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Supporting Information

1,6-addition of 1,2,3-NH triazoles to *para*-quinone methides: Facile access to highly N¹ and N² selective substituted triazoles

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Material and Methods General Information

All reactions were carried out in oven-dried glassware, all compounds were fully characterized by spectroscopic data. The NMR spectra were recorded on JEOL - 400 spectrometers, (¹H: 400 MHz, ¹³C: 100 MHz and ¹⁹F: 376 MHz), and were referenced to the residual peaks of CDCl₃ at 7.26 ppm and CDCl₃ at 77.23 ppm (¹³C NMR). Chemical shifts (δ) are expressed in ppm, and *J* values are given in Hz. Data are reported as follows: Chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, db = doublet broad, m = multiplet), coupling constant (Hz), and integration. The reactions were monitored by thin layer chromatography (TLC) using silica gel GF254. The melting points (m.p.) were determined on digital melting point apparatus and are uncorrected. Mass measurement was performed on Broker Micro TOF QII mass spectrometer with electron spray ionization (ESI) as the ion source. Column chromatography was carried out using commercially available silica gel (230-400 mesh) under pressure. Materials unless otherwise indicated, all reagents were obtained from commercial suppliers used without further purification. PE refers to Petroleum ether (b.p. 60-90 °C) and EA refers to ethyl acetate, and all reaction solvents were freshly distilled prior to use.

All the *p*-QM and 1,2,3 *NH* triazole starting materials were synthesized using the procedure given in literature.^{1,2}

General Procedure for the synthesis of N² substituted triazoles



To a 25 ml reaction flask, was added *p*-quinone methide **1a** (100 mg, 1 equiv. 0.339 mmol), NH-1,2,3 triazole **2a** (49.2 mg, 1 equiv., 0.339 mmol), sodium carbonate (35.9 mg, 1 equiv., 0.339 mmol) and *tert*-butyl ammonium bromide (21.8 mg, 0.2 equiv., 0.067 mmol) in THF:H₂O (1:1) solvent (2 mL). The mixture was stirred at room temperature for 2 hours. The progress of reaction was monitored by TLC. After the completion of reaction, the mixture was quenched with water, extracted with ethyl acetate. The combined organic layers were dried over sodium sulphate, concentrated under reduced pressure and purified by column chromatography to afford product **3a** as white solid (110 mg).

General Procedure for the synthesis of N¹ substituted triazoles



To a 25 ml reaction flask, was added *p*-quinone methide 1a (100 mg, 1 equiv. 0.339 mmol), NH-1,2,3 triazole 2a (49.2 mg, 1 equiv., 0.339 mmol) and monochloroacetic acid (33.8 mg, 1 equiv., 0.339 mmol) in acetonitrile solvent (2 mL). The mixture was stirred at room temperature for 2 hours. The progress of reaction was monitored by TLC. After the completion of reaction, the mixture was quenched with water, extracted with ethyl acetate. The combined organic layers were dried over sodium sulphate, concentrated under reduced pressure and purified by column chromatography to afford product 4a as white solid (116 mg).

Parameters	3a	4a	
CCDC Number	2103494	2103495	
Empirical formula	C ₂₉ H ₃₂ N ₃ O	$C_{29} H_{32} N_3 O$	
Formula weight	438.58	438.58	
Crystal system	Monoclinic	Triclinic	
Space group	$P2_1/n$	$P\overline{1}$	
Temperature (K)	296(2)	296(2) 296(2)	
Unit cell dimensions	a = 11.0143(14) Å	a = 11.8940(13) Å	
	b = 15.747(2) Å	b = 11.7007(13)Å	
	c = 15.541(2) Å	c = 31.479(3)Å	
	$\alpha = 90^{\circ}$	a= 80.990(2)°	
	$\beta = 104.578(4)^{\circ}$	$\beta = 68.5320(10)^{\circ}$	
	$\gamma = 90^{\circ}$	$\gamma = 81.497(2)^{\circ}$	
volume (Å ³)	2608.6(6)	1237.33(11)	
Z	4	2	
Radiation type (Mo-Kα)/Å	0.71073	0.71073	
No. measured reflections	34744	24419	
Calculated density (mg/m ³)	1.117	1.177	
Absorption coefficient (mm ⁻¹)	0.068	0.072	
F(000)	940	470	
θ range for data collection	2.587 to 28.327°	2.671 to 28.255°	
Limiting indices	$-14 \le h \le 14$	$-13 \le h \le 13$	
	$-21 \le k \le 21$	$-14 \le k \le 14$	
	$-20 \le 1 \le 20$	$-15 \le 1 \le 15$	
Refinement method	Full-matrix least-	Full-matrix least-	
	squares on F ²	squares on F ²	
Data / restraints / parameter	6494 / 0 / 305	6117 / 0 / 304	
Final <i>R</i> Indices[I > $2\sigma(I)$]	R1 = 0.0598, wR2 =	R1 = 0.0566, WR2	
	0.1487	= 0.1460	
<i>R</i> indices (all data)	R1 = 0.1382, wR2 =	R1 = 0.0802, wR2	
	0.1957	= 0.1649	
Goodness of fit on F^2	1.019	1.036	
Largest diff. peak and hole	0.241 and -0.160	0.540 and -0.215	
(eA ⁻³)		04410/C117 ED (* 1)	
Reflections collected / unique	34/44/6494 [R(int)	24419/6117 [R(int)	
	= 0.0501]	= 0.0269]	

Table 1: Crystal data and structure refinement of **3a** and **4a**.



Figure 1: ORTEP diagram of compound of **3a** with 50% ellipsoid probability.

Crystal structure determination of 3a

A suitable crystal of compound **3a** was obtained by slowly volatilizing a solution of **3a** in acetonitrile at ambient temperature. A crystal of **3a** was mounted on a cryo loop at a random orientation. The single crystal structure of the ligands as well as the compounds was determined using Bruker D8 Quest Eco X-ray diffractometer. Intensity data were collected at room temperature (RT) using monochromated (MoK α = 0.7107 Å) radiation. The program suite APEX3 (Version 2018.1) was used to integrate the frames, to perform absorption correction and to determine unit cell. The structures were solved with SHELXS and subsequent refinements were performed with SHELXL.³ All non-hydrogen atoms were refined anisotropically. The H atoms attached to the aromatic ring were introduced in the calculated positions and included in the refinement by riding on their respective parent C atoms.

Crystal Data for C₂₉H₃₂N₃O (M =438.58 g/mol): Monoclinic, space group $P2_1/n$ (no. 14), a = 11.0143(14) Å, b = 15.747(2) Å, c = 15.541(2) Å, $\beta = 104.578(4)^\circ$, V = 2608.6(6) Å³, Z = 4, T = 296(2) K, μ (Mo K α) = 0.068 mm-1, Dcalc = 1.117 mg/m³, 34744 reflections measured (2.587° $\leq 2\Theta \leq 28.327^\circ$), 6494 unique (Rint = 0.0501) which were used in all calculations. The final R1 was 0.0598 (I > 2σ (I)) and wR2 was 0.1487 (all data).

