Electronic Supplementary Information

for:

Dynamic optical activity induction in the *N*-alkyl-*N'*-trityl ureas and thioureas

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Experimental details

^{1}H and ^{13}C NMR spectra were recorded on Bruker Ultrashield 300 MHz or Varian VNMR-S 400 MHz instruments. Chemical shifts (δ) are reported in ppm relative to $SiMe_4$. HR-MS spectra were obtained with a Bruker Impact HD, QTOF MS spectrometer. UV and ECD spectra were recorded in spectroscopic grade cyclohexane or acetonitrile using a JASCO J-810 instrument. The UV and ECD measurements were performed in quartz cell (1 mm path length), scanning speed – 50 nm min^{-1} and resolution 0.5 nm. The concentrations of the samples are collected in Table SI_1. FT-IR spectra were measured on a Nicolet iS 50 spectrometer using ATR module. A JASCO P-2000 polarimeter was used for optical rotation ($[\alpha]_D$) measurements (carried out at ca. 20 °C). Column chromatography was performed on J.T. Baker Silica Gel 40µm (chromatography grade). Merck Kieselgel type $60F_{254}$ analytical plates were used for TLC analyses. Melting points were measured on Büchi Melting Point B-545 and uncorrected. All reagents were used as purchased from commercial suppliers. All solvents were provided by a local supplier and were purified by conventional methods prior to use.

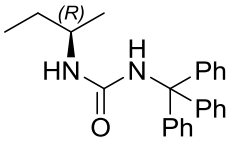
Trityl isocyanate was obtained according the literature procedure.[1]

Trityl isothiocyanate was obtained according the literature procedure.[2]

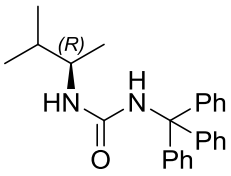
(*R,R*)-1,2-Diisothiocyanatocyclohexane was obtained according the literature procedure.[3]

General procedure for Synthesis of the Urea Derivatives.

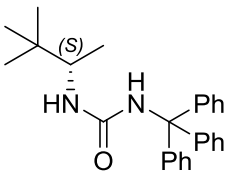
To a solution of the amine (0.4 mmol) in CH_2Cl_2 (3 mL), respective isocyanate (0.4 mmol) was added at room temperature. The whole solution was stirred for 1-2 days. The solvent was evaporated and the crude product was re-disolved in a small amount of CH_2Cl_2 and the obtained urea derivative was either precipitated by adding Et_2O or crystallized.



1a: yield 49 mg (34%). Mp. 240-241 °C; $[\alpha]_D^{20}$ -17 (*c* 1.0, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 0.58 (dt, *J* = 2.0, 7.2 Hz, 3 H), 0.67 (dd, *J* = 2.2, 6.4 Hz, 3 H), 0.91-1.13 (m, 2 H), 1.64 (bs, 1 H), 3.53-3.62 (m, 1 H), 3.70 (d, *J* = 7.6 Hz, 1 H), 5.63 (s, 1 H), 7.29-7.30 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 10.0, 20.3, 29.6, 47.2, 69.6, 127.5, 128.3, 128.8, 144.6, 157.0 ppm;
ATR-IR 3319 (N-H), 3058, 3023 ($=CH_{stretch}$), 2966 (CH_{3asym}), 2931 (CH_{2asym}), 2874 (CH_{3sym}), 1628 (C=O), 1552 (N-H), 1490 (CH_{2def}), 695 ($N\text{-}H_{def}$) cm^{-1};
ESI HRMS *m/z* calcd for $C_{24}H_{26}N_2ONa$ $[M+Na]^+$: 381.1937, found 381.1951.

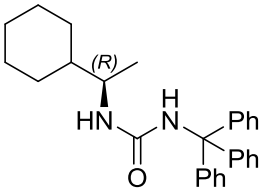


1b: yield 100 mg (67%). Mp. 255-256 °C; $[\alpha]_D^{20}$ -29 (*c* 1.0, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 0.50 (d, *J* = 6.8 Hz, 3 H), 0.59 (t, *J* = 6.9 Hz, 6 H), 1.24-1.39 (m, 1 H), 1.69 (bs, 1 H), 3.51-3.79 (m, 1 H), 3.78 (d, *J* = 8.3 Hz, 1 H), 5.65 (s, 1 H), 7.26-7.31 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 17.4, 17.9, 18.4, 32.8, 50.1, 59.6, 127.5, 128.3, 128.8, 144.5, 157.1 ppm;
ATR-IR 3319 (N-H), 3058 ($=CH_{stretch}$), 3021 ($=CH_{stretch}$), 2973 (CH_{3asym}), 1627 (C=O), 1559 (N-H), 1490 (CH_{2def}), 694 ($N\text{-}H_{def}$) cm^{-1};
ESI HRMS *m/z* calcd for $C_{25}H_{28}N_2ONa$ $[M+Na]^+$: 395.2094, found 395.2101.

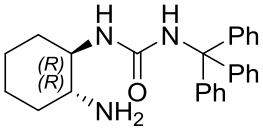


1c: yield 108 mg (71%). Mp. 175-177 °C; $[\alpha]_D^{20}$ +42 (*c* 0.96, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) *δ* 0.55 (s, 9 H), 0.57 (d, *J* = 8.8 Hz, 3 H), 1.74 (bs, 1 H), 3.47-3.59 (m, 1 H), 3.83 (d, *J* = 9.5 Hz, 1 H), 5.67 (s, 1 H), 7.29-7.35 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) *δ* 15.7, 26.0, 33.8, 53.9, 69.5, 127.5, 128.4, 128.8, 144.5,

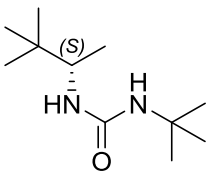
157.2 ppm;
ATR-IR 3368 (N-H), 3313 (N-H), 3060 (=$CH_{stretch}$), 3033 (=$CH_{stretch}$), 2968 (CH_{3asym}), 1638 (C=O), 1541 (N-H), 1492 (CH_{2def}), 1448 (CH_{3def}), 1250 (C-$N_{stretch}$), 694 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{26}H_{30}N_2ONa$ $[M+Na]^+$: 409.2250, found 409.2264.



1d: (0.52 mmol scale) yield 131 mg (61%). Mp.: does not melt up to 305 °C; $[\alpha]_D^{20}$ -25 (*c* 0.9, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.36-0.47 (m, 1 H), 0.66-0.74 (m, 1 H), 0.72 (d, *J* = 12.2 Hz, 3 H), 0.83-1.07 (m, 4 H), 1.25 (d, *J* = 11.7 Hz, 2 H), 1.55-1.62 (m, 3 H), 3.50-3.61 (m, 1 H), 3.80 (d, *J* = 8.9 Hz, 1 H), 5.66 (s, 1 H), 7.27-7.35 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 17.7, 26.16, 26.32, 28.2, 43.1, 50.0, 69.6, 127.5, 128.3, 128.8, 144.5, 157.0 ppm;
ATR-IR 3320 (N-H), 3057 (=$CH_{stretch}$), 3019 (=$CH_{stretch}$), 2968 (CH_{3asym}), 2924 (CH_{2asym}), 2852 (CH_{2sym}), 1633 (C=O), 1549 (N-H), 1489 (CH_{2def}), 1448 (CH_{3def}), 1257 (C-$N_{stretch}$), 699 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{28}H_{32}N_2ONa$ $[M+Na]^+$: 435.2407, found 435.2418.



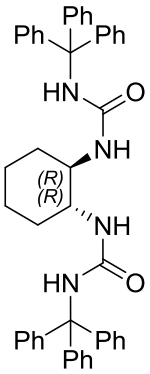
3a: (0.59 mmol scale, 10 mL CH_2Cl_2, during the course of the reaction a solid was formed; the precipitate was filtered out giving analytically pure sample) yield 138 mg (53%). Mp. 235-238 °C; $[\alpha]_D^{20}$ +7 (*c* 0.74, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.58 (dq, *J* = 3.5, 12.6 Hz, 1 H), 0.95-1.20 (m, 3 H), 1.34 (bs, 2 H), 1.51-1.61 (m, 2 H), 1.65-1.78 (m, 3 H), 3.12-3.23 (m, 1 H), 3.79 (d, *J* = 9.1 Hz, 1 H), 5.86 (bs, 1 H), 7.28-7.34 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 24.9, 25.0, 32.5, 34.3, 55.6, 57.4, 69.6, 127.6, 128.4, 128.7, 144.5, 157.5 ppm;
ATR-IR 3315 (N-H), 3088 (=$CH_{stretch}$), 3058 (=$CH_{stretch}$), 3028 (=$CH_{stretch}$), 2931 (CH_{2asym}), 2854 (CH_{2sym}), 1623 (C=O), 1553 (N-H), 1491 (CH_{2def}), 1448 (CH_{2def}), 697 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{26}H_{30}N_3O$ $[M+H]^+$: 400.2383, found 400.2378.



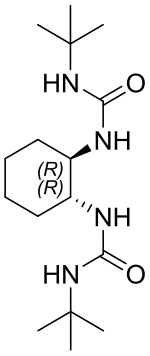
7a: yield 46 mg (57%). Mp.258-260 °C; $[\alpha]_D^{20}$ +25 (*c* 1.1, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.88 (s, 9 H), 1.04 (d, *J* = 6.8 Hz, 3 H), 1.33 (s, 9 H), 3.53-3.63 (m, 1 H), 4.17 (d, *J* = 9.4 Hz, 1 H), 4.30 (bs, 1 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 16.8, 26.3, 29.7, 34.5, 50.2, 53.5, 157.4 ppm;
ATR-IR 3358 (N-H), 3302 (N-H), 2962 (CH_{3asym}), 2935 (CH_{asym}), 2856 (CH_{sym}), 1626 (C=O), 1556 (N-H), 1449 (CH_{3def}), 1271 (C-$N_{stretch}$), 645 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{11}H_{24}N_2ONa$ $[M+Na]^+$: 223.1781, found 223.1796.

General procedure for Synthesis of bis-Urea Derivatives.

To a solution of the amine (1 equiv.) in CH_2Cl_2 (5 mL) was added appropriate isocyanate (2 equiv.) at room temperature. The reaction mixture was stirred for 24 hours. The precipitating white product was filtered out. In the case of the trityl derivative **3b**, the solvent was evaporated and product was crystallized from EtOH.



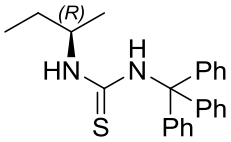
3b: (0.53 mmol scale), yield 167 mg (49%, after column chromatography on silica gel, eluent = DCM:MeOH 1%). Mp. 89-94 °C; $[\alpha]_D^{20}$ -52 (*c* 1.34, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.57 (d, *J* = 8.8 Hz, 1 H), 0.98 (t, *J* = 9.7 Hz, 1 H), 1.42 (d, *J* = 9.5 Hz, 1 H), 1.55 (d, *J* = 11.1 Hz, 1 H), 3.02 (s, 1 H), 4.68 (s, 1 H), 5.62 (s, 1 H), 7.20-7.26 (m, 15 H) ppm;
^{13}C NMR (100 MHz, $CDCl_3$) δ 24.4, 32.4, 53.8, 66.2, 69.8, 126.6, 127.0, 127.9, 128.0, 128.1, 128.8, 145.0, 148.5, 157.3 ppm;
ATR-IR 3422, 3348 (N-H), 3056 (=$CH_{stretch}$), 3022 (=$CH_{stretch}$), 2926 (CH_{2asym}), 2854 (CH_{2sym}), 1634 (C=O), 1530 (N-H), 1489 (CH_{2def}), 1445 (CH_{2def}), 696 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{46}H_{45}N_4O_2$ $[M+H]^+$: 685.3537, found 685.3524.



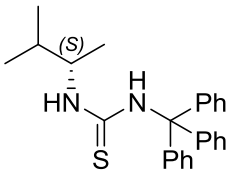
8a: (1.0 mmol scale), yield 191 mg (61%). Mp. 230-232 °C; $[\alpha]_D^{20}$ -2 (*c* 1.24, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 1.10-1.24 (m, 2 H), 1.31 (s, 9 H), 1.69 (d, *J* = 7.7 Hz, 1 H), 1.99 (d, *J* = 12.2 Hz, 1 H), 3.38 (t, *J* = 7.7 Hz, 1 H), 4.36 (bs, 1 H), 4.91 (d, *J* = 6.5 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 25.0, 29.6, 33.4, 50.3, 54.4, 158.1 ppm;
ATR-IR 3354 (N-H), 3298 (N-H), 2966 (CH_{2asym}), 2927 (CH_{3sym}), 2856 (CH_{2sym}), 1630 (C=O), 1557 (N-H), 1494 (CH_{2def}), 1445 (CH_{2def}), 644 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{16}H_{32}N_4O_2Na$ $[M+Na]^+$: 335.2417, found 335.2439.

General procedure for Synthesis of the Thiourea Derivatives.

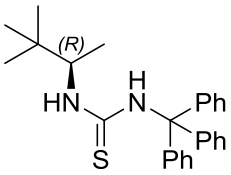
To a solution of the amine (1 mmol) in CH_2Cl_2 (5 mL) was added respective isothiocyanate (1 mmol) at room temperature. The reaction mixture was stirred for 24 hours. The solvent was evaporated and the crude product was crystallized from EtOH.



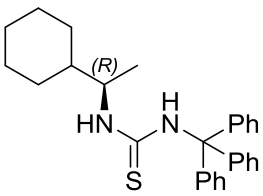
2a: yield 236 mg (63%). Mp. 96-114 °C; $[\alpha]_D^{20}$ -6.5 (*c* 0.92, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.56 (t, *J* = 7.4 Hz, 3H), 0.67 (d, *J* = 6.6 Hz, 3H), 0.97-1.13 (m, 1H), 4.08-4.22 (m, 1H), 4.97 (d, *J* = 8.3 Hz, 1H), 7.19 (bs, 1H), 7.26-7.38 (m, 15H) ppm;
^{13}C NMR (76 MHz, $CDCl_3$) δ 9.9, 19.1, 28.8, 53.1, 72.4, 128.0, 128.7, 142.9, 179.5 ppm;
ATR-IR 3423 (N-H), 3380 (N-H), 3086 ($=CH_{stretch}$), 3066 ($=CH_{stretch}$), 3034 ($=CH_{stretch}$), 2964 (CH_{3asym}), 2922 (CH_{2asym}) 2882 (CH_{3sym}), 1528 (N-H), 1491 (CH_{2def}), 1477 (CH_{3def}), 1444 (CH_{3def}), 1385 ($C\text{-}N_{stretch}$), 1207, 1180, 1151 ($C\text{=}S_{stretch}$), 754 ($=CH_{def}$), 696 ($N\text{-}H_{def}$) cm^{-1};
ESI HRMS *m/z* calcd for $C_{24}H_{26}N_2SNa$ $[M+Na]^+$: 397.1709, found 397.1702.



2b: (0.8 mmol scale) yield 193 mg (61%). Mp. 118-124, 142-158 °C; $[\alpha]_D^{20}$ +9 (*c* 1.06, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.50 (d, *J* = 6.9 Hz, 3H), 0.53 (d, *J* = 6.8 Hz, 3H), 0.59 (d, *J* = 6.7 Hz, 3H), 1.36-1.59 (m, 1H), 4.13-4.20 (m, 1H), 5.07 (d, *J* = 9.0 Hz, 1H), 7.21 (bs, 1H), 7.26-7.46 (m, 15H) ppm;
^{13}C NMR (76 MHz, $CDCl_3$) δ 16.0, 18.0, 18.2, 32.3, 56.8, 72.3, 126.8, 127.7, 128.0, 128.05, 128.1, 128.3, 128.6, 128.7, 142.9, 143.1, 179.8 ppm;
ATR-IR 3423 (N-H), 3386 (N-H), 3086 ($=CH_{stretch}$), 3058 ($=CH_{stretch}$), 3023 ($=CH_{stretch}$), 2962 (CH_{3asym}), 2931 (CH_{3sym}), 2879 (CH_{3sym}), 1525 (N-H), 1476 (CH_{3def}), 1445 (CH_{3def}), 1386 ($C\text{-}N_{stretch}$), 1227, 1191, 1154 ($C\text{=}S_{stretch}$), 770 ($=CH_{def}$), 699 ($N\text{-}H_{def}$) cm^{-1};
ESI HRMS *m/z* calcd for $C_{25}H_{28}N_2SNa$ $[M+Na]^+$: 411.1865, found 411.1854.

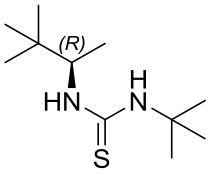


2c: yield 279 mg (70%). Mp. 201-204 °C; $[\alpha]_D^{20}$ -23.5 (*c* 1.02, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.54 (s, 9 H), 0.56 (d, *J* = 6.8 Hz, 3 H), 4.18 (dq, *J* = 6.7, 9.4 Hz, 1 H), 5.12 (d, *J* = 9.4 Hz, 1 H), 7.23 (s, 1 H), 7.26-7.38 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 14.7, 26.2, 33.9, 60.4, 72.2, 128.1, 128.7, 142.9, 180.1 ppm;
ATR-IR 3422 (N-H), 3381 (N-H), 3058 ($=CH_{stretch}$), 3024 ($=CH_{stretch}$), 2962 (CH_{3asym}), 2870 (CH_{3sym}), 1526 (N-H), 1471 (CH_{3def}), 1445 (CH_{3def}), 1380 ($C\text{-}N_{stretch}$), 1237, 1180, 1140 ($C\text{=}S_{stretch}$), 647 ($N\text{-}H_{def}$) cm^{-1};
ESI HRMS *m/z* calcd for $C_{26}H_{30}N_2SNa$ $[M+Na]^+$: 425.2022, found 425.2013.



2d: yield 269 mg (63%). Mp. 166-169 °C; $[\alpha]_D^{20}$ -7 (*c* 0.92, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.36-0.48 (m, 1 H), 0.65 (d, *J* = 6.7 Hz, 3 H), 0.66-0.77 (m, 1 H), 0.90-1.05 (m, 4 H), 1.16-1.20 (m, 2 H), 1.54-1.61 (m, 3 H), 4.12-4.27 (m, 1 H), 5.09 (d, *J* = 8.9 Hz, 1 H), 7.20 (s, 1 H), 7.27-7.38 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 16.5, 26.0, 26.1, 26.2, 28.52, 28.58, 42.7, 56.3, 72.3, 128.0, 128.7, 142.9, 179.6 ppm,
ATR-IR 3422 (N-H), 3388 (N-H), 3057 ($=CH_{stretch}$), 3022 ($=CH_{stretch}$), 2969 (CH_{3asym}), 2926 (CH_{2asym}), 2854 (CH_{2sym}), 1525 (N-H), 1477 (CH_{2def}), 1445 (CH_{3def}), 1379 ($C\text{-}N_{stretch}$), 1249, 1225, 1211, 1188 ($C\text{=}S_{stretch}$), 697 ($N\text{-}H_{def}$) cm^{-1},
ESI HRMS *m/z* calcd for $C_{28}H_{33}N_2S$ $[M+H]^+$: 429.2359, found 429.2349.

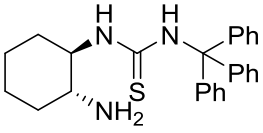
ent-**2d** was obtained analogously (0.4 mmol scale), yield 109 mg (67%).



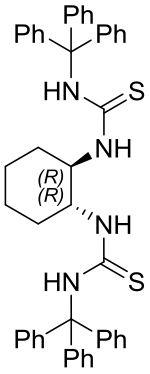
7b: yield 137 mg (64%). Mp. 176-178°C; $[\alpha]_D^{20}$ -40.5 (*c* 0.97, $CHCl_3$);
^{1}H NMR (401 MHz, $CDCl_3$) δ 0.98 (s, 9 H), 1.17 (d, *J* = 6.7 Hz, 3 H), 1.42 (s, 9 H), 4.35 (bs, 1 H), 5.53 (d, *J* = 8.8 Hz, 1 H), 5.99 (bs, 1 H) ppm;
^{13}C NMR (101 MHz, $CDCl_3$) δ 15.7, 26.5, 29.8, 34.5, 52.3, 59.9, 180.6 ppm;
ATR-IR 3261 (N-H), 3120 (N-H), 2959 (CH_{3asym}), 2872 (CH_{sym}), 1534 (N-H), 1476 (CH_{3def}), 1321 (C-$N_{stretch}$), 1197, 1149 (C=$S_{stretch}$), 687 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{11}H_{24}N_2SNa$ $[M+Na]^+$: 239.1552, found 239.1556.

Synthesis of Thiourea Derivatives 4a, 4b and 5

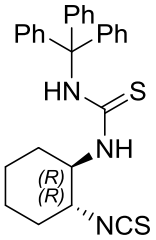
To a solution of (*R,R*)-diaminocyclohexane (0.8 g, 7 mmol) in CH_2Cl_2 (22 mL) was added a solution of trityl isothiocyanate (2.088g, 7 mmol, 1 equiv.) in CH_2Cl_2 (56 mL) at room temperature. The reaction mixture was stirred for a few days. The solvent was evaporated and the crude product was crystallized from MeOH. Crystals of bis-thiourea derivative **4b** precipitated first (the first and the second crop of crystals, white needles, 0.448 g). mono-Derivative **4a** crystallized from the filtrate (1.476 g).



4a: yield 1.476 g (51%). Mp. 171-172 °C; $[\alpha]_D^{20}$ +19 (*c* 1.02, $CHCl_3$);
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.44 (dq, *J* = 3.8, 12.7 Hz, 1 H), 0.95-1.04 (m, 2 H), 1.13-1.26 (m, 3 H), 1.49-1.82 (m, 5 H), 3.89 (dq, *J* = 4.1, 9.4 Hz, 1 H), 5.00 (d, *J* = 9.0 Hz, 1 H), 7.29-7.41 (m, 16 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 24.7, 24.8, 31.3, 34.2, 55.5, 63.2, 72.4, 128.2, 128.6, 128.8, 142.8, 180.5 ppm;
ATR-IR 3424 (N-H), 3389 (N-H), 3368 (N-H), 3059 (=$CH_{stretch}$), 3021 (=$CH_{stretch}$), 2927 (CH_{2asym}), 2852 (CH_{2sym}), 1526 (N-H), 1473 (CH_{2def}), 1445 (CH_{2def}), 1378 (C-$N_{stretch}$), 1220, 1181 (C=$S_{stretch}$), 761 (=CH_{def}), 699 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{26}H_{30}N_3S$ $[M+H]^+$: 416.2155, found 416.2168.



4b: yield 448 mg (9%). Mp. 205-208 °C; $[\alpha]_D^{20}$ 0 (*c* 1.18, $CHCl_3$),
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.82 (t, *J* = 9.1 Hz, 1 H), 1.25 (d, *J* = 12.1 Hz, 2 H), 1.56 (bs, 1 H), 3.71 (bs, 1 H), 5.37 (d, *J* = 4.9 Hz, 1 H), 7.18 (s, 1 H), 7.25-7.42 (m, 15 H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 24.0, 30.7, 58.3, 72.8, 128.0, 128.7, 143.0, 180.4 ppm;
ATR-IR 3409 (N-H), 3391 (N-H), 3313 (N-H), 3056 (=$CH_{stretch}$), 3018 (=$CH_{stretch}$), 2931 (CH_{2asym}), 2917, 2851 (CH_{2sym}), 1526 (N-H), 1474 (CH_{2def}), 1444 (CH_{2def}), 1390 (C-$N_{stretch}$), 1254, 1217, 1184 (C=$S_{stretch}$), 698 (N-H_{def}) cm^{-1};
ESI HRMS *m/z* calcd for $C_{46}H_{44}N_4S_2Na$ $[M+Na]^+$: 739.2900, found 739.2924.



5: To a solution of (*R,R*)-1,2-diisothiocyanatocyclohexane (219 mg, 1.1 mmol) in CH_2Cl_2 (10 mL) was added tritylamine (1.1 mmol) at room temperature. The reaction mixture was stirred for 2 days (the progress of the reaction was monitored by TLC). To the mixture silica gel was added (ca 2 g) and all volatiles was removed by evaporation. The crude product was purified by column chromatography (silica gel, eluent CH_2Cl_2). Traces of the remaining tritylamine was removed by precipitation with the use of Et_2O. Yield 355 mg (70%).

Mp. 195-200 °C; $[\alpha]_D^{20}$ -126 (*c* 1.0, $CHCl_3$);

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.36-0.48 (m, 1 H), 0.96-1.28 (m, 3 H), 1.47-1.72 (m, 4 H), 3.14 (bs, 1 H), 4.35 (dq, *J* = 4.1, 8.6 Hz, 1 H), 5.11 (d, *J* = 8.4 Hz, 1 H), 7.27-7.42 (m, 16 H) ppm;

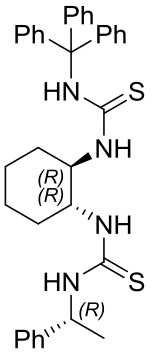
^{13}C NMR (75 MHz, $CDCl_3$) δ 22.4, 22.7, 28.9, 31.1, 57.0, 58.2, 72.7, 128.2, 128.7, 128.8, 131.9, 142.7, 180.6 ppm;

ATR-IR 3385 (N-H), 3230 (N-H), 3055 (=$CH_{stretch}$), 3044 (=$CH_{stretch}$), 2934 (CH_{2asym}), 2859 (CH_{2sym}), 2118 (N=C=S), 2080 (N=C=S), 1544 (N-H), 1490 (CH_{2def}), 1446 (CH_{2def}), 1387, 1356 (C-$N_{stretch}$), 1289, 1227 (C=$S_{stretch}$), 750 (=CH_{def}), 701 (N-H_{def}) cm^{-1};

ESI HRMS *m/z* calcd for $C_{27}H_{28}N_3S_2$ $[M+H]^+$: 458.1719, found 458.1732.

Synthesis of the Non-symmetrical bis-Thiourea Derivatives 6a and 6b

To a solution of **5** (1 equiv.) in CH_2Cl_2 (2 mL) the respective enantiomer of 1-phenylethylamine (1.2 equiv.) was added in one portion at room temperature. The reaction mixture was stirred for 24 hours. The solvent was evaporated *in vacuo* to give pure sample of respective bis-thiourea derivative **6a** or **6b**. Crystals suitable for X-ray measurements were obtained by re-crystallization from MeOH/CH_2Cl_2.



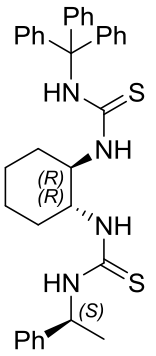
6a: (0.066 mmol scale, crystallization from Et_2O), yield 30 mg (79%). Mp. 194-196 °C; $[\alpha]_D^{20}$ -10.5 (*c* 0.47, $CHCl_3$);

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.51 (bs, 2 H), 1.14 (bs, 4 H), 1.54 (bs, 2 H), 1.60 (d, *J* = 6.8 Hz, 3 H), 2.50 (bs, 1 H), 3.65 (bs, 1 H), 4.20 (bs, 1 H), 5.07 (bs 1 H), 5.51 (bs, 1 H), 6.16 (bs, 1 H), 7.14 - 7.23 (m, 7 H), 7.28-7.41 (m, 11 H), 7.47 (d, *J* = 7.4 Hz, 2 H), 7.61 (bs, 1 H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 22.6, 23.8, 24.7, 31.1, 31.9, 52.8, 57.1, 61.2, 72.8, 126.5, 127.3, 128.3, 128.4, 128.6, 128.9, 142.3, 142.9, 179.8, 180.3 ppm;

ATR-IR 3420 (N-H), 3375 (N-H), 3241 (N-H), 3062 (=$CH_{stretch}$), 3028 (=$CH_{stretch}$), 2938 (CH_{2asym}), 2856 (CH_{2sym}), 1532 (N-H), 1475 (CH_{2def}), 1445 (CH_{2def}), 1388, 1344 (C-$N_{stretch}$), 1257, 1222 (C=$S_{stretch}$), 749 (=CH_{def}), 694 (N-H_{def}) cm^{-1};

ESI HRMS *m/z* calcd for $C_{35}H_{39}N_4S_2$ $[M+H]^+$: 579.2611, found 579.2606.



6b: (0.066 mmol scale, the crude product was washed with Et_2O), yield 32 mg (86%). Mp. 221-229 °C; $[\alpha]_D^{20}$ +53.5 (*c* 0.52, $CHCl_3$);

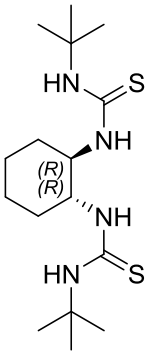
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.40-0.54 (m, 2 H), 1.00 (bs, 3 H), 1.42 (bs, 2 H), 1.55 (d, *J* = 6.5 Hz, 3 H), 1.63 (bs, 1 H), 2.10 (bs, 1 H), 3.65 (bs, 1 H), 4.01-4.09 (m, 1 H), 5.07 (bs, 1 H), 5.27 (bs, 1 H), 6.30 (bs, 1 H), 7.10 (bs, 1 H), 7.17-7.24 (m, 8 H), 7.29-7.41 (m, 12 H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 23.8, 24.5, 31.0, 31.6, 53.0, 57.0, 60.9, 72.9, 125.9, 127.3, 127.9, 128.2, 128.5, 128.6, 128.9, 142.4, 180.0 ppm;

ATR-IR 3422 (N-H), 3372 (N-H), 3362 (N-H), 3251 (N-H), 3063 (=$CH_{stretch}$), 2970 (CH_{3asym}), 2937 (CH_{2asym}), 2924 (CH_{3sym}), 2855 (CH_{2sym}), 1538 (N-H), 1520 (N-H), 1474 (CH_{2def}), 1446 (CH_{2def}), 1387, 1364 (C-$N_{stretch}$), 1256, 1220 (C=$S_{stretch}$), 757 (=CH_{def}), 696 (N-H_{def}) cm^{-1};

ESI HRMS *m/z* calcd for $C_{35}H_{38}N_4S_2Na$ $[M+Na]^+$: 601.2430, found 601.2438.

Synthesis of 8b



To a solution of the (*R,R*)-diaminocyclohexane (102 mg, 0.89 mmol, 1 equiv.) in CH_2Cl_2 (5 mL) *tert*-butyl isocyanate (0.22 ml, 200 mg, 1.7 mmol, 2 equiv.) was added at room temperature. The reaction mixture was stirred for 24 hours. The solvent was evaporated *in vacuo* and the crude product was crystallized from EtOH; yield 253 mg (82%).

Mp. 178-182 °C; $[\alpha]_D^{20}$ +105.5 (*c* 1.1, $CHCl_3$);

^{1}H NMR (300 MHz, $CDCl_3$) δ 1.21-1.37 (m, 2 H), 1.42 (s, 9 H), 1.78 (bs, 1 H), 2.28 (d, *J* = 10.4 Hz, 1 H), 4.50 (s, 1 H), 6.02 (s, 1 H), 6.11 (d, *J* = 5.7 Hz, 1 H) ppm;

^{13}C NMR (75 MHz, $CDCl_3$) δ 24.7, 29.6, 32.6, 53.1, 59.2, 180.6 ppm;

ATR-IR 3267 (N-H), 3210 (N-H), 3112 (N-H), 3044, 2968 (CH_{3asym}), 2931 (CH_{2asym}), 2861 (CH_{2sym}), 1527 (N-H), 1508, 1344 (C-$N_{stretch}$), 1281, 1243, 1193 (C=$S_{stretch}$), 693 (N-H_{def}) cm^{-1};

ESI HRMS *m/z* calcd for $C_{16}H_{32}N_4S_2Na$ $[M+Na]^+$: 367.1961, found 367.1971.

Calculation details

Starting geometries of **1c**, **2c**, **3b**, **4b**, **6a**, **6b**, **7a** and **7b** were obtained by conformational search with the use of a Scigress[4] software and pre-optimization of all conformers at the B3LYP/6-31G(d) level. The conformational searches were done by systematic changes of all rotatable torsion angles with 30° steps. This allowed to identify the minimum energy structures which were further re-optimized with the use of B3LYP functional[5] in conjunction with the enhanced 6-311++G(d,p) basis set.[6] The structures thus obtained were the real minimum energy conformers (no imaginary frequencies were found). The total and free energy values were used to obtain the Boltzmann population of conformers at 298.15 K. For density functional theory calculations, only the results for conformers that differ from the most stable one by less than 2 kcal mol^{-1} were taken into account, following a generally accepted protocol. Relative energies (unit kcal mol^{-1}) discussed in the main text refer to Gibbs free energies ($\Delta\Delta G$) computed at the B3LYP/6-311++G(d,p) level of theory. The same procedure but with the use of IEFPCM solvent model of acetonitrile has been applied additionally for compound **3b**.

ECD spectra for all structures optimized at the B3LYP/6-311++G(d,p) level were calculated employing M06-2X[7] and CAM-B3LYP,[8] hybrid functionals, all in conjunction with 6-311++G(d,p) basis set.**[6]** Additionally, for the compounds **3b**, the ECD spectra for all structures optimized at the B3LYP/6-311++G(d,p) level were calculated employing M06-2X[7] and CAM-B3LYP,[8] hybrid functionals, in conjunction with 6-311++G(d,p) basis set and IEFPCM solvent model of acetonitrile.**[6]** The calculated ECD spectra were Boltzmann averaged by taking into account conformers ranging from 0 to 2.0 kcal mol^{-1} in relative energies, following a generally accepted protocol.[9] Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity calculated values of rotatory strengths were quite small, and for this reason, only the velocity representations were further used. The ECD spectra were simulated by overlapping Gaussian functions for each transition, according to the procedure previously described by Harada and Stephens.[10]

The solvent effect on structure and ECD spectra was not taken into account (with the exception of compound **3b**), since the experimental ECD measurements were done in non-polar cyclohexane.

Since there are no significant differences between results obtained with the use of M06-2X and CAM-B3LYP functionals, we limited our discussion to the results obtained with the use of CAM-B3LYP functional only.

Single crystal X-ray analysis

The colourless single crystals of compounds **2a**-**2d**, **4a**, **4b, 5, 6a, 6b, 7b** and **9** suitable for X-ray structural analysis were obtained by slow evaporation of solvent. The diffraction data were collected at 130K with an Oxford Diffraction SuperNova diffractometer using Cu Kα radiation (λ = 1.54184 Å). The intensity data were collected and processed using CrysAlisPro software.[11] The structures were solved by direct methods with the program SHELXT 2018/2[12] and refined by full-matrix least-squares method on F^2 with SHELXL 2018/3.[13] 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. The hydrogen atoms of NH groups were located in electron-density difference maps. In the final cycles of refinement they were included in calculated position and treated as riding atoms, their displacement parameters were set equal to 1.5Ueq(N). Absolute structures of the compounds were specified by the synthetic procedure and confirmed using Flack parameter.[14]

A summary of the crystallographic data is given in **Table SI_9-SI_10.** The analysis of intermolecular interactions was carried out using the Crystal Explorer.[15] Molecular graphics were generated with Crystal Explorer, Olex2[16] and Mercury CSD 4.1.0 software.[17] ORTEP representation of the molecular structures of the reported compounds are presented in **Figure SI_33**-**SI_43**. The **Figure SI_44** presents the contribution to the Hirshfeld surface area for various intermolecular interactions for molecules in the studied crystal structures.

In the crystal structure of the hydrate of compound **4a** the thermal movements of the 4a molecules are significant (slight dynamic disorder is observed). The molecules of water are also disordered – the occupancy is not integer. The site occupancy of the water molecules was refined and the final cycles of refinement they were fixed (0.84 and 0.15 respectively).

The asymmetric unit in the crystal structure of compound **5** consists two symmetrically independent molecules and one of them is disordered (in the figures the minor position of this molecule is omitted for clarity). The refined site occupancy for major positions is 0.54. The RESI instruction was used in the refinement.

The compound **6a** crystallizes in hydrated form. The site occupancy of the water molecule was refined and the final value is 0.16. Additionally, the PEA part of the molecule is disordered and refined site occupancy for major positions is 0.62 (see **Figure SI_41c**). The RESI instruction was used in the refinement.

Table SI_1. Concentrations (*c*, in mol L^{-1}) of the samples used for UV and ECD measurements.

Compound	*c* (cyclohexane)	*c* (acetonitrile)
(*R*)-1a	1.073×10^{-4}	1.4153×10^{-4}
(*R*)-1b	1.4077×10^{-4}	1.3728×10^{-4}
(*S*)-1c	1.3126×10^{-4}	1.3152×10^{-4}
(*R*)-1d	1.2177×10^{-4}	1.2225×10^{-4}
(*R*)-2a	1.3816×10^{-4}	1.3603×10^{-4}
(*S*)-2b	1.288×10^{-4}	1.3369×10^{-4}
(*R*)-2c	1.2804×10^{-4}	1.2555×10^{-4}
(*R*)-2d	1.1932×10^{-4}	1.2516×10^{-4}
3a	4.21×10^{-5}	1.2674×10^{-4}
3b	1.2499×10^{-4}	1.315×10^{-4}
4a	1.4743×10^{-4}	1.5439×10^{-4}
4b	6.88×10^{-5}	1.4211×10^{-4}
5	7.15×10^{-5}	1.1068×10^{-4}
6a	8.871×10^{-5}	8.646×10^{-5}
6b	3.2×10^{-6}	3.1×10^{-6}
(*S*)-7a	2.5326×10^{-4}	2.6225×10^{-4}
(*R*)-7b	5.87×10^{-5}	2.3778×10^{-4}
8a	1.795×10^{-5}	1.6653×10^{-4}
8b	4.22×10^{-5}	1.499×10^{-4}

Table SI_2. ECD ($\Delta\varepsilon$) and UV (ε) data for urea and thiourea derivatives **1**-**8** measured in acetonitrile solution.

Compd	$\Delta\varepsilon$ (nm)	ε (nm)
(*R*)-1a	-1.4 (214); -0.5 (208); -1.6 (201); 1.6 (185)	81800 (192)
(*R*)-1b	-2.0 (213); -1.2 (207); -3.4 (199); 2.7 (185)	82800 (193)
(*S*)-1c	1.7 (213); 3.3 (197); -1.0 (185)	82500 (192)
(*R*)-1d	-1.2 (214); -0.2 (207); -1.5 (200); 4.2 (185)	79900 (192)
(*R*)-2a	-0.7 (285); 0.8 (266); 2.9 (218); -6.5 (198); 4.7 (185)	15000 (259); 84200 (194)
(*S*)-2b	-2.2 (260); -3.1 (221); 13.7 (197); -15.6 (185)	10700 (259); 97200 (194)
(*R*)-2c	3.2 (260); 0.2 (240); 5.0 (219); -31.4 (199); 25.0 (185)	16300 (260); 92200 (194)
(*R*)-2d	-0.8 (286); 3.0 (260); -2.0 9229); 3.6 (205); 0.1 (198); 4.4 (190)	15500 (259); 85300 (194)
3a	0.2 (225); -5.1 (200); 5.8 (185)	78000 (192)
3b	21.6 (206); -16.1 (194); -17.5 (188)	158700 (194)
4a	0.3 (273); -1.1 (259); 0.9 (241); -2.8 (226); 17.6 (200); -7.2 (185)	14100 (260); 78600 (194)
4b	44.8 (263); -137 (203); 137 (185)	24600 (261); 162700 (194)
5	22.1 (261); -102 (200); 27.2 (185)	15600 (261); 99800 (192)
6a	26.4 (258); -39.9 (223); -58 (202); 36.9 (185)	24400 (254); 117000 (189)
6b	42.4 (257); -90.4 (204); 71.9 (187)	23700 (254); 117300 (190)
(*S*)-7a	-1.5 (194); 2.1 (185)	6900 (190)
(*R*)-7b	1.0 (306); 1.2 (294); -1.4 (245); 0.8 (225); -1.4 (214); 1.4 (200)	12900 (251); 12400 (219)
8a	-5.7 (187)	14483 (192)
8b	32 (250); -32.7 (219); 7.7 (197)	24368 (251); 22078 (214)

Table SI_3. Total and free energies (*E*, *ΔG*, in Hartree), relative energies (*ΔE*, *ΔΔG* in kcal mol^{-1}), percentage populations and number of imaginary frequencies (#ImFreq) calculated at the B3LYP/6-311++G(d,p) level for individual conformers of **1c**, **2a**, **3b**, **4b, 6a, 6b, 7a** and **7b**.

Compound[a]	*E*	*ΔG*	*ΔE*	Pop.	*ΔΔG*	Pop	#ImFreq
1c (1)	-1193.901798	-1193.46093	0.81	13.14	0.00	53.83	0
1c (13)	-1193.903096	-1193.46039	0.00	51.98	0.34	30.34	0
1c (37)	-1193.90272	-1193.45977	0.24	34.88	0.72	15.83	0
2c (1)	-1516.8579	-1516.4178	0.00	100	0.00	100	0
3b (6)	-2149.433577	-2148.71705	0.00	28.88	0.36	16.28	0
3b (12)	-2149.433181	-2148.71692	0.25	18.98	0.44	14.17	0
3b (13)	-2149.433154	-2148.71669	0.27	18.46	0.58	11.13	0
3b (32)	-2149.433	-2148.71762	0.35	15.94	0.00	29.78	0
3b (33)	-2149.433116	-2148.71753	0.29	17.74	0.06	26.9	0
3b (3)[b]	-2149.45545	-2148.74129	0.00	16.26	0.15	14.76	0
3b (6)[b]	-2149.45483	-2148.74002	0.39	8.36	0.95	3.88	0
3b (11)[b]	-2149.45484	-2148.74086	0.39	8.48	0.42	9.44	0
3b (12)[b]	-2149.45504	-2148.74062	0.26	10.44	0.57	7.3	0
3b (13)[b]	-2149.45538	-2148.74075	0.05	15.06	0.49	8.39	0
3b (17)[b]	-2149.45463	-2148.74153	0.52	6.77	0.00	19.16	0
3b (18)[b]	-2149.45402	-2148.73958	0.9	3.55	1.22	2.42	0
3b (32)[b]	-2149.45523	-2148.74141	0.14	12.78	0.08	16.86	0
3b (33)[b]	-2149.45542	-2148.74142	0.02	15.59	0.07	17.11	0
3b (75)[b]	-2149.4527	-2148.73809	1.73	0.88	2.16	-	0
3b (76)[b]	-2149.45275	-2148.73737	1.69	0.93	2.61	-	0
3b (96)[b]	-2149.45273	-2148.73838	1.71	0.9	1.98	0.68	0
4b (1)	-2795.340261	-2794.62837	0.15	23.9	1.16	5.18	0
4b (4)	-2795.337938	-2794.62814	1.61	2.04	1.30	4.09	0
4b (30)	-2795.339964	-2794.63022	0.34	17.45	0.00	36.94	0
4b (40)	-2795.340328	-2794.62979	0.11	25.66	0.27	23.49	0
4b (48)	-2795.340505	-2794.63003	0.00	30.95	0.12	30.3	0
6a (1)	-2372.4825	-2371.89454	1.31	7.8	1.94	3.23	0
6a (12)	-2372.48344	-2371.8957	0.72	21.11	1.21	11.06	0
6a (31)	-2372.484586	-2371.89763	0.00	71.09	0.00	85.71	0
6b (6)	-2372.48529	-2371.89696	0.00	49.16	0.46	15.86	0
6b (15)	-2372.48461	-2371.8977	0.43	23.91	0.00	34.49	0
6b (16)	-2372.48432	-2371.89763	0.61	17.45	0.04	32.27	0
6b (24)	-2372.48374	-2371.89705	0.97	9.48	0.41	17.38	0
7a (1)	-618.5735281	-618.275343	0.00	94.43	0.00	100	0
7a (2)	-618.5708564	-618.271027	1.68	5.57	2.71	-	0
7b (1)	-941.5244515	-941.229166	0.00	41.06	0.00	45.09	0
7b (2)	-941.5240733	-941.226992	0.24	27.5	1.36	4.5	0

7b (3)	-941.5237031	-941.228846	0.47	18.58	0.20	32.12	0
7b (4)	-941.5233562	-941.228314	0.69	12.86	0.53	18.28	0

[a] Conformers are numbered according to their appearance during conformational search; in parentheses is given the conformer number. [b] Calculated at the IEFPCM/B3LYP/6-311++G(d,p) level.

Table SI_4. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) calculated at the B3LYP/6-311++G(d,p) level for individual low-energy conformers of **1c** and **2c** (conformers are numbered according to their appearance during conformational search).

	α^a	α'^b	$\beta_1{}^c$	$\beta_2{}^c$	$\beta_3{}^c$	$\gamma_1{}^d$	$\gamma_2{}^d$	$\gamma_3{}^d$	δ^e	$l_1{}^f$	$l_2{}^g$	$l_3{}^h$	Helicity
1c (1)[k]	-168.77	-165.50	-10.52	-125.64	109.24	-53.01	-17.41	-50.39	12.18	2.37	–	2.32	*MMM*
1c (13)[k]	4.99	-168.55	-0.48	-115.37	119.01	-52.93	-7.94	-49.74	4.05	2.41	2.43	2.31	*MMM*
1c (37)[k]	-0.50	179.48	-13.80	-132.85	101.28	55.08	48.57	7.26	-3.25	2.43	2.40	2.32	*PPP*
2c (1)[k]	-176.13	10.30	-5.95	-125.11	108.84	53.18	49.02	6.05	-15.38	2.41	2.36	2.55	*PPP*

[a] – α = C_{Tr}-N_{Tr}-C=X; [b] – α' = C-N-C=X; [c] – β = H-N-C-C_{ipso}; [d] – γ = N-C_{Tr}-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – δ = C(=X)-N-C*-H; [f] – l_1 = (N_{Tr})H···$C_{ipso\ (1)}$; [g] – l_3 = (N_{alkyl})H···C_{ipso} ; [h] – l_2 = (C=)X···H(C*); X = S, O; [k] – in parentheses are provided the conformer numbers.

Table SI_5. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) calculated at the B3LYP/6-311++G(d,p) level for individual low-energy conformers of **3b** (conformers are numbered according to their appearance during conformational search).

		α^a	α'^b	β_1^c	β_2^c	β_3^c	γ_1^d	γ_2^d	γ_3^d	δ^e	l_1^f	l_2^g	l_3^h	l_4^i	Helicity
3b (6)[k]	C_1-R	-159.84	170.97	-34.32	-147.63	86.66	-29.83	17.43	-77.04	35.26	2.49	–	2.57	1.95	*MMP*
	C_2-R	-0.90	168.89	-18.79	-138.00	96.93	56.70	46.81	12.84	-33.80	2.44	2.27	2.53	–	*PPP*
3b (12)[k]	C_1-R	-160.41	173.51	-33.58	146.95	-27.75	-31.42	15.89	-75.32	39.07	2.49	–	2.60	1.95	*MMP*
	C_2-R	3.26	-178.04	-2.08	-117.32	117.42	-53.02	-9.61	-48.79	-28.20	2.40	2.55	2.52	–	*MMM*
3b (13)[k]	C_1-R	158.46	157.71	42.40	-78.21	155.68	18.08	85.27	-29.90	23.10	2.53	–	2.43	1.99	*MPP*
	C_2-R	3.72	-178.87	-1.22	-116.71	118.23	-53.65	-11.40	-47.84	-30.39	2.40	2.53	2.51	–	*MMM*
3b (32)[k]	C_1-R	158.65	158.54	42.36	-78.26	155.62	18.69	84.61	-29.68	25.82	2.53	–	2.45	1.99	*MPP*
	C_2-R	-0.83	167.85	-16.61	-135.82	99.34	58.52	44.52	16.00	-35.16	2.42	2.28	2.52	–	*PPP*
3b (33)[k]	C_1-R	175.55	171.27	3.35	-115.45	120.55	51.98	42.38	42.86	31.77	2.35	–	2.52	1.98	*PPP*
	C_2-R	-1.14	-174.61	15.08	-100.46	134.25	-56.27	-11.55	-47.90	-26.83	2.43	2.36	2.48	–	*MMM*

[a] – α = C_{Tr}-N_{Tr}-C=O; [b] – α' = C-N-C=O; [c] – β = H-N-C-C_{ipso}; [d] – γ = N-C_{Tr}-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – δ = C(=O)-N-C*-H; [f] – l_1 = $(N_{Tr})H\cdots C_{ipso\ (1)}$; [g] – l_2 = $(N_{alkyl})H\cdots C_{ipso}$; [h] – l_3 = (C=)O···H(C*); [i] – l_4 = $(C_2=)O\cdots H(N_1)$; [k] – in parentheses are provided the conformer numbers.

Table SI_6. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) calculated at the B3LYP/6-311++G(d,p) level for individual low-energy conformers of **4b** (conformers are numbered according to their appearance during conformational search).

		α^a	α'^b	$\beta_1{}^c$	$\beta_2{}^c$	$\beta_3{}^c$	$\gamma_1{}^d$	$\gamma_2{}^d$	$\gamma_3{}^d$	δ^e	$l_1{}^f$	$l_2{}^g$	$l_3{}^h$	$l_4{}^i$	Helicity
4b (1)[k]	C_1-R	-9.68	-174.27	29.64	-89.66	142.37	31.78	69.55	-21.66	36.09	2.47	–	2.63	3.81	*MPP*
	C_2-R	2.21	-179.64	-7.44	-122.67	111.73	-54.40	-9.83	-47.78	13.17	2.38	2.72	2.57	4.49	*MMM*
4b (4)[k]	C_1-R	-2.95	175.03	-3.92	-128.38	111.11	54.48	46.94	7.85	29.94	2.41	2.37	2.68	–	*PPP*
	C_2-R	3.38	-173.51	5.33	-109.87	124.24	-54.50	-8.32	-47.15	26.17	2.41	3.37	2.63	–	*MMM*
4b (30)[k]	C_1-R	-175.42	170.71	-2.51	-115.81	116.62	-51.35	-3.95	-52.60	31.82	2.37	–	2.70	2.42	*MM0*
	C_2-R	1.10	177.94	-2.26	-117.71	116.97	-53.62	-9.96	-47.01	-22.16	2.40	2.56	2.69	–	*MMM*
4b (40)[k]	C_1-R	-171.25	170.95	-17.32	-129.82	102.26	-41.43	9.41	-63.79	31.08	2.39	–	2.70	2.42	*MMP*
	C_2-R	-2.61	172.62	-18.56	-137.90	96.93	57.61	45.63	13.06	-24.56	2.42	2.21	2.70	–	*PPP*
4b (48)[k]	C_1-R	-178.97	172.46	4.39	-114.69	117.83	48.38	54.35	1.39	23.87	2.36	–	2.67	2.44	*PP0*
	C_2-R	1.62	179.55	-0.70	-116.25	118.55	-54.98	-11.95	-46.42	-23.98	2.39	2.52	2.69	–	*MMM*

[a] – α = C_{Tr}-N_{Tr}-C=S; [b] – α' = C-N-C=S; [c] – β = H-N-C-C_{ipso}; [d] – γ = N-C_{Tr}-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – δ = C(=S)-N-C*-H; [f] – l_1 = $(N_{Tr})H\cdots C_{ipso\ (1)}$; [g] – l_2 = $(N_{alkyl})H\cdots C_{ipso}$; [h] – l_3 = (C=)S···H(C*); [i] – l_4 = $(C_2{=})S\cdots H(N_1)$; [k] – in parentheses are provided the conformer numbers.

Table SI_7. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) calculated at the B3LYP/6-311++G(d,p) level for individual low-energy conformers of **6a** (conformers are numbered according to their appearance during conformational search).

		α^a	α'^b	$\beta_1{}^c$	$\beta_2{}^c$ / β'^j	$\beta_3{}^c$ / β''^l	$\gamma_1{}^d$	$\gamma_2{}^d$	$\gamma_3{}^d$	δ^e	$l_1{}^f$	$l_2{}^g$	$l_3{}^h$	$l_4{}^i$	Helicity
6a (1)[k]	C_1-(Tr)	0.43	178.87	0.82	-114.72	120.05	-54.26	-9.73	-47.31	-21.30	2.41	2.51	2.61	–	*MMM*
	C_2-(PEA)	1.93	177.71	-75.87	47.84	164.55	22.74	–	–	37.45	–	–	2.71	2.56	
6a (4)[k]	C_1-(Tr)	-1.98	172.71	-15.23	-134.58	100.19	57.16	45.64	12.20	-20.79	2.42	2.25	2.63	–	*PPP*
	C_2-(PEA)	2.87	173.67	-34.54	90.79	-149.98	66.19	–	–	29.22	2.58	–	2.68	2.55	
6a (30)[k]	C_1-(Tr)	1.53	-179.93	3.81	-111.88	122.95	-55.86	-13.34	-46.08	-23.53	2.40	2.44	2.68	–	*MMM*
	C_2-(PEA)	-179.34	172.69	-51.42	76.80	-167.08	-58.82	–	–	27.67	2.67	–	2.70	2.44	

[a] – α = C_{Tr}-N_{Tr}-C=S; [b] – α' = C-N-C=S; [c] – β = H-N-C-C_{ipso}; [d] – γ = N-C_{Tr}-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – δ = C(=S)-N-C*-H; [f] – l_1 = $(N_{Tr})H\cdots C_{ipso\ (1)}$; [g] – l_2 = $(N_{alkyl})H\cdots C_{ipso}$; [h] – l_3 = (C=)S···H(C*); [i] – l_4 = $(C_1{=})S\cdots H(N_2)$; [j] – β' = H-N-C*-CH_3; [l] – β'' = H-N-C*-H; [k] – in parentheses are provided the conformer numbers.

Table SI_8. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) calculated at the B3LYP/6-311++G(d,p) level for individual low-energy conformers of **6b** (conformers are numbered according to their appearance during conformational search).

		α^a	α'^b	β_1^c	β_2^c / β''^j	β_3^c / β'''^l	γ_1^d	γ_2^d	γ_3^d	δ^e	l_1^f	l_2^g	l_3^h	l_4^i	Helicity
6b (6)[k]	C_1-(Tr)	-2.01	173.39	-17.92	-137.20	97.57	56.56	46.03	13.26	-22.22	2.42	2.23	2.64	–	*PPP*
	C_2-(PEA)	2.73	177.02	98.81	-24.99	-141.07	-30.52	–	–	31.86	–	2.84	2.64	2.60	
6b (15)[k]	C_1-(Tr)	-2.82	172.52	-15.05	-134.41	100.37	57.32	46.38	12.59	-25.07	2.42	2.24	2.69	–	*PPP*
	C_2-(PEA)	-175.34	173.80	79.18	-45.75	-163.21	-52.43	–	–	27.27	–	–	2.72	2.40	
6b (16)[k]	C_1-(Tr)	0.99	177.70	-0.91	-116.08	118.31	-55.32	-7.47	-47.39	-23.43	2.40	2.53	2.69	–	*MMM*
	C_2-(PEA)	-175.98	171.52	77.92	-47.07	-164.43	-52.57	–	–	-142.31	–	–	2.68	2.43	
6b (24)[k]	C_1-(Tr)	-3.20	172.51	-13.40	-132.74	102.05	56.89	45.24	12.08	-24.11	2.42	2.25	2.67	–	*PPP*
	C_2-(PEA)	-176.54	177.00	45.42	-81.02	162.04	-69.80	–	–	-139.36	2.64	–	2.74	2.42	

[a] – α = C_{Tr}-N_{Tr}-C=S; [b] – α' = C-N-C=S; [c] – β = H-N-C-C_{ipso}; [d] – γ = N-C_{Tr}-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – δ = C(=S)-N-C*-H; [f] – l_1 = $(N_{Tr})H\cdots C_{ipso\ (1)}$; [g] – l_2 = $(N_{alkyl})H\cdots C_{ipso}$; [h] – l_3 = (C=)S···H(C*); [i] – l_4 = $(C_1{=})S\cdots H(N_2)$; [j] – β' = H-N-C*-CH_3; [l] – β'' = H-N-C*-H; [k] – in parentheses are provided the conformer numbers.

Table SI_9. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) calculated at the B3LYP/6-311++G(d,p) level for individual low-energy conformers of **7a** and **7b** (in parentheses conformer number; conformers are numbered according to their appearance during conformational search).

	α^a	α'^b	$\beta_1{}^c$	$\beta_2{}^c$	$\beta_3{}^c$	δ^d	l^e
7a (1)[k]	159.46	158.78	-93.02	144.43	26.34	-10.85	2.29
7a (2)[k]	-5.19	-158.44	-142.92	94.54	-24.77	-9.52	2.08
7b (1)[k]	-0.28	-174.20	117.26	0.02	-117.37	11.86	2.55
7b (2)[k]	168.53	3.05	128.74	11.08	-107.05	2.20	–
7b (3)[k]	177.90	6.85	122.31	4.58	-113.41	40.18	–
7b (4)[k]	-168.59	-163.93	106.02	-12.02	-129.53	18.54	2.57

[a] – α = $C_{t\mathrm{Bu}}$-$N_{t\mathrm{Bu}}$-C=X; [b] – α' = C-N-C=X; [c] – β = H-N-C-$C_{t\mathrm{Bu}}$; [d]– δ = C(=X)-N-C*-H; [e] – l = (C=)X···H(C*); X = S, O; [k] – in parentheses are provided the conformer numbers.

Table SI_10. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) calculated at the IEFPCM/B3LYP/6-311++G(d,p) level for individual low-energy conformers of **3b** (conformers are numbered according to their appearance during conformational search).

		α^a	α''^b	$\beta_1{}^c$	$\beta_2{}^c$	$\beta_3{}^c$	$\gamma_1{}^d$	$\gamma_2{}^d$	$\gamma_3{}^d$	δ^e	$l_1{}^f$	$l_2{}^g$	$l_3{}^h$	$l_4{}^i$	Helicity
3b (3)[k]	C_1-R	18.8	5.3	15.3	-104.3	130.1	44.6	55.1	6.5	37.9	2.407		2.572	1.982	*PPP*
	C_2-R	8.3	-15.8	13.4	-106.4	127.1	44.7	57.0	-1.0	-26.7	2.412		2.556		*PP0*
3b (6)[k]	C_1-R	-15.8	5.9	-28.3	92.2	-141.5	-34.5	-69.5	12.8	38.2	2.463		2.602	1.956	*MMP*
	C_2-R	167.6	-6.5	-18.7	96.7	-137.9	54.2	9.6	48.3	-30.9	2.439		2.521		*PPP*
3b (11)[k]	C_1-R	22.7	-7.5	19.6	133.8	-100.3	44.9	1.2	58.1	-24.9	2.420		2.558	2.122	*PP0*
	C_2-R	-13.2	3.7	-11.4	-125.5	108.6	-46.0	-1.7	-56.1	39.1	2.406		2.450		*MM0*
3b (12)[k]	C_1-R	-17.7	5.6	-25.3	95.0	-138.7	-37.5	-65.7	9.5	38.4	2.447		2.596	1.958	*PMM*
	C_2-R	155.6	-10.1	-12.3	107.4	-126.6	-45.6	-54.0	0.0	-28.7	2.415	2.719	2.515		*MM0*
3b (13)[k]	C_1-R	23.6	11.9	21.6	-98.6	135.5	41.7	61.2	-3.0	29.9	2.421		2.528	1.971	*PP0*
	C_2-R	163.5	-10.7	-3.2	116.3	-118.2	-50.6	-50.6	-6.6	-27.5	2.409		2.495		*MMM*
3b (17)[k]	C_1-R	-17.0	-23.6	0.4	119.6	-114.7	-53.1	-48.5	-13.7	-21.8	2.382		2.550	2021	*MMM*
	C_2-R	19.0	3.0	15.9	130.8	-103.6	43.5	5.9	55.7	41.0	2.413		2.590		*PPP*

3b (18)[k]	C_1-R	-13.5	-25.1	-9.0	111.0	-122.8	-44.8	-59.1	2.1	-19.8	2.419		2.507	2.024	*MM0*
	C_2-R	-10.5	4.9	-13.8	106.2	-127.7	-44.2	-56.6	-0.1	46.3	2.429		2.662		*MM0*
3b (32)[k]	C_1-R	24.4	13.4	16.2	-103.7	130.8	45.1	56.5	5.7	30.8	2.400		2.544	1.964	*PPP*
	C_2-R	172.4	-9.6	-11.6	-130.9	103.6	53.0	50.1	7.2	-28.6	2.430		2.501		*PPP*
3b (33)[k]	C_1-R	22.7	12.0	16.0	-103.9	130.4	45.8	55.8	4.7	29.6	2.399		2.525	1.974	*PP0*
	C_2-R	163.1	-10.5	-3.8	115.8	-118.6	-50.3	-50.8	-6.2	-27.6	2.409		2.495		*MMM*
3b (75)[k]	C_1-R	17.2	0.4	-16.1	-103.7	130.5	45.6	56.7	3.3	-26.5	2.407		2.424	2.167	*PP0*
	C_2-R	-12.7	-164.8	-15.9	-130.0	104.0	-45.7	-0.8	-56.8	25.0	2.401				*MM0*
3b (76)[k]	C_1-R	17.0	-0.1	15.8	-130.3	-104.0	45.6	3.3	56.5	-26.5	2.407		2.426	2.156	*PP0*
	C_2-R	-14.5	-164.9	-21.0	99.1	-134.7	-42.0	-61.2	4.4	25.8	2.427				*MM0*
3b (96)[k]	C_1-R	17.3	-0.5	17.6	-102.3	131.8	45.1	57.5	1.2	-26.1	2.411		2.417	2.170	*PP0*
	C_2-R	16.5	-170.2	10.4	-109.3	124.8	48.3	54.3	4.6	32.1	2.403				*PP0*

[a] – α = C_{Tr}-N_{Tr}-C=O; [b] – α' = C-N-C=O; [c] – β = H-N-C-C_{ipso}; [d] – γ = N-C_{Tr}-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – δ = C(=O)-N-C*-H; [f] – I_1 = (N_{Tr})H···$C_{ipso\ (1)}$; [g] – I_2 = (N_{alkyl})H···C_{ipso} ; [h] – I_3 = (C=)O···H(C*); [i] – I_4 = (C_2=)O···H(N_1); [k] – in parentheses are provided the conformer numbers.

Table SI_11. Selected crystal data and structure refinement details.

	2a	**2b**	**2c**	**2d**	**4a**	**4a**
Chemical formula	$C_{24}H_{26}N_2S$	$C_{25}H_{28}N_2S$	$C_{26}H_{30}N_2S$	$C_{28}H_{32}N_2S$	$C_{26}H_{29}N_3S$ $2CH_3OH$	$C_{26}H_{29}N_3S$ $0.5H_2O$
Mr	374.53	388.55	402.58	428.61	479.66	424.60
Crystal system, space group	Monoclinic, *C*2	Tetragonal, $P4_32_12$	Monoclinic, $P2_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P222_1$	Monoclinic, *C*2
Temperature (K)	130	130	130	130	130	130
a, *b*, *c* (Å)	11.1159 (1), 13.1734 (1), 28.2695 (3)	8.73671 (17), 56.4484 (10)	17.6143 (4), 8.86240 (16), 29.0155 (6)	9.60290 (7), 10.57062 (6), 23.07870 (13)	11.09166 (8), 13.89141 (9), 34.8221 (3)	14.3834 (2), 10.6941 (1), 29.8026 (6)
α, β, γ (°)	96.402 (1)		98.484 (2)			98.643 (2)
V (Å^3)	4113.81 (7)	4308.71 (19)	4479.89 (15)	2342.69 (3)	5365.35 (7)	4532.10 (12)
Z	8	8	8	4	8	8
D_x (Mg m^{-3})	1.209	1.198	1.194	1.215	1.188	
Radiation type	Cu *K*α	Cu *K*α	Cu *K*α	Cu *K*α	Cu *K*α	Cu *K*α
μ (mm^{-1})	1.46	1.41	1.37	1.34	1.29	1.41
Crystal size (mm)	0.3 × 0.2 × 0.05	0.45 × 0.1 × 0.1	0.4 × 0.02 × 0.01	0.2 × 0.2 × 0.05	0.2 × 0.2 × 0.15	0.20 × 0.15 × 0.01
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30651, 7817, 7774	23415, 3954, 3851	48848, 16367, 12337	38669, 4605, 4574	24975, 4925, 4904	28813, 8563, 7400
R_{int}	0.018	0.030	0.090	0.025	0.018	0.040
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.025, 0.068, 1.04	0.036, 0.085, 1.06	0.051, 0.120, 0.96	0.023, 0.064, 1.06	0.038, 0.088, 1.24	0.052, 0.144, 1.06
No. of parameters	491	256	1069	289	322	557
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.16, -0.18	0.21, -0.22	0.31, -0.27	0.17, -0.18	0.21, -0.20	0.32, -0.30
Absolute structure parameter	-0.016 (5)	0.002 (7)	0.02 (2)	-0.002 (3)	0.025 (4)	-0.008 (10)

Table SI_12. Selected crystal data and structure refinement details.

	4b	**5**	**6a**	**6b**	**7b**
Chemical formula	$C_{46}H_{44}N_4S_2$	$C_{27}H_{27}N_3S_2$	$C_{35}H_{38}N_4S_2{\cdot}0.16(H_2O)$	$C_{35}H_{38}N_4S_2$	$C_{11}H_{24}N_2S$
Mr	716.97	457.63	581.69	578.81	216.38
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Triclinic, $P1$	Tetragonal, $P4_32_12$
Temperature (K)	130	130	130	130	130
a, *b*, *c* (Å)	9.16773 (5), 14.33308 (8), 15.08193 (8)	10.16800 (5), 14.93848 (8), 16.29099 (8)	8.81055 (10), 20.08758 (17), 9.52368 (11)	9.0135 (2), 9.2173 (2), 10.0939 (2)	12.9053 (1), 16.0870 (1)
α, β, γ (°)	104.0927 (5)	99.1361 (5)	112.3547 (13)	100.231 (2), 94.540 (2), 112.553 (2)	
V (Å^3)	1922.15 (2)	2443.12 (2)	1558.85 (3)	752.08 (3)	2679.24 (4)
Z	2	4	2	1	8
D_x (Mg m^{-3})	1.239	1.244	1.239	1.278	1.073
Radiation type	Cu *K*α	Cu *K*α	Cu *K*α	Cu *K*α	Cu *K*α
M (mm^{-1})	1.54	2.11	1.78	1.84	1.89
Crystal size (mm)	0.35 × 0.08 × 0.02	0.3 × 0.2 × 0.1	0.4 × 0.3 × 0.1	0.35 × 0.18 × 0.07	0.45 × 0.2 × 0.1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31439, 6960, 6854	31443, 8935, 8544	14705, 5686, 5509	25562, 5038, 5012	18425, 2774, 2687
R_{int}	0.027	0.027	0.024	0.032	0.038
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.027, 0.069, 1.02	0.029, 0.075, 1.05	0.032, 0.085, 1.04	0.037, 0.099, 1.13	0.027, 0.071, 1.07
No. of parameters	485	650	475	372	134
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.16, -0.16	0.23, -0.30	0.17, -0.21	0.21, -0.19	0.15, -0.14
Absolute structure parameter	-0.009 (7)	-0.013 (5)	-0.029 (11)	-0.006 (17)	-0.022 (6)

Table SI_13. Dihedral angles α, β, γ and δ (in degrees) and selected interatomic distances l1, l2 and l3 (in Å) fragments observed in the crystal structures **2a-2d**, **4a**, **4b, 5, 6a, 6b, 7b** and **9**.

		α^a	α'^b	$\beta_1{}^c$	$\beta_2{}^c$	$\beta_3{}^c$	$\gamma_1{}^d$	$\gamma_2{}^d$	$\gamma_3{}^d$	δ^e	$l_1{}^f$	$l_2{}^g$	$l_3{}^h$	Helicity
2a	mol A	-169.1 (1)	4.2 (3)	-124.8	-5.0	109.6	46.4 (2)	54.9 (2)	4.9 (2)	33.6	2.420	2.394	2.774	*PP0*
	mol B	-179.9 (1)	-2.9 (3)	-126.8	-7.2	106.9	48.1 (2)	58.1 (2)	5.5 (2)	37.6	2.416	2.433	2.765	*PPP*
2b		178.1 (2)	10.1 (3)	129.7	-104.3	11.0	-43.0 (3)	-8.9 (3)	-57.7 (2)	-24.4	2.397	2.346	2.673	*MMM*
2c	mol A	-176.5 (4)	-11.9 (7)	-126.9	-7.4	107.6	41.7 (7)	57.0 (6)	9.9 (7)	25.6	2.404	2.543	2.624	*PPP*
	mol B	179.5 (4)	-10.2 (8)	128.4	-105.1	9.1	-43.5 (7)	-10.0 (7)	-54.8 (6)	32.1	2.392	2.322	2.685	*MMM*
	mol C	174.6 (4)	-8.9 (7)	135.0	-99.7	16.5	-43.6 (6)	-11.0 (7)	-58.2 (6)	1.7	2.318	2.353	2.674	*MMM*
	mol D	-173.4 (4)	-12.5 (8)	-126.1	106.9	-7.7	41.3 (7)	10.2 (7)	60.8 (6)	18.8	2.415	2.504	2.636	*PPP*
2d		-161.3 (1)	5.6 (2)	-107.0	11.8	127.5	55.43 (17)	40.66 (18)	3.60 (19)	12.2	2.381	2.569	2.676	*PP0*
4a MeOH		-171.3 (3)	4.5 (5)	-123.6	-5.8	109.2	48.6 (4)	53.1 (4)	4.5 (4)	29.0	2.424	2.472	2.730	*PP0*
4a H_2O	mol A	172.5 (3)	-13.0 (7)	134.4	−100.1	16.1	-42.6 (5)	-8.8 (5)	-57.9 (5)	2.5	2.411	2.501	2.621	*MMM*
	mol B	178.0 (3)	-1.6 (7)	−129.9	−11.6	104.0	48.0 (4)	54.5 (4)	7.5 (5)	17.6	2.363	2.298	2.685	*PPP*
4b		156.6 (2)	-9.4 (3)	110.5	-124.5	-6.5	-54.9 (2)	-5.4 (3)	-34.3 (2)	-11.5	2.404	2.572	2.614	*PPP*

		167.7 (2)	-13.1 (3)	132.5	-103.1	11.9	-55.6 (2)	-12.6 (3)	-54.2 (2)	31.6	2.329	2.494	2.621	*MMM*
	mol A	-170.9 (2)	4.7 (4)	-102.7	17.2	131.1	53.6 (3)	49.8 (3)	-1.7 (3)	-14.0	2.414	2.482	2.629	*PP0*
5														
	mol B	166.6 (2)	-12.6 (3)	106.5	-126.7	-13.0	-54.4 (3)	0.8 (3)	-48.9 (3)	41.0	2.361	2.401	2.649	*MM0*
		167.9 (2)	-12.2 (4)	15.0	-100.5	133.2	-58.1 (3)	-11.8 (3)	-41.7 (3)	-17.5	2.425	2.427	2.719	*MMM*
6a		3 (4)	15 (3)	60.3	-63.8	176.8	-35 (3)	-	-	5.3	-	-	2.648	-
	PEA													
		-23 (3)	31 (4)	70.8	-61.2	-174.2	-28 (2)	-	-	-9.0	-	-	2.576	-
		174.5 (2)	-7.3 (5)	135.8	-99.0	17.5	-42.0 (3)	-16.4 (4)	-65.6 (4)	-18.2	2.342	2.382	2.724	*MMM*
6b														
	PEA	-19.5 (5)	5.9 (5)	102.7	-137.8	-20.5	-40.1 (4)	-	-	15.6	2.545	-	2.695	-
7b		3.2 (3)	1.2 (3)	118.2	-117.1	0.9	-	-	-	1.5	-	-	2.634	-

[a] – α = C_{Tr}-N_{Tr}-C=S; [b] – α' = C-N-C=S; [c] – β = H-N-C-C_{ipso}; [d] – γ = N-C_{Tr}-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [e] – δ = C(=S)-N-C*-H; [f] – l_1 = (N_{Tr})H···$C_{ipso\ (1)}$; [g] – l_2 = (N_{alkyl})H···C_{ipso} ; [h] – l_3 = (C=)S···H(C*).

