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Multi-step Synthesis and Characterization of a series different 4-substituted -1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole hybrids

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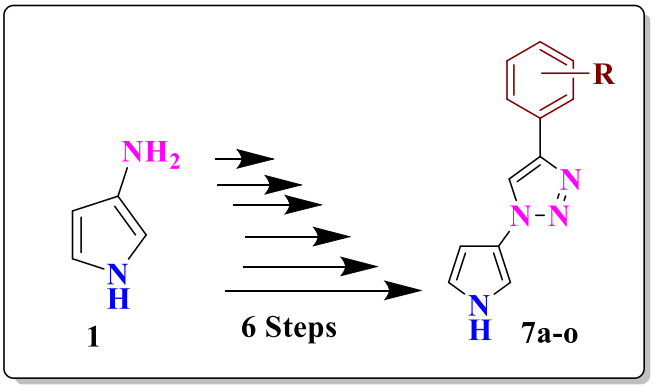
Abstract: Herein, we report the synthesis of 4-Aryl-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazoles from sequential synthesis. N-H activation, Boc protection, Deprotection, azide formation, [3+2] cycloaddition under Cu $^{+2}$ to Cu $^{+1}$ by means of sodium ascorbate leads to 1,2,3-triazole formation and subsequently *tert*-butyl 1*H*-pyrrole-1-carboxylate deprotection to obtain target 4-substituted -1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazoles**7a-o**. Compounds are further charecterized by spectral analysis.

Keywords:N-H activation, terminal alkyne, copper (II) sulphate, cyclo addition,1,2,3-triazoles, Pyrrole, TFA.



Graphical Abstract

1. INTRODUCTION

N-containing heterocycles are commonly embedded within polycyclic frameworks, among which polycycles [1-5] Traditionally, diazo compounds have been most commonly used as the carbene precursors.[6-7] Gevorgyan and Fokin showed that Nsulfonyl-1,2,3-triazoles are proficient of undergoing ring-to-chain isomerization to expose the diazo moiety.[8] As a result, these components can act as masked diazo compounds and serve as an alternative source of carbene precursors.[9] Since these initial reports, several groups have demonstrated the utilitiy of triazoles as carbene precursors for the development of useful transformations,[10] including trans annulation reactions for the direct synthesis of heterocycles.[11]

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Herein, we report the multi-step synthesis of 4-substituted -1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole are shown below.

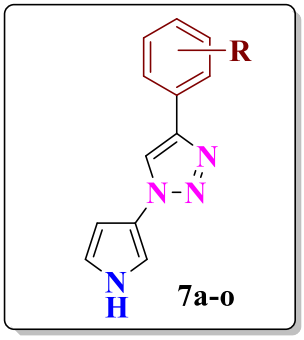


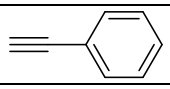
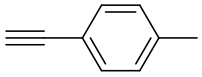
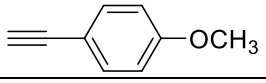
Fig: 14-Aryl-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazoles

2. EXPERIMENTAL SECTION

2.1General information

All reactions were carried out in a round bottom flask under room temperature. All the reagents and solvents were purchased from S.D. Fine chemicals limited and used without further purification. Thin-layer chromatography (TLC) was performed using Merck silica gel 60F254 precoated plates (0.25 mm) and silica gel (particle size 60-120 mesh) was used for column chromatography.^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz & 100 MHz instrument. Chemical shift values are given in δ (ppm) with tetramethyl silane as an internal standard and the coupling constant values (J) are in Hz. Mass spectral measurements were carried out by EI method on a Jeol JMC-300 spectrometer at 70eV. Elemental analyses were performed on a Carlo Erba 106 and Perkin Elmer model 240 analyzers. Mass spectra were recorded on ESI-MS. The purchased chemical are tabulated below.

Table: 1 List of Compounds purchase from Aldrich chemical company

Entry	Name	Structure	CAS Number
1	ethynylbenzene		117706
2	1-ethynyl-4-methylbenzene		206504
3	1-ethynyl-4-methoxybenzene		206490

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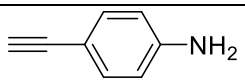
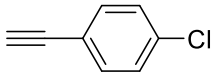
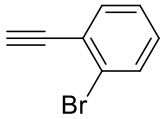
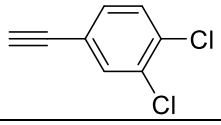
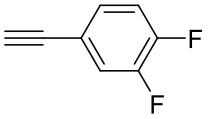
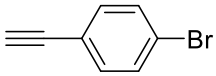
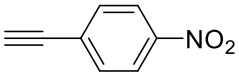
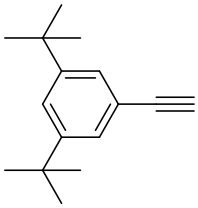
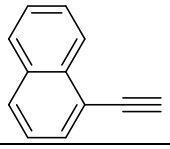
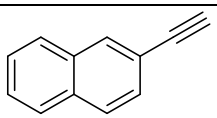
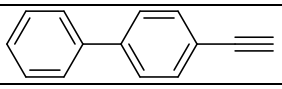
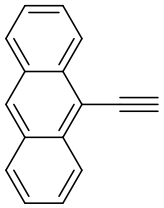
4	4-Ethynylaniline		14235-81-5
5	1-Chloro-4-ethynylbenzene		873-73-4
6	1-Bromo-2-ethynylbenzene		766-46-1
7	3,4-Dichlorophenylacetylene		556112-20-0
8	3,4-Difluorophenylacetylene		143874-13-9
9	1-Bromo-4-ethynylbenzene		766-96-1
10	1-Ethynyl-4-nitrobenzene		937-31-5
11	1,3-di-tert-butyl-5-ethynylbenzene		36720-94-2
12	1-ethynylnaphthalene		557923
13	2-ethynylnaphthalene		CDS008002
14	4-ethynyl-1,1'-biphenyl		521175
15	9-ethynylanthracene		13752-40-4

2.2.1 Synthesis of 2-(1*H*-pyrrol-3-yl) isoindoline-1,3-dione 2

the reaction of isobenzofuran-1,3-dione (PA) and 1H-pyrrol-3-amine **1** in DCM at 15-20 ^{0}C to obtain 2-(1*H*-pyrrol-3-yl) isoindoline-1,3-dione **2.**[12-13]

