Supporting Information

Directing Group-Enabled Cycloaddition of Azides and Alkynes Toward Functionalized Triazoles

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Contents

1 General Information S2
2 Starting Materials S3 – S9
3 Typical Procedure for the Synthesis of 3a S10
4 Gram-scale Synthesis of 3a S10
5 Typical Procedure for the One-Pot Synthesis of 4a S11
6 Procedure for the Synthesis of 5 S11–S12
7 Procedure for the Synthesis of 6 S12
8 Procedure for the Synthesis of 7 S12 – S13
9 Procedure for the Synthesis of 8 S13
10 Procedure for the Synthesis of 9 S14
11 Characterization of Compounds S14 – S44
12 X-ray Crystallographic Data S44 – S47
13 References S48
14 Copies of NMR Spectra S49 – S175
1. General Information

The reaction temperatures are reported corresponding to the oil bath temperature. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Column chromatography was performed over silica gel (200–300 mesh).

Melting points were measured with X-4 micro melting point apparatus. HRMS were performed on Waters GCT premier time of flight mass spectrometer (EI-TOF). $^1$H NMR spectra and $^{13}$C NMR spectra were recorded on a Bruker AV-600 spectrometer or a WNMRI-400 spectrometer in chloroform-$d$ (contain internal TMS). Chemical shifts of $^1$H NMR spectra were reported in ppm with the internal TMS signal at 0 ppm as a standard, and chemical shifts of $^{13}$C NMR spectra were reported in ppm with the chloroform signal at 77.16 ppm as a standard.$^1$ The data is being reported as (s = singlet, d = doublet, t = triplet, q = quartet, hept = heptet, dd = double doublet, dt = double of triplet, m = multiplet or unresolved, br = broad singlet, coupling constant(s) in Hz, integration).

Chloro(1,5-cyclooctadiene)iridium(I) dimer ([Ir(cod)Cl]$_2$, CAS: 12112-67-3, 98% purity) was purchased from Sinocompound Technology Co., Ltd. Solvents, such as ethyl acetate (EA), petroleum ether (PE), dichloromethane (DCM), 1,2-dichloroethane (DCE), $N, N$-dimethylformamide (DMF), tetrahydrofuran (THF), acetonitrile (MeCN) toluene (PhMe) and methanol (MeOH) were obtained commercially and used without further purification unless otherwise noted.
2. Starting Materials

All starting 1-alkynyltriazenes were shown in Figure S1. These 1-alkynyltriazenes were synthesized according to the procedure of reported method (Scheme S1).²

**Scheme S1.** Synthesis of the 1-alkynyltriazenes

*General procedure for the synthesis of alkynyl Grignard reagents:*

An oven-dried two-neck flask equipped with magnetic stirrer bar was charged with
terminal alkynes (15 mmol) and 10 mL anhydrous THF under an argon atmosphere. Ethylmagnesium bromide (15 mL, 1 mol/L in THF) was added dropwise via a syringe through the septum at room temperature. After the end of addition, the solution was stirred for 1 h at room temperature. Then the mixture was heated to 50 °C and stirred for another 1 h. The solution was allowed to cool to room temperature and used directly in next step.

**General Procedure for the synthesis of 1-alkynyltriazenes with nitrous oxide:**

The corresponding lithium amide (10 mmol, 1.0 eq.) was dissolved in 20 mL of anhydrous THF and the resulting solution was stirred vigorously under an atmosphere of N₂O for 3 h at room temperature. A white precipitate formed. The N₂O atmosphere was then replaced by an atmosphere of argon and the corresponding alkynyl Grignard reagent (15 mmol, 1.5 eq.) in THF was added. The solution was heated to 50 °C and stirred for 8 h. The reaction was quenched with water (5 mL), filtered through a layer of diatomite, extracted with ethyl acetate (3 × 40 mL) and the combined organic phases were dried over anhydrous magnesium sulfate, filtered, evaporated to obtain the crude products which were purified by a basic Al₂O₃ column chromatography (PE/EA system) to give corresponding 1-alkynyltriazenes. For some compounds, followed recrystallization from cold pentane is necessary.

**Characterization of new 1-alkynyltriazenes:**

![1b](image)

**1-((2-chlorophenyl)ethynyl)-3,3-diisopropyltriaz-1-ene (1b):** Orange solid. (recrystallized from cold pentane: 1.1 g, 42% yield)

**¹H NMR (400 MHz, CDCl₃)** δ 7.51 – 7.46 (m, 1H), 7.42 – 7.36 (m, 1H), 7.21 – 7.13 (m, 2H), 5.18 (hept, J = 6.8 Hz, 1H), 4.06 (hept, J = 6.8 Hz, 1H), 1.38 (d, J = 6.8 Hz, 6H), 1.25 (d, J = 6.8 Hz, 6H).

**¹³C NMR (100 MHz, CDCl₃)** δ 135.2, 132.9, 129.2, 128.0, 126.4, 124.9, 98.9,
77.0, 50.6, 47.7, 23.5, 19.2.

**HRMS (EI-TOF) m/z**: calcd for C$_{14}$H$_{18}$ClN$_3$(M)$^+$ 263.1189; Found 263.1185.

![Diagram](image)

1-((3-methylphenyl)ethynyl)-3,3-diisopropyltriaz-1-ene (1c): Yellow solid (recrystallized from cold pentane: 1.2 g, 50% yield).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.30 – 7.23 (m, 2H), 7.21 – 7.15 (m, 1H), 7.08 – 7.01 (m, 1H), 5.11 (hept, $J =$ 6.8 Hz, 1H), 4.03 (hept, $J =$ 6.8 Hz, 1H), 2.32 (s, 3H), 1.36 (d, $J =$ 6.8 Hz, 6H), 1.24 (d, $J =$ 6.8 Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 137.8, 131.8, 128.3, 128.1, 128.0, 124.7, 93.7, 80.3, 50.4, 47.5, 23.5, 21.4, 19.2.

**HRMS (EI-TOF) m/z**: calcd for C$_{15}$H$_{21}$N$_3$(M)$^+$ 243.1735; Found 243.1731.

![Diagram](image)

3,3-diisopropyl-1-((trimethylsilyl)ethynyl)triaz-1-ene (1k): Light yellow solid (recrystallized from cold pentane: 720 g, 32% yield).

$^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 5.05 (hept, $J =$ 6.6 Hz, 1H), 4.03 (hept, $J =$ 6.6 Hz, 1H), 1.34 (d, $J =$ 6.6 Hz, 6H), 1.21 (d, $J =$ 6.6 Hz, 6H), 0.22 (s, 9H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 106.6, 81.1, 50.6, 47.4, 23.4, 19.1, 0.6.

**HRMS (EI-TOF) m/z**: calcd for C$_{11}$H$_{23}$N$_3$Si(M)$^+$ 225.1661; Found 225.1667.

![Diagram](image)

1-((phenylethynyl)diazenyl)pyrrolidine (1m): Yellow solid (recrystallized
from cold pentane: 455 mg, 23% yield).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.50 – 7.38 (m, 2H), 7.33 – 7.19 (m, 3H), 3.99 – 3.86 (m, 2H), 3.66 – 3.54 (m, 2H), 2.12 – 1.94 (m, 4H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 131.2, 128.3, 127.2, 124.6, 93.8, 79.8, 51.9, 47.2, 24.0, 23.5.

HRMS (EI-TOF) $m/z$: calcd for C$_{12}$H$_{13}$N$_3$(M)$^+$ 199.1109; Found 199.1102.

1-((phenylethynyl)diazenyl)piperidine (1n) Yellow solid (recrystallized from cold pentane: 470 mg, 22% yield).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.52 – 7.40 (m, 2H), 7.34 – 7.20 (m, 3H), 3.94 – 3.68 (m, 4H), 1.83 – 1.60 (m, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 131.2, 128.4, 127.3, 124.5, 93.1, 81.5, 53.6, 44.0, 26.4, 24.5, 24.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{13}$H$_{15}$N$_3$(M)$^+$ 213.1266; Found 213.1267.

4-((phenylethynyl)diazenyl)morpholine (1o) Orange solid (580 mg, 27% yield).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.59 – 7.41 (m, 2H), 7.39 – 7.20 (m, 3H), 4.19 – 3.44 (m, 8H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 131.3, 128.4, 127.7, 123.9, 92.3, 83.6, 67.1, 65.5, 52.2, 44.4.

HRMS (EI-TOF) $m/z$: calcd for C$_{12}$H$_{13}$N$_3$O(M)$^+$ 215.1059; Found 215.1052.
1-isopropyl-4-((phenylethynyl)diazenyl)piperazine (1p): Brown oil (610 mg, 24% yield).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.47 – 7.42 (m, 2H), 7.35 – 7.22 (m, 3H), 3.89 – 3.82 (m, 4H), 2.81 (hept, $J = 6.8$ Hz, 1H), 2.74 – 2.53 (m, 4H), 1.06 (d, $J = 6.8$ Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 131.3, 128.3, 127.5, 124.3, 92.8, 82.4, 54.6, 52.6, 48.6, 47.1, 44.0, 18.5.

HRMS (EI-TOF) $m/z$: calcd for C$_{15}$H$_{20}$N$_4$(M)$^+$ 256.1688; Found 256.1689.

1-((m-toly lethynyl)diazenyl)pyrrolidine (1q): Light yellow solid (recrystallized from cold pentane: 425 mg, 20% yield).

$^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.29 – 7.23 (m, 2H), 7.20 – 7.15 (m, 1H), 7.10 – 7.02 (m, 1H), 3.93 (t, $J = 7.2$ Hz, 2H), 3.60 (t, $J = 7.2$ Hz, 2H), 2.31 (s, 3H), 2.11 – 1.99 (m, 4H).

$^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 137.9, 131.9, 128.3, 128.2 (128.20), 128.2 (128.18), 124.3, 93.4, 80.0, 51.9, 47.2, 24.0, 23.6, 21.4.

HRMS (EI-TOF) $m/z$: calcd for C$_{13}$H$_{15}$N$_3$(M)$^+$ 213.1266; Found 213.1261.

