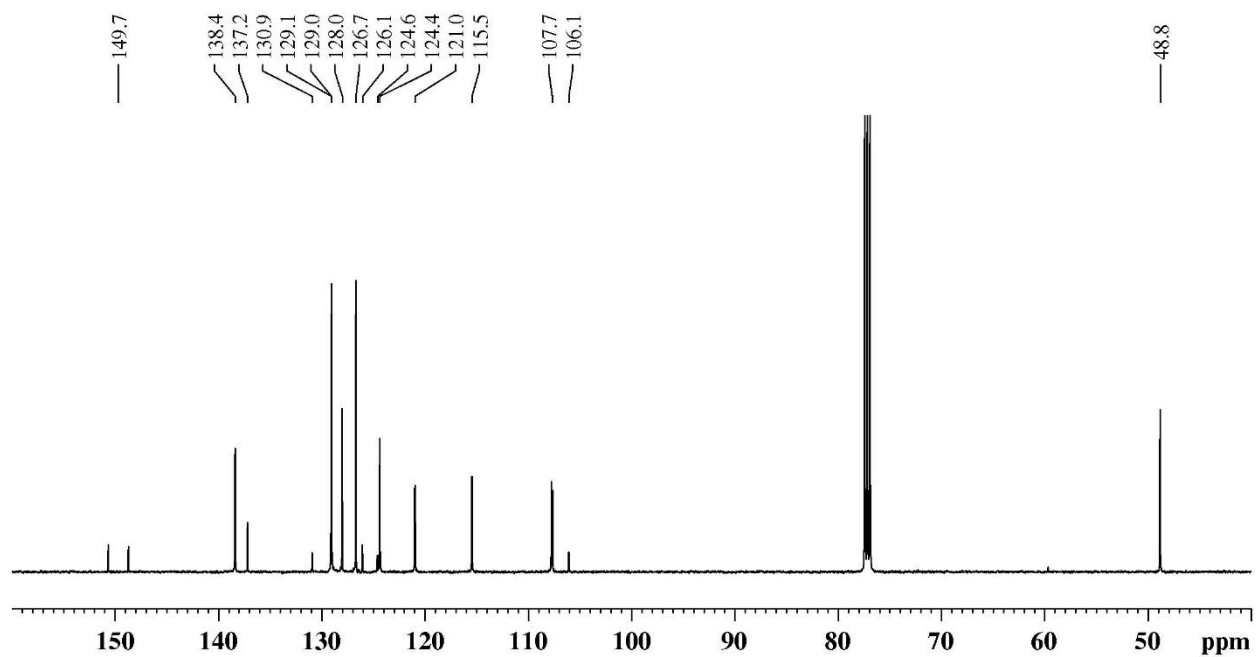
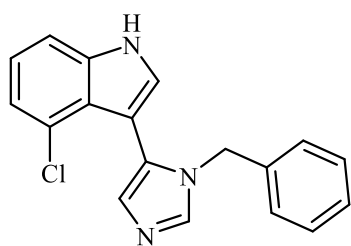
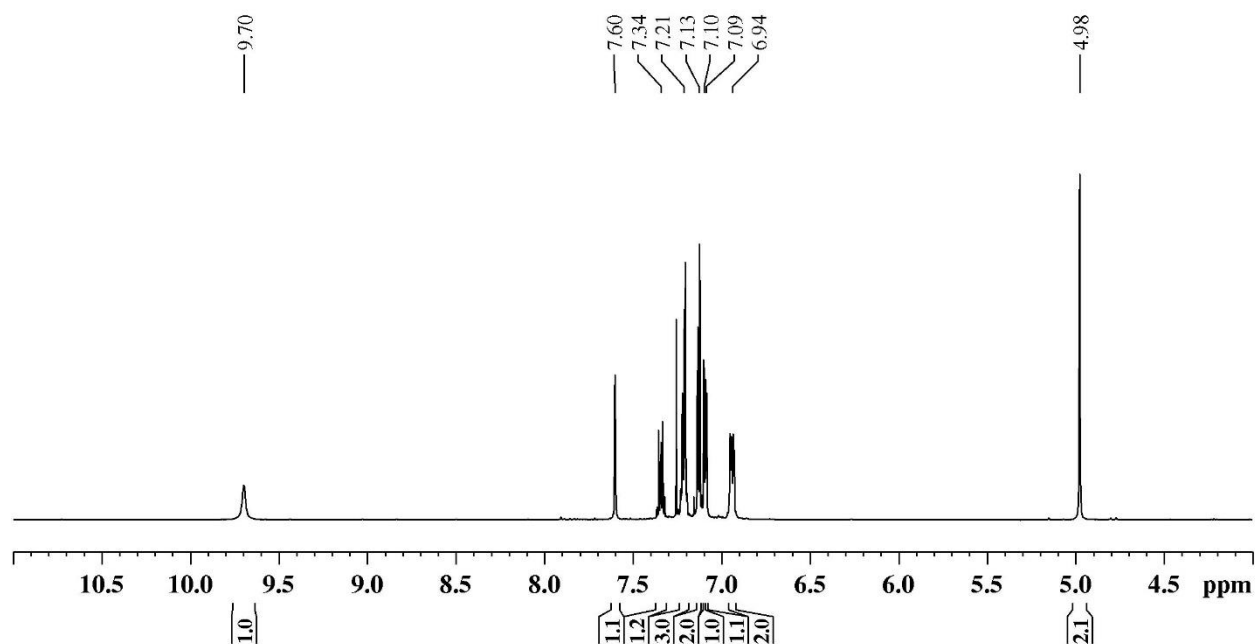


Figure S45. 3-(1-Benzyl-1H-imidazol-5-yl)-4-chloro-1H-indole (45)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

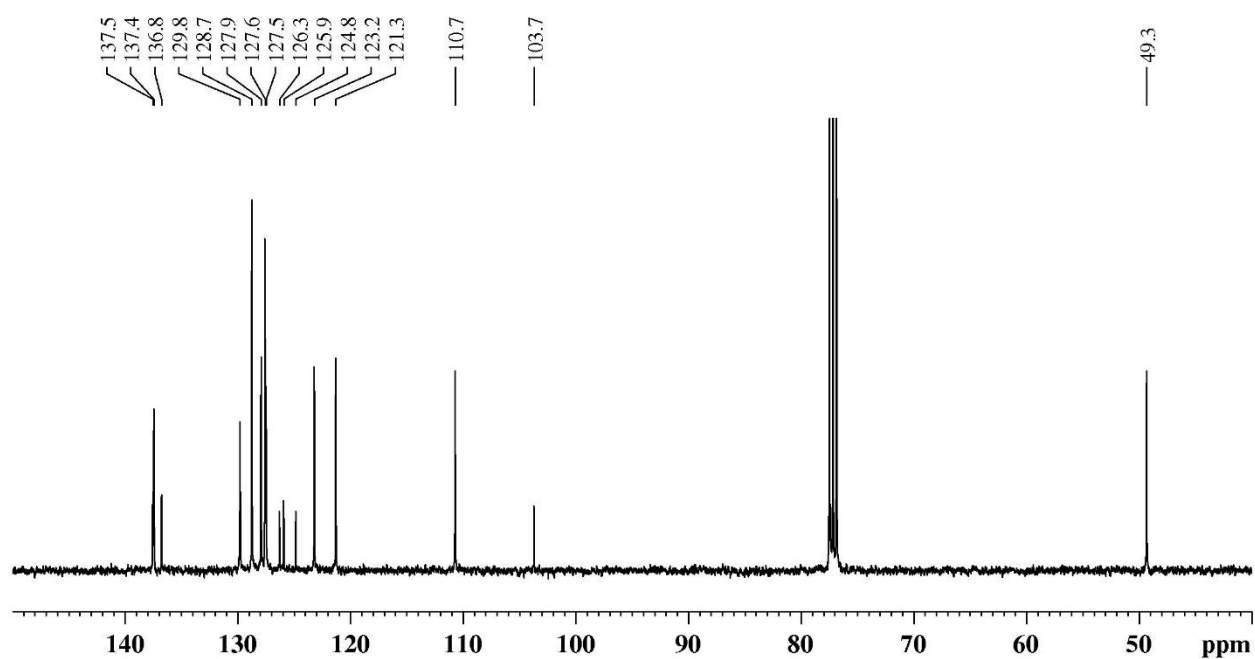
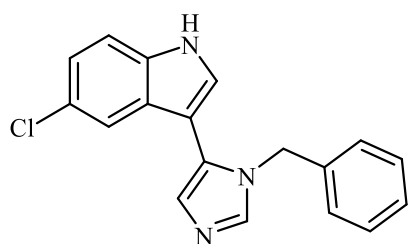
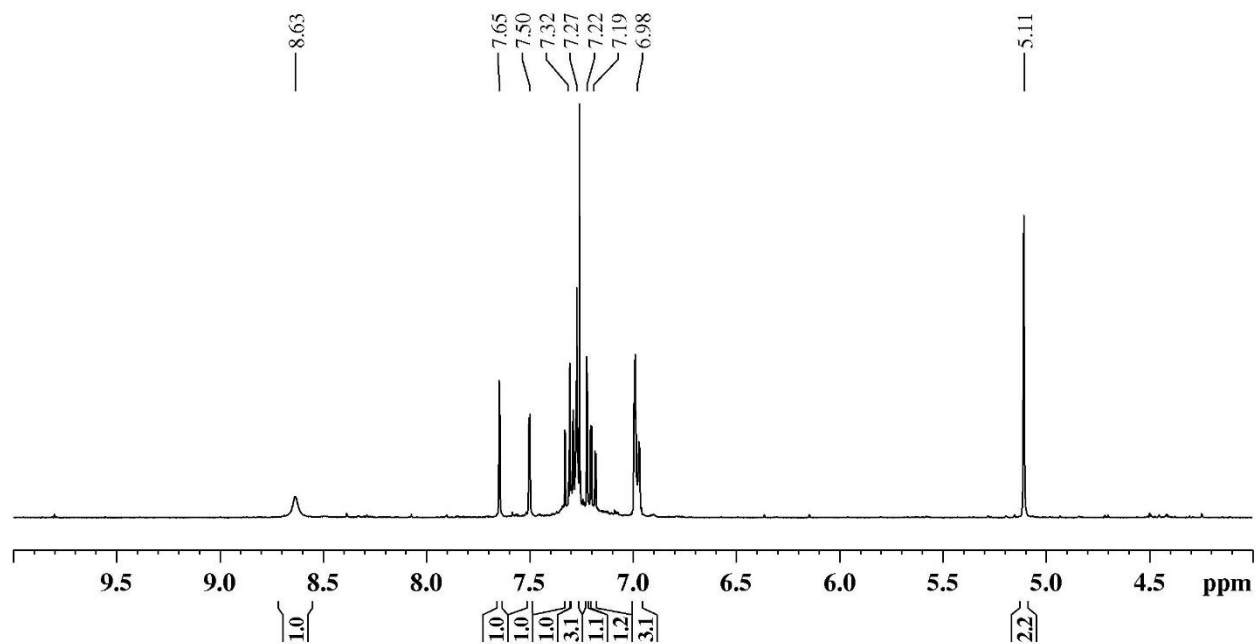


Figure S46. 3-(1-Benzyl-1H-imidazol-5-yl)-5-chloro-1H-indole (46)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

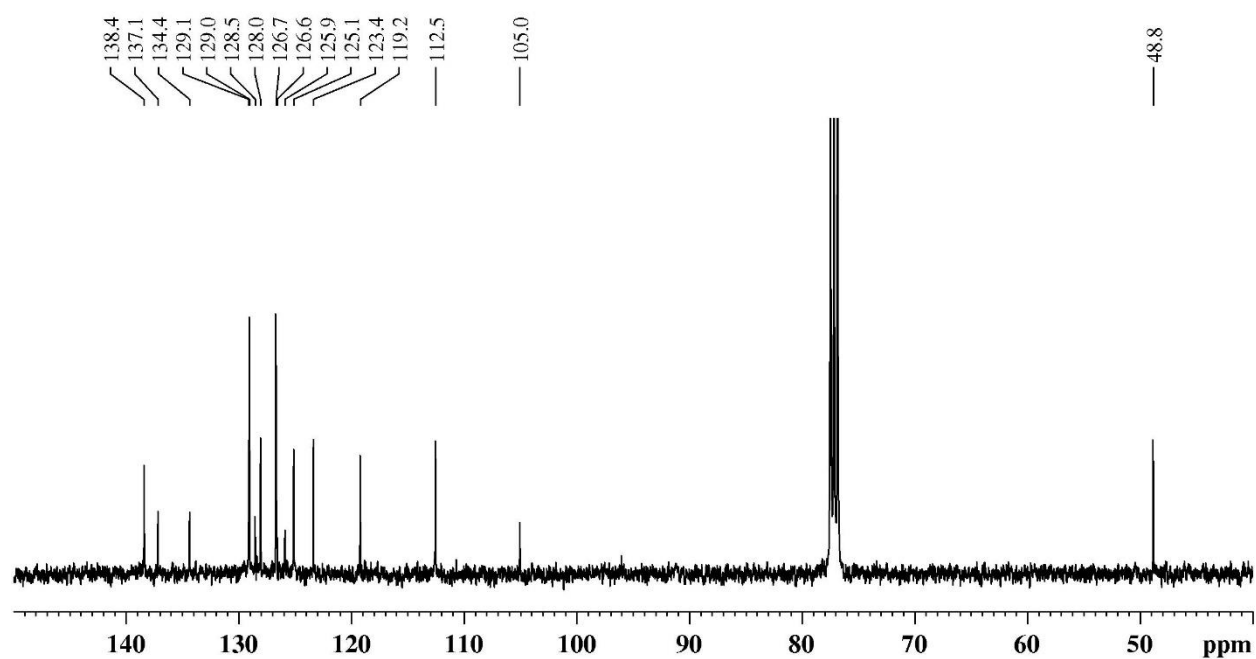
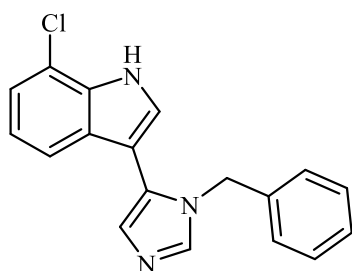
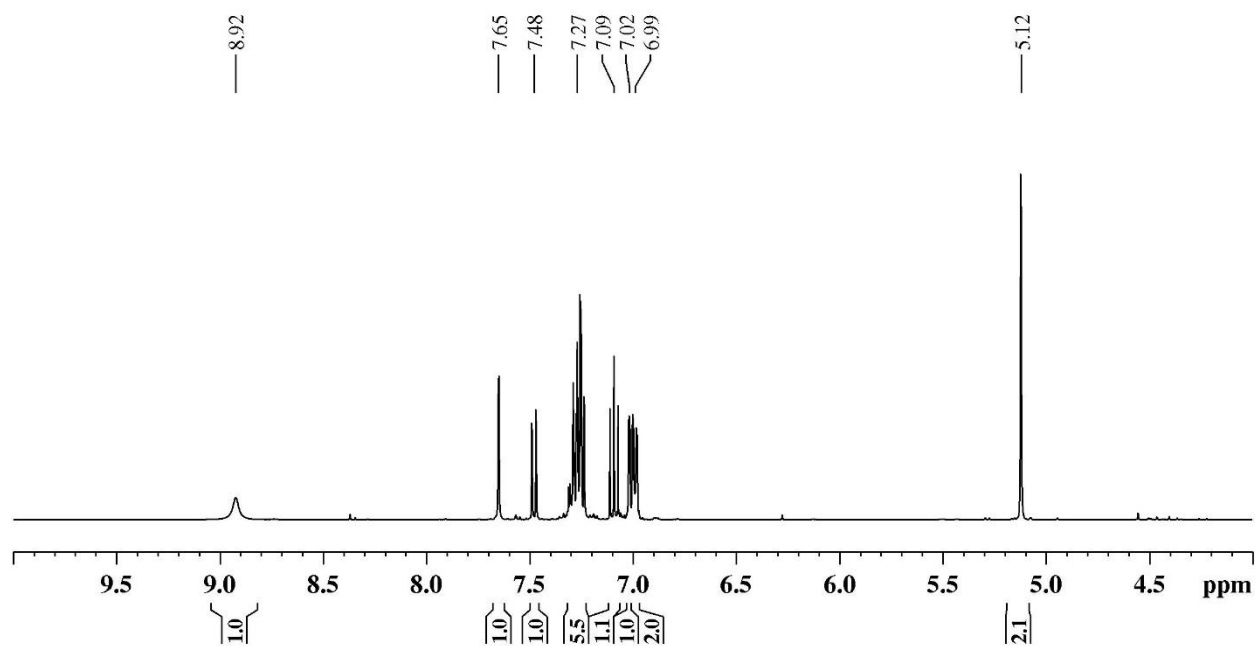


Figure S47. 3-(1-Benzyl-1H-imidazol-5-yl)-7-chloro-1H-indole (47)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

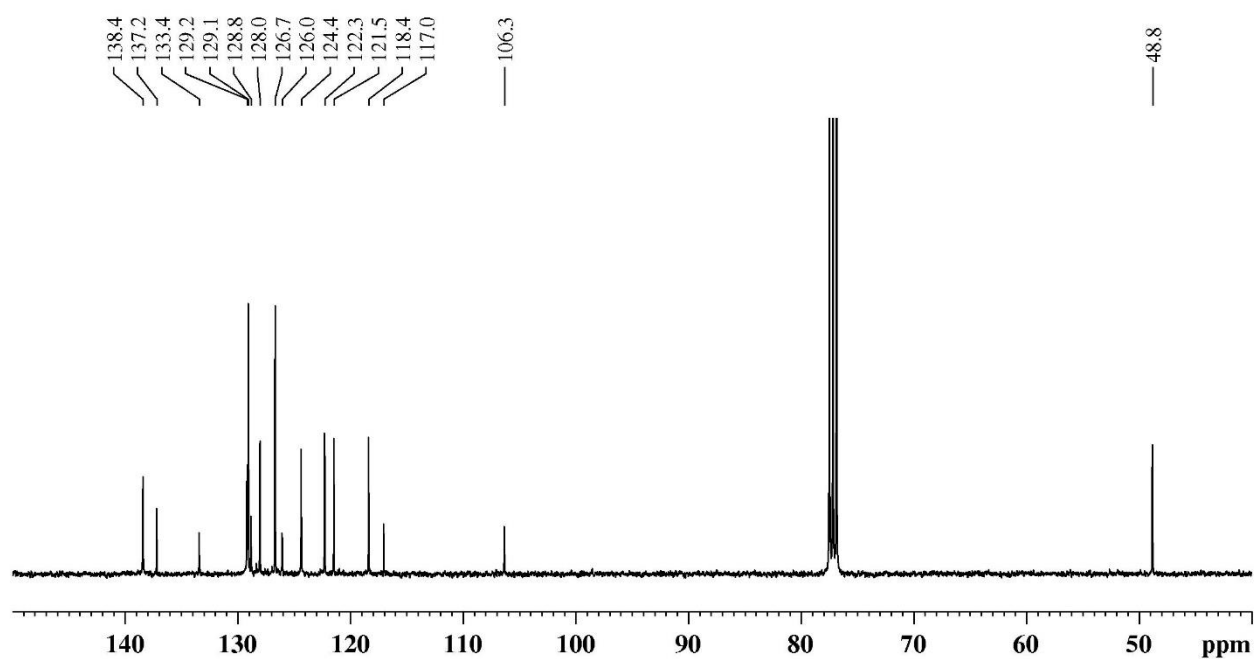
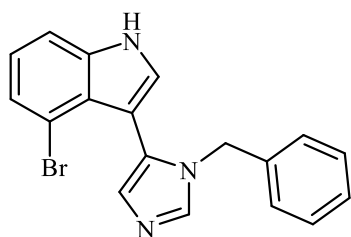
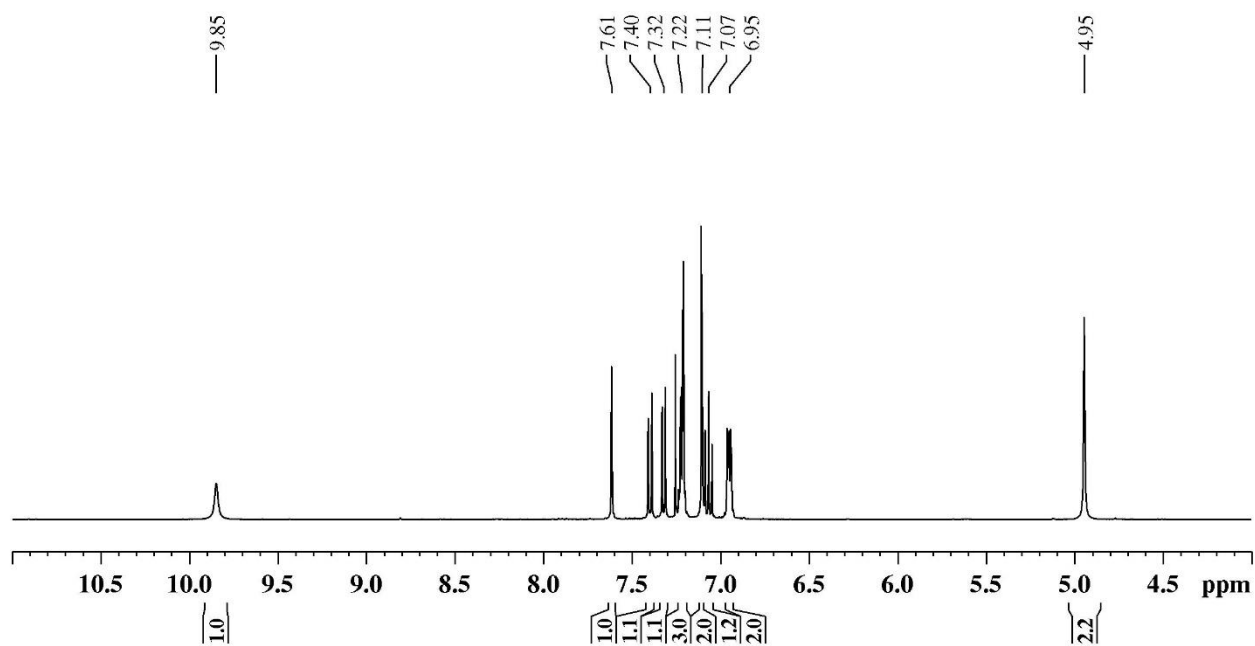


Figure S48. 3-(1-Benzyl-1H-imidazol-5-yl)-4-bromo-1H-indole (48)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

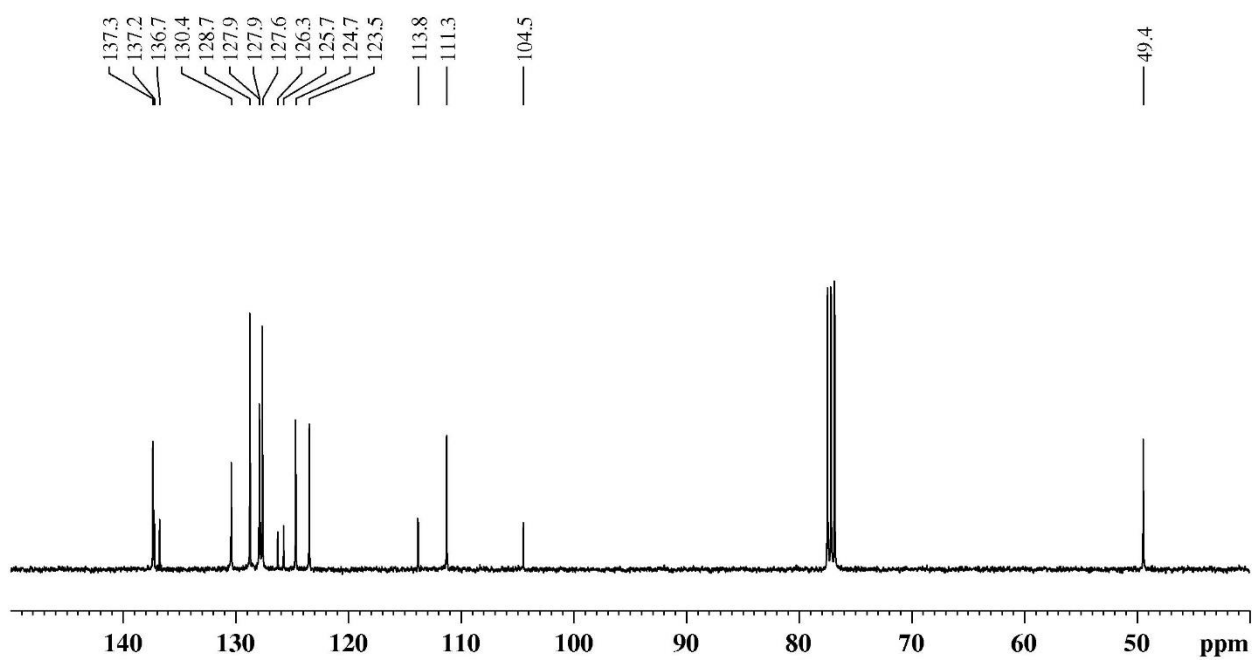
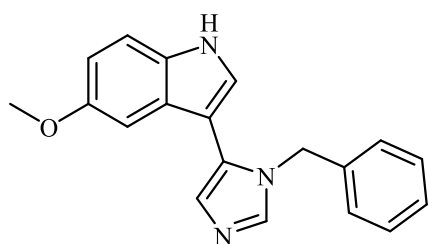
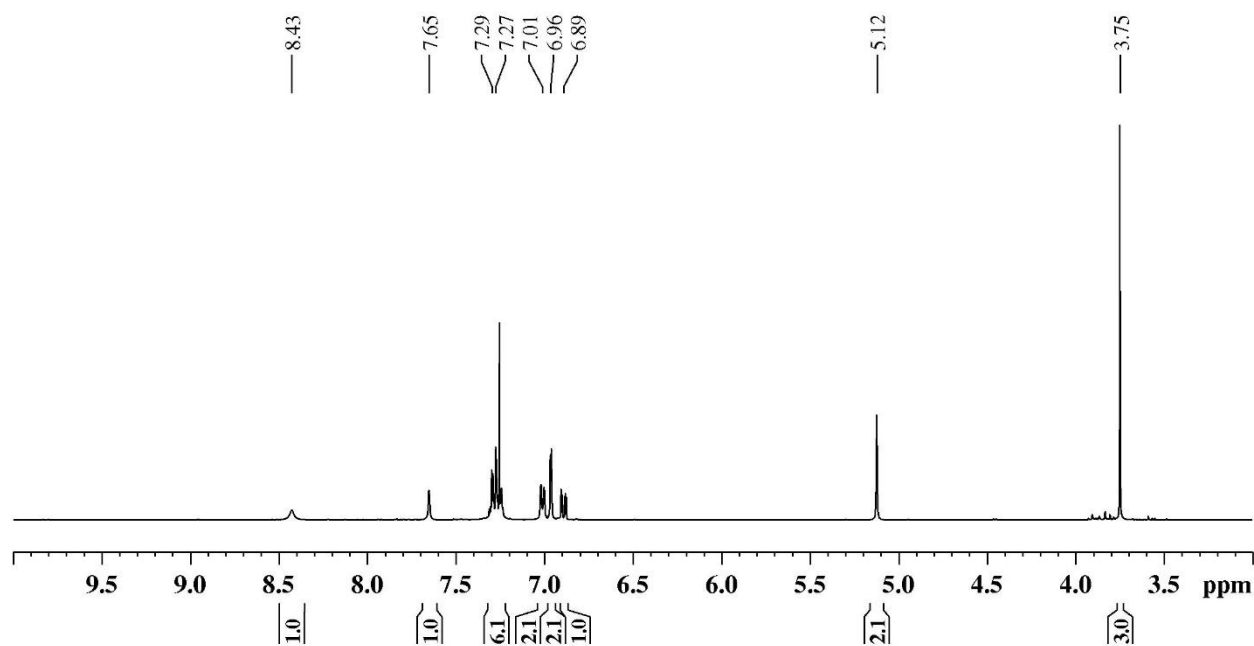


Figure S49. 3-(1-Benzyl-1H-imidazol-5-yl)-5-methoxy-1H-indole (**49**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

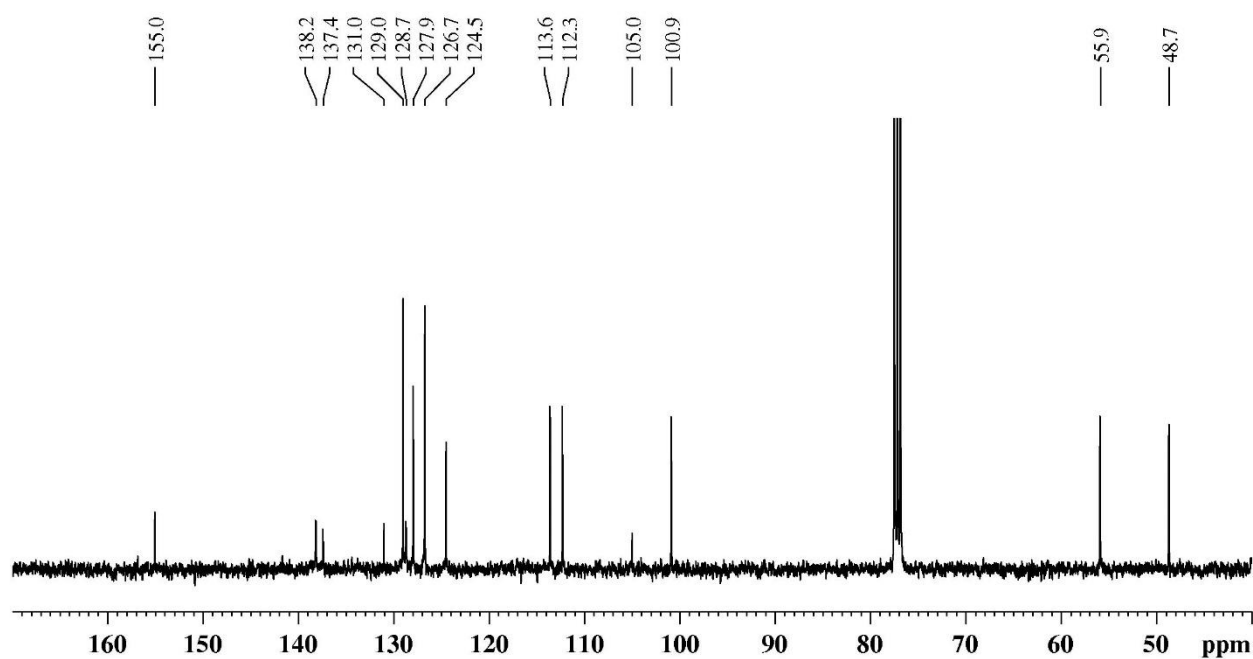
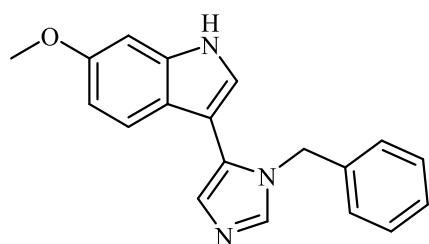
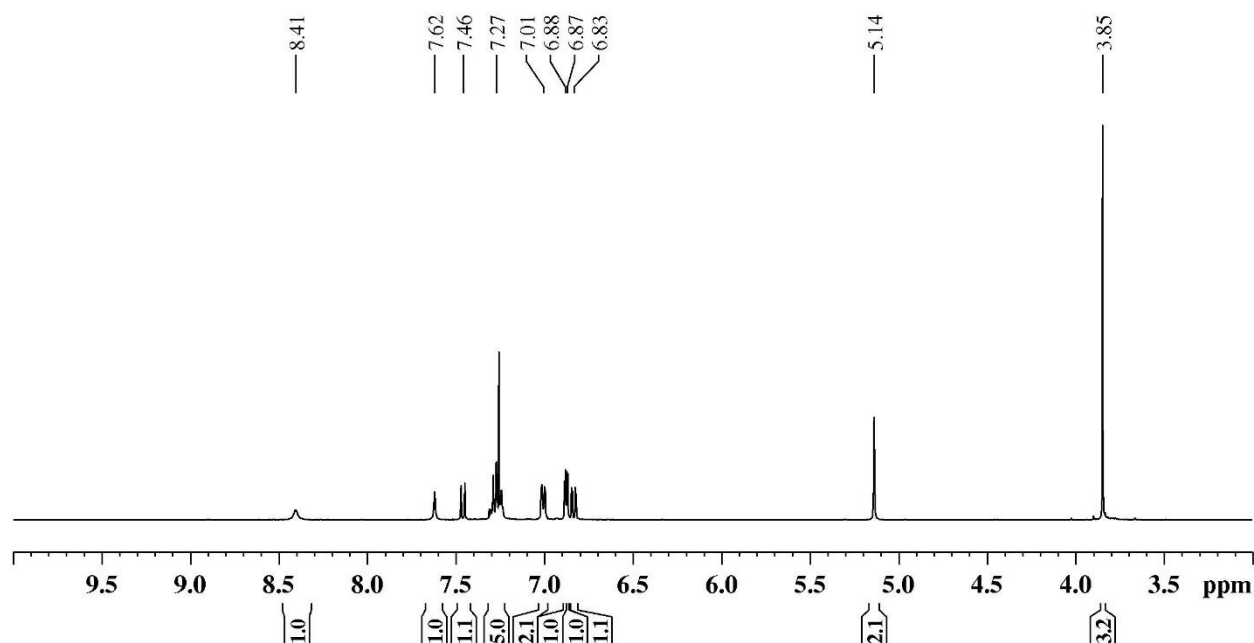


Figure S50. 3-(1-Benzyl-1H-imidazol-5-yl)-6-methoxy-1H-indole (50)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

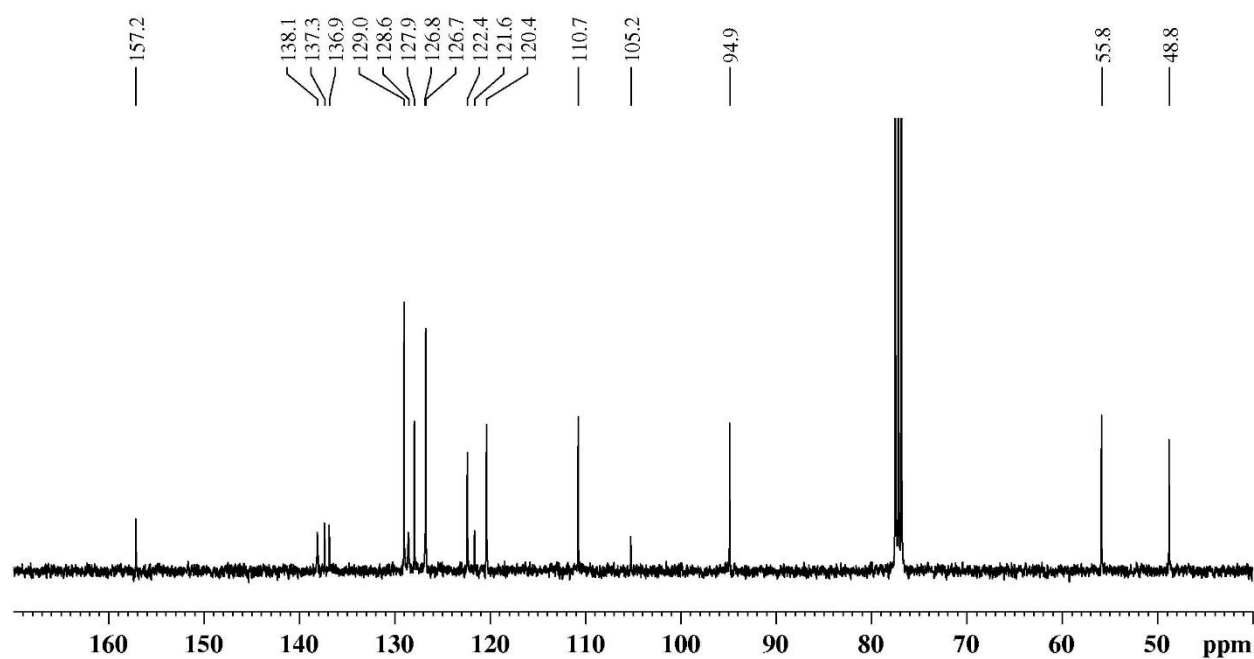
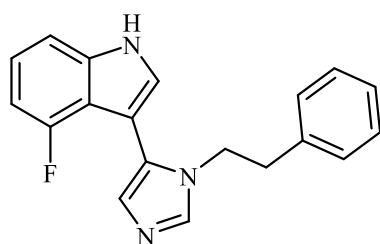
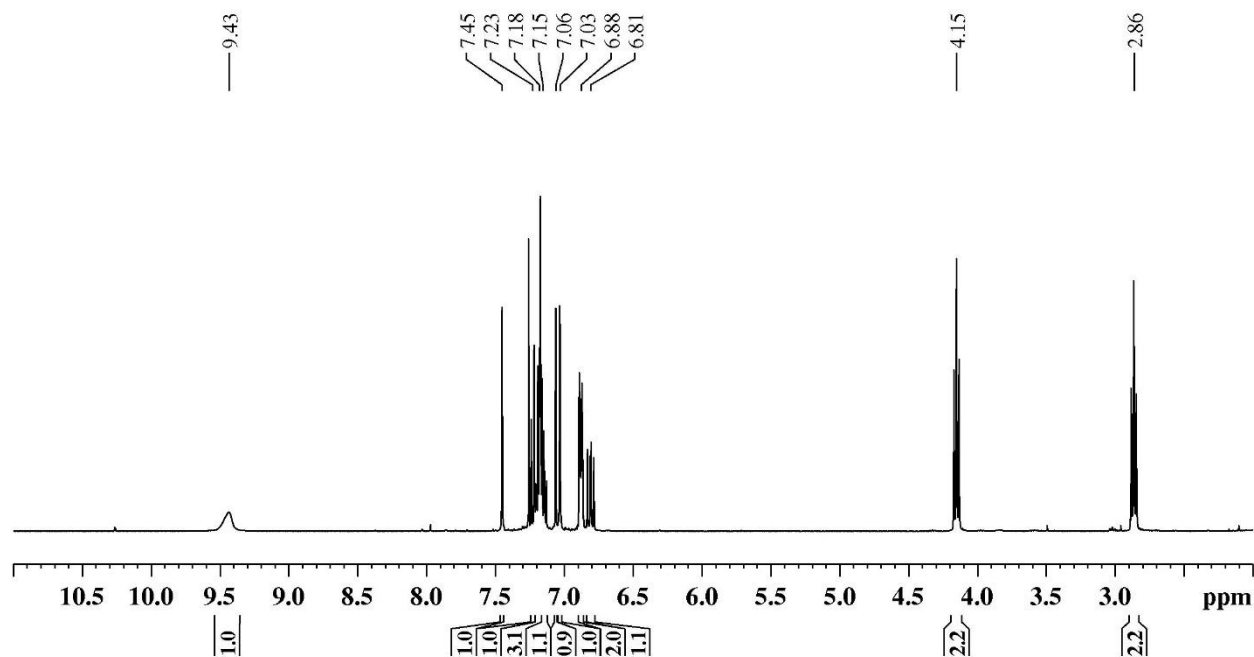


Figure S51. 4-Fluoro-3-(1-phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (**51**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

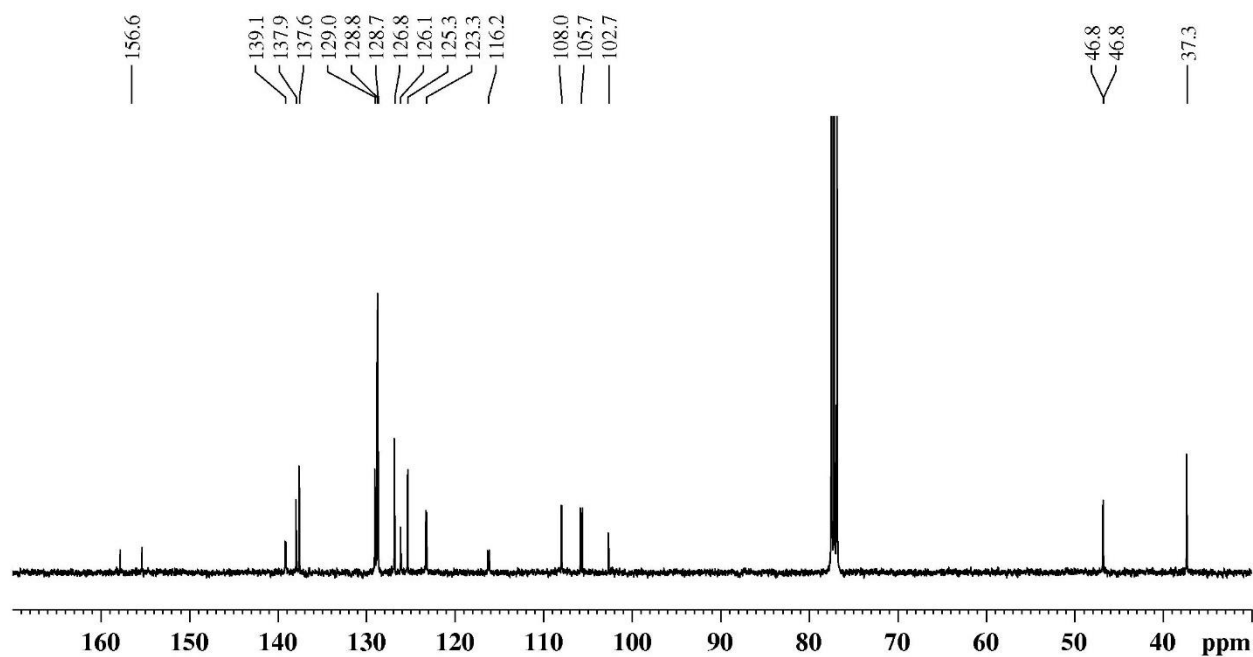
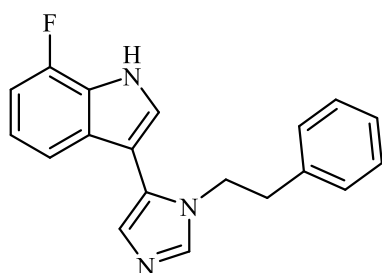
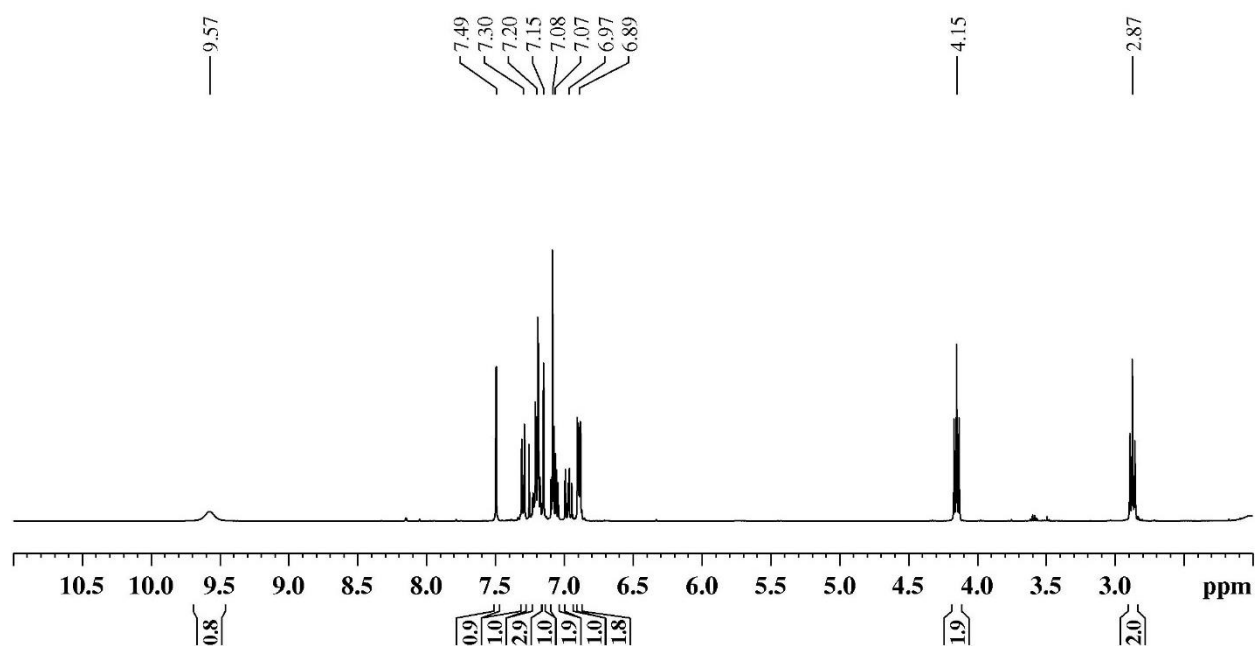


Figure S52. 7-Fluoro-3-(1-phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (**52**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

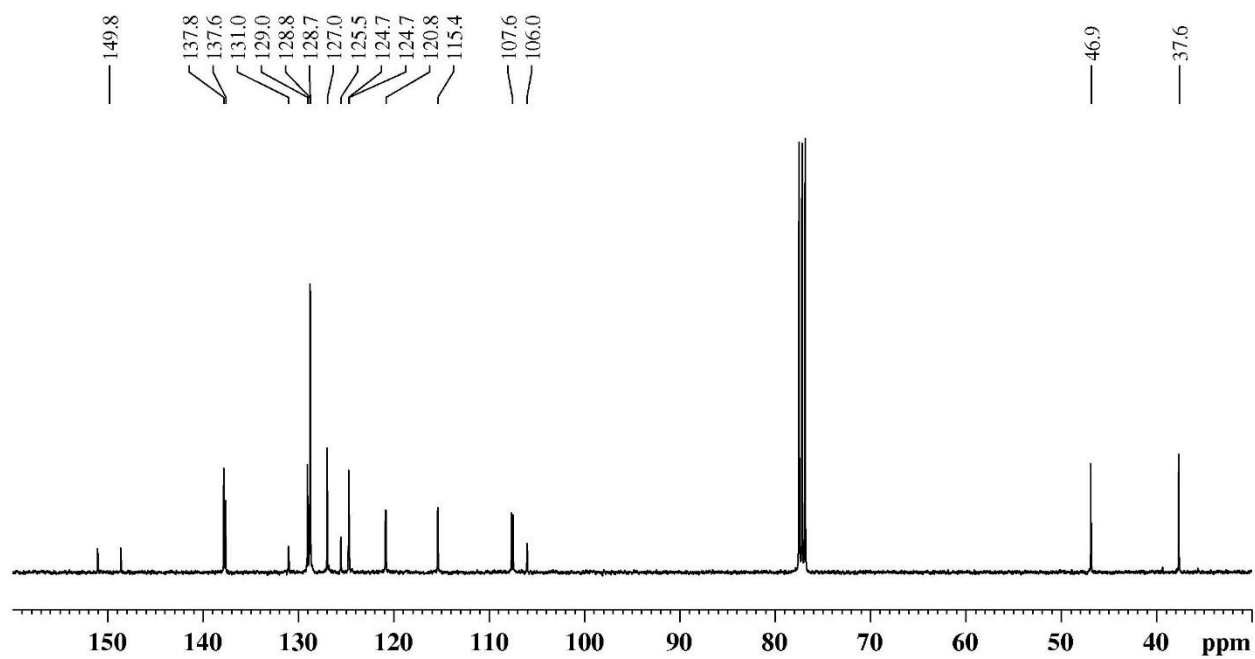
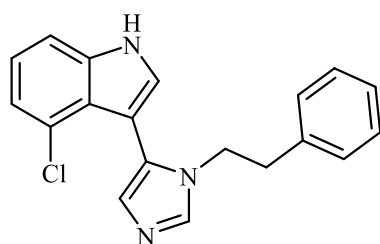
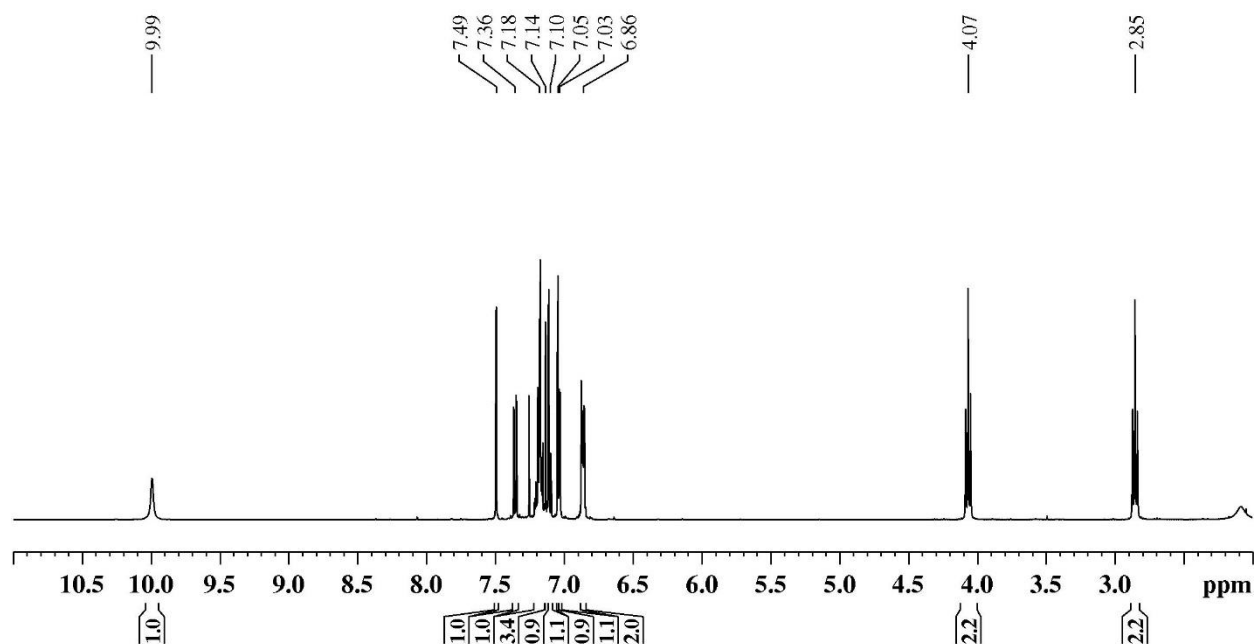


