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Supporting information for article:

Structural verification of a tetrahydrotetrazole compound

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S1. Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: *ShelXS* (Sheldrick, 2015); program(s) used to refine structure: *shelXle* (Hübschle *et al.*, 2011) and *Olex2* (Dolomanov *et al.*, 2009); molecular graphics: *Olex2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *Olex2* (Dolomanov *et al.*, 2009).

S2. 1,2-bis(1,1-dimethylethyl)-3-phenyl-tetrazolo[5,1-a]isoquinoline-1,2(3H,10bH)-dicarboxylic acid

Crystal data

$C_{25}H_{30}N_4O_4$
M_r = 450.53
Monoclinic, $P2_1/c$
a = 9.2613 (19) Å
b = 10.882 (2) Å
c = 23.583 (5) Å
β = 95.54 (3) °
V = 2365.7 (8) Å^3
Z = 4
$F(000)$ = 960.0
D_x = 1.265 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 79687 reflections
θ = 1.731 – 49.236 °
μ = 0.087 mm^{-1}
T = 90.0 (3) K
Block, colourless
0.544 × 0.329 × 0.277 mm

Data collection

Rigaku XtaLAB Synergy-S, Dualflex, HyPix-6000HE diffractometer
Detector resolution: 100 μm × 100 μm pixel size
ω-scans
Absorption correction: gaussian (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min} = 0.372, T_{max} = 1.000
183544 measured reflections
24326 independent reflections
reflections with $I > 2\sigma(I)$
R_{int} = 0.0355
θ_{max} = 1.735°, θ_{min} = 49.836°
h = -19 → 19
k = -21 → 23
l = -45 → 50

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.0419
Hydrogen site location: difference Fourier map
H-atom coordinates and isotropic

$wR(F^2)$ = 0.1159
S = 1.035
24326 reflections
418 parameters
0 restraints
displacement parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.2083P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = -0.25 e Å^{-3}

S3. Geometry.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates, isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}^* / U_{eq}
O(1)	0.27581 (3)	0.73921 (3)	0.78541 (2)	0.01366 (4)
O(2)	0.42718 (3)	0.60049 (3)	0.83311 (2)	0.01571 (5)
O(3)	0.31619 (3)	0.67435 (3)	0.96733 (2)	0.01277 (4)
O(4)	0.20284 (4)	0.49959 (3)	0.99317 (2)	0.01693 (5)
N(1)	0.02413 (3)	0.52644 (3)	0.82967 (2)	0.01196 (4)
N(2)	0.05946 (3)	0.65338 (3)	0.83777 (2)	0.01109 (4)
N(3)	0.20532 (3)	0.65133 (3)	0.86364 (2)	0.01050 (4)
N(4)	0.21584 (3)	0.54738 (3)	0.89982 (2)	0.01086 (4)
C(1)	0.06390 (4)	0.48733 (4)	0.77611 (2)	0.01436 (5)
C(2)	0.12033 (4)	0.37654 (4)	0.76764 (2)	0.01607 (6)
C(3)	0.15273 (4)	0.29276 (3)	0.81520 (2)	0.01501 (5)
C(4)	0.20068 (5)	0.17264 (4)	0.80703 (2)	0.01941 (7)
C(5)	0.22737 (5)	0.09330 (4)	0.85290 (2)	0.02194 (7)
C(6)	0.20595 (5)	0.13303 (4)	0.90772 (2)	0.02048 (7)
C(7)	0.15994 (4)	0.25292 (3)	0.91666 (2)	0.01655 (6)
C(8)	0.13412 (4)	0.33298 (3)	0.87069 (2)	0.01338 (5)
C(9)	0.09017 (4)	0.46394 (3)	0.88103 (2)	0.01160 (4)

C(10)	-0.03570 (4)	0.71725 (3)	0.87237 (2)	0.01151 (4)
C(11)	-0.17551 (4)	0.67480 (4)	0.87762 (2)	0.01539 (5)
C(12)	-0.27025 (5)	0.74630 (4)	0.90630 (2)	0.01872 (6)
C(13)	-0.22630 (5)	0.85958 (4)	0.92885 (2)	0.02054 (7)
C(14)	-0.08583 (5)	0.90087 (4)	0.92372 (2)	0.02242 (8)
C(15)	0.00991 (5)	0.82997 (4)	0.89583 (2)	0.01805 (6)
C(16)	0.31477 (4)	0.65636 (3)	0.82525 (2)	0.01128 (4)
C(17)	0.37557 (4)	0.77151 (3)	0.74242 (2)	0.01410 (5)
C(18)	0.29049 (5)	0.86999 (4)	0.70787 (2)	0.02097 (7)
C(19)	0.51594 (5)	0.82367 (5)	0.77147 (2)	0.02137 (7)
C(20)	0.40079 (6)	0.65914 (4)	0.70642 (2)	0.02022 (7)
C(21)	0.24080 (4)	0.57102 (3)	0.95807 (2)	0.01159 (4)
C(22)	0.35314 (4)	0.71857 (3)	1.02605 (2)	0.01257 (5)
C(23)	0.21485 (5)	0.73970 (5)	1.05462 (2)	0.02044 (7)
C(24)	0.42713 (5)	0.84033 (4)	1.01594 (2)	0.01948 (6)
C(25)	0.45844 (5)	0.62985 (4)	1.05809 (2)	0.01855 (6)
H(1)	0.0390 (9)	0.5467 (8)	0.7462 (4)	0.0192 (18)*
H(2)	0.1349 (10)	0.3516 (8)	0.7285 (4)	0.024 (2)*
H(4)	0.2127 (11)	0.1439 (9)	0.7668 (4)	0.030 (2)*
H(5)	0.2610 (11)	0.0096 (9)	0.8470 (4)	0.032 (2)*
H(6)	0.2238 (11)	0.0772 (10)	0.9406 (4)	0.033 (2)*
H(7)	0.1493 (10)	0.2814 (8)	0.9553 (4)	0.0203 (18)*
H(9)	0.0233 (8)	0.4678 (7)	0.9109 (3)	0.0129 (15)*
H(11)	-0.2052 (10)	0.5941 (9)	0.8611 (4)	0.025 (2)*
H(12)	-0.3665 (11)	0.7162 (9)	0.9081 (4)	0.029 (2)*
H(13)	-0.2939 (11)	0.9094 (9)	0.9488 (4)	0.030 (2)*
H(14)	-0.0504 (12)	0.9823 (10)	0.9386 (5)	0.042 (3)*
H(15)	0.1076 (11)	0.8593 (9)	0.8916 (4)	0.028 (2)*
H(18A)	0.2746 (11)	0.9417(10)	0.7332 (4)	0.034 (2)*
H(18B)	0.3474 (11)	0.9002 (10)	0.6766 (4)	0.035 (2)*
H(18C)	0.2004 (10)	0.8343 (9)	0.6905 (4)	0.027 (2)*
H(19A)	0.5774 (10)	0.7599 (9)	0.7902 (4)	0.028 (2)*
H(19B)	0.4928 (11)	0.8866 (9)	0.8007 (4)	0.033 (2)*
H(19C)	0.5667 (12)	0.8615 (9)	0.7433 (4)	0.034 (2)*

