Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Transfer of chirality in *N*-triphenylacetylamino acids and chiral derivatives of *N*-triphenylacetyl *Gly*-*Gly*-dipetide, and control of their assembly with steric constraints

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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) were 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. FT-IR spectra were measured on a Nicolet iS 50 spectrometer using the ATR module. A JASCO P-2000 polarimeter was used for optical rotation ($[\alpha]_D$) measurements (ca. 20 °C). Flash column chromatography was performed on J.T. Baker Silica Gel 40µm (flash chromatography grade). Merck Kieselgel type $60F_{254}$ analytical plates were employed for TLC. Melting points were measured on a Büchi Melting Point B-545 apparatus 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.

General procedure of synthesis

Method A:

Triphenylacetic acid (288 mg, 1 mmol) was suspended in 10 mL of toluene and two drops of DMF were added. The mixture was stirred and cooled to 0°C and thionyl chloride (0.35 ml, 5 mmol) was added dropwise. After addition of the reagent mixture, the temperature was heated under reflux at 60°C for 3 hours. The resulting clear solution was evaporated and then washed with *n*-hexane and evaporated again. This cycle was performed three times. Acyl chloride obtained as white solid was used in the reaction without further purification.

The chosen amino acid or dipeptide (1 mmol) was suspended in mixture of NaOH (80 mg, 2 mmol) in water (3 mL) and THF (1 mL), and stirred until dissolved. The solution was cooled to 0°C and stirred vigorously. Upon stirring triphenylacetyl chloride was added in small portions over 20 minutes. The resulting suspension was stirred overnight. The following day reaction was quenched using 10% hydrochloric acid (4 mL). The mixture was then diluted with distilled water to twofold volume and extracted three times using ethyl acetate (3x 20 mL). The organic phase was subsequently washed with distilled water and brine. The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated by a rotary evaporator. The crude product was purified by crystallization from ethyl acetate or acetone, or by column chromatography on silica gel (hexane:ethyl acetate mixture).

Method B:

Amino acid methyl ester hydrochloride (1.5 mmol) was dissolved in 30 mL of dichloromethane. The mixture was cooled to 0°C and triethylamine (0.42 mL, 3 mmol) was introduced. After stirring for 20 minutes freshly prepared triphenylacetyl chloride (method A; 552 mg, 1.8 mmol) was added. The solution was stirred overnight. The next day mixture was washed with 1M HCl solution (10 mL), H_2O (10 mL), saturated Na_2CO_3 solution and brine. The organic phase was dried over anhydrous Na_2SO_4. Evaporation using rotary evaporator gave a colourless syrup. Purification by column chromatography on silica gel (hexane:dichloromethane mixture) gave colourless syrup solidifying over time.

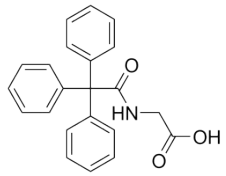
Method C:

N-triphenylacetylglycine (345 mg, 1 mmol) was dissolved in 5 mL of anhydrous THF and triethylamine (0.14 mL, 1 mmol) was added. The mixture was cooled to 0°C and ethyl chloroformate (0.11 mL, 1.1 mmol) was introduced. The solution was stirred until precipitation occurred. Stirring was maintained for 15 minutes and chiral amine (1.1 mmol) along with triethylamine (0.14 ml, 1 mmol) was added dropwise. After addition of reagents the mixture was left to achieve room temperature and stirred overnight. The following day, the reaction was quenched by evaporation and addition of water

(20 mL). Subsequently, the mixture was extracted with methylene chloride (3x 15 mL). The organic layers were collected and washed with 10% HCl solution, H_2O, 10% $NaHCO_3$ solution and brine. The organic phase was dried over anhydrous Na_2SO_4 and evaporated. The pure product was obtained by crystallization (ethyl acetate) or by column chromatography on silica gel (hexane:ethyl acetate mixture).

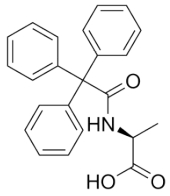
Table S1. Synthetic methods and yields of products **1**-**18**.

Compound	Yield	Method used
1	91%	A
2a	90%	A
2b	72%	B
3a	81%	A
3b	55%	B
4a	91%	A
4b	80%	B
5	58%	A
6	70%	A
7	74%	A
8	57%	A
9	52%	A
10	65%	A
11	65%	A
12	80%	A
13a	69%	A
13b	95%	B
14	57%	C
15	37%	C
16	26%	C
17	57%	A
18	31%	C



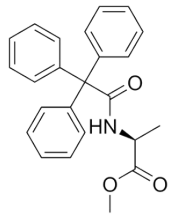
1

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29 (m, 15H), 6.39 (t, 1H), 4.24 (br s, 1H), 4.10 (d,2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.72, 164.39, 142.89, 130.53, 128.05, 127.21, 67.65, 31.40. FT-IR (ATR) cm^{-1} 3421, 3387, 3088, 3023, 2985, 1743, 1729, 1652, 1623, 1494, 1208. ESI-HRMS calc mass: 345.1365 found: 346.1443 $[M+H]^+$, mp 217-220°C



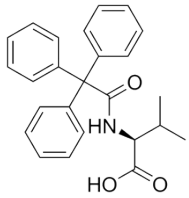
2a

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.27 (m, 15H), 6.28 (d, 1H), 4.64 (quin, 1H), 1.38 (d 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.96, 173.65, 142.94, 130.50, 128.02, 127.18, 67.56, 48.85, 17.53. FT-IR (ATR) cm^{-1} 3410, 3086, 3058, 2917, 1736, 1717, 1663, 1639, 1598, 1509, 1492, 1446, 1207. ESI-HRMS calc mass: 359.1521 found: 360.1596 $[M+H]^+$, $[\alpha]_D^{20}$(c=1, $CHCl_3$) -7° mp 141-144°C



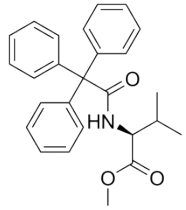
2b

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 (m, 15H), 6.31 (d, 1H), 4.67 (quin, 1H), 3.71 (s, 3H), 1.35 (d, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.23, 172.90, 143.18, 130.56, 127.95, 127.09, 67.55, 52.40, 48.77, 17.96. FT-IR (ATR) cm^{-1} 3429, 3083, 3059, 3031, 2998, 2952, 1746, 1674, 1598, 1494, 1447, 1373, 1338, 1213, 1150. ESI-HRMS calc mass: 373.1678 found: 374.1750 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.25, $CHCl_3$) -4°, colorless syrup



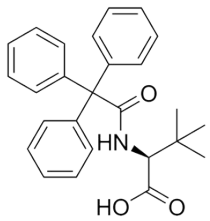
3a

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (br s, 1H), 7.30 (m, 15H), 6.18 (d, 1H), 4.61 (dd,1H), 2.18 (m, 1H), 0.85 (d, 3H), 0.69 (d,3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.58, 173.80, 143.06, 130.54, 128.01, 127.12, 67.88, 57.78, 30.47, 19.24, 17.31. FT-IR (ATR) cm^{-1} 3383, 3090, 3065, 3033, 2967, 1736, 1723, 1646, 1514, 1489, 1407, 1208. ESI-HRMS calc mass: 387.1834 found: 388.1911 $[M+H]^+$, $[\alpha]_D^{20}$(c=1, $CHCl_3$) +19° mp 145-149°C



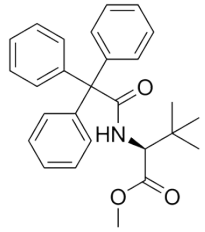
3b

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (m, 15H), 6.18 (d, 1H), 4.60 (m, 1H), 3.71(s, 1H), 2.14 (m, 1H), 0.82 (d, 3H), 0.66 (d, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.33, 172.17, 143.23, 130.58, 127.96, 127.05, 67.85, 57.88, 52.11, 30.80, 19.15, 17.51. FT-IR (ATR) cm^{-1} 3429, 3062, 3038, 3001, 2970, 2892, 2877, 1740, 1675, 1598, 1487, 1445, 1435, 1392, 1374, 1319, 1274, 1202. ESI-HRMS calc mass: 401.1991 found: 402.2052 $[M+H]^+$, $[\alpha]_D^{20}$(c=1, $CHCl_3$) +22° mp 82-85°C



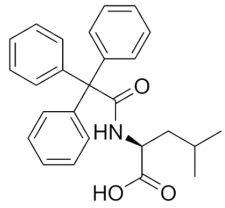
4a

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (br s, 1H), 7.30 (m,15H), 6.24 (d, 1H), 4.41 (d,1H), 0.84 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.99, 173.54, 143.11, 130.56, 128.06, 127.15, 67.86, 61.24, 33.97, 26.63. FT-IR (ATR) cm^{-1} 3424, 3392, 3092, 3060, 2983, 2966, 1731, 1717, 1692, 1637, 1509, 1491, 1443, 1405, 1209. ESI-HRMS calc mass: 401. 1991 found: 402.2065 $[M+H]^+$, $[\alpha]_D^{20}$(c=1, $CHCl_3$) +10° mp 132-134°C



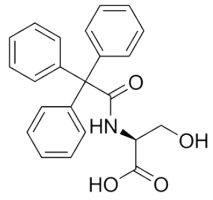
4b

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29 (m, 15H), 6.21 (d, 1H), 4.40 (d, 1H), 3.70 (s, 3H), 0.80 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.14, 171.68, 143.22, 130.55, 127.97, 127.06, 67.80, 61.21, 51.72, 34.10, 26.57. FT-IR (ATR) cm^{-1} 3439, 3091, 3055, 2995, 2963, 2901, 1740, 1666, 1505, 1495, 1442, 1434, 1322, 1283, 1270, 1243, 1215. ESI-HRMS calc mass: 415.2147 found: 416.2217 $[M+H]^+$, $[\alpha]_D^{20}$(c=1, $CHCl_3$) +10° mp 94-96°C



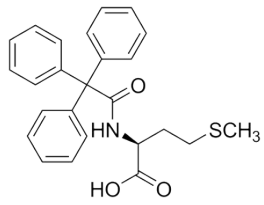
5

^{1}H NMR (403 MHz, $CDCl_3$) δ 7.30 (m, 15H), 6.02(d, 1H), 4.62 (m, 1H), 1.63(m, 1H), 1.45 (m, 1H), 1.38 (m, 1H), 0.85 (d, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.62, 174.01, 142.98, 130.50, 128.01, 127.13, 67.65, 51.58, 40.30, 24.81, 22.83, 21.49. FT-IR (ATR) cm^{-1} 3423, 3058, 2954, 2924, 2854, 1686, 1663, 1655, 1560, 1543, 1491, 1459, 1449, 1421, 1376, 1342, 1190, 1151. ESI-HRMS calc mass: 401.1991 found: 402.2067 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.81, $AcCH_3$) +14° mp 217-220°C colorless syrup



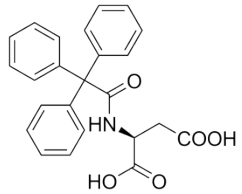
6

^{1}H NMR (401 MHz, $CDCl_3$) δ 7.24 (m, 15H), 6.85 (d, 1H), 4.59 (m, 1H), 3.81 (dd, 1H), 3.70 (dd, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.52, 172.80, 142.70, 130.36, 127.97, 127.11, 67.74, 62.22, 55.00. FT-IR (ATR) cm^{-1} 3410, 3057, 3030, 2924, 2851, 1730, 1643, 1597, 1491, 1444, 1326, 1188. ESI-HRMS calc mass: 375.1471 found: 376.1535 $[M+H]^+$, $[\alpha]_D^{20}$(c=1.17, $AcCH_3$) +17° colorless syrup



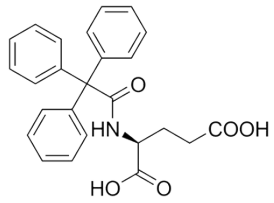
7

^{1}H NMR (403 MHz, $CDCl_3$) δ 7.29 (m, 15H), 6.46 (d, 1H), 4.77 (m, 1H), 2.32 (m, 2H), 2.13 (m, 1H), 1.98 (s, 3H), 1.93 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.10, 174.07, 142.92, 130.47, 128.07, 127.17, 67.72, 52.32, 30.41, 29.84, 15.36. FT-IR (ATR) cm^{-1} 3300, 3063, 3034, 2978, 2946, 1740, 1693, 1642, 1597, 1541, 1492, 1445, 1398, 1293, 1210. ESI-HRMS calc mass: 419.1555 found: 420.1636 $[M+H]^+$, $[\alpha]_D^{20}$(c=1.25, $AcCH_3$) +6° mp 179-184°C



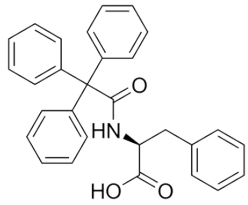
8

^{1}H NMR (401 MHz, DMSO-d_6) δ 12.70 (br s, 1H), 7.28 (m, 15H), 4.72 (m, 1H), 2.72 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 172.24, 172.12, 171.83, 143.29, 130.26, 127.70, 126.75, 67.03, 49.18, 35.32. FT-IR (ATR) cm^{-1} 3479, 3320, 3204, 3027, 2937, 1716, 1663, 1493, 1446, 1331, 1280, 1224. ESI-HRMS calc mass: 403.1420 found: 404.1508 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.7, $AcCH_3$) +19° mp 191-194°C



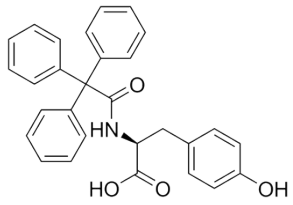
9

^{1}H NMR (401 MHz, $CDCl_3$) δ 9.29 (br s, 1.6H (not internally H-bonded)), 7.27 (m, 15H), 6.96 (m, 0.4H internally H-bonded COOH proton), 6.45 (d, 1H), 4.66 (quart. 1H), 2.28 (m, 1H), 2.22 (m, 1H), 2.14 (m, 1H), 2.01 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.99, 175.91, 173.95, 142.75, 130.35, 128.03, 127.13, 67.75, 52.14, 29.61, 26.28. FT-IR (ATR) cm^{-1} 3416, 3360, 3269, 3086, 3064, 2969, 2925, 1732, 1705, 1657, 1598, 1520, 1496, 1443, 1418, 1348, 1275. ESI-HRMS calc mass: 417.1576 found: 418.1649 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.25, $AcCH_3$) +9° mp 145-150°C



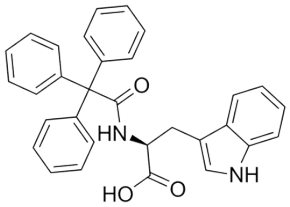
10

^{1}H NMR (401 MHz, $CDCl_3$) δ 10.17 (br s, 1H), 7.23 (m, 13H), 7.13 (m, 5H), 6.91 (m, 2H), 6.18 (d, 1H), 4.93 (m, 1H), 3.17 (dd, 1H), 2.92 (dd, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.42, 173.98, 142.74, 135.41, 130.41, 128.95, 128.80, 128.30, 127.92, 127.13, 127.01, 67.53, 53.92, 36.97. FT-IR (ATR) cm^{-1} 3407, 3086, 3061, 3032, 2930, 1743, 1669, 1620, 1515, 1492, 1442, 1410, 1213, 1193. ESI-HRMS calc mass: 435.1834 found: 436.1908 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.21, $AcCH_3$) +25° mp 139-144°C



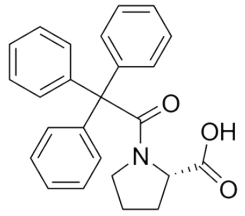
11

^{1}H NMR (300 MHz, DMSO-d_6) δ 9.28 (s, 1H), 7.26 (m, 10H), 7.08 (m, 5H), 6.77 (d, 2H), 6.70 (d, 1H), 6.62 (d, 2H), 4.59 (m, 1H) , 2.90 (m, 2H) ^{13}C NMR (75 MHz, DMSO-d_6) δ 173.16, 172.35, 156.44, 143.63, 130.63, 130.41, 128.16, 127.35, 127.17, 115.57, 67.48, 54.50, 35.75, 25.59. FT-IR (ATR) cm^{-1} 3389, 3261, 3087, 3057, 3029, 2976, 2926, 1745, 1738, 1644, 1614, 1600, 1515, 1492, 1445, 1275, 1246, 1231, 1210, 1171. ESI-HRMS calc mass: 451.1784 found: 452.1856 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.62, $AcCH_3$) +12° mp 197-203°C



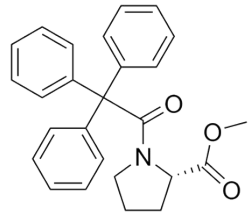
12

^{1}H NMR (401 MHz, DMSO-d_6) δ 12.87 (s, 1H), 10.84 (s, 1H), 7.38 (m, 2H), 7.21 (m, 10H), 7.06 (m, 1H), 7.01 (m, 5H), 6.90 (m, 1H), 6.78 (d, 1H) 6.70 (d, 1H), 4.66 (m, 1H), 3.16 (ddd, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 172.98, 171.89, 143.10, 136.13, 130.07, 127.59, 126.99, 126.64, 123.72, 120.94, 118.39, 118.07, 111.32, 108.85, 66.91, 53.23, 26.30. FT-IR (ATR) cm^{-1} 3402, 3344, 3060, 3023, 2968, 2949, 1715, 1609, 1532, 1491, 1457, 1443, 1248, 1221. ESI-HRMS calc mass: 474.1943 found: 475.2024 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.5, $AcCH_3$) +22° mp 232-235°C



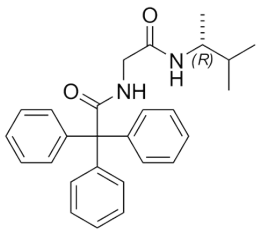
13a

^{1}H NMR (403 MHz, $CDCl_3$) δ 7.27 (m, 15H), 4.66 (t, 1H), 2.61 (m, 2H), 2.04 (m, 2H), 1.77 (sept. 1H), 1.54 (sept. 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.27, 172.56, 142.14, 130.39, 127.71, 126.67, 67.29, 60.91, 49.00, 27.85, 25.43. FT-IR (ATR) cm^{-1} 3168, 3061, 3039, 2996, 2959, 1747, 1697, 1609, 1599, 1494, 1445, 1418, 1205, 1182. ESI-HRMS calc mass: 385.1678 found: 386.1746 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.51, $AcCH_3$) +16° mp 206-210°C



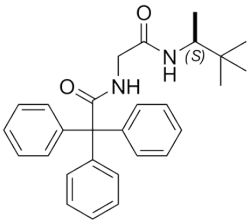
13b

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 (m, 15H), 4.59 (m, 1H), 3.76 (s, 3H), 2.61 (m,2H), 2.06 (m, 1H), 1.74 (m, 2H), 1.54 (m,1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.25, 171.60, 142.43, 130.49, 127.72, 126.61, 67.26, 60.68, 52.15, 48.87, 28.34, 25.58. FT-IR (ATR) cm^{-1} 3172, 3163, 3165, 2954, 2939, 2727, 1746, 1708, 1703, 1654, 1648, 1630, 1463, 1377, 1304, 1208, 1196, 1165, 1156, 1113, 1019 ESI-HRMS calc mass: 399.1834 found: 400.1912 $[M+H]^+$, $[\alpha]_D^{20}$(c=1.1, $AcCH_3$) -5° colorless syrup



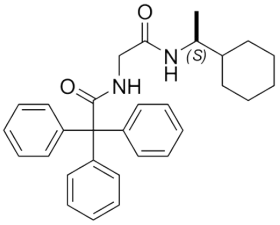
14

^{1}H NMR (403 MHz, $CDCl_3$) δ 7.26 (m, 15H), 6.64 (t, 1H), 6.11 (d, 1H), 3.99 (m, 2H), 3.76 (m, 1H), 1.55 (m, 1H), 0.97 (d, 3H), 0.81 (dd, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.16, 167.70, 143.04, 130.39, 128.09, 127.17, 67.77, 50.30, 44.54, 32.78, 18.74, 18.36, 17.31. FT-IR (ATR) cm^{-1} 3393, 3336, 3071, 3033, 2969, 2930, 2873, 1690, 1643, 1596, 1549, 1505, 1494, 1460, 1446, 1370, 1252. ESI-HRMS calc mass: 414.2307 found: 415.2384 $[M+H]^+$, $[\alpha]_D^{20}$(c=1.14, $AcCH_3$) -4°, mp 141-143°C



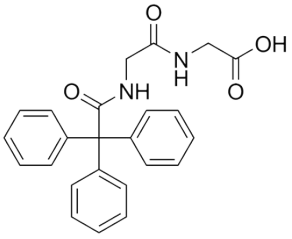
15

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 (m, 15H), 6.63 (br s, 1H), 6.12 (d, 1H), 3.96 (m, 2H), 3.81 (m, 1H), 1.00 (d, 3H), 0.82 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.46, 167.94, 142.96, 130.37, 128.08, 127.18, 67.69, 53.05, 44.77, 34.06, 26.09, 15.98. FT-IR (ATR) cm^{-1} 3374, 3354, 3331, 3090, 3058, 2967, 1688, 1683, 1643, 1597, 1578, 1543, 1493, 1446, 1397, 1366, 1251, 1138. ESI-HRMS calc mass: 428.2464 found: 429.2541 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.9, $AcCH_3$) +5°, mp 155-157°C



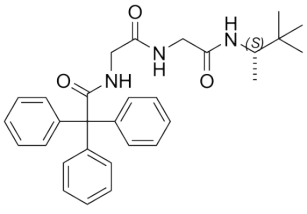
16

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29(m, 15H), 6.62 (br s, 1H), 6.07 (d, 1H), 3.98 (m, 2H), 3.77 (m, 1H), 1.65 (m, 6H), 1.11 (m, 4H), 0.98 (d, 3H), 0.88 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.05, 167.58, 143.08, 130.39, 128.08, 127.16, 67.81, 49.58, 44.53, 42.69, 29.10, 28.88, 26.33, 26.07, 17.61. FT-IR (ATR) cm^{-1} 3389, 3328, 3085, 3060, 3025, 2963, 2925, 2850, 1688, 1641, 1598, 1578, 1548, 1486, 1446, 1368, 1253. ESI-HRMS calc mass: 454.2620 found: 455.2697 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.3, $AcCH_3$) -5°, mp 164-169°C



17

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 (m, 15H), 6.80 (br s, 1H), 6.62 (br s, 1H), 4.06 (d, 2H), 3.95 (d, 2H). ^{13}C NMR (75 MHz, DMSO) δ 172.91, 171.62, 169.51, 144.05, 130.71, 128.18, 127.07, 67.56, 43.26, 41.09. FT-IR (ATR) cm^{-1} 3389, 3323, 3099, 3065, 2964, 2923, 1754, 1745, 1654, 1641, 1581, 1558, 1445, 1421, 1411, 1259, 1240, 1182. ESI-HRMS calc mass: 402.1580 found: 403.1658 $[M+H]^+$, mp 227-235°C (dec.)