1-(hex-1-yn-1-yldiazenyl)pyrrolidine (1r): Yellow oil (555 mg, 31% yield).
$^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 3.87 (t, $J = 6.6$ Hz, 2H), 3.51 (t, $J = 6.6$ Hz, 2H), 2.45 (t, $J = 7.2$ Hz, 2H), 2.07 – 1.94 (m, 4H), 1.59 – 1.51 (m, 2H), 1.48 – 1.41 (m, 2H), 0.91 (t, $J = 7.2$ Hz, 3H).

$^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 85.2, 79.7, 51.5, 46.7, 31.4, 23.9, 23.6, 22.1, 19.1, 13.7.

HRMS (EI-TOF) $m/z$: calcd for C$_{10}$H$_{17}$N$_3$(M)$^+$ 179.1422; Found: 179.1425.

![Diagram of 1s]

1-((3-methoxyprop-1-yn-1-yl)diazenyl)pyrrolidine (1s): Yellow oil (420 mg, 25% yield).

$^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 4.39 (s, 2H), 3.97 – 3.83 (m, 2H), 3.59 – 3.52 (m, 2H), 3.41 (s, 3H), 2.11 – 1.98 (m, 4H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 90.4, 73.9, 60.7, 57.4, 51.8, 47.0, 23.9, 23.5.

HRMS (EI-TOF) $m/z$: calcd for C$_8$H$_{13}$N$_3$O(M)$^+$ 167.1059; Found 167.1055.

![Diagram of 1t]

1-((3-((tetrahydro-2H-pyran-2-yl)oxy)prop-1-yn-1-yl)diazenyl)pyrrolidine (1t): Yellow oil (640 mg, 27 yield).

$^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 4.89 (t, $J = 3.6$ Hz, 1H), 4.58 – 4.67 (m, 2H), 3.94 – 3.82 (m, 3H), 3.60 – 3.48 (m, 3H), 2.10 – 1.98 (m, 4H), 1.88 – 1.80 (m, 1H), 1.77 – 1.70 (m, 1H), 1.65 – 1.50 (m, 4H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 96.4, 89.7, 74.0, 62.0, 54.9, 51.7, 46.9, 30.4, 25.4, 23.8, 23.4, 19.2.

HRMS (EI-TOF) $m/z$: calcd for C$_{12}$H$_{19}$N$_3$O$_2$(M)$^+$ 237.1477; Found 237.1475.
Figure S2. Staring azides

All staring azides were shown in Figure S2. These azides were prepared according to the reported methods.3
3. Typical Procedure for the Synthesis of 3a

To CH₂Cl₂ (2 mL) solution of 3,3-diisopropyl-1-(phenylethynyl)triaz-1-ene 1a (46 mg, 0.2 mmol) and benzyl azide 2a (30 mg, 0.22 mmol) was added [Ir(cod)Cl]₂ (2.7 mg, 2 mol %), and the reaction was stirred at ambient temperature for 12 h. The solvent was evaporated and the residue was purified by silica gel column chromatography using ethyl acetate/petroleum ether (v/v, 1/3) as eluent to give 1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazole 3a (71 mg, 98% yield) as a white solid.

4. Gram-scale Synthesis of 3a

To CH₂Cl₂ (50 mL) solution of 3,3-diisopropyl-1-(phenylethynyl)triaz-1-ene 1a (1.15 g, 5 mmol) and benzyl azide 2a (735 mg, 5.5 mmol) was added [Ir(cod)Cl]₂ (68 mg, 2 mol %), then the reaction was stirred at ambient temperature for 12 h. The solvent was evaporated and the residue was purified by recrystallization from ethyl acetate/petroleum ether (v/v, 1/5) to give 1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazole 3a (1.7 g, 94% yield) as a white solid.
5. Typical Procedure for the One-pot Synthesis of 4a

![Chemical Reaction Diagram]

To CH$_2$Cl$_2$ (2 mL) solution of 1-((phenylethynyl)diazenyl)pyrroolidine 1m (40 mg, 0.2 mmol), benzyl azide 2a (30 mg, 0.22 mmol) was added [Ir(cod)Cl]$_2$ (2.7 mg, 2 mol %), and the reaction was stirred at ambient temperature for 12 h. The solvent was concentrated and the crude triazole product was dissolved in MeOH (2 mL). Raney Ni (approximately 10 equiv.) was added and the mixture was stirred at 60 ℃ until the reaction complete. Raney Ni was carefully filtered and the filtrate was concentrated to obtain the crude product, which was further purified by flash column chromatography using ethyl acetate/petroleum ether (v/v, 1/1) to give 1-benzyl-4-phenyl-1H-1,2,3-triazol-5-amine 4a (44 mg, 88% yield) as a white solid.

6. Procedure for the Synthesis of 5

![Chemical Reaction Diagram]

An oven-dried Schlenk tube equipped with a magnetic stirrer bar was charged with 1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-amine 4e (49 mg, 0.2 mmol), CuCl (58 mg, 0.6 mmol) and CuCl$_2$ (80 mg, 0.6 mmol) under argon atmosphere. Then MeCN (2 mL) was added as solvent. The solution was cooled to 0 ℃ and t-BuONO (26 mg, 0.24 mmol) was added dropwise. Afterwards, the solution was stirred at this temperature for another 1 h. Water was added to quench the reaction and the solution was extracted with EtOAc (3×10 mL). The combined organic layer was washed by brine, dried over anhydrous Na$_2$SO$_4$, filtered and concentrated in vacuum to obtain the residue, which was further purified by silica gel column chromatography using ethyl acetate/petroleum ether (v/v,
1/20) as eluent to give 5-chloro-1-cyclohexyl-4-phenyl-1H-1,2,3-triazole 5 (43 mg, 82% yield) as a white solid.

7. Procedure for the Synthesis of 6

An oven-dried Schlenk tube equipped with a magnetic stirrer bar was charged with 1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-amine 4e (49 mg, 0.2 mmol) and CuBr₂ (98 mg, 0.44 mmol) under argon atmosphere. Then MeCN (2 mL) was added as solvent. The reaction was cooled to 0 °C and t-BuONO (26 mg, 0.24 mmol) was added dropwise. Afterwards, the mixture was stirred at this temperature for another 1 h. Water was added to quench the reaction and the solution was extracted with EtOAc (3×10 mL). The combined organic layer was washed by brine, dried over anhydrous Na₂SO₄, filtered and concentrated in vacuum to obtain the residue, which was further purified by silica gel column chromatography using ethyl acetate/petroleum ether (v/v, 1/20) as eluent to give 5-bromo-1-cyclohexyl-4-phenyl-1H-1,2,3-triazole 6 (53 mg, 86% yield) as a white solid.

8. Procedure for the Synthesis of 7

An oven-dried Schlenk tube equipped with a magnetic stirrer bar was charged with 1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-amine 4e (49 mg, 0.2 mmol) under argon atmosphere. MeCN (0.5 mL) and TMSN₃ (0.3 mmol) were added and the mixture was cooled to 0 °C. Then t-BuONO (26 mg, 0.24 mmol) was added dropwise via a syringe.
After the end of addition, the reaction was stirred at this temperature for 30 mins. The mixture was extracted with EtOAc (3×5 mL). The combined organic layer was concentrated to obtain the crude azide, which was dissolved in DCM (2 mL). 1-((phenylethynyl)diazeny)pyrrolidine \textbf{1m} (40 mg, 0.2 mmol) and [Ir(cod)Cl]$_2$ (2.7 mg, 2 mol %) was then added, the reaction was stirred at ambient temperature for 12 h. The solvent was evaporated and the residue was purified by silica gel column chromatography using ethyl acetate/petroleum ether (v/v, 1/3) as eluent to give 3’-cyclohexyl-4,5’-diphenyl-5-(pyrrolidin-1-yl)diazeny)-3’H-1,4’-bi(1,2,3-triazole) \textbf{7} (50 mg, 53% yield) as a light yellow solid.

9. Procedure for the Synthesis of \textbf{8}

\begin{center}
\includegraphics[width=0.8\textwidth]{diagram.png}
\end{center}

N-Cbz-L-proline (75 mg, 0.3 mmol) was dissolved in SOCl$_2$ and reflux for 2 h, the solvent was removed in vacuum to obtain the acyl chloride which was used directly in next step.

An oven-dried Schlenk tube equipped with a magnetic stirrer bar was charged with 1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-amine \textbf{4e} (49 mg, 0.2 mmol) under argon atmosphere. Pyridine (1 mL) was added as solvent. Then acyl chloride was added and the reaction was heated at 80 °C for 2 h. Aqueous HCl (2N) was carefully added and the mixture was extracted with EtOAc (3×10 mL). The combined organic layer was washed by brine, dried over anhydrous Na$_2$SO$_4$, filtered and concentrated in vacuum to obtain the residue, which was further purified by silica gel column chromatography using ethyl acetate/petroleum ether (v/v, 1:1) to give benzyl 2-((1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-yl)carbamoyl)pyrrolidine-1-carboxylate \textbf{8} (79 mg, 84% yield) as yellow oil.
10. Procedure for the Synthesis of 9

![Reaction Scheme]

An oven dried Schlenk tube equipped with a magnetic stirrer bar was charged with 1-phenethyl-4-phenyl-1H-1,2,3-triazol-5-amine 4b (27 mg, 0.1 mmol) under argon atmosphere. MeCN (1 mL) was added and the mixture was cooled to 0 °C. Then t-BuONO (14 mg, 0.12 mmol) was added dropwise. After the end of addition, the reaction was stirred at this temperature for 30 mins. Water was added to quench the reaction and the solution was extracted with EtOAc (3×10 mL). The combined organic layer was washed by brine, dried over anhydrous Na₂SO₄, filtered and concentrated in vacuum to obtain the residue which was further purified by silica gel column chromatography using ethyl acetate/petroleum ether (v/v, 1:10) as eluent to give 1-phenyl-5,6-dihydro-[1,2,3]triazolo[5,1-a]isoquinoline 9 (24 mg, 95% yield) as a white solid.

11. Characterization of Compounds

![Compound Image]

1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazole

3a: White solid, m.p. 87 – 89 °C, 71 mg (98% yield).

TLC: Rf = 0.44 (PE: EA = 3:1).

