‘Double-twist’-based dynamic induction of optical activity in multichromophoric system

Tomasz Mądry[1], Agnieszka Czapik *[1] and Marcin Kwit*[1,2]

[1] Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland.
[2] Center for Advanced Technologies, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland.
e-mail: agnieszka.czapik@amu.edu.pl or marcin.kwit@amu.edu.pl

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I. Experimental details

General information

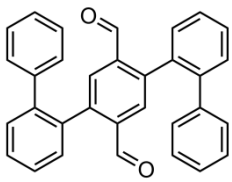
All reactions were carried out in air, unless otherwise noted. Solvents, deuterated chloroform ($CDCl_3$), and other chemicals were purchased from commercial suppliers and used as received without further purification. 2,5-Dibromoterephthalaldehyde used as precursor of **1** was synthesized according to the literature procedure.[1]

^1H and $^{13}C\{H\}$ NMR spectra were recorded on a Varian 400 MHz spectrometer at room temperature. Chemical shifts are reported in parts per million (ppm). Spectra are referenced using trimethylsilane or $CDCl_3$ residual solvent peak as an internal reference. Data is described as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, dq = doublet of quartets, dquint = doublet of quintets and br = broad), coupling constants (Hz), and integration. Column chromatography was performed on silica gel of pore size 60 Å, 70-230 mesh, 63-200 μm (Fluka). Thin-layer chromatography (TLC) was carried out using Sigma-Aldrich precoated TLC plates (60 Å medium pore diameter with a 254 nm fluorescence indicator).

Melting point were measured on a BUCHI B-545 apparatus. High-resolution mass spectra (HRMS) were measured using a Bruker Impact HD spectrometer. Optical rotations were recorded on a Jasco P-2000 polarimeter at 20 °C.

The ECD and UV spectra were measured using a Jasco J-810 spectropolarimeter at room temperature in cyclohexane and acetonitrile solutions and with the use of a quartz cell of 0.1 cm optical lengths. The concentration of analytes ranged from 0.5 to 1.8×10^{-4} mol L^{-1}.

IR spectra were recorded on a Jasco FT-IR 4600 spectrophotometer with ATR PRO ONE using a diamond crystal.



Synthesis of 2,5-di-(binaphthyl)-terephthalaldehyde (1)

The synthesis method was based on the procedure described by Prusinowska et al. and Frederickson et al.[2] In 50 mL round bottom flask, K_2CO_3 (1.90 g, 13.70 mmol, 5 equiv) was dissolved in 17 mL of H_2O and the resulting mixture was sparged with argon for 30 min. A 100 mL round-bottom flask containing a mixture of toluene (27 mL) and EtOH (17 mL) was sparged with argon for 30 min. Subsequently, 2,5-dibromoterephthalaldehyde (0.8 g, 2.74 mmol, 1 equiv), 2-biphenyl boronic acid (1.36 g, 6.87 mmol, 2.5 equiv), $Pd(PPh_3)_4$ (443 mg, 0.38 mmol, 14 mol %), and water solution of K_2CO_3 were added to the flask. The resulting mixture was refluxed overnight in an argon atmosphere. After cooling to room

temperature, the resulting dark mixture was diluted with $CHCl_3$, and filtered through Celite. The filtrate was washed twice with water and brine, dried (Na_2SO_4), and concentrated under reduced pressure, resulting in dark thick oil. The product was separated using column chromatography ($CHCl_3$) and subsequent crystallization ($CHCl_3$/*n*-hexane).

Green-to-yellow crystals, mp 239-241 °C, 54% yield (650 mg).

IR (thin film, cm^{-1}): 3368, 3057, 3028, 2853, 2747, 2359, 2308, 1982, 1961, 1745, 1684, 1579, 1487, 1468, 1447, 1431, 1398, 1379, 1277, 1263, 1250, 1219, 1148, 1073, 1025, 1009, 974, 958, 917, 886, 832, 784, 767, 741, 702, 671, 613, 569, 548, 528, 487, 462, 411.

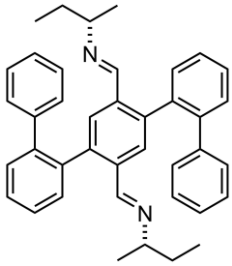
^{1}H NMR (400 MHz, $CDCl_3$): δ 9.70 (d, J = 8.0 Hz, 2H), 7.78 (d, J = 17.4 Hz, 2H), 7.56 – 7.50 (m, 2H), 7.49 – 7.44 (m, 4H), 7.45 – 7.36 (m, 2H), 7.27 – 7.18 (m, 4H), 7.19 – 7.15 (m, 2H), 7.08 – 6.95 (m, 4H).

^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 190.44, 190.24, 143.83, 141.78, 139.57, 136.05, 134.99, 131.13, 130.98, 130.22, 130.17, 130.10, 129.94, 129.12, 128.21, 128.18, 127.78, 127.64, 127.12, 127.10.

HRMS (ESI-Q-TOF), *m/z*: $[M + Na]^+$ calcd for $C_{32}H_{22}NaO_2$, 461.1517; found, 461.1506.

General Procedure for the Synthesis of diimines 2a-2k

To a 25 mL round-bottom flask containing dialdehyde **1** (1 equiv, 0.23 mmol) and chiral amine (2.3 equiv, 0.53 mmol), toluene (14 mL) was added. The resulting mixture was stirred overnight under reflux using a Dean-Stark apparatus. Then, the solvent was removed *in vacuo* and the product was crystallized if necessary.



Diimine **2a**

Colorless crystals, mp 207-209 °C, 57% yield (71 mg).

IR (thin film, cm^{-1}): 3256, 3055, 3023, 2962, 2922, 2873, 2846, 2607, 2570, 2314, 1949, 1826, 1748, 1685, 1627, 1596, 1490, 1471, 1448, 1430, 1386, 1327, 1248, 1221, 1181, 1140, 1073, 1027, 1007, 964, 912, 876, 822, 776, 763, 741, 700, 614, 562, 529, 472, 438, 418.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 – 7.65 (m, 4H), 7.51 – 7.32 (m, 8H), 7.24 – 7.03 (m, 10H), 3.03 – 2.71 (m, 2H), 1.50 – 1.28 (m, 4H), 1.14 – 0.90 (m, 6H), 0.77 – 0.54 (m, 6H).

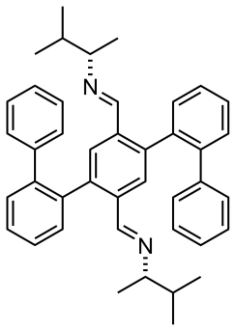
^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 156.88, 156.81, 156.55, 156.41, 141.52, 141.27, 141.23, 141.22, 141.01, 140.99, 140.75, 140.72, 140.59, 140.55, 137.45, 137.43, 134.84, 134.76, 134.59, 134.50, 131.78, 131.69, 131.64, 131.44, 130.01, 129.86, 129.78, 129.77, 129.68, 129.63, 129.56, 129.32, 129.24, 128.87, 128.83, 128.13, 128.09, 127.97, 127.87, 127.80, 127.29, 127.10, 127.07, 126.94,

126.67, 126.60, 126.53, 126.49, 68.31, 68.11, 68.09, 68.07, 30.60, 30.51, 30.46, 22.05, 21.78, 21.60, 21.48, 11.09, 10.99, 10.93, 10.88.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{40}H_{41}N_2$, 549.3270; found, 549.3274.

Optical rotation $[\alpha]_D^{20}$ +51.3 (c = 1.00, $CHCl_3$).

Diimine **2b**



Colorless crystals, mp 222-223 °C, 83% yield (110 mg).

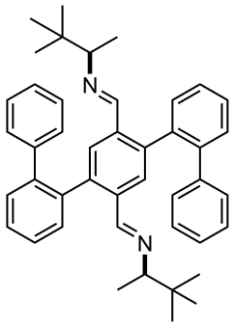
IR (thin film, cm^{-1}): 3256, 3056, 3023, 2962, 2925, 2868, 2827, 2583, 1948, 1825, 1628, 1596, 1490, 1472, 1447, 1430, 1390, 1342, 1303, 1251, 1222, 1156, 1137, 1107, 1074, 1050, 1029, 1009, 983, 966, 912, 863, 776, 763, 741, 699, 614, 583, 560, 530, 445.

^1H NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 0.3H), 7.98 (s, 0.3H), 7.95 (s, 0.7H), 7.91 (s, 0.7H), 7.78 (s, 0.7H), 7.67 (s, 0.7H), 7.66 (s, 0.3H), 7.57 (s, 0.3H), 7.50 – 7.40 (m, 6H), 7.39 – 7.32 (m, 1.3H), 7.29 – 7.26 (m, 0.7H), 7.24 – 7.03 (m, 10H), 2.80 (quint, J = 6.4 Hz, 0.3H), 2.65 (dquint, J = 30.0, 6.4 Hz, 1.4H), 2.54 (quint, J = 6.5 Hz, 0.3H), 1.73 – 1.44 (m, 2H), 1.10 (d, J = 6.4 Hz, 1H), 1.07 (d, J = 6.4 Hz, 2H), 0.92 (d, J = 6.3 Hz, 2H), 0.89 (d, J = 6.3 Hz, 1H), 0.85 (d, J = 6.8 Hz, 1H), 0.80 (d, J = 6.7 Hz, 2H), 0.78 – 0.67 (m, 6H), 0.62 (d, J = 6.7 Hz, 2H), 0.60 (d, J = 6.7 Hz, 1H).

$^{13}C\{H\}$ NMR (101 MHz, $CDCl_3$): δ 157.05, 156.97, 156.30, 156.24, 141.54, 141.33, 141.30, 141.19, 141.12, 140.88, 140.84, 140.65, 140.60, 140.48, 137.57, 137.48, 135.12, 134.79, 134.64, 134.23, 131.90, 131.83, 131.60, 131.40, 129.99, 129.97, 129.78, 129.61, 129.57, 129.54, 128.93, 128.88, 128.11, 128.08, 128.01, 127.88, 127.85, 127.80, 127.31, 127.14, 126.88, 126.81, 126.66, 126.61, 126.41, 72.69, 72.33, 72.28, 72.26, 34.29, 34.19, 34.16, 34.09, 19.84, 19.68, 19.50, 19.48, 19.33, 19.20, 19.15, 19.07, 19.03.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{42}H_{45}N_2$, 577.3583; found, 577.3597.

Optical rotation $[\alpha]_D^{20}$ +76.4 (c = 1.01, $CHCl_3$).



Diimine **2c**

Colorless crystals, mp 263-266 °C, 77% yield (106 mg).

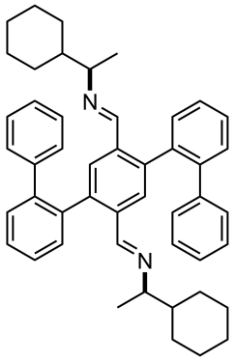
IR (thin film, cm^{-1}): 3059, 3025, 2975, 2955, 2900, 2865, 2311, 1948, 1747, 1625, 1597, 1489, 1472, 1447, 1430, 1392, 1380, 1359, 1330, 1317, 1250, 1223, 1203, 1180, 1168, 1118, 1074, 1056, 1029, 1008, 966, 912, 889, 840, 777, 760, 741, 699, 614, 594, 560, 538, 513, 455, 406.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (s, 0.3H), 8.01 (s, 0.3H), 7.97 (s, 0.8H), 7.95 (s, 0.6H), 7.76 (s, 0.5H), 7.61 – 7.58 (m, 1H), 7.50 – 7.31 (m, 7.5H), 7.24 – 7.01 (m, 11H), 2.81 (q, J = 6.6 Hz, 0.3H), 2.62 (dq, J = 30.4, 6.5 Hz, 1.4H), 2.44 (q, J = 6.6 Hz, 0.3H), 1.26 (s, 0.6H), 1.08 (d, J = 6.5 Hz, 1H), 1.02 (d, J = 6.5 Hz, 2.4H), 0.85 (t, J = 3.2 Hz, 4.5H), 0.81 – 0.75 (m, 6H), 0.70 (s, 7H), 0.62 (s, 2.5H).

^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 157.16, 156.97, 156.02, 141.62, 141.59, 141.45, 141.37, 141.14, 141.04, 140.94, 140.65, 140.62, 140.47, 140.41, 137.68, 137.61, 137.50, 135.47, 134.78, 134.67, 133.87, 132.08, 131.90, 131.64, 131.35, 130.24, 130.20, 130.10, 129.92, 129.87, 129.81, 129.63, 129.54, 129.15, 129.01, 128.92, 128.20, 128.07, 127.91, 127.82, 127.79, 127.75, 127.37, 127.21, 126.78, 126.72, 126.66, 126.63, 126.38, 126.36, 125.27, 75.56, 75.32, 75.26, 34.34, 34.31, 26.71, 26.60, 26.54, 26.49, 17.30, 17.21, 16.44, 16.38.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{44}H_{49}N_2$, 605.3896; found, 605.3881.

Optical rotation $[\alpha]_D^{20}$ -290.0 (c = 0.97, $CHCl_3$).



Diimine **2d**

Colorless crystals, mp 169-171 °C, 82% yield (123 mg).

IR (thin film, cm^{-1}): 3055, 3024, 2977, 2921, 2849, 1624, 1597, 1489, 1471, 1446, 1429, 1387, 1323, 1260, 1220, 1150, 1125, 1101, 1072, 1029, 1008, 964, 912, 890, 852, 777, 763, 741, 699, 614, 578, 557, 526, 447, 410.

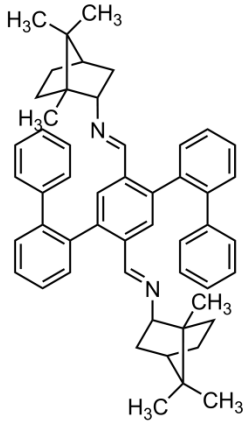
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (s, 0.3H), 7.95 (s, 0.3H), 7.92 (s, 0.7H), 7.88 (s, 0.7H), 7.76 (s, 0.7H), 7.66 (s, 0.7H), 7.65 (s, 0.3H), 7.57 (s, 0.3H), 7.47 – 7.33 (m, 7H), 7.29 – 7.26 (m, 0.7H), 7.24 – 7.02 (m, 10.3H), 2.78 (quint, J = 6.4 Hz, 0.3H), 2.65 (dquint, J = 26.0, 6.4 Hz, 1.4H), 2.54 (quint, J = 6.4 Hz, 0.3H), 1.74 – 1.56 (m, 8H), 1.50 (d, J = 12.8 Hz, 1H), 1.33 – 1.01 (m, 12H), 0.92 (d, J = 6.4 Hz, 2H), 0.89 (d, J = 6.4 Hz, 1H), 0.86 – 0.52 (m, 4H).

^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 157.03, 156.92, 156.30, 141.53, 141.46, 141.29, 141.27, 141.18, 141.15, 140.85, 140.81, 140.79, 140.66, 140.61, 140.48, 137.55, 137.50, 137.44, 135.05, 134.72, 134.59, 134.20, 131.90, 131.84, 131.60, 131.43, 129.99, 129.77, 129.70, 129.61, 129.57, 129.46, 128.89, 128.82, 128.09, 127.99, 127.87, 127.85, 127.74, 127.29, 127.11, 126.87, 126.80, 126.64, 126.58, 126.31, 72.03, 71.84, 71.75, 43.87, 43.67, 43.63, 43.57, 30.22, 29.95, 29.68, 29.61, 29.54, 29.51, 26.58, 26.53, 26.52, 26.36, 26.32, 26.24, 26.15, 19.80, 19.58, 19.09, 19.06.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{48}H_{53}N_2$, 657.4209; found, 657.4207.

Optical rotation $[\alpha]_D^{20}$ -62.1 (c = 0.97, $CHCl_3$).

Diimine **2e**



Colorless crystals, mp 293-295 °C, 84% yield (136 mg).

IR (thin film, cm^{-1}): 3054, 3022, 2984, 2947, 2923, 2870, 2311, 1747, 1625, 1597, 1489, 1471, 1448, 1431, 1388, 1366, 1339, 1249, 1223, 1163, 1110, 1069, 1025, 1008, 944, 911, 863, 774, 754, 741, 699, 614, 573, 555, 521, 437.

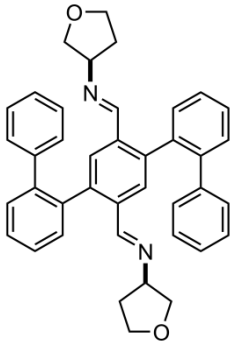
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (s, 0.1H), 8.02 (s, 0.1H), 7.95 – 7.88 (m, 0.5H), 7.86 – 7.80 (m, 0.7H), 7.79 – 7.70 (m, 1H), 7.69 – 7.52 (m, 1.6H), 7.50 – 7.28 (m, 8H), 7.22 – 6.98 (m, 10H), 3.24 – 2.99 (m, 1H), 2.97 – 2.72 (m, 1H), 2.16 – 1.78 (m, 2.5H), 1.78 – 1.39 (m, 7.5H), 1.36 – 0.95 (m, 8H), 0.94 – 0.77 (m, 10H), 0.62 – 0.21 (m, 6H).

^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 157.32, 157.22, 157.08, 156.97, 156.90, 156.49, 155.81, 155.59, 155.44, 155.23, 155.01, 141.89, 141.71, 141.64, 141.48, 141.35, 141.24, 141.06, 140.94, 140.86, 140.82, 140.79, 140.71, 140.64, 140.58, 140.47, 140.43, 140.39, 140.36, 140.24, 138.01, 137.97, 137.94, 137.85, 137.80, 137.73, 135.17, 135.04, 134.98, 134.94, 134.71, 134.64, 134.57, 134.48, 134.37, 134.27, 132.05, 131.87, 131.76, 131.71, 131.66, 131.62, 131.60, 131.33, 130.55, 130.31, 130.12, 130.09, 130.06, 130.01, 129.95, 129.93, 129.86, 129.76, 129.72, 129.65, 129.63, 129.56, 129.52, 129.38, 129.24, 129.20, 129.01, 128.20, 128.05, 128.01, 127.97, 127.88, 127.86, 127.84, 127.82, 127.78, 127.74, 127.34, 127.27, 127.21, 127.12, 127.04, 126.95, 126.92, 126.83, 126.55, 126.47, 126.41, 126.37, 126.35, 125.27, 79.14, 78.98, 78.96, 78.92, 78.89, 75.71, 75.59, 75.57, 75.37, 75.34, 50.93, 50.87, 50.82, 50.73, 50.68, 50.64, 50.62, 50.54, 50.43, 50.37, 48.30, 48.28, 48.25, 48.17, 48.16, 46.96, 46.93, 46.90, 45.50, 45.46, 38.75, 38.68, 38.61, 38.51, 37.19, 37.15, 37.10, 36.45, 36.37, 28.54, 28.43, 28.34, 28.30, 27.64, 27.57, 20.78, 20.74, 20.69, 20.66, 20.60, 19.72, 19.69, 19.65, 18.81, 18.77, 13.71, 13.51, 13.48, 13.40, 13.31, 12.76, 12.73, 12.53, 12.35.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{52}H_{57}N_2$, 709.4522; found, 709.4535.

Optical rotation $[\alpha]_D^{20}$ -8.3 (c = 1.00, $CHCl_3$).

Diimine **2f**



Pale yellow crystals, mp 233-235 °C, 70% yield (93 mg).

IR (thin film, cm^{-1}): 3054, 2971, 2946, 2862, 2310, 1943, 1746, 1630, 1542, 1472, 1447, 1431, 1396, 1362, 1259, 1223, 1168, 1124, 1073, 1008, 975, 916, 781, 770, 744, 702, 672, 613, 536, 427.

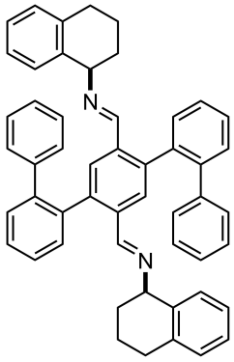
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (s, 0.5H), 7.94 (s, 0.5H), 7.87 (d, J = 2.4 Hz, 0.5H), 7.86 (d, J = 3.6 Hz, 0.5H), 7.82 (s, 1H), 7.53 – 7.34 (m, 8H), 7.27 – 6.99 (m,

11H), 3.99 – 3.88 (m, 2H), 3.86 – 3.63 (m, 6H), 3.58 (dd, J = 8.9, 4.4 Hz, 0.7H), 3.55 – 3.52 (m, 0.3H), 3.40 (dd, J = 8.8, 4.2 Hz, 0.3H), 3.33 (dd, J = 8.8, 4.3 Hz, 0.7H), 2.12 – 1.94 (m, 2H), 1.88 – 1.74 (m, 1H), 1.73 – 1.55 (m, 1H).

$^{13}C\{H\}$ NMR (101 MHz, $CDCl_3$): δ 158.17, 158.04, 157.82, 157.80, 141.55, 141.50, 141.38, 141.36, 141.29, 141.24, 140.63, 140.55, 140.51, 140.44, 137.20, 137.18, 137.16, 134.59, 134.55, 134.52, 131.67, 131.59, 131.34, 131.25, 129.85, 129.81, 129.77, 129.69, 129.63, 129.06, 129.02, 128.87, 128.85, 128.42, 128.37, 128.02, 127.99, 127.91, 127.62, 127.55, 127.42, 127.35, 126.92, 126.82, 126.77, 126.70, 73.74, 73.65, 73.62, 70.19, 70.15, 70.12, 70.07, 67.94, 67.86, 34.39, 34.29, 34.27.

HRMS (ESI), *m/z*: $[M + Na]^+$ calcd for $C_{40}H_{36}N_2NaO_2$, 599.2674; found, 599.2687.

Optical rotation $[\alpha]_D^{20}$ +17.1 (c = 0.91, $CHCl_3$).



Diimine **2g**

Pale yellow crystals, mp 220-221 °C, 80% yield (127 mg).

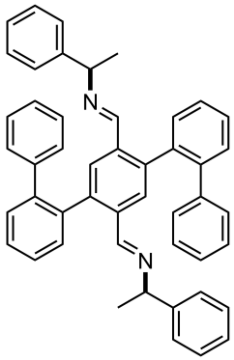
IR (thin film, cm^{-1}): 3050, 3018, 2930, 2860, 2836, 2320, 1949, 1746, 1623, 1542, 1489, 1471, 1448, 1429, 1378, 1308, 1219, 1158, 1116, 1073, 1029, 1008, 967, 917, 879, 757, 740, 701, 614, 556, 518, 479, 445, 410.

^1H NMR (400 MHz, $CDCl_3$): δ 8.08 – 8.03 (m, 2H), 8.02 (s, 1H), 7.94 (s, 0.3H), 7.93 (s, 0.4H), 7.89 (s, 0.3H), 7.48 – 7.37 (m, 8H), 7.30 – 7.16 (m, 6H), 7.14 – 7.01 (m, 10H), 6.81 – 6.73 (m, 0.8H), 6.44 (d, J = 7.6 Hz, 0.2H), 6.32 (d, J = 7.6 Hz, 1H), 4.12 (dt, J = 12.2, 6.4 Hz, 2H), 2.88 – 2.70 (m, 4H), 2.04 – 1.66 (m, 8H).

$^{13}C\{H\}$ NMR (101 MHz, $CDCl_3$): δ 158.91, 158.67, 158.51, 158.25, 141.62, 141.39, 141.22, 141.03, 140.73, 140.69, 140.67, 137.40, 137.32, 137.22, 137.18, 136.95, 136.84, 136.73, 136.60, 134.82, 134.78, 134.42, 134.34, 131.78, 131.73, 131.65, 129.86, 129.81, 129.79, 129.71, 129.66, 129.25, 129.15, 129.02, 128.94, 128.92, 128.87, 128.81, 128.75, 128.34, 128.25, 128.18, 128.16, 128.13, 127.95, 127.90, 127.36, 127.30, 127.14, 127.11, 126.69, 126.66, 126.63, 126.58, 126.53, 125.58, 125.52, 125.50, 68.85, 68.72, 68.70, 31.65, 31.54, 31.00, 30.90, 29.43, 29.37, 20.56, 20.34, 20.28, 20.09.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{52}H_{45}N_2$, 697.3583; found, 697.3595.

Optical rotation $[\alpha]_D^{20}$ +43.5 (c = 0.98, $CHCl_3$).



Diimine **2h**

Colorless crystals, mp 160.5-161.5 °C, 82% yield (120 mg).

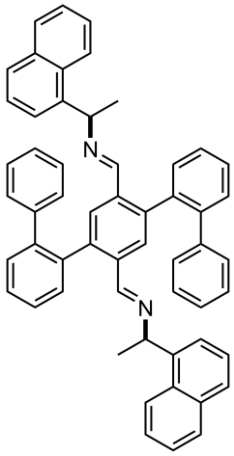
IR (thin film, cm^{-1}): 3050, 3027, 2966, 2922, 2862, 2318, 1956, 1814, 1748, 1632, 1599, 1490, 1471, 1448, 1431, 1379, 1312, 1249, 1220, 1172, 1120, 1078, 1061, 1028, 1009, 968, 913, 896, 864, 778, 765, 743, 699, 615, 551, 530, 510, 480, 432, 410.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (s, 0.4H), 8.04 – 7.99 (m, 1.6H), 7.93 – 7.90 (m, 1.2H), 7.87 (s, 0.4H), 7.83 (s, 0.4H), 7.50 – 7.34 (m, 8H), 7.32 – 7.09 (m, 15.5H), 7.00 – 6.85 (m, 4.5H), 4.28 – 4.05 (m, 2H), 1.58 (s, 0.3H), 1.41 (dd, J = 8.8, 6.6 Hz, 2.7H), 1.28 (d, J = 6.6 Hz, 3H).

^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 157.46, 157.35, 157.09, 145.62, 145.22, 145.16, 145.05, 141.79, 141.60, 141.45, 141.42, 141.39, 141.23, 141.18, 140.62, 140.44, 140.37, 137.44, 137.42, 135.09, 134.79, 134.74, 134.40, 131.77, 131.65, 131.53, 131.41, 129.94, 129.91, 129.88, 129.76, 129.71, 129.47, 129.27, 129.20, 128.98, 128.27, 128.23, 128.20, 128.10, 128.07, 127.97, 127.82, 127.78, 127.50, 127.32, 127.18, 127.06, 126.76, 126.71, 126.68, 126.63, 126.60, 126.51, 126.47, 126.44, 126.30, 70.07, 70.01, 69.95, 69.65, 25.01, 24.87, 24.35.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{48}H_{41}N_2$, 645.3270; found, 645.3272.

Optical rotation $[\alpha]_D^{20}$ -29.6 (c = 1.05, $CHCl_3$).



Diimine **2i**

Light brown solid, mp 195-197 °C, 93% yield (158 mg).

IR (thin film, cm^{-1}): 3054, 3020, 2971, 2925, 2864, 2321, 1942, 1746, 1635, 1595, 1509, 1489, 1472, 1448, 1432, 1393, 1255, 1223, 1165, 1117, 1072, 1010, 969, 914, 799, 774, 738, 700, 614, 554, 506, 472, 443, 410.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (s, 0.3H), 8.15 – 8.02 (m, 4.2H), 7.99 (s, 0.3H), 7.96 (s, 0.7H), 7.90 – 7.85 (m, 1.5H), 7.84 – 7.79 (m, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.71 – 7.65 (m, 1H), 7.62 – 7.52 (m, 1H), 7.51 – 7.33 (m, 15H), 7.30 – 7.18 (m, 3H), 7.17 – 7.12 (m, 2H), 6.85 – 6.80 (m, 2H), 6.80 – 6.72 (m, 1H), 6.67 – 6.59 (m, 2H), 5.06 (q, J = 6.6 Hz, 0.3H), 4.96 (dq, J = 21.4, 6.5 Hz, 1.4H), 4.86 (q, J = 6.5 Hz, 0.3H), 1.57 – 1.51 (m, 3H), 1.43 (d, J = 6.6 Hz, 3H).

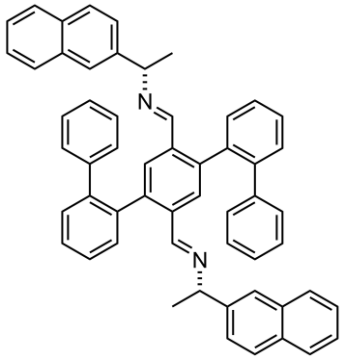
^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 157.60, 157.49, 157.33, 141.81, 141.65, 141.60, 141.48, 141.40, 141.35, 141.31, 141.27, 141.23, 141.18, 141.16, 141.14, 140.68, 140.31, 140.20, 137.49, 137.43, 137.42, 135.26, 134.94, 134.51, 133.83, 133.81, 133.73, 131.76, 131.61, 131.52, 131.41, 130.51, 130.43, 130.35, 130.18, 129.97, 129.92, 129.87, 129.82, 129.74, 129.38, 129.34, 129.31, 129.21, 128.94, 128.85, 128.83, 128.23, 128.10, 128.07, 127.99, 127.63, 127.57, 127.50, 127.36, 127.21, 127.17, 127.04, 126.95, 126.91, 126.83, 126.74, 126.31, 126.25, 125.72, 125.69, 125.66, 125.64,

125.62, 125.58, 125.18, 125.15, 125.09, 124.08, 123.98, 123.78, 123.66, 123.49, 123.36, 123.30, 123.25, 66.17, 66.04, 65.74, 24.72, 24.68, 24.46, 24.19.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{56}H_{45}N_2$, 745.3583; found, 745.3586.

Optical rotation $[\alpha]_D^{20}$ -63.4 (c = 1.02, $CHCl_3$).

Diimine **2j**



Colorless crystals, mp 202-204 °C, 88% yield (150 mg).

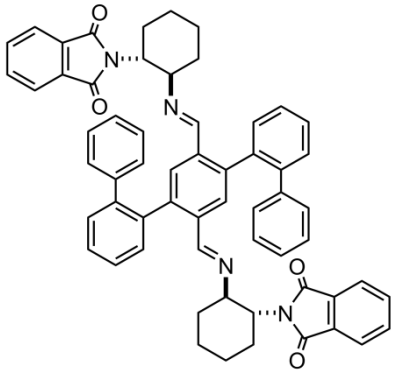
IR (thin film, cm^{-1}): 3056, 3020, 2976, 2926, 2883, 2839, 2321, 1922, 1746, 1636, 1601, 1507, 1489, 1471, 1447, 1431, 1389, 1361, 1287, 1266, 1223, 1162, 1127, 1110, 1073, 1026, 1008, 970, 951, 912, 886, 851, 816, 774, 741, 700, 685, 656, 614, 602, 533, 471, 440, 420.

^1H NMR (400 MHz, $CDCl_3$): δ 8.12 (s, 0.3H), 8.07 (s, 0.6H), 8.03 (s, 0.7H), 8.02 – 7.96 (m, 2H), 7.89 (s, 0.4H), 7.84 – 7.71 (m, 6H), 7.65 – 7.60 (m, 1.4H), 7.56 (s, 0.6H), 7.51 – 7.34 (m, 13H), 7.32 – 7.10 (m, 6H), 6.96 – 6.88 (m, 2H), 6.85 – 6.68 (m, 3H), 4.42 – 4.22 (m, 2H), 1.57 (s, 1H), 1.48 (dd, J = 6.6, 4.3 Hz, 2H), 1.37 (dd, J = 6.6, 3.6 Hz, 3H).

$^{13}C\{H\}$ NMR (101 MHz, $CDCl_3$): δ 157.66, 157.58, 157.55, 157.32, 142.96, 142.62, 142.50, 141.83, 141.63, 141.52, 141.49, 141.45, 141.36, 141.22, 140.68, 140.37, 140.32, 137.51, 137.48, 135.08, 134.91, 134.87, 134.60, 133.44, 133.42, 133.39, 133.36, 132.56, 132.52, 132.50, 131.71, 131.69, 131.52, 131.47, 129.91, 129.80, 129.75, 129.44, 129.38, 129.28, 129.23, 129.21, 129.11, 128.26, 128.22, 128.16, 128.14, 128.09, 128.00, 127.91, 127.88, 127.82, 127.78, 127.75, 127.64, 127.56, 127.53, 127.51, 127.32, 127.25, 127.10, 126.79, 126.74, 126.41, 125.80, 125.78, 125.74, 125.49, 125.40, 125.37, 125.32, 125.25, 125.18, 124.88, 124.73, 124.70, 124.56, 70.26, 70.15, 70.03, 69.82, 24.93, 24.74, 24.70, 24.19.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{56}H_{45}N_2$, 745.3583; found, 745.3600.

Optical rotation $[\alpha]_D^{20}$ +15.5 (c = 0.98, $CHCl_3$).



Diimine **2k**

Colorless crystals, mp 216-217 °C, 79% yield (160 mg).

IR (thin film, cm^{-1}): 3059, 3022, 2923, 2857, 2310, 1765, 1705, 1636, 1611, 1467, 1444, 1432, 1390, 1366, 1328, 1251, 1226,

1190, 1156, 1096, 1050, 1016, 973, 945, 903, 876, 861, 840, 781, 770, 747, 716, 703, 637, 613, 558, 528, 500, 454, 430, 403.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (s, 0.2H), 7.85 (s, 0.3H), 7.69 – 7.57 (m, 9H), 7.51 (s, 1.5H), 7.46 – 7.27 (m, 5H), 7.25 – 7.08 (m, 7H), 7.06 – 6.95 (m, 3H), 6.71 (dd, J = 7.6, 0.8 Hz, 1.4H), 6.64 (d, J = 7.8 Hz, 0.2H), 6.61 – 6.45 (m, 2.4H), 4.25 – 4.05 (m, 2H), 3.81 – 3.68 (m, 0.7H), 3.58 (m, 1.3H), 2.22 – 2.04 (m, 2H), 1.86 – 1.67 (m, 6H), 1.64 (s, 3H), 1.54 – 1.30 (m, 7H).

^{13}C{H} NMR (101 MHz, $CDCl_3$): δ 168.11, 167.98, 159.16, 158.93, 158.75, 158.59, 141.15, 141.01, 140.97, 140.91, 140.49, 140.45, 137.18, 136.77, 134.60, 134.51, 133.77, 133.56, 133.51, 133.46, 133.37, 131.75, 131.66, 131.22, 131.00, 129.83, 129.81, 129.72, 129.64, 128.95, 128.92, 128.58, 128.39, 128.14, 128.04, 127.87, 127.83, 127.79, 127.37, 127.20, 126.99, 126.88, 126.82, 126.60, 125.66, 125.42, 122.93, 122.90, 122.84, 68.90, 68.79, 68.32, 68.14, 55.58, 55.44, 34.04, 33.60, 33.45, 33.30, 28.69, 28.48, 25.45, 25.36, 24.09, 24.00.