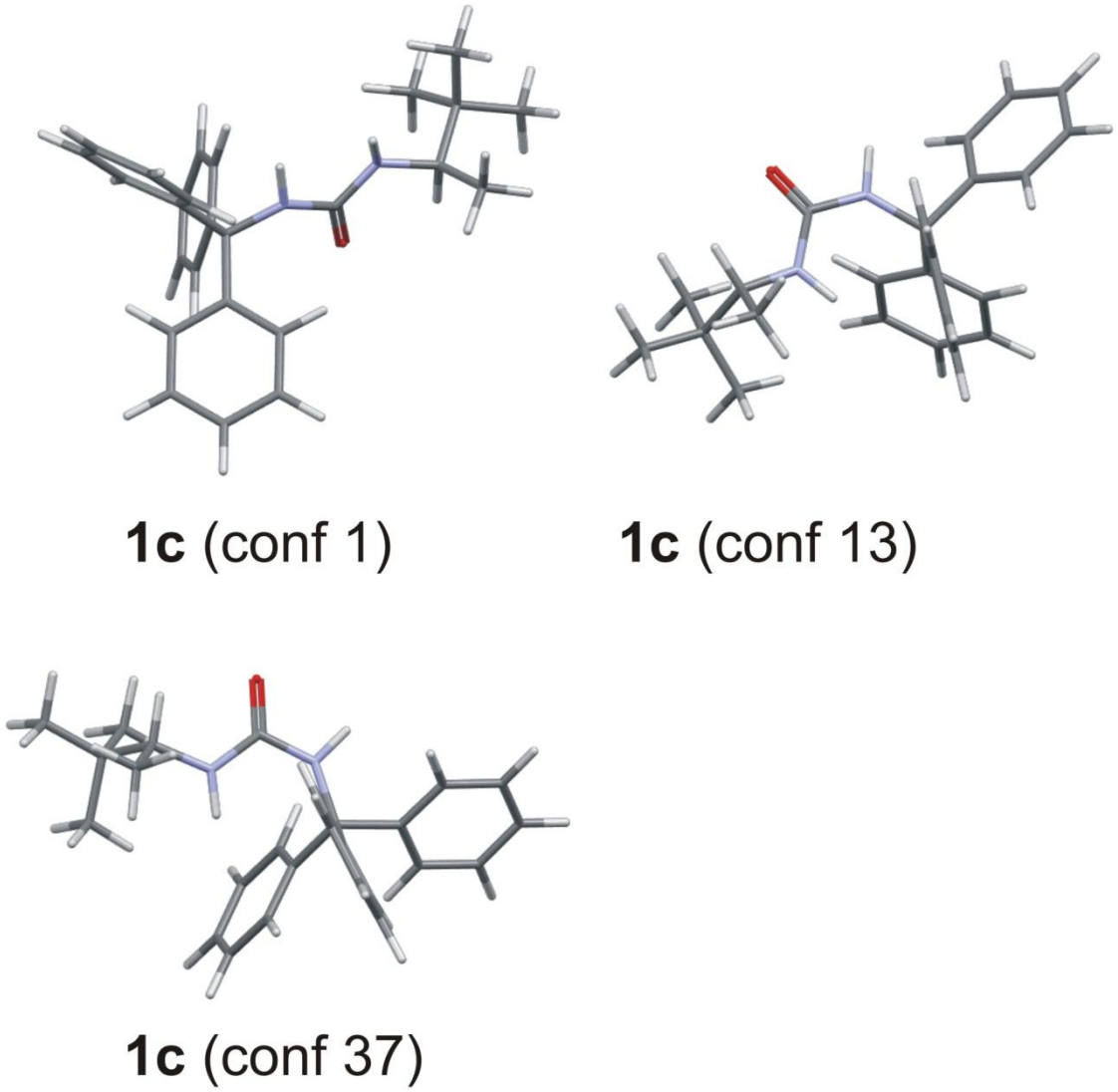
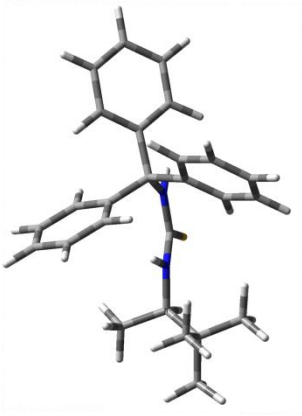


Figure SI_1. Structures of individual, low-energy conformers of **1c**, calculated at the B3LYP/6-311++G(d,p) level of theory.



2c (conf 1)

Figure SI_2. Structure of the lowest-energy conformer of **2c**, calculated at the B3LYP/6-311++G(d,p) level of theory.

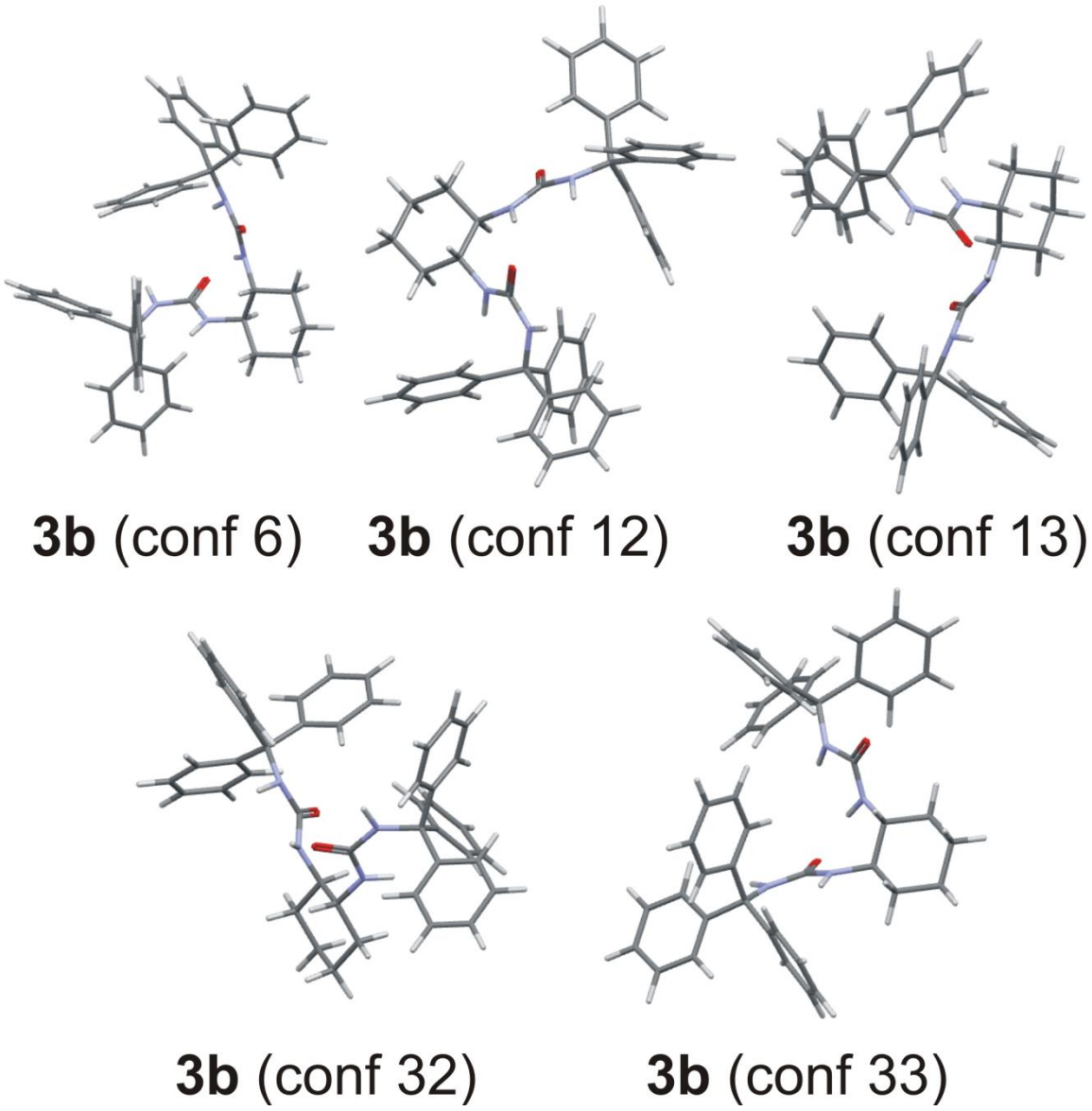


Figure SI_3. Structures of individual, low-energy conformers of **3b**, calculated at the B3LYP/6-311++G(d,p) level of theory.

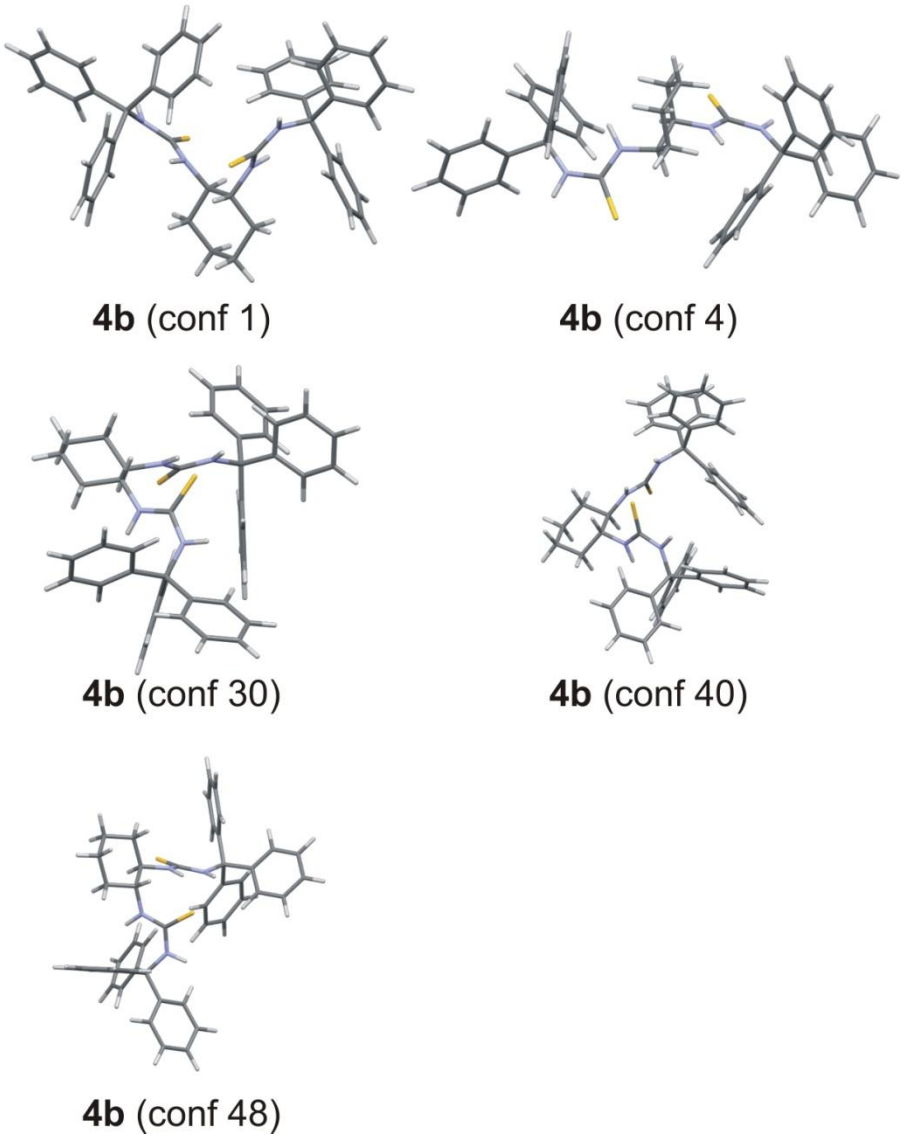


Figure SI_4. Structures of individual, low-energy conformers of **4b**, calculated at the B3LYP/6-311++G(d,p) level of theory.

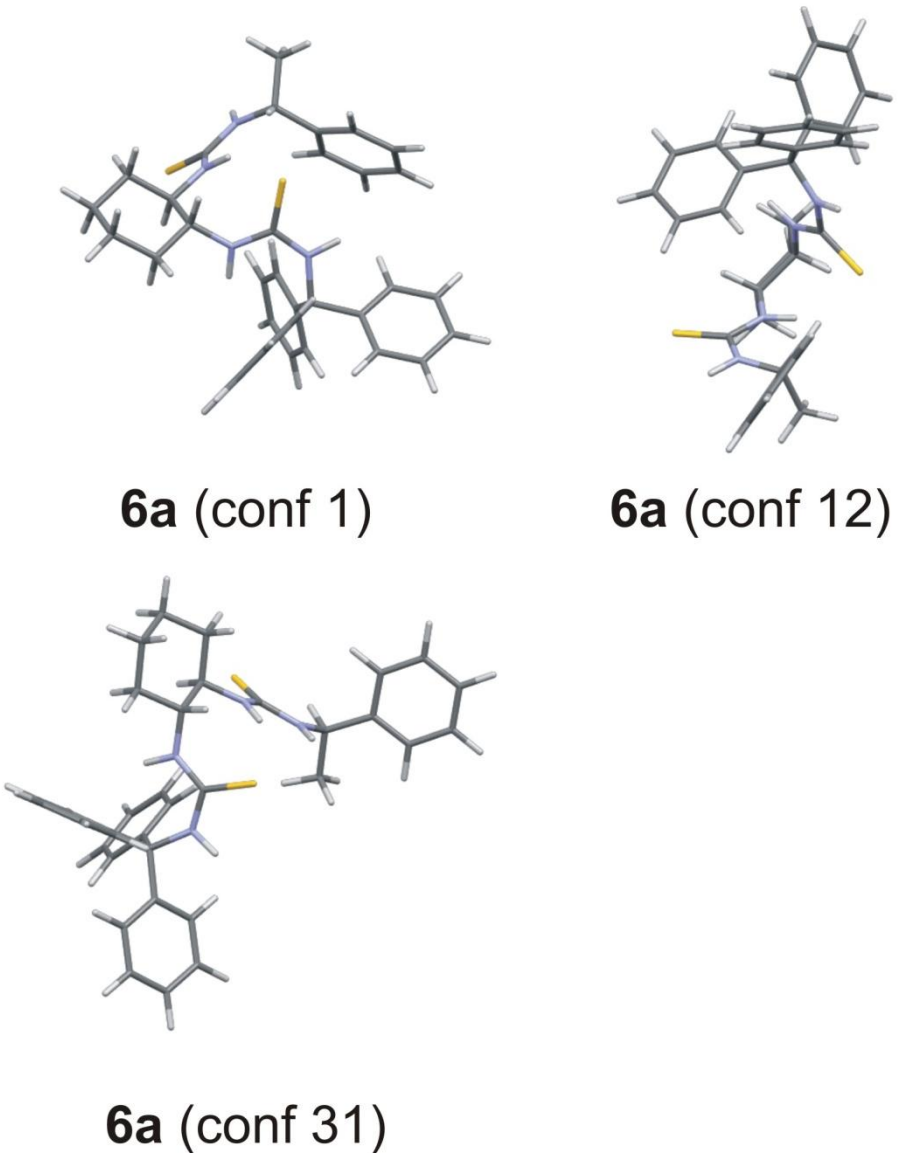


Figure SI_5. Structures of individual, low-energy conformers of **6a**, calculated at the B3LYP/6-311++G(d,p) level of theory.

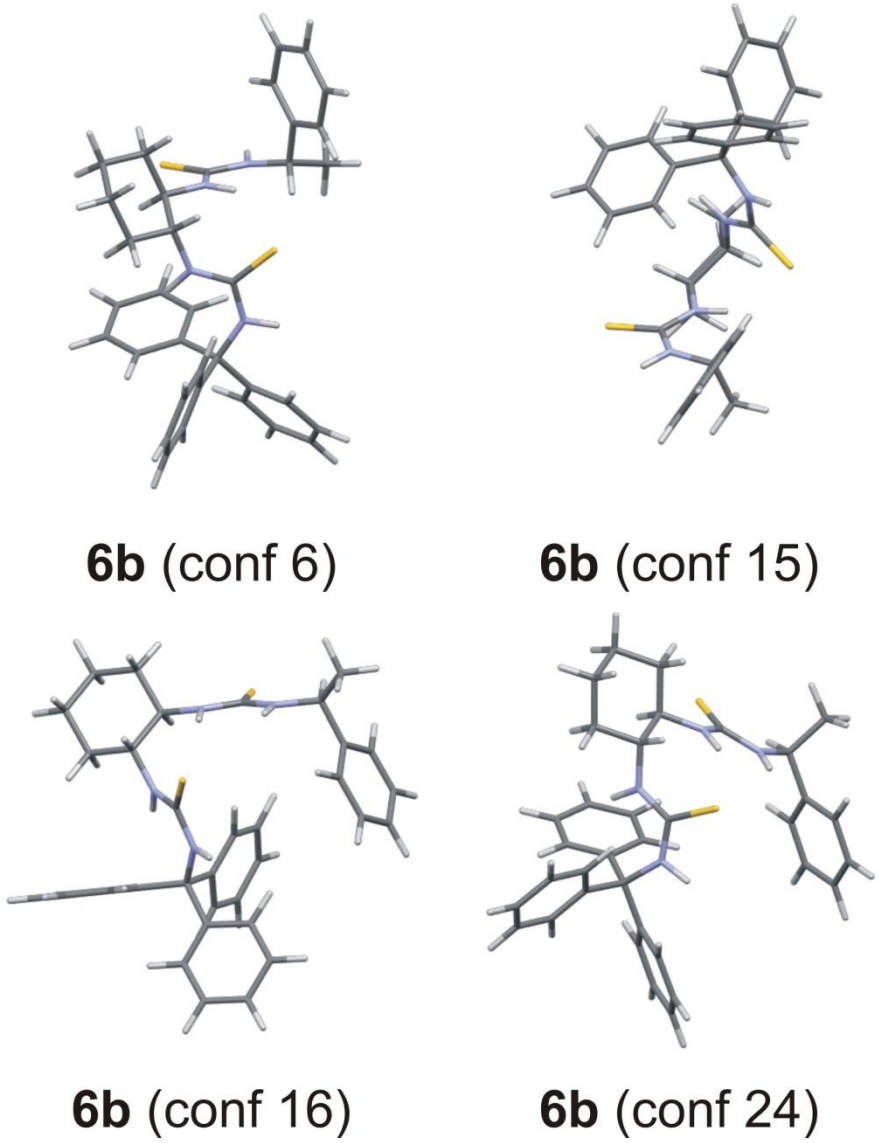


Figure SI_6. Structures of individual, low-energy conformers of **6b**, calculated at the B3LYP/6-311++G(d,p) level of theory.

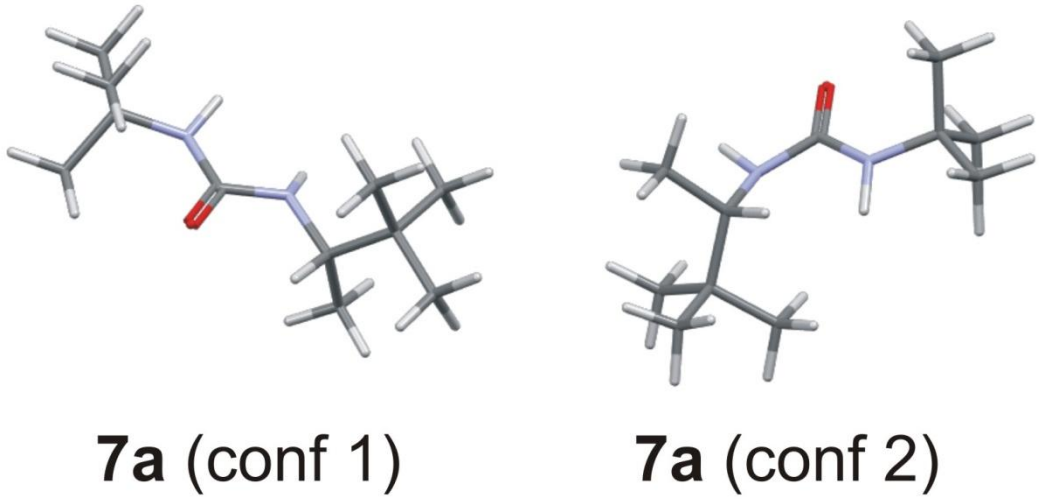


Figure SI_7. Structures of individual, low-energy conformers of **7a**, calculated at the B3LYP/6-311++G(d,p) level of theory.

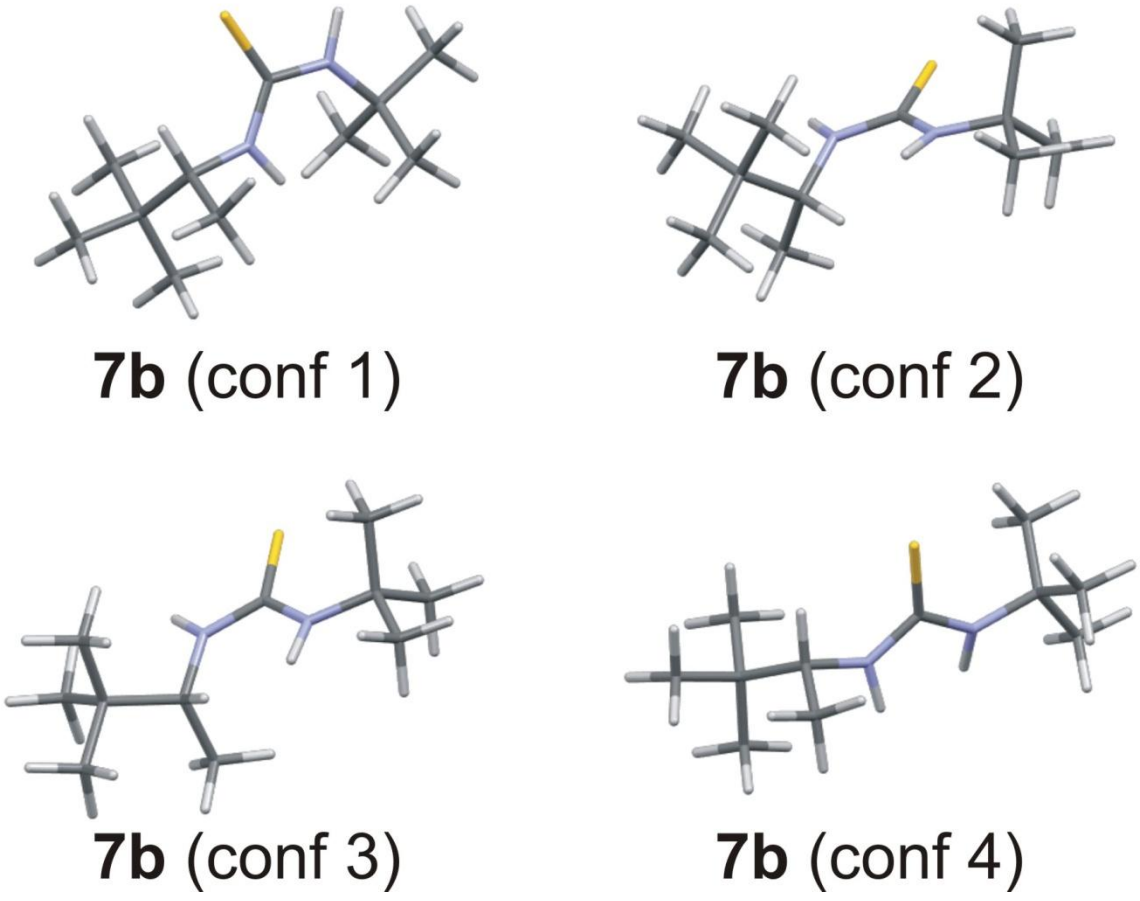


Figure SI_8. Structures of individual, low-energy conformers of **7b**, calculated at the B3LYP/6-311++G(d,p) level of theory.

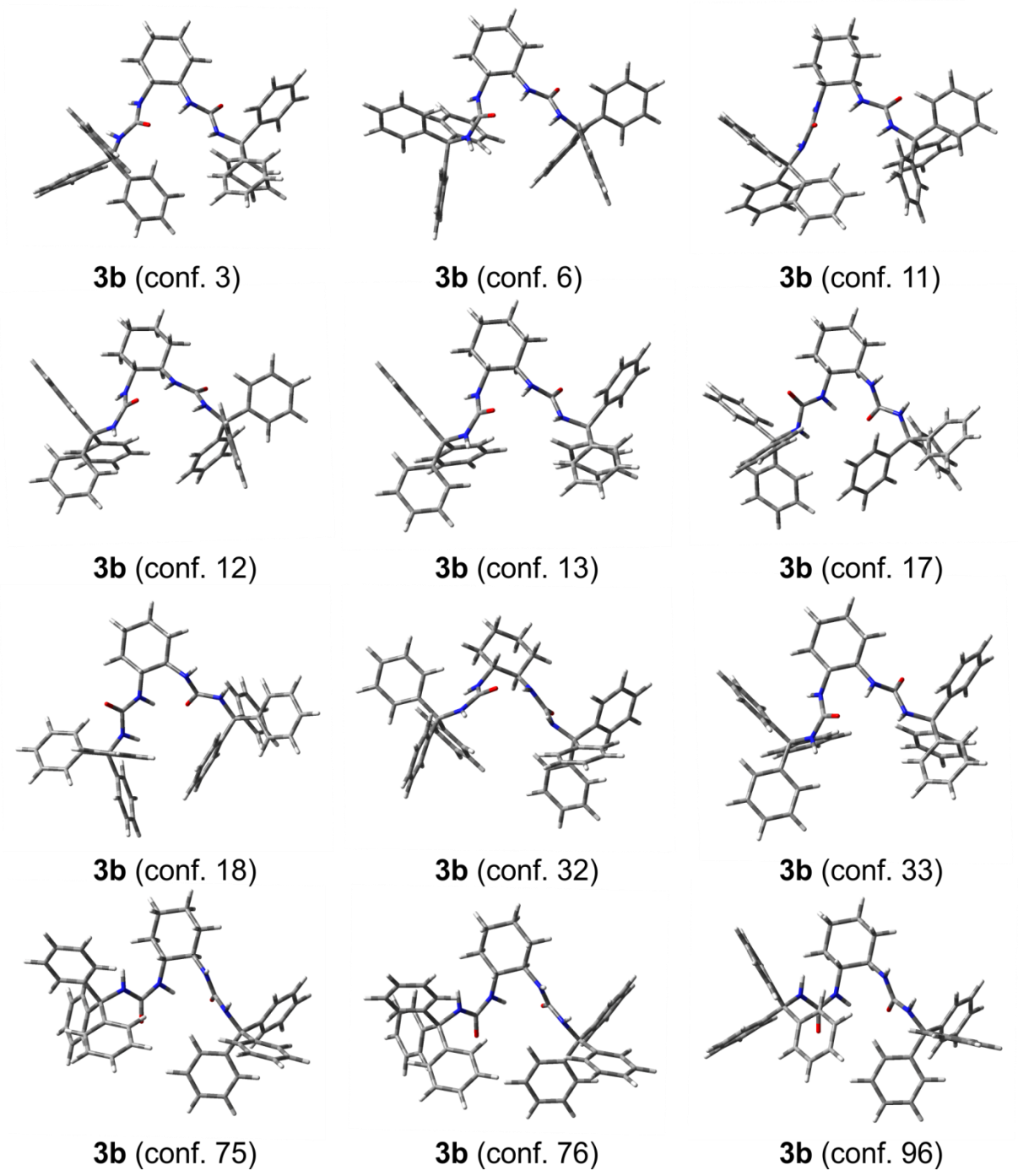


Figure SI_9. Structures of individual, low-energy conformers of **3b**, calculated at the IEFPCM/B3LYP/6-311++G(d,p) level of theory.

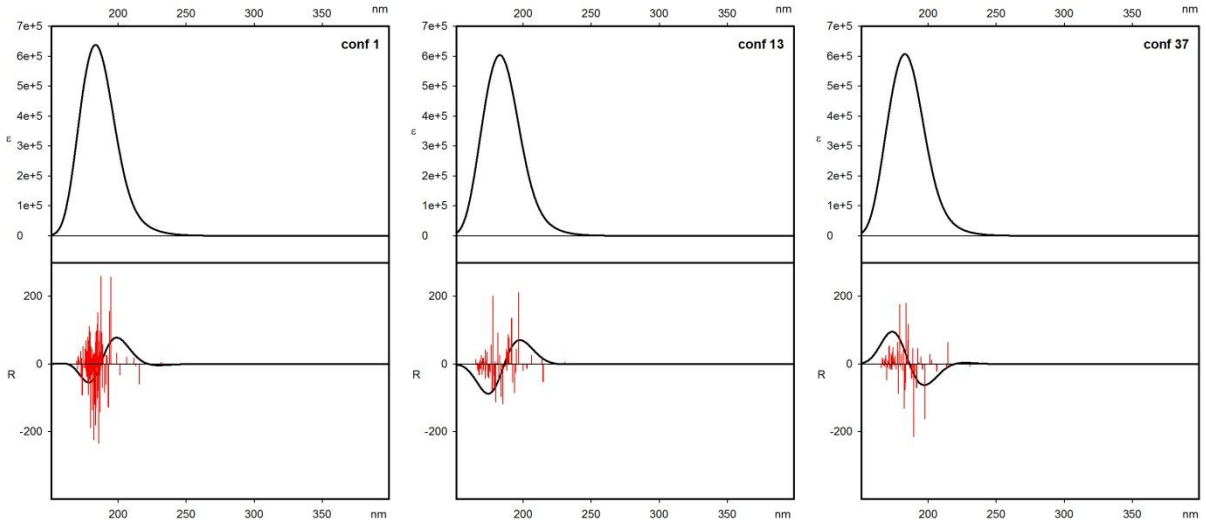


Figure SI_10. ECD spectra of the low-energy conformers of compound (*S*)-**1c** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

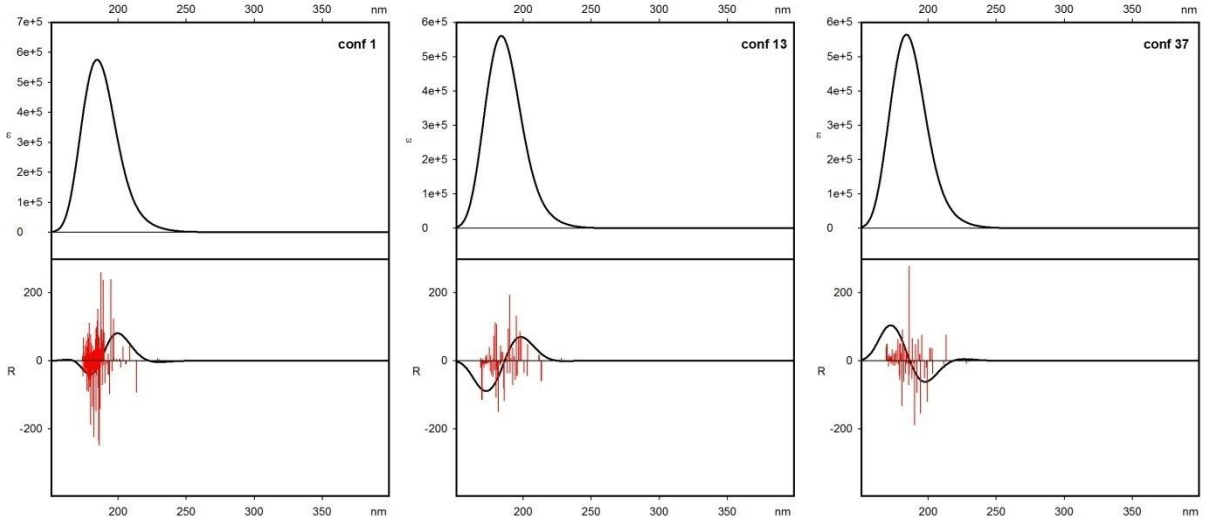


Figure SI_11. ECD spectra of the low-energy conformers of compound (*S*)-**1c** calculated at TD-M06-2X/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

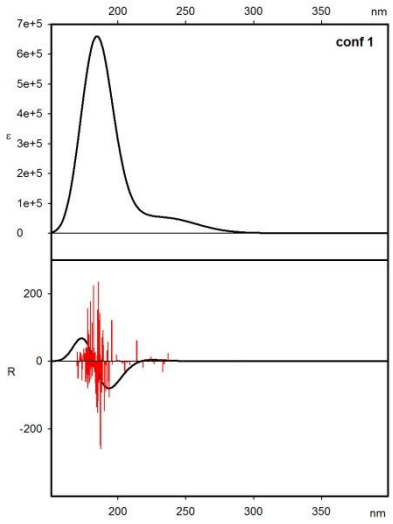


Figure SI_12. ECD spectra of the lowest energy conformer of compound (*R*)-**2c** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structure optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

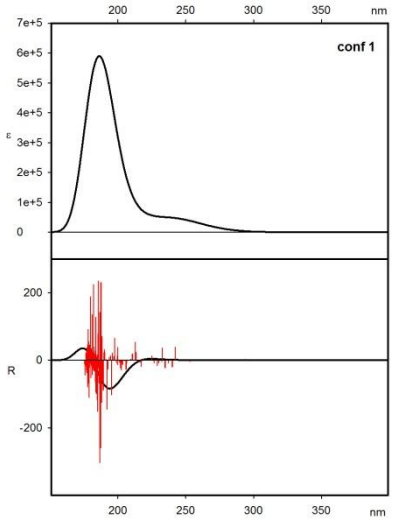


Figure SI_13. ECD spectra of the lowest energy conformer of compound (*R*)-**2c** calculated at TD-M06-2X/6-311++G(d,p) level for structure optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

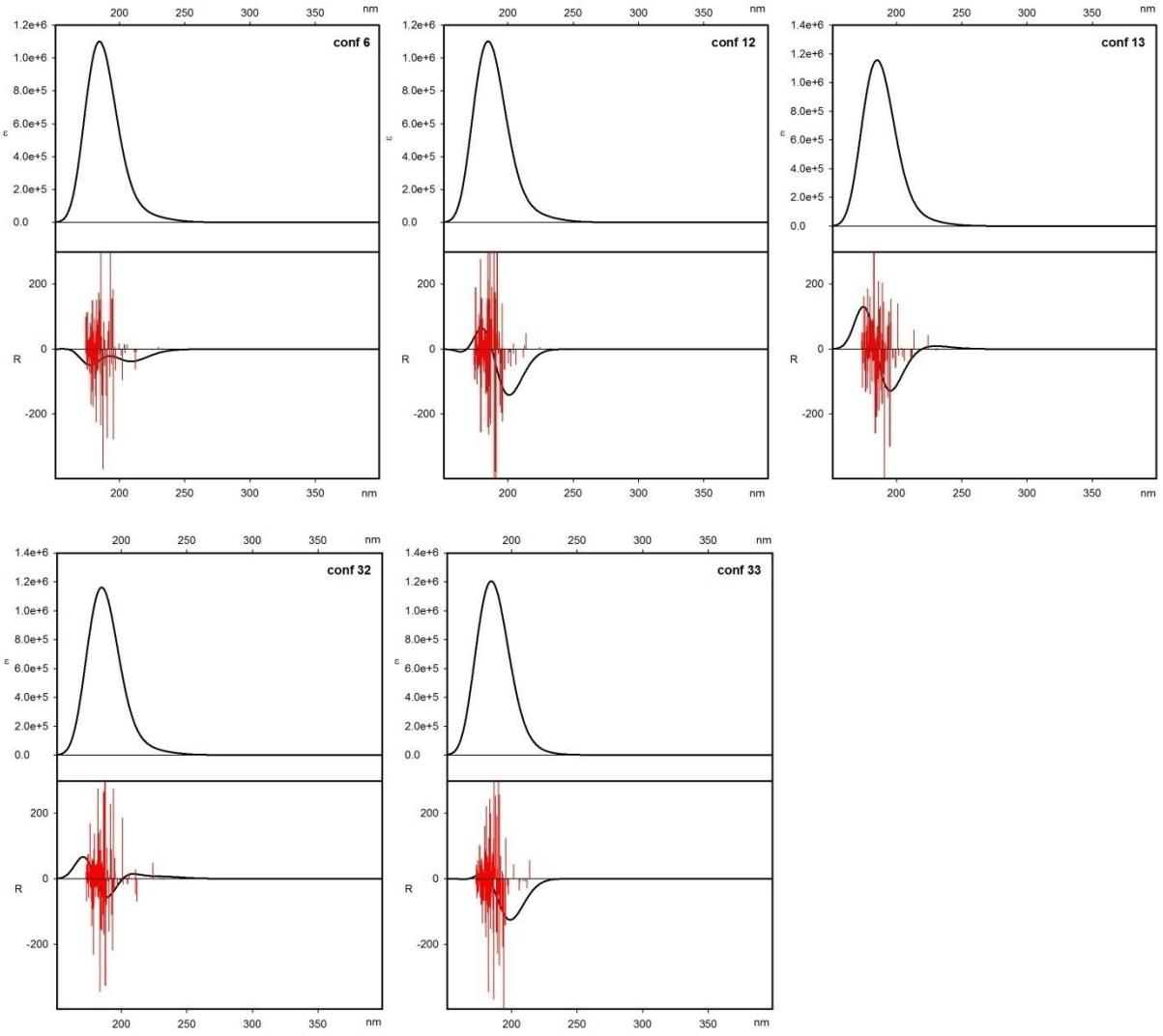


Figure SI_14. ECD spectra of the low-energy conformers of compound **3b** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

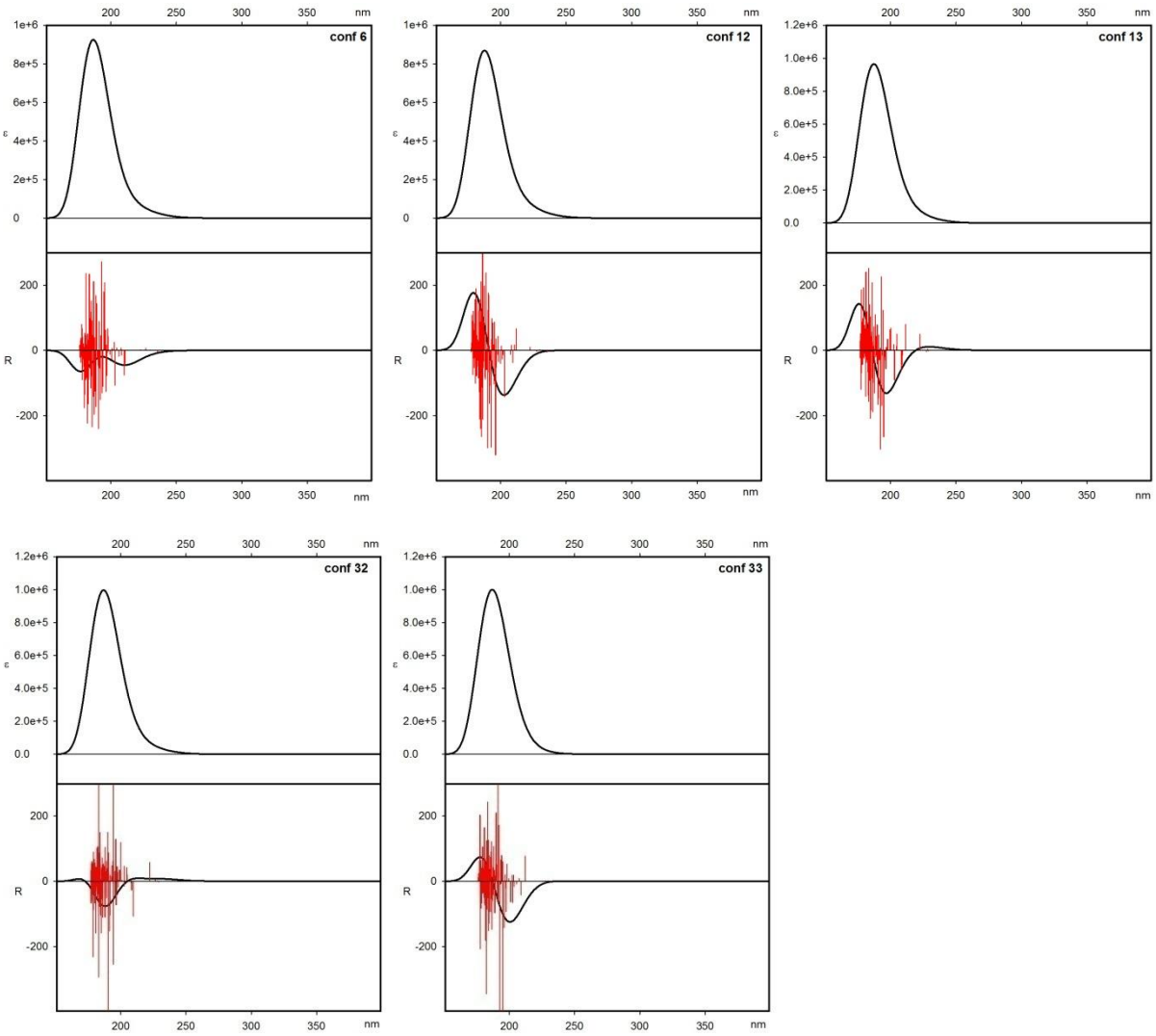


Figure SI_15. ECD spectra of the low-energy conformers of compound **3b** calculated at TD-M06-2X/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

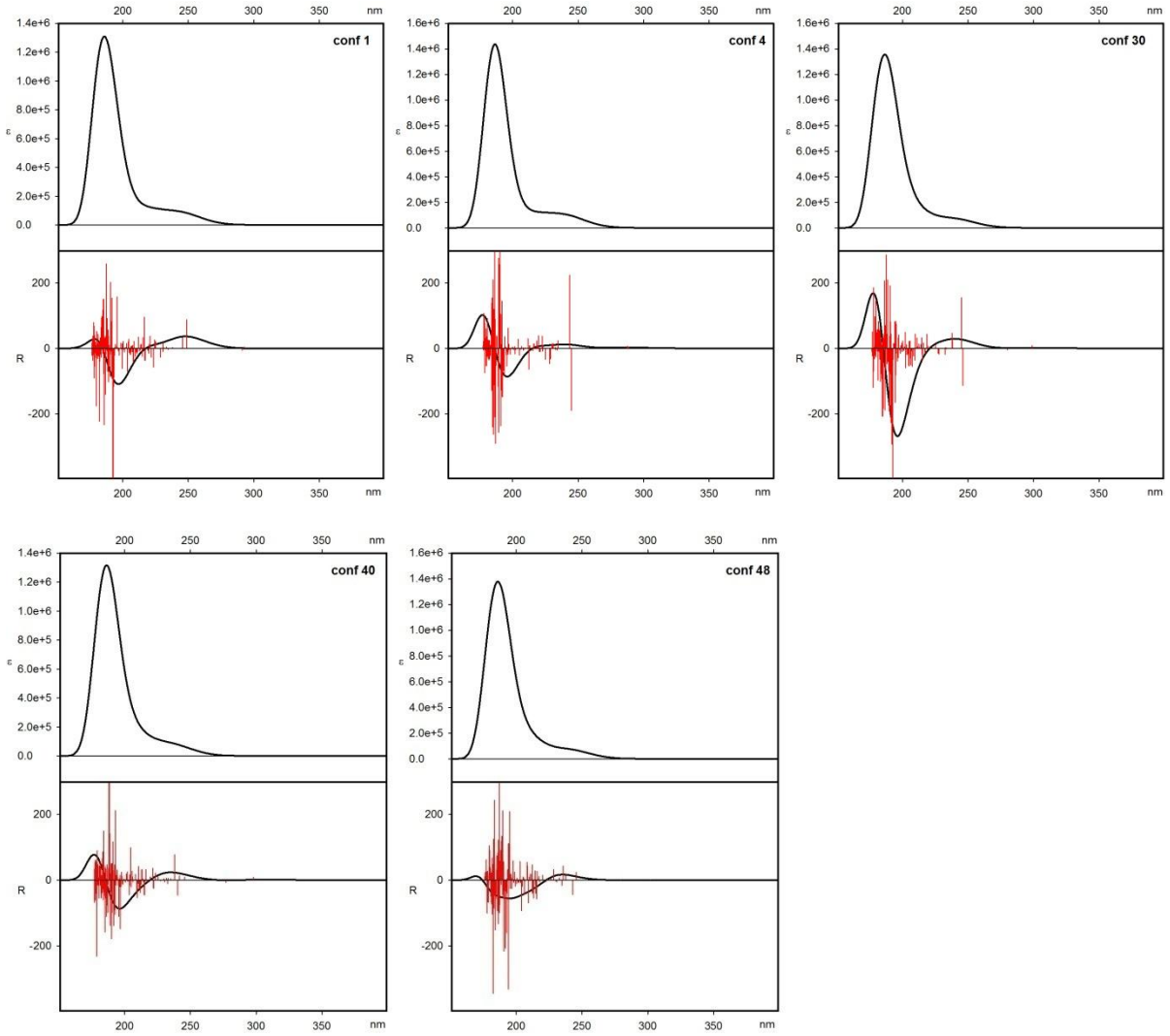


Figure SI_16. ECD spectra of the low-energy conformers of compound **4b** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

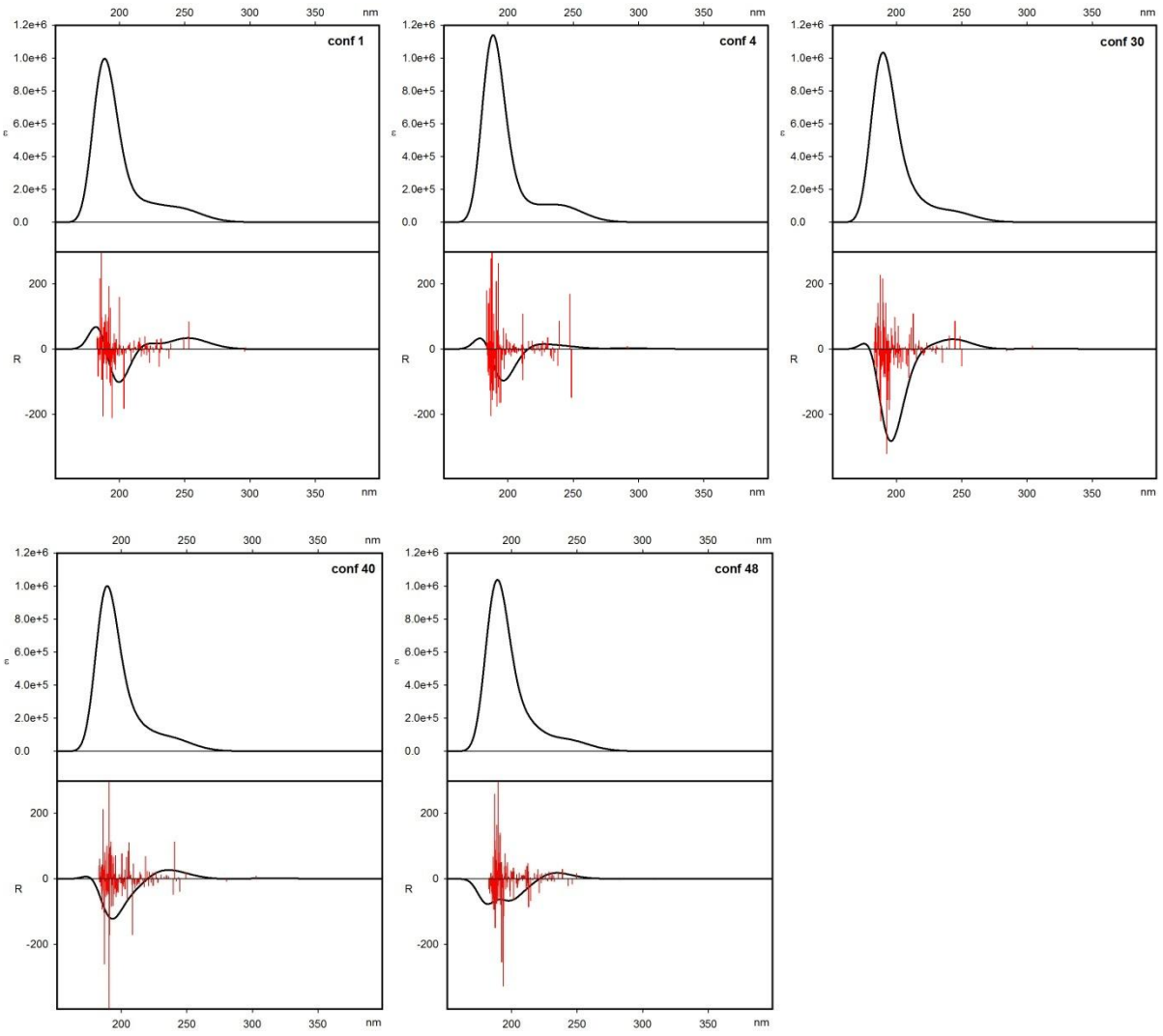


Figure SI_17. ECD spectra of the low-energy conformers of compound **4b** calculated at TD-M06-2X/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

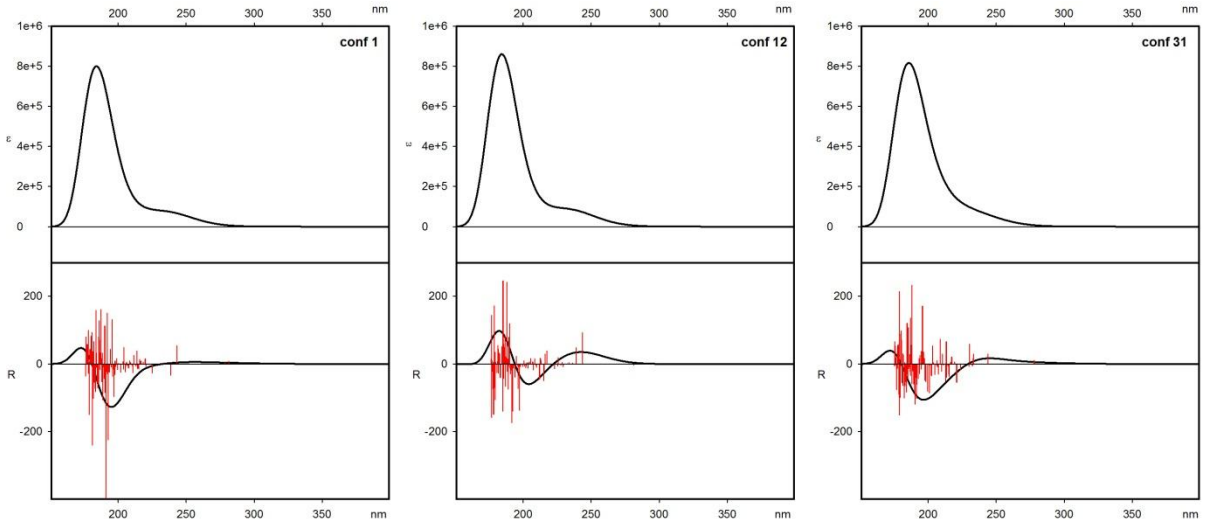


Figure SI_18. ECD spectra of the low-energy conformers of compound **6a** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

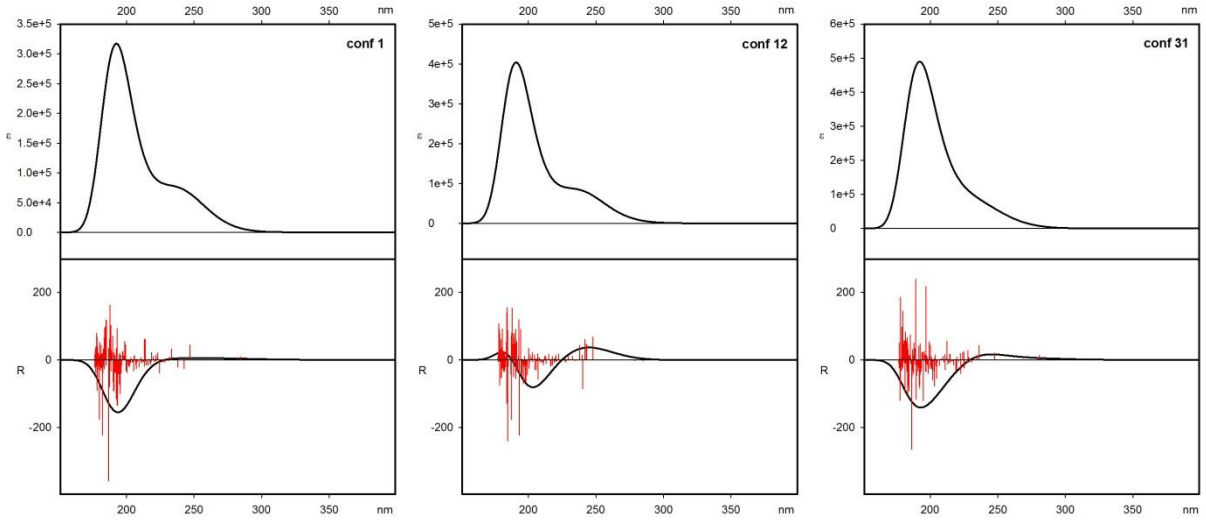


Figure SI_19. ECD spectra of the low-energy conformers of compound **6a** calculated at TD-M06-2X/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

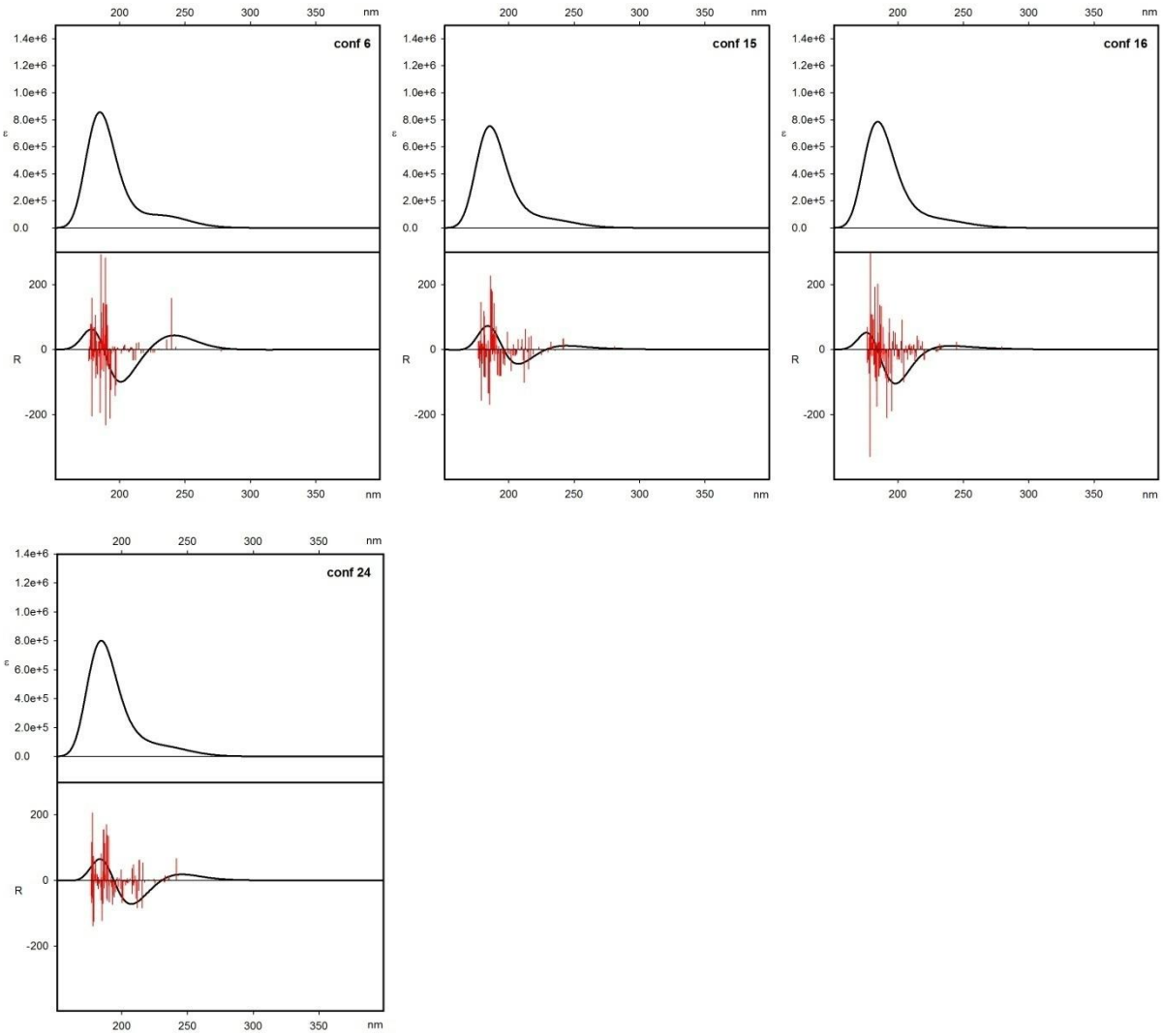


Figure SI_20. ECD spectra of the low-energy conformers of compound **6b** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

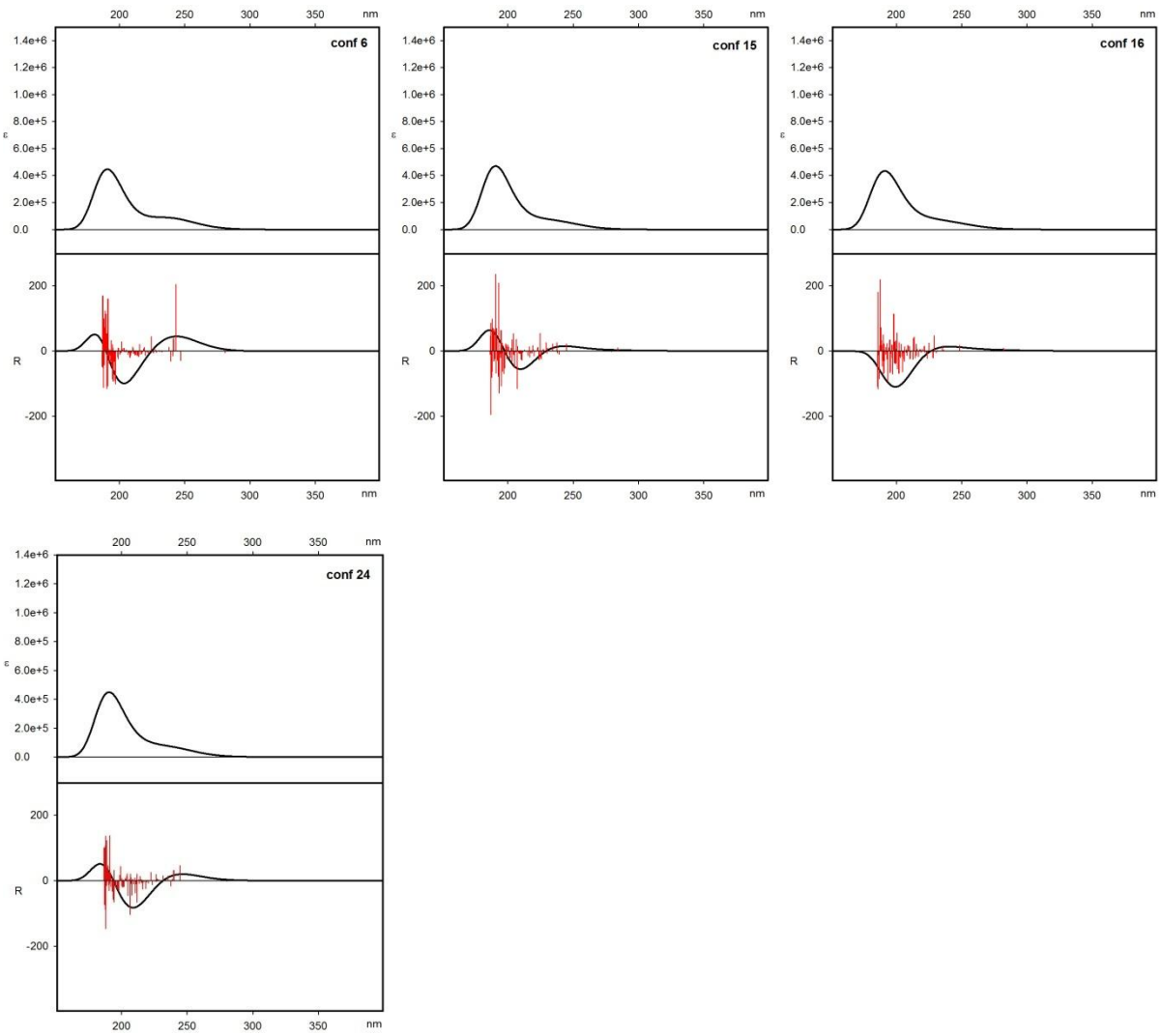


Figure SI_21. ECD spectra of the low-energy conformers of compound **6b** calculated at TD-M06-2X/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

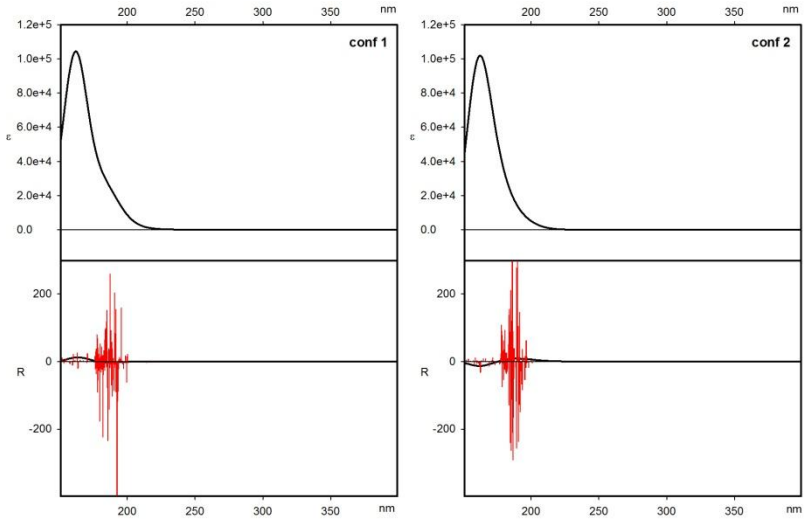


Figure SI_22. ECD spectra of the low-energy conformers of compound **7a** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

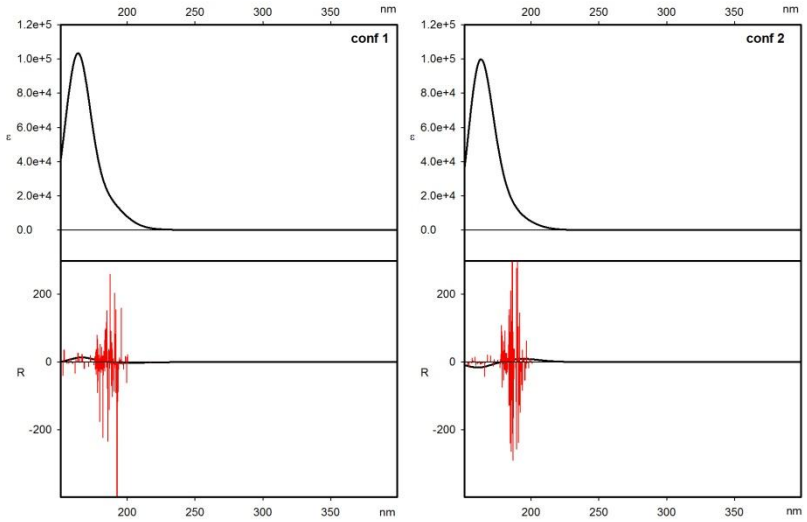


Figure SI_23. ECD spectra of the low-energy conformers of compound **7a** calculated at TD-M06-2X/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

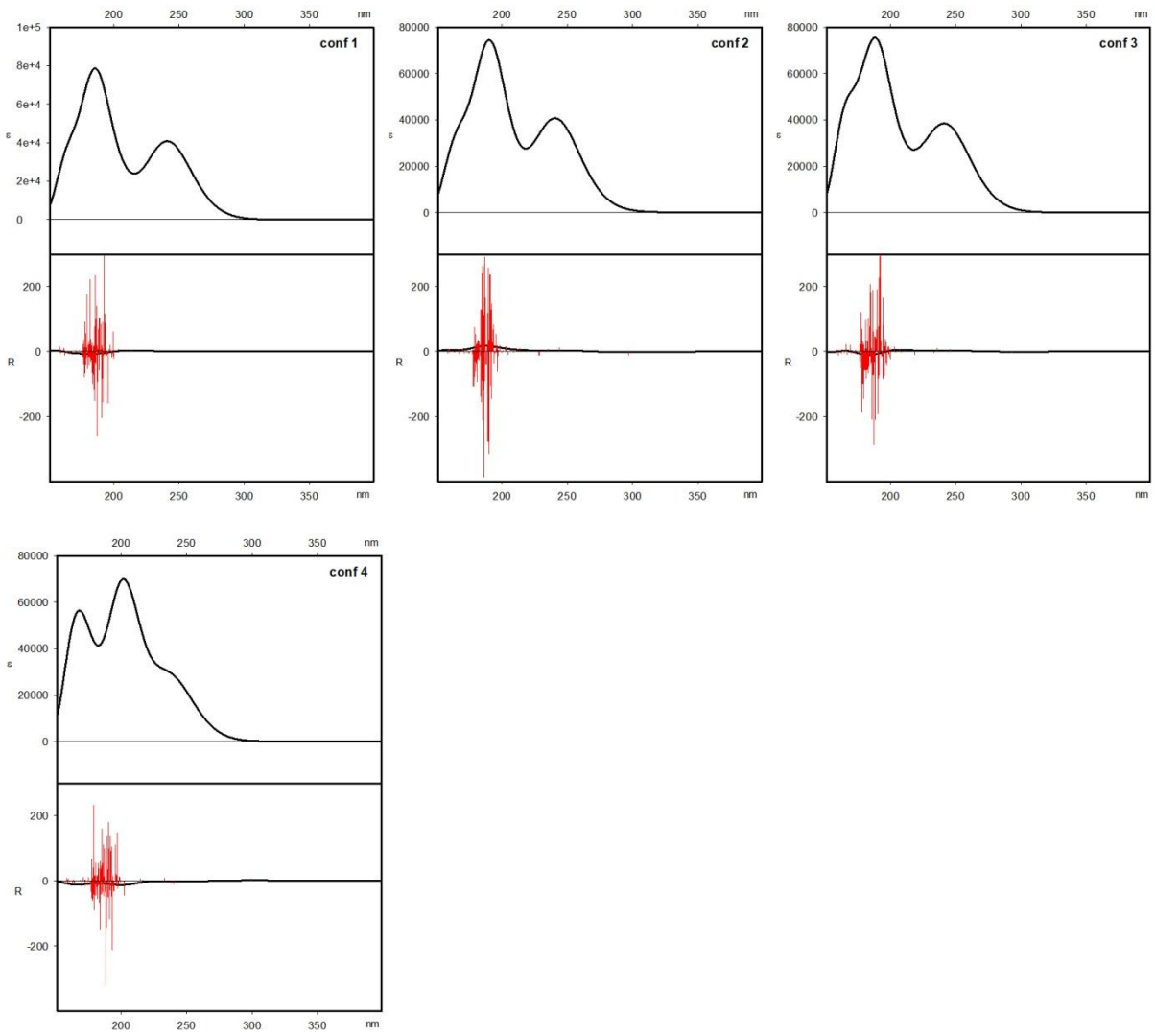


Figure SI_24. ECD spectra of the low-energy conformers of compound **7b** calculated at TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

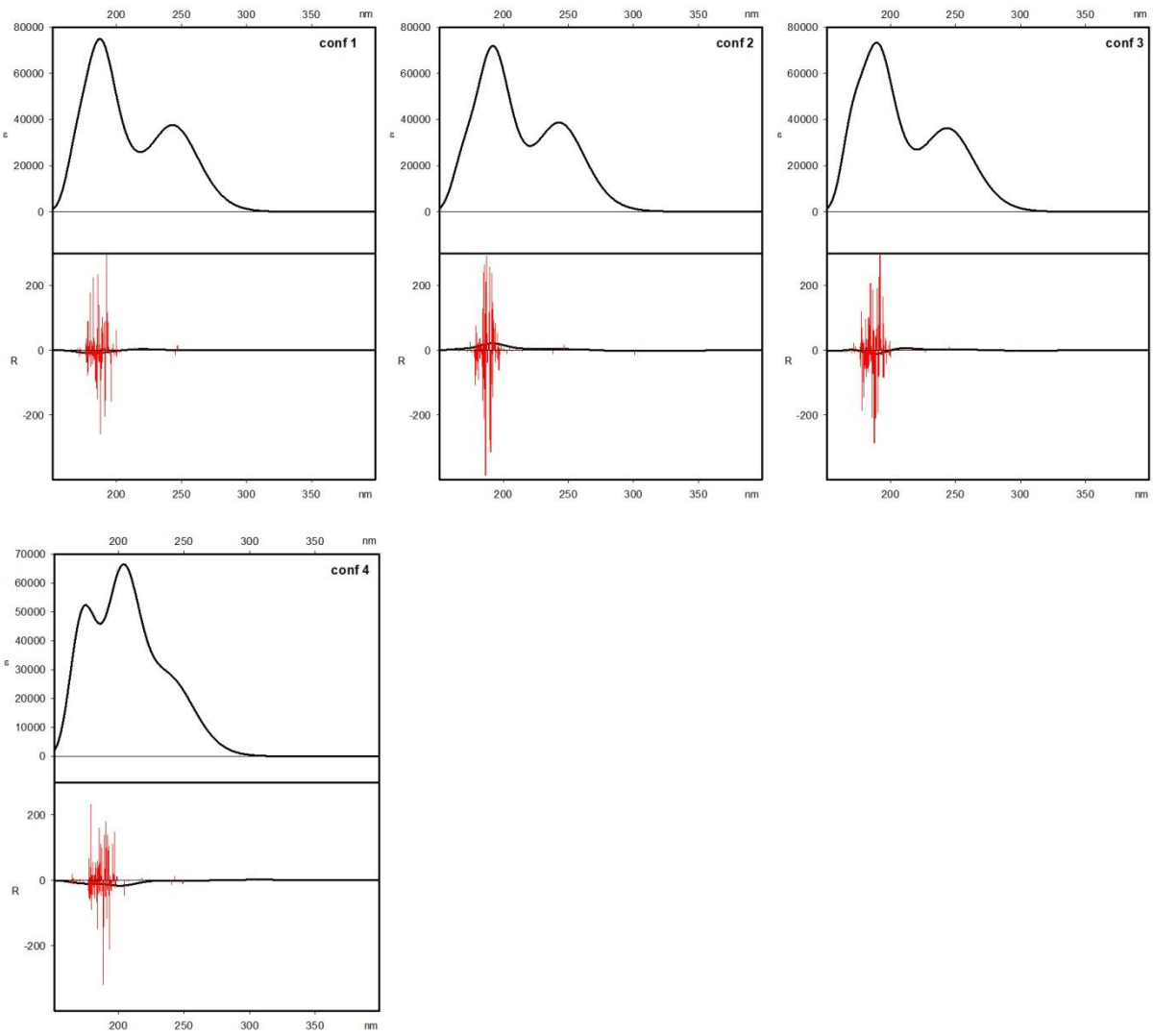


Figure SI_25. ECD spectra of the low-energy conformers of compound **7b** calculated at TD-M06-2X/6-311++G(d,p) level for structures optimized at B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

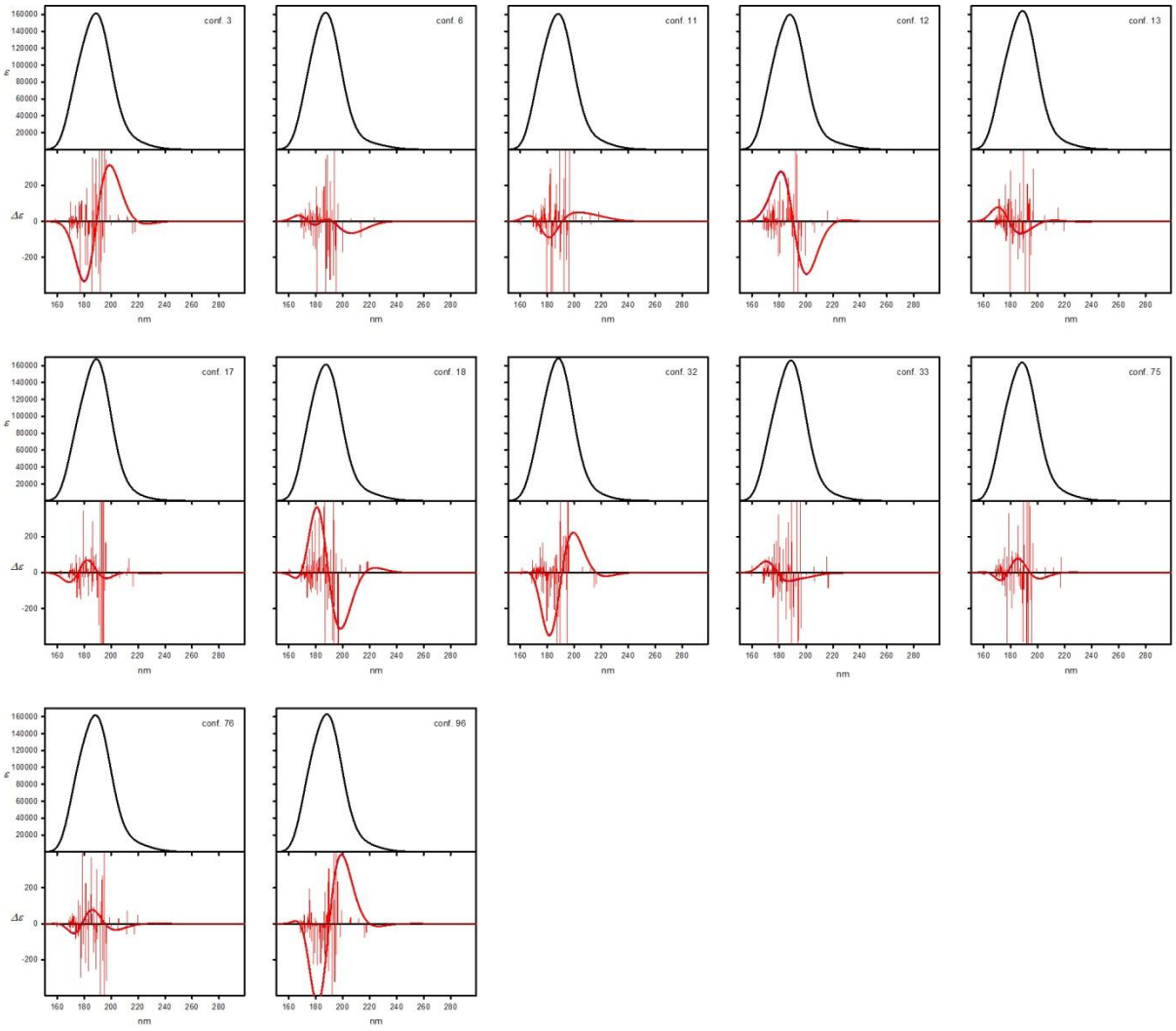


Figure SI_26. ECD spectra of the low-energy conformers of compound **3b** calculated at IEFPCM/TD-CAM-B3LYP/6-311++G(d,p) level for structures optimized at IEFPCM/B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

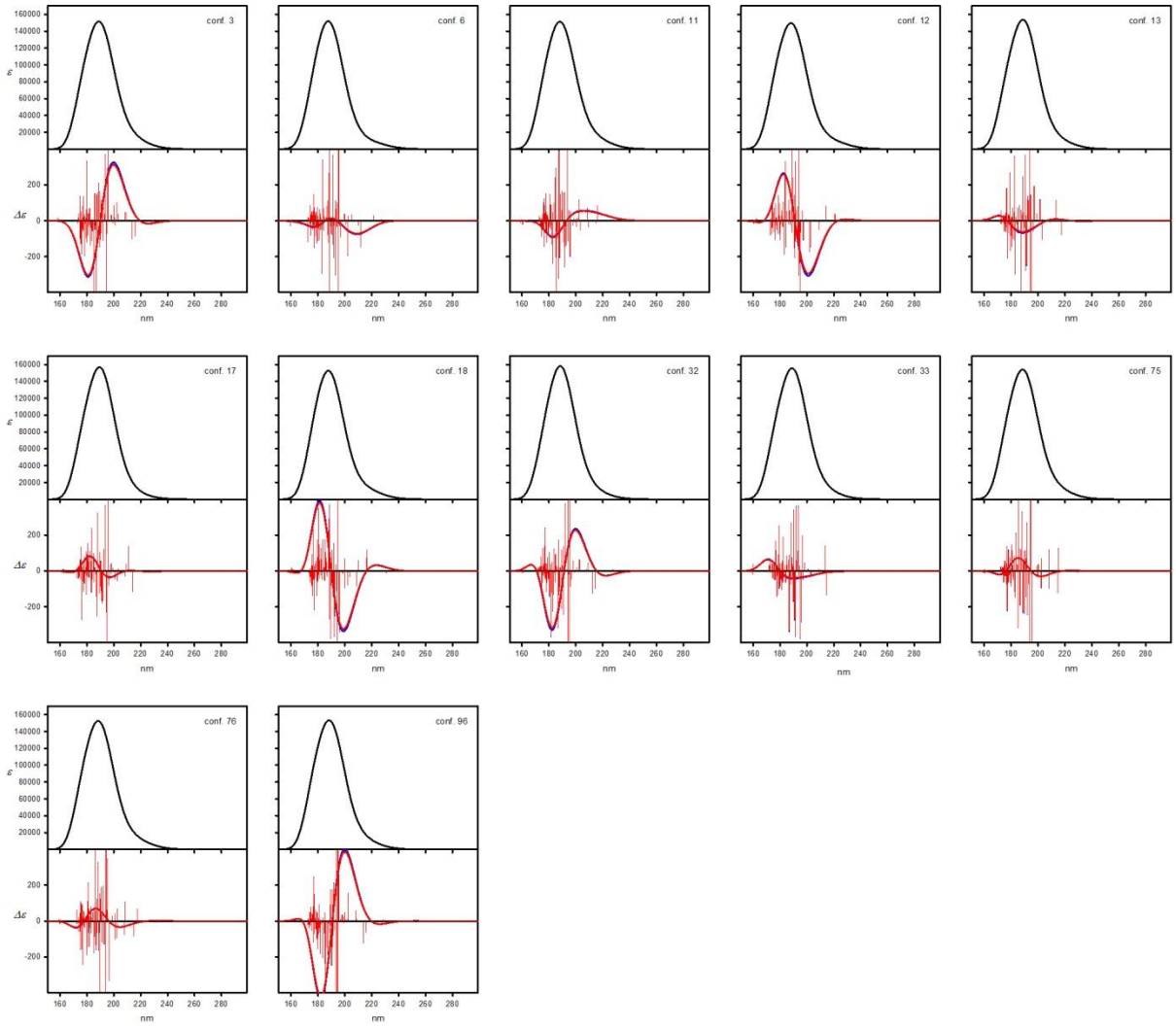


Figure SI_27. ECD spectra of the low-energy conformers of compound **3b** calculated at IEFPCM/TD-M06-2X/6-311++G(d,p) level for structures optimized at IEFPCM/B3LYP/6-311++G(d,p) level. Wavelengths have not been corrected.