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2.2.2 Synthesis of *tert*-butyl (S)-(1-amino-1-oxopropan-2-yl) carbamate 3

To a stirred solution of 2-(1*H*-pyrrol-3-yl) isoindoline-1,3-dione **2**(811 mmol) in Dichloromethane (700 ml) was added triethylamine (1622 mmol) and Boc-anhydride (892 mmol) at 0 °C. The reaction mixture was stirred at 25 °C for 16h. Reaction was monitored by TLC. After completion of reaction, it was diluted with water (400 ml) and extracted with DCM (500ml X 2). The organic layer was concentrated under reduced pressure to obtained *tert*-butyl 3-(1,3-dioxoisoindolin-2-yl)-1H-pyrrole-1-carboxylate**3***viz*boc protection. It is treated with methyl amine to yield *tert*-butyl 3-amino-1*H*-pyrrole-1-carboxylate **4.**

2.2.3 Synthesis of *tert*-butyl 3-azido-1*H*-pyrrole-1-carboxylate 5: *tert*-butyl 3-amino-1*H*-pyrrole-1-carboxylate **4** 1.48 mmol containing amine functionality was dissolved in CH_3CN (2 mL) in a RB flask and cooled to 0°C in an ice bath. To this stirred mixture was added 2.22 mmol of *t*-BuONO followed by 1.77 mmol $TMSN_3$ drop-wise. The subsequent solution was stirred at RT for 1 h further followed by reaction mixture was focused under vacuum and the crude product was purified by silica gel chromatography (hexane) to give *tert*-butyl 3-azido-1*H*-pyrrole-1-carboxylate **5.**

2.2.4 Synthesis of*tert*-butyl 3-(4-substituted-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6a-o: *tert*-butyl 3-azido-1*H*-pyrrole-1-carboxylate 5 was stirred at RT for 2 h in the presence of 0.54 mmol series of substituted Phenyl acetylenes, aq. solution (0.2 mL) 0.036 mmol of $CuSO_4.5H_2O$ and 0.108 mmol sodium ascorbate which is namely Sharpless catalyst were then added and the reaction was stirred the product was then precipitated with methanol to give the product an off white solid of 6a-o viz 1,3- dipolar cyclo addition as click protocols**.**

2.2.5 Synthesis of 4-substituted -1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7a-o from 6a-o:

To a stirred solution of compounds 6a-o (500 mg, 1.68 mmol) in DCM (10 mL) was added TFA (2mL) at 0 ^{O}C and stirred the reaction mixture at RT for 3 h. The progress of the reaction was monitored by TLC and the reaction mixture was concentrated under reduced pressure. The residue is washed with diethyl ether to afford solid 4-substituted -1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole **7a-o** TFA salt as off white solid (650 mg, crude wt).

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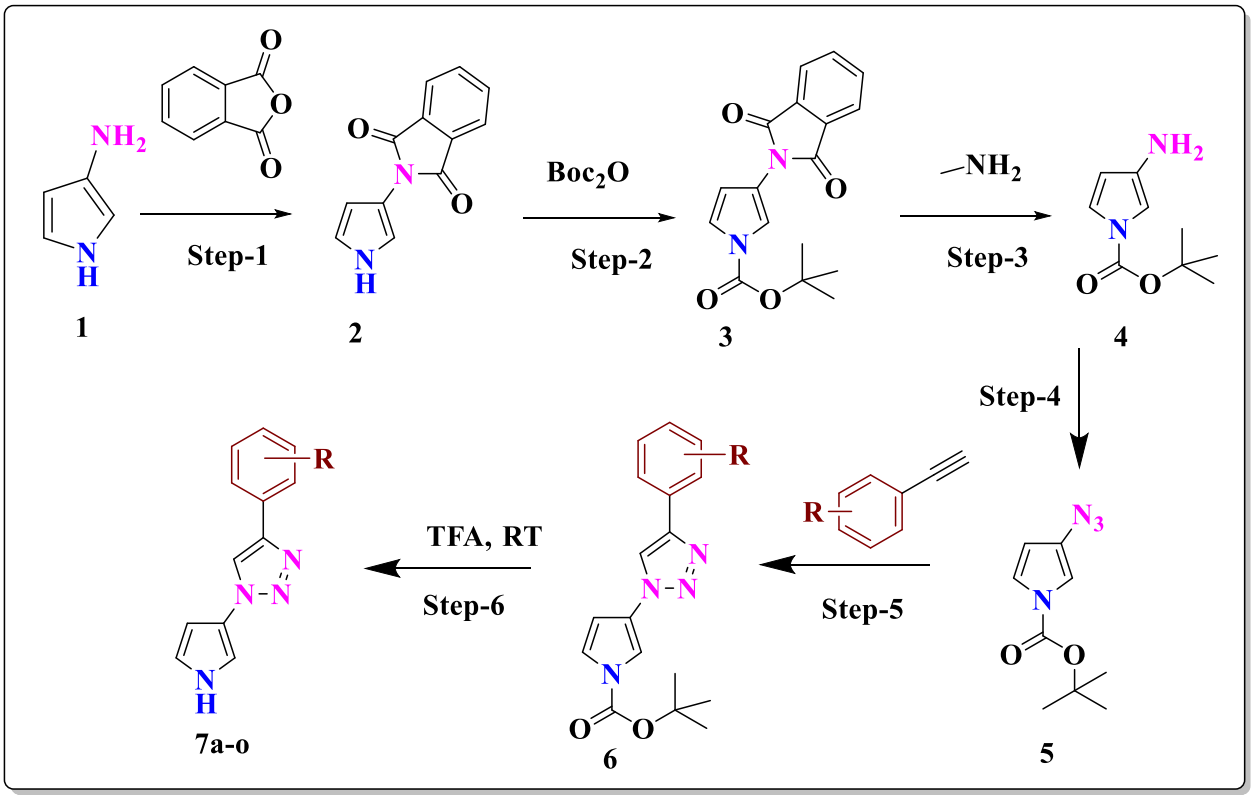
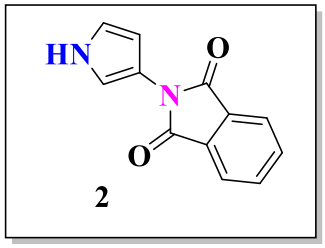
3. RESULTS AND DISCUSSIONS

A different series of 4-substituted -1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazoles**7a-o**synthesis led to promising yields described in Scheme I.