H(20A)	0.4617 (11)	0.6004 (9)	0.7289 (4)	0.032 (2)*
H(20B)	0.4554 (10)	0.6840 (9)	0.6749 (4)	0.026 (2)*
H(20C)	0.3125 (10)	0.6246 (9)	0.6886 (4)	0.026 (2)*
H(23A)	0.2402 (11)	0.7858 (9)	1.0910 (4)	0.031 (2)*
H(23B)	0.1726 (12)	0.6633 (10)	1.0646 (5)	0.037 (3)*
H(23C)	0.1452 (10)	0.7857 (9)	1.0287 (4)	0.028 (2)*
H(24A)	0.4558 (11)	0.8803 (9)	1.0528 (4)	0.030 (2)*
H(24B)	0.5160 (12)	0.8251 (10)	0.9961 (4)	0.035 (2)*
H(24C)	0.3600 (12)	0.8944 (10)	0.9927 (5)	0.036 (2)*
H(25A)	0.4965 (10)	0.6665 (9)	1.0944 (4)	0.028 (2)*
H(25B)	0.4113 (11)	0.5510 (9)	1.0645 (4)	0.028 (2)*
H(25C)	0.5397 (11)	0.6167 (9)	1.0358 (4)	0.031 (2)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O(1)	0.01323 (9)	0.01518 (10)	0.01316 (9)	0.00325 (7)	0.00428 (7)	0.00513 (7)
O(2)	0.01207 (9)	0.01753 (11)	0.01774 (10)	0.00354 (8)	0.00256 (8)	0.00487 (8)
O(3)	0.01592 (10)	0.01261 (9)	0.00963 (8)	-0.00433 (7)	0.00040 (7)	-0.00066 (7)
O(4)	0.02262 (12)	0.01558 (11)	0.01255 (9)	-0.00587 (9)	0.00139 (8)	0.00363 (8)
N(1)	0.01166 (9)	0.01191 (10)	0.01202 (9)	0.00010 (7)	-0.00027 (7)	-0.00217 (7)
N(2)	0.01000 (9)	0.01155 (9)	0.01165 (9)	0.00056 (7)	0.00063 (7)	-0.00086 (7)
N(3)	0.01013 (9)	0.01134 (9)	0.00999 (8)	-0.00032 (7)	0.00076 (7)	0.00175 (7)
N(4)	0.01248 (9)	0.01003 (9)	0.00980 (8)	-0.00225 (7)	-0.00029 (7)	0.00090 (7)
C(1)	0.01354 (12)	0.01697 (13)	0.01221 (11)	0.00117 (10)	-0.00055 (9)	-0.00345 (9)
C(2)	0.01536 (13)	0.01701 (13)	0.01575 (12)	0.00058 (10)	0.00109 (10)	-0.00531 (10)
C(3)	0.01249 (11)	0.01263 (12)	0.01995 (13)	-0.00107 (9)	0.00180 (10)	-0.00415 (10)
C(4)	0.01706 (14)	0.01319 (13)	0.02859 (18)	-0.00098 (10)	0.00533 (13)	-0.00574 (12)
C(5)	0.01895 (15)	0.01170 (13)	0.0358 (2)	-0.00012 (11)	0.00599 (15)	-0.00189 (13)
C(6)	0.01834 (15)	0.01174 (13)	0.0312 (2)	-0.00076 (11)	0.00164 (13)	0.00242 (12)
C(7)	0.01558 (13)	0.01189 (12)	0.02187 (15)	-0.00184 (10)	0.00032 (11)	0.00124 (10)
C(8)	0.01170 (11)	0.01050 (11)	0.01775 (12)	-0.00152 (8)	0.00054 (9)	-0.00148 (9)
C(9)	0.01114 (10)	0.01069 (10)	0.01283 (10)	-0.00145 (8)	0.00041 (8)	-0.00070 (8)
C(10)	0.01197 (10)	0.01124 (10)	0.01148 (10)	0.00070 (8)	0.00191 (8)	0.00019 (8)
C(11)	0.01255 (11)	0.01596 (13)	0.01807 (13)	-0.00103 (9)	0.00365 (9)	-0.00334 (10)
C(12)	0.01477 (13)	0.02046 (16)	0.02190 (15)	-0.00054 (11)	0.00680 (11)	-0.00420 (12)