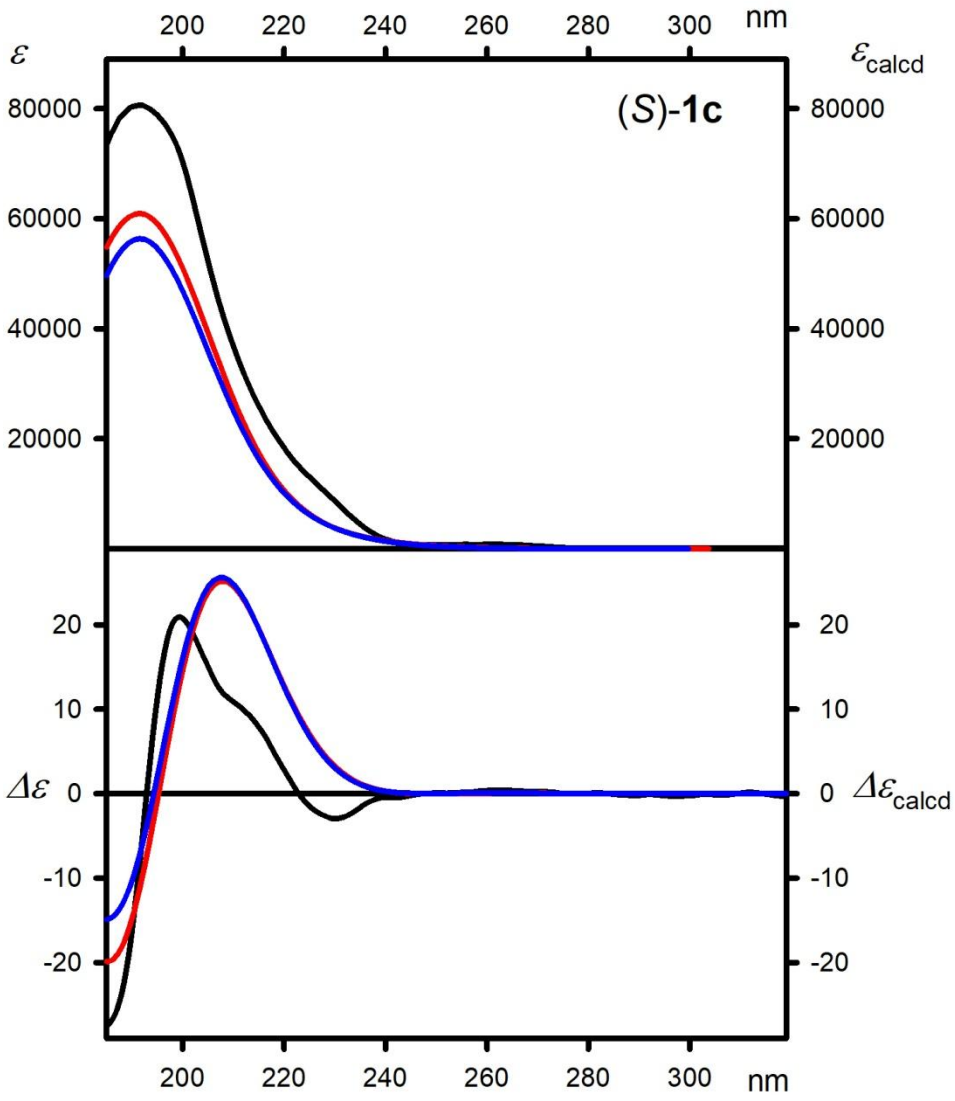


Figure S_28. UV (upper panel) and ECD (lower panel) spectra of **1c**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

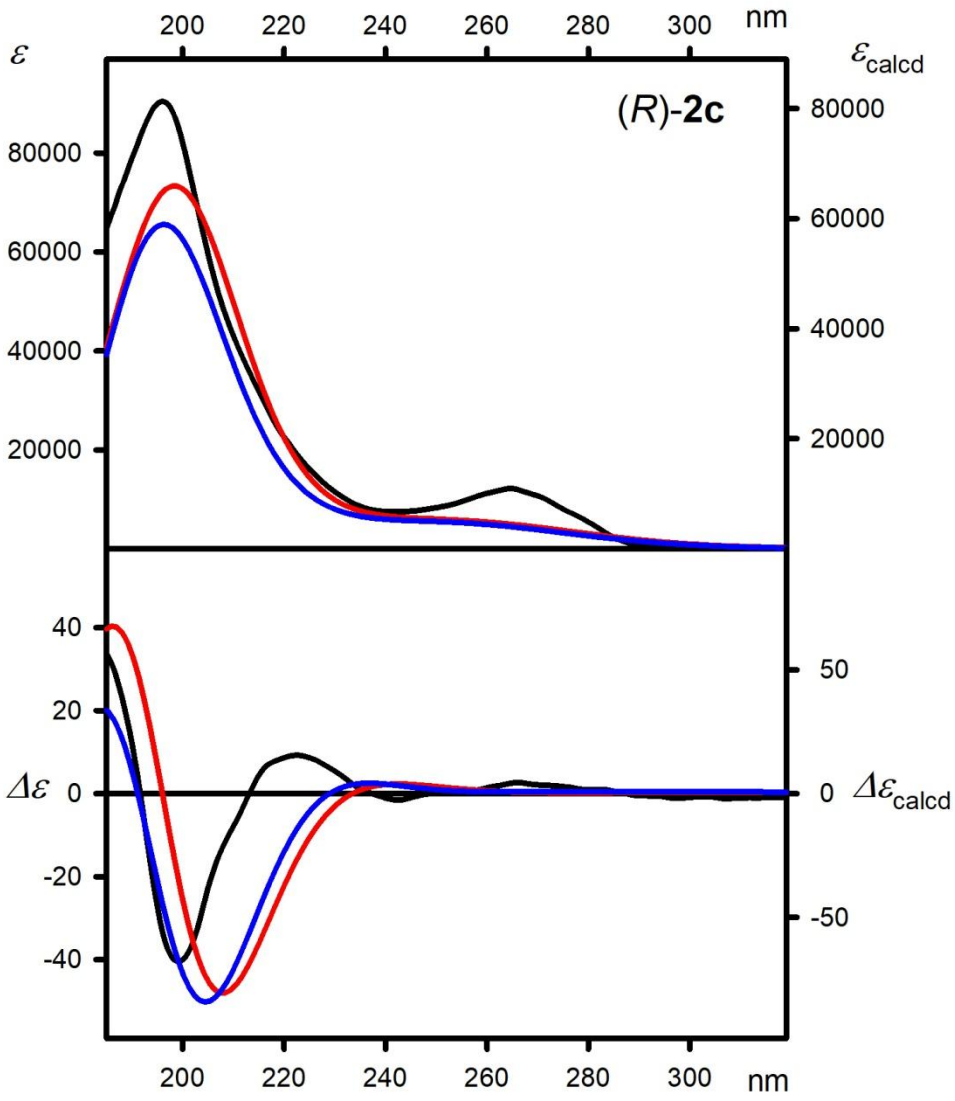


Figure S_29. UV (upper panel) and ECD (lower panel) spectra of **2c**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

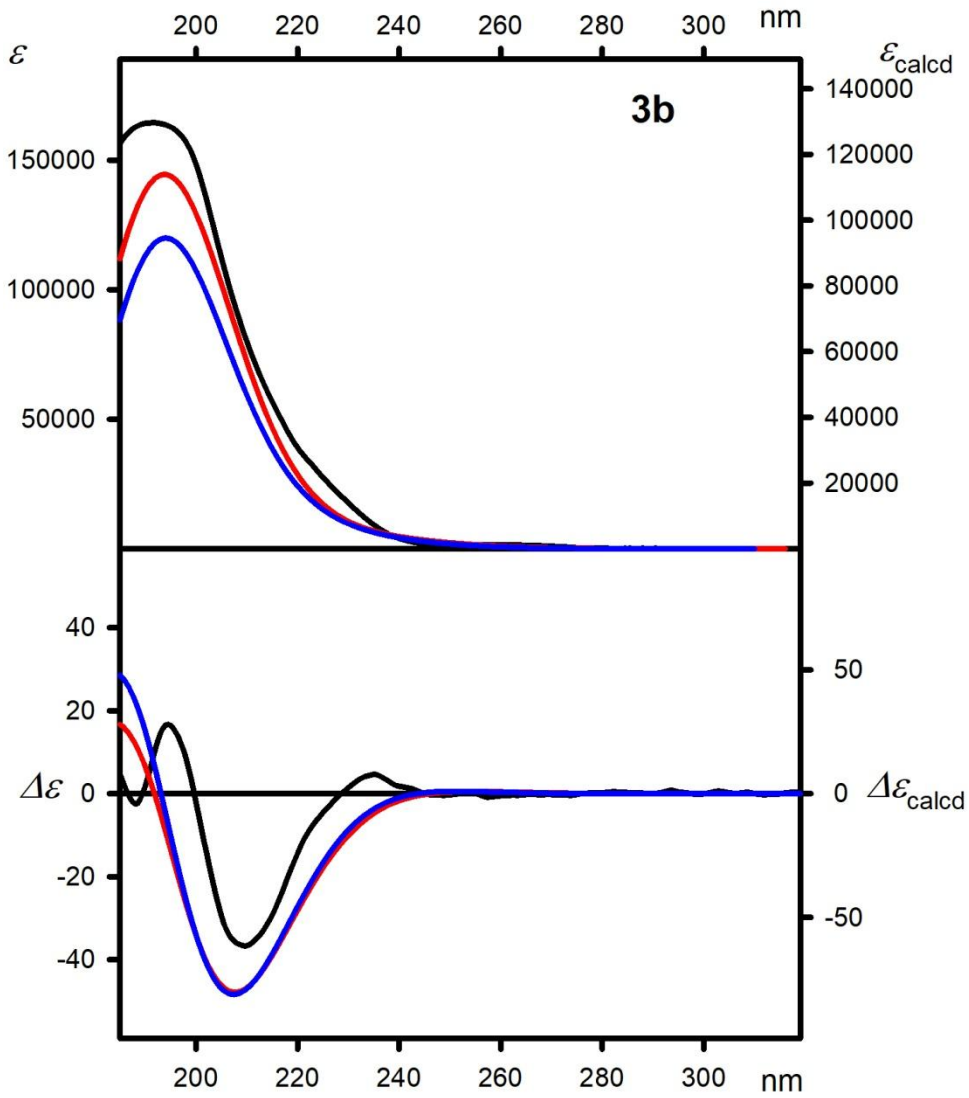


Figure S_30. UV (upper panel) and ECD (lower panel) spectra of **3b**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

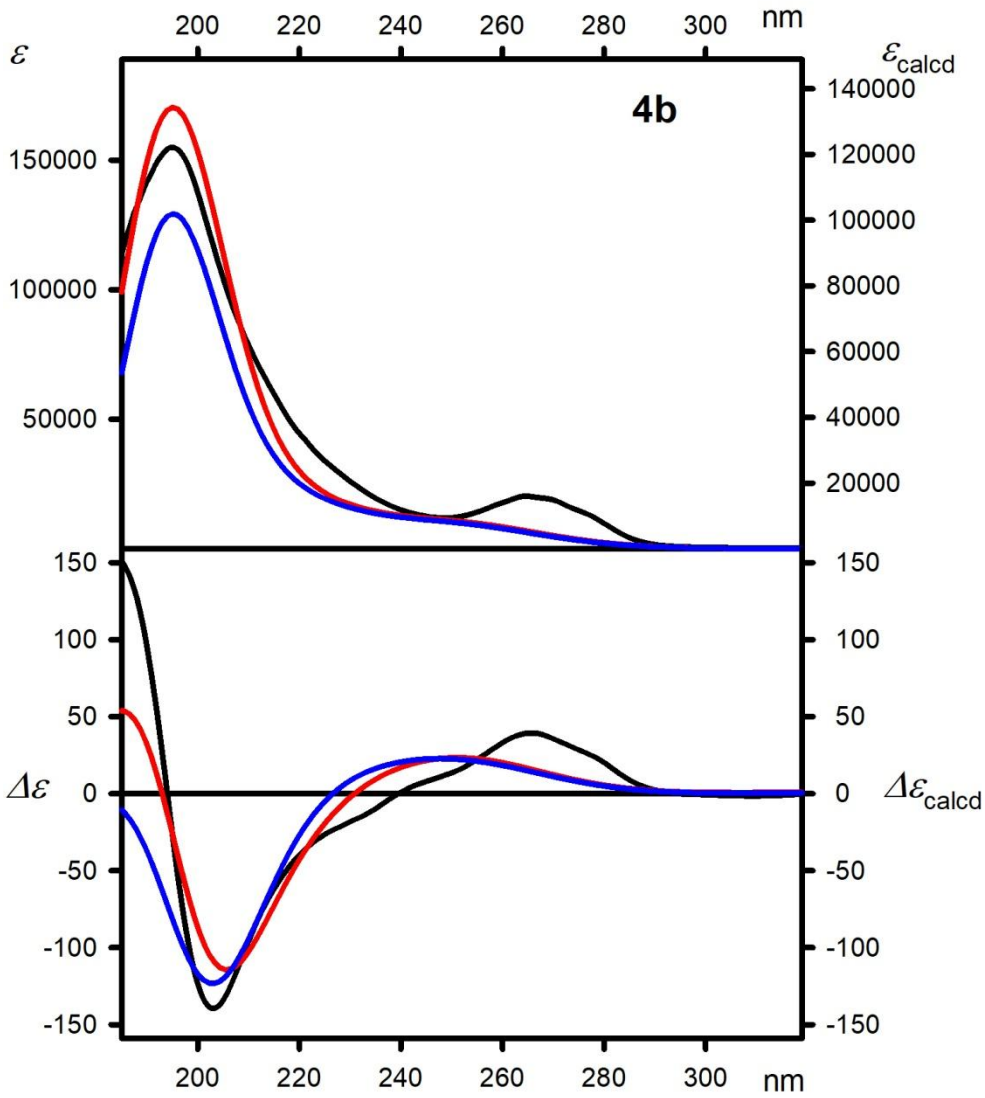


Figure S_31. UV (upper panel) and ECD (lower panel) spectra of **4b**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

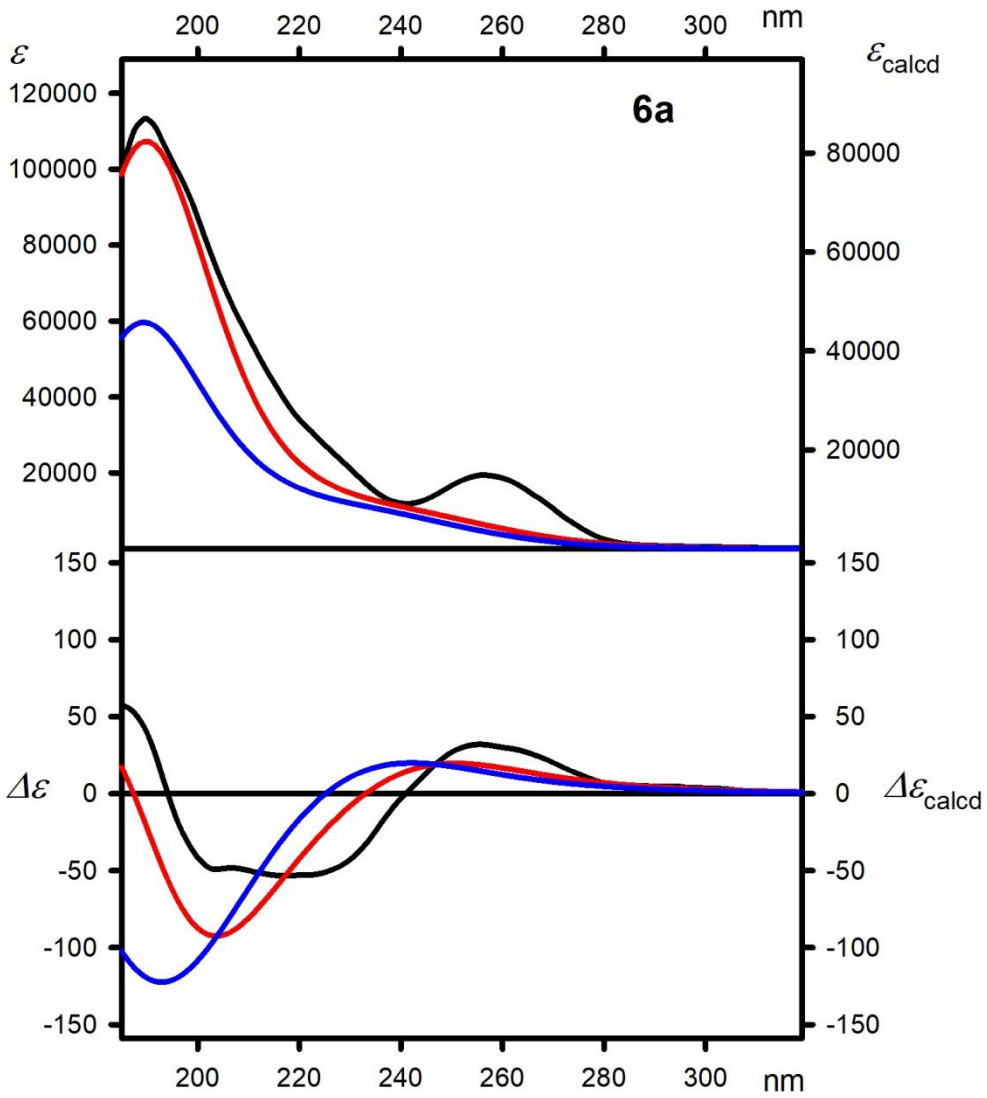


Figure S_32. UV (upper panel) and ECD (lower panel) spectra of **6a**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

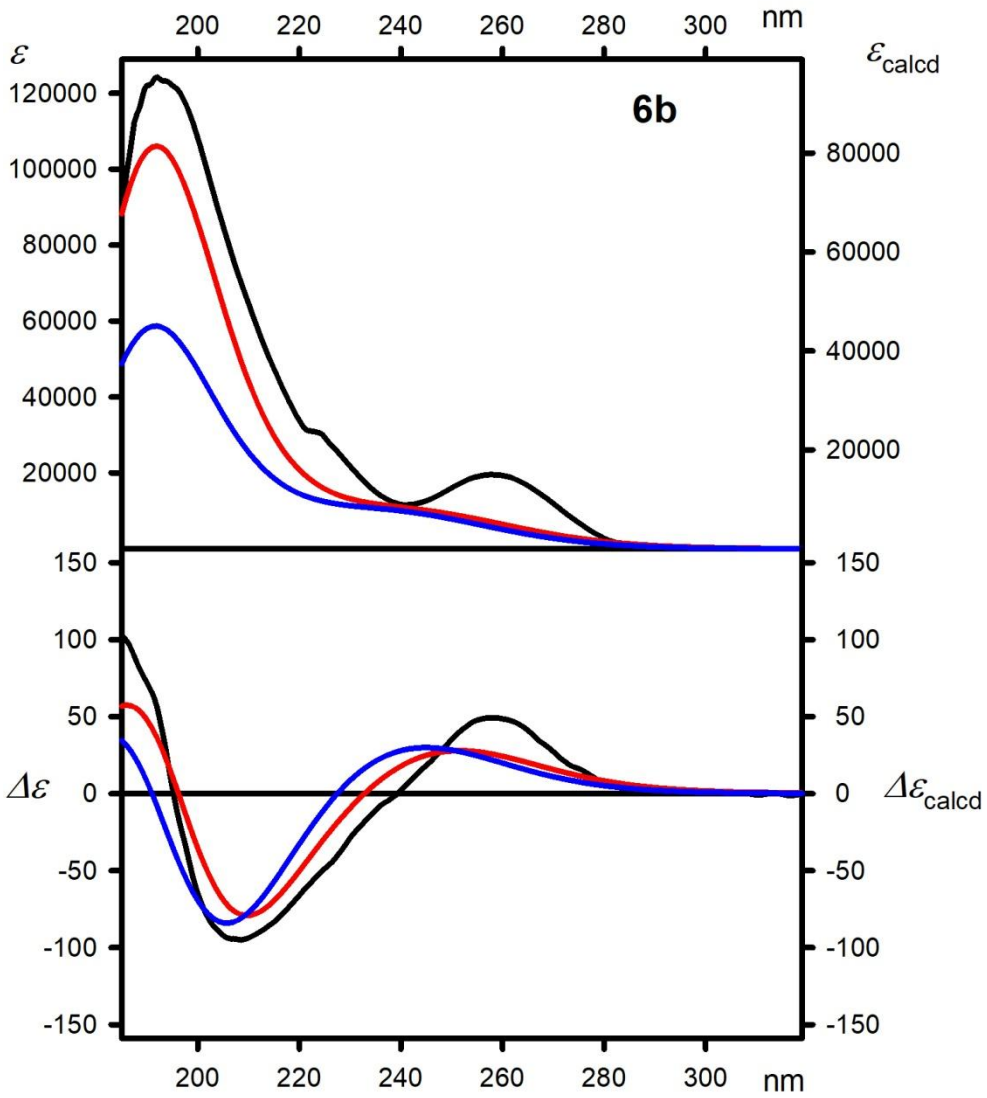


Figure S_33. UV (upper panel) and ECD (lower panel) spectra of **6b**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

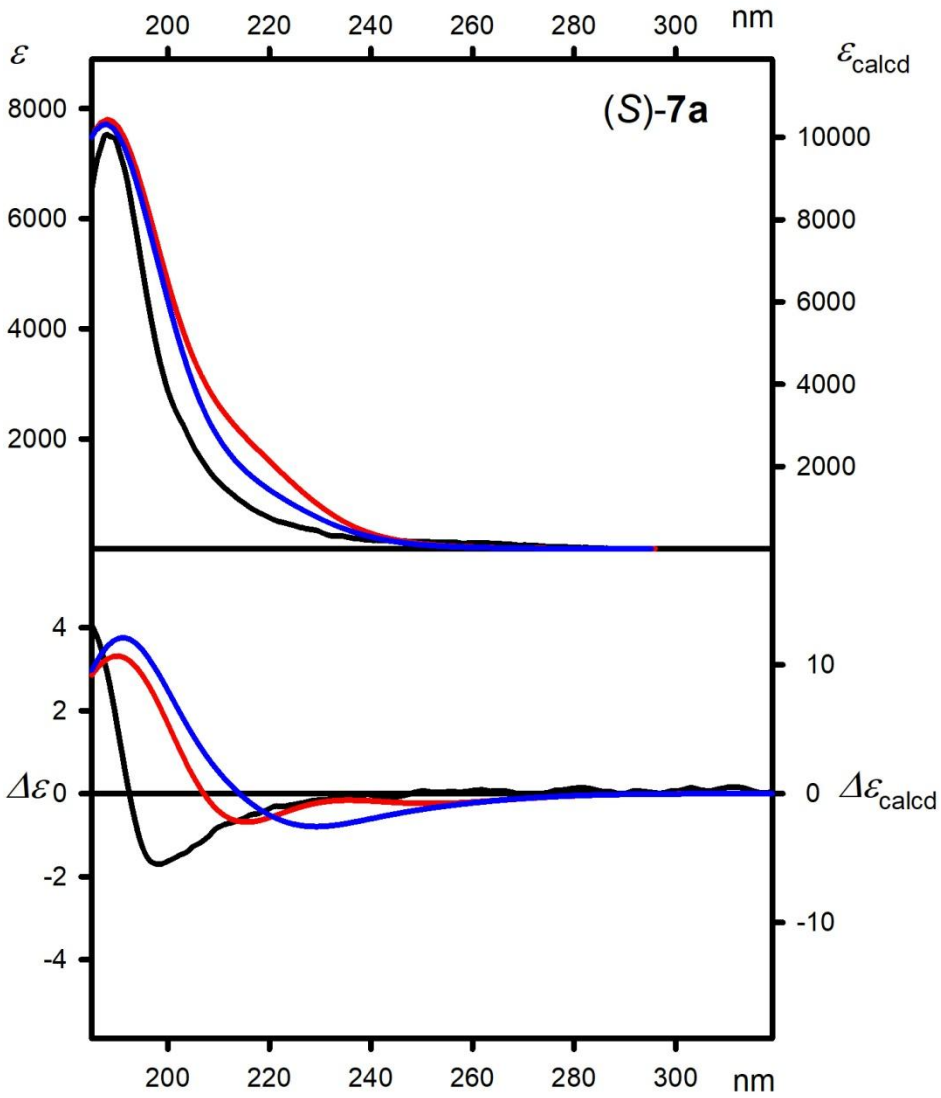


Figure S_34. UV (upper panel) and ECD (lower panel) spectra of **7a**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

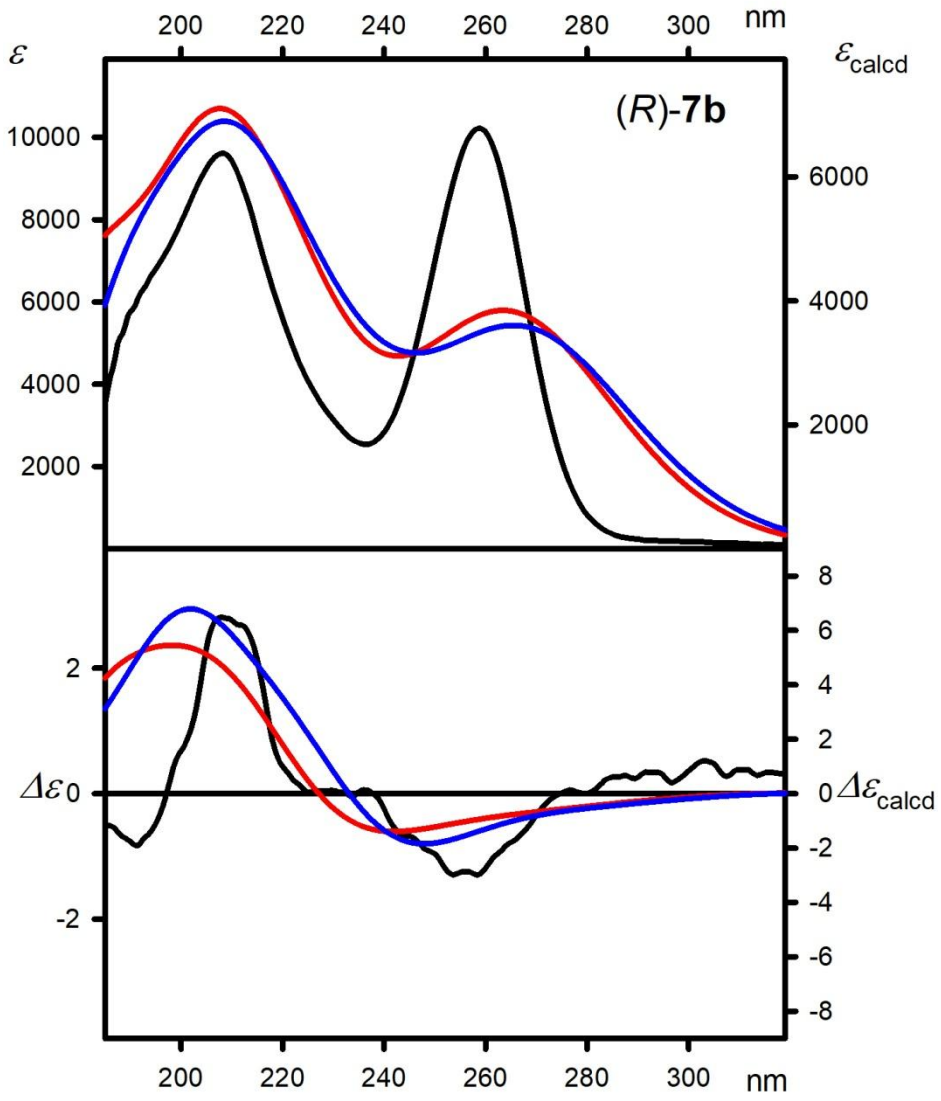


Figure S_35. UV (upper panel) and ECD (lower panel) spectra of **7b**, measured in cyclohexane (solid black line), calculated at TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

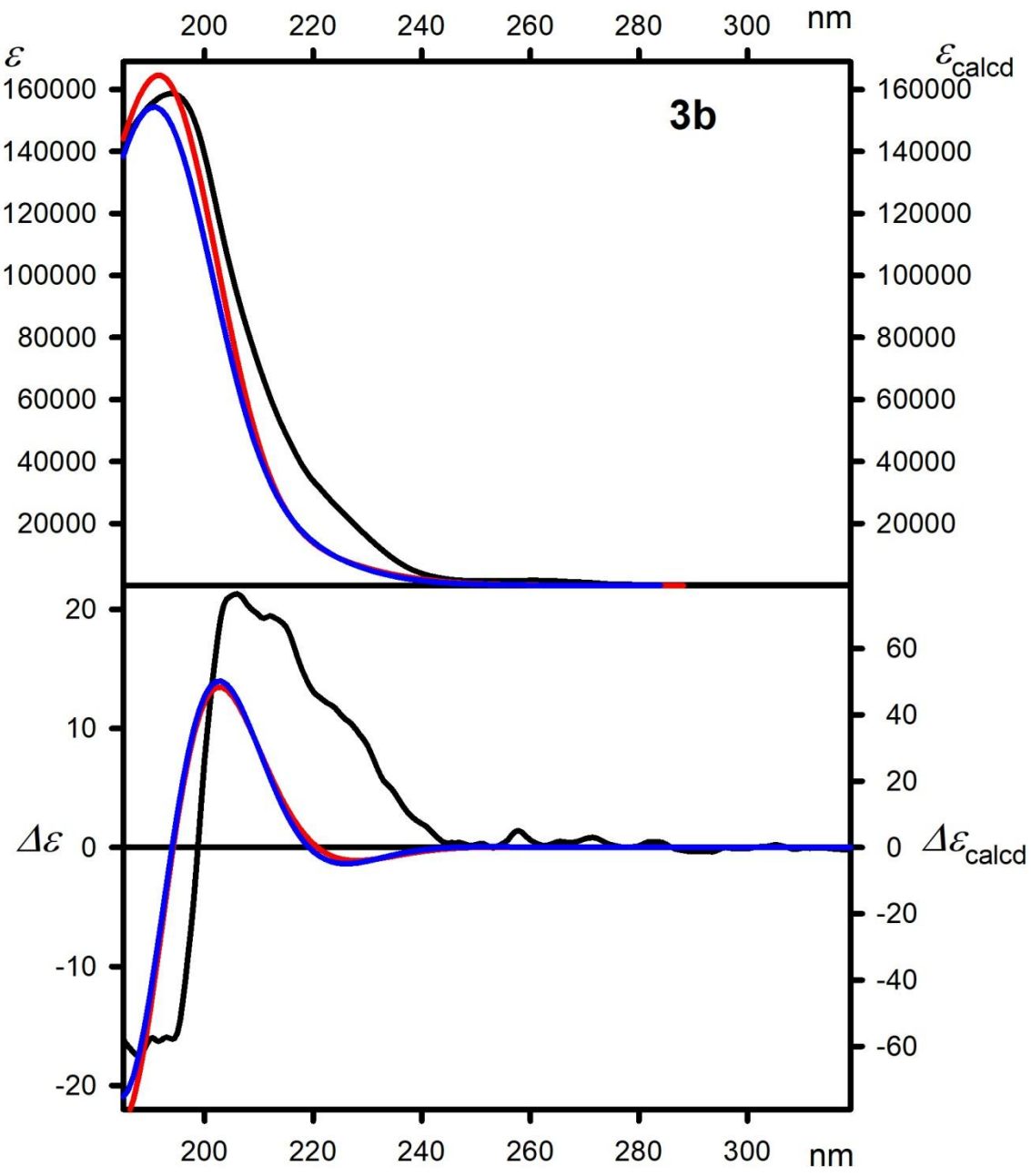


Figure S_36. UV (upper panel) and ECD (lower panel) spectra of **3b**, measured in acetonitrile (solid black line), calculated at IEFPCM/TD-CAM-B3LYP/6-311++G(d,p) level and *ΔΔG*-based (solid red lines) and calculated at IEFPCM/TD-M06-2X/6-311++G(d,p) level and *ΔΔG*-based (solid blue lines). Wavelengths have been corrected to match experimental UV maximum.

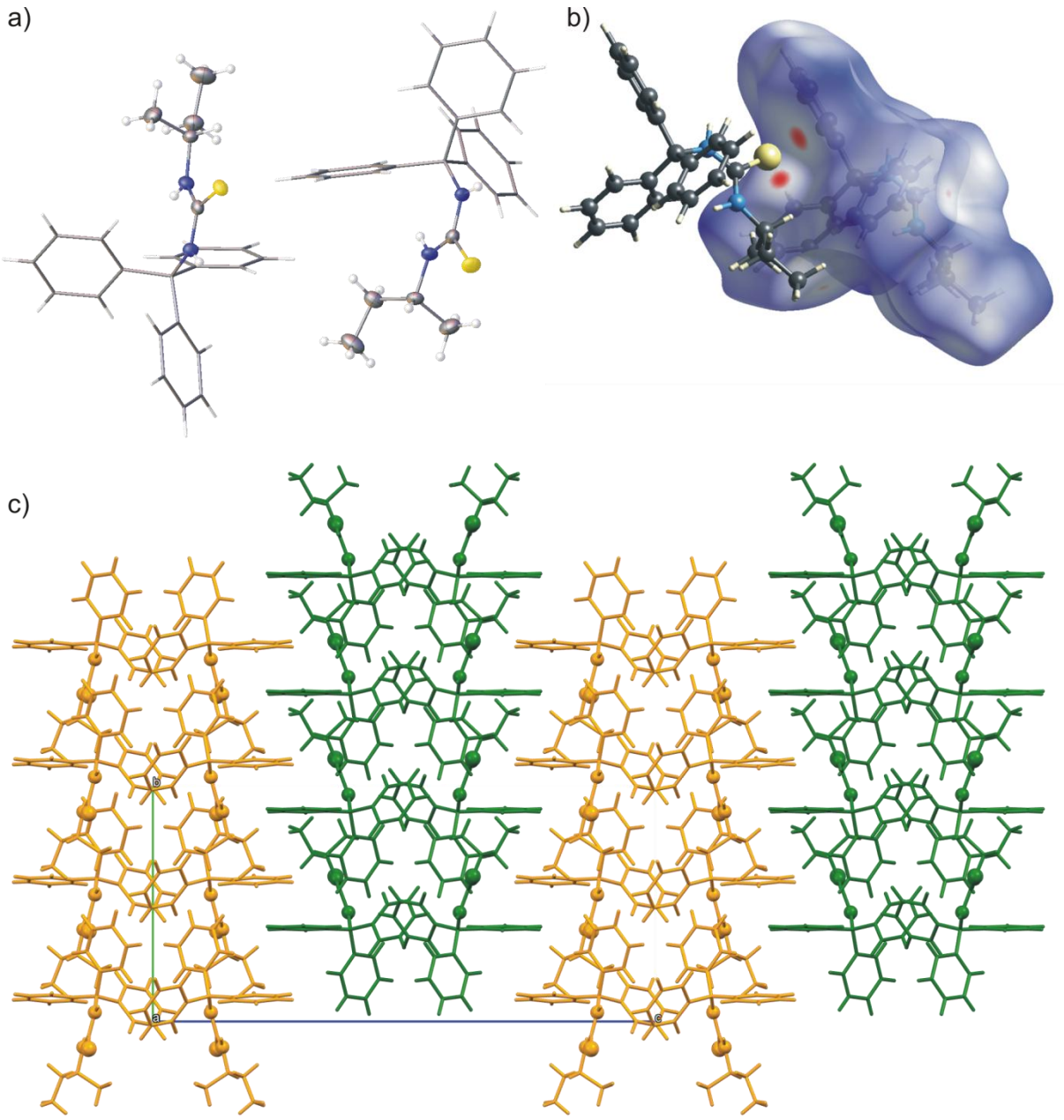


Figure SI_37. a) The molecular structure of **2a**. Displacement ellipsoids are drawn at 50% probability level, trytyl groups are shown as stick model for clarity; b) Hirshfeld surface mapped over d_{norm} displaying the intermolecular interactions; c) molecular packing in crystal structure of compound **2a** (view along a axis), symmetrically independent molecules are indicated with different colors, the S and N atoms are shown as balls.

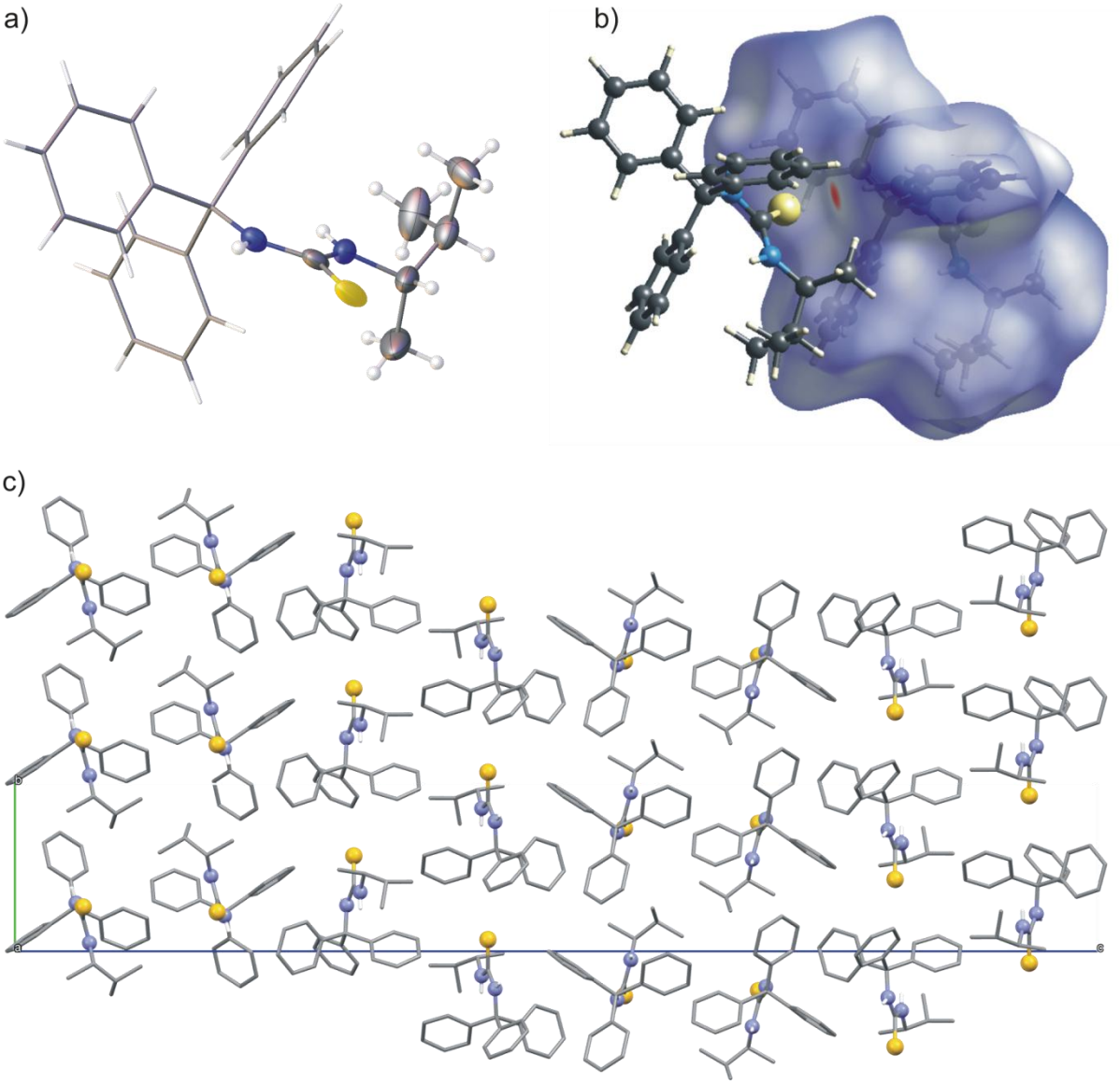


Figure SI_38. a) The molecular structure of **2b** (displacement ellipsoids are drawn at 50% probability level, trytyl group is shown as stick model for clarity); b) Hirshfeld surface mapped over d_{norm} displaying the intermolecular interactions; c) molecular packing in crystal structure of compound **2b** (view along a axis), the S and N atoms are shown as balls, C-bound hydrogen atoms have been omitted for clarity.

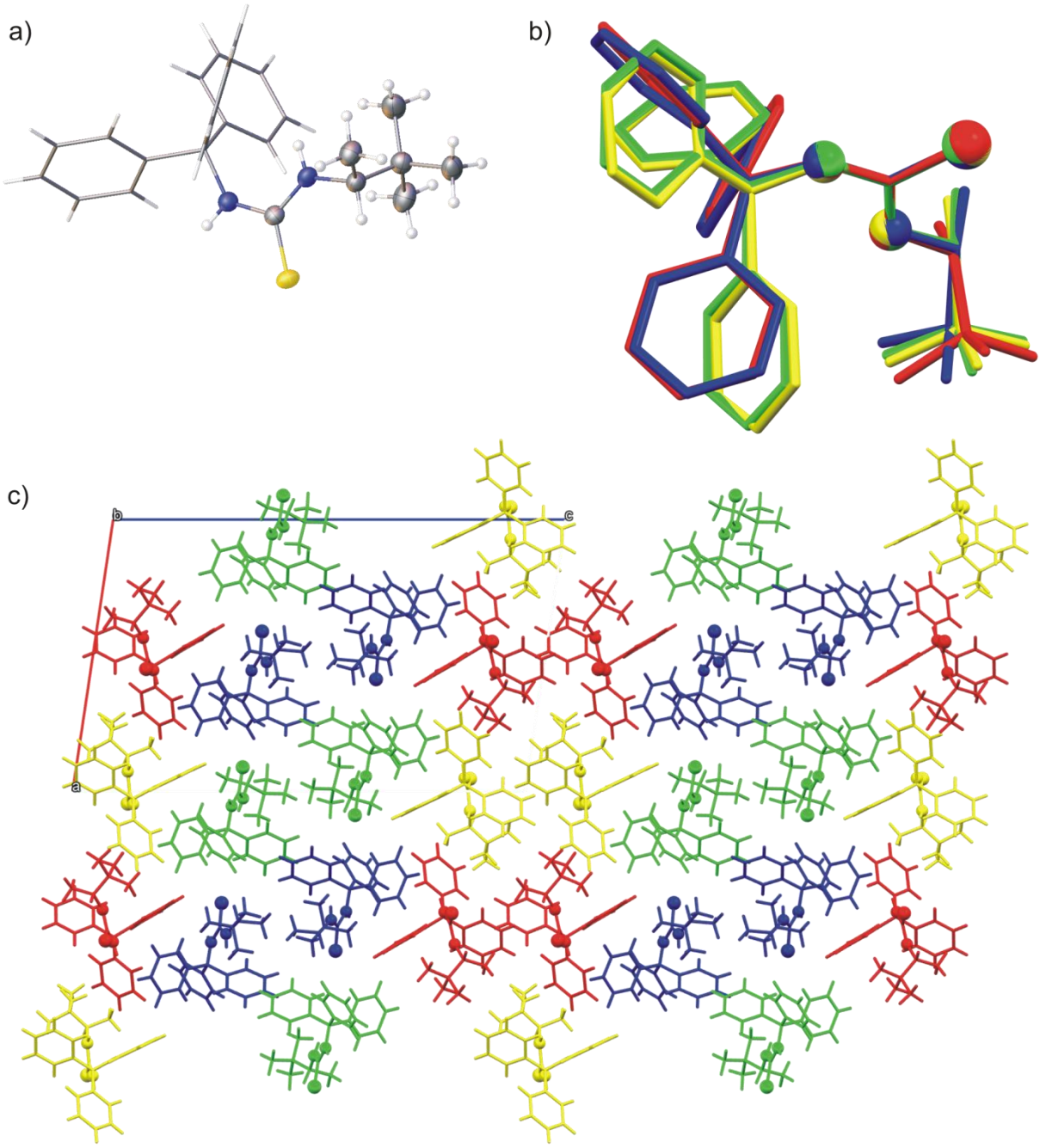


Figure SI_39. a) The molecular structure of selected symmetrically independent molecule of compound **2c**. Displacement ellipsoids are drawn at 50% probability level, trytyl group is shown as stick model for clarity; b) overlapping of symmetrically independent molecules of compound **2c** (green – molecule A, blue – molecule B, red – molecule C, yellow – molecule D), hydrogen atoms have been omitted for clarity; c) molecular packing in crystal structure of compound **2c** (view along b axis), symmetrically independent molecules are indicated with different colors, the S and N atoms are shown as balls.

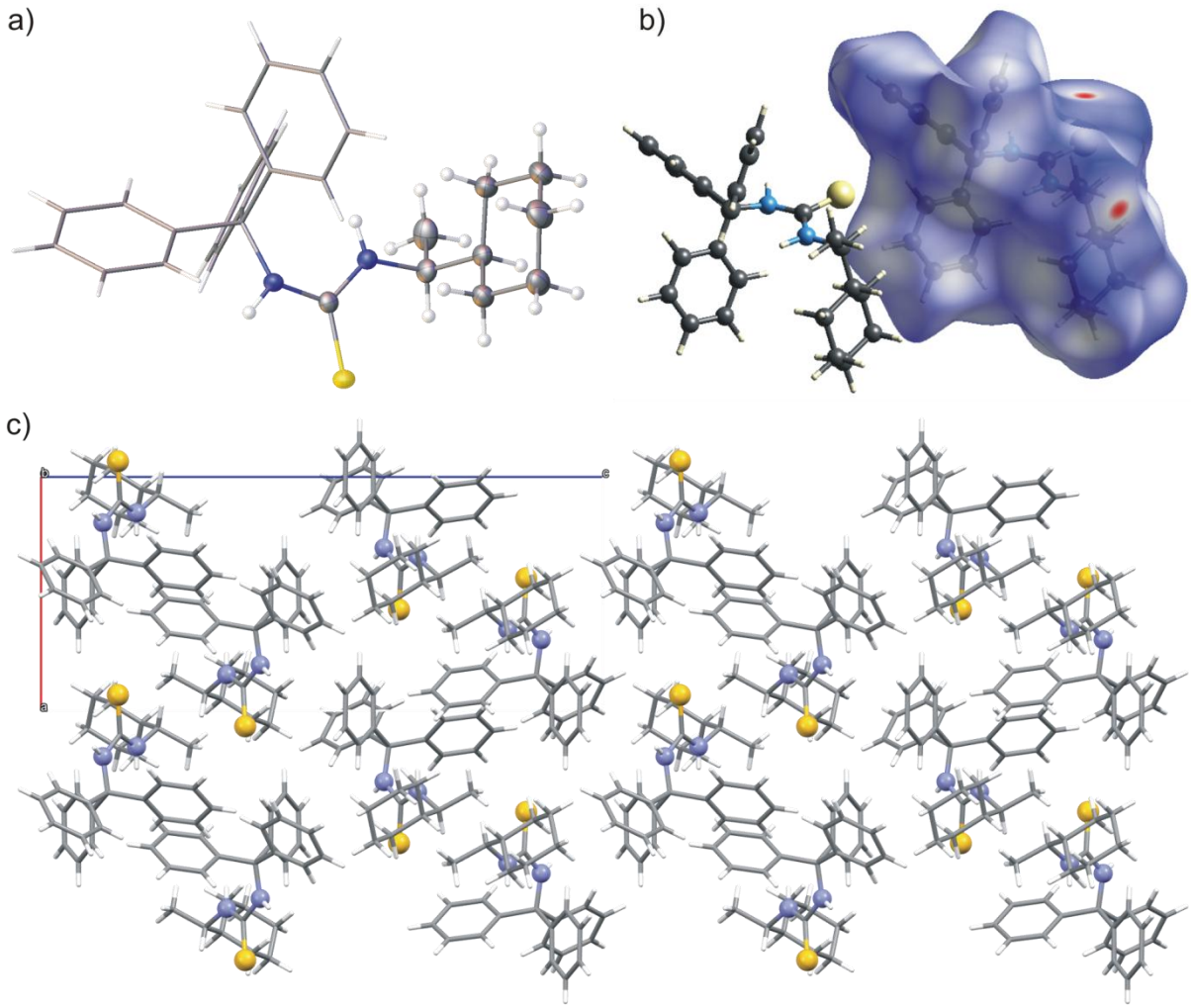


Figure SI_40. a) The molecular structure of **2d**. Displacement ellipsoids are drawn at 50% probability level, trytyl group is shown as stick model for clarity; b) Hirshfeld surface mapped over d_{norm} displaying the intermolecular interactions; c) molecular packing in crystal structure of compound **2d** (view along b axis), the S and N atoms are shown as balls, C-bound hydrogen atoms have been omitted for clarity.

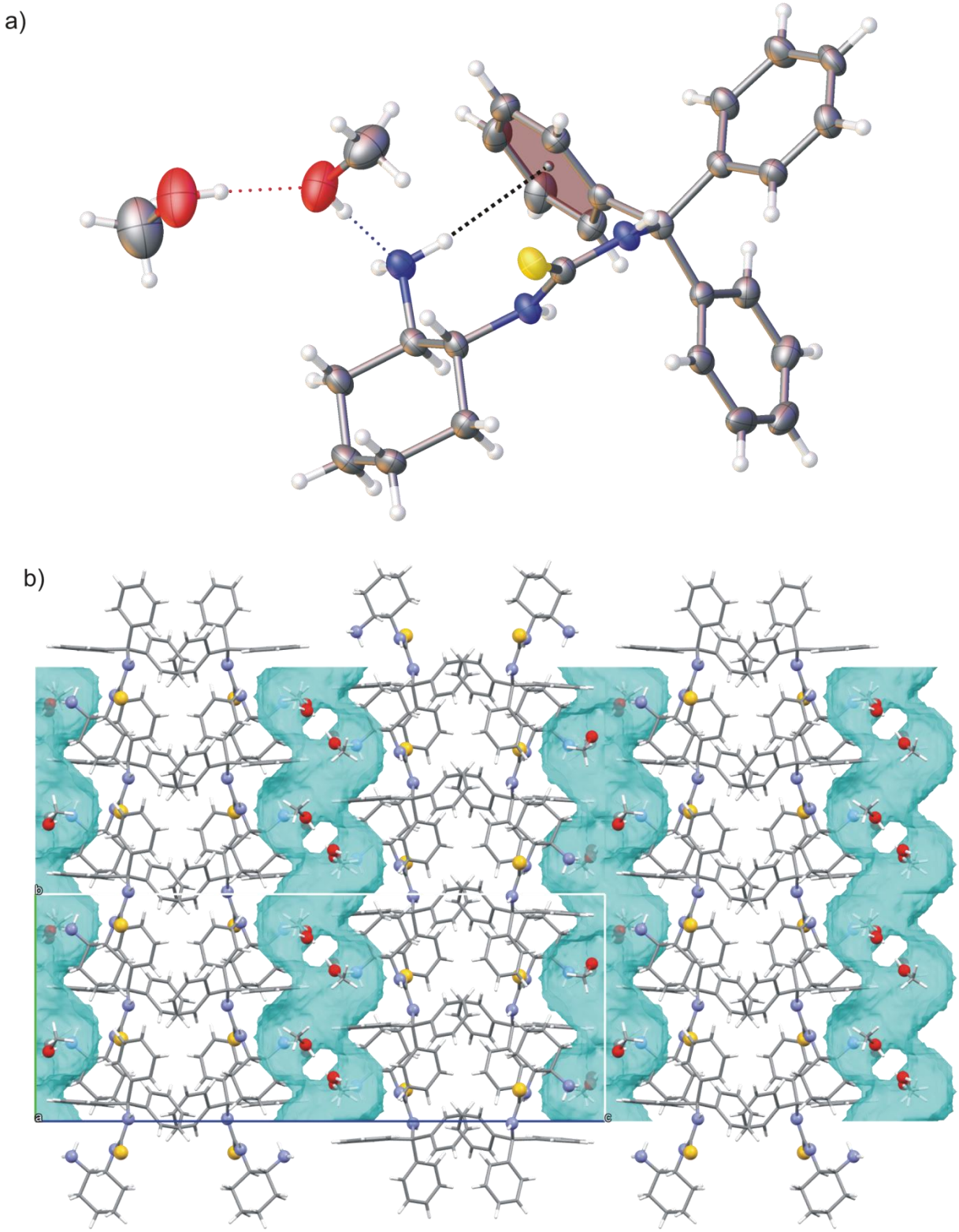


Figure SI_41. a) The molecular structure of asymmetric unit of **4a** solvate. Displacement ellipsoids are drawn at 50% probability level, hydrogen bonds are presented as dashed lines; b) molecular packing in crystal structure (view along a axis), the S, N and O atoms are shown as balls, the area accessible for the solvent molecules is marked with the blue surface.

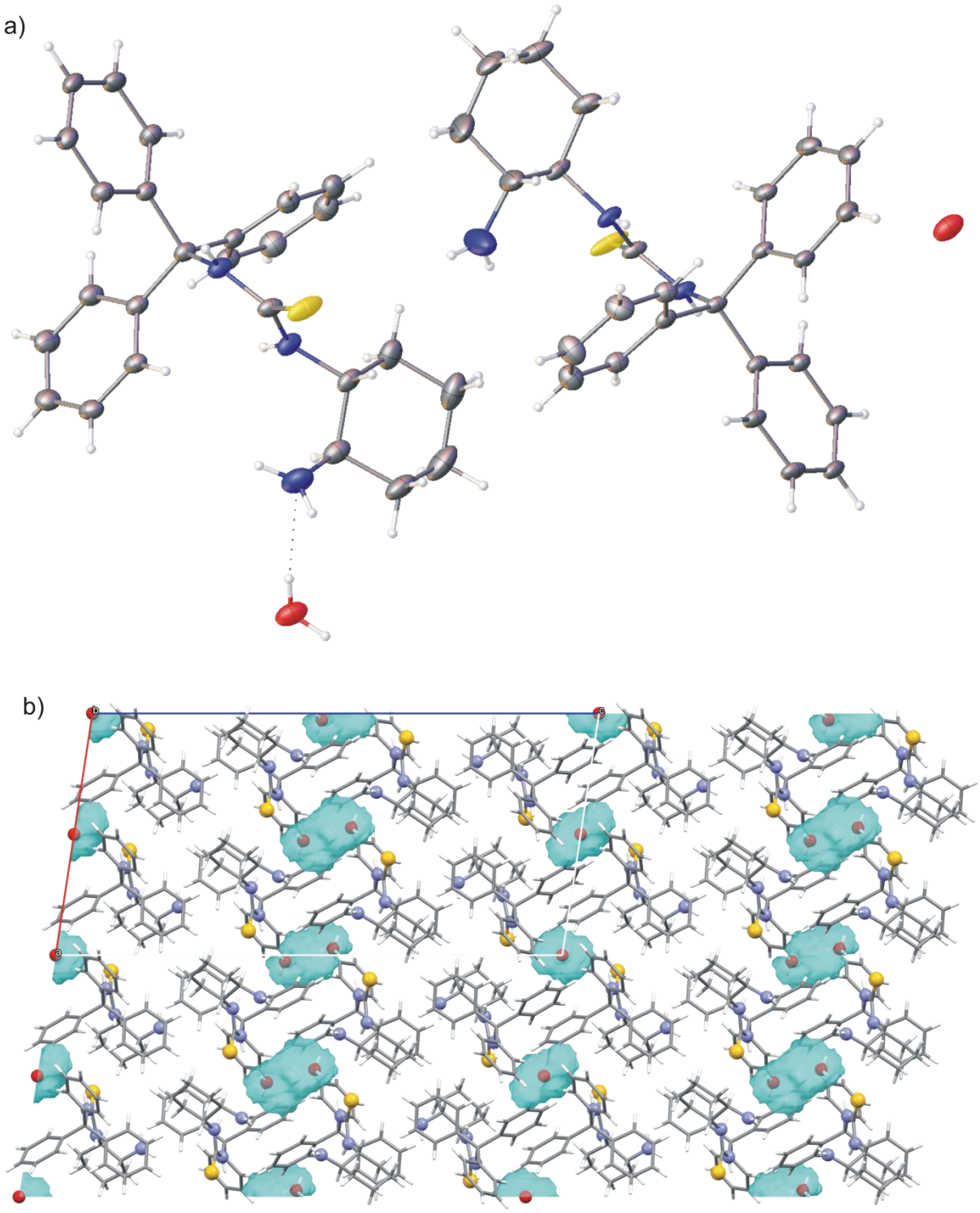


Figure SI_42. a) The molecular structure of asymmetric unit of **4a** hydrate. Displacement ellipsoids are drawn at 50% probability level, hydrogen bond is presented as dashed lines; b) molecular packing in crystal structure (view along b axis), the S, N and O atoms are shown as balls, the area accessible for the solvent molecules is marked with the blue surface.

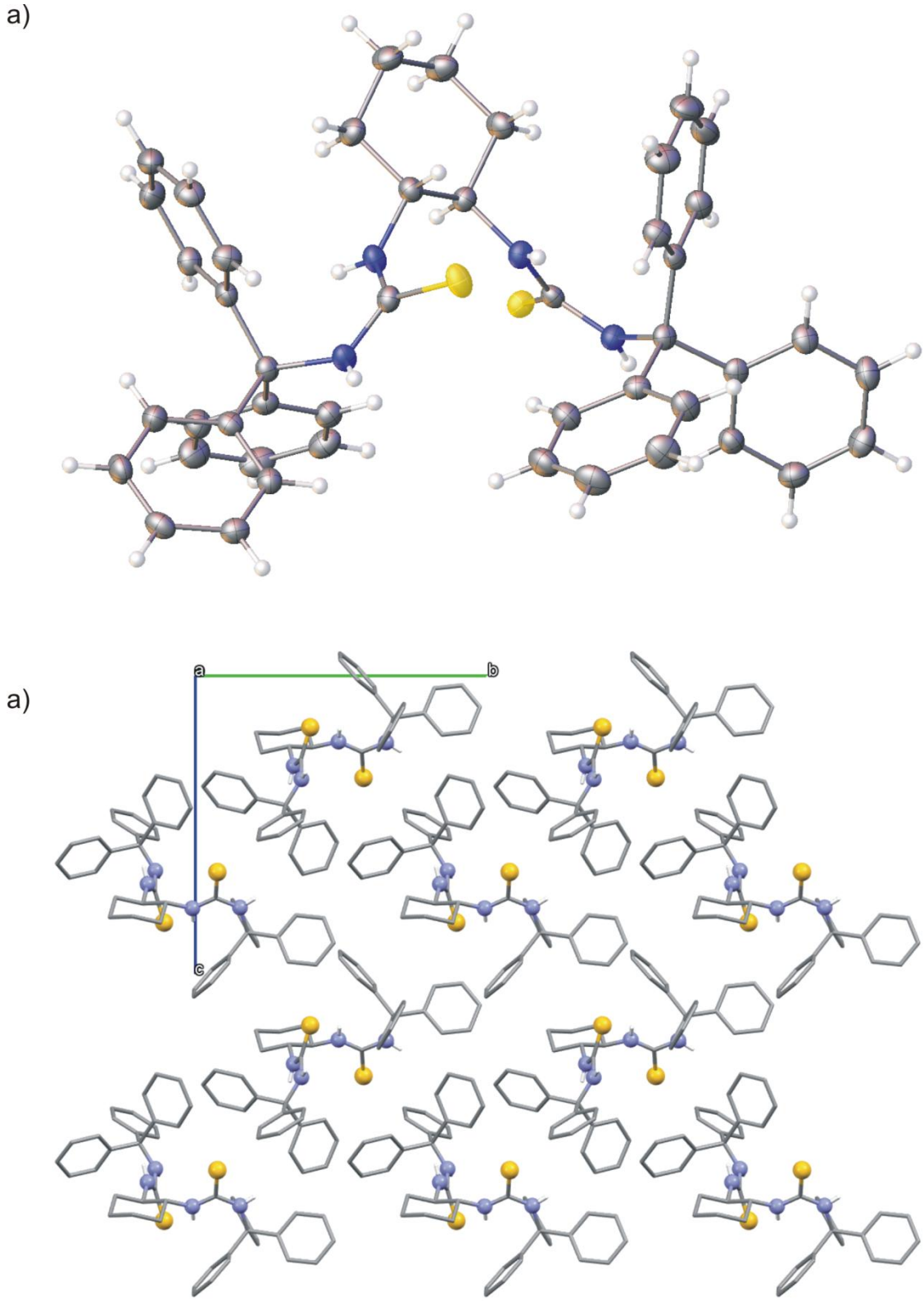


Figure SI_43. a) The molecular structure of **4b**. Displacement ellipsoids are drawn at 50% probability level; b) molecular packing in the crystal structure (view along a axis), the S and N atoms are shown as balls.