Figure S53. 4-Chloro-3-(1-phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (53)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

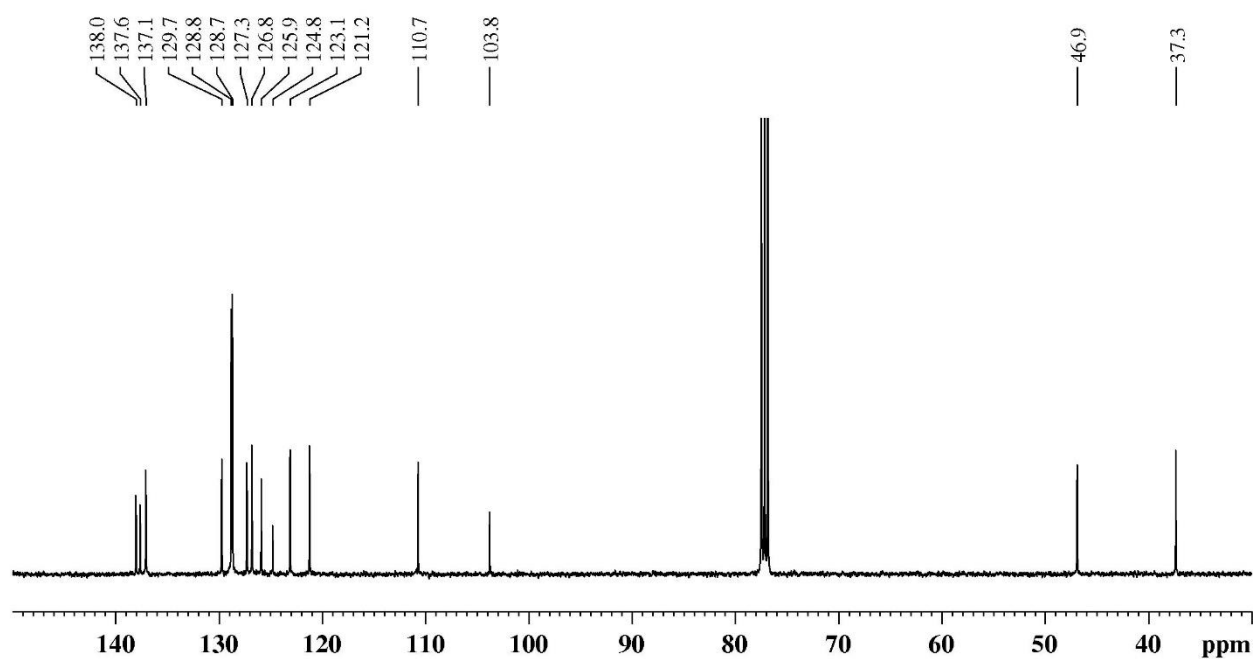
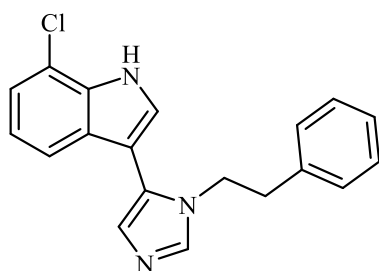
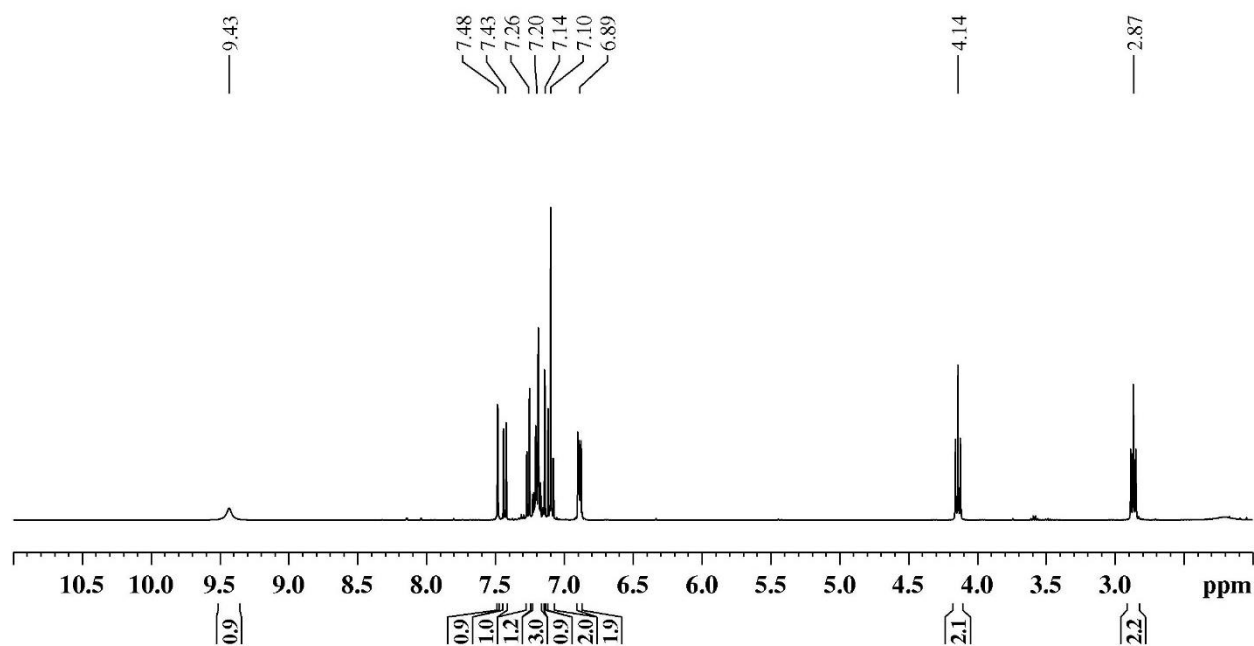


Figure S54. 7-Chloro-3-(1-phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (**54**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

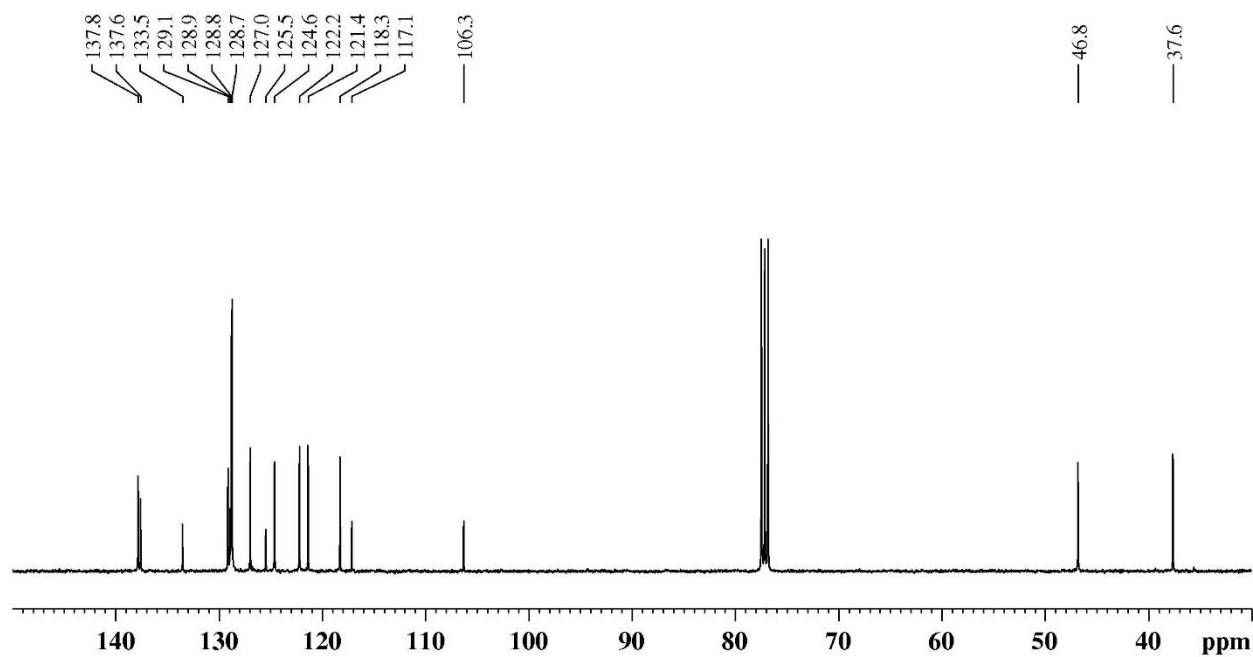
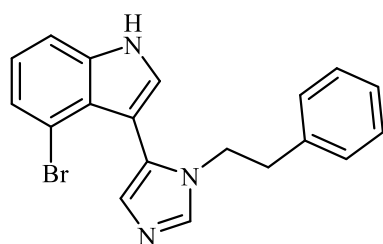
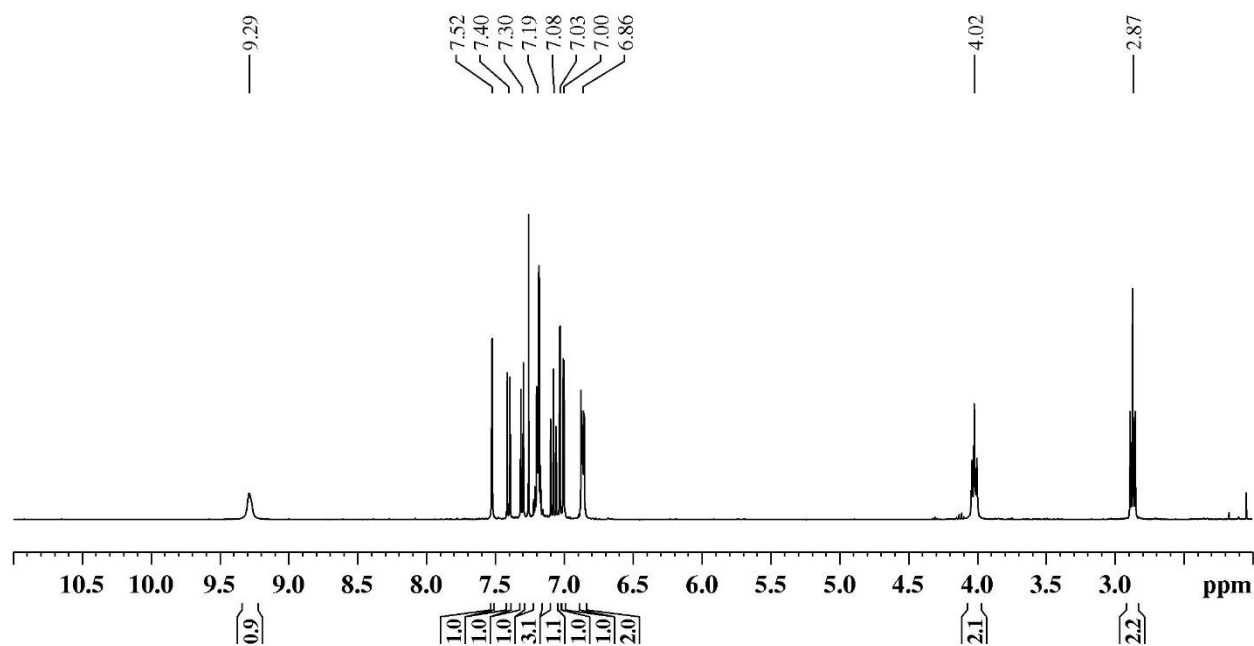


Figure S55. 4-Bromo-3-(1-phenethyl-1H-imidazol-5-yl)-1H-indole (55)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

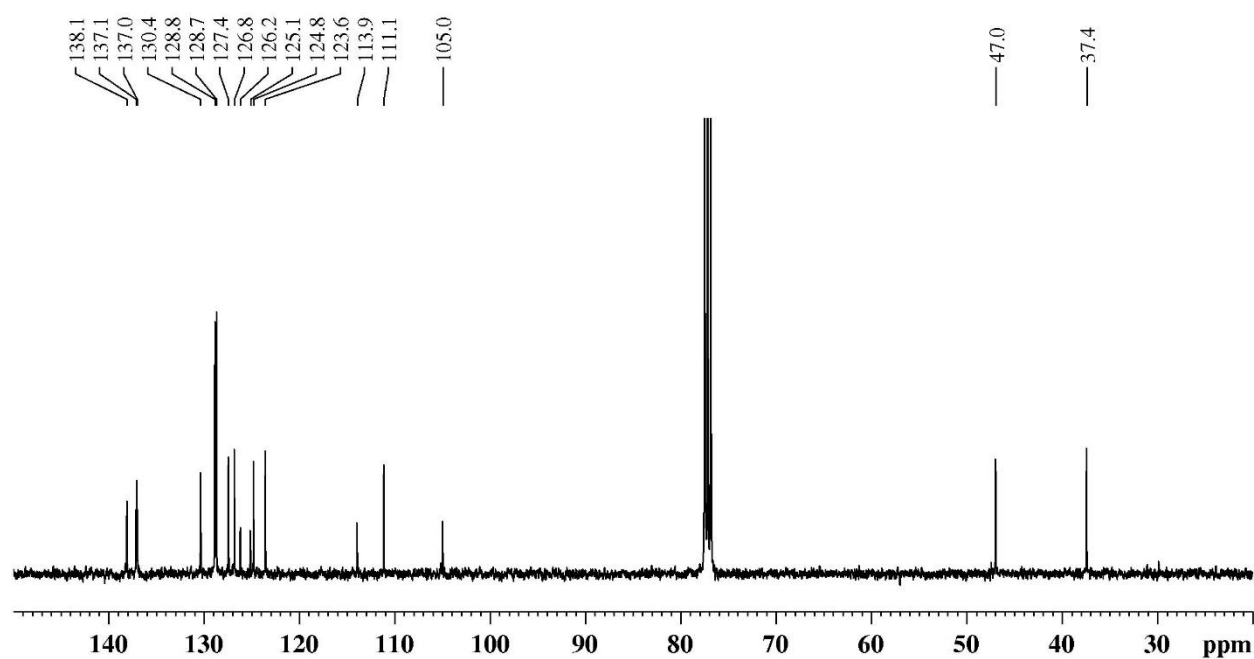
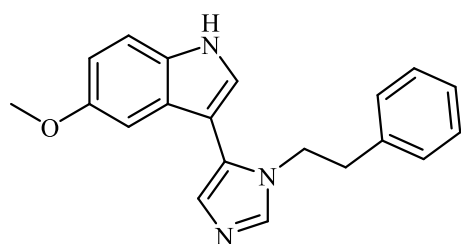
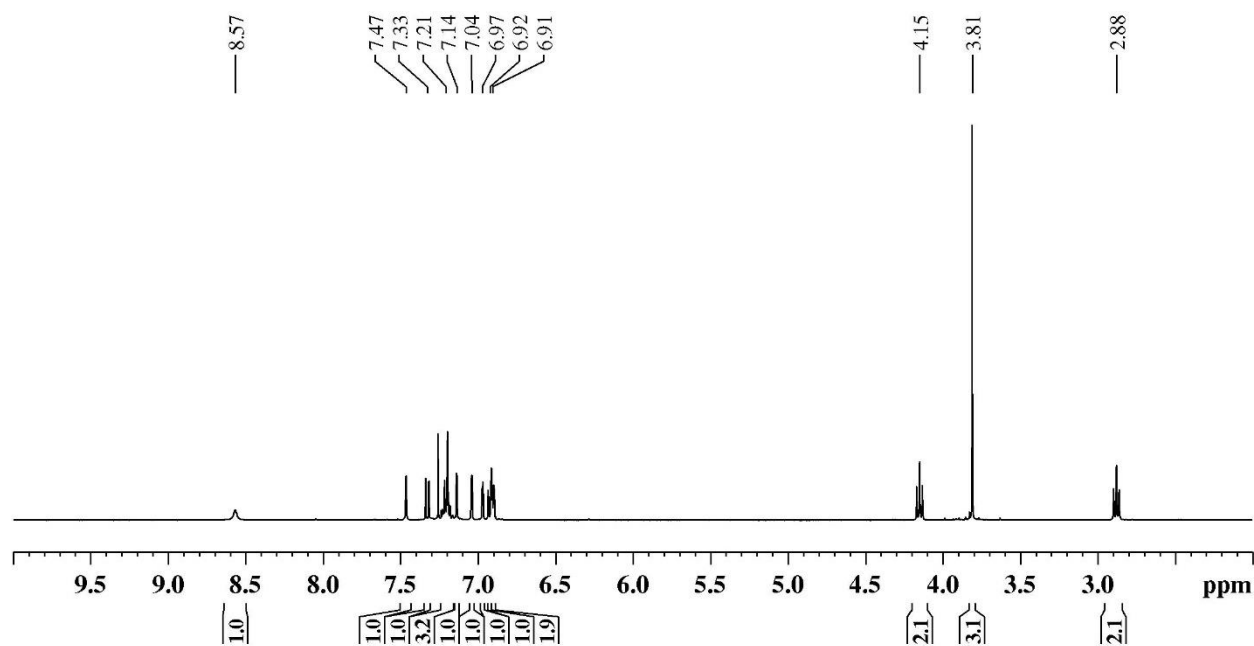


Figure S56. 5-Methoxy-3-(1-phenethyl-1*H*-imidazol-5-yl)-1*H*-indole (**56**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

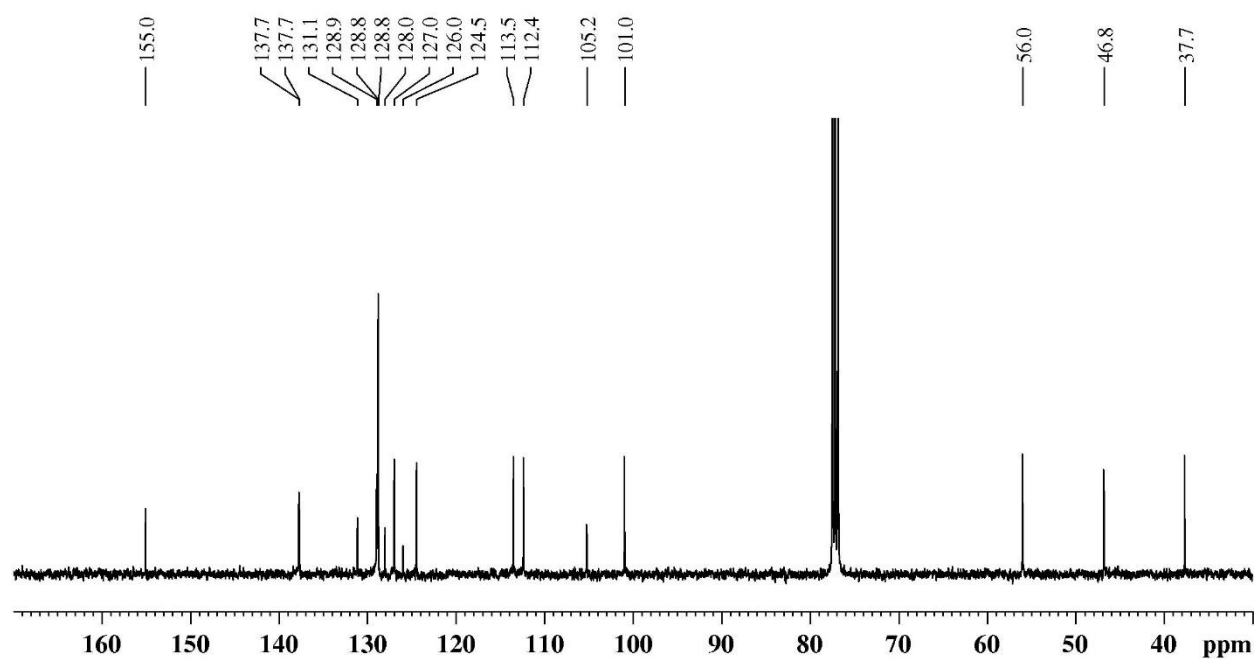
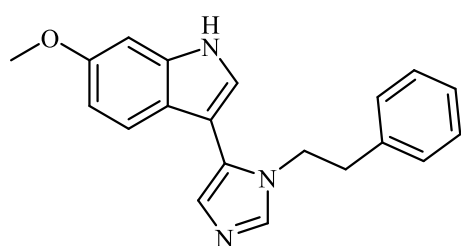
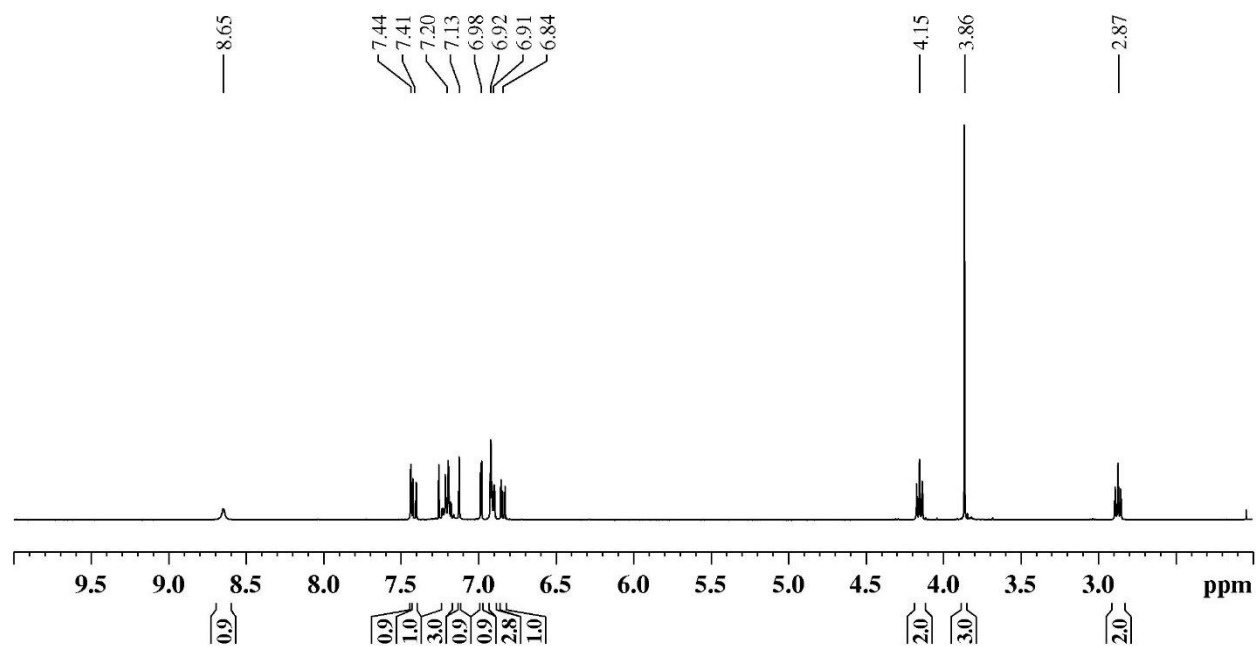


Figure S57. 6-Methoxy-3-(1-phenethyl-1H-imidazol-5-yl)-1H-indole (57)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

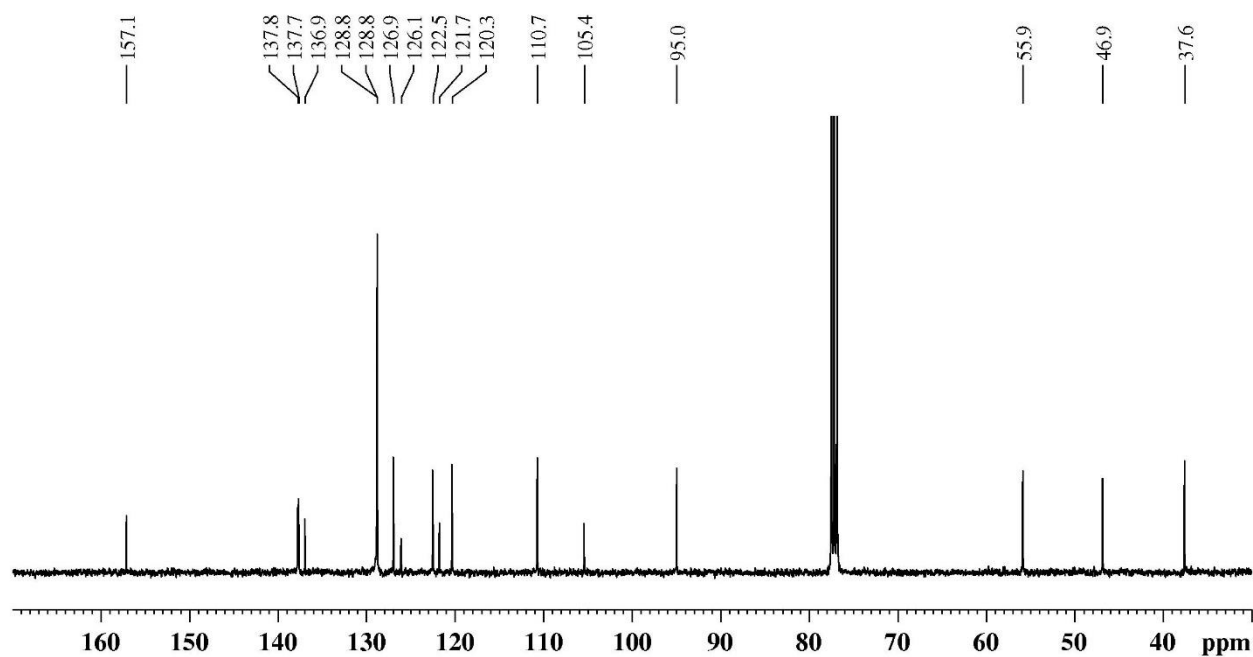
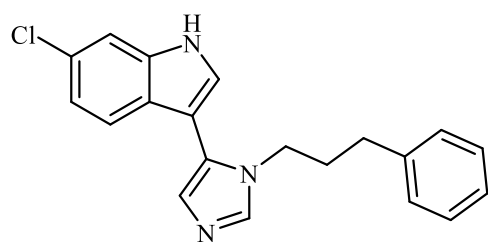
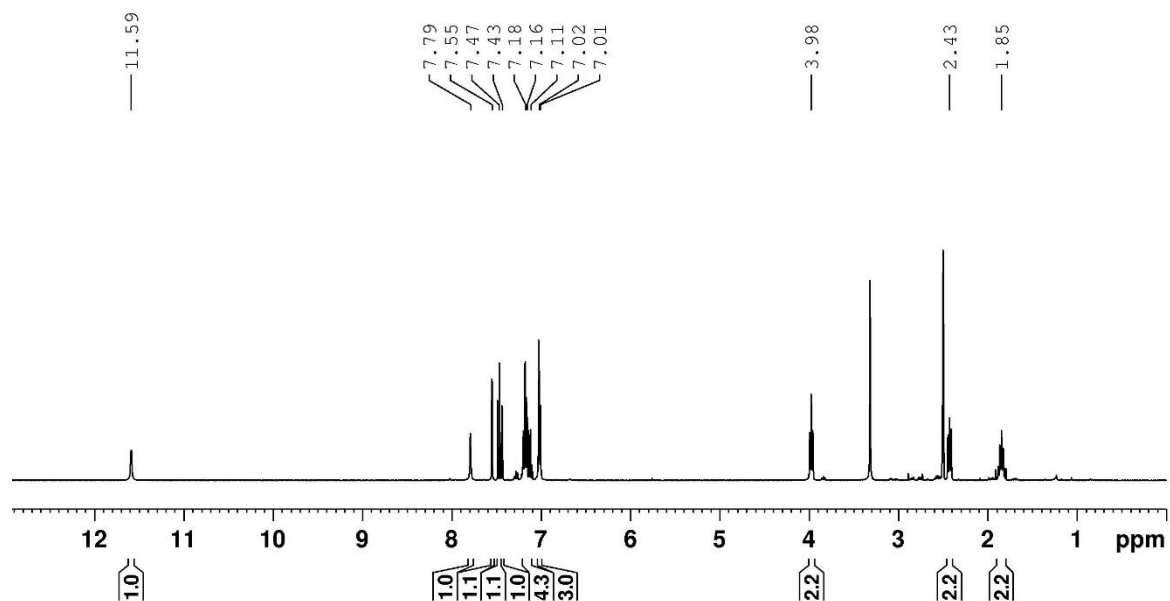


Figure S58. 5-Chloro-3-(1-(3-phenylpropyl)-1H-imidazol-5-yl)-1H-indole (58)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

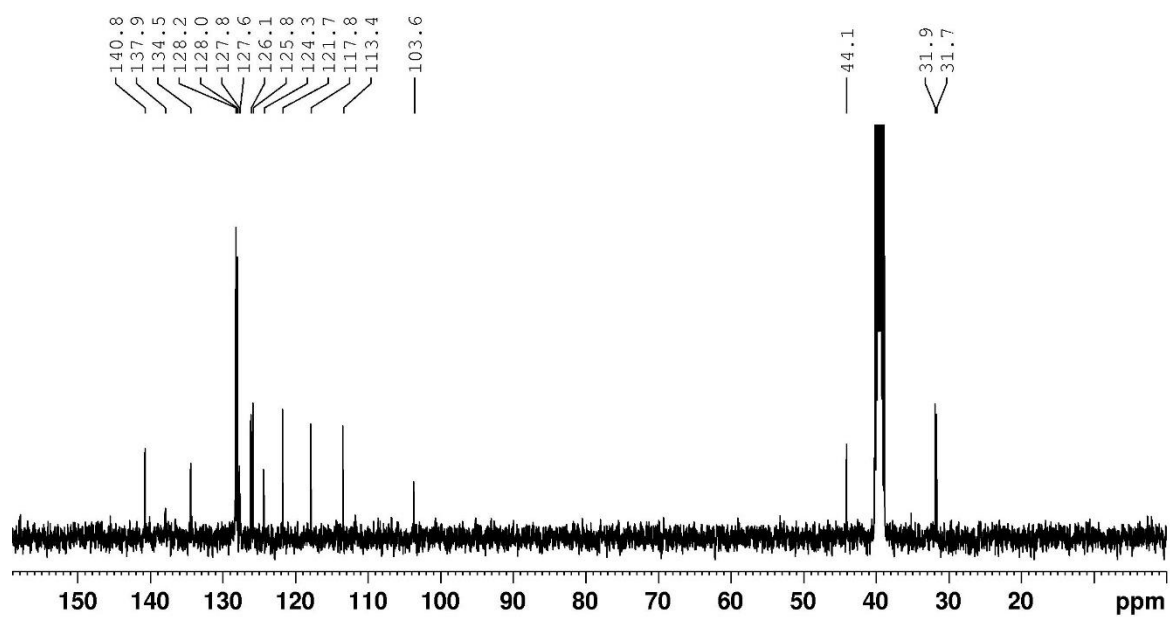
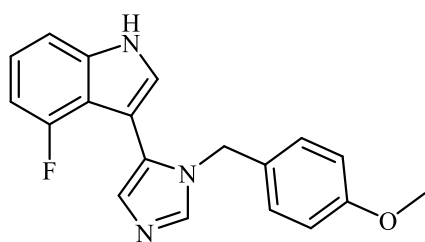
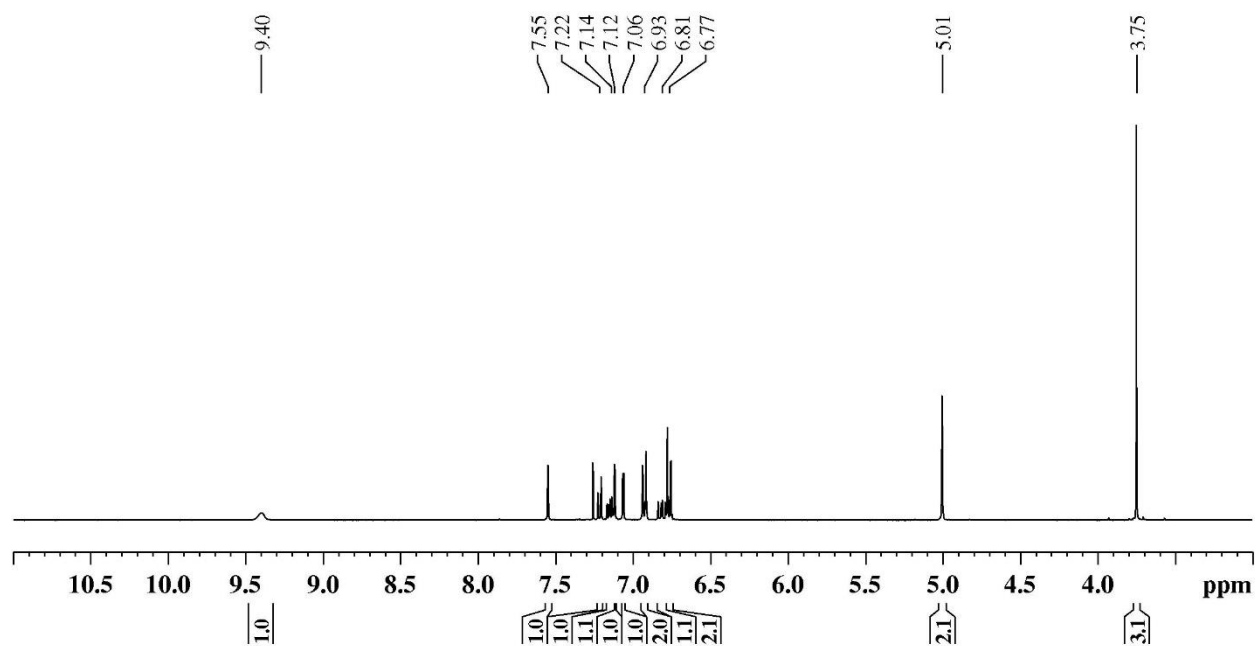


Figure S59. 4-Fluoro-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (59)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

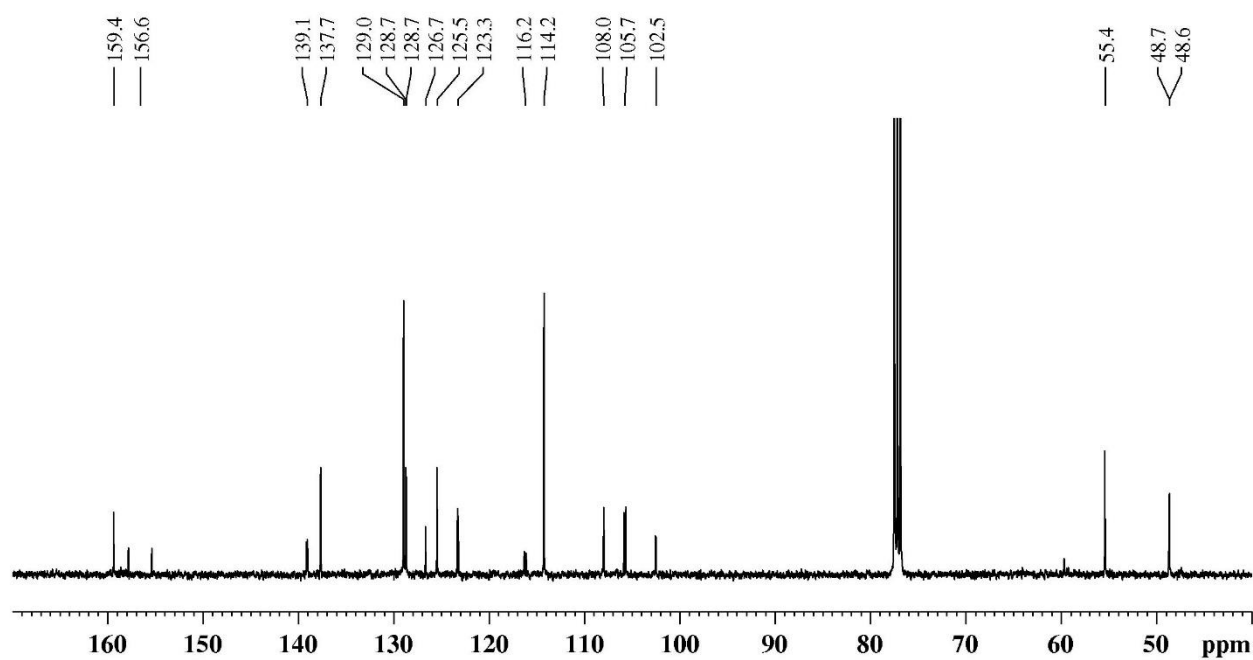
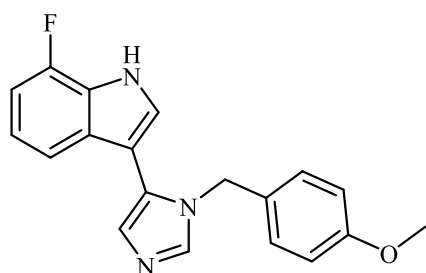
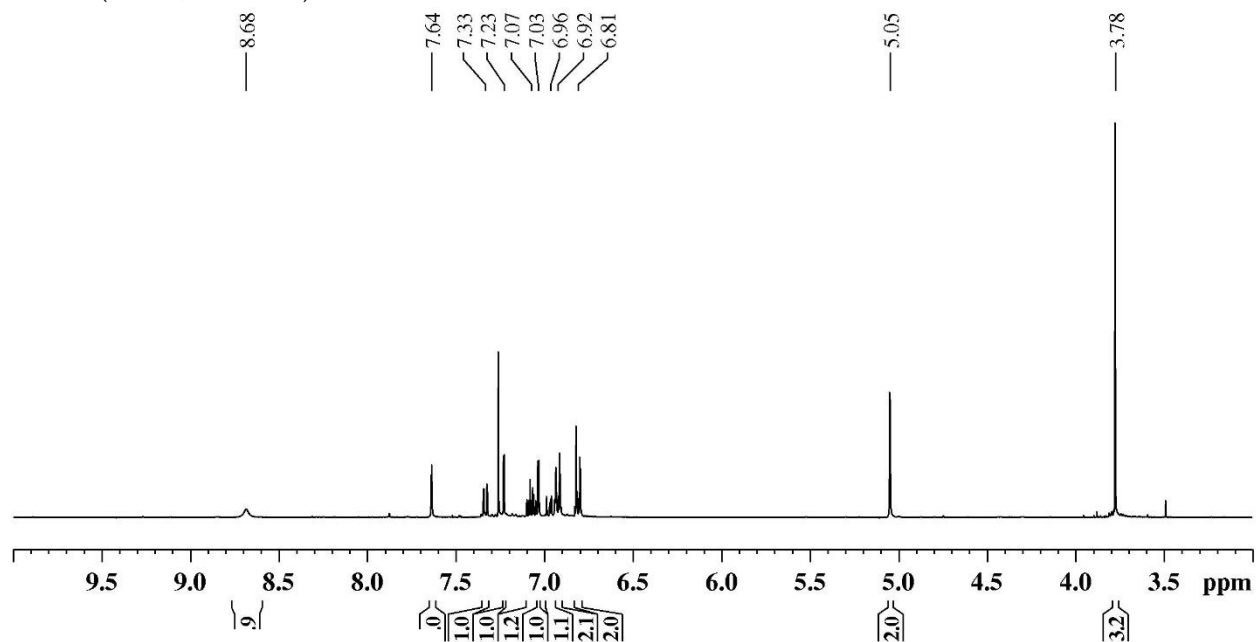


Figure S60. 7-Fluoro-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (60)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

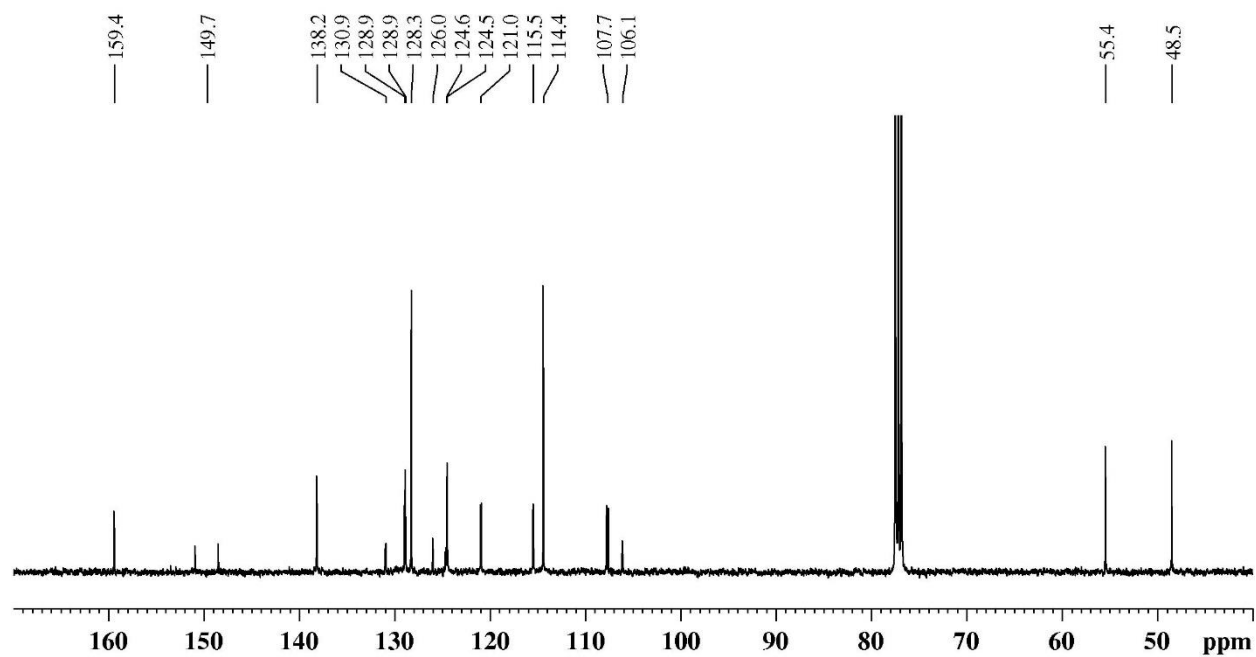
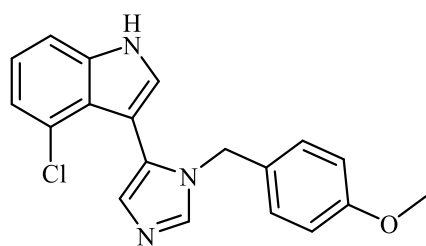
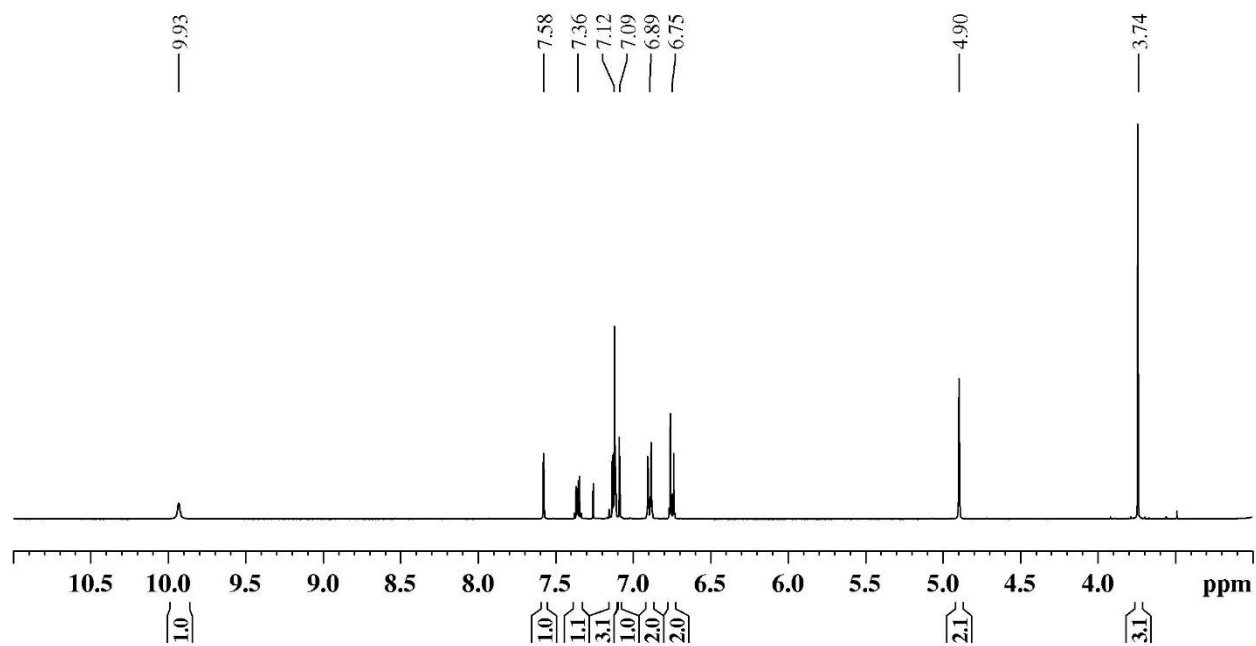


Figure S61. 4-Chloro-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (**61**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