C(13)	0.01936 (15)	0.01922 (16)	0.02430 (17)	0.00141 (12)	0.00862 (13)	-0.00541 (13)
C(14)	0.02111 (17)	0.01592 (15)	0.0315 (2)	-0.00126 (12)	0.00915 (15)	-0.00849 (14)
C(15)	0.01639 (13)	0.01323 (13)	0.02544 (16)	-0.00203 (10)	0.00671 (12)	-0.00486 (11)
C(16)	0.01117 (10)	0.01158 (10)	0.01117 (10)	0.00015 (8)	0.00149 (8)	0.00151 (8)
C(17)	0.01572 (12)	0.01339 (12)	0.01403 (11)	0.00324 (9)	0.00582 (9)	0.00371 (9)
C(18)	0.02573 (18)	0.02020 (16)	0.01822 (14)	0.01002 (14)	0.00849 (13)	0.00857 (12)
C(19)	0.01873 (15)	0.02050 (16)	0.02546 (18)	-0.00404 (12)	0.00518 (13)	0.00382 (13)
C(20)	0.02767 (19)	0.01729 (15)	0.01667 (14)	0.00551 (13)	0.00709 (13)	0.00060 (11)
C(21)	0.01299 (11)	0.01130 (10)	0.01033 (9)	-0.00198 (8)	0.00034 (8)	0.00086 (8)
C(22)	0.01253 (11)	0.01427 (12)	0.01080 (10)	-0.00043 (9)	0.00060 (8)	-0.00206 (8)
C(23)	0.01573 (14)	0.02806 (19)	0.01812 (14)	0.00095 (13)	0.00463 (11)	-0.00534 (13)
C(24)	0.02259 (16)	0.01579 (14)	0.01981 (15)	-0.00553 (12)	0.00075 (12)	-0.00359 (11)
C(25)	0.01928 (15)	0.02031 (16)	0.01514 (13)	0.00355 (12)	-0.00306 (11)	-0.00109 (11)

Geometric parameters (Å, º)

O(1)—C(16)	1.3268 (5)	C(3)— C(8)	1.4062 (6)
O(1)—C(17)	1.4784 (6)	C(4) — C(5)	1.3875 (8)
O(2)—C(16)	1.2044 (5)	C(5) — C(6)	1.3953 (8)
O(3)—C(21)	1.3305 (5)	C(6) — C(7)	1.3948 (6)
O(3)—C(22)	1.4748 (5)	C(7) — C(8)	1.3933 (6)
O(4)—C(21)	1.2120 (5)	C(8) — C(9)	1.5085 (6)
N(1)—N(2)	1.4282 (5)	C(10) — C(11)	1.3915 (6)
N(1)—C(1)	1.4148 (6)	C(10) — C(15)	1.3943 (6)
N(1)—C(9)	1.4700 (6)	C(11) — C(12)	1.3955 (6)
N(2)—N(3)	1.4277 (6)	C(12) — C(13)	1.3879 (7)
N(2)—C(10)	1.4369 (5)	C(13) — C(14)	1.3926 (7)
N(3)—N(4)	1.4146 (4)	C(14) — C(15)	1.3880 (6)
N(3)—C(16)	1.4237 (6)	C(17) — C(18)	1.5196 (6)
N(4)—C(9)	1.5086 (5)	C(17) — C(19)	1.5197 (7)
N(4)—C(21)	1.3949 (5)	C(17) — C(20)	1.5195 (6)
C(1)—C(2)	1.3367 (6)	C(22) — C(23)	1.5211 (7)
C(2)—C(3)	1.4541 (6)	C(22) — C(24)	1.5210 (6)
C(3)—C(4)	1.3998 (6)	C(22) — C(25)	1.5204 (6)

C(16)-O(1)-C(17)	120.13 (3)	C(8)-C(9)-N(4)	113.80 (3)