18

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 (m, 15H), 6.79 (t, 1H), 6.58 (t, 1H), 6.15 (d,1H), 3.95 (m, 2H), 3.77 (m, 2H), 1.89 (br s, 1H), 0.97 (d, 3H), 0.82 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.42, 169.22, 167.71, 142.96, 130.41, 128.10, 127.18, 67.73, 53.07, 43.91, 43.44, 34.21, 26.11, 15.82. FT-IR (ATR) cm^{-1} 3517, 3438, 3305, 3059, 2973, 2871, 1685, 1668, 1652, 1630, 1564, 1505, 1493, 1448, 1428, 1407, 1378, 1367, 1264. ESI-HRMS calc mass: 485.2678 found: 486.2761 $[M+H]^+$, $[\alpha]_D^{20}$(c=0.33, $AcCH_3$) +14°, mp 168-172°C

Calculation details

Starting geometries of triphenylacetamides **2b**, **3b**, **4b** and **15** with assumed *S* absolute configuration of all stereogenic elements were obtained by a conformational search with the use of Scigress[1] software and pre-optimization of all conformers were calculated 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 one to identify the minimum energy structures which were further re-optimized with the use of a B3LYP functional[2] in conjunction with an enhanced 6-311++G(d,p) basis set.[3] 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 were different 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.

ECD spectra for all structures optimized at the B3LYP/6-311++G(d,p) level were calculated employing M06-2X[4] and CAM-B3LYP,[5] hybrid functionals, all in conjunction with the 6-311++G(d,p) basis set.[3] The calculated ECD spectra were Boltzmann averaged by taking into account conformers of **2b**, **3b**, **4b** and **15** ranging from 0 to 2.0 kcal mol^{-1} in relative energies, following a generally accepted protocol.[6] Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity calculated values of the 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.[7]

The solvent effect on the structure and ECD spectra was not taken into account, since all measurements for amides **2b**, **3b**, **4b** and **15** were done in non-polar cyclohexane.

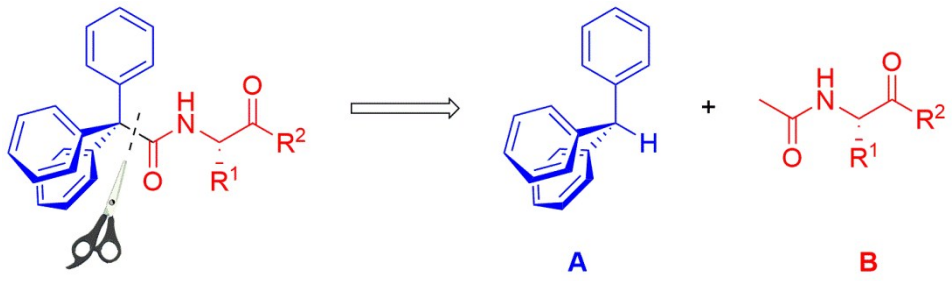
Since there are no significant differences between results obtained with the use of M06-2X and CAM-B3LYP functionals, we limited our discussion to the results obtained with the use of CAM-B3LYP functional only.

Depuzzling of the ECD spectra

A more detailed look into the calculated ECD spectra allowed us to determine the factors that are responsible for the observed CE's. We were particularly interested whether the observed ECD spectra result from intrachromophoric or interchromophoric interactions and wished to clarify to what extent the amino acid backbone affected the overall ECD spectrum of a given amide.[8]

To solve this problem we divided ("cut") each conformer into two moieties, denoted here as **A** and **B** (see Scheme S1). Each of the A subunits consisted of a triphenylmethane group. The subunits B consisted of the rest of the molecule. For B subunits, the triphenylacetyl fragments were replaced by simple acetamide fragments. The other structural parameters remained the same as in the parent structure. For each of the sub-structures the ECD spectra were calculated at the CAM-B3LYP/6-311++G(d,p) level (see **Figures S14-S17**). Additionally, the results of summation of the ECD spectra calculated for the **A** and **B** subunits were compared with ECD spectra calculated for the given, "whole" conformer.

In general, the effects of summation are in good to perfect agreement with the ECD spectra calculated for the whole structures. Therefore, in the amides under study, there were no significant trityl-amide-carboxylate interactions and each part of the molecule contributed to the overall spectrum independently. Influence of the amino acid backbone on the overall ECD spectrum is negligible in the cases of **2b**-**4b**. The presence of a *bis*-amide system in **15**, resulted in the generation of stronger rotatory strengths than in the cases mentioned earlier. However, according to the computational results these rotary strengths were overwhelmed by the rotatory strengths originated from the trityl chromophore. The discrepancy between the postulated model and the experimental results are clearly due to the dominant influence of higher-energy conformers of **15**, characterized by PPP helicities, on the averaged ECD spectrum.



Scheme S1.

Table S2. ECD ($\Delta\varepsilon$) and UV (ε) data for *N*-triphenylacetylamino acids **2**-**16** and **18** measured in cyclohexane and acetonitrile solution.

	Cyclohexane		Acetonitrile	
Compd	$\Delta\varepsilon$ (nm)	ε (nm)	$\Delta\varepsilon$ (nm)	ε (nm)
2a	-[a]	-[a]	-1.9 (229); 4.6 (202); 4.9 (195)	76596 (194)
2b	2.1 (221); -2.2 (207); 6.9 (191)	76500 (192)	-1.4 (217); 5.5 (201)	72700 (194)
3a	-[a]	-[a]	-4.2 (230); 20.3 (201)	77122 (194)
3b	-4.5 (229); 23.6 (202); -27.0 (185)	80477 (192)	-4.7 (228); 21.3 (200)	77070 (194)
4a	-3.7 (232); 13.9 (203)	77906 (192)	-3.4 (230); 18.2 (201)	78626 (194)
4b	-4.6 (228); 17.8 (201); -36.0 (183)	80700 (192)	-3.0 (227); 17.1 (199); -26.8 (184)	76800 (193)
5	-5.7(231); 20.8 (202); -22.5 (185)	79890(192)	-4.4 (229); 20.6 (200)	79075 (194)
6	-[a]	-[a]	1.3 (223); 3.9 (197)	71200 (194)
7	-0.9 (223); 1.52 (202)	81300 (193)	-2.9 (229); 17.2 (200)	81400 (194)
8	-[a]	-[a]	-2.0 (222); 5.2 (199)	78000 (194)
9	-[a]	-[a]	-0.6 (230); 7.0 (200)	77300 (194)
10	-1.7 (228); 7.4 (205); 16.6 (195)	91400 (189)	8.4 (212); 14.5 (201); 29.3 (194)	116400 (189)
11	-[a]	-[a]	4.2 (214); 15.5 (198)	107800 (194)
12	-[a]	-[a]	-4.6 (233); 18.7 (203)	79500 (194)
13a	-4.6 (233); 18.7 (203)	79500 (194)	-4.6 (233); 18.7 (203)	79500 (194)
13b	-[a]	-[a]	-3.1 (233); 14.0 (204); -12.2 (185)	80439 (195)
14	1.0 (229); -3.5 (206)	81700 (192)	-[a]	-[a]
15	-2.3 (227); 6.0 (205)	79300 (192)	-[a]	-[a]
16	-3.1 (227); 8.4 (203)	79200 (193)	-0.1 (227); 1.5 (205); -3.3 (189)	71900 (191)
18	-[a]	-[a]	1.4 (220); -3.4 (192)	82800 (194)

[a] data not available.

Table S3. Total energies (in Hartree), relative energies (*ΔE*, *ΔΔG* in kcal mol^{-1}) and percentage populations calculated at the B3LYP/6-311++G(d,p) level for individual conformers of **2b**, **3b**, **4b** and **15**.

Compound[a]	Energy	*ΔE*	Pop.	*ΔΔG*	Pop
2b (conf. 2)	-1209.16752	1.68	5	1.50	7
2b (conf. 25)	-1209.17021	0.00	95	0.00	93
3b (conf. 9)	-1287.81732	0.00	35	0.00	37
3b (conf. 13)	-1287.81655	0.49	15	0.61	13
3b (conf. 16)	-1287.81698	0.21	24	0.00	37
3b (conf. 17)	-1287.81497	1.48	3	1.81	2
3b (conf. 27)	-1287.81659	0.46	17	0.80	9
3b (conf. 32)	-1287.81564	1.05	6	1.77	2
4b (conf. 8)	-1327.13745	0.00	94	0.00	90
4b (conf. 15)	-1327.1349	1.60	6	1.33	10
15 (conf. 15)	-1346.60134	0.00	28	0.00	29
15 (conf. 18)	-1346.60098	0.22	18	0.37	15
15 (conf. 21)	-1346.60035	0.62	10	0.74	8
15 (conf. 22)	-1346.59984	0.94	5	1.10	4
15 (conf. 30)	-1346.60097	0.23	18	0.44	13
15 (conf. 35)	-1346.59942	1.21	3	1.33	3
15 (conf. 36)	-1346.60094	0.25	18	0.02	27
15 (conf. 42)	-1346.59777	2.24		1.99	1

[a] Conformers are numbered according to their appearance during conformational search.

Table S4. Dihedral angles α, β, γ, δ and φ (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) observed in the crystal structures of amino acids **1**, **2a**, **3a**, **4a**, **7**, **11**, **12**, **13a** and **13b** and calculated for individual conformers of **2b**, **3b** and **4b** at the B3LYP/6-311++G(d,p) level

Amino acid		α^a	$\beta_1{}^b$	$\beta_2{}^b$	$\beta_3{}^b$	$\gamma_1{}^c$	$\gamma_2{}^c$	$\gamma_3{}^c$	δ^d	φ^e	$l_1{}^f$	$l_2{}^f$	$l_3{}^f$	Helicity
1	A	10.4 -108.5	66.3(2)	-52.7(2)	-173.2(1)	-26.5(2)	-41.6(2)	-71.7(2)	-49.0	131.0(2)	2.27	2.39[h]	2.26	*MMM*
	B	-16.6 -134.7	67.1(2)	-172.4(2)	-51.3(2)	31.7(2)	55.1(2)	57.7(2)	-75.7	104.3(2)	2.39	2.43[h]	2.35	*PPP*
2a	A	-6.7	110.6(3)	-6.9(4)	-127.2(3)	-4.9(3)	53.8(3)	60.4(3)	57.1 (0.3)[g]	-123.0(3) (179.9(2))[g]	2.50	2.40	2.49	*0PP*
	B	-37.7	-95.2(2)	143.5(2)	22.6(3)	-25.8(3)	-53.2(2)	-59.5(3)	24.3	-155.8(2)	2.39	2.58	2.46	*MMM*
3a		-15.2	-86.0(2)	153.9(2)	32.8(2)	-43.7(3)	-46.6(2)	-59.9(2)	47.6	-132.5(2)	2.42	2. 47	2.41	*MMM*
4a		-15.6	158.3(1)	-83.0(2)	36.7(2)	-40.4(2)	-54.1(2)	-61.5(2)	48.3	-131.7(2)	2.49	2.43	2.41	*MMM*
7		9.6	134.7(5)	16.6(6)	-102.0(5)	-26.7(6)	49.7(6)	67.7(5)	72.3	-107.7(5)	2.61	2.45	2.63	*MPP*
11		8.6	-81.0(3)	157.2(3)	34.0(4)	-17.7(4)	-54.1(4)	-66.4(4)	68.0	-112.1(3)	2.36	2.40	2.57	*MMM*
12		16.5	60.3(4)	-59.2(4)	179.5(3)	-17.3(4)	-59.6(4)	-64.0(4)	78.9	-101.1(4)	2.35	2.33	2.20	*MMM*
13a		58.7	115.9(2)	-119.0(2)	-0.3(2)	-10.6(2)	51.0(2)	58.4(2)	---	-63.5(2)	---	2.59	2.64	*MPP*
13b	A	52.9	-117.0(3)	119.7(3)	0.9(2)	-2.8(4)	-41.9(4)	-57.7(4)	---	-69.4(4)	---	2.56	2.61	*0MM*
	B	60.8	108.6(3)	-128.2(3)	-8.2(4)	8.7(4)	48.1(4)	66.3(4)		-62.0(4)		2.62	2.70	*PPP*
	C	58.7	113.4(3)	-121.9(3)	-3.9(4)	2.5(4)	49.3(4)	53.9(4)		-65.3(4)		2.60	2.96	*0PP*
	D	50.5	-115.7(3)	121.3(3)	2.2(4)	-6.0(4)	-40.8(4)	-64.0(4)		-71.8(4)		2.54	2.90	*0MM*
2b (conf. 2)[h]		44	-77	40	162	-28	-54	-58	94	-71	2.31	2.52	2.28	*MMM*

2b (conf. 25)[h]	-39	83	-34	-157	24	56	58	21	-157	2.37	2.51	2.32	*PPP*
3b (conf. 9)[h]	-9	-52	61	-178	24	48	67	37	-126	2.31	2.31	2.11	*PPP*
3b (conf. 13)[h]	36	-79	160	-38	-27	-55	-57	78	-79	2.31	2.40	2.33	*MMM*
3b (conf. 16)[h]	-8	79	-39	-161	34	53	58	157	-125	2.34	2.30	2.26	*PPP*
3b (conf. 17)[h]	-34	82	-35	-158	22	56	59	27	-151	2.34	2.46	2.32	*PPP*
3b (conf. 27)[h]	-36	83	-34	-156	23	55	58	22	-153	2.36	2.48	2.32	*PPP*
3b (conf. 32)[h]	50	87	-30	-152	21	57	58	109	-67	2.37	2.62	2.37	*PPP*
4b (conf. 8)[h]	48	87	-30	-152	22	57	58	108	-68	2.37	2.58	2.36	*PPP*
4b (conf. 15)[h]	-7	-103	135	14	-12	-55	-59	68	-88	2.42	2.38	2.37	*MMM*

[a] – α = H-C$_\alpha$-N-C(=O); [b] – β = O=C-C-C$_{ipso}$; [c] – γ = C(=O)-C-C$_{ipso}$-C$_{ortho}$ (of the two possibilities the absolute values ≤90° has been chosen); [d] δ – H-N-C$_\alpha$-C(=O); [e] φ – C(=O)-N-C$_\alpha$-C(=O); [f] – l_1 = (N)H···C$_{ipso}$; l_2 = (C=)O···H(C$_\alpha$) (of the two possibilities the smaller absolute value has been chosen); l_3 = (C=)O···H(C$_{ortho}$); [g] – disordered fragment; [h] calculated structure.

Table S5. Dihedral angles α, β, γ, δ, ζ, φ, χ, ψ, and ω (in degrees) and selected interatomic distances l_1, l_2 and l_3 (in Å) observed in the crystal structures of **15 – 17** and calculated at the B3LYP/6-311++G(d,p) level for individual low-energy conformers of **15**.

		α_1[a]	α_2[a]	β_1[b]	β_2[b]	β_3[b]	γ_1[c]	γ_2[c]	γ_3[c]	δ[d]	ζ[e]	φ[f]	χ[g]	ψ[h]	ω[i]	l_1[j]	l_2[j]	l_3[j]	Helicity
15	A	-54.1 64.9	15.9	-77.9(2)	43.1(2)	162.8(2)	13.7(2)	39.7(2)	73.0(2)	5.4	-177.0(2)	-174.6(2)	174.7(2)	-170.3(2)	-102.4(2)	2.39	2.53	2.36	*PPP*
	B	73.7 -45.9	-29.8	76.3(2)	-43.8(2)	-164.4(2)	-12.1(2)	-44.2(2)	-71.3(2)	14.0	173.5(2)	-166.1(2)	171.0(2)	175.8(2)	-145.3(2)	2.38	2.45	2.36	*MMM*
16	A	69.8 -48.5	-28.3	65.9(4)	-54.8(3)	-175.9(3)	-3.3(4)	-51.8(3)	-68.6(3)	10.6	-178.2(3)	-169.4(3)	170.7(3)	-173.8(3)	-145.5(3)	2.42	2.56	2.41	*0MM*
	B	72.7 -46.0	35.8	-66.1(4)	55.6(4)	176.0(3)	0.7(4)	47.4(4)	70.5(4)	13.7	176.6(3)	-166.3(3)	168.6(3)	-179.8(3)	-79.5(4)	2.40	2.61	2.43	*0PP*
	C	72.1 -46.0	14.1	-64.7(4)	57.0(4)	177.5(3)	-0.4(4)	46.7(4)	70.5(4)	13.0	176.1(3)	-167.0(3)	170.3(3)	173.3(5)	-104.0(3)	2.39	2.64	2.44	*0PP*
	D	69.6 -48.5	-30.2	62.8(4)	-57.8(3)	-177.3(3)	-7.7(4)	-49.9(3)	-68.4(3)	10.6	-177.0(3)	-169.4(3)	172.4(3)	-173.5(3)	-147.8(3)	2.40	2.57	2.36	*MMM*
17		148.1 30.0	3.4 -114.2	-90.8(2)	148.3(1)	28.1(2)	-34.3(2)	-48.5(2)	-56.7(2)	89.0 -55.3	176.8(1)	-91.0(2)	140.3(1)	175.8(1)	124.6(2)	2.44	2.45	2.43	*MMM*
15 (15)[k]		157 39	-2	-82	157	35	-25	-57	-57	91	-174	-84	68	-176	-117	2.32	2.53	2.34	*MMM*
15 (18)[k]		156 38	-5	-65	54	175	25	45	69	98	-174	-85	67	-178	-121	2.31	2.56	2.16	*PPP*
15 (21)[k]		155 37	1	84	-156	-34	27	56	57	104	-174	-86	69	-179	-115	2.33	2.56	2.36	*PPP*
15 (22)[k]		-155 -37	-1	67	-52	-173	-25	-45	-70	-102	168	86	-64	-170	-116	2.31	2.58	2.18	*MMM*

15 (30)[k]	-157 -39	-1	79	-39	-161	27	55	58	-94	172	84	-66	-176	-116	2.30	2.55	2.31	*PPP*
15 (35)[k]	-155 -37	3	-91	148	26	-24	-55	-59	-109	170	86	-61	-170	-112	2.36	2.59	2.42	*MMM*
15 (36)[k]	-157 -39	4	79	-38	-160	26	55	58	-95	171	84	-62	-174	-112	2.30	2.55	2.31	*PPP*
15 (42)[k]	-127 -10	5	99.316	-17.134	-139	2	54	62	-84	169	116	-7	-173	-107	2.43	2.37	2.39	*0PP*

[a] – α = H-C_{α}-N-C(=O); [b] – β = O=C-C-C_{ipso}; [c] – γ = C(=O)-C-C_{ipso}-C_{ortho} (of the two possibilities the absolute values ≤90° has been chosen); [d] – δ = H-N-C_{α}-C(=O) (two possibilities in **17**); [e] – ζ = C_{Tr}-C(=O)-N-C_{α}; [f] – φ = C(=O)-N-C_{α}-C(=O); [g] – χ = N-C_{α}-C(=O)-N; [h] – ψ = C_{α}-C(=O)-N-$C_{\alpha'}$; [i] – ω = C(=O)-N-$C_{\alpha'}$-C_{alkyl} (C(=O)-N-C_{sp3}-$C_{carboxyl}$ for **17**); [j] – l_1 = (N)H···C_{ipso}; l_2 = (C=)O···H(C_{α}); l_3 = (C=)O···H(C_{ortho}); [k] calculated structure, in parentheses conformer number; conformers are numbered according to their appearance during conformational search.

Table S6. Geometry of intramolecular hydrogen bonds and weak intramolecular interactions in the investigated crystal structures.