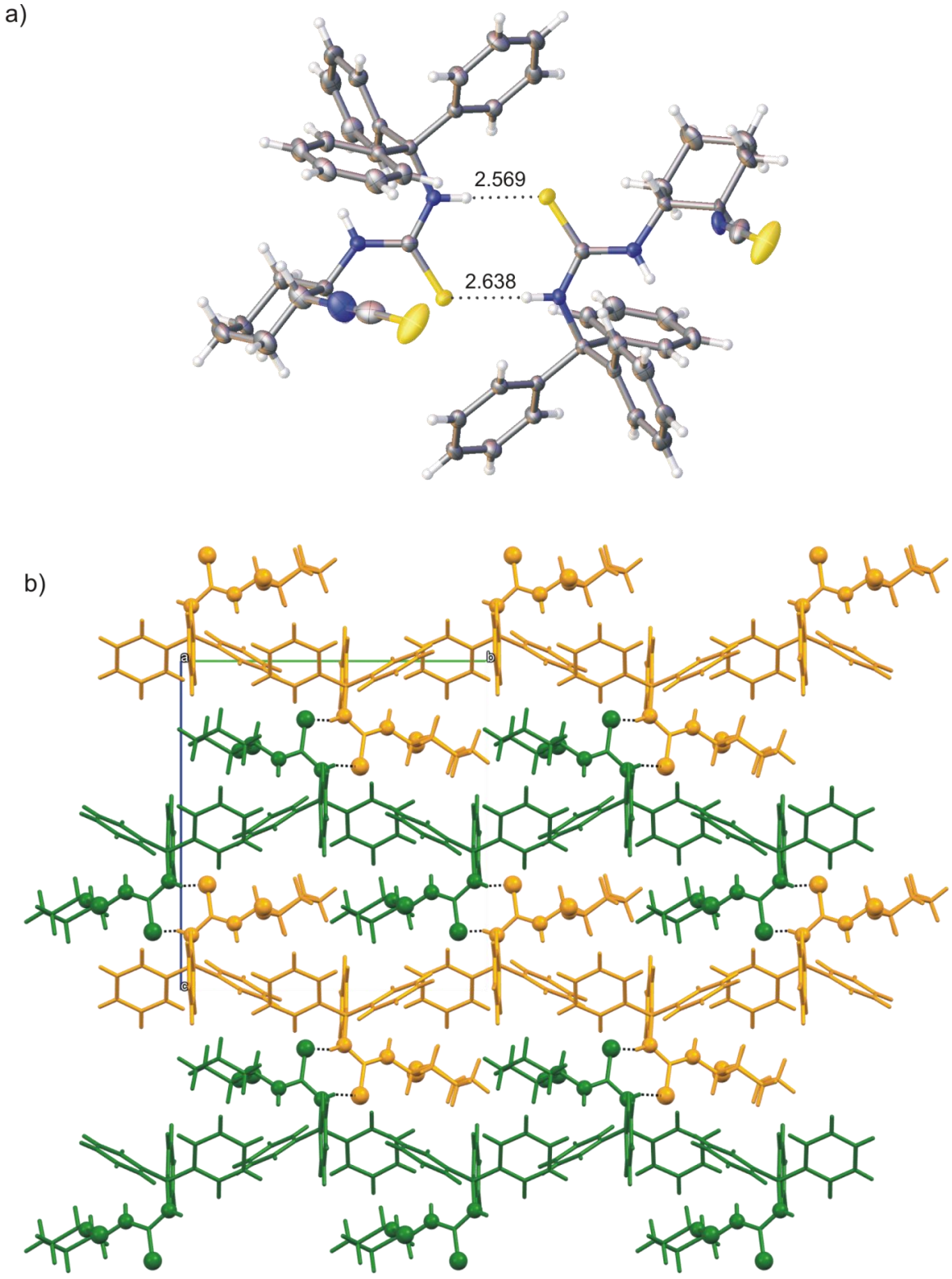


Figure SI_44. a) The molecular structure of **5**. Displacement ellipsoids are drawn at 50% probability level; hydrogen bonds are presented as dashed lines b) molecular packing in crystal structure of compound (view along a axis), the S and N atoms are shown as balls, hydrogen bonds are presented as dashed lines.

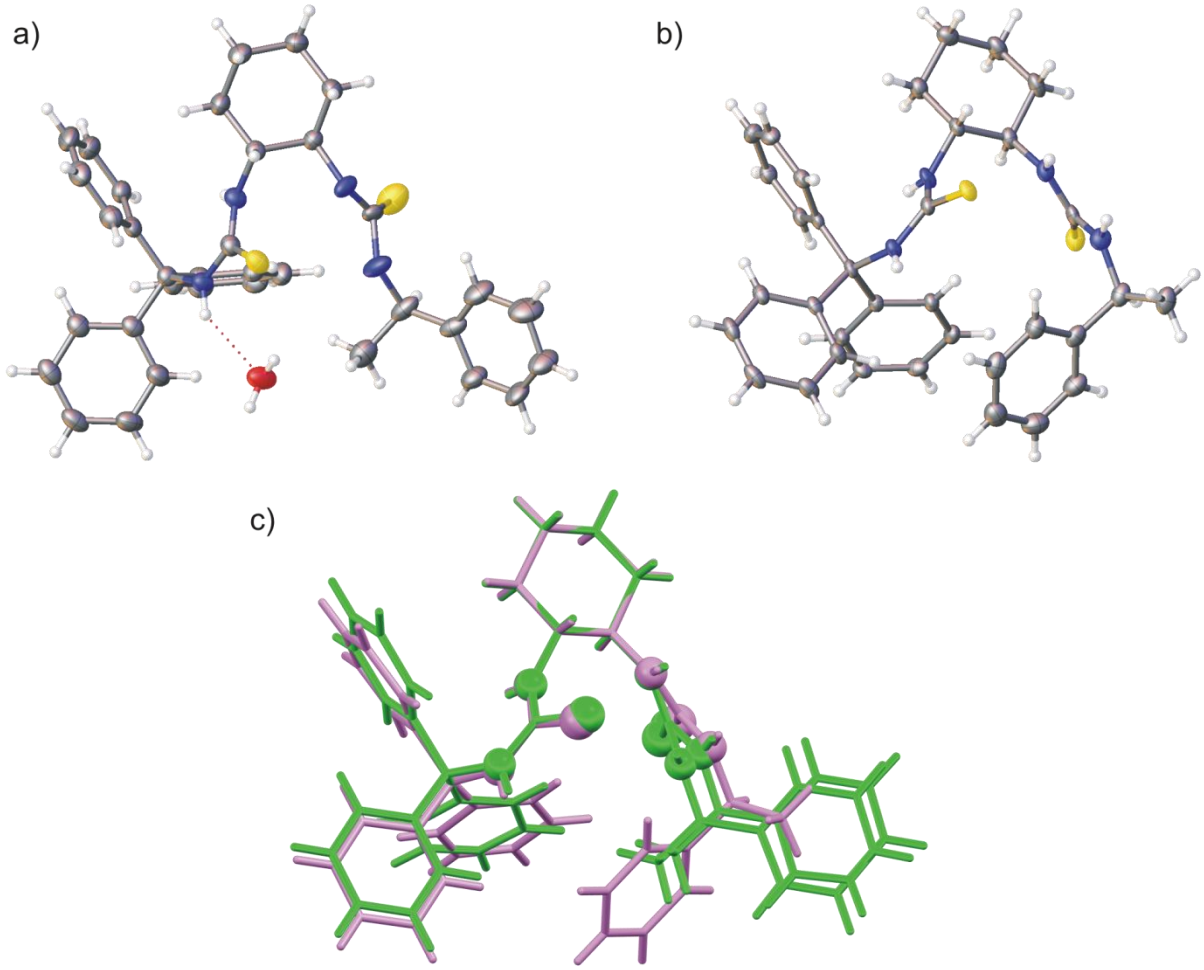


Figure SI_45. The molecular structure of a) compound **6a** and b) compound **6b**. Displacement ellipsoids are drawn at 50% probability level, hydrogen bond is presented as dashed line. c) Overlapping of molecules of compound **6a** (green; molecule is disordered over two positions) and compound **6b** (pink). The S and N atoms are shown as balls.

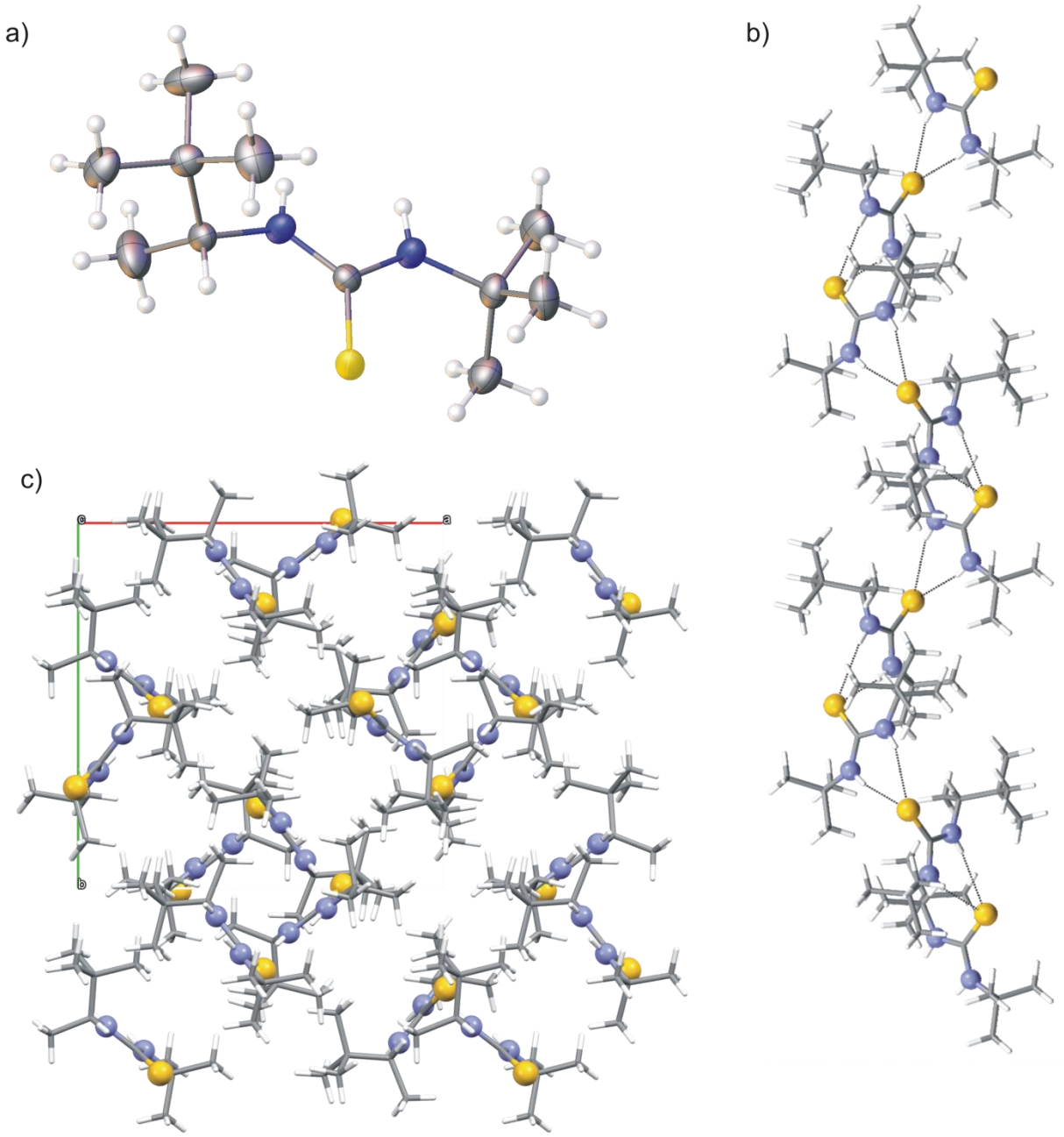


Figure SI_46. a) The molecular structure of **7b**. Displacement ellipsoids are drawn at 50% probability level, b) molecular ribbon twisted around four-fold axis, hydrogen bonds are presented as dashed lines; c) molecular packing in crystal structure of compound **7b** (view along c axis), the S and N atoms are shown as balls.

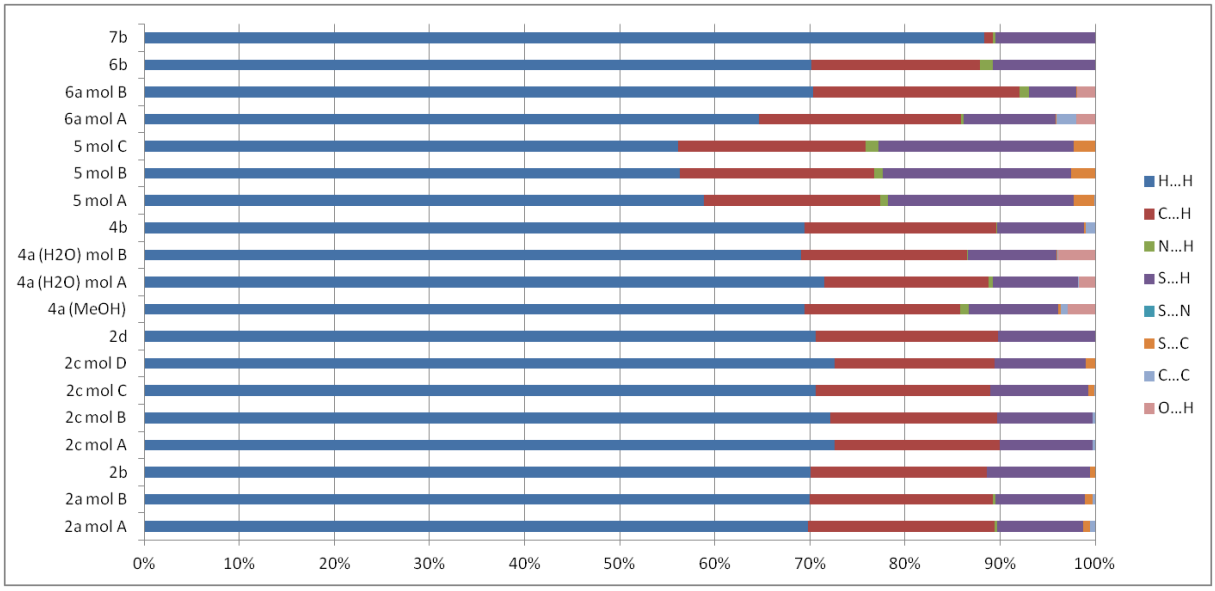


Figure SI_47. Contribution to the Hirshfeld surface area for various intermolecular interactions for molecules in crystal structures of compounds **2a**-**2d**, **4a**, **4b**, **5**, **6a**, **6b** and **7b**.

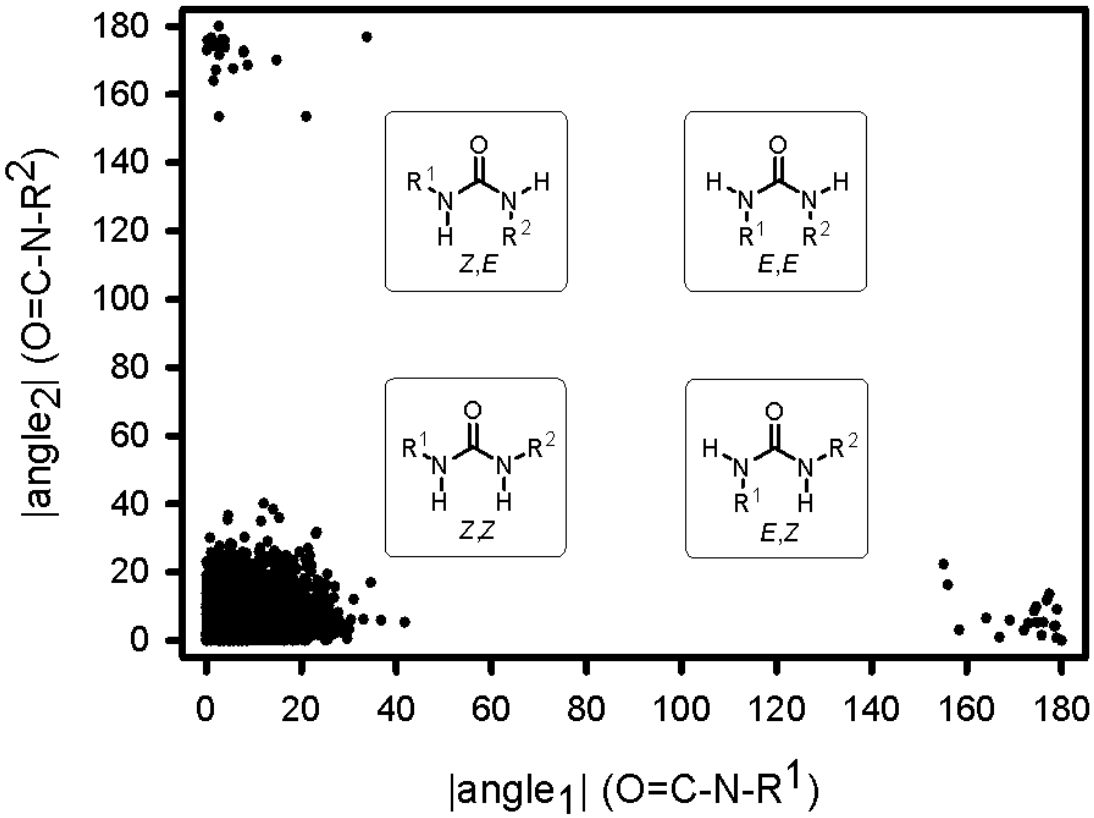
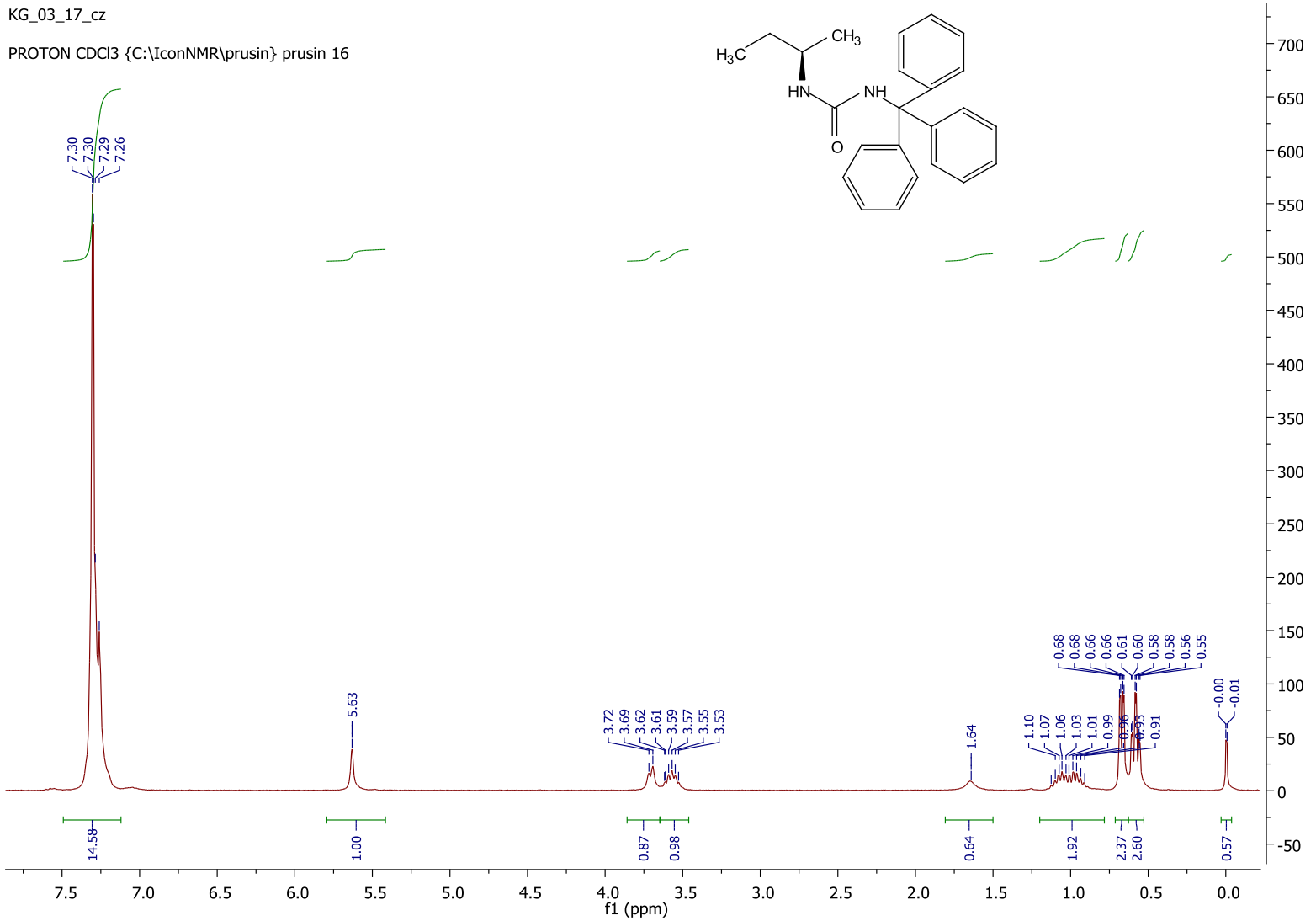
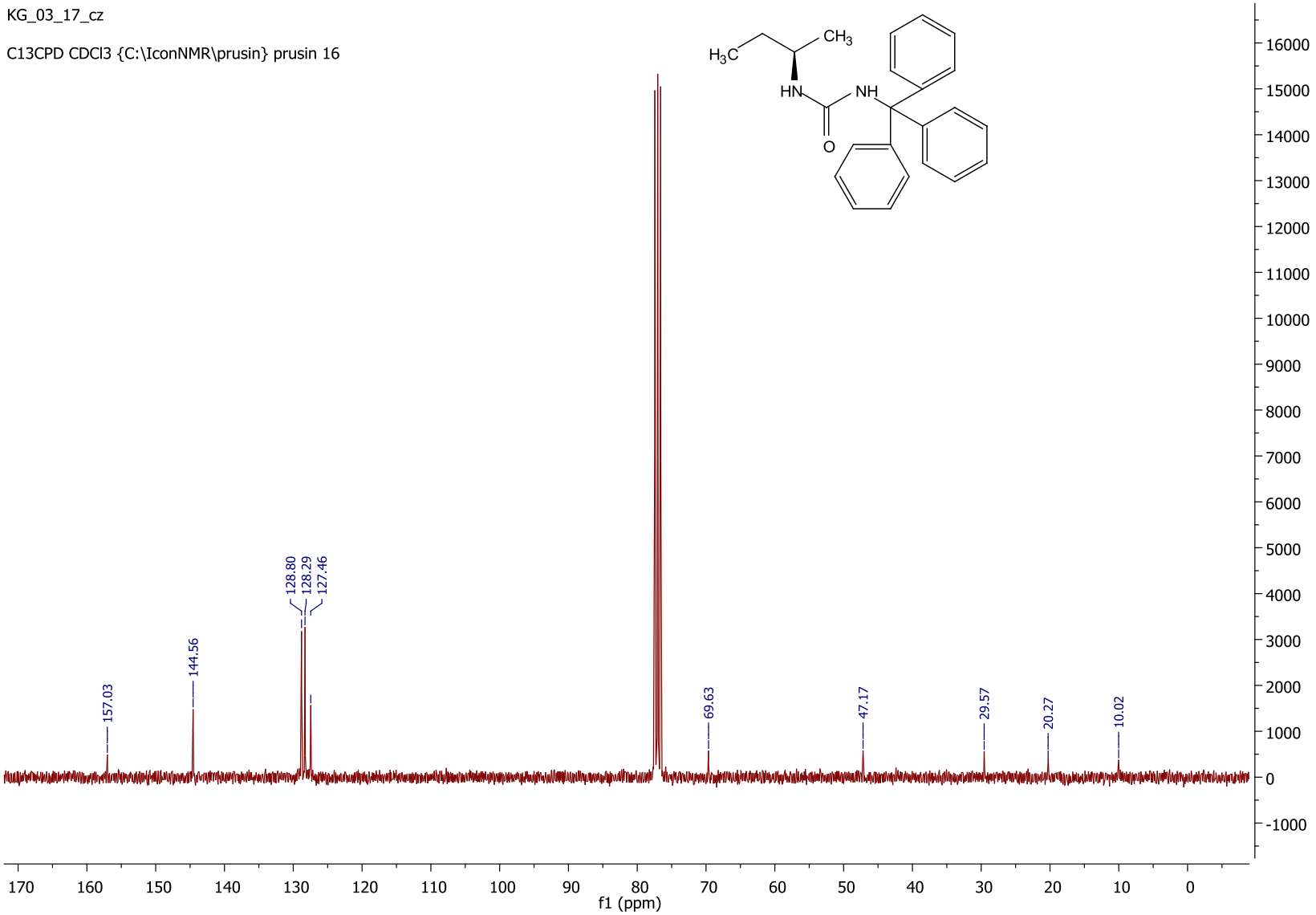


Figure SI_48**.** Scatter plot showing the distribution of conformation of the urea group in the crystal structures (black circles – data taken from the Cambridge Structural Database,[18] red triangles – this study).

Copies of ^{1}H, ^{13}C NMR, ECD and UV spectra

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CH3
HN
NH
O
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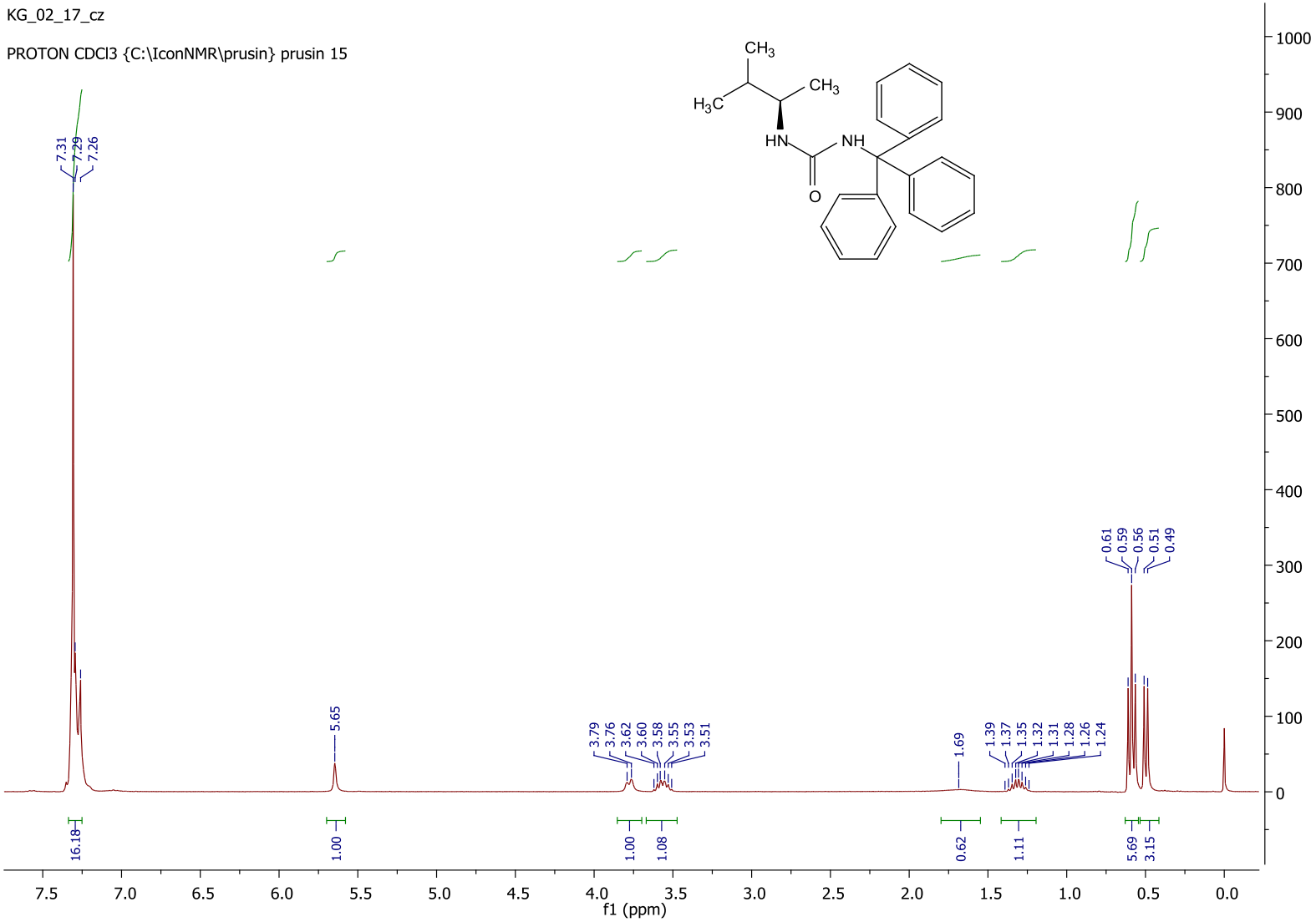
128.29
127.46
69.63
47.17
29.57
20.27
10.02
f1 (ppm)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HN
NH
O
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5.65
3.79
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3.62
3.60
3.58
3.55
3.53
3.51
1.69
1.39
1.37
1.35
1.32
1.31
1.28
1.26
1.24
0.61
0.59
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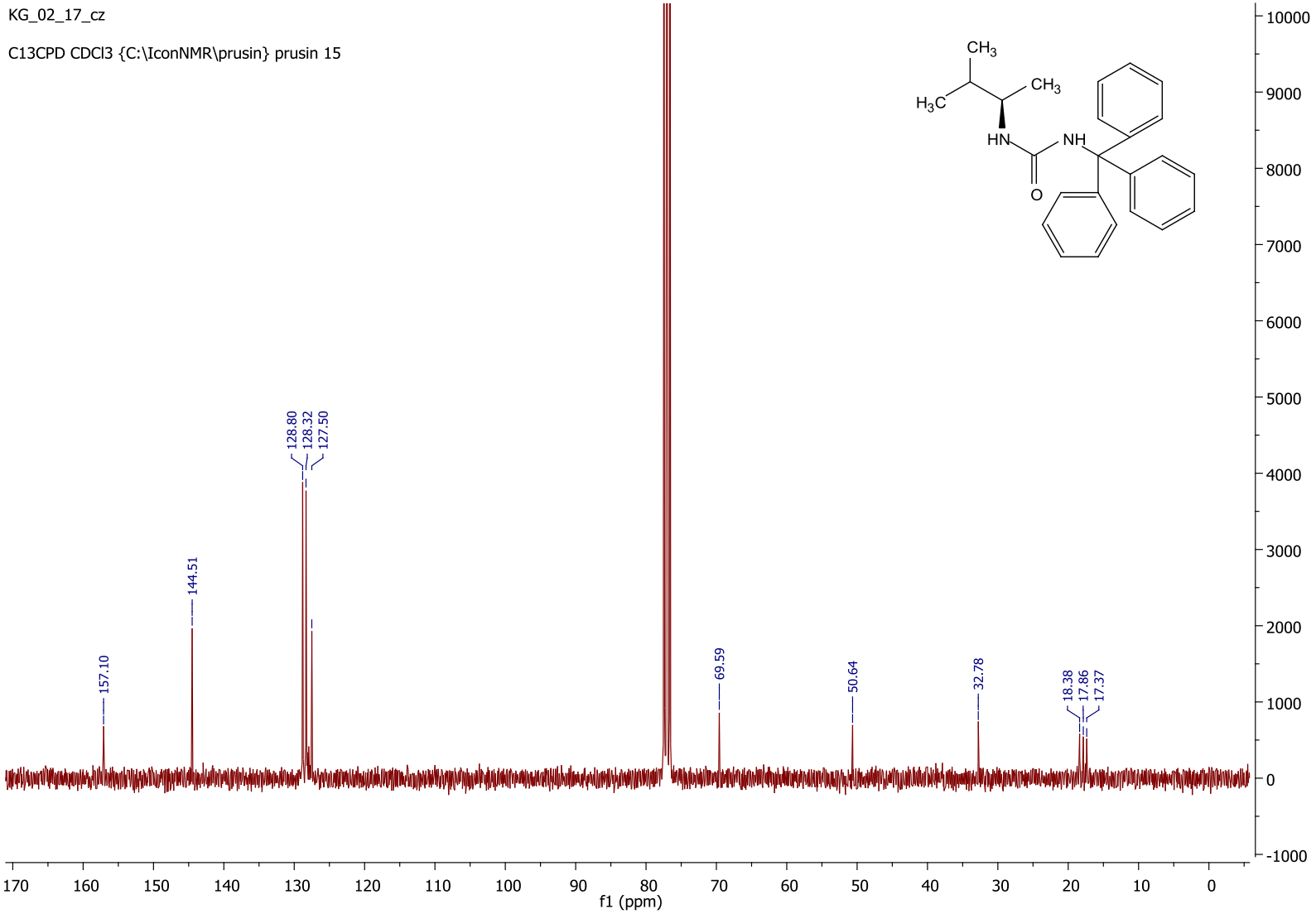
1.00
1.00
1.08
0.62
1.11
5.69
3.15
f1 (ppm)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CH3
H3C
HN
NH
O
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157.10
69.59
50.64
32.78
18.38
17.86
17.37
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
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120
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100
90
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50
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20
10
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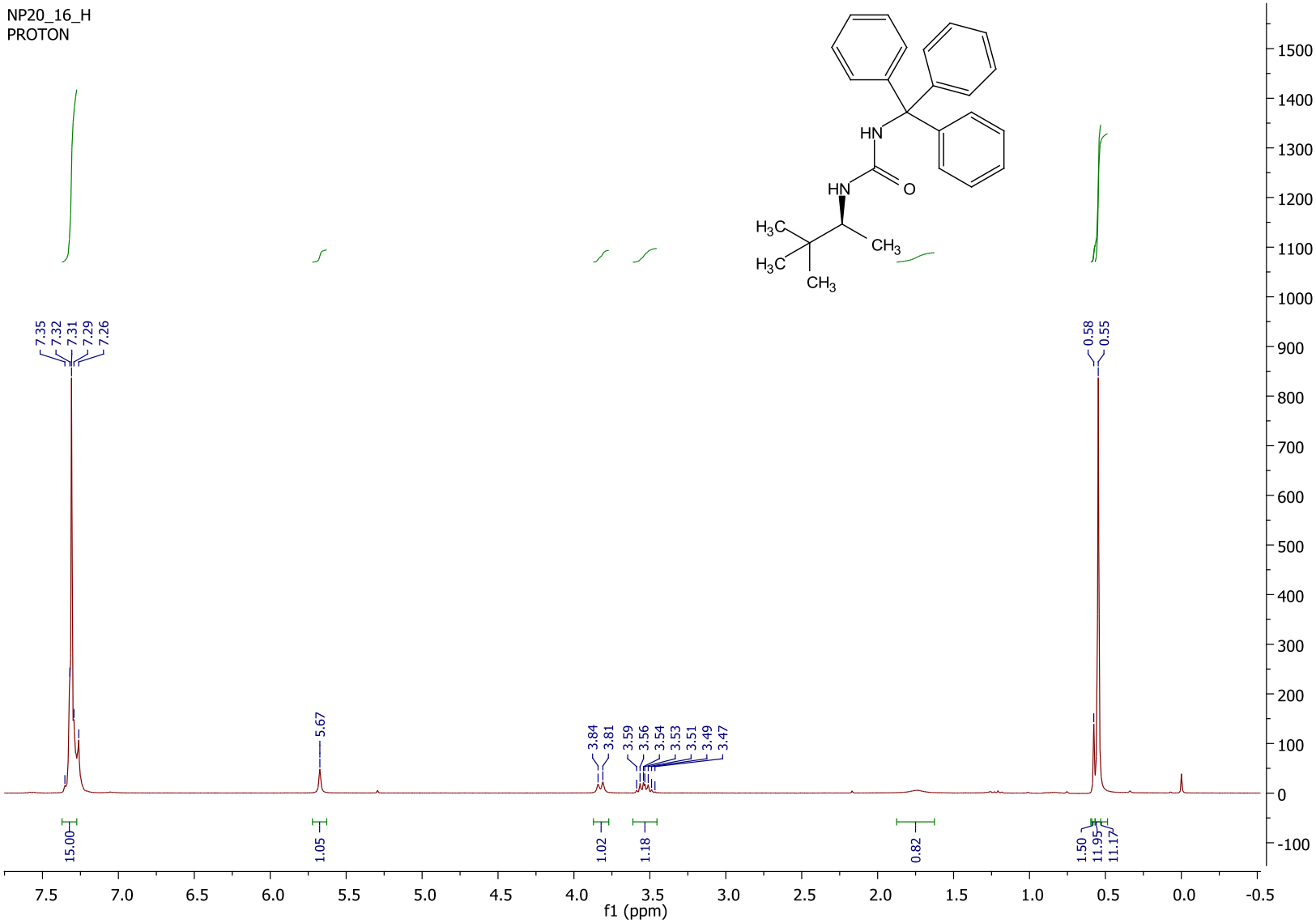
f1 (ppm)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O
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H3C
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5.67
3.84
3.81
3.59
3.56
3.54
3.53
3.51
3.49
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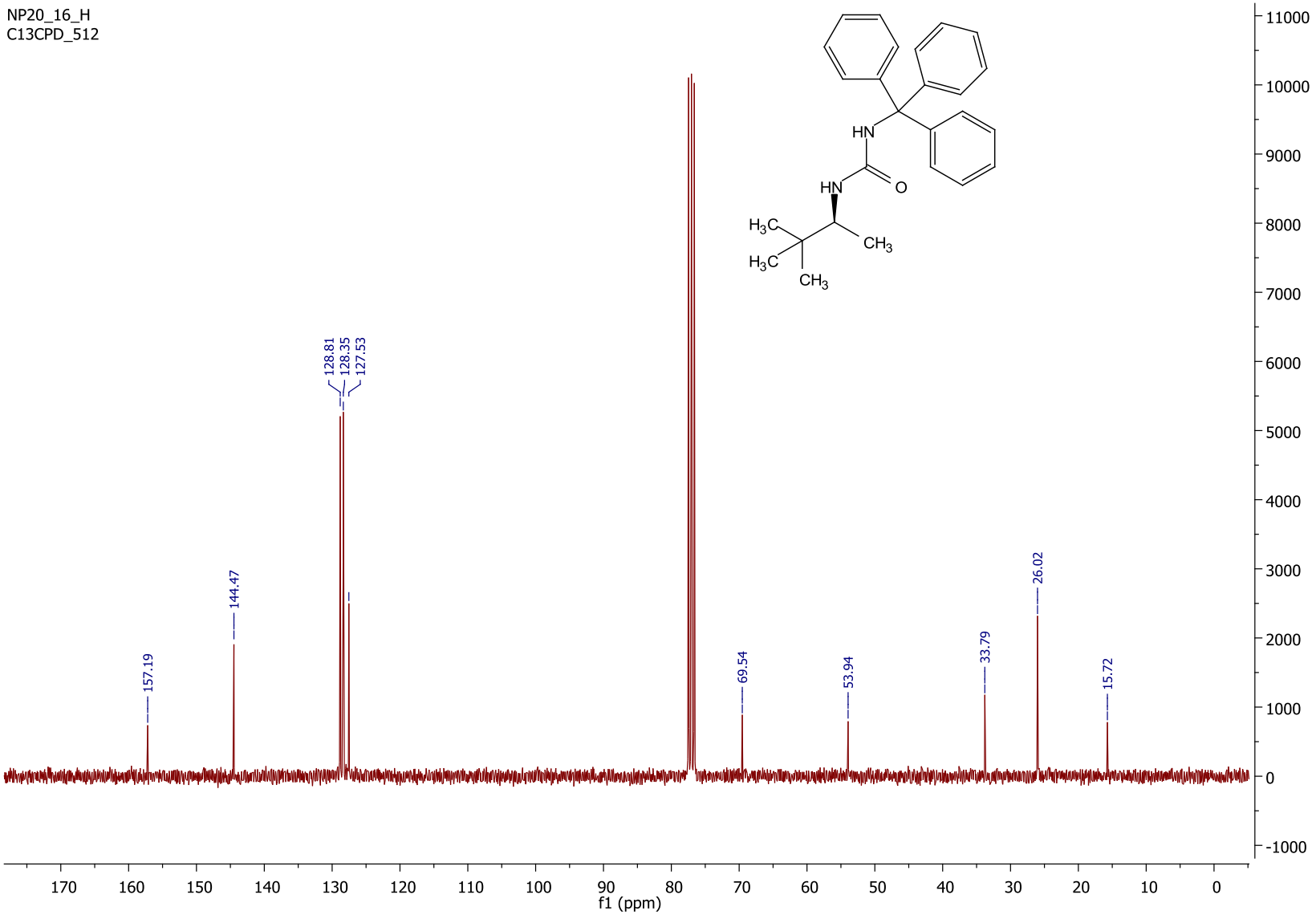
11.17
f1 (ppm)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69.54
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33.79
26.02
15.72
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
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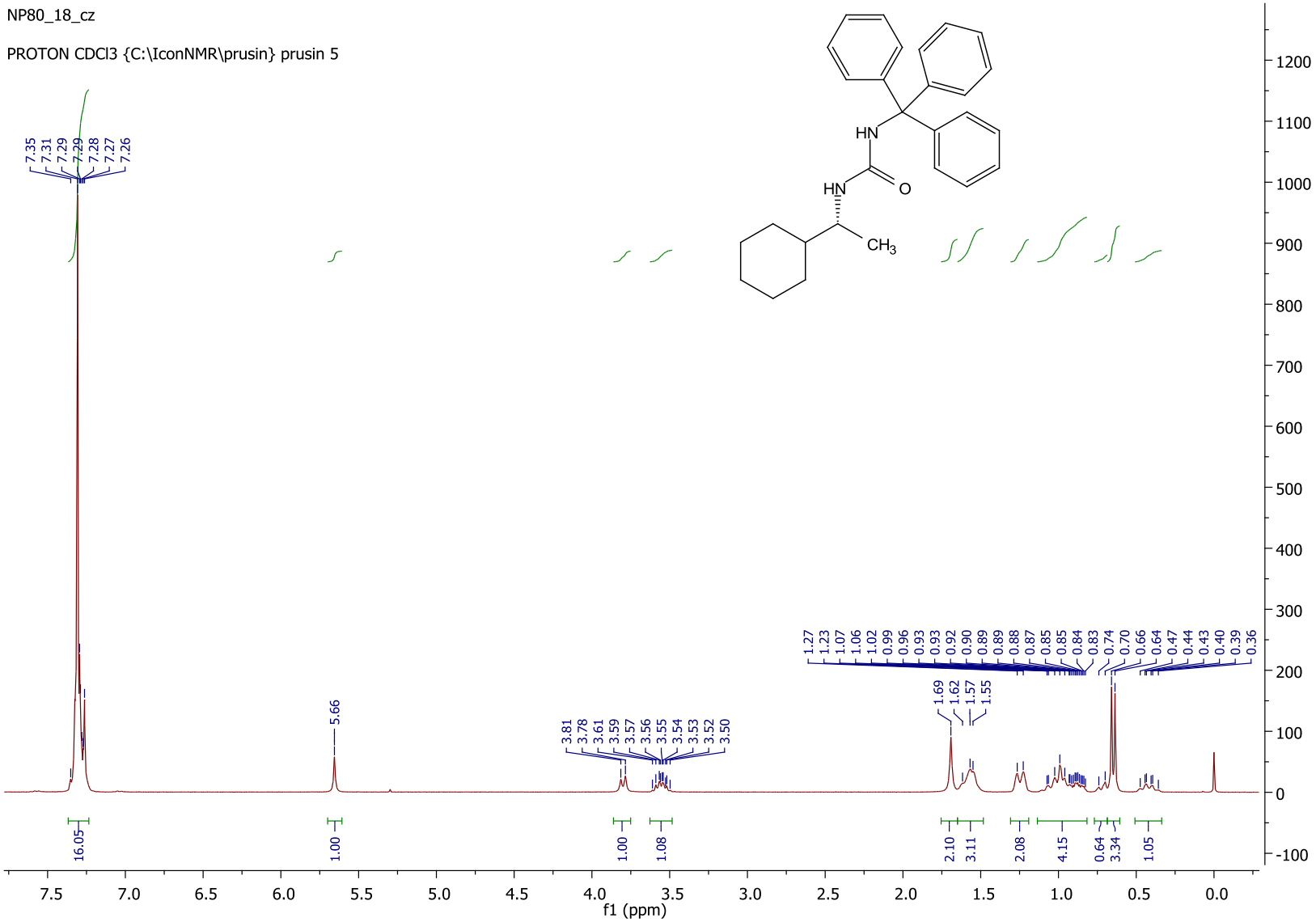
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HN
O
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3.78
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3.55
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3.53
3.52
3.50
1.69
1.62
1.57
1.55
1.27
1.23
1.07
1.06
1.02
0.99
0.96
0.93
0.93
0.92
0.90
0.89
0.89
0.88
0.87
0.85
0.85
0.84
0.83
0.74
0.70
0.66
0.64
0.47
0.44
0.43
0.40
0.39
0.36
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3.11
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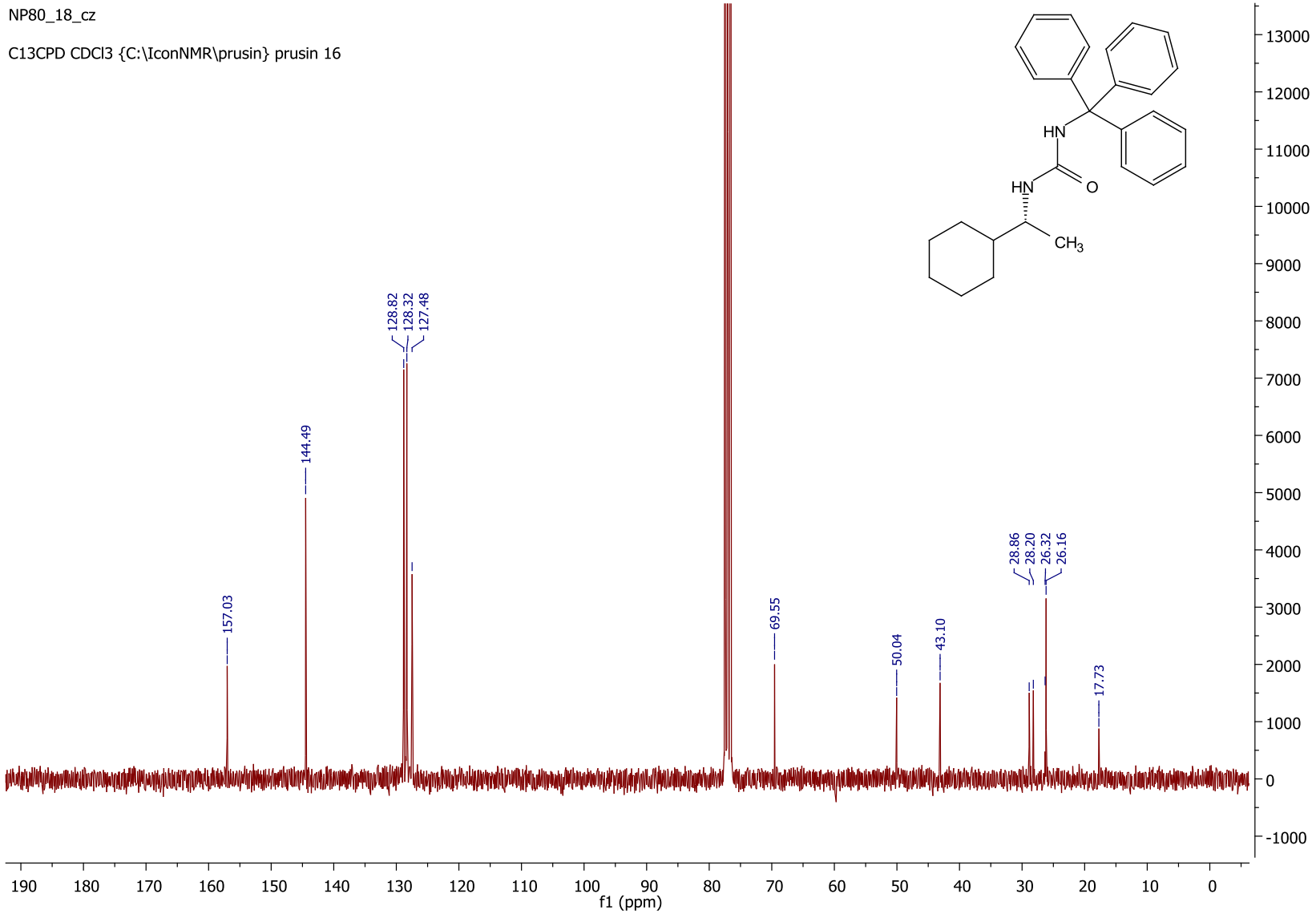
1.05
f1 (ppm)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O
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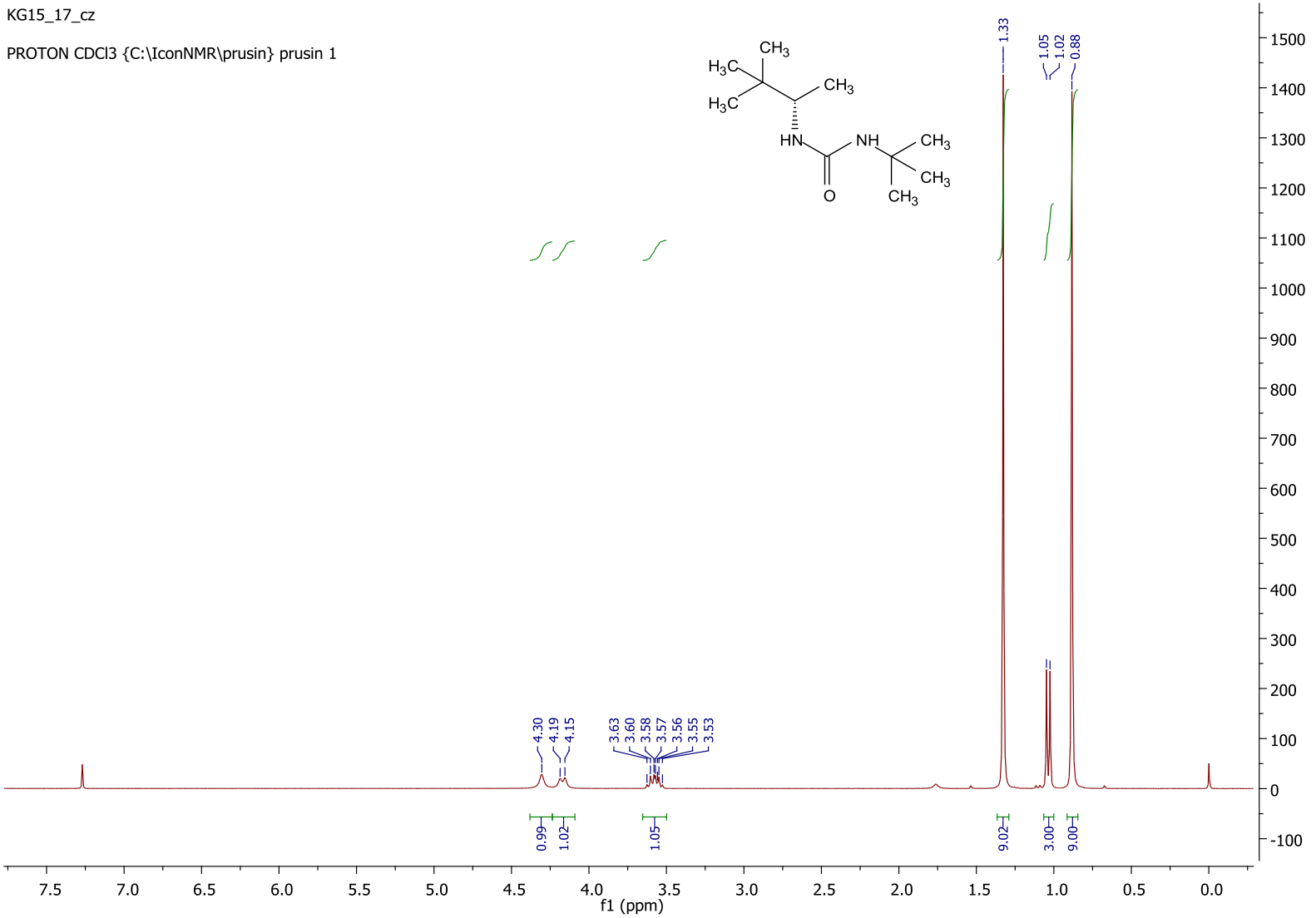
f1 (ppm)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1.02
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4.15
3.63
3.60
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3.57
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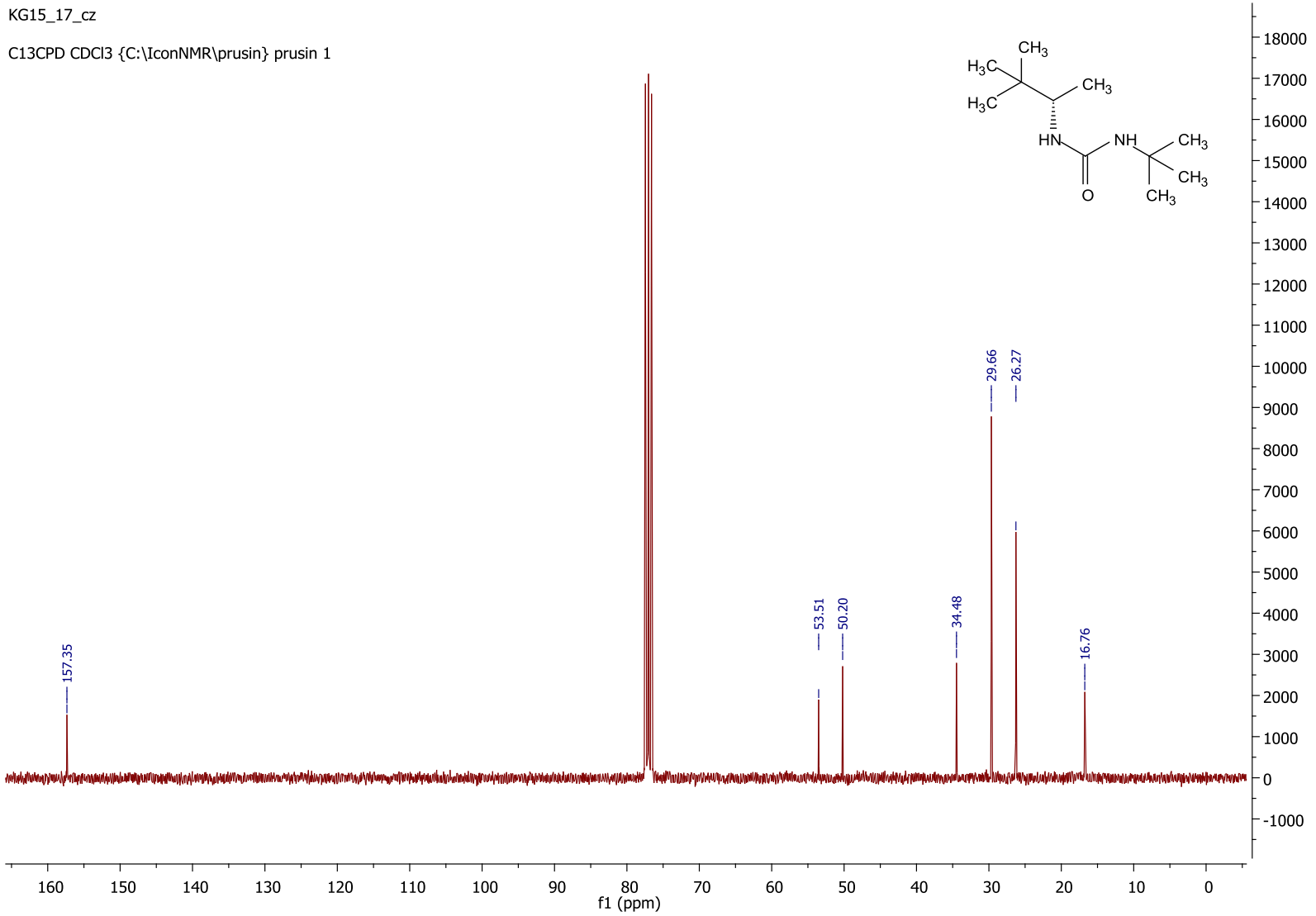
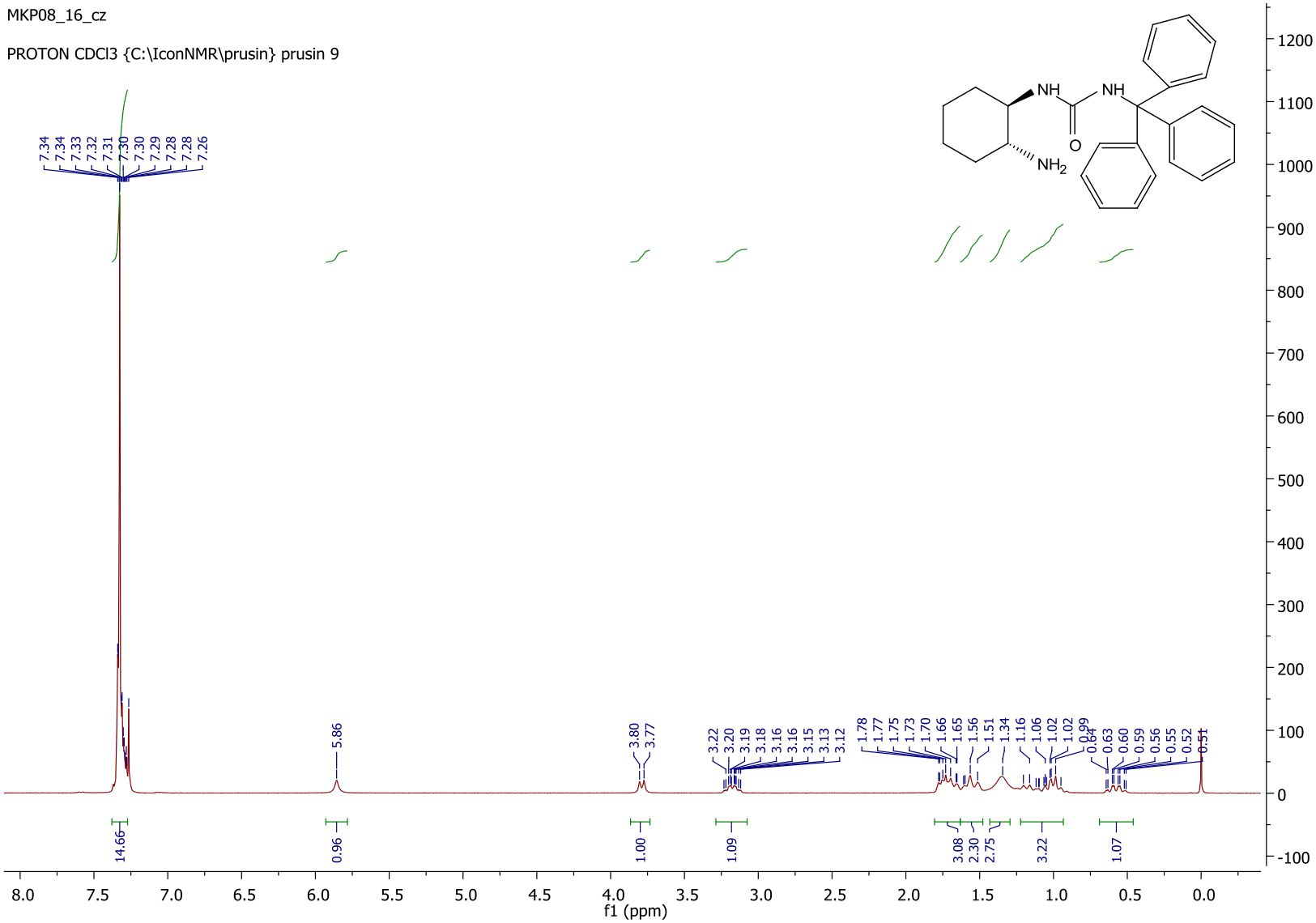
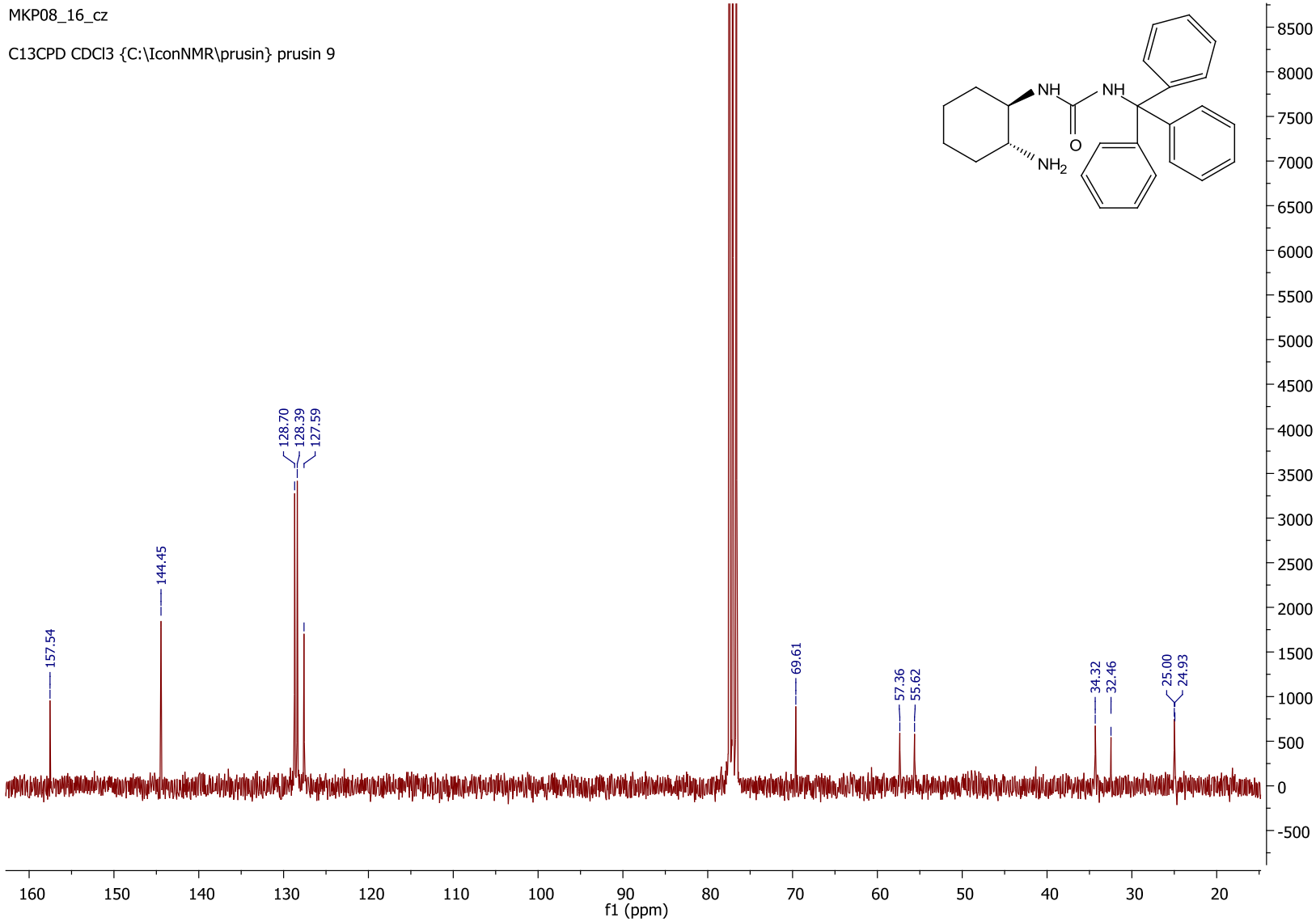
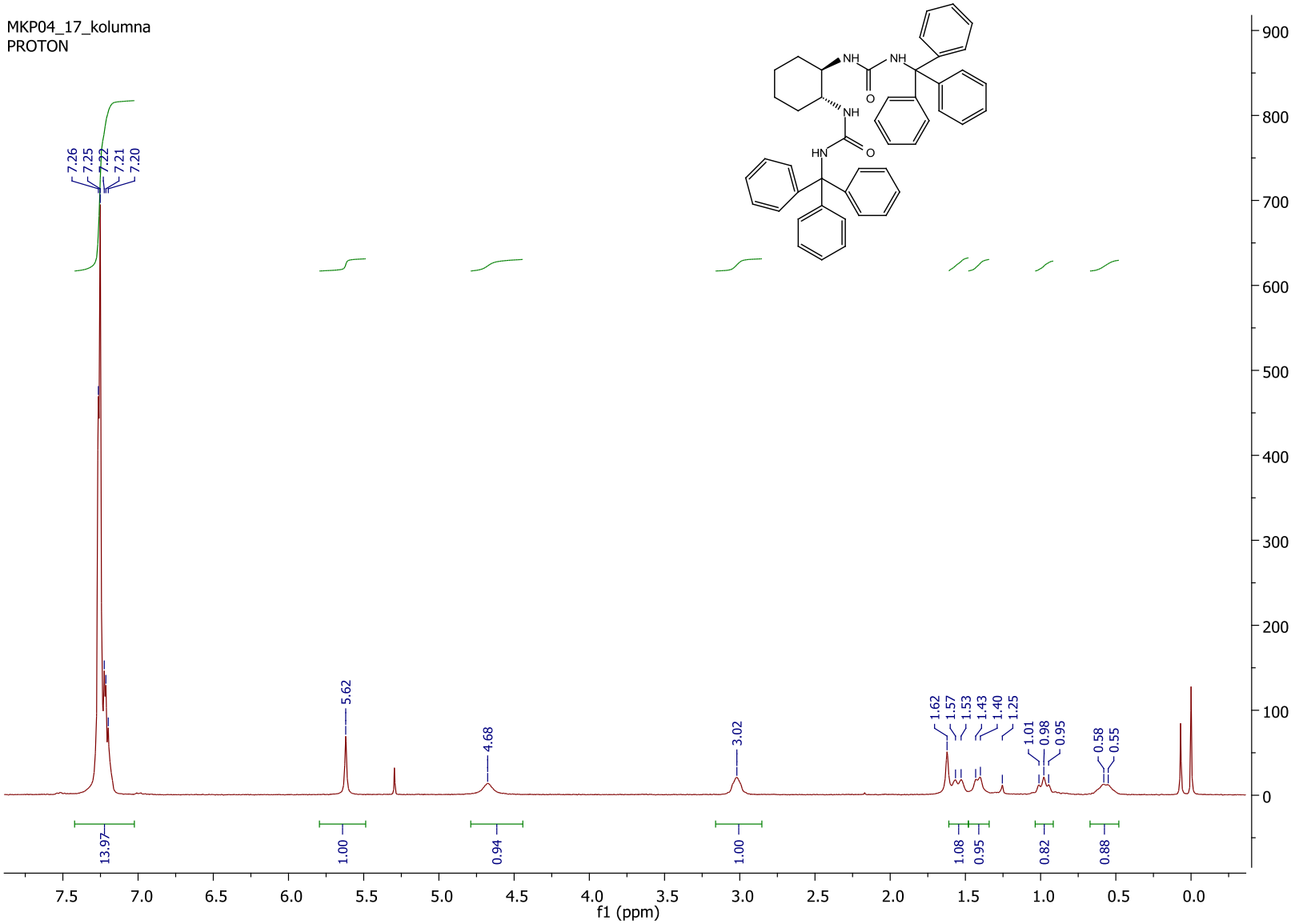
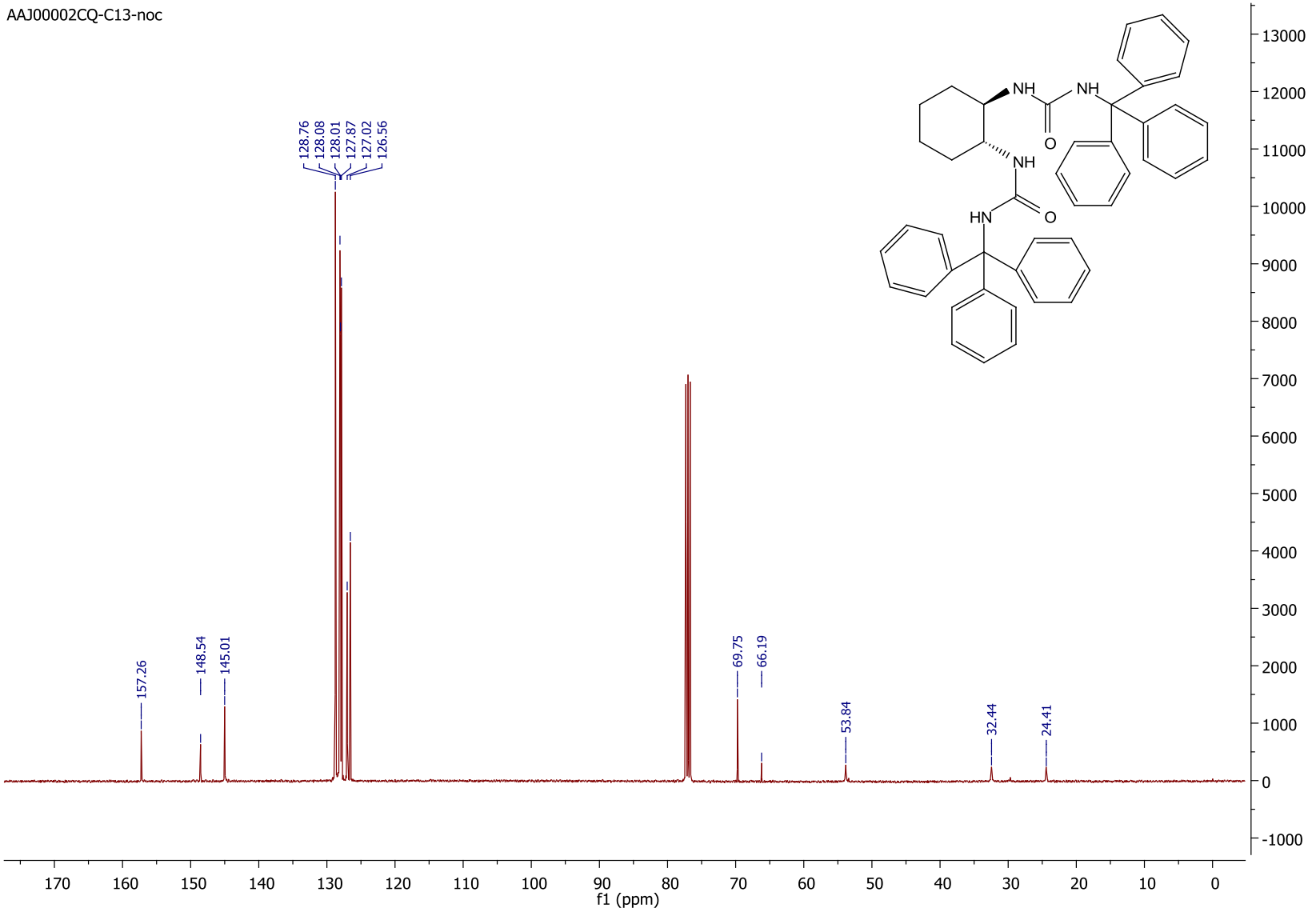
3.55
3.53
0.99
1.02
1.05
9.02
3.00
9.00
f1 (ppm)