C(21)-O(3)-C(22)	120.02 (3)	C(11)-C(10)-N(2)	121.12 (4)
N(2)-N(1)-C(9)	105.40 (3)	C(11)-C(10)-C(15)	120.38 (3)
C(1)-N(1)-N(2)	109.53 (3)	C(15)-C(10)-N(2)	118.16 (3)
C(1)-N(1)-C(9)	118.23 (3)	C(10)-C(11)-C(12)	119.47 (4)
N(1)-N(2)-C(10)	113.49 (3)	C(13)-C(12)-C(11)	120.41 (4)
N(3)-N(2)-N(1)	103.72 (3)	C(12)-C(13)-C(14)	119.68 (4)
N(3)-N(2)-C(10)	111.82 (3)	C(15)-C(14)-C(13)	120.44 (4)
N(4)-N(3)-N(2)	106.11 (3)	C(14)-C(15)-C(10)	119.61 (4)
N(4)-N(3)-C(16)	113.73 (3)	O(1)-C(16)-N(3)	108.34 (3)
C(16)-N(3)-N(2)	115.47 (3)	O(2)-C(16)-O(1)	128.61 (4)
N(3)-N(4)-C(9)	107.33 (3)	O(2)-C(16)-N(3)	122.73 (3)
C(21)-N(4)-N(3)	116.22 (3)	O(1)-C(17)-C(18)	102.08 (3)
C(21)-N(4)-C(9)	116.75 (3)	O(1)-C(17)-C(19)	110.10 (4)
C(2)-C(1)-N(1)	122.96 (4)	O(1)-C(17)-C(20)	109.37 (4)
C(1)-C(2)-C(3)	120.32 (4)	C(18)-C(17)-C(19)	110.80 (4)
C(4)-C(3)-C(2)	121.60 (4)	C(20)-C(17)-C(18)	111.58 (4)
C(4)-C(3)-C(8)	119.19 (4)	C(20)-C(17)-C(19)	112.42 (4)
C(8)-C(3)-C(2)	119.21 (4)	O(3)-C(21)-N(4)	110.60 (3)
C(5)-C(4)-C(3)	120.59 (4)	O(4)-C(21)-O(3)	127.75 (3)
C(4)-C(5)-C(6)	119.92 (4)	O(4)-C(21)-N(4)	121.53 (3)
C(7)-C(6)-C(5)	120.18 (4)	O(3)-C(22)-C(23)	109.65 (4)
C(8)-C(7)-C(6)	119.95 (4)	O(3)-C(22)-C(24)	101.79 (3)
C(3)-C(8)-C(9)	120.25 (3)	O(3)-C(22)-C(25)	109.81 (4)
C(7)-C(8)-C(3)	120.14 (4)	C(24)-C(22)-C(23)	110.43 (4)
C(7)-C(8)-C(9)	119.59 (4)	C(25)-C(22)-C(23)	113.77 (4)
N(1)-C(9)-N(4)	102.20 (3)	C(25)-C(22)-C(24)	110.73 (4)
N(1)-C(9)-C(8)	113.65 (3)		

N(1)-N(2)-N(3)-N(4)	-35.80(3)	C(4)-C(3)-C(8)-C(9)	176.78(3)
N(1)-N(2)-N(3)-C(16)	91.19(3)	C(4)-C(5)-C(6)-C(7)	-1.01(7)
N(1)-N(2)-C(10)-C(11)	-23.78(5)	C(5)-C(6)-C(7)-C(8)	0.53(6)
N(1)-N(2)-C(10)-C(15)	162.85(3)	C(6)-C(7)-C(8)-C(3)	0.73(6)
N(1)-C(1)-C(2)-C(3)	-4.16(6)	C(6)-C(7)-C(8)-C(9)	-177.57(3)
N(2)-N(1)-C(1)-C(2)	141.94(4)	C(7)-C(8)-C(9)-N(1)	-162.30(3)
N(2)-N(1)-C(9)-N(4)	-27.23(3)	C(7)-C(8)-C(9)-N(4)	81.25(5)
N(2)-N(1)-C(9)-C(8)	-150.29(3)	C(8)-C(3)-C(4)-C(5)	1.04(6)
N(2)-N(3)-N(4)-C(9)	18.43(3)	C(9)-N(1)-N(2)-N(3)	39.42(4)

N(2)-N(3)-N(4)-C(21)	-114.35(4)	C(9)-N(1)-N(2)-C(10)	-82.14(4)
N(2)-N(3)-C(16)-O(1)	42.68(4)	C(9)-N(1)-C(1)-C(2)	21.26(5)
N(2)-N(3)-C(16)-O(2)	-143.34(4)	C(9)-N(4)-C(21)-O(3)	-158.24(3)
N(2)-C(10)-C(11)-C(12)	-172.86(4)	C(9)-N(4)-C(21)-O(4)	25.47(5)
N(2)-C(10)-C(15)-C(14)	172.36(4)	C(10)-N(2)-N(3)-N(4)	86.87(4)
N(3)-N(2)-C(10)-C(11)	-140.69(3)	C(10)-N(2)-N(3)-C(16)	-146.14(3)
N(3)-N(2)-C(10)-C(15)	45.94(4)	C(10)-C(11)-C(12)-C(13)	0.80(7)
N(3)-N(4)-C(9)-N(1)	5.38(3)	C(11)-C(10)-C(15)-C(14)	-1.06(7)
N(3)-N(4)-C(9)-C(8)	128.33(3)	C(11)-C(12)-C(13)-C(14)	-1.24(8)
N(3)-N(4)-C(21)-O(3)	-29.91(4)	C(12)-C(13)-C(14)-C(15)	0.53(8)
N(3)-N(4)-C(21)-O(4)	153.80(4)	C(13)-C(14)-C(15)-C(10)	0.62(8)
N(4)-N(3)-C(16)-O(1)	165.71(3)	C(15)-C(10)-C(11)-C(12)	0.36(6)
N(4)-N(3)-C(16)-O(2)	-20.31(5)	C(16)-O(1)-C(17)-C(18)	-178.18(4)
C(1)-N(1)-N(2)-N(3)	-88.77(4)	C(16)-O(1)-C(17)-C(19)	-60.47(5)
C(1)-N(1)-N(2)-C(10)	149.67(3)	C(16)-O(1)-C(17)-C(20)	63.53(5)
C(1)-N(1)-C(9)-N(4)	95.55(4)	C(16)-N(3)-N(4)-C(9)	-109.59(3)
C(1)-N(1)-C(9)-C(8)	-27.50(4)	C(16)-N(3)-N(4)-C(21)	117.63(4)
C(1)-C(2)-C(3)-C(4)	174.71(4)	C(17)-O(1)-C(16)-O(2)	1.27(6)
C(1)-C(2)-C(3)-C(8)	-4.67(6)	C(17)-O(1)-C(16)-N(3)	174.78(3)
C(2)-C(3)-C(4)-C(5)	-178.34(4)	C(21)-O(3)-C(22)-C(23)	-59.09(5)
C(2)-C(3)-C(8)-C(7)	177.88(3)	C(21)-O(3)-C(22)-C(24)	-176.04(3)
C(2)-C(3)-C(8)-C(9)	-3.83(5)	C(21)-O(3)-C(22)-C(25)	66.61(4)
C(3)-C(4)-C(5)-C(6)	0.21(7)	C(21)-N(4)-C(9)-N(1)	137.87(3)
C(3)-C(8)-C(9)-N(1)	19.40(5)	C(21)-N(4)-C(9)-C(8)	-99.17(4)
C(3)-C(8)-C(9)-N(4)	-97.05(5)	C(22)-O(3)-C(21)-O(4)	-5.01(6)
C(4)-C(3)-C(8)-C(7)	-1.51(5)	C(22)-O(3)-C(21)-N(4)	178.99(3)