HRMS (ESI), *m/z*: $[M + H]^+$ calcd for $C_{60}H_{51}N_4O_4$, 891.3910; found, 891.3889.

Optical rotation $[\alpha]_D^{20}$ -79.0 (c = 1.00, $CHCl_3$).

I. Calculation details

The theoretical approach applied for compound **2c** follow the standard routine that includes (i) conformational search at molecular mechanics level (MM3); (ii) pre-optimization at the B3LYP/6-31G(d) level to reduce the number of thermally accessible conformers; (iii) re-optimization of conformers found at low-DFT level at B3LYP/6-311++G(d,p) level followed by frequency calculations to confirm stability of received structures; (iv) calculations on relative energies (ΔEDFT and $\Delta\Delta$GDFT) using Boltzmann distribution at T = 298.15 K; (v) rotatory strengths calculations at the TD-DFT/6-311++G(d,p) level for all stable conformers of relative energies ranging from 0.0 to 2.0 kcal mol^{-1}.

Preliminary conformer distribution search was performed by the Scigress package[1] using the MM3 molecular mechanics force field. Minimum energy conformers of relative steric energies (ΔE_{SE}) up to 10 kcal mol^{-1} found by molecular mechanics were further fully optimized at the B3LYP/6-31G(d) level as implemented in the Gaussian09 package,[2] which significantly reduced the number of conformers.

Calculations of higher accuracy were performed at the B3LYP/6-311++G(d,p) level with the inclusion of empirical dispersion correction *via* GD3BJ schemes. Resulting conformers were the real minima (no imaginary frequencies have been found). Total and free energy values have been calculated and used to obtain the Boltzmann population of conformers at 298.15 K. Apart from B3LPY with GD3BJ, we also tested it without GD3BJ correction likewise other functionals namely: M062X, wB97XD but results were far from satisfying.

For further calculations, only conformers with up to 2 kcal mol^{-1} above most stable one were used following a generally accepted protocol.[3]

The TD-DFT/6-311++G(d,p) calculations of ECD of **2c** were performed for all structures re-optimized at higher levels of theory. We used CAM-B3LYP[4] density functional for calculations of rotatory strengths because among other tested density functionals (B3LYP, M062X and wB97XD) the results were more consistent with experimental. Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity representations of the calculated values of rotatory strengths were quite small, and for this reason only the velocity representations were further used. The CD spectra were simulated by overlapping Gaussian functions for each transition according to the procedure previously described.[6]

II. Calculation results

Table S1. Total and Gibbs free energies (E, ΔG, in Hartree), relative energies (ΔE, ΔΔG, in kcal mol^{-1}), ΔE and ΔΔG-based percentage populations (% ΔE, % ΔΔG) and numbers of imaginary frequencies (#Imfreq) calculated at B3LYP-GD3BJ/6-311++G(d,p) level for individual conformers of diimine **2c**.

Compound	E	ΔG	ΔE	% ΔE	ΔΔG	% ΔΔG	#Imfreq
2c (conformer 1)	-1815.80601	-1815.08228	0.75	10.91	1.41	2.88	0
2c (conformer 2)	-1815.80508	-1815.08333	1.33	4.08	0.75	8.78	0
2c (conformer 4)	-1815.80721	-1815.08356	0.00	38.77	0.61	11.14	0
2c (conformer 5)	-1815.80578	-1815.08301	0.90	8.50	0.95	6.24	0
2c (conformer 9)	-1815.80505	-1815.08371	1.35	3.94	0.51	13.16	0
2c (conformer 12)	-1815.80421	-1815.08266	1.88	1.62	1.18	4.29	0
2c (conformer 13)	-1815.80656	-1815.07930	0.40	19.57	3.28	0.00	0
2c (conformer 35)	-1815.80293	-1815.08236	2.68	0.00	1.36	3.14	0
2c (conformer 47)	-1815.80510	-1815.08028	1.32	4.17	2.67	0.00	0
2c (conformer 59)	-1815.80287	-1815.08453	2.72	0.00	0.00	31.27	0
2c (conformer 69)	-1815.80429	-1815.07849	1.83	1.75	3.79	0.00	0
2c (conformer 77)	-1815.80463	-1815.08406	1.62	2.53	0.29	19.10	0

Table S2. Dihedral angles *α*, *β*, *γ*, *ω* (in degrees) of calculated at the B3LYP-GD3BJ/6-311++G(d,p) level for each low-energy conformer of diimine **2c**.

Compound	α_1[1]	α_2[2]	β_1[3]	β_2[4]	γ[5]	γ[6]	ω[7]
2c (conformer 1)	-62	-62	-46	-46	-177	-177	54
2c (conformer 2)	60	-67	48	-48	-174	-180	173
2c (conformer 4)	59	-59	47	47	-175	-175	-57
2c (conformer 5)	-128	-74	52	-55	-172	179	-24
2c (conformer 9)	-120	59	54	49	-178	-175	117
2c (conformer 12)	66	134	50	-54	-168	160	22
2c (conformer 13)	-123	-123	52	53	-176	-176	-69
2c (conformer 35)	70	130	52	-51	-179	163	21
2c (conformer 47)	-115	-65	58	-44	22	-180	-2
2c (conformer 59)	126	119	-52	-53	166	-26	68
2c (conformer 69)	59	110	45	-53	-175	-22	-11
2c (conformer 77)	-118	59	55	49	23	-176	118

[1] α_1 = C2-C1-C1'$_A$-C2'$_A$
[2] α_2 = C4-C5-C1'$_B$-C2'$_B$
[3] β_1 = C1'$_A$-C2'$_A$-C1''$_A$-C2''$_A$
[4] β_2 = C1'$_B$-C2'$_B$-C1''$_B$-C2''$_B$
[5] γ = C1-C2-C=N
[6] γ = C5-C4-C=N
[7] ω = C2'$_A$-C1'$_A$-C1'$_B$-C2''$_B$

Table S3. Steric energies (E_{SE}, kcal mol^{-1}), relative steric energies (ΔE_{SE}, kcal mol^{-1}) and percentage populations (% ΔE_{SE}) calculated for low-energy conformers of imine **2c** at the molecular mechanics level.

Conformer	E_{SE}	ΔE_{SE}	% ΔE_{SE}
M0001	0.00	203.13	33.3
M0002	0.28	203.41	20.7
M0003	0.28	203.41	20.7
M0004	0.87	204.00	7.7
M0005	1.48	204.61	2.7
M0006	1.48	204.61	2.7
M0007	1.52	204.65	2.6
M0008	1.52	204.65	2.6
M0009	1.79	204.91	1.6
M0010	1.79	204.91	1.6
M0011	2.13	205.26	0.9
M0012	2.13	205.26	0.9
M0013	2.28	205.41	0.7
M0014	2.66	205.79	0.4
M0015	2.68	205.81	0.4
M0016	2.68	205.81	0.4
M0017	4.26	207.39	0.0
M0018	4.26	207.39	0.0
M0019	4.61	207.74	0.0
M0020	4.61	207.74	0.0
M0021	4.87	208.00	0.0
M0022	4.87	208.00	0.0
M0023	4.94	208.07	0.0
M0024	4.94	208.07	0.0
M0025	5.58	208.71	0.0
M0026	5.58	208.71	0.0
M0027	5.78	208.90	0.0
M0028	5.78	208.90	0.0
M0029	5.96	209.09	0.0
M0030	5.96	209.09	0.0
M0031	5.98	209.11	0.0
M0032	5.98	209.11	0.0
M0033	5.98	209.11	0.0
M0034	5.98	209.11	0.0
M0035	6.02	209.15	0.0
M0036	6.02	209.15	0.0
M0037	6.05	209.18	0.0
M0038	6.07	209.20	0.0
M0039	6.10	209.23	0.0
M0040	6.10	209.23	0.0
M0041	6.18	209.31	0.0
M0042	6.18	209.31	0.0

M0043	6.55	209.68	0.0
M0044	6.55	209.68	0.0
M0045	6.63	209.76	0.0
M0046	6.63	209.76	0.0
M0047	6.64	209.77	0.0
M0048	6.64	209.77	0.0
M0049	6.76	209.89	0.0
M0050	6.76	209.89	0.0
M0051	6.78	209.91	0.0
M0052	6.78	209.91	0.0
M0053	6.88	210.01	0.0
M0054	6.88	210.01	0.0
M0055	7.02	210.15	0.0
M0056	7.02	210.15	0.0
M0057	7.19	210.32	0.0
M0058	7.19	210.32	0.0
M0059	7.20	210.33	0.0
M0060	7.20	210.33	0.0
M0061	7.31	210.43	0.0
M0062	7.31	210.43	0.0
M0063	7.37	210.50	0.0
M0064	7.37	210.50	0.0
M0065	7.49	210.62	0.0
M0066	7.49	210.62	0.0
M0067	7.52	210.65	0.0
M0068	7.52	210.65	0.0
M0069	7.60	210.73	0.0
M0070	7.60	210.73	0.0
M0071	7.84	210.97	0.0
M0072	7.84	210.97	0.0
M0073	7.94	211.06	0.0
M0074	7.94	211.06	0.0
M0075	7.99	211.11	0.0
M0076	7.99	211.11	0.0
M0077	8.16	211.29	0.0
M0078	8.16	211.29	0.0
M0079	8.51	211.64	0.0
M0080	8.51	211.64	0.0
M0081	8.54	211.66	0.0
M0082	8.54	211.66	0.0
M0083	8.69	211.81	0.0
M0084	8.75	211.88	0.0
M0085	8.83	211.96	0.0
M0086	8.83	211.96	0.0
M0087	8.87	211.99	0.0
M0088	8.87	211.99	0.0

M0089	8.88	212.01	0.0
M0090	8.88	212.01	0.0
M0091	8.89	212.02	0.0
M0092	8.89	212.02	0.0
M0093	9.04	212.17	0.0
M0094	9.22	212.35	0.0
M0095	9.23	212.36	0.0
M0096	9.24	212.37	0.0
M0097	9.24	212.37	0.0
M0098	9.71	212.84	0.0
M0099	9.99	213.12	0.0
M0100	9.99	213.12	0.0

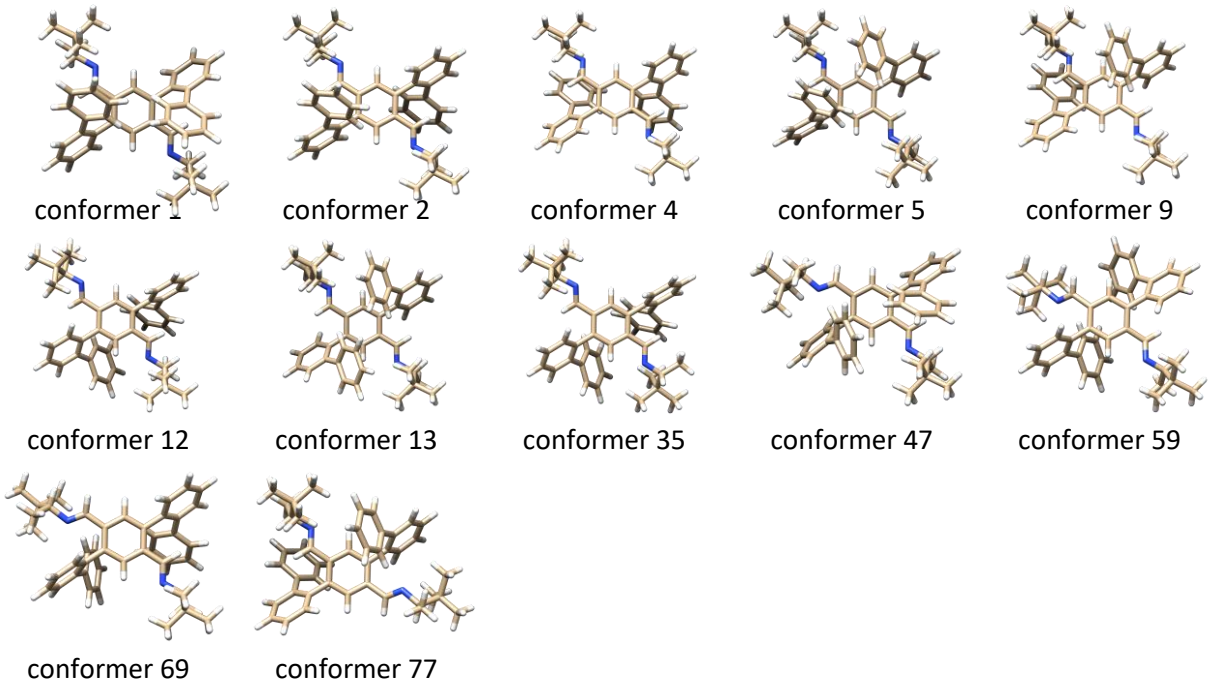


Figure S1. Calculated at the B3LYP-GD3BJ/6-311++G(d,p) level structures of thermally accessible conformers of compound **2c**.

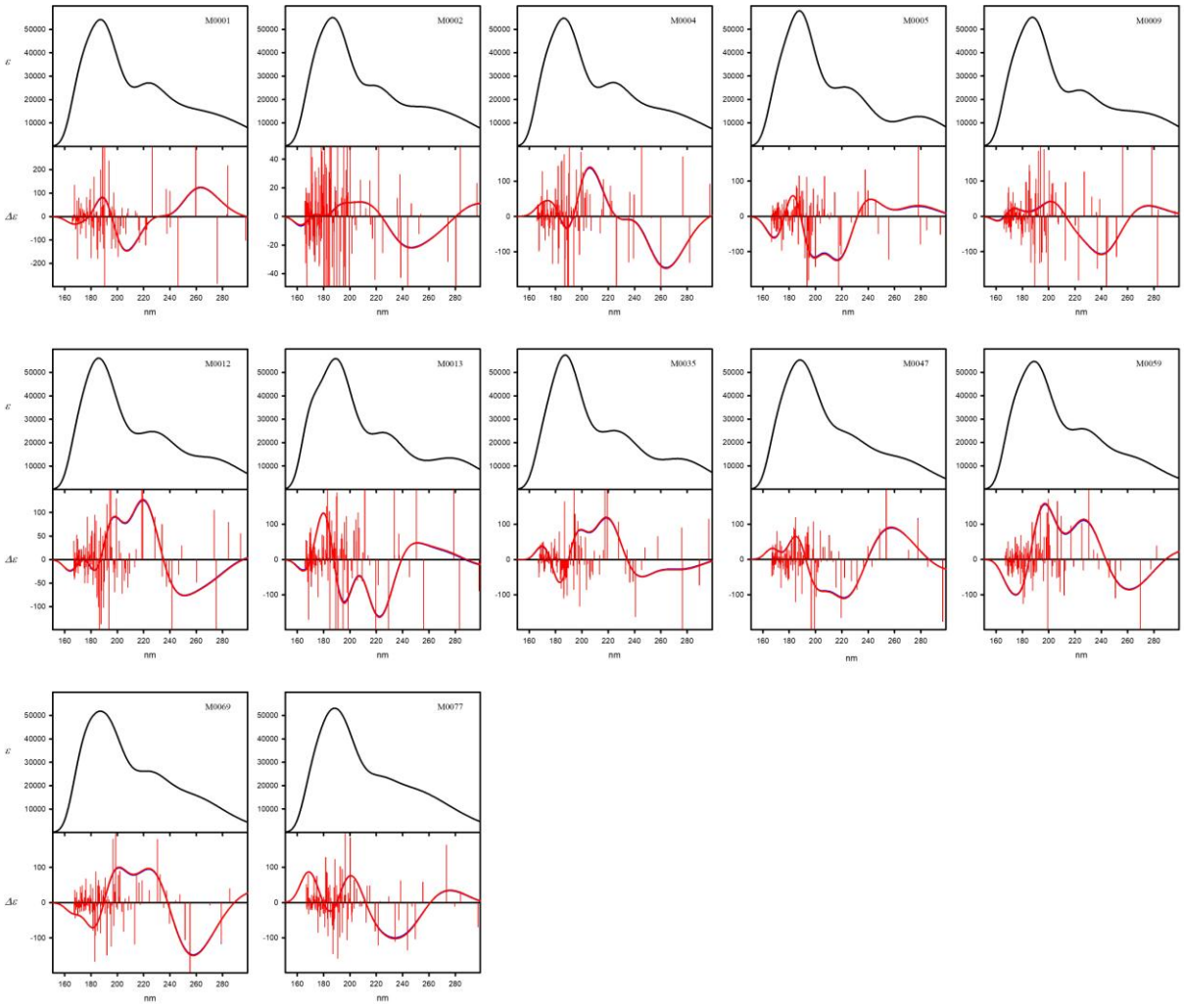


Figure S2. ECD spectra of low-energy conformers of imine **2c** calculated at TD-CAM-B3LYP/6-311++g(d,p) level. Wavelengths have not been corrected.

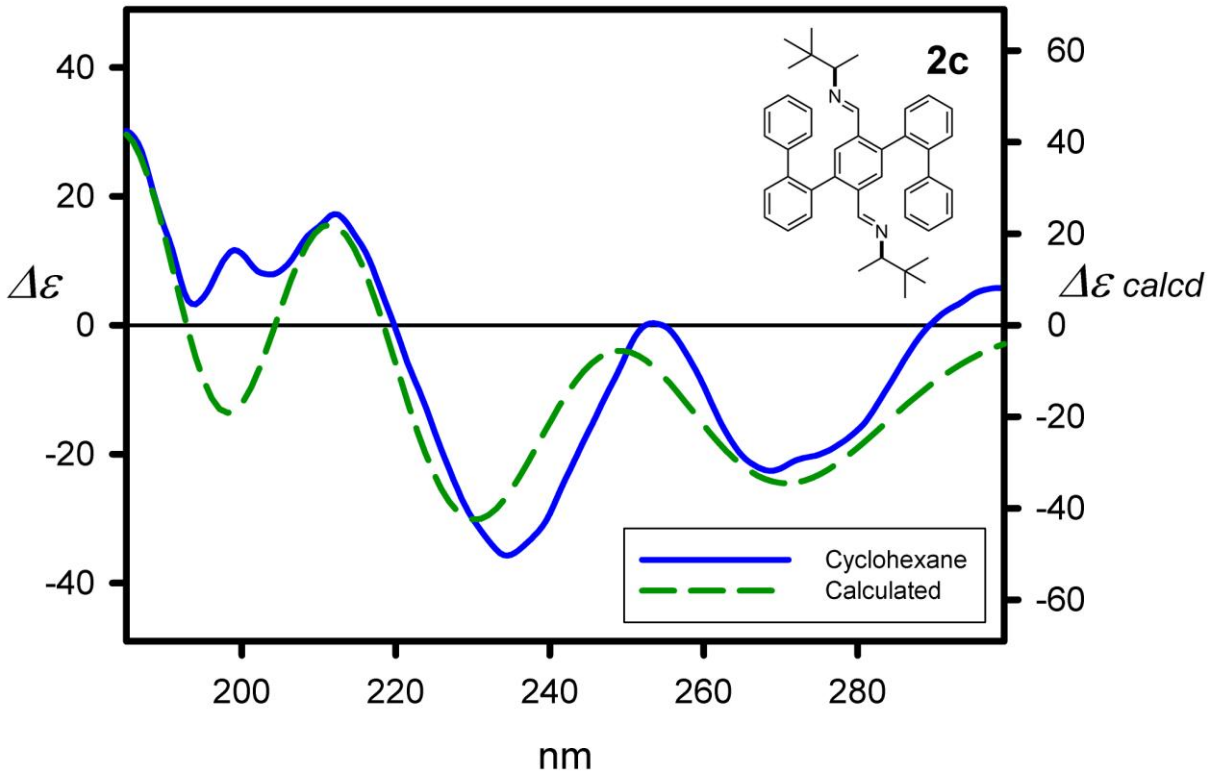


Figure S3. Measured in cyclohexane (solid blue line) and calculated (dashed green line) at TD-CAM-B3LYP/6-311++g(d,p) level spectra of diimine **2c**. Wavelengths have been corrected to match experimental UV maxima.

III. Single crystals X-ray analysis

A colourless single crystals of **1**, **2a**-**2f**, **2h** and **2k** suitable for X-ray structural analysis were obtained by slow evaporation of solution. The diffraction data for **1**, **2a**, **2c**, **2f**, **2k** were collected at 130 K with an Oxford Diffraction SuperNova diffractometer and for **2b**, **2d**, **2e**, **2h**, at 100 K with Rigaku XtaLAB Synergy-R diffractometer, both using Cu Kα radiation (λ = 1.54184 Å). The intensity data were collected and processed using CrysAlis PRO software [8,9]. The structures were solved by direct methods with the program SHELXT 2018/2 [10] and refined by full-matrix least-squares method on F^2 with SHELXL 2018/3 [11]. The carbon-bound hydrogen atoms were refined as riding on their carriers and their displacement parameters were set equal to 1.5Ueq(C) for the methyl groups and 1.2Ueq(C) for the remaining H atoms. Absolute structures of the compounds were specified by the synthetic procedure and confirmed using Flack parameter [12].

A summary of the crystallographic data is given in **Table S4**. Molecular graphics were generated with Olex2 [13] and Mercury CSD 4.3.1 software [14]. ORTEP representation of the molecular structures of the reported compounds are presented in **Figure S4**-**S11**.

The molecule of compound **2a** is disordered. One of the 2-buthyl substituent can adapts either extended or bent conformation, while the second one is in an extended conformation. Refined occupation factors for alternative orientation are 0.63 for extended and 0.36 for bent chain (see **Figure S5**). In refinement process for atoms C36 C33 C34 C35 C35A RIGU restrain was used.

Also in crystal structure of **2b** the molecule is slightly disordered and one of the alkyl chain can adopt two alternative orientation (see **Figure S6**). Refined occupancy factor for those chains are 0.82 and 0.18. For atom C34A in refinement process ISOR 0.005 0.01 restrain was used.

The crystal of **2c** used for diffraction measurement was twinned and this was taken into account in data reduction process. The refined BASF factor was 0.261.

The alkyl substituents of compound **2e** in crystal structure are strongly disordered. For disordered fragments substituent geometrical restrains was used: DFIX 1.54 for all C-C bonds, ISOR 0.01 0.02 for atom C34A, and RIGU for both position of disordered part. The ratio of refined occupancy factors was 0.56/0.44 and 0.68/0.32 for substituents on both sides of molecule.

Compound **2f** crystallizes as a solvate. There are two symmetrically independent voids filled with a solvent, which are strongly disordered ethanol molecules. The SQUEEZ procedure was used in the refinement process. Additionally, the following constraints were used for the atoms O1A, C11A, C12A, C13A and C14A: DELU 0.005 0.005 and RIGU 0.003 0.003.

Compound **2k** crystallizes as a solvate, with disordered 2-propanol molecules located in channels. For 2-propanol molecules geometrical restrains was used: DFIX 1.54 for all C-C bonds, DFIX 1.43 for C-O bonds, RIGU 0.002 0.002 and additionally ISOR 0.05 0.02 for some atoms.

Table S4. Selected crystal data and structure refinement details for **1**, **2a** – **2f**, **2h** and **2k**.

	1	**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2h**	**2k**
Chemical formula	$C_{32}H_{22}O_2$	$C_{40}H_{40}N_2$	$C_{42}H_{44}N_2$	$C_{48}H_{48}N_2$	$C_{48}H_{54}N_2$	$C_{52}H_{56}N_2$	$C_{40}H_{36}N_2O_2$ 2[C_2H_5OH]	$C_{48}H_{40}N_2$	$C_{60}H_{50}N_4O_4$ 2[C_3H_7OH]
Mr	438.49	548.74	576.79	604.84	658.93	708.98	576.71	644.82	995.10
Crystal system, space group	Triclinic, $P\overline{1}$	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Monoclinic, $C2$	Monoclinic, $P2_1$	Monoclinic, $P2_1$
Temperature (K)	130	130	100	130	100	100	130	100	130
a, *b*, *c* (Å)	8.1728 (4), 8.3473 (3), 9.4540 (4)	9.1325 (3), 13.4292 (5), 26.0931 (11)	13.4156 (1), 8.9957 (1), 14.3921 (1)	13.1433 (2), 9.34771 (16), 14.5023 (3)	13.7099 (3), 9.1714 (2), 15.9916 (4)	13.1850 (5), 9.8466 (4), 15.6192 (6)	17.7649 (7), 12.5517 (5), 16.5841 (8)	12.9567 (2), 10.2150 (1), 14.0973 (2)	12.93432 (13), 13.85518 (17), 16.61444 (16)
α,β,γ (°)	78.344 (3), 74.283 (4), 64.517 (4)		98.140 (1)	97.5242 (18)	108.914 (3)	97.853 (4)	110.403 (5)	105.680 (1)	102.318 (1)
V (Å^3)	557.73 (5)	3200.1 (2)	1719.38 (3)	1766.40 (5)	1902.20 (9)	2008.78 (14)	3465.9 (3)	1796.38 (4)	2908.88 (5)
Z	1	4	2	2	2	2	4	2	2
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu K?	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.63	0.50	0.48	0.49	0.49	0.50	0.53	0.52	0.58
Crystal size (mm)	0.41 × 0.11 × 0.09	0.35 × 0.05 × 0.01	0.36 × 0.12 × 0.02	0.4 × 0.2 × 0.03	0.2 × 0.1 × 0.02	0.1 × 0.05 × 0.02	0.25 × 0.2 × 0.07	0.22 × 0.18 × 0.05	0.22 × 0.2 × 0.07
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11515, 2300, 2120	18862, 6590, 5100	26193, 6868, 6478	11621, 11621, 10100	34691, 7517, 6732	33663, 7879, 5850	20211, 6583, 6119	31683, 7264, 7032	51987, 11992, 10983
R_{int}	0.030	0.058	0.033	0.056	0.058	0.055	0.033	0.035	0.030
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.037, 0.098, 1.04	0.064, 0.178, 1.02	0.036, 0.093, 1.06	0.051, 0.146, 1.06	0.053, 0.151, 1.07	0.050, 0.138, 1.02	0.067, 0.209, 1.05	0.030, 0.077, 1.05	0.055, 0.154, 1.07
No. of parameters	154	394	452	424	454	700	397	453	796
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.19, -0.19	0.35, -0.22	0.17, -0.20	0.18, -0.20	0.37, -0.31	0.32, -0.15	0.29, -0.25	0.15, -0.19	0.51, -0.29
Absolute structure parameter	-	-0.3 (9)	-0.39 (18)	0.5 (6)	-0.6 (4)	-0.3 (6)	2.1 (5)	0.08 (17)	-0.09 (7)

Table S5. Selected dihedral angles *α*, *β*, *γ*, and *ω* (in degrees) observed in the crystal structures of compounds **1**, **2a** – **2f**, **2h** and **2k**.

		α1	*α2*	*β1*	*β2*	*γ1*	*γ2*	*ω*
1		-63.03 (15)	-	-53.20 (15)	-	176.81 (11)	-	180.00
2a		-64.3 (5)	65.1 (5)	-50.0 (5)	47.0 (5)	-176.0 (4)	166.7 (4)	-179.3 (4)
2b		-61.1 (3)	63.3 (3)	-48.2 (3)	49.4 (3)	176.17 (18)	162.6 (2)	-179.9 (2)
2c		-64.1 (6)	63.7 (6)	-50.4 (6)	46.8 (6)	-166.3 (4)	-177.1 (4)	-177.9 (5)
2d		-69.7 (4)	63.1 (4)	-52.0 (4)	46.3 (4)	-163.8 (3)	-174.6 (3)	175.2 (3)
2e		-66.2 (5)	64.7 (5)	-54.2 (5)	52.3 (5)	170.1 (5) -157.2 (8)	-163.0 (6) -155.4 (9)	179.8 (4)
2f	**mol A**	-58.7 (7)	-	-49.3 (8)	-	171.7 (6)	-	58.9 (7)
	mol B	62.2 (7)	-	49.4 (8)	-	-172.5 (6)	-	-55.7 (7)
2h		-65.2 (2)	60.9 (2)	-54.0 (2)	55.7 (2)	171.75 (17)	-171.87 (15)	173.51 (16)
2k		59.4 (5)	59.8 (5)	44.7 (5)	45.3 (5)	-163.5 (4)	-163.4 (3)	-61.3 (3)

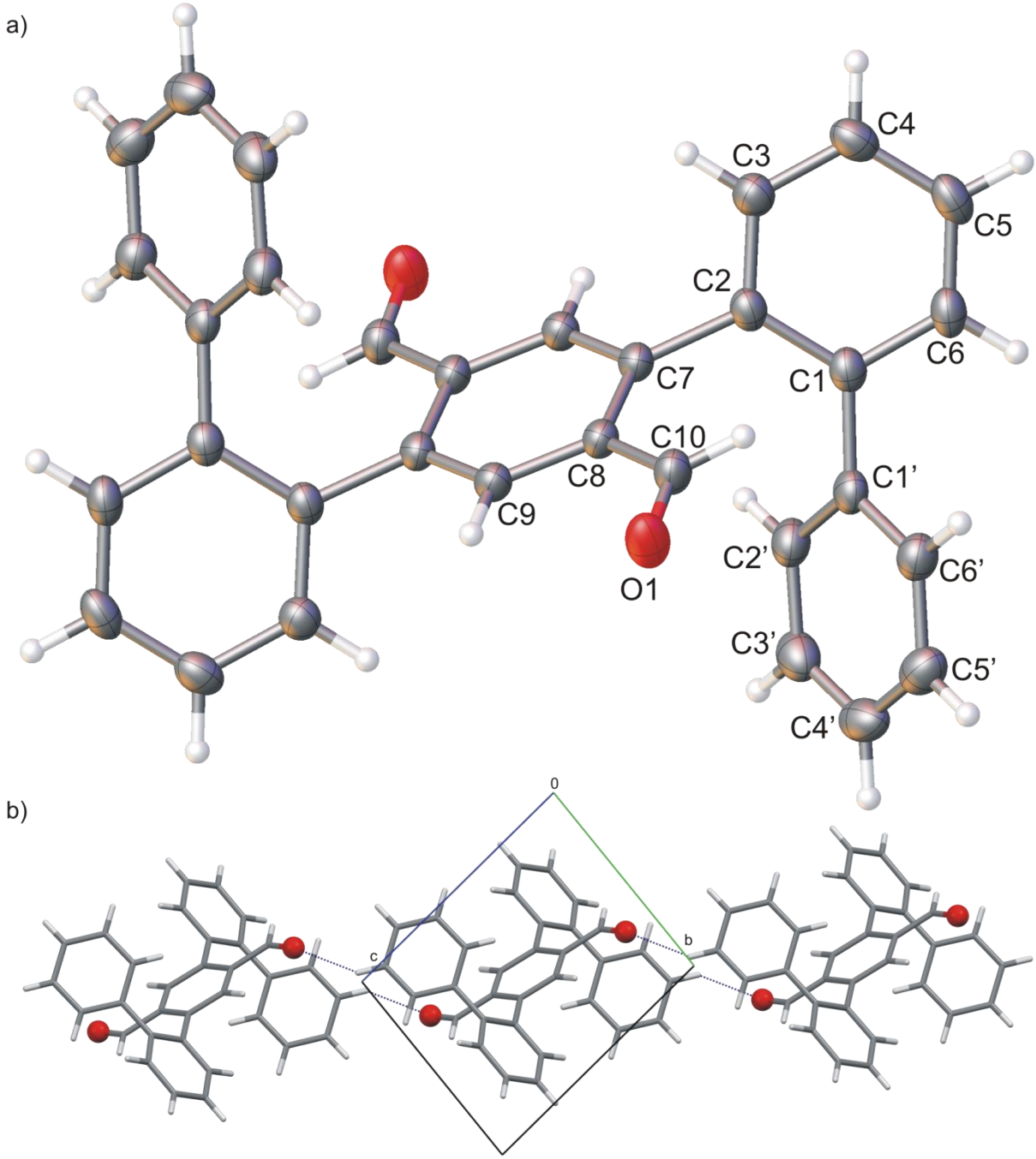


Figure S4. a) Molecular structure of compound **1** (numbering scheme shown for asymmetric part for clarity) and b) C-H···O interactions in crystal structure (O-atoms shown as balls).