Scheme I. Synthetic path way for target compounds**7a-o**

2-(1H-pyrrol-3-yl) isoindoline-1,3-dione 2 :



MF: $C_{12}H_8N_2O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 7.91 (dt, *J* = 7.5, 3.7 Hz, 2H), 7.60 (dd, *J* = 8.2, 4.7 Hz, 2H), 6.91 – 6.66 (m, 1H), 5.99 (d, *J* = 7.5 Hz, 1H), 5.88 (s, 1H), 5.52 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 167.28 (2C), 134.26, 131.88 (2C), 127.22, 124.98 (2C), 121.76, 118.55 (2C), 111.99; **ESI $[M+H]^+$:** 212.06; **Elemental Analysis (%):**Found:C, 68.04; H, 3.81; N, 13.22 , (Calcd): (C, 67.92; H, 3.80; N, 13.20).

***tert*-butyl 3-(1,3-dioxoisoindolin-2-yl)-1H-pyrrole-1-carboxylate 3 :**

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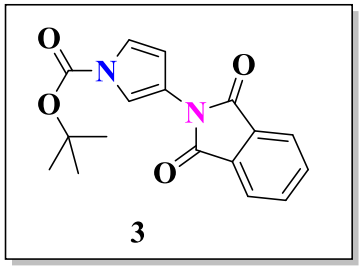
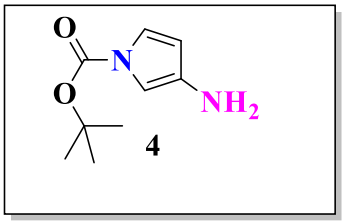


3

MF:$C_{17}H_{16}N_2O_4$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.10 (d, *J* = 7.4 Hz, 1H), 7.87 (d, *J* = 13.0 Hz, 2H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.63 (d, *J* = 9.0 Hz, 2H), 7.41 (s, 1H), 1.51 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 167.28 (2C), 150.87 , 134.26 (2C), 131.88 (2C), 131.25 , 124.98 (2C), 121.33,118 108.71, 80.96, 28.41 (3C);**ESI [M+H]$^+$:** 312.11; **Elemental Analysis (%):**Found:C, 65.50; H, 5.17; N, 8.99, (Calcd): (C, 65.38; H, 5.16; N, 8.97).

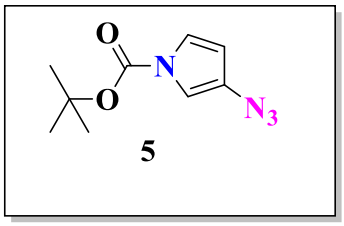
***tert*-butyl 3-amino-1H-pyrrole-1-carboxylate 4 :**



4

MF:$C_9H_{14}N_2O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.90 (d, *J* = 7.5 Hz, 1H), 7.66 (s, 2H), 6.87 (d, *J* = 9.1 Hz, 1H), 6.16 (s, 1H), 1.49 (s, 9H)**; ^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 133.32, 127.32, 109.31, 101.81, 80.96, 28.41 (3C);**ESI [M+H]$^+$:** 182.11; **Elemental Analysis (%):**Found: C, 59.44; H, 7.75; N, 15.39, (Calcd): (C, 59.32; H, 7.74; N, 15.37).

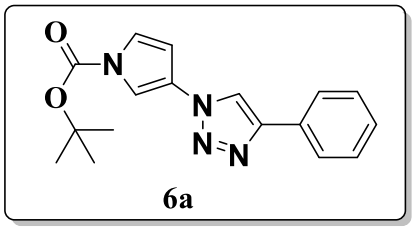
***tert*-butyl 3-azido-1H-pyrrole-1-carboxylate 5 :**



5

MF:$C_9H_{12}N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.84 (s, 1H), 8.12 (s, 1H), 7.57 (s, 1H), 1.49 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** δ 150.87, 130.98, 121.87, 120.80, 106.05, 80.96, 28.41 (3C); **ESI [M+H]$^+$:** 208.10; **Elemental Analysis (%):**Found: C, 52.06; H, 5.82; N, 26.95 , (Calcd): (C, 51.92; H, 5.81; N, 26.91).

***tert*-butyl 3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6a :**



6a

MF:$C_{17}H_{18}N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.24 – 7.95 (m, 2H), 7.69 (s, 1H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.32 (d, *J* = 8.9 Hz, 1H), 1.50 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 148.94, 130.41, 129.53, 128.86 (2C), 126.28, 125.77 (2C), 124.90, 119.77, 117.46, 104.63, 80.96, 28.41 (3C);**ESI [M+H]$^+$:** 310.14;

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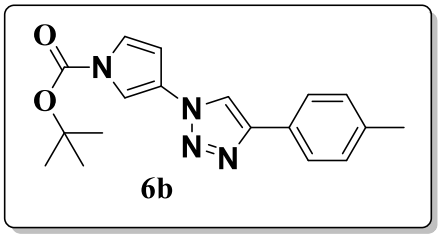
Elemental Analysis (%): Found: C, 65.91; H, 5.86; N, 18.07, (Calcd): (C, 65.79; H, 5.85; N, 18.05).

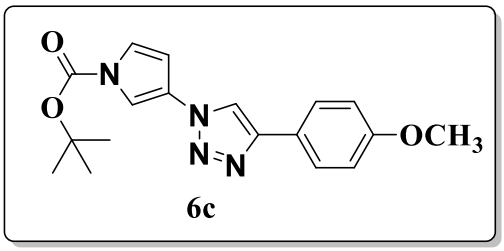
***tert*-butyl 3-(4-(p-tolyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6b :**



6b

MF: C18H20N4O2, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.08 (s, 1H), 7.85 (s, 1H), 7.72 (s, 1H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.39 (d, *J* = 8.9 Hz, 1H), 7.31 (d, *J* = 7.5 Hz, 2H), 2.35 (s, 3H), 1.49 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 148.94, 136.14, 130.31, 129.53 , 128.90 (2C), 126.37 (2C), 124.90, 119.77, 117.46, 104.63, 80.96, 28.41 (3C), 21.12;**ESI [M+H]$^{+}$:** 324.16; **Elemental Analysis (%):**Found: C, 66.77; H, 6.22; N, 17.29, (Calcd): (C, 66.65; H, 6.21; N, 17.27).