S4. References

Rigaku Oxford Diffraction, (2018), CrysAlisPro Software system, version 1.171.40.15a, Rigaku Corporation, Oxford, UK.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K., Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

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Figure S1 ^{1}H NMR of Compound 3 in $CDCl_3$ (–20 °C)

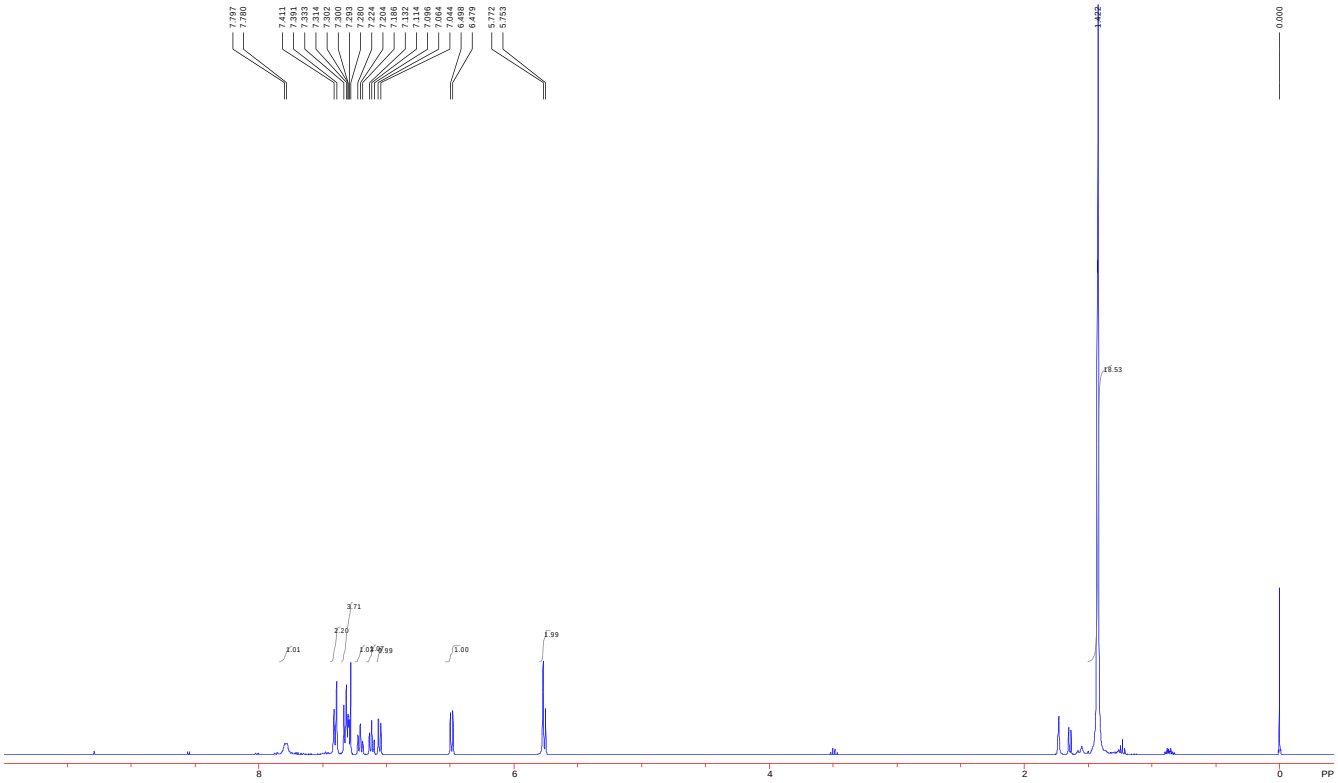


Figure S2 ^{13}C NMR of Compound 3 in $CDCl_3$ (–30 °C)