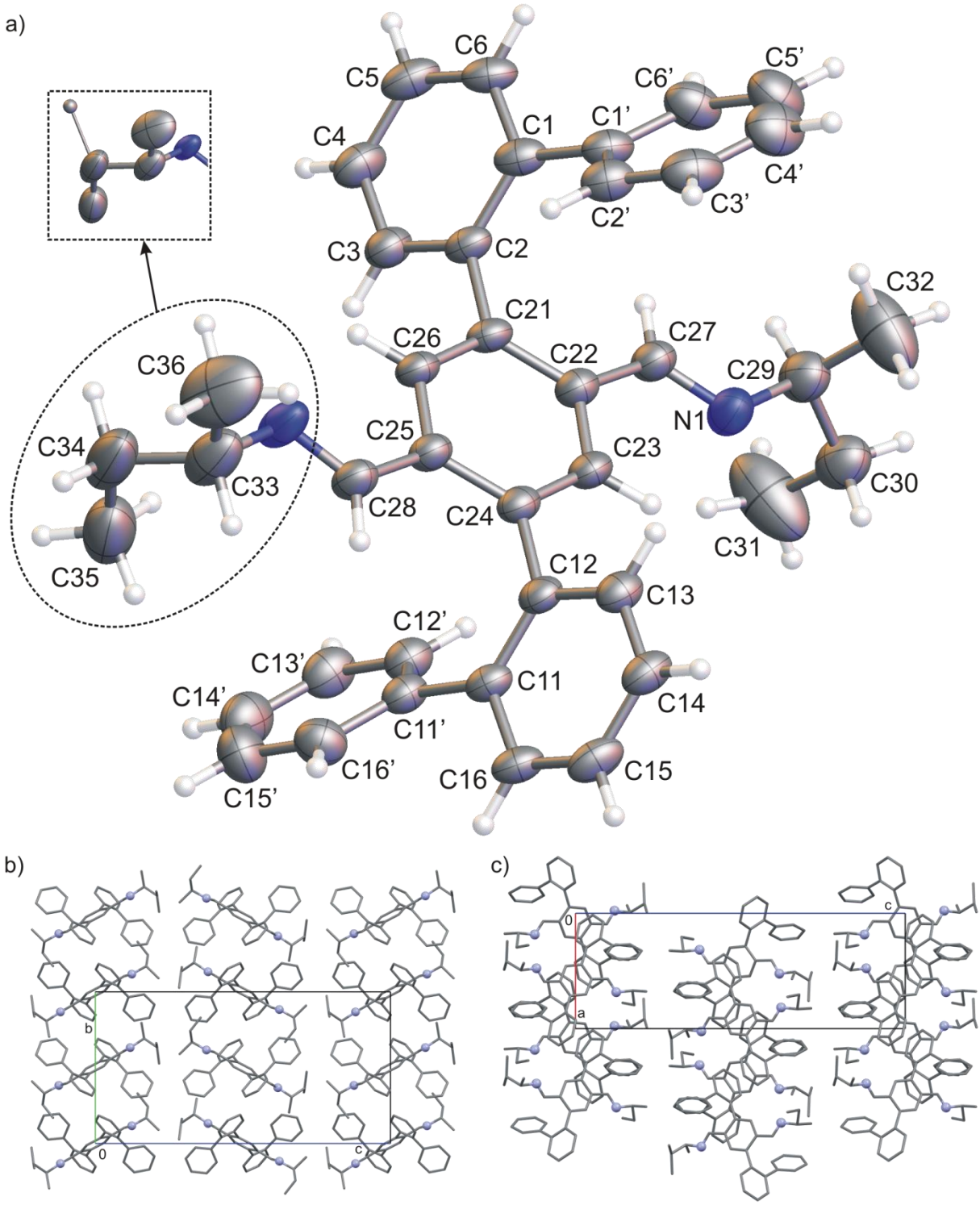


Figure S5. a) Molecular structure of **2a** and atoms numbering scheme. The disorder model shown in the box (minor occupancy fragment shown as a balls with thinner bonds). Crystal packing b) view along a axis and c) view along b axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

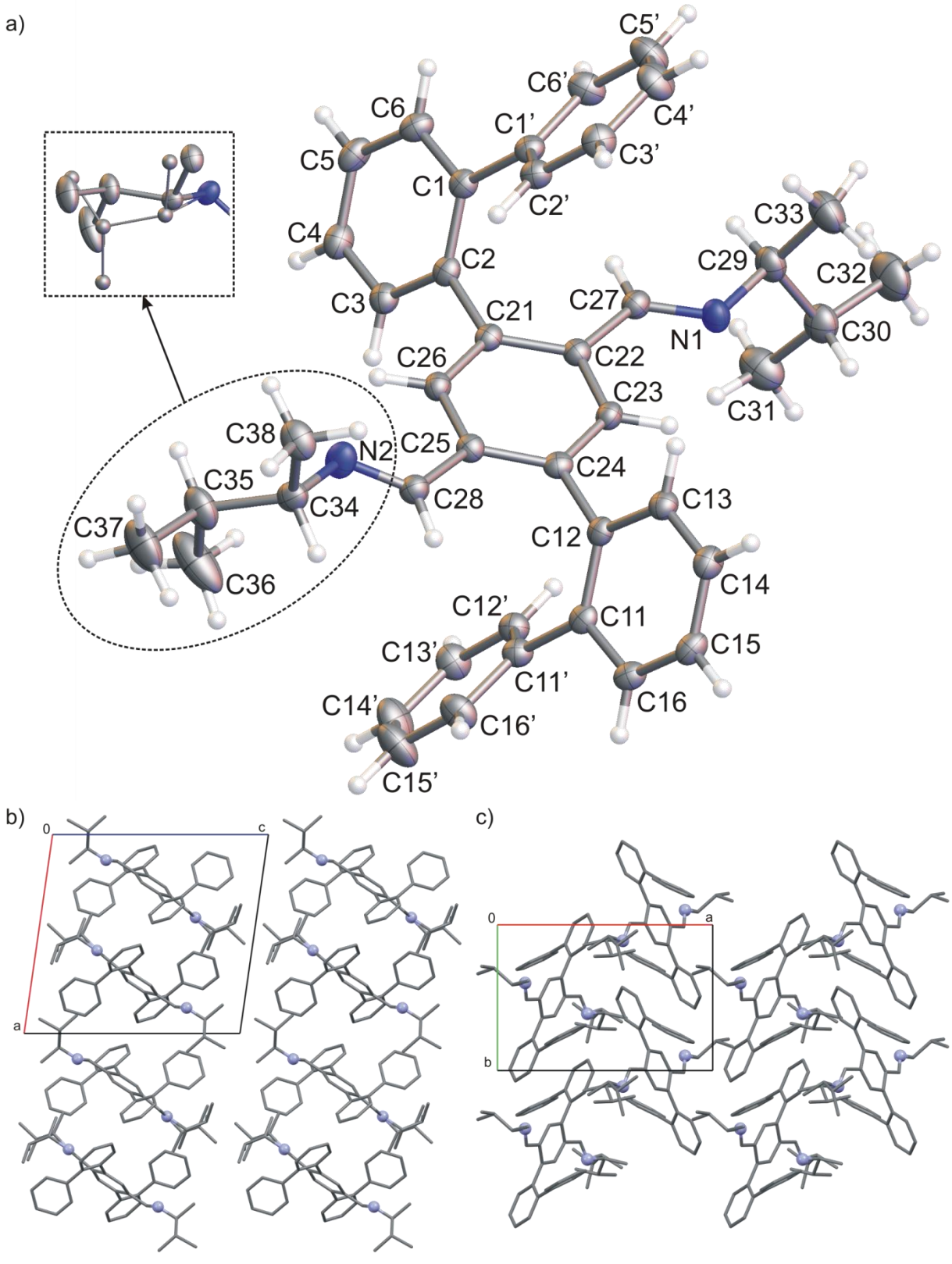


Figure S6. a) Molecular structure of **2b** and atoms numbering scheme. The disorder model shown in the box (minor occupancy fragment shown as a balls with thinner bonds). Crystal packing b) view along b axis and c) view along c axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

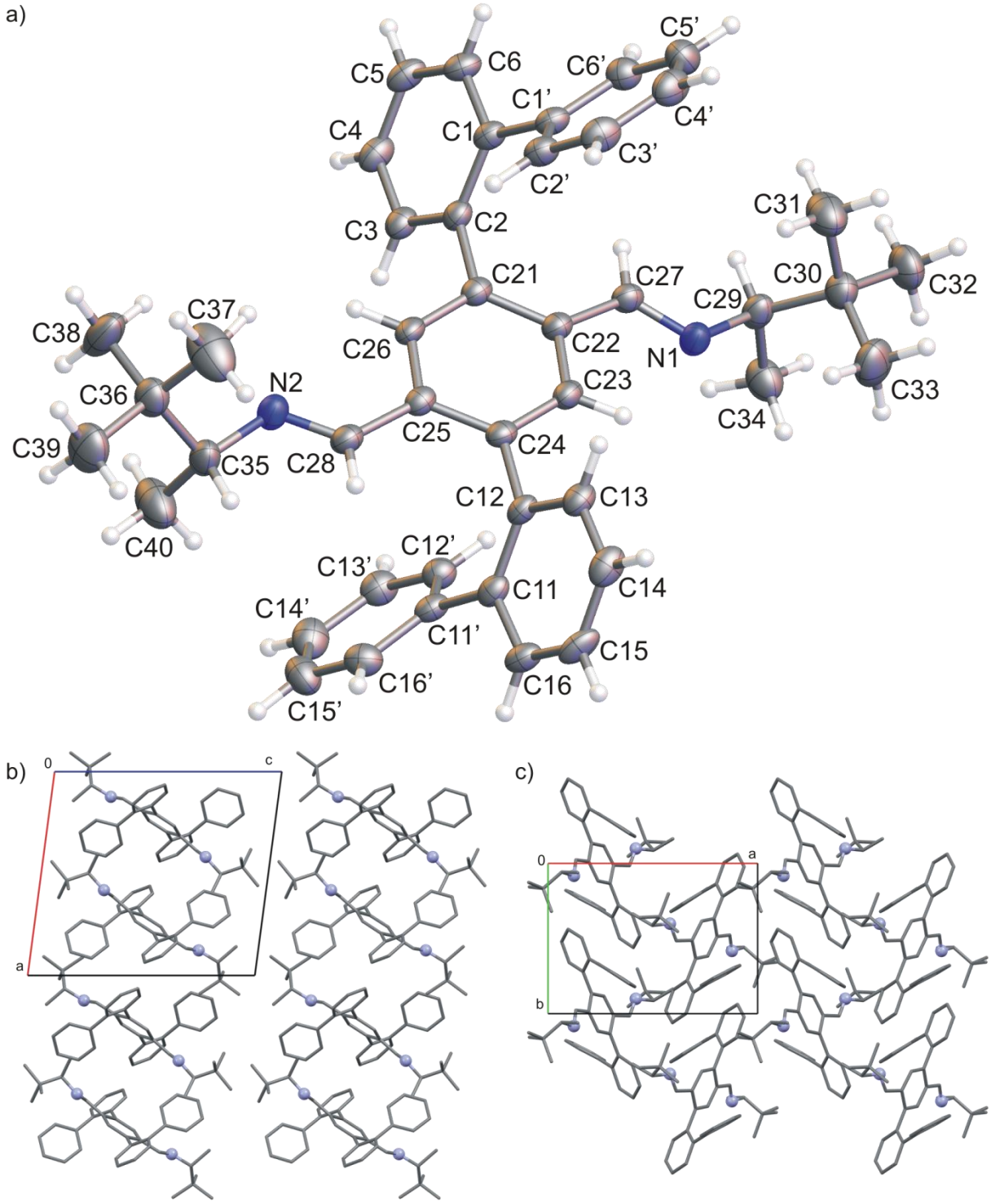


Figure S7. a) Molecular structure of **2c** and atoms numbering scheme. Crystal packing b) view along b axis and c) view along c axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

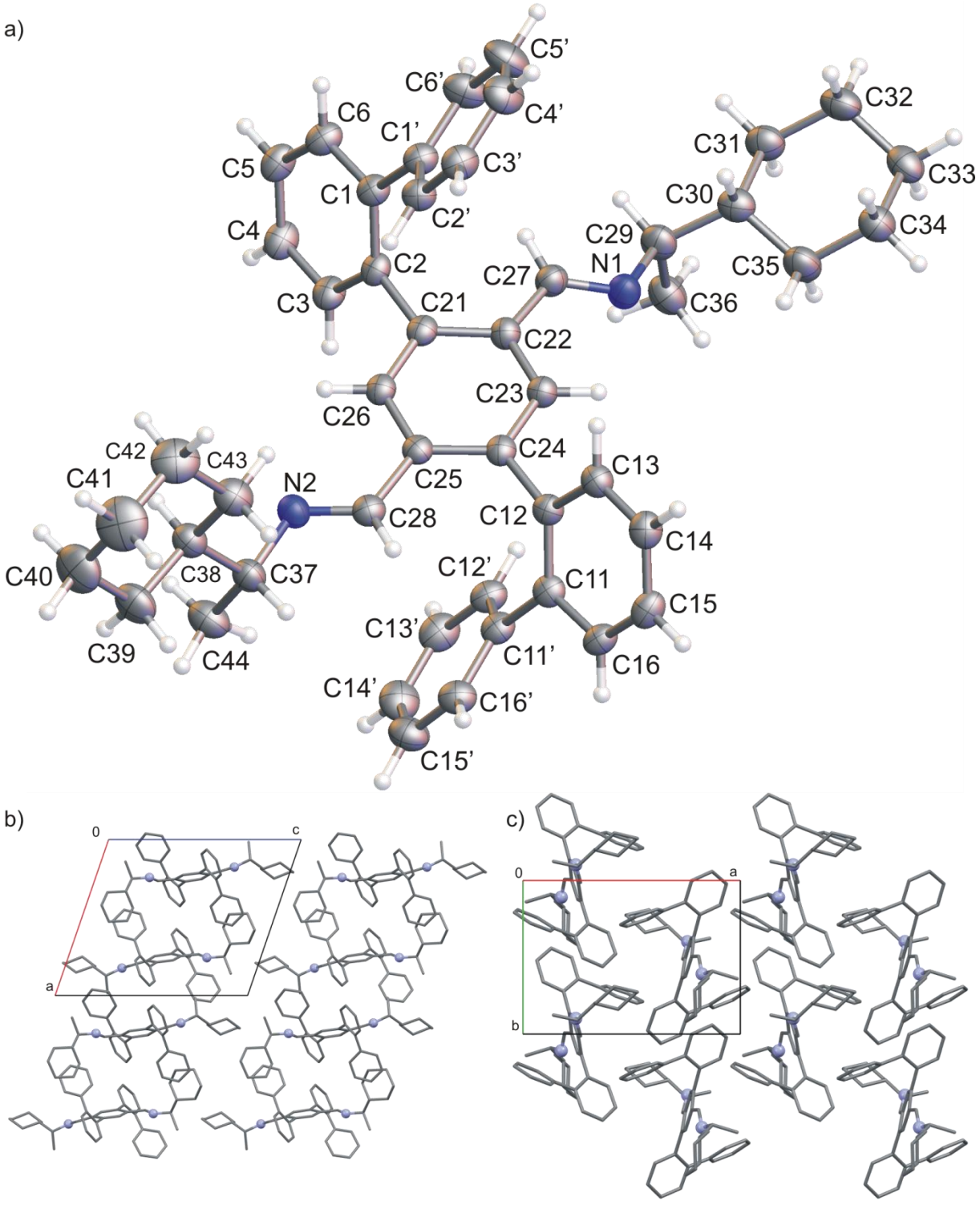


Figure S8. a) Molecular structure of **2d** and atoms numbering scheme. Crystal packing b) view along b axis and c) view along c axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

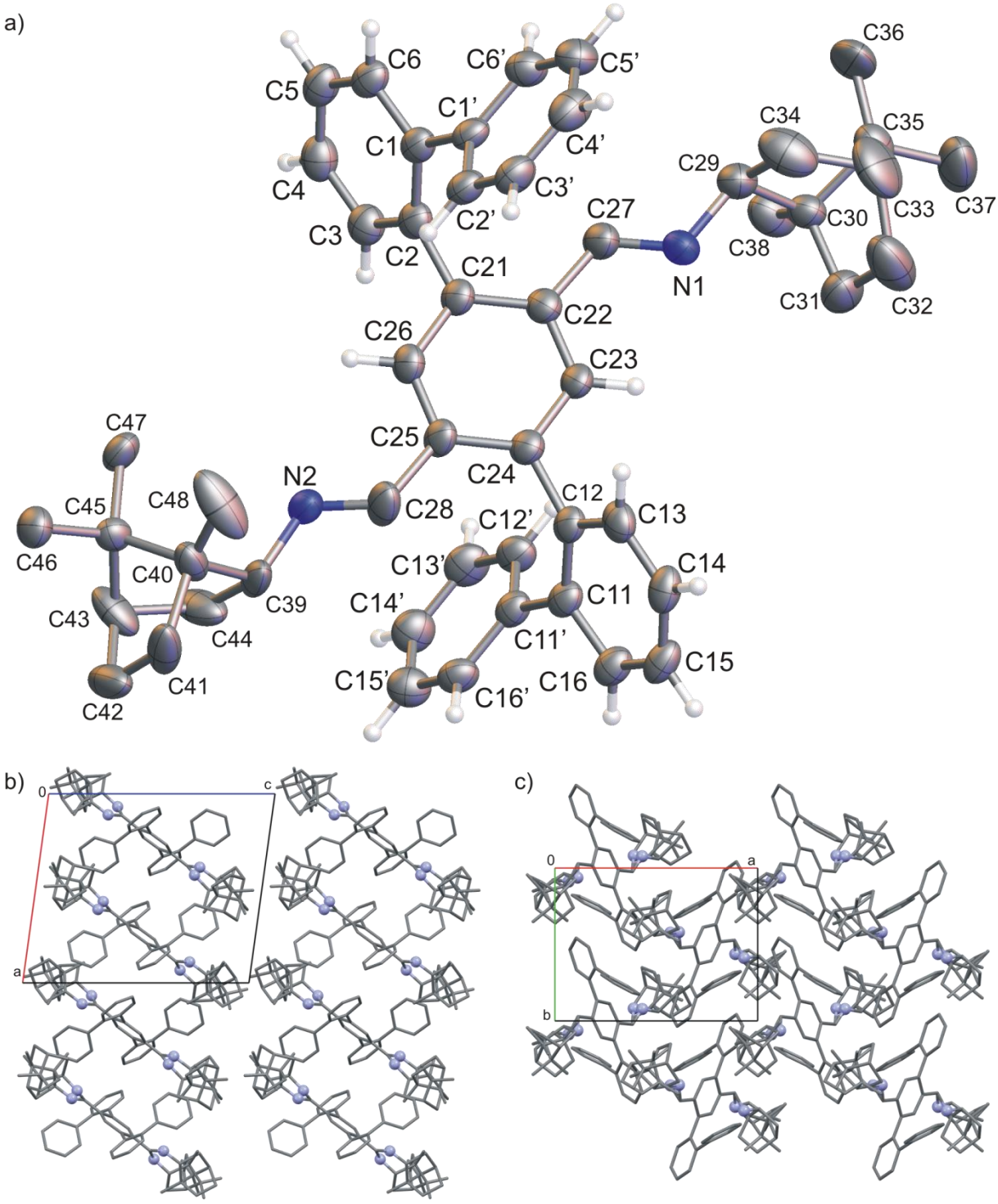


Figure S9. a) Molecular structure of **2e** and atoms numbering scheme. Crystal packing b) view along b axis and c) view along c axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

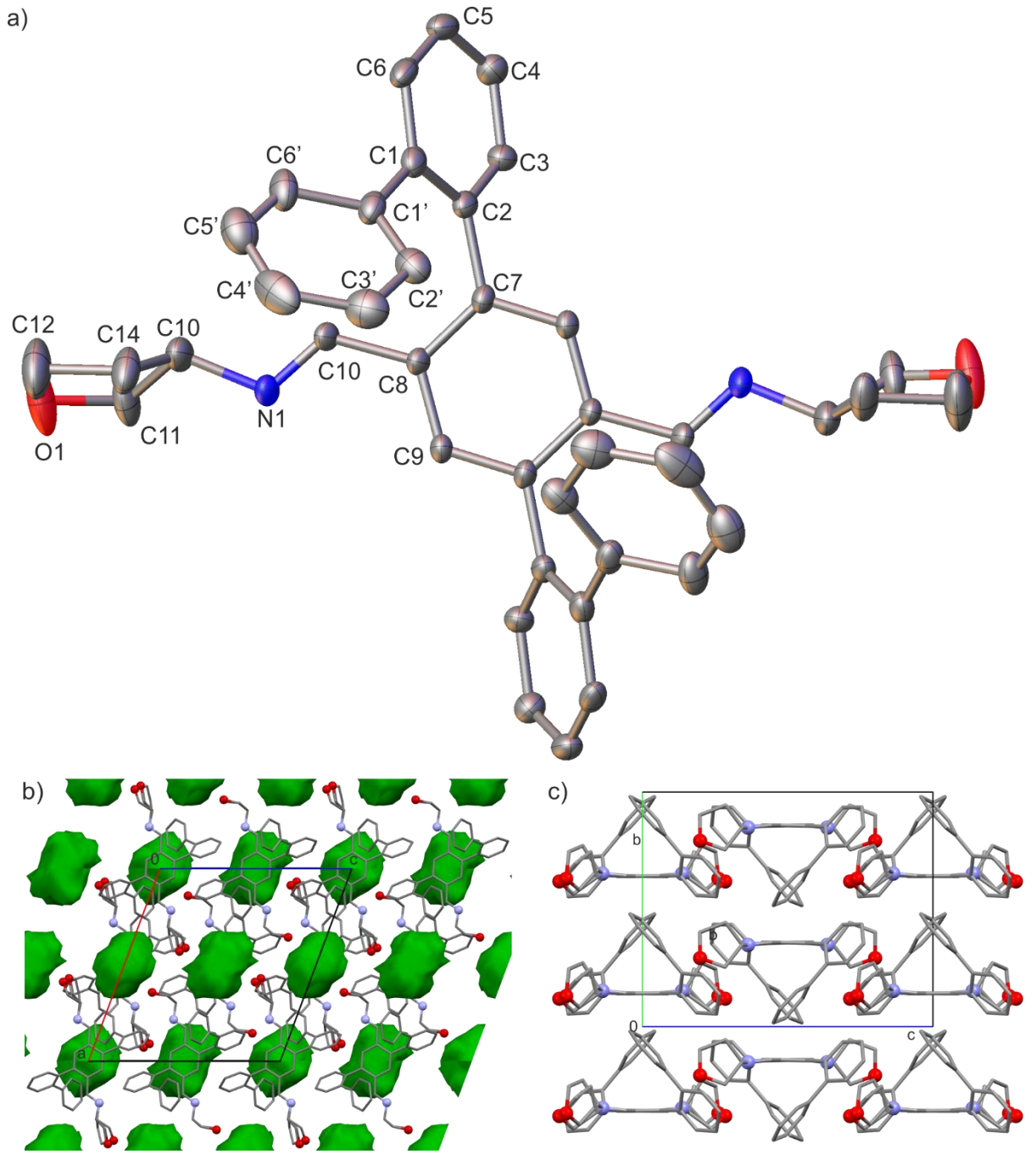


Figure S10. a) Molecular structure of one of the independent molecules in crystal structure of **2f** and atoms numbering scheme (shown for asymmetric part), b) voids in crystal structure, view along b axis and c) molecular packing, view along a axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

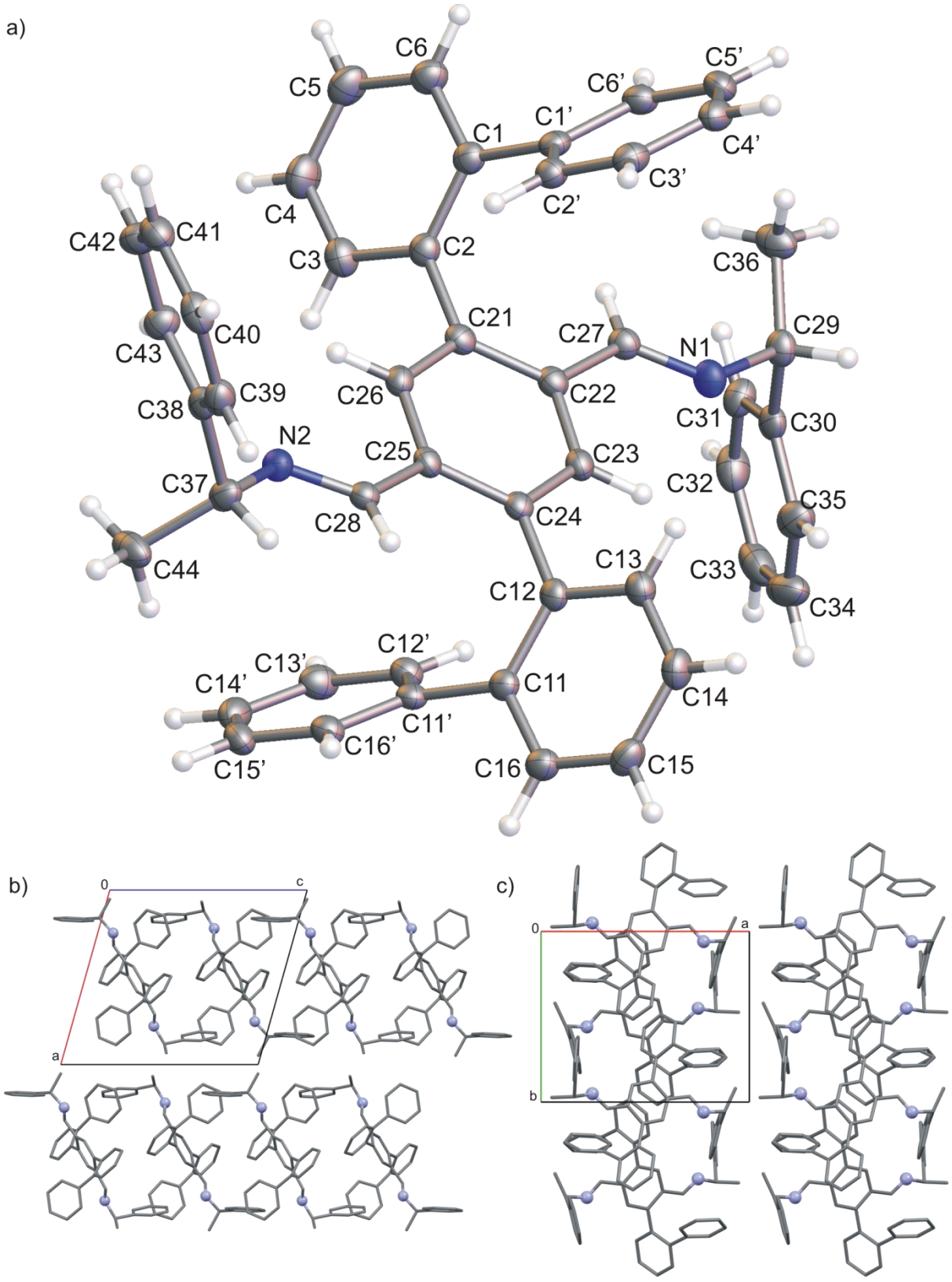


Figure S11. a) Molecular structure of **2h** and atoms numbering scheme. Crystal packing b) view along b axis and c) view along c axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

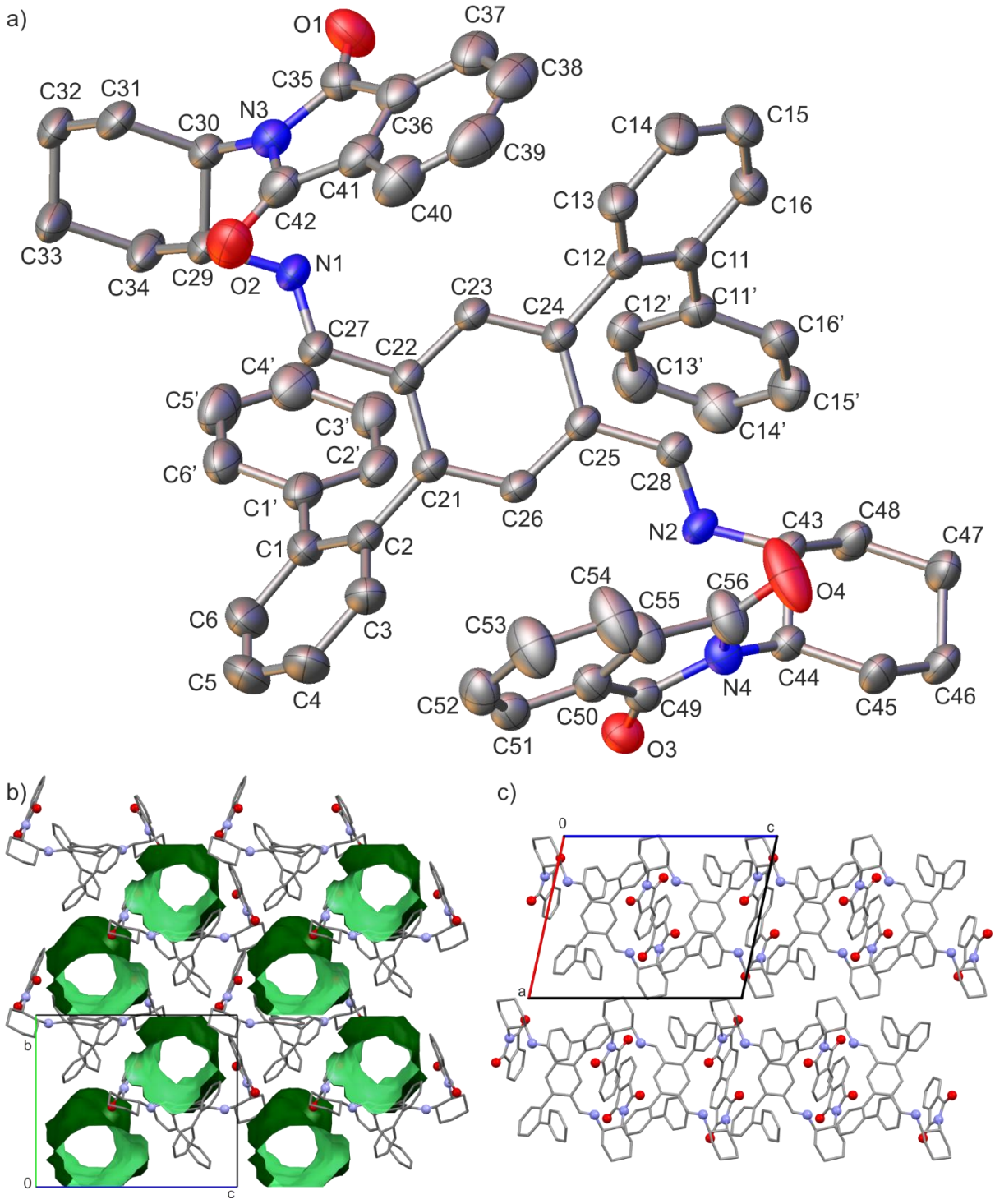


Figure S12. a) Molecular structure of **2k** and atoms numbering scheme, b) structural channels in crystal structure, view along a axis and c) molecular packing, view along c axis. N-atoms shown as balls and hydrogen atoms are omitted for clarity.

IV. Measured NMR spectra of studied compounds

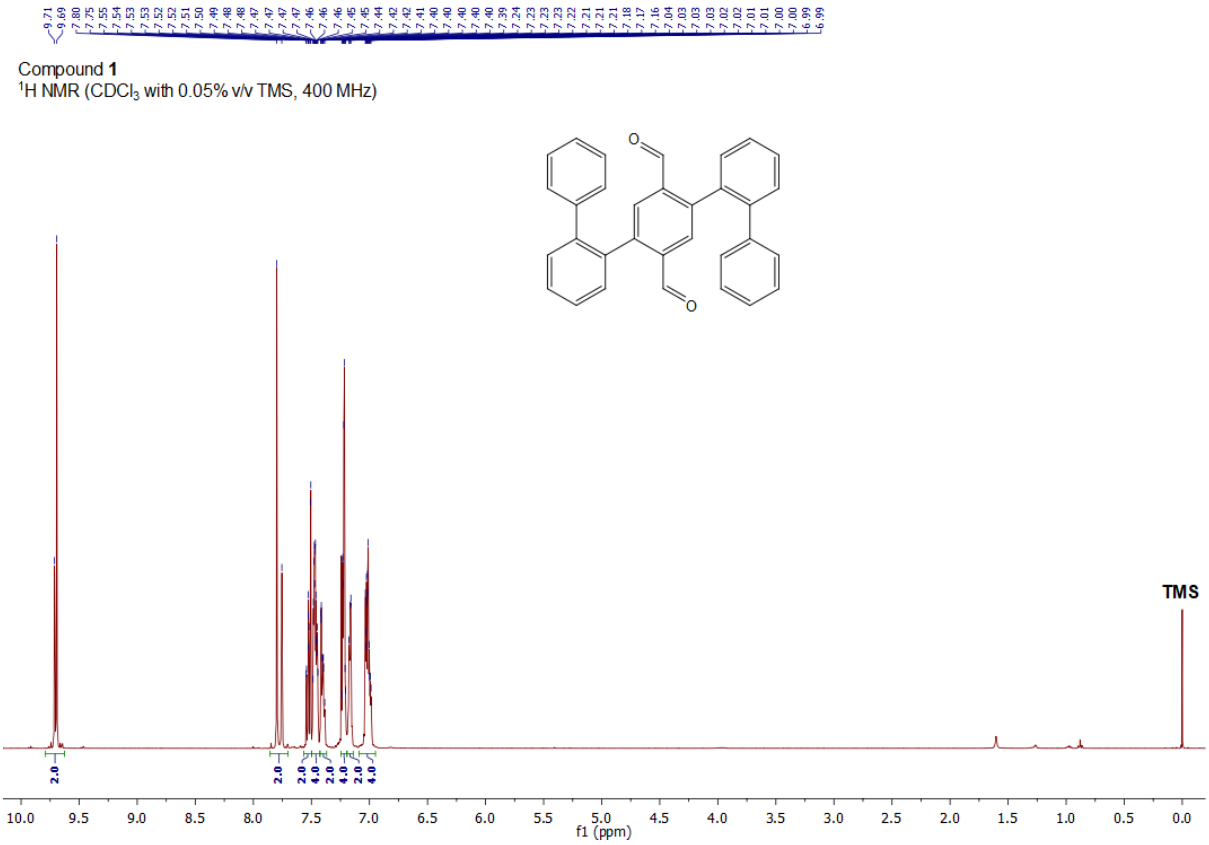


Figure S13. Copy of ^{1}H NMR spectrum of studied dialdehyde **1** measured in $CDCl_3$.

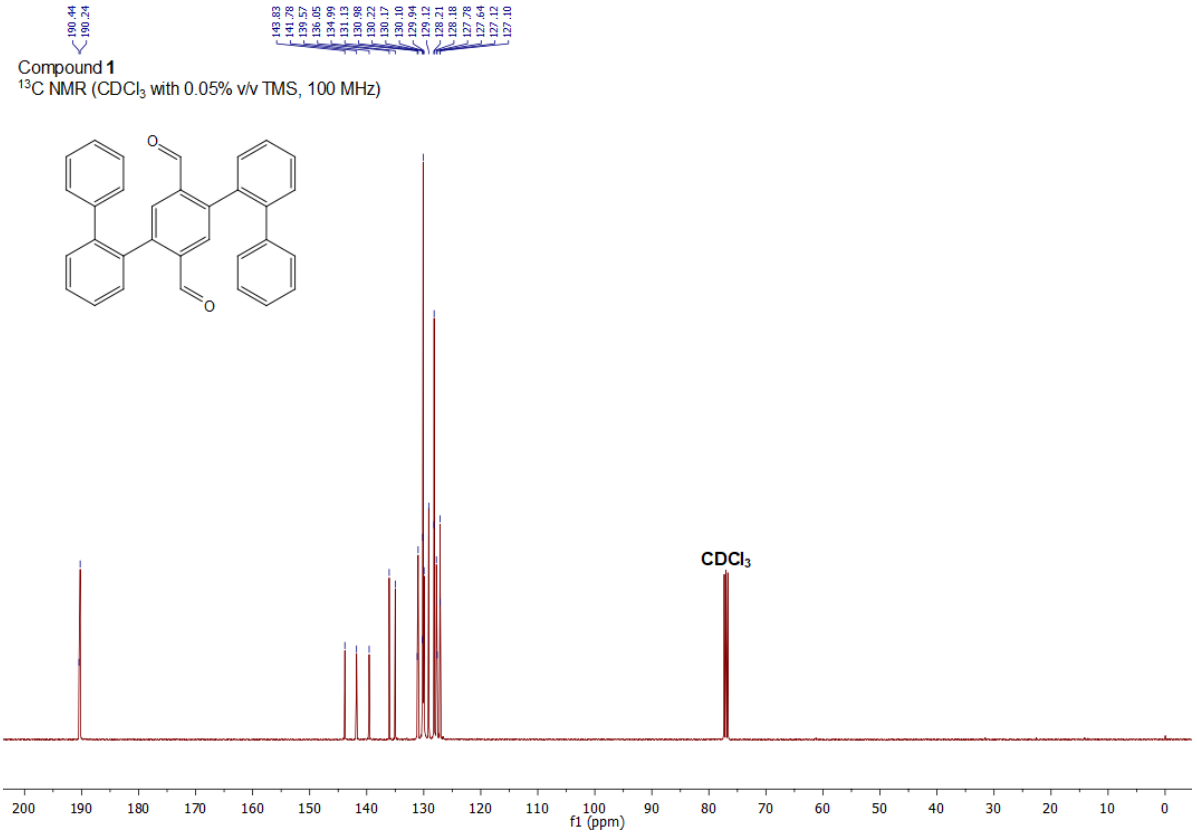


Figure S14. Copy of ^{13}C NMR spectrum of studied dialdehyde **1** measured in $CDCl_3$.