Crystal structure determination of 4a

A suitable crystal of compound **4a** was obtained by slowly volatilizing a solution of **4a** in acetonitrile at ambient temperature. A crystal of **4a** was mounted on a cryo loop at a random orientation. The single crystal structure of the ligands as well as the compounds was determined using Bruker D8 Quest Eco X-ray diffractometer. Intensity data were collected at room temperature (RT) using monochromated (MoK α = 0.7107 Å) radiation. The program suite APEX3 (Version 2018.1) was used to integrate the frames, to perform absorption correction and to determine unit cell. The structures were solved with SHELXS and subsequent refinements were performed with SHELXL.⁴ II non-hydrogen atoms were refined anisotropically. The H atoms attached to the aromatic ring were introduced in the calculated positions and included in the refinement by riding on their respective parent C atoms.

Crystal Data for C₂₉H₃₂N₃O (M =438.58 g/mol): Triclinic, space group *P*ī (no. 2), a = 11.8940(13) Å, b = 11.7007(13) Å, c = 31.479(3) Å, α = 80.990(2)°, β = 68.5320(10)°, γ = 81.497(2)°, V = 1237.33(11) Å³, Z = 2, T = 296(2) K, μ (Mo K α) = 0.072 mm-1, Dcalc = 1.177 mg/m³, 24419 reflections measured (2.671° ≤ 2 Θ ≤ 28.255°), 6117 unique (Rint = 0.0269) which were used in all calculations. The final R1 was 0.0566 (I > 2 σ (I)) and wR2 was 0.1460 (all data).



Figure 1: ORTEP diagram of compound of 4a with 50% ellipsoid probability.

References

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Spectroscopic Data

2,6-di-tert-butyl-4-(phenyl(4-phenyl-2H-1,2,3-triazol-2-yl)methyl)phenol (3a):

White solid; m.p. 167-169 °C; Yield – 74% (110 mg); $R_f = 0.8$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.30$ (s, 18H), 5.16 (s, 1H), 6.89 1H), 7.08 (s, 2H), 7.16 - 7.32 (m, 8H), 7.62 – 7.68 (m, 2H), 7.80 (s, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 68.4, 125.3, 125.9, 127.8, 128.1, 128.2,



6-di-tert-butyl-4-((4-(4-chlorophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)phenol (3b):

White semi solid; Yield – 81% (130 mg); $R_f = 0.6$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.34$ (s, 18H), 5.20 (s, 1H), 6.93 (s, 1H), 7.13 (s, 2H), 7.20 - 7.24 (m, 2H), 7.26 - 7.36 (m, 5H), 7.70 (s, 2H), 7.84 (s, 1H); ¹³C-NMR

 $(100 \text{ MHz}, \text{CDCl}_3); \delta = 30.1, 34.3, 72.8, 125.2, 127.1, 127.9, 128.1, 128.4, 128.8, 128.9, 129.0, 131.0, 134.0, 135.7, 139.3, 146.5, 153.6; HRMS (ESI): m/z calcd for C₂₉H₃₂ClN₃NaO [M+Na] 496.2131, found 496.2133$

2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)phenol (3c):

Pale yellow liquid; Yield – 74% (128 mg); $R_f = 0.7$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ (s, 18H), 5.25 (s, 1H), 6.97 (s, 1H), 7.15 (s, 2H), 7.23 - 7.27 (m, 2H), 7.29 - 7.38 (m, 3H), 7.47 (d, J = 8.3 Hz, 1H), 7.61 (dd, $J_I = 8.3$ Hz, $J_I = 2.1$ Hz, 1H), 7.88 (s, 1H), 7.90 (d, J = 1.9 Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 72.9, 125.0, 125.2, 127.7, 127.9, 128.0, 128.4, 128.6, 130.5, 130.7, 131.1, 132.1, 133.0, 135.7, 139.1

72.9, 125.0, 125.2, 127.7, 127.9, 128.0, 128.4, 128.6, 130.5, 130.7, 131.1, 132.1, 133.0, 135.7, 139.1, 145.4, 153.7; HRMS (ESI): m/z calcd for C₂₉H₃₁Cl₂N₃NaO [M+Na] 530.1741, found 530.1743.

2,6-di-tert-butyl-4-((4-(3-bromo-4-fluorophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)phenol (3d):

Semi solid; Yield – 72% (120 mg); $R_f = 0.5$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.52$ (s, 18H), 5.38 (s, 1H), 7.11 (s, 1H), 7.27 - 7.31 (m, 3H), 7.37 - 7.42 (m, 2H), 7.42 - 7.51 (m, 3H), 7.82 (dq, $J_1 = 8.6$ Hz, $J_2 = 2.2$ Hz, 1H), 7.99 (s, 1H), 8.14 (dd, $J_1 = 6.6$ Hz, $J_2 = 2.1$ Hz, 1H); ¹³C-NMR (100 MHz,

CDCl₃); δ = 30.1, 34.3, 72.9, 109.5 (d, *J* = 21.6 Hz), 116.7 (d, *J* = 22.5 Hz), 119.5, 125.2, 126.4 (d, *J* = 7.2 Hz), 127.9, 128.0, 128.2(d, *J* = 3.8 Hz), 128.4, 128.7, 130.9 (d, *J* = 3.3 Hz), 135.7, 139.2, 145.4, 153.7, 158.9 (d, *J* = 247.3 Hz); ¹⁹F-NMR (376 MHz, CDCl₃); δ = -107.6; HRMS (ESI): m/z calcd for C₂₉H₃₁BrFN₃NaO [M+Na] 558.1532, found 558.1537.

henol (3c):
$$00 \text{ MHz}$$
 CDCL):

Ph

N=





2,6-di-tert-butyl-4-((4-(3-nitrophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)phenol (3e):

Pale yellow solid; m.p. 140-142 °C; Yield – 70% (148 mg); $R_f = 0.8$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.41$ (s, 18H), 5.29 (s, 1H), 7.03 (s, 1H), 7.22 (s, 2H), 7.28 - 7.40 (m, 5H), 7.59 (t, J = 7.9 Hz, 1H), 8.01 (s, 1H), 8.11 -8.21 (m, 2H), 8.67 (s, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1, 34.3, 73.1,$

120.7, 122.8, 125.3, 128.0, 128.4, 128.5, 129.7, 131.3, 131.5, 132.3, 135.8, 139.0, 145.4, 148.6, 153.7; HRMS (ESI): m/z calcd for C₂₉H₃₂N₄NaO₃ [M+Na] 507.2371 found 507.2374.