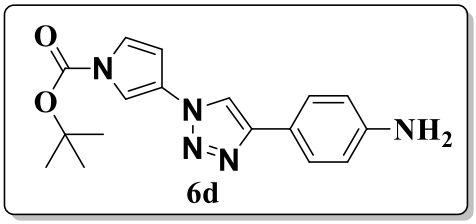
***tert*-butyl 3-(4-(4-methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6c :**



6c

MF:$C_{18}H_{20}N_4O_3$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.08 (s, 2H), 7.86 (s, 2H), 7.60 (s, 3H), 7.40 (s, 2H), 7.05 (s, 4H), 3.81 (s, 6H), 1.49 (s, 18H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 159.63, 150.87, 148.94, 129.53, 125.92 (2C), 124.90 , 124.61, 119.77, 117.46, 114.40 (2C), 104.63, 80.96, 56.03, 28.41 (3C);**ESI [M+H]$^{+}$:** 340.15; **Elemental Analysis (%):**Found:C, 63.64; H, 5.93; N, 16.48 , (Calcd): (C, 63.52; H, 5.92; N, 16.46).

***tert*-butyl 3-(4-(4-aminophenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6d :**



6d

MF:$C_{17}H_{19}N_5O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.08 (s, 1H), 7.86 (s, 1H), 7.71 (s, 1H), 7.42 (d, *J* = 7.5 Hz, 3H), 6.74 (d, *J* = 7.5 Hz, 2H), 3.95 (s, 2H), 1.49 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 148.94, 148.53, 129.53, 124.98 (2C), 122.55, 119.77 (2C), 117.46 , 111.31 (2C), 104.63, 80.96, 28.40 (3C);**ESI [M+H]$^{+}$:**325.15;**Elemental Analysis (%):**Found: C, 62.87; H, 5.90; N, 21.54 , (Calcd): (C, 62.75; H, 5.89; N, 21.52).

***tert*-butyl 3-(4-(4-chlorophenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6e :**

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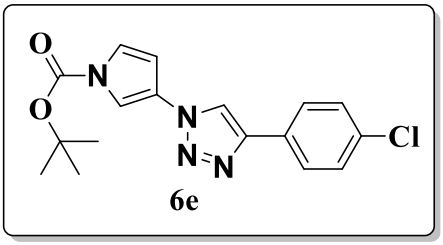
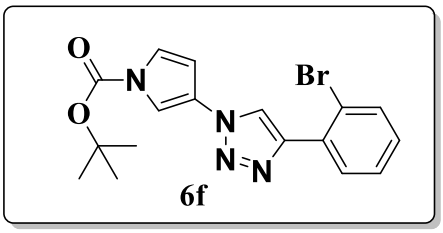


6e

MF:$C_{17}H_{17}ClN_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.08 (s, 1H), 7.85 (s, 1H), 7.73 (s, 1H), 7.62 – 7.29 (m, 5H), 1.49 (s, 9H)**;^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 148.94, 134.14, 129.53, 129.20 (2C), 128.28 (2C), 124.90 (2C), 119.77, 117.46, 104.63, 80.96 , 28.41 (3C); **ESI [M+H]$^+$:**344.10; **Elemental Analysis (%):**Found: C, 59.22; H, 4.97;N, 16.25, (Calcd): (C, 59.22; H, 4.97;N, 16.25).

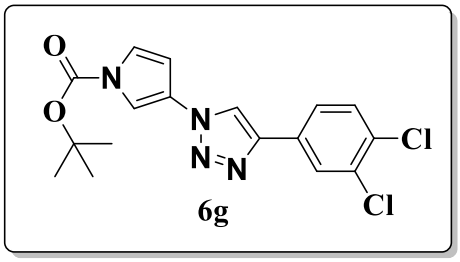
***tert*-butyl 3-(4-(2-bromophenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6f :**



6f

MF:$C_{17}H_{17}BrN_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.08 (d, *J* = 3.8 Hz, 2H), 7.68 (s, 1H), 7.62 (d, *J* = 6.0 Hz, 1H), 7.54 (d, *J* = 7.5 Hz, 2H), 7.39 (s, 1H), 7.25 (d, *J* = 8.9 Hz, 1H), 1.50 (s, 9H)**;^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 149.26, 133.46, 132.19, 129.53, 128.78, 127.02, 126.31, 124.73, 122.38, 119.77, 117.46, 104.63, 80.96, 28.41 (3C); **ESI [M+H]$^+$:** 388.05;**Elemental Analysis (%):**Found:C, 52.58; H, 4.41; N, 14.41, (Calcd): (C, 52.46; H, 4.40; N, 14.39).

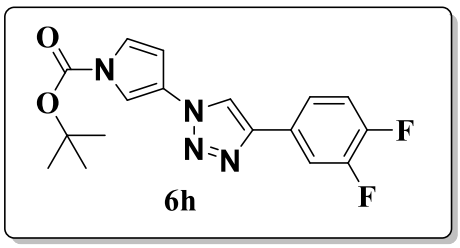
***tert*-butyl 3-(4-(3,4-dichlorophenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6g :**



6g

MF: $C_{17}H_{16}Cl_2N_4O_2$,^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.09 (d, *J* = 10.3 Hz, 2H), 7.68 (s, 2H), 7.45 (d, *J* = 26.9 Hz, 3H), 1.50 (s, 9H)**;^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 149.06, 132.78, 132.06, 131.41, 129.53, 129.16, 128.79 , 125.86 (2C), 119.77, 117.46, 104.63, 80.96, 28.41 (3C);**ESI [M+H]$^+$:** 378.07, **Elemental Analysis (%):**Found: C, 53.96; H, 4.26; N, 14.79 , (Calcd): (C, 53.84; H, 4.25; N, 14.77).

***tert*-butyl 3-(4-(3,4-difluorophenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6h :**

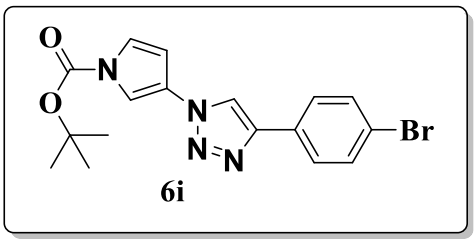


6h

ISSN: 2366-1313

MF: $C_{17}H_{16}F_2N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.10 (d, *J* = 15.8 Hz, 2H), 7.67 (s, 1H), 7.51 (s, 1H), 7.35 (s, 2H), 7.14 (s, 1H), 1.50 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 151.48 , 148.60, 129.53, 126.42, 125.42, 120.64, 119.77, 118.40, 118.19, 117.46, 116.89, 116.68, 104.63, 80.96, 28.41 (3C);**ESI [M+H]$^+$:** 346.12, **Elemental Analysis (%):**Found:C, 59.08; H, 4.67; N, 16.20, (Calcd): (C, 58.96; H, 4.66; N, 16.18).