¹H NMR (600 MHz, CDCl₃) δ 7.95 – 7.89 (m, 2H), 7.41 – 7.34 (m, 2H), 7.31 – 7.21 (m, 4H), 7.20 – 7.13 (m, 2H), 5.64 (s, 2H), 5.14 (hept, J = 6.6 Hz, 1H), 3.92 (hept, J = 6.6 Hz, 1H), 1.20 (d, J = 7.2 Hz, 6H), 1.10 (d, J = 6.6 Hz, 6H).
$^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 142.0, 136.3, 135.9, 132.2, 128.6, 128.1, 127.7 (127.71), 127.7 (127.68), 127.2, 127.1, 52.1, 50.0, 47.0, 23.3, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{21}$H$_{26}$N$_6$ (M)$^+$ 362.2219; Found 362.2215.

1-benzyl-4-(2-chlorophenyl)-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-1,2,3-triazole

3b: White solid, m.p. 135 – 137 °C, 70 mg (89% yield).

TLC: Rf = 0.38 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.53 – 7.45 (m, 1H), 7.42 – 7.13 (m, 8H), 5.61 (s, 2H), 5.08 (hept, $J$ = 6.8 Hz, 1H), 3.77 (hept, $J$ = 6.8 Hz, 1H), 1.15 (d, $J$ = 6.8 Hz, 6H), 0.85 (d, $J$ = 6.8 Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 143.6, 136.2, 134.5, 132.6, 132.3, 131.0, 129.1, 128.9, 128.6, 127.9, 127.8, 126.4, 51.0, 49.9, 47.0, 22.8, 18.9.

HRMS (EI-TOF) $m/z$: calcd for C$_{21}$H$_{25}$ClN$_6$ (M)$^+$ 396.1829; Found 396.1828.

1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-(m-tolyl)-1H-1,2,3-triazole

3c: White solid, m.p. 106 – 108 °C, 73 mg (97% yield).
**TLC:** $R_f = 0.44$ (PE: EA = 3:1).

**$^{1}H$ NMR (400 MHz, CDCl$_3$)** $\delta$ 7.78 – 7.69 (m, 2H), 7.31 – 7.20 (m, 4H), 7.19 – 7.12 (m, 2H), 7.11 – 7.06 (m, 1H), 5.64 (s, 2H), 5.13 (hept, $J = 6.8$ Hz, 1H), 3.93 (hept, $J = 6.8$ Hz, 1H), 2.36 (s, 3H), 1.21 (d, $J = 6.8$ Hz, 6H), 1.10 (d, $J = 6.6$ Hz, 6H).

**$^{13}C$ NMR (100 MHz, CDCl$_3$)** $\delta$ 141.9, 137.5, 136.3, 136.1, 132.0, 128.6, 128.3, 128.0 (128.05), 128.0 (127.98), 127.7, 127.0, 124.8, 52.1, 50.0, 47.0, 23.3, 21.6, 19.1.

**HRMS (EI-TOF) m/z:** calcd for C$_{22}$H$_{28}$N$_6$ (M$^+$) 376.2375; Found 376.2378.

![NMR Spectrum](image)

1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-(4-fluorophenyl)-1H-1,2,3-triazole

**3d:** White solid, m.p. 104 – 106 °C, 71 mg (93% yield).

**TLC:** $R_f = 0.41$ (PE: EA = 3:1).

**$^{1}H$ NMR (400 MHz, CDCl$_3$)** $\delta$ 7.94 – 7.82 (m, 2H), 7.32 – 7.22 (m, 3H), 7.20 – 7.13 (m, 2H), 7.10 – 7.02 (m, 2H), 5.64 (s, 2H), 5.14 (hept, $J = 6.8$ Hz, 1H), 3.94 (hept, $J = 6.8$ Hz, 1H), 1.21 (d, $J = 6.8$ Hz, 6H), 1.11 (d, $J = 6.8$ Hz, 6H).

**$^{13}C$ NMR (100 MHz, CDCl$_3$)** $\delta$ 162.2 (d, $J = 246.0$ Hz), 141.8, 136.2, 135.0, 129.5 (d, $J = 7.9$ Hz), 128.7, 128.4 (d, $J = 3.1$ Hz), 127.7, 127.1, 115.0 (d, $J = 21.4$ Hz), 52.1, 50.0, 47.1, 23.3, 19.0.

**HRMS (EI-TOF) m/z:** calcd for C$_{21}$H$_{25}$FN$_6$ (M$^+$) 380.2125; Found 380.2129.
1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-(4-methoxyphenyl)-1H-1,2,3-triazole

3e: White solid, m.p. 95 – 96 ℃, 71 mg (91% yield).

TLC: Rf = 0.28 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.93 – 7.80 (m, 2H), 7.33 – 7.20 (m, 3H), 7.18 – 7.13 (m, 2H), 6.95 – 6.88 (m, 2H), 5.64 (s, 2H), 5.13 (hept, $J$ = 6.8 Hz, 1H), 3.93 (hept, $J$ = 6.8 Hz, 1H), 3.83 (s, 3H), 1.20 (d, $J$ = 6.8 Hz, 6H), 1.12 (d, $J$ = 6.8 Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 159.0, 141.4, 136.4, 135.8, 129.0, 128.6, 127.7, 127.1, 124.9, 113.6, 55.4, 52.1, 49.9, 46.9, 23.3, 19.1.

HRMS (EI-TOF) $m/z$: calcd for C$_{22}$H$_{28}$N$_6$O (M)$^+$ 392.2325; Found 392.2321.

1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-(thiophen-3-yl)-1H-1,2,3-triazole

3f: White solid, m.p. 86 – 88 ℃, 66 mg (90% yield).

TLC: Rf = 0.41 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.81 – 7.74 (m, 1H), 7.71 – 7.65 (m, 1H), 7.35 – 7.17 (m, 4H), 7.14 – 7.06 (m, 2H), 5.65 (s, 2H), 5.14 (hept, $J$ = 6.8 Hz, 1H), 3.94 (hept, $J$ = 6.8 Hz, 1H), 1.20 (d, $J$ = 6.8 Hz, 6H), 1.12 (d, $J$ = 6.8 Hz, 6H).
**13C NMR (100 MHz, CDCl₃)** δ 141.2, 136.1, 132.9, 132.8, 128.5, 127.5, 127.3, 126.7, 124.8, 121.6, 52.1, 49.9, 46.9, 23.1, 18.9.

**HRMS (EI-TOF) m/z:** calcd for C₁₉H₂₄N₆S (M)+ 368.1783; Found 368.1786.

![Diagram of 3g](image)

**11-benzyl-4-butyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-1,2,3-triazole**

**3g:** White solid, m.p. 82 – 84 °C, 64 mg (94% yield).

**TLC:** Rf = 0.38 (PE: EA = 3:1).

**1H NMR (400 MHz, CDCl₃)** δ 7.35 – 7.19 (m, 5H), 5.52 (s, 2H), 5.10 (hept, J = 6.8 Hz, 1H), 4.00 (hept, J = 6.8 Hz, 1H), 2.82 – 2.77 (m, 2H), 1.70 – 1.59 (m, 2H), 1.44 – 1.36 (m, 2H), 1.32 (d, J = 6.8 Hz, 6H), 1.19 (d, J = 6.8 Hz, 6H), 0.92 (t, J = 7.2 Hz, 3H).

**13C NMR (100 MHz, CDCl₃)** δ 142.0, 136.4, 134.5, 128.5, 127.8, 127.7, 51.0, 49.5, 46.5, 31.5, 26.3, 23.4, 22.7, 19.0, 14.1.

**HRMS (EI-TOF) m/z:** calcd for C₁₉H₃₀N₆ (M)+ 342.2532; Found 342.2537.

![Diagram of 3h](image)

**11-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenethyl-1H-1,2,3-triazole**

**3h:** White solid, m.p. 67 – 69 °C, 68 mg (87% yield).

**TLC:** Rf = 0.32 (PE: EA = 3:1).
$^1\text{H NMR (400 MHz, CDCl}_3$) δ 7.39 – 7.08 (m, 10H), 5.53 (s, 2H), 5.04 (hept, $J = 6.8$ Hz, 1H), 3.99 (hept, $J = 6.8$ Hz, 1H), 3.17 – 3.10 (m, 2H), 3.04 – 2.98 (m, 2H), 1.29 (d, $J = 6.8$ Hz, 6H), 1.18 (d, $J = 6.8$ Hz, 6H).

$^{13}\text{C NMR (100 MHz, CDCl}_3$) δ 142.2, 142.1, 136.4, 133.7, 128.6, 128.5, 128.3, 127.8, 125.8, 51.1, 49.8, 46.7, 35.4, 28.1, 23.5, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{23}$H$_{30}$N$_6$ (M)$^+$ 390.2532; Found 390.2534.

1-benzyl-4-cyclopropyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-1,2,3-triazole

3i: White solid, m.p. 78 – 79 °C, 60 mg (92% yield).

TLC: Rf = 0.47 (PE: EA = 3:1).

$^1\text{H NMR (400 MHz, CDCl}_3$) δ 7.38 – 7.16 (m, 5H), 5.51 (s, 2H), 5.10 (hept, $J = 6.8$ Hz, 1H), 4.00 (hept, $J = 6.8$ Hz, 1H), 2.18 – 2.07 (m, 1H), 1.31 (d, $J = 6.6$ Hz, 6H), 1.20 (d, $J = 6.8$ Hz, 6H), 1.06 – 1.00 (m, 2H), 0.89 – 0.83 (m, 2H).

$^{13}\text{C NMR (100 MHz, CDCl}_3$) δ 142.9, 136.3, 135.4, 128.5, 127.8, 127.7, 51.1, 49.7, 46.5, 23.5, 19.0, 7.5, 7.2.

HRMS (EI-TOF) $m/z$: calcd for C$_{18}$H$_{26}$N$_6$ (M)$^+$ 326.2219; Found 326.2215.

1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-(methoxymethyl)-1H-1,2,3-triazole
3j: White solid, m.p. 60 – 62 °C, 61 mg (93% yield).

**TLC:** Rf = 0.13 (PE: EA = 3:1).

**1H NMR (400 MHz, CDCl₃)** δ 7.37 – 7.20 (m, 5H), 5.54 (s, 2H), 5.12 (hept, J = 6.8 Hz, 1H), 4.64 (s, 2H), 4.04 (hept, J = 6.8 Hz, 1H), 3.40 (s, 3H), 1.35 (d, J = 6.8 Hz, 6H), 1.21 (d, J = 6.8 Hz, 6H).