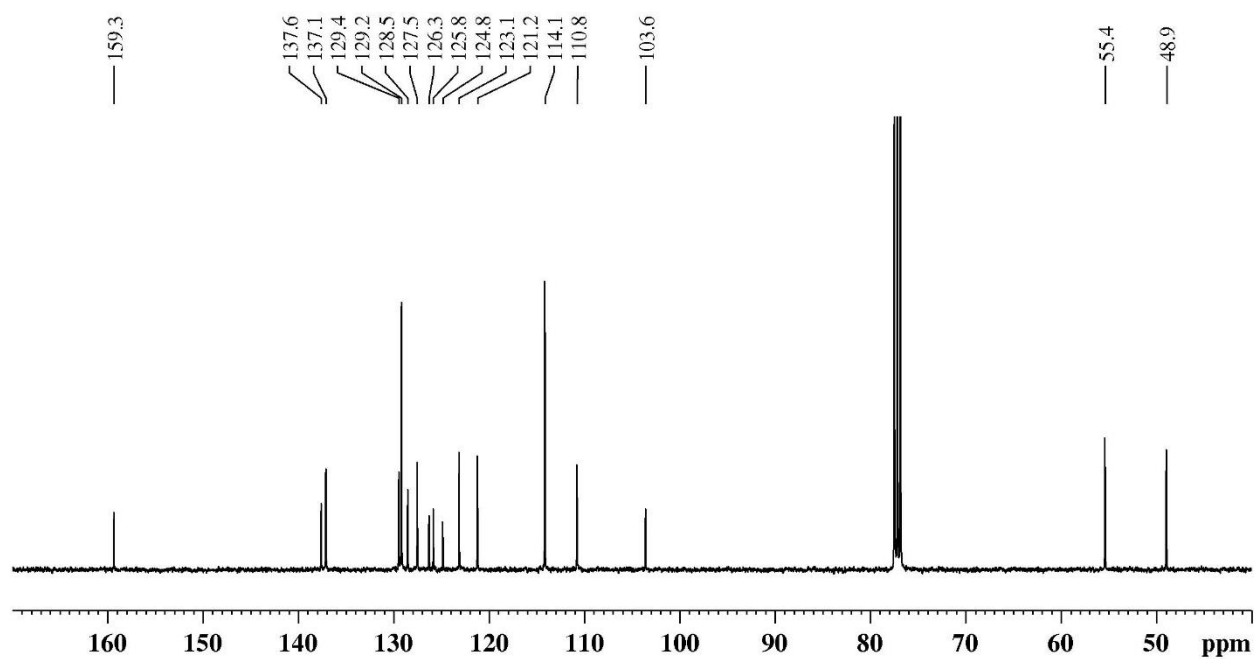
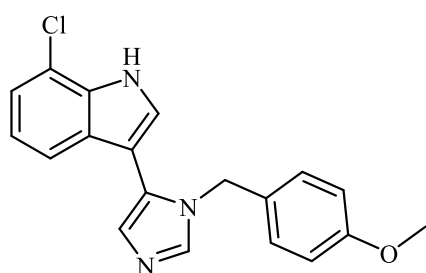
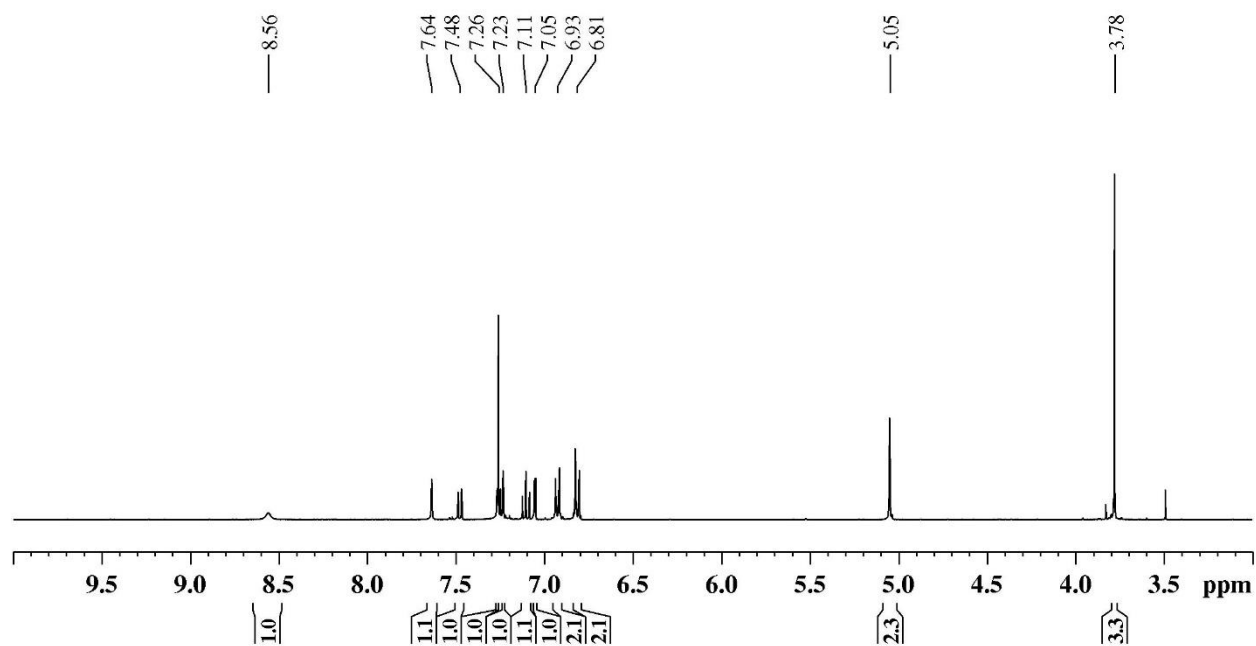


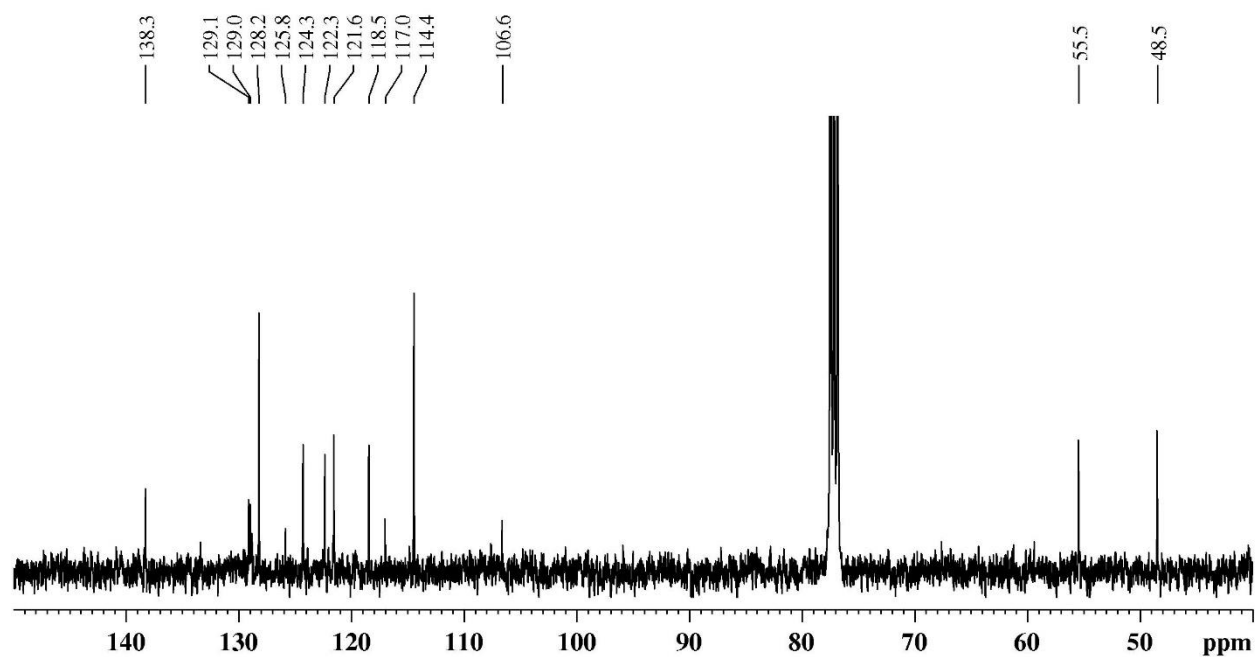
Figure S62. 7-Chloro-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (**62**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):



COC1=CC=C(C=C1)CNc2nc3ccccc3n2

¹H NMR (CDCl₃, 400 MHz):

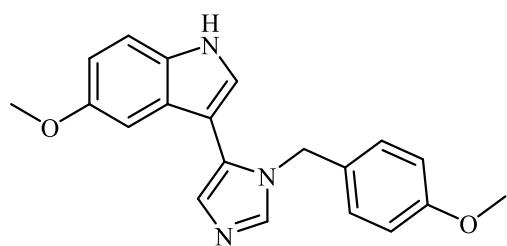
The ¹H NMR spectrum shows several peaks corresponding to the compound. The aromatic region contains a multiplet between 6.7 and 7.8 ppm, with integration values of 1.0, 1.0, 1.0, 1.0, 2.1, 2.1, and 2.1. A singlet at 9.74 ppm has an integration of 1.0. A singlet at 4.86 ppm has an integration of 2.1. A singlet at 3.75 ppm has an integration of 3.2.

| Chemical Shift (ppm) | Integration |
|----------------------|-------------|
| 9.74 | 1.0 |
| 7.59 | 1.0 |
| 7.42 | 1.0 |
| 7.32 | 1.0 |
| 7.13 | 1.0 |
| 7.08 | 2.1 |
| 7.07 | 2.1 |
| 6.90 | 2.1 |
| 6.75 | 2.1 |
| 4.86 | 2.1 |
| 3.75 | 3.2 |

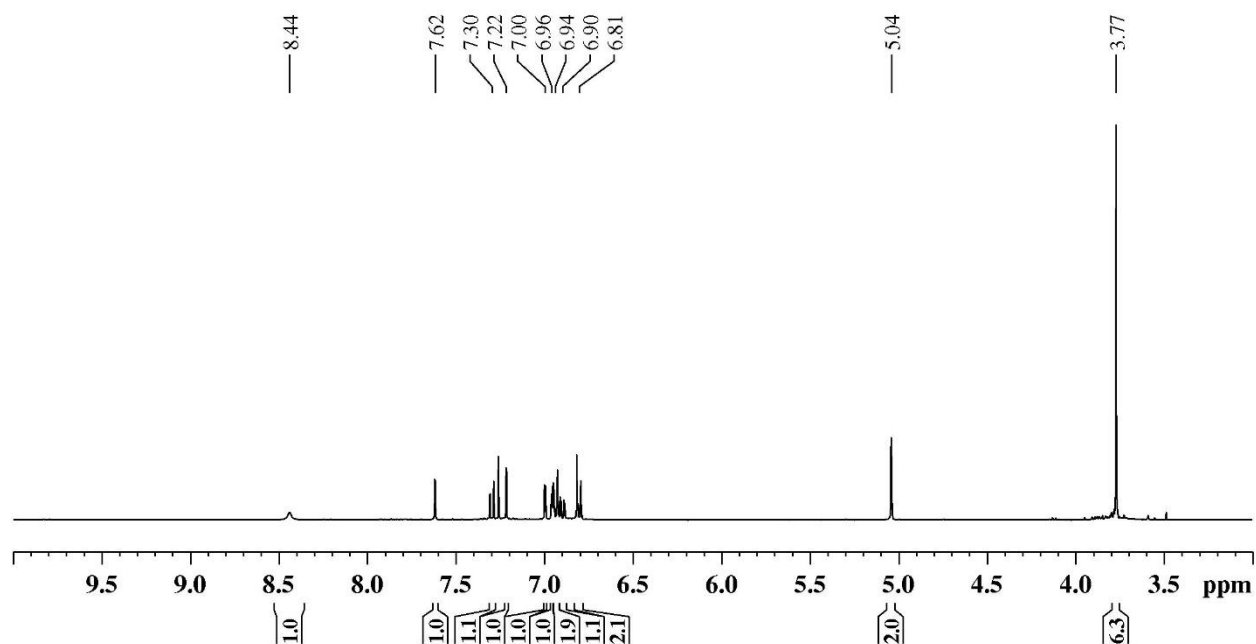
159.4
137.2
137.0
129.9
129.3
128.4
127.8
126.2
125.7
124.7
123.5
114.2
113.8
111.3
104.4
55.4
49.1

160 150 140 130 120 110 100 90 80 70 60 50 ppm

Figure S64. 5-Methoxy-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (64)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

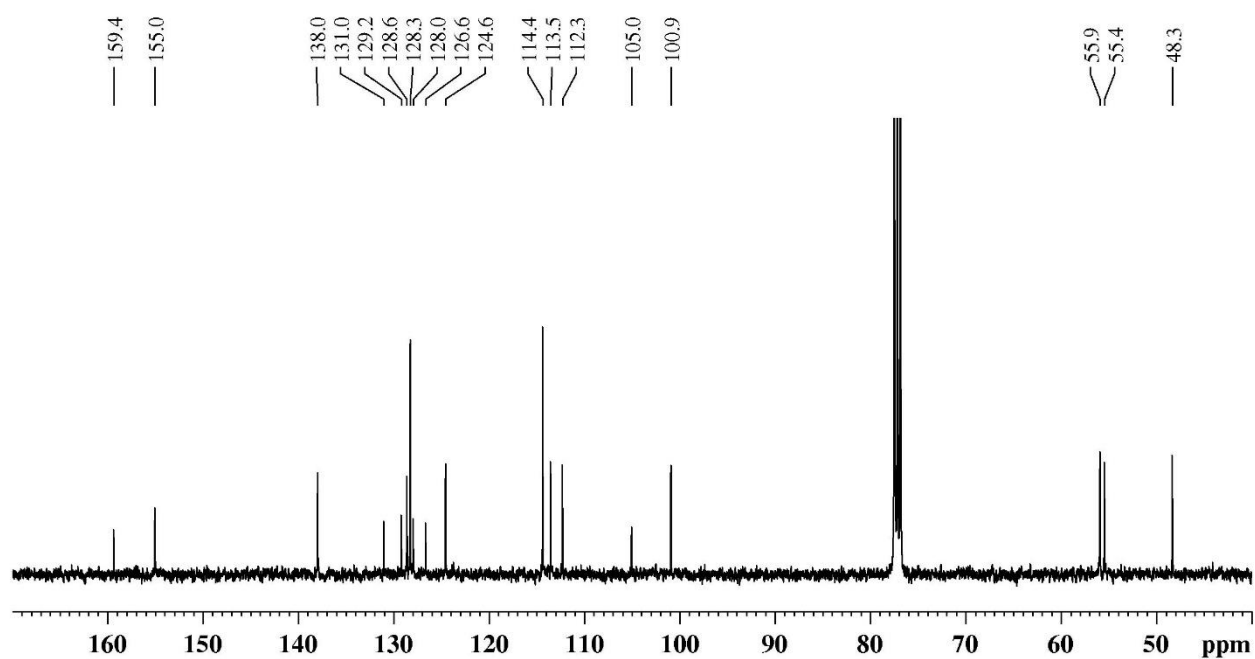
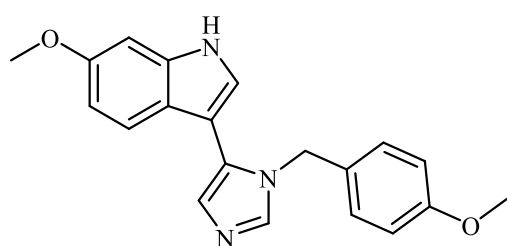
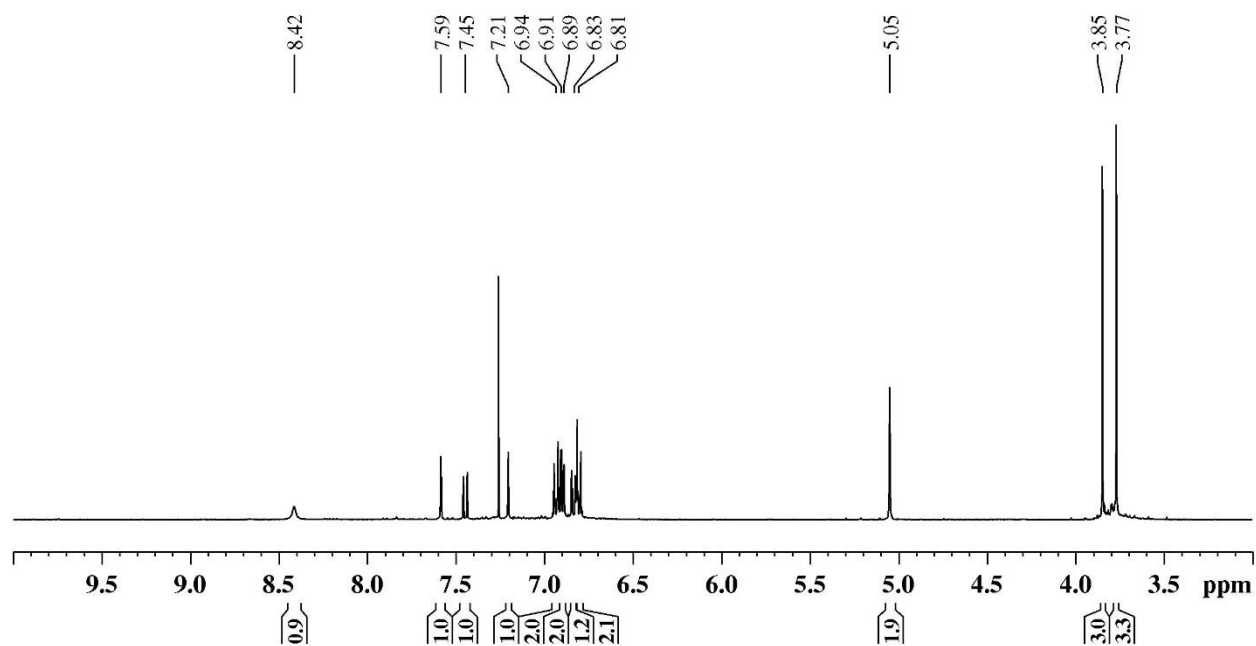


Figure S65. 6-Methoxy-3-(1-(4-methoxybenzyl)-1H-imidazol-5-yl)-1H-indole (65)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

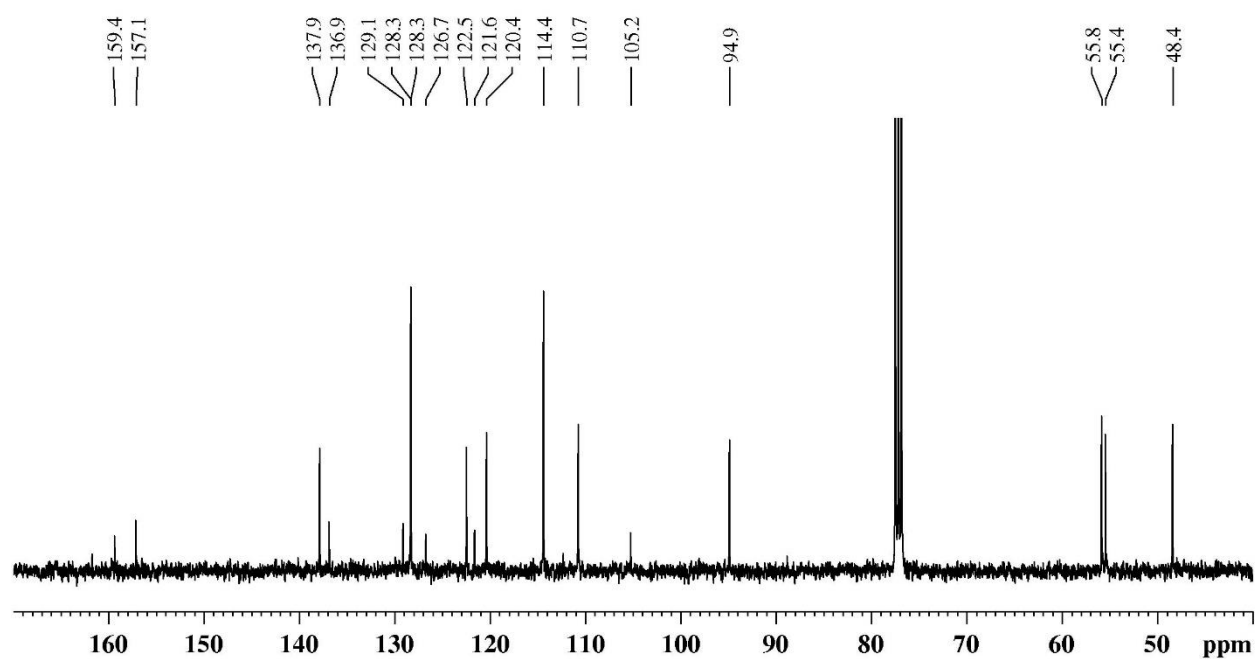
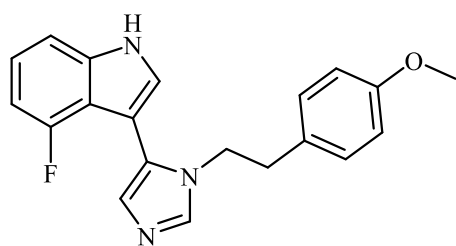
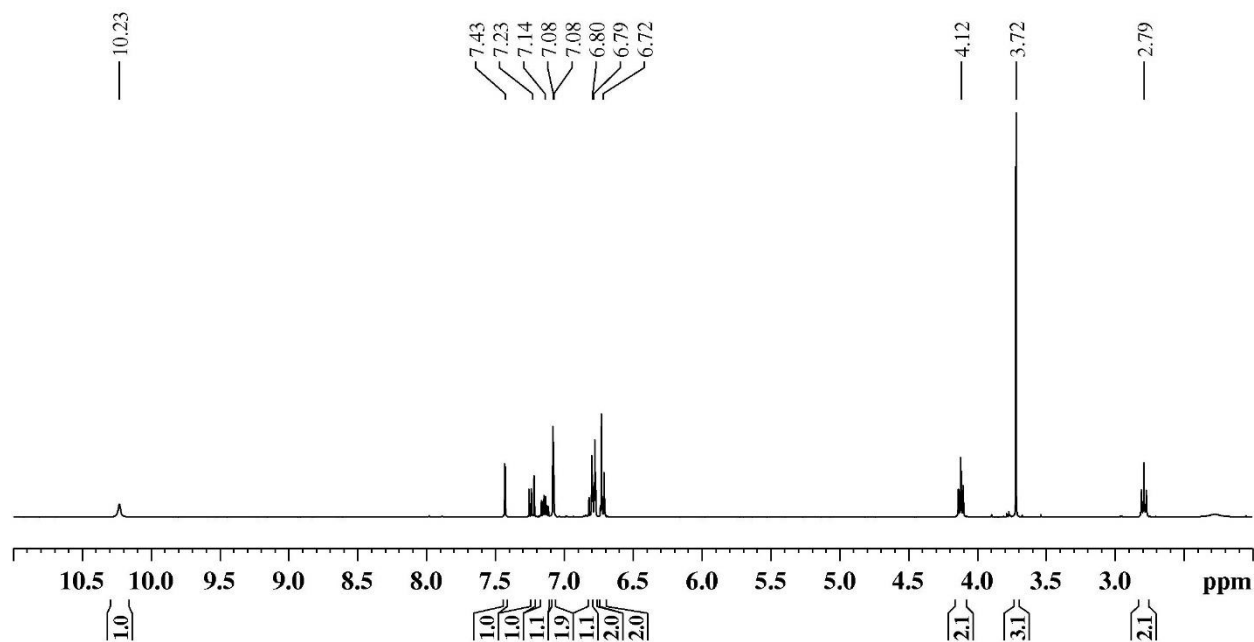


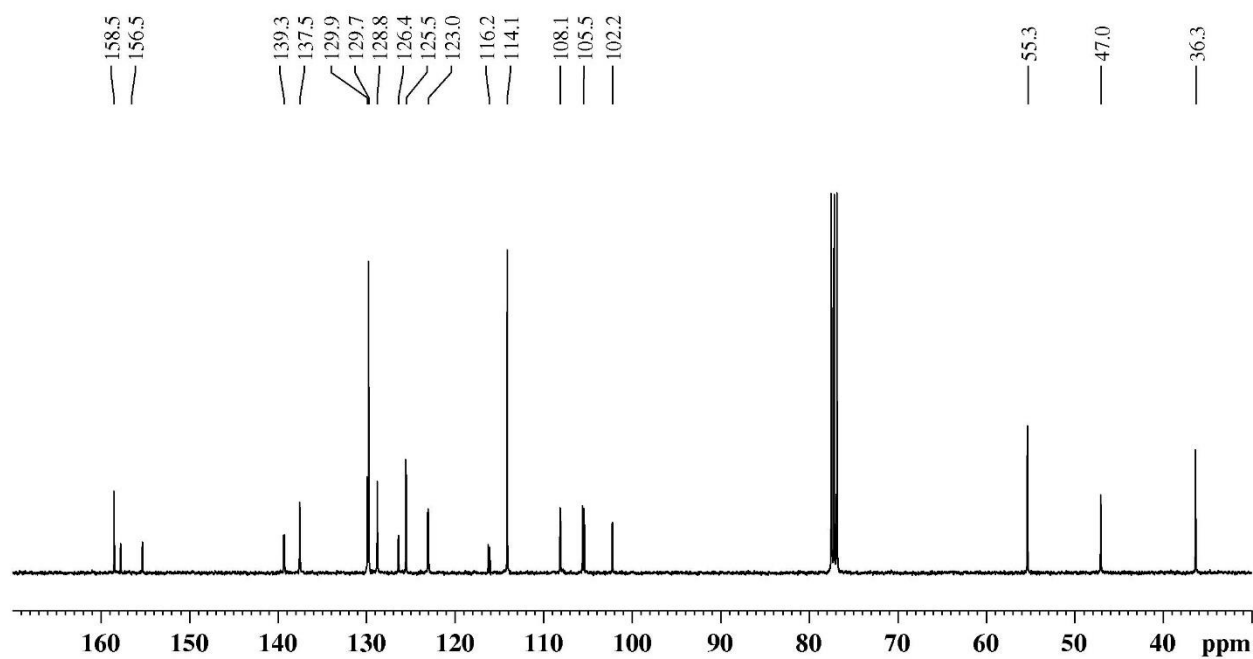
Figure S66. 4-Fluoro-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (66)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):



COc1ccc(cc1)CCN2C=CN=C2c3c[nH]c4cc(F)ccc34

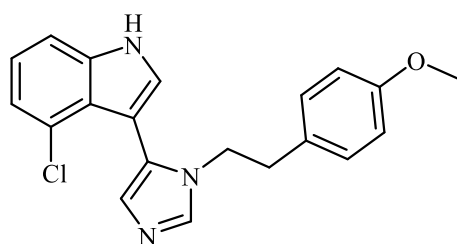
¹H NMR (CDCl₃, 400 MHz):

8.87, 7.48, 7.29, 7.14, 7.09, 7.08, 6.98, 6.80, 6.74, 4.11, 3.75, 2.81

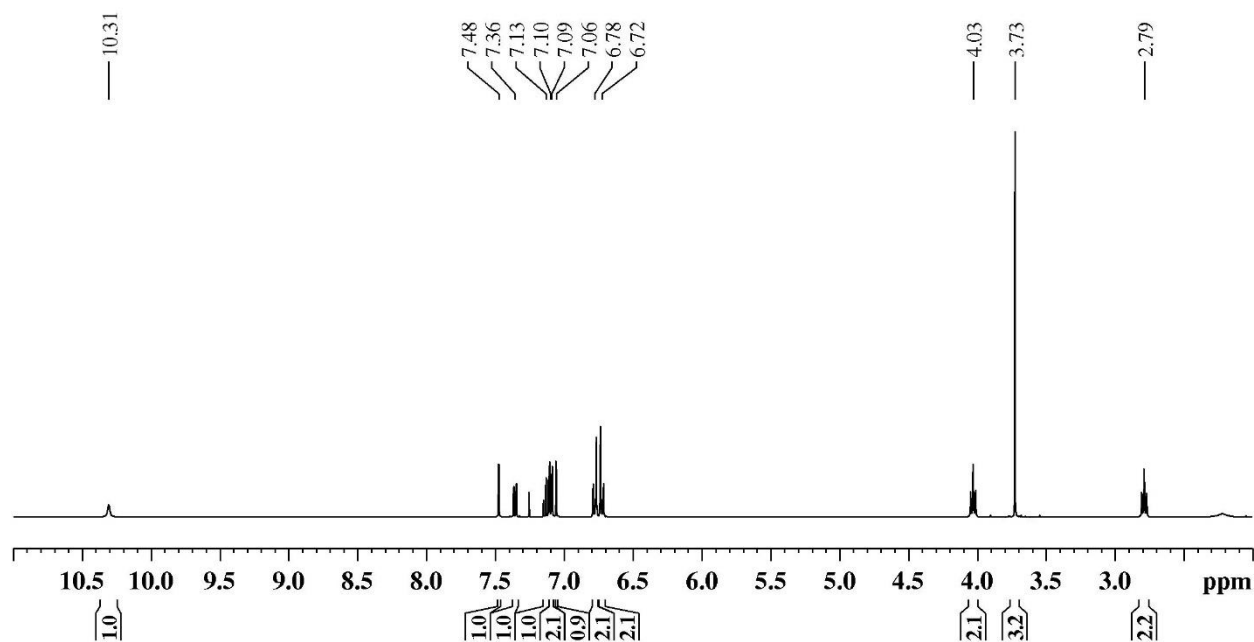
¹³C NMR (CDCl₃, 100 MHz):

158.6, 149.7, 137.9, 131.0, 129.7, 129.6, 129.1, 125.3, 124.6, 124.4, 121.0, 115.5, 114.2, 107.7, 106.4, 55.4, 47.1, 36.8

Figure S68. 4-Chloro-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (68)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

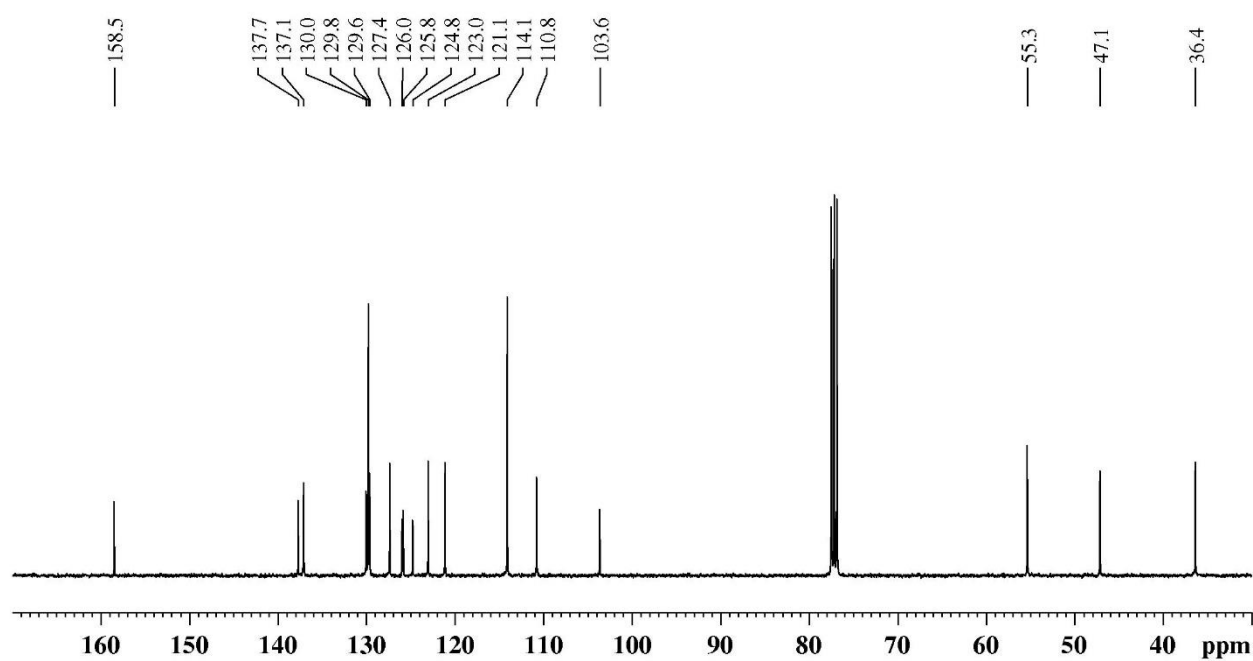
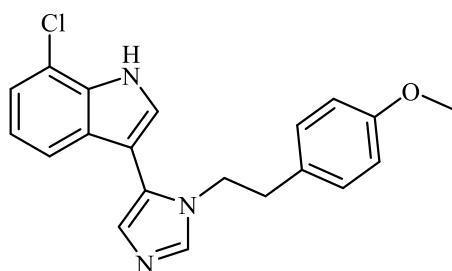
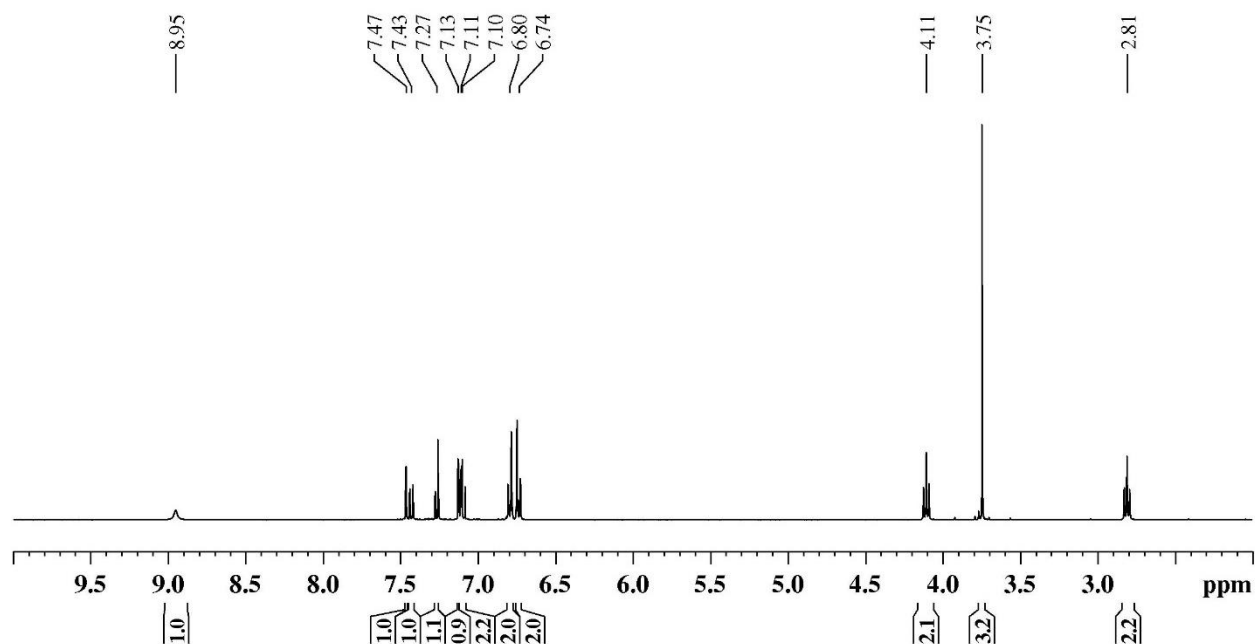


Figure S69. 7-Chloro-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (69)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

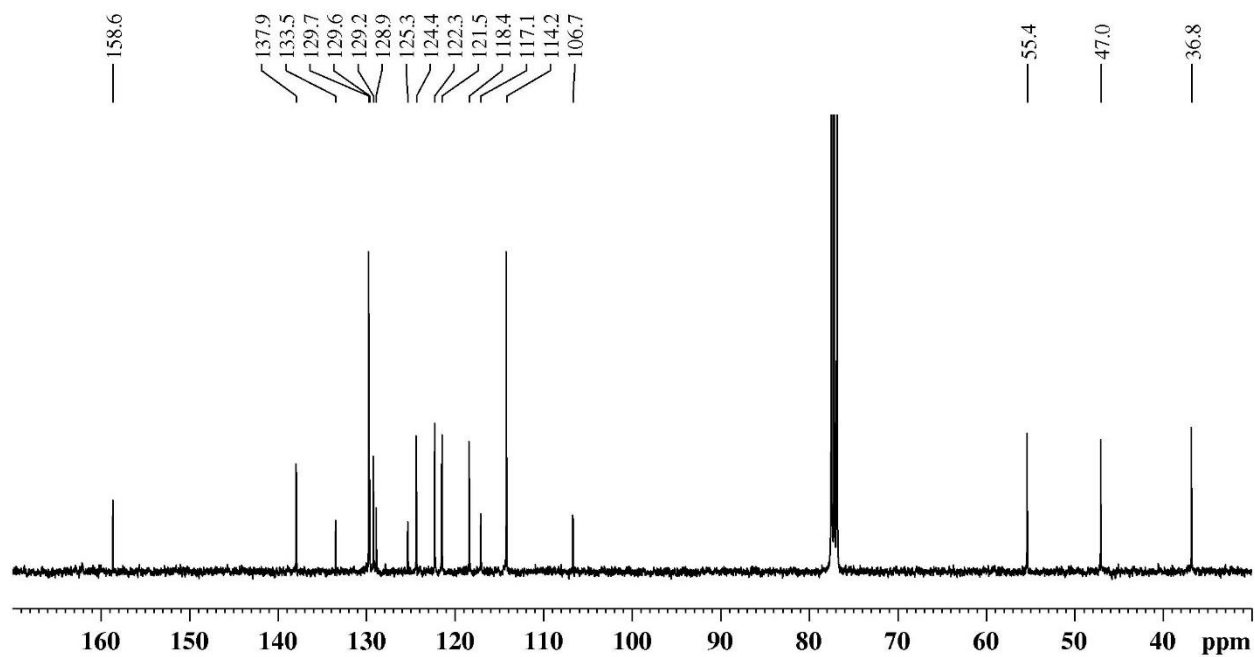
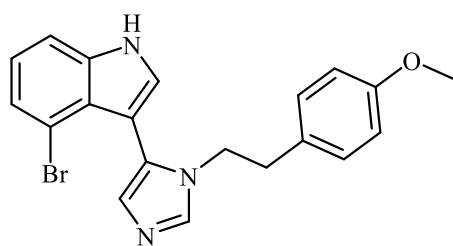
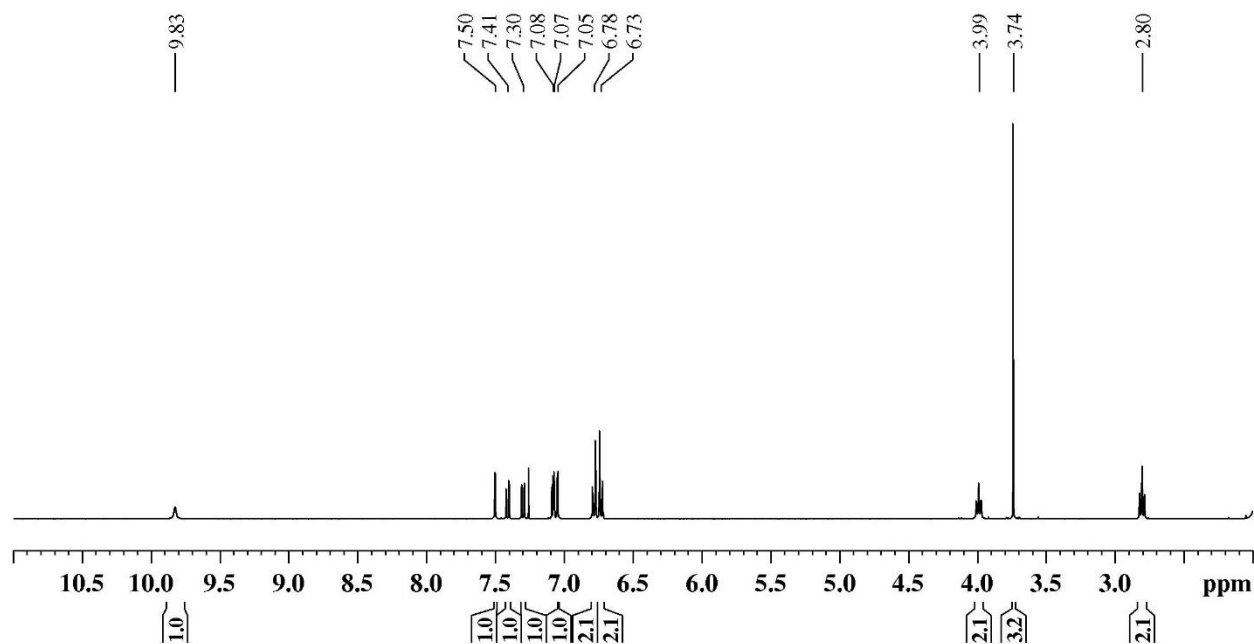


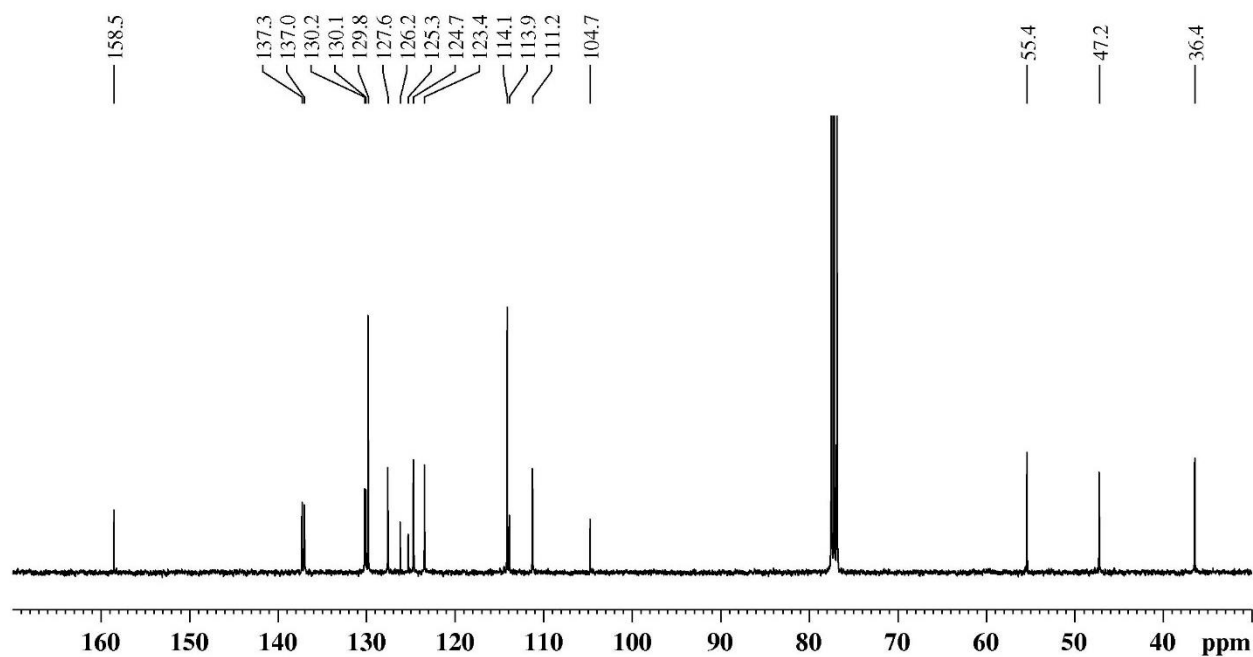
Figure S70. 4-Bromo-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (70)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

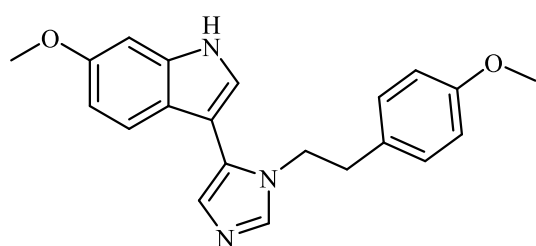


COc1ccc(OCCc2c[nH]c3cc(OC)ccc23)cc1

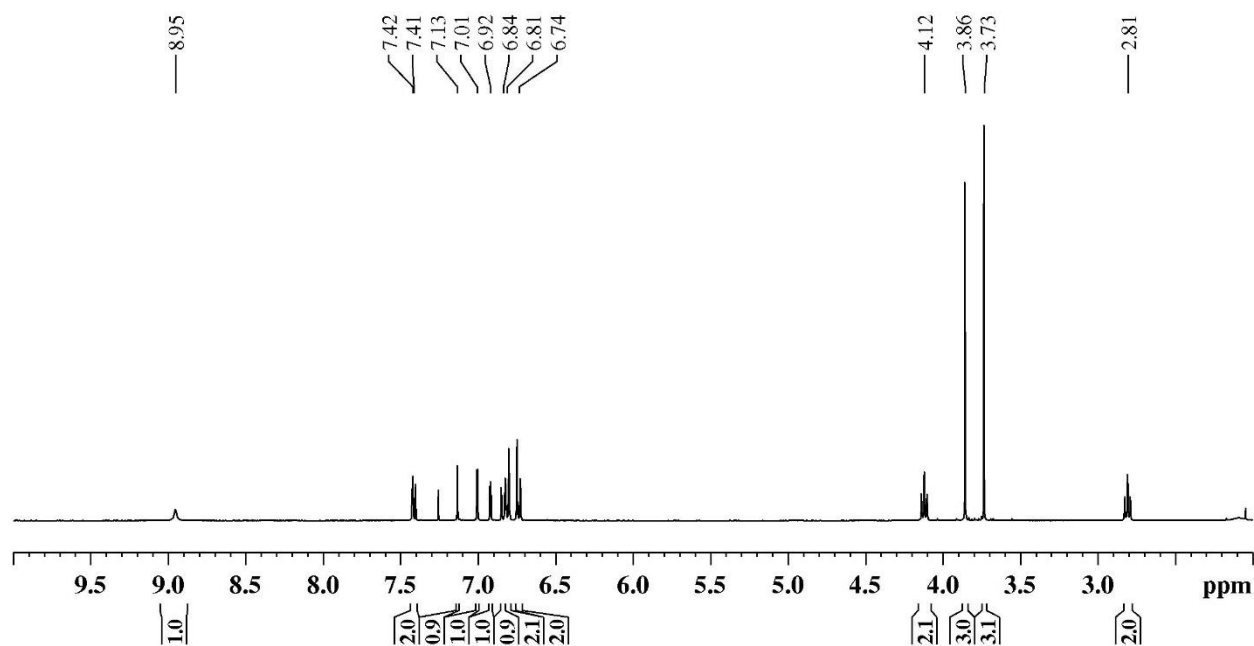
¹H NMR spectrum of compound **1** in CDCl₃. The spectrum shows peaks at 8.85, 7.45, 7.32, 7.14, 7.07, 6.97, 6.92, 6.81, 6.74, 4.12, 3.81, 3.74, and 2.82 ppm. Integration values are shown below the baseline: 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 2.1, 2.1, 2.1, 2.1, 2.1, 2.1, 3.0, 3.1, 2.1.