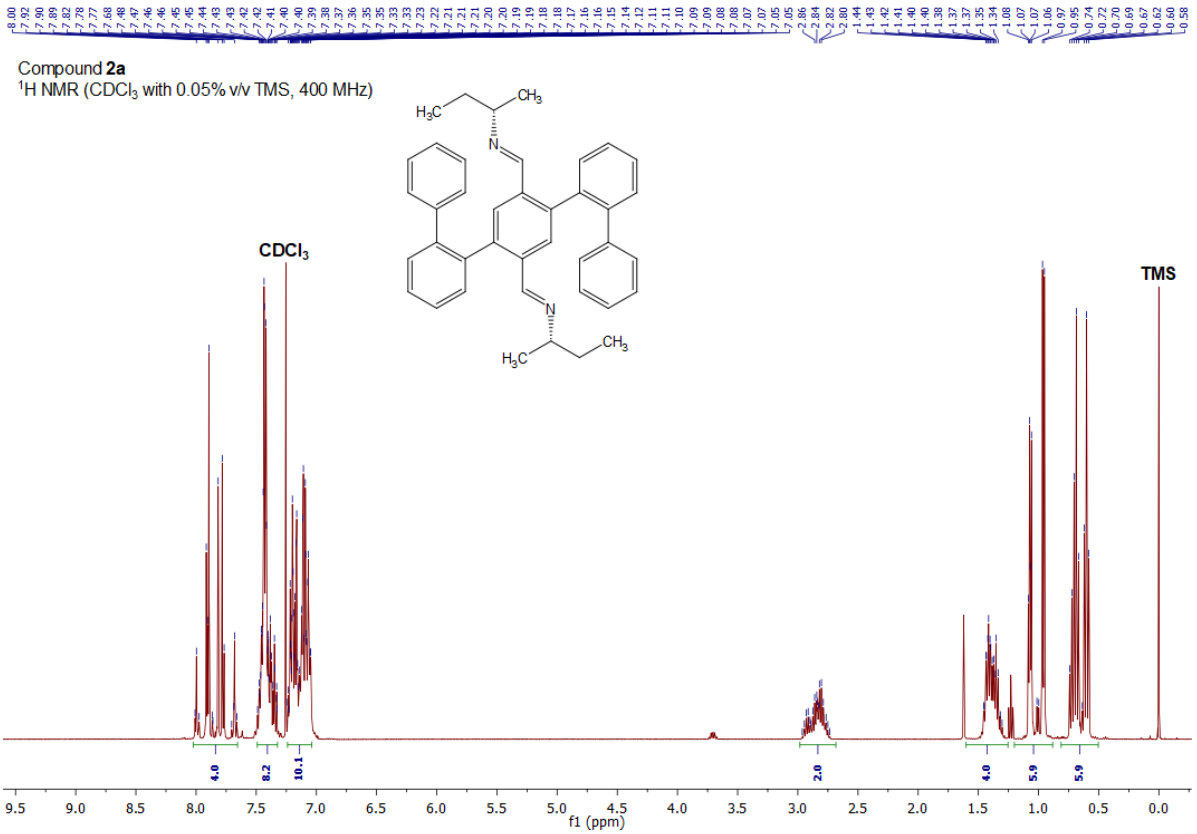


Figure S15. Copy of ^{1}H NMR spectrum of studied diimine **2a** measured in $CDCl_3$.

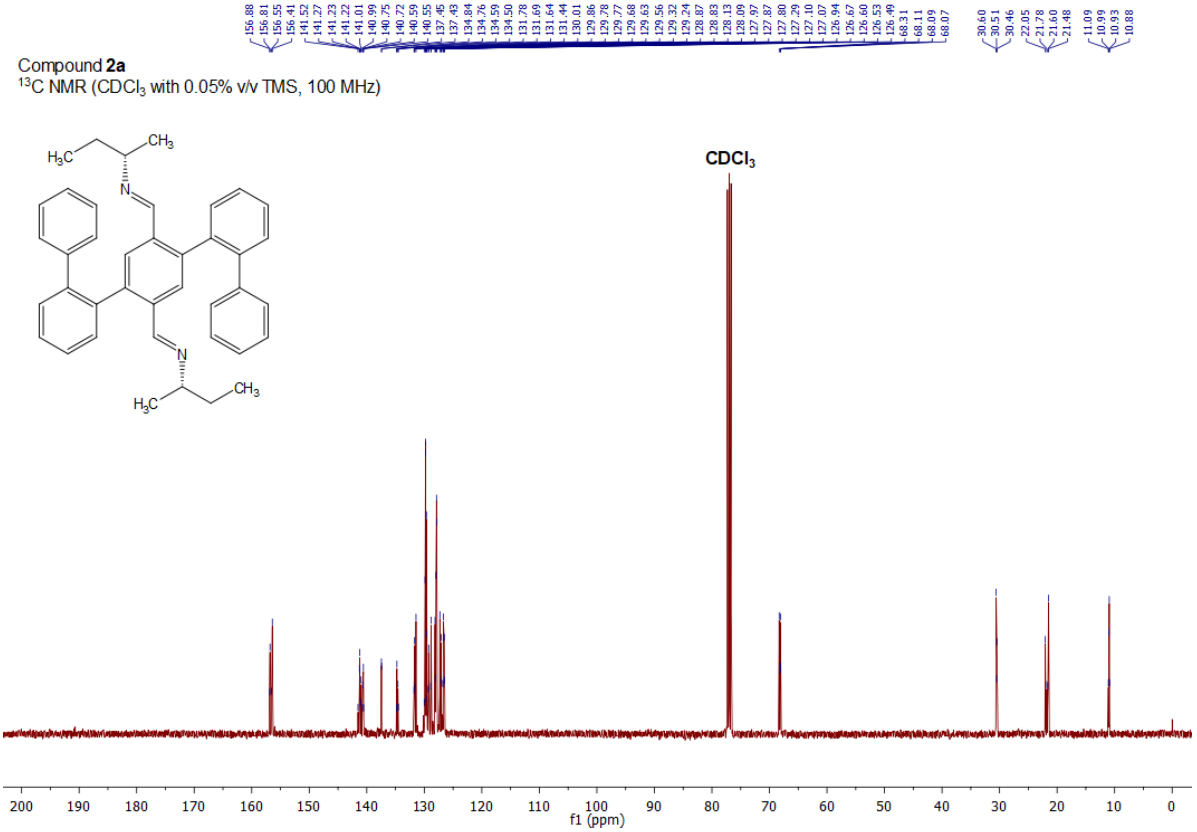


Figure S16. Copy of ^{13}C NMR spectrum of studied diimine **2a** measured in $CDCl_3$.

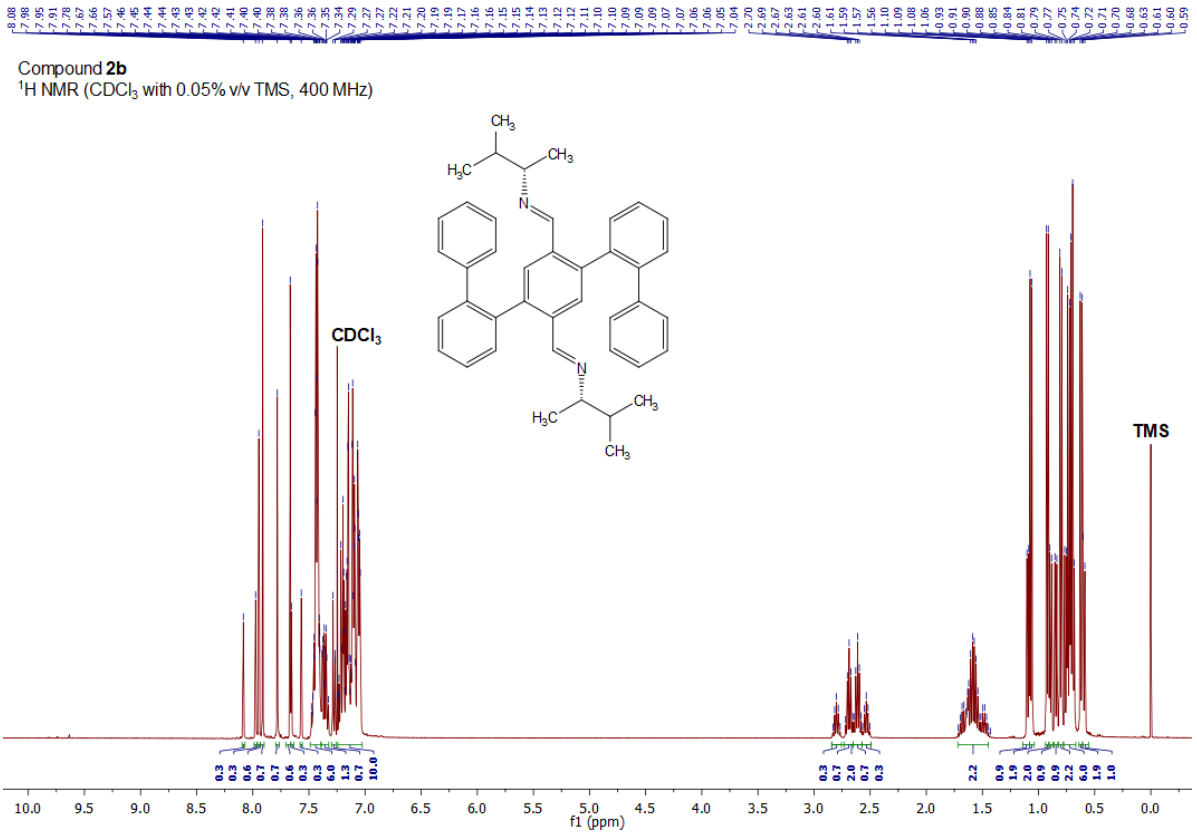


Figure S17. Copy of ^{1}H NMR spectrum of studied diimine **2b** measured in $CDCl_3$.

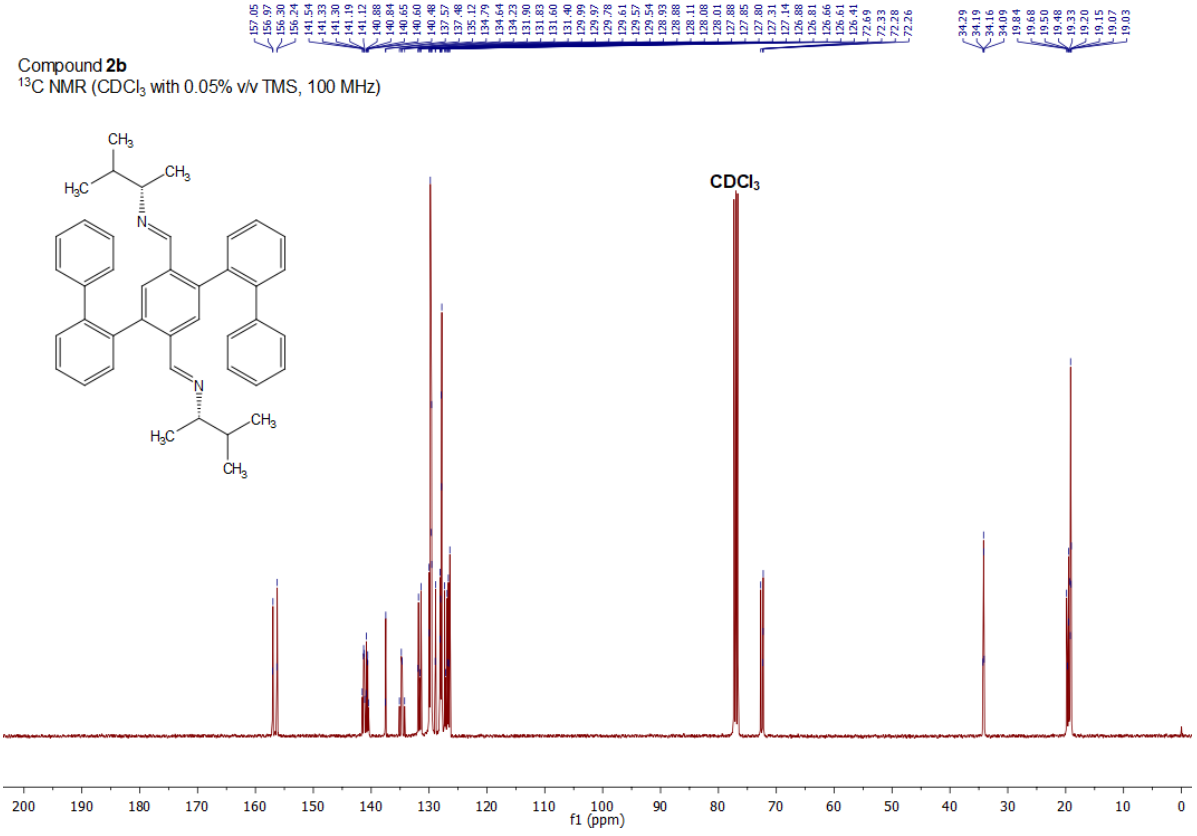


Figure S18. Copy of ^{13}C NMR spectrum of studied diimine **2b** measured in $CDCl_3$.

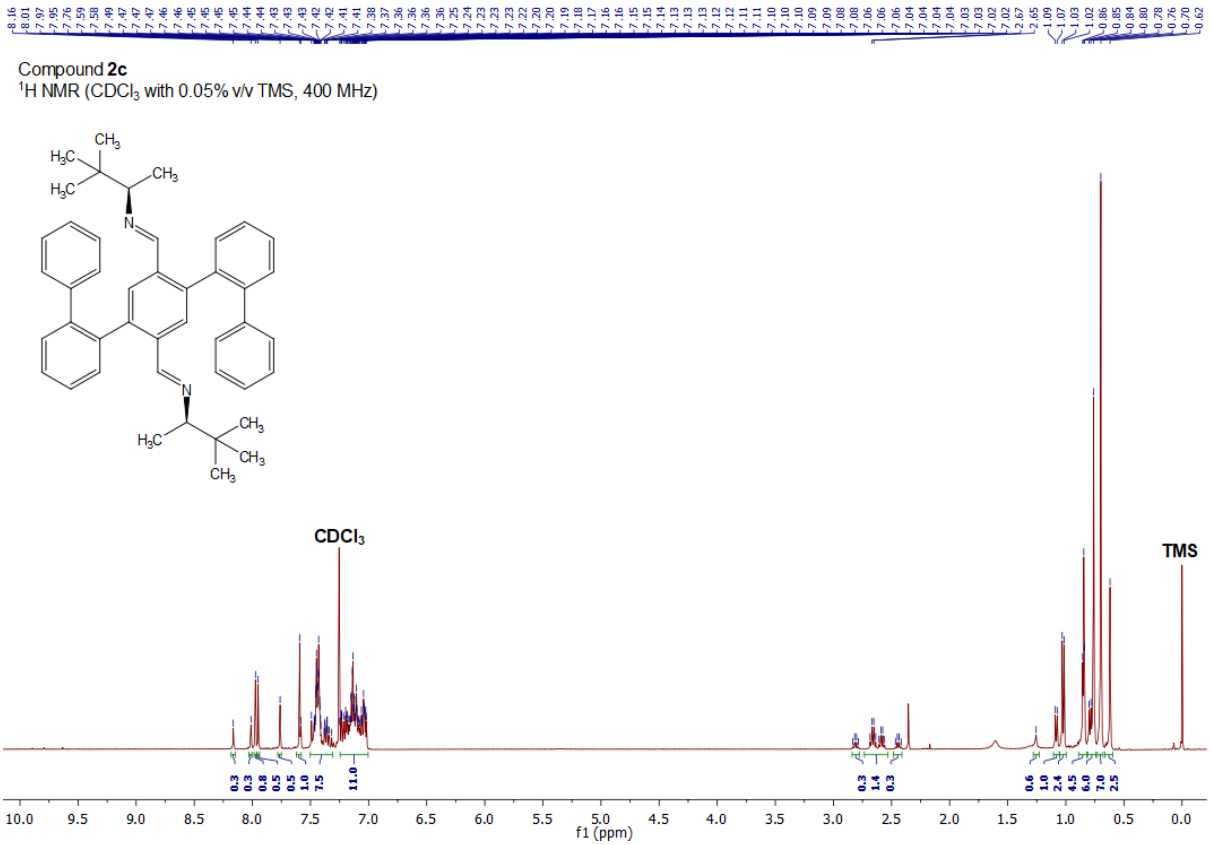


Figure S19. Copy of ^{1}H NMR spectrum of studied diimine **2c** measured in $CDCl_3$.

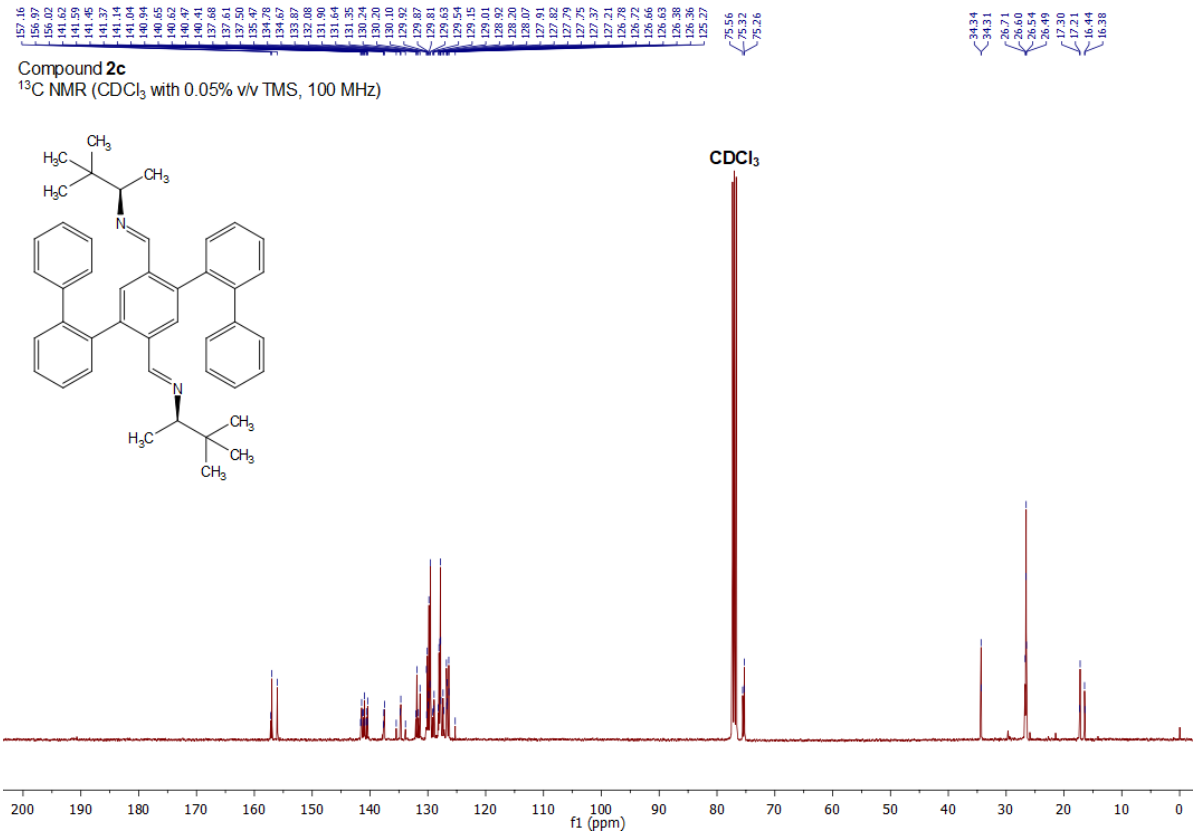


Figure S20. Copy of ^{13}C NMR spectrum of studied diimine **2c** measured in $CDCl_3$.

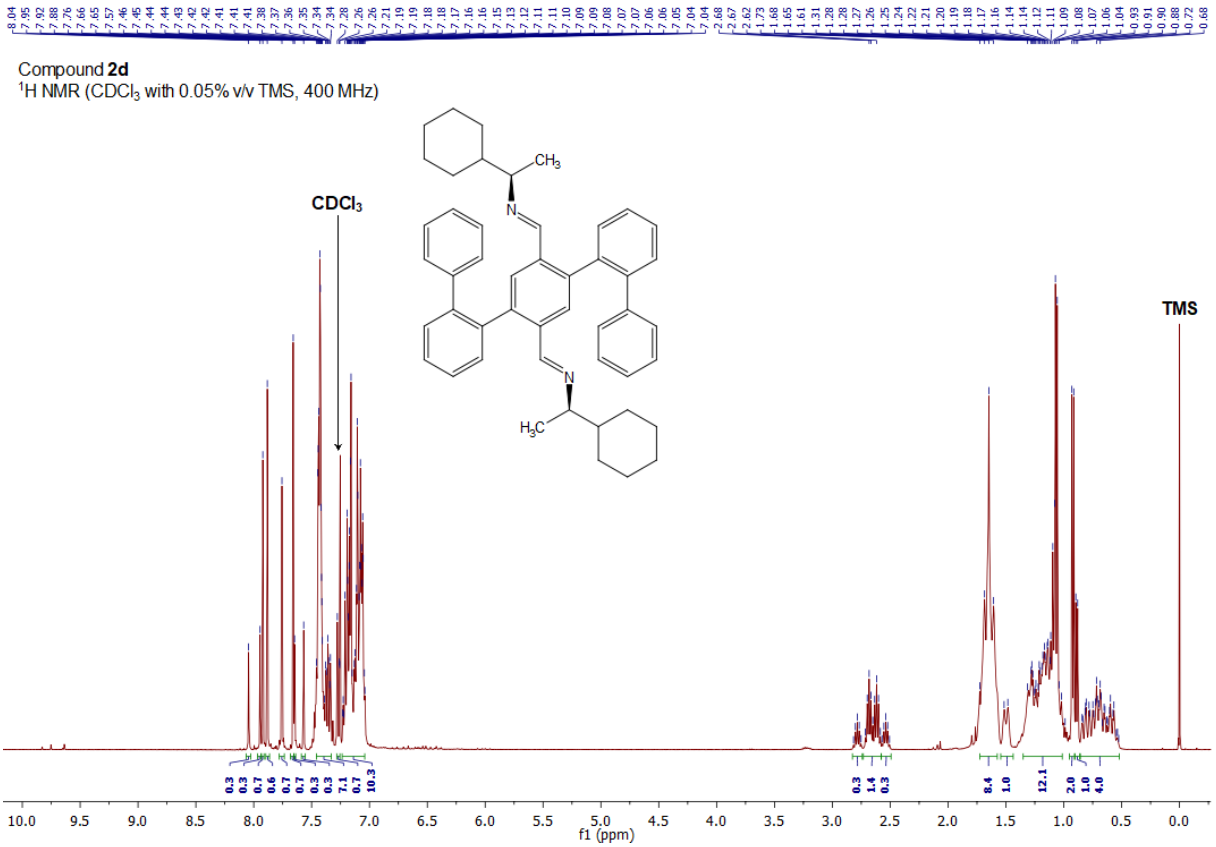


Figure S21. Copy of ^{1}H NMR spectrum of studied diimine **2d** measured in $CDCl_3$.

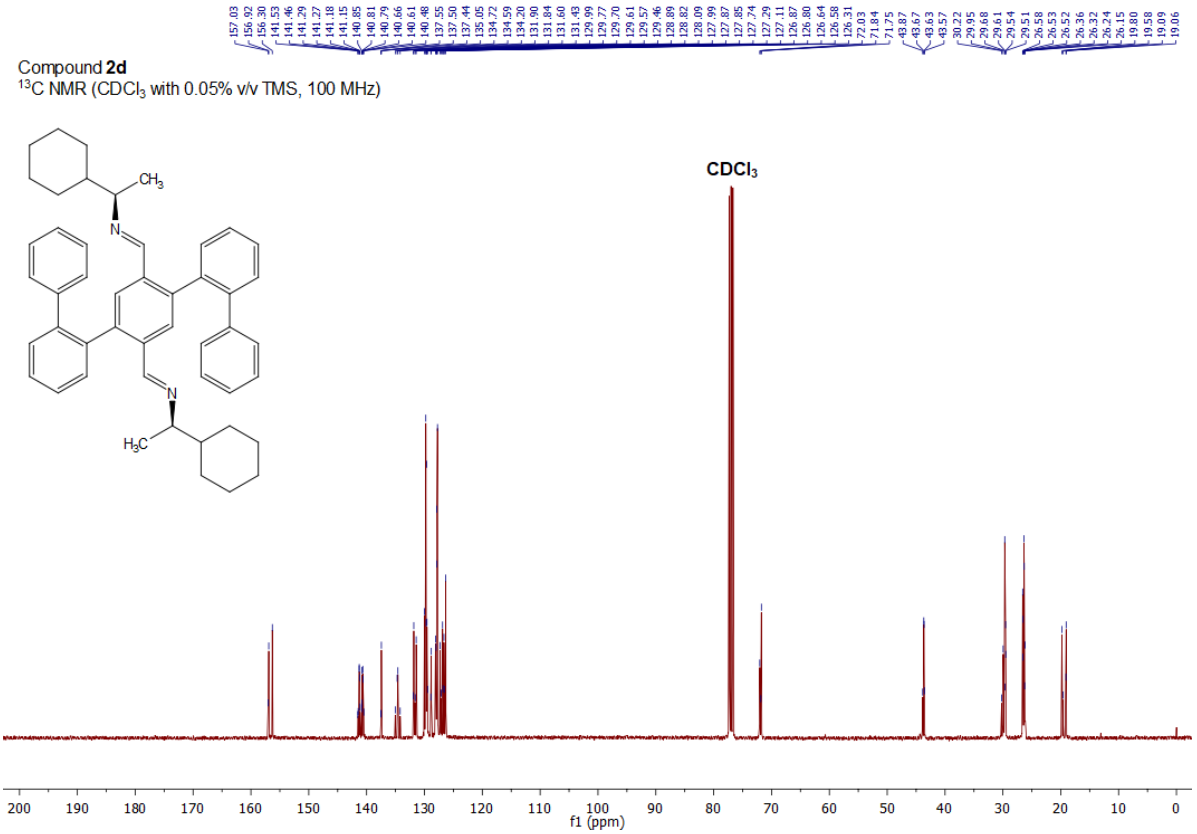


Figure S22. Copy of ^{13}C NMR spectrum of studied diimine **2d** measured in $CDCl_3$.

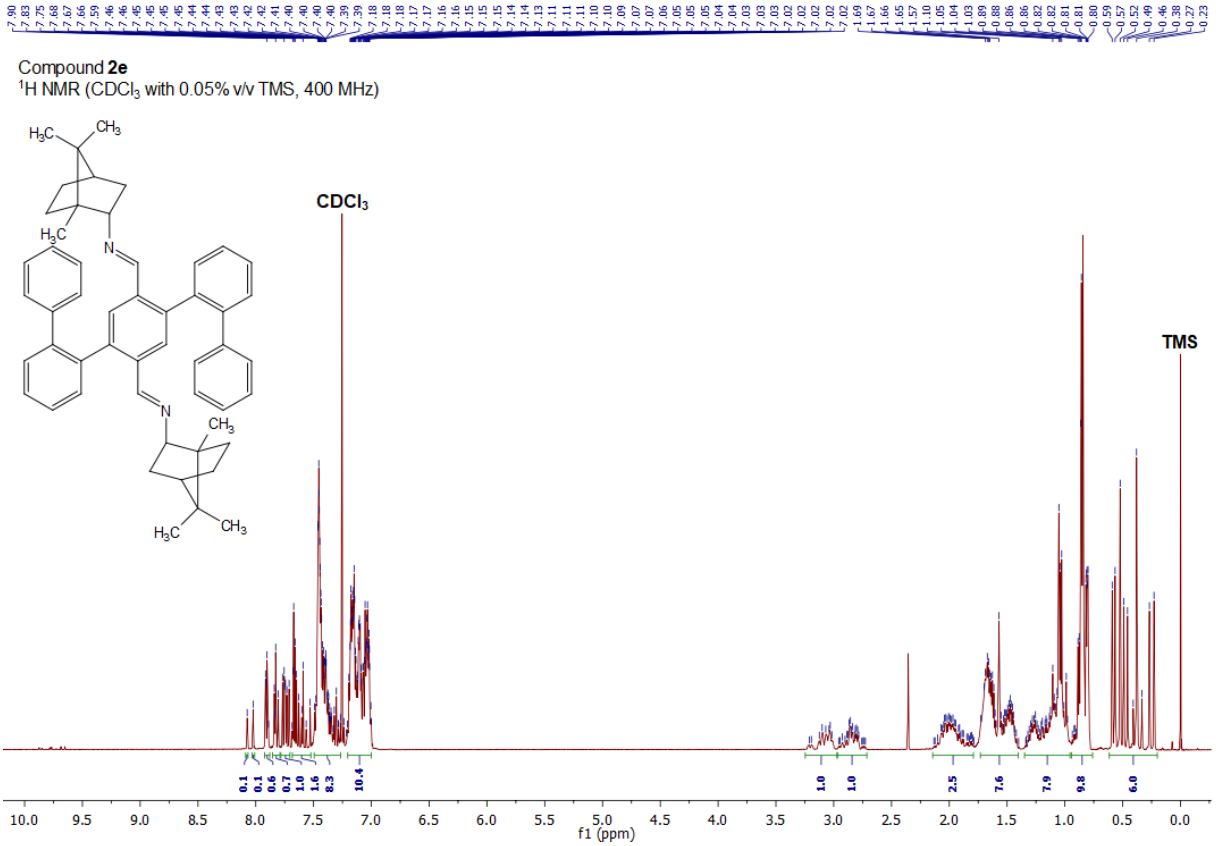


Figure S23. Copy of ^{1}H NMR spectrum of studied diimine **2e** measured in $CDCl_3$

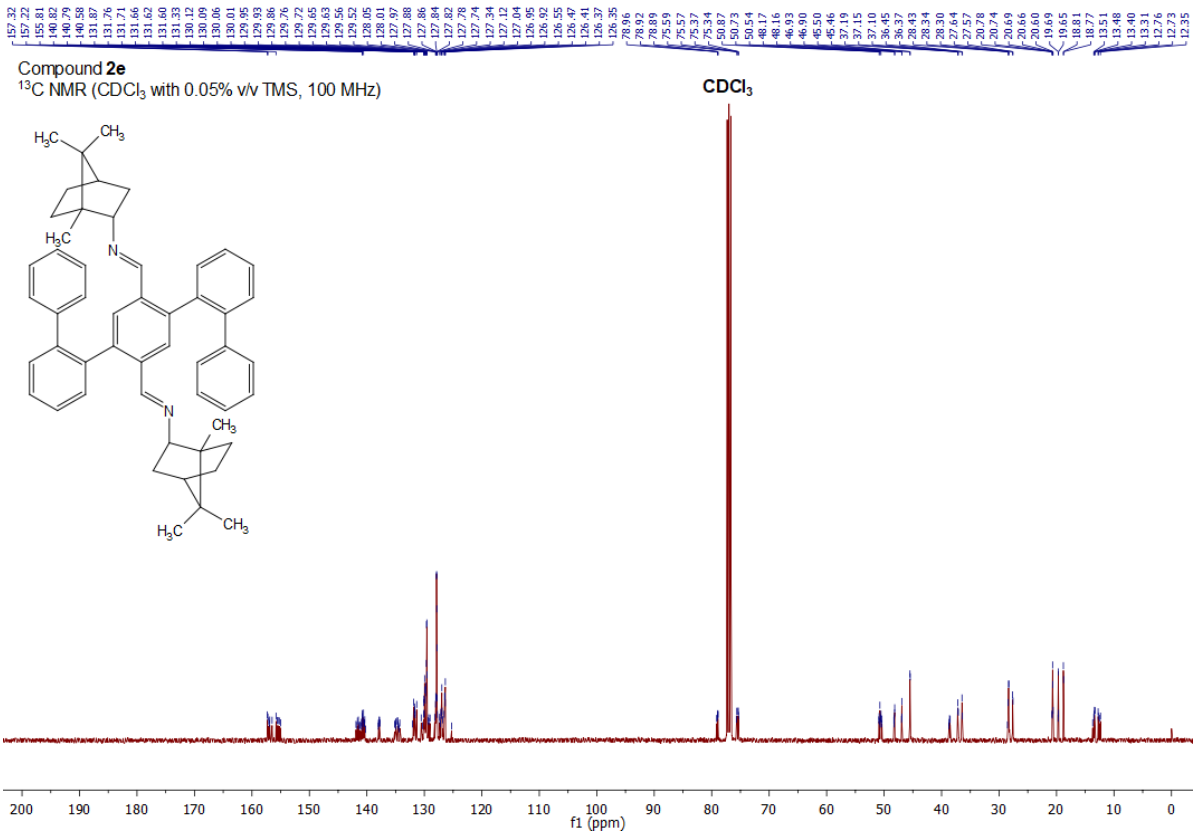


Figure S24. Copy of ^{13}C NMR spectrum of studied diimine **2e** measured in $CDCl_3$.