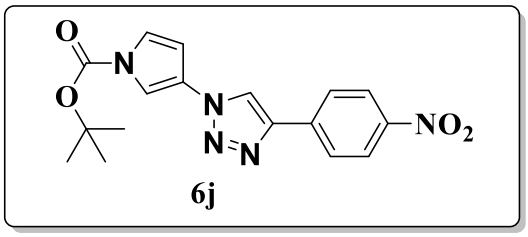
***tert*-butyl 3-(4-(4-bromophenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6i :**



6i

MF:$C_{17}H_{17}BrN_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.08 (s, 1H), 7.85 (d, *J* = 7.5 Hz, 1H), 7.73 (s, 1H), 7.56 (dd, *J* = 55.9, 7.5 Hz, 4H), 7.37 (d, *J* = 8.9 Hz, 1H), 1.49 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):**150.87, 148.94, 132.37, 129.53, 128.37, 127.48 (2C), 124.90 (2C), 123.35, 119.77, 117.46, 104.63, 80.96, 28.41 (3C);**ESI [M+H]$^+$:** 388.05;**Elemental Analysis (%):**Found: C, 52.58; H, 4.41; N, 14.41 , (Calcd): (C, 52.46; H, 4.40; N, 14.39).

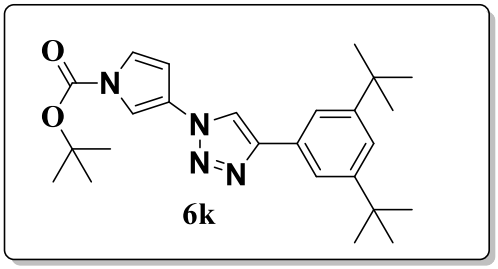
***tert*-butyl 3-(4-(4-nitrophenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6j :**



6j

MF:$C_{17}H_{17}N_5O_4$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.32 (s, 2H), 8.19 – 8.03 (m, 2H), 7.88 (d, *J* = 7.5 Hz, 2H), 7.73 (s, 1H), 7.52 (s, 1H), 1.50 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 148.94, 146.40, 134.60 (2C), 129.53 (2C), 124.86 , 124.45 (2C), 119.77, 117.46 ,104.63, 80.96, 28.41 (3C);**ESI [M]$^+$:** 355.13**; Elemental Analysis (%):**Found:C, 57.58; H, 4.83; N, 19.73,(Calcd): (C, 57.46; H, 4.82; N, 19.71).

***tert*-butyl 3-(4-(3,5-di-tert-butylphenyl)-1H-1,2,3-triazol-1-yl)-1H-pyrrole-1-carboxylate 6k:**



6k

MF:$C_{25}H_{34}N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):8.34 (s, 1H), 8.08 (s, 1H), 7.75 (s, 1H), 7.58 (s, 1H), 7.45 (d, *J* = 51.4 Hz, 3H), 1.51 (s, 9H), 1.41 (s, 18H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 159.39, 150.87, 148.11 (2C), 130.72, 129.53, 121.48 (2C), 120.22, 119.77, 118.28 (2C), 117.46, 104.63, 80.96, 35.22, 31.43 (3C), 28.41 (6C); **ESI [M+H]$^+$:** 422.27;**Elemental Analysis (%)**:Found: C, 71.18; H, 8.12; N, 13.28 , (Calcd): (C, 71.06; H, 8.11; N, 13.26).

***tert*-butyl 3-(4-(naphthalen-1-yl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6l:**

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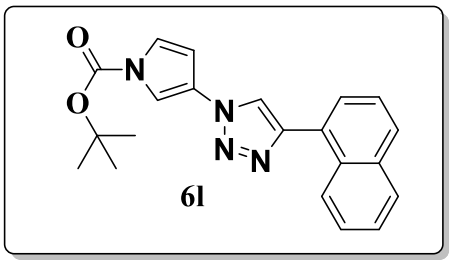
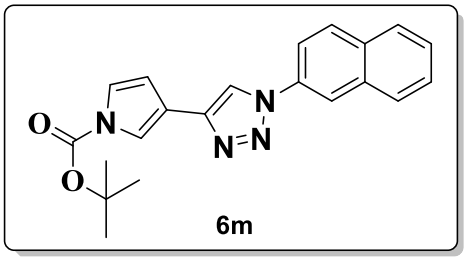


6l

MF:$C_{21}H_{20}N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.10 (d, *J* = 17.8 Hz, 2H), 8.00 – 7.75 (m, 4H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.50 (dd, *J* = 29.0, 5.7 Hz, 3H), 1.51 (s, 9H)**;^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 145.49, 131.78 (2C), 131.43, 129.88 (2C), 128.63, 127.64, 126.99, 125.47 (2C), 125.09, 123.89, 119.77, 117.46 , 104.63, 80.96, 28.41 (3C);**ESI [M+H]$^+$:** 360.16; **Elemental Analysis (%):**Found:C, 70.10; H, 5.60; N, 15.57, (Calcd): (C, 69.98; H, 5.59; N, 15.55).

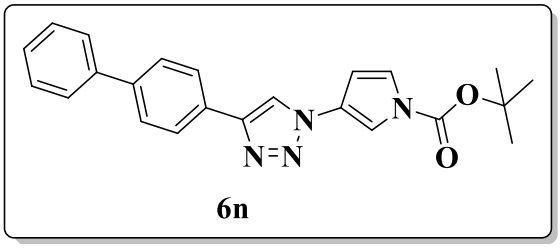
***tert* -butyl 3-(1-(naphthalen-2-yl)-1 *H* -1,2,3-triazol-4-yl)-1 *H* -pyrrole-1-carboxylate 6m :**



6m

MF:$C_{21}H_{20}N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.24 – 7.78 (m, 8H), 7.63 (d, *J* = 6.1 Hz, 1H), 7.49 (dd, *J* = 25.0, 6.7 Hz, 2H), 1.51 (s, 9H)**;^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 145.08, 138.30, 134.85, 130.56, 130.28, 128.80 (2C), 127.62, 126.94 (2C), 125.37 (2C), 125.07, 123.65, 121.74, 120.35, 115.03, 110.28, 80.96, 28.41 (3C); **ESI [M+H]$^+$:** 360.16;**Elemental Analysis (%):**Found: C, 69.98; H, 5.60; N, 15.57, (Calcd): (C, 69.98; H, 5.59; N, 15.55).