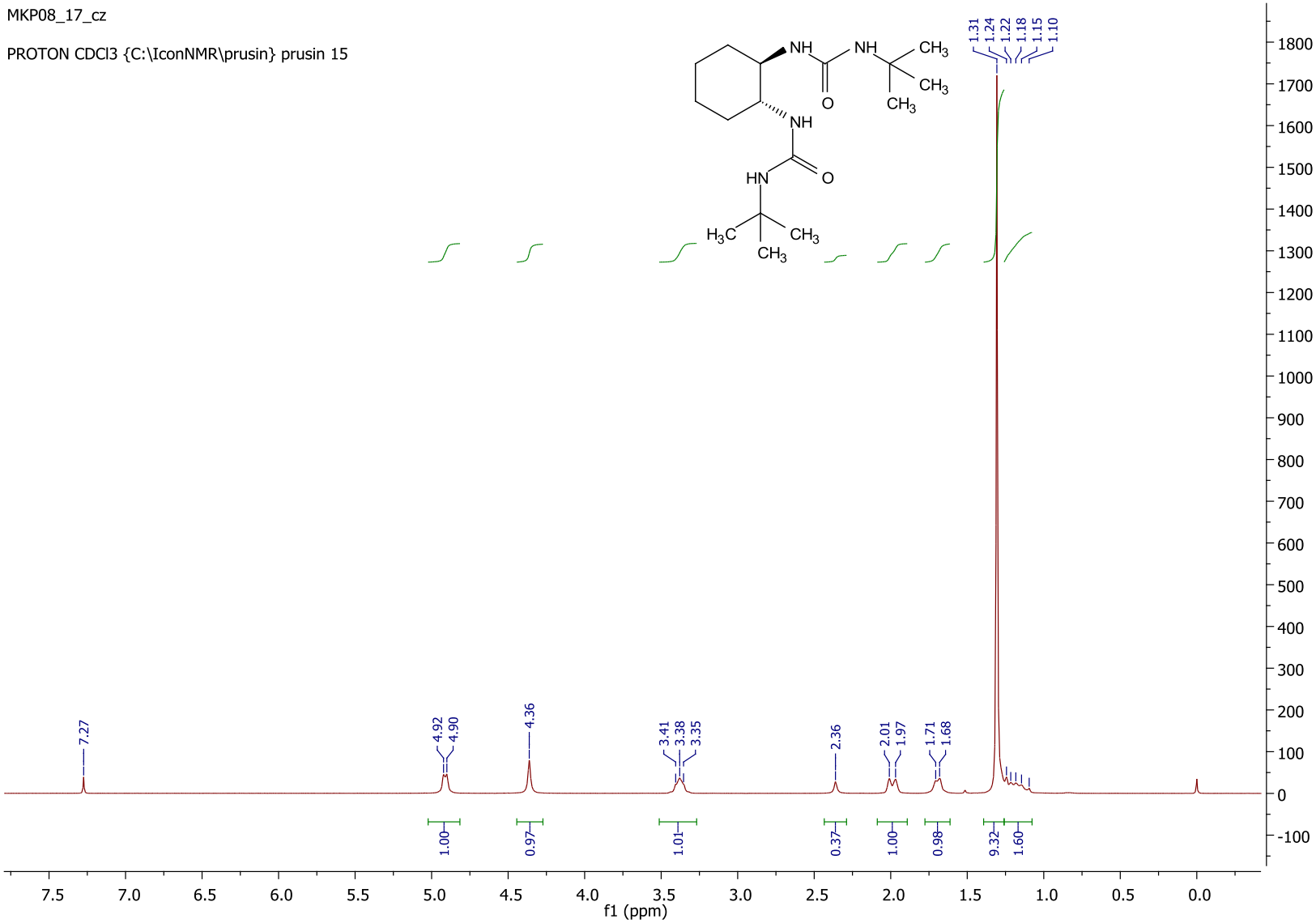

KG15_17_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 1
157.35
53.51
50.20
34.48
29.66
26.27
16.76
f1 (ppm)

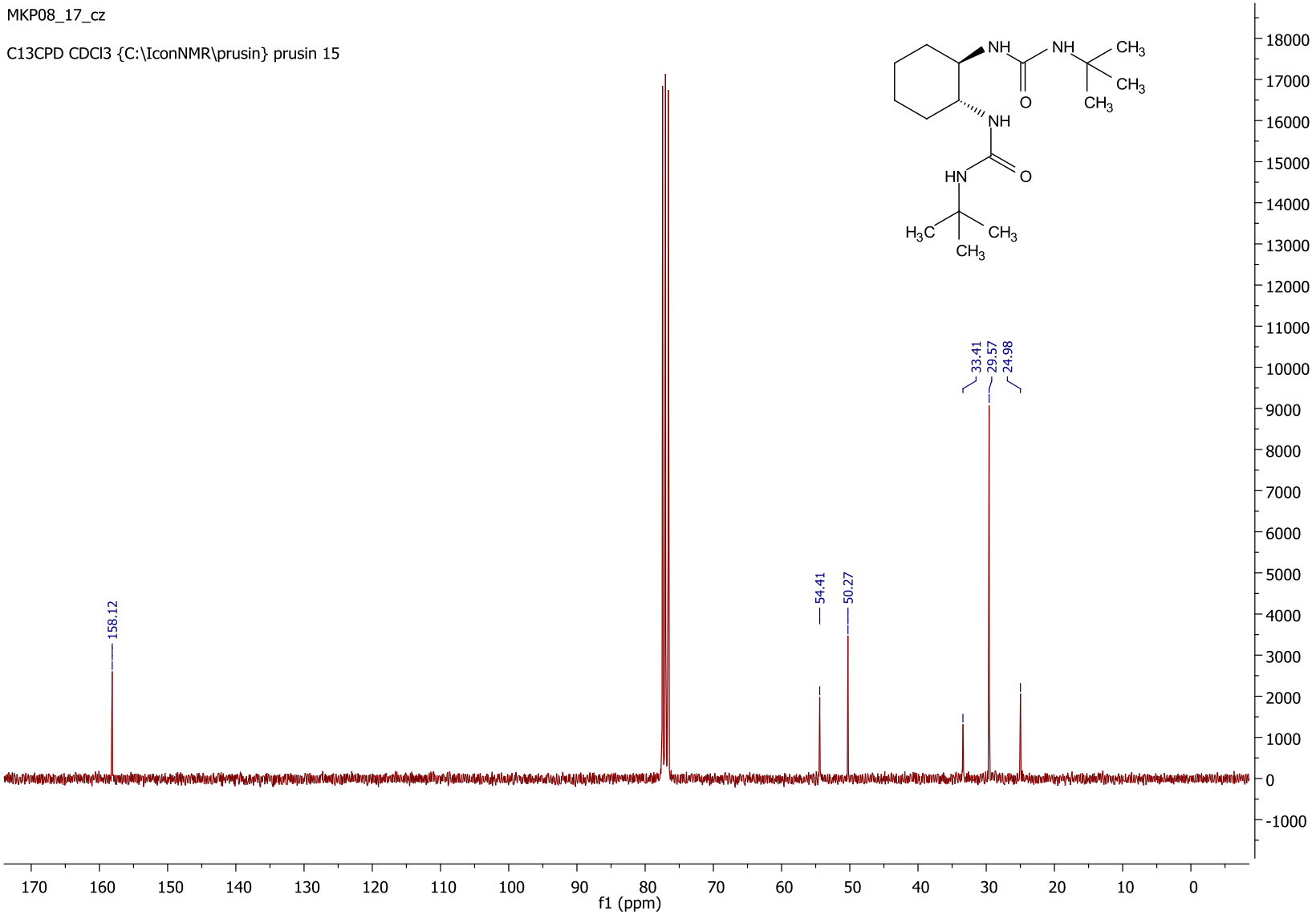

MKP08_16_cz
PROTON CDCl3 {C:\IconNMR\prusin} prusin 9
NH
NH
O
NH2
f1 (ppm)

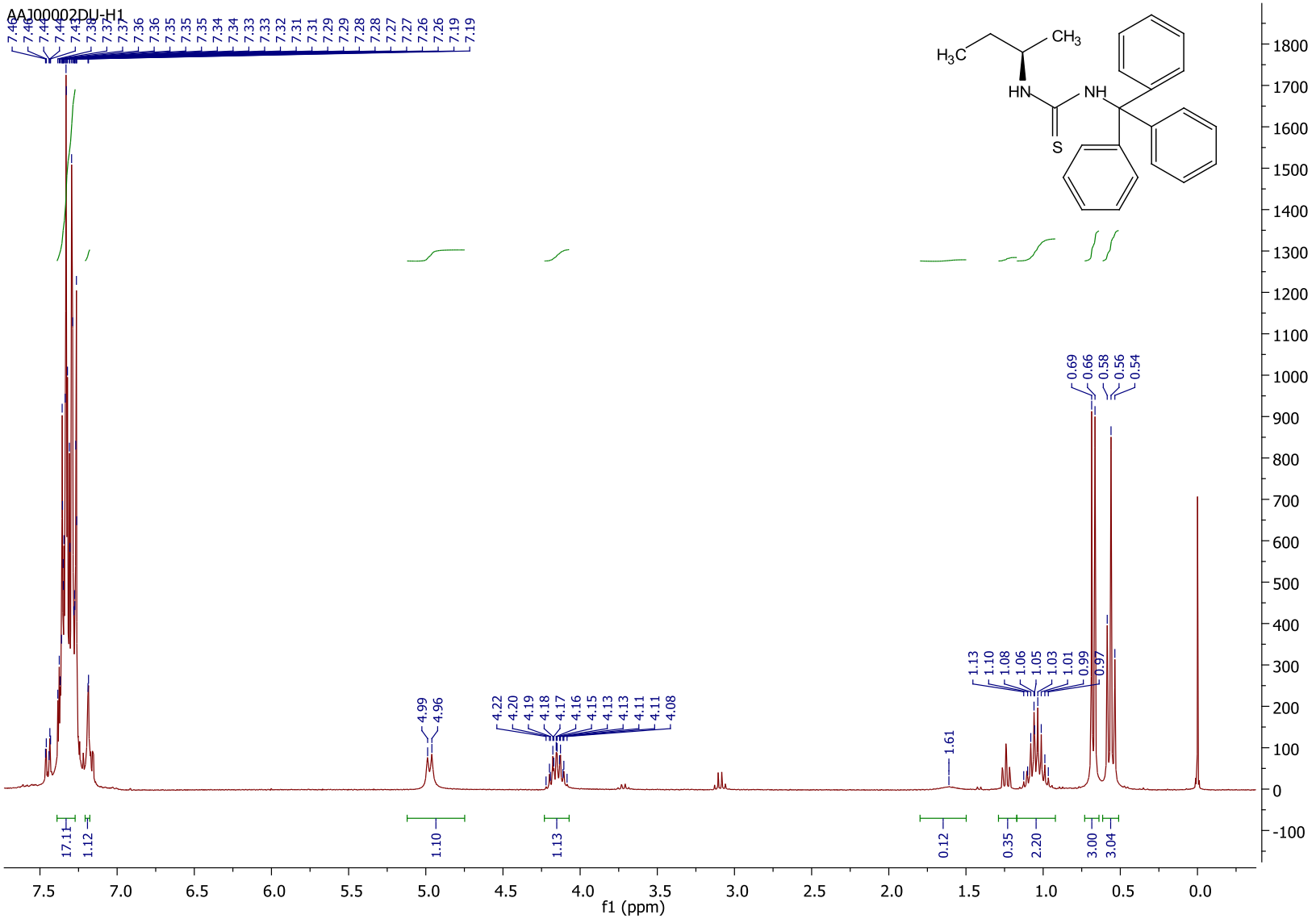

MKP08_16_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 9
NH
NH
O
NH2
157.54
144.45
128.70
128.39
127.59
69.61
57.36
55.62
34.32
32.46
25.00
24.93
f1 (ppm)

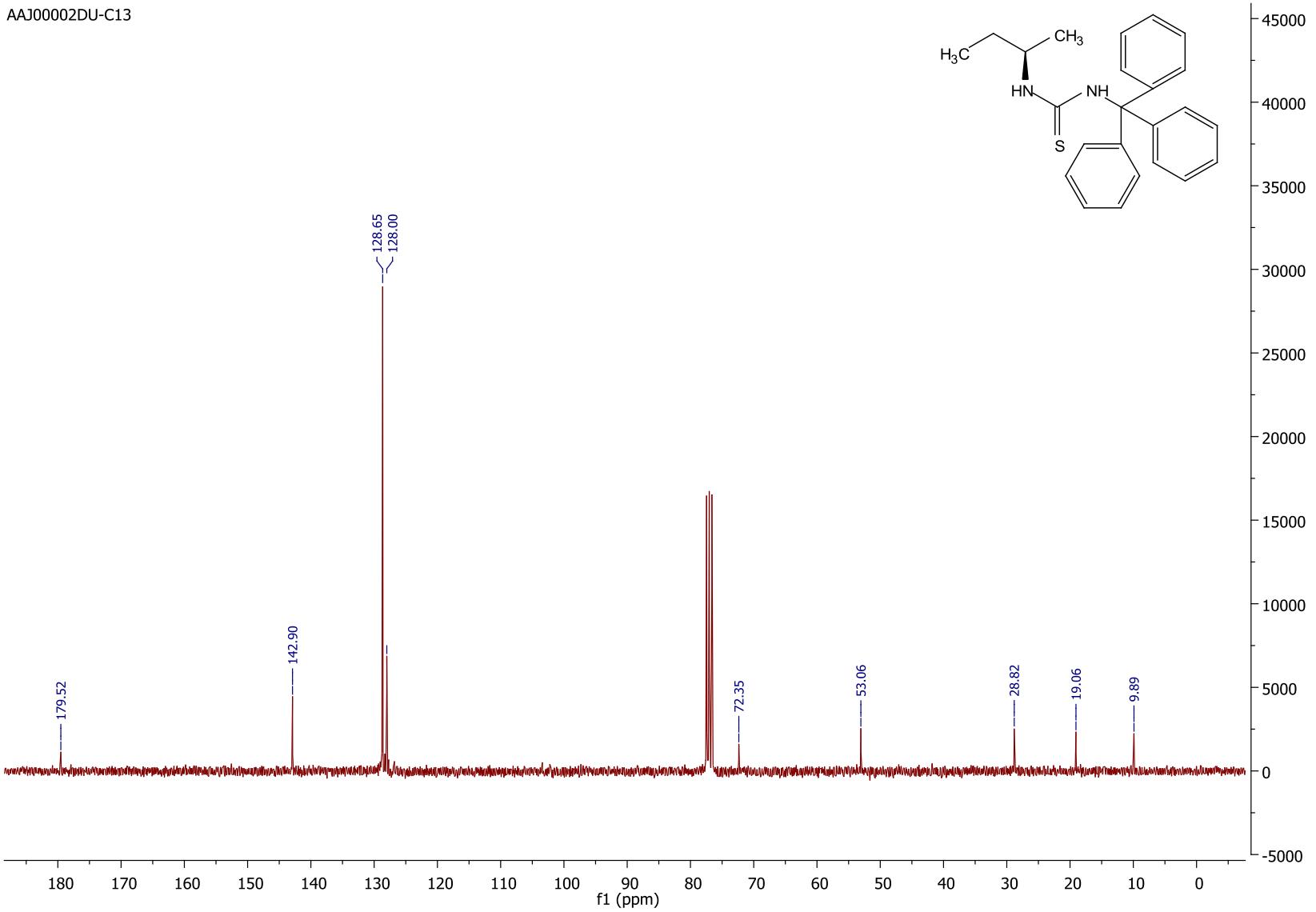

MKP04_17_kolumna
PROTON
NH
NH
NH
HN
O
O
7.26
7.25
7.22
7.21
7.20
5.62
4.68
3.02
1.62
1.57
1.53
1.43
1.40
1.25
1.01
0.98
0.95
0.58
0.55
13.97
1.00
0.94
1.00
1.08
0.95
0.82
0.88
f1 (ppm)

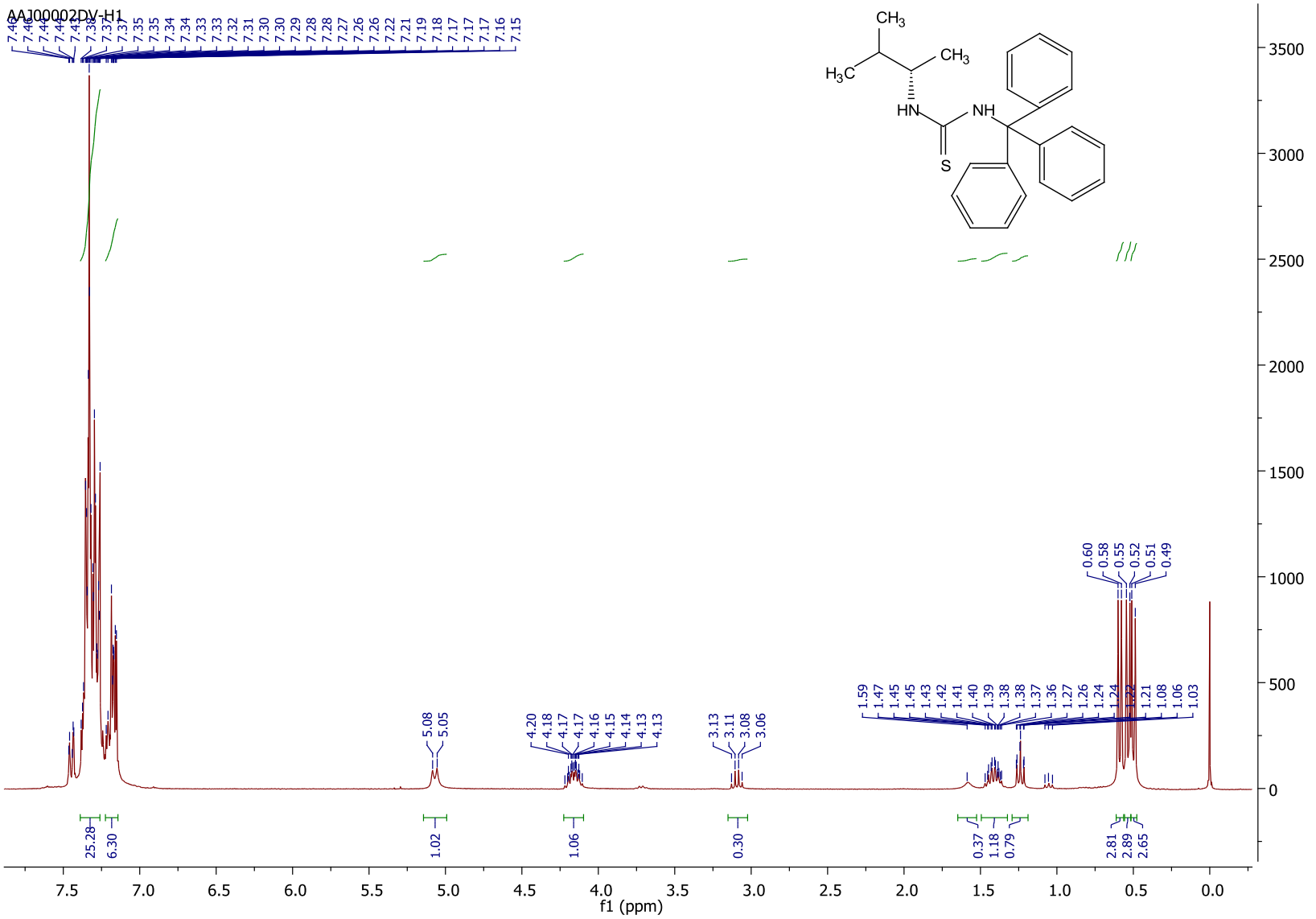

AAJ00002CQ-C13-noc
128.76
128.08
128.01
127.87
127.02
126.56
157.26
148.54
145.01
69.75
66.19
53.84
32.44
24.41
NH
NH
O
NH
HN
O
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

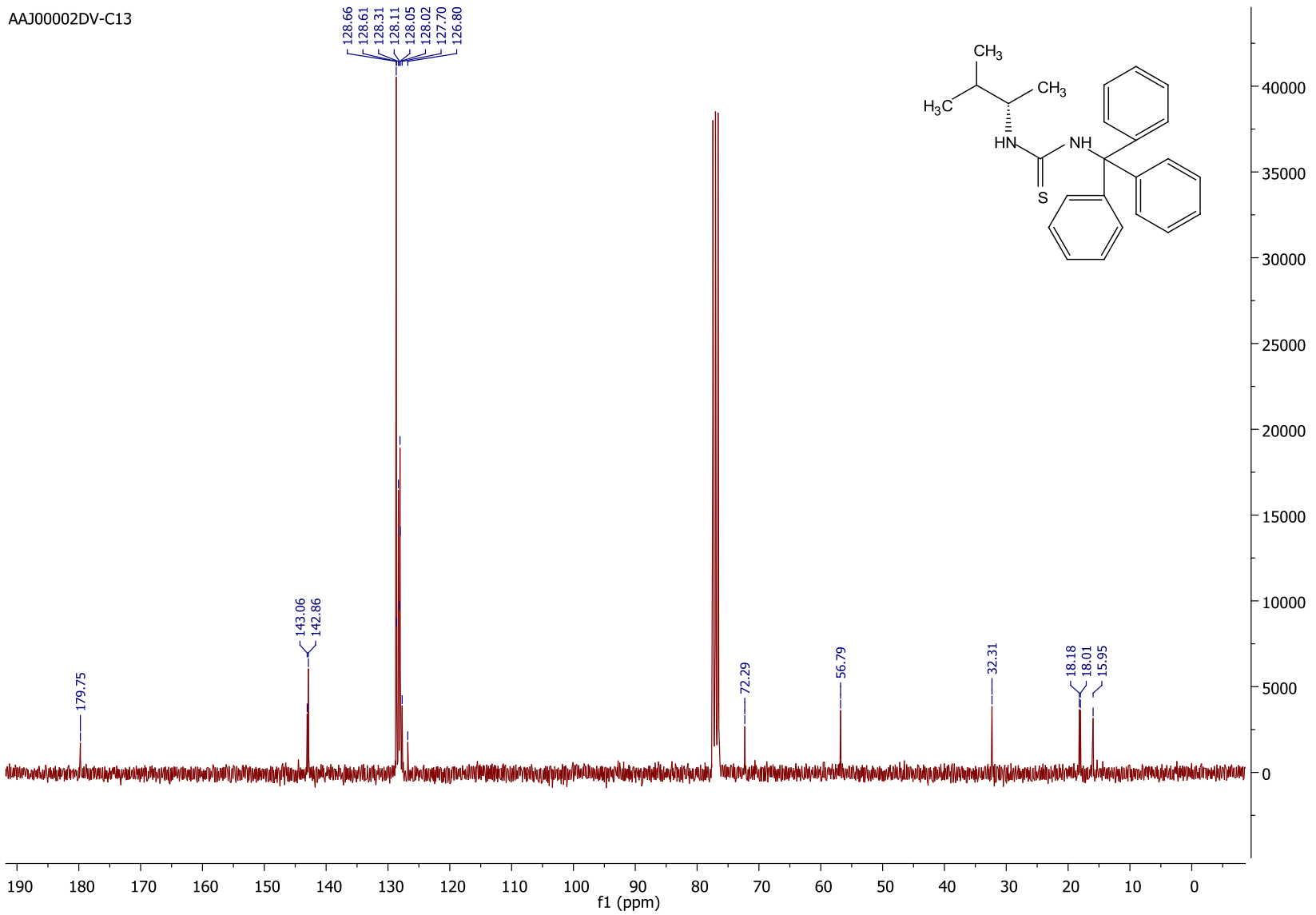

MKP08_17_cz
PROTON CDCl3 {C:\IconNMR\prusin} prusin 15
NH
NH
CH3
CH3
CH3
O
NH
HN
O
H3C
CH3
CH3
1.31
1.24
1.22
1.18
1.15
1.10
7.27
4.92
4.90
4.36
3.41
3.38
3.35
2.36
2.01
1.97
1.71
1.68
1.00
0.97
1.01
0.37
1.00
0.98
9.32
1.60
f1 (ppm)


MKP08_17_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 15
158.12
54.41
50.27
33.41
29.57
24.98
f1 (ppm)


AA100002DU-H1
H3C
CH3
HN
NH
S
f1 (ppm)


AAJ00002DU-C13
H3C
CH3
HN
NH
S
128.65
128.00
179.52
142.90
72.35
53.06
28.82
19.06
9.89
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


AAJ00002DV-H1
CH3
CH3
H3C
HN
NH
S
f1 (ppm)


AAJ00002DV-C13
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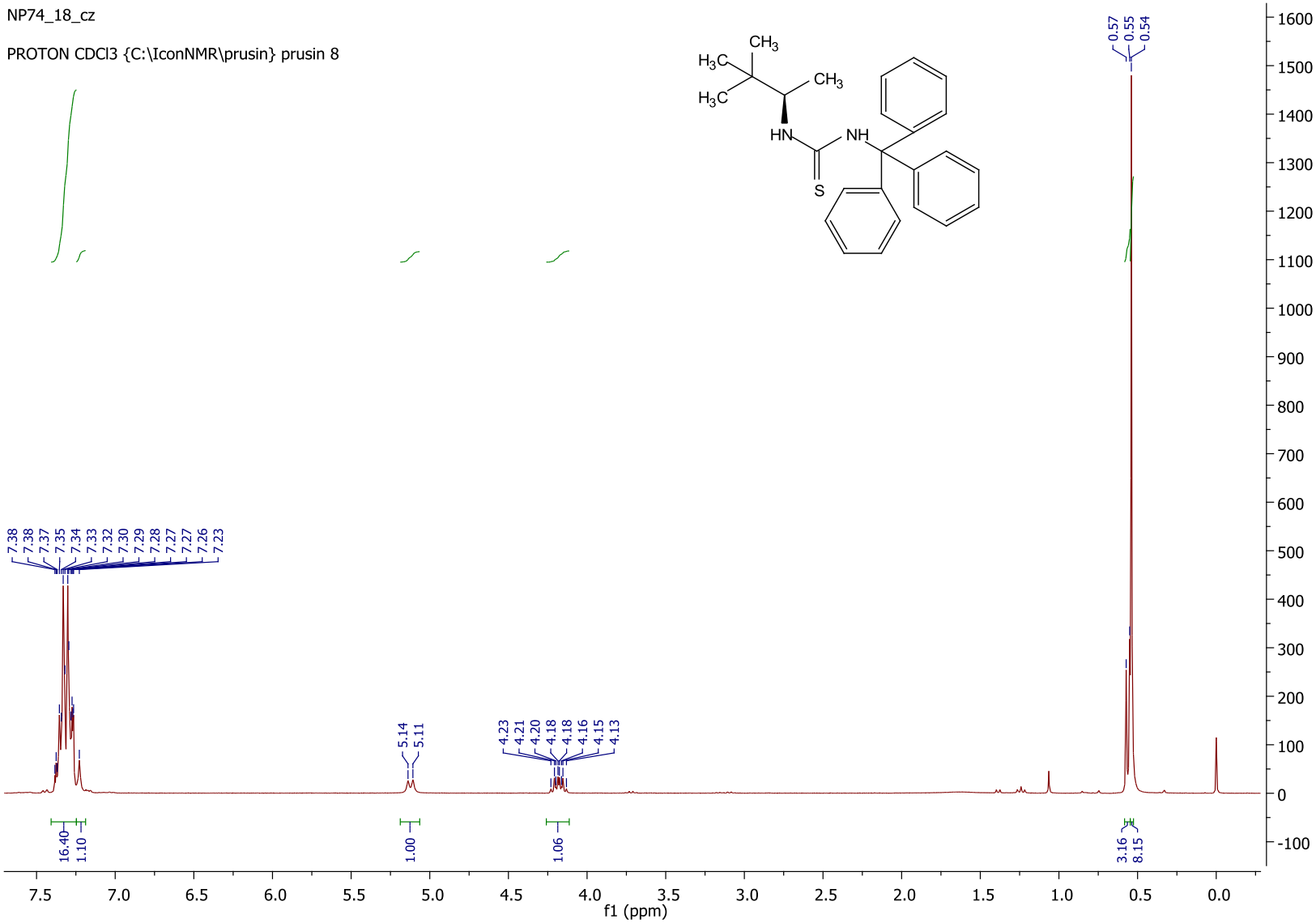
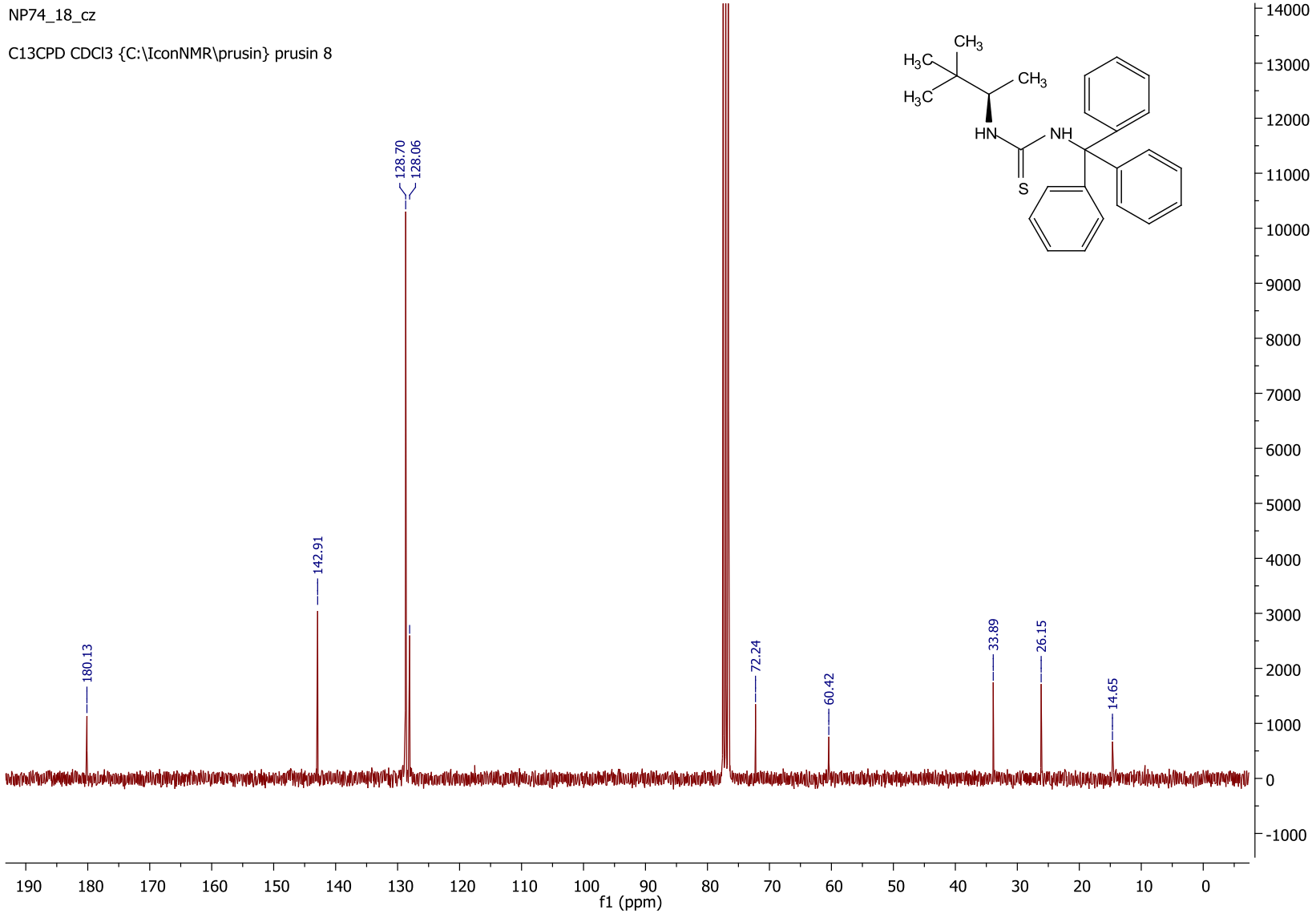
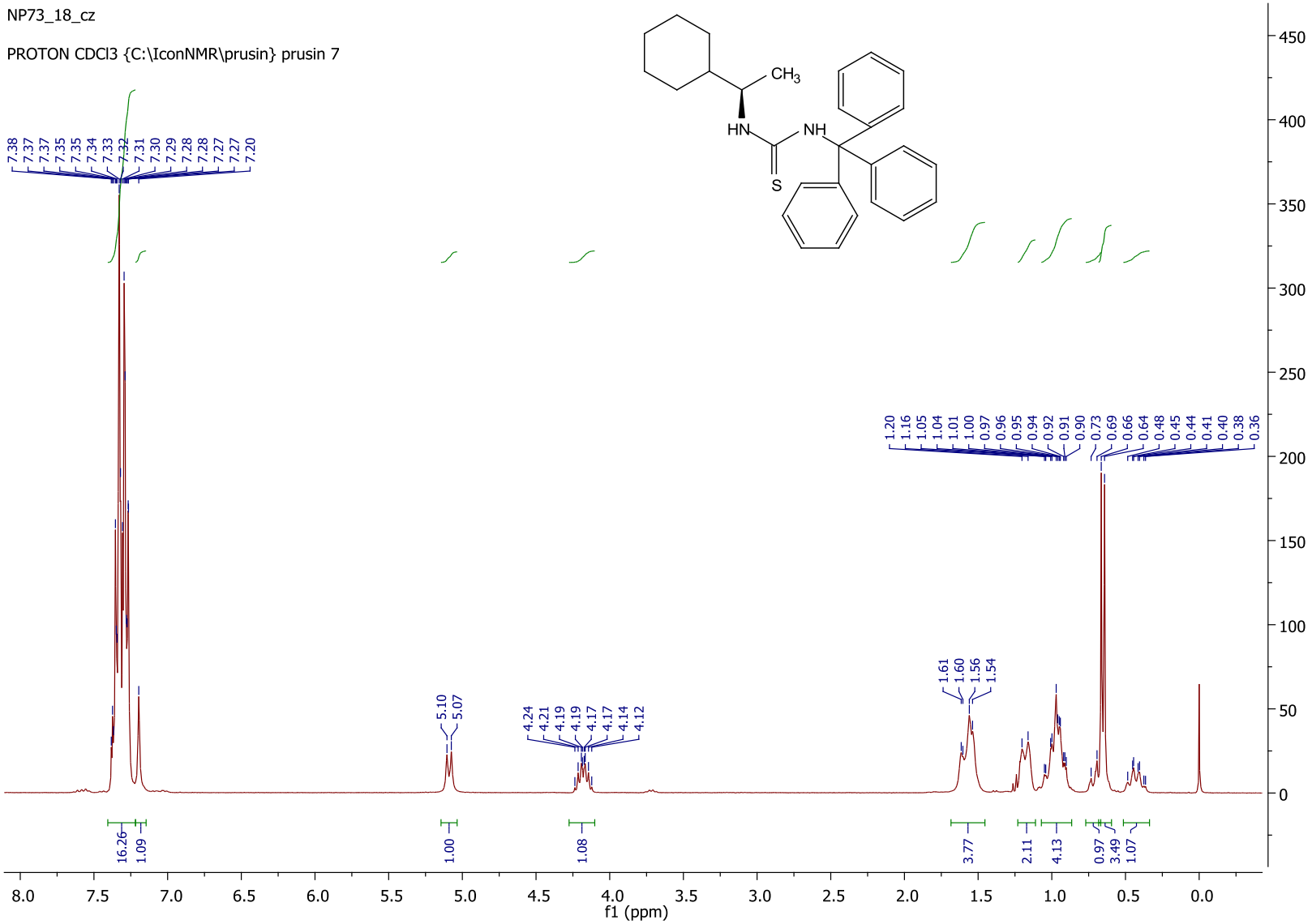
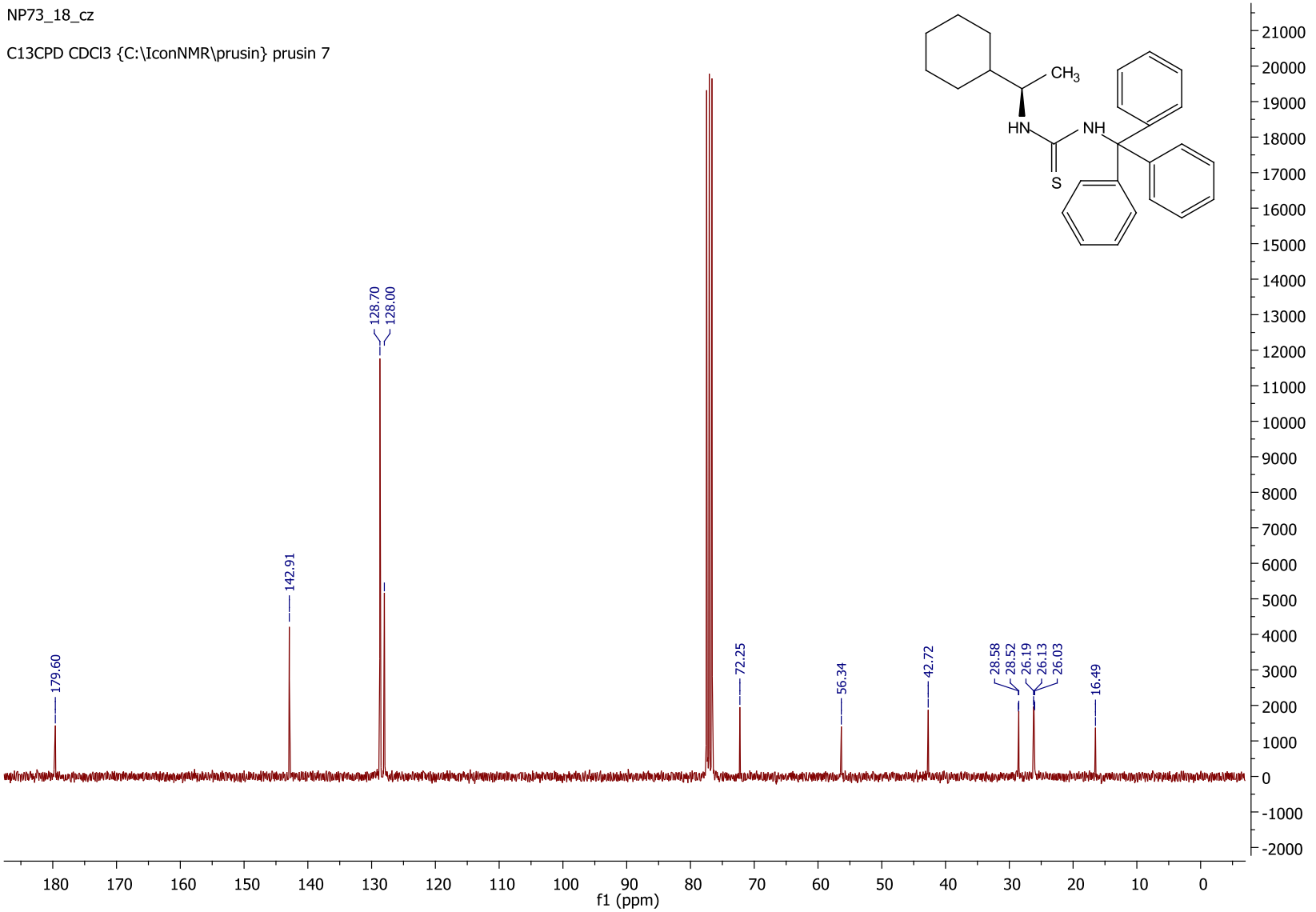
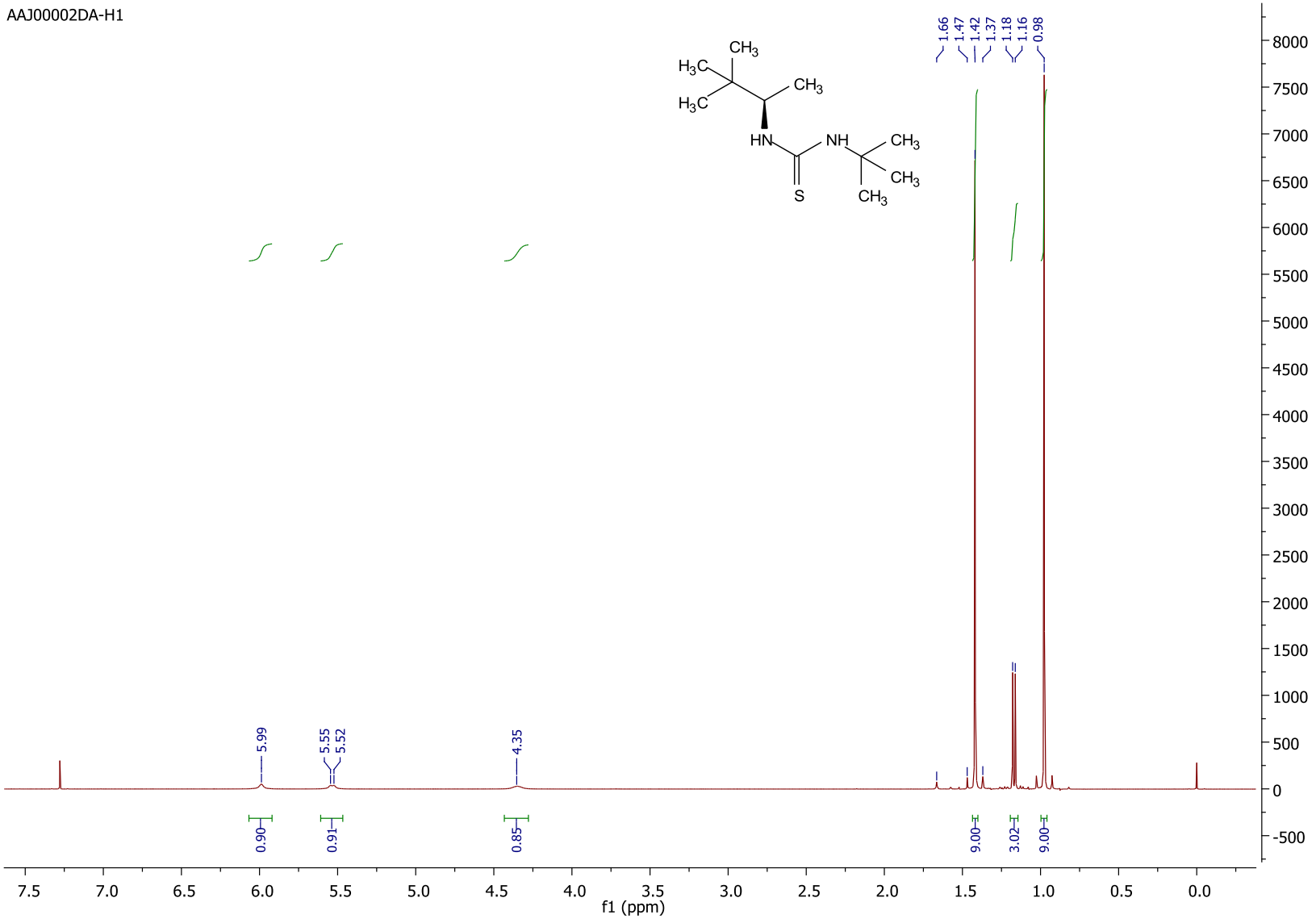
128.61
128.31
128.11
128.05
128.02
127.70
126.80
179.75
143.06
142.86
72.29
56.79
32.31
18.18
18.01
15.95
CH3
CH3
H3C
HN
NH
S
40000
35000
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

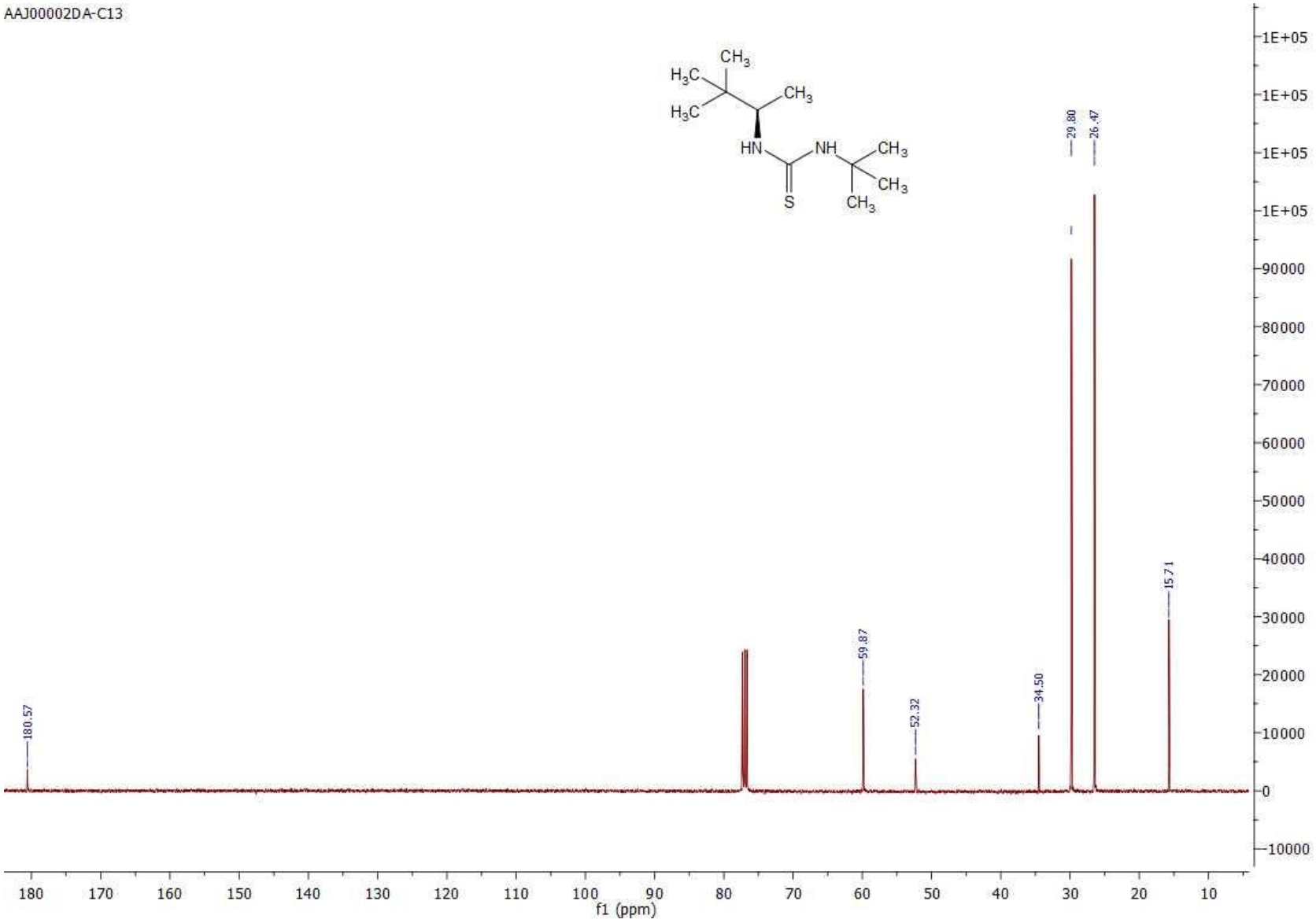

NP74_18_cz
PROTON CDCl3 {C:\IconNMR\prusin} prusin 8
CH3
H3C
CH3
H3C
HN
NH
S
0.57
0.55
0.54
7.38
7.38
7.37
7.35
7.34
7.33
7.32
7.30
7.29
7.28
7.27
7.27
7.26
7.23
5.14
5.11
4.23
4.21
4.20
4.18
4.18
4.16
4.15
4.13
16.40
1.10
1.00
1.06
3.16
8.15
f1 (ppm)

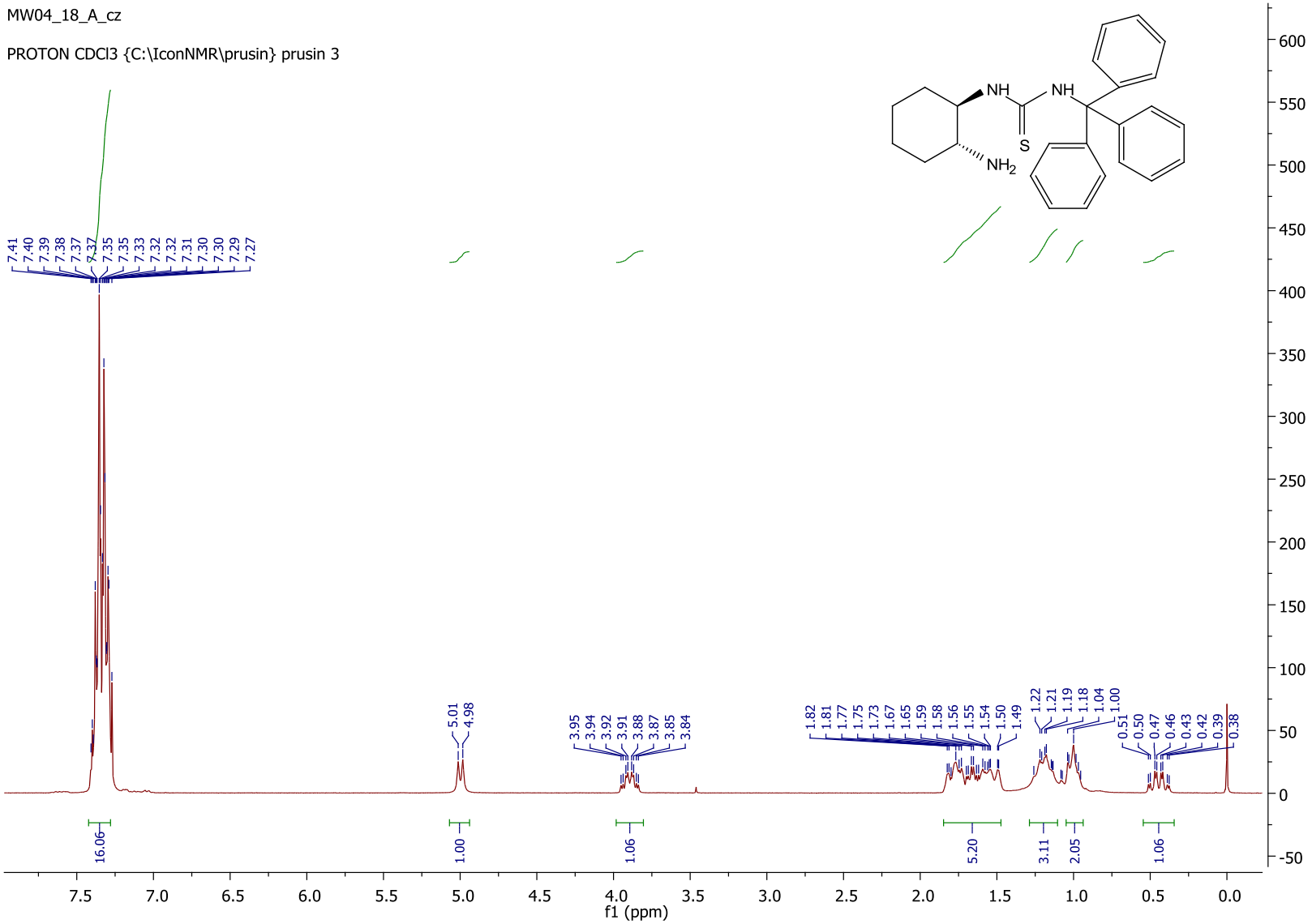

NP74_18_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 8
180.13
142.91
128.70
128.06
72.24
60.42
33.89
26.15
14.65
f1 (ppm)

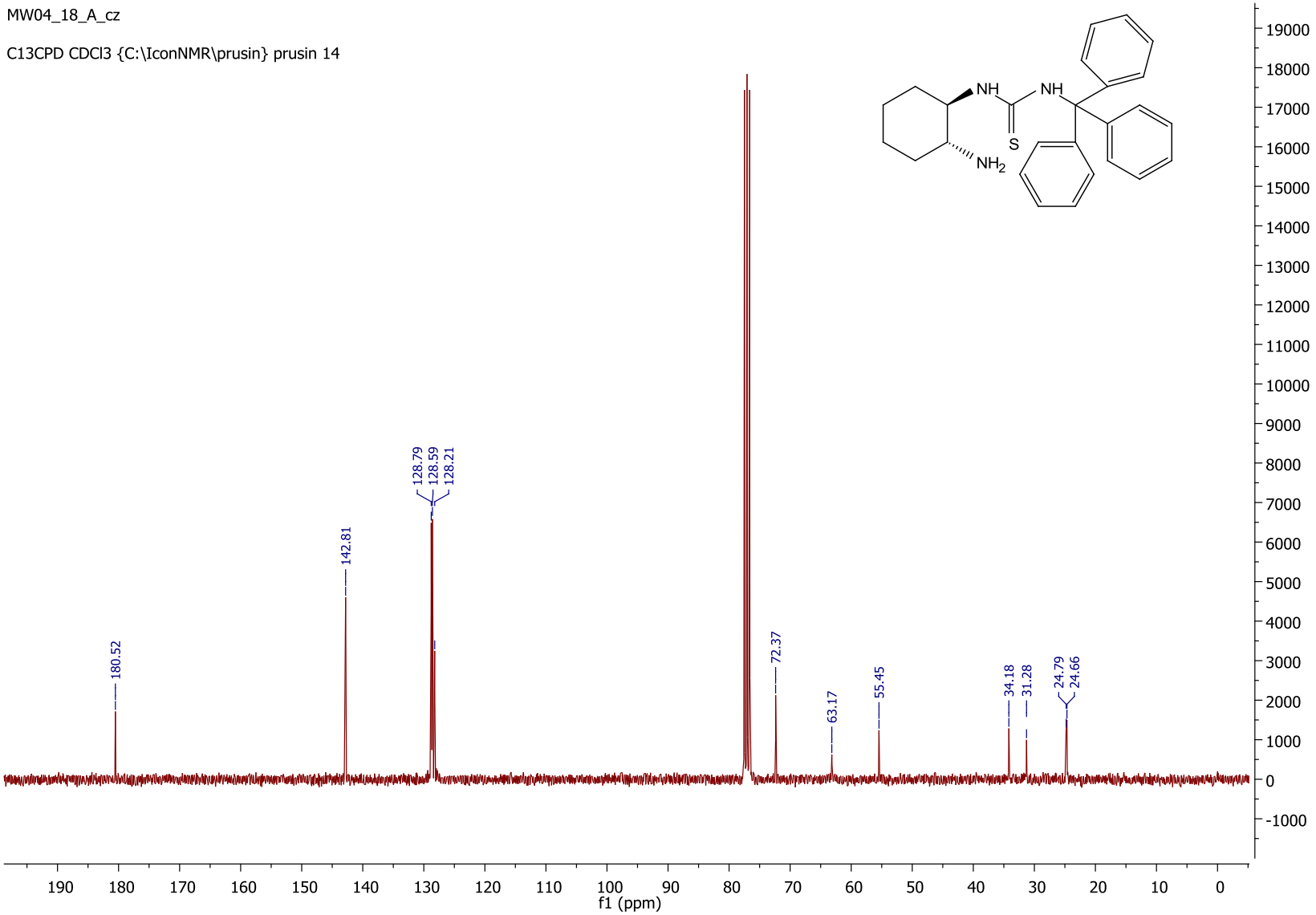

NP73_18_cz
PROTON CDCl3 {C:\IconNMR\prusin} prusin 7
CH3
HN
NH
S
7.38 7.37 7.37 7.35 7.35 7.34 7.33 7.32 7.31 7.30 7.29 7.28 7.28 7.27 7.27 7.20
5.10 5.07
4.24 4.21 4.19 4.19 4.17 4.17 4.14 4.12
1.61 1.60 1.56 1.54
1.20 1.16 1.05 1.04 1.01 1.00 0.97 0.96 0.95 0.94 0.92 0.91 0.90 0.73 0.69 0.66 0.64 0.48 0.45 0.44 0.41 0.40 0.38 0.36
16.26 1.09 1.00 1.08 3.77 2.11 4.13 0.97 3.49 1.07
f1 (ppm)

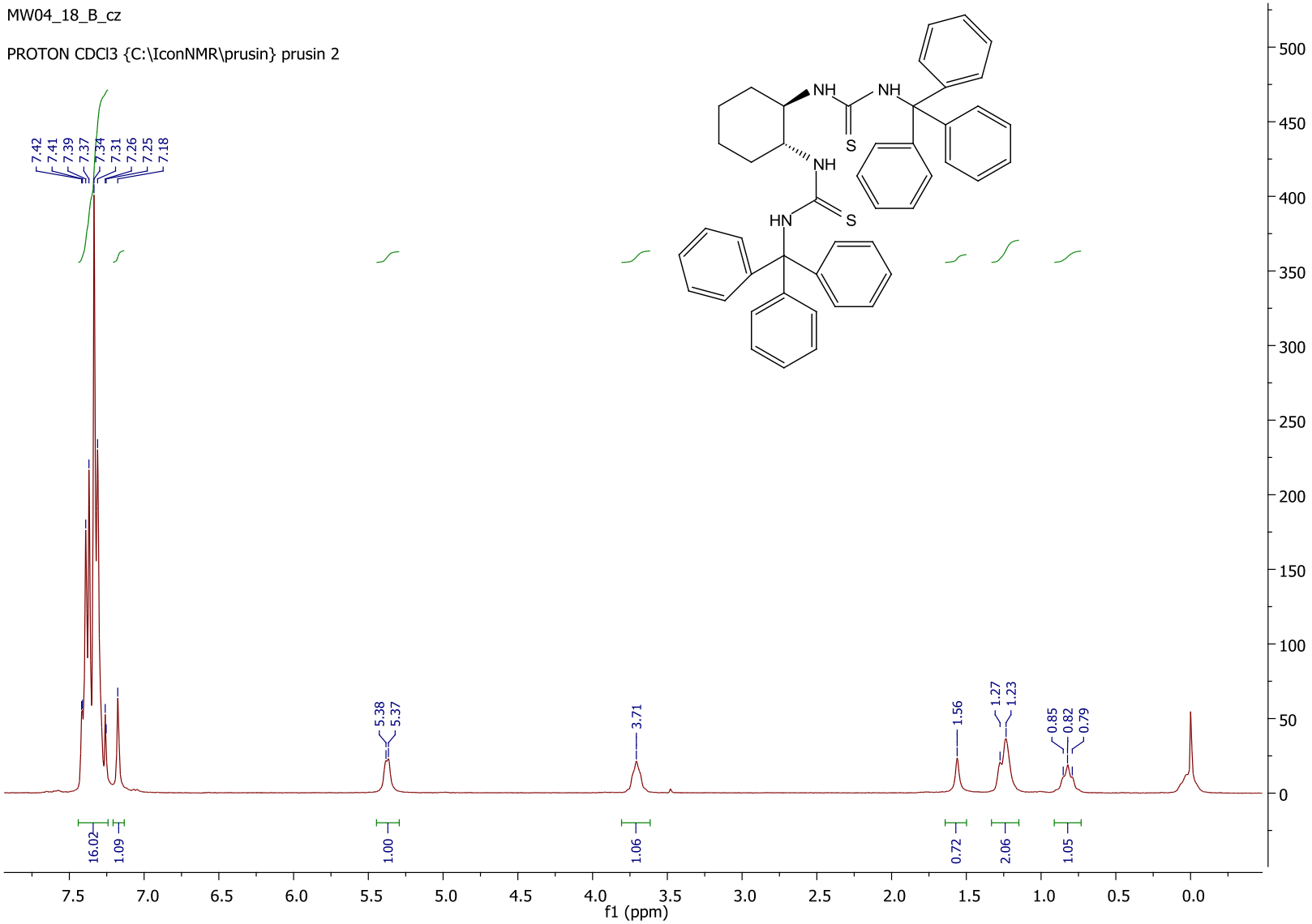

NP73_18_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 7
CH3
HN
NH
S
179.60
142.91
128.70
128.00
72.25
56.34
42.72
28.58
28.52
26.19
26.13
26.03
16.49
f1 (ppm)

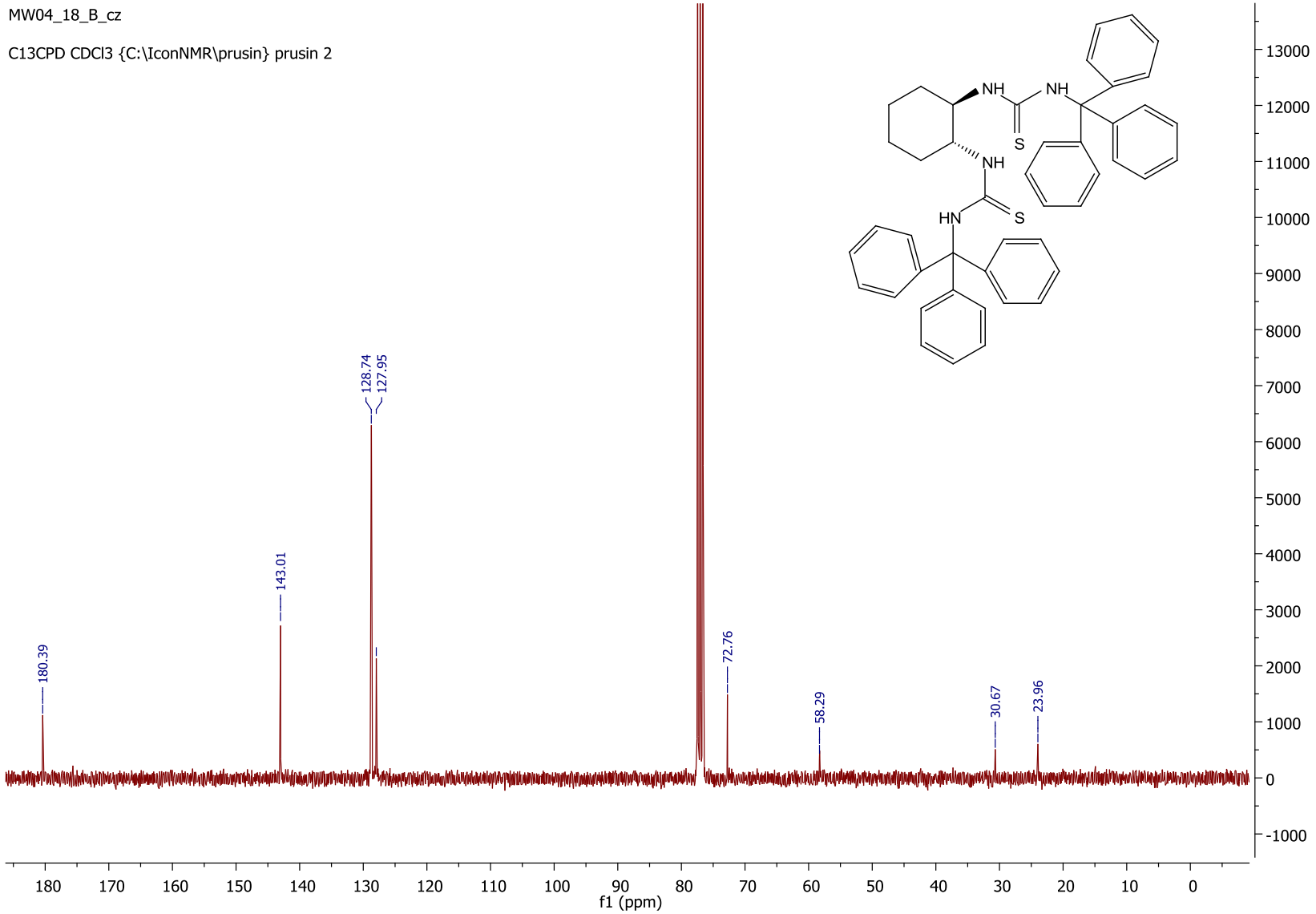

AAJ00002DA-H1
1.66
1.47
1.42
1.37
1.18
1.16
0.98
5.99
5.55
5.52
4.35
0.90
0.91
0.85
9.00
3.02
9.00
f1 (ppm)

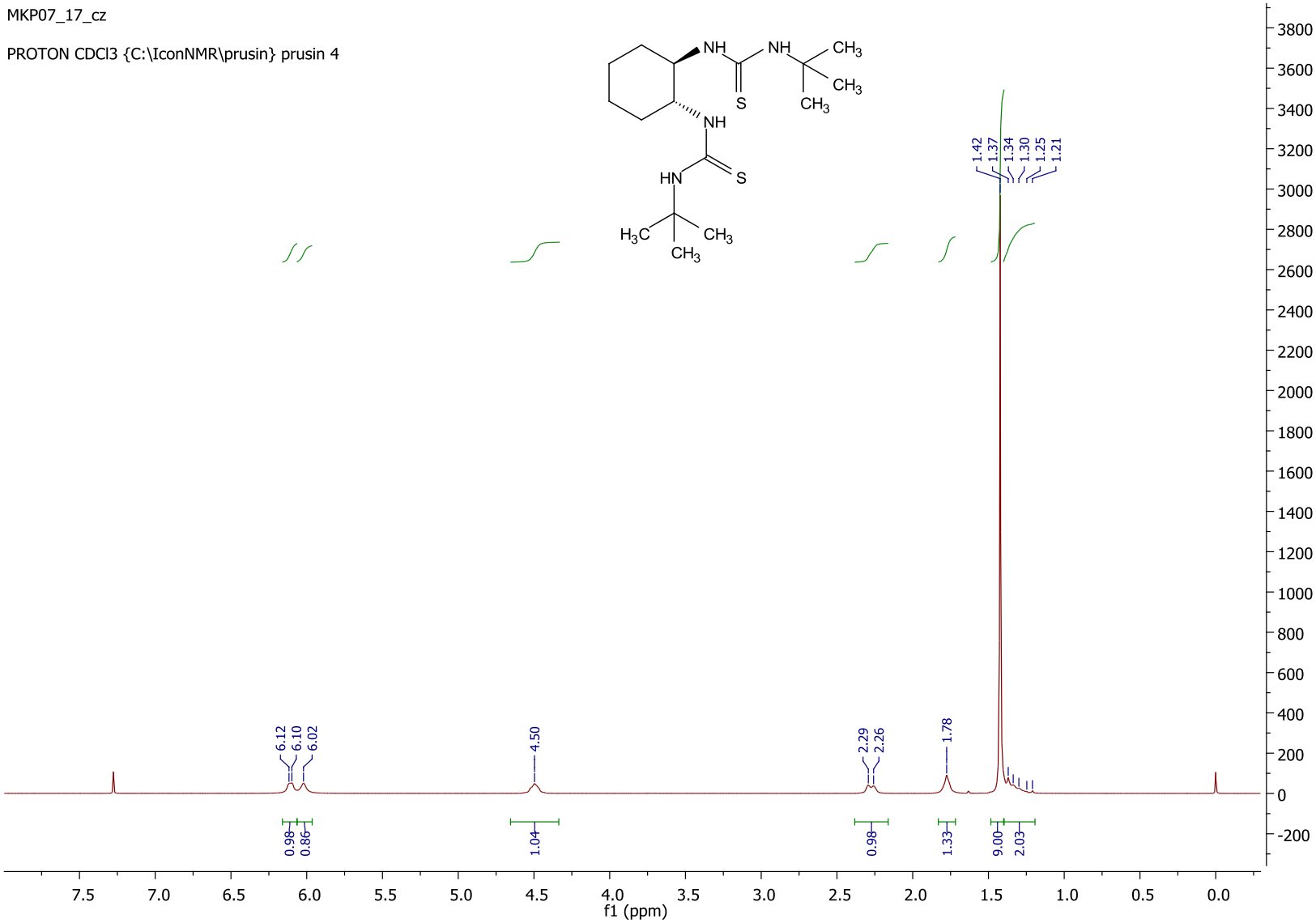

AAJ00002DA-C13
180.57
59.87
52.32
34.50
29.80
26.47
15.71
f1 (ppm)

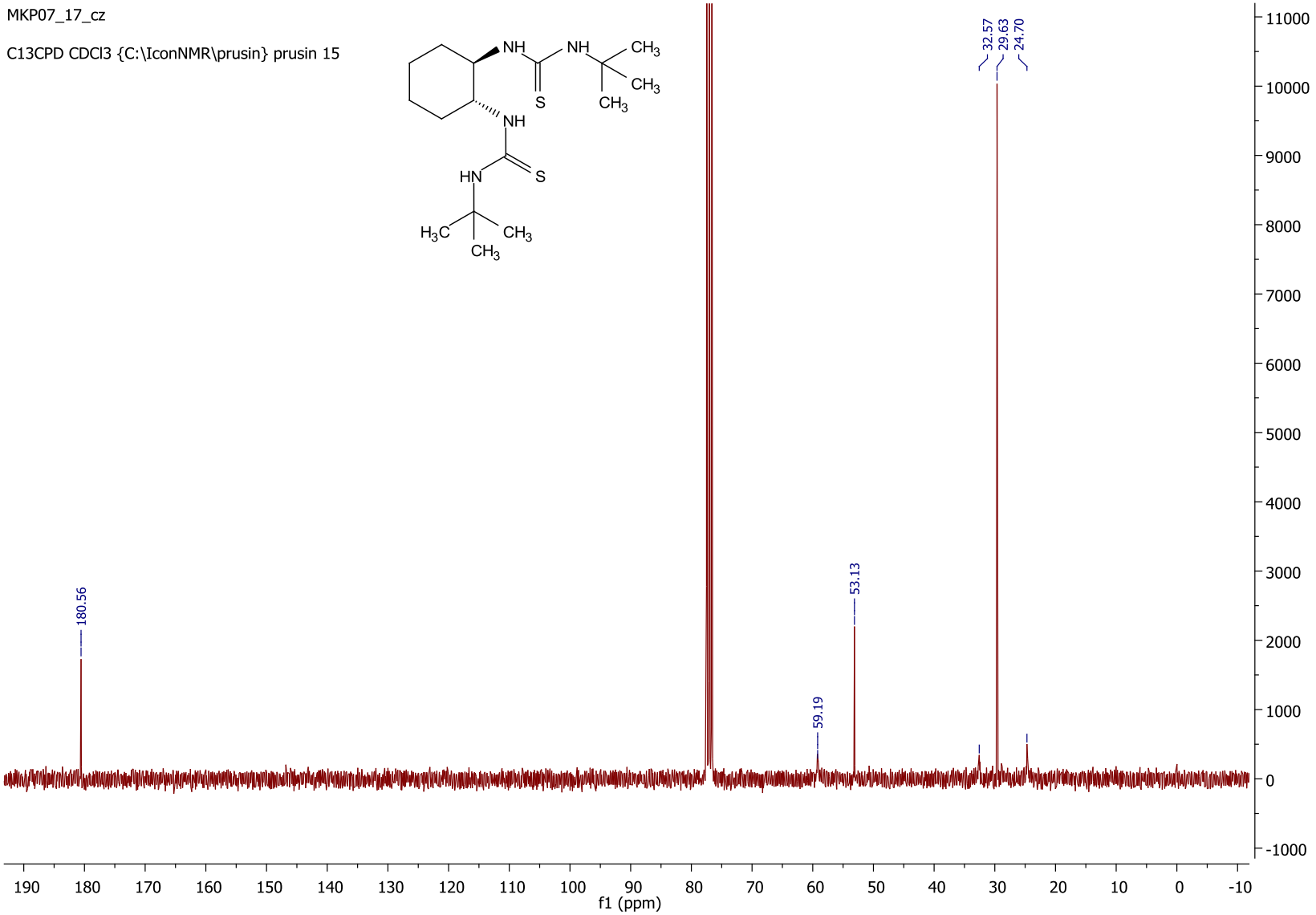

MW04_18_A_cz
PROTON CDCl3 {C:\IconNMR\prusin} prusin 3
NH
NH
S
NH2
7.41 7.40 7.39 7.38 7.37 7.37 7.35 7.35 7.33 7.32 7.32 7.31 7.30 7.30 7.29 7.27
5.01 4.98
3.95 3.94 3.92 3.91 3.88 3.87 3.85 3.84
1.82 1.81 1.77 1.75 1.73 1.67 1.65 1.59 1.58 1.56 1.55 1.54 1.50 1.49
1.22 1.21 1.19 1.18 1.04 1.00
0.51 0.50 0.47 0.46 0.43 0.42 0.39 0.38
16.06
1.00
1.06
5.20
3.11
2.05
1.06
f1 (ppm)