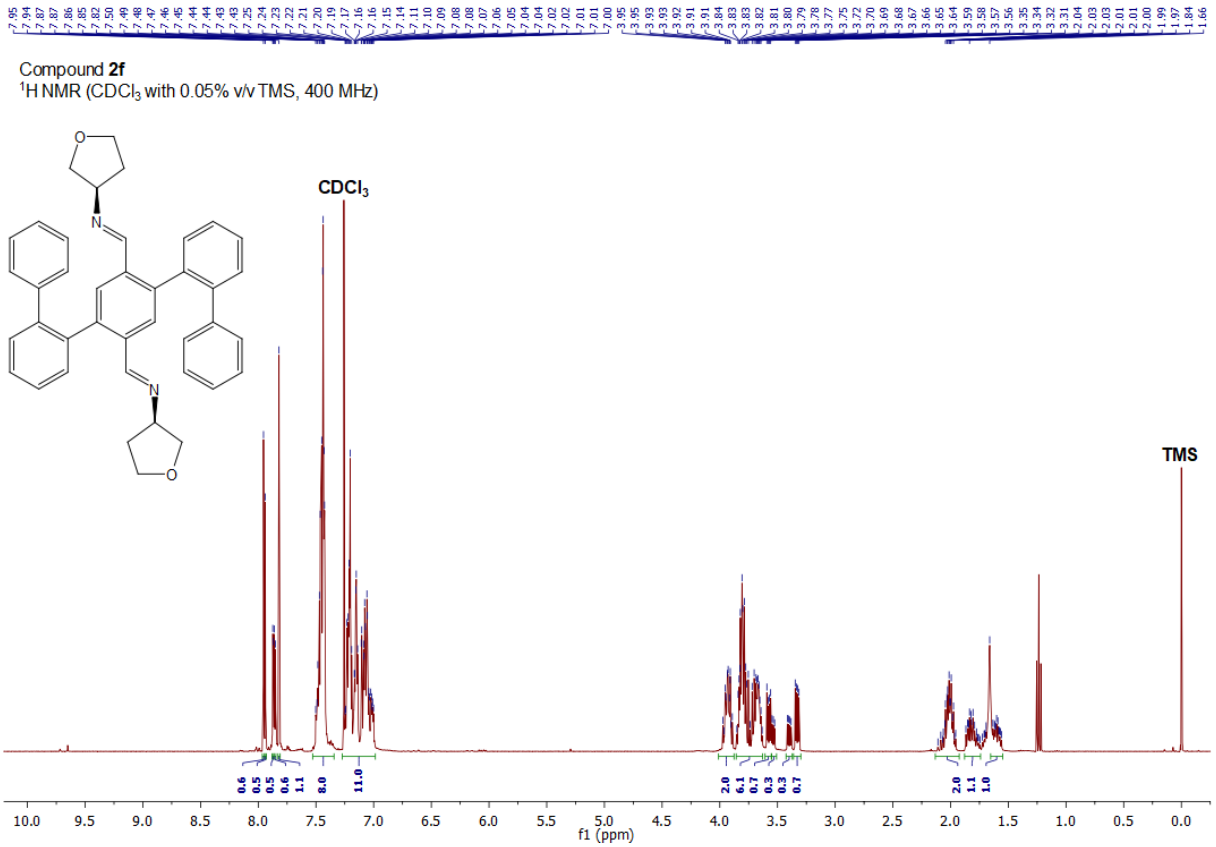


Figure S25. Copy of ^{1}H NMR spectrum of studied diimine **2f** measured in $CDCl_3$

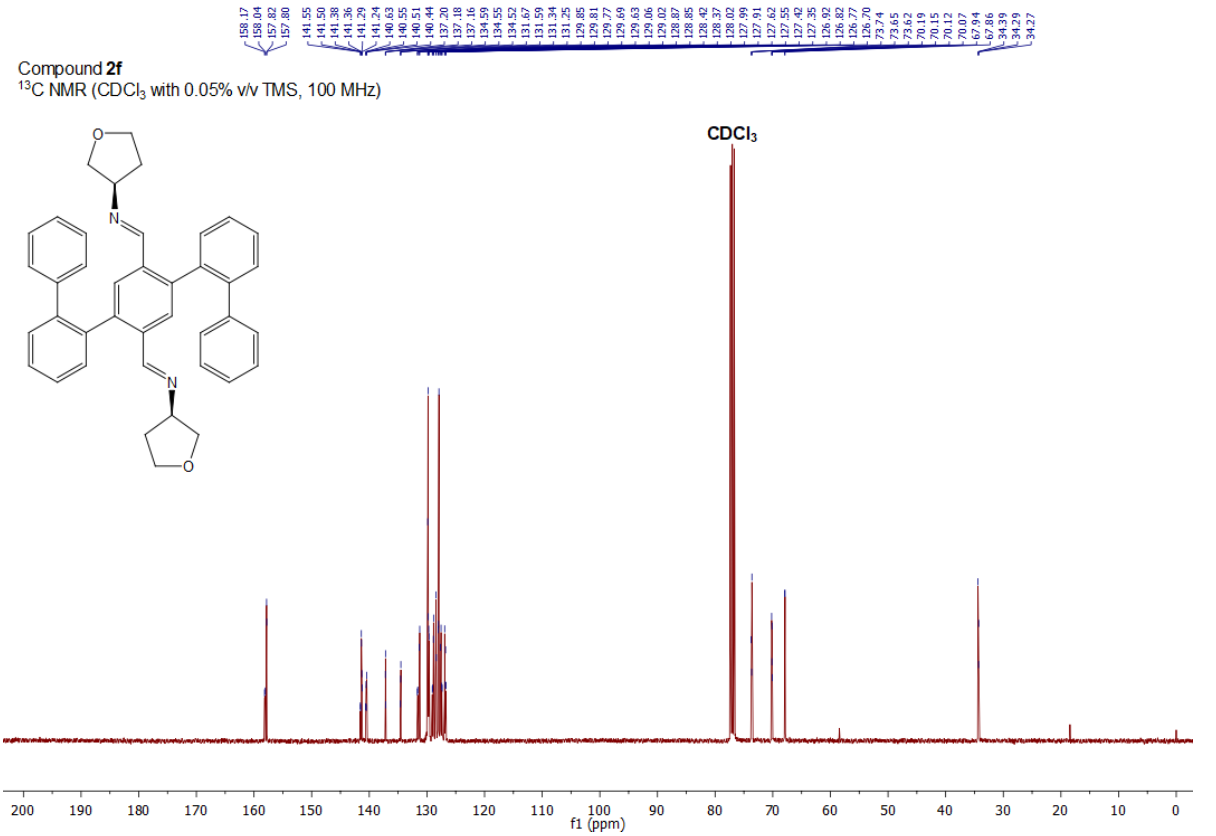


Figure S26. Copy of ^{13}C NMR spectrum of studied diimine **2f** measured in $CDCl_3$.

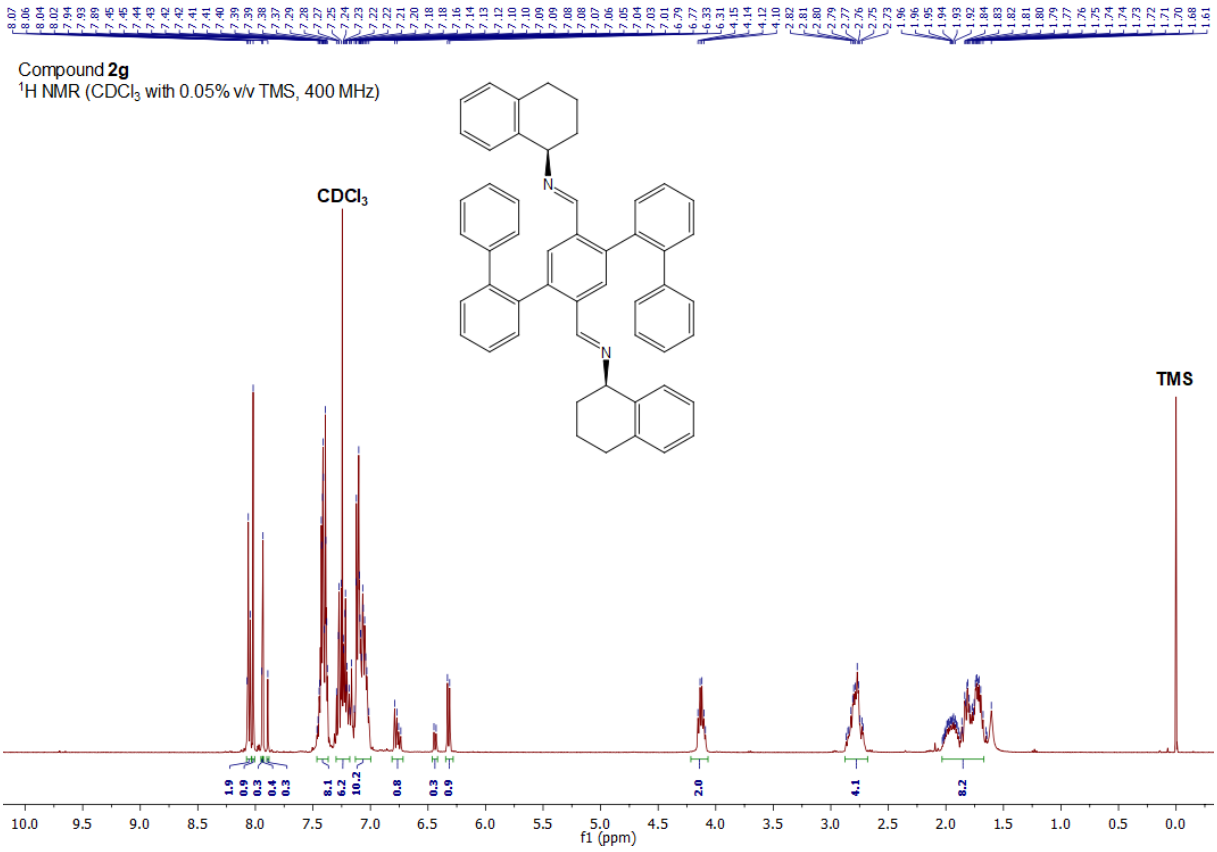


Figure S27. Copy of ^{1}H NMR spectrum of studied diimine **2g** measured in $CDCl_3$

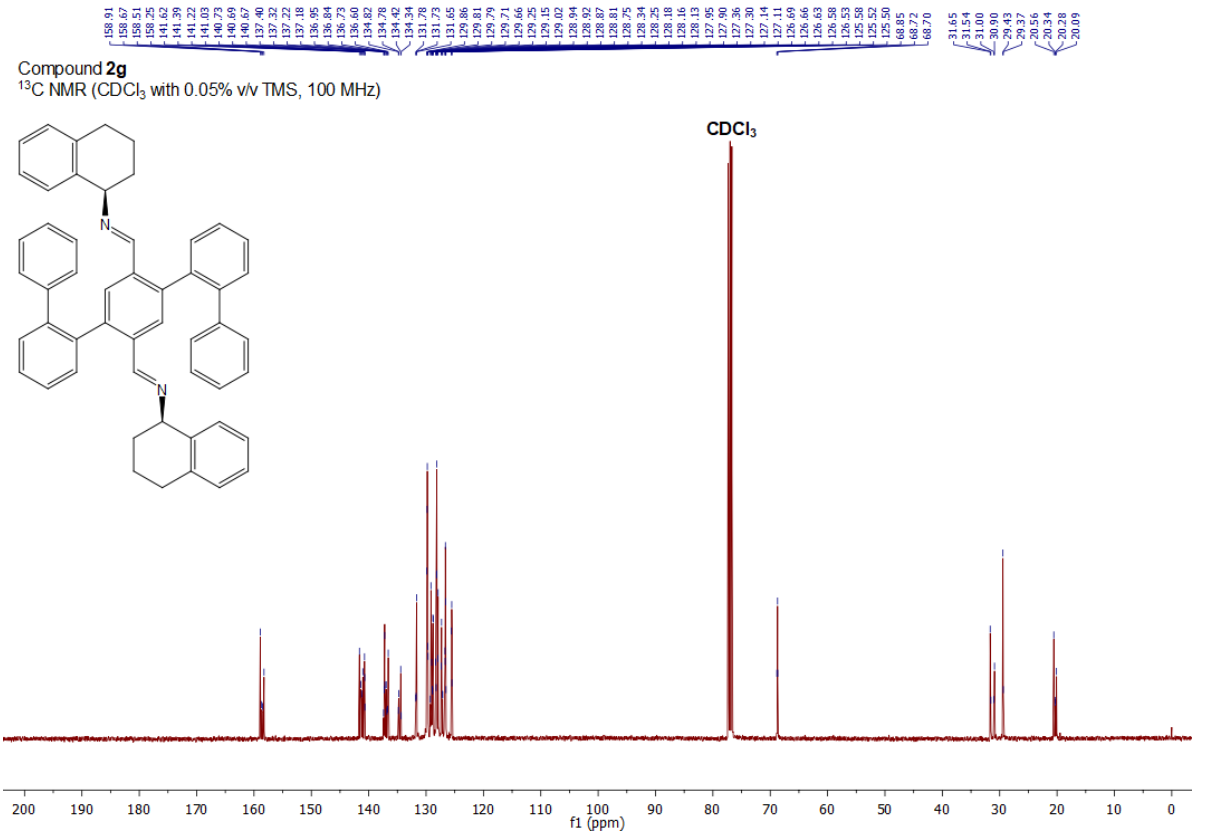


Figure S28. Copy of ^{13}C NMR spectrum of studied diimine **2g** measured in $CDCl_3$.

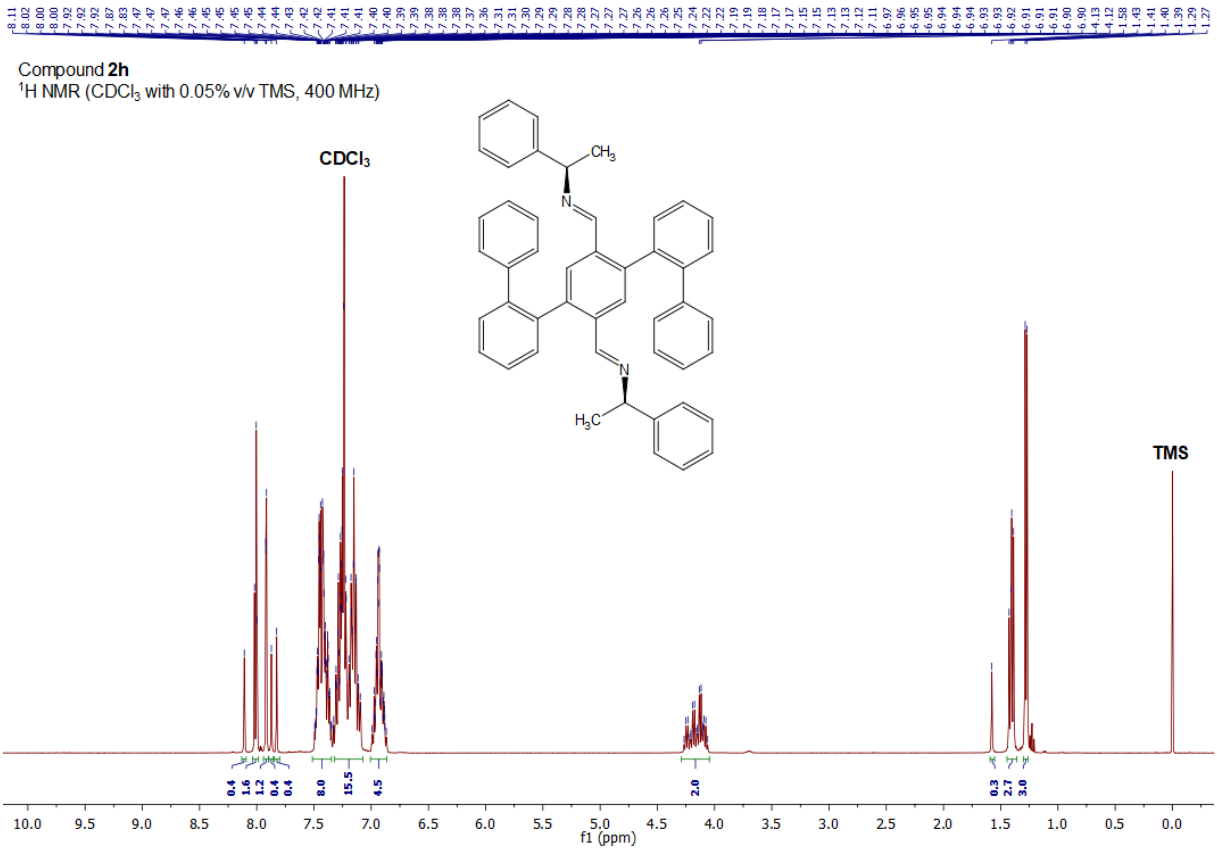


Figure S29. Copy of ^{1}H NMR spectrum of studied diimine **2h** measured in $CDCl_3$

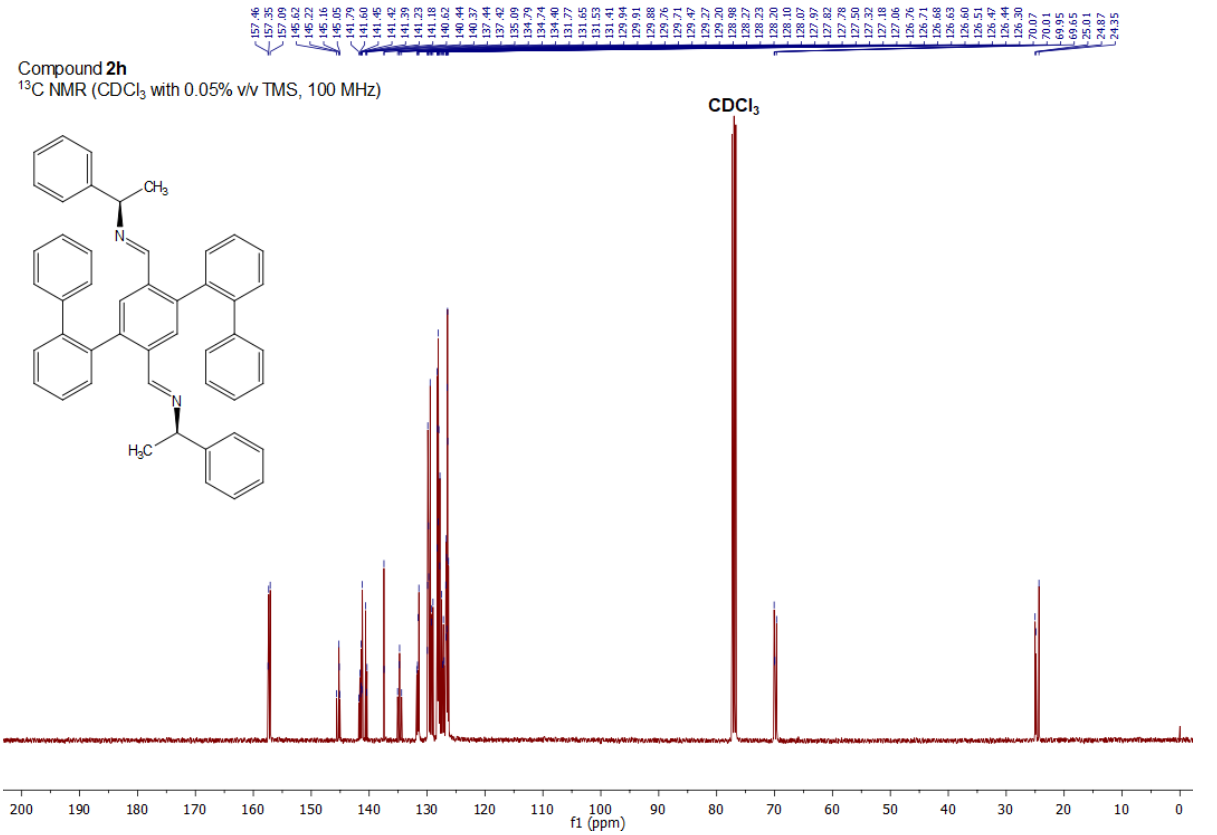


Figure S30. Copy of ^{13}C NMR spectrum of studied diimine **2h** measured in $CDCl_3$.

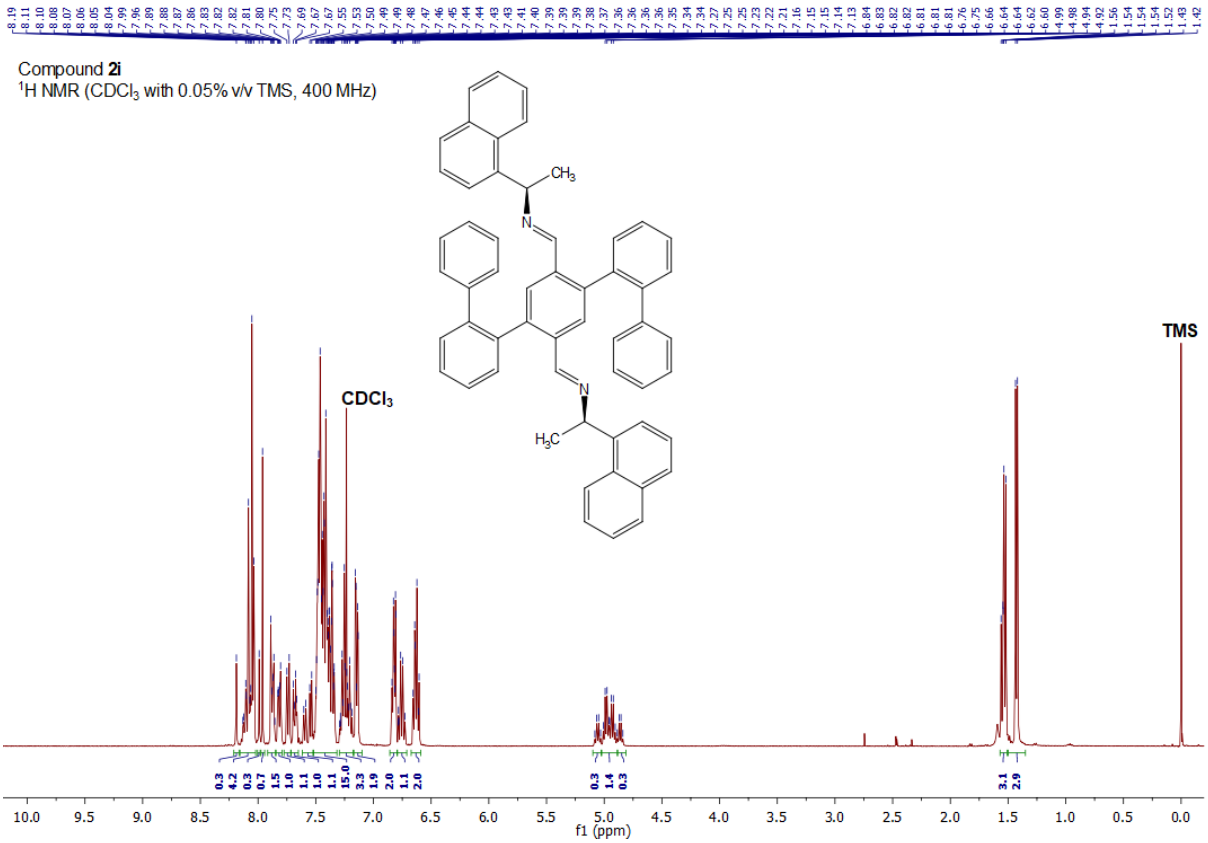


Figure S31. Copy of ^{1}H NMR spectrum of studied diimine **2i** measured in $CDCl_3$.

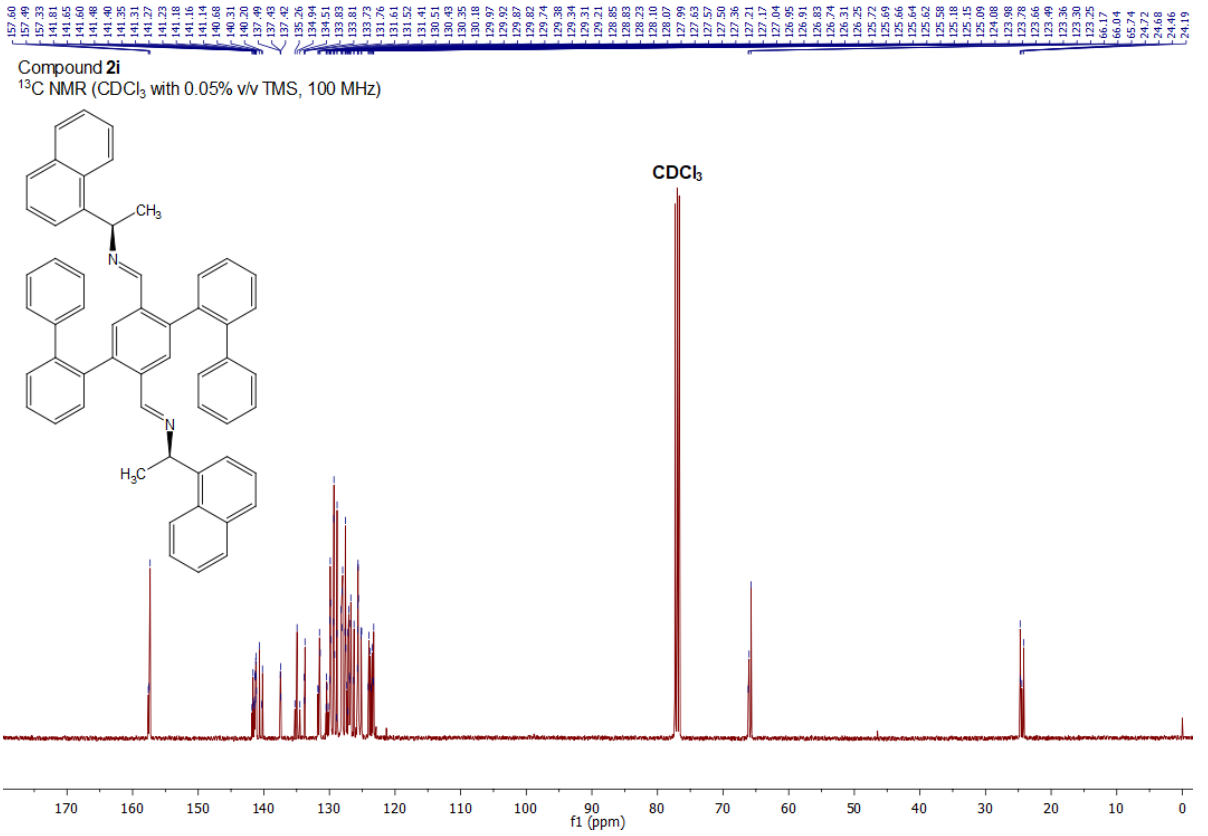


Figure S32. Copy of ^{13}C NMR spectrum of studied diimine **2i** measured in $CDCl_3$.

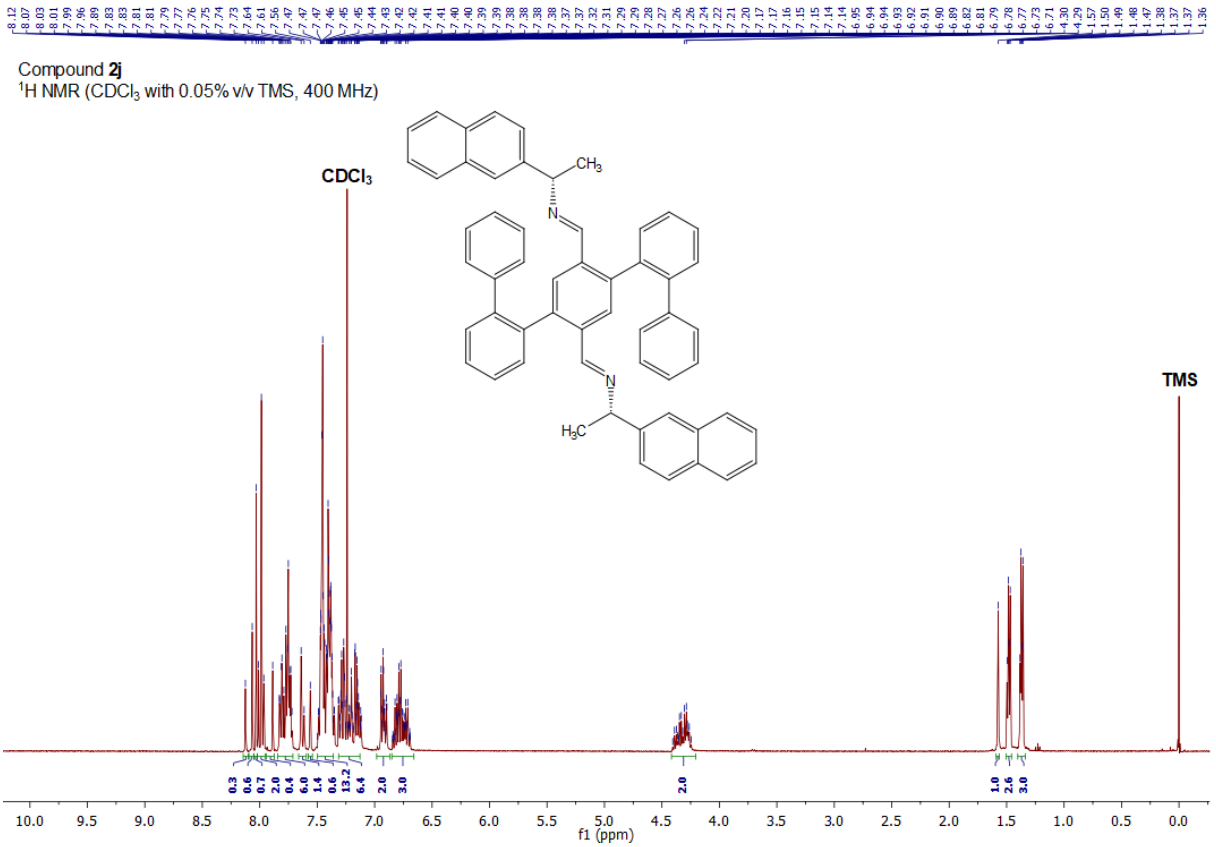


Figure S33. Copy of ^{1}H NMR spectrum of studied diimine **2j** measured in $CDCl_3$.

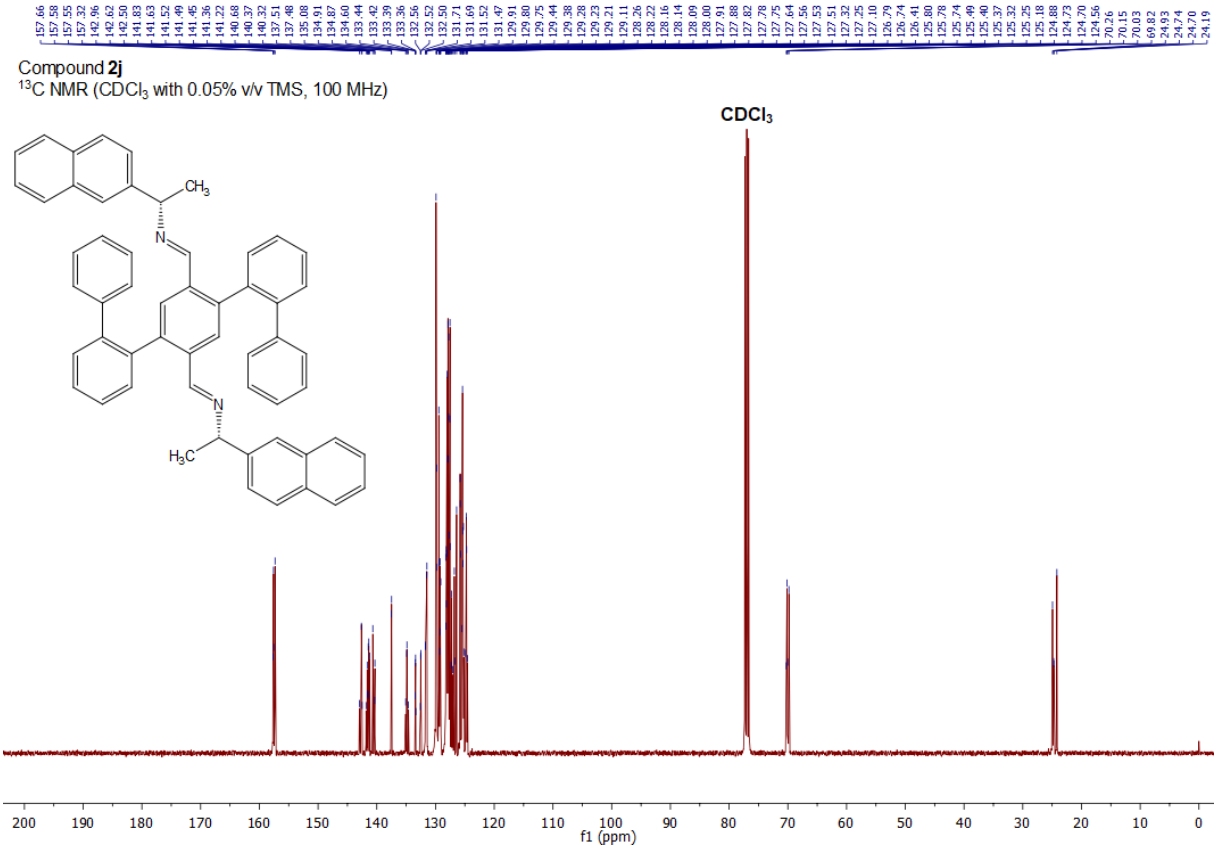


Figure S34. Copy of ^{13}C NMR spectrum of studied diimine **2j** measured in $CDCl_3$.

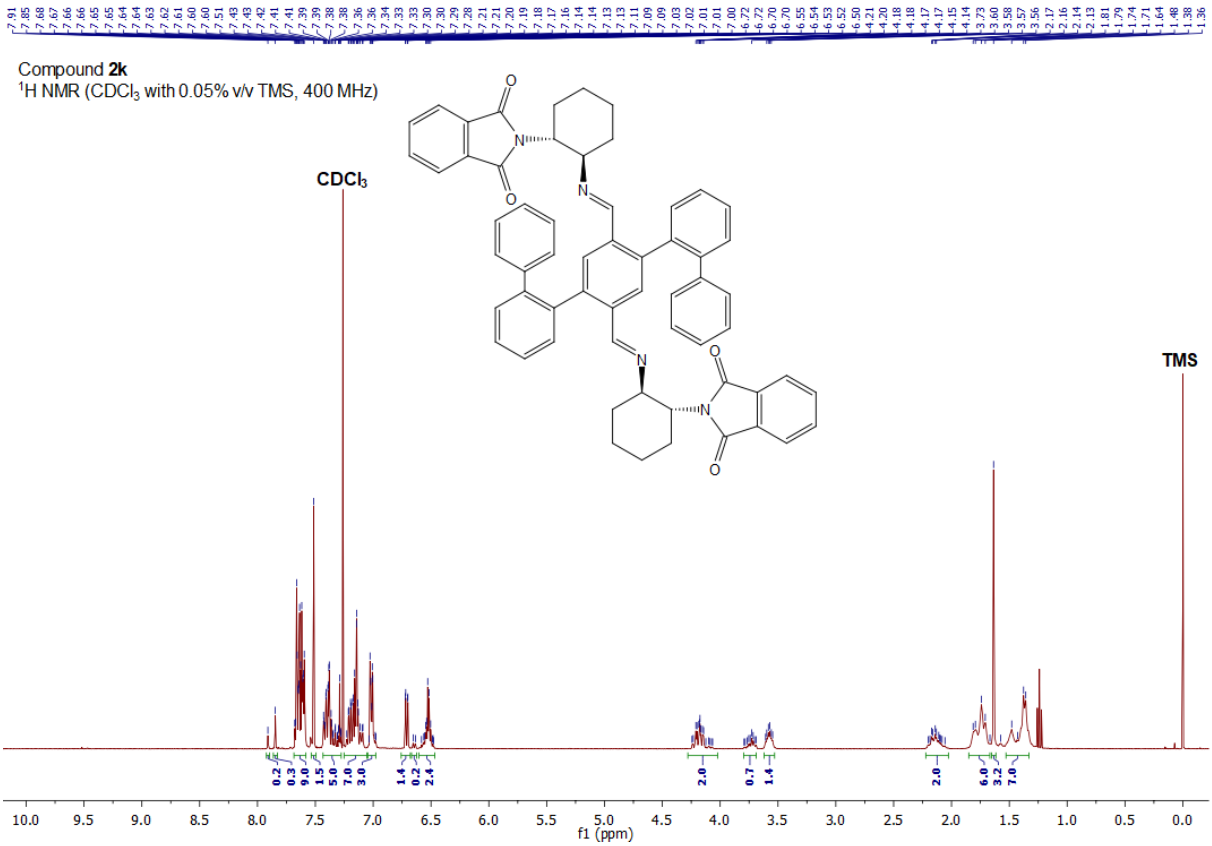


Figure S35. Copy of ^{1}H NMR spectrum of studied diimine **2k** measured in $CDCl_3$.