***tert* -butyl 3-(4-([1,1'-biphenyl]-4-yl)-1 *H* -1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6n :**



6n

MF:$C_{23}H_{22}N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.08 (s, 1H), 8.02 – 7.81 (m, 2H), 7.76 (d, *J* = 7.7 Hz, 4H), 7.58 (d, *J* = 22.6 Hz, 3H), 7.50 – 7.29 (m, 3H), 1.50 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.87, 148.94, 140.41, 138.77, 130.36,129.53,128.92 (4C),128.33, 127.32 (2C), 125.44 (2C), 124.90, 119.77, 117.46 , 104.63, 80.96,28.41 (3C);**ESI [M+H]$^+$:** 386.17; **Elemental Analysis (%):**Found: C, 71.60; H, 5.75; N, 14.52 , (Calcd): (C, 71.48; H, 5.74; N, 14.50).

***tert*-butyl 3-(4-(anthracen-9-yl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-1-carboxylate 6o :**

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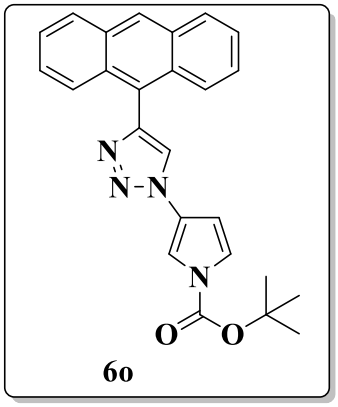
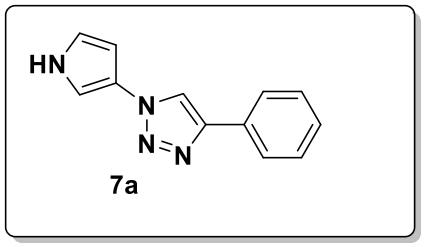


6o

MF:$C_{25}H_{22}N_4O_2$, ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.39 (s, 1H), 8.13 – 7.78 (m, 7H), 7.57 (d, *J* = 8.9 Hz, 1H), 7.43 (d, *J* = 16.7 Hz, 4H), 1.51 (s, 9H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** δ 150.87, 145.90,133.03 (2C),131.38 (2C), 129.53, 128.88 (2C), 128.45 (2C), 128.23, 127.54 (2C), 126.53, 125.69 (2C), 119.77, 117.46, 104.63, 80.96, 28.41 (3C); **ESI [M+H]$^+$:** 410.17, **Elemental Analysis (%):**Found: C, 73.27; H, 5.41; N, 13.67 , (Calcd): (C, 73.15; H, 5.40; N, 13.65).

Analysis data for Target compounds 7a-o:

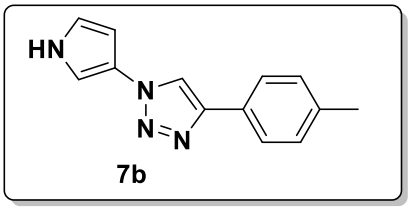
4-phenyl-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7a:



7a

MF:$C_{12}H_{10}N_4$,Light white, yield: 90%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.52 – 7.25 (m, 3H), 7.01 (d, *J* = 9.5 Hz, 1H), 6.90 – 6.66 (m, 2H), 6.13 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):**148.94, 130.41, 128.86, 126.28, 125.77, 124.90, 123.48, 119.36, 113.05, 108.37;**ESI [M+H]$^+$:** 210.09;**Elemental Analysis (%):** Found: C, 68.67; H, 4.80; N, 26.67, (Calcd): (C, 68.56; H, 4.79; N, 26.65).

1-(1*H*-pyrrol-3-yl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole 7b:



7b

MF:$C_{13}H_{12}N_4$,Pale white, yield: 84%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.56 (d, *J* = 7.5 Hz, 2H), 7.31 (s, 2H), 7.01 (d, *J* = 9.5 Hz, 1H), 6.75 (dd, *J* = 16.4, 5.3 Hz, 2H), 6.13 (s, 1H), 2.35 (s, 3H),**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 148.94, 136.14, 130.31, 128.90, 126.37, 124.90, 123.48, 119.36, 113.05, 108.37, 21.12;**ESI [M+H]$^+$:** 224.11, **Elemental Analysis (%):** Found:C, 69.74; H, 5.40; N, 25.00,(Calcd): (C, 69.62; H, 5.39; N, 24.98).

4-(4-methoxyphenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7c:

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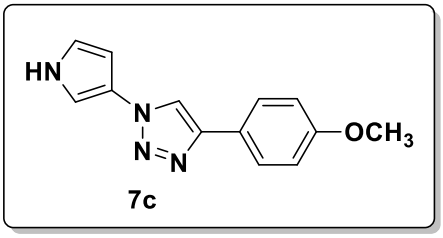
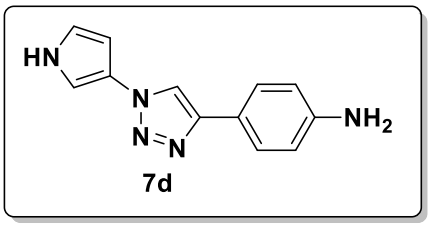


7c

MF:$C_{13}H_{12}N_4O$,Off white, yield: 90%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.60 (s, 2H), 7.03 (dd, *J* = 21.4, 7.5 Hz, 3H), 6.75 (dd, *J* = 18.7, 4.6 Hz, 2H), 6.13 (s, 1H), 3.82 (s, 3H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 159.63, 148.94, 125.92, 124.90, 124.61 , 123.48 , 119.36, 114.40 , 113.05, 108.37, 56.03;**ESI [M+H]$^+$:** 240.10;**Elemental Analysis (%):** Found:C, 65.02; H, 5.04; N, 23.35, (Calcd): (C, 64.99; H, 5.03; N, 23.32).