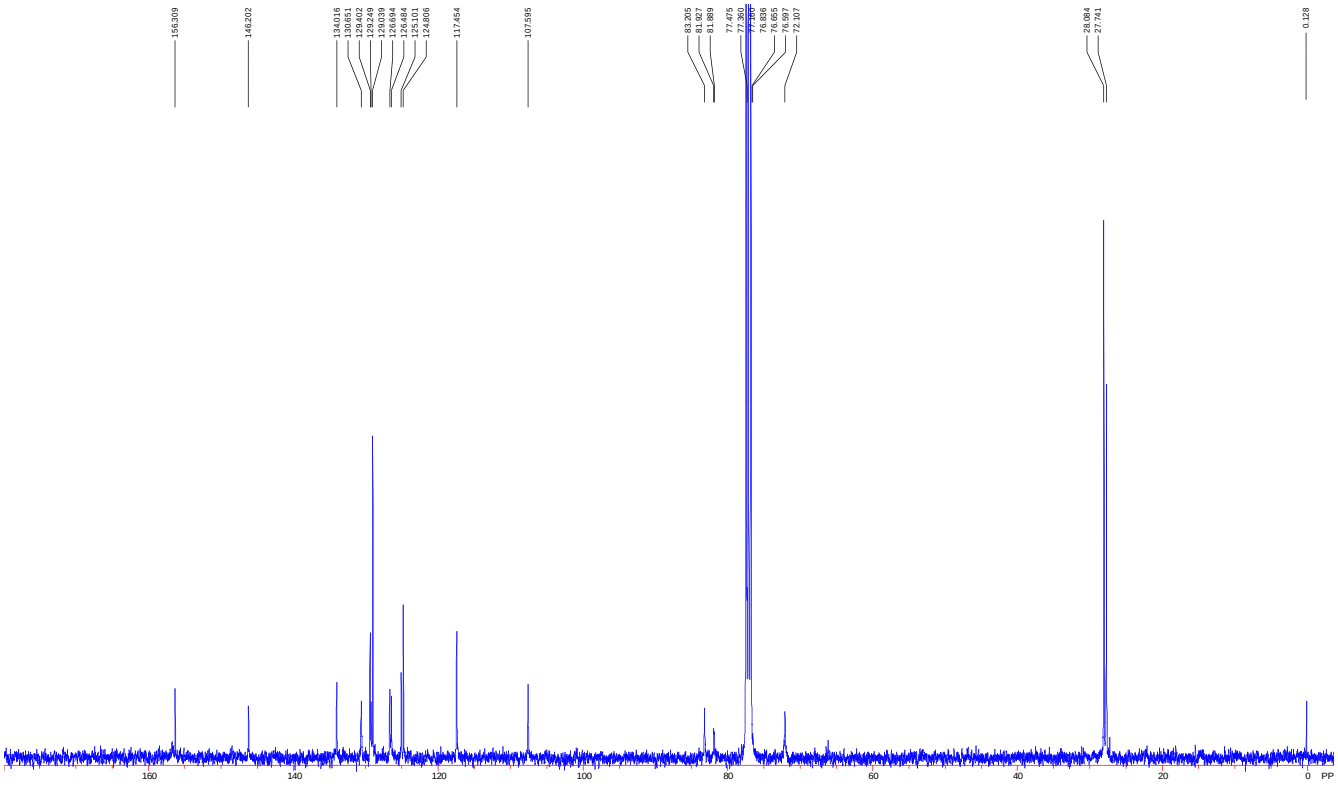


Figure S3 ^{1}H NMR of Proposed Compound 13 (with isoquinoline) in $CDCl_3$ (20 °C)