158.6
155.0
137.7
131.2
129.7
128.8
128.0
126.1
124.5
114.2
113.4
112.4
105.1
100.9
56.0
55.3
47.0
36.8

Figure S72. 6-Methoxy-3-(1-(4-methoxyphenethyl)-1H-imidazol-5-yl)-1H-indole (72)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

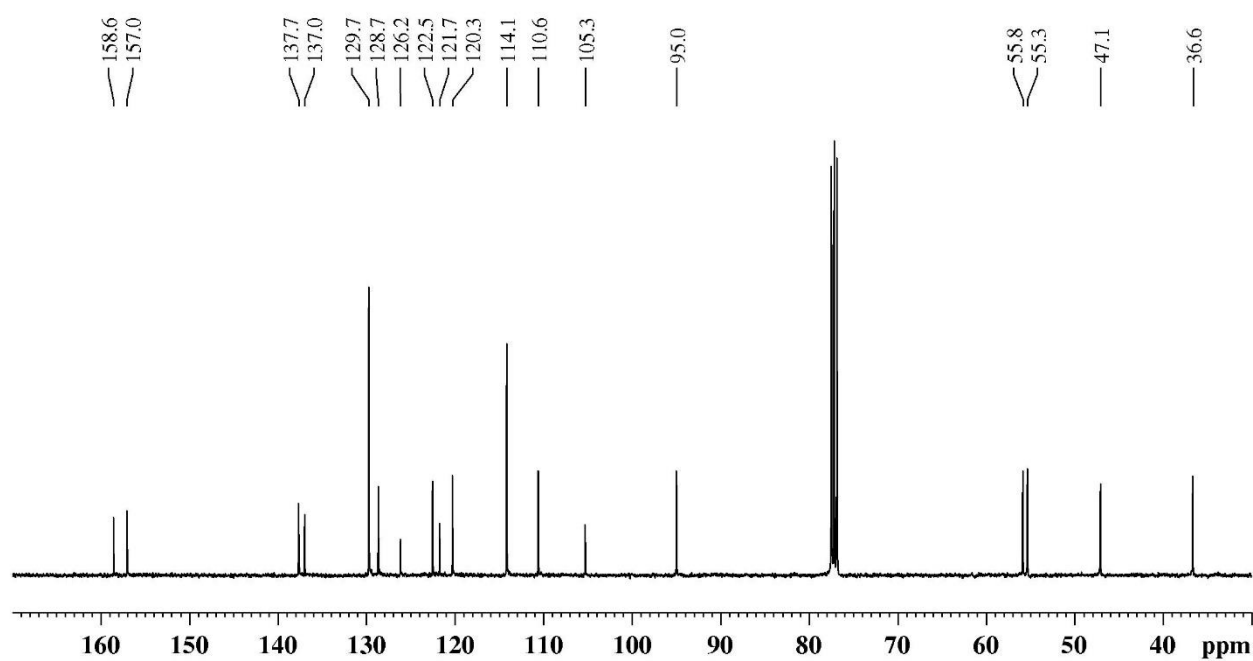
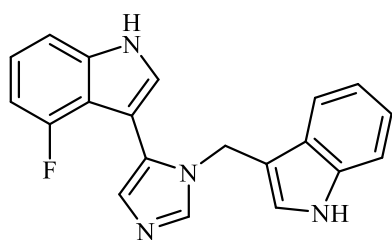
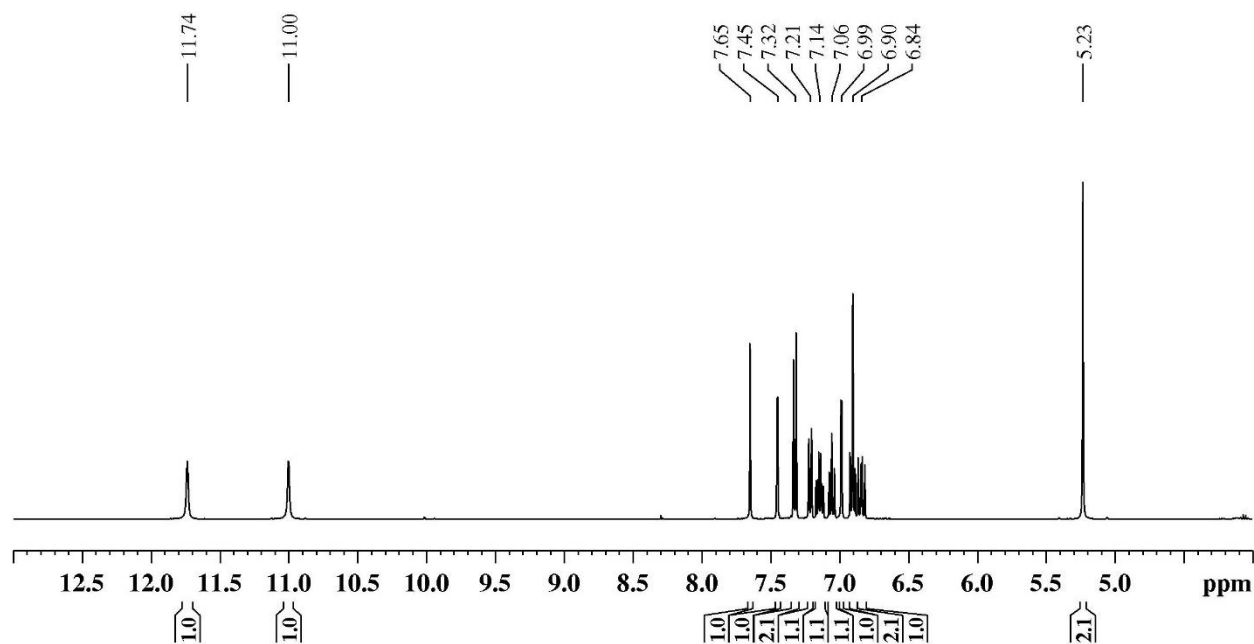


Figure S73. 3-(1-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-4-fluoro-1*H*-indole (73)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

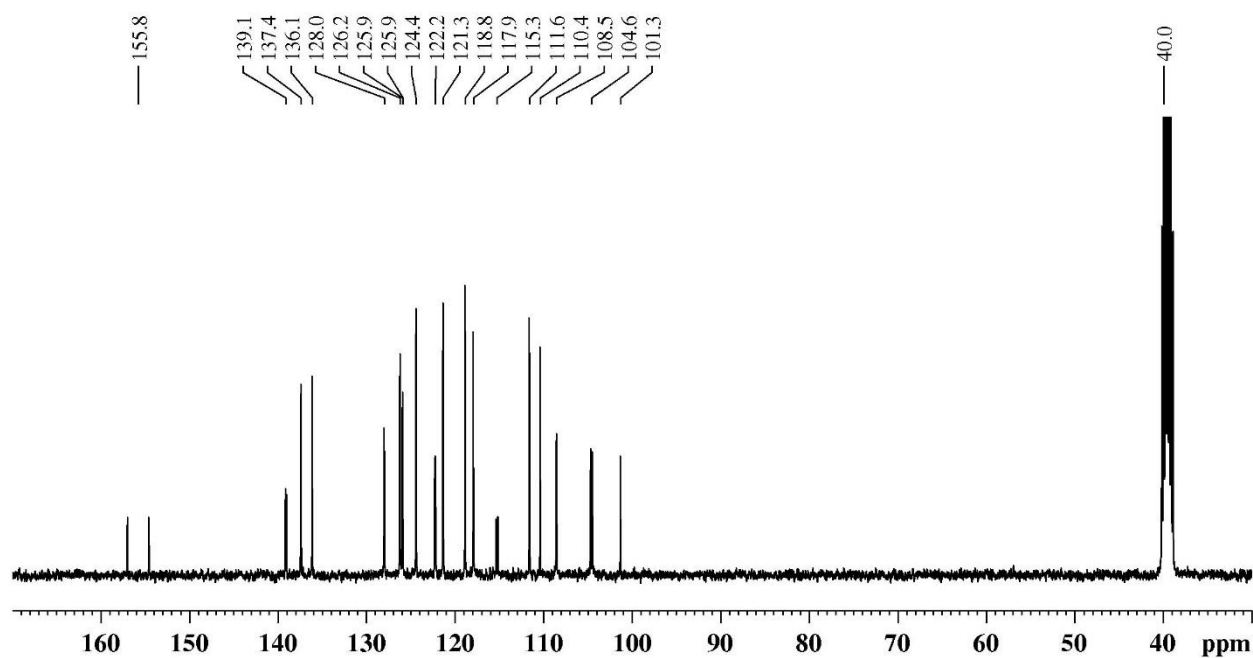
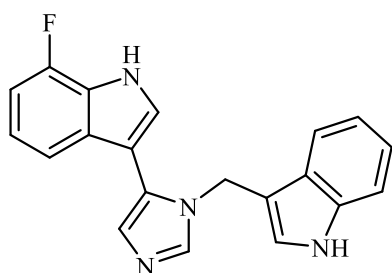
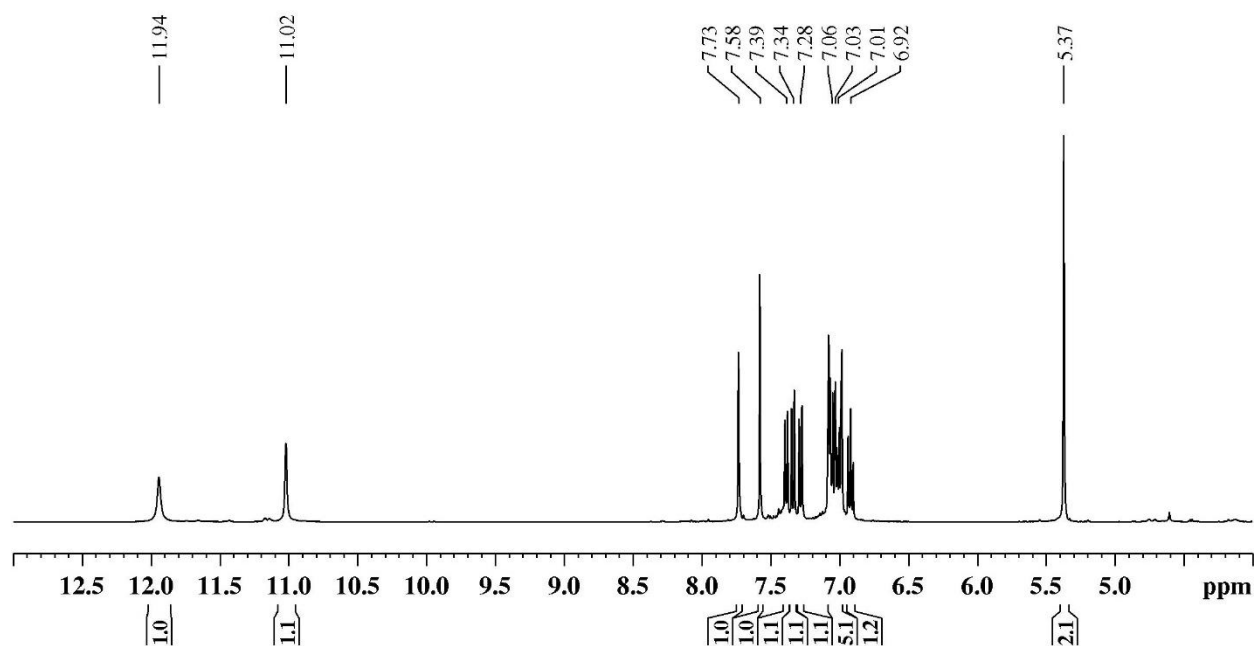


Figure S74. 3-(1-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-7-fluoro-1*H*-indole (74)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

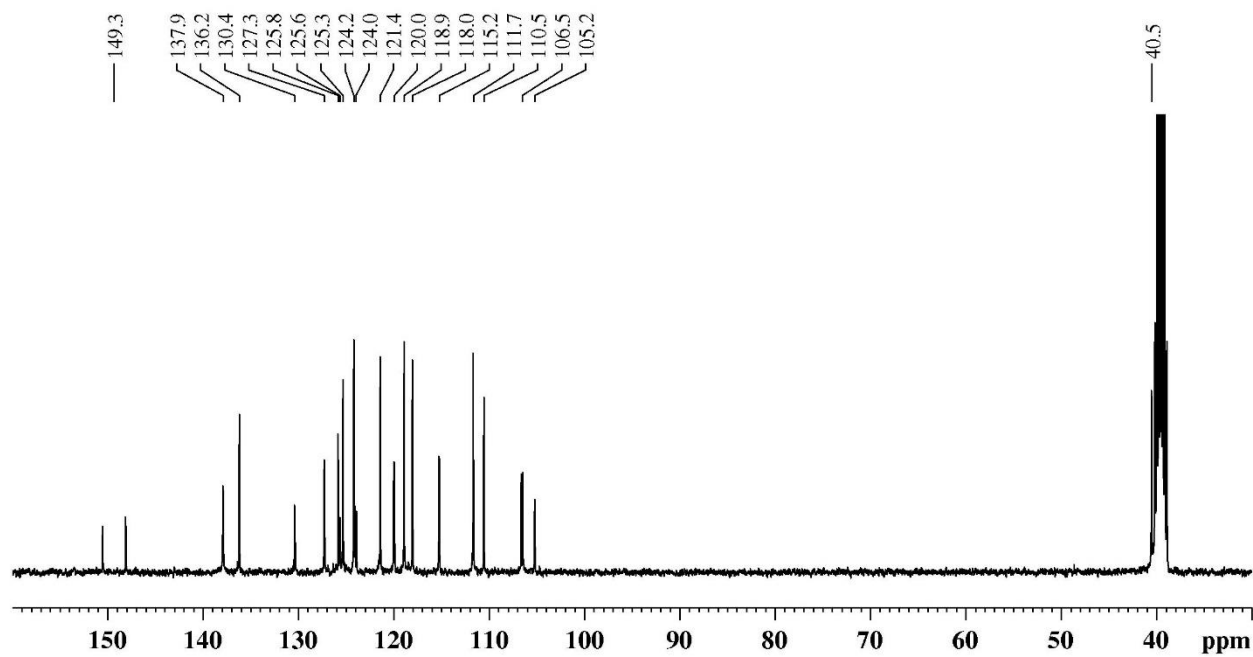
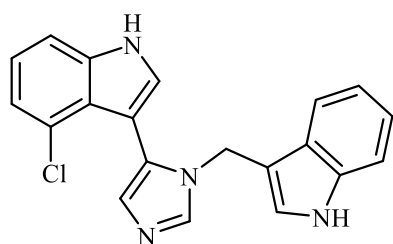
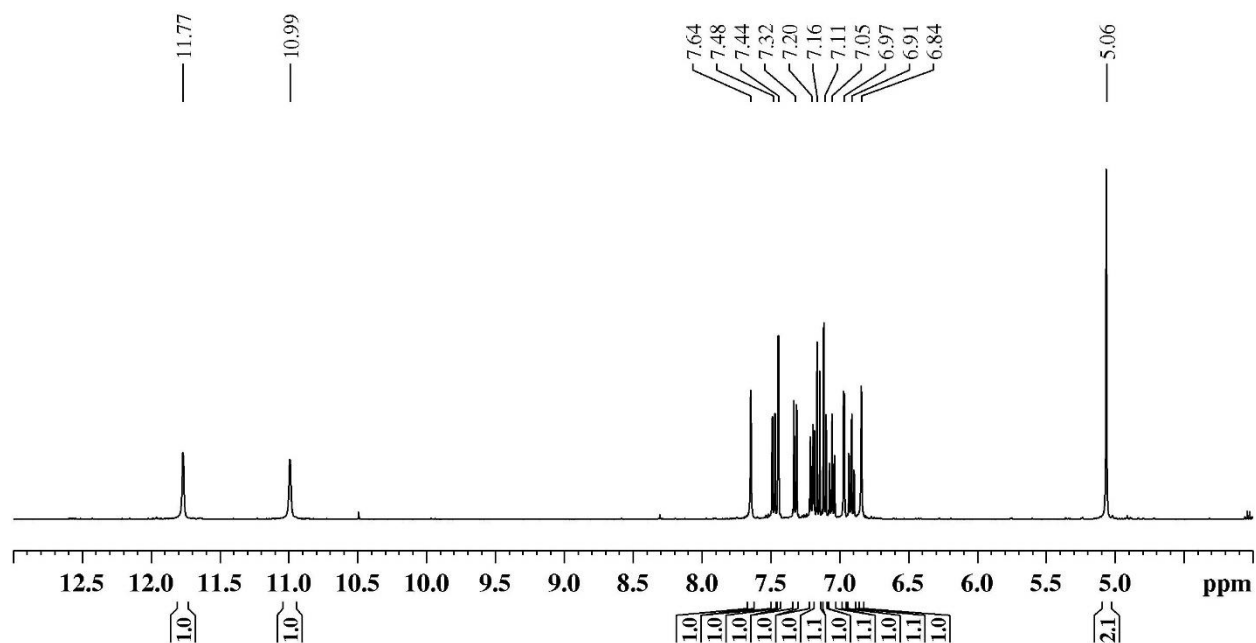


Figure S75. 3-(1-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-4-chloro-1*H*-indole (75)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

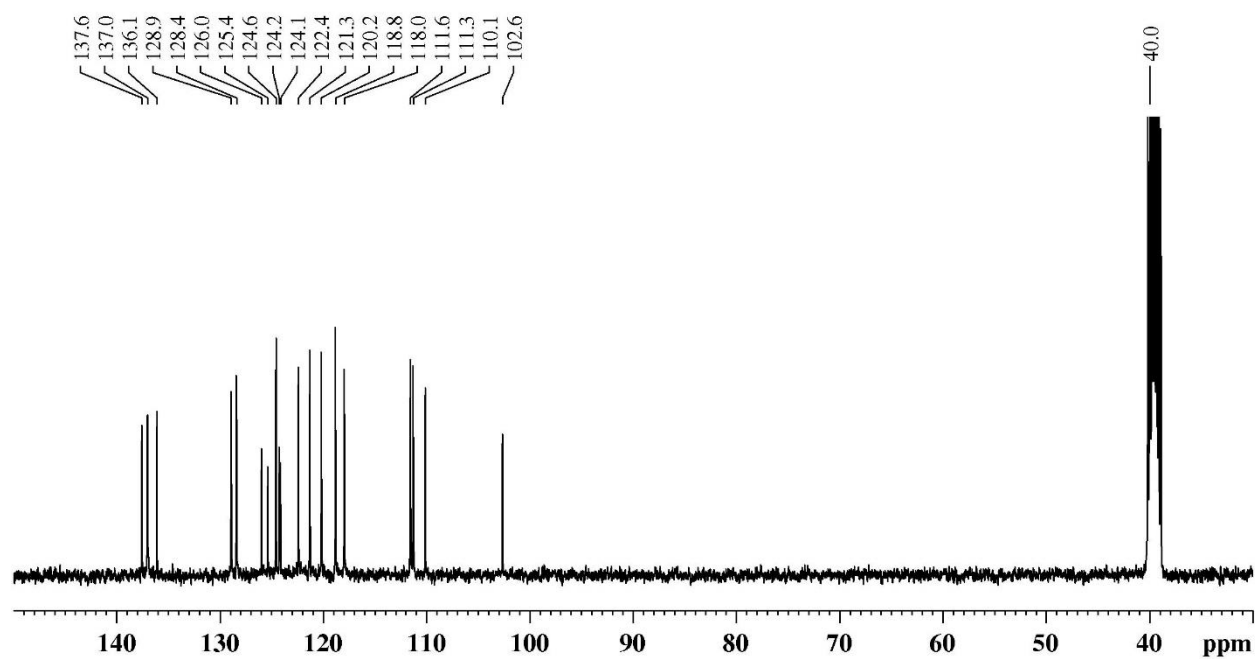
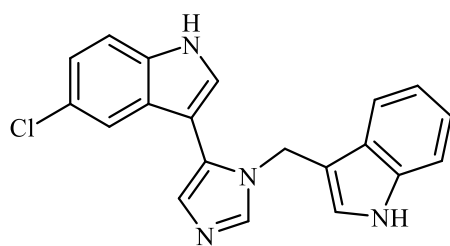
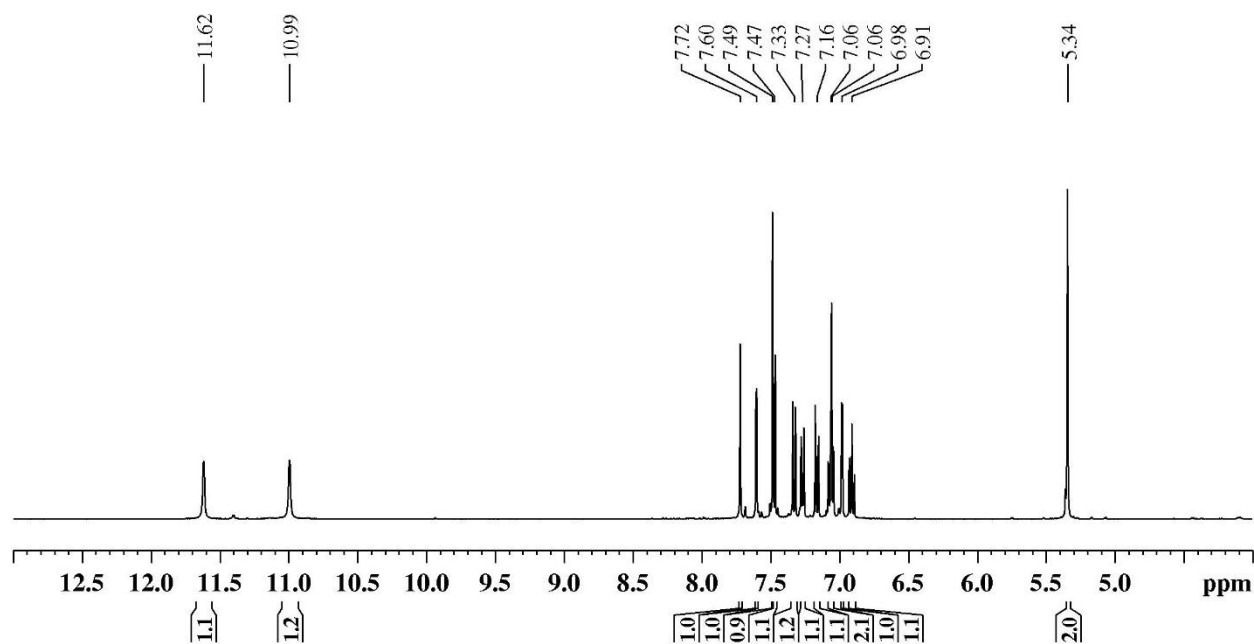


Figure S76. 3-(1-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-5-chloro-1*H*-indole (76)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

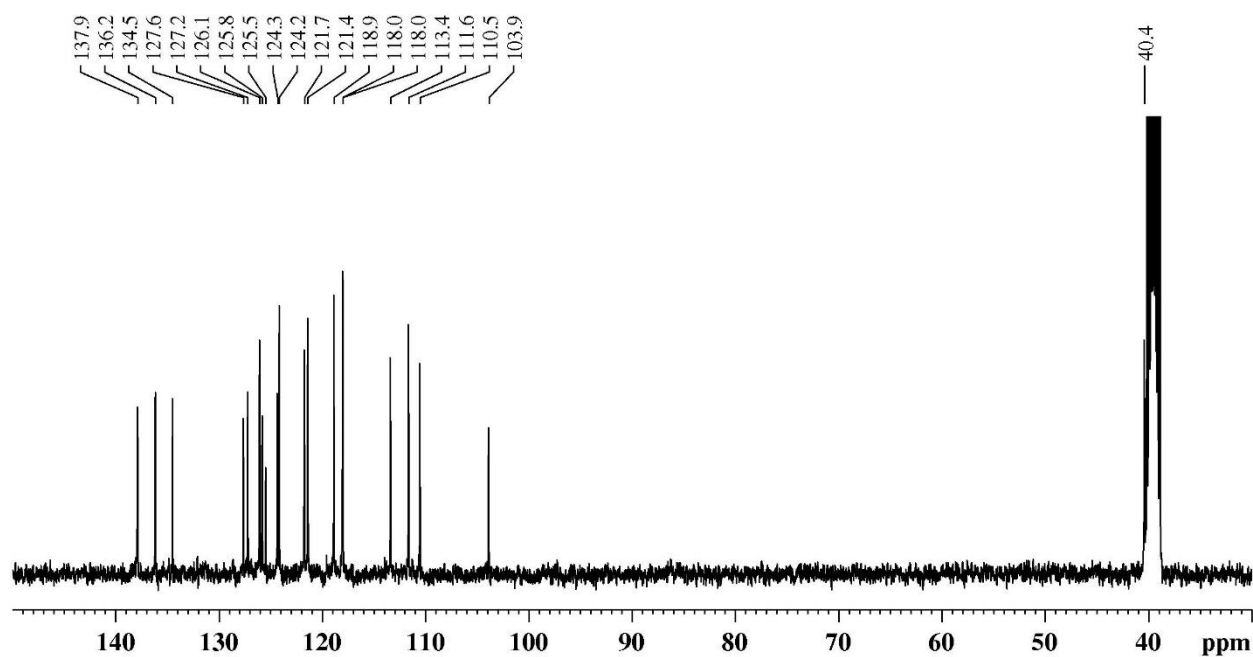
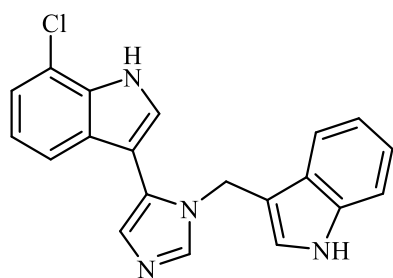
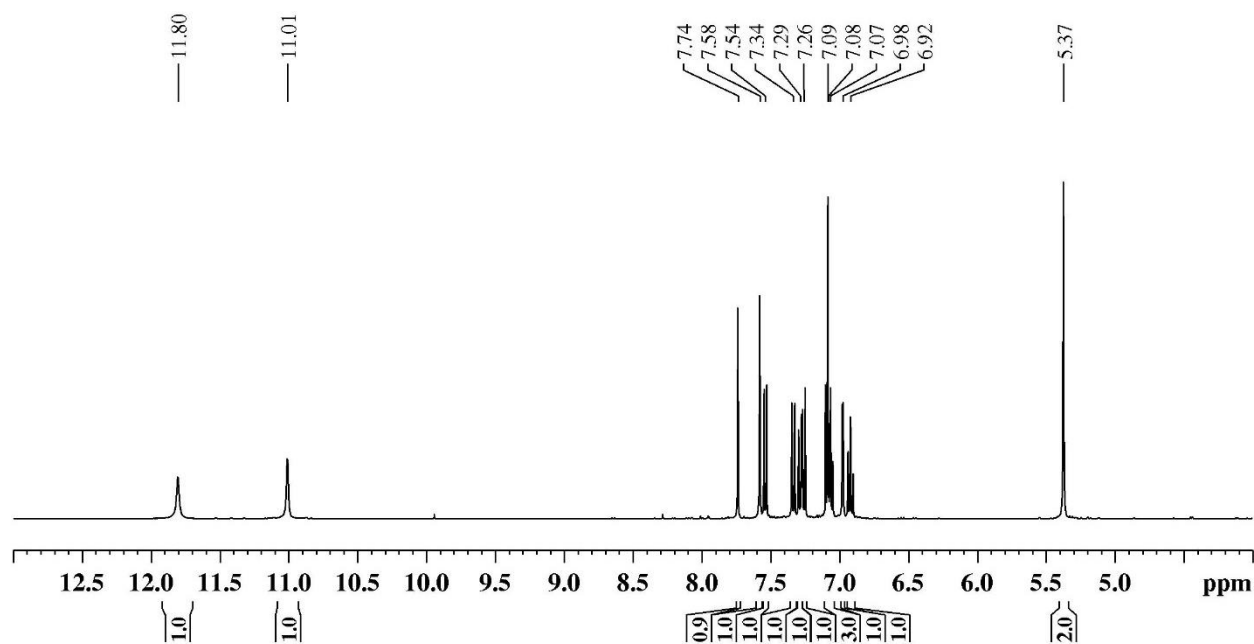


Figure S77. 3-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-7-chloro-1*H*-indole (77)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

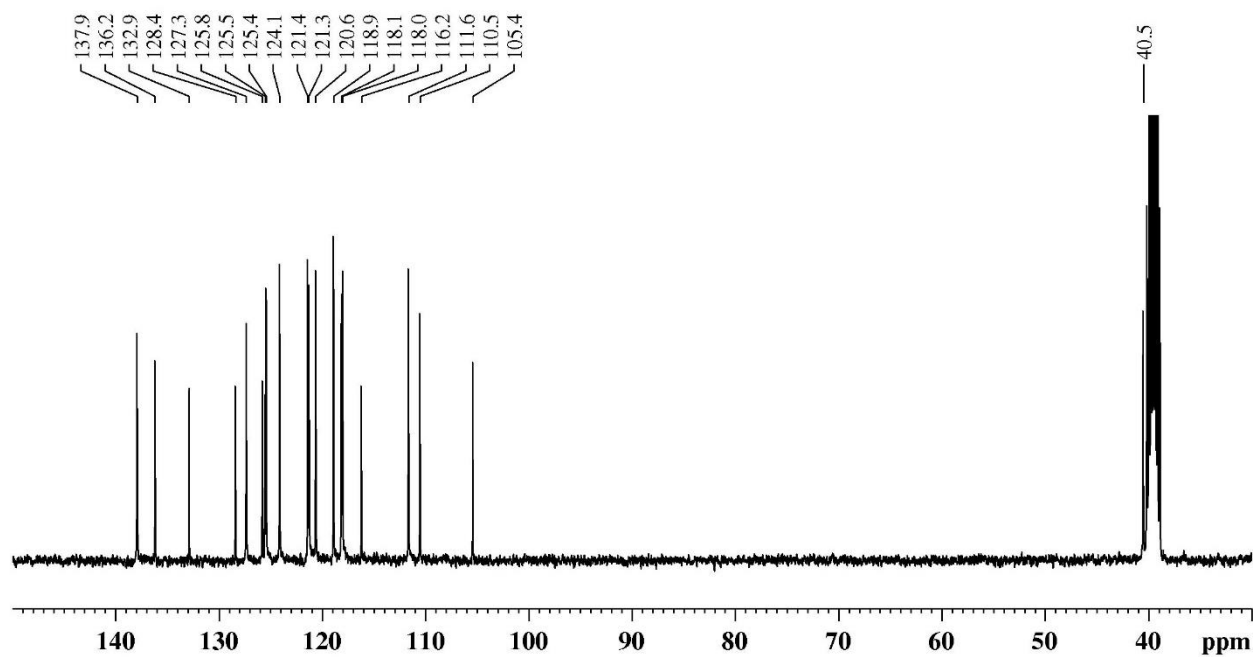
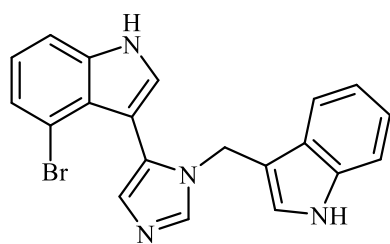
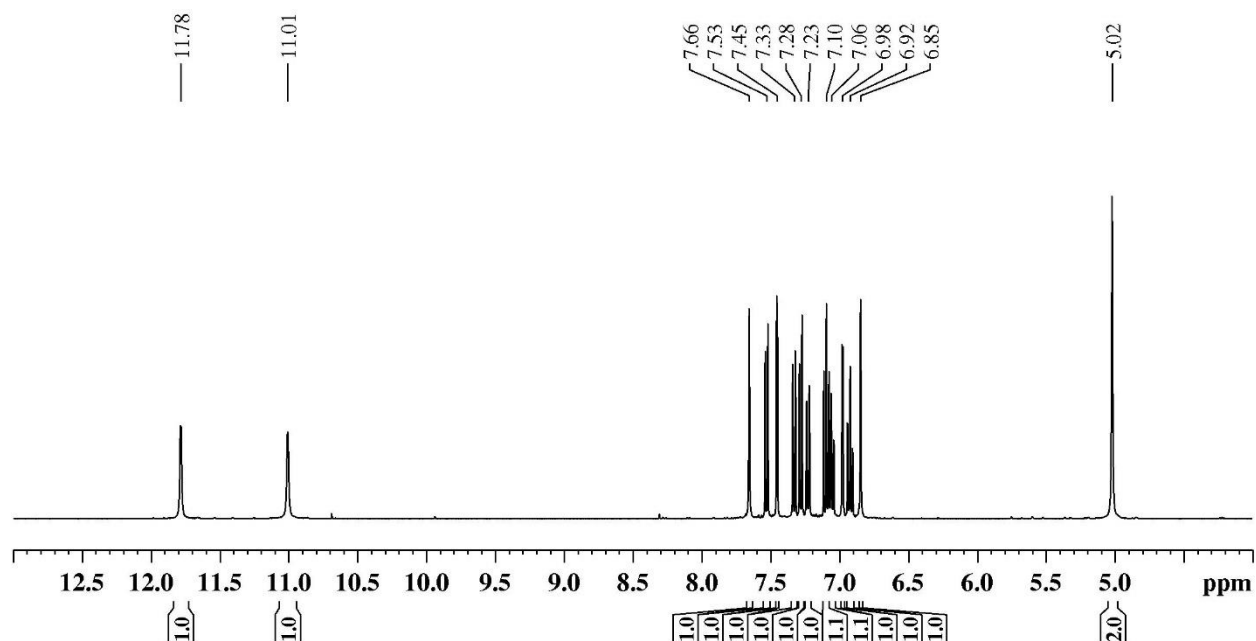


Figure S78. 3-(1-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-4-bromo-1*H*-indole (78)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

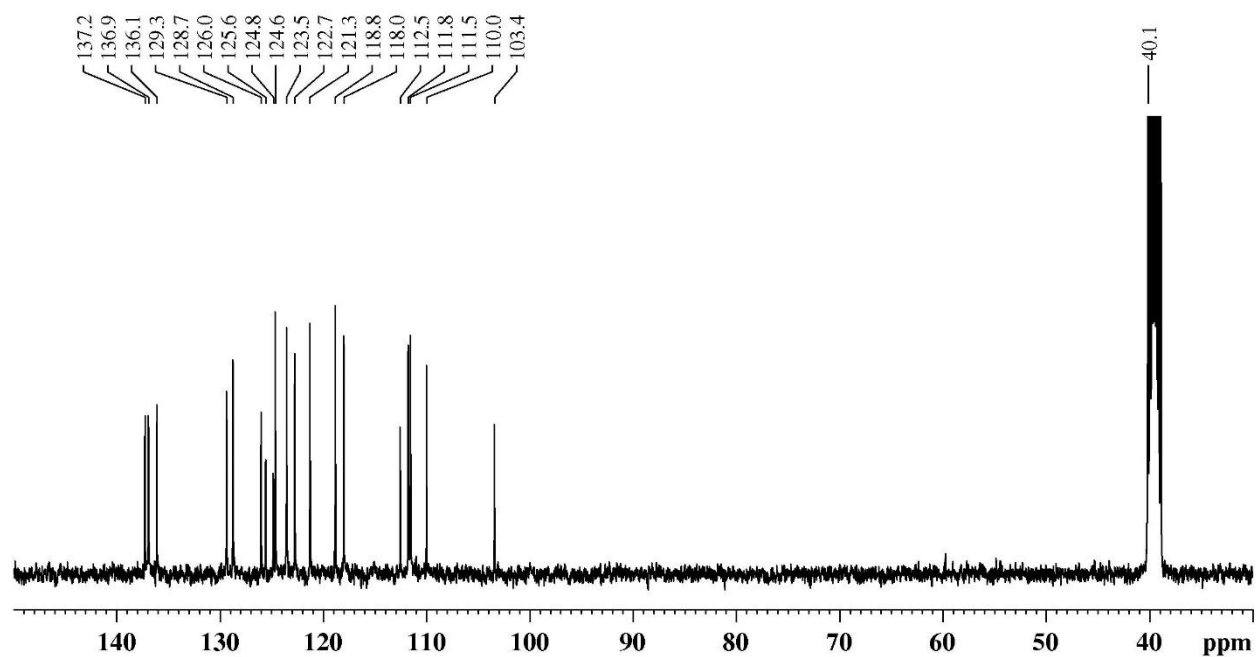
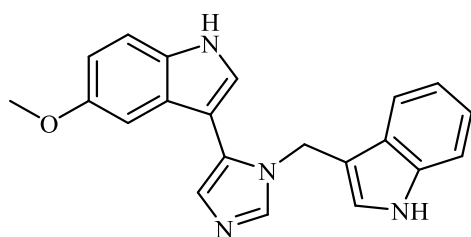
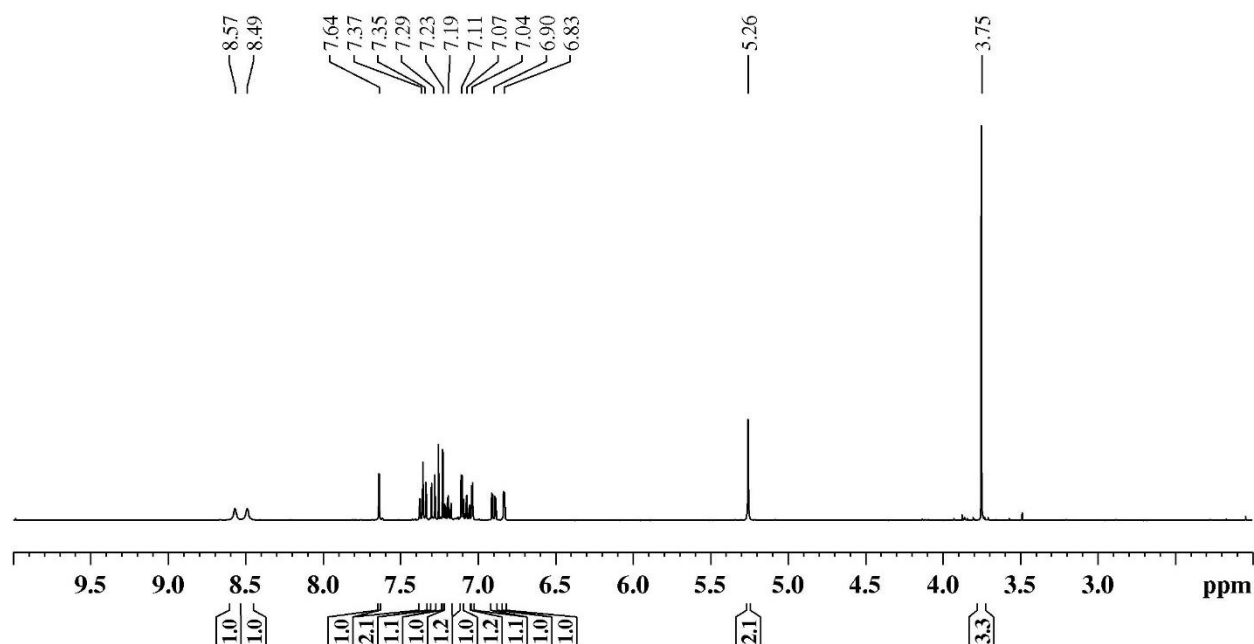


Figure S79. 3-(1-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-5-methoxy-1*H*-indole (**79**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

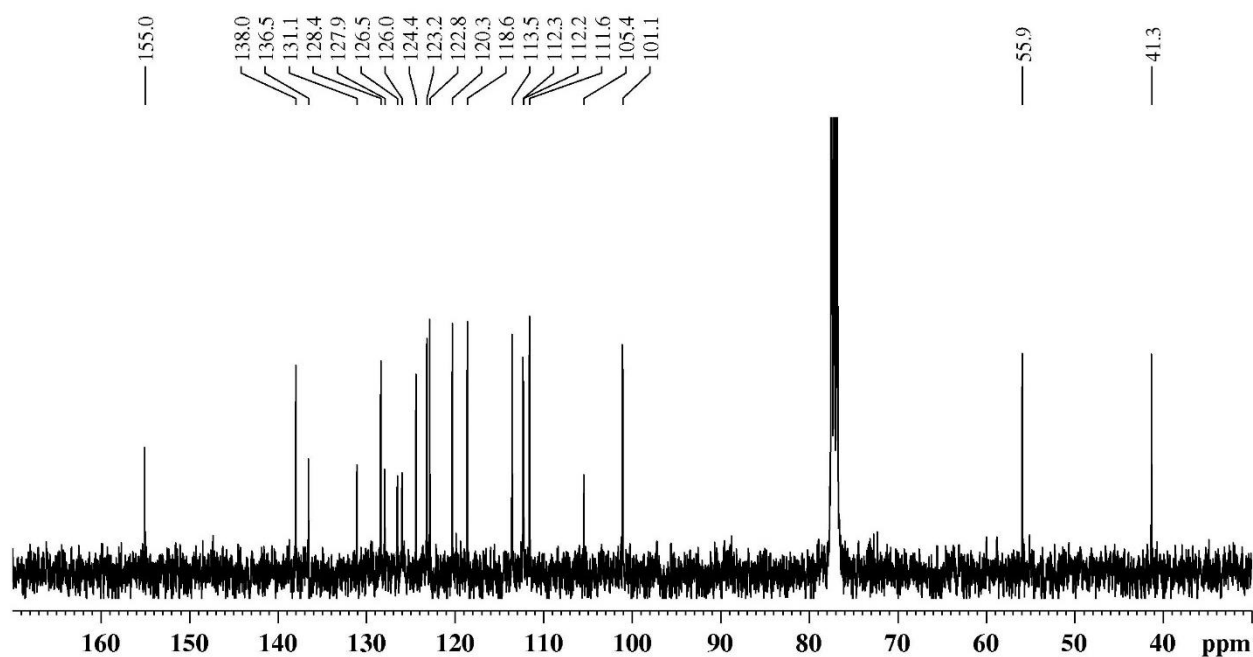
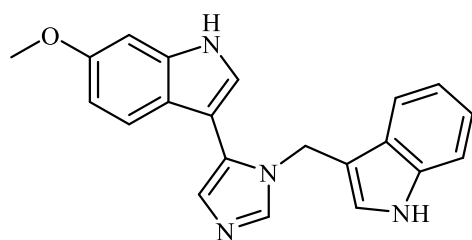
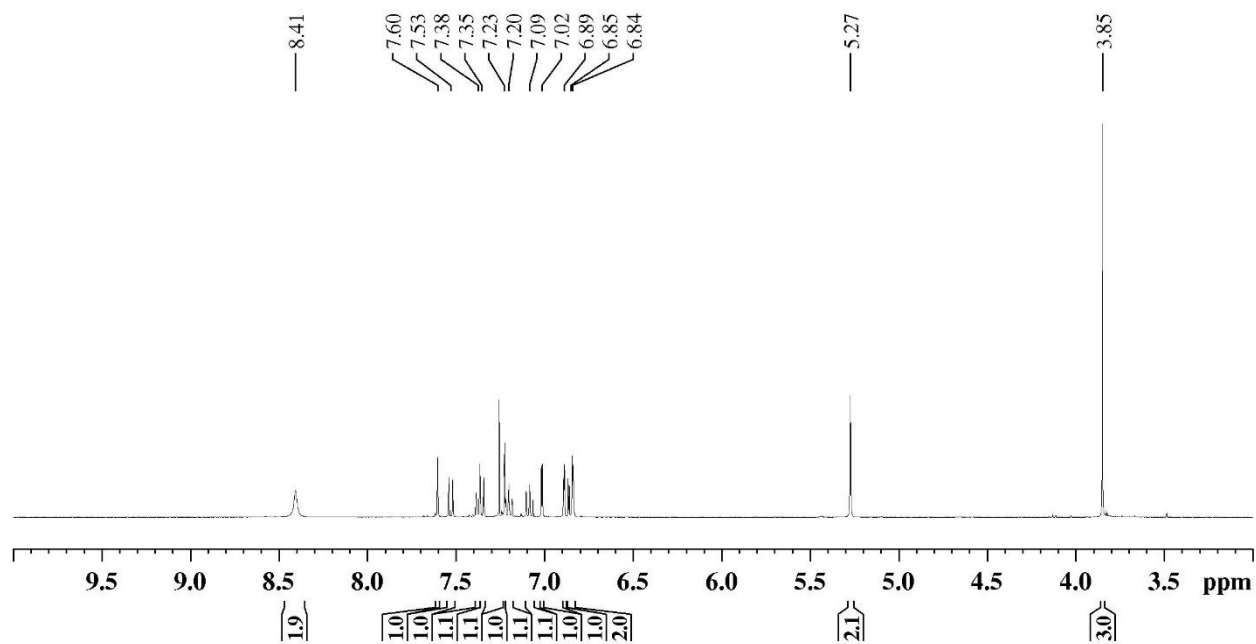


Figure S80. 3-(1-((1*H*-Indol-3-yl)methyl)-1*H*-imidazol-5-yl)-6-methoxy-1*H*-indole (**80**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

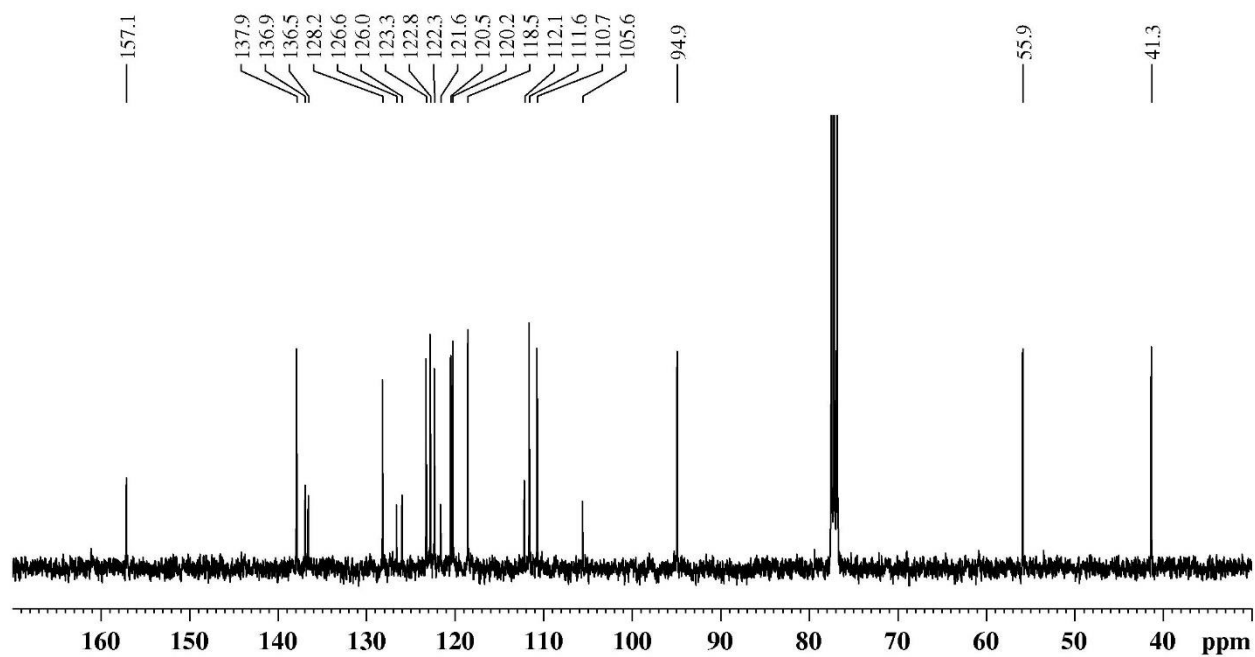
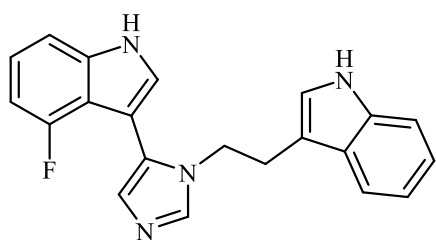
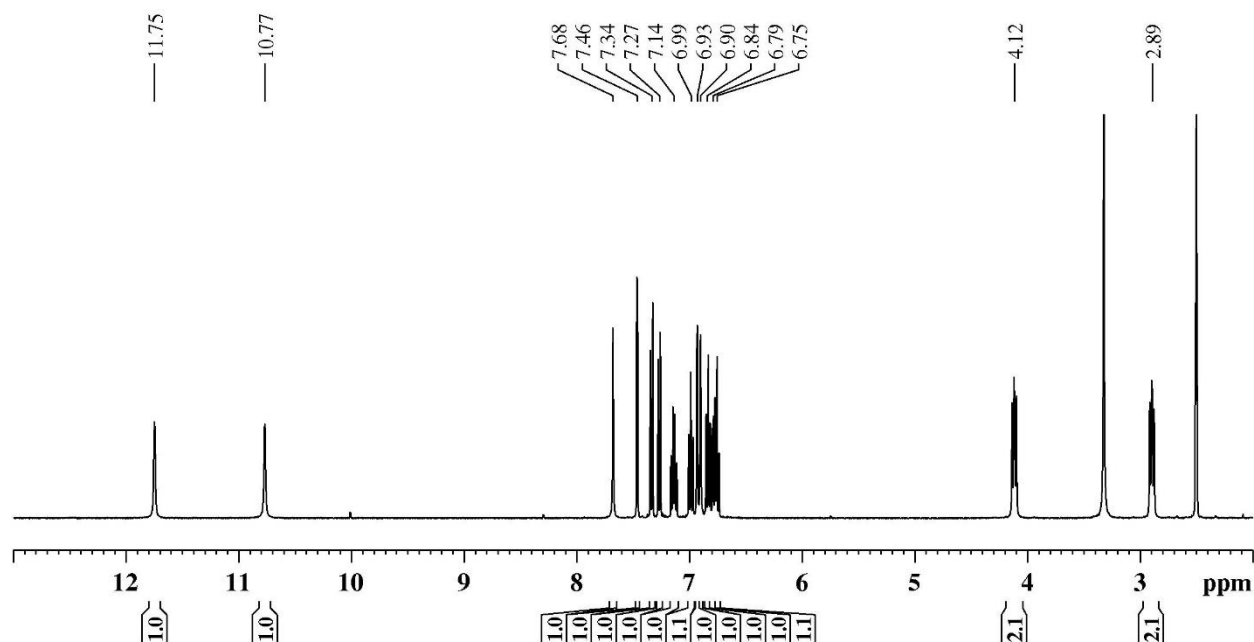


Figure S81. 3-(1-(2-(1*H*-Indol-3-yl)ethyl)-1*H*-imidazol-5-yl)-4-fluoro-1*H*-indole (**81**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