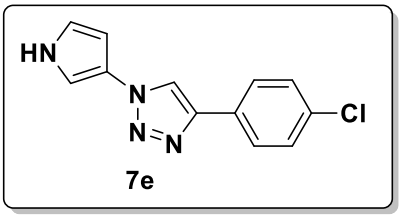
4-(1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazol-4-yl)aniline 7d:



7d

MF: $C_{12}H_{11}N_5$, Light yellow, yield: 82%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.42 (s, 2H), 7.01 (d, *J* = 9.5 Hz, 1H), 6.90 – 6.60 (m, 4H), 6.12 (s, 1H), 3.89 (s, 2H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 148.94, 148.53, 124.98, 123.48, 122.55(2C), 119.36, 113.05, 111.31, 108.37;**ESI [M+H]$^+$:** 225.10; **Elemental Analysis (%):** Found:C, 64.12; H, 4.93; N, 31.11, (Calcd): (C, 63.99; H, 4.92; N, 31.09).

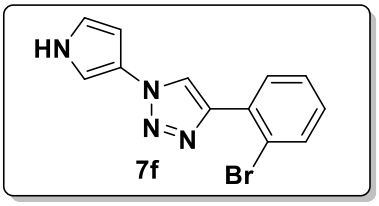
4-(4-chlorophenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7e:



7e

MF: $C_{12}H_9ClN_4$, Pale yellow, yield: 81%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.50 (dd, *J* = 50.7, 7.5 Hz, 4H), 7.00 (s, 1H), 6.75 (dd, *J* = 11.8, 5.2 Hz, 2H), 6.13 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 148.94, 134.14(2C), 129.56, 129.20, 128.28, 124.90, 123.48(2C), 119.36, 113.05 , 108.37;**ESI [M+H]$^+$:** 244.05;**Elemental Analysis (%):** Found:C, 59.01; H, 3.72; N, 22.92, (Calcd): (C, 58.91; H, 3.71; N, 22.90).

4-(2-bromophenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7f:

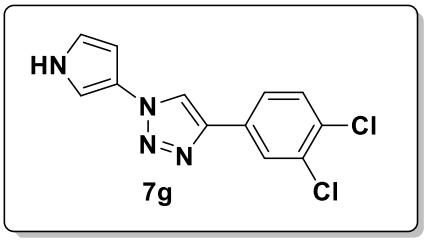


7f

ISSN: 2366-1313

MF:$C_{12}H_9BrN_4$,Dirty white, yield: 90%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.62 (d, *J* = 8.9 Hz, 1H), 7.54 (d, *J* = 8.9 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 9.7 Hz, 1H), 6.82 (s, 1H), 6.74 (s, 1H), 6.13 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 149.26, 133.46, 132.19, 128.78, 127.02, 126.31, 124.73, 123.48, 122.38 , 119.36, 113.05, 108.37;**ESI $[M+H]^+$:** 288.00; **Elemental Analysis (%):** Found: C, 49.97; H, 3.15; N, 19.40, (Calcd): (C, 49.85; H, 3.14; N, 19.38).

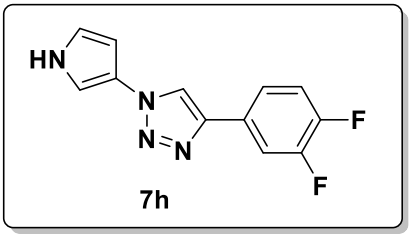
4-(3,4-dichlorophenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7g:



7g

MF:$C_{12}H_8Cl_2N_4$, Light yellow, yield: 90%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.66 (s, 1H), 7.42 (q, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 9.5 Hz, 1H), 6.75 (d, *J* = 9.1 Hz, 2H), 6.13 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 149.06, 132.78 , 132.06, 131.41, 129.16, 128.79, 125.86, 125.42, 123.48, 119.36, 113.05 , 108.37;**ESI $[M+H]^+$:** 278.01;**Elemental Analysis (%):** Found:C, 51.76; H, 2.90; N, 20.09, (Calcd): (C, 51.64; H, 2.89; N, 20.07).

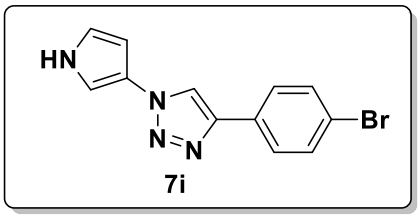
4-(3,4-difluorophenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7h:



7h

MF: $C_{12}H_8F_2N_4$, Light white, yield: 89%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.59 – 7.29 (m, 2H), 7.28 – 7.10 (m, 1H), 7.01 (d, *J* = 7.5 Hz, 1H), 6.75 (dd, *J* = 13.9, 5.4 Hz, 2H), 6.14 (s, 1H),**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 150.33, 149.54, 149.06, 126.38 , 125.42, 123.48 , 120.69, 119.36, 118.32, 116.76, 113.05, 108.38;**ESI $[M+H]^+$:** 246.07;**Elemental Analysis (%):** Found:C, 58.66; H, 3.29; N, 22.78, (Calcd): (C, 58.54; H, 3.28; N, 22.76).

4-(4-bromophenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7i:



7i

MF:$C_{12}H_9BrN_4$,White, yield: 90%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.56 (dd, *J* = 55.5, 7.5 Hz, 4H), 7.00 (d, *J* = 9.5 Hz, 1H), 6.87 – 6.60 (m, 2H), 6.13 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 148.94, 132.37, 128.37, 127.48, 124.90, 123.42, 119.36 , 113.05, 108.37;**ESI $[M+H]^+$:** 288.00; **Elemental Analysis (%):** Found:C, 49.97; H, 3.15; N, 19.40, (Calcd): (C, 49.85; H, 3.14; N, 19.38).

4-(4-nitrophenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7j:

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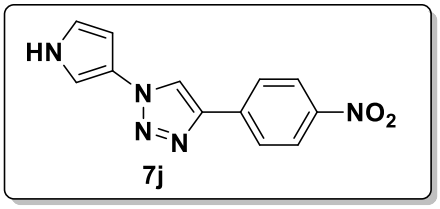
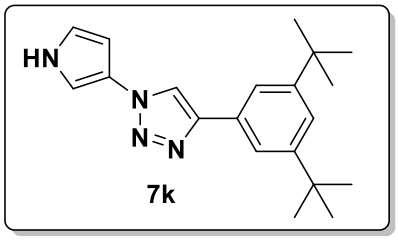


7j

MF: $C_{12}H_9N_5O_2$, White, yield: 86%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.32 (d, *J* = 7.5 Hz, 2H), 8.08 (s, 1H), 7.88 (s, 2H), 7.02 (d, *J* = 9.5 Hz, 1H), 6.78 (d, *J* = 9.9 Hz, 2H), 6.15 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 148.94, 146.40, 134.60, 124.86, 124.45, 123.48, 119.36, 113.05, 108.37;**ESI [M]$^+$:** 255.08;**Elemental Analysis (%):** Found:C, 56.59; H, 3.56; N, 27.12, (Calcd):(C, 56.47; H, 3.55; N, 27.44).