	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [°]
1				
mol A				
C2A–H28A···O1A	0.97	2.43	2.794(2)	102
C12A–H12A···O1A	0.93	2.27	2.931(2)	128
C26A–H26A···Cg(C11A-C16A)	0.93	3.05	3.70	129
C36A–H36A···Cg(C21A-C26A)	0.93	3.04	3.73	132
N1A–H1A···Cg(C31A-C36A)	0.86	2.80	3.52	142
mol B				
C2B–H22B···O1B	0.97	2.39	2.771(2)	103
C32B–H32B···O1B	0.93	2.35	2.816(2)	111
C22B–H22B···O2B	0.93	2.72	3.446(2)	135
C26B–H26B···Cg(C11B-C16B)	0.93	2.93	3.63	133
C36B–H36B···Cg(C21B-C26B)	0.93	2.94	3.65	133
N1B–H1B···Cg(C21B-C26B)	0.86	3.03	3.67	133
2a				
mol A				
C2A–H2A···O1A	1.00	2.40	2.807(4)	104
C22A–H22A···O1A	0.95	2.48	2.804(4)	100
C12A–H12A···O2A	0.95	2.77	3.403(5)	125
C26A–H26A···Cg(C31A-C36A)	0.95	3.08	3.75	130
C4'–H4'C···O3'*	0.98	2.19	2.666(34)	109
N1A–H1A···O2'*	0.88	2.45	2.805(18)	105
mol B				
C32B–H32B···O1B	0.95	2.46	2.850(3)	105
N1B–H1B···O2B	0.88	2.30	2.660(3)	105
C26B–H26B···Cg(C11B-C16B)	0.95	2.99	3.69	131
C16B–H16B···Cg(C31B-C36B)	0.95	2.95	3.54	122
C36B–H36B···Cg(C21B-C26B)	0.95	2.95	3.66	133
N1B–H1B···Cg(C21B-C26B)	0.88	3.07	3.61	121
3a				
C2–H2···O1	0.98	2.47	2.821(2)	101
C32–H32···O1	0.93	2.41	2.785(2)	104
C16–H16···Cg(C31-C36)	0.93	3.01	3.68	129
C36–H36···Cg(C21-C26)	0.93	2.96	3.66	133
C26–H26···Cg(C11-C16)	0.93	2.97	3.64	131
N1–H1···Cg(C21-C26)	0.86	3.08	3.66	126
4a				
C2-H2···O1	1.00	2.43	2.805(1)	101
C32–H32···O1	0.95	2.41	2.783(1)	103
C7–H7B···O3	0.98	2.50	2.965(2)	109
C16–H16···Cg(C21-C26)	0.95	2.88	3.55	129
C36–H36···Cg(C11-C16)	0.95	2.85	3.58	134
C26–H26···Cg(C31-C36)	0.95	3.06	3.75	131
7				
C2-H2···O1	1.00	2.45	2.845(5)	103
C12-H12···O2	0.95	2.57	3.323(6)	137
C4-H4B···O3	0.99	2.38	2.740(6)	101
11				
C2-H2···O1	1.00	2.40	2.796(4)	103
C32-H32···O1	0.95	2.57	2.916(4)	102
C4-H4B···O3	0.99	2.68	2.978(4)	98
C36-H36···Cg(C21-C26)	0.95	3.03	3.73	132
C12-H12···Cg(C1'-C6')	0.95	2.76	3.54	139
12				
C2-H2···O1	1.00	2.33	2.742(5)	104
C12-H12···O1	0.95	2.20	2.872(4)	127
N1-H1···Cg(C31-C36)	0.88	2.96	3.65	138

C22-H22···Cg(C4',C9')	0.95	2.77	3.57	142
13a				
C22-H22···O1	0.93	2.87	3.423(2)	119
C12-H12···O3	0.93	2.68	3.601(3)	173
C5-H5B···Cg(C21-C26)	0.97	2.91	3.55	124
C36-H36···Cg(C21-C26)	0.93	3.08	3.75	130
13b				
mol A				
C22A-H22A···O1A	0.95	2.84	3.431(4)	122
C22A-H22A···O2A	0.95	2.79	3.223(4)	108
C5A-H5A1···Cg(C21A-C26A)	0.99	3.04	3.52	111
C36A-H36A···Cg(C21A-C26A)	0.95	3.06	3.74	130
mol B				
C4B-H4B1···O2B	0.99	2.88	3.338(4)	109
C12B-H12B···O2B	0.95	2.47	3.393(4)	163
C7B-H7B1···O3B	0.99	2.23	2.659(5)	105
C26B-H26B···Cg(C11B-C16B)	0.95	3.05	3.74	130
C5B-H5B2···Cg(C21B-C26B)	0.99	2.97	3.56	119
C36B-H36B···Cg(C21B-C26B)	0.95	3.04	3.74	132
mol C				
C12C-H12C···O2C	0.95	2.46	3.391(4)	168
C5C-H5C2···Cg(C21C-C26C)	0.99	2.92	3.55	122
C36C-H36C···Cg(C21C-C26C)	0.95	2.99	3.67	130
mol D				
C22D-H22D···O2D	0.95	2.76	3.288(4)	116
C36D-H36D···Cg(C21D-C26D)	0.95	3.03	3.73	132
15				
mol A				
C12A-H12A···O1A	0.95	2.36	3.012(3)	125
N1A-H1A···O2A	0.88	2.26	2.645(3)	107
C36A-H36A···Cg(C21A-C26A)	0.95	2.89	3.60	133
N1A-H1A···Cg(C31A-C36A)	0.88	2.97	3.65	135
mol B				
C12B-H12B···O1B	0.95	2.36	2.999(3)	124
N1B-H1B···O2B	0.88	2.22	2.607(3)	106
C36B-H36B···Cg(C21B-C26B)	0.95	2.92	3.63	132
N1B-H1B···Cg(C31B-C36B)	0.88	2.95	3.65	138
16				
mol A				
C12A-H12A···O1A	0.95	2.41	3.019(4)	122
N1A-H1A···O2A	0.88	2.34	2.690(4)	104
C36A-H36A···Cg(C21A-C26A)	0.95	3.04	3.74	131
N1A-H1A···Cg(C31A-C36A)	0.88	2.97	3.65	135
mol B				
C12B-H12B···O1B	0.95	2.42	3.019(4)	121
C1'B-H1'B···O2B	1.00	2.83	3.381(6)	115
N1B-H1B···O2B	0.88	2.34	2.687(4)	103
C36B-H36B···Cg(C21B-C26B)	0.95	3.01	3.71	132
N1B-H1B···Cg(C31B-C36B)	0.88	2.96	3.64	136
mol C				
C12C-H12C···O1C	0.95	2.44	3.026(5)	120
C4C-H4C···O2C	1.00	2.63	2.983(5)	100
N1C-H1C···O2C	0.88	2.34	2.683(4)	103
C36C-H36C···Cg(C21C-C26C)	0.95	3.05	3.74	131
N1C-H1C···Cg(C31C-C36C)	0.88	2.94	3.62	136
mol D				
C12D-H12D···O1D	0.95	2.36	2.985(4)	123
N1D-H1D···O2D	0.88	2.35	2.694(3)	104
C36D-H36D···Cg(C21D-C26D)	0.95	2.97	3.67	132
N1D-H1D···Cg(C31D-C36D)	0.88	2.96	3.64	136
17				
C32-H32···O1	0.95	2.43	2.818(2)	104
C4-H4A···O2	0.99	2.39	2.802(2)	104

C16–H16···Cg(C31-C36)	0.95	3.03	3.68	126
C26–H26···Cg(C11-C16)	0.95	2.92	3.62	132
C36–H36···Cg(C21-C26)	0.95	2.75	3.49	135

*disordered fragment

Table S7. Geometry of intermolecular hydrogen bonds and weak intermolecular interactions in the investigated crystal structures.

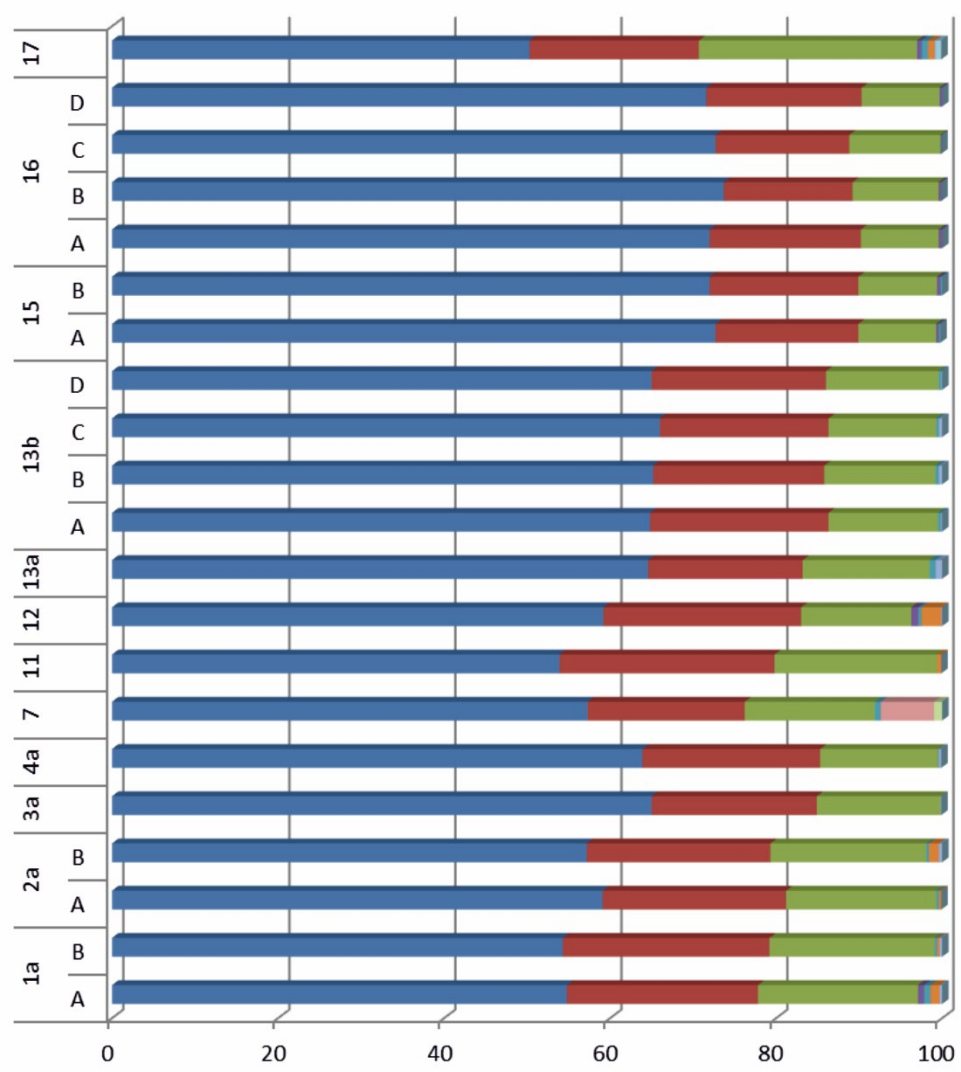
	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [°]	Symmetry operation on A
1					
mol A					
C34A–H34A···O1A	0.93	2.95	3.658(2)	134	-1+x, y, z
O3A–H3A···O1B	0.89	1.73	2.611(2)	166	x, y, z
C2A–H28A···O2B	0.97	2.33	3.267(2)	163	1+x, y, z
C14A–H14A···O2B	0.93	2.81	3.459(2)	128	1-x, 1-y, 1-z
mol B					
O3B–H3B···O1A	0.88	1.83	2.705(2)	170	-1+x, y, z
C2B–H27B···O2A	0.97	2.46	3.390(2)	160	x, y, z
C34B–H34B···O2A	0.93	2.75	3.599(2)	153	x, 1+y, z
C23B-H23B···O3A	0.93	2.60	3.440(2)	151	-1+x, y, z
C35B–H35B···O3B	0.93	2.59	3.404(2)	146	x, 1+y, z
C24B-H24B···Cg(C11B-C16B)	0.93	2.70	3.58	158	-1+x, y, z
2a					
mol A					
O3A–H3A···O1A	0.92	1.77	2.670(3)	165	1-x, 1/2+y, 1-z
C2A–H2A···O2A	0.98	2.62	3.596(5)	173	1-x, -1/2+y, 1-z
C13A–H13A···O3A	0.95	2.80	3.494(4)	130	1-x, 1/2+y, 1-z
C23A–H23A···O1B	0.95	2.67	3.555(4)	155	-1+x, -1+y, z
C24A–H24A···Cg(C31B-C36B)	0.95	2.62	3.47	151	-1+x, -1+y, z
O3'-H3'A···O2B*	0.85	2.05	2.889(23)	171	x, y, z
mol B					
O3B–H3B···O1B	0.92	1.84	2.677(2)	164	2-x, -1/2+y, 1-z
C2B–H2B···O2B	0.98	2.33	3.126(4)	147	2-x, 1/2+y, 1-z
C13B–H13B···O2A	0.95	2.92	3.321(6)	107	x, y, z
C13B–H13B···O3A	0.95	2.63	3.507(5)	154	1-x, 1/2+y, 1-z
3a					
C14–H14···O1	0.93	2.85	3.653(3)	146	-1+x, y, z
O3–H3···O1	0.82	1.87	2.679(2)	170	2-x, -1/2+y, 2-z
C2–H2···O2	0.98	2.47	3.436(3)	167	2-x, 1/2+y, 2-z
C13–H13···O2	0.93	2.97	3.660(4)	132	1-x, 1/2+y, 2-z
C23–H23···O3	0.93	2.83	3.459(3)	126	2-x, -1/2+y, 2-z
4a					
O3–H3···O1	0.87	1.82	2.676(2)	166	2-x, -1/2+y, 1-z
C24–H24···O1	0.95	2.59	3.446(2)	150	-1+x, y, z
C2–H2···O2	1.00	2.54	3.522(2)	167	2-x, 1/2+y, 1-z
C23–H232···O2	0.95	2.84	3.365(2)	116	1-x, 1/2+y, 1-z
C6–H6C···Cg(C21-C26)	0.98	2.94	3.79	146	1-x, -1/2+y, 1-z
C15–H15···Cg(C31-C36)	0.95	2.69	3.56	152	1-x, -1/2+y, -z
7					
O3-H3···O1	0.88	1.77	2.619(5)	160	1.5-x, -1/2+y, ¾-z
C34-H34···O1	0.95	2.77	3.655(7)	156	-1+x, y, z
C2–H2···O2	1.00	2.33	3.281(6)	159	1.5-x, 1/2+y, ¾-z
C6–H6B···O3	0.98	2.60	3.381(7)	137	-1+x, y, z
C13-H13···O3	0.95	2.79	3.536(6)	137	1.5-x, -1/2+y, ¾-z
C34-H34···O3	0.95	2.59	3.394(7)	142	1/2-x, 1/2+y, 3/4-z
N1-H1···S1	0.88	2.57	3.423(4)	165	1/2-x, -1/2+y, 3/4-z
C36-H36···S1	0.95	2.81	3.523(5)	132	1/2-x, -1/2+y, 3/4-z
C14-H14···Cg(C21-C26)	0.95	2.82	3.75	168	x, -1+y, z
C15-H15···Cg(C21-C26)	0.95	2.97	3.73	137	1-y, 1-x, 1/2-z
11					
O4'-H4'···O1	0.90	1.85	2.736(3)	168	1/2+x, 1/2-y, 1-z
C2-H2···O2	1.00	2.78	3.751(4)	164	-1/2+x, 1.5-y, 1-z
C14-H14···O2	0.95	2.63	3.280(4)	126	x, -1+y, z
C13-H13···O2	0.95	2.73	3.335(4)	122	x, -1+y, z
N1-H1···O3	0.88	2.64	3.454(3)	155	1/2+x, 1.5-y, 1-z
C4-H4A···O3	0.99	2.88	3.680(4)	138	1/2+x, 1.5-y, 1-z
O3-H3···O4'	0.91	1.81	2.694(3)	163	x, 1+y, z

C25-H25···O4'	0.95	2.86	3.219(4)	104	1/2+x, 1.5-y, 1-z
C5'-H5'···Cg(C11-C16)	0.95	3.01	3.69	130	-1/2+x, 1/2-y, 1-z
C15-H15···Cg(C21-C26)	0.95	3.06	3.78	134	1-x, -1/2+y, 1/2-z
C35-H35···Cg(C1'-C6')	0.95	2.87	3.67	143	1/2-x, 1-y, -1/2+z
12					
C2'-H2'···O1	0.95	2.67	3.174(4)	114	-x, -1/2+y, -z
N1'-H1'···O1	0.88	2.62	3.128(4)	118	-x, -1/2+y, -z
O3-H3···O1	0.89	1.72	2.609(3)	173	-x, 1/2+y, -z
C2'-H2'···O2	0.95	2.96	3.628(5)	129	-x, -1/2+y, -z
C2-H2···O2	1.00	2.89	3.875(4)	169	-x, -1/2+y, -z
C14-H14···O2	0.95	2.78	3.448(5)	128	1+x, y, z
N1'-H1'···O2	0.88	2.08	2.910(4)	157	x, -1+y, z
C13-H13···O3	0.95	2.85	3.284(5)	109	1+x, y, z
C4-H4A···Cg(C11-C16)	0.99	2.92	3.62	128	-1+x, y, z
C24-H24···Cg(C11-C16)	0.95	2.73	3.66	166	x, -1+y, z
C34-H34···Cg(C21-C26)	0.95	3.02	3.60	121	1-x, 1/2+y, 1-z
13a					
O2-H1···O1	0.82	1.84	2.642(2)	166	2-x, 2-y, z
C14-H14···O1	0.93	2.65	3.525(3)	156	x, y, 1+z
C23-H23···O2	0.93	2.59	3.195(3)	124	1.5-x, -1/2+y, -z
C24-H24···O2	0.93	2.60	3.196(3)	123	1.5-x, -1/2+y, -z
C25-H25···O3	0.93	2.45	3.322(3)	157	1.5-x, -1/2+y, 1-z
C32-H32···O3	0.93	2.79	3.660(2)	156	2-x, 2-y, z
13b					
mol A					
C7A-H7A3···O1C	0.98	2.50	3.377(5)	149	x, y, 1+z
C2A-H2A···O3D	1.00	2.44	3.140(5)	126	-1+x, y, z
C4A-H4A2···O3D	0.99	2.88	3.512(5)	123	-1+x, y, z
C12A-H12A···O3D	0.95	2.41	3.283(5)	153	-1+x, y, z
C24A-H24A···Cg(C11B-C16B)	0.95	2.75	3.62	152	1-x, -1/2+y, 1-z
C5A-H5A1···Cg(C11C-C16C)	0.99	3.03	3.85	142	-1+x, y, 1+z
C33A-H33A···Cg(C11C-C16C)	0.95	2.95	3.73	140	-1+x, y, z
mol B					
C14B-H14B···O1B	0.95	2.61	3.319(5)	131	1+x, y, z
C14B-H14B···O3B	0.95	2.72	3.391(5)	128	1+x, y, z
C4B-H4B1···O3C	0.99	2.56	3.546(5)	176	x, y, z
C7B-H7B3···O3C	0.98	2.83	3.762(5)	121	x, y, z
C4B-H4B2···Cg(C11D-C16D)	0.99	2.97	3.72	134	x, y, -1+z
C33B-H33B···Cg(C11D-C16D)	0.95	2.84	3.74	159	x, y, z
mol C					
C14C-H14C···O3C	0.95	2.73	3.408(4)	129	1+x, y, z
C4C-H4C1···O3B	0.99	2.50	3.490(5)	177	1+x, y, z
C14C-H14C···O1C	0.95	2.63	3.305(4)	129	1+x, y, z
C15C-H15C···O1C	0.95	2.91	3.445(4)	117	1+x, y, z
C33C-H33C···Cg(C11A-C16A)	0.95	2.86	3.72	150	1-x, y, -1+z
C24C-H24C···Cg(C21D-C26D)	0.95	2.92	3.71	141	2-x, -1/2+y, 1-z
mol D					
C2D-H2D···O3A	1.00	2.46	3.117(5)	123	x, y, z
C4AD-H4D2···O3A	0.99	2.78	3.414(5)	122	x, y, z
C12D-H12D···O3A	0.95	2.37	3.219(5)	149	x, y, z
C7D-H7D1···O1B	0.98	2.49	3.323(5)	142	1+x, z, y
C5D-H5D1···Cg(C11B-C16B)	0.99	2.92	3.73	140	x, z, y
C33D-H33D···Cg(C11B-C16B)	0.95	2.96	3.73	139	x, y, 1+z
C23D-H23D···Cg(C31B-C36B)	0.95	3.08	4.00	163	1+x, y, z
15					
mol A					
N2A-H2A···O1B	0.88	2.05	2.908(3)	165	x, y, z
C3A-H3AA···O1B	0.99	2.75	3.166(3)	106	x, y, z
C34A-H34A···O2B	0.95	2.35	3.272(3)	162	1+x, 1+y, z
C6A-H6AB···Cg(C11B-C16B)	0.98	3.00	3.86	147	x, 1+y, z
C8A-H8AC···Cg(C21B-C26B)	0.98	3.00	3.44	108	x, y, z
mol B					
N2B-H2B···O1A	0.88	2.21	3.054(3)	161	x, y, z

C3B-H3BB···O1A	0.99	2.73	3.241(3)	113	x, y, z
C6B-H6BA···O1A	0.98	2.87	3.822(3)	163	x, y, z
C23B-H23B···O2A	0.95	2.60	3.150(3)	117	-1+x, y, z
C34B-H34B···O2A	0.95	2.49	3.384(3)	157	-1+x, -1+y, z
C25B-H25B···Cg(C11A-C16A)	0.95	3.02	3.77	137	-1+x, y, -1+z
C6B-H6BA···Cg(C21A-C26A)	0.98	2.85	3.37	114	x, y, z
C23B-H23B···Cg(C31A-C36A)	0.95	3.09	3.86	140	-1+x, y, z
16					
mol A					
C23A-H23A···O2A	0.95	2.66	3.237(4)	120	-1+x, y, z
C24A-H24A···O2A	0.95	2.63	3.227(4)	121	-1+x, y, z
N2A-H2A···O1B	0.88	2.04	2.874(4)	158	x, y, z
C2A-H2A1···O1B	0.99	2.69	3.101(4)	105	x, y, z
C5'A-H5'5···O2D	0.99	2.72	3.549(5)	142	x, y, 1+z
C3'A-H3'5···Cg(C11B-C16B)	0.99	2.94	3.72	137	x, y, z
mol B					
N2B-H2B···O1A	0.88	2.02	2.879(4)	165	x, y, z
C2B-H2B2···O1A	0.99	2.66	3.183(4)	113	x, y, z
C24B-H24B···O2B	0.95	2.81	3.507(4)	131	1+x, y, z
C13B-H13B···O2D	0.95	2.78	3.641(4)	152	-1+x, y, 1+z
C33B-H33B···Cg(C11A-C16A)	0.95	3.08	3.38	138	-1+x, 1+y, z
mol C					
C13C-H13C···O2A	0.95	2.70	3.553(4)	151	x, y, -1+z
N2C-H2C···O1D	0.88	2.07	2.930(4)	166	x, y, z
C2C-H2C2···O1D	0.99	2.66	3.193(4)	114	x, y, z
C6'C-H6'7···O2B	0.99	2.44	3.305(7)	146	x, y, z
C4C-H4C···O2B	1.00	2.79	3.481(8)	127	x, y, z
mol D					
C5'D-H5'1···O2A	0.99	2.69	3.535(4)	144	1-x, y, -1+z
N2D-H2D···O1C	0.88	2.04	2.878(4)	158	x, y, z
C2D-H2D1···O1C	0.99	2.64	3.075(4)	107	x, y, z
C23D-H23D···O2D	0.95	2.76	3.285(5)	116	-1+x, y, z
C24D-H24D···O2D	0.95	2.55	3.190(6)	125	-1+x, y, z
C3'D-H3'1···Cg(C11C-C16C)	0.99	2.86	3.64	136	x, y, z
C25D-H25D···Cg(C1C-C36C)	0.95	3.06	3.75	131	-1+x, 1+y, z
17					
N2-H2···O1	0.88	2.17	2.963(2)	149	1-x, 2-y, 1-z
N1-H1···O2	0.88	2.27	3.055(2)	149	1-x, 1-y, 1-z
O4-H4···O2	0.93	1.74	2.640(2)	162	1-x, 1/2+y, 1.5-z
C3-H3B···O3	0.99	2.63	3.279(2)	124	1-x, 2-y, 1-z
C4-H4A···O3	0.99	2.72	3.667(2)	160	1-x, -1/2+y, 1.5-z
C12-H12···O3	0.95	2.87	3.702(2)	124	1-x, 2-y, 1-z
C3-H3A···O4	0.99	2.78	3.586(2)	139	x, 1.5-y, -1/2+z
C23-H23···O4	0.95	2.76	3.415(2)	127	1-x, -1/2+y, 1.5-z
C14-H14···Cg(C31-C36)	0.95	2.85	3.62	138	x, 1.5-y, -1/2+z

*disordered fragment

Table S8. Relative contributions to the Hirshfeld surface areas of the various intermolecular contacts (H···H, H···O, H···C and C···C) in the investigated crystal structures



	1		2a		3a	4a	7	11	12	13a	13b				15		16				17
H···H	54.8	54.3	59.1	57.2	65.0	63.9	57.3	53.9	59.2	64.6	64.8	65.2	66.0	65.0	72.7	72.0	72.0	73.7	72.7	71.6	50.3
H···C	23.0	24.9	22.1	22.1	19.9	21.4	18.9	25.9	23.8	18.6	21.5	20.6	20.3	21.0	17.2	17.9	18.2	15.5	16.1	18.7	20.4
H···O	19.3	19.9	18.1	18.8	14.9	14.2	15.7	19.6	13.3	15.3	13.2	13.4	13.0	13.6	9.4	9.5	9.4	10.4	11.0	9.4	26.3
H···N	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.0	0.0	0.0	0.0	0.0	0.3	0.4	0.4	0.3	0.1	0.3	0.5
C···C	0.8	0.3	0.3	0.3	0.0	0.1	0.7	0.0	0.4	0.7	0.4	0.4	0.3	0.3	0.2	0.2	0.0	0.0	0.0	0.0	0.8
O···C	1.1	0.3	0.3	1.2	0.0	0.0	0.0	0.5	2.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8
O···O	0.4	0.4	0.0	0.4	0.1	0.3	0.0	0.0	0.0	0.8	0.1	0.4	0.4	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1
H···S	---	---	---	---	---	---	6.4	---	---	---	---	---	---	---	---	---	---	---	---	---	---
S···C	---	---	---	---	---	---	1.0	---	---	---	---	---	---	---	---	---	---	---	---	---	---
O···N	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C···N	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7

Table S9. Selected crystal data and structure refinement details.