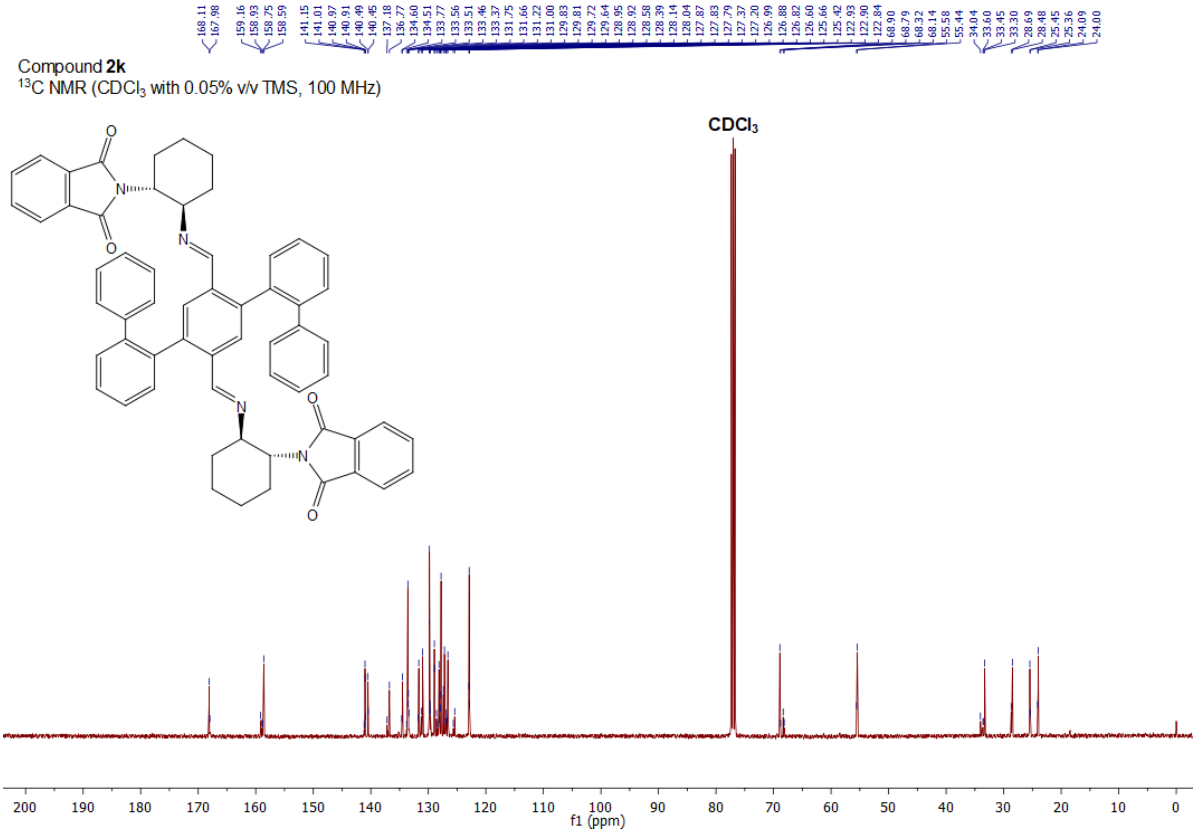


Figure S36. Copy of ^{13}C NMR spectrum of studied diimine **2k** measured in $CDCl_3$.

V. Measured ECD spectra of studied inductor-reporter systems

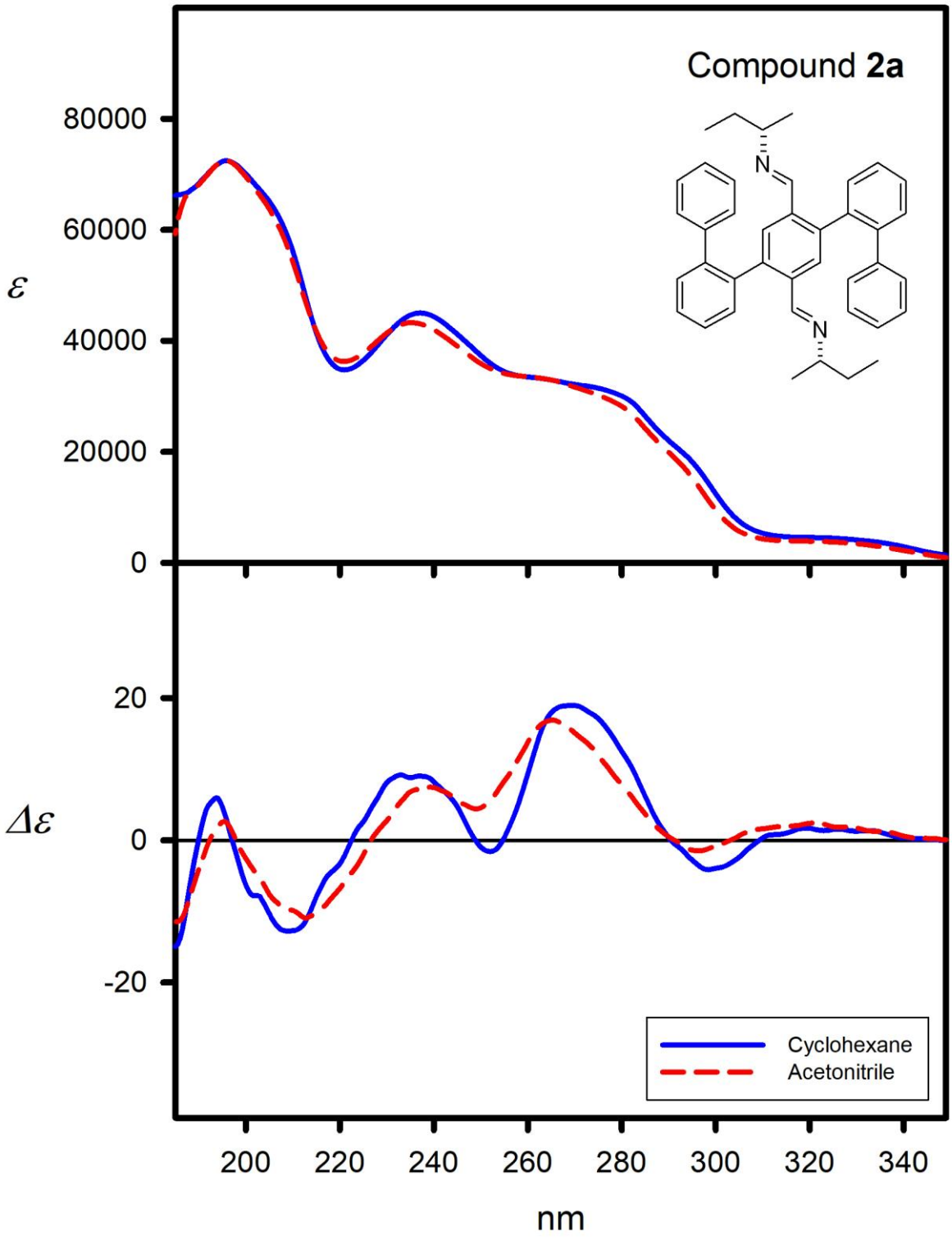


Figure S37. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2a** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

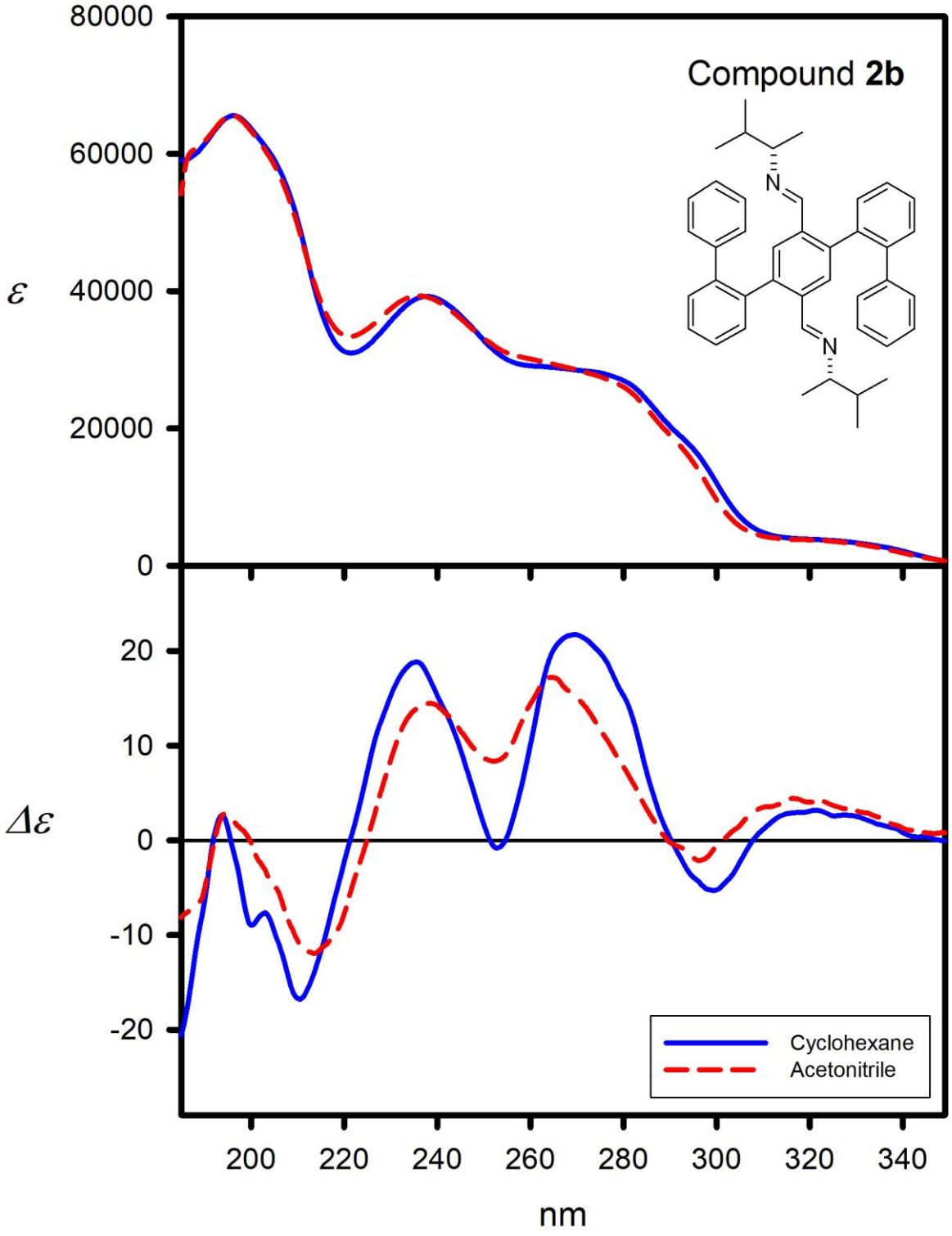


Figure S38. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2b** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

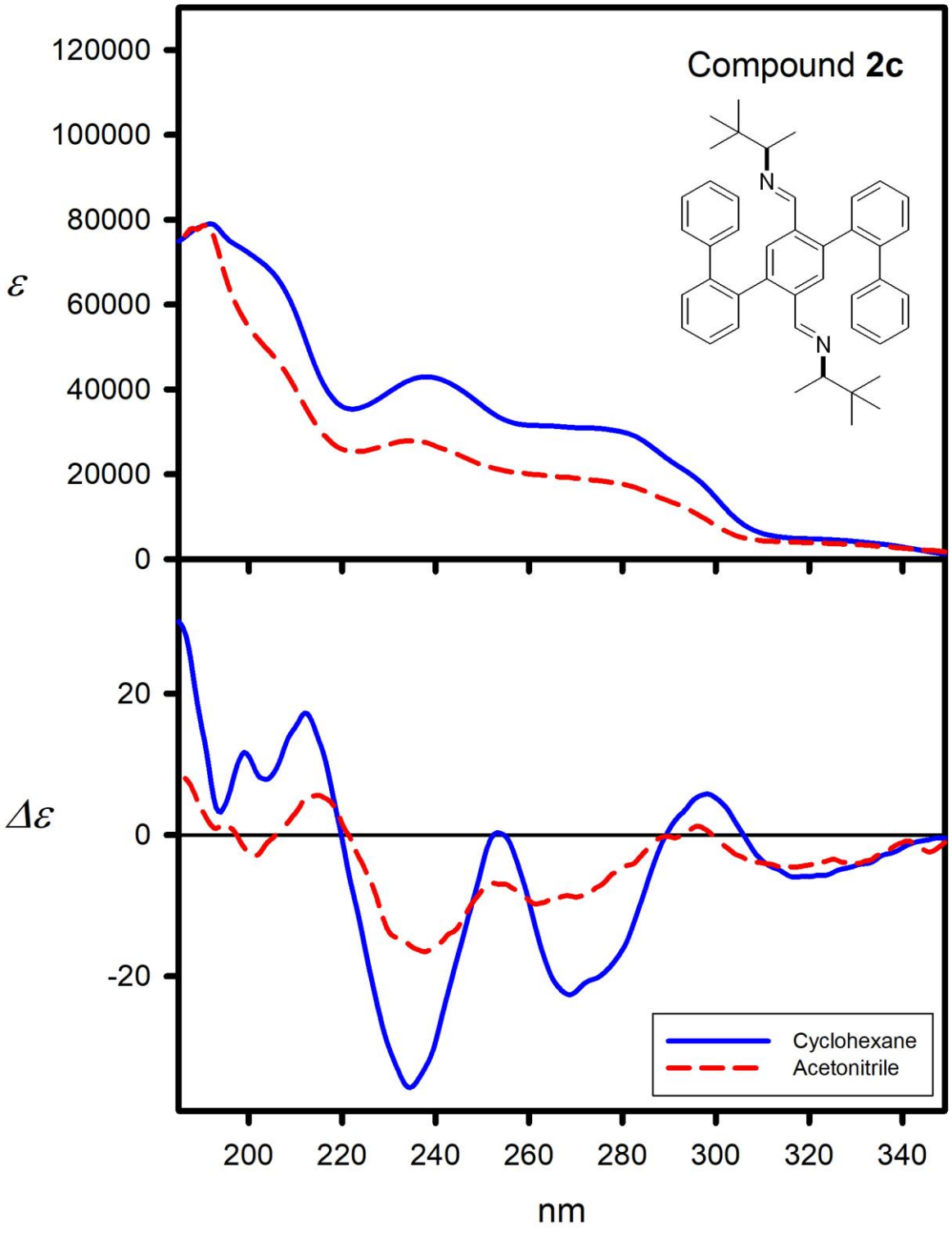


Figure S39. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2c** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

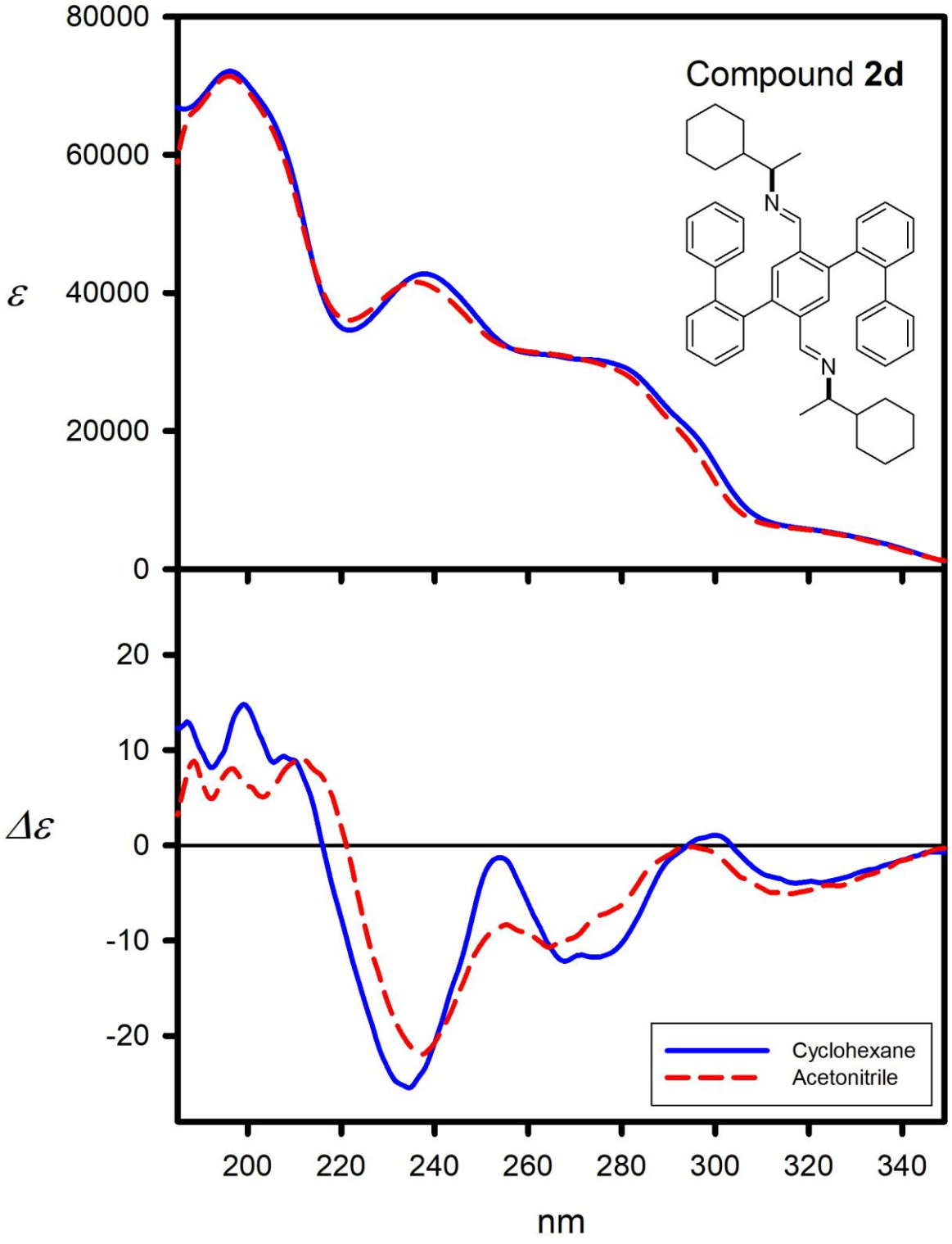


Figure S40. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2d** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

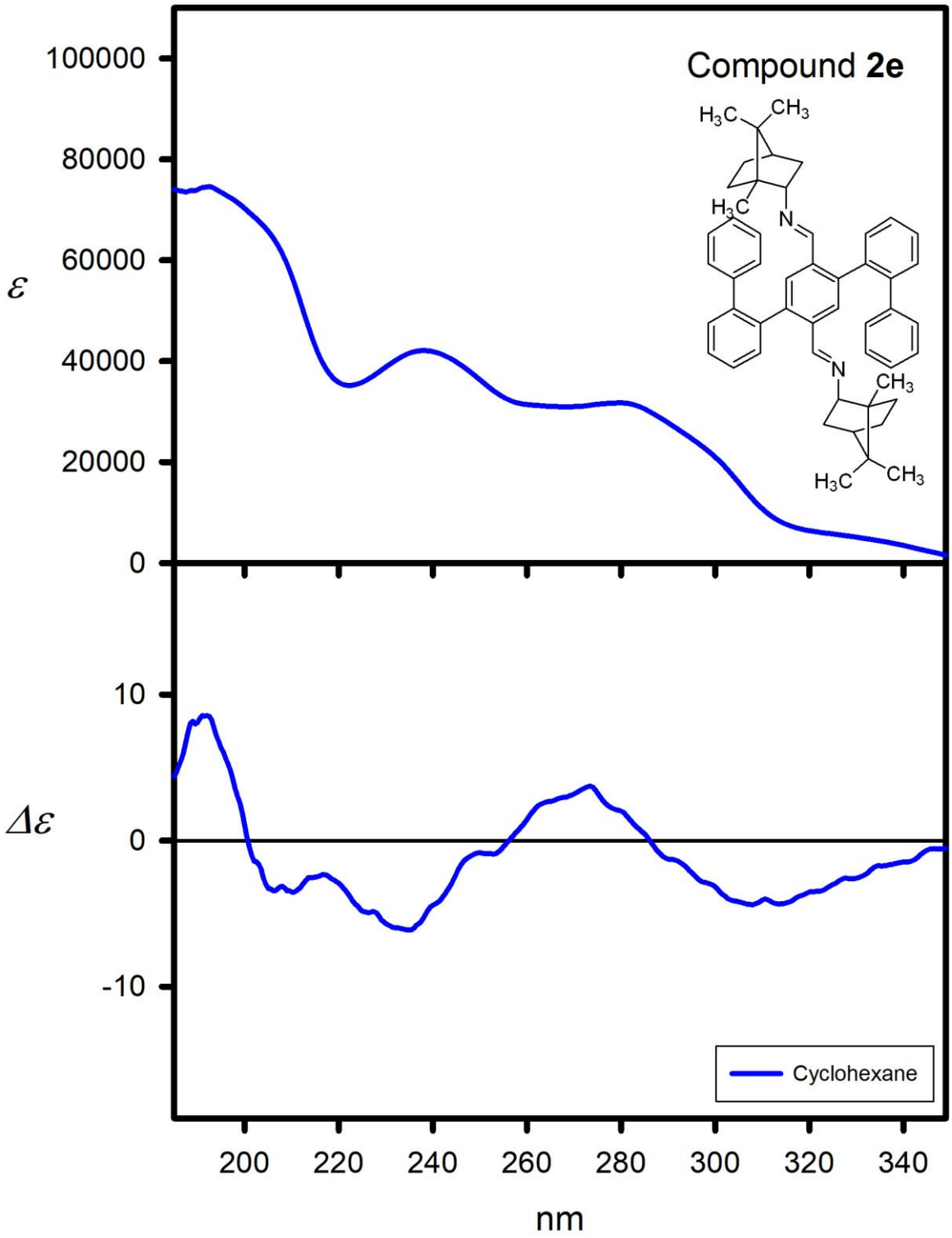


Figure S41. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2e** measured in cyclohexane (solid blue line) Sample was insoluble in acetonitrile.

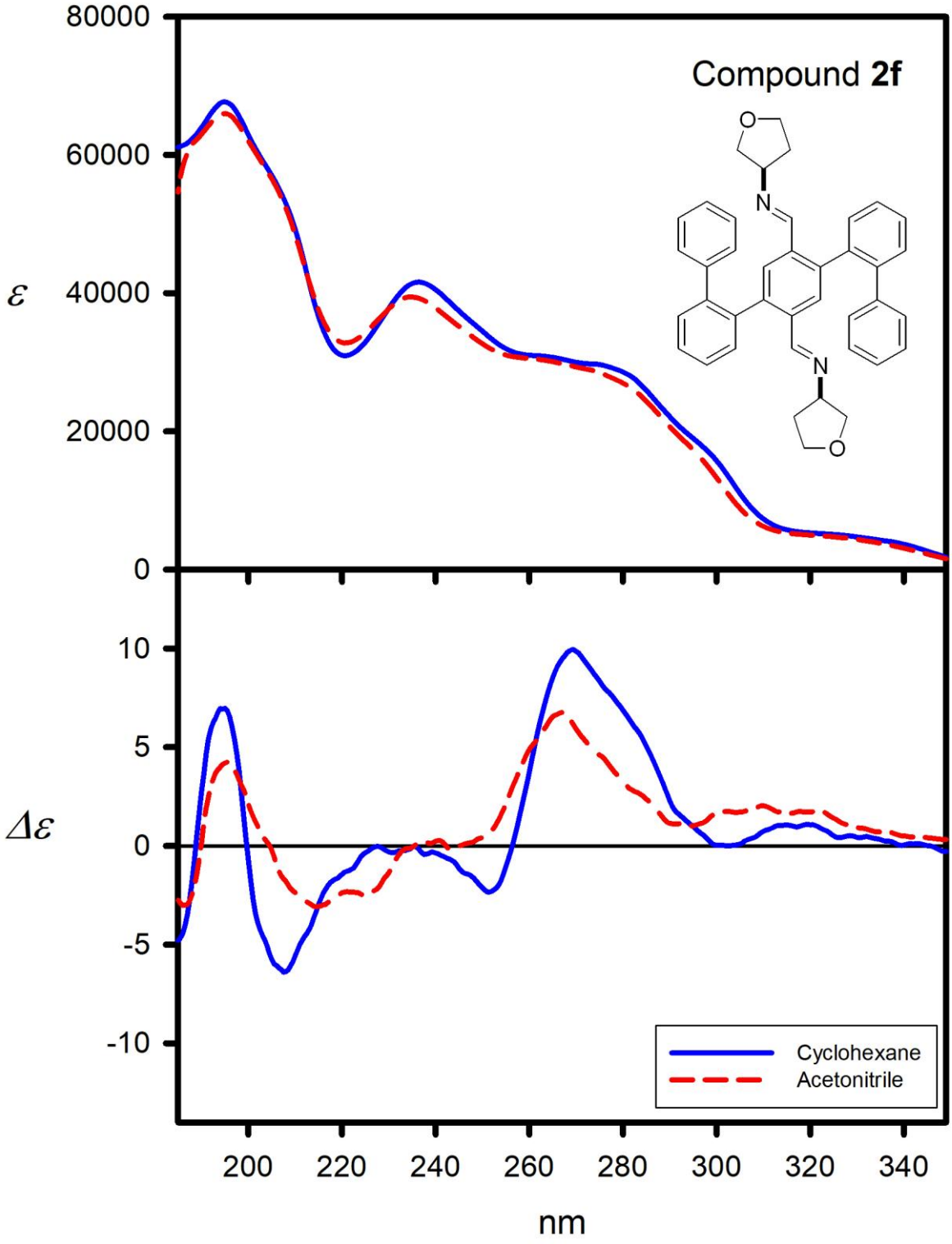


Figure S42. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2f** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

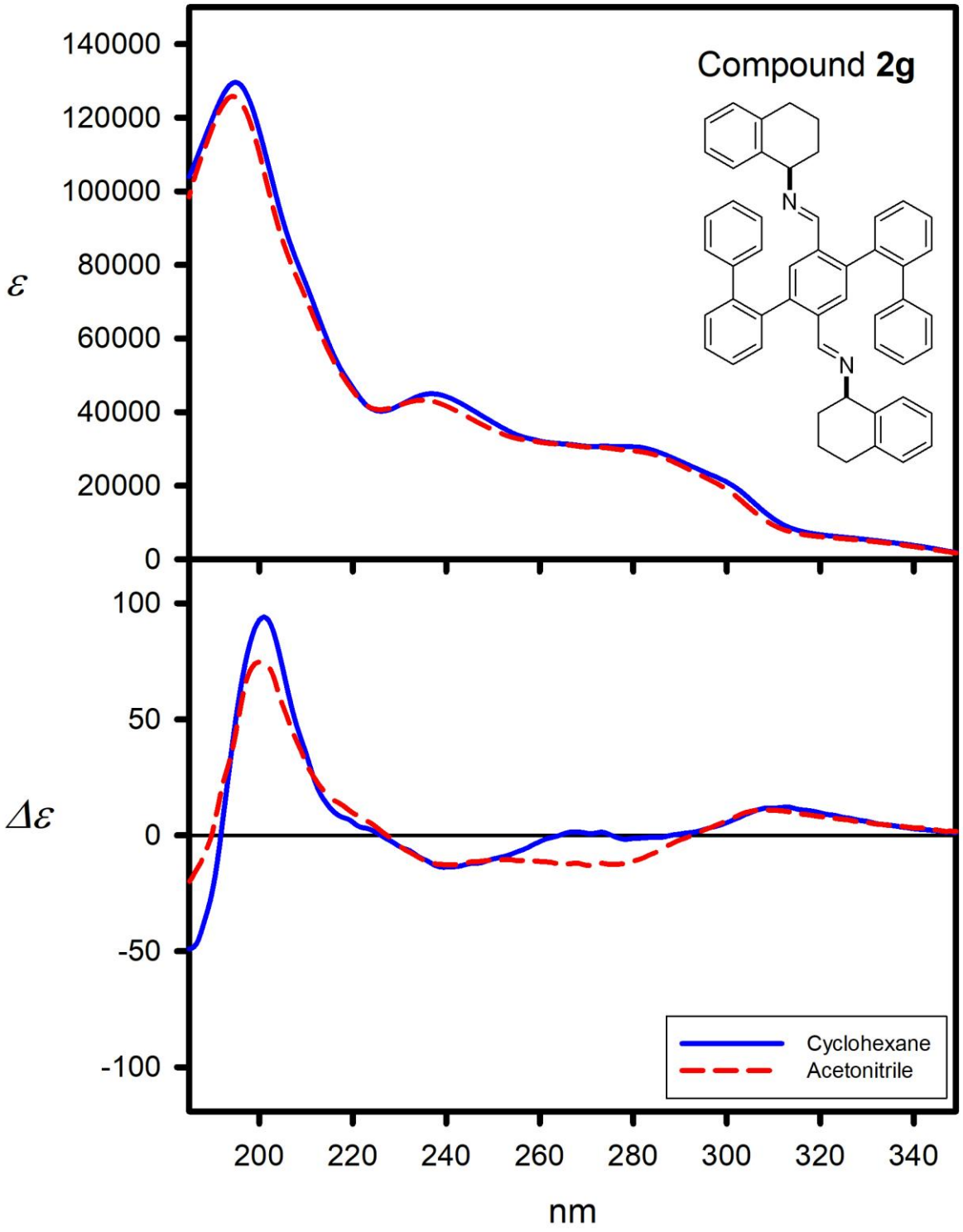


Figure S43. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2g** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

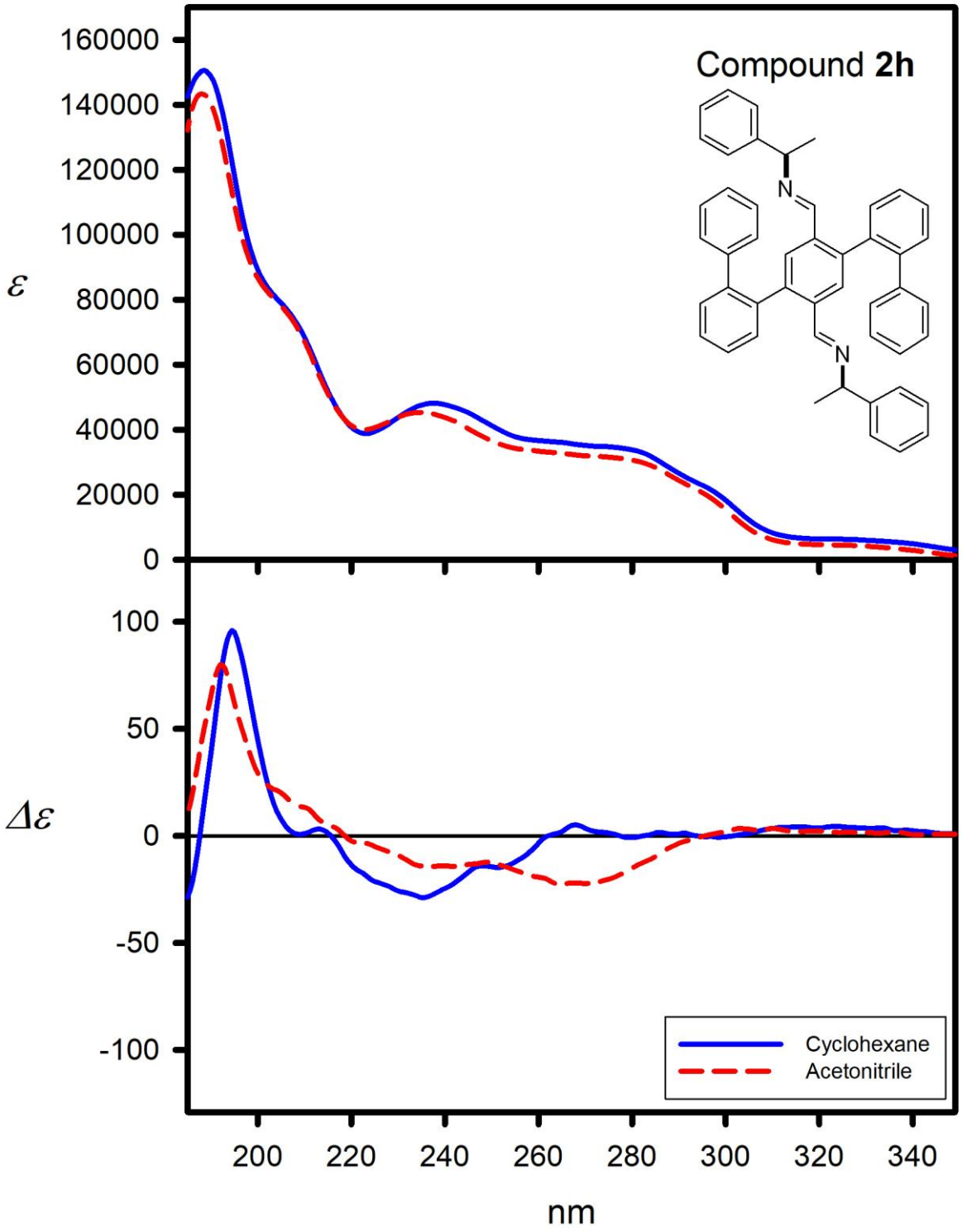


Figure S44. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2h** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