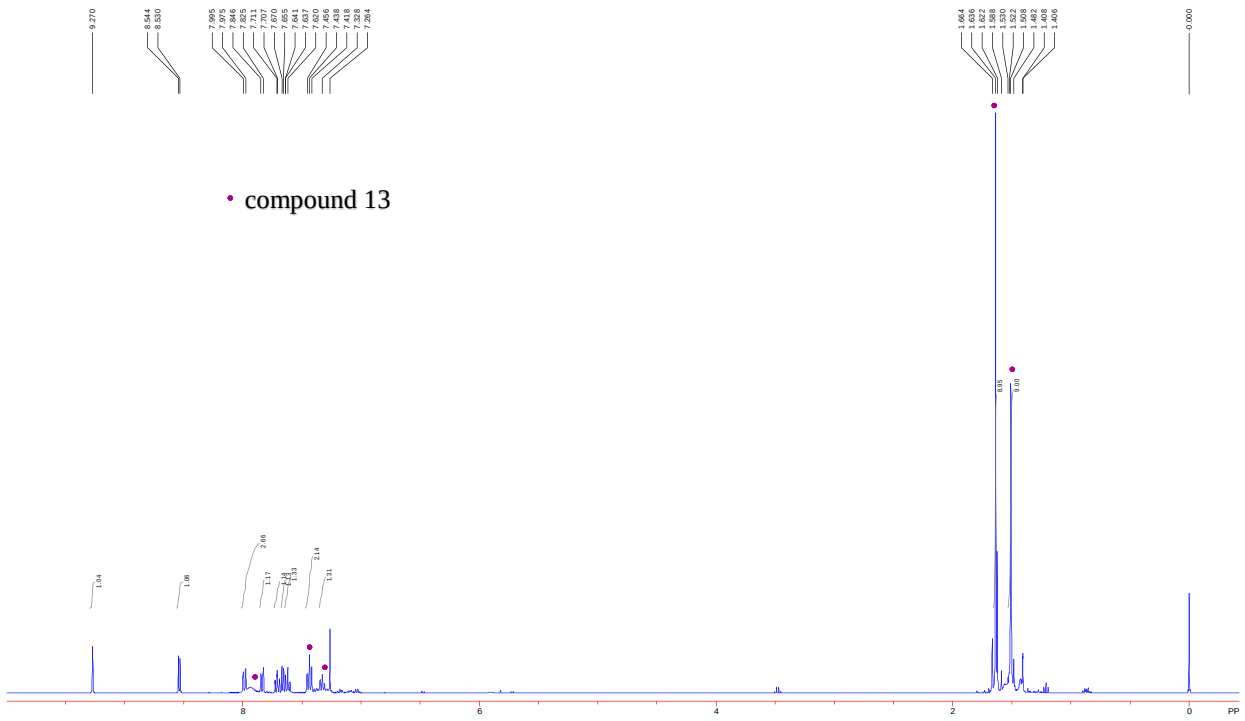
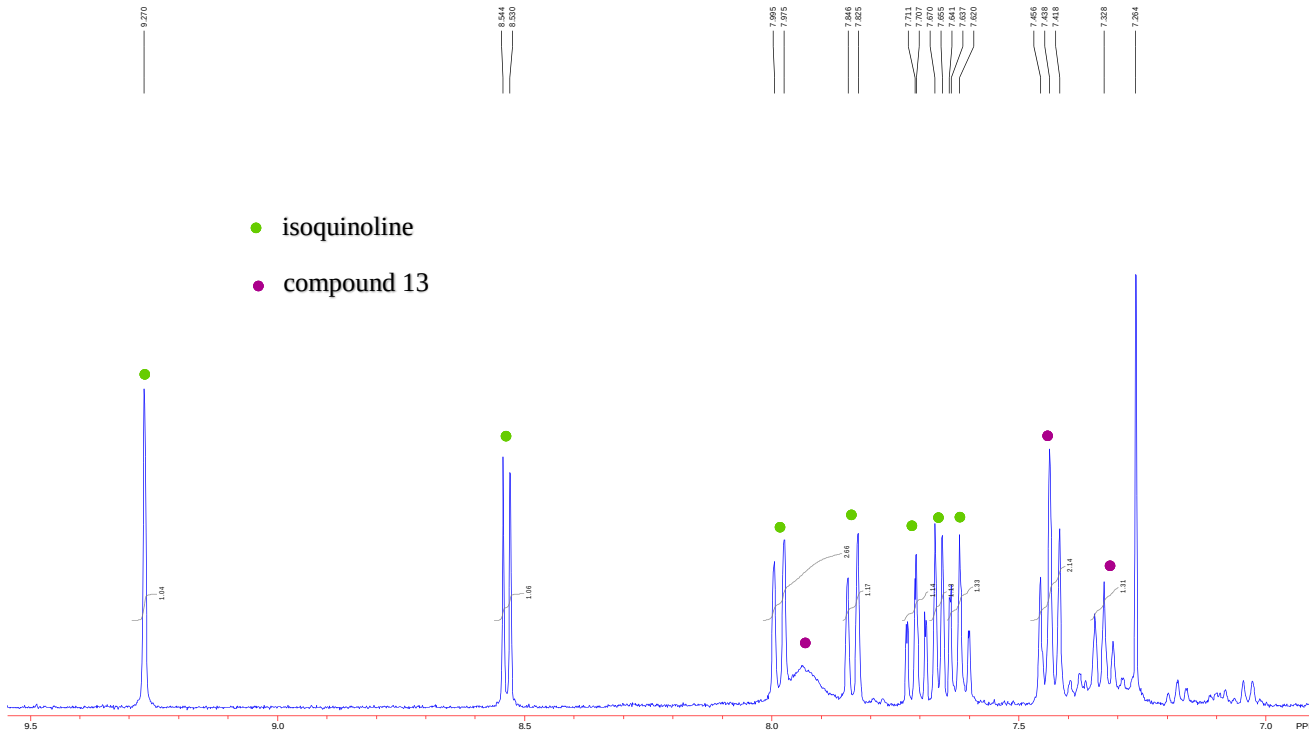


Figure S4 Inset of ^{1}H NMR of Proposed Compound 13 in $CDCl_3$ (20 °C)



S5. Energies and coordinates for calculations

Calculations carried out at the M062X/6-311G(d,p) level of theory

S5.1. Data for tetrahydrotetrazole 3

E = –1490.338575 Hartrees

G (298.15 K)= –1489.874640 Hartrees

Coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.886382	-0.277432	1.688621
2	1	0	-2.397312	1.087064	2.125612
3	8	0	-1.271933	2.508876	-0.239428
4	6	0	-2.239624	0.115239	1.676258
5	7	0	-0.046277	0.811710	1.328298
6	1	0	-4.251304	-0.337205	1.306518
7	8	0	-1.310703	0.966946	-1.901133
8	6	0	-3.221494	-0.659669	1.212553
9	7	0	0.055799	0.701907	-0.076405
10	8	0	2.022761	-0.247423	-1.490518
11	6	0	-2.924747	-1.957773	0.616561
12	7	0	0.137206	-0.671476	-0.344047
13	1	0	-4.970991	-2.547806	0.352149
14	8	0	1.627352	-2.339290	-0.707333
15	6	0	-3.617532	-4.073191	-0.328031
16	1	0	-4.410048	-4.748773	-0.629630
17	6	0	-2.285728	-4.443171	-0.488913
18	1	0	-2.035191	-5.407827	-0.914546
19	6	0	-1.272380	-3.572953	-0.102157
20	1	0	-0.230194	-3.839882	-0.236810
21	6	0	-1.587562	-2.335747	0.447723
22	6	0	-0.470839	-1.393505	0.823943
23	1	0	0.341133	-1.940197	1.308022
24	6	0	1.244253	0.761838	1.956917
25	6	0	1.388263	0.179395	3.213485
26	1	0	0.532363	-0.284496	3.686625