**13C NMR (100 MHz, CDCl₃)** δ 143.9, 136.0, 130.4, 128.6, 127.9, 127.8, 66.1, 58.0, 51.0, 50.0, 47.0, 23.5, 19.0.

**HRMS (EI-TOF) m/z:** calcd for C₁₇H₂₆N₆O (M)⁺ 330.2168; Found 330.2165.

1-benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-(trimethylsilyl)-1H-1,2,3-triazole

3k: Grey solid, m.p. 73 – 75 °C, 66 mg (92% yield).

**TLC:** Rf = 0.54 (PE: EA = 3:1).

**1H NMR (400 MHz, CDCl₃)** δ 7.31 – 7.18 (m, 5H), 5.56 (s, 2H), 4.91 (hept, J = 6.8 Hz, 1H), 4.06 (hept, J = 6.8 Hz, 1H), 1.29 (d, J = 6.8 Hz, 6H), 1.23 (d, J = 6.8 Hz, 6H), 0.32 (s, 9H).

**13C NMR (100 MHz, CDCl₃)** δ 151.5, 136.4, 132.6, 128.5, 127.6, 127.4, 51.2, 50.8, 47.3, 23.1, 18.9, -0.7.

**HRMS (EI-TOF) m/z:** calcd for C₁₈H₃₀N₆Si (M)⁺ 358.2301; Found 358.2308.
1-benzyl-5-(3,3-dimethyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazole

3l: White solid, m.p. 125 – 127 °C, 57 mg (93% yield).

TLC: Rf = 0.30 (PE: EA = 3:1).

$^1$H NMR (600 MHz, CDCl$_3$) δ 8.02 – 7.98 (m, 2H), 7.40 – 7.34 (m, 2H), 7.31 – 7.22 (m, 4H), 7.21 – 7.17 (m, 2H), 5.64 (s, 2H), 3.40 (s, 3H), 3.14 (s, 3H).

$^{13}$C NMR (150 MHz, CDCl$_3$) δ 140.9, 136.7, 136.3, 131.9, 128.6, 128.2, 127.8, 127.4 (127.44), 127.4 (127.37), 127.3, 52.8, 43.3, 36.2.

HRMS (EI-TOF) m/z: calcd for C$_{17}$H$_{18}$N$_6$ (M)$^+$ 306.1593; Found 306.1591.

1-benzyl-4-phenyl-5-(pyrrolidin-1-yldiazenyl)-1H-1,2,3-triazole

3m: White solid, m.p. 129 – 130 °C, 63 mg (95% yield).

TLC: Rf = 0.33 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.10 – 7.93 (m, 2H), 7.40 – 7.34 (m, 2H), 7.31 – 7.17 (m, 6H), 5.63 (s, 2H), 3.79 (t, $J = 6.8$ Hz, 2H), 3.56 (t, $J = 6.8$ Hz, 2H), 2.04 – 1.90 (m, 4H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 141.2, 136.6, 136.4, 132.0, 128.6, 128.2, 127.7, 127.5, 127.3, 127.2, 52.9, 51.3, 46.8, 24.0, 23.4.

HRMS (EI-TOF) m/z: calcd for C$_{19}$H$_{20}$N$_6$ (M)$^+$ 332.1749; Found 332.1745.
1-((1-benzyl-4-phenyl-1H-1,2,3-triazol-5-yl)diazenyl)piperidine

3n: White solid, m.p. 127 – 129 °C, 66 mg (96% yield).

TLC: Rf = 0.46 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.02 – 7.96 (m, 2H), 7.39 – 7.34 (m, 2H), 7.30 – 7.20 (m, 4H), 7.19 – 7.13 (m, 2H), 5.64 (s, 2H), 3.83 – 3.55 (m, 4H), 1.70 – 1.54 (m, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 140.9, 136.8, 136.3, 131.8, 128.6, 128.2, 127.7, 127.5 (127.33), 127.3 (127.26), 53.1, 52.8, 43.4, 26.3, 24.2, 24.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{20}$H$_{22}$N$_6$ (M$^+$) 346.1906; Found 346.1909.

4-((1-benzyl-4-phenyl-1H-1,2,3-triazol-5-yl)diazenyl)morpholine

3o: Light yellow solid, m.p. 99 – 101 °C, 65 mg (94% yield).

TLC: Rf = 0.2 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.02 – 7.91 (m, 2H), 7.43 – 7.31 (m, 2H), 7.29 – 7.17 (m, 4H), 7.15 – 7.05 (m, 2H), 5.61 (s, 2H), 3.83 – 3.50 (m, 8H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 140.1, 137.4, 135.9, 131.4, 128.5, 128.1, 127.7, 127.5, 127.3, 127.0, 66.7, 65.3, 52.9, 51.6, 43.8.

HRMS (EI-TOF) $m/z$: calcd for C$_{19}$H$_{20}$N$_6$O (M$^+$) 348.1699; Found 348.1696.
1-((1-benzyl-4-phenyl-1H-1,2,3-triazol-5-yl)diazenyl)-4-isopropylpiperazine

**3p**: Orange oil, 69 mg (89% yield).

**TLC**: Rf = 0.15 (PE: EA = 1:1).

**H NMR (400 MHz, CDCl₃)** δ 8.01 – 7.96 (m, 2H), 7.40 – 7.34 (m, 2H), 7.30 – 7.19 (m, 4H), 7.18 – 7.11 (m, 2H), 5.63 (s, 2H), 3.86 – 3.58 (m, 4H), 2.82 – 2.71 (m, 1H), 2.63 – 2.45 (m, 4H), 1.03 (d, J = 6.8 Hz, 6H).

**C NMR (100 MHz, CDCl₃)** δ 140.6, 137.1, 136.1, 131.6, 128.6, 128.1, 127.7, 127.4, 127.3, 127.2, 54.5, 52.9, 52.1, 48.5, 46.9, 43.5, 18.4.

**HRMS (EI-TOF) m/z**: calcd for C₂₂H₂₇N₇ (M)+ 389.2328; Found 389.2326.

5-(3,3-diisopropyltriaz-1-en-1-yl)-1,4-diphenyl-1H-1,2,3-triazole

**3q**: Brown solid, m.p. 131 – 133 °C, 62 mg (89% yield).

**TLC**: Rf = 0.49 (PE: EA = 3:1).

**H NMR (400 MHz, CDCl₃)** δ 8.01 – 7.92 (m, 2H), 7.58 – 7.52 (m, 2H), 7.50 – 7.44 (m, 2H), 7.43 – 7.36 (m, 3H), 7.33 – 7.25 (m, 1H), 5.13 (hept, J = 6.8 Hz, 1H), 3.84 (hept, J = 6.8 Hz, 1H), 1.22 (d, J = 6.8 Hz, 6H), 0.94 (d, J = 6.8 Hz, 6H).
$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 142.9, 137.8, 135.7, 132.0, 129.0, 128.4, 128.3, 127.5, 127.2, 125.4, 50.0, 47.3, 23.1, 19.1.

HRMS (EI-TOF) $m/z$: calcd for C$_{20}$H$_{24}$N$_6$ (M)$^+$ 348.2062; Found 348.2067.

5-(3,3-diisopropyltriaz-1-en-1-yl)-1-(2-iodophenyl)-4-phenyl-1H-1,2,3-triazole

3r: Light yellow solid, m.p. 121 – 123 °C, 80 mg (84% yield).

TLC: Rf = 0.51 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.24 – 8.18 (m, 2H), 7.97 – 7.89 (m, 1H), 7.52 – 7.38 (m, 4H), 7.34 – 7.25 (m, 1H), 7.19 – 7.11 (m, 1H), 5.21 (hept, $J = 6.8$ Hz, 1H), 3.78 (hept, $J = 6.8$ Hz, 1H), 1.22 (dd, $J_1 = 6.8$ Hz, $J_2 = 1.2$ Hz, 6H), 0.81 (d, $J = 6.8$ Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 142.2, 141.9, 139.6, 136.2, 131.8, 130.6, 129.1, 129.0, 128.4, 127.2, 126.9, 97.5, 49.6, 47.4, 22.9, 19.1.

HRMS (EI-TOF) $m/z$: calcd for C$_{20}$H$_{23}$IN$_6$ (M)$^+$ 474.1029; Found 474.1027.

5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1-(m-tolyl)-1H-1,2,3-triazole
3s: White solid, m.p. 83 – 85 °C, 61 mg (84% yield).

TLC: Rf = 0.59 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.96 (d, $J = 8.0$ Hz, 2H), 7.46 – 7.15 (m, 7H), 5.13 (hept, $J = 6.8$ Hz, 1H), 3.85 (hept, $J = 6.8$ Hz, 1H), 2.39 (s, 3H), 1.23 (d, $J = 6.8$ Hz, 6H), 0.95 (d, $J = 6.8$ Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 142.8, 138.9, 137.6, 135.7, 132.0, 129.1, 128.8, 128.2, 127.5, 127.2, 126.0, 122.4, 50.0, 47.3, 23.1, 21.4, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{21}$H$_{26}$N$_6$ (M)$^+$ 362.2219; Found 362.2217.

![Diagram](image)

5-((3,3-diisopropyltriaz-1-en-1-yl)-1-(4-methoxyphenyl)-4-phenyl-1H-1,2,3-triazole

3t: Grown solid, m.p. 109 – 111 °C, 60 mg (80% yield).

TLC: Rf = 0.35 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.97 – 7.91 (m, 2H), 7.51 – 7.43 (m, 2H), 7.42 – 7.35 (m, 2H), 7.32 – 7.24 (m, 1H), 7.03 – 6.91 (m, 2H), 5.10 (hept, $J = 6.8$ Hz, 1H), 3.90 – 3.78 (m, 4H), 1.21 (d, $J = 6.8$ Hz, 6H), 0.98 (d, $J = 6.8$ Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 159.5, 142.8, 135.5, 132.0, 130.8, 128.2, 127.6, 127.2, 126.7, 114.1, 55.7, 50.0, 47.2, 23.1, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{21}$H$_{26}$N$_6$O (M)$^+$ 378.2168; Found 378.2160.
1-(4-bromophenyl)-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazole

3u: White solid, m.p. 146 – 147 °C, 78 mg (92% yield).