	1	**2a**	**3a**	**4a**	**7**	**11**	**12**	**13a**	**13b**	**15**	**16**	**17**
Chemical formula	$C_{22}H_{19}NO_3$	$C_{23}H_{21}NO_3$	$C_{25}H_{25}NO_3$	$C_{26}H_{27}NO_3$	$C_{25}H_{25}NO_3S$	$C_{29}H_{25}NO_4$	$C_{31}H_{26}N_2O_3$	$C_{25}H_{23}NO_3$	$C_{26}H_{25}NO_3$	$C_{28}H_{32}N_2O_2$	$C_{30}H_{34}N_2O_2$	$C_{24}H_{22}N_2O_4$
M_r	345.38	359.41	387.46	401.48	419.52	451.50	474.54	385.44	399.47	428.55	454.59	402.43
Crystal system, space group	Triclinic, *P*-1	Monoclinic , $P2_1$	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Tetragonal, $P4_32_12$	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1$	Orthorhombic, $P2_12_12$	Monoclinic , $P2_1$	Triclinic, *P*1	Triclinic, *P*1	Monoclinic , $P2_1/c$
Temperature (K)	294	130	291	130	100	100	100	294	130	130	130	100
a, *b*, *c* (Å)	8.9568 (1), 10.4462 (2), 19.2221 (3)	13.1517 (2), 9.5286 (1), 15.2352 (2)	8.5896 (1), 9.9657 (1), 12.7116 (2)	8.5012 (1), 9.8952 (1), 12.8936 (2)	8.9410 (2), 8.9410 (2), 54.361 (2)	9.1939 (4), 10.3126 (4), 24.1891 (8)	9.7079 (12), 9.4265 (8), 13.9926 (13)	14.3139 (2), 15.9294 (2), 9.1186 (1)	9.1720 (2), 32.8820 (5), 13.5380 (3)	9.8268 (2), 10.7524 (2), 12.3034 (3)	9.6669 (3), 14.8741 (6), 19.1839 (6)	13.3958 (6), 9.2202 (3), 16.7458 (7)
α, β, γ (°)	95.594 (2), 91.222 (1), 92.512 (2)	90, 91.793 (1), 90	90, 94.914 (1), 90	90, 92.270 (1), 90	90, 90, 90	90, 90, 90	90, 107.665 (12), 90	90, 90, 90	90, 90.126 (2), 90	104.385 (2), 99.112 (2), 92.482 (2)	86.367 (4), 81.808 (3), 71.038 (3)	90, 108.447 (5), 90
V (Å^3)	1787.63 (5)	1908.30 (4)	1084.13 (2)	1083.77 (2)	4345.7 (3)	2293.44 (15)	1220.1 (2)	2079.15 (5)	4082.97 (14)	1238.70 (5)	2581.65 (16)	1962.03 (15)
Z	4	4	2	2	8	4	2	4	8	2	4	4
D_x (Mg m^{-3})	1.283	1.251	1.187	1.230	1.282	1.308	1.292	1.231	1.300	1.149	1.170	1.362
Radiation type	Cu *Kα*	Cu *Kα*	Cu *Kα*	Cu *Kα*	Mo *Kα*	Mo *Kα*	Mo *Kα*	Cu *Kα*	Cu *Kα*	Cu *Kα*	Cu *Kα*	Mo *Kα*
μ (mm^{-1})	0.69	0.66	0.62	0.64	0.18	0.09	0.08	0.64	0.67	0.56	0.57	0.09
Crystal size (mm)	0.60 × 0.08 × 0.08	0.20 × 0.20 × 0.05	0.4 × 0.1 × 0.1	0.40 × 0.20 × 0.10	0.40 × 0.20 × 0.10	0.60 × 0.30 × 0.20	0.40 × 0.20 × 0.20	0.50 × 0.15 × 0.05	0.50 × 0.20 × 0.05	0.10 × 0.10 × 0.05	0.10 × 0.10 × 0.04	0.20 × 0.20 × 0.20
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38100, 6312, 5972	16711, 6742, 6649	9544, 3795, 3739	16818, 3828, 3818	15833, 3844, 3284	12387, 4037, 3378	7328, 4306, 3753	9282, 3675, 3589	21842, 11829, 11807	24231, 9684, 9586	25609, 25609, 24126	13534, 3450, 2883
R_{int}	0.048	0.019	0.025	0.019	0.079	0.040	0.040	0.014	0.023	0.018	0.05	0.037
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.119, 1.04	0.035, 0.095, 1.06	0.035, 0.092, 1.03	0.024, 0.063, 1.08	0.065, 0.116, 1.12	0.043, 0.093, 1.06	0.045, 0.096, 1.04	0.031, 0.083, 1.06	0.039, 0.106, 1.04	0.032, 0.086, 1.08	0.040, 0.109, 1.05	0.038, 0.094, 1.05
No. of parameters	471	527	265	274	273	307	325	262	1087	586	1300	271
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, -0.25	0.33, -0.26	0.12, -0.17	0.14, -0.19	0.24, -0.24	0.20, -0.20	0.16, -0.21	0.13, -0.15	0. 34, -0.22	0.24, -0.20	0.33, -0.17	0.21, -0.23
Absolute structure parameter	---	0.07 (5)	-0.04 (11)	-0.03 (4)	0.09 (9)	0.2 (8)	0.2 (10)	0.05 (6)	0.08 (10)	0.00 (7)	-0.07 (10)	---

Single crystal X-ray investigations

Crystal data for 1: $C_{22}H_{19}NO_3$, M_r = 345.38, T = 294 K, colourless needle, 0.60 x 0.08 x 0.08 mm, triclinic, space group *P*-1, a = 8.9568(1), b = 10.4462(2), c = 19.2221(3) Å, α = 95.594(2), β = 91.222(1), γ = 92.512(2)°, V = 1787.63(5) Å^3, Z = 4, ρ_{calcd} = 1.283 Mgm^{-3}, $Cu_{K\alpha}$ (λ = 1.54178 Å, ω-scan), μ = 0.69 mm^{-1}, 38100 reflections collected, 6312 unique (R_{int} = 0.048) and 5972 considered as observed with I>2σ(I), theta range 2.3 to 76.2°, no. of parameters 471, Δ_{max} = 0.28, Δ_{min} = -0.25 eÅ^{-3}, R_1 = 0.043, wR_2 = 0.119.

Crystal data for 2a: $C_{23}H_{21}NO_3$, M_r = 359.41, T = 130 K, colourless plate, 0.20 x 0.20 x 0.05 mm, monoclinic, space group $P2_1$, a = 13.1517(2), b = 9.5286(1), c = 15.2352(2) Å, β = 91.793(1)°, V = 1908.30(4) Å^3, Z = 4, ρ_{calcd} = 1.251 Mgm^{-3}, $Cu_{K\alpha}$ (λ = 1.54178 Å, ω-scan), μ = 0.66 mm^{-1}, 16711 reflections collected, 6742 unique (R_{int} = 0.019) and 6649 considered as observed with I>2σ(I), theta range 2.9 to 76.2°, no. of parameters: 527, Δ_{max} = 0.33, Δ_{min} = -0.26 eÅ^{-3}, R_1 = 0.035, wR_2 = 0.095.

Crystal data for 3a: $C_{25}H_{25}NO_3$, M_r = 387.46, T = 291 K, colourless block, 0.4 x 0.1 x 0.1 mm, monoclinic, space group $P2_1$, a = 8.5896(1), b = 9.9657(1), c = 12.7116(2) Å, β = 94.914(1)°, V = 1084.13(2) Å^3, Z = 2, ρ_{calcd} = 1.187 Mgm^{-3},$Cu_{K\alpha}$ (λ = 1.54178 Å, ω-scan), μ = 0.62 mm^{-1}, 9544 reflections collected, 3795 unique (R_{int} = 0.025) and 3739 considered as observed with I>2σ(I), theta range 5.2 to 76.2°, no. of parameters: 265, Δ_{max} = 0.12, Δ_{min} = -0.17 eÅ^{-3}, R_1 = 0.035, wR_2 = 0.092.

Crystal data for 4a: $C_{26}H_{27}NO_3$, M_r = 401.48, T = 130 K, colourless plate, 0.40 x 0.20 x 0.10 mm, monoclinic, space group $P2_1$, a = 8.5012(1), b = 9.8952(1), c = 12.8936(2) Å, β = 92.270(1)°, V = 1083.77(2) Å^3, Z = 2, ρ_{calcd} = 1.230 Mgm^{-3}, $Cu_{K\alpha}$ (λ = 1.54178 Å, ω-scan), μ = 0.64 mm^{-1}, 16818 reflections collected, 3828 unique (R_{int} = 0.019) and 3818 considered as observed with I>2σ(I), theta range 3.4 to 76.4°, no. of parameters: 274, Δ_{max} = 0.14, Δ_{min} = -0.19 eÅ^{-3}, R_1 = 0.024, wR_2 = 0.063.

Crystal data for 7: $C_{25}H_{25}NO_3S$, M_r = 419.52, T = 100 K, colourless plate, 0.40 x 0.20 x 0.10 mm, tetragonal, space group $P4_32_12$, a = b = 8.9410(2), c = 54.361(2) Å, V = 4345.7(3) Å^3, Z = 8, ρ_{calcd} = 1.282 Mgm^{-3}, $Mo_{K\alpha}$ (λ = 0.71073 Å, ω-scan), μ = 0.18 mm^{-1}, 15833 reflections collected, 3844 unique (R_{int} = 0.079) and 3284 considered as observed with I>2σ(I), theta range 3.2 to 25.2°, no. of parameters: 273, Δ_{max} = 0.24, Δ_{min} = -0.24 eÅ^{-3}, R_1 = 0.065, wR_2 = 0.116.

Crystal data for 11: $C_{29}H_{25}NO_4$, M_r = 451.50, T = 100 K, colourless block, 0.60 x 0.20 x 0.10 mm, orthorhombic, space group $P2_12_12_1$, a = 9.1939(4), b = 10.3126(4), c = 24.1891(8) Å, V = 2293.44(15) Å^3, Z = 4, ρ_{calcd} = 1.308 Mgm^{-3}, $Mo_{K\alpha}$ (λ = 0.71073 Å, ω-scan), μ = 0.09 mm^{-1}, 12387 reflections collected, 4037 unique (R_{int} = 0.040) and 3378 considered as observed with I>2σ(I), theta range 3.2 to 27.0°, no. of parameters: 307, Δ_{max} = 0.20, Δ_{min} = -0.20 eÅ^{-3}, R_1 = 0.043, wR_2 = 0.093.

Crystal data for 12: $C_{31}H_{26}N_2O_3$, M_r = 474.54, T = 100 K, colourless block, 0.40 x 0.20 x 0.20 mm, monoclinic, space group $P2_1$, a = 9.7079(12), b = 9.4265(8), c = 13.9926(13) Å, β = 107.665(12)°, V = 1220.1(2) Å^3, Z = 2, ρ_{calcd} = 1.292 Mgm^{-3}, $Mo_{K\alpha}$ (λ = 0.71073 Å, ω-scan), μ = 0.08 mm^{-1}, 7328 reflections collected, 4306 unique (R_{int} = 0.040) and 3753 considered as observed with I>2σ(I), theta range 3.1 to 26.9°, no. of parameters: 325, Δ_{max} = 0.16, Δ_{min} = -0.21 eÅ^{-3}, R_1 = 0.045, wR_2 = 0.096.

Crystal data for 13a: $C_{25}H_{23}NO_3$, M_r = 385.44, T = 294 K, colourless block, 0.50 x 0.15 x 0.05 mm, orthorhombic, space group $P2_12_12$, a = 14.3139(2), b = 15.9294(2), c = 9.1186(1), V = 2079.15(5) Å^3, Z = 4, ρ_{calcd} = 1.231 Mgm^{-3}, $Cu_{K\alpha}$ (λ = 1.54184 Å, ω-scan), μ = 0.64 mm^{-1}, 9282 reflections collected, 3675 unique (R_{int} = 0.014) and 3589 considered as observed with I>2σ(I), theta range 2.8 to 76.3°, no. of parameters: 262, Δ_{max} = 0.13, Δ_{min} = -0.15 eÅ^{-3}, R_1 = 0.031, wR_2 = 0.083.

Crystal data for 13b: $C_{26}H_{25}NO_3$, M_r = 399.47, T = 130 K, colourless block, 0.50 x 0.20 x 0.05 mm, monoclinic, space group $P2_1$, a = 9.1720(2), b = 32.8820(5), c = 13.5380(3), β = 90.126(2)°, V = 4082.97(14) Å^3, Z = 8, ρ_{calcd} = 1.300 Mgm^{-3}, $Cu_{K\alpha}$ (λ = 1.54184

Å, ω-scan), μ = 0.67 mm^{-1}, 21842 reflections collected, 11829 unique (R_{int} = 0.023) and 11807 considered as observed with I>2σ(I), theta range 3.3 to 76.4°, no. of parameters: 1087, Δ_{max} = 0.34, Δ_{min} = -0.22 eÅ^{-3}, R_1 = 0.039, wR_2 = 0.105.

Crystal data for 15: $C_{28}H_{32}N_2O_2$, M_r = 428.55, T = 130 K, colourless plate, 0.10 x 0.10 x 0.05 mm, triclinic, space group *P*1, *a* = 9.8268(2), *b* = 10.7524(2), *c* = 12.3034(3) Å, *α* = 104.385(2), *β* = 99.112(2), *γ* = 92.482(2)°, *V* = 1238.70(5) Å^3, *Z* = 2, ρ_{calcd} = 1.149 Mgm^{-3}, $Cu_{K\alpha}$ (λ = 1.54178 Å, ω-scan), μ = 0.56 mm^{-1}, 24231 reflections collected, 9684 unique (R_{int} = 0.018) and 9586 considered as observed with I>2σ(I), theta range 3.8 to 76.3°, no. of parameters: 586, Δ_{max} = 0.24, Δ_{min} = -0.21 Å^{-3}, R_1 = 0.032, wR_2 = 0.086.

Crystal data for 16: $C_{30}H_{34}N_2O_2$, M_r = 454.59, T = 130 K, colourless plate, 0.10 x 0.10 x 0.04 mm, triclinic, space group *P*1, *a* = 9.6669(3), *b* = 14.8741(6), *c* = 19.1839(6) Å, *α* = 86.367(4), *β* = 81.808(3), *γ* = 71.038(3)°, *V* = 2581.65(16) Å^3, *Z* = 4, ρ_{calcd} = 1.170 Mgm^{-3}, $Cu_{K\alpha}$ (λ = 1.54178 Å, ω-scan), μ = 0.57 mm^{-1}, 25609 reflections collected, 25609 unique (R_{int} = 0.05) and 24126 considered as observed with I>2σ(I), theta range 4.9 to 75.4°, no. of parameters: 1300, Δ_{max} = 0.33, Δ_{min} = -0.17 eÅ^{-3}, R_1 = 0.040, wR_2 = 0.109.

Crystal data for 17: $C_{24}H_{22}N_2O_4$, M_r = 402.43, T = 100 K, colourless block, 0.20 x 0.20 x 0.20 mm, monoclinic, space group $P2_1/c$, *a* = 13.3958(6), *b* = 9.2202(3), *c* = 16.7458(7), *β* = 108.447(5), *V* = 1962.03(15) Å^3, *Z* = 4, ρ_{calcd} = 1.362 Mgm^{-3}, $Mo_{K\alpha}$ (λ = 0.71073 Å, ω-scan), μ = 0.09 mm^{-1}, 13534 reflections collected, 3450 unique (R_{int} = 0.037) and 2883 considered as observed with I>2σ(I), theta range 3.2 to 28.3°, no. of parameters: 271, Δ_{max} = 0.21, Δ_{min} = -0.23 eÅ^{-3}, R_1 = 0.038, wR_2 = 0.094.

Reflection intensities for crystals **1**-**4a**, **13a**-**16** were measured on a SuperNova diffractometer equipped with a Cu microfocus source and 135 mm Atlas CCD. Diffraction data for **7-12** and **17** were measured with a Xcalibur kappa-geometry diffractometer and monochromated Mo Kα radiation. Data reduction and analysis for all structures were carried out with CrysAlisRED[9]. The structures were solved in SHELXT and refined with SHELXL from the SHELX-2014 package.[10-12] Non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed at calculated positions and refined using the riding model, and their isotropic displacement parameters were assigned a value 20% higher than the isotropic equivalent for the atom to which they were attached. Methyl hydrogen atoms were positioned using SHELXL HFIX 137 instruction. Where necessary, restraints for the 1,2- and 1,3-distances as well as the ADP restraint (SIMU) and rigid-bond restraint (DELU) were applied. In cases where the Flack parameter value[13] was meaningless, the absolute structure of the investigated crystals was assumed from the known absolute configurations of the compounds used in the syntheses. Crystals of **16** appeared to be twinned. The twinning matrix (100, 0-10, 00-1) corresponds to a rotation of 180° about the [100] direct lattice direction. Subsequent refinement indicated that the twin fraction of the second domain was 0.472(1). In structure of **2a** the carboxyl group disordered over two positions. The occupancies of the two positions were assigned as 0.84 and 0.16, respectively, summing up to the total occupancy of 1.0. In structure of **16** the position of the cyclohexyl and methyl groups display disorder over two positions. The occupancies of the two positions were assigned as 0.60 and 0.40, respectively, summing up to the total occupancy of 1.0. The absolute structures of the crystals were assumed from the known absolute configurations of the compounds used in the syntheses. The Mercury[14] program was used to prepare drawings. The CIFs files have been deposited with the Cambridge Crystallographic Data Centre (www.ccdc.cam.ac.uk, deposition numbers 1901218-1901229).

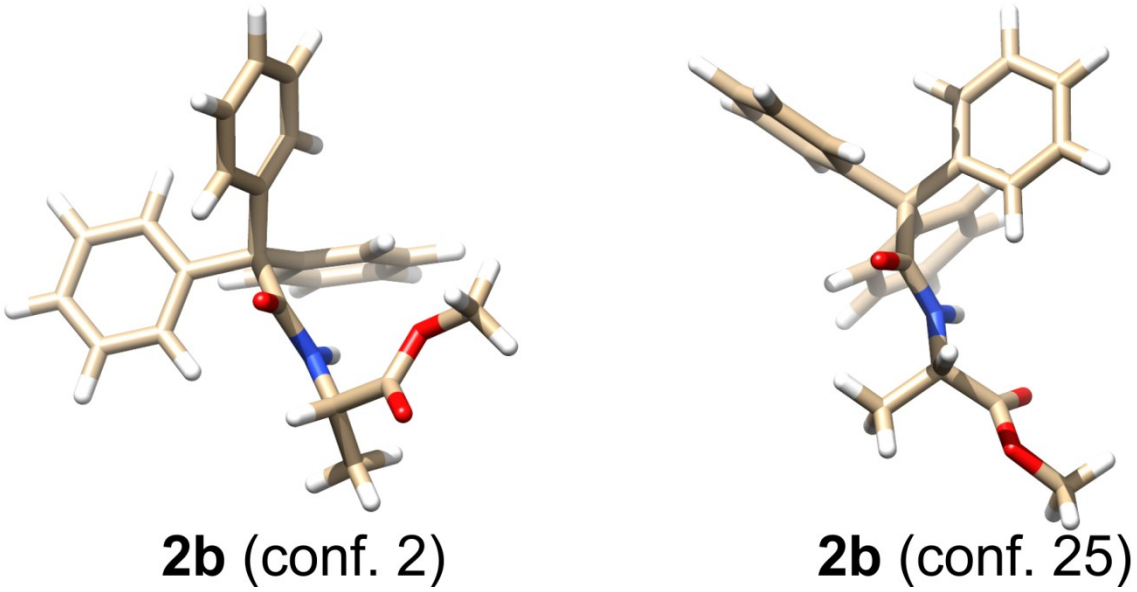


Fig. S1. Structures of individual, low-energy conformers of **2b**, calculated at the B3LYP/6-311++G(d,p) level of theory.