27	6	0	2.629307	0.200195	3.839908
28	1	0	2.737298	-0.259276	4.815806
29	6	0	3.723185	0.799227	3.226494
30	1	0	4.688028	0.812186	3.719449
31	6	0	3.566383	1.383028	1.973559
32	1	0	4.411366	1.856047	1.484802
33	6	0	2.334214	1.366178	1.332356
34	1	0	2.207230	1.806831	0.351901
35	6	0	-0.939420	1.375396	-0.841426
36	6	0	-2.254878	3.397524	-0.858655
37	6	0	-2.349022	4.536353	0.146426
38	1	0	-1.376451	5.015122	0.271678
39	1	0	-3.066556	5.283197	-0.198220
40	1	0	-2.674456	4.160509	1.118186
41	6	0	-1.735715	3.902362	-2.199838
42	1	0	-1.684985	3.101704	-2.934896
43	1	0	-0.741281	4.337364	-2.077141
44	1	0	-2.403471	4.681339	-2.574679
45	6	0	-3.592557	2.678140	-0.987775
46	1	0	-3.537988	1.858303	-1.701745
47	1	0	-4.352692	3.386899	-1.324034
48	1	0	-3.900083	2.280250	-0.018064
49	6	0	1.333299	-1.175869	-0.841675
50	6	0	3.304707	-0.582936	-2.107071
51	6	0	4.281176	-1.103858	-1.057722
52	1	0	5.283581	-1.145230	-1.490337
53	1	0	4.006882	-2.098411	-0.712913
54	1	0	4.304866	-0.428736	-0.198892
55	6	0	3.767997	0.763087	-2.646423
56	1	0	4.716614	0.650878	-3.174524
57	1	0	3.027106	1.170972	-3.335978
58	1	0	3.906930	1.472574	-1.827684
59	6	0	3.084986	-1.576483	-3.241016
60	1	0	4.022652	-1.724305	-3.781710
61	1	0	2.746847	-2.538783	-2.860627
62	1	0	2.341792	-1.189206	-3.941172
63	6	0	-3.933594	-2.838967	0.221997

S5.2. Data for isoquinoline

E = –401.850229 Hartrees

G (298.15 K)= –401.744694 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.404700	-0.707747	0.000002
2	6	0	-1.221323	-1.395208	0.000003
3	6	0	0.008380	-0.692529	-0.000002
4	6	0	0.009179	0.722675	-0.000001
5	6	0	-1.230951	1.410685	-0.000002
6	6	0	-2.406268	0.708813	0.000000
7	1	0	1.284355	-2.442395	0.000006
8	1	0	-3.347063	-1.241672	0.000003
9	1	0	-1.207535	-2.479780	0.000003
10	6	0	1.266344	-1.353924	-0.000009
11	6	0	1.268756	1.371269	-0.000001
12	1	0	-1.231587	2.494928	-0.000003
13	1	0	-3.352008	1.237615	0.000000
14	6	0	2.409799	0.617490	0.000007
15	1	0	1.322426	2.453751	-0.000004
16	1	0	3.386064	1.089533	0.000002
17	7	0	2.421435	-0.743019	0.000001

S5.3. Data for azo imide 13

E = –1088.488453 Hartrees

G (298.15 K) = –1088.158509 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.721856	1.597563	0.303664
2	7	0	1.666940	0.583144	-0.136602

3	8	0	-1.108959	0.636912	-1.712885
4	7	0	0.652739	-0.125826	-0.389152
5	8	0	-1.405994	-1.380582	0.369915
6	7	0	0.617792	-1.395696	-0.657819
7	8	0	-0.927777	-2.994035	-1.152932
8	6	0	2.946514	0.032484	0.020831
9	6	0	3.887541	1.003452	0.408626
10	1	0	3.537161	2.020179	0.535451
11	6	0	5.209550	0.666229	0.623678
12	1	0	5.919165	1.426319	0.926524
13	6	0	5.624351	-0.653052	0.444592
14	1	0	6.660292	-0.924393	0.608549
15	6	0	4.705545	-1.615914	0.050517
16	1	0	5.026481	-2.640092	-0.096315
17	6	0	3.368588	-1.294839	-0.165306
18	1	0	2.670366	-2.050571	-0.479733
19	6	0	-0.550827	0.760838	-0.674067
20	6	0	-1.445079	2.867012	0.062678
21	6	0	-0.633031	-1.999762	-0.551825
22	6	0	-2.788585	-1.793007	0.585616
23	6	0	-1.355423	3.552572	1.415773
24	1	0	-0.311695	3.686935	1.702607
25	1	0	-1.839824	4.529174	1.365439
26	1	0	-1.853340	2.951105	2.178337
27	6	0	-2.892874	2.607653	-0.331764
28	1	0	-2.963156	2.108876	-1.296614
29	1	0	-3.399809	2.005915	0.424040
30	1	0	-3.407606	3.568950	-0.396795
31	6	0	-0.685311	3.638103	-1.008184
32	1	0	-1.116030	4.636465	-1.104774
33	1	0	0.364645	3.733764	-0.725327
34	1	0	-0.751881	3.139875	-1.976002
35	6	0	-3.225396	-0.888886	1.731094
36	1	0	-2.660059	-1.124407	2.634636
37	1	0	-3.038059	0.154463	1.473783
38	1	0	-4.289663	-1.023330	1.933037
39	6	0	-2.861214	-3.255971	1.012650

40	1	0	-3.869167	-3.464958	1.379324
41	1	0	-2.632913	-3.926053	0.187591
42	1	0	-2.155928	-3.440148	1.826211
43	6	0	-3.594642	-1.516364	-0.677962
44	1	0	-3.230672	-2.123239	-1.506704
45	1	0	-4.645273	-1.756842	-0.500499
46	1	0	-3.516881	-0.461490	-0.951531