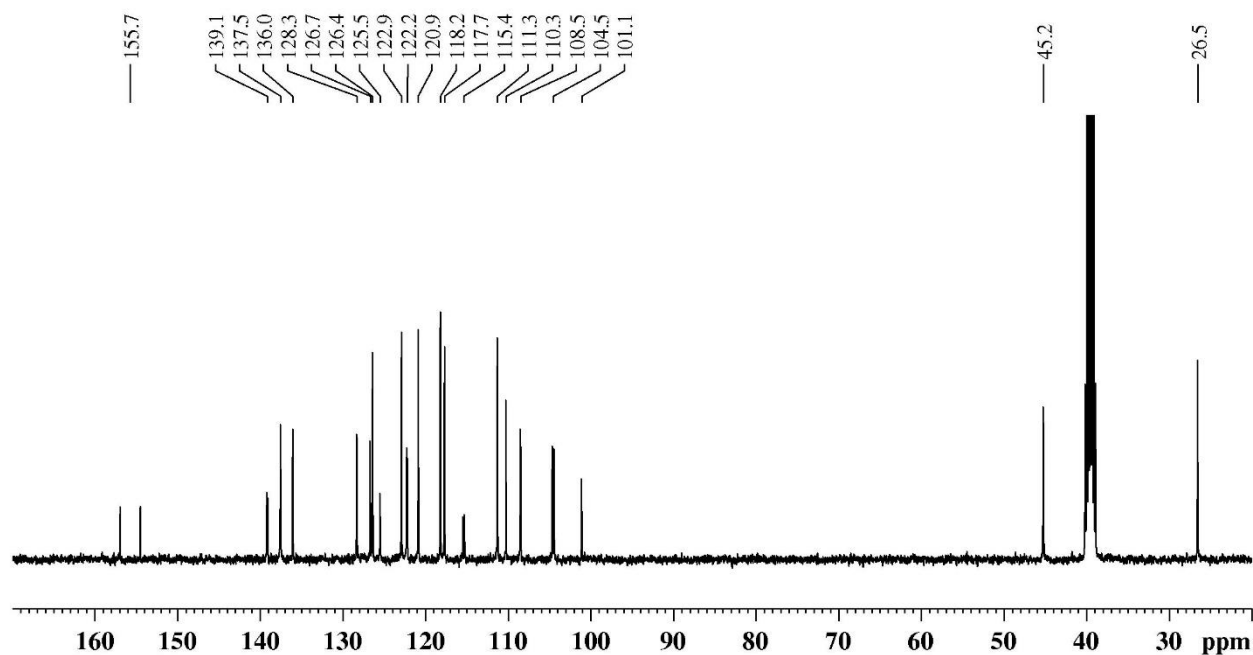
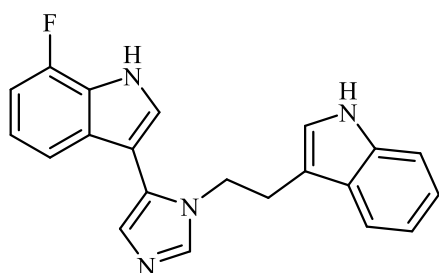
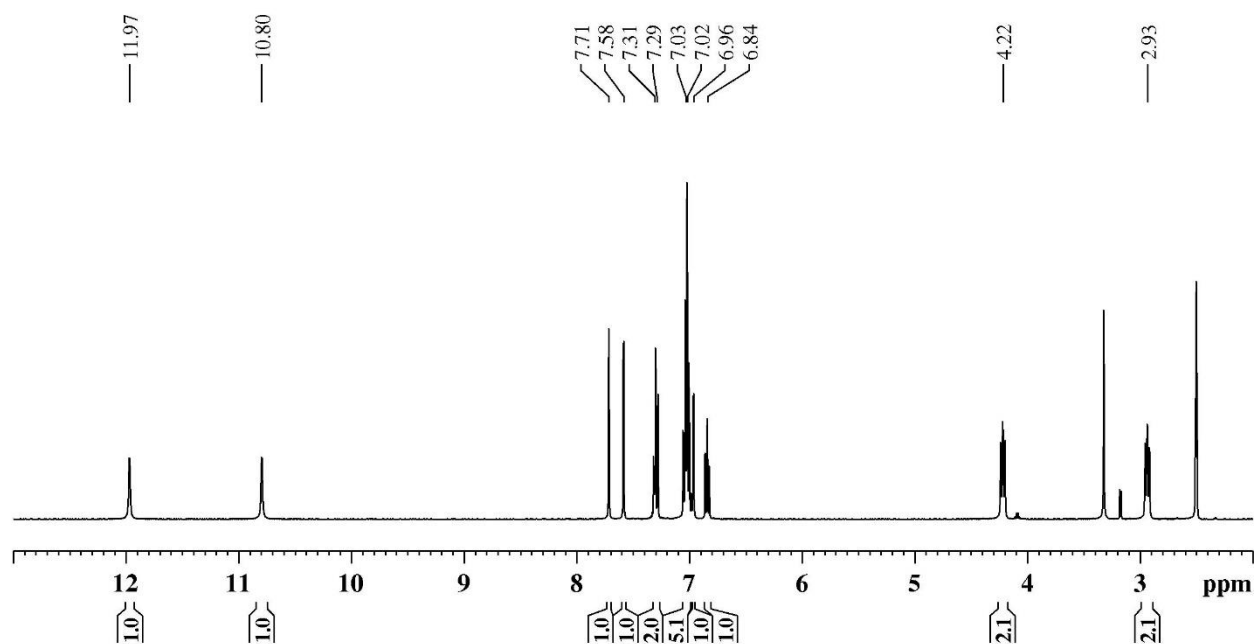


Figure S82. 3-(1-(2-(1*H*-Indol-3-yl)ethyl)-1*H*-imidazol-5-yl)-7-fluoro-1*H*-indole (**82**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

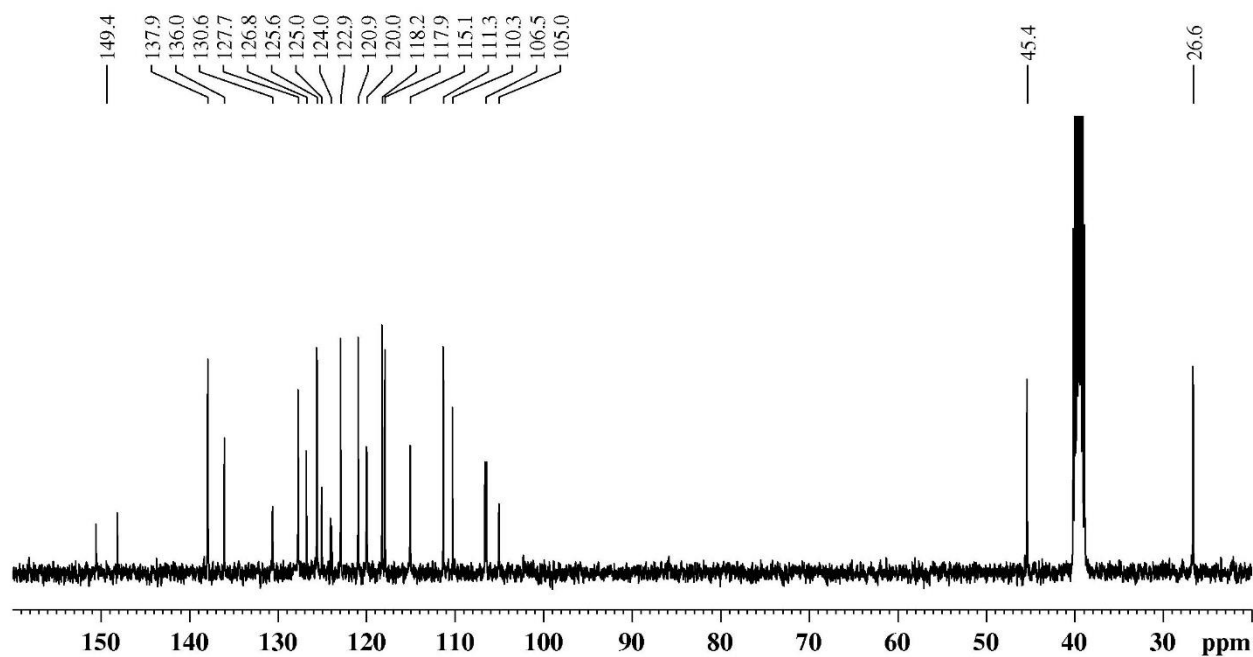
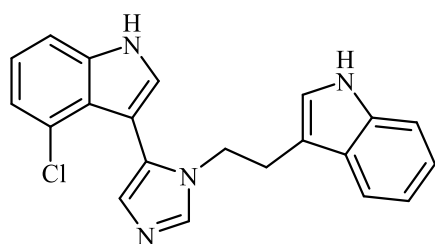
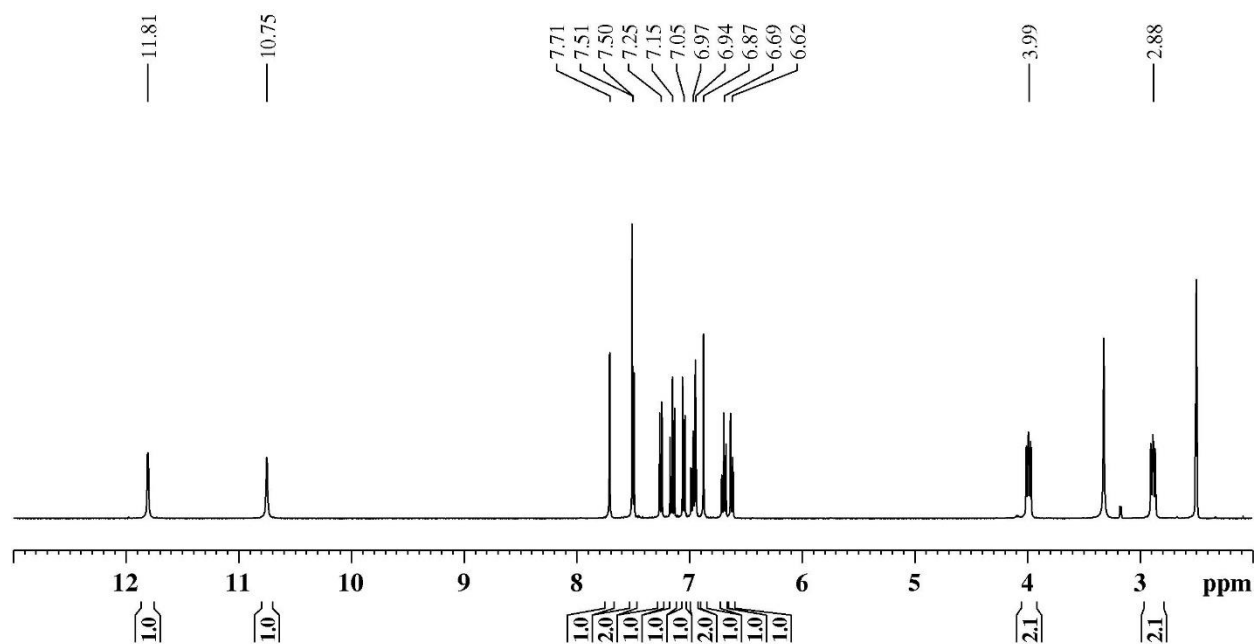


Figure S83. 3-(1-(2-(1*H*-Indol-3-yl)ethyl)-1*H*-imidazol-5-yl)-4-chloro-1*H*-indole (**83**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

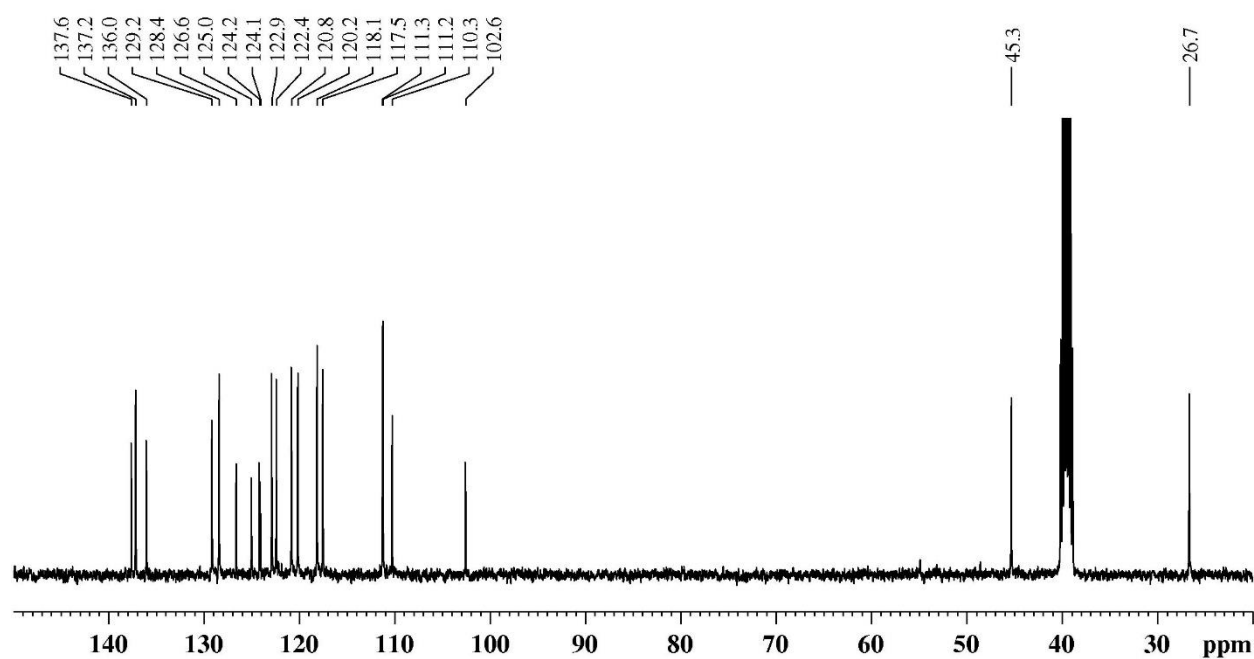
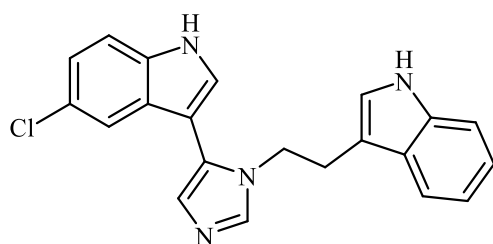
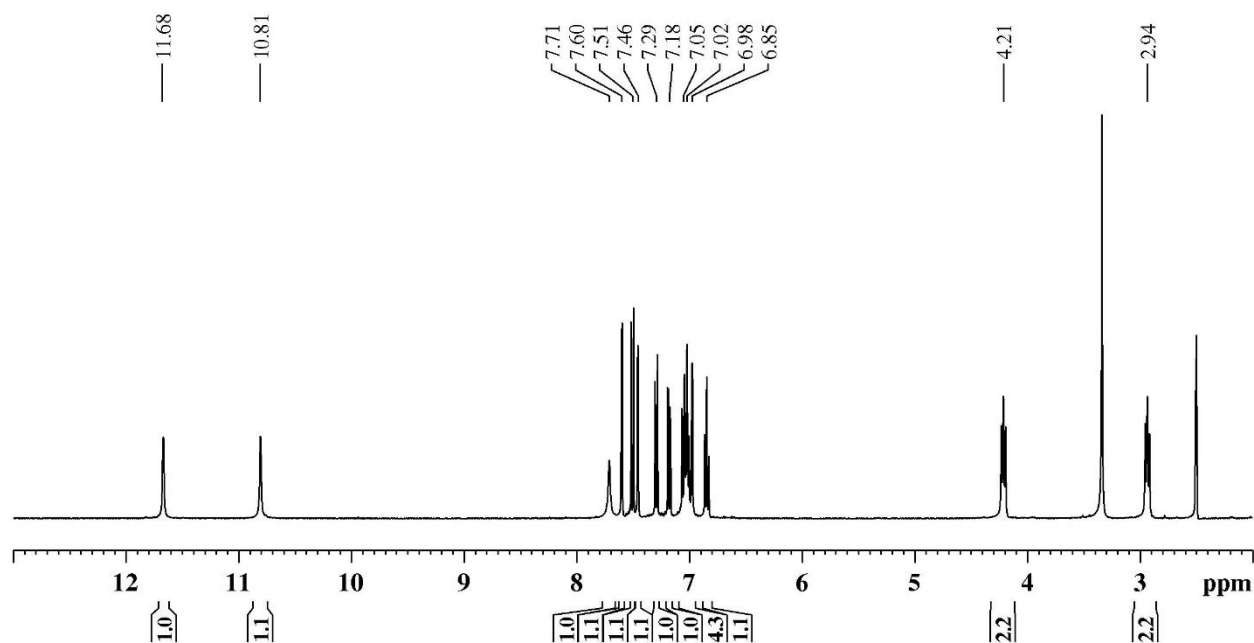


Figure S84. 3-(1-(2-(1*H*-Indol-3-yl)ethyl)-1*H*-imidazol-5-yl)-5-chloro-1*H*-indole (**84**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

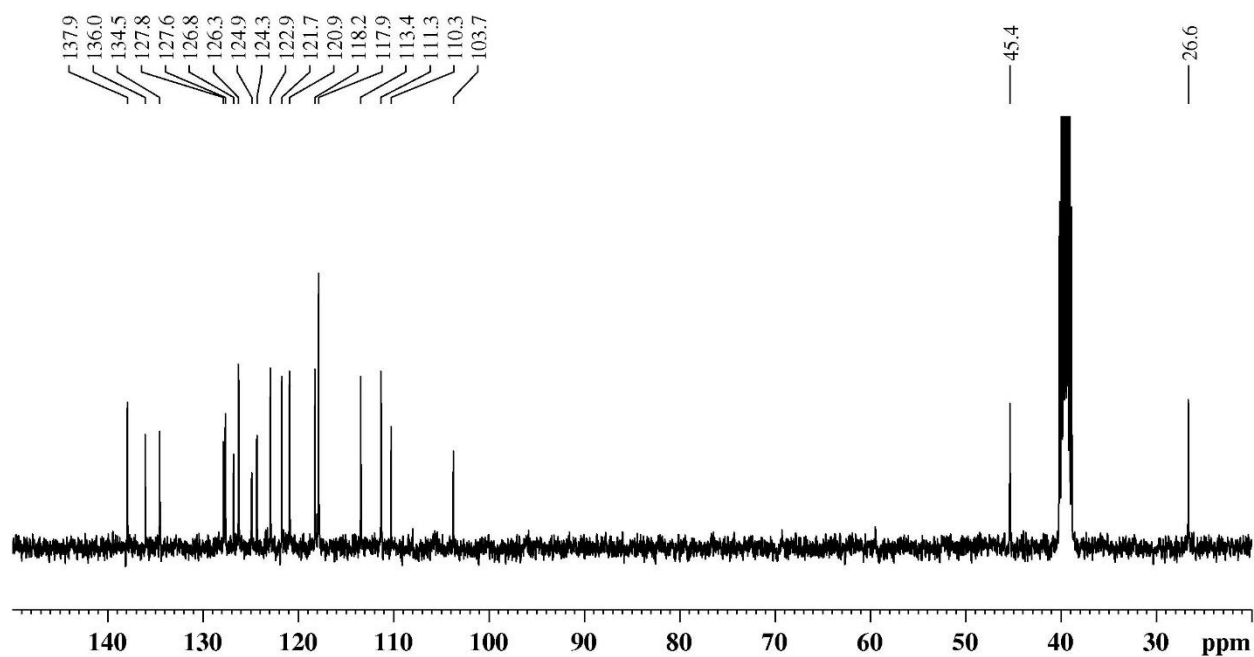
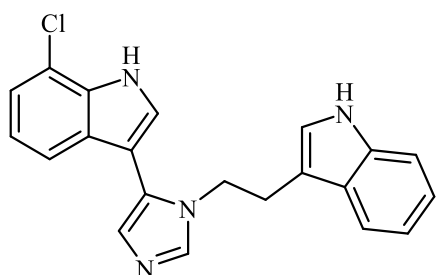
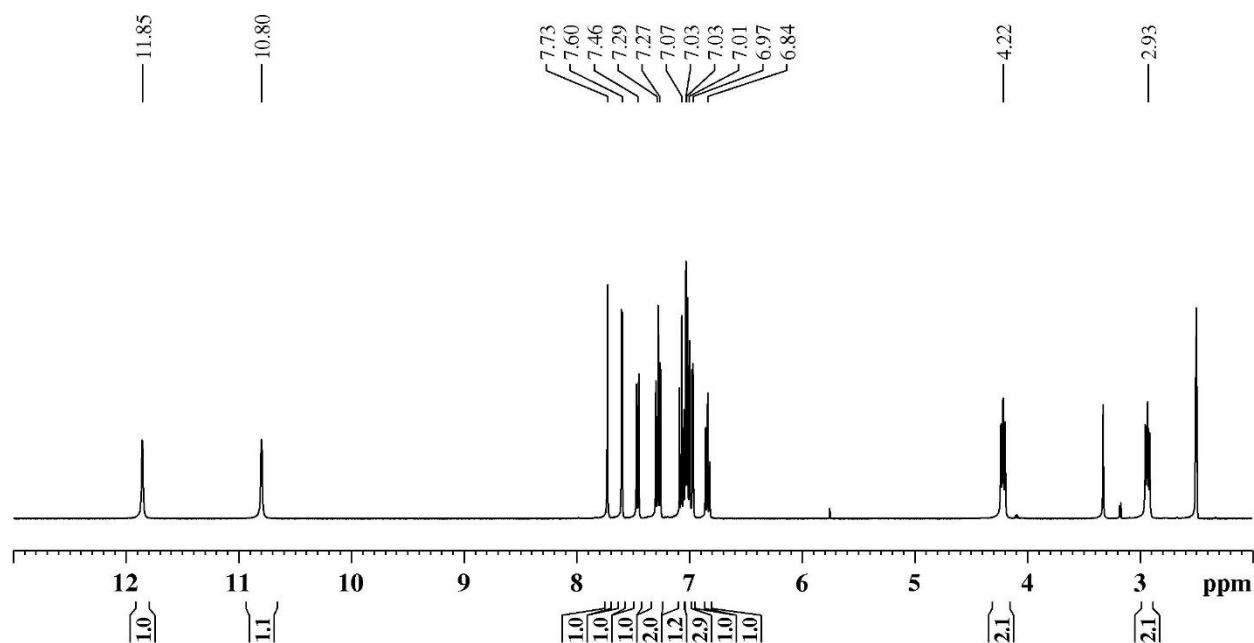


Figure S85. 3-(1-(2-(1*H*-Indol-3-yl)ethyl)-1*H*-imidazol-5-yl)-7-chloro-1*H*-indole (85)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

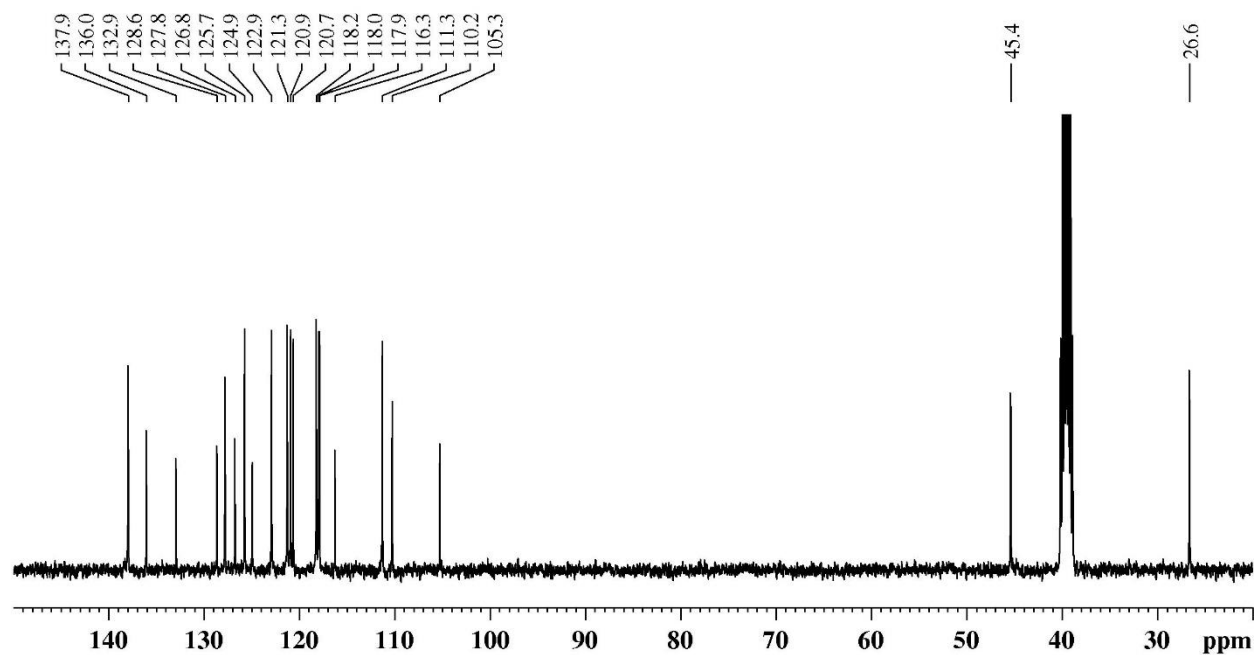
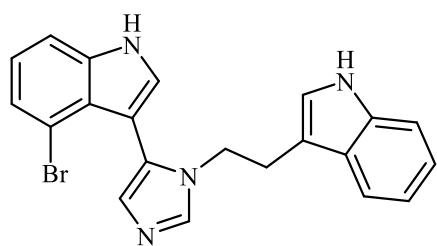
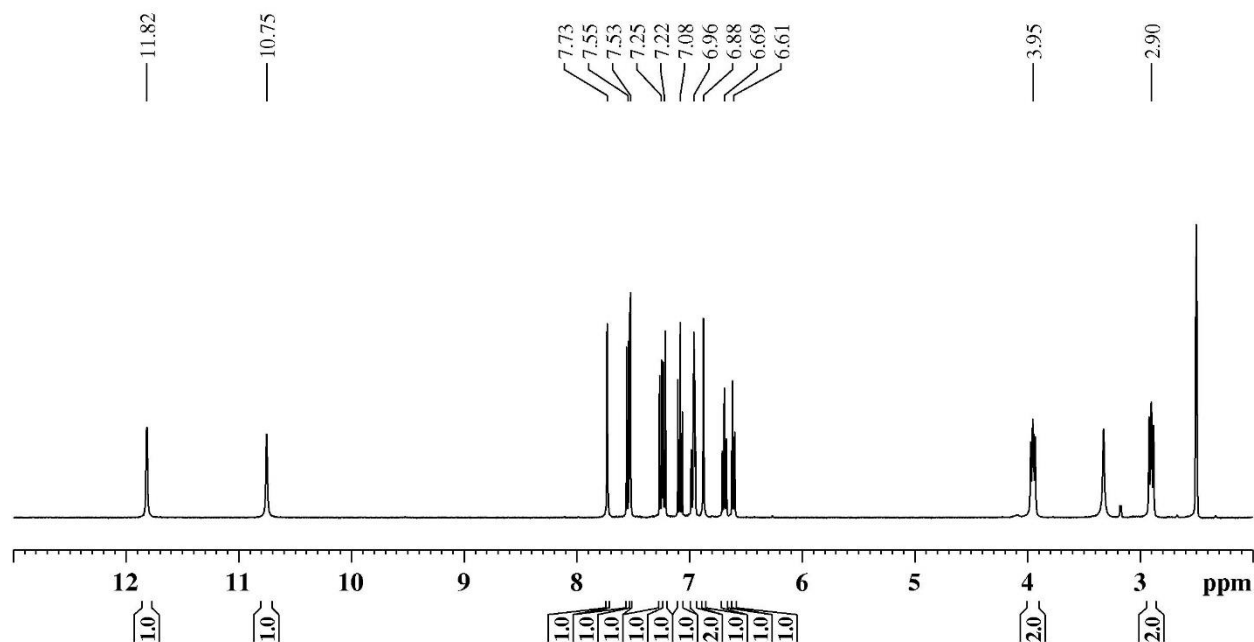


Figure S86. 3-(1-(2-(1H-Indol-3-yl)ethyl)-1H-imidazol-5-yl)-4-bromo-1H-indole (**86**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

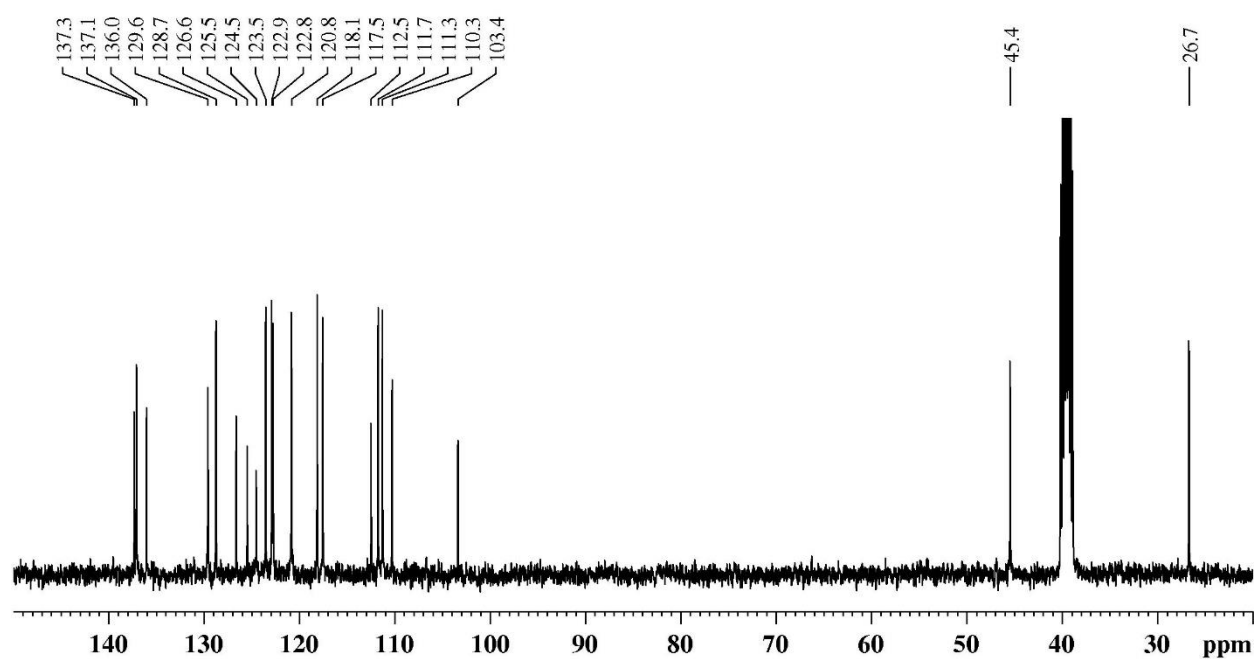
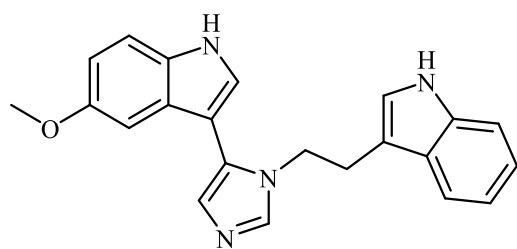
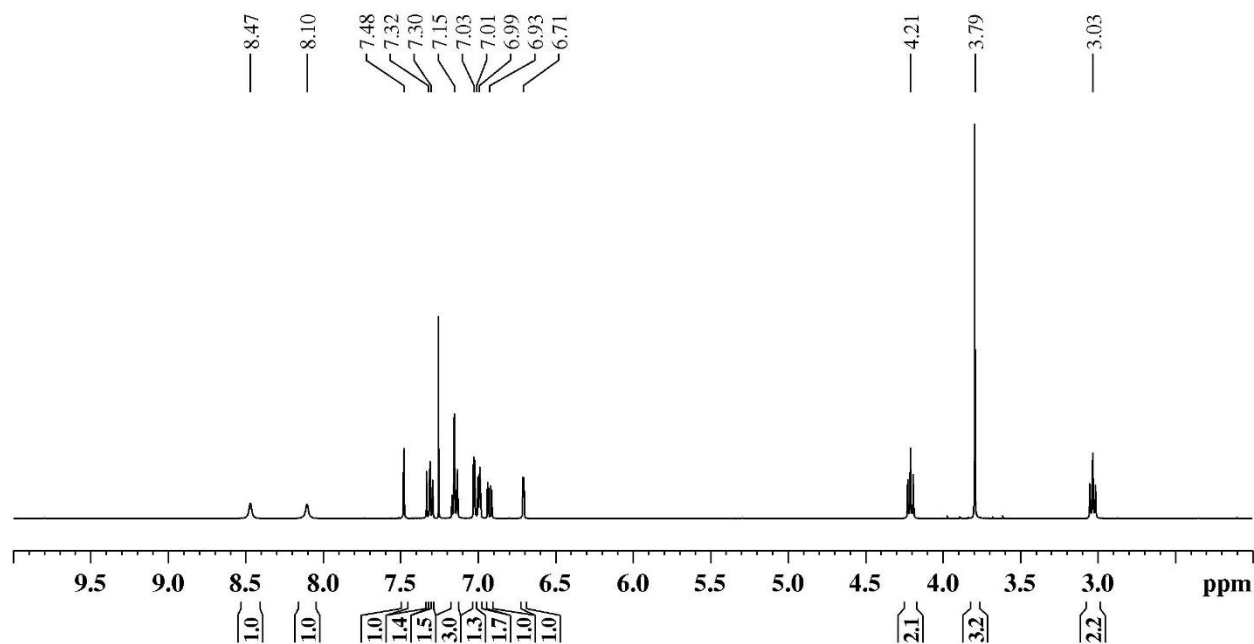


Figure S87. 3-(1-(2-(1*H*-Indol-3-yl)ethyl)-1*H*-imidazol-5-yl)-5-methoxy-1*H*-indole (**87**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

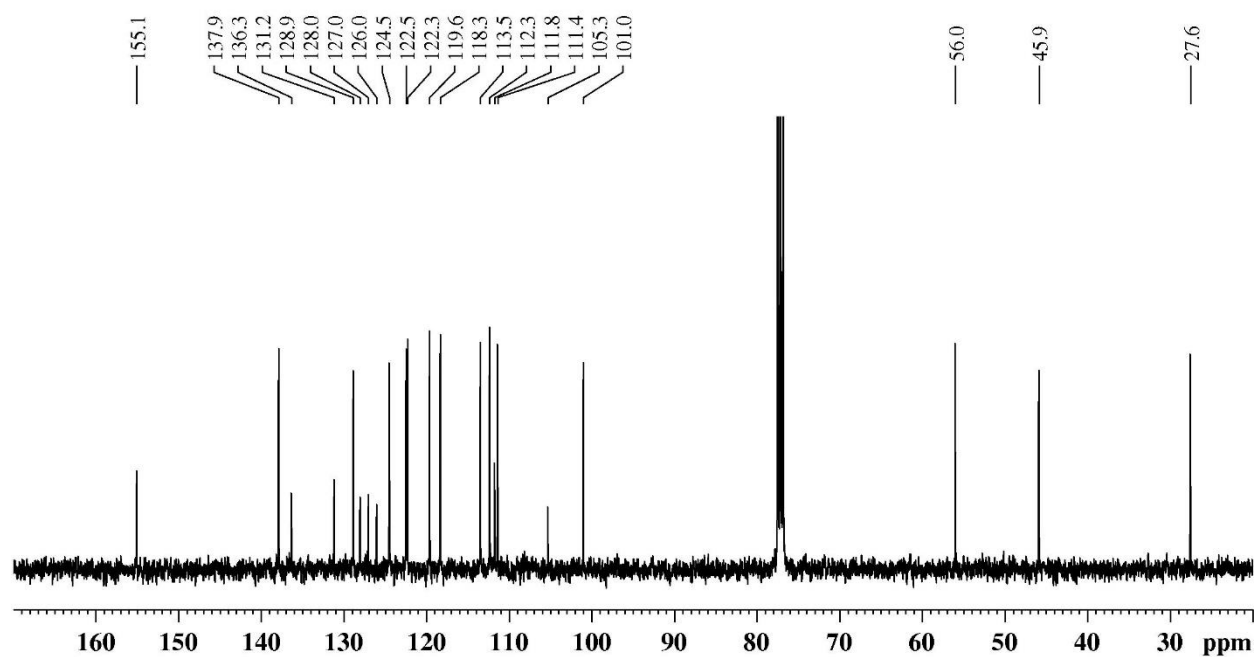
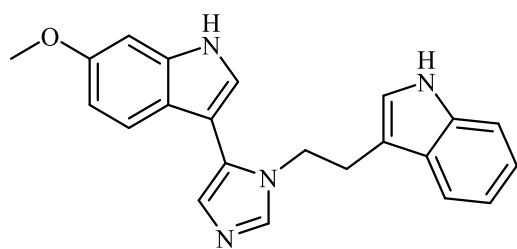
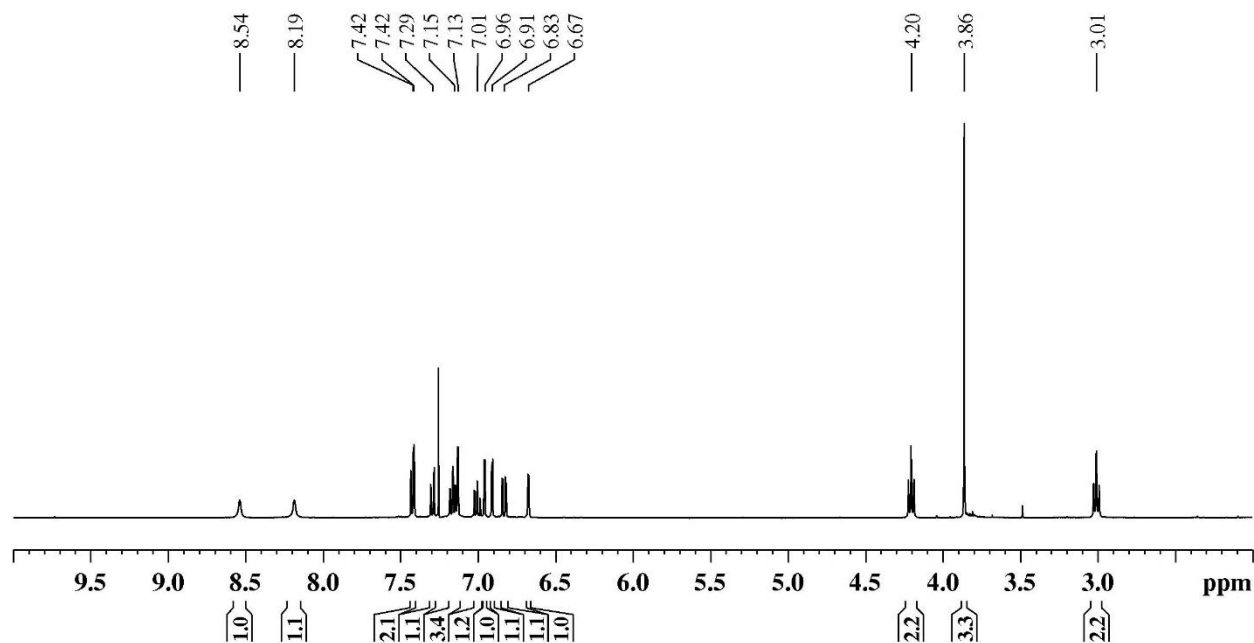


Figure S88. 3-(1-(2-(1*H*-Indol-3-yl)ethyl)-1*H*-imidazol-5-yl)-6-methoxy-1*H*-indole (**88**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

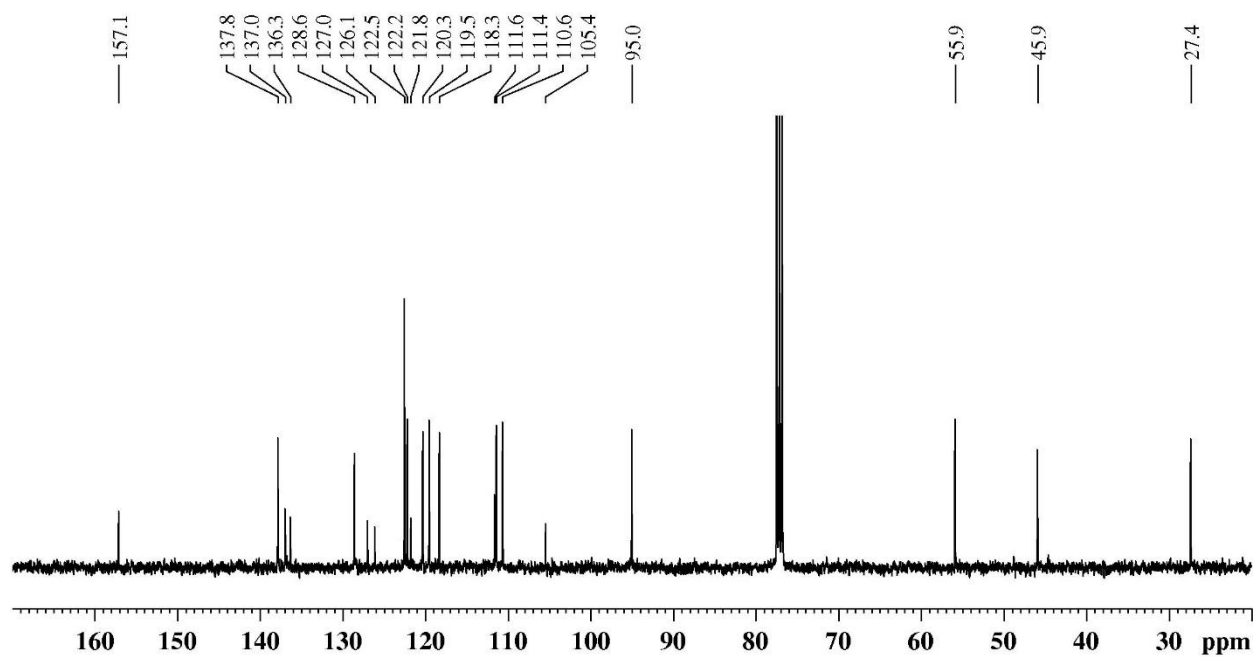
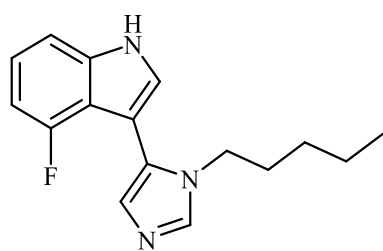
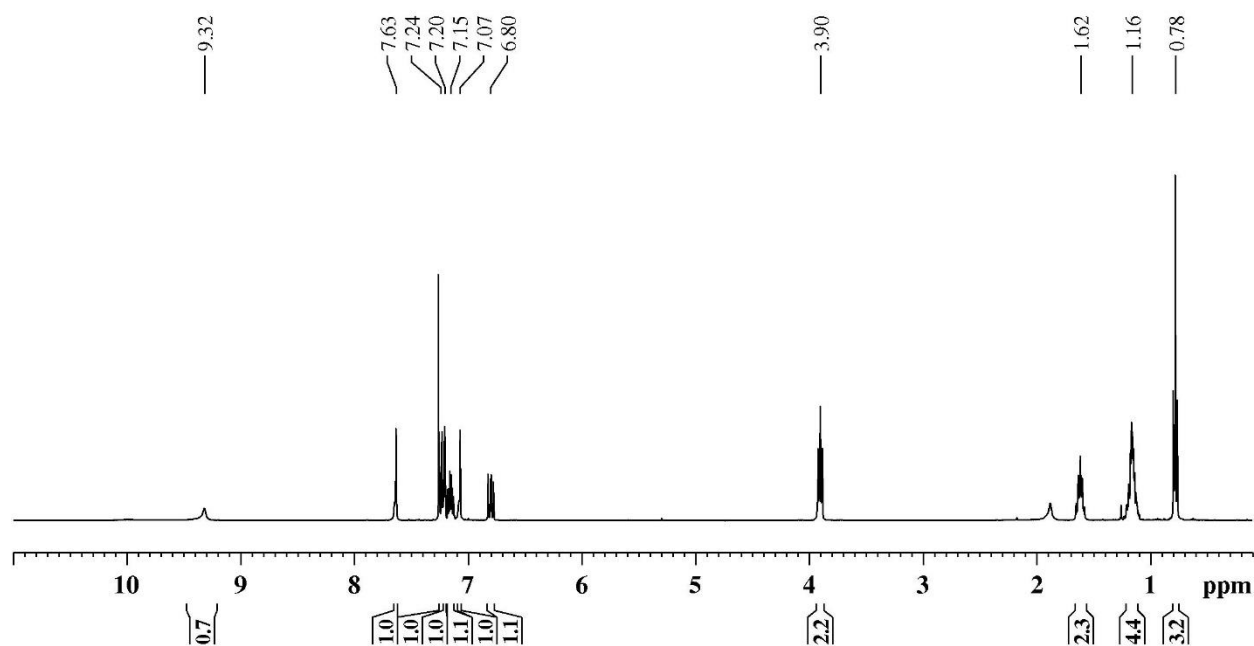


Figure S89. 4-Fluoro-3-(1-pentyl-1H-imidazol-5-yl)-1H-indole (**89**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

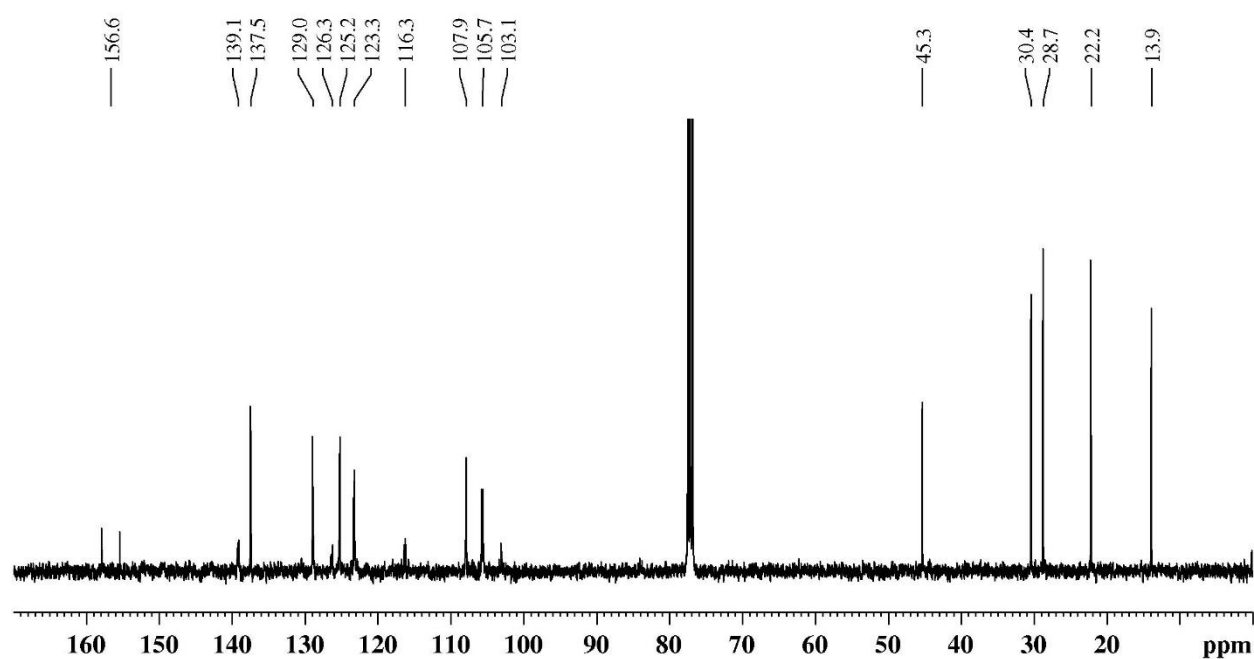
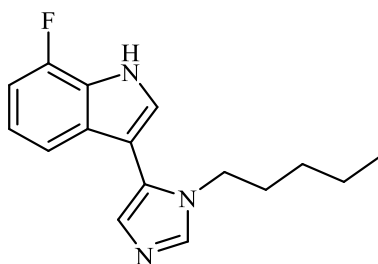
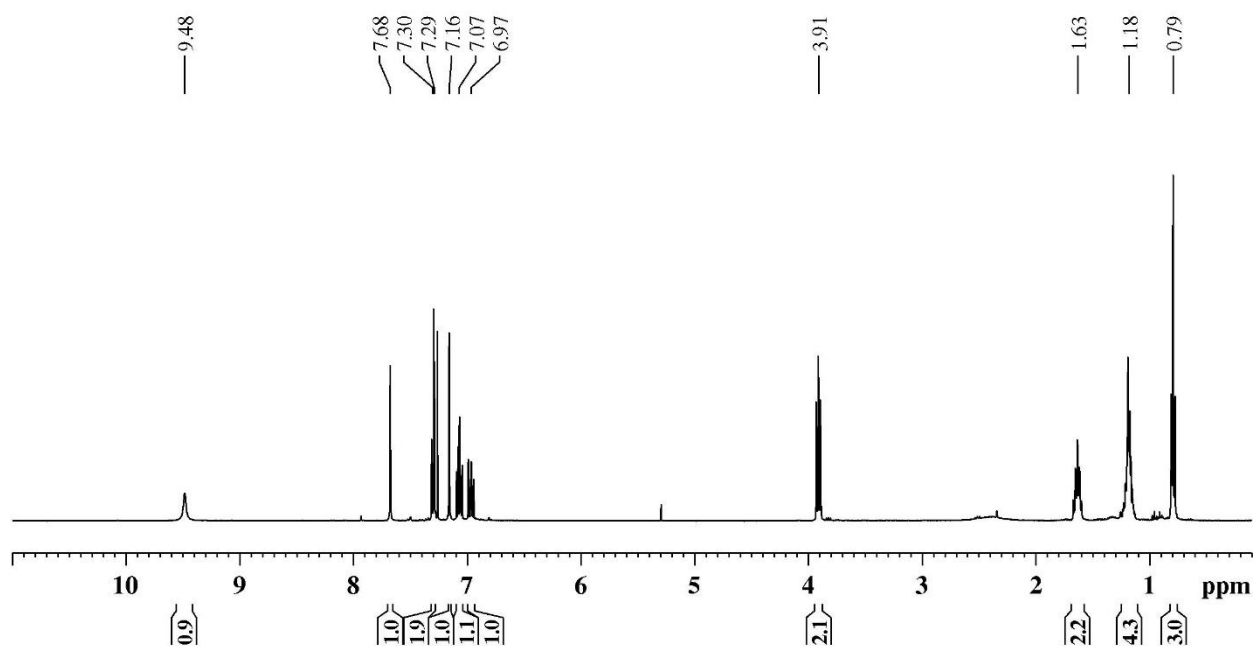