TLC: Rf = 0.65 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.94 – 7.85 (m, 2H), 7.64 – 7.56 (m, 2H), 7.53 – 7.45 (m, 2H), 7.43 – 7.36 (m, 2H), 7.33 – 7.27 (m, 1H), 5.12 (hept, $J = 6.8$ Hz, 1H), 3.88 (hept, $J = 6.8$ Hz, 1H), 1.24 (d, $J = 6.8$ Hz, 6H), 0.99 (d, $J = 6.8$ Hz, 6H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 142.9, 136.8, 135.7, 132.2, 131.8, 128.3, 127.8, 127.4, 126.8, 122.2, 50.2, 47.5, 23.2, 19.1.

HRMS (EI-TOF) m/z: calcd for C$_{20}$H$_{23}$BrN$_6$ (M)$^+$ 426.1168; Found 426.1162.

5-(3,3-diisopropyltriaz-1-en-1-yl)-1-(naphthalen-2-yl)-4-phenyl-1H-1,2,3-triazole

3v: White solid, m.p. 129 – 131 °C, 71 mg (89% yield).

TLC: Rf = 0.54 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.07 (d, $J = 1.6$ Hz, 1H), 7.99 – 7.83 (m, 5H), 7.70 (dd, $J_1 = 8.8$ Hz, $J_2 = 2.0$ Hz, 1H), 7.56 – 7.50 (m, 2H), 7.44 – 7.38 (m, 2H), 7.34 – 7.27
(m, 1H), 5.14 (hept, \( J = 6.8 \) Hz, 1H), 3.80 (hept, \( J = 6.8 \) Hz, 1H), 1.21 (d, \( J = 6.8 \) Hz, 6H), 0.86 (d, \( J = 6.8 \) Hz, 6H).

\( ^{13} \text{C NMR (100 MHz, CDCl}_3) \) \( \delta \) 143.1, 135.7, 135.1, 133.2, 132.7, 132.0, 128.9, 128.3, 127.9, 127.7, 127.3, 127.0, 126.8, 123.7, 123.4, 50.1, 47.4, 23.0, 19.1.

HRMS (EI-TOF) \( m/z \): calcd for C\(_{24}\)H\(_{26}\)N\(_6\) (M)\(^+\) 398.2219; Found 398.2217.

5-(3,3-diisopropyltriaz-1-en-1-yl)-1-phenethyl-4-phenyl-1\( H \)-1,2,3-triazole

\( 3w \): Light yellow solid, m.p. 92 – 94 °C, 69 mg (92% yield).

TLC: \( R_f = 0.43 \) (PE: EA = 3:1).

\( ^{1} \text{H NMR (400 MHz, CDCl}_3) \) \( \delta \) 7.92 – 7.75 (m, 2H), 7.40 – 7.33 (m, 2H), 7.30 – 7.13 (m, 6H), 5.16 (hept, \( J = 6.8 \) Hz, 1H), 4.70 – 4.59 (m, 2H), 3.99 (hept, \( J = 6.8 \) Hz, 1H), 3.25 – 3.17 (m, 2H), 1.28 (d, \( J = 6.8 \) Hz, 6H), 1.21 (d, \( J = 6.8 \) Hz, 6H).

\( ^{13} \text{C NMR (100 MHz, CDCl}_3) \) \( \delta \) 142.0, 137.9, 135.4, 132.2, 128.8, 128.6, 128.0, 127.9, 127.1, 126.8, 50.0, 49.4, 47.0, 36.4, 23.5, 19.1.

HRMS (EI-TOF) \( m/z \): calcd for C\(_{22}\)H\(_{28}\)N\(_6\) (M)\(^+\) 376.2375; Found 376.2372.

3-(2-(5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1\( H \)-1,2,3-triazol-1-yl)ethyl)-1\( H \)-indole
3x: Grey solid, m.p. 150 – 152 °C, 65 mg (78% yield).

TLC: Rf = 0.16 (PE: EA = 3:1).

\(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 8.41\) (s, 1H), 7.89 – 7.80 (m, 2H), 7.58 (d, \(J = 8.0\) Hz, 1H), 7.39 – 7.31 (m, 3H), 7.30 – 7.24 (m, 1H), 7.19 – 7.14 (m, 1H), 7.12 – 7.04 (m, 1H), 6.92 (d, \(J = 1.6\) Hz, 1H), 5.12 (hept, \(J = 6.8\) Hz, 1H), 4.70 (t, \(J = 7.6\) Hz, 2H), 3.94 (hept, \(J = 6.8\) Hz, 1H), 3.37 (t, \(J = 7.6\) Hz, 2H), 1.22 (d, \(J = 6.8\) Hz, 6H), 1.17 (d, \(J = 6.8\) Hz, 6H).

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta 142.2, 136.4, 135.4, 132.4, 128.1, 128.0, 127.4, 127.2, 122.4, 122.0, 119.3, 118.5, 111.9, 111.4, 49.9, 48.7, 46.9, 26.3, 23.6, 19.1.

HRMS (EI-TOF) \(m/z\): calcd for C\(_{24}\)H\(_{29}\)N\(_7\) (M)\(^+\) 415.2484; Found 415.2483.

1-cyclohexyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1\(H\)-1,2,3-triazole

3y: Light yellow solid, m.p. 98 – 100 °C, 63 mg (89% yield).

TLC: Rf = 0.65 (PE: EA = 3:1).

\(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 7.94 – 7.84\) (m, 2H), 7.42 – 7.35 (m, 2H), 7.31 – 7.24 (m, 1H), 5.25 (hept, \(J = 6.8\) Hz, 1H), 4.54 – 4.44 (m, 1H), 4.04 (hept, \(J = 6.8\) Hz, 1H), 2.20 – 2.09 (m, 4H), 2.04 – 1.93 (m, 2H), 1.82 – 1.72 (m, 1H), 1.50 – 1.36 (m, 3H), 1.33 (d, \(J = 6.8\) Hz, 6H), 1.28 (d, \(J = 6.8\) Hz, 6H).

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta 141.4, 135.4, 132.4, 128.0, 127.7, 126.9, 58.2, 49.8, 46.9, 32.6, 25.8, 25.4, 23.5, 19.1.

HRMS (EI-TOF) \(m/z\): calcd for C\(_{20}\)H\(_{30}\)N\(_6\) (M)\(^+\) 354.2532; Found 354.2534.
1-cinnamyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazole

3z: Light yellow solid, m.p. 88 – 90 °C, 72 mg (93% yield).

TLC: Rf = 0.50 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.02 – 7.90 (m, 2H), 7.41 – 7.15 (m, 8H), 6.48 (d, $J = 16.0$ Hz, 1H), 6.34 (dt, $J_1 = 16.0$ Hz, $J_2 = 5.6$ Hz, 1H), 5.34 – 5.07 (m, 3H), 3.98 (hept, $J = 6.8$ Hz, 1H), 1.28 – 1.18 (m, 12H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 141.7, 136.1, 135.8, 132.9, 132.1, 128.5, 128.0, 127.8, 127.5, 127.0, 126.4, 123.5, 50.6, 49.9, 47.0, 23.4, 18.9.

HRMS (EI-TOF) $m/z$: calcd for C$_{23}$H$_{28}$N$_6$ (M)$^+$ 388.2375; Found 388.2377.

5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1-(4-phenylbut-3-yn-1-yl)-1H-1,2,3-triazole

3a': Light yellow solid, m.p. 87 – 88 °C, 72 mg (90% yield).

TLC: Rf = 0.47 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.00 – 7.93 (m, 2H), 7.41 – 7.33 (m, 4H), 7.30 – 7.23 (m, 4H), 5.25 (hept, $J = 6.8$ Hz, 1H), 4.73 – 4.62 (m, 2H), 4.03 (hept, $J = 6.8$ Hz, 1H), 3.06 – 2.96 (m, 2H), 1.31 (d, $J = 6.8$ Hz, 6H), 1.28 (d, $J = 6.8$ Hz, 6H).
$^{13}$C NMR (100 MHz, CDCl$_3$) δ 141.5, 136.2, 132.1, 131.6, 128.3, 128.1, 128.0, 127.5, 127.1, 123.2, 85.4, 82.8, 49.9, 47.6, 47.2, 23.5, 21.2, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{24}$H$_{30}$N$_6$ (M)$^+$ 400.2375; Found 400.2371.

4-(5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazol-1-yl)-1-phenylbutan-1-one

3b': Light yellow oil, 76 mg (91% yield).

TLC: Rf = 0.29 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.95 – 7.85 (m, 4H), 7.57 – 7.50 (m, 1H), 7.47 – 7.40 (m, 2H), 7.39 – 7.34 (m, 2H), 7.30 – 7.24 (m, 1H), 5.18 (hept, $J$ = 6.8 Hz, 1H), 4.56 (t, $J$ = 6.4 Hz, 2H), 4.00 (hept, $J$ = 6.8 Hz, 1H), 3.07 (t, $J$ = 7.2 Hz, 2H), 2.40 – 2.27 (m, 2H), 1.25 (d, $J$ = 6.8 Hz, 12H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 199.1, 142.0, 136.8, 135.8, 133.2 (133.24), 133.2 (132.18), 128.7, 128.1, 127.8, 127.2, 50.0, 47.8, 47.1, 35.1, 24.0, 23.6, 19.1.

HRMS (EI-TOF) $m/z$: calcd for C$_{24}$H$_{30}$N$_6$O (M)$^+$ 418.2481; Found 418.2487.

2-(5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazol-1-yl)ethyl 4-methylbenzenesulfonate

3c': White solid, m.p. 97 – 99 °C, 90 mg (96% yield).
TLC: Rf = 0.18 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.87 (d, $J = 8.0$ Hz, 2H), 7.61 (d, $J = 7.6$ Hz, 2H), 7.42 – 7.35 (m, 2H), 7.32 – 7.25 (m, 1H), 7.22 – 7.14 (m, 2H), 5.19 (hept, $J = 6.8$ Hz, 1H), 4.69 (t, $J = 6.0$ Hz, 2H), 4.42 (t, $J = 6.0$ Hz, 2H), 4.04 (hept, $J = 6.8$ Hz, 1H), 2.27 (s, 3H), 1.33 – 1.24 (m, 12H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 145.1, 141.9, 135.6, 132.0, 131.8, 129.9, 128.1, 127.7, 127.5, 127.2, 67.4, 50.1, 47.3, 46.9, 23.6, 21.5, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C\textsubscript{23}H\textsubscript{30}N\textsubscript{6}O\textsubscript{3}S (M)$^+$ 470.2100; Found 470.2103.