2,6-di-tert-butyl-4-((4-(naphthalen-1-yl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)phenol (3f):

White semi solid; Yield – 85% (141 mg); $R_f = 0.6$ (5% in EtOAc/PE); ¹H-NMR $(400 \text{ MHz}, \text{CDCl}_3); \delta = 1.40 \text{ (s, 18H)}, 5.25 \text{ (s, 1H)}, 7.09 \text{ (s, 1H)}, 7.19 \text{ (s, 2H)}, 7.29 \text{ -}$ 7.40 (m, 5H), 7.46 - 7.55 (m, 3H), 7.70 (dd, $J_1 = 7.1$ Hz, $J_2 = 1.1$ Hz, 1H), 7.89 (dd, $J_1 = 9.5$ Hz, $J_2 = 2.9$ Hz, 2H), 7.95 (s, 1H), 8.35 - 8.50 (m, 1H); ¹³C-NMR (100)

MHz, CDCl₃); $\delta = 30.2, 34.3, 72.8, 125.2, 125.6, 125.9, 126.6, 127.2, 127.9, 128.0, 128.2, 128.4, 129.0, 128.2, 128.4, 128.4, 129.0, 128.2, 128.4, 129.0, 128.2, 128.4, 129.0, 128.2, 128.4$ 129.3, 131.0, 133.8, 134.0, 135.7, 139.3, 147.0, 153.6; HRMS (ESI): m/z calcd for C₃₃H₃₅N₃NaO [M+Na] 512.2677, found 512.2676

2,6-di-tert-butyl-4-((4-ethoxyphenyl)(4-phenyl-2H-1,2,3-triazol-2-yl)methyl)phenol (3g):

White solid; m.p. 120-122 °C; Yield – 85% (121 mg); $R_f = 0.7$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ -1.43 (m, 21H), 4.02 (q, J = 7.0 Hz, 2H), 5.22 (s, 1H), 6.87 (d, J = 8.7 Hz, 2H), 6.95 (s, 1H), 7.14 (s, 2H), 7.22 (d, J = 8.8 Hz, 2H), 7.33 (t, J = 7.4 Hz, 1H), 7.39 - 7.45 (m, 2H), 7.79 - 7.83 (m, 2H), 7.90 (s,

1H); 13 C-NMR (100 MHz, CDCl₃); $\delta = 14.7, 30.1, 34.3, 63.3, 72.2, 114.2, 124.9, 125.9, 128.2, 128.2, 128$ 128.2, 128.7, 129.4, 129.5, 130.5, 131.0, 131.3, 135.6, 147.4, 153.4, 158.5; HRMS (ESI): m/z calcd for C₃₁H₃₇N₃NaO₂ [M+Na] 506.2783, found 506.2782.

4-((3-bromophenyl)(4-phenyl-2H-1,2,3-triazol-2-yl)methyl)-2,6-di-tert-butylphenol (3s):

White solid; m.p. 158-160 °C; Yield – 78% (108 mg); $R_f = 0.8$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.37$ (s, 18H), 5.34 (s, 1H), 6.98 - 7.04 (m, 4H), 7.19 - 7.34 (m, 3H), 7.40 (t, J = 7.4 Hz, 2H), 7.46 (d, J = 7.9 Hz, 1H), 7.58 (s, 1H), 7.79 - 7.83 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.4, 67.9, 119.4,

122.8, 125.3, 125.7, 126.2, 127.6, 128.2, 128.8, 130.2, 130.4, 130.7, 131.3, 136.5, 141.0, 147.4, 154.2; HRMS (ESI): m/z calcd for C₂₉H₃₂BrN₃NaO [M+Na] 540.1626 found 540.1628.









2,6-di-tert-butyl-4-((4-nitrophenyl)(4-phenyl-2H-1,2,3-triazol-2-yl)methyl)phenol (3i):

Pale yellow solid; m.p. 182-184 °C; Yield – 72% (103 mg); $R_f = 0.6$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.49$ (s, 18H), 5.31 (s, 1H), 7.03 (s, 1H), 7.18 (s, 2H), 7.32 - 7.46 (m, 5H), 7.77 - 7.82 (m, 2H), 7.93 (s, 1H), 8.19 (dd, $J_I = 6.9$ Hz, $J_2 = 2.0$ Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 71.9,

123.6, 125.3, 125.9, 127.7, 128.6, 128.8, 128.9, 130.1, 131.5, 136.1, 146.7, 147.4, 148.1, 154.1; HRMS (ESI): m/z calcd for C₂₉H₃₂N₄NaO₃ [M+Na] 507.2371, found 507.2369.

4-((4-(4-(benzyloxy)phenyl)-2H-1,2,3-triazol-2-yl)(4-ethoxyphenyl)methyl)-2,6-di-tert-butylphenol (3j):

White solid; m.p. 140-142 °C; Yield – 87% (152 mg); $R_f = 0.8$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ (s, 18H), 1.39 - 1.42 (m, 3H), 4.02 (q, J = 7.0 Hz, 2H), 5.10 (s, 2H), 5.21 (s, 1H), 6.85 (d, J = 8.6 Hz,

2H), 6.91 (s, 1H), 7.02 (d, J = 8.6 Hz, 2H), 7.12 (s, 2H), 7.20 (d, J = 8.8 Hz, 2H), 7.30 - 7.46 (m, 5H), 7.72 (d, J = 8.6 Hz, 2H), 7.81 (s, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 14.7$, 30.1, 34.3, 63.4, 72.7, 72.8, 114.3, 122.6, 124.9, 126.2, 127.8, 128.8, 129.5, 130.0, 130.8, 131.0, 131.2, 131.9, 132.2, 135.8 144.4, 148.2, 153.6, 158.7; HRMS (ESI) m/z: calcd for C₃₈H₄₃N₃NaO₃ [M+Na] 612.3201, found 612.3205.

2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-2H-1,2,3-triazol-2-yl)(4-ethoxyphenyl)methyl)phenol (3k):

White solid; m.p. 89-71 °C; Yield – 81% (132 mg); $R_f = 0.7$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38 - 1.43$ (m, 21H), 4.02 (q, J = 7.0 Hz, 2H), 5.24 (s, 1H), 6.87 (d, J = 8.8 Hz, 2H), 6.93 (s, 1H), 7.12 (s, 2H), 7.20 (d, J = 8.8 Hz,



2H), 7.47 (d, J = 8.3 Hz, 1H), 7.61 (dd, $J_1 = 8.3$ Hz, $J_2 = 1.9$ Hz, 1H), 7.88 (s, 1H), 7.90 (d, J = 1.8 Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 14.7$, 30.1, 34.3, 63.4, 114.3, 124.9 125.0, 127.7, 129.1, 129.5, 130.6, 1307, 131.0, 131.1, 132.0, 133.0, 135.7, 145.3, 153.5, 158.6; HRMS (ESI): m/z calcd for C₃₁H₃₅Cl₂N₃NaO₂ [M+Na] 574.2003, found 574.2005.

4-((4-(3-bromo-4-fluorophenyl)-2H-1,2,3-triazol-2-yl)(3-bromophenyl)methyl)-2,6-di-tertbutylphenol (3l):

Yellow liquid; Yield – 78% (129 mg); $R_f = 0.6$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.35$ (s, 18H), 5.25 (s, 1H), 6.87 (s, 1H), 7.9 - 7.23 (m, 5H), 7.35 - 7.42 (m, 2H), 7.62 - 7.68 (m, 1H), 7.82 (s, 1H), 7.97 (s, 1H); ¹³C-NMR (100 MHz,



 $CDCl_3$); $\delta = 30.1$, 34.7, 72.2, 109.5 (d, J = 21.5 Hz), 116.8 (d, J = 22.5 Hz), 119.5, 122.5, 125.2, 126.4(d, J = 7.2 Hz), 126.7, 128.0, 129.9, 131.0, 131.1, 135.1, 135.1, 135.9, 141.9, 145.6, 153.9, 159.0



BnO

(d, J = 247.2 Hz), 189.2; HRMS (ESI): m/z calcd for $C_{29}H_{30}Br_2FN_3NaO$ [M+Na] 636.0637, found 636.0635.