Figure S90. 7-Fluoro-3-(1-pentyl-1H-imidazol-5-yl)-1H-indole (90)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

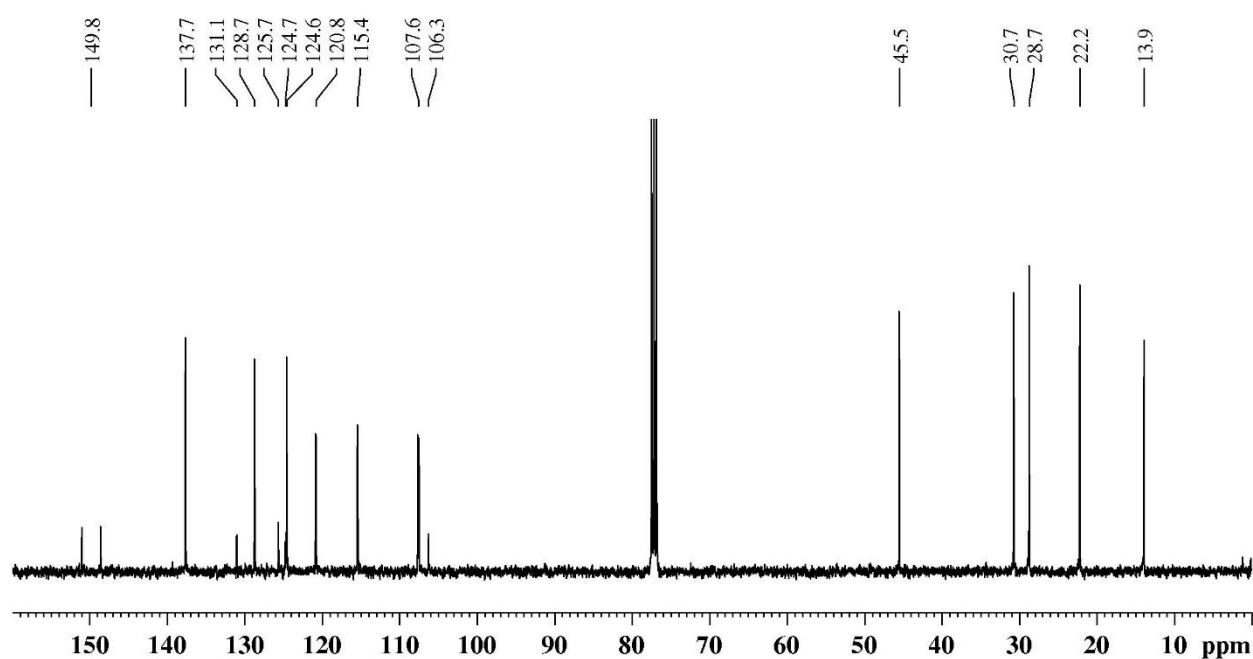
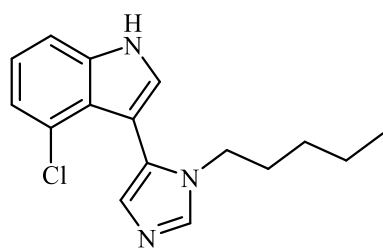
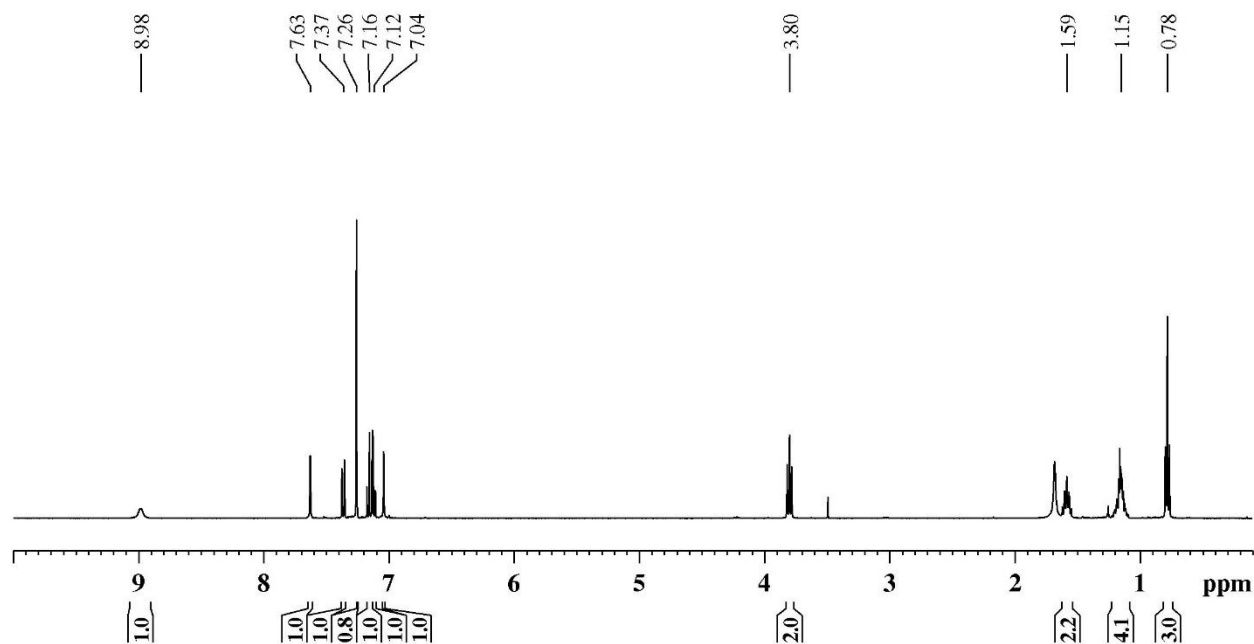


Figure S91. 4-Chloro-3-(1-pentyl-1*H*-imidazol-5-yl)-1*H*-indole (**91**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

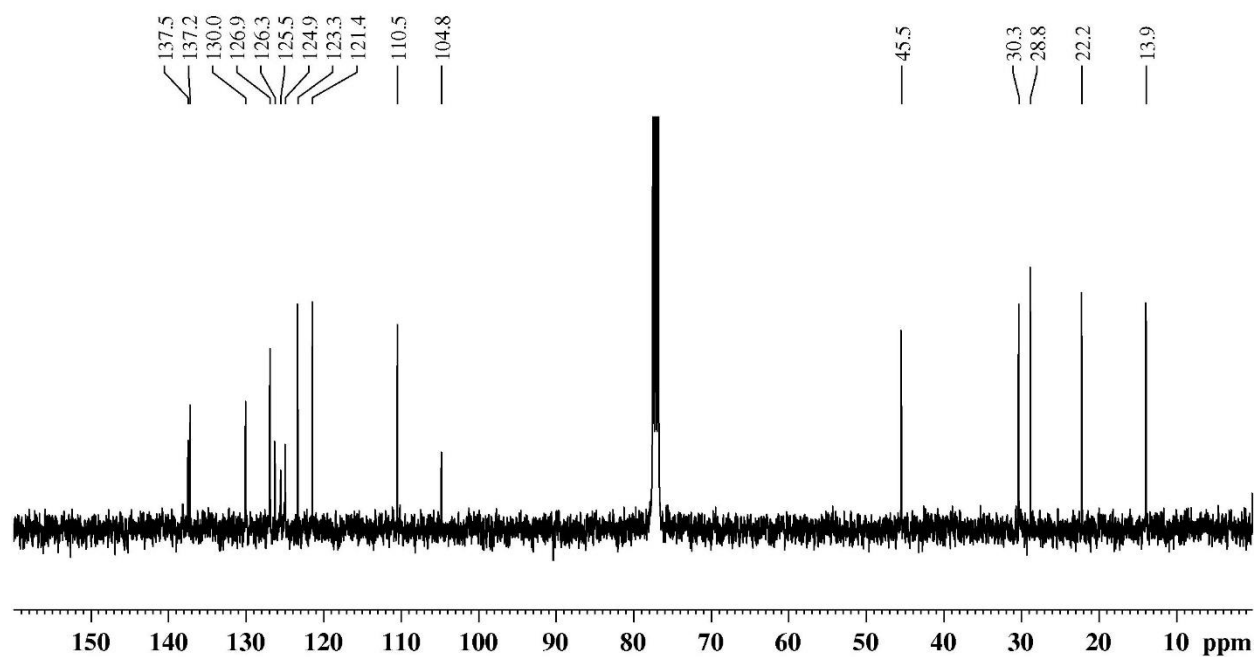
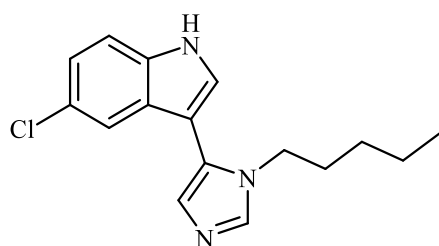
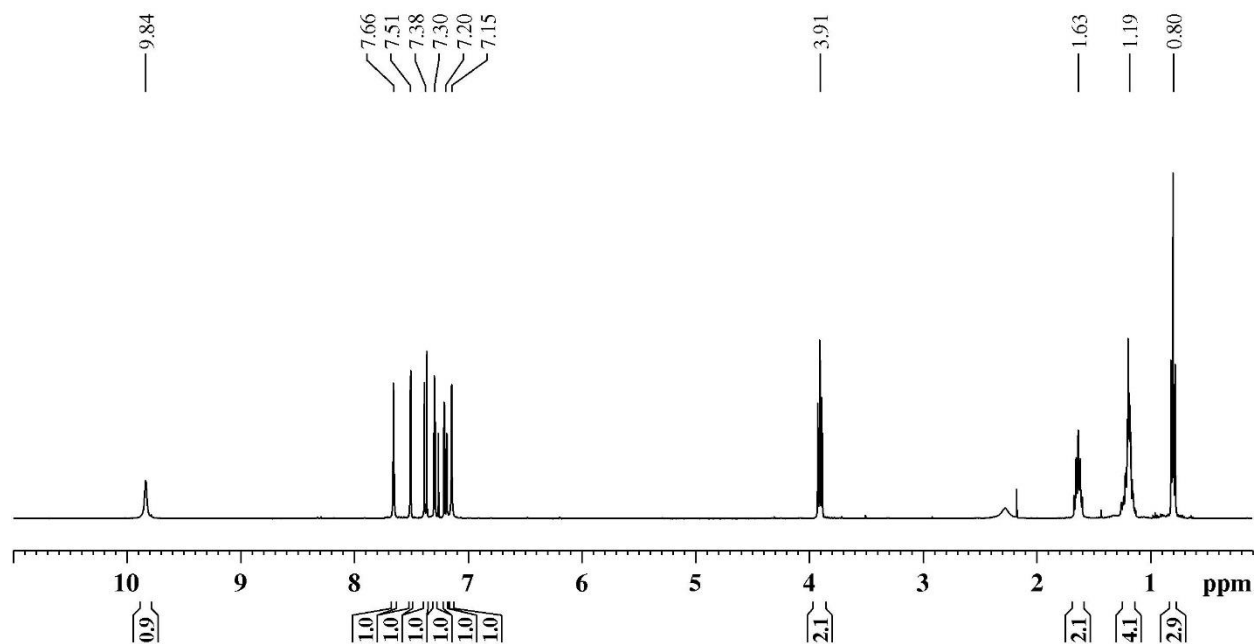


Figure S92. 5-Chloro-3-(1-pentyl-1H-imidazol-5-yl)-1H-indole (**92**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

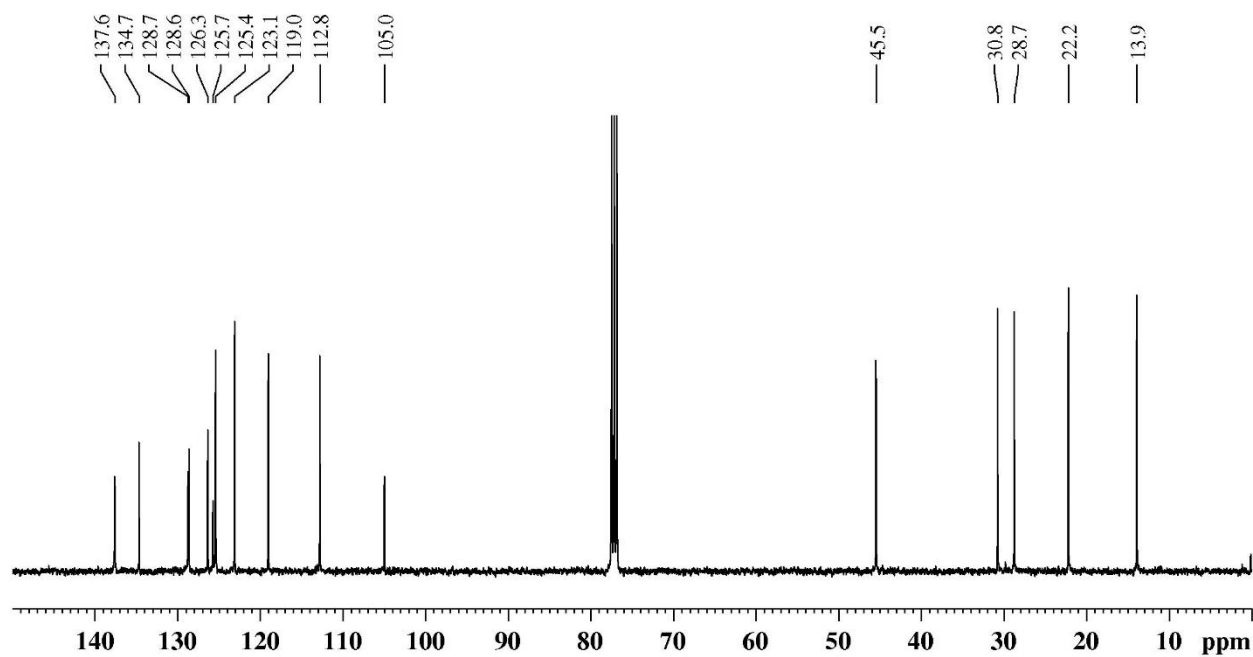
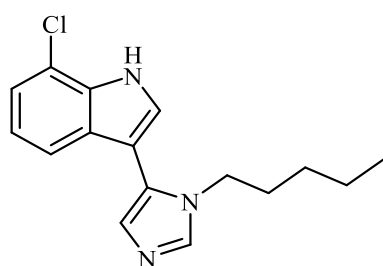
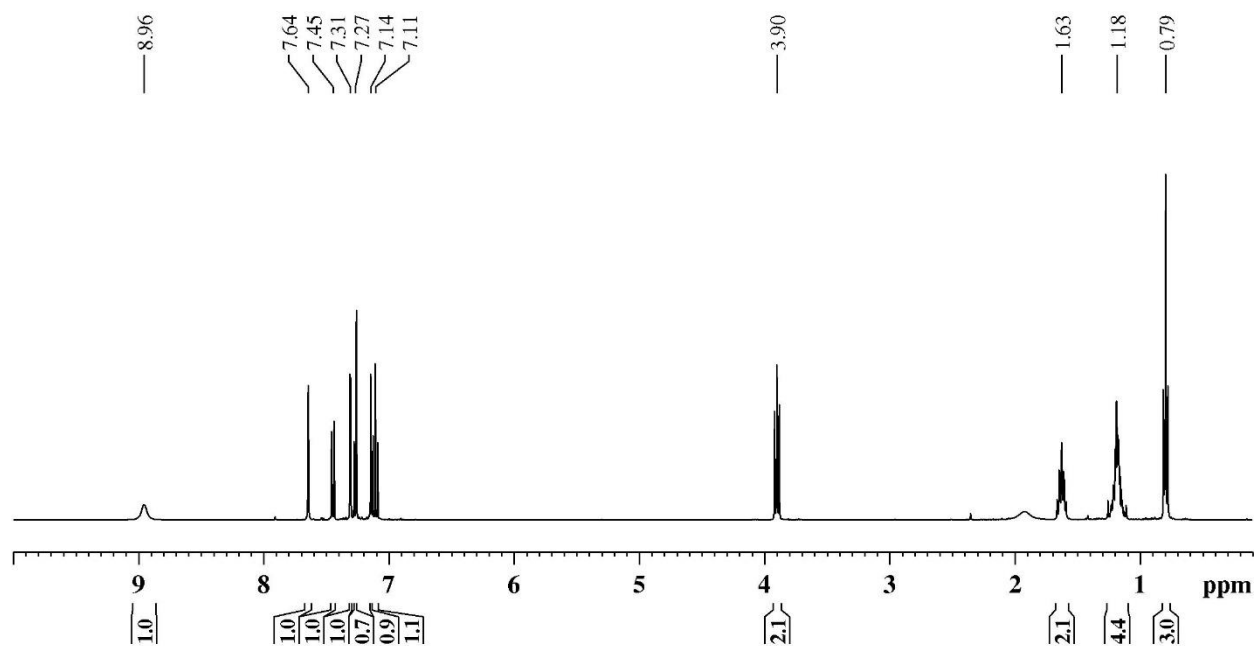


Figure S93. 7-Chloro-3-(1-pentyl-1H-imidazol-5-yl)-1H-indole (93)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

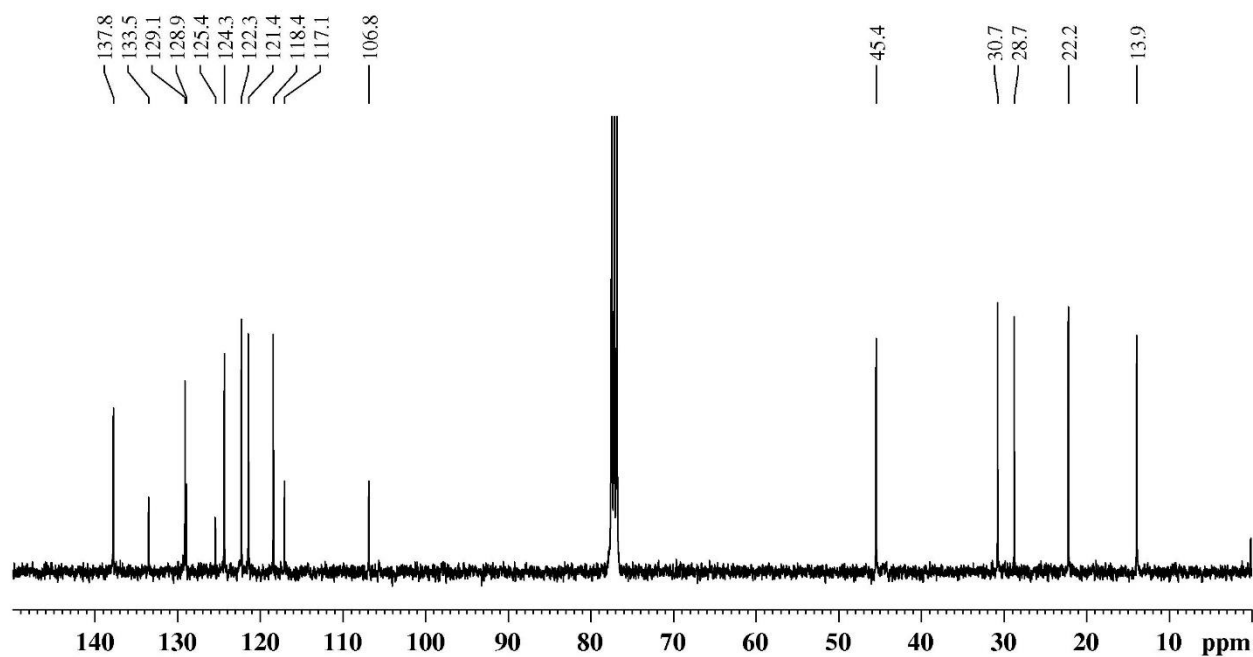
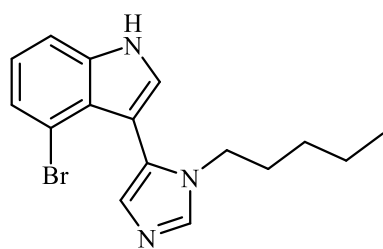
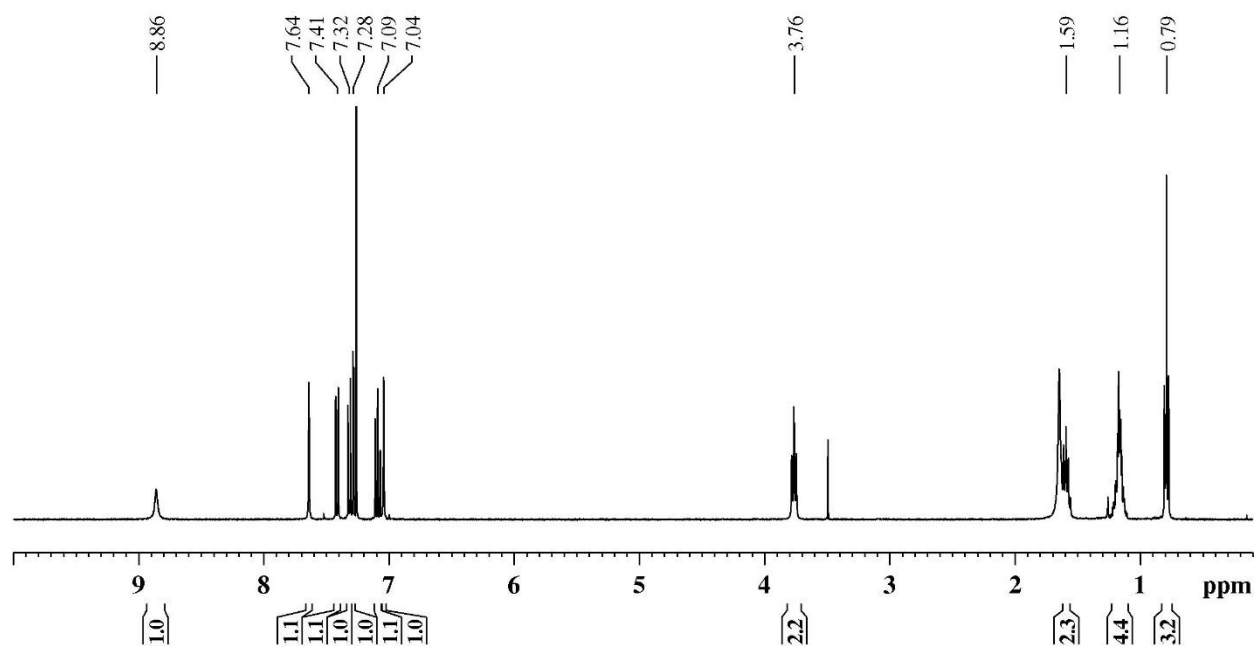


Figure S94. 4-Bromo-3-(1-pentyl-1H-imidazol-5-yl)-1H-indole (94)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

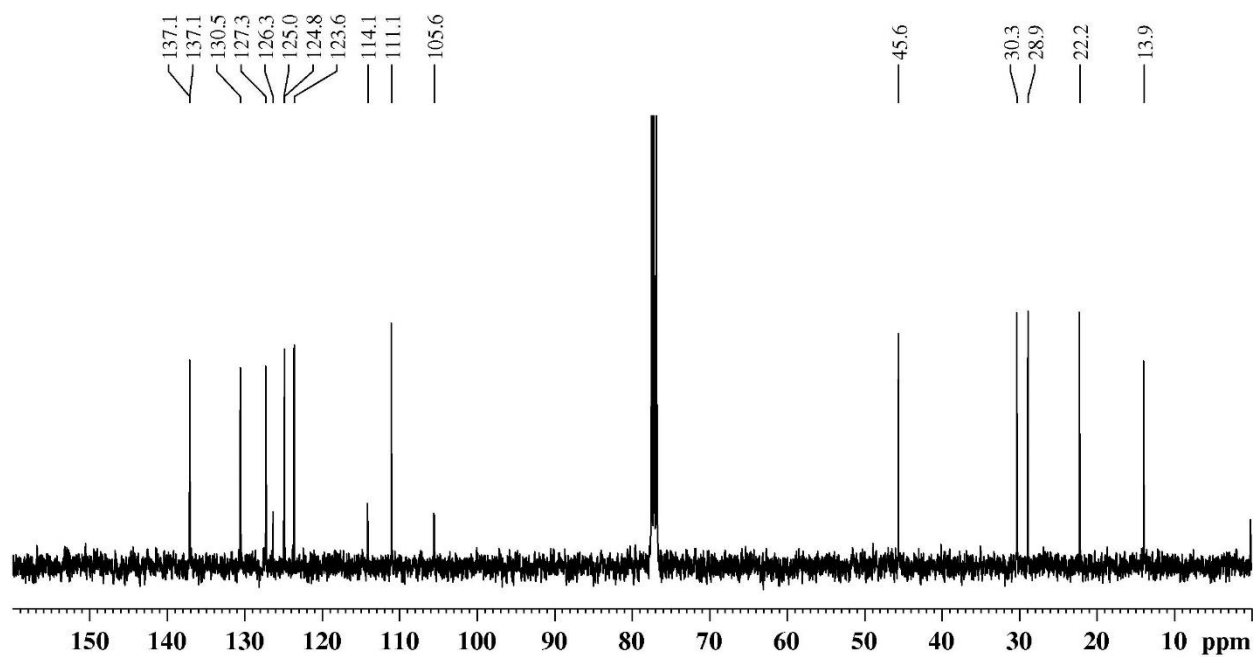
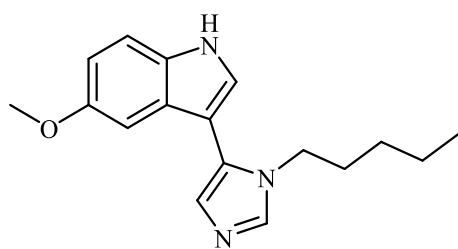
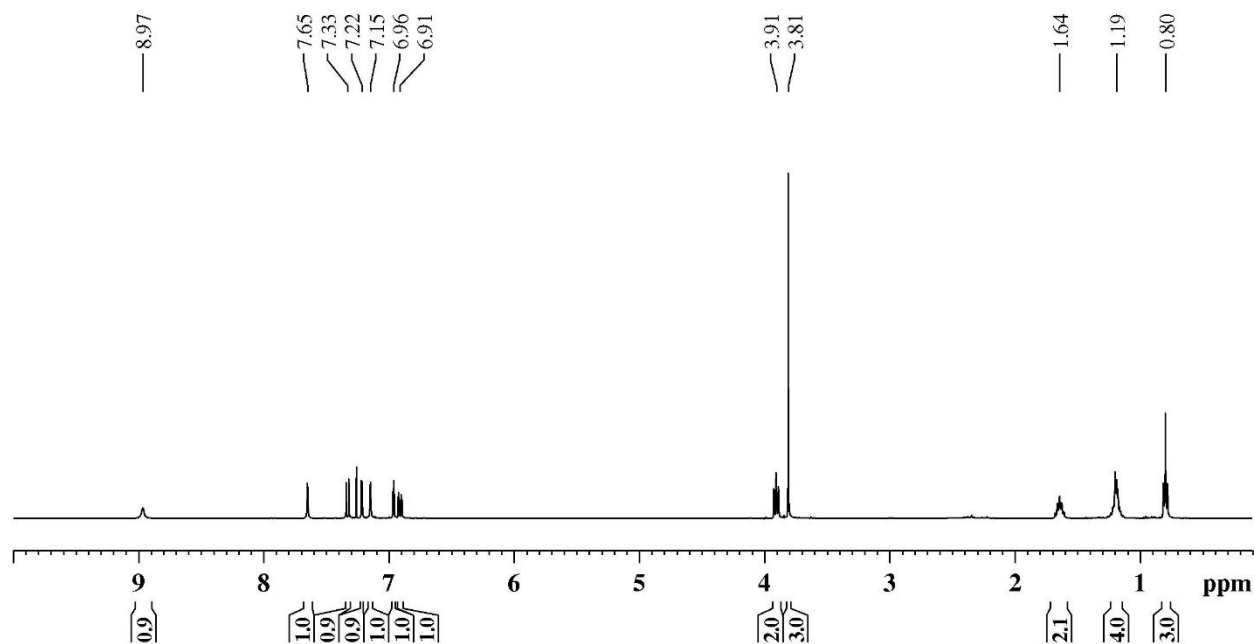


Figure S95. 5-Methoxy-3-(1-pentyl-1H-imidazol-5-yl)-1H-indole (**95**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

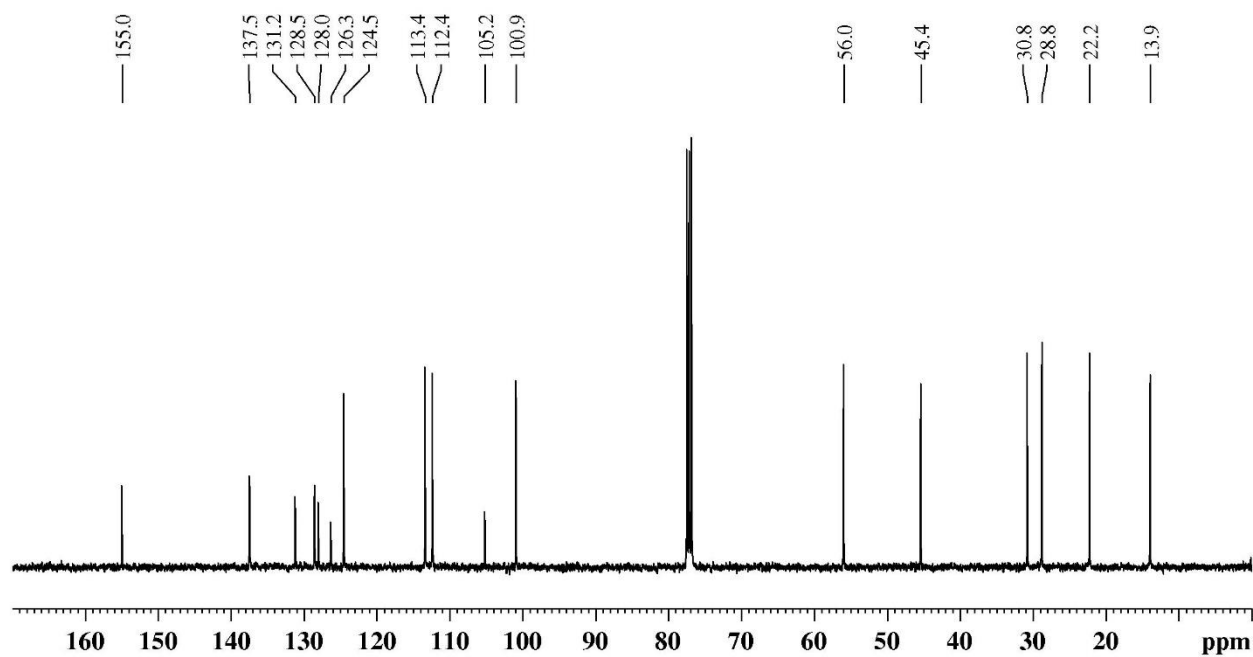
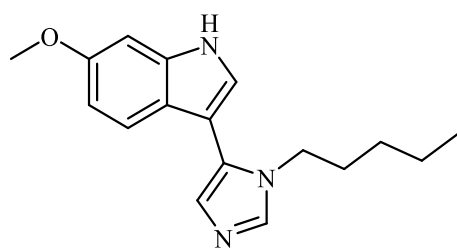
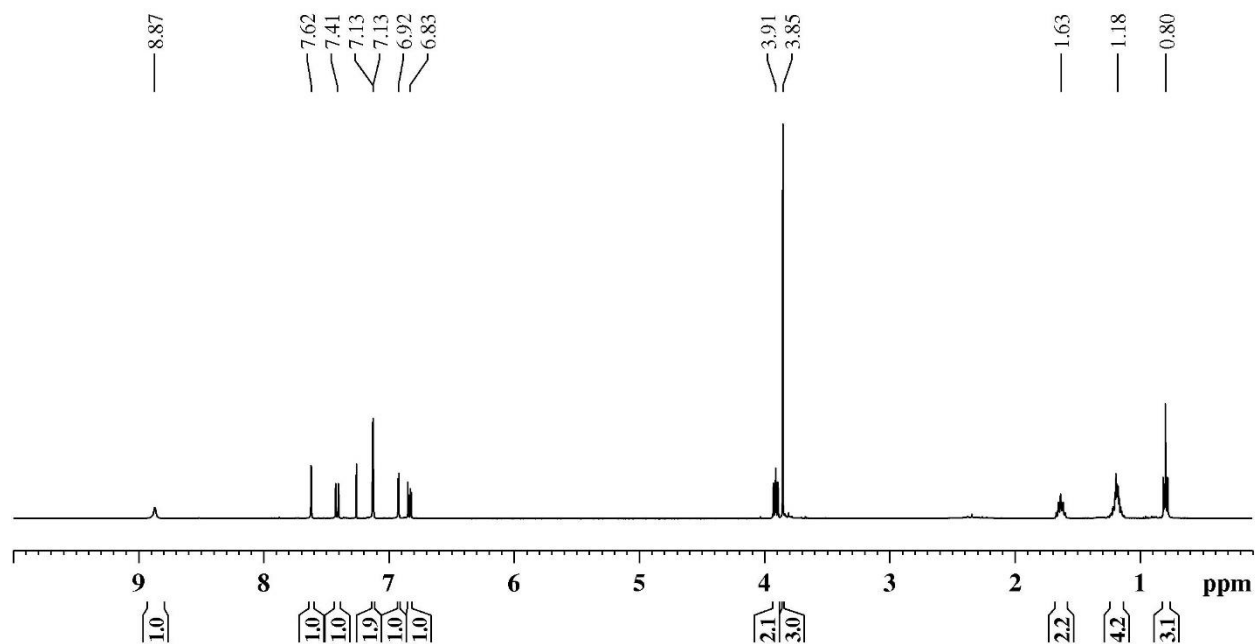


Figure S96. 6-Methoxy-3-(1-pentyl-1H-imidazol-5-yl)-1H-indole (96)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

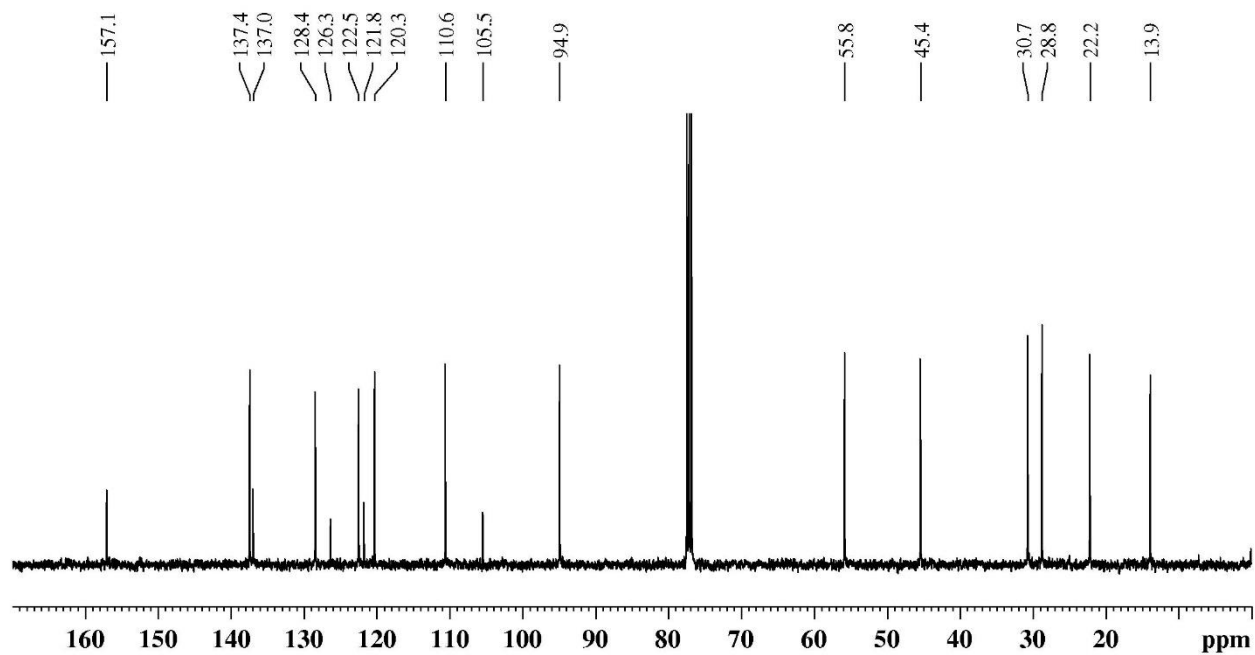
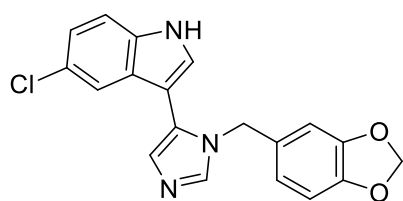
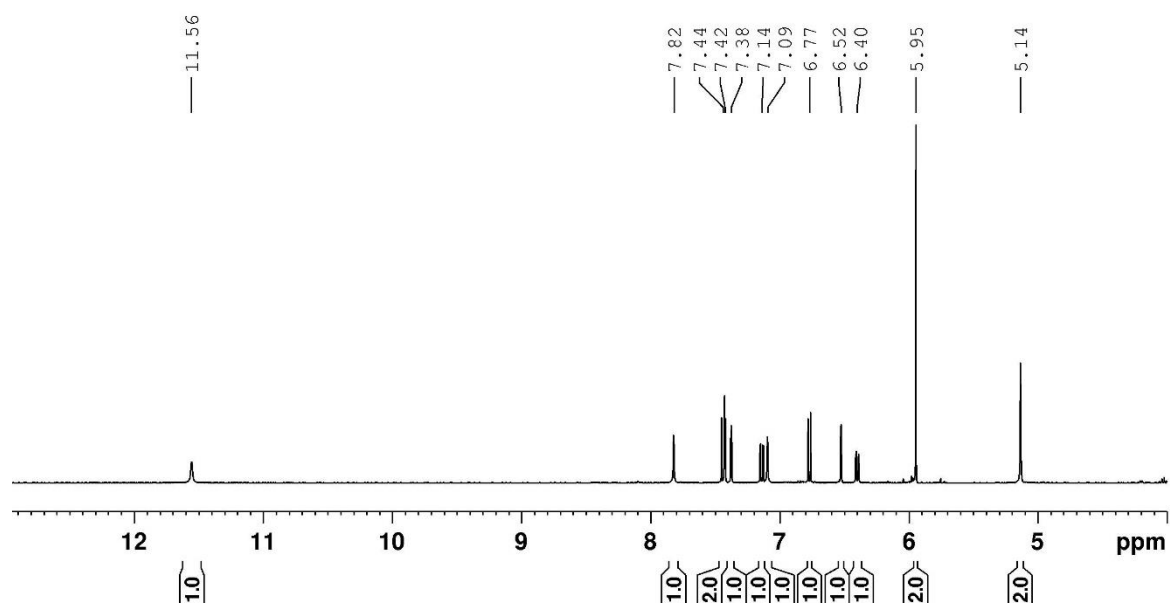


Figure S97. 3-(1-(Benzo[d][1,3]dioxol-5-ylmethyl)-1H-imidazol-5-yl)-5-chloro-1H-indole (97)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

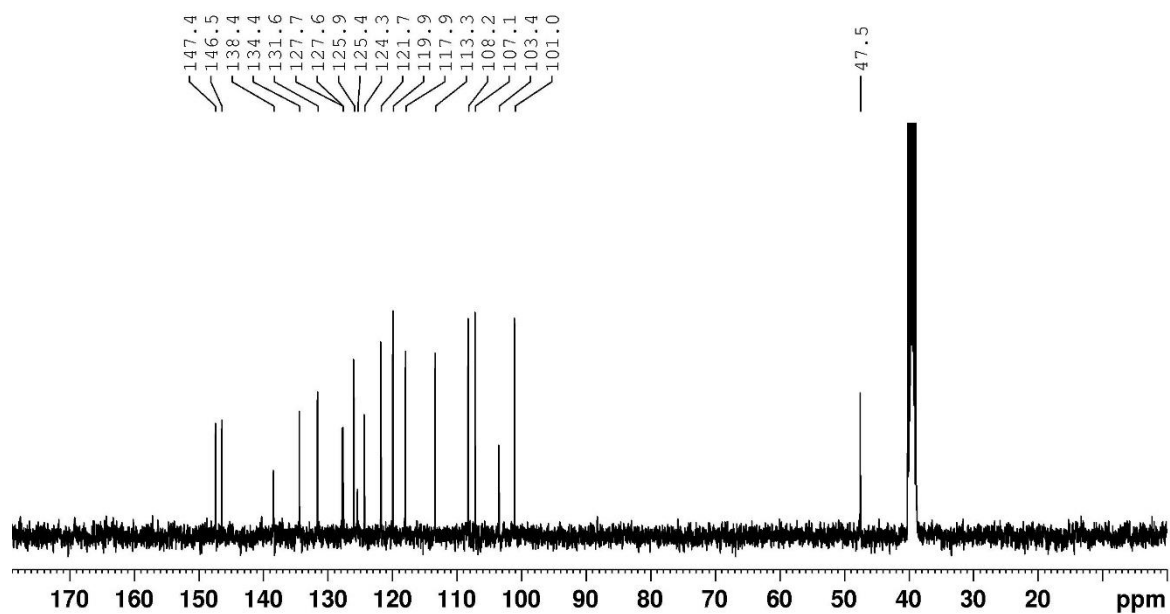
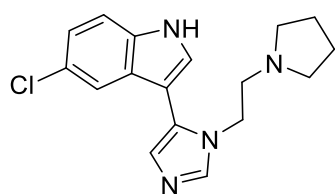
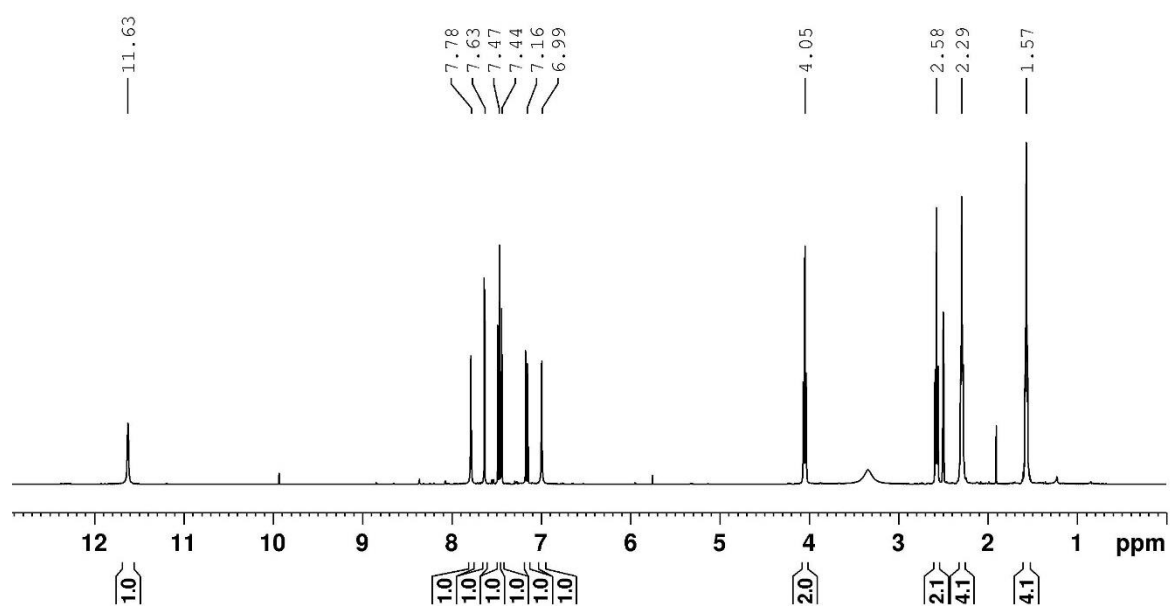


Figure S98. 5-Chloro-3-(1-(2-(pyrrolidin-1-yl)ethyl)-1H-imidazol-5-yl)-1H-indole (98)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

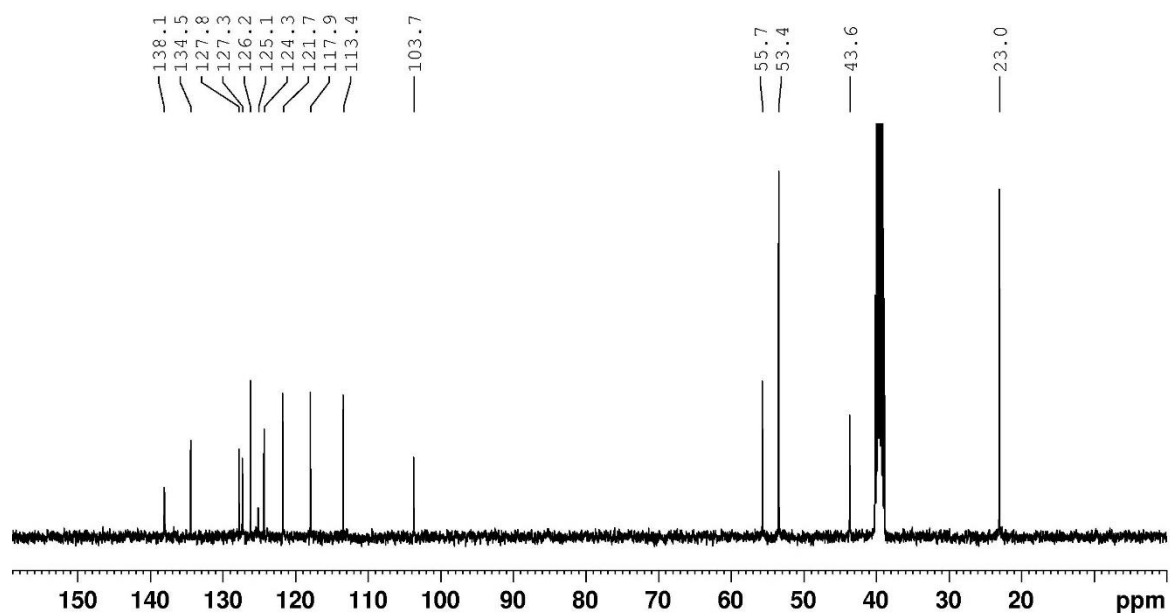
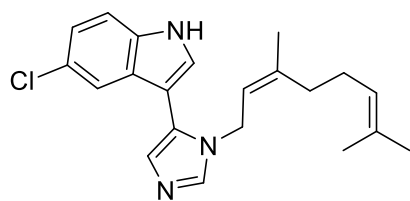
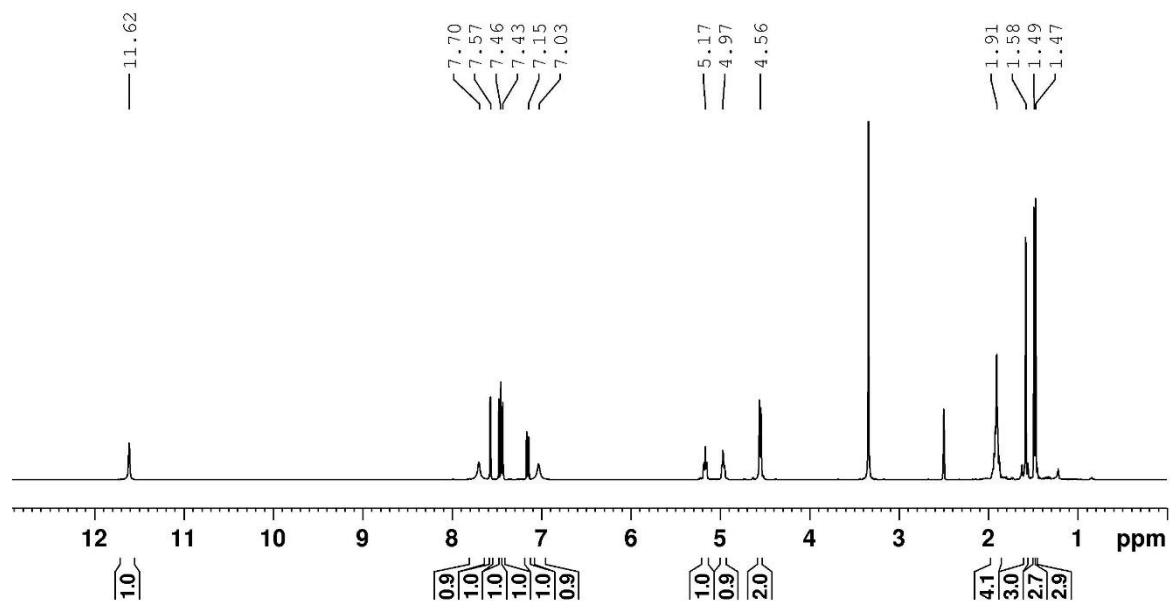