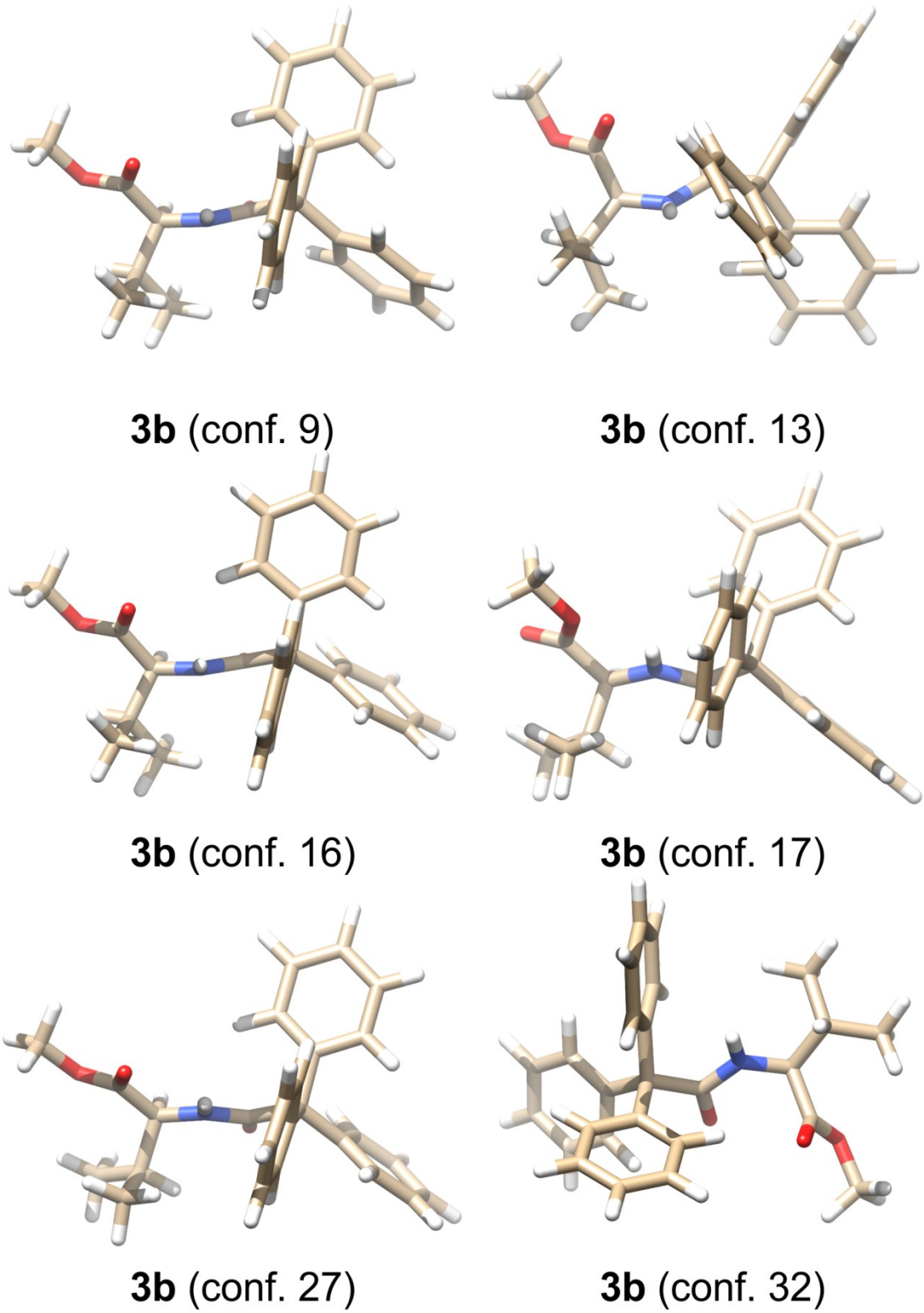


Fig. S2. Structures of individual, low-energy conformers of **3b**, calculated at the B3LYP/6-311++G(d,p) level of theory.

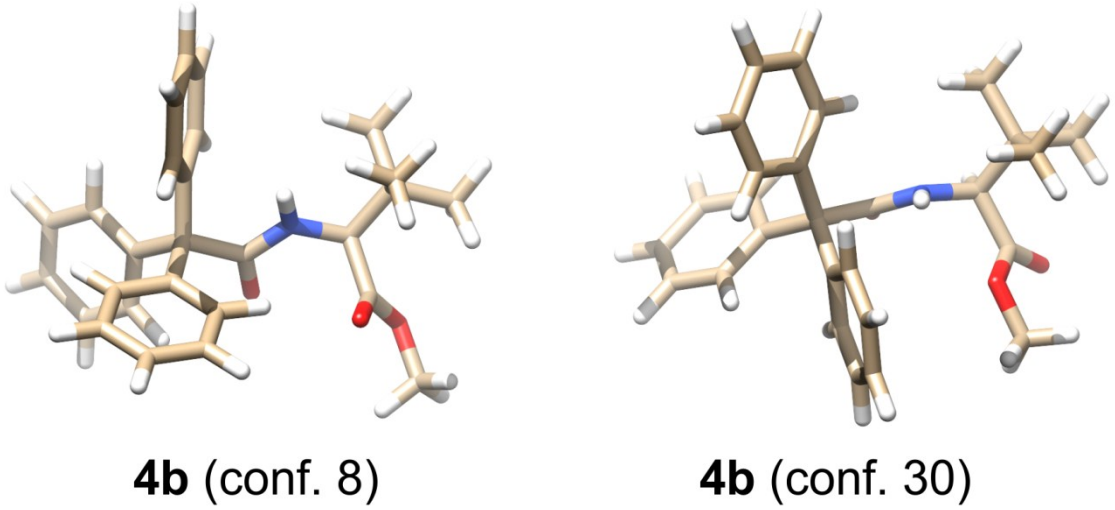


Fig. S3. Structures of individual, low-energy conformers of **4b**, calculated at the B3LYP/6-311++G(d,p) level of theory.

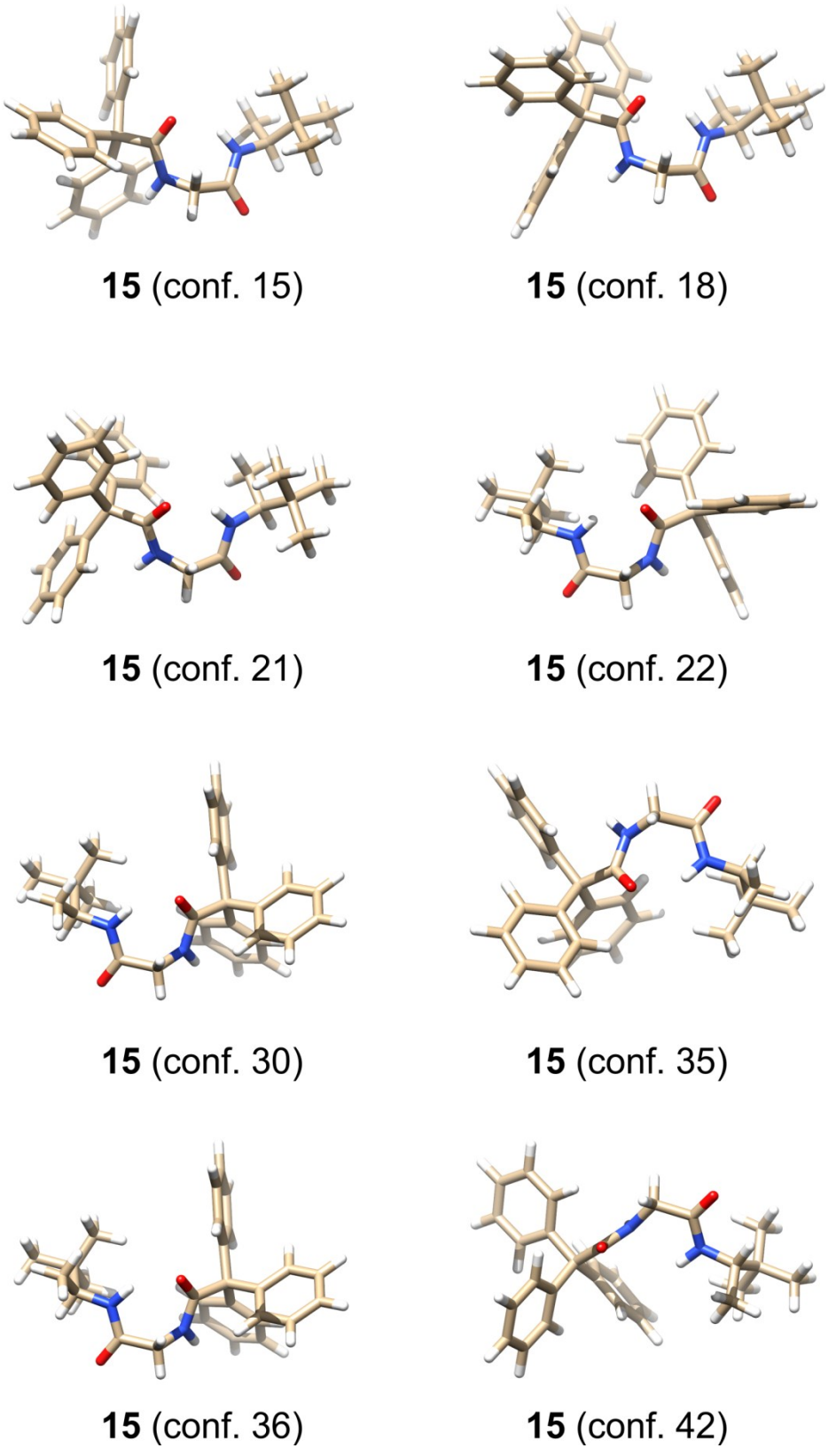


Fig. S4. Structures of individual, low-energy conformers of **15**, calculated at the B3LYP/6-311++G(d,p) level of theory.

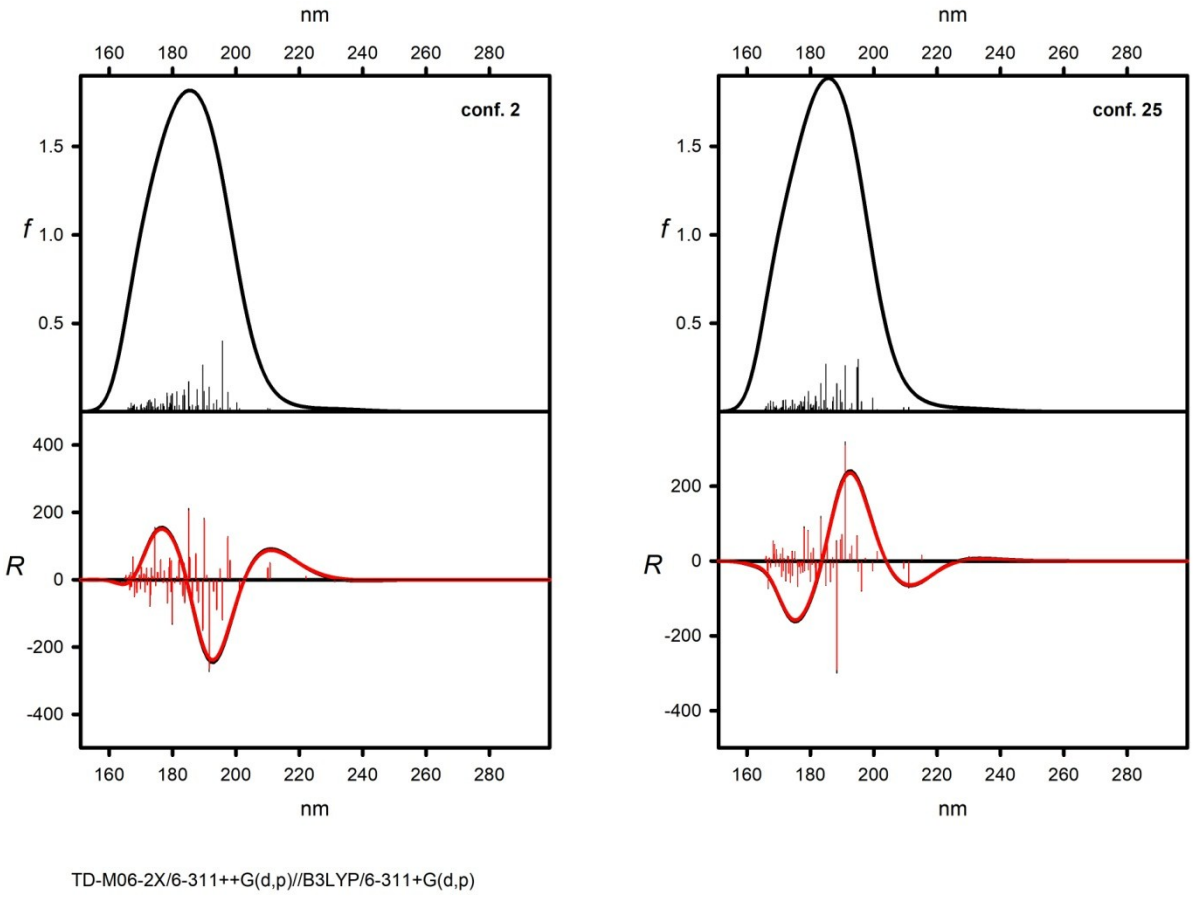


Fig. S5. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-M06-2X/6-311++G(d,p) level for individual conformers of **2b**. Wavelengths were not corrected.

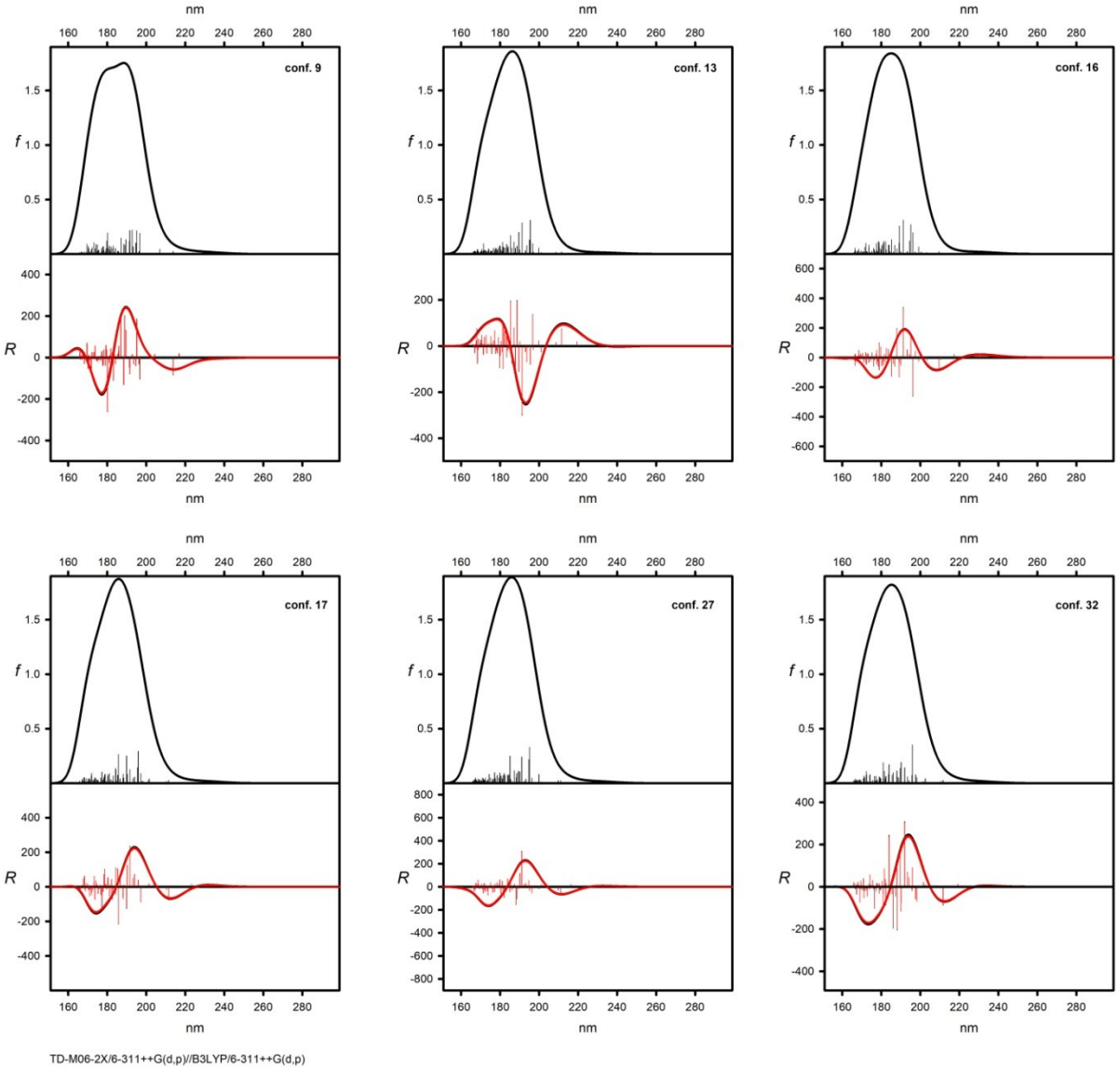


Fig. S6. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-M06-2X/6-311++G(d,p) level for individual conformers of **3b**. Wavelengths were not corrected.

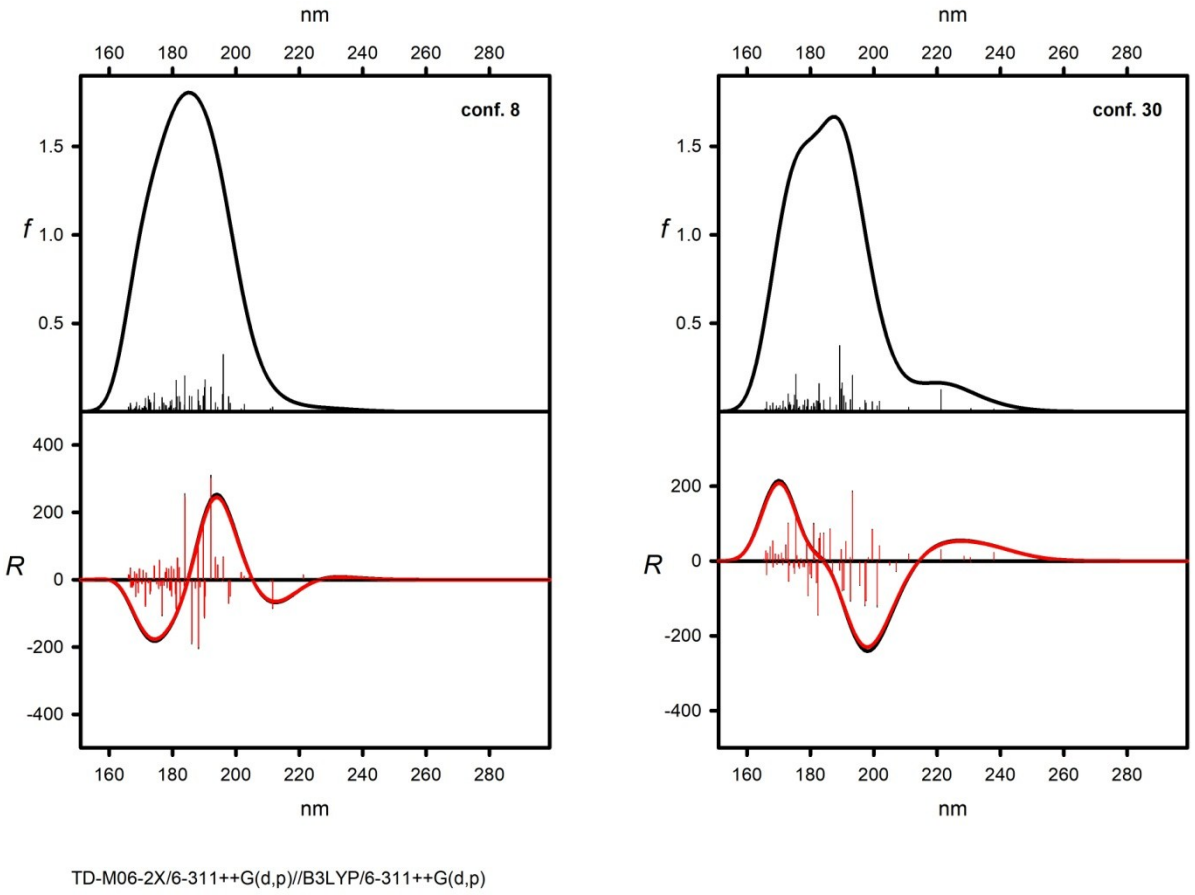
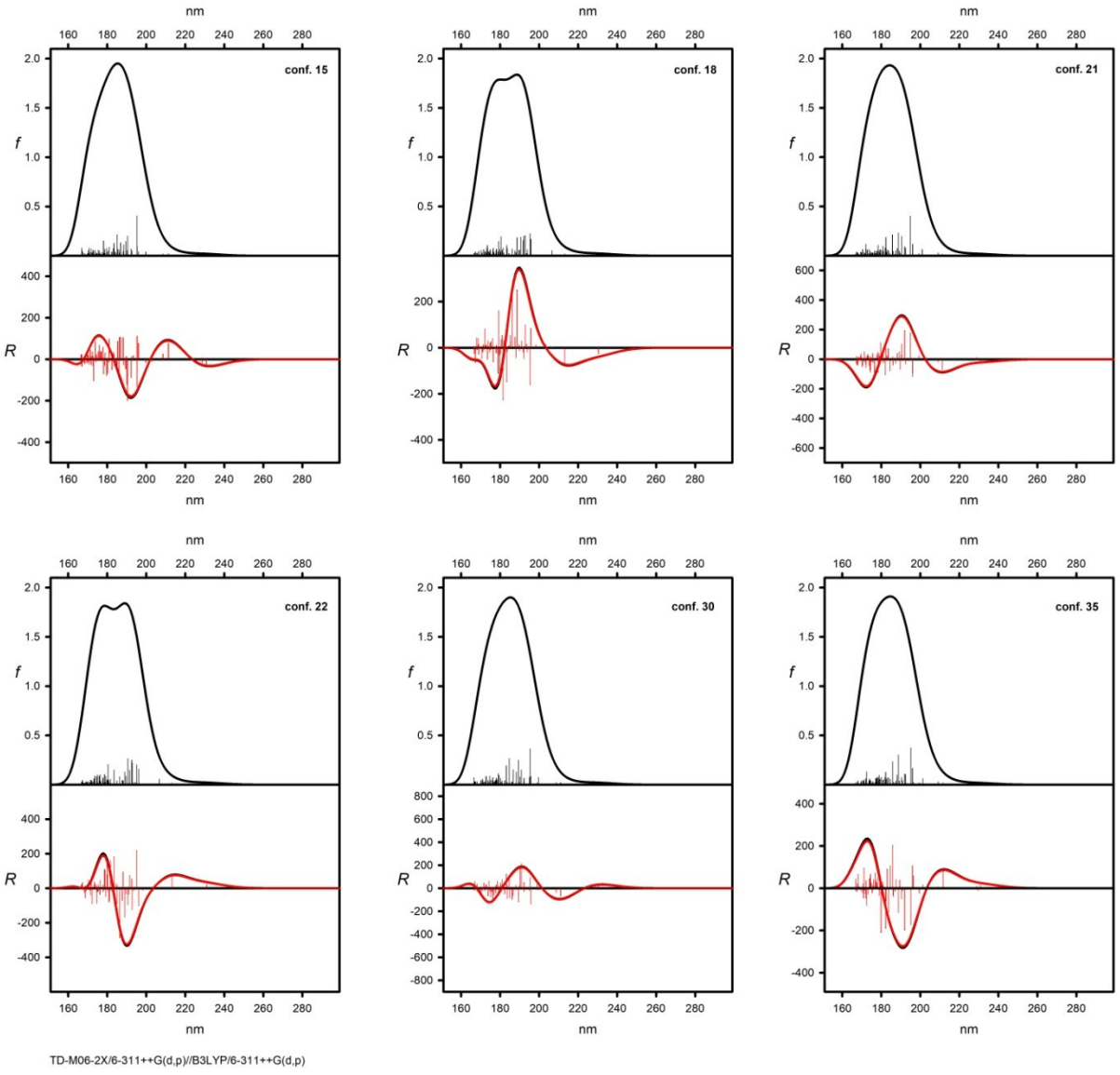


Fig. S7. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-M06-2X/6-311++G(d,p) level for individual conformers of **4b**. Wavelengths were not corrected.