2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-2H-1,2,3-triazol-2-yl)(4-nitrophenyl)methyl)phenol (3m):

White semi solid; Yield – 70% (114 mg); $R_f = 0.8$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.39$ (s, 18H), 5.33 (s, 1H), 7.02 (s, 1H), 7.16 (s, 2H), 7.38 (d, J = 8.6 Hz, 2H), 7.49 (d, J = 8.4 Hz, 1H), 7.61 (dd, $J_1 = 8.3$ Hz, $J_2 = 2.1$ Hz, 1H), 7.88 - 7.93 (m, 2H), 8.20 (d, J = 8.9 Hz, 2H); ¹³C-NMR (100

MHz, CDCl₃); $\delta = 30.1$, 34.4, 67.9, 119.4, 122.8, 125.3, 125.7, 126.2, 127.6, 128.2, 128.8, 130.2, 130.4, 130.7, 131.3, 136.5, 141.0, 147.4, 154.2; HRMS (ESI): m/z calcd for C₂₉H₃₀Cl₂N₄NaO₃ [M+Na] 575.1592, found 575.1593.

4-((4-(benzyloxy)phenyl)(4-(thiophen-2-yl)-2H-1,2,3-triazol-2-yl)methyl)-2,6-di-tert-butylphenol (3n):

Orange liquid; Yield – 80% (110 mg); $R_f = 0.7$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.42$ (s, 18H), 5.05 (s, 2H), 5.23 (s, 1H), 6.91 – 6.96 (m, 3H), 7.05 - 7.09 (m, 1H), 7.15 (s, , 2H), 7.21 (d, J = 8.8 Hz, 2H), 7.29 – 7.44 (m, 7H), 7.79 (s, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 69.9, 72.209,

114.6, 124.6, 125.0, 125.3, 127.4, 127.5, 127.9, 128.5, 129.1, 129.5, 130.8, 131.7, 132.8, 135.6, 136.8, 142.6, 153.5, 158.4; HRMS (ESI): m/z calcd for $C_{34}H_{37}N_3NaO_2S$ [M+Na] 574.2503, found 574.2502.

4-((4-bromo-5-(2-bromo-4-methoxyphenyl)-2H-1,2,3-triazol-2-yl)(thiophen-2-yl)methyl)-2,6-di-tertbutylphenol (30):

Yellow liquid; Yield – 75% (158 mg); $R_f = 0.6$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.42$ (s, 18H), 3.93 (s, 3H), 5.29 (s, 1H), 6.94 - 7.04 (m, 4H), 7.30 - 7.36 (m, 3H), 7.85 - 7.91 (m, 1H), 8.13 - 8.15 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.4, 56.2, 69.4, 111.5, 111.8, 119.4, 123.1, 124.9, 126.5,

126.6, 127.4, 127.5, 128.3, 132.2, 135.9, 141.7, 143.9, 154.0, 156.1; HRMS (ESI): m/z calcd for $C_{28}H_{31}$ Br₂N₃NaO₂S [M+Na] 654.0401, found 654.0402.

4-((5-bromo-4-phenyl-2H-1,2,3-triazol-2-yl)(phenyl)methyl)-2,6-di-tert-butylphenol (3p):

Colourless liquid; Yield – 82% (144 mg); $R_f = 0.6$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.30$ (s, 18H), 5.18 (s, 1H), 6.83 (s, 1H), 7.13 - 7.39 (m, 10H), 7.84 - 7.88 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 73. 6, 119.6, 125.4, 127.2, 128.0, 128.0, 128.4, 128.5, 128.6, 128.7, 129.2, 131.7, 135.8, 138.8,

145.2, 153.8; HRMS (ESI): m/z calcd for $C_{29}H_{32}BrN_3NaO$ [M+Na] 540.1626, found 540.1628



ОН

OBn



$\label{eq:constraint} 4-((4-brom o-5-phenyl-2H-1,2,3-triazol-2-yl)(thiophen-2-yl)methyl)-2, 6-di-tert-butylphenol~(3q):$

Yellow liquid; Yield – 77% (134 mg); $R_f = 0.7$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.45$ (s, 18H), 5.32 (s, 1H), 6.97 - 7.04 (m, 2H), 7.10 (s, 1H), 7.32 - 7.50 (m, 6H), 7.98 (d, J = 8.6 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.0$, 34.3, 69.3, 119.8, 124.8, 126.5, 126.5, 127.2, 127.5, 128.4,

128.7, 129.2, 131.7, 135.8, 141.7, 145.3, 154.0; HRMS (ESI): m/z calcd for C₂₇H₃₀ BrN₃NaOS [M+Na] 546.1190, found 546.1191.

2,6-di-tert-butyl-4-((4-(2-fluorophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)phenol (3r):

White solid; m.p. 138-140 °C; Yield – 74% (115 mg); $R_f = 0.6$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.31$ (s, 18H), 5.16 (s, 1H), 6.93 (s, 1H), 7.02 - 7.13 (m, 4H), 7.15 - 7.29 (m, 6H), 7.90 - 7.97 (m, 2H); ¹³C-NMR

(100 MHz, CDCl₃); δ = 30.1, 34.3, 72.8, 115.9 (d, *J* = 21.5 Hz), 118.5 (d, *J* = 12.5 Hz), 124.3, (d, *J* = 2.9 Hz), 125.3, 127.8, 128.1, 128.3, 128.9, 129.5, (d, *J* = 8.2 Hz), 133.8, 133.9, 135.7, 139.3, 142.0, 153.6, 159.9 (d, *J* = 248.7 Hz); ¹⁹F-NMR (376 MHz, CDCl₃); δ = -114.5; HRMS (ESI): m/z calcd for C₂₉H₃₂FN₃NaO [M+Na] 480.2426, found 480.2425.

$\label{eq:constraint} 4-((4-(4-bromophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)-2,6-di-tert-butylphenol~(3s):$

Yellow liquid; Yield – 80% (141 mg); $R_f = 0.6$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.32$ (s, 18H), 5.19 (s, 1H), 6.85 (s, 1H), 7.08 (s, 2H), 7.11 - 7.16 (m, 1H), 7.19 (s, 1H), 7.24 - 7.30 (m, 1H), 7.32 - 7.39 (m, 4H), 7.71

7.75 (m, 2H), 7.84 (s, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 72.0, 122.4, 125.3, 125.9, 126.7, 128.4, 128.8, 128.9, 131.0, 131.2, 131.3, 135.8, 141.7, 147.7, 153.8; HRMS (ESI): m/z calcd for C₂₉H₃₂BrN₃NaO [M+Na] 540.1626 found 540.1624.