2-(3-(5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazol-1-yl)propyl)isoindoline-1,3-dionene

3d$: Yellow solid, m.p. 79 – 81 °C, 88 mg (98% yield).

TLC: Rf = 0.12 (PE: EA = 3:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.88 – 7.79 (m, 4H), 7.74 – 7.68 (m, 2H), 7.39 – 7.23 (m, 3H), 5.16 (hept, $J = 6.8$ Hz, 1H), 4.50 (t, $J = 7.6$ Hz, 2H), 4.00 (hept, $J = 6.8$ Hz, 1H), 3.83 (t, $J = 7.2$ Hz, 2H), 2.39 – 2.25 (m, 2H), 1.29 – 1.20 (m, 12H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 168.1, 141.6, 135.7, 134.1, 132.1, 132.0, 128.0, 127.7, 127.1, 123.3, 50.0, 47.1, 46.6, 35.7, 28.9, 23.5, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C\textsubscript{25}H\textsubscript{29}N\textsubscript{7}O\textsubscript{2} (M)$^+$ 459.2383; Found 459.2388.
2-(5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1H-1,2,3-triazol-1-yl)ethyl (S)-2-(1,3-dioxoisindolin-2-yl)-3-phenylpropanoate

3e': White solid, m.p. 109 – 110 °C, 111 mg (94% yield).

TLC: Rf = 0.47 (PE: EA = 1:1).

\[^1\text{H NMR (400 MHz, CDCl}_3\text{)} \delta \] 7.91 – 7.84 (m, 2H), 7.74 – 7.66 (m, 2H), 7.63 – 7.56 (m, 2H), 7.40 – 7.32 (m, 2H), 7.29 – 7.22 (m, 1H), 7.19 – 7.06 (m, 5H), 5.29 – 5.10 (m, 2H), 4.78 – 4.56 (m, 4H), 4.02 (hept, J = 6.8 Hz, 1H), 3.60 – 3.43 (m, 2H), 1.28 (d, J = 6.8 Hz, 6H), 1.24 (d, J = 6.8 Hz, 6H).

\[^{13}\text{C NMR (100 MHz, CDCl}_3\text{)} \delta \] 168.6, 167.2, 141.8, 136.5, 135.7, 134.1, 131.9, 131.4, 128.8, 128.5, 128.0, 127.6, 127.1, 126.8, 123.4, 63.2, 53.1, 49.9, 47.2, 46.8, 34.6, 23.5, 23.5, 19.0.

HRMS (EI-TOF) m/z: calcd for C\text{33}H\text{35}N\text{7}O\text{4} (M)\text{+} 593.2751; Found 593.2756.

5-(3,3-diisopropyltriaz-1-en-1-yl)-4-phenyl-1-(2,2,3,3-tetramethyl-4,7,10,13-tetraoxa-3-silapentadecan-15-yl)-1H-1,2,3-triazole

3f': Yellow oil, 89 mg (79% yield).

TLC: Rf = 0.44 (PE: EA = 1:1).
**1H NMR** (400 MHz, CDCl₃) δ 7.92 – 7.87 (m, 2H), 7.40 – 7.34 (m, 2H), 7.30 – 7.23 (m, 1H), 5.25 (hept, J = 6.8 Hz, 1H), 4.61 (t, J = 6.8 Hz, 2H), 4.03 (hept, J = 6.8 Hz, 1H), 3.93 (t, J = 6.8 Hz, 2H), 3.75 (t, J = 5.6 Hz, 2H), 3.66 – 3.58 (m, 8H), 3.53 (t, J = 5.6 Hz, 2H), 1.33 – 1.24 (m, 12H), 0.89 (s, 9H), 0.06 (s, 6H).

**13C NMR** (100 MHz, CDCl₃) δ 141.9, 135.7, 132.2, 128.1, 127.7, 127.1, 72.7, 70.8, 70.7 (70.74), 70.7 (70.70), 70.5, 69.3, 62.8, 49.9, 48.0, 47.0, 26.0, 23.6, 19.1, 18.4, -5.2.

**HRMS (EI-TOF)** m/z: calcd for C₂₈H₅₀N₆O₄Si (M)⁺ 562.3663; Found 562.3667.

(2R,3R,4S,5R)-2-(acetoxy methyl)-6-(5-(3,3-diisopropyl triaz 1-enyl)-4-phenyl-1H-1,2,3-triazol-1-yl) tetrahydro-2H-pyran-3,4,5-triyl triacetate

**3g’:** Light yellow solid, 116 mg (96% yield).

**TLC:** Rf = 0.41 (PE: EA = 1:1).

**1H NMR** (400 MHz, CDCl₃) δ 7.84 – 7.75 (m, 1.5H), 7.53 – 7.43 (m, 1.25H), 7.39 – 7.33 (m, 1.5H), 7.31 – 7.25 (m, 0.75H), 6.18 (t, J = 9.6 Hz, 0.75H), 6.04 – 5.94 (m, 1H), 5.49 (d, J = 9.6 Hz, 0.25H), 5.41 (t, J = 9.6 Hz, 0.75H), 5.33 – 5.10 (m, 2.25H), 4.31 – 3.77 (m, 4H), 2.12 (s, 0.75H), 2.07 (s, 2.25H), 2.06 – 2.02 (m, 5.25H), 2.00 (s, 0.75H), 1.90 – 1.83 (m, 3H), 1.37 (dd, J₁ = 6.8 Hz, J₂ = 4.0 Hz, 4.5H), 1.27 – 1.23 (m, 4.5H), 1.17 (d, J = 6.4 Hz, 1.5H), 1.05 (d, J = 6.4 Hz, 1.5H).

**13C NMR** (100 MHz, CDCl₃) δ 170.6, 170.5, 170.4 (170.43), 170.4 (170.36), 169.3, 169.2, 168.6, 168.4, 154.4, 142.7, 134.9, 131.6, 130.4, 129.1, 128.5, 128.3, 128.0,
127.5, 127.3, 126.5, 83.8, 83.6, 74.7, 74.5, 73.8, 73.6, 69.4, 69.2, 67.9, 67.8, 62.0, 61.9, 50.5, 49.3, 47.7, 45.9, 23.6, 23.5, 23.2, 23.1, 20.7 (20.74), 20.7 (20.71), 20.7 (20.66), 20.6 (20.61), 20.6 (20.56), 20.4, 19.2, 19.1, 19.0.

HRMS (EI-TOF) $m/z$: calcd for C$_{28}$H$_{38}$N$_6$O$_9$ (M)$^+$ 602.2700; Found 602.2706.

1-benzyl-4-phenyl-1H-1,2,3-triazol-5-amine

4a: White solid, m.p. 155 – 157 °C, 44 mg, (88% yield).


TLC: Rf = 0.46 (PE: EA = 1:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.68 – 7.63 (m, 2H), 7.45 – 7.32 (m, 5H), 7.31 – 7.24 (m, 3H), 5.45 (s, 2H), 3.67 (s, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 137.4, 134.3, 131.8, 131.6, 129.4, 129.1, 128.7, 127.4, 127.2, 125.8, 50.9.

HRMS (EI-TOF) $m/z$: calcd for C$_{15}$H$_{14}$N$_4$ (M)$^+$ 250.1218; Found 250.1216.

1-phenethyl-4-phenyl-1H-1,2,3-triazol-5-amine


TLC: Rf = 0.43 (PE: EA = 1:1).
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.60 – 7.55 (m, 2H), 7.42 – 7.36 (m, 2H), 7.30 – 7.20 (m, 4H), 7.11 – 7.05 (m, 2H), 4.37 (t, $J$ = 6.8 Hz, 2H), 3.33 (s, 2H), 3.16 (t, $J$ = 6.8 Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 137.9, 137.5, 131.8, 131.3, 129.0, 127.3, 127.1, 125.9, 48.2, 36.2.

HRMS (EI-TOF) $m/z$: calcd for C$_{16}$H$_{16}$N$_4$ (M)$^+$ 264.1375; Found 264.1377.

4-phenyl-1-(3-phenylpropyl)-1H-1,2,3-triazol-5-amine

4c: White solid, m.p. 113 – 115°C, 41 mg, (74% yield).


TLC: Rf = 0.43 (PE: EA=1:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.70 – 7.64 (m, 2H), 7.47 – 7.40 (m, 2H), 7.33 – 7.27 (m, 3H), 7.23 – 7.19 (m, 3H), 4.15 (t, $J$ = 7.2 Hz, 2H), 3.71 (s, 2H), 2.72 (t, $J$ = 7.2 Hz, 2H), 2.26 (p, $J$ = 7.2 Hz, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 140.5, 136.9, 131.9, 131.3, 129.1, 128.8, 128.6, 127.2, 126.5, 125.9, 45.7, 32.6, 30.3.

HRMS (EI-TOF) $m/z$: calcd for C$_{17}$H$_{18}$N$_4$ (M)$^+$ 278.1531; Found 278.1537.

4-phenyl-1-(4-phenylbutyl)-1H-1,2,3-triazol-5-amine

4d: White solid, m.p. 121-123°C, 53 mg, (90% yield).

TLC: Rf = 0.43 (PE: EA=1:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.70 – 7.64 (m, 2H), 7.46 – 7.40 (m, 2H), 7.33 – 7.25 (m, 3H), 7.21 – 7.14 (m, 3H), 4.16 (t, $J$ = 7.2 Hz, 2H), 3.71 (s, 2H), 2.67 (t, $J$ = 7.6 Hz, 2H), 1.98 – 1.89 (m, 2H), 1.78 – 1.68 (m, 2H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 141.7, 136.7, 131.9, 131.5, 129.1, 128.6 (128.58), 128.6 (128.56), 127.2, 126.2, 125.9, 46.5, 35.3, 28.7, 28.3.