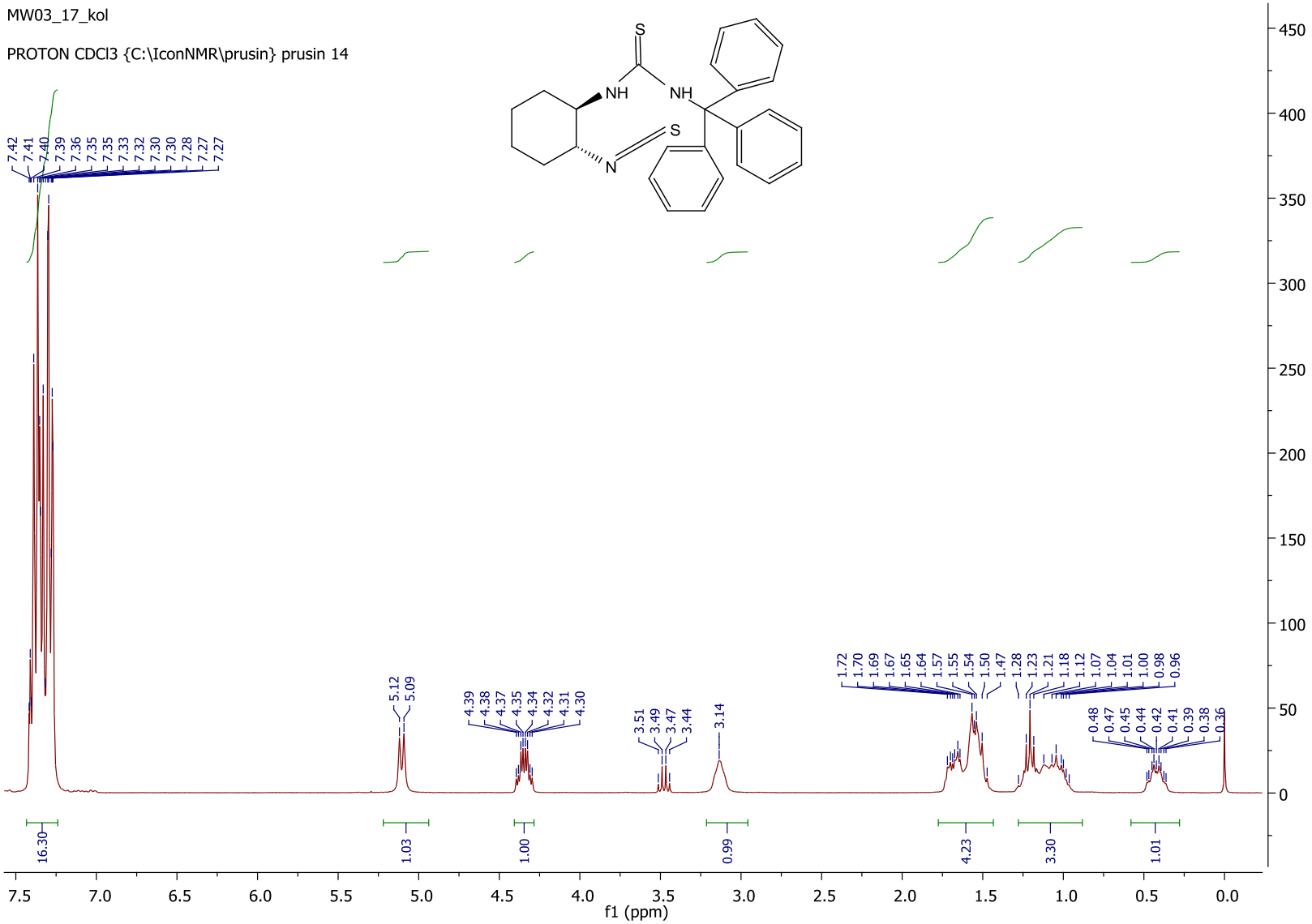

MW04_18_A_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 14
NH
NH
S
NH2
180.52
142.81
128.79
128.59
128.21
72.37
63.17
55.45
34.18
31.28
24.79
24.66
f1 (ppm)

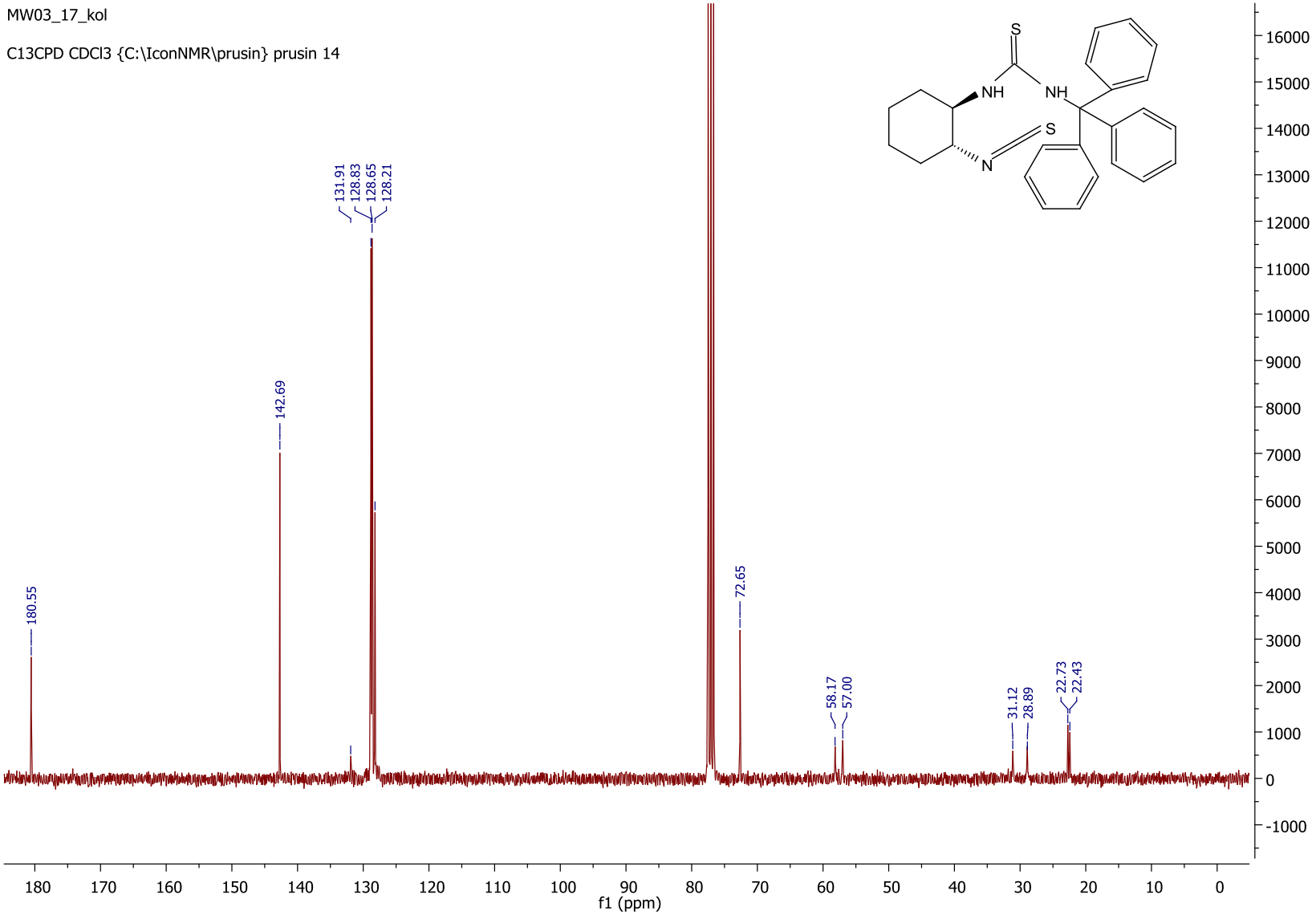

MW04_18_B_cz
PROTON CDCl3 {C:\IconNMR\prusin} prusin 2
7.42
7.41
7.39
7.37
7.34
7.31
7.26
7.25
7.18
5.38
5.37
3.71
1.56
1.27
1.23
0.85
0.82
0.79
16.02
1.09
1.00
1.06
0.72
2.06
1.05
NH
NH
S
NH
HN
S
f1 (ppm)

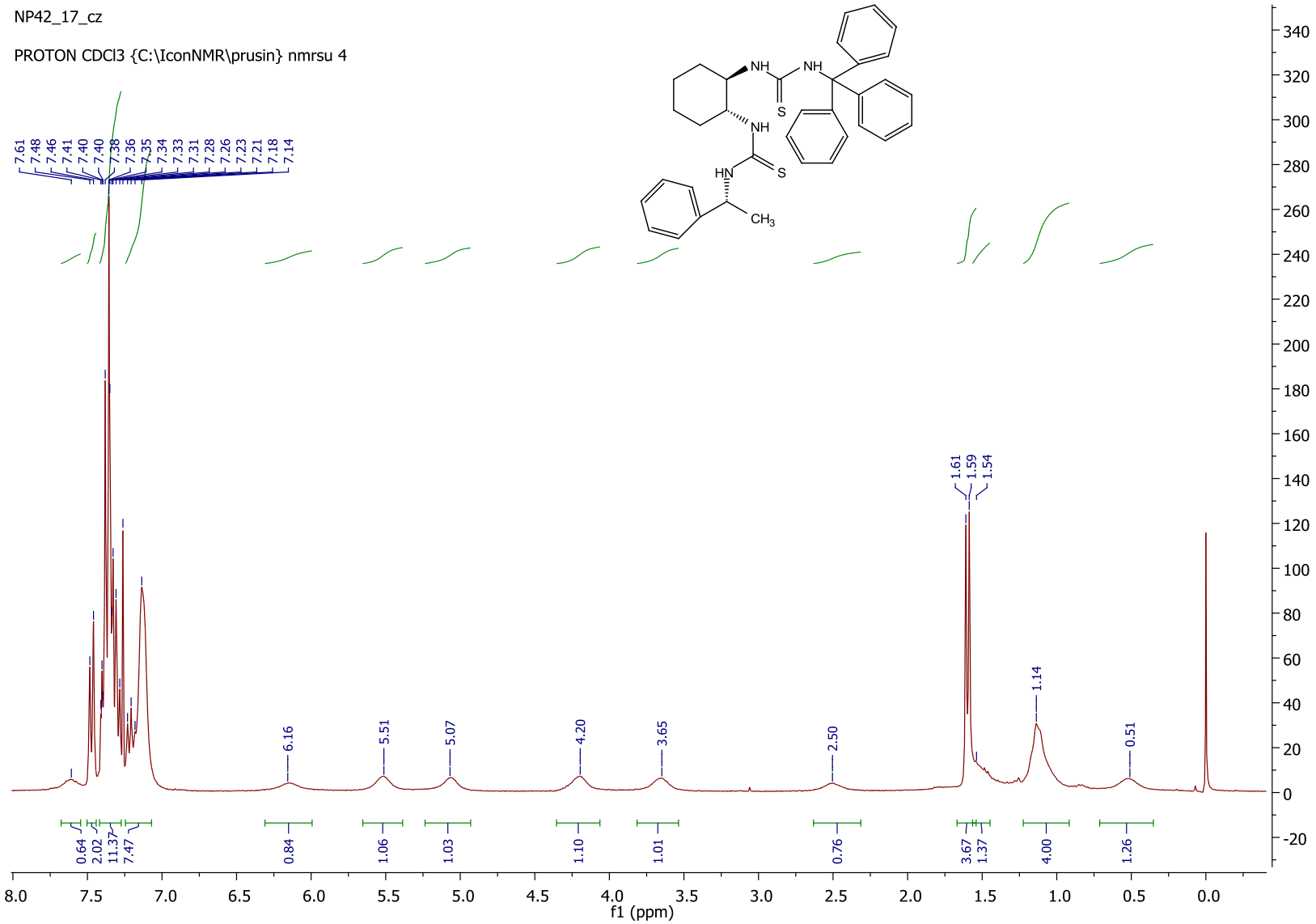

MW04_18_B_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 2
NH
NH
S
NH
HN
S
180.39
143.01
128.74
127.95
72.76
58.29
30.67
23.96
f1 (ppm)

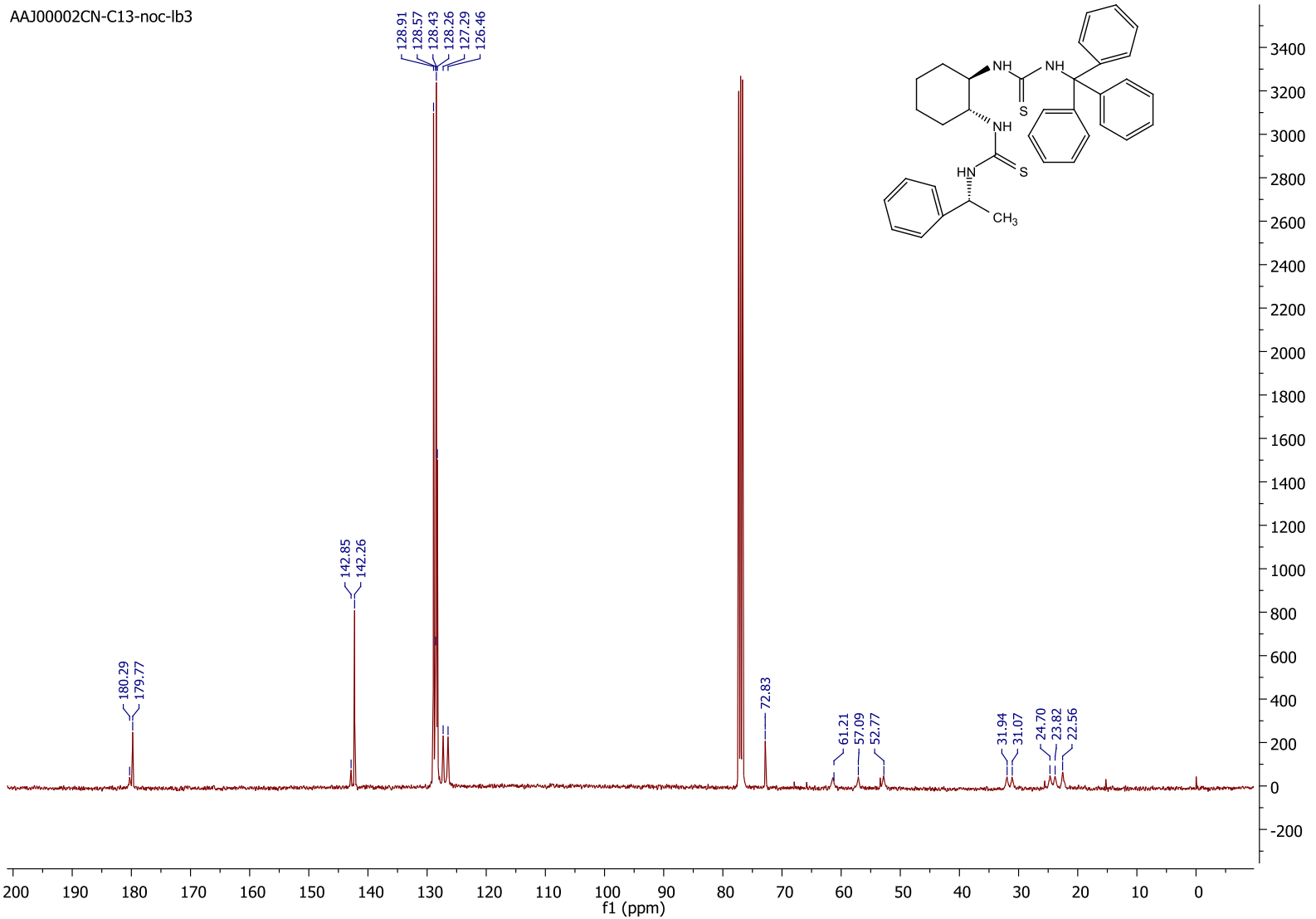

MKP07_17_cz
PROTON CDCl3 {C:\IconNMR\prusin} prusin 4
NH
NH
CH3
CH3
CH3
S
NH
HN
S
H3C
CH3
CH3
1.42
1.37
1.34
1.30
1.25
1.21
6.12
6.10
6.02
4.50
2.29
2.26
1.78
0.98
0.86
1.04
0.98
1.33
9.00
2.03
f1 (ppm)

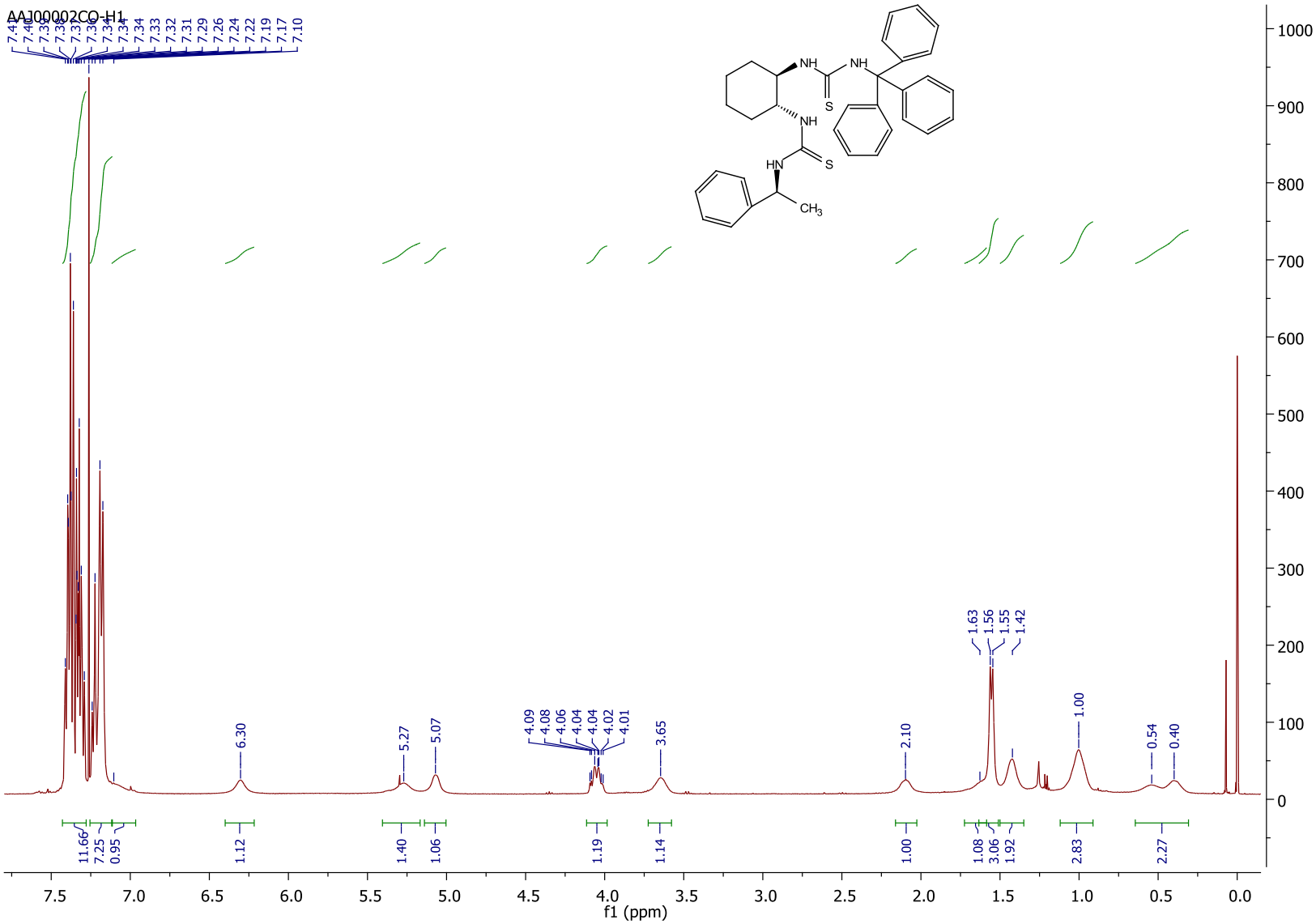

MKP07_17_cz
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 15
NH
NH
CH3
CH3
CH3
S
NH
HN
S
H3C
CH3
CH3
180.56
59.19
53.13
32.57
29.63
24.70
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

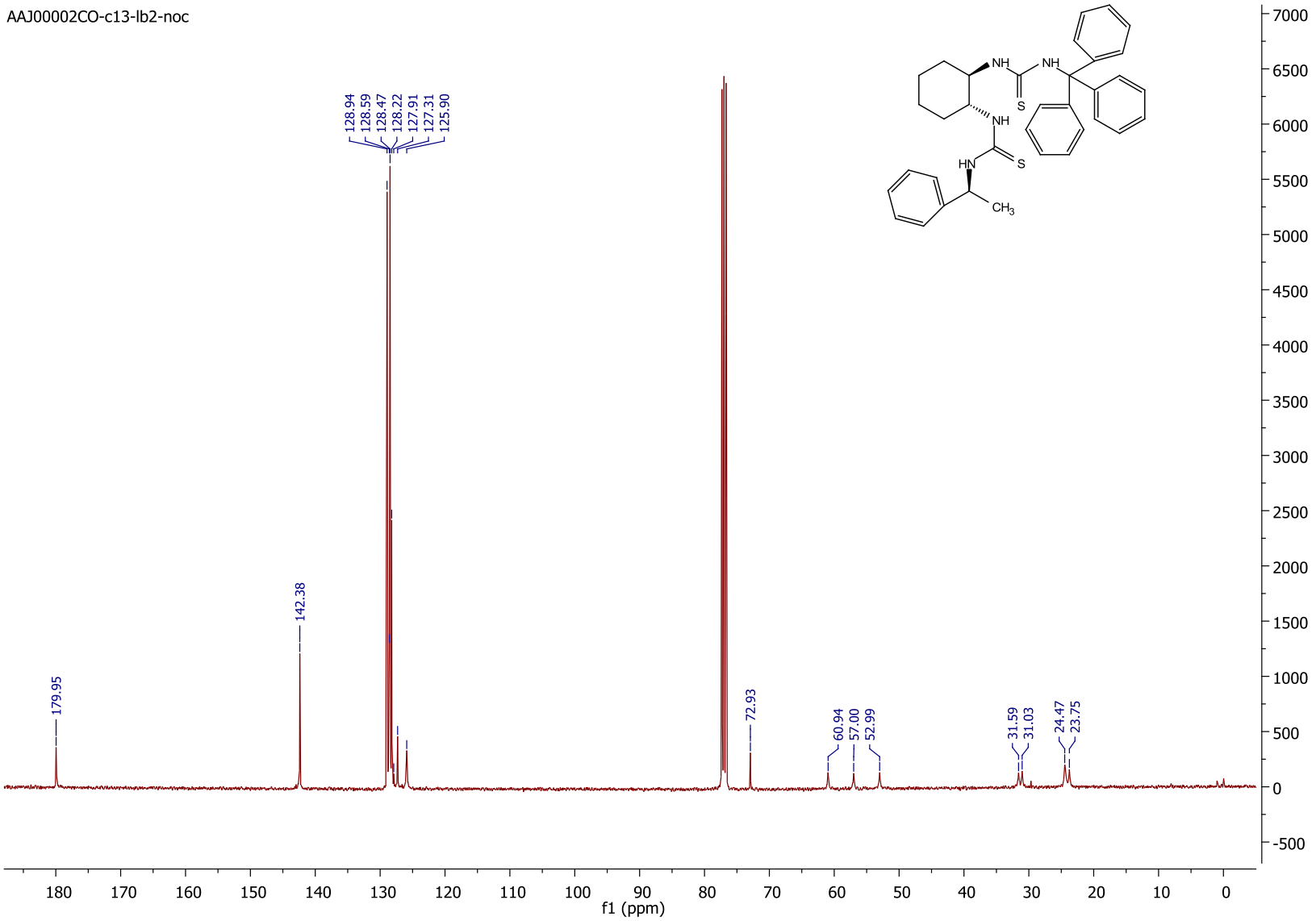

MW03_17_kol
PROTON CDCl3 {C:\IconNMR\prusin} prusin 14
S
NH
NH
S
N
7.42
7.41
7.40
7.39
7.36
7.35
7.35
7.33
7.32
7.30
7.30
7.28
7.27
7.27
5.12
5.09
4.39
4.38
4.37
4.35
4.34
4.32
4.31
4.30
3.51
3.49
3.47
3.44
3.14
1.72
1.70
1.69
1.67
1.65
1.64
1.57
1.55
1.54
1.50
1.47
1.28
1.23
1.21
1.18
1.12
1.07
1.04
1.01
1.00
0.98
0.96
0.48
0.47
0.45
0.44
0.42
0.41
0.39
0.38
0.36
16.30
1.03
1.00
0.99
4.23
3.30
1.01
f1 (ppm)

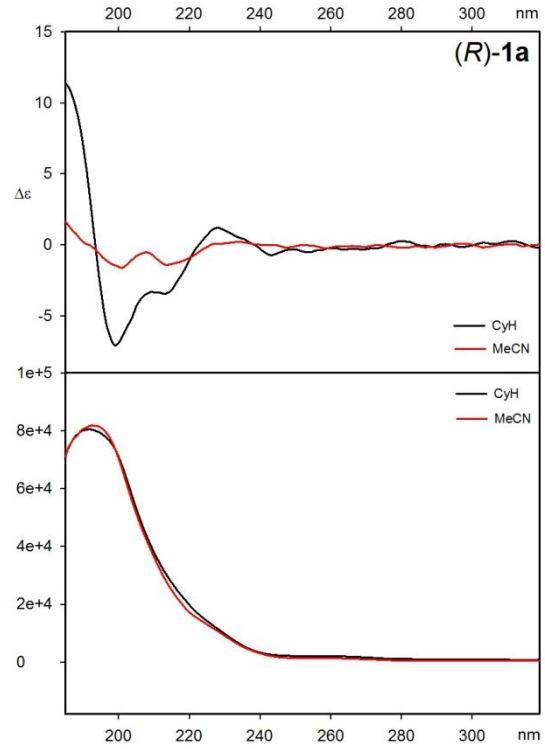

MW03_17_kol
C13CPD CDCl3 {C:\IconNMR\prusin} prusin 14
S
NH
NH
S
N
131.91
128.83
128.65
128.21
142.69
180.55
72.65
58.17
57.00
31.12
28.89
22.73
22.43
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


NP42_17_cz
PROTON CDCl3 {C:\IconNMR\prusin} nmrsu 4
NH
NH
S
NH
HN
S
CH3
7.61
7.48
7.46
7.41
7.40
7.40
7.38
7.36
7.35
7.34
7.33
7.31
7.28
7.26
7.23
7.21
7.18
7.14
6.16
5.51
5.07
4.20
3.65
2.50
1.61
1.59
1.54
1.14
0.51
0.64
2.02
11.37
7.47
0.84
1.06
1.03
1.10
1.01
0.76
3.67
1.37
4.00
1.26
f1 (ppm)


AAJ00002CN-C13-noc-lb3
128.91
128.57
128.43
128.26
127.29
126.46
142.85
142.26
180.29
179.77
72.83
61.21
57.09
52.77
31.94
31.07
24.70
23.82
22.56
NH
NH
S
NH
HN
S
CH3
f1 (ppm)


AA100002CO-H1
NH
NH
S
NH
HN
S
CH3
f1 (ppm)


AAJ00002CO-c13-lb2-noc
128.94
128.59
128.47
128.22
127.91
127.31
125.90
179.95
142.38
72.93
60.94
57.00
52.99
31.59
31.03
24.47
23.75
NH
NH
S
NH
HN
S
CH3
f1 (ppm)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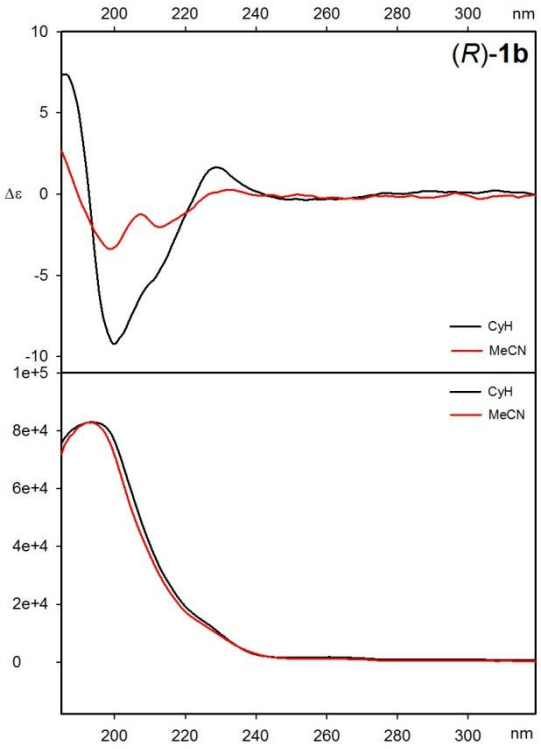
Δε
nm
CyH
MeCN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Δε
nm
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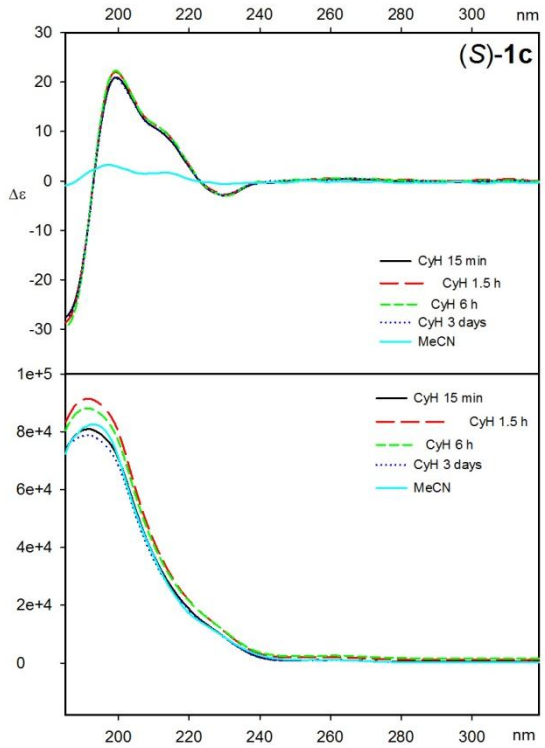
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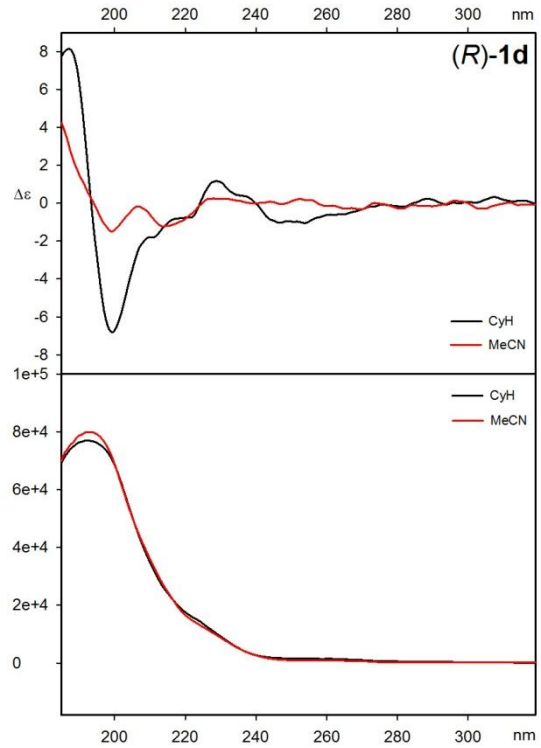
Δε
nm
CyH 15 min
CyH 1.5 h
CyH 6 h
CyH 3 days
MeCN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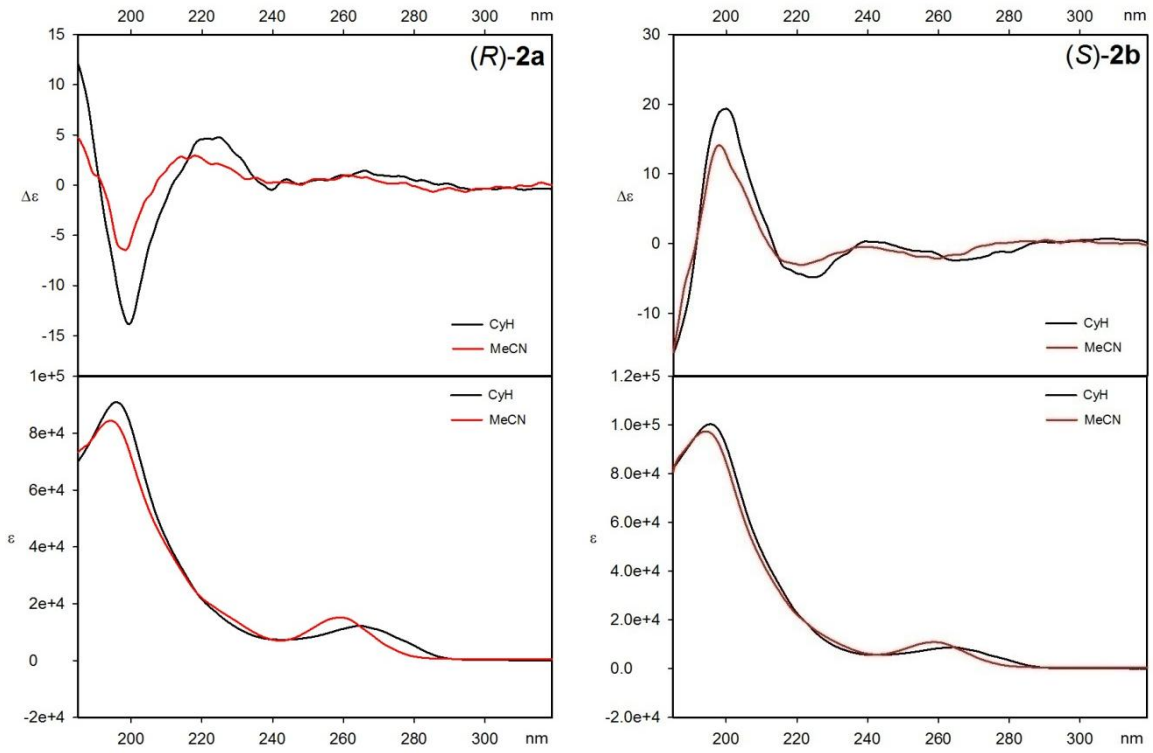
Δε
nm
CyH
MeCN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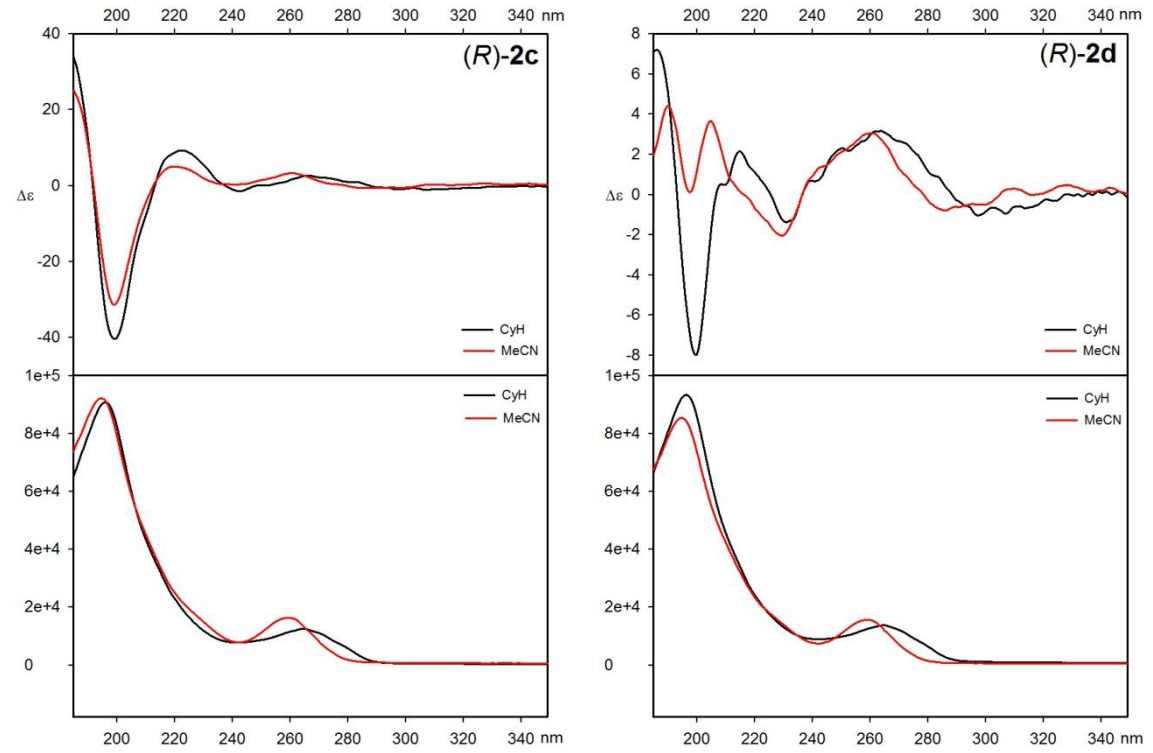
(S)-2b
CyH
MeCN
Δε
ε
nm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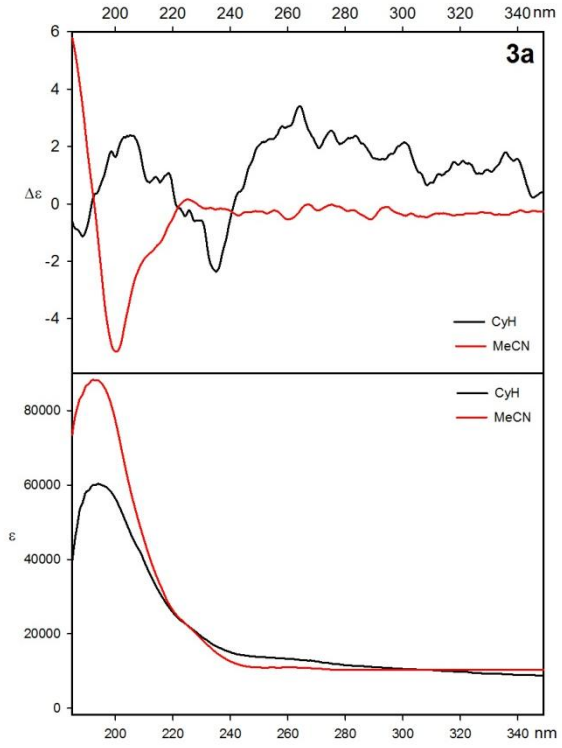
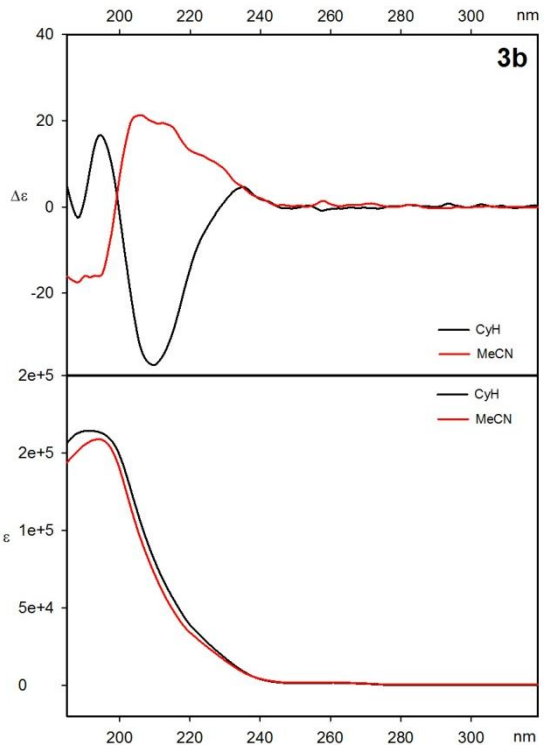
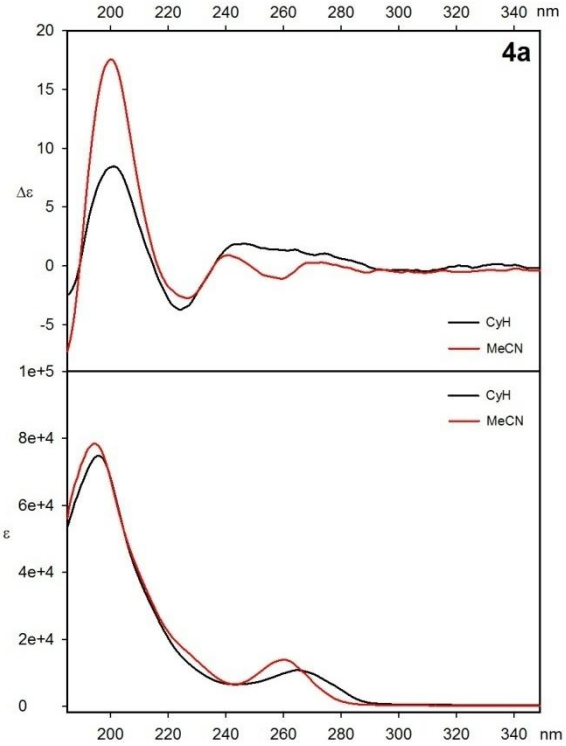
(R)-2d
CyH
MeCN
Δε
ε
nm


3a
Δε
ε
CyH
MeCN
nm


3b
Δε
ε
CyH
MeCN
nm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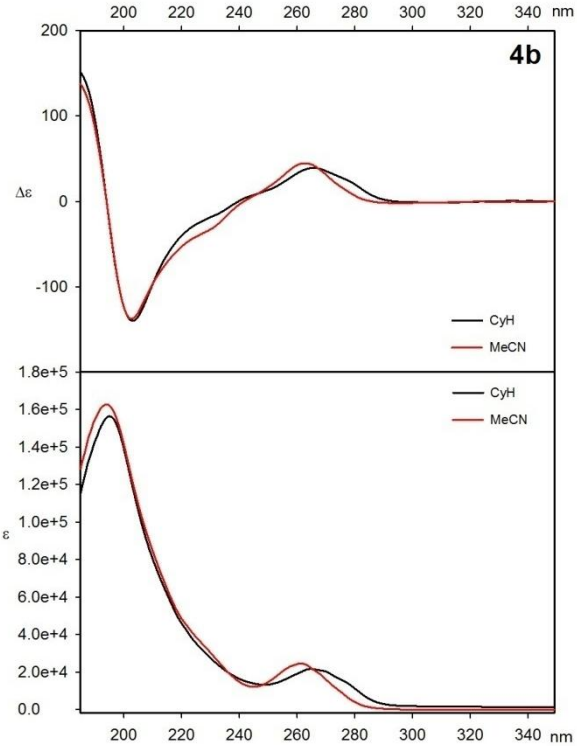
Δε
ε
CyH
MeCN
nm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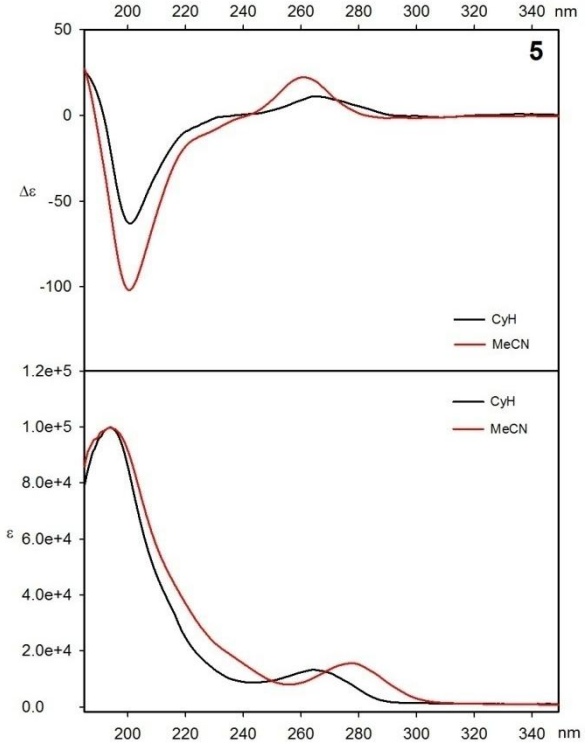
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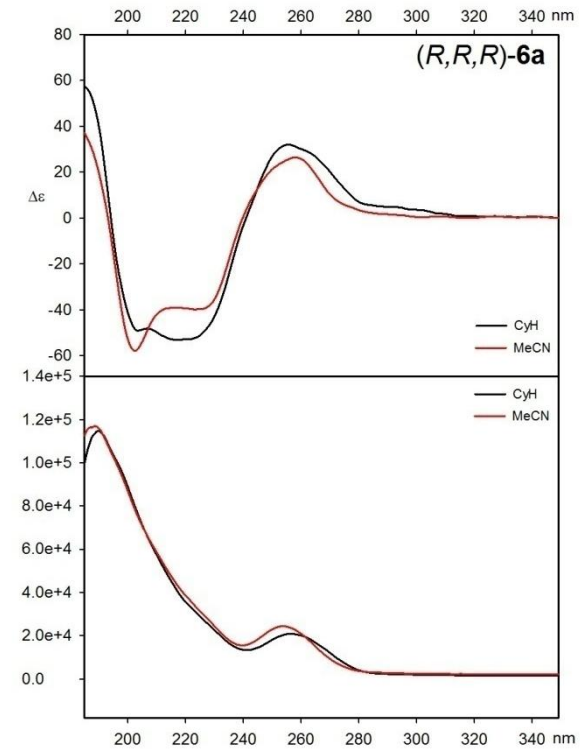
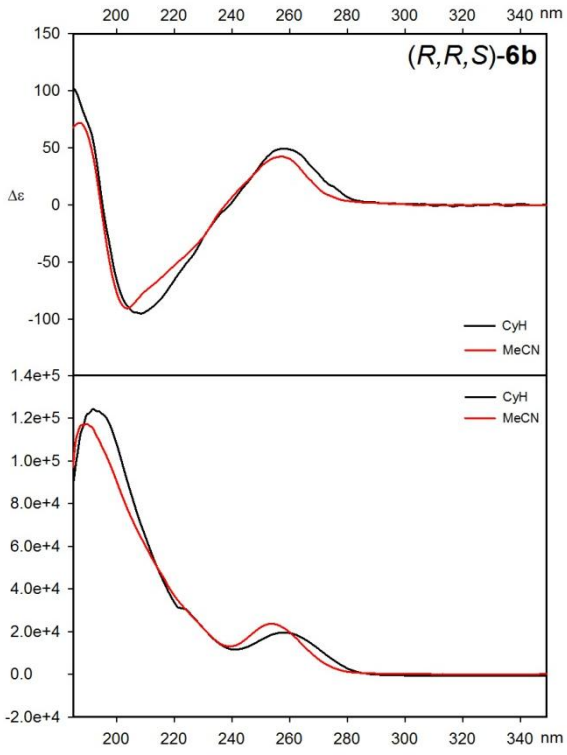
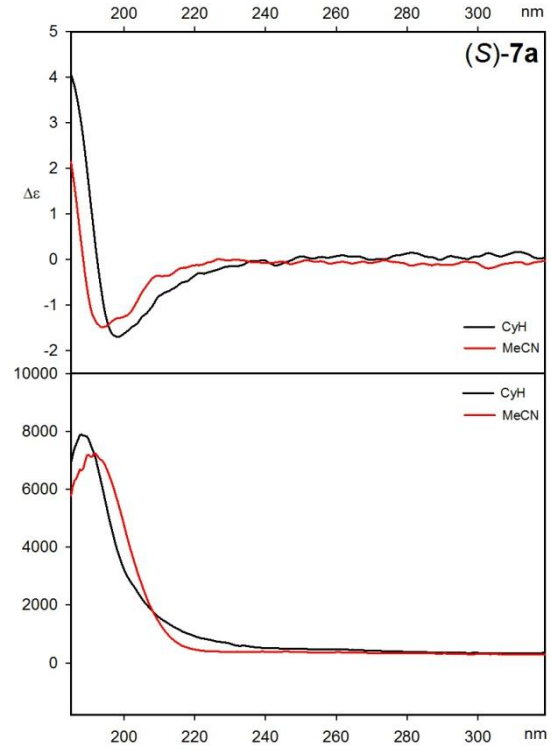
Δε
ε
CyH
MeCN
nm


(R,R,R)-6a
Δε
CyH
MeCN
nm


(R,R,S)-6b
Δε
CyH
MeCN
nm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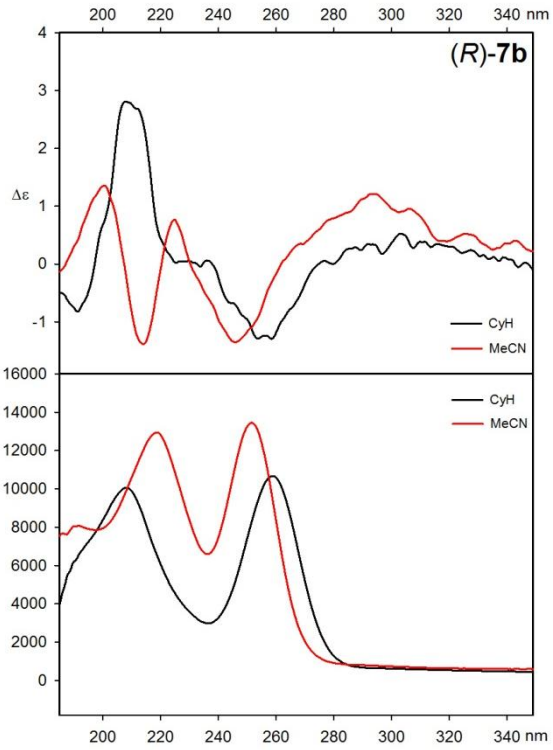
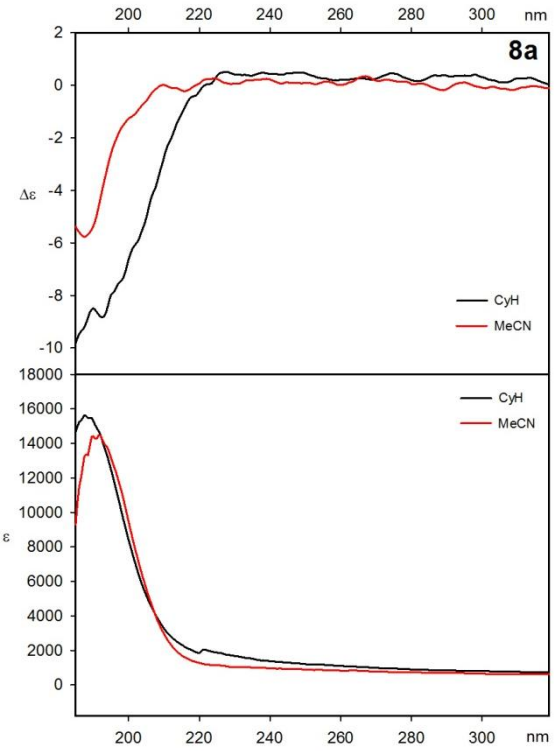
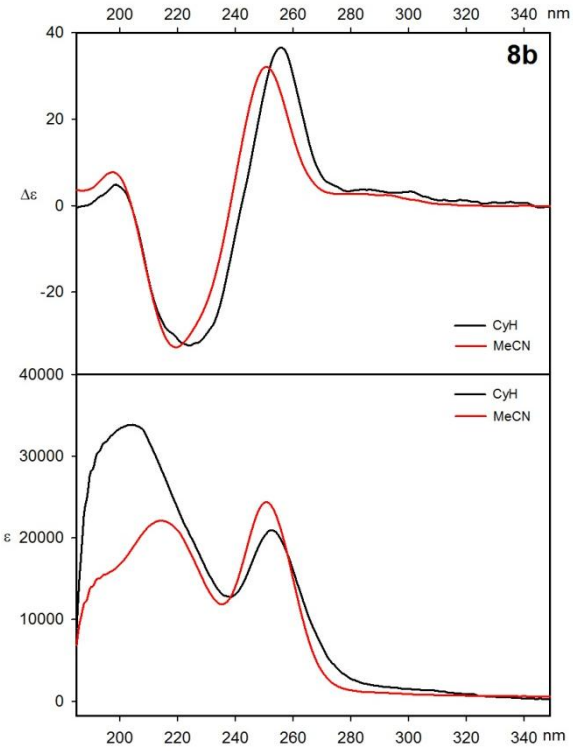
Δε
ε
nm
CyH
MeCN


(R)-7b
Δε
ε
nm
CyH
MeCN


8a
Δε
ε
nm
CyH
MeCN


8b
Δε
ε
nm
CyH
MeCN

Cartesian coordinates for all calculated structures

1c (conf. 1)

C	-4.36777800	1.38163700	-0.40539600
C	-4.80078900	0.12406500	0.37221000
C	-5.03462900	0.49689800	1.84871900
C	-6.11961900	-0.39261000	-0.23574600
C	-3.69200000	-0.96860500	0.21797200
C	-4.02683700	-2.33483300	0.83607100
N	-2.39928000	-0.49701600	0.72780500
C	-1.25391300	-0.55849300	-0.04823700
O	-1.27188600	-0.79292600	-1.24581100
C	1.22722700	0.01230600	0.06493100
C	1.97199200	-1.24969000	-0.43713100
C	1.32426800	-2.46807200	-0.64814700
C	2.03223100	-3.58679900	-1.09001300
C	3.40010900	-3.50809700	-1.33281400
C	4.05829200	-2.29663700	-1.12622100
C	3.35138300	-1.18402100	-0.67913500
C	2.06207200	0.58875300	1.24329000
C	2.18225700	-0.17341800	2.41606500
C	2.93323900	0.28275400	3.49479400
C	3.59920100	1.50608800	3.41791900
C	3.50539300	2.25983500	2.25271200
C	2.74158900	1.80675600	1.17471900
C	1.02074000	1.06233200	-1.05456700
C	0.26648300	2.20949500	-0.77222500
C	0.05378100	3.18828500	-1.73679900
C	0.59257000	3.04028700	-3.01486900
C	1.33607600	1.90279300	-3.31000000
C	1.54694900	0.92235700	-2.33878600
N	-0.08735400	-0.33504300	0.66924600
H	-3.43056100	1.78682400	-0.01914300
H	-4.21975500	1.15741900	-1.46578100
H	-5.13359300	2.15950400	-0.32823500
H	-5.36578200	-0.35990900	2.44247200
H	-4.13009200	0.90627800	2.30891000
H	-5.80976800	1.26501000	1.92626500
H	-5.97252600	-0.73953300	-1.26354400
H	-6.54857700	-1.21488600	0.34202300
H	-6.86163300	0.41070400	-0.26094200
H	-3.53152700	-1.10901500	-0.85294700
H	-4.15025000	-2.27298000	1.92207300
H	-4.94297600	-2.75611000	0.41870900
H	-3.21491200	-3.03646000	0.63050200
H	-2.28005600	-0.52243100	1.72996800
H	0.26014000	-2.54972200	-0.48691700
H	1.50461200	-4.52104000	-1.24836600
H	3.94827000	-4.37843300	-1.67600500
H	5.12515100	-2.21761300	-1.30440900

H	3.88480500	-0.25614200	-0.50910600
H	1.70342800	-1.14449700	2.47404000
H	3.01038400	-0.32419400	4.39018500
H	4.18995000	1.86132000	4.25474200
H	4.02589600	3.20800900	2.17468900
H	2.68094900	2.41021900	0.27918000
H	-0.16416200	2.34023500	0.21418700
H	-0.53582800	4.06508000	-1.49202500
H	0.42546900	3.79912700	-3.77112100
H	1.74807100	1.76456400	-4.30359500
H	2.10965600	0.03706500	-2.60060900
H	-0.20496900	0.01923200	1.60605500

1c (conf. 13)

C	-3.96134000	1.75041800	-1.28523700
C	-4.22550400	0.53849400	-0.37150400
C	-4.05184200	0.96440400	1.09827500
C	-5.67726700	0.07104400	-0.59823400
C	-3.24134700	-0.61381900	-0.76209100
C	-3.46185200	-1.93886800	-0.01739800
N	-1.83669500	-0.20528300	-0.61882900
C	-0.98065000	-0.19705300	-1.68859600
O	-1.35600200	-0.32346800	-2.85073500
C	1.17879900	-0.01360700	-0.19680500
C	1.07385000	1.31915600	0.59239600
C	1.94249900	1.56482700	1.66626800
C	1.89319200	2.76359500	2.37033500
C	0.97910300	3.75338400	2.00802200
C	0.12634200	3.52963800	0.93251200
C	0.17579300	2.32386000	0.22926300
C	2.65719300	-0.12296900	-0.66628000
C	3.13770600	0.81288300	-1.59469100
C	4.45758000	0.77525000	-2.03200900
C	5.33505000	-0.18813500	-1.53457000
C	4.87565000	-1.10658700	-0.59692200
C	3.54724000	-1.07581900	-0.16706100
C	0.76721600	-1.24904000	0.64739100
C	0.71114000	-2.49946100	0.01165000
C	0.34693000	-3.64542000	0.70810800
C	0.01824400	-3.57024600	2.06295400
C	0.05682500	-2.33743500	2.70300000
C	0.42930300	-1.18656000	2.00163100
N	0.37214900	0.01889300	-1.43808900
H	-2.94614800	2.13137400	-1.15895400
H	-4.08771100	1.48634100	-2.33886900
H	-4.65771400	2.56169300	-1.05174300
H	-4.26048600	0.14310000	1.78953700
H	-3.03952600	1.32966300	1.29341900
H	-4.74326700	1.77723200	1.34033200
H	-5.81695000	-0.31094700	-1.61472600
H	-5.97480900	-0.71244400	0.10275400
H	-6.36693400	0.90935700	-0.46260400

H	-3.37363100	-0.79308200	-1.83070000
H	-3.30092400	-1.83571300	1.05984000
H	-4.47155500	-2.32269500	-0.17196700
H	-2.75815900	-2.68759900	-0.38718400
H	-1.43589300	-0.27273600	0.30434000
H	2.67855500	0.81961100	1.94489900
H	2.57758600	2.92962000	3.19500300
H	0.94274700	4.69061600	2.55180900
H	-0.57938200	4.29486200	0.62858000
H	-0.48059300	2.17614500	-0.61634900
H	2.47980800	1.59020000	-1.96679300
H	4.80307600	1.50628600	-2.75443500
H	6.36502900	-0.21665300	-1.87151600
H	5.54734700	-1.85729800	-0.19540800
H	3.21368600	-1.80462500	0.55953500
H	0.94839600	-2.57109800	-1.04322800
H	0.31409100	-4.59849600	0.19192400
H	-0.27000000	-4.46263100	2.60695700
H	-0.20438400	-2.25948700	3.75261500
H	0.44576900	-0.23982100	2.52441800
H	0.89270000	-0.03991600	-2.29960500

1c (conf. 37)

C	3.95094700	-1.41396300	-1.33962100
C	4.23115000	-0.21496800	-0.41332300
C	4.14644700	-0.67599400	1.05341900
C	5.65663400	0.29698700	-0.70385600
C	3.20147000	0.92300500	-0.72657700
C	3.39235700	2.21034600	0.08949400
N	1.81167500	0.47332000	-0.59207700
C	0.97308100	0.35859300	-1.66506900
O	1.34270900	0.51818100	-2.82601200
C	-1.16593200	-0.06167700	-0.19060100
C	-0.47220900	-1.05634900	0.77721400
C	-0.21971600	-0.78360600	2.12410000
C	0.40333500	-1.73013200	2.94367200
C	0.78458200	-2.96386100	2.42996900
C	0.55089800	-3.24302800	1.08217100
C	-0.06330900	-2.29884800	0.26813100
C	-2.55260200	-0.60222900	-0.64677700
C	-3.16353900	-1.71910400	-0.07400900
C	-4.42414300	-2.14214900	-0.50146800
C	-5.09321900	-1.45842500	-1.51055600
C	-4.49828300	-0.33362100	-2.08175500
C	-3.24859100	0.09426100	-1.64622900
C	-1.43730200	1.32464200	0.45651000
C	-0.83455000	2.49396100	-0.01052400
C	-1.12908900	3.73226000	0.56480700
C	-2.03626100	3.82426000	1.61464900
C	-2.65916100	2.66567900	2.07928900
C	-2.36724600	1.43441500	1.50166800
N	-0.35980100	0.03876300	-1.42376200

H	3.99476000	-1.11986500	-2.39176500
H	4.69335000	-2.20080300	-1.17371700
H	2.96262900	-1.83945900	-1.15508500
H	4.85827200	-1.48721500	1.23437500
H	3.15252800	-1.05861900	1.30166000
H	4.38824700	0.13059400	1.75120100
H	5.73470500	0.69720900	-1.71986500
H	5.96764500	1.07821500	-0.00608800
H	6.37534700	-0.52304400	-0.61598400
H	3.31322700	1.16459700	-1.78512800
H	3.21876400	2.04724100	1.15717900
H	4.39810600	2.61679500	-0.02892900
H	2.68340900	2.96858100	-0.24985400
H	1.44691200	0.32207100	0.33526600
H	-0.50066300	0.17042800	2.54904800
H	0.59013700	-1.49162300	3.98487000
H	1.26726900	-3.69758800	3.06557400
H	0.85355000	-4.19628900	0.66326300
H	-0.22610600	-2.51960100	-0.77978500
H	-2.66304700	-2.27224500	0.70936300
H	-4.87692600	-3.01339400	-0.04116700
H	-6.06906200	-1.79128400	-1.84540500
H	-5.01207800	0.21923200	-2.86022200
H	-2.82249400	0.99403500	-2.07660000
H	-0.14180100	2.45398900	-0.83934500
H	-0.64831700	4.62521800	0.18076600
H	-2.26658100	4.78602100	2.05887500
H	-3.38335600	2.72170300	2.88456300
H	-2.88412800	0.55069000	1.85764700
H	-0.86357400	-0.02834800	-2.29409900

2c

C	3.82598400	1.91260300	-0.64344200
C	4.05979000	0.55033100	0.03773700
C	3.72406100	0.66738900	1.53718000
C	5.54945800	0.18269400	-0.11792000
C	3.19055200	-0.53218200	-0.67969300
C	3.41764200	-1.97747400	-0.21289900
N	1.75478900	-0.21712000	-0.58906700
C	0.89556400	-0.22243300	-1.63289500
S	1.36817100	-0.34766100	-3.25682900
C	-1.21420800	-0.02931400	-0.09998300
C	-2.70327000	-0.19310400	-0.51743700
C	-3.22450100	0.66178400	-1.50007900
C	-4.55599500	0.57349200	-1.89238700
C	-5.40352800	-0.35844100	-1.29396900
C	-4.90324300	-1.19499700	-0.30203100
C	-3.56311100	-1.11518100	0.08225400
C	-0.75953300	-1.19508900	0.81611700
C	-0.39472400	-1.03576600	2.15561800
C	0.00817900	-2.13200700	2.92427800
C	0.05118400	-3.40458200	2.36713800

C	-0.30246600	-3.57521700	1.02734400
C	-0.69726700	-2.48403800	0.26315600
C	-1.10302000	1.36484900	0.57055600
C	-1.92305900	1.67909500	1.66469900
C	-1.87455700	2.93532900	2.25996700
C	-1.01235900	3.91423800	1.76497000
C	-0.21157300	3.62184100	0.66646000
C	-0.25890800	2.35871500	0.07235000
N	-0.44401800	-0.08869500	-1.36865600
H	2.78590400	2.23083600	-0.55481600
H	4.07244600	1.86828400	-1.70789000
H	4.45344800	2.68082800	-0.18128800
H	3.87481100	-0.27713500	2.06694700
H	2.69199400	0.99200200	1.69995700
H	4.37046300	1.41327600	2.00932500
H	5.80866400	0.01313400	-1.16771100
H	5.81639800	-0.71364700	0.44674300
H	6.17591600	1.00019600	0.25039600
H	3.42165800	-0.47837000	-1.74435300
H	3.16271700	-2.11507100	0.84171500
H	4.45544400	-2.28302100	-0.35558000
H	2.78911100	-2.64856500	-0.80178200
H	1.35332000	-0.27303600	0.33690900
H	-2.59175600	1.41726700	-1.95288300
H	-4.93316700	1.24017800	-2.65965100
H	-6.44241200	-0.42640500	-1.59600900
H	-5.55169300	-1.92009500	0.17709300
H	-3.19667600	-1.78152000	0.85161500
H	-0.41406400	-0.05629000	2.61406100
H	0.28861300	-1.98035700	3.96070900
H	0.36227400	-4.25458100	2.96384500
H	-0.26483600	-4.56007200	0.57540500
H	-0.95384900	-2.62870300	-0.77954300
H	-2.62160900	0.94229600	2.04404500
H	-2.52041600	3.15398800	3.10316600
H	-0.97769900	4.89588300	2.22374000
H	0.45100800	4.37696100	0.25832900
H	0.35473300	2.16125500	-0.79544400
H	-0.98943300	-0.12144700	-2.21626300

3b (conf. 6)

C	1.37795600	5.55365500	-0.56404500
C	-0.03096600	5.61344500	0.03853200
C	-0.90283200	4.47241600	-0.49648900
C	-0.26761200	3.09155000	-0.24829800
C	1.15512400	3.02821600	-0.85025100
C	2.02460100	4.18307100	-0.32902600
H	1.31944100	5.74598100	-1.64270100
H	2.01416700	6.33762500	-0.14162400
H	0.03674400	5.54156000	1.13148500
H	-0.49815100	6.57851500	-0.18022000
H	-1.88948500	4.47789600	-0.02874200

H	-1.05602200	4.59394000	-1.57629400
H	-0.19928000	2.93293600	0.83501900
N	-1.07600900	2.01952400	-0.81489100
N	1.84269100	1.76277000	-0.58381300
H	1.06370900	3.11131800	-1.93831500
H	2.18882000	4.04275000	0.74792200
H	3.00679700	4.12946700	-0.80767300
C	-2.13982800	1.48917200	-0.13367200
O	-2.57966200	1.96260700	0.90405200
C	1.68285700	0.65188800	-1.35564400
N	2.42049100	-0.47560700	-1.04760500
O	0.90847100	0.61231500	-2.31982100
C	3.55734900	-0.71098900	-0.12919800
C	3.17730400	-0.18235000	1.27775500
C	4.01176700	0.63720400	2.04332100
C	3.60619800	1.09639900	3.29922700
C	2.36052400	0.74752100	3.80760600
C	1.51506800	-0.06422800	3.05051900
C	1.92034400	-0.52169000	1.80236500
C	3.75668600	-2.25335000	-0.11727600
C	3.98294400	-2.90825200	-1.33707300
C	4.17356200	-4.28438000	-1.38757700
C	4.16279800	-5.03676600	-0.21383600
C	3.96386800	-4.39553600	1.00311100
C	3.76040200	-3.01500100	1.05189000
N	-2.70801000	0.39278600	-0.78549000
C	-3.70299900	-0.49837200	-0.15580300
C	-5.02878700	0.25326400	0.12116800
C	-5.32389900	1.46121400	-0.51398800
C	-6.55859100	2.08010500	-0.33475700
C	-7.52624100	1.50279400	0.48210800
C	-7.24742500	0.29313700	1.11300400
C	-6.01374800	-0.32526500	0.92967400
C	-4.07932500	-1.57036000	-1.21499800
C	-4.03548300	-1.27180600	-2.58185300
C	-4.44208900	-2.20441000	-3.53446300
C	-4.91442800	-3.45212800	-3.14082100
C	-4.98070200	-3.75494000	-1.78282700
C	-4.56895300	-2.82523700	-0.83255200
C	-3.06330600	-1.12612500	1.10926700
C	-2.14571800	-2.17762600	0.97723700
C	-1.49743600	-2.71399500	2.08679000
C	-1.74743300	-2.20042300	3.35839000
C	-2.63124500	-1.13387400	3.49891600
C	-3.27541800	-0.59620000	2.38547200
H	-0.66635000	1.51120000	-1.59315000
H	2.35457700	1.68437600	0.28185700
H	2.20080500	-1.22596700	-1.68375200
H	4.97900200	0.93557300	1.66303900
H	4.27059600	1.73394700	3.87184100
H	2.04363100	1.11069700	4.77866900
H	0.53260800	-0.33348600	3.41971600

H	1.24585400	-1.13576900	1.21860800
H	4.03668400	-2.33543900	-2.25674700
H	4.34202500	-4.76734400	-2.34351600
H	4.31566900	-6.10931200	-0.25018400
H	3.96305600	-4.96587800	1.92531400
H	3.60470900	-2.53866300	2.01024500
H	-2.09018000	-0.08540100	-1.42677400
H	-4.58502300	1.92232700	-1.15436200
H	-6.75990000	3.02165800	-0.83400700
H	-8.48587600	1.98725300	0.62399200
H	-7.99082800	-0.17478900	1.74914200
H	-5.82168100	-1.26814800	1.42646300
H	-3.69965500	-0.29608900	-2.90870000
H	-4.39344400	-1.94683300	-4.58671800
H	-5.23171400	-4.17805000	-3.88092000
H	-5.35191800	-4.72078100	-1.45803900
H	-4.62223200	-3.08672500	0.21628500
H	-1.94215400	-2.59552900	-0.00170800
H	-0.80404100	-3.53787000	1.95666300
H	-1.25597000	-2.62522000	4.22702700
H	-2.82088600	-0.70960700	4.47894700
H	-3.93079600	0.25383100	2.50694600
C	4.87639000	-0.09036100	-0.66278900
C	4.89847100	0.81540900	-1.72463800
C	6.10386000	1.34350600	-2.19026800
C	7.30886400	0.97413200	-1.60377300
C	7.30166500	0.06057800	-0.55065300
C	6.10020900	-0.46809200	-0.09117000
H	3.97871400	1.10688900	-2.21094000
H	6.09345500	2.04160900	-3.01995000
H	8.24454500	1.38294300	-1.96795300
H	8.23393000	-0.25023100	-0.09229200
H	6.11535700	-1.19433100	0.71315400