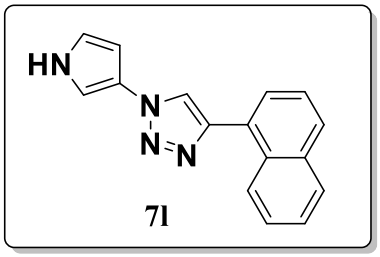
4-(3,5-di-tert-butylphenyl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7k:



7k

MF: $C_{20}H_{26}N_4$, Off white, yield: 88%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.44 (d, *J* = 51.9 Hz, 3H), 7.08 (s, 1H), 6.82 (d, *J* = 54.7 Hz, 2H), 6.12 (s, 1H), 1.41 (s, 18H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 159.39, 148.11, 130.72, 123.48, 121.48, 120.22, 119.36, 118.28, 113.05, 108.37, 35.22, 31.43;**ESI [M+H]$^+$:** 322.22;**Elemental Analysis (%):** Found:C, 74.50; H, 8.14; N, 17.40, (Calcd)(C, 74.50; H, 8.13; N, 17.38).

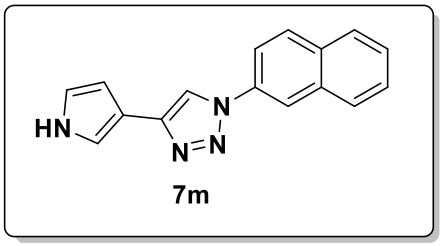
4-(naphthalen-1-yl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7l:



7l

MF:$C_{16}H_{12}N_4$, Yellow, yield: 85%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.98 (s, 1H), 7.88 – 7.72 (m, 3H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.45 (d, *J* = 12.6 Hz, 2H), 7.03 (s, 1H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.15 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 145.49, 131.78, 131.43, 129.88, 128.63, 127.64, 126.99, 125.47, 125.09, 123.89, 123.48, 119.36, 113.05, 108.37;**ESI [M+H]$^+$:** 260.11; **Elemental Analysis (%):** Found:C, 73.95; H, 4.66; N, 21.54, (Calcd)(C, 73.83; H, 4.65; N, 21.52).

1-(naphthalen-2-yl)-4-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7m:



7m

MF:$C_{16}H_{12}N_4$,Light yellow, yield: 90%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H),

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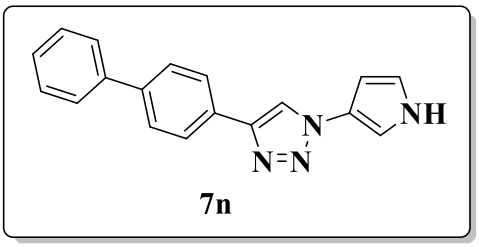
7.82 (d, *J* = 37.3 Hz, 5H), 7.43 (dt, *J* = 14.8, 8.2 Hz, 2H), 7.03 (s, 1H), 6.80 (dd, *J* = 18.4, 4.7 Hz, 2H), 6.17 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 144.32, 138.30, 134.85, 130.28, 128.80 , 128.34 , 127.62, 126.94, 125.07, 123.65, 122.93, 120.69, 120.35, 110.78, 106.15;
ESI [M+H]$^+$: 260.11;**Elemental Analysis (%):** Found:C, 73.95; H, 4.66; N, 21.54, (Calcd): (C, 73.83; H, 4.65; N, 21.52).

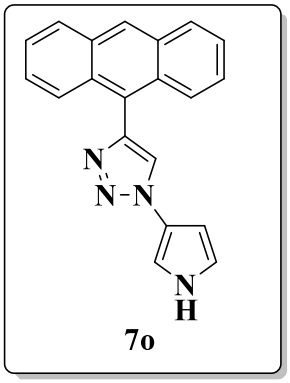
4-([1,1'-biphenyl]-4-yl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7n:



7n

MF: $C_{18}H_{14}N_4$,Palewhite, yield: 89%;**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.08 (s, 1H), 7.73 (d, *J* = 38.1 Hz, 4H), 7.46 (d, *J* = 56.5 Hz, 5H), 7.01 (d, *J* = 7.5 Hz, 1H), 6.87 – 6.65 (m, 2H), 6.14 (s, 1H),**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 148.94, 140.41, 138.77, 130.36, 128.92, 128.33, 127.32, 125.44, 124.90 , 123.48 , 119.36, 113.05, 108.37;**ESI [M+H]$^+$:** 286.12; **Elemental Analysis (%):** Found:C, 75.12; H, 4.94; N, 19.59, (Calcd)(C, 75.50; H, 4.93; N, 19.57).

4-(anthracen-9-yl)-1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazole 7o:



7o

MF:$C_{20}H_{14}N_4$,Light orange, yield: 90%,**^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm):** 8.39 (s, 1H), 8.16 – 7.84 (m, 5H), 7.44 (s, 4H), 7.02 (d, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 13.9 Hz, 2H), 6.17 (s, 1H);**^{13}CNMR(100 MHz, $CDCl_3$) δ(ppm):** 145.90, 133.03, 131.38, 128.88, 128.45, 128.23, 127.54, 126.53, 125.69, 123.48, 119.36, 113.05, 108.37;**ESI [M+H]$^+$:** 310.12,**Elemental Analysis (%):** Found:C, 77.52; H, 4.56; N, 18.07, (Calcd)(C, 77.40; H, 4.55; N, 18.05).

4. CONCLUSION

In summary, a novel, cost-effective and practical method was developed to synthesize the series of 4-substituted -1-(1*H*-pyrrol-3-yl)-1*H*-1,2,3-triazoles **7a-o.**The advantages of this method include a simple reaction set-up not requiring specialized equipment's, low-toxicity of the reagent, moderate reaction times, and high product yields with excellent purity.

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