TD-M06-2X/6-311++G(d,p)//B3LYP/6-311++G(d,p)

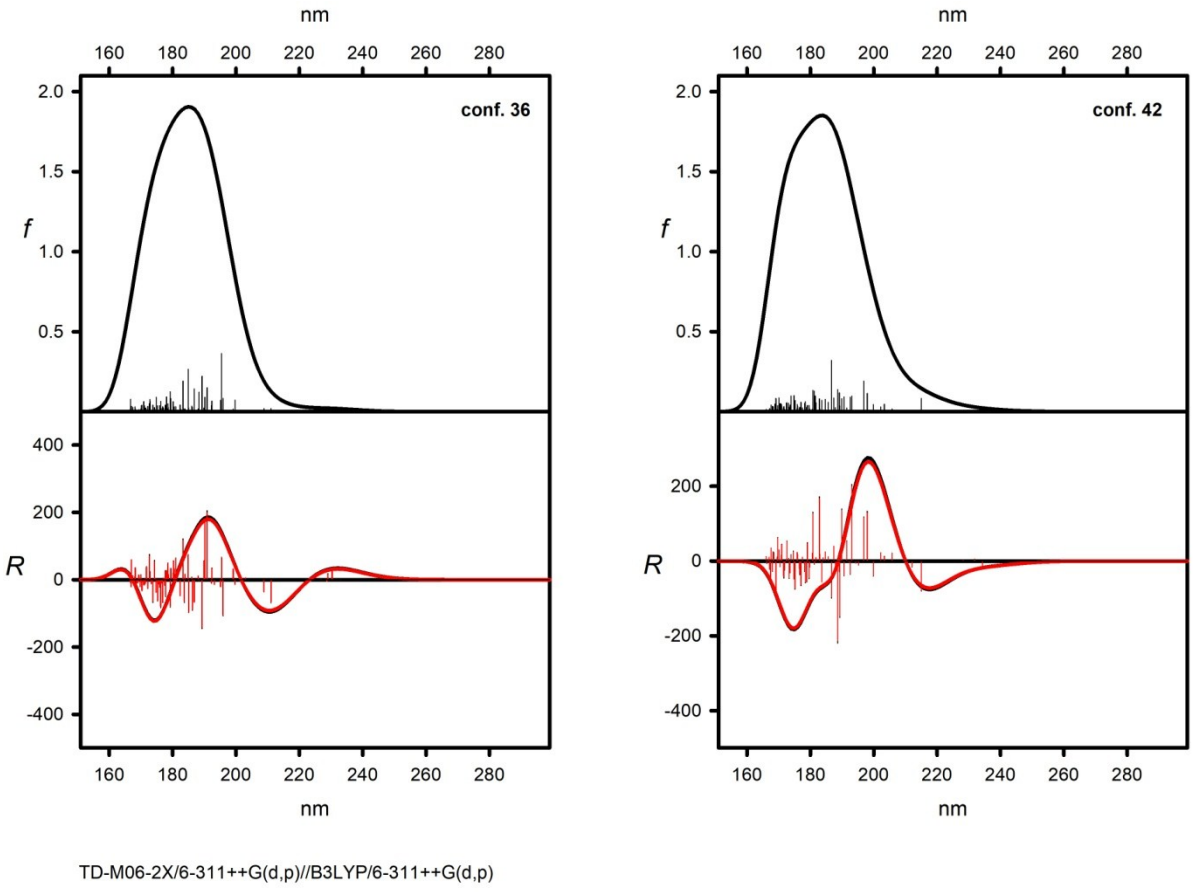


Fig. S8. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for individual conformers of **15**. Wavelengths were not corrected.

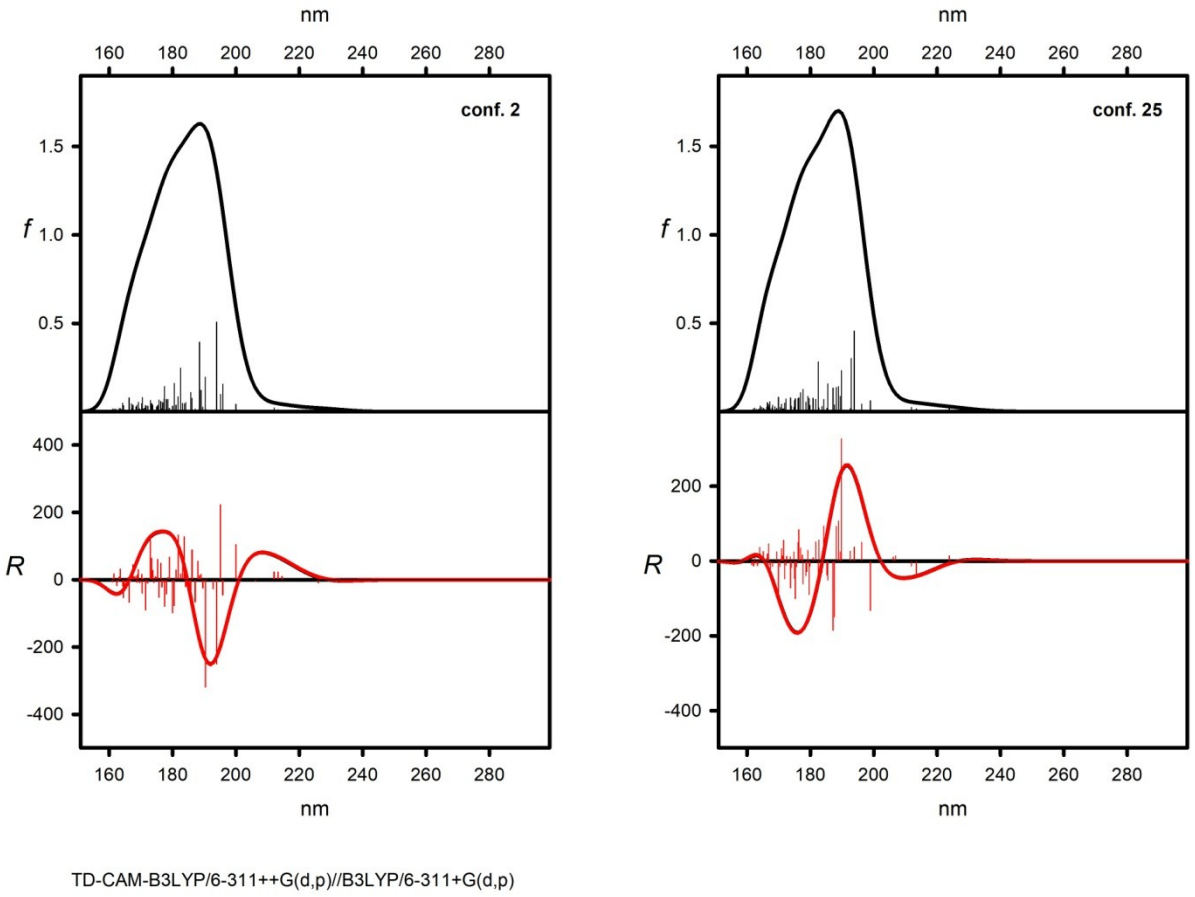


Fig. S9. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for individual conformers of **2b**. Wavelengths were not corrected.

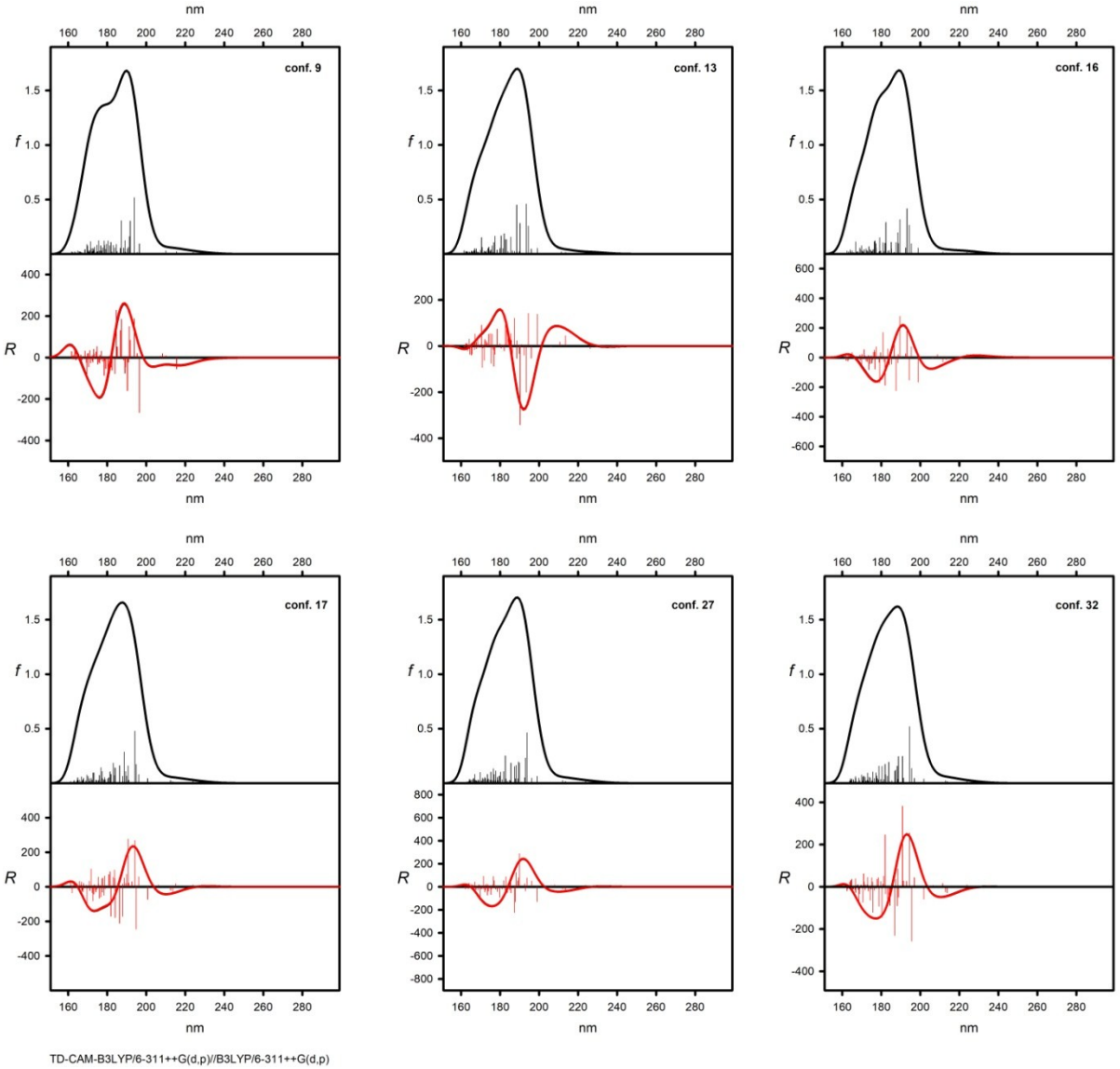


Fig. S10. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for individual conformers of **3b**. Wavelengths were not corrected.

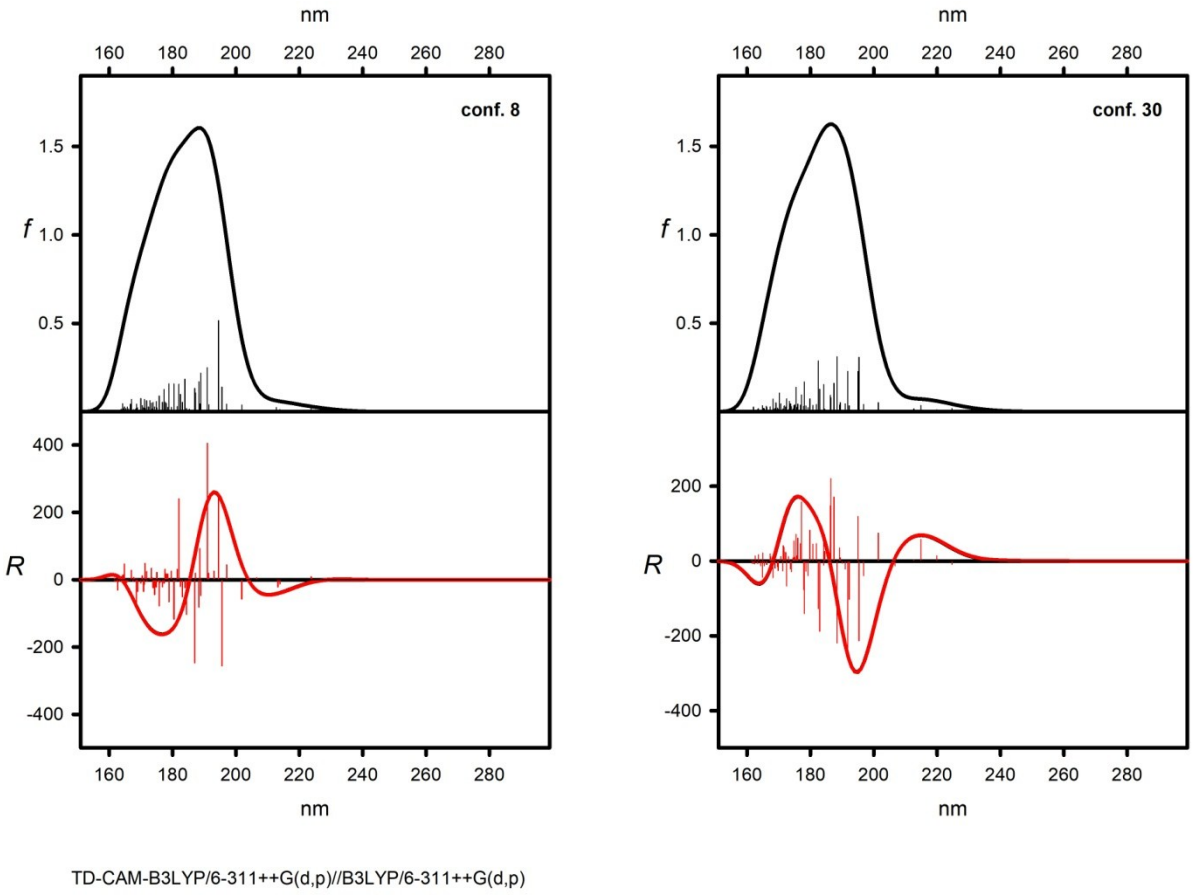
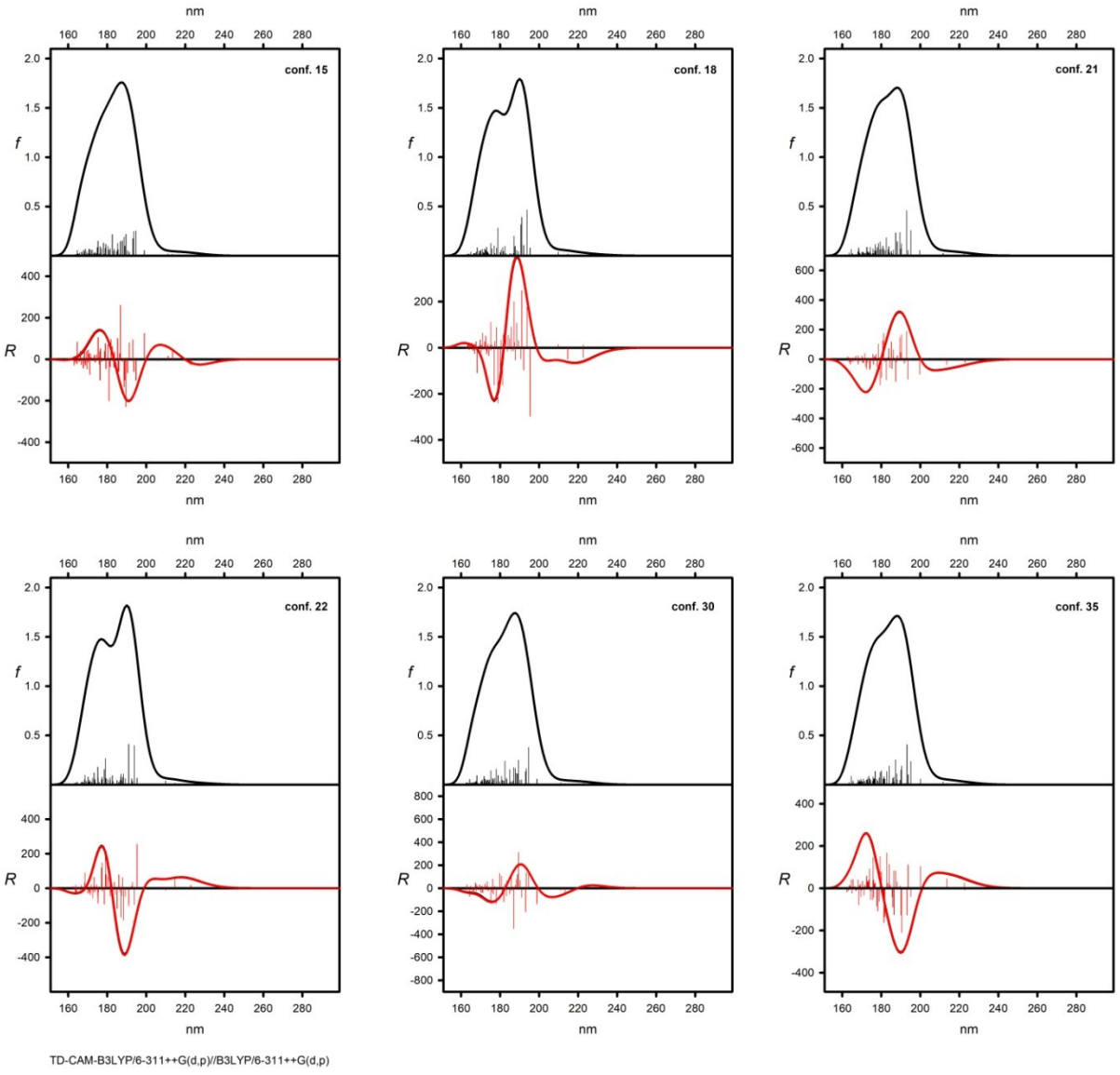


Fig. S11. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for individual conformers of **4b**. Wavelengths were not corrected.



TD-CAM-B3LYP/6-311++G(d,p)//B3LYP/6-311++G(d,p)

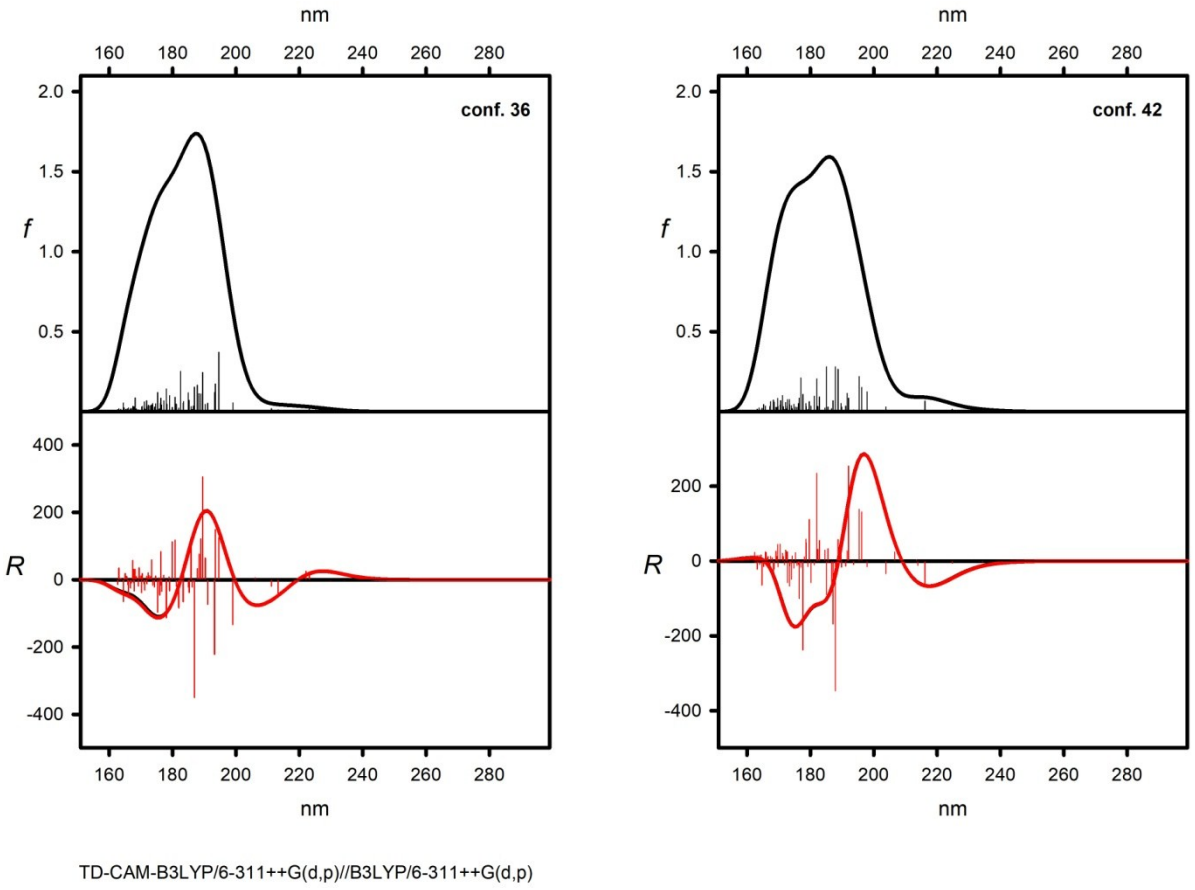


Fig. S12. UV (upper panels) and ECD (lower panels) spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for individual conformers of **15**. Wavelengths were not corrected.