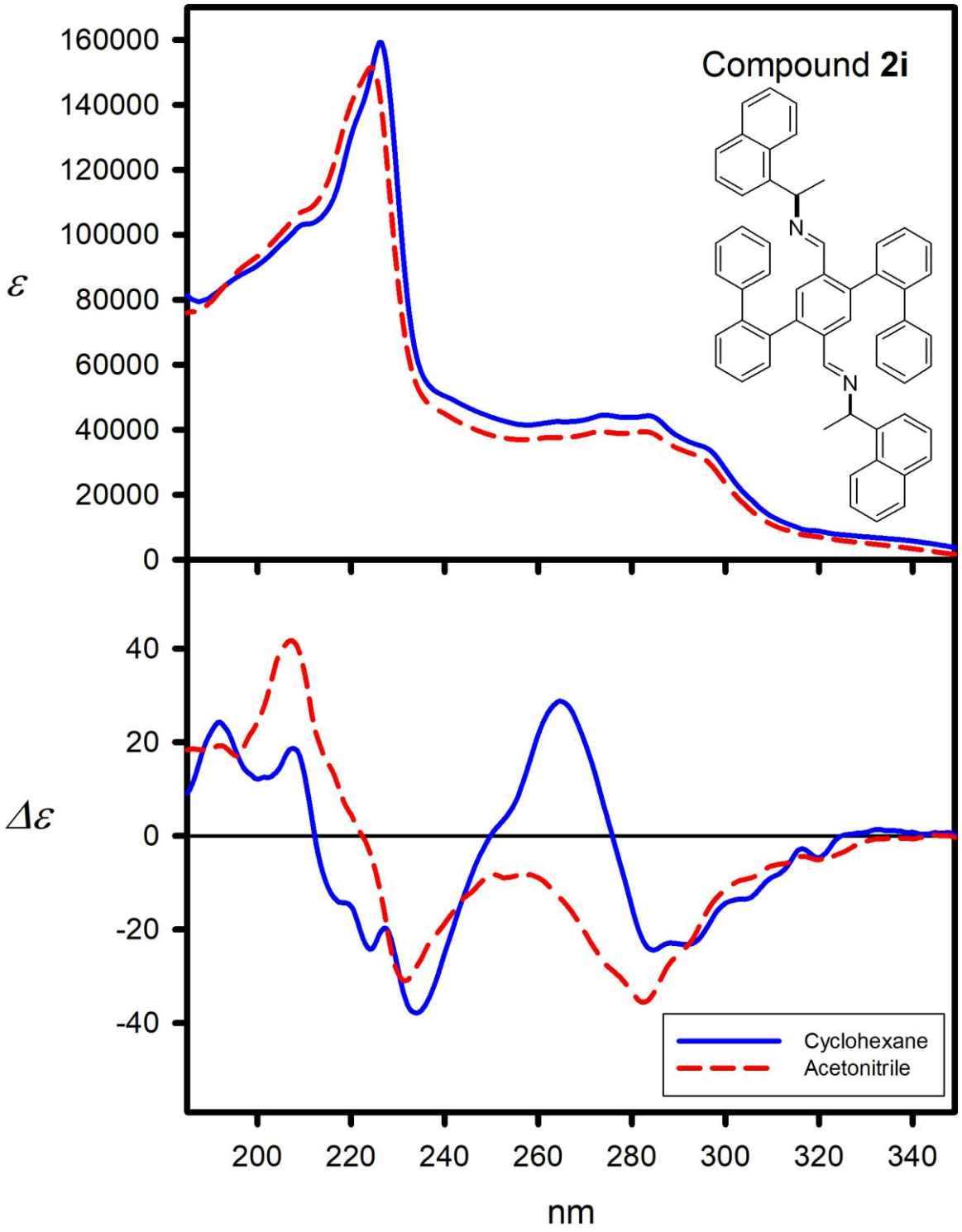


Figure S45. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2i** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

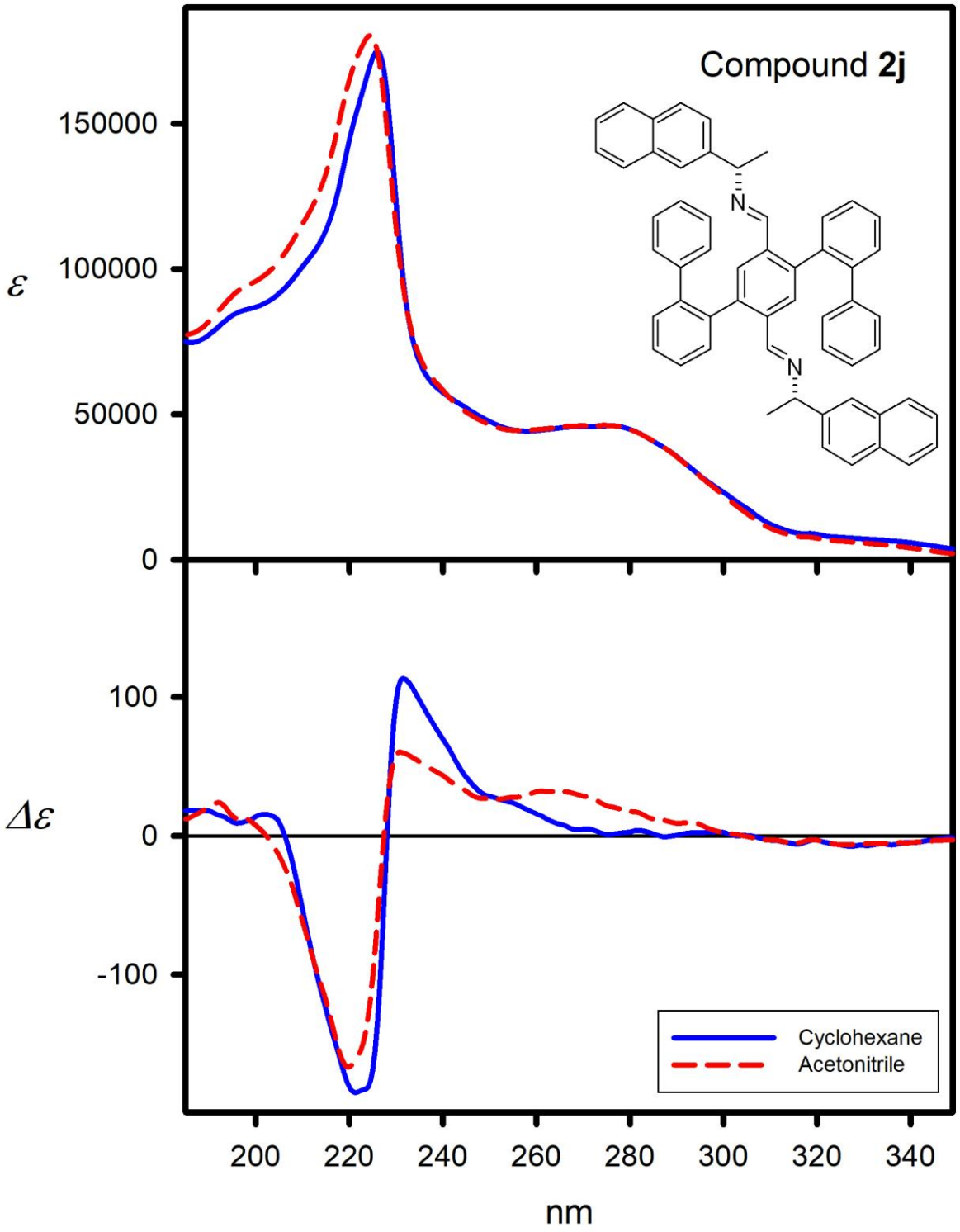


Figure S46. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2j** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

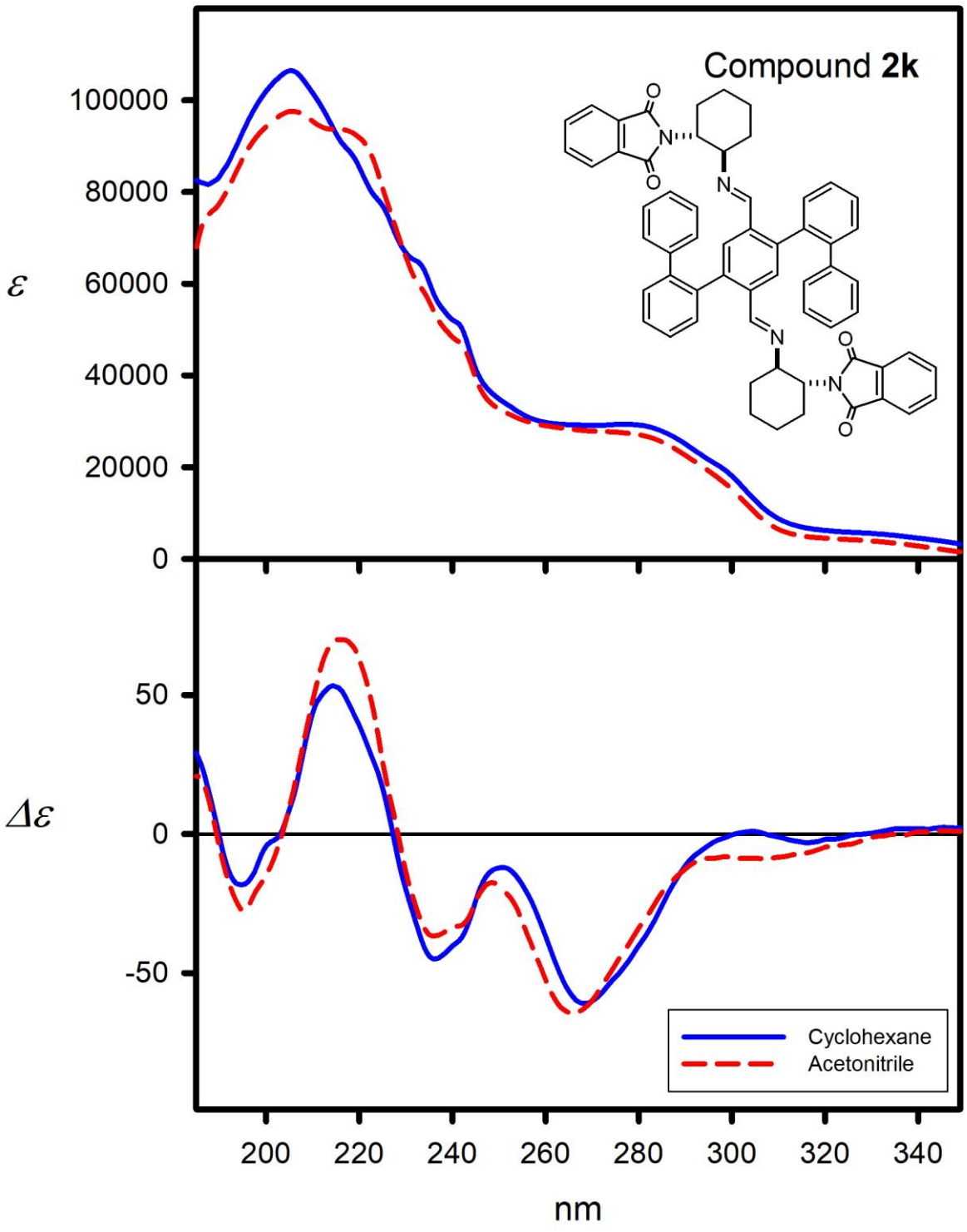


Figure S47. Copy of UV (upper chart) and ECD (bottom chart) spectra of studied diamine **2k** measured in cyclohexane (solid blue line) and acetonitrile (dashed red line).

VI. Cartesian coordinates

2c (conformer 1)	C -1.40261200 0.16842500 -0.89007500 C -0.54491900 1.26472500 -0.92844900 C 0.84506400 1.12591200 -0.94202100 C 1.40261200 -0.16842500 -0.89007500 C 0.54491900 -1.26472500 -0.92844900 C -0.84506400 -1.12591200 -0.94202100 C 2.86794900 -0.42551900 -0.80837500 C 3.46391900 -1.16424400 -1.83792600 C 4.82087000 -1.46557500 -1.82581700 C 5.60889800 -1.03187400 -0.76322800 C 5.03015300 -0.30367100 0.26914900 C 3.66387800 0.01393100 0.27244000 C -2.86794900 0.42551900 -0.80837500 C -3.66387800 -0.01393100 0.27244000 C -5.03015300 0.30367100 0.26914900 C -5.60889800 1.03187400 -0.76322800 C -4.82087000 1.46557500 -1.82581700 C -3.46391900 1.16424400 -1.83792600 C 1.69214400 2.32732200 -1.04584000 N 1.19759100 3.49143000 -1.15684300 C 2.10774700 4.61578900 -1.32804000 C 1.69214400 5.78081700 -0.38002600 C 2.71629900 6.92225200 -0.48669800 C 0.29014600 6.30708400 -0.72282800 C 1.69760700 5.25173700 1.06247800 C 2.11694100 4.98156700 -2.81827400 C -1.69214400 -2.32732200 -1.04584000 N -1.19759100 -3.49143000 -1.15684300 C -2.10774700 -4.61578900 -1.32804000 C -1.69214400 -5.78081700 -0.38002600 C -2.11694100 -4.98156700 -2.81827400 C -2.71629900 -6.92225200 -0.48669800 C -0.29014600 -6.30708400 -0.72282800 C -1.69760700 -5.25173700 1.06247800 H -0.95075800 2.26835600 -0.93293100 H 0.95075800 -2.26835600 -0.93293100 H 2.84499700 -1.49029300 -2.66565900 H 5.25729400 -2.03468900 -2.63823600 H 6.66613200 -1.26817300 -0.73143300 H -6.66613200 1.26817300 -0.73143300 H -5.25729400 2.03468900 -2.63823600 H -2.84499700 1.49029300 -2.66565900 H 2.77542900 2.16247600 -1.05186500

	H 3.13180700 4.32082000 -1.04221700 H 2.49319400 7.69683900 0.25254700 H 3.73212900 6.56177100 -0.29468900 H 2.70428400 7.39583500 -1.47084700 H -0.01584500 7.06134500 0.00809600 H 0.26341300 6.77531700 -1.70998100 H -0.44024900 5.49634000 -0.70860400 H 1.44800600 6.05260400 1.76469700 H 0.97567700 4.44383200 1.19277500 H 2.68203000 4.86048800 1.33130400 H 2.49913400 4.14002700 -3.40064400 H 1.10763600 5.20016700 -3.17145500 H 2.75394000 5.84585100 -3.01313500 H -2.77542900 -2.16247600 -1.05186500 H -3.13180700 -4.32082000 -1.04221700 H -2.49913400 -4.14002700 -3.40064400 H -1.10763600 -5.20016700 -3.17145500 H -2.75394000 -5.84585100 -3.01313500 H -2.49319400 -7.69683900 0.25254700 H -3.73212900 -6.56177100 -0.29468900 H -2.70428400 -7.39583500 -1.47084700 H 0.01584500 -7.06134500 0.00809600 H -0.26341300 -6.77531700 -1.70998100 H 0.44024900 -5.49634000 -0.70860400 H -1.44800600 -6.05260400 1.76469700 H -0.97567700 -4.44383200 1.19277500 H -2.68203000 -4.86048800 1.33130400 C 3.12344500 0.80291000 1.41118300 C 3.83641500 1.91762100 1.87413400 C 1.92689200 0.46514100 2.05830100 C 3.37373500 2.67213700 2.94721500 H 4.75292000 2.20582100 1.37246700 C 1.45849100 1.22824600 3.12327200 H 1.36325200 -0.39697200 1.72725500 C 2.17730500 2.33417800 3.57260500 H 3.93895000 3.53368300 3.28316300 H 0.52747200 0.96145500 3.60864000 H 1.80486700 2.92793900 4.39900000 C -3.12344500 -0.80291000 1.41118300 C -3.83641500 -1.91762100 1.87413400 C -1.92689200 -0.46514100 2.05830100 C -3.37373500 -2.67213700 2.94721500 H -4.75292000 -2.20582100 1.37246700 C -1.45849100 -1.22824600 3.12327200 H -1.36325200 0.39697200 1.72725500

	C -2.17730500 -2.33417800 3.57260500 H -3.93895000 -3.53368300 3.28316300 H -0.52747200 -0.96145500 3.60864000 H -1.80486700 -2.92793900 4.39900000 H 5.63811600 0.00654900 1.11057800 H -5.63811600 -0.00654900 1.11057800
2c (conformer 2)	C 0.65844000 0.99547200 0.79996700 C -0.70551000 1.05767400 0.53104500 C -1.39498900 -0.00139700 -0.06358000 C -0.69501600 -1.18454800 -0.38012400 C 0.66745200 -1.24906400 -0.10233400 C 1.35891500 -0.18691000 0.48651500 C -1.35338000 -2.37484200 -0.98862300 C -0.89273000 -2.81890200 -2.23390800 C -1.45988000 -3.91947000 -2.86693500 C -2.50653100 -4.60075700 -2.25144700 C -2.96700900 -4.17792700 -1.00980600 C -2.40510400 -3.07275600 -0.35599100 C 1.32399800 2.18456600 1.40404000 C 2.28514200 2.94496900 0.70528400 C 2.87837200 4.03637600 1.35483700 C 2.53214500 4.38358600 2.65581300 C 1.57016600 3.64134700 3.33584500 C 0.97376500 2.55322800 2.70721700 C -2.82407100 0.15323900 -0.38399600 N -3.49653900 1.16291200 -0.01037900 C -4.89847000 1.23375500 -0.39075200 C -5.13117300 2.45624800 -1.33539500 C -6.59946200 2.47614600 -1.79020600 C -4.78608500 3.78024900 -0.63681300 C -4.23587900 2.29358200 -2.57588200 C -5.72687600 1.25432400 0.89818300 C 2.78634500 -0.34336800 0.81855600 N 3.42956100 -1.40418600 0.54773100 C 4.81602900 -1.50549900 0.97869000 C 5.71969900 -1.91041100 -0.22600000 C 4.85995000 -2.48126000 2.16185400 C 7.18905500 -1.95322500 0.22340400 C 5.31236200 -3.27667800 -0.79840300 C 5.57242900 -0.83841900 -1.31679800 H -1.25986100 1.96107300 0.75260400 H 1.21942000 -2.15694000 -0.31041100 H -0.08764600 -2.27358000 -2.71266600 H -1.08849200 -4.23984000 -3.83330400 H -2.95474800 -5.46439800 -2.72880600

	H 3.00143900 5.23773600 3.13004100 H 1.28679000 3.90532400 4.34800600 H 0.23346600 1.96081500 3.23244700 H -3.27684800 -0.64366300 -0.98403500 H -5.18116300 0.33636800 -0.96839600 H -6.75266300 3.26740900 -2.52950900 H -6.88442700 1.52645500 -2.25423400 H -7.28179500 2.66699300 -0.95933300 H -4.87740400 4.61148800 -1.34227200 H -5.45904000 3.98305700 0.19961700 H -3.76388400 3.76180400 -0.25515700 H -4.43857000 3.08987500 -3.29754400 H -3.17789500 2.33789500 -2.31082900 H -4.41959100 1.33506200 -3.07274700 H -5.49979100 0.36444900 1.48775300 H -5.48224100 2.12729200 1.50553600 H -6.79720100 1.26044400 0.68425000 H 3.26117100 0.49809600 1.33697900 H 5.17881500 -0.52447700 1.33173500 H 4.24732900 -2.09401300 2.97924000 H 4.45989800 -3.45626400 1.87808600 H 5.87755800 -2.61115100 2.53380700 H 7.83952600 -2.11943800 -0.64001000 H 7.48948600 -1.00917000 0.68937700 H 7.37794900 -2.75919700 0.93577500 H 4.25705700 -3.28026500 -1.07585000 H 5.90581800 -3.50127300 -1.68970100 H 5.48007200 -4.08321700 -0.08032200 H 4.54592400 -0.77601000 -1.68122100 H 5.84698300 0.14795600 -0.93295500 H 6.22465300 -1.06339900 -2.16577200 C -2.93673700 -2.68393000 0.97628400 C -4.31998100 -2.58819400 1.17558500 C -2.08742900 -2.41863600 2.05827500 C -4.84089500 -2.23152600 2.41603200 H -4.98999500 -2.77292600 0.34368400 C -2.60706900 -2.05928900 3.29713700 H -1.01604300 -2.49522400 1.92780400 C -3.98540000 -1.96066700 3.48099900 H -5.91422400 -2.15528400 2.54698500 H -1.93341700 -1.85846400 4.12223900 H -4.38830700 -1.67494800 4.44564700 C 2.68299500 2.63717400 -0.69315500 C 4.03767600 2.60825500 -1.04619000 C 1.72935000 2.39975300 -1.69241900

	C 4.43067200 2.34688900 -2.35563600 H 4.78837600 2.77238900 -0.28157800 C 2.12137000 2.13575900 -3.00016000 H 0.67677000 2.42948700 -1.44567300 C 3.47384100 2.10575200 -3.33747400 H 5.48491500 2.31567400 -2.60463200 H 1.36781300 1.95793700 -3.75886800 H 3.77817400 1.89526200 -4.35613200 H -3.75972900 -4.72747400 -0.51588000 H 3.60147600 4.63519200 0.81356900
2c (conformer 4)	C 1.25925400 -0.64004900 -0.53922100 C 1.15775300 0.74827200 -0.57297700 C -0.07513600 1.40467000 -0.58400300 C -1.25925400 0.64004900 -0.53922100 C -1.15775300 -0.74827200 -0.57297700 C 0.07513600 -1.40467000 -0.58400300 C -2.61586300 1.24785500 -0.44534000 C -3.54561600 0.95304100 -1.44988200 C -4.83527900 1.47123800 -1.42093700 C -5.21872200 2.29718700 -0.36768800 C -4.30910300 2.59283300 0.64080500 C -3.00390300 2.08115900 0.62707600 C 2.61586300 -1.24785500 -0.44534000 C 3.00390300 -2.08115900 0.62707600 C 4.30910300 -2.59283300 0.64080500 C 5.21872200 -2.29718700 -0.36768800 C 4.83527900 -1.47123800 -1.42093700 C 3.54561600 -0.95304100 -1.44988200 C -0.11383200 2.87469300 -0.66158800 N 0.93771400 3.58359400 -0.60873800 C 0.80120200 5.02734500 -0.71949800 C 1.51808000 5.53122300 -2.01292600 C 1.30353700 7.04686200 -2.15623200 C 3.02242000 5.22143000 -1.97901900 C 0.88453400 4.83089800 -3.22718800 C 1.32490300 5.64378400 0.58201100 C 0.11383200 -2.87469300 -0.66158800 N -0.93771400 -3.58359400 -0.60873800 C -0.80120200 -5.02734500 -0.71949800 C -1.51808000 -5.53122300 -2.01292600 C -1.32490300 -5.64378400 0.58201100 C -1.30353700 -7.04686200 -2.15623200 C -3.02242000 -5.22143000 -1.97901900 C -0.88453400 -4.83089800 -3.22718800 H 2.05288400 1.35735500 -0.56361000

	H -2.05288400 -1.35735500 -0.56361000 H -3.23554100 0.31847800 -2.27188000 H -5.53376200 1.23164000 -2.21410400 H -6.22356200 2.70101600 -0.32496700 H 6.22356200 -2.70101600 -0.32496700 H 5.53376200 -1.23164000 -2.21410400 H 3.23554100 -0.31847800 -2.27188000 H -1.10238300 3.32862200 -0.79439000 H -0.26302000 5.30107000 -0.82721000 H 1.70682300 7.39448700 -3.11159900 H 0.23895000 7.30078000 -2.13186500 H 1.80490100 7.60790700 -1.36478800 H 3.48709100 5.51615900 -2.92465100 H 3.52897800 5.76677400 -1.17920900 H 3.19488800 4.15483900 -1.82580600 H 1.30760000 5.22344400 -4.15605400 H 1.06147000 3.75415000 -3.20290700 H -0.19788900 4.99499300 -3.25553700 H 0.75100500 5.25391700 1.42404400 H 2.37169200 5.38132000 0.74370300 H 1.22917700 6.73100500 0.57539700 H 1.10238300 -3.32862200 -0.79439000 H 0.26302000 -5.30107000 -0.82721000 H -0.75100500 -5.25391700 1.42404400 H -2.37169200 -5.38132000 0.74370300 H -1.22917700 -6.73100500 0.57539700 H -1.70682300 -7.39448700 -3.11159900 H -0.23895000 -7.30078000 -2.13186500 H -1.80490100 -7.60790700 -1.36478800 H -3.19488800 -4.15483900 -1.82580600 H -3.48709100 -5.51615900 -2.92465100 H -3.52897800 -5.76677400 -1.17920900 H -1.06147000 -3.75415000 -3.20290700 H 0.19788900 -4.99499300 -3.25553700 H -1.30760000 -5.22344400 -4.15605400 C -2.08445300 2.44644400 1.73714900 C -1.98761400 3.78444300 2.14156500 C -1.30353700 1.49170100 2.40254800 C -1.13285100 4.16242200 3.17272200 H -2.57075200 4.53754000 1.62414900 C -0.44253800 1.87126300 3.42658100 H -1.36824000 0.45094100 2.11343300 C -0.35044400 3.20674000 3.81487100 H -1.06888200 5.20454500 3.46390600 H 0.16169300 1.12415900 3.92742100

	H 0.32656600 3.49800900 4.60932400 C 2.08445300 -2.44644400 1.73714900 C 1.98761400 -3.78444300 2.14156500 C 1.30353700 -1.49170100 2.40254800 C 1.13285100 -4.16242200 3.17272200 H 2.57075200 -4.53754000 1.62414900 C 0.44253800 -1.87126300 3.42658100 H 1.36824000 -0.45094100 2.11343300 C 0.35044400 -3.20674000 3.81487100 H 1.06888200 -5.20454500 3.46390600 H -0.16169300 -1.12415900 3.92742100 H -0.32656600 -3.49800900 4.60932400 H -4.61644000 3.21188300 1.47540500 H 4.61644000 -3.21188300 1.47540500
2c (conformer 5)	C -0.93943000 1.25037100 -1.04857700 C 0.40830200 0.93029400 -1.18868500 C 0.85920000 -0.38937200 -1.21782600 C -0.08051600 -1.43949200 -1.15140300 C -1.42732100 -1.12470400 -1.02602500 C -1.87446500 0.19915000 -0.93863000 C 0.33659100 -2.87062400 -1.21854900 C 0.12209700 -3.57657500 -2.40632100 C 0.53636200 -4.89791000 -2.54389800 C 1.17892800 -5.53118700 -1.48332500 C 1.38714700 -4.84272200 -0.29287800 C 0.96593800 -3.51580900 -0.13630800 C -1.35201800 2.68040300 -1.05264500 C -0.77009300 3.63067600 -0.18603300 C -1.16310100 4.97133500 -0.29270100 C -2.10775700 5.38023600 -1.22719500 C -2.67799400 4.44319900 -2.08518700 C -2.29758800 3.10940100 -1.99361100 C 2.30546700 -0.65534300 -1.31111500 N 3.15816800 0.28445100 -1.34358900 C 4.56935200 -0.05567300 -1.41942800 C 5.33277500 0.63426200 -0.24555900 C 6.81176300 0.21835700 -0.27928700 C 5.21816300 2.16416700 -0.32824100 C 4.71660100 0.15161900 1.07745700 C 5.06929900 0.32750300 -2.81750600 C -3.29006500 0.45857900 -0.62356500 N -4.17600600 -0.45101800 -0.66177800 C -5.52775400 -0.11110000 -0.24446400 C -5.94117900 -1.00966700 0.96473500 C -6.44347700 -0.22690600 -1.46794000

	C -7.31236200 -0.55673900 1.49155900 C -6.00018300 -2.49218300 0.56688300 C -4.90210100 -0.82772900 2.08507200 H 1.14772800 1.71521600 -1.26926000 H -2.16308800 -1.91496500 -0.94387400 H -0.35976900 -3.06861500 -3.23378900 H 0.36284100 -5.42603900 -3.47422300 H 1.50631200 -6.56012600 -1.57718600 H -2.39791100 6.42299900 -1.28306800 H -3.40784400 4.74864300 -2.82579300 H -2.71849100 2.38166500 -2.67773500 H 2.61063800 -1.70829500 -1.33730900 H 4.70749000 -1.14341100 -1.29081800 H 7.33103600 0.60971700 0.60024800 H 6.91772400 -0.87137500 -0.27092300 H 7.32705000 0.60288900 -1.16226200 H 5.68922800 2.62136900 0.54724000 H 5.71886600 2.56006000 -1.21540900 H 4.17210100 2.47112900 -0.35497300 H 5.26025900 0.57529900 1.92720500 H 3.66983900 0.44469600 1.16424000 H 4.76753600 -0.93824900 1.15532500 H 4.51694000 -0.23757100 -3.57183500 H 4.90749800 1.38915500 -3.01184600 H 6.13069100 0.10380200 -2.93693200 H -3.53598000 1.47879500 -0.30486300 H -5.56385800 0.93175400 0.11561700 H -6.12327500 0.48396100 -2.23327100 H -6.39079500 -1.22742200 -1.90036700 H -7.48132900 -0.00516600 -1.21371100 H -7.57277300 -1.11886600 2.39286800 H -7.30577000 0.50639700 1.75209100 H -8.10736900 -0.72262900 0.76144200 H -5.05602100 -2.81139600 0.12209100 H -6.19407200 -3.11088600 1.44804800 H -6.79951200 -2.68498500 -0.15267900 H -4.79091900 0.22873900 2.35107000 H -5.21199700 -1.36975000 2.98274800 H -3.92309400 -1.20348000 1.78167200 C 1.18799600 -2.83889500 1.16811200 C 2.46462100 -2.81178000 1.73958000 C 0.12507800 -2.26227400 1.87554900 C 2.67694300 -2.22616700 2.98503800 H 3.29782100 -3.24081800 1.19479200 C 0.33402200 -1.68820700 3.12434100

	H -0.87048600 -2.28160300 1.45231300 C 1.61101000 -1.66703700 3.68382300 H 3.67560700 -2.20179200 3.40513700 H -0.50397000 -1.26096200 3.66362700 H 1.77367000 -1.21717900 4.65661800 C 0.24943300 3.26276900 0.83153200 C 1.45879400 3.96604700 0.89169900 C 0.03605600 2.21988100 1.74056100 C 2.43438800 3.62846100 1.82582400 H 1.64529000 4.76201900 0.17986400 C 1.00709400 1.88699300 2.67791100 H -0.89226600 1.66317900 1.70625100 C 2.21224300 2.58544900 2.72063500 H 3.37337000 4.16918700 1.84196500 H 0.83019000 1.06993100 3.36426500 H 2.97490000 2.31151200 3.44003700 H 1.86122100 -5.34175300 0.54439000 H -0.72992300 5.69483800 0.38807400
2c (conformer 9)	C -0.15791800 -1.49665500 -0.27056200 C 1.21386300 -1.39550600 -0.06320200 C 1.79913000 -0.25976600 0.50971800 C 0.97222300 0.80738200 0.91370000 C -0.39786600 0.71326700 0.68705000 C -0.97692700 -0.40317700 0.08759900 C 1.50619200 2.04589700 1.54487700 C 2.15427700 1.97103200 2.78282400 C 2.60105500 3.11623400 3.43342100 C 2.39845300 4.36388900 2.84800300 C 1.75487900 4.45255200 1.61815700 C 1.30638700 3.30788600 0.94791600 C -0.70301900 -2.74403500 -0.87513500 C -1.67664900 -3.53935900 -0.23230500 C -2.14285100 -4.68978700 -0.88278100 C -1.66209600 -5.06477900 -2.13214900 C -0.69253700 -4.28632800 -2.75891700 C -0.22208600 -3.13938200 -2.12942600 C 3.26599600 -0.16070900 0.59349300 N 4.03711500 -1.11644300 0.26747900 C 5.47301400 -0.88566000 0.31803800 C 6.07547600 -1.01537700 -1.11783000 C 7.57366900 -0.67302100 -1.07641600 C 5.88258800 -2.43082800 -1.68355700 C 5.36862500 -0.00417400 -2.03717600 C 6.06997300 -1.84761400 1.35050400 C -2.41641400 -0.37993400 -0.22310000

	N -3.17274000 0.55863200 0.17292300 C -4.56635900 0.54574200 -0.23660200 C -4.84310300 1.76207100 -1.18013400 C -5.42548500 0.50934500 1.03136600 C -6.30533600 1.71813200 -1.65149300 C -4.56481000 3.09652400 -0.47114400 C -3.92473800 1.64755500 -2.40889200 H 1.86729000 -2.21072400 -0.34786600 H -1.04863200 1.53523400 0.95286200 H 2.28556300 0.99924100 3.24497900 H 3.09627000 3.03520400 4.39400700 H 2.74329300 5.26362700 3.34419000 H -2.03471000 -5.96469100 -2.60746900 H -0.30747100 -4.56680200 -3.73233300 H 0.51853000 -2.51833800 -2.61971800 H 3.66753000 0.80644300 0.91903600 H 5.68030100 0.14693500 0.64858200 H 7.98376800 -0.66337100 -2.09029100 H 7.74359900 0.31605400 -0.63936100 H 8.14490600 -1.40288600 -0.49893100 H 6.23739500 -2.47247900 -2.71766700 H 6.44481700 -3.17405900 -1.11319100 H 4.82883200 -2.71453000 -1.66801800 H 5.82836500 -0.00732600 -3.02935400 H 4.31037900 -0.24517600 -2.15304300 H 5.44255200 1.01227600 -1.63637900 H 5.62758200 -1.65344200 2.33035600 H 5.85429100 -2.88464100 1.08815300 H 7.15039400 -1.72115400 1.43732100 H -2.79423100 -1.19456700 -0.85098500 H -4.78325400 -0.36109600 -0.82789300 H -5.16096300 -0.36976300 1.62196600 H -5.24586800 1.39078000 1.64903500 H -6.48897900 0.45468800 0.79205100 H -6.48405200 2.50224800 -2.39280500 H -6.54351000 0.75717200 -2.11877700 H -7.00499900 1.87870300 -0.82850900 H -3.54022600 3.12939400 -0.09859600 H -4.70496500 3.92664600 -1.17027300 H -5.24334900 3.25633700 0.37016600 H -4.05680500 0.68343000 -2.91128400 H -4.15932200 2.43573300 -3.13032000 H -2.87429700 1.74822100 -2.13362100 C 0.63468800 3.44870100 -0.37113900 C -0.47460400 4.28990900 -0.51142400