HRMS (EI-TOF) m/z: calcd for C$_{18}$H$_{20}$N$_4$ (M) $^+$ 292.1688; Found 292.1687.

1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-amine

4e: White solid, m.p. 135 – 137°C, 43 mg, (88% yield).


TLC: Rf = 0.52 (PE: EA=1:1).

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.68 – 7.62 (m, 2H), 7.42 – 7.36 (m, 2H), 7.30 – 7.22 (m, 1H), 4.18 (s, 2H), 4.10 – 4.00 (m, 1H), 2.07 – 1.85 (m, 6H), 1.73 – 1.66 (m, 1H), 1.39 – 1.23 (m, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$) δ 136.7, 132.0, 130.8, 128.9, 126.9, 125.8, 56.6, 32.2, 25.5, 25.1.

HRMS (EI-TOF) m/z: calcd for C$_{14}$H$_{18}$N$_4$ (M) $^+$ 242.1531; Found 242.1533.
2-(5-amino-4-phenyl-1H-1,2,3-triazol-1-yl)ethan-1-ol

4f: White solid, 76 – 78 °C, 26 mg, (63% yield).

Flash chromatography: CH₂Cl₂: MeOH = 1:0 – 20:1, v:v.

TLC: Rf = 0.18 (CH₂Cl₂: MeOH = 30:1).

¹H NMR (600 MHz, CDCl₃) δ 7.55 – 7.51 (m, 2H), 7.42 – 7.37 (m, 2H), 7.30 – 7.26 (m, 1H), 4.46 – 4.20 (m, 4H), 4.11 – 4.06 (m, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 139.2, 131.6, 130.4, 129.1, 127.1, 125.7, 62.4, 49.4.

HRMS (EI-TOF) m/z: calcd for C₁₀H₁₂N₄O (M)⁺ 204.1011; Found 204.1013.

4-phenyl-1-(2-(piperidin-1-yl)ethyl)-1H-1,2,3-triazol-5-amine

4g: White solid, m.p. 186 – 187°C, 44 mg, (82% yield).


TLC: Rf = 0.48 (CH₂Cl₂: MeOH = 10:1).

¹H NMR (600 MHz, CDCl₃) δ 7.71 – 7.62 (m, 2H), 7.47 – 7.40 (m, 2H), 7.33 – 7.23 (m, 1H), 5.62 (s, 2H), 4.40 – 4.36 (m, 2H), 2.77 – 2.73 (m, 2H), 2.68 – 2.32 (m, 4H), 1.62 – 1.54 (m, 4H), 1.52 – 1.40 (m, 2H).

¹³C NMR (150 MHz, CDCl₃) δ 139.7, 132.4, 130.1, 129.0, 126.7, 125.6, 59.8, 55.0, 46.1, 26.2, 24.0.

HRMS (EI-TOF) m/z: calcd for C₁₅H₂₁N₅ (M)⁺ 271.1797; Found 271.1793.
1-(2-(4-methylpiperazin-1-yl)ethyl)-4-phenyl-1H-1,2,3-triazol-5-amine

4h: Colourless oil, 47 mg, (83% yield).

**Flash chromatography:** CH$_2$Cl$_2$: MeOH = 20:1 – 10:1, v:v.

**TLC:** Rf = 0.15 (CH$_2$Cl$_2$: MeOH = 10:1).

$^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.69 – 7.64 (m, 2H), 7.46 – 7.40 (m, 2H), 7.31 – 7.25 (m, 1H), 5.40 (s, 2H), 4.41 – 4.34 (m, 2H), 2.84 – 2.79 (m, 2H), 2.76 – 2.30 (m, 8H), 2.28 (s, 3H).

$^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 139.3, 132.2, 130.2, 129.0, 126.7, 125.6, 58.9, 55.2, 53.4, 45.9, 45.6.

**HRMS (EI-TOF) m/z:** calcd for C$_{15}$H$_{22}$N$_6$ (M)$^+$ 286.1906; Found 286.1907.

1-(2-morpholinoethyl)-4-phenyl-1H-1,2,3-triazol-5-amine

4i: White solid, m.p. 185 – 187 °C, 43 mg, (79% yield).

**Flash chromatography:** CH$_2$Cl$_2$: MeOH = 1:0 – 20:1, v:v.

**TLC:** Rf = 0.29 (CH$_2$Cl$_2$: MeOH = 30:1).
\[\text{H NMR (600 MHz, CDCl}_3\] \delta 7.71 – 7.62 (m, 2H), 7.48 – 7.41 (m, 2H), 7.32 – 7.27 (m, 1H), 5.30 (s, 2H), 4.41 – 4.36 (m, 2H), 3.80 – 3.62 (m, 4H), 2.89 – 2.78 (m, 2H), 2.68 – 2.47 (m, 4H).

\[\text{13C NMR (100 MHz, CDCl}_3\] \delta 139.1, 132.1, 130.5, 129.1, 126.9, 125.7, 67.0, 59.5, 54.0, 45.3.

HRMS (EI-TOF) \(m/z\): calcd for C\(_{14}\)H\(_{19}\)N\(_5\)O (M)\(^+\) 273.1590; Found 273.1593.

\[\text{1,4-diphenyl-1H-1,2,3-triazol-5-amine} 4j: \text{White solid, m.p. 167 – 169 °C, 25 mg, (54\% yield).} \]

Flash chromatography: CH\(_2\)Cl\(_2\): MeOH = 30:1, v:v.

TLC: R\(_f\) = 0.50 (CH\(_2\)Cl\(_2\): MeOH = 30:1).

\[\text{H NMR (600 MHz, CDCl}_3\] \delta 7.75 – 7.71 (m, 2H), 7.60 – 7.54 (m, 4H), 7.52 – 7.47 (m, 1H), 7.47 – 7.43 (m, 2H), 7.33 – 7.28 (m, 1H), 4.14 (s, 2H).

\[\text{13C NMR (150 MHz, CDCl}_3\] \delta 137.6, 135.3, 131.6, 130.1, 129.9, 129.1, 127.2, 125.8, 124.5.

HRMS (EI-TOF) \(m/z\): calcd for C\(_{14}\)H\(_{12}\)N\(_4\) (M)\(^+\) 236.1062; Found 236.1063.

\[\text{1-phenethyl-4-(m-tolyl)-1H-1,2,3-triazol-5-amine} 4k: \text{White solid, m.p. 116 – 118 °C, 45 mg, (81\% yield).} \]
TLC: Rf = 0.60 (PE: EA=1:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.45 (s, 1H), 7.37 – 7.22 (m, 5H), 7.15 – 7.06 (m, 3H), 4.41 (t, $J = 6.8$ Hz, 2H), 3.20 (t, $J = 6.8$ Hz, 2H), 3.11 (s, 2H), 2.38 (s, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 138.8, 138.0, 137.4, 131.7, 131.5, 129.1 (129.12), 129.1 (129.07), 128.9, 128.0, 127.4, 126.8, 122.8, 48.4, 36.4, 21.6.

HRMS (EI-TOF) $m/z$: calcd for C$_{17}$H$_{18}$N$_4$ (M)$^+ 278.1531$; Found 278.1530.

4-butyl-1-phenethyl-1H-1,2,3-triazol-5-amine

4l: Colourless oil, 35 mg, (71% yield).

TLC: Rf = 0.26 (PE: EA=1:1).

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.36 – 7.17 (m, 3H), 7.10 – 6.95 (m, 2H), 4.34 (t, $J = 6.8$ Hz, 2H), 3.13 (t, $J = 6.8$ Hz, 2H), 2.79 (s, 2H), 2.47 (t, $J = 7.2$ Hz, 2H), 1.62 – 1.49 (m, 2H), 1.38 – 1.24 (m, 2H), 0.90 (t, $J = 7.2$ Hz, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 138.0, 137.0, 132.7, 129.0, 128.8, 127.1, 47.9, 36.4, 31.2, 24.2, 22.3, 13.9.

HRMS (EI-TOF) $m/z$: calcd for C$_{14}$H$_{20}$N$_4$ (M)$^+ 244.1688$; Found 244.1685.
4-(methoxymethyl)-1-phenethyl-1H-1,2,3-triazol-5-amine

4m: White solid, m.p. 115 – 117 °C, 35 mg, (75% yield).

Flash chromatography: CH₂Cl₂: MeOH = 1:0 – 30:1, v:v.

TLC: Rf = 0.35 (CH₂Cl₂: MeOH = 30:1).

¹H NMR (600 MHz, CDCl₃) δ 7.32 – 7.24 (m, 3H), 7.10 – 7.06 (m, 2H), 4.51 (s, 2H), 4.35 (t, J = 6.8 Hz, 2H), 3.30 (s, 3H), 3.16 (t, J = 6.8 Hz, 2H), 3.09 (s, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 139.4, 137.9, 129.1, 129.0, 128.2, 127.4, 66.3, 57.9, 48.1, 36.4.

HRMS (EI-TOF) m/z: calcd for C₁₂H₁₆N₄O (M)⁺ 232.1324; Found 232.1327.

1-phenethyl-4-(((tetrahydro-2H-pyran-2-yl)oxy)methyl)-1H-1,2,3-triazol-5-amine


Flash chromatography: CH₂Cl₂: MeOH = 1:0 – 30:1, v:v.

TLC: Rf = 0.21 (CH₂Cl₂: MeOH = 30:1).

¹H NMR (600 MHz, CDCl₃) δ 7.31 – 7.22 (m, 3H), 7.13 – 7.03 (m, 2H), 4.69 (d, J = 12.6 Hz, 1H), 4.62 (d, J = 12.6 Hz, 1H), 4.56 (t, J = 4.2 Hz, 1H), 4.38 – 4.28 (m, 2H), 3.86 – 3.79 (m, 1H), 3.57 – 3.44 (m, 3H), 3.15 (t, J = 7.2 Hz, 2H), 1.83 – 1.75 (m, 1H), 1.72 – 1.65 (m, 1H), 1.61 – 1.45 (m, 4H).

¹³C NMR (150 MHz, CDCl₃) δ 140.1, 137.9, 128.9 (128.93), 128.9 (128.91), 127.7, 127.1, 97.5, 62.7, 60.2, 47.9, 36.1, 30.4, 25.3, 19.6.