(2-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (3t):

White semi solid; Yield – 73% (106 mg); $R_f = 0.6$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.31$ (s, 18H), 5.20 (s, 1H), 6.97 (s, 1H), 7.10 – 7.19 (m, 4H), 7.23 - 7.30 (m, 3H), 7.40 (t, J = 7.7 Hz, 2H), 7.49 - 7.55 (m, 1H), 8.21 - 8.23 (m, 3H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 73.5, 125.4,

127.9, 127.9, 128.1, 128.3, 128.5, 130.3, 133.2, 135.9, 136.6, 137.6, 138.8, 146.4, 153.9, 185.6; HRMS (ESI): m/z calcd for C₃₀H₃₃N₃NaO₂ [M+Na] 490.2470, found 490.2472.





OH



(2-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-2H-1,2,3-triazol-4*vl)(phenvl)methanone (3u):*

White semi solid; Yield – 72% (105 mg); $R_f = 0.6$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); δ 1.59 (s, 18H), 5.49 (s, 1H), 7.39 - 7.45 (m, 4H), 7.49 - 7.57 (m, 3H), 7.63 - 7.69 (m, 2H), 7.78 (t, J = 7.4 Hz, 1H), 8.46 - 8.50 (m, 3H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1, 34.3, 73.5, 125.4, 127.8, 128.0, 128.2, 128.4,$

130.3, 133.1, 135.9, 136.6, 137.6, 138.8, 146.4, 153.8, 185.6; HRMS (ESI): m/z calcd for C₃₀H₃₂ BrN₃NaO₂ [M+Na] 568.1575, found 568.1577.

2,6-di-tert-butyl-4-(phenyl(4-phenyl-1H-1,2,3-triazol-1-yl)methyl)phenol (4a):

White solid; m.p. 164-166 °C; Yield – 78% (116 mg); $R_f = 0.6$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ (s, 18H), 5.32 (s, 1H), 7.01 (s, 2H), 7.06 (s, 1H), 7.14 (d, J = 7.9 Hz, 2H), 7.29 - 7.43 (m, 6H), 7.61 (s, 1H), 7.79 - 7.85 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3,72.7 125.3,

OH Ρĥ

125.9, 127.8, 128.1, 128.2, 128.3, 128.7, 129.0, 130.5, 131.0, 135.6, 139.4, 147.5, 153.6; HRMS (ESI): m/z calcd for C₂₉H₃₃N₃NaO [M+Na] 462.2521, found 462.2523

2,6-di-tert-butyl-4-((4-(4-chlorophenyl)-1H-1,2,3-triazol-1-yl)(phenyl)methyl)phenol (4b):

White solid; m.p. 190-192 °C; Yield – 81% (130 mg); $R_f = 0.5$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.37$ (s, 19H), 5.32 (s, 1H), 6.99 (s, 2H), 7.05 (s, 1H), 7.13 (d, *J* = 7.3 Hz, 2H), 7.35 - 7.39 (m, 5H), 7.60

(s, 1H), 7.75 (dd, J = 8.3, 1.3 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 68.5, 119.5, 125.2, 126.9, 127.7, 128.2, 128.7, 128.9, 129.2, 133.7, 136.3, 138.6, 146.3, 154.0; HRMS (ESI): m/z calcd for C₂₉H₃₂ClN₃NaO [M+Na] 496.2131, found 496.2133.

2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-1H-1,2,3-triazol-1-yl)(phenyl)methyl)phenol (4c):

White solid; m.p. 180-182 °C; Yield – 76% (131 mg); $R_f = 0.5$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.37$ (s, 18H), 5.33 (s, 1H), 6.98 (s, 2H), 7.05 (s, 1H), 7.11 - 7.15 (m, 2H), 7.34 - 7.41 (m, 3H), 7.46 (d, J = 8.3 Hz, 1H), 7.61 (s, 1H), 7.67 (dd, $J_1 = 8.3$ Hz, $J_2 =$

1.9 Hz, 1H), 7.91 (d, J = 1.9 Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1, 34.3, 68.6, 119.9, 124.8,$ 125.1, 127.4, 127.7, 128.1, 128.3, 128.7, 130.7, 131.8, 132.9, 136.3, 138.4, 145.2, 154.0; HRMS (ESI): m/z calcd for C₂₉H₃₁Cl₂N₃NaO [M+Na] 530.1741, found 530.1744.



N=N



2,6-di-tert-butyl-4-((4-(3-bromo-4-fluorophenyl)-1H-1,2,3-triazol-1-yl)(phenyl)methyl)phenol (4d):

White solid; m.p. 198-200 °C; Yield – 73% (122 mg); $R_f = 0.5$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.37$ (s, 18H), 5.32 (s, 1H), 6.98 (s, 2H), 7.05 (s, 1H), 7.10 - 7.18 (m, 3H), 7.32 - 7.41 (m, 3H), 7.57 (s, 1H), 7.74 (dq, $J_I = 8.6$ Hz, $J_2 = 2.2$ Hz, 1H), 8.01 (dd, $J_I =$

6.6 Hz, $J_2 = 2.1$ Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 68.6, 109.4 (d, J = 21.1 Hz), 116.7, 119.5, 125.1, 126.2(d, J = 22.6 Hz), 127.6, 128.2, 128.3, 128.4, 128.7, 130.6, 136.3, 138.5, 145.2, 154.0, 158.7(d, J = 247.2 Hz); HRMS (ESI): m/z calcd for C₂₉H₃₁BrFN₃NaO [M+Na] 558.1532, found 558.1535.

2,6-di-tert-butyl-4-((4-(3-nitrophenyl)-1H-1,2,3-triazol-1-yl)(phenyl)methyl)phenol (4e):

Pale yellow solid; m.p. 138-140 °C; Yield – 71% (117 mg); $R_f = 0.7$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.41$ (s, 18H), 5.33 (s, 1H), 6.99 (s, 2H), 7.08 (s, 1H), 7.13 - 7.17 (m, 2H), 7.26 (s, 1H), 7.38 (d, J = 7.3 Hz, 2H), 7.60 (t, J = 8.0 Hz, 1H), 7.72 (s, 1H),

8.16 (dq, J_1 = 8.2 Hz, J_2 = 1.1 Hz, 1H), 8.24 - 8.28 (m, 1H), 8.56 (t, J = 1.8 Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃); δ = 30.1, 34.3, 68.7, 120.3, 120.4, 122.6, 125.1, 127.7, 128.0, 128.4, 128.8, 129.8, 131.5, 132.5, 136.4, 138.3, 145.2, 148.5, 154.1; HRMS (ESI): m/z calcd for C₂₉H₃₂N₄NaO₃ [M+Na] 507.2371, found 507.2372.