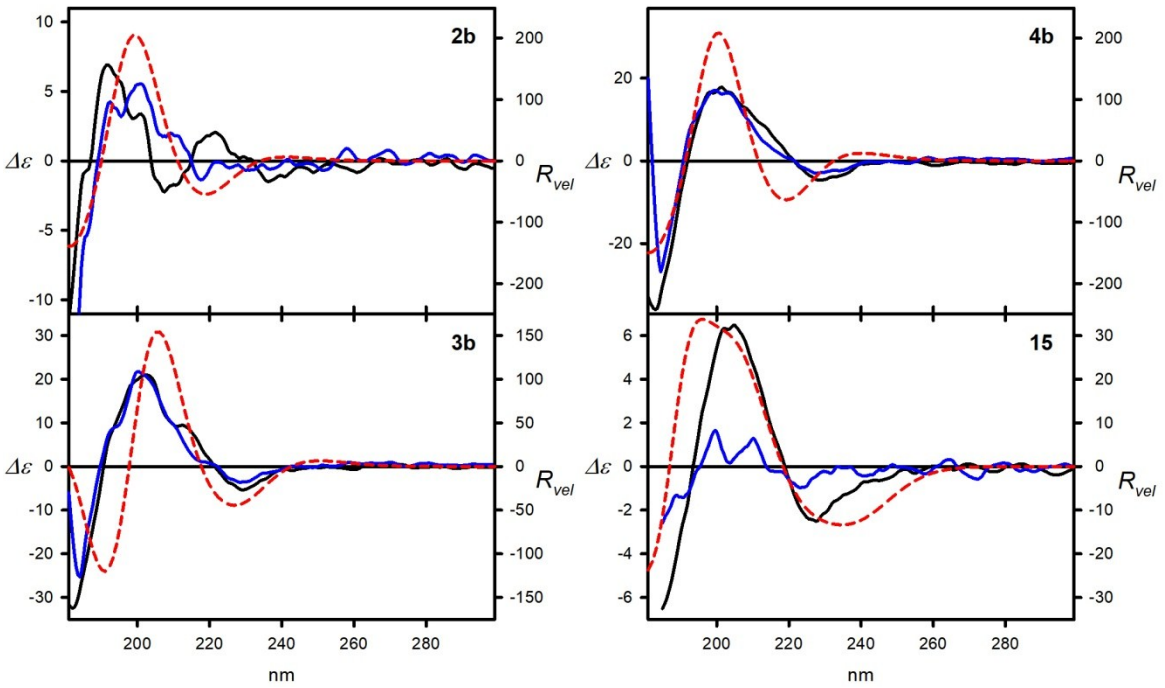


Fig. S13. Exemplary ECD spectra of amides **2b**, **3b**, **4b** and **15**, measured in cyclohexane (solid black lines), acetonitrile (solid blue line) and calculated at the TD-M06-2X/6-311++G(d,p) level for geometries optimized at the B3LYP/6-311++G(d,p) level (dashed red lines). The calculated ECD spectra were Boltzman-averaged based on *ΔΔG* values. Wavelengths were corrected to match experimental UV maxima.

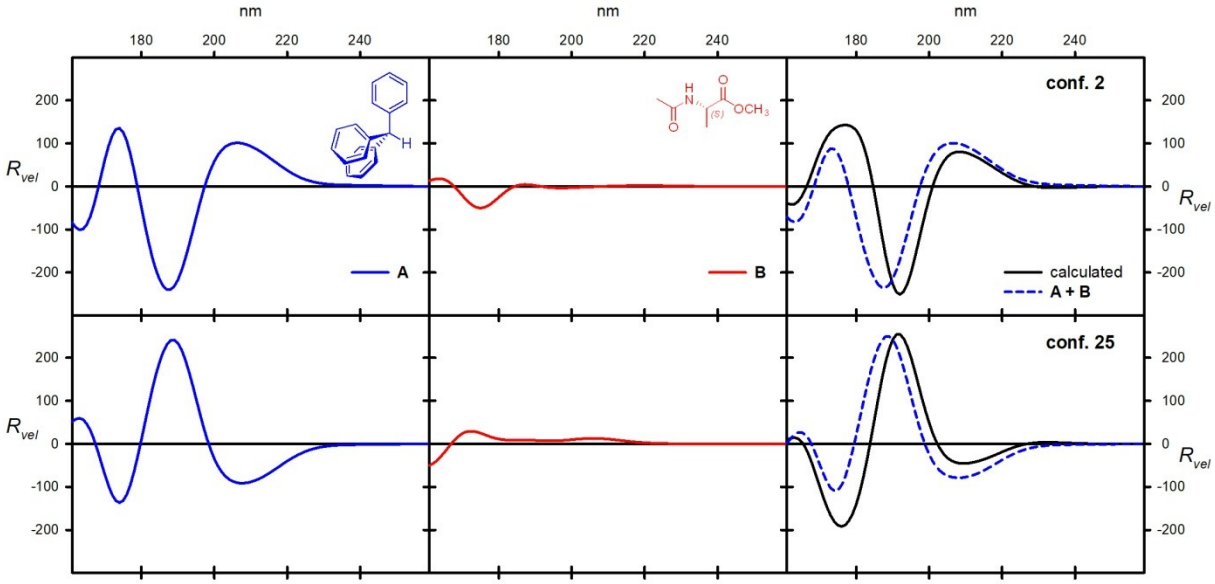
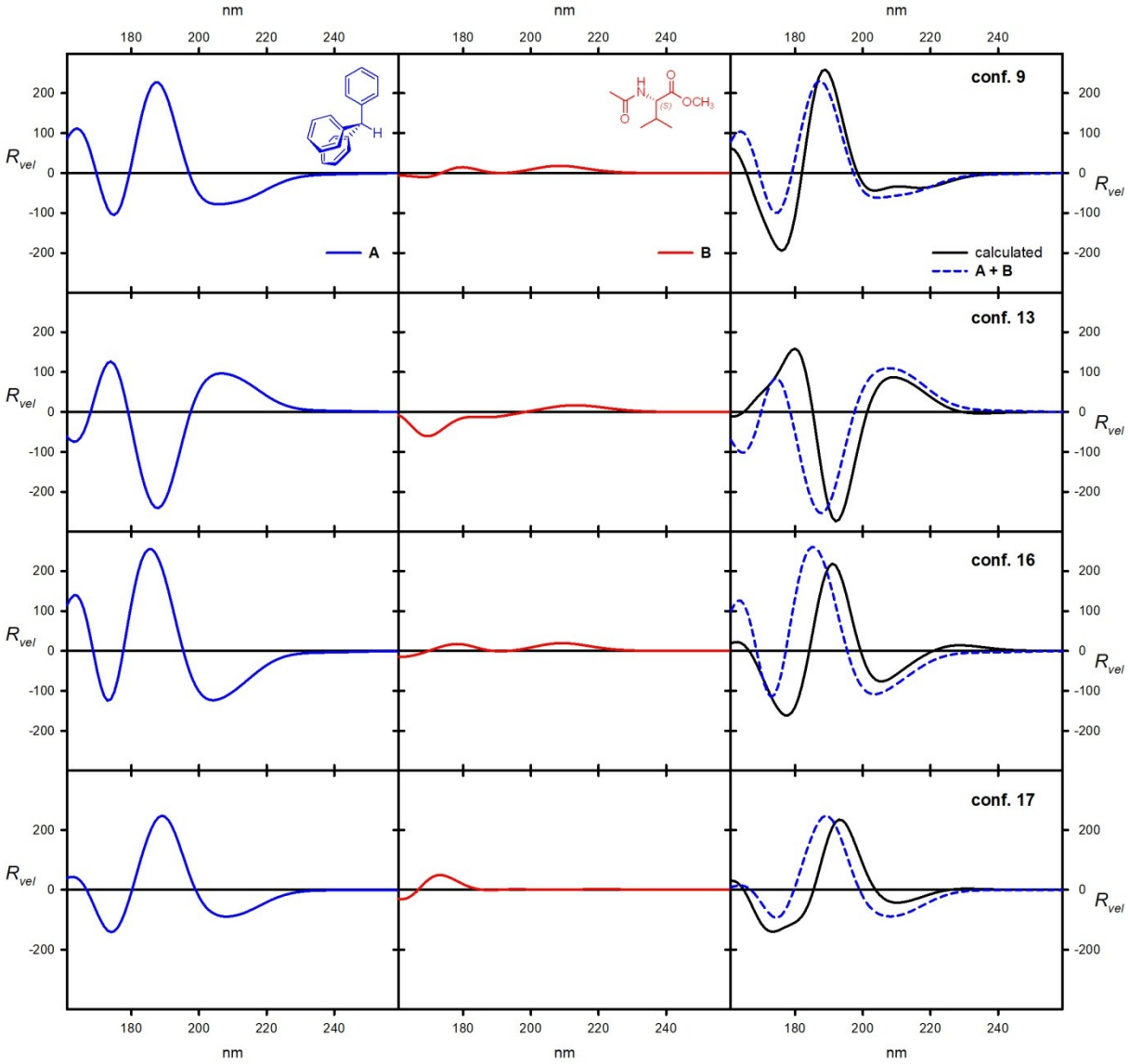


Fig. S14. ECD spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for the model compounds **A** (left column) and **B** (middle column) derived from low-energy conformers of amide **2b**. Last column shows effect of summation of ECD spectra of **A** and **B** (blue dashed lines) in comparison with ECD spectra calculated for a given low-energy conformer (black solid lines). Wavelengths were not corrected.


nm
180
200
220
240
R_{vel}
200
100
0
-100
-200
A
B
conf. 9
conf. 13
conf. 16
conf. 17
calculated
A + B

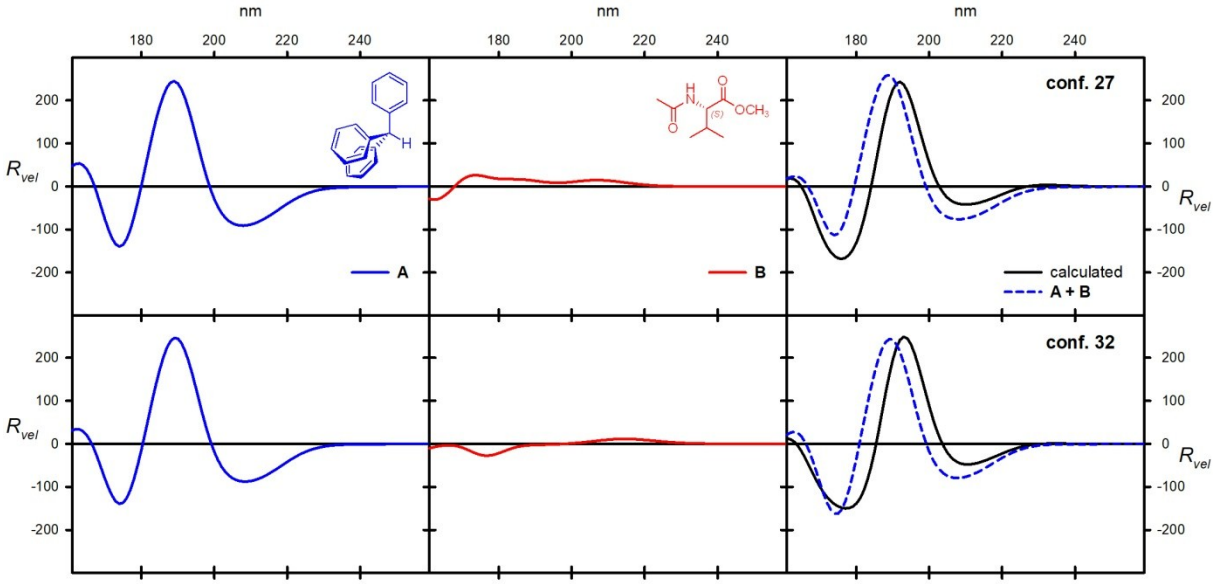


Fig. S15. ECD spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for the model compounds **A** (left column) and **B** (middle column) derived from low-energy conformers of amide **3b**. Last column shows effect of summation of ECD spectra of **A** and **B** (blue dashed lines) in comparison with ECD spectra calculated for a given low-energy conformer (black solid lines). Wavelengths were not corrected.

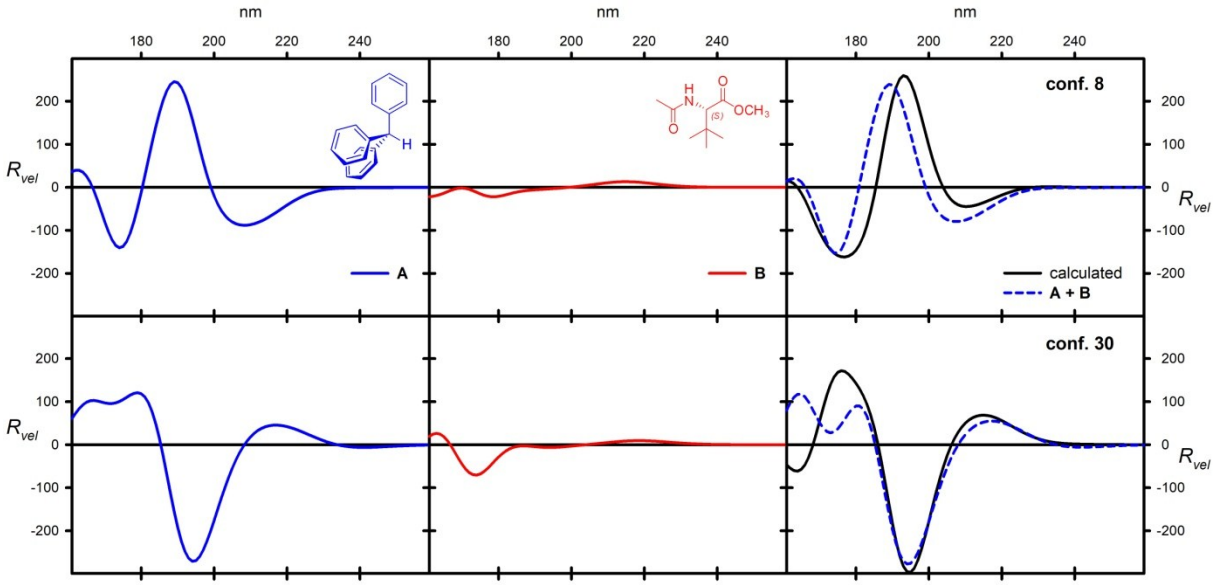
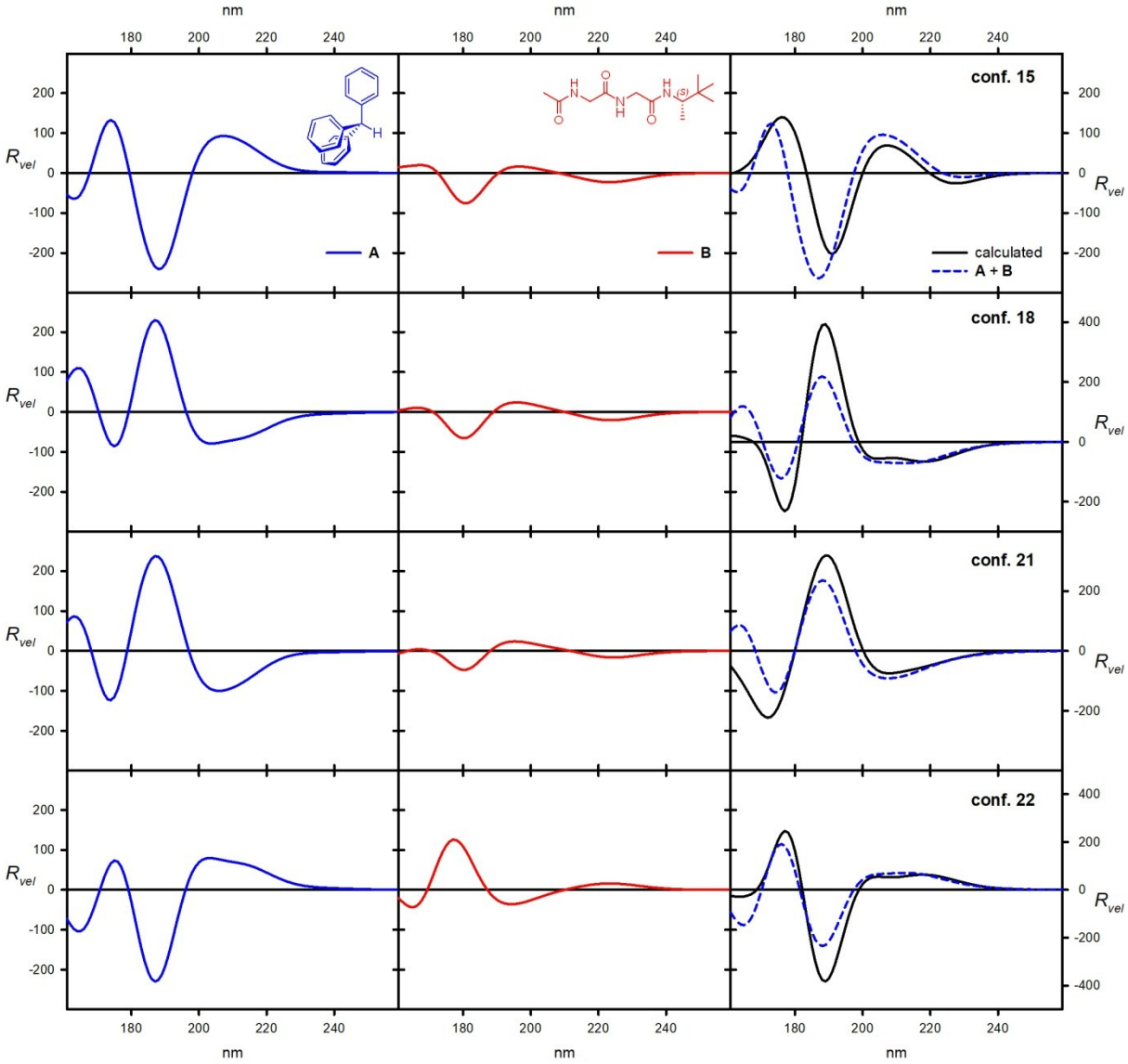


Fig. S16. ECD spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for the model compounds **A** (left column) and **B** (middle column) derived from low-energy conformers of amide **4b**. Last column shows effect of summation of ECD spectra of **A** and **B** (blue dashed lines) in comparison with ECD spectra calculated for a given low-energy conformer (black solid lines). Wavelengths were not corrected.


nm
180
200
220
240
R_{vel}
A
B
conf. 15
calculated
A + B
conf. 18
conf. 21
conf. 22

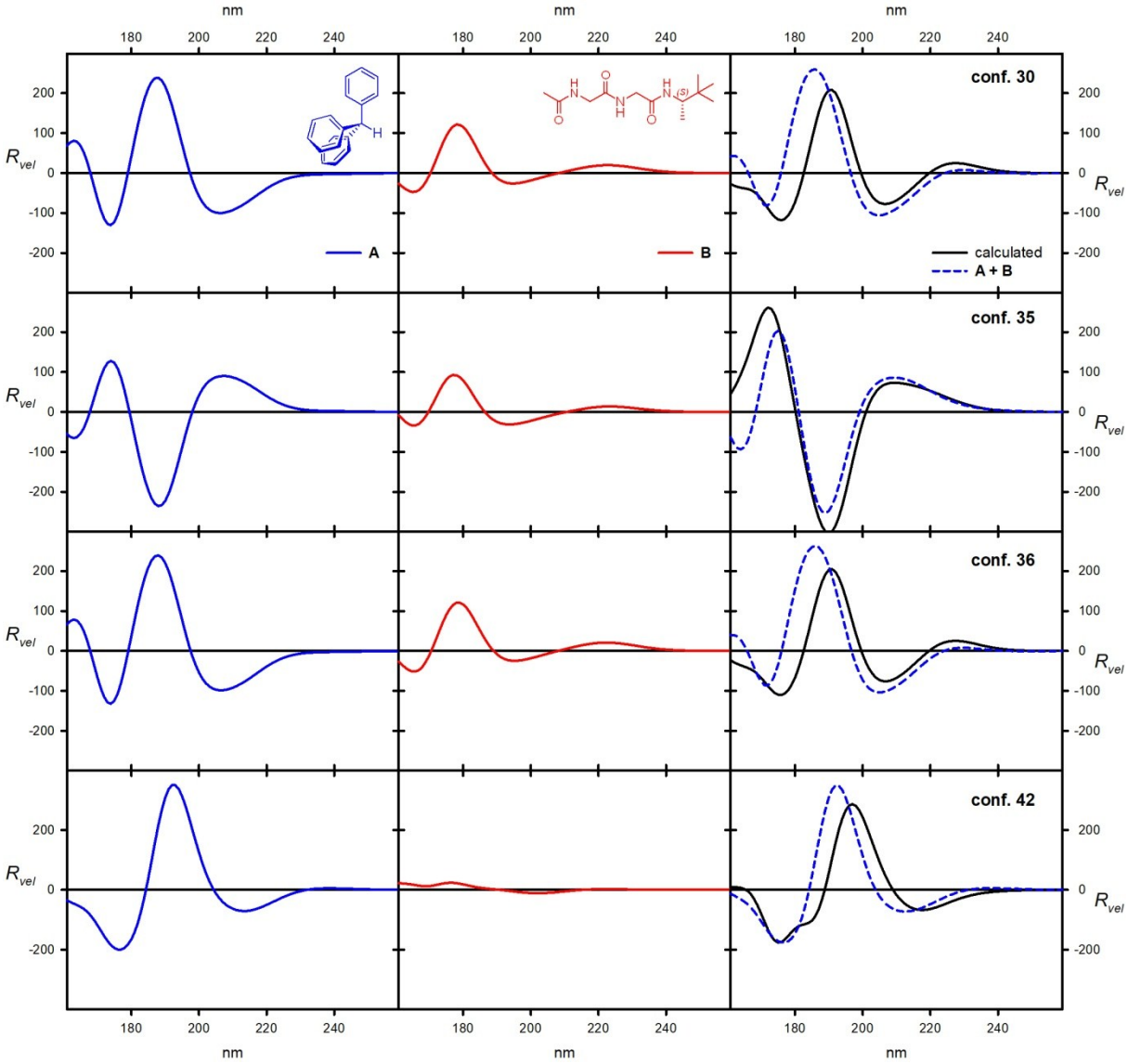
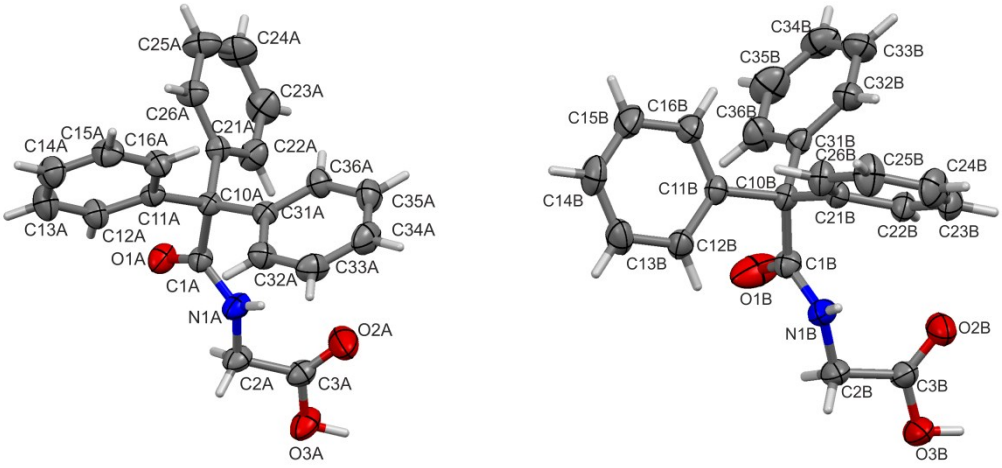


Fig. S17. ECD spectra calculated at the TD-CAM-B3LYP/6-311++G(d,p) level for the model compounds **A** (left column) and **B** (middle column) derived from low-energy conformers of amide **15**. Last column shows effect of summation of ECD spectra of **A** and **B** (blue dashed lines) in comparison with ECD spectra calculated for a given low-energy conformer (black solid lines). Wavelengths were not corrected.