	C 1.08551500 2.74021600 -1.49174600 C -1.12718400 4.40888400 -1.73584800 H -0.84501700 4.82846600 0.35343400 C 0.43856200 2.86357000 -2.71642500 H 1.94404500 2.08651500 -1.39956800 C -0.67415700 3.69448200 -2.84166900 H -1.99943700 5.04632700 -1.82010900 H 0.80093800 2.30784500 -3.57367300 H -1.18740100 3.77853100 -3.79237600 C -2.22344800 -3.20420900 1.10831200 C -3.60783400 -3.21448600 1.32101900 C -1.38522300 -2.88155300 2.18299100 C -4.14141400 -2.90253100 2.56803900 H -4.27014000 -3.44426800 0.49416700 C -1.91772900 -2.56768700 3.42863800 H -0.31247900 -2.87592400 2.03993400 C -3.29772100 -2.57314900 3.62589100 H -5.21607300 -2.90686700 2.70992100 H -1.25323400 -2.31892300 4.24801800 H -3.71110900 -2.32148400 4.59557000 H 1.61213000 5.42010900 1.15082700 H -2.87519900 -5.31034100 -0.37987900
2c (conformer 12)	C -0.04013600 1.61695700 -0.57821100 C -1.38754500 1.40085700 -0.30578900 C -1.92013300 0.11381100 -0.16956700 C -1.08707000 -1.00603000 -0.38321500 C 0.25628500 -0.78251500 -0.67286000 C 0.80228800 0.49820700 -0.74223700 C -1.61185700 -2.39816400 -0.36410700 C -2.75298400 -2.70229700 -1.12023500 C -3.26257700 -3.99364600 -1.18355200 C -2.62571800 -5.01825700 -0.48848900 C -1.48383300 -4.73741100 0.25388600 C -0.95957000 -3.44104900 0.33128300 C 0.46455000 3.01515500 -0.69042300 C 1.38270800 3.56837500 0.22556100 C 1.84023400 4.87622600 0.01509900 C 1.39723000 5.63520600 -1.06230300 C 0.47427100 5.09422700 -1.95348200 C 0.01621700 3.79476500 -1.76247900 C -3.32017700 -0.04176000 0.26440800 N -4.18977600 0.87161700 0.11591900 C -5.53262200 0.62489300 0.62239300 C -6.55536100 0.64009500 -0.55750000 C -7.94912400 0.26460600 -0.02854700

	C -6.60991800 2.01728000 -1.23628400 C -6.12387700 -0.41562000 -1.59047100 C -5.81347000 1.65342800 1.72309800 C 2.25097400 0.63678500 -0.97839600 N 3.02666600 -0.36351900 -0.89406400 C 4.45085400 -0.17494300 -1.10253000 C 4.93842600 -1.10652200 -2.25605400 C 5.14153200 -0.41856900 0.24514600 C 6.41979400 -0.82358900 -2.55131800 C 4.75309100 -2.58783500 -1.89007000 C 4.11711500 -0.78933000 -3.51722100 H -2.04785300 2.24349000 -0.14170700 H 0.92215600 -1.61575300 -0.84352600 H -3.22994000 -1.91226700 -1.68738800 H -4.14425800 -4.19785200 -1.77975900 H -3.01302300 -6.02986300 -0.52481600 H 1.76079400 6.64733400 -1.19663500 H 0.11594100 5.67688200 -2.79406700 H -0.68698400 3.35852200 -2.46247600 H -3.57331300 -0.99647800 0.74255800 H -5.59063400 -0.38258600 1.06950900 H -8.65506200 0.18115700 -0.85969600 H -7.93026100 -0.69856100 0.49125200 H -8.34165100 1.01526000 0.66059400 H -7.25952900 1.97723500 -2.11562700 H -7.01084000 2.78154600 -0.56620500 H -5.61447300 2.33042400 -1.55605600 H -6.87055500 -0.49817900 -2.38514300 H -5.16909100 -0.15132800 -2.04893700 H -6.01648600 -1.40112600 -1.12526600 H -5.08736800 1.53349100 2.53055300 H -5.71904700 2.67051700 1.33921600 H -6.81139100 1.52605800 2.14590600 H 2.62375200 1.64005700 -1.21650400 H 4.66101800 0.86151100 -1.42041300 H 4.78284600 0.30839200 0.97533300 H 4.89942400 -1.41212100 0.62509600 H 6.22554100 -0.32002200 0.16329800 H 6.75030200 -1.41092000 -3.41279500 H 6.58202500 0.23313900 -2.78667100 H 7.06349800 -1.08598400 -1.70883600 H 4.99555400 -3.22041700 -2.74915000 H 5.40854500 -2.88405100 -1.06740200 H 3.72243300 -2.78673500 -1.59155600 H 4.48975800 -1.36414500 -4.36970400

	H 3.06316400 -1.03487300 -3.37540100 H 4.18431800 0.27343900 -3.77280500 C 0.27977400 -3.21933200 1.12357000 C 1.42408700 -3.97518800 0.84337100 C 0.34616800 -2.25137100 2.13204000 C 2.61085700 -3.75618300 1.53780400 H 1.38986500 -4.71418200 0.05097300 C 1.52908600 -2.03707300 2.83004000 H -0.52973700 -1.65453300 2.35634500 C 2.66755300 -2.78299400 2.53121300 H 3.49313000 -4.33498400 1.28985400 H 1.56862100 -1.27496200 3.59701200 H 3.59288700 -2.59999500 3.06486600 C 1.86564200 2.82463500 1.41751000 C 3.23388800 2.77052000 1.70883000 C 0.97027100 2.20204200 2.29659700 C 3.69628600 2.11438200 2.84644500 H 3.94003900 3.23262800 1.02837900 C 1.43112400 1.55293900 3.43613200 H -0.09124200 2.23984300 2.09106600 C 2.79582700 1.50371700 3.71530500 H 4.76011000 2.07677200 3.05102800 H 0.72050000 1.08933300 4.11093000 H 3.15453700 0.99393200 4.60207000 H -0.98928900 -5.52954900 0.80405000 H 2.53208400 5.30725600 0.72932100
2c (conformer 13)	C -1.40107300 -0.18097600 -1.18831100 C -0.84274100 1.09279200 -1.18665100 C 0.53873900 1.29804300 -1.16509100 C 1.40107300 0.18097600 -1.18831100 C 0.84274100 -1.09279200 -1.18665100 C -0.53873900 -1.29804300 -1.16509100 C 2.88262700 0.32138800 -1.20935400 C 3.48982000 1.00098300 -2.27248800 C 4.87281100 1.10516800 -2.36909000 C 5.67612000 0.52074800 -1.39286300 C 5.08684600 -0.15896100 -0.33263700 C 3.69471800 -0.26845700 -0.21872200 C -2.88262700 -0.32138800 -1.20935400 C -3.69471800 0.26845700 -0.21872200 C -5.08684600 0.15896100 -0.33263700 C -5.67612000 -0.52074800 -1.39286300 C -4.87281100 -1.10516800 -2.36909000 C -3.48982000 -1.00098300 -2.27248800 C 1.05747600 2.66819300 -1.00773500

	N 0.30279200 3.68847900 -1.05618000 C 0.88749400 4.99405500 -0.79711800 C 0.26200600 5.59457400 0.50365000 C 0.93003700 6.94360200 0.81451200 C -1.25579100 5.78579100 0.36079700 C 0.53873900 4.62800700 1.66778000 C 0.70018500 5.85275800 -2.05220500 C -1.05747600 -2.66819300 -1.00773500 N -0.30279200 -3.68847900 -1.05618000 C -0.88749400 -4.99405500 -0.79711800 C -0.26200600 -5.59457400 0.50365000 C -0.70018500 -5.85275800 -2.05220500 C -0.93003700 -6.94360200 0.81451200 C 1.25579100 -5.78579100 0.36079700 C -0.53873900 -4.62800700 1.66778000 H -1.48184600 1.96528700 -1.16790900 H 1.48184600 -1.96528700 -1.16790900 H 2.86044600 1.43238000 -3.04242100 H 5.31924300 1.63203400 -3.20431200 H 6.75553000 0.59692000 -1.45367000 H -6.75553000 -0.59692000 -1.45367000 H -5.31924300 -1.63203400 -3.20431200 H -2.86044600 -1.43238000 -3.04242100 H 2.13007200 2.76209000 -0.79957300 H 1.96998700 4.89701000 -0.60310400 H 0.57412400 7.32538300 1.77572300 H 2.01824600 6.84282100 0.87874200 H 0.70222200 7.69712400 0.05763700 H -1.67913300 6.12995300 1.30925700 H -1.49958600 6.53228200 -0.39907200 H -1.73968100 4.84665200 0.08999000 H 0.19563000 5.06385300 2.61044600 H 0.01979500 3.67886700 1.53063600 H 1.61030700 4.42300700 1.76309900 H 1.19502500 5.37370500 -2.90025200 H -0.35744200 5.95657000 -2.30051300 H 1.13392800 6.84611400 -1.92604400 H -2.13007200 -2.76209000 -0.79957300 H -1.96998700 -4.89701000 -0.60310400 H -1.19502500 -5.37370500 -2.90025200 H 0.35744200 -5.95657000 -2.30051300 H -1.13392800 -6.84611400 -1.92604400 H -0.57412400 -7.32538300 1.77572300 H -2.01824600 -6.84282100 0.87874200 H -0.70222200 -7.69712400 0.05763700

	H 1.67913300 -6.12995300 1.30925700 H 1.49958600 -6.53228200 -0.39907200 H 1.73968100 -4.84665200 0.08999000 H -1.61030700 -4.42300700 1.76309900 H -0.19563000 -5.06385300 2.61044600 H -0.01979500 -3.67886700 1.53063600 C 3.12358300 -0.99922600 0.94355700 C 3.56443700 -2.29462400 1.23911300 C 2.15260800 -0.41762800 1.76855100 C 3.04699100 -2.99478900 2.32551700 H 4.30012900 -2.76332500 0.59558500 C 1.64268500 -1.11418400 2.85875800 H 1.79668500 0.58261900 1.55515800 C 2.08437900 -2.40586600 3.14047100 H 3.38615700 -4.00428800 2.52571800 H 0.89806700 -0.64825700 3.49255000 H 1.67546900 -2.95008600 3.98351400 C -3.12358300 0.99922600 0.94355700 C -3.56443700 2.29462400 1.23911300 C -2.15260800 0.41762800 1.76855100 C -3.04699100 2.99478900 2.32551700 H -4.30012900 2.76332500 0.59558500 C -1.64268500 1.11418400 2.85875800 H -1.79668500 -0.58261900 1.55515800 C -2.08437900 2.40586600 3.14047100 H -3.38615700 4.00428800 2.52571800 H -0.89806700 0.64825700 3.49255000 H -1.67546900 2.95008600 3.98351400 H 5.70839600 -0.59746500 0.43942600 H -5.70839600 0.59746500 0.43942600
2c (conformer 35)	C -0.05381900 1.61748500 -0.67440100 C -1.37701100 1.39554300 -0.30963200 C -1.92273000 0.10827700 -0.25300900 C -1.12765600 -0.99564300 -0.62839200 C 0.19285400 -0.76741500 -1.00549200 C 0.75039900 0.51104600 -1.02069400 C -1.68016700 -2.37602500 -0.69346000 C -2.83143100 -2.60301400 -1.46012500 C -3.36650600 -3.87684600 -1.60965300 C -2.74661500 -4.95855900 -0.98933100 C -1.59969200 -4.75111300 -0.23148600 C -1.04867500 -3.47289600 -0.06864200 C 0.46822000 3.01500000 -0.70595300 C 1.41747300 3.48853000 0.22238600 C 1.89657100 4.79851000 0.08940000

	C 1.44322500 5.63641700 -0.92366700 C 0.48974200 5.17340700 -1.82640000 C 0.01122100 3.87184800 -1.71270000 C -3.29161600 -0.07436400 0.26055400 N -4.13537000 0.87336500 0.31516400 C -5.44812500 0.58831400 0.87670700 C -6.54926600 0.83338200 -0.20275400 C -7.91951000 0.43029600 0.36611200 C -6.58239900 2.30325000 -0.64821200 C -6.24300300 -0.05706100 -1.41974300 C -5.60425500 1.42713500 2.14988300 C 2.16503300 0.68270800 -1.40397900 N 2.89206300 -0.31551400 -1.69725000 C 4.30406400 -0.16709600 -2.03032900 C 5.10975900 -1.18629600 -1.15268400 C 4.85502400 1.26224400 -2.00347800 C 6.60644600 -1.10942300 -1.49385100 C 4.90518900 -0.89077400 0.34060900 C 4.61001800 -2.60755300 -1.46214900 H -2.00596100 2.22795800 -0.01896000 H 0.82463200 -1.59337000 -1.30202400 H -3.29631500 -1.76353700 -1.96330500 H -4.25539800 -4.02295900 -2.21212900 H -3.15414200 -5.95758700 -1.09198700 H 1.82367700 6.64844300 -0.99921500 H 0.12366100 5.81798400 -2.61699600 H -0.71547400 3.49627900 -2.42384400 H -3.54683800 -1.08308300 0.60858700 H -5.51829300 -0.47742000 1.15561100 H -8.68513600 0.50423100 -0.41137000 H -7.91068300 -0.60285500 0.72793100 H -8.22691500 1.07630000 1.19125400 H -7.29591300 2.43094900 -1.46764500 H -6.89331700 2.96430200 0.16429700 H -5.59827000 2.62482900 -0.99345600 H -7.04568000 0.01904000 -2.15845500 H -5.30960100 0.24065800 -1.90087400 H -6.15378400 -1.10838800 -1.12641500 H -4.82606800 1.15425000 2.86652500 H -5.49750000 2.49095600 1.93119700 H -6.57285200 1.25911400 2.62371000 H 2.53189100 1.71015200 -1.40783800 H 4.39396300 -0.53771200 -3.06101900 H 4.26941500 1.91758200 -2.65296900 H 4.84390800 1.68921300 -0.99795600

	H 5.88150100 1.28166300 -2.36917600 H 7.14324300 -1.92064700 -0.99399000 H 6.77523200 -1.21367100 -2.57060900 H 7.05612200 -0.16906300 -1.16744900 H 3.85342600 -0.96679100 0.61929200 H 5.46667200 -1.60881300 0.94586400 H 5.25557400 0.10924800 0.60562800 H 4.77416900 -2.85729300 -2.51557500 H 5.15360800 -3.33824200 -0.85555800 H 3.54646600 -2.70327200 -1.24995200 C 0.18019200 -3.32688000 0.75518500 C 1.28874000 -4.14461100 0.50388200 C 0.26254900 -2.38937900 1.79168300 C 2.45077000 -4.02438500 1.26096900 H 1.24693600 -4.85879100 -0.31044000 C 1.42111600 -2.27261900 2.55097300 H -0.58394200 -1.74619400 1.99801300 C 2.52114700 -3.08613700 2.28671200 H 3.30557100 -4.65135500 1.03640000 H 1.47152200 -1.53553400 3.34126400 H 3.42877900 -2.98052000 2.86912600 C 1.91750400 2.65147200 1.34352500 C 3.29285500 2.52855300 1.57290500 C 1.03383000 2.00792500 2.21942400 C 3.77476100 1.78112200 2.64395800 H 3.98760700 3.01330100 0.89680100 C 1.51452000 1.27184500 3.29622800 H -0.03277200 2.09989000 2.06372000 C 2.88644100 1.15096000 3.51092300 H 4.84339200 1.68718900 2.79770700 H 0.81383000 0.79625900 3.97309900 H 3.25996000 0.57100900 4.34699400 H -1.12529400 -5.58802700 0.26759900 H 2.61541600 5.16628100 0.81238000
2c (conformer 47)	C 1.19588700 -0.00925500 -0.96330000 C -0.13263200 -0.36175100 -1.15779400 C -1.18086400 0.56158000 -1.07715800 C -0.88411800 1.91140200 -0.81809500 C 0.45240800 2.26918700 -0.63095000 C 1.49321200 1.33597600 -0.65848900 C -1.91709800 2.98578900 -0.75810300 C -1.85146500 3.99246800 -1.72968500 C -2.76011100 5.04427200 -1.75267000 C -3.75741700 5.10604300 -0.78348700 C -3.83152700 4.11748400 0.19018300

	C -2.92688000 3.04529000 0.22685100 C 2.22577900 -1.06749900 -1.17248500 C 2.33383100 -2.16472900 -0.30102900 C 3.20863300 -3.20747300 -0.62632400 C 3.97771000 -3.16658900 -1.78468800 C 3.87784400 -2.07205500 -2.63998900 C 3.00198600 -1.03606700 -2.33371600 C -2.56310500 0.08952600 -1.27559800 N -2.81822400 -1.13036200 -1.51466000 C -4.20652000 -1.53759500 -1.66330700 C -4.46378100 -2.80084700 -0.78412800 C -5.96361800 -3.13546800 -0.79694200 C -3.65533100 -4.00536700 -1.28988400 C -4.04180900 -2.48159800 0.65949500 C -4.48462000 -1.73422500 -3.15861000 C 2.83027900 1.81039300 -0.26403200 N 3.72127900 1.04900000 0.21842300 C 4.97702700 1.62653800 0.67128700 C 6.16917300 0.93021400 -0.05418700 C 5.00610200 1.51034800 2.20063900 C 7.49215700 1.55540100 0.41633100 C 6.17945100 -0.58215300 0.21678100 C 6.02122700 1.17330400 -1.56557300 H -0.38569300 -1.38779900 -1.38971200 H 0.68533800 3.30442800 -0.40364800 H -1.07934600 3.92869000 -2.48774700 H -2.68922800 5.80656800 -2.51966400 H -4.46785400 5.92448300 -0.77772200 H 4.65712800 -3.97956200 -2.01284600 H 4.47348300 -2.02722300 -3.54436500 H 2.90004900 -0.19381400 -3.00854700 H -3.35875200 0.83744000 -1.19149300 H -4.87660900 -0.74503600 -1.28900200 H -6.16754500 -3.97211300 -0.12262500 H -6.56122200 -2.28258200 -0.45950800 H -6.31337800 -3.42314000 -1.79107600 H -3.76644800 -4.84688500 -0.59955500 H -3.99434400 -4.34019200 -2.27346800 H -2.59523900 -3.75437400 -1.35866300 H -4.29362500 -3.31539400 1.32176100 H -2.96759300 -2.30304900 0.72987700 H -4.55026400 -1.58877500 1.03152500 H -4.37257400 -0.78163000 -3.68188700 H -3.77648300 -2.44010800 -3.59587900 H -5.49864800 -2.09877800 -3.33254500

	H 2.98935500 2.89749100 -0.35164100 H 5.02403300 2.69756400 0.40651100 H 4.15889200 2.05355700 2.62626400 H 4.92689400 0.46827000 2.51467200 H 5.92150200 1.93500800 2.61514100 H 8.32257800 1.16099400 -0.17576900 H 7.48467900 2.64364100 0.29590000 H 7.70157300 1.33039300 1.46436100 H 5.23389300 -1.03844500 -0.07497000 H 6.98074300 -1.05874000 -0.35555700 H 6.35588800 -0.80045000 1.27303100 H 5.97923700 2.24467800 -1.78968500 H 6.87469900 0.75133200 -2.10357100 H 5.11537500 0.70578800 -1.95182900 C -3.07839800 2.02918200 1.30101500 C -4.35686600 1.55696600 1.63189200 C -1.98327800 1.53799800 2.02320700 C -4.53750000 0.63300900 2.65591700 H -5.21414000 1.90509700 1.06746900 C -2.16330300 0.60875600 3.04229200 H -0.98535100 1.88347200 1.78989800 C -3.43904500 0.15306400 3.36463100 H -5.53454900 0.27713200 2.88920500 H -1.30121300 0.23417000 3.57743800 H -3.57464200 -0.57704200 4.15397200 C 1.56459800 -2.21607200 0.96900400 C 1.72125300 -1.20319700 1.92294400 C 0.69336300 -3.27502400 1.24150800 C 1.02813300 -1.25884000 3.12744700 H 2.40442400 -0.38974200 1.71058600 C -0.01450600 -3.31972100 2.44085400 H 0.55532500 -4.05433400 0.50039800 C 0.15483700 -2.31414500 3.38943900 H 1.17324100 -0.47736300 3.86563300 H -0.69975400 -4.13773000 2.63140200 H -0.39166200 -2.35215800 4.32499200 H -4.58872700 4.18413600 0.96209200 H 3.29858700 -4.04544400 0.05554000
2c (conformer 59)	C 1.18833100 1.33466100 -0.95106400 C -0.13855100 1.45087500 -1.36826900 C -1.00569400 0.36009500 -1.39914600 C -0.51080600 -0.92795800 -1.09695000 C 0.81403200 -1.04744500 -0.70137400 C 1.66338900 0.06062100 -0.58861300 C -1.34369000 -2.15705500 -1.21629900

	C -1.80018300 -2.54450700 -2.47922900 C -2.52738400 -3.71537200 -2.65289300 C -2.80175800 -4.52626400 -1.55320100 C -2.34461800 -4.15486200 -0.29375300 C -1.61752300 -2.97316100 -0.10446400 C 2.05059300 2.54544000 -0.90161900 C 1.66448500 3.70301800 -0.19174700 C 2.49700200 4.82899600 -0.23074800 C 3.69018400 4.82428100 -0.94488100 C 4.07155400 3.68117400 -1.64316100 C 3.25416100 2.55706800 -1.61861700 C -2.43567600 0.64469300 -1.60970700 N -3.34642400 -0.06917600 -1.09511600 C -4.73749200 0.29744600 -1.29344800 C -5.43070600 0.46518500 0.09456200 C -6.86477500 0.97899200 -0.10889500 C -5.45705600 -0.86273900 0.86793900 C -4.64687300 1.51128800 0.90575400 C -5.36582000 -0.77235000 -2.19509600 C 3.00798000 -0.12349700 -0.01410500 N 3.56880500 -1.25996200 0.05495200 C 4.86647600 -1.34772800 0.70737500 C 5.92684700 -1.90039300 -0.29502100 C 4.68648200 -2.18643400 1.97815300 C 7.31080600 -1.90031000 0.37391900 C 5.57312000 -3.32094200 -0.76059700 C 5.97251900 -0.96466400 -1.51584000 H -0.52440500 2.43131200 -1.62149700 H 1.21074800 -2.01769700 -0.43259300 H -1.57547000 -1.91391500 -3.33183600 H -2.87424700 -3.99643900 -3.64062600 H -3.37137500 -5.44035400 -1.67512700 H 4.32001600 5.70626500 -0.95187200 H 4.99582700 3.66579900 -2.20875900 H 3.53685900 1.67327800 -2.17856400 H -2.66574700 1.56152900 -2.17559100 H -4.80864700 1.27360400 -1.80505000 H -7.33274100 1.17760200 0.85951500 H -6.87482100 1.91212400 -0.68119900 H -7.49049300 0.25285100 -0.63230800 H -5.84647900 -0.70098100 1.87746300 H -6.10049200 -1.59912300 0.38077300 H -4.45606500 -1.28842300 0.94943000 H -5.15509600 1.71638900 1.85237200 H -3.63638500 1.16888500 1.13166800

	H -4.56035300 2.45538000 0.35810600 H -4.88396800 -0.75557900 -3.17533600 H -5.21747900 -1.76734800 -1.77293300 H -6.43356100 -0.59862700 -2.33863100 H 3.49545000 0.77830300 0.37739800 H 5.21261800 -0.34242500 1.00488200 H 3.96014300 -1.70321700 2.63552800 H 4.30498400 -3.18013800 1.73804700 H 5.62505400 -2.28907200 2.52550900 H 8.07746900 -2.19075800 -0.34994100 H 7.56873000 -0.90579900 0.75191300 H 7.36300900 -2.60444200 1.20705400 H 6.28044000 -3.65201200 -1.52675300 H 5.61979200 -4.03827400 0.06236400 H 4.56704000 -3.35031800 -1.18237300 H 6.76549300 -1.27324000 -2.20269700 H 5.02638700 -0.98078700 -2.06019600 H 6.17274100 0.06856600 -1.21258100 C -1.18612000 -2.59286500 1.26497000 C -0.45659900 -3.48716400 2.05583700 C -1.51367800 -1.33814700 1.79364000 C -0.05382700 -3.13535000 3.34211700 H -0.18577000 -4.45501700 1.64917800 C -1.12178500 -0.99271200 3.08228500 H -2.08688400 -0.64770200 1.18835100 C -0.38631600 -1.88608500 3.86050900 H 0.52270200 -3.83528200 3.93623700 H -1.39770800 -0.02637500 3.48700700 H -0.07727600 -1.61108500 4.86243400 C 0.40282100 3.76691800 0.59334600 C -0.50047600 4.81473200 0.37889900 C 0.08263800 2.79204400 1.54704100 C -1.69999600 4.88008200 1.08430900 H -0.27008800 5.56788600 -0.36612900 C -1.11110100 2.86187800 2.25594500 H 0.76685700 1.97236600 1.72765400 C -2.01091100 3.90066400 2.02386400 H -2.39312200 5.69145400 0.89345800 H -1.34305500 2.10072400 2.99018100 H -2.94687800 3.94246000 2.56805500 H -2.57226700 -4.77129800 0.56838300 H 2.20779000 5.71004300 0.33041000
2c (conformer 69)	C 0.99590500 1.57971200 -1.05231500 C -0.35039400 1.88283000 -1.26244300 C -1.35443500 0.91156400 -1.22966800

	C -0.99738800 -0.43550600 -1.00322900 C 0.34486300 -0.74066000 -0.81866400 C 1.34934500 0.23341200 -0.84557200 C -1.97735300 -1.56040400 -1.04997400 C -2.43773400 -1.98830700 -2.29783400 C -3.29118600 -3.07899800 -2.41472400 C -3.68709200 -3.76850600 -1.27073900 C -3.22580600 -3.35658900 -0.02556800 C -2.37430400 -2.25226700 0.10688000 C 1.97794600 2.70046800 -1.05514700 C 2.80703800 3.00533800 0.04799200 C 3.67116000 4.10579200 -0.04971200 C 3.73152500 4.89030200 -1.19512600 C 2.91613800 4.58588400 -2.28157500 C 2.04896800 3.50249300 -2.20168100 C -2.74599700 1.36571900 -1.39020100 N -3.74151900 0.70994900 -0.96093800 C -5.08315000 1.21703800 -1.19415900 C -5.84995600 1.32947000 0.15906600 C -7.24392900 1.92824800 -0.08978900 C -5.98786500 -0.04243300 0.83803300 C -5.07238300 2.28220600 1.08332000 C -5.74013000 0.28639400 -2.22237000 C 2.75687400 -0.17761100 -0.70192500 N 3.08475100 -1.36956400 -0.41631900 C 4.49948400 -1.68802300 -0.30858900 C 4.89757500 -2.72137500 -1.41059900 C 4.75883500 -2.15428000 1.12793900 C 6.40891200 -2.99099100 -1.33288100 C 4.12503700 -4.03971600 -1.25129400 C 4.57930400 -2.11433400 -2.78771800 H -0.63231100 2.91934500 -1.41563700 H 0.64522200 -1.76908100 -0.66510300 H -2.11633700 -1.45309400 -3.18414000 H -3.64060200 -3.39171000 -3.39200100 H -4.35410700 -4.61949400 -1.34683300 H 4.40524900 5.73833100 -1.23475000 H 2.95474100 5.18478900 -3.18393300 H 1.42123700 3.25078600 -3.04874100 H -2.86934000 2.34157100 -1.88765500 H -5.04078900 2.23397300 -1.62286900 H -7.74829100 2.10960900 0.86351300 H -7.17811700 2.88455000 -0.61861500 H -7.87892100 1.25914500 -0.67408900 H -6.45695400 0.07121300 1.81976200

	H -6.61241300 -0.71923900 0.25011100 H -5.01445700 -0.51427000 0.97504400 H -5.61615700 2.43124600 2.02013400 H -4.08588800 1.88628100 1.32815700 H -4.93665200 3.26209100 0.61355300 H -5.17979000 0.32217800 -3.15940200 H -5.72911600 -0.74655000 -1.87175600 H -6.76887600 0.58417800 -2.43103300 H 3.51156500 0.59733500 -0.87447000 H 5.10719100 -0.78507400 -0.49441400 H 4.46241100 -1.36730500 1.82261100 H 4.17036800 -3.04308900 1.36143200 H 5.81537700 -2.37537200 1.29057200 H 6.71792000 -3.63533500 -2.16083300 H 6.98134400 -2.06042400 -1.40285000 H 6.68770900 -3.49295700 -0.40407300 H 4.35805800 -4.71321300 -2.08141900 H 4.39055900 -4.55482600 -0.32502300 H 3.04879700 -3.85957700 -1.24425800 H 4.93001500 -2.77577700 -3.58489600 H 3.50592100 -1.96618200 -2.91892200 H 5.07228100 -1.14464800 -2.91454600 C -1.96435500 -1.81841300 1.46723700 C -1.40026400 -2.72624700 2.37033600 C -2.19342900 -0.50384900 1.89090700 C -1.07929400 -2.33272500 3.66751000 H -1.20331800 -3.74245100 2.04798400 C -1.88513200 -0.11338900 3.18956600 H -2.64951500 0.19156600 1.20061200 C -1.32769200 -1.02664300 4.08394500 H -0.63616000 -3.04674000 4.35238600 H -2.08930300 0.90332900 3.50736800 H -1.08888700 -0.72316400 5.09709400 C 2.81764000 2.20490400 1.30066100 C 4.04429400 1.84274200 1.87490700 C 1.63950000 1.78798700 1.93328500 C 4.09398000 1.08662900 3.04174700 H 4.96629200 2.13506200 1.38585600 C 1.68814900 1.02103000 3.09222600 H 0.67888400 2.05443700 1.51302900 C 2.91426200 0.66668100 3.65116900 H 5.05407800 0.81134100 3.46315000 H 0.76541500 0.68742400 3.54798600 H 2.94866900 0.06094900 4.54926200 H -3.54769200 -3.87667600 0.86938000

	H 4.28728900 4.35936500 0.80469400
2c (conformer 77)	C 0.99073400 -1.65617900 0.69692900 C -0.33317300 -2.09485400 0.73883900 C -1.38840300 -1.35261900 0.19809700 C -1.10041500 -0.15610600 -0.49161200 C 0.21578000 0.28595700 -0.51854200 C 1.25907900 -0.41523400 0.09023300 C -2.11940600 0.65597800 -1.21475900 C -2.71109900 0.14306700 -2.37141800 C -3.57397100 0.91699500 -3.13976800 C -3.85022700 2.22778500 -2.75856400 C -3.26317900 2.74985900 -1.61042600 C -2.39931600 1.97860700 -0.82522200 C 2.05270400 -2.50229400 1.30722600 C 3.16130800 -2.97761000 0.57283400 C 4.11999200 -3.75879300 1.23237400 C 3.99785400 -4.07729400 2.58007100 C 2.89955300 -3.61536800 3.30046200 C 1.94041200 -2.83654600 2.66258200 C -2.75397400 -1.81372300 0.50287800 N -3.74629000 -1.02857000 0.57266000 C -5.03479600 -1.55407600 0.99776800 C -6.11489900 -1.24549800 -0.08427000 C -7.47026700 -1.81596100 0.36283200 C -6.23853500 0.26603100 -0.33023000 C -5.70034100 -1.94121600 -1.39159200 C -5.33232600 -0.96184800 2.38116300 C 2.59660300 0.19975700 0.13883300 N 2.85753200 1.27916300 -0.47419200 C 4.17199500 1.87358000 -0.30783400 C 4.02672400 3.25739900 0.40448800 C 4.83945000 1.92582800 -1.68585400 C 5.42129600 3.86119300 0.63573200 C 3.16943900 4.22842800 -0.42229000 C 3.35330900 3.03685400 1.77027400 H -0.55490300 -3.03681900 1.23000600 H 0.45820000 1.22256500 -1.00250800 H -2.47475100 -0.87045600 -2.67479100 H -4.02510400 0.49998900 -4.03267800 H -4.52441400 2.83839700 -3.34785400 H 4.75143100 -4.68958400 3.06155200 H 2.79266700 -3.85362500 4.35225800 H 1.09573400 -2.45270400 3.22298300 H -2.84785200 -2.88369700 0.75047500 H -4.98680700 -2.65289300 1.09696600

	H -8.20271900 -1.71140400 -0.44246900 H -7.39415500 -2.88075300 0.60650200 H -7.86737300 -1.29386700 1.23594200 H -6.94261600 0.45548700 -1.14578200 H -6.61218400 0.78764900 0.55456800 H -5.27588300 0.69834100 -0.60180600 H -6.46585200 -1.79487500 -2.15879600 H -4.76194100 -1.53806200 -1.77200600 H -5.57694700 -3.01921200 -1.24149700 H -4.54623000 -1.25289300 3.08202600 H -5.35720700 0.12832400 2.34132700 H -6.28432000 -1.32298500 2.77301800 H 3.34146100 -0.29621800 0.77178500 H 4.79465000 1.24631900 0.35428100 H 4.90029900 0.91608100 -2.09626000 H 4.25438800 2.53079700 -2.38045800 H 5.85039100 2.33256500 -1.62547900 H 5.33935000 4.77551500 1.23029400 H 6.06905900 3.16669100 1.18037600 H 5.91585700 4.12363700 -0.30199800 H 2.18567000 3.80145900 -0.62218600 H 3.03398300 5.16543500 0.12644300 H 3.64017100 4.47192600 -1.37784300 H 3.90981600 2.30961600 2.37094000 H 3.31789100 3.97599100 2.32981700 H 2.32988500 2.67584300 1.65926400 C -1.79341700 2.55171300 0.40389000 C -1.03722100 3.72680500 0.34562300 C -1.94501800 1.90394000 1.63608600 C -0.42722100 4.23519500 1.49002600 H -0.90086900 4.22405000 -0.60820600 C -1.34213300 2.41679500 2.77999500 H -2.54244600 1.00111300 1.68148300 C -0.57507700 3.57968900 2.71000000 H 0.17617300 5.13315600 1.42431900 H -1.46880300 1.90753700 3.72890500 H -0.09373000 3.96988500 3.59935100 C 3.35083900 -2.68127000 -0.87119100 C 4.58978700 -2.21788500 -1.33139000 C 2.31829500 -2.85984100 -1.80042400 C 4.79059400 -1.93300600 -2.67892100 H 5.39300900 -2.05657900 -0.62153200 C 2.51726700 -2.57345500 -3.14649100 H 1.35525900 -3.22274500 -1.46545100 C 3.75282900 -2.10552500 -3.59122600

	H 5.75421800 -1.56627900 -3.01343800 H 1.70509900 -2.71485000 -3.85014400 H 3.90379400 -1.87581400 -4.63949700 H -3.48815500 3.76341200 -1.29849300 H 4.95953500 -4.14114900 0.66377600

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