4-((3-bromophenyl)(4-phenyl-1H-1,2,3-triazol-1-yl)methyl)-2,6-di-tert-butylphenol (4f):

White solid; m.p. 170-172 °C; Yield – 76% (106 mg); $R_f = 0.6$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ (s, 18H), 5.36 (s, 1H), 7.00 - 7.06 (m, 4H), 7.21 - 7.27 (m, 1H), 7.30 (d, J = 5.8 Hz, 1H), 7.33 (d, J = 7.2 Hz, 1H), 7.41 (t, J = 7.4 Hz, 2H), 7.48 (d, J = 8.7 Hz, 1H), 7.59 (s, 1H), 7.80 - 7.84

(m, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 67.8, 119.4, 122.8, 125.3, 125.7, 126.2, 127.6, 128.1, 128.7, 130.2, 130.5, 130.6, 131.3, 136.5, 141.1, 147.5, 154.2; HRMS (ESI): m/z calcd for C₂₉H₃₂BrN₃NaO [M+Na] 540.1626 found 540.1625

2,6-di-tert-butyl-4-((4-nitrophenyl)(4-phenyl-1H-1,2,3-triazol-1-yl)methyl)phenol (4g):

Yellow solid; m.p. 180-182 °C; Yield – 65% (93 mg); $R_f = 0.4$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ (s, 18H), 5.41 (s, 1H), 7.02 (s, 2H), 7.08 (s, 1H), 7.23 - 7.27 (m, 2H), 7.30 - 7.36 (m, 1H), 7.41 (t, J = 7.5 Hz, 2H), 7.61 (s, 1H), 7.79 - 7.83 (m, 2H), 8.21 (dd, $J_I = 6.9$ Hz, $J_2 = 1.8$ Hz, 2H); ¹³C-

NMR (100 MHz, CDCl₃); δ = 30.0, 34.4, 67.8, 76.6, 119.4, 123.8, 125.5, 125.7, 126.9, 128.3, 128.8,



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130.2, 136.8, 146.1, 147.5, 147.7, 154.5; HRMS (ESI): m/z calcd for C₂₉H₃₂N₄NaO₃ [M+Na] 507.2372 found 507.2375.

2,6-di-tert-butyl-4-((4-(naphthalen-1-yl)-1H-1,2,3-triazol-1-yl)(phenyl)methyl)phenol (4h):

Pale yellow liquid; Yield – 74% (123 mg); $R_f = 0.6$ (20% in EtOAc/PE); ¹H-NMR $(400 \text{ MHz}, \text{CDCl}_3); \delta = 1.41 \text{ (s, 18H)}, 5.36 \text{ (s, 1H)}, 7.07 \text{ (s, 2H)}, 7.18 \text{ (s, 1H)}, 7.23 \text{ -}$ 7.27 (m, 2H), 7.36 - 7.44 (m, 3H), 7.48 - 7.55 (m, 3H), 7.70 - 7.75 (m, 2H), 7.86 -7.90 (m, 2H), 8.37 (dd, $J_1 = 6.3$ Hz, $J_2 = 3.4$ Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃);

 $\delta = 30.1, 34.3, 68.6, 109.3, 109.5, 116.6, 116.8, 119.5, 125.1, 126.1, 126.3, 127.6, 128.2, 128.3, 128.4, 109.5, 126.1,$ 128.7, 130.6, 136.3, 138.5, 145.2, 154.0, 157.5, 159.9; HRMS (ESI): m/z calcd for C₃₃H₃₅N₃NaO [M+Na] 512.2677, found 512.2678.

4-((3-bromophenyl)(4-(naphthalen-1-yl)-1H-1,2,3-triazol-1-yl)methyl)-2,6-di-tert-butylphenol (4i):

Yellow liquid; Yield – 71% (108 mg); $R_f = 0.6$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.40$ (s, 18H), 5.29 (s, 1H), 7.04 (s, 2H), 7.08 - 7.15 (m, 2H), 7.27 (d, J = 4.7 Hz, 1H), 7.38 (s, 1H), 7.48 - 7.55 (m, 4H), 7.66 - 7.74 (m, 2H), 7.84 7.94 (m, 2H), 8.30 - 8.35 (m, 1H)¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1, 34.4,$

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67.9, 76.6, 122.5, 122.9, 124.9, 125.1, 125.2, 125.9, 126.4, 126.5, 127.2, 127.8, 128.0, 128.4, 128.9, 130.3, 130.9, 131.1, 131.4, 133.8, 136.5, 141.1, 146.6, 154.2; HRMS (ESI): m/z calcd for C₃₃H₃₄BrN₃NaO [M+Na] 590.1782, found 590.1780.

4-((4-(3-bromo-4-fluorophenyl)-1H-1,2,3-triazol-1-yl)(3-bromophenyl)methyl)-2,6-di-tert-butylphenol (4j):

Yellow liquid; Yield – 70% (115 mg); $R_f = 0.5$ (10% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.31$ (s, 18H), 5.22 (s, 1H), 6.91 (s, 3H), 6.95 (d, J =7.8 Hz, 1H), 7.08 (t, J = 8.5 Hz, 1H), 7.14 - 7.22 (m, 2H), 7.41 (d, J = 9.8 Hz, 1H), 7.49 (s, 1H), 7.67 (dq, $J_1 = 8.6$ Hz, $J_2 = 2.3$ Hz, 1H), 7.94 (dd, $J_1 = 6.6$



2,6-di-tert-butyl-4-((4-(2-fluorophenyl)-1H-1,2,3-triazol-1-yl)(phenyl)methyl)phenol (4k):

Yellow liquid; Yield – 73% (113 mg); $R_f = 0.7$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ (s, 18H), 5.30 (s, 1H), 7.03 - 7.17 (m, 6H), 7.25 -7.39 (m, 5H), 7.84 - 7.81 (m, 1H), 8.33 (t, J = 7.5 Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 68.6, 115.5 (d, J = 21.5 Hz), 118.6 (d, J = 13 Hz), 122.7, (d, J = 13 Hz),



124.5, 125.2, 127.6, 127.8, 128.2, 128.3, 128.7, 129.2, (d, *J* = 8.2 Hz), 136.3, 138.7, 140.7, 153.9, 159.1 (d, J = 246.2 Hz); ¹⁹F-NMR (376 MHz, CDCl₃); $\delta = -114.54$; HRMS (ESI): m/z calcd for C₂₉H₃₂FN₃NaO [M+Na] 480.2426, found 480.2427.

2,6-di-tert-butyl-4-((4-phenyl-1H-1,2,3-triazol-1-yl)(thiophen-2-yl)methyl)phenol (4l):

Pale yellow liquid; Yield – 79% (117 mg); $R_f = 0.6$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.42$ (s, 18H), 5.27 (s, 1H), 6.96 - 7.01 (m, 2H), 7.17 (s, 1H), 7.31 - 7.38 (m, 4H), 7.43 (t, J = 7.3 Hz, 2H), 7.81 - 7.85 (m, 2H), 7.92 (s, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.1$, 34.3, 68.4, 124.7, 125.9,

126.3, 126.4, 127.3, 128.3, 128.7, 129.1, 130.4, 131.2, 135.7, 142.4, 147.6, 153.8; HRMS (ESI): m/z calcd for C₂₇H₃₁N₃NaOS [M+Na] 468.2085, found 468.2081.