3b (conf. 12)

C	1.37530000	5.40867900	-0.25354000
C	-0.06210900	5.48214100	0.27517400
C	-0.92399300	4.36433900	-0.32154800
C	-0.32080900	2.97110000	-0.06266100
C	1.12294200	2.89757000	-0.60498000
C	1.98713500	4.02207900	-0.01494900
H	1.37790800	5.62322800	-1.32953000
H	2.00172000	6.17219700	0.21815100
H	-0.05312200	5.39262600	1.36888200
H	-0.50131200	6.45830600	0.04797200
H	-1.93165800	4.37812100	0.09765500
H	-1.02081300	4.50430500	-1.40566800
H	-0.29744100	2.80196900	1.02116700
N	-1.11770700	1.91441600	-0.67154900
N	1.76727600	1.60535300	-0.34154300
H	1.07841000	3.01308700	-1.69359900
H	2.09182200	3.85661700	1.06602900

H	2.99132000	3.96247600	-0.44467100
C	-2.25603800	1.44725800	-0.07092700
O	-2.75299300	1.96229800	0.92029700
C	1.69343000	0.56122100	-1.21339200
N	2.49794100	-0.54123300	-0.98958300
O	0.90967800	0.54737700	-2.16930800
C	3.72755400	-0.71039600	-0.17684600
C	3.39082900	-0.98015400	1.31294500
C	2.09515400	-0.85236500	1.81623200
C	1.81825800	-1.11703800	3.15925500
C	2.83224500	-1.52256900	4.01896200
C	4.12735700	-1.67432300	3.52382500
C	4.40081800	-1.41134900	2.18621000
C	4.40406500	-1.99898200	-0.72004000
C	3.64278100	-3.17489900	-0.79530700
C	4.20256000	-4.36022700	-1.25840400
C	5.54341100	-4.40125100	-1.63826700
C	6.31294100	-3.24735700	-1.54616700
C	5.74821100	-2.05414100	-1.09223700
N	-2.82325500	0.36164600	-0.74153400
C	-3.87894400	-0.48522300	-0.14758500
C	-5.20225900	0.30350300	0.01308200
C	-5.41769400	1.50902700	-0.65724000
C	-6.64666400	2.16020400	-0.58017200
C	-7.68767600	1.61794100	0.16737000
C	-7.48812000	0.41050900	0.83215300
C	-6.26030100	-0.24002000	0.75072300
C	-4.20733800	-1.58793000	-1.19016100
C	-4.09608100	-1.32836400	-2.56145700
C	-4.45904400	-2.28665700	-3.50580300
C	-4.95414900	-3.52197000	-3.10023600
C	-5.08689800	-3.78600300	-1.73916600
C	-4.71830700	-2.83049100	-0.79636400
C	-3.33703200	-1.07619600	1.17934200
C	-2.40857700	-2.12568400	1.14193700
C	-1.83705100	-2.62542700	2.30887300
C	-2.17615800	-2.07576100	3.54407700
C	-3.07317200	-1.01258400	3.59222900
C	-3.64135000	-0.51237300	2.42175100
H	-0.68417100	1.40026900	-1.43326700
H	2.44653500	1.57423900	0.40228800
H	2.35761400	-1.22639400	-1.71591800
H	1.28438700	-0.56031400	1.16426400
H	0.80127100	-1.01109900	3.51845600
H	2.61730500	-1.73110200	5.06093500
H	4.92520100	-2.00886200	4.17763700
H	5.40764400	-1.55905100	1.81334500
H	2.60853100	-3.16737900	-0.47038200
H	3.59312600	-5.25529000	-1.31240200
H	5.98240400	-5.32568700	-1.99572400
H	7.35902200	-3.26650200	-1.83083300
H	6.36461100	-1.16724500	-1.03341400

H	-2.18336400	-0.15293900	-1.33077400
H	-4.62104600	1.94255200	-1.24533700
H	-6.78560000	3.09913400	-1.10498500
H	-8.64290000	2.12724800	0.22974900
H	-8.28944100	-0.03048400	1.41499700
H	-6.12983000	-1.18098700	1.27083000
H	-3.74103000	-0.36286700	-2.89847700
H	-4.35909500	-2.05915000	-4.56138200
H	-5.23799300	-4.26784300	-3.83406800
H	-5.47658700	-4.74154100	-1.40560000
H	-4.82219000	-3.06188200	0.25575600
H	-2.13447500	-2.56840300	0.19134800
H	-1.12988400	-3.44569500	2.25232300
H	-1.74205200	-2.47006300	4.45653600
H	-3.32946100	-0.55930800	4.54354500
H	-4.30654700	0.33705600	2.47322500
C	4.63766300	0.53067200	-0.37486800
C	4.89565300	0.96577200	-1.68392800
C	5.69885100	2.07252700	-1.92858300
C	6.26185100	2.78090500	-0.86592500
C	6.00746700	2.36738900	0.43570000
C	5.20261600	1.25130500	0.67940100
H	4.45584600	0.43360500	-2.51892000
H	5.88281800	2.38562200	-2.95022300
H	6.88677000	3.64632900	-1.05495500
H	6.43031700	2.91113700	1.27306600
H	5.01620700	0.95486600	1.70260800

3b (conf. 32)

C	-0.02146200	5.54052100	0.40182800
C	1.38764100	5.51094100	-0.20323600
C	2.03463600	4.13032300	-0.03844400
C	1.16361500	3.00794800	-0.62228500
C	-0.25833000	3.03787600	-0.01805700
C	-0.89483600	4.42868300	-0.19016000
H	0.04685600	5.41232600	1.48958200
H	-0.48788800	6.51594400	0.23294000
H	1.32954100	5.75788100	-1.27066300
H	2.02337800	6.27246800	0.25896100
H	3.01814900	4.10229700	-0.51633700
H	2.19403100	3.93452500	1.03076600
H	1.07652800	3.14874500	-1.70512700
N	1.83214300	1.72133500	-0.41459800
N	-1.07924100	2.00123800	-0.63644500
H	-0.19016400	2.81513800	1.05272900
H	-1.05456400	4.60821300	-1.26071900
H	-1.88169800	4.41312400	0.27871500
C	1.70892900	0.67757200	-1.28030600
O	0.93989600	0.70143200	-2.24729200
C	-1.97867500	1.27845100	0.11350000
N	-2.54727300	0.22835800	-0.60989800
O	-2.23136100	1.51864400	1.28404600

C	-3.78309600	-0.47104200	-0.19445400
C	-4.93837100	0.56328700	-0.19369000
C	-5.21155200	1.34658300	0.93529100
C	-6.17655800	2.35052700	0.89012900
C	-6.88087200	2.60364000	-0.28398000
C	-6.60234400	1.84864400	-1.41989200
C	-5.64012000	0.84247000	-1.37381500
C	-4.02866600	-1.61241900	-1.21862400
C	-3.01745800	-2.08535600	-2.06088500
C	-3.24935400	-3.15163100	-2.93136300
C	-4.49175200	-3.77277900	-2.96999400
C	-5.50327200	-3.32028900	-2.12348900
C	-5.27261300	-2.25645500	-1.25945800
N	2.44913300	-0.46498300	-1.03603800
C	3.61598400	-0.71585700	-0.15611600
C	3.18296100	-0.95006400	1.31531800
C	1.88486700	-0.69229300	1.76054600
C	1.52512300	-0.91166100	3.09198000
C	2.45567000	-1.40643100	3.99843100
C	3.74906700	-1.69132300	3.56157300
C	4.10561100	-1.46922700	2.23579200
C	4.22860100	-2.05040100	-0.66208300
C	3.39371700	-3.17293100	-0.76734900
C	3.89226400	-4.39623400	-1.20058500
C	5.24282000	-4.52996500	-1.52022300
C	6.08345700	-3.42968800	-1.39851100
C	5.58092100	-2.19827100	-0.97421900
C	4.62125000	0.45773100	-0.30359800
C	4.96597200	0.88070800	-1.59639800
C	5.85503900	1.92912500	-1.79683900
C	6.41956000	2.59026300	-0.70503700
C	6.08093600	2.18809900	0.58084200
C	5.18994700	1.13017500	0.78035100
H	2.48683000	1.65717900	0.34843700
H	-0.67390500	1.55264600	-1.45406100
H	-2.50978900	0.36967400	-1.61003300
H	-4.64514700	1.18934300	1.84146500
H	-6.37018800	2.94151300	1.77867900
H	-7.63260800	3.38462600	-0.31551300
H	-7.13397700	2.03868300	-2.34596100
H	-5.44099200	0.26669400	-2.26935900
H	-2.03220500	-1.63859200	-2.03420900
H	-2.44774100	-3.49446800	-3.57633300
H	-4.67168300	-4.60138200	-3.64560400
H	-6.47706400	-3.79740000	-2.13543400
H	-6.07247900	-1.91982700	-0.61218300
H	2.29168500	-1.14710200	-1.76141600
H	1.13578200	-0.32534600	1.07399400
H	0.51084300	-0.69467600	3.40653800
H	2.17597500	-1.57938700	5.03143100
H	4.48070700	-2.09647900	4.25183200
H	5.10887000	-1.71723500	1.90964600

H	2.34882500	-3.09466100	-0.48908600
H	3.22670500	-5.24859600	-1.27774700
H	5.63384800	-5.48431900	-1.85396500
H	7.13741600	-3.52068100	-1.63639800
H	6.25289900	-1.35472100	-0.89092000
H	4.52546100	0.38598300	-2.45365700
H	6.10460200	2.23439600	-2.80689100
H	7.11083400	3.41093700	-0.85958700
H	6.50450400	2.69567300	1.44028100
H	4.93994600	0.84177300	1.79224100
C	-3.57473700	-1.20183800	1.15284300
C	-2.31007500	-1.68502500	1.50067900
C	-2.12651400	-2.45151200	2.64711500
C	-3.20717100	-2.75532700	3.47270000
C	-4.47230400	-2.28830800	3.13165900
C	-4.65433400	-1.52375200	1.98053900
H	-1.46461500	-1.46170300	0.86336800
H	-1.13459700	-2.81432700	2.89314900
H	-3.06457900	-3.35123000	4.36729200
H	-5.32599600	-2.51753800	3.76015300
H	-5.64867500	-1.17328600	1.73569600

3b (conf. 33)

C	1.38349600	5.52458400	-0.25902000
C	-0.03284800	5.54156000	0.32986000
C	-0.87925200	4.39764500	-0.24011900
C	-0.21340600	3.02774200	-0.02101200
C	1.20501600	3.01150700	-0.62942300
C	2.05353900	4.15881100	-0.06152400
H	1.33300500	5.74935900	-1.33171100
H	2.00098000	6.30599800	0.19480700
H	0.02521600	5.44369900	1.42133500
H	-0.51582300	6.50307400	0.13049900
H	-1.86793600	4.37069400	0.22210700
H	-1.02903300	4.54308600	-1.31747800
H	-0.13360500	2.85237700	1.05854400
N	-1.00396600	1.94362500	-0.59488600
N	1.90127000	1.73727200	-0.41330900
H	1.10799300	3.13997700	-1.71296600
H	2.21049600	3.98628700	1.01175400
H	3.04022200	4.14051400	-0.53377800
C	-1.99966900	1.34816200	0.13873400
O	-2.42937400	1.82896300	1.18009900
C	1.83473800	0.72002700	-1.31894900
N	2.68587300	-0.35737800	-1.17298100
O	1.03010100	0.72297100	-2.25771200
C	3.70506800	-0.70419100	-0.15797600
C	3.06191300	-1.19532200	1.16673100
C	1.69652000	-1.06418900	1.42601800
C	1.14338400	-1.54442400	2.61459000
C	1.94788400	-2.16263800	3.56464400
C	3.31194800	-2.30817800	3.31453800

C	3.85945700	-1.83617000	2.12664100
C	4.47942800	-1.91349200	-0.75511900
C	3.75229100	-3.05506500	-1.12443600
C	4.39008600	-4.17024600	-1.65526400
C	5.77576300	-4.17794900	-1.80984500
C	6.50921400	-3.06230900	-1.42399700
C	5.86691200	-1.93771500	-0.90234300
N	-2.44645400	0.15248600	-0.40918000
C	-3.75119100	-0.51606900	-0.14235700
C	-3.68261700	-1.40252900	1.13133500
C	-3.04030900	-0.94699400	2.29002600
C	-3.01620100	-1.72755300	3.44377800
C	-3.63653600	-2.97508700	3.47204500
C	-4.29013900	-3.43095700	2.33228200
C	-4.31239400	-2.65180100	1.17560800
C	-4.88471500	0.53072600	-0.03208600
C	-4.93152900	1.59758400	-0.93835700
C	-5.96559200	2.52589300	-0.90124800
C	-6.98250000	2.40654500	0.04520100
C	-6.94788200	1.35109000	0.94927700
C	-5.90797500	0.42150900	0.91051900
C	-3.97231100	-1.43041500	-1.37839600
C	-5.15758600	-1.43727900	-2.11593800
C	-5.31291300	-2.28865200	-3.21133300
C	-4.28608000	-3.14572400	-3.59053300
C	-3.10086200	-3.15584700	-2.85655500
C	-2.95035600	-2.31404200	-1.75988300
H	-0.58225100	1.45259700	-1.37856500
H	2.63015300	1.72256100	0.28322600
H	2.51272200	-1.04708000	-1.88716400
H	1.04247300	-0.59909700	0.70233600
H	0.07787100	-1.43948300	2.78287500
H	1.51687300	-2.53912900	4.48536500
H	3.94965700	-2.80267600	4.03896900
H	4.91636200	-1.98290600	1.93646900
H	2.67902000	-3.08463300	-0.97098000
H	3.80521800	-5.03872600	-1.93654800
H	6.27574000	-5.04840600	-2.21891100
H	7.58848700	-3.05755300	-1.52822600
H	6.45965400	-1.08122100	-0.61118100
H	-2.04988600	-0.08195900	-1.30625800
H	-2.59190400	0.03725800	2.29240500
H	-2.51828700	-1.34871500	4.33029600
H	-3.61611000	-3.57952400	4.37228700
H	-4.78441300	-4.39641200	2.33510100
H	-4.82832100	-3.02955300	0.30239200
H	-4.14591800	1.70782900	-1.67649600
H	-5.97447100	3.34680500	-1.60992700
H	-7.78760900	3.13212500	0.07856500
H	-7.72743100	1.24792600	1.69619900
H	-5.89591000	-0.38629800	1.62980400
H	-5.96885500	-0.77788700	-1.83950700

H	-6.24306500	-2.27366500	-3.76863400
H	-4.40667100	-3.80223400	-4.44489400
H	-2.29445500	-3.82613900	-3.13285900
H	-2.03560200	-2.35733000	-1.17975700
C	4.63992900	0.51582200	0.04395200
C	5.16210000	1.15450700	-1.09185000
C	6.00667800	2.25119200	-0.97355500
C	6.34551500	2.74480800	0.28740100
C	5.82721700	2.12942500	1.42002800
C	4.98166900	1.02308800	1.29994700
H	4.89370300	0.78784600	-2.07516100
H	6.39833200	2.72503400	-1.86675100
H	7.00135300	3.60290900	0.38090500
H	6.07381800	2.50573500	2.40647300
H	4.58594100	0.56510100	2.19621800

4b (conf. 1)

C	-0.39680500	5.04071100	1.09587000
C	0.65876700	5.08305100	-0.01365600
C	1.44001100	3.76638200	-0.07065800
C	0.52355900	2.53843600	-0.23941300
C	-0.56017200	2.50107100	0.85510600
C	-1.32747500	3.83774600	0.91253300
H	0.09884000	4.97331300	2.07220900
H	-0.98356600	5.96435800	1.10726400
H	0.16801900	5.26001400	-0.97877900
H	1.35135500	5.91594600	0.14168600
H	2.15799100	3.77104100	-0.89407000
H	2.02120500	3.64897500	0.85250000
H	0.04985800	2.57967500	-1.22314800
N	1.32529400	1.31611200	-0.23050700
N	-1.49061500	1.38484500	0.64021000
H	-0.09341900	2.32407500	1.82749500
H	-1.89586100	3.95479000	-0.01865800
H	-2.04955300	3.77884700	1.73045300
C	1.63858600	0.57298500	-1.30898900
S	0.96701700	0.81214800	-2.85137800
C	-2.20661100	0.81369900	1.63508100
N	-3.30355300	0.05706400	1.30957000
S	-1.84713200	1.01639500	3.28185000
C	-3.72275100	-0.58305700	0.03306000
C	-5.10350100	-1.24208000	0.30843900
C	-5.99953200	-0.68388100	1.22668600
C	-7.26556400	-1.23549600	1.41527500
C	-7.66635300	-2.34520500	0.67832300
C	-6.78903900	-2.89699500	-0.25226000
C	-5.52185600	-2.35156300	-0.43498200
C	-4.02302800	0.47034200	-1.06157400
C	-4.33217600	1.78989000	-0.71270400
C	-4.71938000	2.71580300	-1.67972000
C	-4.81684100	2.33845300	-3.01517300
C	-4.53501700	1.02197000	-3.37211100

C	-4.14936200	0.09751300	-2.40617800
N	2.53117600	-0.45240100	-1.13495300
C	3.61699800	-0.61762800	-0.12040300
C	4.57849700	-1.66868300	-0.73892900
C	4.04662000	-2.90167200	-1.14475100
C	4.86190100	-3.88580700	-1.69172300
C	6.23220500	-3.66629200	-1.82690100
C	6.77268000	-2.45609300	-1.40813700
C	5.95264600	-1.46262500	-0.87006100
C	4.32347600	0.74924500	0.07822900
C	4.59553800	1.30505800	1.33045000
C	5.24632600	2.53617800	1.44200200
C	5.63499400	3.23303100	0.30437800
C	5.35920000	2.69382600	-0.95250600
C	4.70887400	1.47080100	-1.06227000
C	3.08448700	-1.22382300	1.20047200
C	3.99819500	-1.67443300	2.16604600
C	3.55950600	-2.22275900	3.36529000
C	2.19395600	-2.33995800	3.62575100
C	1.27954300	-1.92067000	2.66787000
C	1.72127300	-1.37682800	1.45930100
H	1.78362300	1.09924500	0.64401500
H	-1.83252800	1.27918100	-0.30574900
H	-3.65708500	-0.40868300	2.13304100
H	-5.72083900	0.19568700	1.79347000
H	-7.93853500	-0.78853400	2.13832000
H	-8.65128900	-2.77377200	0.82418800
H	-7.08772500	-3.75960400	-0.83740100
H	-4.85214400	-2.80257900	-1.15592900
H	-4.28108400	2.09377500	0.32456700
H	-4.94999400	3.73248800	-1.38168300
H	-5.11537300	3.05822000	-3.76861600
H	-4.61671200	0.70877900	-4.40670100
H	-3.95427200	-0.92342600	-2.70675400
H	2.70215600	-0.93094400	-2.00623000
H	2.98821200	-3.09686200	-1.01493200
H	4.42808300	-4.82923400	-2.00368200
H	6.86991000	-4.43424000	-2.24960300
H	7.83754900	-2.27417200	-1.50084700
H	6.39448900	-0.52653200	-0.55633300
H	4.29972700	0.78684200	2.23230900
H	5.44404100	2.94528000	2.42654600
H	6.14147100	4.18758500	0.39174700
H	5.64681200	3.22875100	-1.85064700
H	4.48981000	1.07485200	-2.04652100
H	5.06235000	-1.60771400	1.97207500
H	4.28524600	-2.56396100	4.09528300
H	1.84976000	-2.76011200	4.56387700
H	0.21514300	-2.00323800	2.85061900
H	0.98763000	-1.08928900	0.71956400
C	-2.65553200	-1.64487900	-0.33024900
C	-1.71078300	-1.47926600	-1.34442800

C	-0.73911200	-2.45356700	-1.58536300
C	-0.68724900	-3.60337100	-0.80753200
C	-1.60291300	-3.76615600	0.23236100
C	-2.57010700	-2.79747300	0.46777700
H	-1.70413700	-0.59373900	-1.96517300
H	-0.02472900	-2.28869600	-2.38293900
H	0.06175000	-4.36352000	-0.99924700
H	-1.56501000	-4.64962200	0.85978200
H	-3.27550600	-2.94485700	1.27706700

4b (conf. 4)

C	0.34158700	3.06843700	-0.43130100
C	-0.32555300	2.96547600	0.94798100
C	0.02066800	1.64044100	1.63897200
C	-0.32232800	0.41163400	0.77328200
C	0.28096000	0.51518000	-0.65006900
C	-0.02433800	1.87143000	-1.31891200
H	0.04825900	3.99828100	-0.92847400
H	1.42946800	3.11628000	-0.30826800
H	-0.01922400	3.80328200	1.58202700
H	-1.41318600	3.04464500	0.83434600
H	1.09366600	1.61875000	1.86940800
H	-0.49393800	1.53925700	2.59669200
H	0.06665400	-0.48485400	1.25746700
N	-1.77419400	0.22222000	0.65822600
N	1.72328100	0.26089100	-0.56368400
H	-0.12483100	-0.28711500	-1.26702000
H	0.50125000	1.90601700	-2.27582700
H	-1.09446800	1.91012500	-1.55887600
C	-2.51658200	-0.50275200	1.52298100
S	-1.89179900	-1.20152900	2.93596800
C	2.43912100	-0.41171100	-1.49066800
N	3.76508800	-0.63726600	-1.23988700
S	1.78153500	-1.01494700	-2.93280700
C	4.64012100	-0.26476600	-0.09957900
C	6.07817100	-0.64048600	-0.55499800
C	6.32160500	-1.95248600	-0.98754300
C	7.59244800	-2.34846400	-1.38829000
C	8.65435000	-1.44608600	-1.34563700
C	8.42877500	-0.14993300	-0.89735800
C	7.15025200	0.25183400	-0.50679600
C	4.51336300	1.26213900	0.14431100
C	4.59857300	2.11916200	-0.96414300
C	4.51853300	3.49793800	-0.81300200
C	4.33920800	4.05712300	0.45310200
C	4.23274700	3.22001900	1.55679600
C	4.31888300	1.83328700	1.40453800
N	-3.84970100	-0.66127100	1.25422300
C	-4.66492600	-0.32731300	0.05588300
C	-3.90056900	-0.78803900	-1.21124500
C	-3.34775100	-2.07819800	-1.21753500
C	-2.62922400	-2.54416900	-2.31099000

C	-2.43914100	-1.72867200	-3.42714000
C	-2.98053000	-0.44966000	-3.43445500
C	-3.70567500	0.01848200	-2.33532200
C	-5.99270600	-1.11376100	0.23476000
C	-6.72293800	-0.93782300	1.41939400
C	-7.92583300	-1.60438500	1.62291400
C	-8.43588600	-2.44730200	0.63648000
C	-7.73086800	-2.61195900	-0.55010400
C	-6.51688400	-1.95246400	-0.74992800
C	-5.04011500	1.17688400	0.03402600
C	-5.99248100	1.64333500	-0.88404300
C	-6.36984300	2.98140800	-0.90853000
C	-5.81387400	3.88467800	-0.00327600
C	-4.88711500	3.42974300	0.92737900
C	-4.50512200	2.08677700	0.94768900
H	-2.21385900	0.53479700	-0.19500600
H	2.22039900	0.66801800	0.21513300
H	4.21521200	-1.11164900	-2.00681600
H	5.51522400	-2.67747800	-0.99397300
H	7.75457500	-3.36632100	-1.72435400
H	9.64681800	-1.75457300	-1.65366400
H	9.24654700	0.56059500	-0.85187700
H	6.99896300	1.26717400	-0.16598800
H	4.72421300	1.69649100	-1.95348600
H	4.59100100	4.13724300	-1.68564500
H	4.27461500	5.13268000	0.57210100
H	4.08073300	3.63753900	2.54576200
H	4.22985300	1.20373900	2.27927500
H	-4.30015000	-1.24168500	1.94465400
H	-3.46771500	-2.71262200	-0.34768800
H	-2.19996700	-3.53907100	-2.28618800
H	-1.85820700	-2.08291600	-4.26995400
H	-2.83092200	0.19963700	-4.28950200
H	-4.10493000	1.02319200	-2.36141800
H	-6.35813000	-0.26018300	2.18334000
H	-8.46931900	-1.45756400	2.54942600
H	-9.37538400	-2.96518900	0.79211100
H	-8.11854800	-3.25959700	-1.32849600
H	-5.98211400	-2.10017700	-1.67847900
H	-6.45749600	0.95028800	-1.57531400
H	-7.10912800	3.31606000	-1.62771900
H	-6.11186800	4.92688000	-0.01697800
H	-4.45954200	4.11474600	1.65101300
H	-3.80112500	1.75033900	1.69589500
C	4.33966100	-1.11606000	1.16174500
C	3.24763800	-1.98328400	1.23437900
C	3.01657600	-2.74776300	2.37946700
C	3.88047100	-2.66844100	3.46514300
C	4.98973800	-1.82672900	3.39445200
C	5.21831400	-1.06451900	2.25411000
H	2.57281100	-2.08176100	0.39634600
H	2.15478300	-3.40401900	2.41431500

H	3.69906700	-3.26199300	4.35378400
H	5.68448700	-1.76929000	4.22502200
H	6.09947100	-0.43549900	2.20664800

4b (conf. 30)

C	0.22841800	5.50131800	0.43571100
C	1.59389900	5.40159100	-0.25503300
C	2.19149900	3.99642300	-0.10866400
C	1.23249200	2.91097700	-0.62241500
C	-0.13514200	3.00554400	0.09203600
C	-0.72738900	4.41752500	-0.07533600
H	0.35727000	5.39024800	1.51949700
H	-0.20815300	6.49156900	0.27470700
H	1.48104800	5.63633000	-1.32073100
H	2.28949000	6.14025500	0.15472000
H	3.13861700	3.91692300	-0.64894800
H	2.41175900	3.80723500	0.95067300
H	1.08062100	3.04392800	-1.69687400
N	1.85524900	1.59544100	-0.45405900
N	-1.02853900	1.97956100	-0.43000900
H	0.00096500	2.80704700	1.16046000
H	-0.94439900	4.58173500	-1.13837400
H	-1.67865300	4.45276500	0.45955300
C	1.80612600	0.56988700	-1.32231000
S	0.88984200	0.58412100	-2.76300700
C	-2.03108600	1.37592300	0.26482300
N	-2.73317500	0.48808800	-0.50892000
S	-2.36778000	1.72447600	1.87864000
C	-3.79977400	-0.47274000	-0.13349900
C	-3.32634400	-1.32137200	1.07061800
C	-2.09156200	-1.97624200	0.97303700
C	-1.61880000	-2.77845800	2.00565500
C	-2.37238500	-2.93988000	3.16758500
C	-3.59201800	-2.28158200	3.28226800
C	-4.06276000	-1.47770500	2.24439700
C	-5.16450800	0.22829900	0.08428500
C	-5.31366200	1.61337500	0.01421800
C	-6.56967600	2.20500400	0.14931100
C	-7.70065900	1.42308800	0.35556800
C	-7.56724200	0.03702300	0.41218800
C	-6.31505000	-0.55124700	0.26911900
N	2.51903700	-0.55538700	-1.02669700
C	3.66518500	-0.75932300	-0.09197400
C	4.64912800	0.42961700	-0.25118600
C	5.18593400	1.13748500	0.82650400
C	6.06627000	2.20187600	0.61722500
C	6.42299500	2.57707900	-0.67214100
C	5.88850100	1.88160400	-1.75733400
C	5.01206600	0.82400100	-1.54801400
C	3.18081800	-0.95833900	1.36593100
C	1.85610000	-0.74197800	1.75225000
C	1.45460800	-0.93036100	3.07693700

C	2.37006900	-1.35305200	4.03314600
C	3.68967700	-1.60089200	3.65474700
C	4.08788000	-1.41065600	2.33655800
C	4.31460000	-2.09623100	-0.53935700
C	5.68019000	-2.22749900	-0.79636300
C	6.21924100	-3.46181100	-1.16275400
C	5.40235100	-4.58011900	-1.28284900
C	4.03822400	-4.46161900	-1.02028400
C	3.50288800	-3.23547500	-0.64263800
H	2.40290900	1.47628900	0.38665100
H	-0.78946900	1.62019700	-1.35321200
H	-2.36350200	0.33525900	-1.43707700
H	-1.49349800	-1.85640100	0.07687100
H	-0.65974600	-3.27404500	1.90523600
H	-2.00714300	-3.56491300	3.97496400
H	-4.18038700	-2.37935600	4.18795200
H	-4.99744400	-0.95016500	2.36985500
H	-4.44983300	2.24192900	-0.14223500
H	-6.65633500	3.28468300	0.09684400
H	-8.67582800	1.88482000	0.46294100
H	-8.44009700	-0.59017900	0.55653700
H	-6.23615300	-1.63173100	0.28761900
H	2.41829700	-1.25844400	-1.74303400
H	4.91902500	0.87207000	1.84027400
H	6.46676100	2.73636100	1.47133900
H	7.10550400	3.40359000	-0.83423800
H	6.15102700	2.16603300	-2.77003100
H	4.59677500	0.30347100	-2.40241500
H	1.11436100	-0.43801800	1.02703400
H	0.42000300	-0.74961400	3.34324300
H	2.05848900	-1.50084700	5.06084900
H	4.40958300	-1.95242000	4.38552600
H	5.11093900	-1.63139300	2.05561500
H	6.33340900	-1.36924900	-0.71443800
H	7.28279900	-3.54089300	-1.35800000
H	5.82199300	-5.53652100	-1.57291300
H	3.39040800	-5.32723300	-1.09961100
H	2.44619100	-3.16782100	-0.40932200
C	-3.99891400	-1.35950500	-1.40110500
C	-4.20560900	-0.73318500	-2.63938100
C	-4.42130700	-1.47765600	-3.79388400
C	-4.45927900	-2.86945700	-3.73366800
C	-4.28262200	-3.50099700	-2.50793700
C	-4.05216100	-2.75404600	-1.35191900
H	-4.22399400	0.34926100	-2.69927200
H	-4.57146500	-0.96817000	-4.73910000
H	-4.63135700	-3.45190800	-4.63165100
H	-4.31809800	-4.58291500	-2.44289200
H	-3.91096500	-3.26850000	-0.41136300

4b (conf. 40)

C	1.55457800	5.48724300	-0.56563600

C	0.19714000	5.59504400	0.13928700
C	-0.75006200	4.48105500	-0.31965700
C	-0.13850200	3.08338100	-0.10727500
C	1.22313500	2.97616200	-0.83305100
C	2.17180000	4.09617200	-0.37477800
H	1.42474700	5.68113500	-1.63761100
H	2.24583100	6.24918800	-0.19281400
H	0.34147200	5.52540600	1.22457600
H	-0.25450400	6.57307200	-0.05191000
H	-1.69594000	4.52377700	0.22422000
H	-0.98108400	4.60299600	-1.38541100
H	0.01108500	2.92488100	0.96602200
N	-1.02680900	2.03055600	-0.58247000
N	1.87288100	1.68188100	-0.61327600
H	1.05825100	3.06151600	-1.91029300
H	2.41010300	3.94951200	0.68712900
H	3.11254000	4.00992400	-0.92577500
C	-2.00549200	1.43226000	0.14722400
S	-2.34271100	1.84494300	1.74528600
C	1.80244300	0.60121600	-1.41109300
N	2.51198000	-0.51001000	-1.06440200
S	0.88758800	0.54219400	-2.85508700
C	3.57405700	-0.73778600	-0.04439000
C	3.78553000	-2.27802600	-0.02897900
C	3.67380000	-3.05098800	1.12728200
C	3.89388000	-4.42912900	1.08592500
C	4.22378000	-5.05533900	-0.11040900
C	4.34836600	-4.29098300	-1.26974900
C	4.14187200	-2.91689700	-1.22584500
C	4.91752600	-0.09525600	-0.47878000
C	5.00695500	0.81437000	-1.53421700
C	6.23779800	1.35856000	-1.90565700
C	7.39949600	1.00213900	-1.23074900
C	7.32509400	0.08303700	-0.18507900
C	6.09965200	-0.46310700	0.18050700
N	-2.69899600	0.50044300	-0.58573400
C	-3.67979000	-0.51441100	-0.13030700
C	-3.01023300	-1.40035800	0.94906600
C	-3.40142300	-1.40833800	2.28829500
C	-2.74166100	-2.20802100	3.22181800
C	-1.66833200	-3.00422700	2.83601500
C	-1.24886300	-2.98440500	1.50619800
C	-1.91073800	-2.18655100	0.57796400
C	-5.02499300	0.12314700	0.29726600
C	-5.30895200	1.46918400	0.06266200
C	-6.56325400	1.99774500	0.36086900
C	-7.56041700	1.19003900	0.89811500
C	-7.29451000	-0.15893200	1.12130200
C	-6.04367900	-0.68642300	0.81520100
C	-4.04358900	-1.34091300	-1.39963000
C	-4.28374400	-2.71719900	-1.34278000
C	-4.68524900	-3.42089800	-2.47672800

C	-4.85321000	-2.76506100	-3.69225500
C	-4.63077400	-1.39226400	-3.75937100
C	-4.24134800	-0.68777400	-2.62388800
H	-0.78786300	1.63589300	-1.49105700
H	2.34822800	1.57534700	0.27352600
H	2.36468600	-1.26736900	-1.71371200
H	3.41462500	-2.58598300	2.06854800
H	3.80294000	-5.00954000	1.99722100
H	4.38935300	-6.12614000	-0.14114400
H	4.61742800	-4.76246600	-2.20809300
H	4.28292300	-2.33419300	-2.12993500
H	4.12509400	1.09632500	-2.09169100
H	6.28084100	2.05781700	-2.73314400
H	8.35467700	1.42385900	-1.52211500
H	8.22421600	-0.21926500	0.34016300
H	6.06359400	-1.19518700	0.97879100
H	-2.28478200	0.27131900	-1.47964300
H	-4.21076800	-0.77185900	2.61549500
H	-3.06620100	-2.19515700	4.25646300
H	-1.15895500	-3.62894000	3.56149200
H	-0.40978800	-3.59417400	1.18929700
H	-1.57233300	-2.18478400	-0.45201600
H	-4.54733000	2.11380800	-0.35136100
H	-6.75454700	3.04916800	0.17685700
H	-8.53463400	1.60333800	1.13408900
H	-8.06366700	-0.80724700	1.52652100
H	-5.86719200	-1.74319100	0.97402600
H	-4.15121700	-3.25152700	-0.41144500
H	-4.86158700	-4.48850100	-2.40541700
H	-5.15900900	-3.31483300	-4.57509200
H	-4.76923700	-0.86220600	-4.69502500
H	-4.11392400	0.38601000	-2.69104500
C	3.07607900	-0.22288200	1.32864000
C	1.77543400	-0.55585800	1.73844100
C	1.26783200	-0.10926700	2.95273400
C	2.05608900	0.67841600	3.79209300
C	3.34566800	1.01806700	3.39916300
C	3.85237500	0.57501800	2.17504700
H	1.14445100	-1.15067800	1.09009100
H	0.25104500	-0.36107200	3.22778500
H	1.65904700	1.03403900	4.73587900
H	3.96544700	1.63757300	4.03778500
H	4.85112500	0.86836200	1.88291200

4b (conf. 48)

C	0.18031500	5.50616500	0.41082400
C	1.53886400	5.44399800	-0.29853400
C	2.17792500	4.05587500	-0.16352700
C	1.24207000	2.94596100	-0.66649600
C	-0.11898000	3.00452700	0.06608700
C	-0.75426600	4.39802300	-0.08812700
H	0.32717000	5.39751500	1.49258500

H	-0.28425000	6.48478900	0.25742700
H	1.40542200	5.67721700	-1.36217400
H	2.21921900	6.20100700	0.10316400
H	3.11914200	4.00520100	-0.71749900
H	2.41871800	3.87077800	0.89205400
H	1.07473600	3.07427300	-1.73918300
N	1.89621700	1.64492700	-0.50290300
N	-0.99508000	1.95616000	-0.44032100
H	0.03565100	2.80802900	1.13221900
H	-0.99362900	4.55985800	-1.14673700
H	-1.69887700	4.40338400	0.46004800
C	1.83267000	0.60445300	-1.35248400
S	0.92114000	0.60842200	-2.79793100
C	-1.86586800	1.22452300	0.30677100
N	-2.43908800	0.20371000	-0.41036800
S	-2.16264500	1.53405100	1.93568900
C	-3.70904100	-0.52602700	-0.14723800
C	-4.80043300	0.49731600	0.24892300
C	-5.53960200	0.42520300	1.42888900
C	-6.51221900	1.38110400	1.72216700
C	-6.75669100	2.43180300	0.84505200
C	-6.01246900	2.52493300	-0.32992500
C	-5.04630100	1.56884200	-0.62027000
C	-4.05780100	-1.22697400	-1.49469200
C	-3.06386500	-1.95666600	-2.16373200
C	-3.34233300	-2.62792500	-3.34988500
C	-4.62944300	-2.60606200	-3.88299500
C	-5.62964100	-1.90835000	-3.21470500
C	-5.34696500	-1.22301400	-2.03290200
N	2.52512400	-0.52734100	-1.03776400
C	3.62286000	-0.76461700	-0.05475700
C	3.07364000	-0.95441500	1.38125700
C	1.75138200	-0.66565400	1.72521600
C	1.29501400	-0.83928900	3.03402900
C	2.15140700	-1.32260100	4.01638700
C	3.46691100	-1.64172700	3.67991500
C	3.92031900	-1.46285100	2.37790400
C	4.25288500	-2.11699500	-0.48381600
C	3.41624800	-3.23702800	-0.60018700
C	3.92927600	-4.47574300	-0.96742700
C	5.29465800	-4.62617900	-1.20667200
C	6.13534500	-3.52729100	-1.07316900
C	5.61920300	-2.28016900	-0.71676600
C	4.64422700	0.39800000	-0.16309000
C	5.06676600	0.79793100	-1.44014000
C	5.98223100	1.83051200	-1.60199200
C	6.49658100	2.49501400	-0.48801200
C	6.08103100	2.11430600	0.78200300
C	5.16170400	1.07488600	0.94384800
H	2.45876200	1.54068300	0.32994900
H	-0.78363100	1.63490200	-1.38364700
H	-2.14356000	0.14338100	-1.37527700

H	-5.34229900	-0.36146100	2.14315200
H	-7.06702300	1.30741000	2.65097300
H	-7.51009200	3.17636400	1.07689200
H	-6.18190400	3.34428100	-1.01992200
H	-4.47162200	1.65781400	-1.53504800
H	-2.06450800	-2.01896200	-1.74853200
H	-2.55251800	-3.17553500	-3.85163100
H	-4.84934200	-3.13192400	-4.80518500
H	-6.63828600	-1.88821900	-3.61247200
H	-6.13865400	-0.67950700	-1.53538100
H	2.42219500	-1.23731600	-1.74671800
H	1.05570400	-0.31088800	0.97802700
H	0.26739600	-0.58846200	3.27041100
H	1.79741100	-1.45878400	5.03183800
H	4.14081400	-2.03849400	4.43108700
H	4.93948600	-1.73550700	2.13021200
H	2.35772000	-3.14482900	-0.38360900
H	3.26297600	-5.32624900	-1.05619900
H	5.69681300	-5.59247900	-1.48859800
H	7.20003000	-3.63159700	-1.24950100
H	6.29133800	-1.43785200	-0.62338200
H	4.66709000	0.30130100	-2.31598100
H	6.29097700	2.12000500	-2.60011000
H	7.20924600	3.30226900	-0.61310300
H	6.46573400	2.62492200	1.65767700
H	4.85046000	0.80354300	1.94335800
C	-3.51823500	-1.67936300	0.86662300
C	-2.28537000	-1.94471200	1.46126000
C	-2.12084000	-3.03571200	2.31426800
C	-3.18945000	-3.88207200	2.58970300
C	-4.42383800	-3.63548100	1.99148700
C	-4.58207100	-2.55220300	1.13315300
H	-1.44733200	-1.29454300	1.26015200
H	-1.15068500	-3.21724300	2.76364300
H	-3.06253500	-4.72890100	3.25494600
H	-5.26429600	-4.29342900	2.18350100
H	-5.54217900	-2.39403000	0.65655200

6a (conf. 1)

C	-3.48209400	4.46401500	0.08133200
C	-2.23362700	4.90842700	-0.69098200
C	-1.05407300	3.95700900	-0.44784100
C	-1.42644300	2.50123700	-0.76855800
C	-2.65450000	2.06561600	0.06158000
C	-3.83928100	3.00512800	-0.22760100
H	-4.32853700	5.11430300	-0.15875700
H	-3.30409200	4.57045900	1.15853200
H	-2.45920900	4.93242200	-1.76423300
H	-1.94847000	5.92679200	-0.40991000
H	-0.19214400	4.24296700	-1.05641300
H	-0.73989400	4.02628200	0.60227200

H	-1.66809100	2.41847900	-1.83065200
N	-0.27480600	1.62820000	-0.54671800
N	-2.97996200	0.66515800	-0.21327300
H	-2.41179500	2.13115700	1.12697100
H	-4.12092800	2.90239600	-1.28325200
H	-4.69120600	2.67992500	0.37208900
C	0.09524700	0.60183200	-1.33421400
S	-0.73295800	0.17120400	-2.76479400
C	-3.65565500	-0.13741900	0.63690000
N	-3.96677400	-1.39434700	0.21272800
S	-4.14180800	0.34214200	2.19508200
C	-3.51433200	-2.13375800	-0.96363600
C	-2.32568200	-3.05565400	-0.67993700
C	-2.03944600	-3.52500300	0.60374400
C	-0.99192500	-4.42085000	0.81663700
C	-0.21475300	-4.85783000	-0.25244600
C	-0.48274200	-4.38209000	-1.53596600
C	-1.52696900	-3.48614400	-1.74506600
C	-4.70481700	-2.92901500	-1.52893300
N	1.17792500	-0.13580200	-0.96445200
C	2.23816700	0.12868700	0.05051300
C	3.36775300	-0.88511600	-0.27388800
C	3.04318800	-2.24780300	-0.34681100
C	4.02151900	-3.19869700	-0.61477800
C	5.34855900	-2.81097000	-0.79469600
C	5.68310500	-1.46488700	-0.70276300
C	4.70011000	-0.50737400	-0.44706500
C	2.72202800	1.59274500	-0.12114600
C	3.02119700	2.04596900	-1.41504500
C	3.45589900	3.34670800	-1.63715900
C	3.59645900	4.23284100	-0.56848900
C	3.29468200	3.80025100	0.71686000
C	2.86115700	2.49079500	0.93959900
C	1.74885600	-0.18609700	1.48707500
C	0.41309700	-0.46682700	1.78038800
C	0.00713100	-0.73720700	3.08916500
C	0.93624500	-0.75273600	4.12229900
C	2.27957400	-0.50695100	3.83772100
C	2.68045800	-0.23006600	2.53568100
H	0.26060000	1.80435100	0.29184300
H	-2.68513400	0.31254300	-1.11949500
H	-4.50177300	-1.90640500	0.89814300
H	-2.62298000	-3.18009800	1.44919600
H	-0.78391800	-4.77317100	1.82064800
H	0.59471800	-5.56038100	-0.08761900
H	0.12515100	-4.70372500	-2.37448500
H	-1.71340900	-3.10541500	-2.74326200
H	1.37228200	-0.87979200	-1.61695700
H	2.02281200	-2.57321400	-0.17635700
H	3.74688100	-4.24592400	-0.67193000
H	6.11239000	-3.55263600	-0.99863900
H	6.71206700	-1.14908900	-0.83355900

H	4.98259900	0.53501300	-0.38533100
H	2.90237300	1.37469100	-2.25690000
H	3.68001500	3.67071200	-2.64720900
H	3.93238300	5.24905300	-0.74072700
H	3.39147200	4.47835900	1.55734300
H	2.62681700	2.18244000	1.94940200
H	-0.32730200	-0.49289800	0.99426200
H	-1.04173900	-0.92688500	3.28581000
H	0.62162900	-0.96308800	5.13813100
H	3.01919400	-0.53700700	4.63017300
H	3.73099600	-0.06129100	2.33003600
H	-3.20257000	-1.41843500	-1.72808500
H	-5.07045800	-3.64768200	-0.78919900
H	-5.52161600	-2.25387400	-1.79317800
H	-4.40611200	-3.48991400	-2.41615100

6a (conf. 12)

C	1.08459000	-5.50507600	-0.14598600
C	-0.18808300	-5.34258200	-0.98681800
C	-0.88298000	-4.00538600	-0.69819500
C	0.06827700	-2.81347400	-0.89356200
C	1.32504800	-2.98050600	-0.00896800
C	2.02758200	-4.31094000	-0.33247500
H	1.59920400	-6.43341000	-0.41117900
H	0.81530600	-5.59017800	0.91403500
H	0.07141900	-5.38994900	-2.05161700
H	-0.88340300	-6.16613200	-0.79821800
H	-1.75290000	-3.87341200	-1.34755600
H	-1.25340000	-4.00302500	0.33558700
H	0.37426300	-2.76516500	-1.94115300
N	-0.64768800	-1.56526000	-0.62020300
N	2.21833800	-1.83684400	-0.18102700
H	1.02484100	-2.99435900	1.04328900
H	2.38939000	-4.27649600	-1.36788900
H	2.90167000	-4.40058000	0.31562100
C	-0.54991900	-0.42540100	-1.32860600
S	0.47363100	-0.24293100	-2.68639100
C	3.01480700	-1.33676900	0.79189600
N	3.72738800	-0.21882400	0.49165400
S	3.15219800	-2.02257700	2.34265700
C	3.90665600	0.42077900	-0.82371300
C	4.29799500	1.87582300	-0.61483800
C	3.42894400	2.89755000	-1.00567200
C	3.77188900	4.23520500	-0.81846000
C	4.98922000	4.56926300	-0.23073400
C	5.86336900	3.55830100	0.16438300
C	5.52203300	2.22255200	-0.03106700
C	4.91145500	-0.34702100	-1.70100700
N	-1.31278200	0.64182400	-0.96232100
C	-2.38570600	0.80138000	0.05847900
C	-1.87795800	0.24418300	1.41085700
C	-2.63380900	-0.60825800	2.22076100

C	-2.11783400	-1.08852500	3.42735500
C	-0.83889400	-0.73276200	3.83717300
C	-0.07100500	0.11092700	3.03394600
C	-0.58724600	0.59510400	1.83851800
C	-2.63849700	2.33306900	0.13440800
C	-2.99623100	3.01184500	-1.04000600
C	-3.24144600	4.38019700	-1.02869600
C	-3.15452100	5.09736100	0.16380000
C	-2.82257200	4.43047000	1.33728900
C	-2.56373000	3.05870500	1.32377900
C	-3.70927600	0.14350800	-0.41104900
C	-3.77020600	-0.71069200	-1.51377000
C	-4.98407700	-1.26840000	-1.91932300
C	-6.15716900	-0.98015700	-1.23177500
C	-6.11164700	-0.11581700	-0.13877400
C	-4.90311200	0.44371800	0.26109700
H	-1.19296300	-1.54393400	0.23208600
H	2.11122000	-1.32214600	-1.05022400
H	4.32990800	0.08220500	1.24231700
H	2.47944000	2.64061900	-1.46346600
H	3.08648100	5.01505500	-1.13121100
H	5.25700600	5.60935700	-0.08282400
H	6.81441400	3.80960100	0.62054600
H	6.22034000	1.44868800	0.27192700
H	-1.14390900	1.44526900	-1.54753700
H	-3.62443000	-0.91492000	1.91458400
H	-2.72171000	-1.75136600	4.03699400
H	-0.42987100	-1.12125800	4.76231900
H	0.94070000	0.36500600	3.32431400
H	0.02551900	1.23537900	1.21554500
H	-3.10788300	2.46383700	-1.96951200
H	-3.51181200	4.88363700	-1.94996100
H	-3.35053600	6.16340300	0.17597000
H	-2.75895800	4.97408100	2.27318600
H	-2.30298200	2.56181600	2.24824700
H	-2.87793800	-0.93769600	-2.07968300
H	-5.00521800	-1.92428700	-2.78242600
H	-7.09939200	-1.41203100	-1.54927600
H	-7.02060700	0.13359000	0.39716700
H	-4.88977200	1.13416500	1.09621900
H	2.93810700	0.42593100	-1.32962900
H	4.58590700	-1.38000100	-1.84123200
H	4.99465100	0.12576200	-2.68263200
H	5.90216400	-0.36423400	-1.24118700

6a (conf. 31)

C	-1.14087600	5.15727700	0.41990500
C	0.12255200	5.20567000	-0.44725300
C	0.92003900	3.89814100	-0.34676100
C	0.05653300	2.67634600	-0.69593100
C	-1.20891000	2.62669700	0.19110800
C	-2.00417900	3.93939400	0.07130900

H	-1.72220200	6.07575500	0.29586900
H	-0.85613900	5.10971500	1.47833800
H	-0.15956400	5.37666900	-1.49349900
H	0.75935000	6.04621000	-0.15518300
H	1.78946400	3.91955000	-1.00934400
H	1.30242800	3.78656800	0.67677900
H	-0.24697100	2.73690100	-1.74425400
N	0.85829700	1.45626400	-0.56692900
N	-2.01217400	1.46759500	-0.17986200
H	-0.91019800	2.49322900	1.23602600
H	-2.38155600	4.02941700	-0.95507400
H	-2.87242600	3.87387600	0.73030200
C	0.81162100	0.37921600	-1.37181300
S	-0.23034900	0.24564200	-2.72069200
C	-2.75887500	0.71783200	0.66777600
N	-3.34398100	-0.35804000	0.07545400
S	-2.94559700	1.08620000	2.31431200
C	-4.23051800	-1.32920900	0.72334800
C	-5.51809500	-1.45750000	-0.08830800
C	-5.96500200	-2.66607300	-0.62589500
C	-7.15746600	-2.72849400	-1.34959400
C	-7.91999300	-1.58254900	-1.54485400
C	-7.48377900	-0.36880000	-1.01178000
C	-6.29569800	-0.30888400	-0.29350200
C	-3.48926600	-2.64227000	0.99308700
N	1.63173200	-0.67178200	-1.09312600
C	2.76363800	-0.81538600	-0.13302300
C	3.50456900	-2.10444000	-0.58183300
C	2.77312000	-3.29793100	-0.67190000
C	3.38686600	-4.48406900	-1.05770900
C	4.75170200	-4.50679600	-1.34198600
C	5.49007000	-3.33412500	-1.23434900
C	4.87166700	-2.13999300	-0.85946200
C	3.67743300	0.43176200	-0.25295200
C	4.16081800	1.13933600	0.85039100
C	4.98431600	2.25506400	0.67964000
C	5.33820900	2.68022700	-0.59494300
C	4.85693000	1.98484100	-1.70493200
C	4.03469100	0.87793000	-1.53456800
C	2.25803100	-1.05734100	1.31215800
C	3.15812700	-1.51701000	2.28532800
C	2.74545400	-1.73928600	3.59446200
C	1.41914200	-1.51242600	3.96105500
C	0.51200700	-1.07605900	3.00271100
C	0.92732500	-0.85903700	1.68706400
H	1.50959500	1.44059700	0.20561100
H	-1.85976000	1.11576400	-1.12426200
H	-3.16827300	-0.50478500	-0.91042900
H	-5.38926100	-3.57219800	-0.48373200
H	-7.48616600	-3.67708500	-1.75978800
H	-8.84644700	-1.63123700	-2.10598100
H	-8.07301000	0.53039800	-1.15430800

H	-5.95950000	0.63638800	0.11903600
H	1.53055900	-1.41836000	-1.76346900
H	1.71870500	-3.30423000	-0.41872000
H	2.80046600	-5.39333900	-1.12543200
H	5.23280700	-5.43189600	-1.63810700
H	6.55361600	-3.33907100	-1.44498000
H	5.46524100	-1.23894500	-0.78559500
H	3.89647800	0.83168900	1.85294900
H	5.34438300	2.78857400	1.55212000
H	5.97710600	3.54604000	-0.72657600
H	5.11831500	2.30819000	-2.70618400
H	3.65748100	0.35652700	-2.40596600
H	4.18798000	-1.71732700	2.01381300
H	3.46027800	-2.09752900	4.32698100
H	1.09659800	-1.68236300	4.98193500
H	-0.52375400	-0.88918200	3.26226800
H	0.19142700	-0.54118000	0.96243900
H	-4.48014800	-0.87929200	1.68740600
H	-3.14896300	-3.11411700	0.06661500
H	-2.61483400	-2.43943500	1.61337700
H	-4.12831700	-3.35055700	1.52638400

6b (conf. 6)

C	-2.59485000	4.30948300	0.17511000
C	-1.55225400	4.49752700	-0.93292100
C	-0.38398000	3.51542400	-0.77182400
C	-0.86458900	2.05636900	-0.70442300
C	-1.89864500	1.87927600	0.43003200
C	-3.07447200	2.85527500	0.24106400
H	-3.44664300	4.97662000	0.01268200
H	-2.15805700	4.59165000	1.14114000
H	-1.17140000	5.52334900	-0.93590400
H	-2.02592800	4.33706600	-1.90930800
H	0.32411000	3.61477900	-1.59930100
H	0.16636600	3.75381200	0.14822800
H	-1.32809100	1.78510600	-1.65569200
N	0.29083700	1.17064100	-0.54298700
N	-2.35337200	0.49192400	0.48481900
H	-1.41872100	2.09282600	1.38988000
H	-3.60612600	2.59294200	-0.68199200
H	-3.77212500	2.71201700	1.06863500
C	0.46697700	-0.02141900	-1.14193400
S	-0.64251300	-0.68983000	-2.25658300
C	-2.76292500	-0.13727300	1.60512800
N	-3.16365000	-1.43192400	1.46803600
S	-2.79434100	0.58425100	3.14508400
C	-3.37470000	-2.18226200	0.22833800
C	-4.58841200	-1.71131600	-0.57318900
C	-5.71443900	-1.16759500	0.04948000
C	-6.82912400	-0.79875400	-0.70076200
C	-6.83194800	-0.96687800	-2.08373400
C	-5.70996000	-1.50131400	-2.71379900

C	-4.59611800	-1.86854600	-1.96264300
C	-3.49120800	-3.67010800	0.59073000
N	1.59589800	-0.73305700	-0.86388000
C	2.83707000	-0.39589600	-0.11239900
C	3.75235700	0.54838700	-0.93417600
C	5.08836100	0.72240600	-0.54416000
C	5.94238900	1.55357300	-1.26070400
C	5.48259500	2.22195200	-2.39454500
C	4.16600700	2.04193700	-2.80226300
C	3.30769300	1.21125400	-2.07964500
C	2.45048600	0.18957300	1.26802500
C	1.46418300	-0.46530300	2.02294900
C	1.06546600	0.02288200	3.26110900
C	1.65071300	1.17885900	3.77855000
C	2.62778500	1.83829600	3.04281200
C	3.02340500	1.35107400	1.79443400
C	3.58990700	-1.74788600	0.03861000
C	3.99959700	-2.25777000	1.27118400
C	4.68950800	-3.46916100	1.34637100
C	4.97566600	-4.19083600	0.19350700
C	4.58100200	-3.68529800	-1.04440800
C	3.90624500	-2.47217500	-1.12037400
H	0.95112600	1.43334000	0.17734300
H	-2.32045700	-0.02038500	-0.39118700
H	-3.49402400	-1.83779300	2.33000500
H	-5.71388700	-1.01491600	1.12271300
H	-7.69413000	-0.37434600	-0.20317100
H	-7.69838900	-0.67592300	-2.66702100
H	-5.69705000	-1.62407000	-3.79113200
H	-3.71970100	-2.27075100	-2.46067800
H	1.61133800	-1.61467400	-1.35273500
H	5.46903000	0.19066200	0.31999900
H	6.97134100	1.66961200	-0.93904600
H	6.14848400	2.86513600	-2.95850200
H	3.79787100	2.54107100	-3.69158500
H	2.29519100	1.07582900	-2.43259100
H	0.98859700	-1.35222100	1.62204500
H	0.27653400	-0.47823700	3.80768800
H	1.33005000	1.56676000	4.73826500
H	3.08415600	2.74297100	3.42881800
H	3.77249000	1.89208200	1.23293000
H	3.78371500	-1.71665100	2.18230200
H	4.99793900	-3.84575800	2.31518200
H	5.50636100	-5.13401200	0.25495100
H	4.80841200	-4.22959200	-1.95394500
H	3.64379000	-2.07653300	-2.09588800
H	-2.48613000	-2.06648300	-0.40192800
H	-3.62094600	-4.26921000	-0.31138100
H	-4.35982900	-3.84276600	1.23369100
H	-2.59232800	-4.00969300	1.11136800

6b (conf. 15)

C	-1.87793100	5.34797500	0.62830800
C	-0.45186800	5.54063600	0.09839300
C	0.35019700	4.23335100	0.15875100
C	-0.36510000	3.09035300	-0.57874400
C	-1.79527600	2.89348100	-0.02200500
C	-2.59130300	4.20807800	-0.10734600
H	-2.44906600	6.27549000	0.52615900
H	-1.84156700	5.12113100	1.70100700
H	0.06987900	6.31673000	0.66656600
H	-0.49391300	5.88965100	-0.94082900
H	1.34491500	4.36877800	-0.27518900
H	0.49653300	3.94595300	1.20846700
H	-0.43010000	3.33318300	-1.64237800
N	0.44232100	1.86966500	-0.48248900
N	-2.44643600	1.81039800	-0.74698600
H	-1.73446800	2.59099500	1.02884600
H	-2.72629200	4.46989800	-1.16426200
H	-3.58420600	4.03202500	0.31136300
C	0.60113500	0.93669800	-1.43908600
S	-0.13056500	1.02548200	-2.98545100
C	-3.32787400	0.92550800	-0.22182300
N	-3.68262300	-0.06466200	-1.09015600
S	-3.95195700	1.05083900	1.34848700
C	-4.51315300	-1.22252800	-0.76604800
C	-3.69577200	-2.40704100	-0.25591400
C	-2.60007700	-2.89773500	-0.97484300
C	-1.87984100	-3.99749600	-0.51538200
C	-2.24716800	-4.62731500	0.67327200
C	-3.33487200	-4.14657800	1.39759500
C	-4.05081500	-3.04270800	0.93576600
C	-5.35849700	-1.59582900	-1.99152700
N	1.40211000	-0.13339100	-1.18235400
C	2.28643900	-0.47224500	-0.03152400
C	2.67935600	-1.95911500	-0.25808300
C	2.46400500	-2.95686000	0.69318200
C	2.85376100	-4.27401200	0.44344400
C	3.45903500	-4.61466000	-0.76066500
C	3.68843100	-3.62355800	-1.71419100
C	3.31270300	-2.30940900	-1.45988600
C	3.59533800	0.35781400	-0.06837700
C	4.67635300	-0.02658900	0.73817800
C	5.87072100	0.68539000	0.72391100
C	6.01682100	1.79382100	-0.10914700
C	4.95902800	2.17292100	-0.92726600
C	3.75859900	1.46053500	-0.90884100
C	1.49099300	-0.29122200	1.28511800
C	0.19468600	-0.82446400	1.36492300
C	-0.57244200	-0.67615000	2.51410300
C	-0.05697500	0.00731800	3.61577200
C	1.22455800	0.54132200	3.55114300
C	1.99366300	0.39707200	2.39362600
H	0.82246600	1.66564700	0.43322800

H	-2.05115800	1.60316300	-1.66360000
H	-3.19807600	-0.09116500	-1.97793900
H	-2.29655700	-2.41634000	-1.89912700
H	-1.03171500	-4.36243800	-1.08401700
H	-1.68689600	-5.48339500	1.03211000
H	-3.62390800	-4.62509800	2.32694900
H	-4.88660800	-2.66076100	1.51223200
H	1.42449800	-0.78167700	-1.95426900
H	1.98925800	-2.71683200	1.63456400
H	2.67731700	-5.03223800	1.19809500
H	3.75692500	-5.63881700	-0.95415800
H	4.17159100	-3.87053800	-2.65270600
H	3.53563200	-1.54620800	-2.19785600
H	4.58825000	-0.90056400	1.37285600
H	6.69198200	0.36611100	1.35576800
H	6.94940300	2.34616700	-0.12691000
H	5.06223300	3.02255600	-1.59286800
H	2.96050900	1.76738400	-1.56991800
H	-0.22595300	-1.34564100	0.51362600
H	-1.58010400	-1.07150200	2.53643300
H	-0.65934600	0.13299300	4.50794500
H	1.63418200	1.08178200	4.39724200
H	2.98157900	0.83540700	2.36185500
H	-5.17192400	-0.89797600	0.03988600
H	-6.00437500	-2.44512800	-1.75991400
H	-4.72751200	-1.88339300	-2.83879100
H	-5.98180000	-0.75107100	-2.29385500

6b (conf. 16)

C	-1.15752600	5.53416500	0.70591400
C	0.27206300	5.51307400	0.14980200
C	0.87478600	4.10314300	0.20590300
C	-0.01436000	3.07610900	-0.51125200
C	-1.44783300	3.09138000	0.07108600
C	-2.04485700	4.50700500	-0.00729800
H	-1.58888400	6.53469600	0.60641500
H	-1.13524700	5.31046200	1.77973000
H	0.91129300	6.20701000	0.70395900
H	0.26319500	5.86046600	-0.89071500
H	1.87115900	4.08643400	-0.24372500
H	0.99353200	3.80269100	1.25563500
H	-0.06093400	3.31970200	-1.57585300
N	0.59706600	1.74781000	-0.41930400
N	-2.26398000	2.11331400	-0.63589900
H	-1.41337700	2.78363900	1.12115400
H	-2.16154000	4.78236200	-1.06306100
H	-3.04480300	4.48125600	0.43129600
C	0.62033900	0.80749400	-1.38010000
S	-0.12171800	0.98982600	-2.91101400
C	-3.19356000	1.30143300	-0.07302000
N	-3.70890100	0.38786100	-0.94191700
S	-3.67822000	1.42280500	1.54689800

C	-4.70133300	-0.63692600	-0.62313500
C	-4.07001700	-1.98920000	-0.30420300
C	-3.15684200	-2.59080500	-1.17689300
C	-2.62052100	-3.84404700	-0.89337900
C	-2.98946900	-4.51775400	0.27029700
C	-3.89474000	-3.92656600	1.14732900
C	-4.42834000	-2.67084600	0.86077300
C	-5.71487400	-0.73697000	-1.77225100
N	1.26332900	-0.36384800	-1.11743500
C	2.22620200	-0.72487900	-0.03631400
C	3.27440400	0.41238100	0.08215100
C	3.65311600	0.99330400	1.29448400
C	4.60543000	2.01486300	1.33287200
C	5.19341000	2.47358200	0.16054500
C	4.81676000	1.90767100	-1.05804900
C	3.86801700	0.89339800	-1.09506500
C	1.49708900	-1.03440900	1.29533900
C	0.12716500	-0.82486500	1.46607100
C	-0.50096100	-1.13180700	2.67506700
C	0.23046400	-1.66821200	3.72744700
C	1.59464200	-1.90879900	3.56108800
C	2.21864800	-1.60017200	2.35804300
C	2.87697100	-2.05313400	-0.50904900
C	2.03776200	-3.13269500	-0.82230200
C	2.56683700	-4.35001800	-1.23556500
C	3.94773500	-4.52091900	-1.32538400
C	4.78808000	-3.46408800	-0.99547300
C	4.25781600	-2.23741000	-0.59206300
H	1.03536600	1.52972800	0.46474300
H	-1.94149700	1.88226400	-1.57467200
H	-3.30711300	0.35726100	-1.86976100
H	-2.85263200	-2.07991000	-2.08486800
H	-1.91764700	-4.29706700	-1.58430100
H	-2.57111500	-5.49302800	0.49237600
H	-4.18142300	-4.43818700	2.05949000
H	-5.12170200	-2.20737200	1.55453900
H	1.23151400	-0.99788700	-1.90105600
H	3.20563200	0.66065100	2.22101300
H	4.87996600	2.44996200	2.28728300
H	5.93251100	3.26605900	0.19079700
H	5.25942900	2.26011100	-1.98283800
H	3.57697600	0.47411000	-2.05058100
H	-0.47627500	-0.43840500	0.65716300
H	-1.56352600	-0.94474900	2.77430800
H	-0.25671100	-1.90924600	4.66538400
H	2.17324300	-2.34753400	4.36652000
H	3.27322100	-1.81881200	2.23731500
H	0.96328500	-3.02714600	-0.72062200
H	1.89965600	-5.16991200	-1.47638300
H	4.36144900	-5.47116100	-1.64304900
H	5.86398400	-3.58550000	-1.05260000
H	4.93069200	-1.42772700	-0.34416300

H	-5.20954200	-0.28237700	0.27389500
H	-6.20200900	0.22750200	-1.93376800
H	-6.47818300	-1.48205600	-1.53864300
H	-5.23055800	-1.04323400	-2.70512100

6b (conf. 24)

C	-0.91415800	5.62456100	0.11775400
C	0.46320700	5.51841700	-0.54866400
C	1.08186800	4.12979100	-0.33872700
C	0.14440600	3.01113100	-0.81954100
C	-1.22928000	3.11416200	-0.11454600
C	-1.84631400	4.50339400	-0.35597900
H	-0.79908900	5.56423900	1.20714900
H	-1.36361100	6.59948400	-0.09313200
H	0.36224800	5.70803900	-1.62443100
H	1.14076100	6.28449200	-0.15950200
H	2.03523600	4.04651100	-0.86805900
H	1.29566900	3.98518200	0.72871200
H	-0.00557300	3.10649100	-1.89777000
N	0.78613900	1.71038600	-0.60849300
N	-2.09414900	2.03891500	-0.58570900
H	-1.09343500	2.97471500	0.96314600
H	-2.05216800	4.61414500	-1.42802600
H	-2.80499700	4.54481900	0.16444800
C	0.72121000	0.64715600	-1.43155300
S	-0.14917700	0.63895400	-2.90494400
C	-3.04048800	1.40630800	0.14979100
N	-3.56407800	0.30879000	-0.46216100
S	-3.52303100	1.92925400	1.69087700
C	-4.70414800	-0.47999500	0.01928900
C	-4.42331000	-1.96347300	-0.17451700
C	-4.18675100	-2.77972700	0.93532200
C	-3.91498400	-4.13776400	0.78070700
C	-3.86952900	-4.70023000	-0.49243300
C	-4.10295700	-3.89773600	-1.60743000
C	-4.38216700	-2.54264600	-1.44822700
C	-6.01450700	-0.01344700	-0.63226600
N	1.39731500	-0.48428100	-1.09096400
C	2.32572800	-0.79536700	0.03142000
C	2.50817500	-2.33788600	-0.01796300
C	2.97966900	-2.91854400	-1.20473500
C	3.16967600	-4.29216100	-1.30229600
C	2.91183400	-5.11437600	-0.20623800
C	2.46522900	-4.54672300	0.98129800
C	2.26173800	-3.16885600	1.07546500
C	3.72158900	-0.16277600	-0.20405100
C	3.95343300	0.78752700	-1.20042300
C	5.22834700	1.32154600	-1.39578600
C	6.29350100	0.91280300	-0.60189400
C	6.07808200	-0.04816100	0.38505000
C	4.80893000	-0.58364300	0.57542900
C	1.67296900	-0.34594400	1.36259100

C	2.35522500	0.37882900	2.34425500
C	1.71077500	0.76706200	3.52172300
C	0.37552000	0.44538100	3.73205400
C	-0.31881500	-0.27015900	2.75616100
C	0.32402600	-0.66310900	1.58875600
H	1.22878200	1.57811700	0.29177800
H	-1.83132200	1.63051600	-1.48200300
H	-3.17558900	0.04415400	-1.35810800
H	-4.21825300	-2.34503800	1.92893200
H	-3.73795100	-4.75490200	1.65469500
H	-3.65590200	-5.75595600	-0.61596200
H	-4.07168000	-4.32760700	-2.60243000
H	-4.57255400	-1.93682600	-2.32840300
H	1.25008100	-1.22794400	-1.75586100
H	3.22287900	-2.29095900	-2.05543800
H	3.52966800	-4.71846000	-2.23176200
H	3.06401300	-6.18518600	-0.27847800
H	2.26750300	-5.17333000	1.84371600
H	1.90890300	-2.74995800	2.00802500
H	3.14947600	1.11020300	-1.84652400
H	5.38264200	2.05417800	-2.18003500
H	7.28354800	1.32624100	-0.75674800
H	6.90207200	-0.39186400	1.00032600
H	4.66498600	-1.34916000	1.32877500
H	3.38920500	0.65817100	2.19641600
H	2.26031000	1.33145200	4.26682100
H	-0.12984400	0.76157000	4.63705400
H	-1.36927700	-0.49556400	2.89111200
H	-0.23226300	-1.20205300	0.83151000
H	-4.76370300	-0.27608300	1.08826200
H	-6.85823100	-0.59446200	-0.25096400
H	-5.98710400	-0.12759900	-1.71941900
H	-6.18305500	1.04013900	-0.40025100

7a (conf. 1)

C	4.15170300	-0.04539800	-0.74668500
C	2.87587400	-0.44045900	0.02234500
C	3.21496700	-0.62851300	1.51280000
C	1.77737300	0.65378600	-0.18390600
C	2.35436200	-1.77284200	-0.54841000
N	0.52693900	0.28801400	0.48972200
C	2.18547600	2.07883700	0.21853400
C	-0.67441200	0.25808900	-0.20598000
O	-0.73827400	0.35561100	-1.42322800
N	-1.77671000	0.10635600	0.61353900
C	-3.15346600	-0.12511400	0.11533800
C	-4.03339000	-0.27799400	1.36541000
C	-3.62119000	1.09422400	-0.69673500
C	-3.22612500	-1.40508100	-0.73839400
H	3.92909400	0.17065800	-1.79654500
H	4.64074300	0.83185300	-0.31633400
H	4.87460800	-0.86602800	-0.72418600