HRMS (EI-TOF) m/z: calcd for C₁₆H₂₂N₄O₂ (M)⁺ 302.1743; Found 302.1747.
5-chloro-1-cyclohexyl-4-phenyl-1H-1,2,3-triazole

5: White solid, m.p. 99 – 101 °C, 43 mg, (82% yield).

**TLC:** Rf = 0.27 (PE: EA=20:1).

**1H NMR (400 MHz, CDCl₃)** δ 8.01 – 7.95 (m, 2H), 7.49 – 7.42 (m, 2H), 7.40 – 7.34 (m, 1H), 4.42 – 4.31 (m, 1H), 2.16 – 1.94 (m, 6H), 1.82 – 1.74 (m, 1H), 1.54 – 1.31 (m, 3H).

**13C NMR (100 MHz, CDCl₃)** δ 141.5, 129.7, 128.7, 128.4, 126.5, 120.7, 58.7, 32.3, 25.5, 25.1.

**HRMS (EI-TOF) m/z:** calcd for C₁₄H₁₆ClN₃ (M)⁺ 261.1033; Found 261.1030.

5-bromo-1-cyclohexyl-4-phenyl-1H-1,2,3-triazole


**TLC:** Rf = 0.25 (PE: EA=20:1).

**1H NMR (400 MHz, CDCl₃)** δ 8.00 – 7.95 (m, 2H), 7.49 – 7.42 (m, 2H), 7.41 – 7.35 (m, 1H), 4.44 – 4.31 (m, 1H), 2.17 – 1.94 (m, 6H), 1.81 – 1.74 (m, 1H), 1.53 – 1.30 (m, 3H).

**13C NMR (100 MHz, CDCl₃)** δ 144.2, 130.0, 128.6, 128.5, 127.0, 107.2, 59.6, 32.5, 25.5, 25.1.
HRMS (EI-TOF) m/z: calcd for C_{14}H_{16}BrN_{3} (M)^{+} 305.0528; Found 305.0520.

3'-cyclohexyl-4,5'-diphenyl-5-(pyrrolidin-1-yl)diazenyl)-3'H-1,4'-bi(1,2,3-triazole)

7: Yellow solid, m.p. 201 – 203 °C, 50 mg, (53% yield).

TLC: Rf = 0.24 (PE: EA=3:1).

$^{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.25 – 8.20 (m, 2H), 7.49 – 7.40 (m, 4H), 7.38 – 7.32 (m, 1H), 7.31 – 7.24 (m, 3H), 4.00 – 3.89 (m, 1H), 3.57 – 3.45 (m, 2H), 3.44 – 3.28 (m, 2H), 2.27 – 2.18 (m, 1H), 2.16 – 2.05 (m, 1H), 2.02 – 1.80 (m, 8H), 1.71 – 1.65 (m, 1H), 1.34 – 1.22 (m, 3H).

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 143.0, 141.0, 136.2, 130.9, 129.3, 128.9, 128.7, 128.6, 128.1, 127.9, 126.7, 126.1, 58.6, 51.8, 47.1, 33.3, 32.1, 25.4 (25.44), 25.4 (25.37), 25.1, 23.7, 23.3.

HRMS (EI-TOF) m/z: calcd for C$_{26}$H$_{29}$N$_{9}$ (M)$^{+}$ 467.2546; Found 467.2541.

benzyl (S)-2-((1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-yl)carbamoyl)pyrrolidine-1-carboxylate
8: Yellow oil, 79 mg, (84% yield).

**TLC:** Rf = 0.12 (PE: EA=1:1).

1H NMR (400 MHz, CDCl$_3$) δ 9.17 (s, 1H), 7.73 – 7.57 (m, 2H), 7.39 – 7.17 (m, 8H), 5.26 – 4.81 (m, 2H), 4.64 – 4.52 (m, 1H), 4.16 – 3.84 (m, 1H), 3.57 – 3.39 (m, 2H), 2.41 – 1.80 (m, 10H), 1.74 – 1.61 (m, 1H), 1.44 – 1.19 (m, 3H).

13C NMR (100 MHz, CDCl$_3$) δ 172.2, 156.5, 140.6, 136.1, 130.2, 128.6 (128.62), 128.6 (128.55), 128.3, 128.0, 127.9, 126.9, 126.4, 67.7, 60.6, 57.7, 47.2, 32.7 (32.72), 32.7 (32.66), 28.3, 25.6, 25.2, 24.7.

HRMS (EI-TOF) m/z: calcd for C$_{27}$H$_{31}$N$_5$O$_3$ (M)$^+$ 473.2427; Found 473.2425.

1-phenyl-5,6-dihydro-[1,2,3]triazolo[5,1-a]isoquinoline

9: White solid, m.p. 137 – 139 °C. 24 mg, (95% yield)

**TLC:** Rf = 0.30 (PE: EA=3:1).

1H NMR (400 MHz, CDCl$_3$) δ 7.75 – 7.71 (m, 2H), 7.60 (d, J = 7.6 Hz, 1H), 7.50 – 7.41 (m, 3H), 7.36 – 7.27 (m, 2H), 7.22 – 7.16 (m, 1H), 4.60 (t, J = 6.8 Hz, 2H), 3.26 (t, J = 6.8 Hz, 2H).

13C NMR (100 MHz, CDCl$_3$) δ 143.2, 133.0, 131.8, 129.4, 129.3, 128.8, 128.6 (128.64), 128.6 (128.62), 128.6 (128.56), 127.6, 125.2, 124.6, 45.1, 29.5.

HRMS (EI-TOF) m/z: calcd for C$_{16}$H$_{13}$N$_3$ (M)$^+$ 247.1109; Found 247.1106.

12. X-ray Crystallographic Data

Crystals suitable for X-ray diffraction experiments were obtained by following methods: compound 3a, 3n and 3a’ were crystallized from their solution in PE/EA.
Compound 4e was crystallized from its solution in Hexane/Chloroform. Intensity data for compounds was collected on ‘Bruke Apex2’ diffractometer at 296(2) (MoK/α radiation, radiation wavelength = 0.7107). The structures were solved by direct methods and refined by the full-matrix least-squares method using the SHELX-97 program package. The geometrical parameters and the figures were analyzed using the program OLEX2.

![Figure S3. X-ray crystallographic structure 3a (ORTEP view with 50% thermal ellipsoid contour probability)](image)

![Figure S4. X-ray crystallographic structure 3n (ORTEP view with 50% thermal ellipsoid contour probability)](image)
**Figure S5.** X-ray crystallographic structure 3a' (ORTEP view with 50% thermal ellipsoid contour probability)

**Figure S6.** X-ray crystallographic structure 4e (ORTEP view with 50% thermal ellipsoid contour probability)
## Table S1. Crystal data and structure refinements for 3a, 3n, 3a' and 4e

<table>
<thead>
<tr>
<th>Compounds</th>
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<th>4e</th>
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<td>1945307</td>
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<td>C_{21}H_{26}N_{6}</td>
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<td>P2(1)/c</td>
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<td>P - 1</td>
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<td>-</td>
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<td>23.998(5)</td>
<td>10.3558(11)</td>
<td>12.0903(7)</td>
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<tr>
<td>c/Å</td>
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<td>10.424(2)</td>
<td>11.0250(12)</td>
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<td>90</td>
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<td>γ/°</td>
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<td>90</td>
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<td>909.09(17)</td>
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<td>296(2)</td>
<td>170(2)</td>
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<td>MoKα</td>
<td>MoKα</td>
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<td>2.29 to 21.56</td>
<td>2.58 to 27.56</td>
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<tr>
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<td>5032</td>
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<tr>
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<td>–11 ≤ h ≤ 11</td>
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<tr>
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<td>R₁ = 0.0472</td>
<td>R₁ = 0.0520</td>
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<td>wR₂ = 0.1084</td>
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<td>Final R indexes R [all data]</td>
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<td>R₁ = 0.0954</td>
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<td>wR₂ = 0.1604</td>
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<td>0.121/-0.144</td>
<td>0.219/-0.362</td>
<td>0.391/-0.441</td>
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</table>
13. References


14. Copies of NMR Spectra

$^1$H NMR: 400 MHz
Solvent: CDCl$_3$
$^{13}$C NMR: 100 MHz
Solvent: CDCl$_3$
$^1$H NMR: 400 MHz
Solvent: CDCl$_3$
$^{13}$C NMR: 100 MHz
Solvent: CDCl$_3$
TMS=NN

$^1$H NMR: 600 MHz
Solvent: CDCl$_3$
TMS \equiv \equiv N \quad N \equiv \equiv N

$1k$

$^{13}$C NMR: 100 MHz
Solvent: CDCl$_3$
^1H NMR: 400 MHz
Solvent: CDCl₃
$^{13}$C NMR: 100 MHz
Solvent: CDCl$_3$
$^1$H NMR: 400 MHz
Solvent: CDCl$_3$
13C NMR: 100 MHz
Solvent: CDCl₃
$^{1}{H}$ NMR: 400 MHz
Solvent: CDCl$_3$
$^{13}\text{C NMR: } 100 \text{ MHz}$

**Solvent:** CDCl$_3$
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Solvent: CDCl$_3$
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Solvent: CDCl$_3$
Chemical structure: 

1q

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Solvent: CDCl$_3$
\[
\text{\textsuperscript{1}H NMR: 600 MHz}
\]

\textbf{Solvent: CDCl}_3
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Solvent: CDCl$_3$
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Solvent: CDCl$_3$
MeO
\[ \text{N=}
\]
\[ \text{N=}
\]
1s

$^{13}$C NMR: 100 MHz
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THPO

$\text{N} \quad \text{N}$

1t

$^1\text{H NMR: 600 MHz}$

$\text{Solvent: CDCl}_3$
$^{13}$C NMR: 100 MHz
Solvent: CDCl$_3$
crude $^1$H NMR

$^1$H NMR: 400 MHz

Solvent: CDCl$_3$
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Solvent: CDCl$_3$
3d

$^1$H NMR: 400 MHz
Solvent: CDCl$_3$
\[ \text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{N}^\text{(iPr)}_2 \]

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$3b'$

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$dr \ 3:1$

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