(1-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (4m):

White solid; m.p. 128-130 C; Yield – 72% (114 mg); $R_f = 0.6$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.38$ (s, 18H), 5.32 (s, 1H), 6.98 (s, 2H), 7.08 - 7.13 (m, 3H), 7.34 - 7.41 (m, 3H), 7.51 (t, J = 7.7 Hz, 2H), 7.61

 $(t, J = 7.3 \text{ Hz}, 1\text{H}), 8.12 (s, 1\text{H}), 8.44 - 8.48 (m, 2\text{H}); {}^{13}\text{C-NMR} (100 \text{ MHz}, \text{CDCl}_3); \delta = 30.1, 34.4, 68.8,$ 125.2, 127.5, 127.7, 128.3, 128.4, 128.5, 128.8, 130.6, 133.2, 136.5, 138.0, 147.5, 154.2, 185.6; HRMS (ESI): m/z calcd for C₃₀H₃₃N₃NaO₂ [M+Na] 490.2470, found 490.2471

(1-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-1H-1,2,3-triazol-4yl)(phenyl)methanone (4n):

White semi solid; Yield – 70% (102 mg); $R_f = 0.6$ (20% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.37$ (s, 18H), 5.34 (s, 1H), 6.97 (s, 2H), 7.08 – 7.13 (m, 3H), 7.33 - 7.40 (m, 2H), 7.52 (t, J = 7.7 Hz, 2H), 7.61 (t, J = 7.4 Hz,

1H), 8.12 (s, 1H), 8.45 (d, J = 7.8 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.0, 34.3, 68.7, 125.2,$ 125.4, 127.5, 127.7, 127.8, 128.3, 128.4, 128.8, 130.3, 130.6, 133.2, 136.5, 138.0, 147.5, 154.2, 185.8; HRMS (ESI): m/z calcd for C₃₀H₃₂BrN₃NaO₂ [M+Na] 568.1575, found 568.1578.

1-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)indoline-2,3-dione (6a):

Orange solid; m.p. 218-220 C; Yield – 94% (140 mg); $R_f = 0.4$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.28$ (s, 18H), 5.19 (s, 1H), 6.42 (d, J = 8.1 Hz, 1H), 6.82 (s, 1H), 6.93 - 6.99 (m, 1H), 7.05 (s, 2H), 7.20 - 7.31 (m, 6H), 7.54 (dd, $J_1 = 7.4$ Hz, $J_2 = 1.1$ Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 29.1, 33.3, 58.1, 76.1, 112.8,$







N=N



117.1, 122.3, 124.2, 125.9, 126.9, 127.1, 127.6, 135.1, 136.4, 149.8, 152.6, 157.4, 182.4; HRMS (ESI): m/z calcd for C₂₉H₃₁NNaO₃ [M+Na] 464.2201, found 464.2205.

2,6-di-tert-butyl-4-(morpholino(phenyl)methyl)phenol(6b):

Pale yellow solid; m.p.126 C; Yield – 92% (118 mg); $R_f = 0.3$ (5% in EtOAc/PE); ¹H-NMR (400 MHz, CDCl₃); $\delta = 1.36$ (18H), 2.34 (dd, $J_1 = 8.7$ Hz, $J_2 = 4.9$ Hz, 4H), 3.70 (dd, $J_1 = 8.3$ Hz, $J_2 = 4.6$ Hz, 4H), 5.04 (s, 1H), 7.18 (s, 1H), 7.26 (dd, $J_1 = 1.9$

Hz, $J_2 = 1.3$ Hz, 5H), 7.40 - 7.44 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃); $\delta = 30.3$,



34.2, 52.5, 67.2, 77.2, 124.4 126.6, 127.9, 128.3, 132.4, 135.6, 143.1, 152.6; HRMS (ESI): m/z calcd for C₂₅H₃₅NNaO₂ [M+Na] 404.2565, found 404.2568

¹H and ¹³C NMR Spectra



Fig. 1: ¹H NMR spectrum of 2,6-di-tert-butyl-4-(phenyl(4-phenyl-2H-1,2,3-triazol-2yl)methyl)phenol (3a)



Fig. 2: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-(phenyl(4-phenyl-2H-1,2,3-triazol-2yl)methyl)phenol (3a)



Fig. 3: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(4-chlorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3b)



Fig. 4: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-(4-chlorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3b)



Fig. 5: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-2H-1,2,3-triazol-2-



Fig. 6: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3,4-*dichlorophenyl*)-2H-1,2,3-*triazol*-2yl)(phenyl)methyl)phenol (3c)



Fig. 7: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(3-bromo-4-fluorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3d)



Fig. 8: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-(3-bromo-4-fluorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3d)



Fig. 9: ¹⁹F NMR spectrum of 2,6-di-tert-butyl-4-((4-(3-bromo-4-fluorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3d)



Fig. 10: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(3-nitrophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3e)



Fig. 11: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3-nitrophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3e)



Fig. 12: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(naphthalen-1-yl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3f)



Fig. 13: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(naphthalen-1-yl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3f)



Fig. 14: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-ethoxyphenyl)(4-phenyl-2H-1,2,3-triazol-2yl)methyl)phenol (3g)



Fig. 15: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-ethoxyphenyl)(4-phenyl-2H-1,2,3-triazol-2yl)methyl)phenol (3g)



Fig. 16: ¹H NMR spectrum of 4-((3-bromophenyl)(4-phenyl-2H-1,2,3-triazol-2-yl)methyl)-2,6-ditert-butylphenol (3h)



Fig. 17: ¹³C NMR spectrum of 4-((3-bromophenyl)(4-phenyl-2H-1,2,3-triazol-2-yl)methyl)-2,6-ditert-butylphenol (3h)



Fig. 18: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-nitrophenyl)(4-phenyl-2H-1,2,3-triazol-2yl)methyl)phenol (3i)



Fig. 19: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-*nitrophenyl*)(4-*phenyl*-2H-1,2,3-*triazol*-2yl)methyl)phenol (3i)



Fig. 20: ¹H NMR spectrum of 4-((4-(benzyloxy)phenyl)-2H-1,2,3-triazol-2-yl)(4ethoxyphenyl)methyl)-2,6-di-tert-butylphenol (3j)



Fig. 21: ¹³C NMR spectrum of 4-((4-(benzyloxy)phenyl)-2H-1,2,3-triazol-2-yl)(4ethoxyphenyl)methyl)-2,6-di-tert-butylphenol (3j)



Fig. 22: ¹H NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3,4-*dichlorophenyl*)-2H-1,2,3-*triazol*-2-yl)(4ethoxyphenyl)methyl)phenol (3k)



Fig. 23: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-2H-1,2,3-triazol-2-yl)(4ethoxyphenyl)methyl)phenol (3k)



Fig. 24: ¹H NMR spectrum of 4-((4-(5-bromo-4-fluorophenyl)-2H-1,2,3-triazol-2-yl)(3bromophenyl)methyl)-2,6-di-tert-butylphenol (3l)



Fig. 25: ¹³C NMR spectrum of 4-((4-(3-bromo-4-fluorophenyl)-2H-1,2,3-triazol-2-yl)(3-

bromophenyl)methyl)-2,6-di-tert-butylphenol (3l)



Fig. 26: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-2H-1,2,3-triazol-2-yl)(4nitrophenyl)methyl)phenol (3m)



Fig. 27: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3,4-*dichlorophenyl*)-2H-1,2,3-*triazol*-2-yl)(4nitrophenyl)methyl)phenol (3m)



Fig. 28: ¹H NMR spectrum of *4-((4-(benzyloxy)phenyl)(4-(thiophen-2-yl)-2H-1,2,3-triazol-2-yl)methyl)-2,6-di-tert-butylphenol (3n)*



Fig. 29: ¹³C NMR spectrum of 4-((4-(benzyloxy)phenyl)(4-(thiophen-2-yl)-2H-1,2,3-triazol-2yl)methyl)-2,6-di-tert-butylphenol (3n)