H	2.33540200	-0.94052800	2.08367400
H	3.97392000	-1.40674900	1.63552200
H	3.61079000	0.28622700	1.96326000
H	1.52738700	0.66036100	-1.24689300
H	1.44611200	-2.09253500	-0.03419300
H	2.12036100	-1.68004800	-1.61293900
H	3.10663600	-2.55916500	-0.43444600
H	0.46887700	0.53174800	1.46775000
H	1.37179300	2.76897800	-0.01607600
H	2.39467900	2.15678700	1.29043500
H	3.07239900	2.41589700	-0.32033200
H	-1.59044500	-0.27797900	1.52825100
H	-5.07439500	-0.43850400	1.07743400
H	-3.72009900	-1.13768800	1.96817100
H	-3.98508300	0.61891300	1.98919600
H	-4.65661500	0.95394900	-1.01950800
H	-3.56896400	1.99907800	-0.08547500
H	-2.99255300	1.23082700	-1.57530900
H	-4.25088500	-1.58022000	-1.07855200
H	-2.57831500	-1.31351500	-1.60996200
H	-2.90788700	-2.27500600	-0.15584600

7a (conf. 2)

C	3.52732800	1.16759900	0.90015500
C	2.60154400	0.52969900	-0.15351500
C	3.44403000	-0.25313200	-1.17655700
C	1.55327100	-0.39956300	0.54776000
C	1.84874100	1.65605900	-0.88646300
N	0.63750800	-1.01534300	-0.42379200
C	2.15694600	-1.49902300	1.43634900
C	-0.75363600	-0.97942800	-0.40920300
O	-1.40313400	-1.90058100	-0.88674200
N	-1.31519500	0.14534000	0.15321600
C	-2.77153700	0.42537900	0.15789700
C	-3.32656400	0.49913100	-1.27713900
C	-3.50504000	-0.65837400	0.96573700
C	-2.93680400	1.78517700	0.85309200
H	2.95133100	1.64892900	1.69775000
H	4.19620200	0.43685400	1.36042100
H	4.15314700	1.93543500	0.43664600
H	2.81302200	-0.68709300	-1.95620800
H	4.16148600	0.41242700	-1.66497900
H	4.01549100	-1.05821500	-0.70686200
H	0.95060000	0.24156900	1.19757600
H	1.14811600	1.25111500	-1.61965400
H	1.29281100	2.28476700	-0.18099600
H	2.55067400	2.30753500	-1.41457000
H	0.93888200	-1.90924500	-0.78722700
H	1.35376500	-2.06041900	1.91863300
H	2.75192300	-2.20563500	0.85019900
H	2.79714200	-1.08906400	2.21930000
H	-0.72505400	0.96068600	0.20356100

H	-4.39550900	0.73080600	-1.26048300
H	-2.81779200	1.28285600	-1.84658900
H	-3.18131700	-0.45275700	-1.78723300
H	-4.57360900	-0.43036400	1.01210900
H	-3.37322400	-1.63498900	0.50220100
H	-3.11617600	-0.69916500	1.98674900
H	-3.99334700	2.05639200	0.90451700
H	-2.54164100	1.75406900	1.87232300
H	-2.41771800	2.57701900	0.30210800

7b (conf. 1)

C	4.02531000	-0.18447100	0.04101900
C	2.55596900	-0.54541000	0.33662400
C	2.35078300	-2.05321400	0.09274800
C	1.62476000	0.32990400	-0.56310300
C	2.26647700	-0.22456400	1.81577700
N	0.20773500	0.08920300	-0.25797300
C	1.84184100	0.19150600	-2.07685400
C	-0.70838800	1.04367300	0.03658500
S	-0.32000300	2.67951800	0.27010400
N	-2.01108200	0.65876600	0.16075300
C	-2.69748900	-0.64771000	0.01579800
C	-4.18320100	-0.35043200	0.28490900
C	-2.20348400	-1.66601100	1.06315500
C	-2.56513300	-1.20464400	-1.41719000
H	4.19489300	0.89163100	0.14314800
H	4.33250000	-0.48282100	-0.96411000
H	4.68574100	-0.69290000	0.74912500
H	1.33131400	-2.37333300	0.33244600
H	3.02089800	-2.63276300	0.73419700
H	2.56359100	-2.33686400	-0.94156300
H	1.79656200	1.37123900	-0.28822600
H	1.23860900	-0.47171800	2.08889700
H	2.41468700	0.83840700	2.02296600
H	2.93594200	-0.79510700	2.46634800
H	-0.13387300	-0.83472600	-0.46538700
H	1.17827500	0.88426500	-2.59855200
H	1.62474200	-0.82037800	-2.43266500
H	2.86707600	0.43506300	-2.36009300
H	-2.59997400	1.44392100	0.39227400
H	-4.77302800	-1.26532200	0.20413400
H	-4.57255300	0.37069200	-0.43894700
H	-4.32192300	0.05612000	1.29039500
H	-2.78684000	-2.58800800	0.99287600
H	-2.31972300	-1.25840800	2.06958700
H	-1.15278900	-1.93246100	0.93553300
H	-3.18361500	-2.09934400	-1.52733400
H	-1.54288800	-1.48601800	-1.67919900
H	-2.89881500	-0.46099500	-2.14378000

7b (conf. 2)

C	-3.65832600	-1.40559100	-0.48332000

C	-2.69275600	-0.49421900	0.29869900
C	-3.49397500	0.58492200	1.05013100
C	-1.65782700	0.14890500	-0.68609500
C	-1.93327600	-1.35531500	1.32552200
N	-0.69236200	1.00599500	0.01960000
C	-2.27126000	0.96145700	-1.83700100
C	0.67111100	0.88876200	0.10028300
S	1.57457800	2.27300500	0.47057900
N	1.17146000	-0.35314500	-0.10754000
C	2.58177200	-0.83305700	-0.12064000
C	2.48985200	-2.32906900	-0.46559800
C	3.23390000	-0.66652400	1.26261600
C	3.39203400	-0.11361700	-1.21087400
H	-3.11405200	-2.13072400	-1.09807900
H	-4.32370900	-0.83969300	-1.13908600
H	-4.28754400	-1.97005300	0.21039800
H	-2.83619500	1.22967100	1.63846300
H	-4.19859600	0.11548100	1.74208300
H	-4.07590200	1.21278000	0.37040600
H	-1.10059900	-0.67615100	-1.14037600
H	-1.20329100	-0.76284500	1.88094500
H	-1.41007700	-2.18669200	0.83869700
H	-2.62906600	-1.79301300	2.04649200
H	-0.97675600	1.96603000	0.15399700
H	-1.47706200	1.32392900	-2.49263300
H	-2.81760500	1.83157100	-1.46325800
H	-2.95898700	0.36299000	-2.43606800
H	0.49147300	-1.09690200	-0.13955500
H	3.48889500	-2.76760900	-0.49161100
H	2.02889400	-2.48071400	-1.44635900
H	1.90733700	-2.87339800	0.28509900
H	4.25029800	-1.06974800	1.24334400
H	2.66424700	-1.20818400	2.02296700
H	3.27753800	0.38444000	1.54476400
H	4.40124300	-0.53241700	-1.25233100
H	3.46342300	0.95319300	-1.00587100
H	2.92167500	-0.24989900	-2.18845300

7b (conf. 3)

C	3.83407000	-1.44122800	-0.10782500
C	2.95127400	-0.19443300	-0.31249400
C	3.67567600	1.03071100	0.27985000
C	1.55695400	-0.43522000	0.35767400
C	2.74547500	0.01862800	-1.82517400
N	0.68835600	0.72605400	0.14075700
C	1.59714000	-0.81115700	1.84937100
C	-0.67750700	0.78030000	0.09474200
S	-1.42077400	2.30318200	0.13235700
N	-1.31662100	-0.41160500	0.01534800
C	-2.76533100	-0.71835700	-0.14695700
C	-2.84174000	-2.25308200	-0.21637400
C	-3.31065700	-0.12217900	-1.45542800

C	-3.56748900	-0.22766600	1.06961200
H	3.32773100	-2.34988100	-0.44945300
H	4.11520800	-1.58192800	0.93818200
H	4.75759600	-1.34217600	-0.68456400
H	3.14194600	1.96590300	0.08760600
H	4.66201100	1.13339300	-0.18062300
H	3.82706800	0.93842100	1.35811200
H	1.12974800	-1.27970800	-0.19719200
H	2.10487600	0.87875900	-2.02665200
H	2.28205600	-0.85974900	-2.28604700
H	3.70656200	0.18442000	-2.31977600
H	1.08958000	1.63707600	0.30553100
H	0.57955200	-0.94619700	2.22217700
H	2.06024200	-0.02066100	2.44403800
H	2.14456200	-1.73984600	2.02086300
H	-0.72466600	-1.22636600	-0.03027600
H	-3.87978100	-2.56991300	-0.32957800
H	-2.44918400	-2.70976900	0.69762300
H	-2.27916300	-2.63921700	-1.07266600
H	-4.35758300	-0.41081400	-1.58421800
H	-2.74320000	-0.49654300	-2.31205300
H	-3.24490300	0.96475700	-1.44427000
H	-4.61539800	-0.52118200	0.96084100
H	-3.51317600	0.85575400	1.16121500
H	-3.17862800	-0.67449400	1.98876000

7b (conf. 4)

C	4.29963600	-0.36414900	-0.32986700
C	2.97754400	0.42565000	-0.26901100
C	3.20594100	1.72879900	0.52126200
C	1.87169900	-0.46965200	0.37967100
C	2.55034400	0.77333900	-1.70807200
N	0.58627200	0.23529000	0.41447500
C	2.19275200	-1.01754300	1.77789700
C	-0.62568200	-0.28917400	0.05006400
S	-0.78371300	-1.82526600	-0.63164400
N	-1.65656200	0.57010500	0.29025700
C	-3.11840900	0.42643900	0.05409200
C	-3.73245700	1.73923200	0.57088000
C	-3.69178600	-0.74787000	0.86419600
C	-3.42817700	0.27553400	-1.44555900
H	4.15854400	-1.33365400	-0.81736800
H	4.72192100	-0.54140600	0.66190800
H	5.04288500	0.19240600	-0.90789400
H	2.31122800	2.35981500	0.53608300
H	3.99965500	2.31859200	0.05386700
H	3.50787900	1.53646400	1.55440500
H	1.71068300	-1.31876800	-0.28620300
H	1.60465300	1.31899500	-1.72289500
H	2.41956300	-0.13176500	-2.30768800
H	3.30962400	1.39386000	-2.19327800
H	0.55611500	1.03516600	1.03205300

H	1.37277200	-1.65980500	2.10561100
H	2.31311700	-0.21630700	2.51388000
H	3.10542900	-1.61576200	1.77810900
H	-1.38143500	1.51191800	0.53215000
H	-4.81556500	1.72306000	0.43937500
H	-3.34344500	2.60187600	0.01938000
H	-3.52277600	1.87959100	1.63553200
H	-4.77800900	-0.78082200	0.74179900
H	-3.46843500	-0.62323700	1.92713700
H	-3.27306000	-1.69597600	0.53147100
H	-4.51056700	0.23795800	-1.59835900
H	-2.98572500	-0.63644300	-1.84330500
H	-3.03204400	1.12711600	-2.00589800

3b (conf. 3)[a]

C	1.09930000	5.82470000	-0.76790000
C	-0.37760000	6.09470000	-0.45940000
C	-1.26140000	4.93600000	-0.93510000
C	-0.81720000	3.58010000	-0.36250000
C	0.67350000	3.31340000	-0.66180000
C	1.54330000	4.48560000	-0.17060000
H	1.24770000	5.80960000	-1.85500000
H	1.72440000	6.63360000	-0.37800000
H	-0.50460000	6.22890000	0.62180000
H	-0.70800000	7.02410000	-0.93240000
H	-2.30550000	5.10700000	-0.65770000
H	-1.22590000	4.88260000	-2.03130000
H	-0.94420000	3.59370000	0.72540000
N	-1.70290000	2.53640000	-0.88670000
N	1.08010000	2.05690000	-0.03280000
H	0.79530000	3.21580000	-1.74730000
H	1.47930000	4.52700000	0.92380000
H	2.58400000	4.27040000	-0.42240000
C	-2.09250000	1.44620000	-0.15550000
O	-1.51560000	1.10710000	0.88230000
C	2.14570000	1.34180000	-0.50700000
N	2.31780000	0.11370000	0.11700000
O	2.87640000	1.74260000	-1.41100000
C	3.57780000	-0.66510000	0.07660000
C	4.77090000	0.28870000	0.34700000
C	5.85000000	0.44650000	-0.52350000
C	6.88660000	1.33480000	-0.22910000
C	6.86050000	2.08600000	0.94140000
C	5.78230000	1.94550000	1.81620000
C	4.75230000	1.05880000	1.51910000
C	3.45240000	-1.73570000	1.19590000
C	2.25340000	-2.45010000	1.33530000
C	2.12200000	-3.45010000	2.29520000
C	3.19380000	-3.77120000	3.12710000
C	4.39470000	-3.08190000	2.98570000
C	4.52220000	-2.07220000	2.03070000
N	-3.14650000	0.74550000	-0.69750000
C	-3.83760000	-0.38520000	-0.03840000

C	-5.09650000	-0.67640000	-0.90380000
C	-4.97840000	-0.71530000	-2.30110000
C	-6.07280000	-1.02440000	-3.10430000
C	-7.30640000	-1.32140000	-2.52680000
C	-7.42980000	-1.30760000	-1.14040000
C	-6.33570000	-0.98630000	-0.33620000
C	-2.98910000	-1.67970000	-0.10650000
C	-1.74680000	-1.71790000	-0.74230000
C	-1.03980000	-2.91590000	-0.86330000
C	-1.56020000	-4.09850000	-0.34620000
C	-2.80410000	-4.07480000	0.28470000
C	-3.51140000	-2.88120000	0.39450000
C	-4.22520000	0.04130000	1.40120000
C	-3.78570000	-0.61560000	2.55060000
C	-4.15000000	-0.16230000	3.82000000
C	-4.95590000	0.96270000	3.96240000
C	-5.39050000	1.63780000	2.82110000
C	-5.02620000	1.18160000	1.55860000
H	-2.17720000	2.73740000	-1.75440000
H	0.37400000	1.59060000	0.53190000
H	1.78030000	-0.02050000	0.96040000
H	5.88630000	-0.11080000	-1.44920000
H	7.71120000	1.44060000	-0.92540000
H	7.66500000	2.77600000	1.16950000
H	5.74290000	2.52670000	2.73080000
H	3.92180000	0.96520000	2.20970000
H	1.41540000	-2.23520000	0.68320000
H	1.18210000	-3.98280000	2.38590000
H	3.09370000	-4.55120000	3.87310000
H	5.23920000	-3.32280000	3.62160000
H	5.46350000	-1.54620000	1.94420000
H	-3.69380000	1.22370000	-1.39660000
H	-4.02140000	-0.51910000	-2.77020000
H	-5.95700000	-1.04090000	-4.18210000
H	-8.15860000	-1.56510000	-3.15070000
H	-8.38070000	-1.54270000	-0.67580000
H	-6.45800000	-0.97550000	0.73850000
H	-1.32700000	-0.81620000	-1.16460000
H	-0.08150000	-2.91880000	-1.37060000
H	-1.01080000	-5.02810000	-0.44110000
H	-3.23120000	-4.98830000	0.68320000
H	-4.48700000	-2.89210000	0.86560000
H	-3.13890000	-1.47790000	2.46860000
H	-3.79170000	-0.69010000	4.69690000
H	-5.23820000	1.31500000	4.94810000
H	-6.01320000	2.52070000	2.91390000
H	-5.37000000	1.72060000	0.68310000
C	3.71430000	-1.45040000	-1.25290000
C	2.81050000	-1.29330000	-2.30560000
C	2.93510000	-2.04310000	-3.47680000
C	3.96640000	-2.96700000	-3.61740000
C	4.87220000	-3.13830000	-2.57070000

C	4.74210000	-2.39280000	-1.40230000
H	2.00330000	-0.58160000	-2.21870000
H	2.21950000	-1.90020000	-4.27900000
H	4.06220000	-3.54990000	-4.52650000
H	5.67780000	-3.85880000	-2.65900000
H	5.44760000	-2.55540000	-0.59620000

3b (conf. 6)[a]

C	1.36040000	5.49220000	-0.51450000
C	-0.05360000	5.55840000	0.07440000
C	-0.92000000	4.41150000	-0.45770000
C	-0.28810000	3.03380000	-0.18490000
C	1.13740000	2.96600000	-0.77940000
C	2.00400000	4.12390000	-0.26050000
H	1.31220000	5.67510000	-1.59490000
H	1.99220000	6.27830000	-0.09060000
H	0.00410000	5.49790000	1.16850000
H	-0.52000000	6.51960000	-0.16130000
H	-1.91370000	4.42950000	-0.00460000
H	-1.05730000	4.52060000	-1.54070000
H	-0.21880000	2.88900000	0.90000000
N	-1.09420000	1.95070000	-0.74350000
N	1.81860000	1.69990000	-0.49950000
H	1.05070000	3.04520000	-1.86770000
H	2.16140000	3.99200000	0.81780000
H	2.98750000	4.06590000	-0.73510000
C	-2.19190000	1.45710000	-0.09730000
O	-2.64420000	1.94730000	0.93550000
C	1.70470000	0.60300000	-1.29250000
N	2.48280000	-0.49960000	-1.01710000
O	0.91750000	0.55720000	-2.25390000
C	3.65450000	-0.69430000	-0.13160000
C	3.27960000	-0.21760000	1.29500000
C	4.06910000	0.65250000	2.05180000
C	3.66860000	1.05560000	3.32910000
C	2.47250000	0.59690000	3.86870000
C	1.67090000	-0.26610000	3.11940000
C	2.06930000	-0.66450000	1.84890000
C	3.93980000	-2.22350000	-0.15720000
C	4.11880000	-2.85500000	-1.39740000
C	4.39220000	-4.21670000	-1.47590000
C	4.51450000	-4.97570000	-0.31180000
C	4.36370000	-4.35540000	0.92390000
C	4.07700000	-2.99050000	1.00120000
N	-2.78740000	0.38760000	-0.75620000
C	-3.80750000	-0.49140000	-0.14850000
C	-5.14450000	0.26220000	0.06520000
C	-5.38590000	1.50550000	-0.52500000
C	-6.62750000	2.12880000	-0.40190000
C	-7.65590000	1.52010000	0.31270000
C	-7.43190000	0.27360000	0.89550000
C	-6.19250000	-0.34850000	0.76700000

C	-4.14230000	-1.57950000	-1.20640000
C	-4.13570000	-1.26510000	-2.57180000
C	-4.50710000	-2.20950000	-3.52740000
C	-4.90830000	-3.48490000	-3.13740000
C	-4.93610000	-3.80380000	-1.78130000
C	-4.55690000	-2.86170000	-0.82710000
C	-3.21390000	-1.10730000	1.14460000
C	-2.18350000	-2.05230000	1.03190000
C	-1.56880000	-2.58820000	2.16000000
C	-1.96650000	-2.18180000	3.43420000
C	-2.97080000	-1.22620000	3.55990000
C	-3.58320000	-0.69090000	2.42570000
H	-0.66740000	1.42010000	-1.49890000
H	2.38210000	1.64620000	0.33580000
H	2.28790000	-1.24800000	-1.66400000
H	4.99830000	1.03430000	1.65240000
H	4.29790000	1.73410000	3.89380000
H	2.16100000	0.91180000	4.85800000
H	0.72940000	-0.62360000	3.52010000
H	1.43030000	-1.32160000	1.27180000
H	4.06750000	-2.27910000	-2.31520000
H	4.52010000	-4.68190000	-2.44670000
H	4.73220000	-6.03580000	-0.37040000
H	4.46600000	-4.92960000	1.83780000
H	3.96220000	-2.53300000	1.97440000
H	-2.20570000	-0.07620000	-1.43910000
H	-4.60400000	1.98930000	-1.09330000
H	-6.78670000	3.09540000	-0.86740000
H	-8.62000000	2.00610000	0.41040000
H	-8.22300000	-0.22040000	1.44870000
H	-6.04770000	-1.32250000	1.21780000
H	-3.85260000	-0.27180000	-2.89710000
H	-4.48680000	-1.94160000	-4.57780000
H	-5.19800000	-4.22000000	-3.87950000
H	-5.24940000	-4.79090000	-1.46040000
H	-4.57880000	-3.13680000	0.21930000
H	-1.85880000	-2.38160000	0.05160000
H	-0.78200000	-3.32500000	2.04310000
H	-1.49510000	-2.60230000	4.31540000
H	-3.28000000	-0.88760000	4.54260000
H	-4.34550000	0.06530000	2.54610000
C	4.92580000	0.00290000	-0.68740000
C	4.88350000	0.87800000	-1.77470000
C	6.04980000	1.46980000	-2.26530000
C	7.28020000	1.19530000	-1.67790000
C	7.33820000	0.31230000	-0.59930000
C	6.17580000	-0.27990000	-0.11590000
H	3.94580000	1.09610000	-2.26570000
H	5.98850000	2.14280000	-3.11310000
H	8.18520000	1.65410000	-2.05950000
H	8.29060000	0.07690000	-0.13790000
H	6.24520000	-0.97730000	0.71060000

3b (conf. 11)[a]

C	0.65460000	6.11620000	0.12530000
C	-0.86410000	5.97580000	0.28400000
C	-1.35780000	4.64870000	-0.30400000
C	-0.63350000	3.44260000	0.32200000
C	0.89220000	3.58010000	0.13940000
C	1.39360000	4.91080000	0.72070000
H	0.90140000	6.20030000	-0.94010000
H	1.00800000	7.03500000	0.60260000
H	-1.12560000	6.02320000	1.34860000
H	-1.37550000	6.81300000	-0.20040000
H	-2.43160000	4.52780000	-0.14590000
H	-1.18620000	4.63330000	-1.38750000
H	-0.85370000	3.42280000	1.39570000
N	-1.08400000	2.17590000	-0.25070000
N	1.64160000	2.47210000	0.73040000
H	1.10530000	3.55920000	-0.93390000
H	1.25200000	4.89860000	1.80920000
H	2.46920000	4.99030000	0.53920000
C	-2.24750000	1.58580000	0.16030000
O	-3.00720000	2.10830000	0.97460000
C	2.00700000	1.36700000	0.01240000
N	2.81210000	0.47550000	0.69500000
O	1.61240000	1.17160000	-1.14020000
C	3.67770000	-0.53000000	0.02660000
C	2.86580000	-1.75330000	-0.46220000
C	1.48300000	-1.84720000	-0.29840000
C	0.78920000	-2.98910000	-0.70390000
C	1.46760000	-4.06060000	-1.27700000
C	2.85120000	-3.98390000	-1.43500000
C	3.54010000	-2.84580000	-1.02660000
C	4.46820000	0.17980000	-1.10320000
C	4.36100000	-0.15940000	-2.45250000
C	5.06790000	0.54600000	-3.42850000
C	5.89000000	1.61030000	-3.07250000
C	5.99480000	1.97000000	-1.72850000
C	5.28960000	1.26370000	-0.75930000
N	-2.51970000	0.37520000	-0.45280000
C	-3.57970000	-0.55830000	-0.01730000
C	-4.98320000	-0.06900000	-0.46020000
C	-5.16750000	1.13130000	-1.14910000
C	-6.43520000	1.52050000	-1.58530000
C	-7.54380000	0.71550000	-1.34120000
C	-7.37140000	-0.49210000	-0.66470000
C	-6.10520000	-0.88060000	-0.23680000
C	-3.33640000	-1.87790000	-0.80160000
C	-3.07820000	-1.81830000	-2.17950000
C	-2.90280000	-2.97910000	-2.92740000
C	-3.00070000	-4.22940000	-2.31760000
C	-3.27850000	-4.30190000	-0.95570000
C	-3.44370000	-3.13710000	-0.20430000

C	-3.45590000	-0.77560000	1.51410000
C	-2.23120000	-1.23450000	2.02010000
C	-2.03980000	-1.43000000	3.38410000
C	-3.07450000	-1.16460000	4.28160000
C	-4.29080000	-0.69680000	3.79460000
C	-4.47740000	-0.50160000	2.42450000
H	-0.42700000	1.67650000	-0.84000000
H	1.96990000	2.58440000	1.67790000
H	3.19550000	0.81460000	1.56510000
H	0.93970000	-1.02710000	0.14820000
H	-0.28620000	-3.03640000	-0.57350000
H	0.92760000	-4.94600000	-1.59240000
H	3.39770000	-4.81280000	-1.87090000
H	4.61670000	-2.81390000	-1.14380000
H	3.71290000	-0.96910000	-2.75740000
H	4.96450000	0.26250000	-4.47000000
H	6.43830000	2.15820000	-3.83040000
H	6.62580000	2.80120000	-1.43390000
H	5.38290000	1.56010000	0.27920000
H	-1.77530000	-0.03910000	-0.99200000
H	-4.31900000	1.76520000	-1.36040000
H	-6.55030000	2.45770000	-2.11860000
H	-8.52820000	1.01860000	-1.67960000
H	-8.22180000	-1.13800000	-0.47630000
H	-5.99170000	-1.83170000	0.26970000
H	-3.02690000	-0.85830000	-2.67970000
H	-2.69740000	-2.90500000	-3.98930000
H	-2.86780000	-5.13440000	-2.89920000
H	-3.36500000	-5.26630000	-0.46790000
H	-3.65370000	-3.21950000	0.85370000
H	-1.41420000	-1.44230000	1.33920000
H	-1.08250000	-1.78900000	3.74550000
H	-2.92980000	-1.31520000	5.34550000
H	-5.10110000	-0.47170000	4.47930000
H	-5.42500000	-0.11540000	2.07600000
C	4.62080000	-1.07520000	1.13460000
C	4.08670000	-1.40920000	2.38800000
C	4.88970000	-1.95370000	3.38650000
C	6.24240000	-2.19300000	3.14790000
C	6.77900000	-1.88330000	1.90150000
C	5.97620000	-1.32800000	0.90430000
H	3.03200000	-1.25670000	2.58380000
H	4.45430000	-2.19790000	4.34890000
H	6.86810000	-2.61960000	3.92340000
H	7.82780000	-2.06880000	1.69870000
H	6.41730000	-1.09040000	-0.05450000

3b (conf. 12)[a]

C	1.40000000	5.40880000	-0.16310000
C	-0.03160000	5.49180000	0.37850000
C	-0.90800000	4.38870000	-0.22470000
C	-0.31930000	2.98650000	0.01830000

C	1.12180000	2.90340000	-0.53290000
C	2.00060000	4.01510000	0.06000000
H	1.39540000	5.63250000	-1.23690000
H	2.03660000	6.16120000	0.31170000
H	-0.01430000	5.39030000	1.47100000
H	-0.46410000	6.47320000	0.16250000
H	-1.91550000	4.41640000	0.19620000
H	-1.00570000	4.54050000	-1.30680000
H	-0.28790000	2.80340000	1.09900000
N	-1.13330000	1.94390000	-0.60170000
N	1.75260000	1.60280000	-0.28450000
H	1.07340000	3.02840000	-1.61950000
H	2.11640000	3.83840000	1.13720000
H	2.99800000	3.94980000	-0.38290000
C	-2.26350000	1.46090000	-0.00540000
O	-2.73050000	1.92720000	1.03180000
C	1.66110000	0.56050000	-1.15010000
N	2.42090000	-0.56640000	-0.90440000
O	0.88980000	0.57120000	-2.12330000
C	3.71010000	-0.69970000	-0.17540000
C	3.48550000	-0.80180000	1.35530000
C	2.20840000	-0.76720000	1.91990000
C	2.02820000	-0.91550000	3.29760000
C	3.12210000	-1.11010000	4.13340000
C	4.40170000	-1.16780000	3.57890000
C	4.57910000	-1.02200000	2.20740000
C	4.29840000	-2.07190000	-0.60400000
C	3.46330000	-3.19850000	-0.63180000
C	3.96650000	-4.45310000	-0.96350000
C	5.32070000	-4.61230000	-1.25550000
C	6.16190000	-3.50450000	-1.21070000
C	5.65520000	-2.24440000	-0.88980000
N	-2.86990000	0.43200000	-0.71620000
C	-3.90060000	-0.46240000	-0.14770000
C	-5.25030000	0.27620000	0.03420000
C	-5.46580000	1.55300000	-0.48990000
C	-6.71500000	2.16650000	-0.39270000
C	-7.77600000	1.51410000	0.22940000
C	-7.57730000	0.23400000	0.74530000
C	-6.33080000	-0.37790000	0.64190000
C	-4.18790000	-1.54270000	-1.22690000
C	-4.19930000	-1.19330000	-2.58420000
C	-4.52650000	-2.12950000	-3.56300000
C	-4.86530000	-3.43260000	-3.20470000
C	-4.87460000	-3.78690000	-1.85760000
C	-4.53830000	-2.85220000	-0.87950000
C	-3.33980000	-1.08630000	1.15660000
C	-2.24480000	-1.95800000	1.06290000
C	-1.65190000	-2.49760000	2.20050000
C	-2.13930000	-2.17080000	3.46660000
C	-3.21290000	-1.29210000	3.57480000
C	-3.80250000	-0.75160000	2.43070000

H	-0.69790000	1.42910000	-1.36310000
H	2.35770000	1.52680000	0.51830000
H	2.28080000	-1.24210000	-1.64090000
H	1.34120000	-0.64360000	1.28630000
H	1.02520000	-0.88400000	3.70760000
H	2.98290000	-1.22640000	5.20200000
H	5.26380000	-1.33520000	4.21470000
H	5.57900000	-1.09390000	1.79680000
H	2.41390000	-3.10250000	-0.37900000
H	3.30000000	-5.30780000	-0.98490000
H	5.71440000	-5.58950000	-1.51040000
H	7.21810000	-3.61320000	-1.43000000
H	6.32780000	-1.39730000	-0.86710000
H	-2.29230000	-0.00700000	-1.41850000
H	-4.65800000	2.07140000	-0.98670000
H	-6.85430000	3.15960000	-0.80580000
H	-8.74600000	1.99220000	0.30660000
H	-8.39420000	-0.29400000	1.22450000
H	-6.20580000	-1.37900000	1.03630000
H	-3.96510000	-0.17900000	-2.88340000
H	-4.52160000	-1.83470000	-4.60630000
H	-5.12160000	-4.16130000	-3.96510000
H	-5.13990000	-4.79570000	-1.56180000
H	-4.54440000	-3.15420000	0.15970000
H	-1.85060000	-2.22420000	0.08880000
H	-0.81040000	-3.17350000	2.09800000
H	-1.68280000	-2.59280000	4.35480000
H	-3.59410000	-1.01590000	4.55180000
H	-4.62070000	-0.05420000	2.54170000
C	4.63760000	0.47110000	-0.59650000
C	4.87410000	0.66000000	-1.96730000
C	5.67290000	1.70180000	-2.42310000
C	6.25460000	2.58940000	-1.51560000
C	6.02060000	2.42070000	-0.15590000
C	5.21770000	1.37100000	0.29940000
H	4.42700000	-0.01580000	-2.68700000
H	5.84170000	1.82220000	-3.48730000
H	6.87800000	3.40290000	-1.86860000
H	6.45680000	3.10610000	0.56190000
H	5.04700000	1.27250000	1.36260000

3b (conf. 13)[a]

C	-0.07880000	5.42780000	0.56780000
C	1.34800000	5.40600000	0.00600000
C	1.99550000	4.02650000	0.18000000
C	1.14330000	2.90780000	-0.43740000
C	-0.28860000	2.92670000	0.14220000
C	-0.92860000	4.31250000	-0.05230000
H	-0.04340000	5.29810000	1.65680000
H	-0.54550000	6.40010000	0.38380000
H	1.32210000	5.66110000	-1.06050000
H	1.96610000	6.16450000	0.49530000

H	2.98910000	4.00770000	-0.27580000
H	2.12930000	3.82140000	1.25010000
H	1.07180000	3.06950000	-1.51790000
N	1.81340000	1.61750000	-0.24350000
N	-1.08450000	1.87240000	-0.48530000
H	-0.23070000	2.71520000	1.21600000
H	-1.05040000	4.49060000	-1.12790000
H	-1.93010000	4.29460000	0.38410000
C	1.74910000	0.61540000	-1.16010000
O	0.96620000	0.65140000	-2.12400000
C	-2.07830000	1.23140000	0.20260000
N	-2.53900000	0.07970000	-0.42340000
O	-2.50990000	1.62380000	1.28450000
C	-3.87470000	-0.50920000	-0.16730000
C	-4.93090000	0.62230000	-0.25350000
C	-5.69100000	1.05310000	0.83480000
C	-6.58470000	2.11850000	0.71010000
C	-6.72710000	2.78050000	-0.50550000
C	-5.95990000	2.37250000	-1.59720000
C	-5.07190000	1.30910000	-1.46850000
C	-4.08930000	-1.58410000	-1.26780000
C	-3.02860000	-2.42820000	-1.62730000
C	-3.20580000	-3.44220000	-2.56540000
C	-4.45280000	-3.64580000	-3.15380000
C	-5.51820000	-2.82610000	-2.79080000
C	-5.33790000	-1.80490000	-1.85770000
N	2.54660000	-0.49410000	-0.98420000
C	3.76610000	-0.69850000	-0.16150000
C	3.40750000	-1.01120000	1.31500000
C	2.09650000	-0.94730000	1.79160000
C	1.80050000	-1.26100000	3.12030000
C	2.80930000	-1.65390000	3.99300000
C	4.12070000	-1.74060000	3.52370000
C	4.41350000	-1.42770000	2.20040000
C	4.43860000	-1.97980000	-0.72770000
C	3.66070000	-3.13570000	-0.89300000
C	4.22490000	-4.31510000	-1.36920000
C	5.58540000	-4.37000000	-1.67200000
C	6.37030000	-3.23580000	-1.49050000
C	5.80170000	-2.04900000	-1.02350000
C	4.68710000	0.54040000	-0.31820000
C	4.98970000	0.98010000	-1.61660000
C	5.79980000	2.08890000	-1.82950000
C	6.32530000	2.79370000	-0.74460000
C	6.02650000	2.37500000	0.54650000
C	5.21420000	1.25710000	0.75810000
H	2.47770000	1.55280000	0.51220000
H	-0.64620000	1.40410000	-1.27520000
H	-2.22040000	-0.04840000	-1.37290000
H	-5.58200000	0.56920000	1.79520000
H	-7.16220000	2.43330000	1.57230000
H	-7.42070000	3.60810000	-0.60220000

H	-6.05240000	2.88240000	-2.54970000
H	-4.48160000	1.00920000	-2.32690000
H	-2.05780000	-2.30350000	-1.16320000
H	-2.36790000	-4.07730000	-2.83020000
H	-4.59240000	-4.43590000	-3.88270000
H	-6.49580000	-2.97470000	-3.23540000
H	-6.17940000	-1.17670000	-1.59690000
H	2.41810000	-1.14820000	-1.74120000
H	1.29130000	-0.66700000	1.12740000
H	0.77490000	-1.19740000	3.46570000
H	2.57910000	-1.89970000	5.02330000
H	4.91680000	-2.05970000	4.18680000
H	5.43520000	-1.52050000	1.85160000
H	2.60810000	-3.12200000	-0.63430000
H	3.60230000	-5.19360000	-1.49470000
H	6.02720000	-5.28910000	-2.03940000
H	7.43060000	-3.26530000	-1.71450000
H	6.43150000	-1.17930000	-0.89450000
H	4.58360000	0.44920000	-2.46950000
H	6.02020000	2.40520000	-2.84280000
H	6.95560000	3.66010000	-0.90850000
H	6.41920000	2.91570000	1.40020000
H	4.99350000	0.96030000	1.77420000
C	-3.90510000	-1.28940000	1.17010000
C	-2.76710000	-1.44440000	1.96370000
C	-2.80460000	-2.21360000	3.12770000
C	-3.98150000	-2.84430000	3.52040000
C	-5.12290000	-2.70500000	2.73110000
C	-5.08070000	-1.94270000	1.56710000
H	-1.84380000	-0.96380000	1.67510000
H	-1.90630000	-2.31900000	3.72610000
H	-4.00990000	-3.44110000	4.42510000
H	-6.04670000	-3.19600000	3.01630000
H	-5.97480000	-1.86350000	0.96030000

3b (conf. 17)[a]

C	-1.15750000	5.78630000	0.44620000
C	0.30450000	6.07280000	0.08650000
C	1.22620000	4.96030000	0.59940000
C	0.80030000	3.56530000	0.11270000
C	-0.67390000	3.28250000	0.46550000
C	-1.58170000	4.40720000	-0.06780000
H	-1.28020000	5.82710000	1.53580000
H	-1.81110000	6.55810000	0.02880000
H	0.40150000	6.15170000	-1.00310000
H	0.62510000	7.03300000	0.50120000
H	2.25860000	5.13930000	0.28540000
H	1.21990000	4.96490000	1.69740000
H	0.89830000	3.52120000	-0.97760000
N	1.72220000	2.56920000	0.67300000
N	-1.07070000	1.98610000	-0.08340000
H	-0.76510000	3.24450000	1.55770000

H	-1.54150000	4.39090000	-1.16400000
H	-2.61090000	4.18290000	0.21900000
C	2.18290000	1.50210000	-0.05680000
O	1.56730000	1.06080000	-1.03280000
C	-2.14930000	1.31330000	0.42290000
N	-2.35740000	0.06560000	-0.14830000
O	-2.86730000	1.76980000	1.31080000
C	-3.64420000	-0.66580000	-0.07050000
C	-3.56750000	-1.78620000	-1.14410000
C	-2.39040000	-2.53650000	-1.27840000
C	-2.30730000	-3.58020000	-2.19660000
C	-3.40580000	-3.90990000	-2.98910000
C	-4.58570000	-3.18440000	-2.85110000
C	-4.66470000	-2.13100000	-1.93950000
C	-3.80150000	-1.38880000	1.29170000
C	-2.88070000	-1.22870000	2.32900000
C	-3.02680000	-1.92200000	3.53210000
C	-4.09670000	-2.79160000	3.72090000
C	-5.01930000	-2.96680000	2.68970000
C	-4.86820000	-2.27760000	1.48960000
N	3.37890000	0.98800000	0.37980000
C	3.95530000	-0.33230000	0.03120000
C	4.62630000	-0.32060000	-1.36670000
C	4.42850000	0.71130000	-2.28590000
C	5.06780000	0.69720000	-3.52720000
C	5.91670000	-0.34960000	-3.87350000
C	6.12730000	-1.38380000	-2.96180000
C	5.49440000	-1.36380000	-1.72240000
C	5.09410000	-0.55990000	1.06720000
C	6.07340000	0.43360000	1.22160000
C	7.12350000	0.27150000	2.12000000
C	7.22980000	-0.89930000	2.87080000
C	6.27660000	-1.89980000	2.71060000
C	5.21630000	-1.73120000	1.81760000
C	2.85630000	-1.41470000	0.16300000
C	2.07900000	-1.44060000	1.33050000
C	1.11180000	-2.41980000	1.52990000
C	0.89670000	-3.40070000	0.56050000
C	1.64910000	-3.37550000	-0.60920000
C	2.61750000	-2.38880000	-0.80720000
H	2.25930000	2.86900000	1.47320000
H	-0.36500000	1.48730000	-0.62020000
H	-1.83350000	-0.11450000	-0.99180000
H	-1.53130000	-2.31580000	-0.65640000
H	-1.38310000	-4.13970000	-2.28610000
H	-3.34270000	-4.72410000	-3.70190000
H	-5.45080000	-3.43060000	-3.45660000
H	-5.58980000	-1.57620000	-1.85640000
H	-2.04060000	-0.56240000	2.20320000
H	-2.29730000	-1.77720000	4.32150000
H	-4.20930000	-3.33020000	4.65500000
H	-5.85500000	-3.64630000	2.81500000

H	-5.58820000	-2.44260000	0.69700000
H	3.81570000	1.44860000	1.16260000
H	3.76920000	1.53090000	-2.04450000
H	4.89760000	1.51210000	-4.22220000
H	6.41290000	-0.35870000	-4.83730000
H	6.79220000	-2.20350000	-3.21020000
H	5.68740000	-2.16760000	-1.02180000
H	6.02760000	1.33710000	0.62360000
H	7.86420000	1.05610000	2.22500000
H	8.04990000	-1.02970000	3.56740000
H	6.35010000	-2.81860000	3.28150000
H	4.48640000	-2.52210000	1.71260000
H	2.23590000	-0.68830000	2.09470000
H	0.52660000	-2.41850000	2.44250000
H	0.14790000	-4.16890000	0.71560000
H	1.48680000	-4.12330000	-1.37740000
H	3.18090000	-2.38790000	-1.72990000
C	-4.80450000	0.31750000	-0.37760000
C	-5.86650000	0.56080000	0.49390000
C	-6.87340000	1.47020000	0.16340000
C	-6.83370000	2.15740000	-1.04560000
C	-5.77120000	1.93210000	-1.92190000
C	-4.77080000	1.02460000	-1.58850000
H	-5.91090000	0.05420000	1.44790000
H	-7.68530000	1.64300000	0.86130000
H	-7.61540000	2.86350000	-1.30210000
H	-5.72140000	2.46310000	-2.86610000
H	-3.95250000	0.86340000	-2.28110000

3b (conf. 18)[a]

C	-0.99210000	5.91150000	0.15110000
C	0.51500000	6.10560000	-0.05020000
C	1.31180000	4.95460000	0.57590000
C	0.84910000	3.57900000	0.07070000
C	-0.66390000	3.39080000	0.30030000
C	-1.44250000	4.54120000	-0.36690000
H	-1.23210000	5.99580000	1.21850000
H	-1.54860000	6.70460000	-0.35730000
H	0.73410000	6.15430000	-1.12370000
H	0.84390000	7.05570000	0.38110000
H	2.37870000	5.06650000	0.36160000
H	1.19850000	4.98530000	1.66740000
H	1.02850000	3.51640000	-1.00820000
N	1.66660000	2.53400000	0.70400000
N	-1.07400000	2.08550000	-0.21270000
H	-0.85570000	3.41780000	1.38030000
H	-1.28390000	4.48210000	-1.45120000
H	-2.50740000	4.38690000	-0.18740000
C	2.13800000	1.46410000	-0.01880000
O	1.57200000	1.06940000	-1.04290000
C	-2.27180000	1.52720000	0.13340000
N	-2.48940000	0.26990000	-0.40730000

O	-3.10680000	2.10870000	0.82550000
C	-3.62560000	-0.60030000	-0.04270000
C	-4.94330000	-0.11030000	-0.69820000
C	-6.12050000	-0.85650000	-0.54220000
C	-7.30570000	-0.47060000	-1.16210000
C	-7.33870000	0.66770000	-1.96740000
C	-6.17230000	1.40540000	-2.14600000
C	-4.98700000	1.01920000	-1.51800000
C	-3.33800000	-1.98310000	-0.69190000
C	-2.87410000	-2.04120000	-2.01430000
C	-2.66030000	-3.26320000	-2.64660000
C	-2.92450000	-4.45710000	-1.97650000
C	-3.40450000	-4.41170000	-0.67060000
C	-3.60700000	-3.18660000	-0.03360000
N	3.28660000	0.89500000	0.47220000
C	3.84990000	-0.40490000	0.04480000
C	4.49170000	-0.31660000	-1.36410000
C	4.54890000	0.87840000	-2.08350000
C	5.19670000	0.94220000	-3.31840000
C	5.80170000	-0.18910000	-3.85740000
C	5.76260000	-1.38630000	-3.14270000
C	5.12210000	-1.44510000	-1.90860000
C	5.03450000	-0.69720000	1.00900000
C	5.94220000	0.32720000	1.31670000
C	7.04550000	0.08660000	2.13110000
C	7.27840000	-1.19020000	2.63960000
C	6.39780000	-2.22020000	2.32140000
C	5.28540000	-1.97570000	1.51550000
C	2.73970000	-1.47830000	0.16180000
C	2.15800000	-1.69290000	1.41980000
C	1.15100000	-2.63630000	1.59580000
C	0.69020000	-3.38090000	0.50900000
C	1.24190000	-3.15950000	-0.74880000
C	2.25540000	-2.21430000	-0.92010000
H	2.19090000	2.82490000	1.51650000
H	-0.36580000	1.54420000	-0.70120000
H	-1.68370000	-0.20700000	-0.78220000
H	-6.11500000	-1.75520000	0.06300000
H	-8.20150000	-1.06510000	-1.02100000
H	-8.25950000	0.96850000	-2.45430000
H	-6.17740000	2.28740000	-2.77700000
H	-4.08990000	1.59780000	-1.68330000
H	-2.68980000	-1.12580000	-2.56410000
H	-2.29520000	-3.28000000	-3.66740000
H	-2.76290000	-5.40920000	-2.46880000
H	-3.62120000	-5.33080000	-0.13790000
H	-3.97360000	-3.17750000	0.98420000
H	3.64820000	1.25790000	1.34050000
H	4.09540000	1.77240000	-1.68120000
H	5.22530000	1.88340000	-3.85620000
H	6.30360000	-0.13950000	-4.81700000
H	6.23840000	-2.27530000	-3.54130000

H	5.12300000	-2.38070000	-1.36220000
H	5.80310000	1.32010000	0.90490000
H	7.72810000	0.89740000	2.35930000
H	8.13890000	-1.37970000	3.27090000
H	6.56900000	-3.22050000	2.70260000
H	4.61280000	-2.79170000	1.28740000
H	2.50070000	-1.12040000	2.27410000
H	0.72810000	-2.79210000	2.58200000
H	-0.09440000	-4.11670000	0.64200000
H	0.88200000	-3.71630000	-1.60650000
H	2.65600000	-2.05000000	-1.91060000
C	-3.70200000	-0.70580000	1.50350000
C	-4.81420000	-0.32920000	2.25730000
C	-4.80540000	-0.42870000	3.65010000
C	-3.67890000	-0.90090000	4.31650000
C	-2.55430000	-1.26610000	3.57560000
C	-2.56850000	-1.16650000	2.18800000
H	-5.69320000	0.06490000	1.76700000
H	-5.68250000	-0.12540000	4.21110000
H	-3.67180000	-0.97730000	5.39800000
H	-1.66410000	-1.62740000	4.07860000
H	-1.68280000	-1.44770000	1.63010000

3b (conf. 32)[a]

C	1.32530000	5.45100000	-0.23160000
C	-0.09630000	5.47460000	0.34330000
C	-0.93780000	4.32800000	-0.22890000
C	-0.28010000	2.95710000	0.00930000
C	1.14660000	2.93490000	-0.58400000
C	1.99100000	4.08620000	-0.01700000
H	1.28560000	5.66860000	-1.30590000
H	1.93840000	6.23360000	0.22480000
H	-0.04890000	5.38390000	1.43580000
H	-0.57710000	6.43400000	0.13010000
H	-1.93510000	4.31420000	0.21680000
H	-1.07060000	4.46570000	-1.30920000
H	-0.21030000	2.78630000	1.09000000
N	-1.06790000	1.87080000	-0.57300000
N	1.84450000	1.66650000	-0.35790000
H	1.06060000	3.05690000	-1.66850000
H	2.14100000	3.92000000	1.05760000
H	2.97930000	4.06200000	-0.48420000
C	-2.05940000	1.25540000	0.14080000
O	-2.51270000	1.70790000	1.19030000
C	1.77640000	0.62400000	-1.22740000
N	2.61590000	-0.45080000	-1.04470000
O	0.98070000	0.61050000	-2.18260000
C	3.75030000	-0.68060000	-0.12120000
C	4.14810000	-2.17180000	-0.31510000
C	4.41470000	-2.63650000	-1.61200000
C	4.79820000	-3.95500000	-1.83570000
C	4.94460000	-4.83480000	-0.76320000

C	4.70650000	-4.37820000	0.52900000
C	4.30990000	-3.05790000	0.75170000
C	4.99790000	0.15720000	-0.51050000
C	4.96600000	1.12260000	-1.51850000
C	6.11550000	1.83710000	-1.86400000
C	7.31880000	1.59550000	-1.20980000
C	7.36810000	0.62140000	-0.21210000
C	6.22290000	-0.09180000	0.12720000
N	-2.49190000	0.05980000	-0.41700000
C	-3.82470000	-0.53930000	-0.16440000
C	-4.01230000	-1.62420000	-1.26070000
C	-2.95380000	-2.49930000	-1.54760000
C	-3.09840000	-3.51510000	-2.48860000
C	-4.31200000	-3.69050000	-3.15240000
C	-5.37560000	-2.84120000	-2.86150000
C	-5.22660000	-1.81650000	-1.92570000
C	-3.86770000	-1.29490000	1.18730000
C	-2.79990000	-1.27950000	2.08630000
C	-2.85690000	-2.00420000	3.27830000
C	-3.98200000	-2.76020000	3.59350000
C	-5.05270000	-2.78970000	2.70020000
C	-4.99130000	-2.06990000	1.51050000
C	-4.89880000	0.57330000	-0.27340000
C	-5.76690000	0.91490000	0.76440000
C	-6.69490000	1.94760000	0.61380000
C	-6.76720000	2.66190000	-0.57790000
C	-5.89610000	2.33950000	-1.61930000
C	-4.97330000	1.31010000	-1.46490000
H	-0.62250000	1.37000000	-1.33890000
H	2.42470000	1.58930000	0.46380000
H	2.43630000	-1.17480000	-1.72270000
H	4.34350000	-1.96210000	-2.45830000
H	4.99250000	-4.29130000	-2.84780000
H	5.24760000	-5.86110000	-0.93500000
H	4.82530000	-5.04730000	1.37380000
H	4.12800000	-2.72860000	1.76570000
H	4.05090000	1.31790000	-2.05910000
H	6.06310000	2.57980000	-2.65220000
H	8.21080000	2.14930000	-1.47910000
H	8.30130000	0.40940000	0.29750000
H	6.28730000	-0.85900000	0.88970000
H	-2.12460000	-0.14540000	-1.33440000
H	-2.01060000	-2.39630000	-1.02410000
H	-2.26300000	-4.17410000	-2.69670000
H	-4.42690000	-4.48280000	-3.88330000
H	-6.32750000	-2.96840000	-3.36470000
H	-6.06610000	-1.16570000	-1.72070000
H	-1.92000000	-0.69490000	1.86340000
H	-2.01550000	-1.97280000	3.96200000
H	-4.02450000	-3.32280000	4.51930000
H	-5.93480000	-3.37910000	2.92480000
H	-5.82870000	-2.11980000	0.82470000

H	-5.71820000	0.38710000	1.70670000
H	-7.35570000	2.19440000	1.43740000
H	-7.48760000	3.46360000	-0.69480000
H	-5.93490000	2.89030000	-2.55270000
H	-4.30180000	1.07610000	-2.28320000
C	3.26380000	-0.41120000	1.32650000
C	3.92150000	0.43810000	2.22010000
C	3.41920000	0.65160000	3.50750000
C	2.25420000	0.01740000	3.92210000
C	1.58400000	-0.82810000	3.03560000
C	2.07970000	-1.03260000	1.75360000
H	4.82640000	0.94940000	1.92240000
H	3.94620000	1.31920000	4.17960000
H	1.86560000	0.18180000	4.92050000
H	0.67210000	-1.32680000	3.34250000
H	1.54190000	-1.67880000	1.07060000

3b (conf. 33)[a]

C	1.36250000	5.41160000	-0.01540000
C	-0.06360000	5.44020000	0.54790000
C	-0.91760000	4.32560000	-0.06720000
C	-0.28220000	2.93810000	0.13130000
C	1.14940000	2.91240000	-0.44880000
C	2.00570000	4.03080000	0.16340000
H	1.33620000	5.66250000	-1.08280000
H	1.98360000	6.17010000	0.47020000
H	-0.02720000	5.31440000	1.63740000
H	-0.52720000	6.41340000	0.36100000
H	-1.91880000	4.31250000	0.37020000
H	-1.03990000	4.50040000	-1.14340000
H	-0.22480000	2.72990000	1.20580000
N	-1.08210000	1.88480000	-0.49260000
N	1.81510000	1.62080000	-0.24990000
H	1.07800000	3.06970000	-1.52990000
H	2.14000000	3.82940000	1.23420000
H	2.99880000	4.00690000	-0.29340000
C	-2.07370000	1.24460000	0.19980000
O	-2.50050000	1.63840000	1.28350000
C	1.74630000	0.61440000	-1.16130000
N	2.53790000	-0.49840000	-0.97820000
O	0.96490000	0.64940000	-2.12630000
C	3.75880000	-0.70080000	-0.15720000
C	3.40310000	-0.99710000	1.32340000
C	2.09280000	-0.93000000	1.80140000
C	1.79970000	-1.22920000	3.13410000
C	2.81040000	-1.61100000	4.00940000
C	4.12110000	-1.70150000	3.53880000
C	4.41120000	-1.40280000	2.21170000
C	4.42320000	-1.99160000	-0.71140000
C	3.63790000	-3.14370000	-0.86820000
C	4.19540000	-4.33120000	-1.33190000
C	5.55630000	-4.39830000	-1.63010000

C	6.34840000	-3.26780000	-1.45680000
C	5.78660000	-2.07290000	-1.00250000
N	-2.53960000	0.09570000	-0.42440000
C	-3.86650000	-0.51010000	-0.16000000
C	-3.85840000	-1.36050000	1.13470000
C	-2.74540000	-1.43170000	1.97410000
C	-2.75360000	-2.24830000	3.10660000
C	-3.87530000	-3.00930000	3.42150000
C	-4.99160000	-2.95190000	2.58730000
C	-4.97820000	-2.14210000	1.45550000
C	-4.93430000	0.61380000	-0.14780000
C	-5.04000000	1.44020000	-1.27650000
C	-5.95920000	2.48330000	-1.32310000
C	-6.79550000	2.72980000	-0.23350000
C	-6.69210000	1.92550000	0.89690000
C	-5.76790000	0.87930000	0.93930000
C	-4.10740000	-1.51470000	-1.32080000
C	-5.34340000	-1.64210000	-1.96080000
C	-5.53650000	-2.59850000	-2.95890000
C	-4.49670000	-3.44250000	-3.33780000
C	-3.26150000	-3.33120000	-2.70020000
C	-3.07270000	-2.38420000	-1.69760000
H	-0.64690000	1.41500000	-1.28310000
H	2.47580000	1.55520000	0.50880000
H	2.40800000	-1.15510000	-1.73280000
H	1.28590000	-0.65890000	1.13540000
H	0.77470000	-1.16330000	3.48070000
H	2.58240000	-1.84550000	5.04280000
H	4.91880000	-2.01220000	4.20400000
H	5.43230000	-1.49840000	1.86210000
H	2.58470000	-3.12050000	-0.61260000
H	3.56710000	-5.20650000	-1.45110000
H	5.99290000	-5.32370000	-1.98770000
H	7.40920000	-3.30660000	-1.67740000
H	6.42200000	-1.20630000	-0.87940000
H	-2.20870000	-0.04950000	-1.36670000
H	-1.86620000	-0.84590000	1.75060000
H	-1.87550000	-2.28750000	3.74170000
H	-3.88010000	-3.64330000	4.30100000
H	-5.87180000	-3.54400000	2.81190000
H	-5.84960000	-2.12670000	0.81160000
H	-4.39470000	1.26770000	-2.13030000
H	-6.02180000	3.10440000	-2.20980000
H	-7.51270000	3.54210000	-0.26600000
H	-7.32530000	2.11190000	1.75740000
H	-5.69410000	0.28150000	1.83700000
H	-6.16540000	-0.99430000	-1.68700000
H	-6.50450000	-2.67670000	-3.44100000
H	-4.64630000	-4.18110000	-4.11700000
H	-2.44400000	-3.98740000	-2.97700000
H	-2.11370000	-2.33090000	-1.19590000
C	4.68580000	0.53170000	-0.32960000

C	4.98950000	0.95380000	-1.63340000
C	5.80390000	2.05670000	-1.86060000
C	6.33270000	2.77310000	-0.78490000
C	6.03290000	2.37170000	0.51150000
C	5.21620000	1.25980000	0.73730000
H	4.58120000	0.41390000	-2.47950000
H	6.02510000	2.35930000	-2.87790000
H	6.96640000	3.63480000	-0.96000000
H	6.42810000	2.92150000	1.35810000
H	4.99480000	0.97690000	1.75720000

3b (conf. 75)[a]

C	-1.78430000	5.07050000	0.57400000
C	-0.35620000	5.55560000	0.84910000
C	0.53750000	4.41120000	1.34370000
C	0.53270000	3.21610000	0.37900000
C	-0.91100000	2.72170000	0.11830000
C	-1.78510000	3.88250000	-0.39540000
H	-2.25680000	4.77170000	1.51810000
H	-2.39040000	5.88410000	0.16500000
H	0.06830000	5.97330000	-0.07190000
H	-0.36150000	6.36320000	1.58680000
H	1.56820000	4.75300000	1.47130000
H	0.18780000	4.07570000	2.32890000
H	0.95600000	3.52940000	-0.57950000
N	1.40460000	2.16230000	0.88660000
N	-0.87970000	1.59250000	-0.81460000
H	-1.30550000	2.37060000	1.08020000
H	-1.39810000	4.19490000	-1.37250000
H	-2.80640000	3.52900000	-0.56720000
C	2.15520000	1.36730000	0.05970000
O	2.14470000	1.49920000	-1.16570000
C	-1.65640000	0.46070000	-0.78500000
N	-2.76290000	0.51280000	0.04010000
O	-1.36340000	-0.53580000	-1.44530000
C	-3.85360000	-0.48960000	0.02470000
C	-3.42570000	-1.80200000	0.72810000
C	-4.36210000	-2.83180000	0.90090000
C	-4.02820000	-4.00320000	1.57430000
C	-2.74910000	-4.16730000	2.10570000
C	-1.81700000	-3.14490000	1.95660000
C	-2.15260000	-1.97380000	1.27490000
C	-4.98580000	0.10290000	0.90970000
C	-4.66000000	0.66790000	2.15190000
C	-5.65030000	1.16040000	2.99750000
C	-6.99230000	1.08280000	2.62740000
C	-7.32910000	0.50610000	1.40630000
C	-6.33530000	0.02220000	0.55440000
N	2.88610000	0.39520000	0.70860000
C	4.00600000	-0.35750000	0.09110000
C	3.49320000	-1.45410000	-0.87550000
C	2.13740000	-1.62830000	-1.15800000

C	1.70600000	-2.65660000	-1.99780000
C	2.62310000	-3.53320000	-2.56920000
C	3.98020000	-3.37640000	-2.28670000
C	4.40700000	-2.35290000	-1.44560000
C	4.96860000	0.65600000	-0.58020000
C	5.28260000	0.64060000	-1.93960000
C	6.13160000	1.60220000	-2.49150000
C	6.67750000	2.60200000	-1.69300000
C	6.36190000	2.63680000	-0.33430000
C	5.51670000	1.67610000	0.21140000
C	4.69420000	-1.11580000	1.25970000
C	3.90090000	-1.79870000	2.19380000
C	4.48000000	-2.53200000	3.22570000
C	5.86750000	-2.61440000	3.33610000
C	6.66470000	-1.95770000	2.40310000
C	6.08360000	-1.21350000	1.37530000
H	1.37560000	1.96930000	1.87670000
H	-0.01590000	1.46220000	-1.32990000
H	-3.04340000	1.42330000	0.36700000
H	-5.36760000	-2.71850000	0.51350000
H	-4.77140000	-4.78430000	1.69010000
H	-2.48740000	-5.07700000	2.63410000
H	-0.82030000	-3.25280000	2.37010000
H	-1.41500000	-1.19030000	1.18070000
H	-3.62560000	0.70910000	2.47190000
H	-5.37170000	1.59700000	3.95000000
H	-7.76490000	1.46300000	3.28580000
H	-8.36860000	0.43270000	1.10700000
H	-6.62160000	-0.41630000	-0.39220000
H	2.95120000	0.48120000	1.71190000
H	1.39950000	-0.96750000	-0.72990000
H	0.64600000	-2.75840000	-2.20040000
H	2.28790000	-4.33160000	-3.22170000
H	4.70900000	-4.05530000	-2.71560000
H	5.46440000	-2.26020000	-1.22740000
H	4.85470000	-0.11330000	-2.58560000
H	6.35610000	1.56860000	-3.55180000
H	7.33590000	3.34910000	-2.12170000
H	6.77400000	3.41250000	0.30150000
H	5.28100000	1.72190000	1.26850000
H	2.82100000	-1.77110000	2.10850000
H	3.84500000	-3.04580000	3.93860000
H	6.31990000	-3.18740000	4.13730000
H	7.74510000	-2.01700000	2.47200000
H	6.72420000	-0.70640000	0.66620000
C	-4.32190000	-0.69290000	-1.44010000
C	-4.28660000	-1.92010000	-2.10330000
C	-4.69350000	-2.02940000	-3.43450000
C	-5.13700000	-0.90960000	-4.13090000
C	-5.16530000	0.32630000	-3.48420000
C	-4.76080000	0.42980000	-2.15710000
H	-3.92520000	-2.80210000	-1.59370000

H	-4.65230000	-2.99510000	-3.92610000
H	-5.45140000	-0.99450000	-5.16500000
H	-5.50180000	1.21110000	-4.01310000
H	-4.78890000	1.39970000	-1.67380000

3b (conf. 76)[a]

C	-1.78470000	5.03990000	0.63120000
C	-0.35700000	5.52890000	0.90210000
C	0.54310000	4.38580000	1.38820000
C	0.53750000	3.19430000	0.41910000
C	-0.90580000	2.69540000	0.16510000
C	-1.78530000	3.85500000	-0.34200000
H	-2.25250000	4.73640000	1.57620000
H	-2.39500000	5.85280000	0.22730000
H	0.06200000	5.95160000	-0.01900000
H	-0.36190000	6.33350000	1.64310000
H	1.57320000	4.73090000	1.51170000
H	0.19970000	4.04540000	2.37390000
H	0.95320000	3.51320000	-0.54090000
N	1.41730000	2.14250000	0.91720000
N	-0.87470000	1.56850000	-0.77060000
H	-1.29500000	2.34070000	1.12790000
H	-1.40260000	4.17160000	-1.31950000
H	-2.80630000	3.49950000	-0.51180000
C	2.16650000	1.35430000	0.08280000
O	2.14100000	1.48530000	-1.14270000
C	-1.65700000	0.44080000	-0.74870000
N	-2.76720000	0.49510000	0.07360000
O	-1.36560000	-0.55470000	-1.41060000
C	-3.87650000	-0.48590000	0.01770000
C	-4.36550000	-0.58870000	-1.45080000
C	-4.88110000	0.56330000	-2.06250000
C	-5.28850000	0.55300000	-3.39310000
C	-5.18460000	-0.61500000	-4.14870000
C	-4.66060000	-1.76090000	-3.55840000
C	-4.25050000	-1.74470000	-2.22410000
C	-3.46340000	-1.84290000	0.63980000
C	-2.22270000	-2.03110000	1.25230000
C	-1.90560000	-3.24000000	1.87360000
C	-2.82440000	-4.28510000	1.89560000
C	-4.07150000	-4.10570000	1.29760000
C	-4.38750000	-2.89640000	0.68460000
N	2.91370000	0.38960000	0.72350000
C	4.03040000	-0.35600000	0.09210000
C	4.74150000	-1.10540000	1.25260000
C	3.96750000	-1.79230000	2.19990000
C	4.56750000	-2.51750000	3.22560000
C	5.95710000	-2.58790000	3.31620000
C	6.73520000	-1.92740000	2.37000000
C	6.13320000	-1.19100000	1.34860000
C	3.51210000	-1.45900000	-0.86430000
C	2.15380000	-1.64330000	-1.12820000

C	1.71820000	-2.67690000	-1.95910000
C	2.63350000	-3.54900000	-2.54040000
C	3.99320000	-3.38230000	-2.27640000
C	4.42420000	-2.35340000	-1.44400000
C	4.97540000	0.66320000	-0.59550000
C	5.27410000	0.64420000	-1.95820000
C	6.10820000	1.61070000	-2.52410000
C	6.65430000	2.61900000	-1.73650000
C	6.35410000	2.65720000	-0.37440000
C	5.52360000	1.69170000	0.18530000
H	1.40400000	1.95280000	1.90820000
H	-0.00980000	1.43740000	-1.28410000
H	-3.04950000	1.41080000	0.38560000
H	-4.96930000	1.48230000	-1.49420000
H	-5.68680000	1.45760000	-3.83910000
H	-5.50230000	-0.62710000	-5.18520000
H	-4.55850000	-2.67300000	-4.13590000
H	-3.82340000	-2.64070000	-1.79620000
H	-1.49780000	-1.22990000	1.25670000
H	-0.93380000	-3.36000000	2.33970000
H	-2.57690000	-5.22470000	2.37650000
H	-4.80430000	-4.90470000	1.31350000
H	-5.36930000	-2.77410000	0.24330000
H	2.98910000	0.47550000	1.72610000
H	2.88630000	-1.77410000	2.13020000
H	3.94710000	-3.03440000	3.94900000
H	6.42580000	-3.15470000	4.11240000
H	7.81690000	-1.97740000	2.42350000
H	6.75930000	-0.68060000	0.62890000
H	1.41720000	-0.98670000	-0.69110000
H	0.65640000	-2.78670000	-2.14740000
H	2.29500000	-4.35140000	-3.18610000
H	4.72070000	-4.05750000	-2.71300000
H	5.48370000	-2.25320000	-1.24010000
H	4.84570000	-0.11650000	-2.59590000
H	6.32090000	1.57420000	-3.58680000
H	7.30110000	3.36980000	-2.17620000
H	6.76660000	3.43940000	0.25310000
H	5.29950000	1.74030000	1.24480000
C	-4.98670000	0.06420000	0.95570000
C	-4.63590000	0.61950000	2.19480000
C	-5.61180000	1.06330000	3.08400000
C	-6.96250000	0.94540000	2.76130000
C	-7.32350000	0.37700000	1.54260000
C	-6.34560000	-0.05810000	0.64820000
H	-3.59320000	0.69220000	2.47920000
H	-5.31350000	1.49410000	4.03310000
H	-7.72320000	1.28820000	3.45320000
H	-8.37010000	0.27310000	1.27890000
H	-6.65140000	-0.48990000	-0.29550000

3b (conf. 96)[a]

C	-1.80590000	5.11690000	0.23620000
C	-0.37970000	5.59680000	0.53070000
C	0.48850000	4.46350000	1.09200000
C	0.49190000	3.23120000	0.17510000
C	-0.95210000	2.74180000	-0.09480000
C	-1.79520000	3.89000000	-0.68360000
H	-2.30750000	4.86210000	1.17810000
H	-2.39040000	5.92010000	-0.22170000
H	0.07340000	5.97400000	-0.39410000
H	-0.39500000	6.43240000	1.23640000
H	1.52000000	4.79900000	1.22950000
H	0.11300000	4.17140000	2.08140000
H	0.93380000	3.50410000	-0.78730000
N	1.34820000	2.19230000	0.73580000
N	-0.91230000	1.56970000	-0.96820000
H	-1.37310000	2.44630000	0.87590000
H	-1.37310000	4.15660000	-1.65990000
H	-2.81410000	3.54020000	-0.87130000
C	2.11140000	1.36910000	-0.05120000
O	2.11290000	1.45250000	-1.28090000
C	-1.77190000	0.50200000	-1.00620000
N	-2.94670000	0.64140000	-0.29600000
O	-1.51500000	-0.50100000	-1.67350000
C	-3.85360000	-0.47990000	0.04110000
C	-3.01050000	-1.63860000	0.63410000
C	-3.00880000	-2.93710000	0.12350000
C	-2.21280000	-3.93260000	0.69450000
C	-1.39980000	-3.64590000	1.78650000
C	-1.38450000	-2.34880000	2.30110000
C	-2.17810000	-1.36010000	1.72810000
C	-4.85460000	0.08750000	1.08650000
C	-5.48630000	1.31430000	0.83090000
C	-6.42160000	1.83840000	1.71870000
C	-6.76230000	1.13700000	2.87500000
C	-6.15940000	-0.09130000	3.12770000
C	-5.21300000	-0.61070000	2.24280000
N	2.84190000	0.42800000	0.64290000
C	3.97390000	-0.33810000	0.06530000
C	3.47930000	-1.46530000	-0.87470000
C	2.12500000	-1.67750000	-1.13700000
C	1.70850000	-2.73470000	-1.94770000
C	2.63960000	-3.60300000	-2.50910000
C	3.99560000	-3.40940000	-2.24450000
C	4.40750000	-2.35700000	-1.43220000
C	4.94290000	0.66070000	-0.61910000
C	5.48790000	1.69380000	0.15780000
C	6.33460000	2.64610000	-0.40030000
C	6.65470000	2.58980000	-1.75720000
C	6.11130000	1.57740000	-2.54150000
C	5.26070000	0.62440000	-1.97740000
C	4.64590000	-1.06210000	1.26450000
C	6.03380000	-1.16400000	1.39470000

C	6.60220000	-1.88070000	2.44870000
C	5.79350000	-2.50550000	3.39360000
C	4.40750000	-2.41870000	3.26910000
C	3.84080000	-1.71270000	2.21140000
H	1.30080000	2.03310000	1.73130000
H	-0.04830000	1.40750000	-1.47290000
H	-3.03500000	1.44690000	0.30170000
H	-3.61640000	-3.18260000	-0.73610000
H	-2.22730000	-4.93200000	0.27420000
H	-0.78180000	-4.41860000	2.22940000
H	-0.75440000	-2.10670000	3.14980000
H	-2.14940000	-0.35750000	2.13940000
H	-5.26290000	1.85930000	-0.07890000
H	-6.89120000	2.79090000	1.50040000
H	-7.49330000	1.54170000	3.56550000
H	-6.41950000	-0.65270000	4.01800000
H	-4.75610000	-1.56590000	2.46420000
H	2.90350000	0.56080000	1.64140000
H	1.37980000	-1.02360000	-0.71040000
H	0.64960000	-2.86760000	-2.13770000
H	2.31590000	-4.42340000	-3.13970000
H	4.73510000	-4.08180000	-2.66490000
H	5.46460000	-2.23590000	-1.22710000
H	5.24890000	1.75620000	1.21330000
H	6.74440000	3.43190000	0.22460000
H	7.31440000	3.33010000	-2.19550000
H	6.33890000	1.52740000	-3.60050000
H	4.83430000	-0.13890000	-2.61310000
H	6.68320000	-0.68140000	0.67660000
H	7.68160000	-1.94370000	2.52840000
H	6.23590000	-3.05730000	4.21500000
H	3.76370000	-2.90810000	3.99120000
H	2.76190000	-1.68220000	2.11610000
C	-4.71460000	-0.90480000	-1.17530000
C	-4.54720000	-0.34150000	-2.44150000
C	-5.37430000	-0.70860000	-3.50450000
C	-6.38590000	-1.64650000	-3.32130000
C	-6.56930000	-2.21050000	-2.05890000
C	-5.74720000	-1.83790000	-0.99940000
H	-3.77070000	0.39020000	-2.60710000
H	-5.22250000	-0.25540000	-4.47800000
H	-7.02790000	-1.93090000	-4.14730000
H	-7.35880000	-2.93550000	-1.89470000
H	-5.92070000	-2.27410000	-0.02270000

[a] Calculated at the IEFPCM/6-311++G(d,p) level.

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