Figure S99. (E)-5-Chloro-3-(1-(3,7-dimethylocta-2,6-dien-1-yl)-1H-imidazol-5-yl)-1H-indole (**99**)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

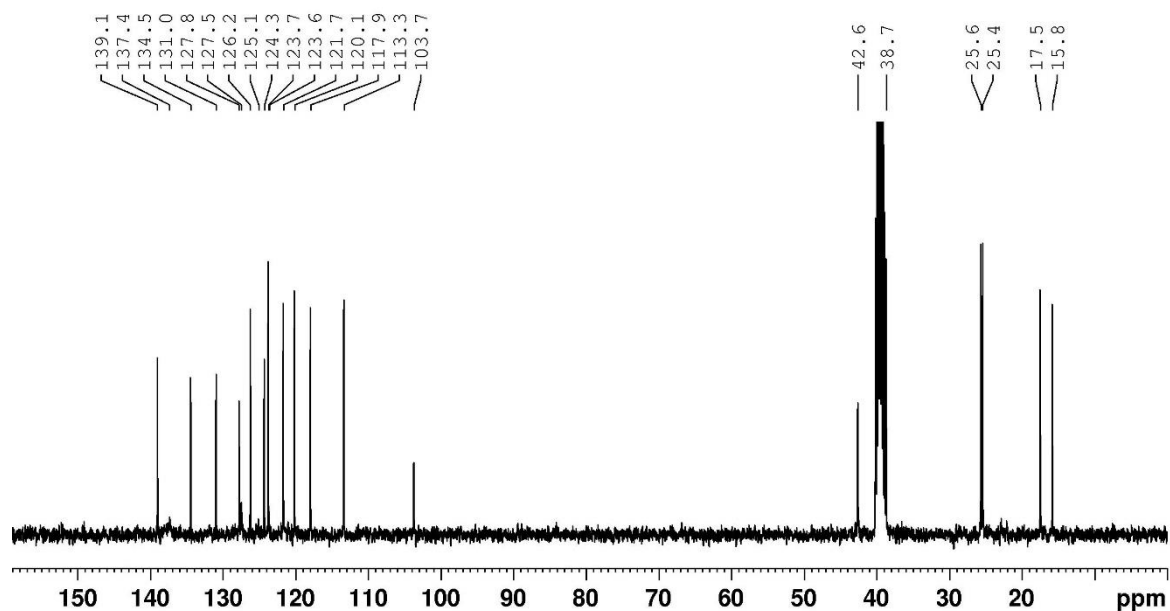
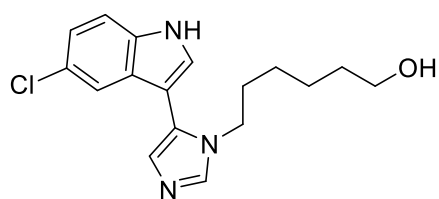
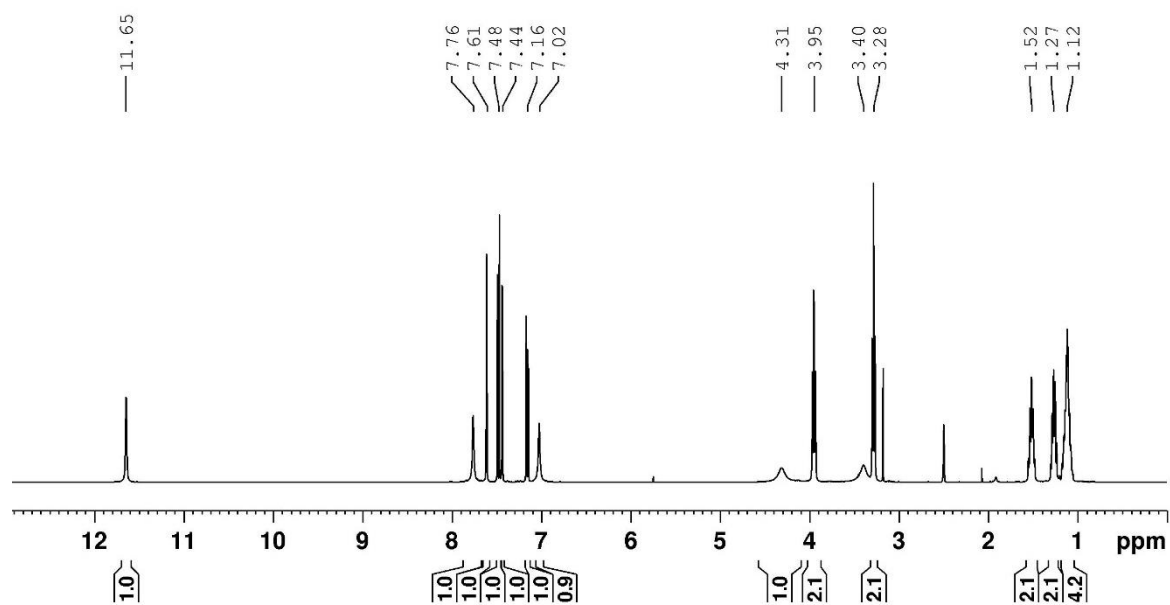


Figure S100. 6-(5-(5-Chloro-1*H*-indol-3-yl)-1*H*-imidazol-1-yl)hexan-1-ol (**100**)



^1H NMR ($\text{DMSO}-d_6$, 400 MHz):



^{13}C NMR ($\text{DMSO}-d_6$, 100 MHz):

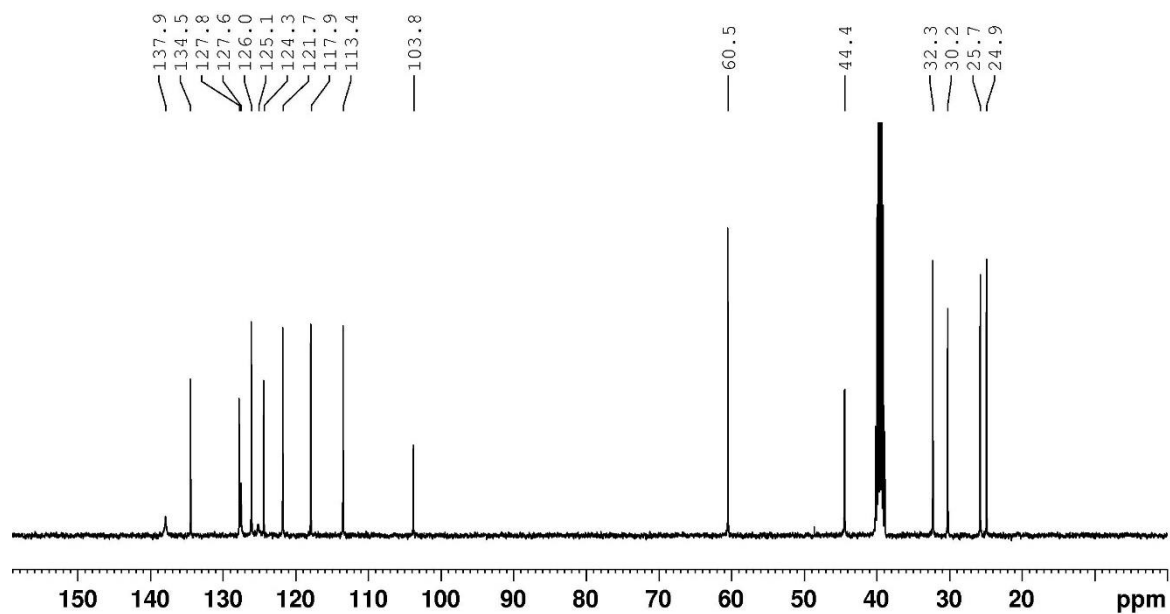
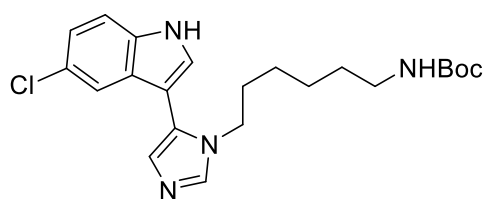
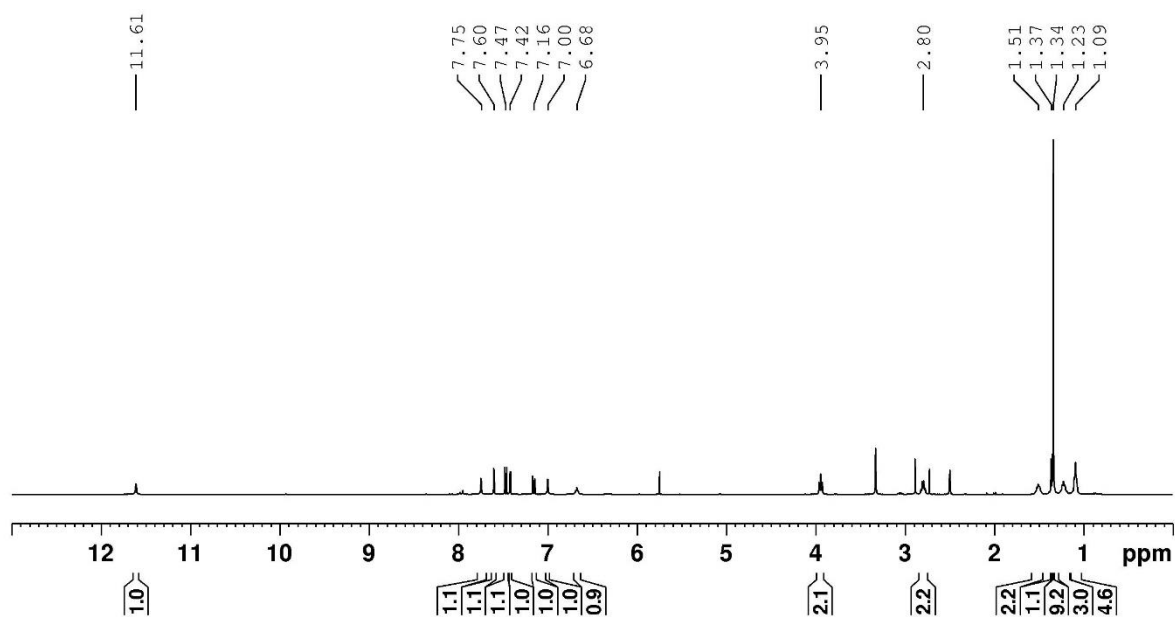


Figure S101. *tert*-Butyl (6-(5-(5-chloro-1*H*-indol-3-yl)-1*H*-imidazol-1-yl)hexyl)carbamate (**101**)



^1H NMR ($\text{DMSO}-d_6$, 400 MHz):



^{13}C NMR ($\text{DMSO}-d_6$, 100 MHz):

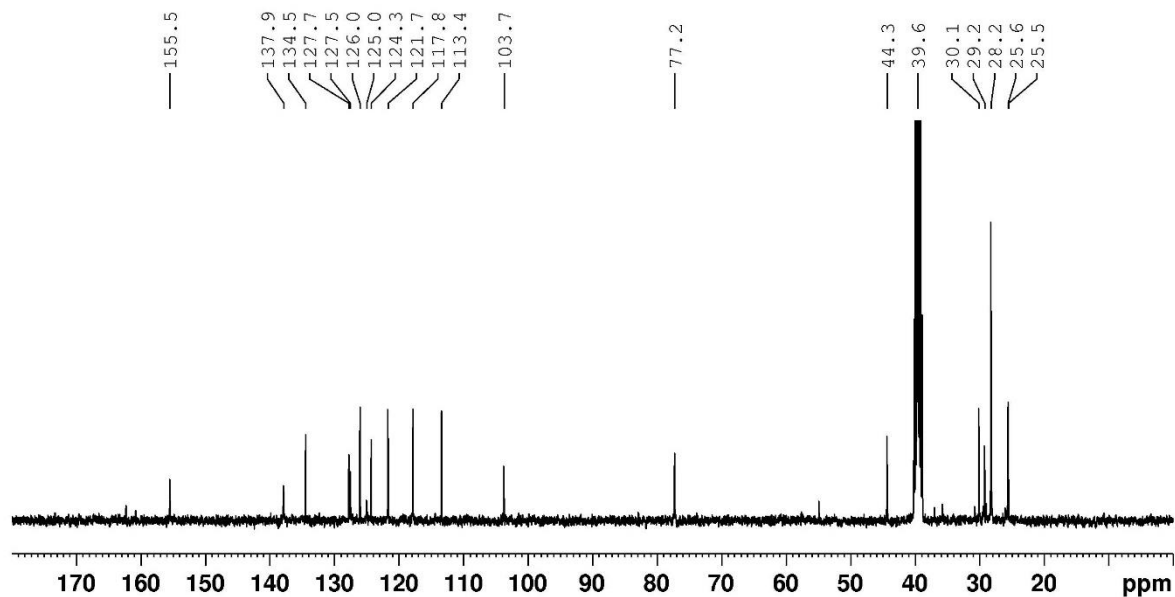
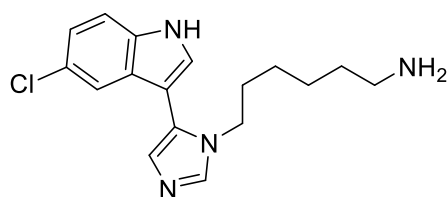
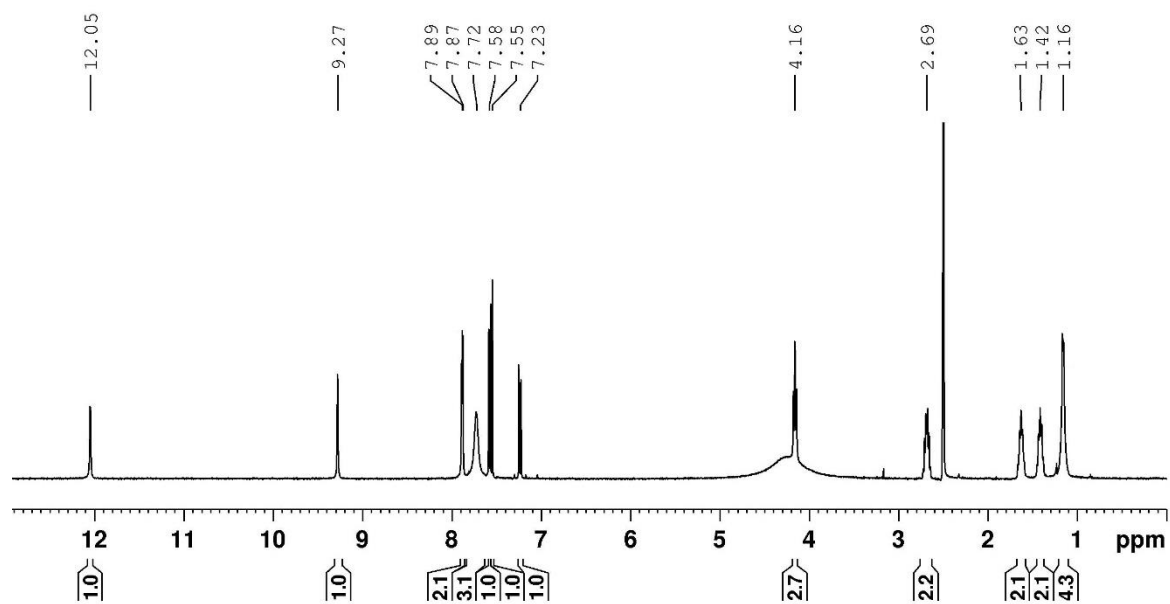


Figure S102. 6-(5-(5-Chloro-1*H*-indol-3-yl)-1*H*-imidazol-1-yl)hexan-1-aminium 2,2,2-trifluoroacetate (102)



^1H NMR (DMSO- d_6 , 400 MHz):



^{13}C NMR (DMSO- d_6 , 100 MHz):

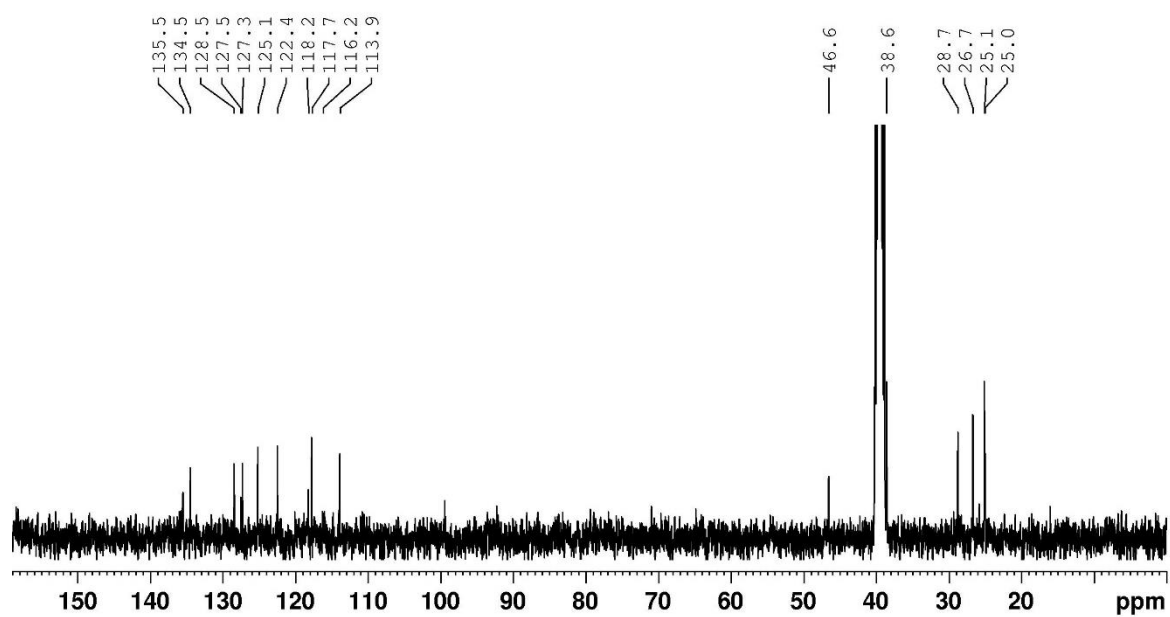
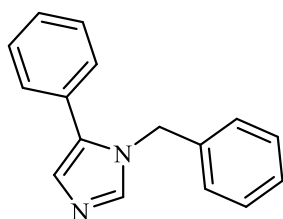
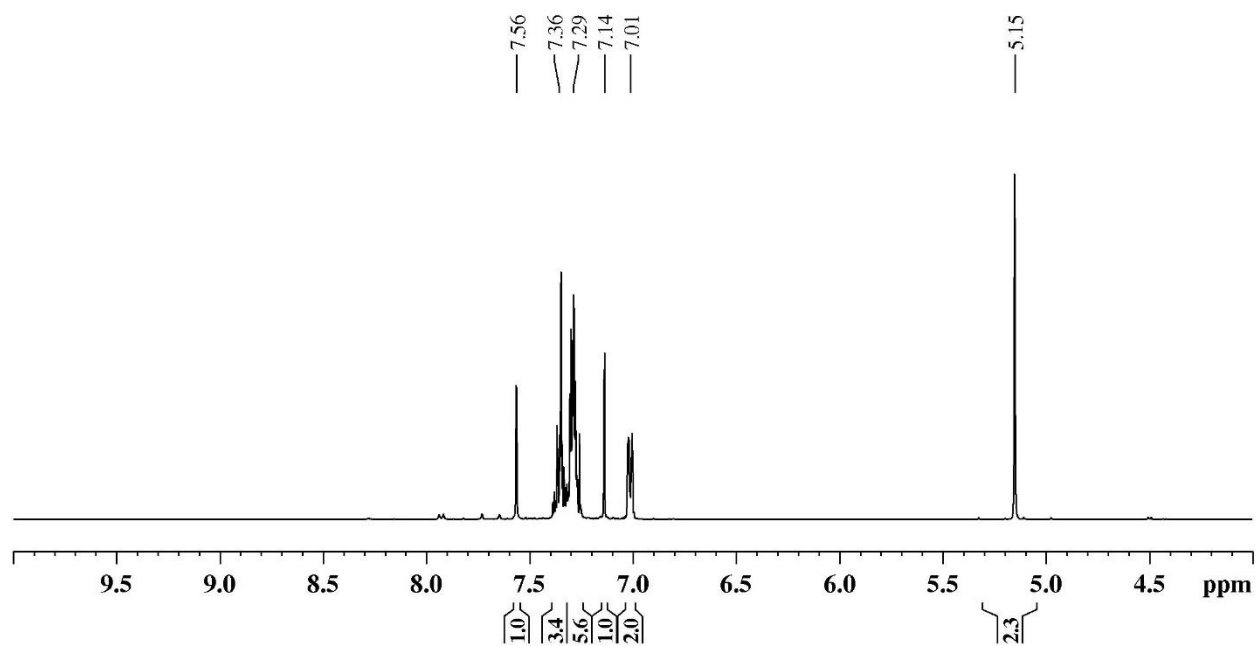


Figure S103. 1-Benzyl-5-phenyl-1H-imidazole (**103**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

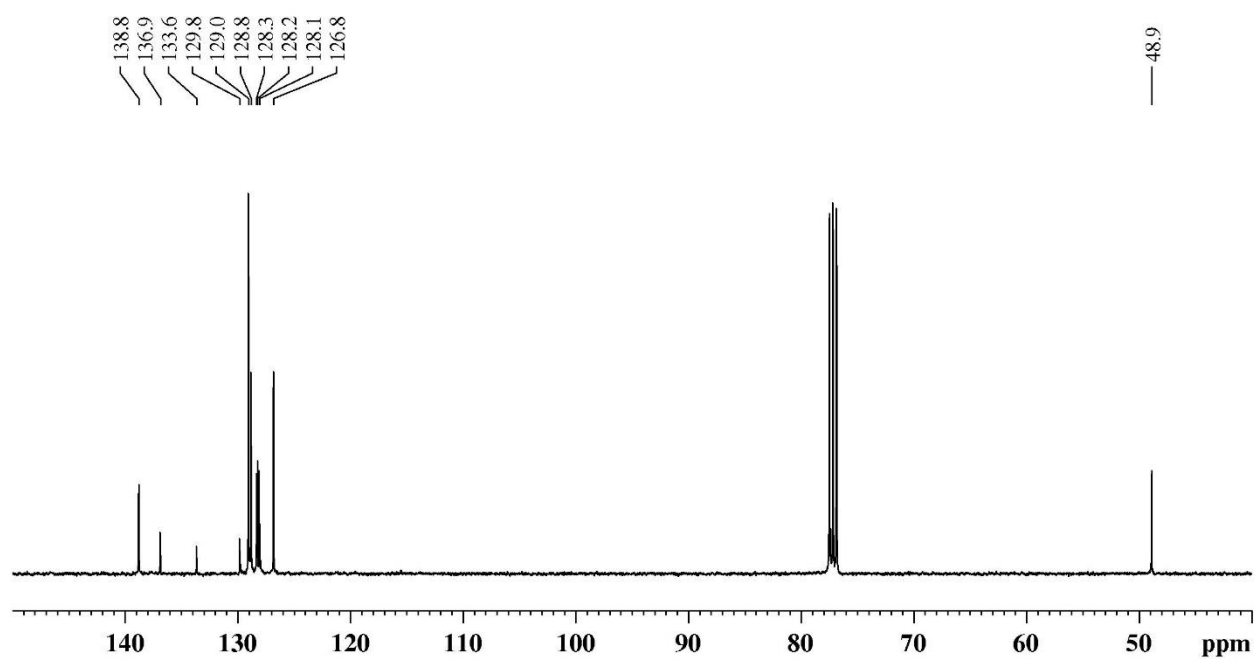
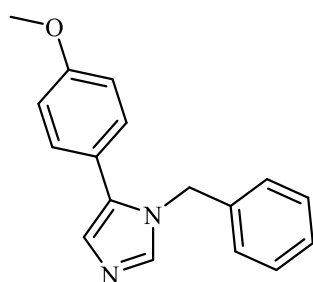
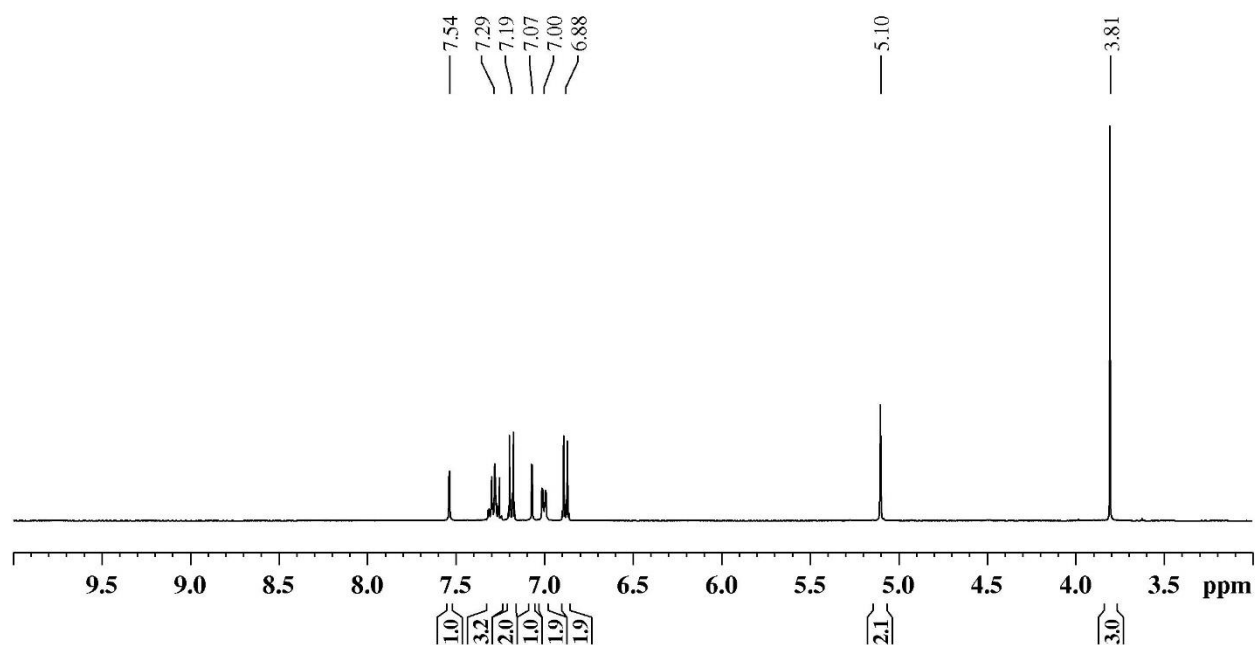


Figure S104. 1-Benzyl-5-(4-methoxyphenyl)-1H-imidazole (**104**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

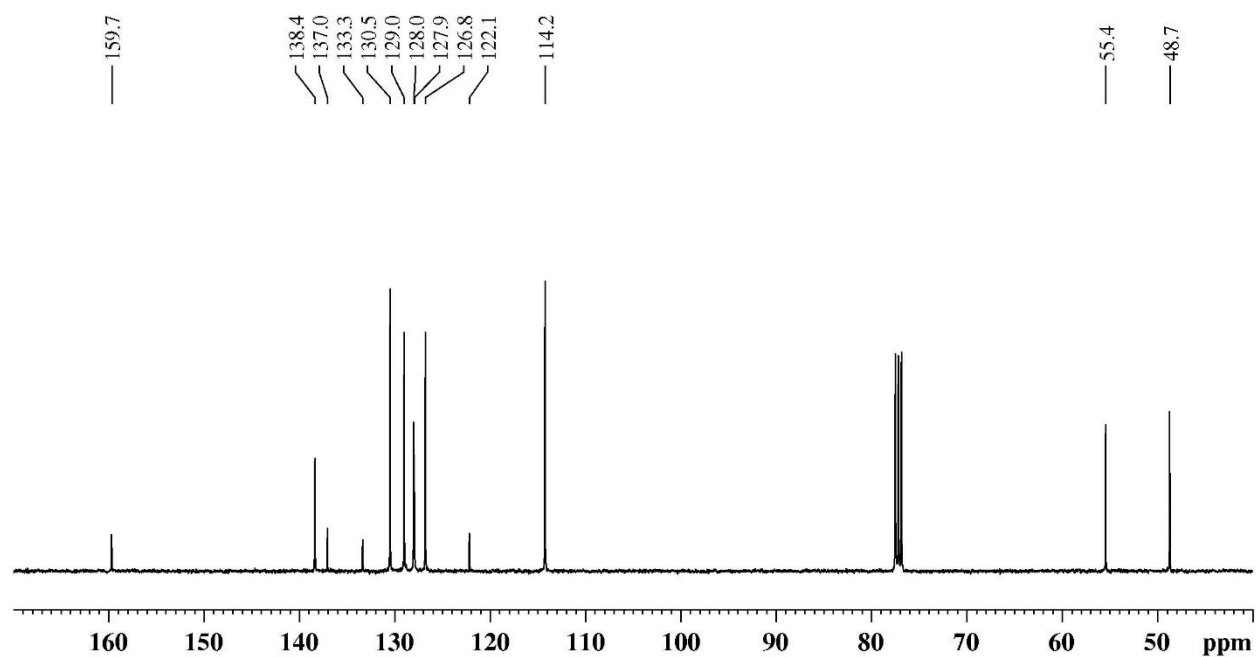
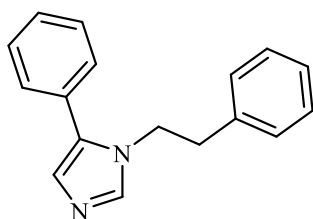
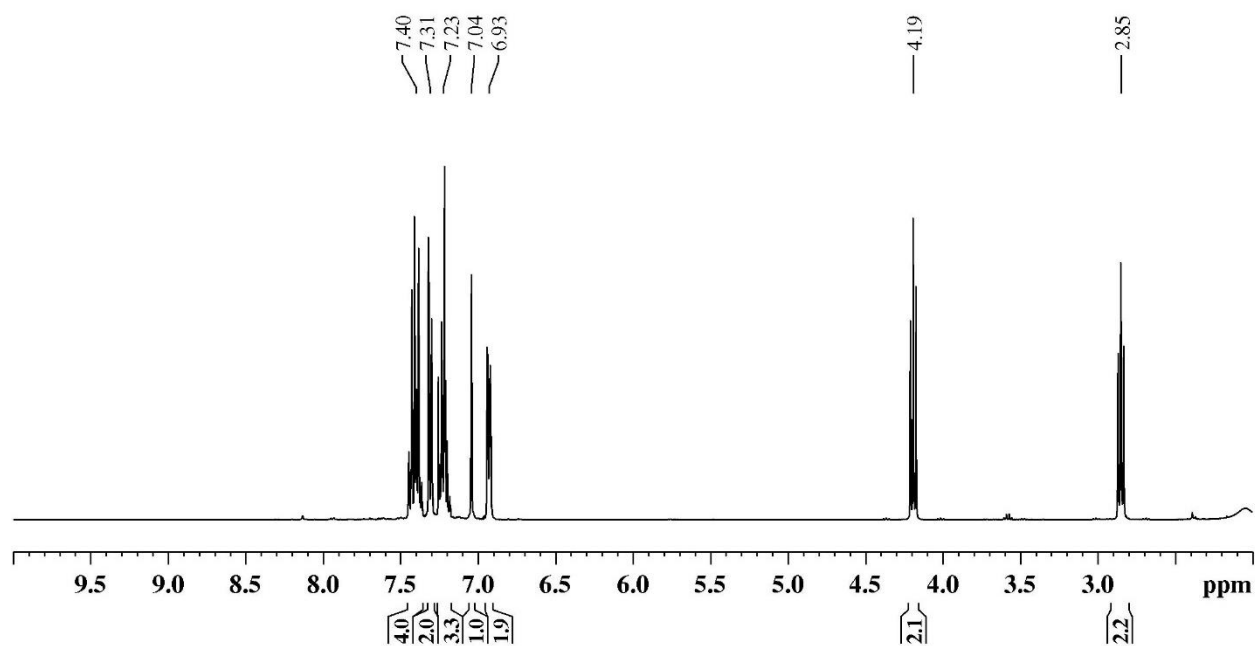


Figure S105. 1-Phenethyl-5-phenyl-1H-imidazole (105)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

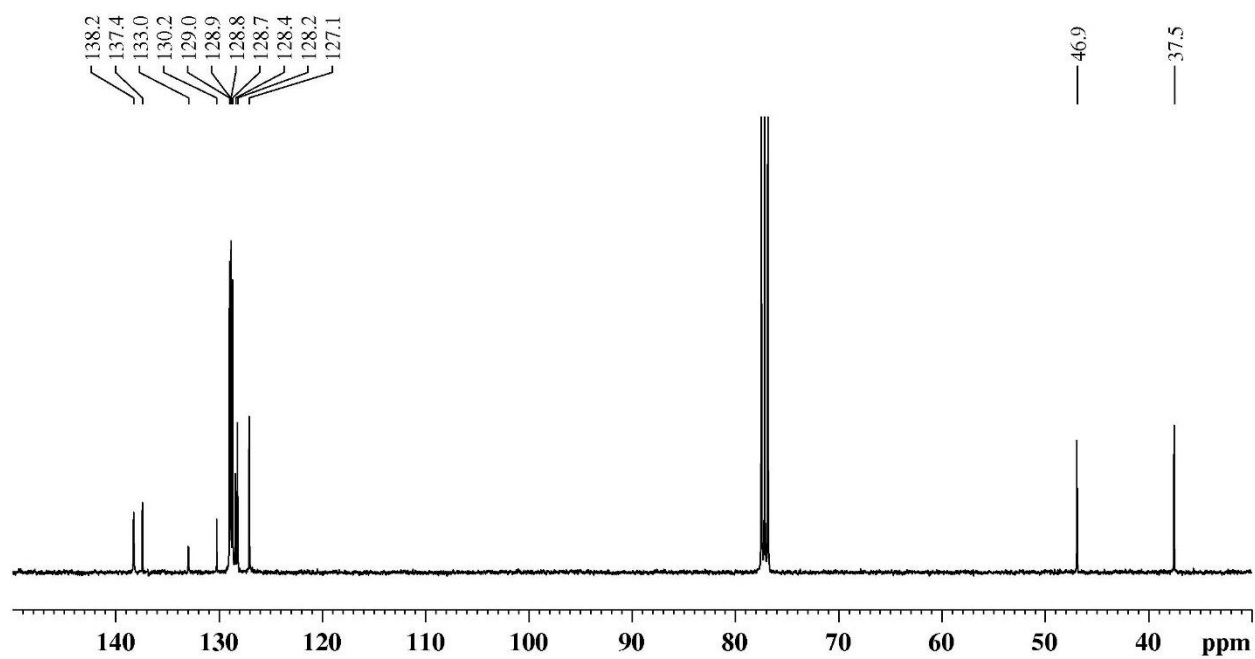
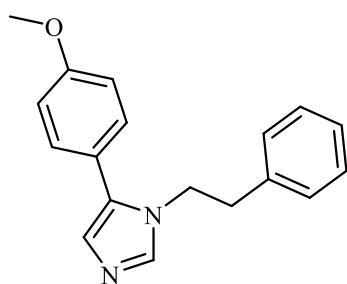
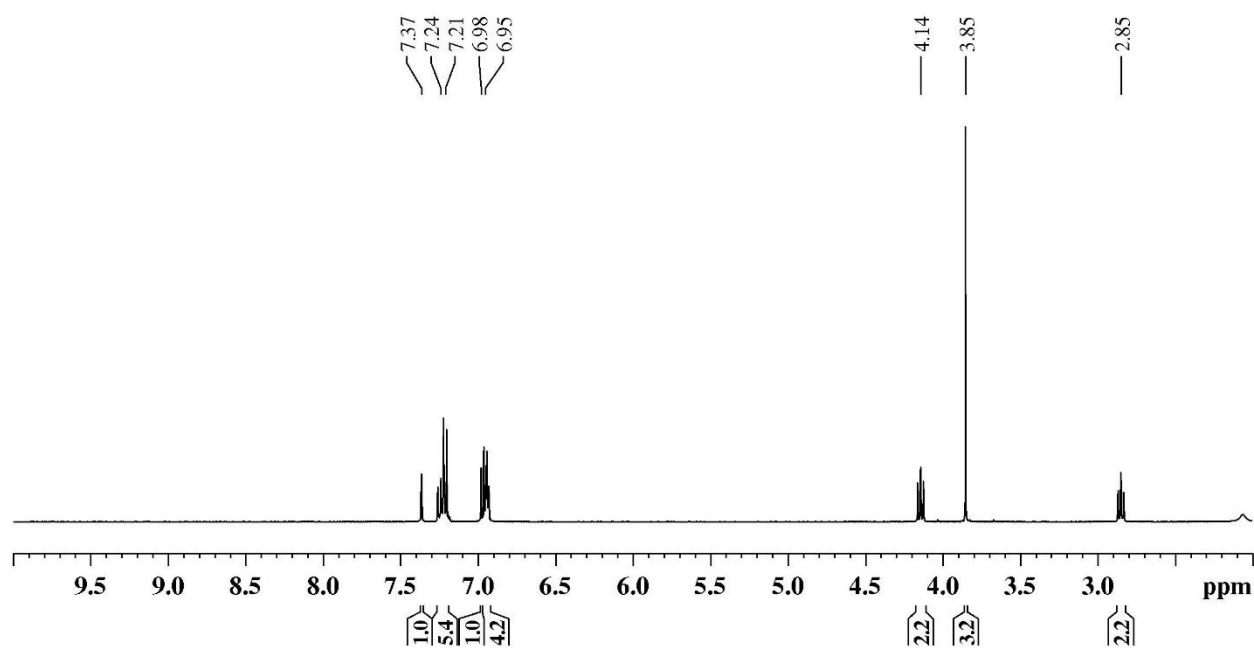


Figure S106. 5-(4-Methoxyphenyl)-1-phenethyl-1H-imidazole (**106**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

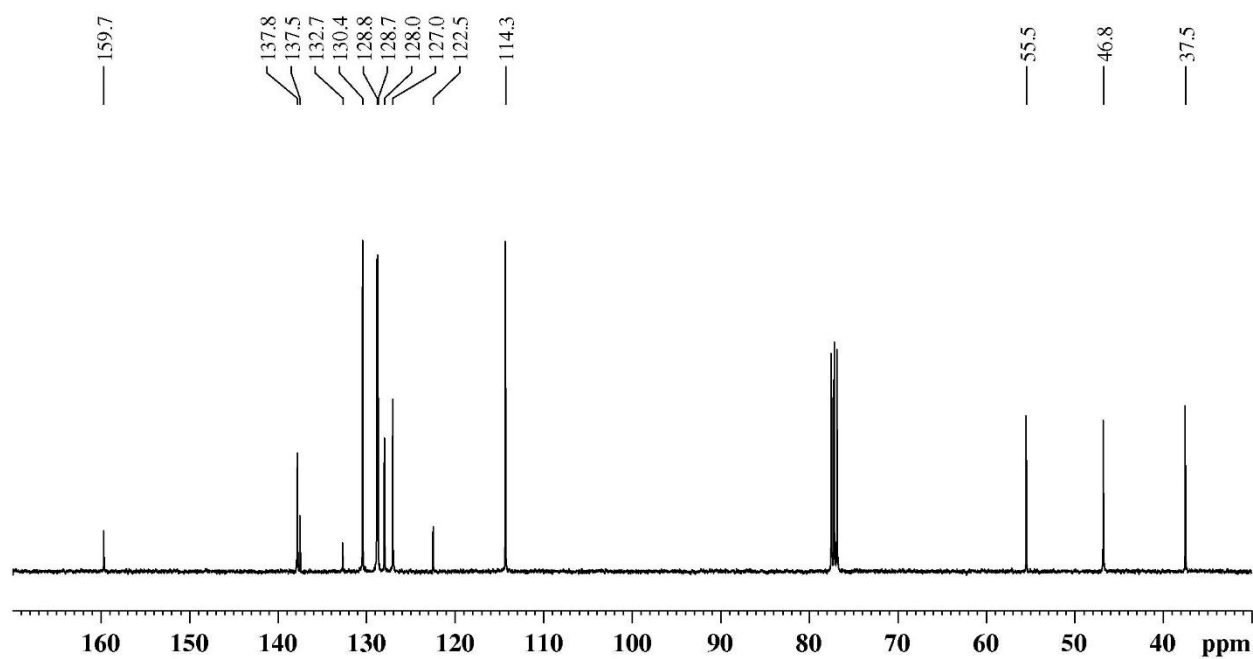
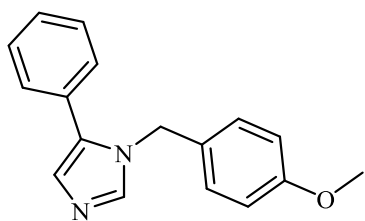
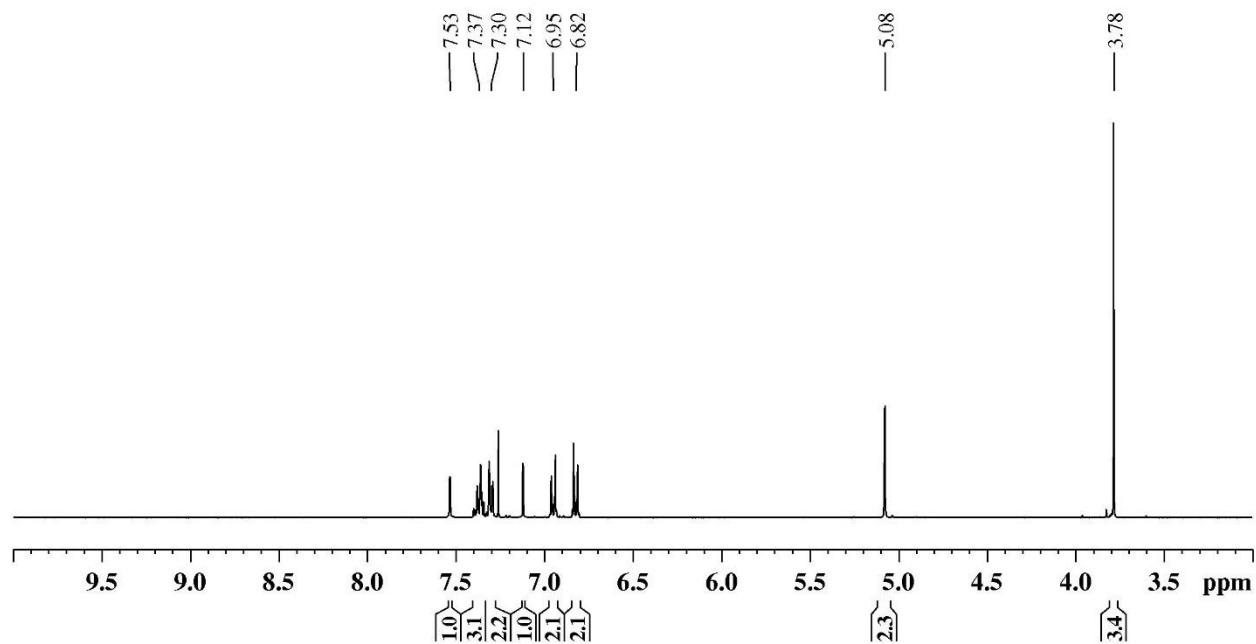


Figure S107. 1-(4-Methoxybenzyl)-5-phenyl-1H-imidazole (**107**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