Fig. 30: ¹H NMR spectrum of 4-((2-bromo-4-methoxyphenyl)(4-bromo-5-(thiophen-2-yl)-2H-1,2,3triazol-2-yl)methyl)-2,6-di-tert-butylphenol (30)



Fig. 31: ¹³C NMR spectrum of 4-((2-bromo-4-methoxyphenyl)(4-bromo-5-(thiophen-2-yl)-2H-1,2,3triazol-2-yl)methyl)-2,6-di-tert-butylphenol (30)



Fig. 32: ¹H NMR spectrum of 4-((4-bromo-5-phenyl-2H-1,2,3-triazol-2-yl)(phenyl)methyl)-2,6-ditert-butylphenol (3p)



Fig. 33: ¹³C NMR spectrum of 4-((4-bromo-5-phenyl-2H-1,2,3-triazol-2-yl)(phenyl)methyl)-2,6-ditert-butylphenol (3p)



Fig. 34: ¹H NMR spectrum of *4-((4-bromo-5-phenyl-2H-1,2,3-triazol-2-yl)(thiophen-2-yl)methyl)-*2,6-di-tert-butylphenol (3q)



Fig. 35: ¹³C NMR spectrum of 4-((4-bromo-5-phenyl-2H-1,2,3-triazol-2-yl)(thiophen-2-yl)methyl)-2,6-di-tert-butylphenol (3q)



Fig. 36: ¹H NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(2-fluorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3r)



Fig. 37: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-(2-fluorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3r)



Fig. 38: ¹⁹F NMR spectrum of 2,6-di-tert-butyl-4-((4-(2-fluorophenyl)-2H-1,2,3-triazol-2yl)(phenyl)methyl)phenol (3r)



Fig. 39: ¹H NMR spectrum of 4-((4-(4-bromophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)-2,6-di-

tert-butylphenol (3s)



Fig. 40: ¹³C NMR spectrum of 4-((4-(4-bromophenyl)-2H-1,2,3-triazol-2-yl)(phenyl)methyl)-2,6-ditert-butylphenol (3s)



Fig. 41: ¹H NMR spectrum of (2-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-2H-1,2,3triazol-4-yl)(phenyl)methanone (3t)



Fig. 42: ¹³C NMR spectrum of (2-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-2H-1,2,3triazol-4-yl)(phenyl)methanone (3t)



Fig. 43: ¹H NMR spectrum of (2-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (3u)



Fig. 44: ¹³C NMR spectrum of (2-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (3u)



Fig. 45: ¹H NMR spectrum of 2,6-di-tert-butyl-4-(phenyl(4-phenyl-1H-1,2,3-triazol-1-

yl)methyl)phenol (4a)



Fig. 46: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-(phenyl(4-phenyl-1H-1,2,3-triazol-1yl)methyl)phenol (4a)



Fig. 47: ¹H NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(4-chlorophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4b)



Fig. 48: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(4-chlorophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4b)



Fig. 49: ¹H NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3,4-*dichlorophenyl*)-1H-1,2,3-*triazol*-1yl)(phenyl)methyl)phenol (4c)



Fig. 50: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-(3,4-dichlorophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4c)



Fig. 51: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(3-bromo-4-fluorophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4d)



Fig. 52: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3-bromo-4-fluorophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4d)



Fig. 53: ¹H NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3-nitrophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4e)



Fig. 54: ¹³C NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(3-nitrophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4e)



Fig. 55: ¹H NMR spectrum of 4-((3-bromophenyl)(4-phenyl-1H-1,2,3-triazol-1-yl)methyl)-2,6-di-

tert-butylphenol (4f)



Fig. 56: ¹³C NMR spectrum of 4-((3-bromophenyl)(4-phenyl-1H-1,2,3-triazol-1-yl)methyl)-2,6-ditert-butylphenol (4f)



Fig. 57: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-nitrophenyl)(4-phenyl-1H-1,2,3-triazol-1-

yl)methyl)phenol (4g)



Fig. 58: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-nitrophenyl)(4-phenyl-1H-1,2,3-triazol-1yl)methyl)phenol (4g)



Fig. 59: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-(naphthalen-1-yl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4h)



Fig. 60: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-(naphthalen-1-yl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4h)



Fig. 61: ¹H NMR spectrum of 4-((3-bromophenyl)(4-(naphthalen-1-yl)-1H-1,2,3-triazol-1yl)methyl)-2,6-di-tert-butylphenol (4i)



Fig. 62: ¹³C NMR spectrum of 4-((3-bromophenyl)(4-(naphthalen-1-yl)-1H-1,2,3-triazol-1yl)methyl)-2,6-di-tert-butylphenol (4i)



Fig. 63: ¹H NMR spectrum of 4-((4-(3-bromo-4-fluorophenyl)-1H-1,2,3-triazol-1-yl)(3bromophenyl)methyl)-2,6-di-tert-butylphenol (4j)



Fig. 64: ¹³C NMR spectrum of 4-((4-(3-bromo-4-fluorophenyl)-1H-1,2,3-triazol-1-yl)(3bromophenyl)methyl)-2,6-di-tert-butylphenol (4j)



Fig. 65: ¹H NMR spectrum of 2,6-*di-tert-butyl*-4-((4-(2-fluorophenyl)-1H-1,2,3-triazol-1yl)(phenyl)methyl)phenol (4k)



Fig. 66: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-(2-fluorophenyl)-1H-1,2,3-triazol-1-

yl)(phenyl)methyl)phenol (4k)



Fig. 67: ¹⁹F NMR spectrum of 2,6-di-tert-butyl-4-((4-(2-fluorophenyl)-1H-1,2,3-triazol-1-



Fig. 68: ¹H NMR spectrum of 2,6-di-tert-butyl-4-((4-phenyl-1H-1,2,3-triazol-1-yl)(thiophen-2yl)methyl)phenol (4l)



Fig. 69: ¹³C NMR spectrum of 2,6-di-tert-butyl-4-((4-phenyl-1H-1,2,3-triazol-1-yl)(thiophen-2yl)methyl)phenol (4l)



Fig. 70: ¹H NMR spectrum of (1-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-1H-1,2,3triazol-4-yl)(phenyl)methanone (4m)



Fig. 71: ¹³C NMR spectrum of (1-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)-1H-1,2,3triazol-4-yl)(phenyl)methanone (4m)



Fig. 72: ¹H NMR spectrum of (1-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (4n)



Fig. 73: ¹³C NMR spectrum of (1-((3-bromophenyl)(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (4n)



Fig. 74: ¹H NMR spectrum of *1-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)indoline-2,3dione (6a)*



Fig. 75: ¹³C NMR spectrum of 1-((3,5-di-tert-butyl-4-hydroxyphenyl)(phenyl)methyl)indoline-2,3dione (6a)



Fig. 76: ¹H NMR spectrum 2,6-di-tert-butyl-4-(morpholino(phenyl)methyl)phenol (6b)



Fig. 77: ¹³C NMR spectrum 2,6-di-tert-butyl-4-(morpholino(phenyl)methyl)phenol (6b)