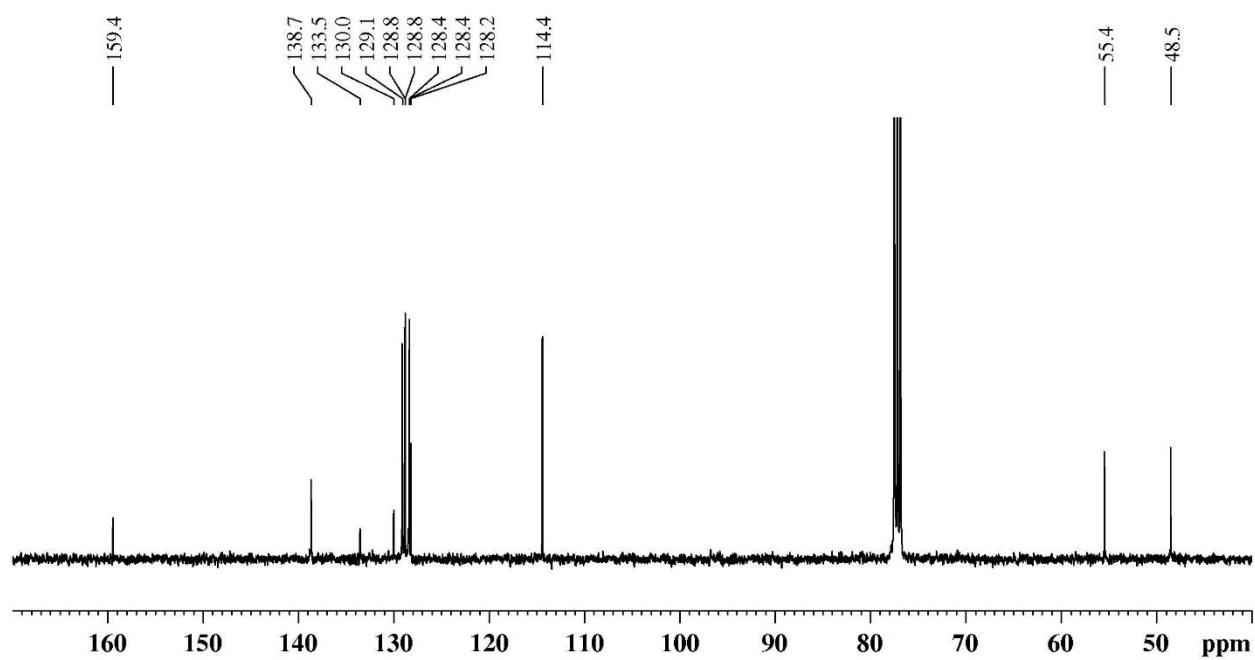
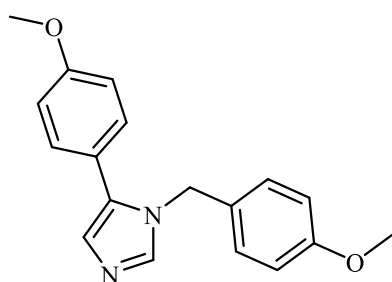
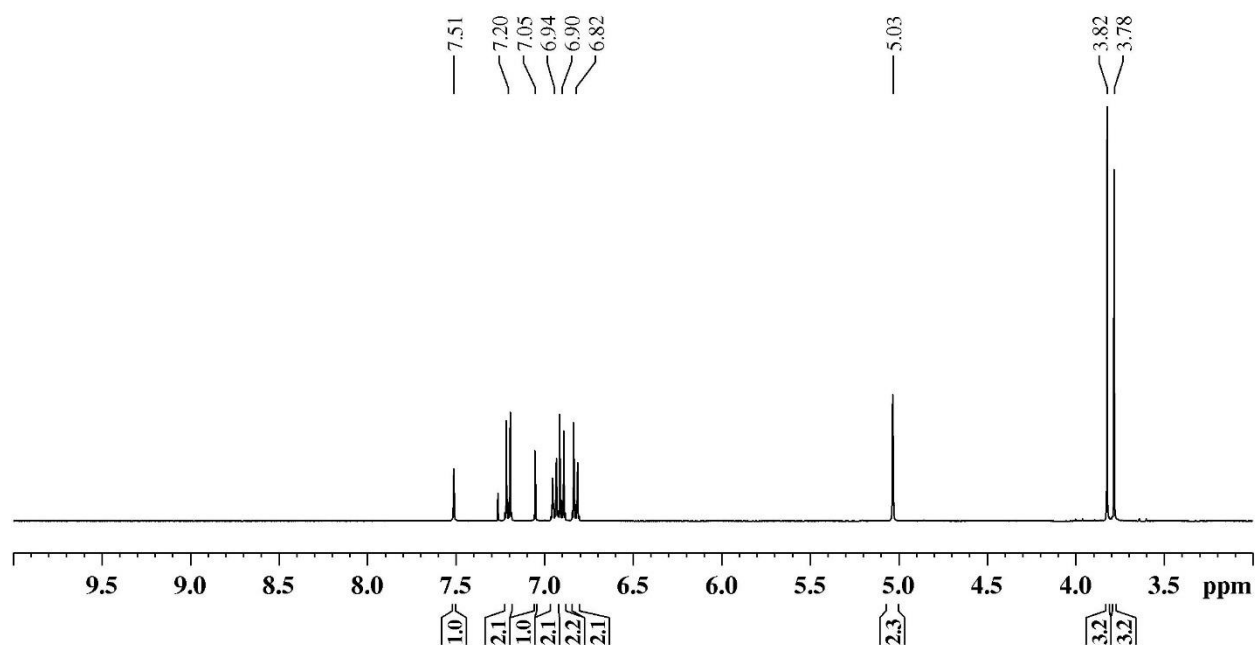


Figure S108. 1-(4-Methoxybenzyl)-5-(4-methoxyphenyl)-1H-imidazole (**108**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

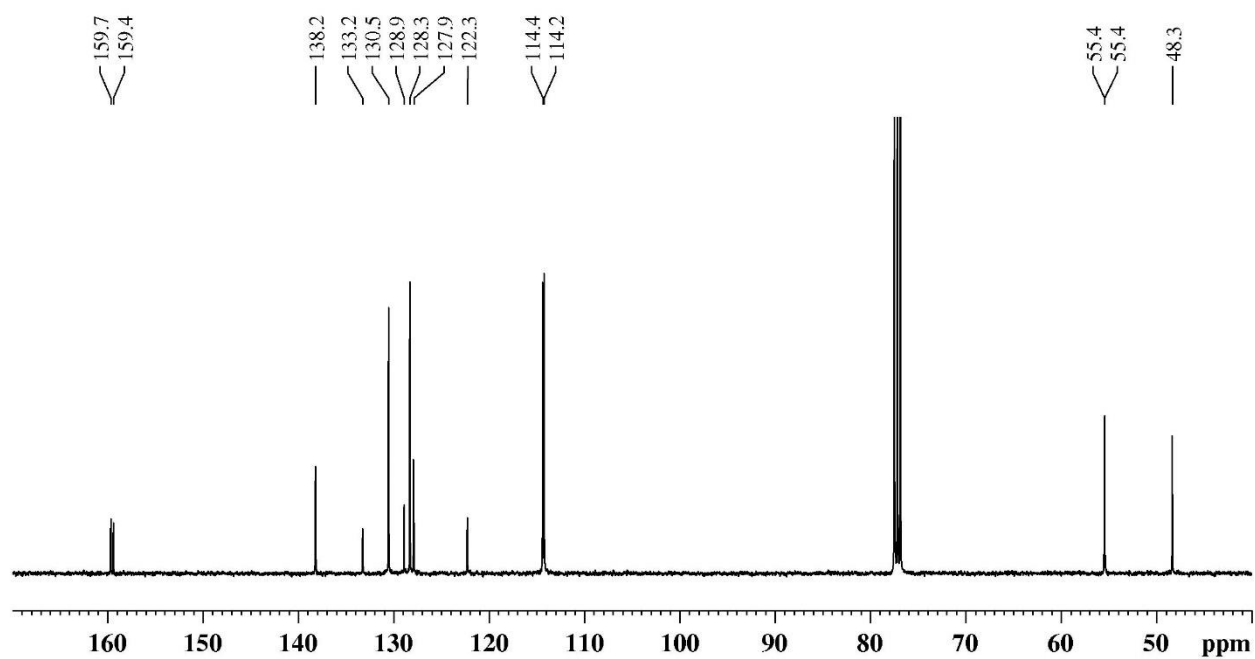
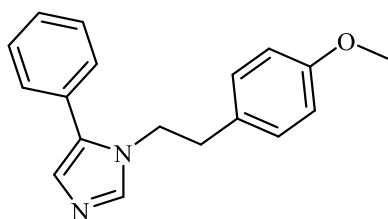
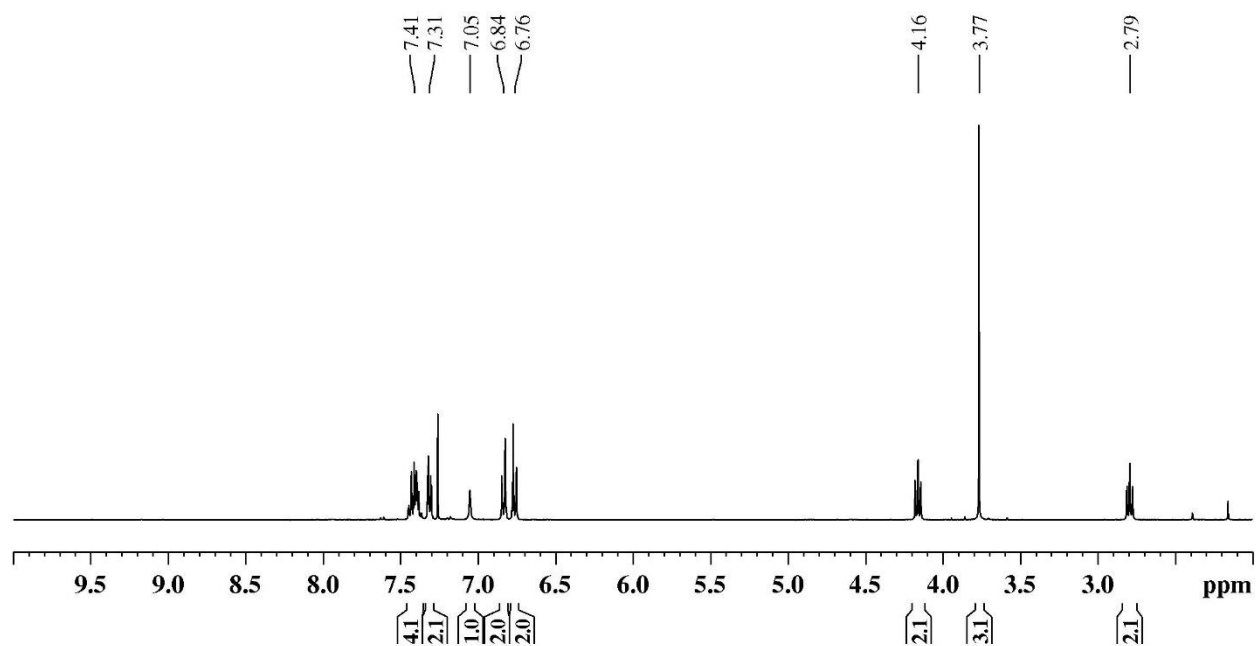


Figure S109. 1-(4-Methoxyphenethyl)-5-phenyl-1*H*-imidazole (**109**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

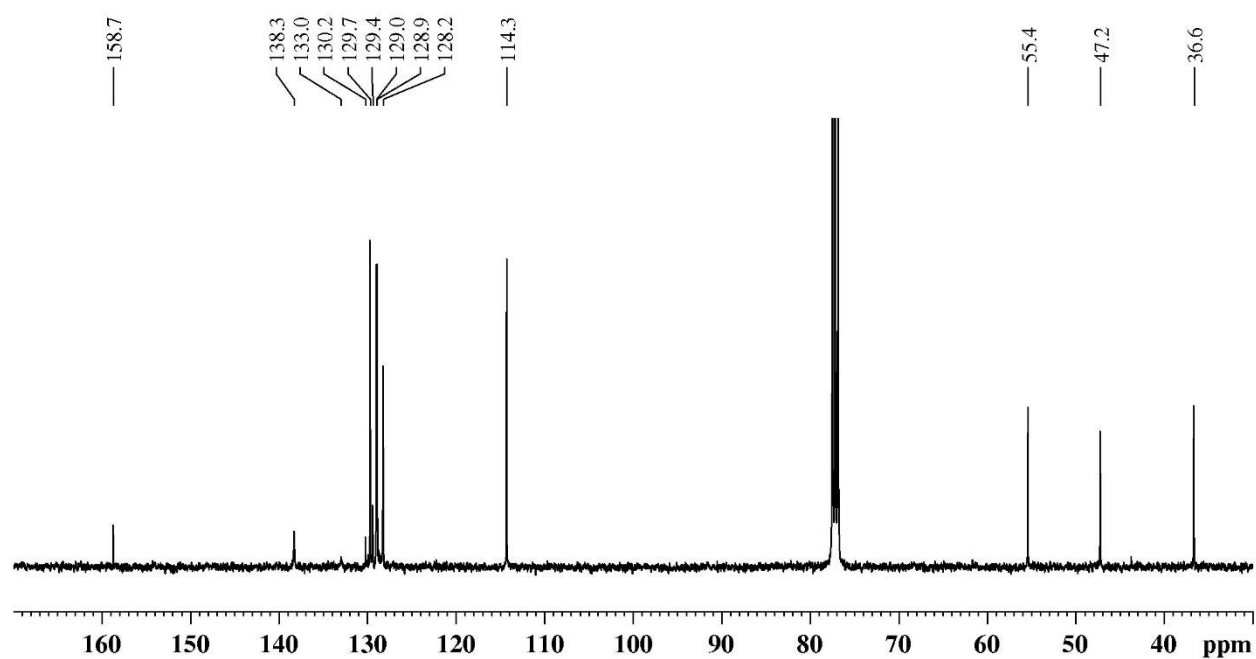
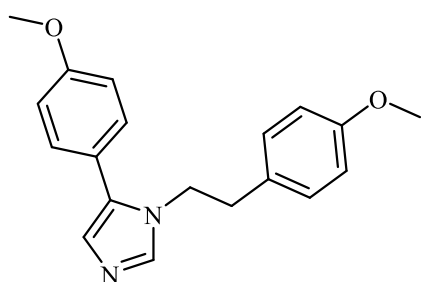
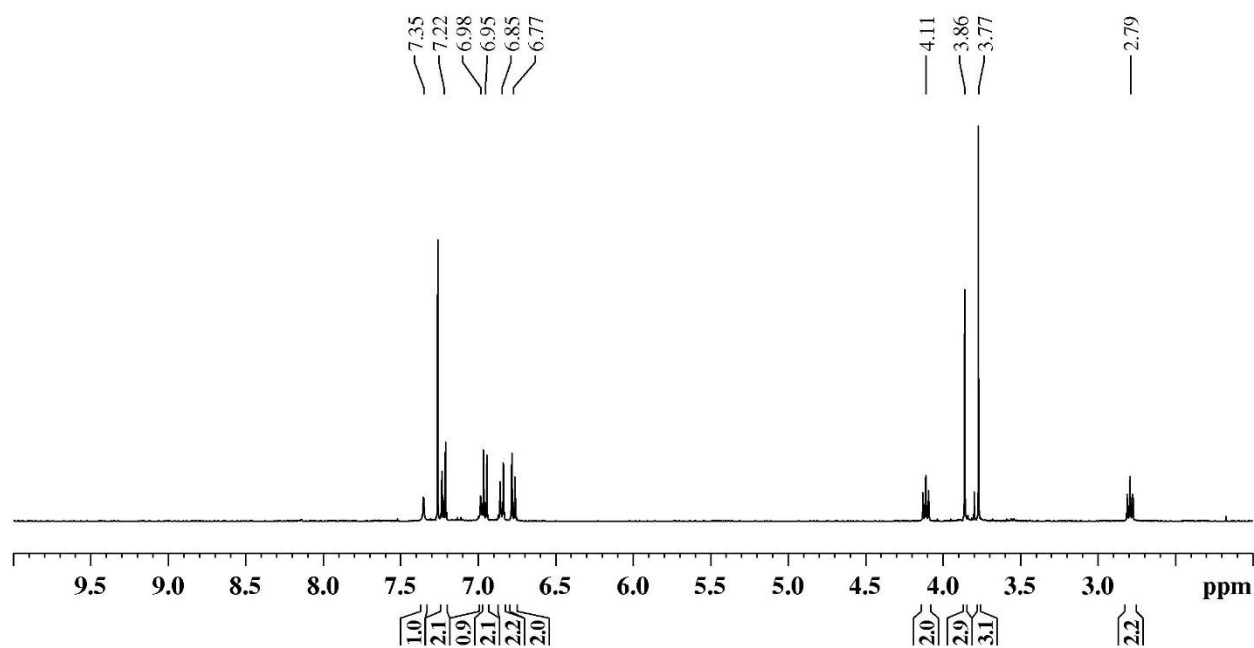


Figure S110. 1-(4-Methoxyphenethyl)-5-(4-methoxyphenyl)-1H-imidazole (**110**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

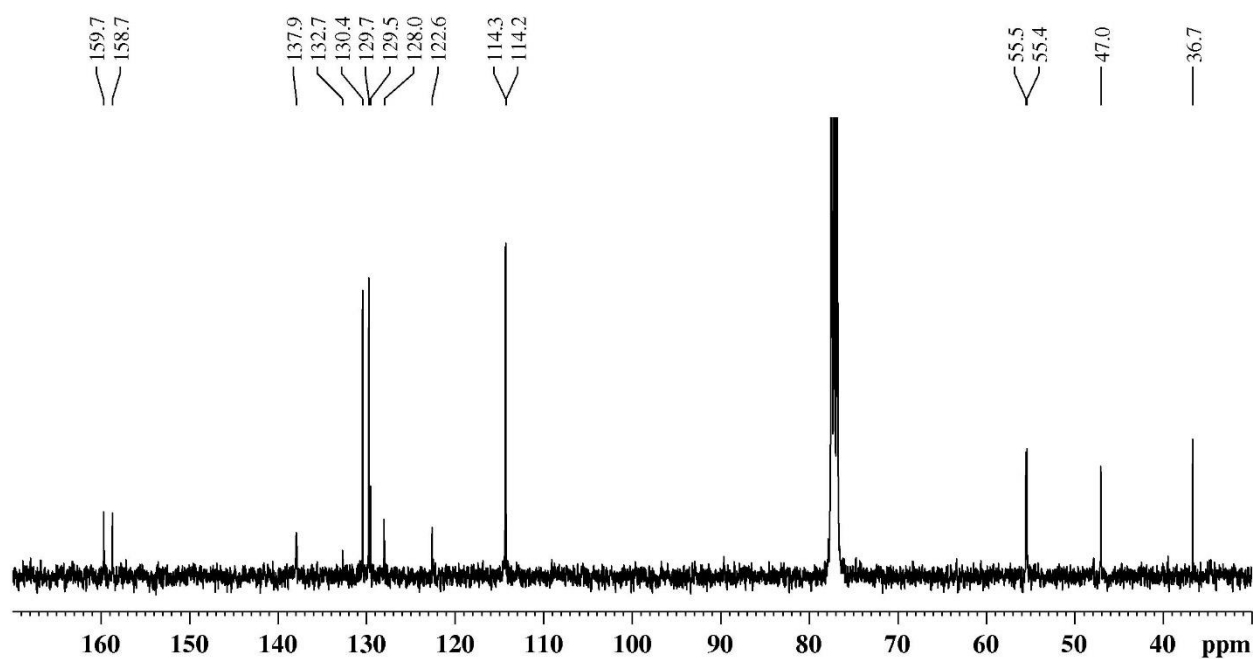
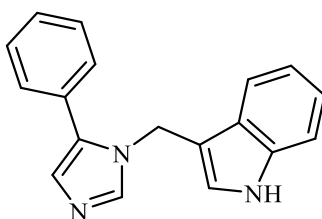
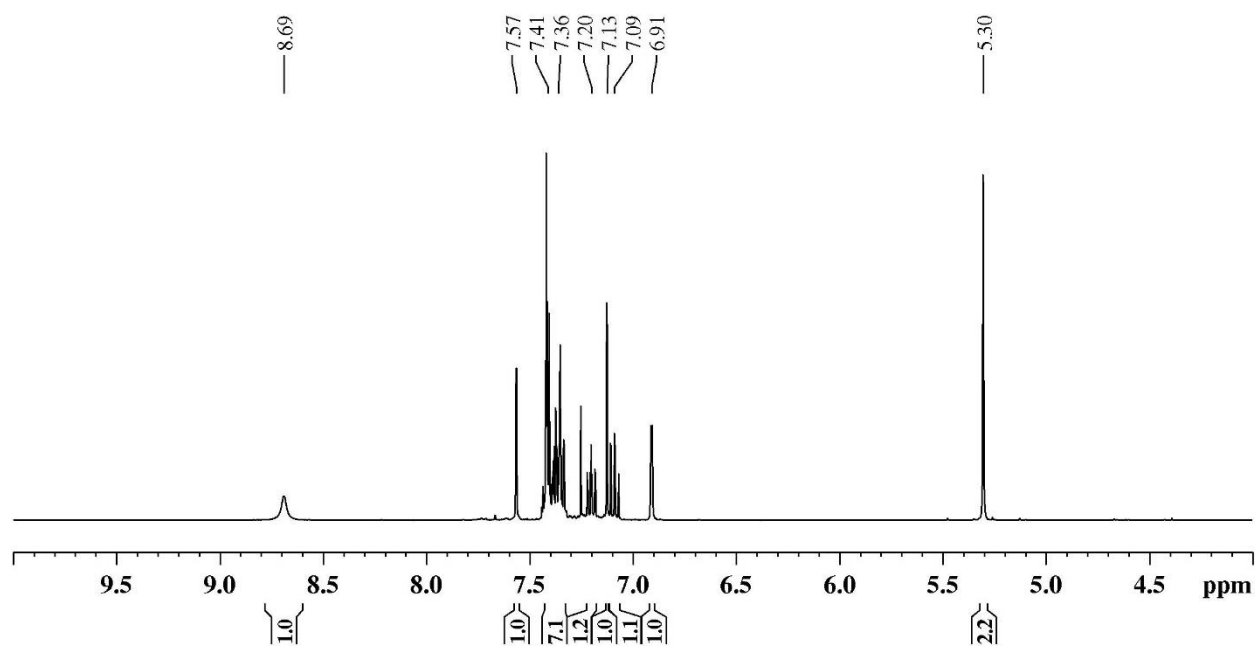


Figure S111. 3-((5-Phenyl-1H-imidazol-1-yl)methyl)-1H-indole (**111**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

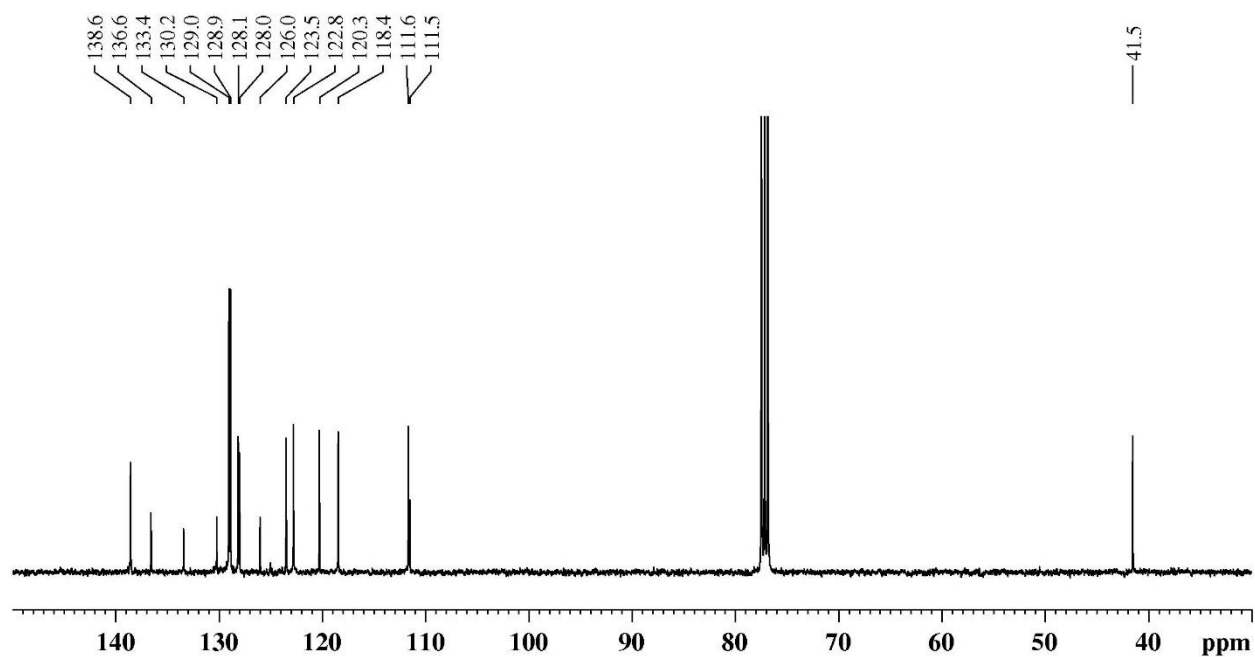
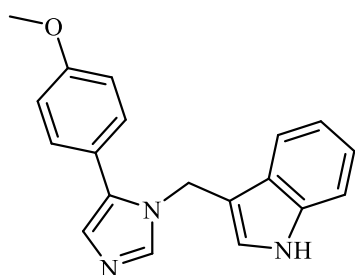
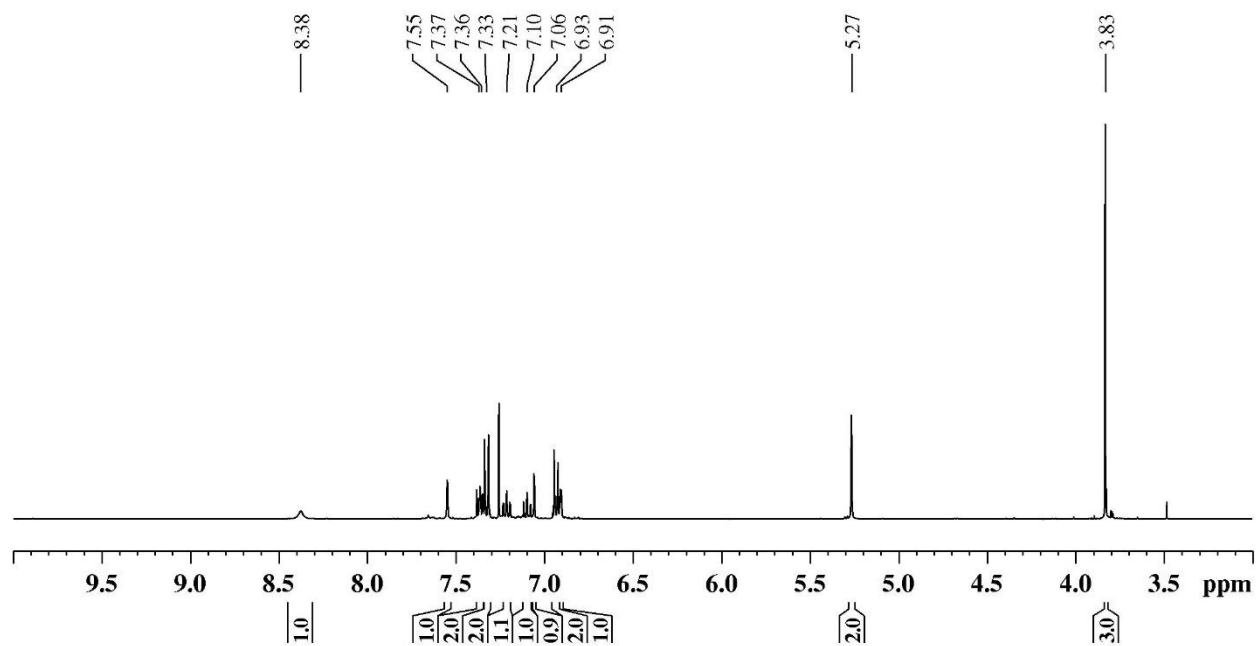


Figure S112. 3-((5-(4-Methoxyphenyl)-1H-imidazol-1-yl)methyl)-1H-indole (**112**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

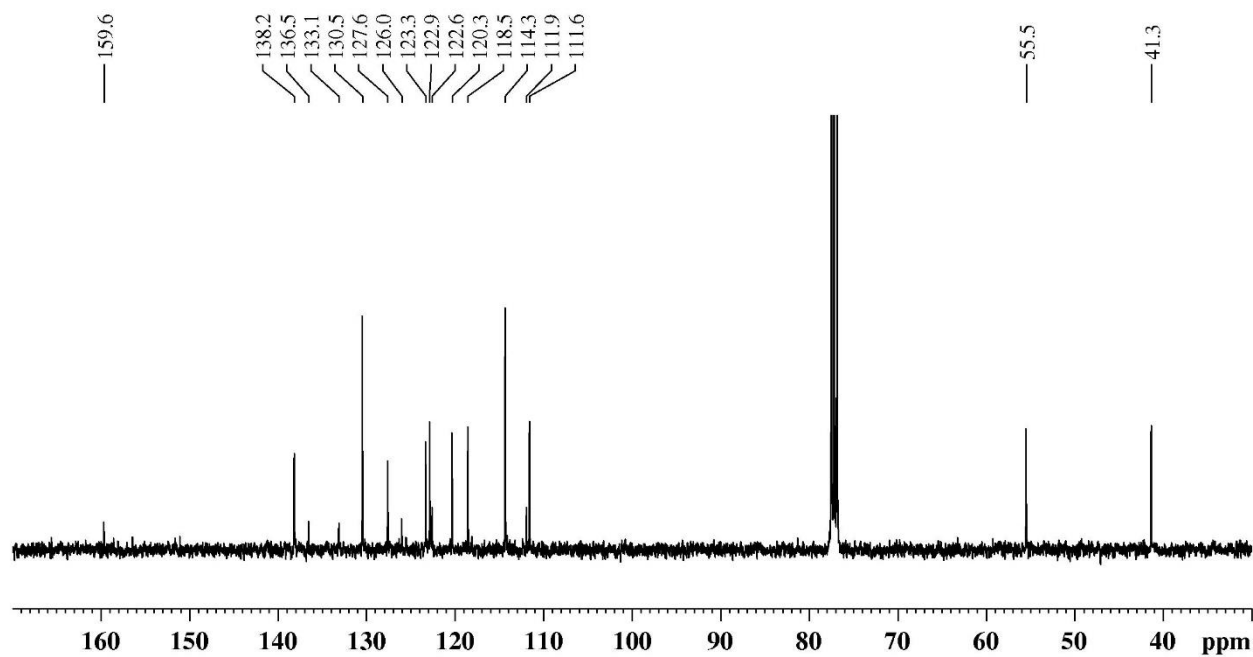
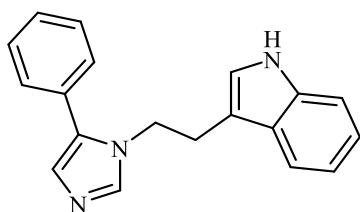
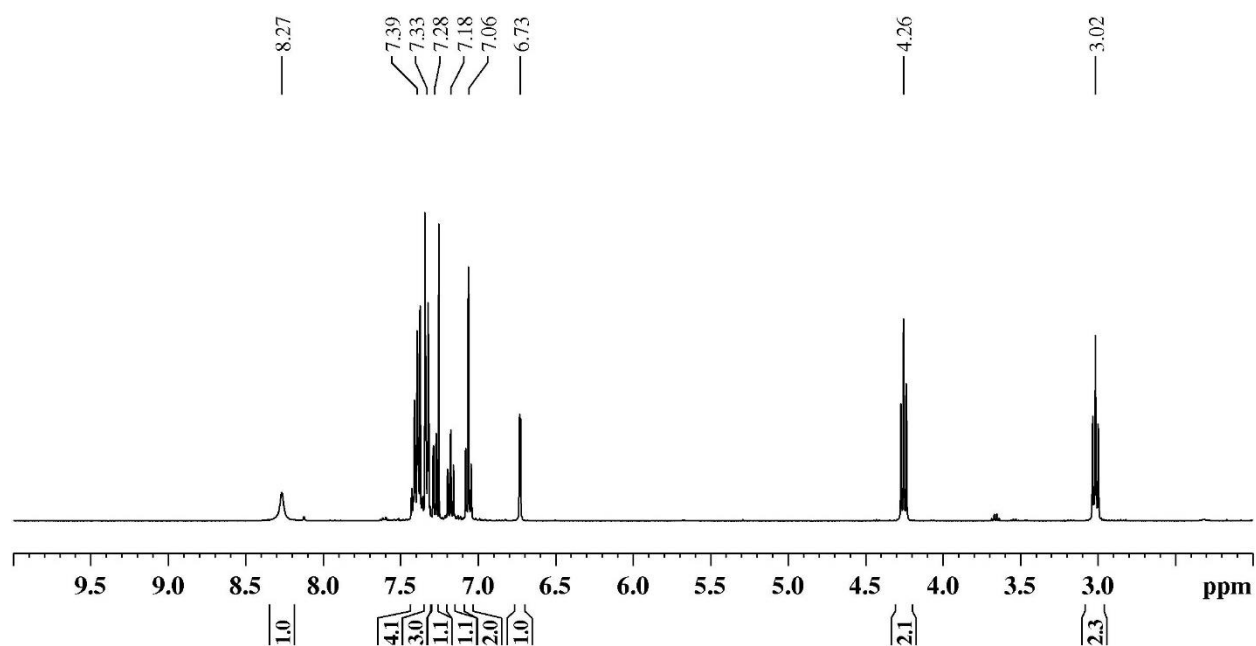


Figure S113. 3-(2-(5-Phenyl-1H-imidazol-1-yl)ethyl)-1H-indole (113)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

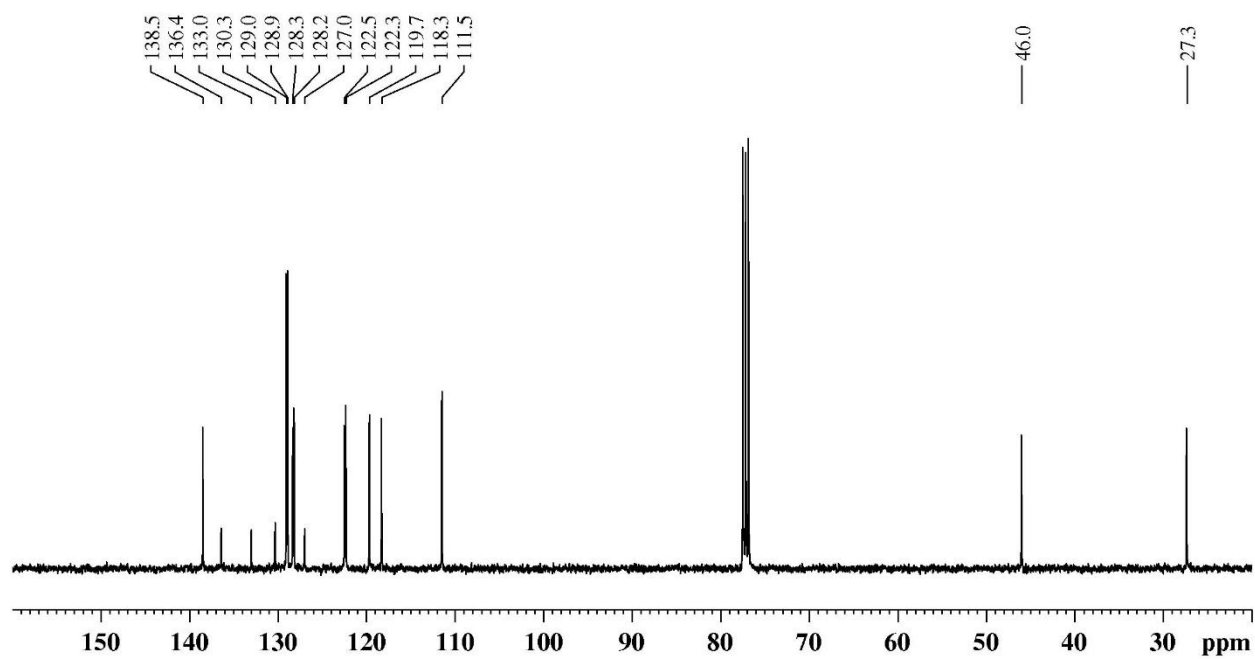
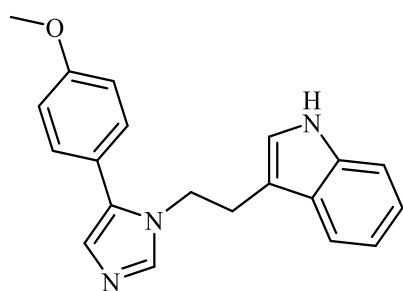
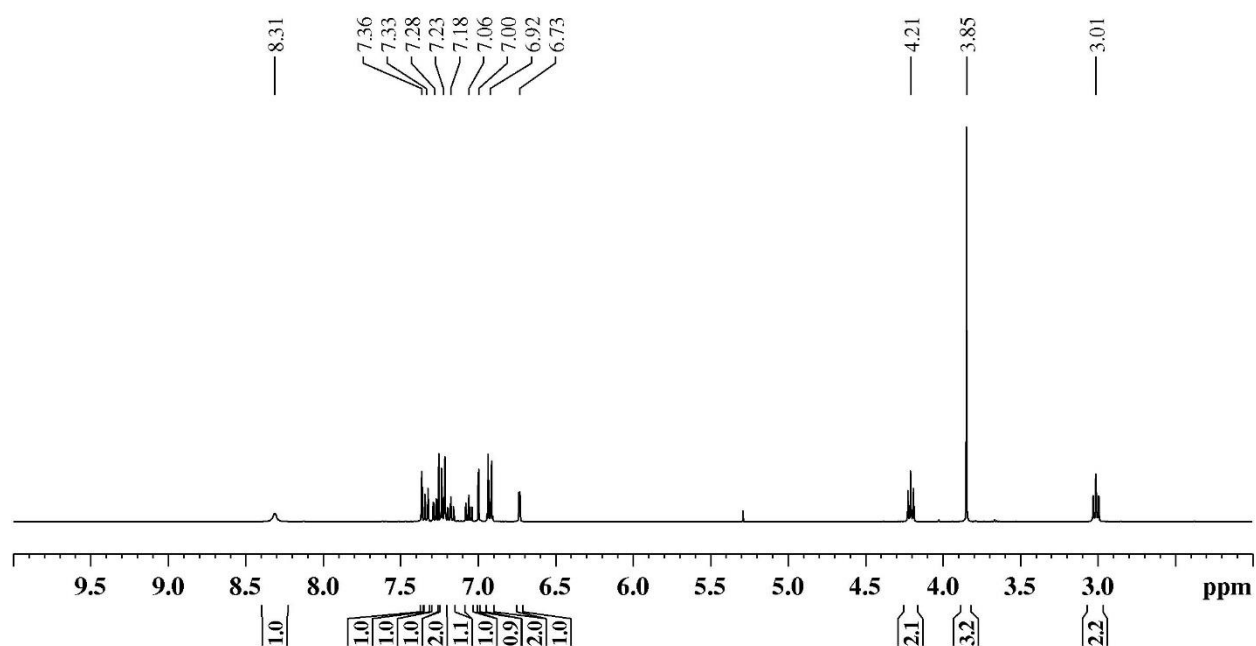


Figure S114. 3-(2-(5-(4-Methoxyphenyl)-1H-imidazol-1-yl)ethyl)-1H-indole (114)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

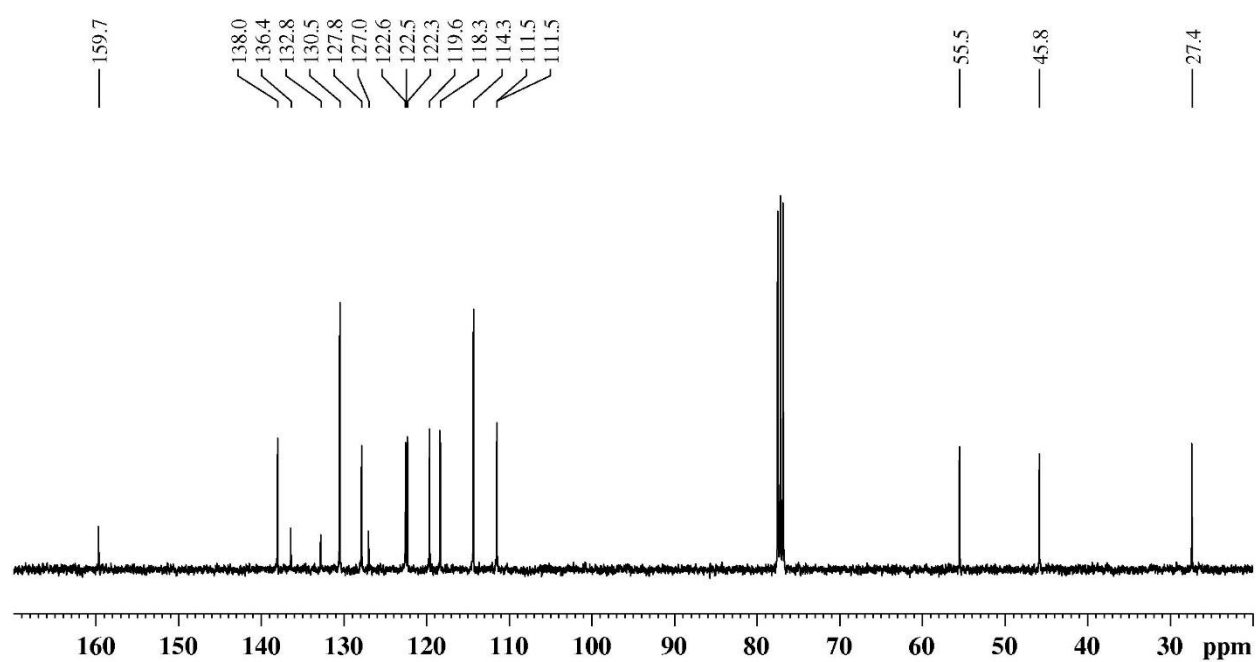
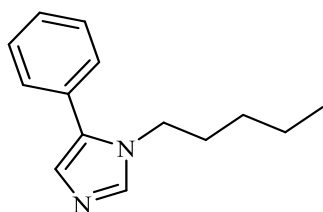
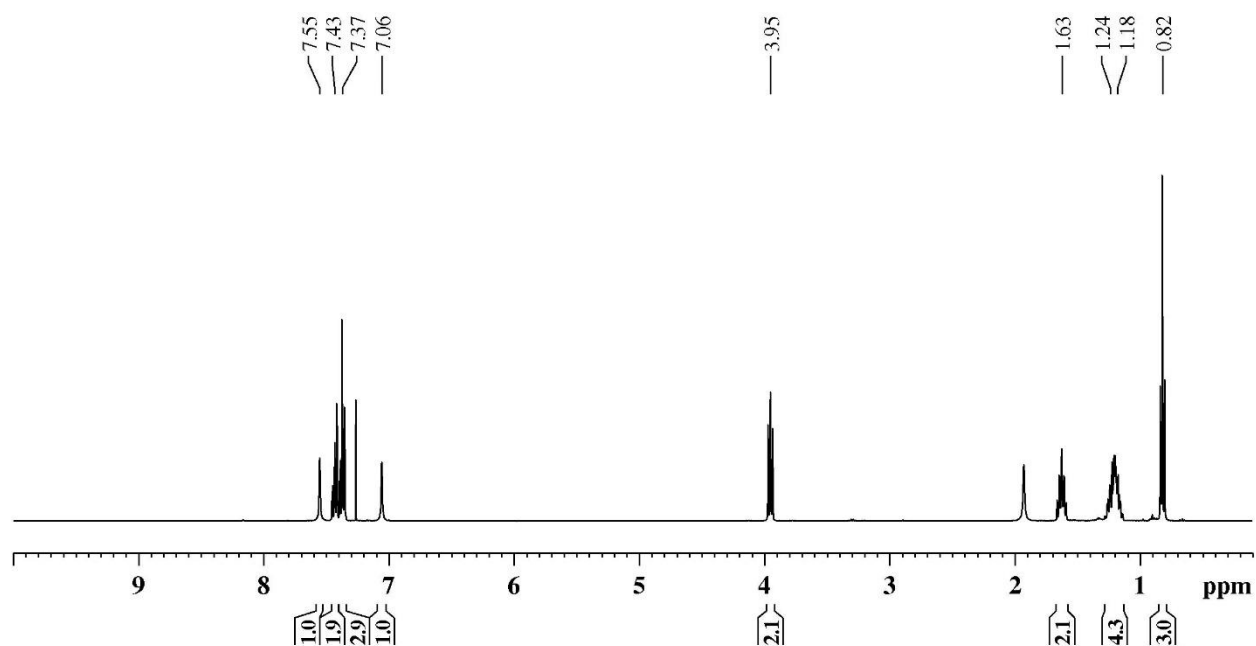


Figure S115. 1-Pentyl-5-phenyl-1*H*-imidazole (115)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

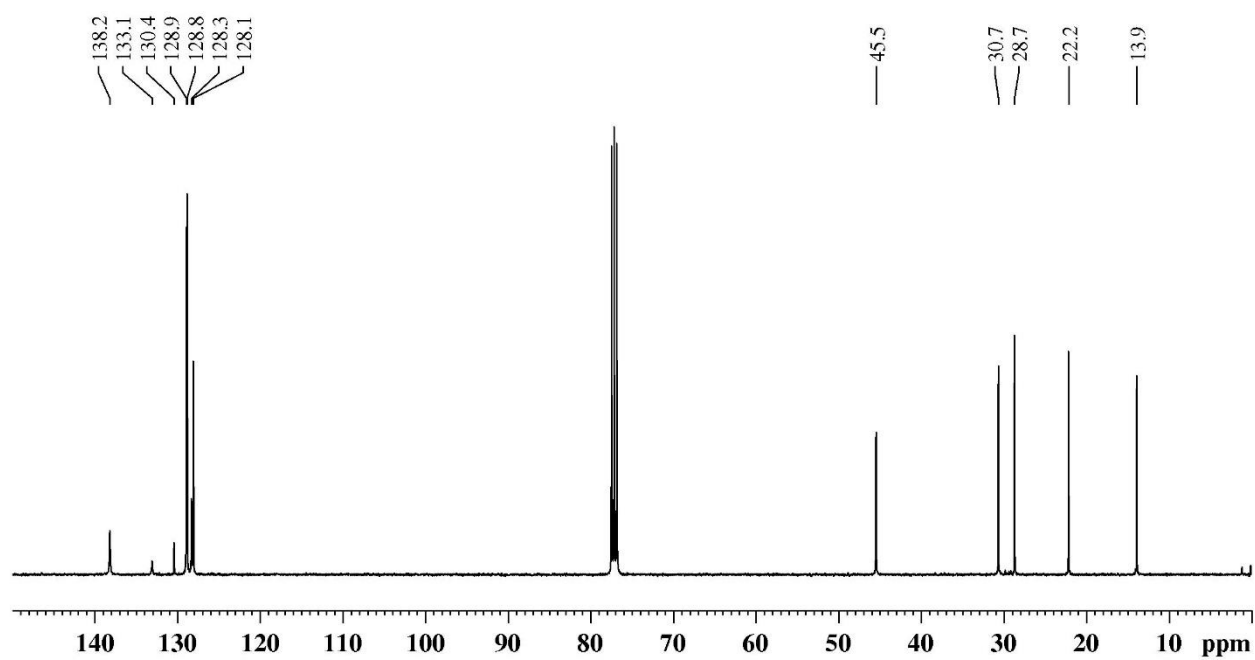
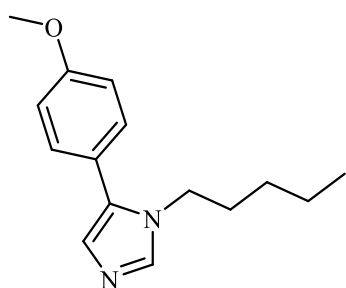
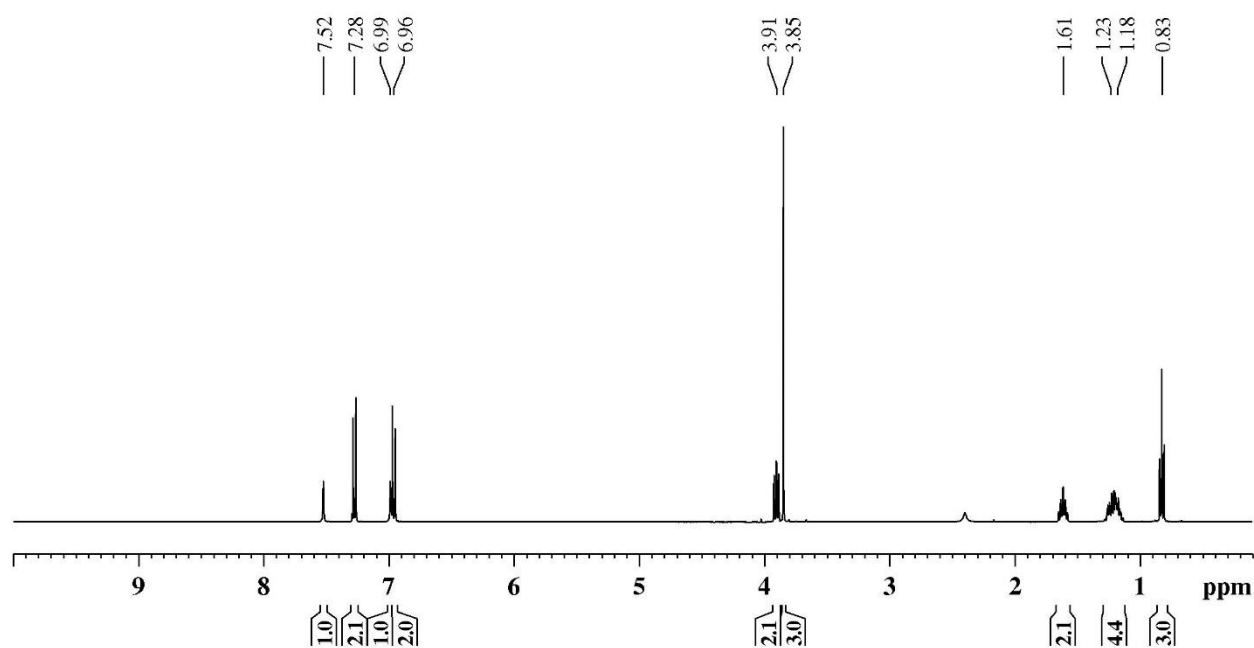


Figure S116. 5-(4-Methoxyphenyl)-1-pentyl-1H-imidazole (**116**)



^1H NMR (CDCl_3 , 400 MHz):



^{13}C NMR (CDCl_3 , 100 MHz):