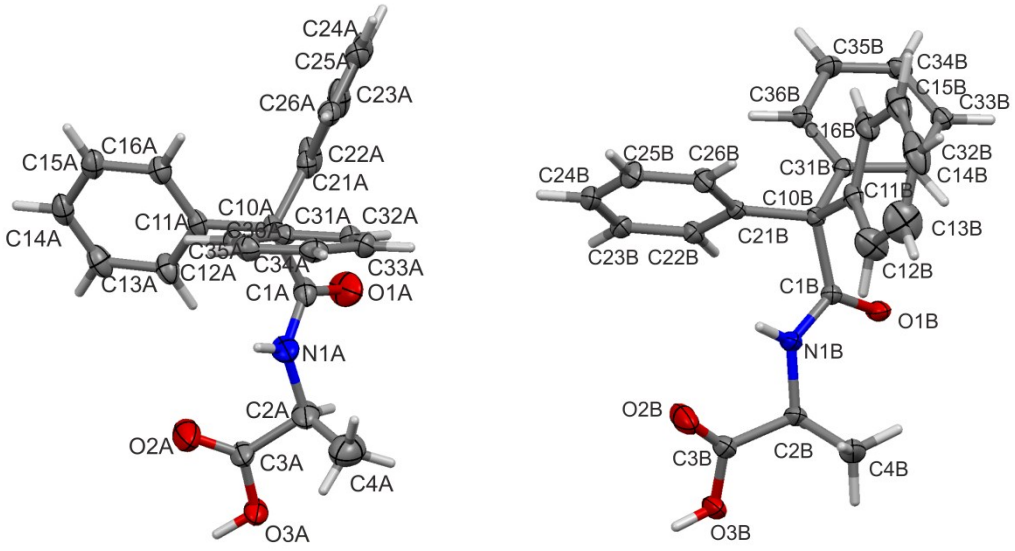
Figs S18 – S29. Perspective views of molecules **1**, **2a**, **3a**, **4a**, **7**, **11**, **12**, **13a**, **13b**, **15**, **16**, **17** as present in their crystal structures.

The phenyl groups constituting the trityl moiety were numbered, respectively, from C11 to C16, C21 to C26 and C31 to C36. For multiple asymmetric units the capital A, B, C and D letters, directly following the above numbers, distinguish the symmetry independent molecules.



mol A *mol B*

Fig. S18. Perspective view of molecule **1** from its crystal structure at 294 K (two independent molecules). Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.



mol A *mol B*

Fig. S19. Perspective view of molecule **2a** from its crystal structure at 130 K (two independent molecules). Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

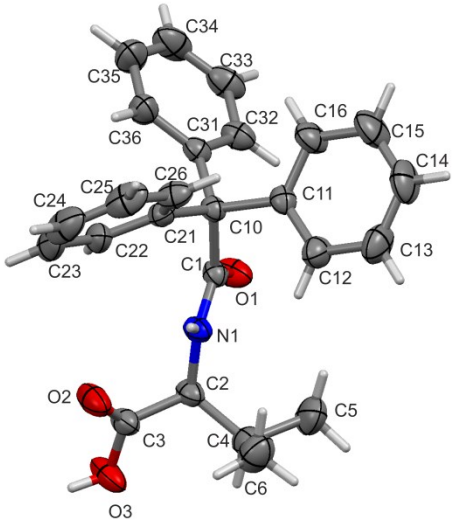


Fig. S20. Perspective view of molecule **3a** from its crystal structure at 291 K. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

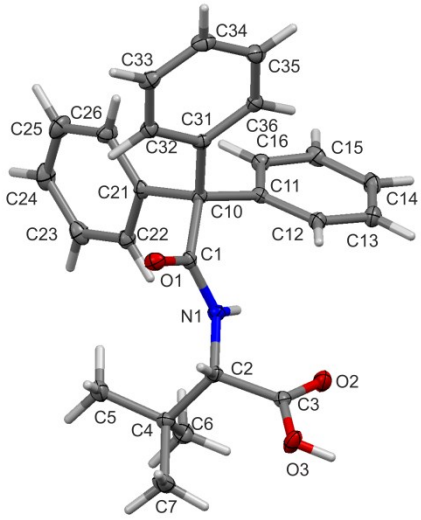


Fig. S21. Perspective view of molecule **4a** from its crystal structure at 130 K. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

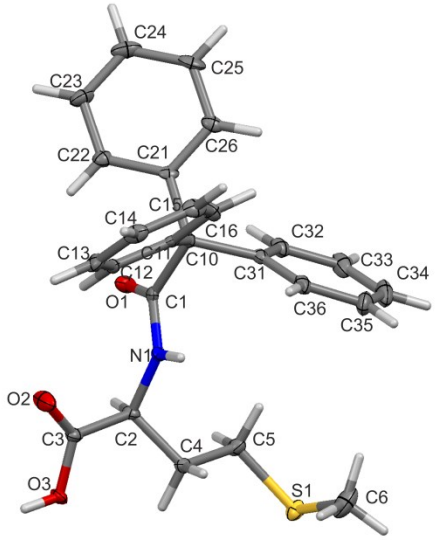


Fig. S22. Perspective view of molecule **7** from its crystal structure at 100 K. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

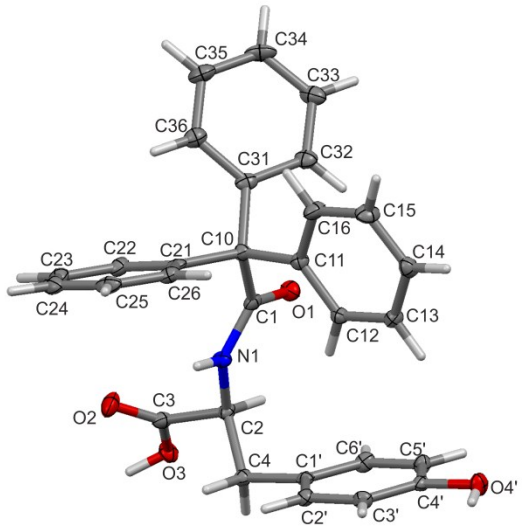


Fig. S23. Perspective view of molecule **11** from its crystal structure at 100 K. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

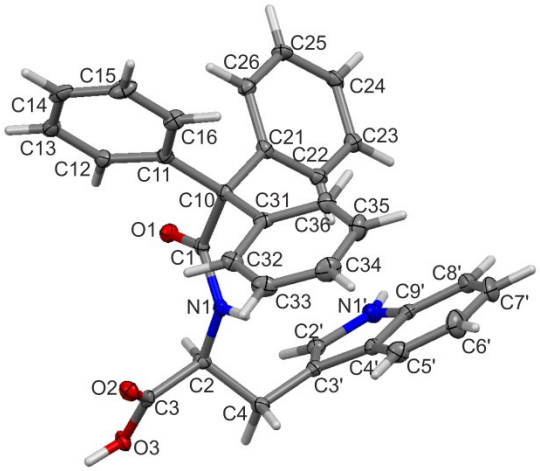


Fig. S24. Perspective view of molecule **12** from its crystal structure at 100 K. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

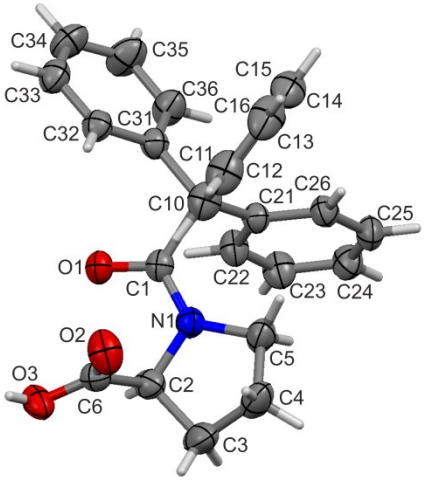
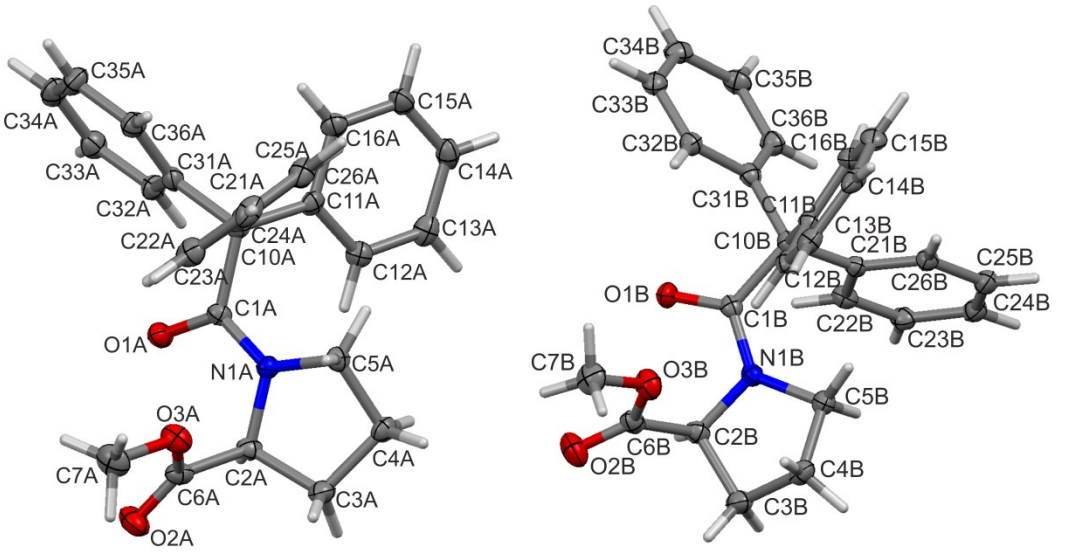
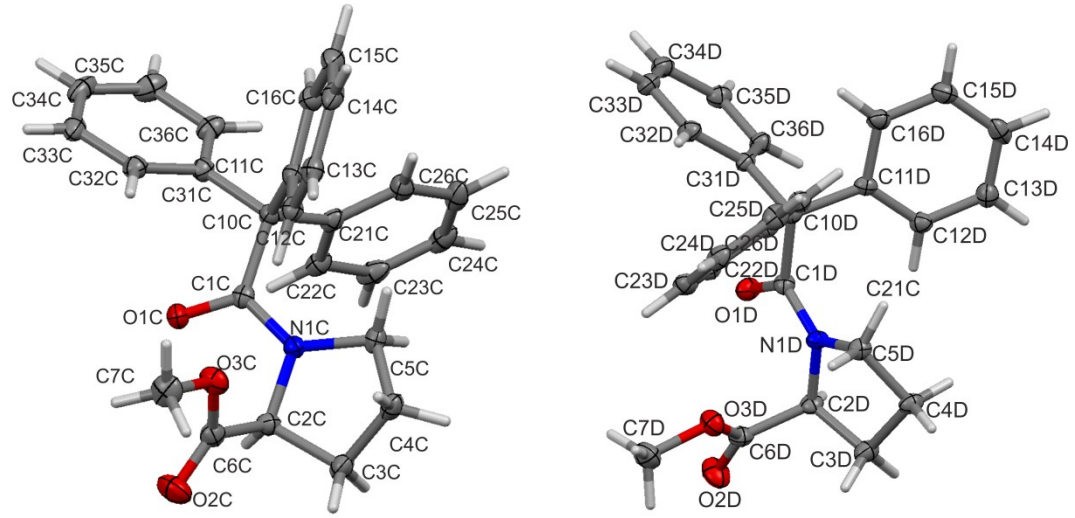


Fig. S25. Perspective view of molecule **13a** from its crystal structure at 294 K. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

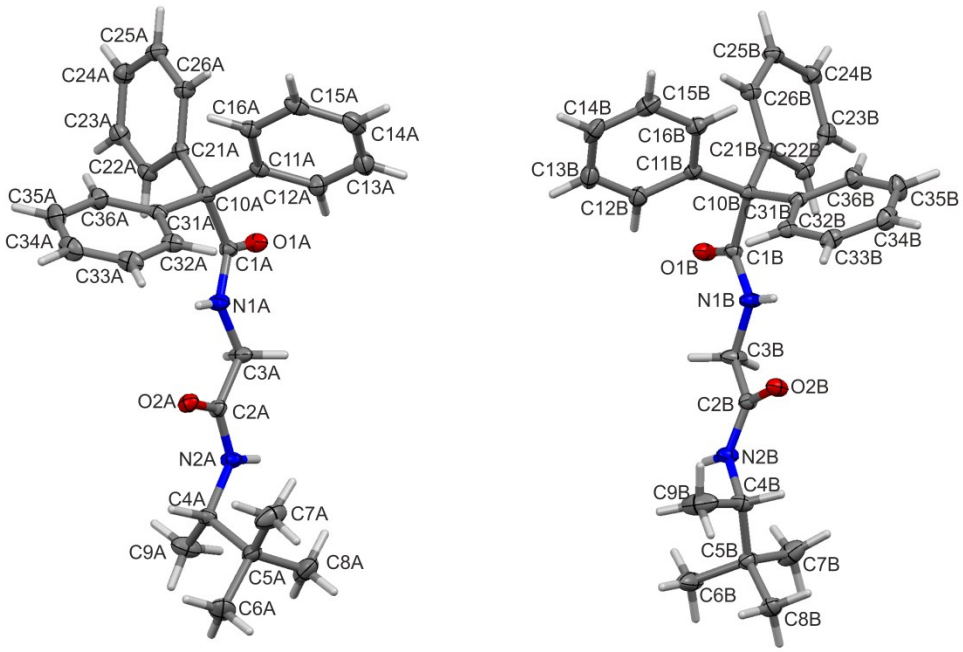


mol A *mol B*



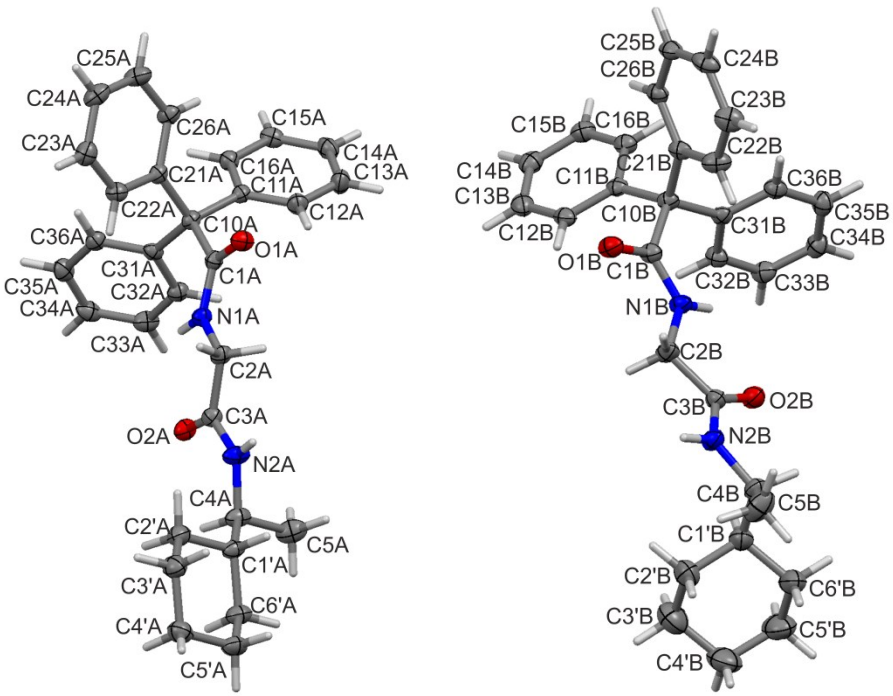
mol C *mol D*

Fig. S26. Perspective view of molecule **13b** from its crystal structure at 130 K (four independent molecules). Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

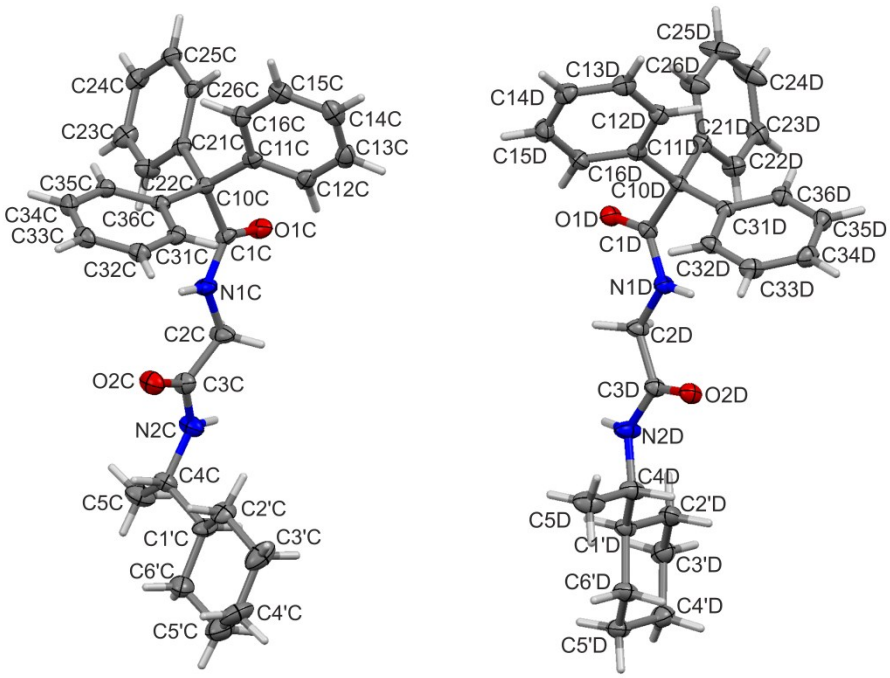


mol A *mol B*

Fig. S27. Perspective view of molecule **15** from its crystal structure at 130 K (two independent molecules). Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.



mol A *mol B*



mol C *mol D*

Fig

. S28. Perspective view of molecules **16** from its crystal structure at 130 K (four independent molecules). Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

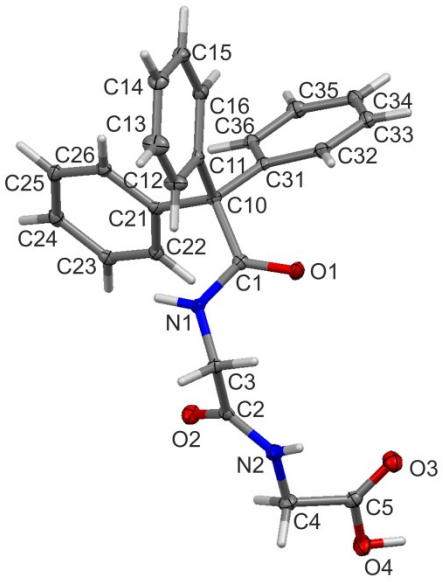
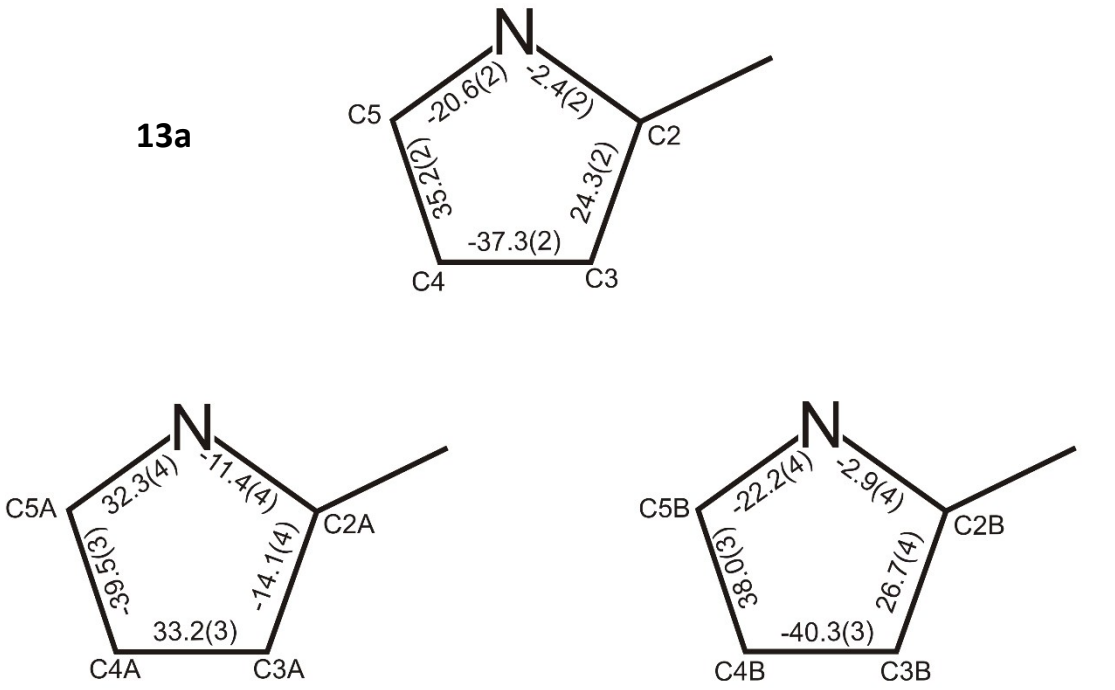


Fig. S29. Perspective view of molecule **17** from its crystal structure at 100 K. Ellipsoids are drawn at the 40% probability level, hydrogen atoms are represented by sticks.

13a



13b

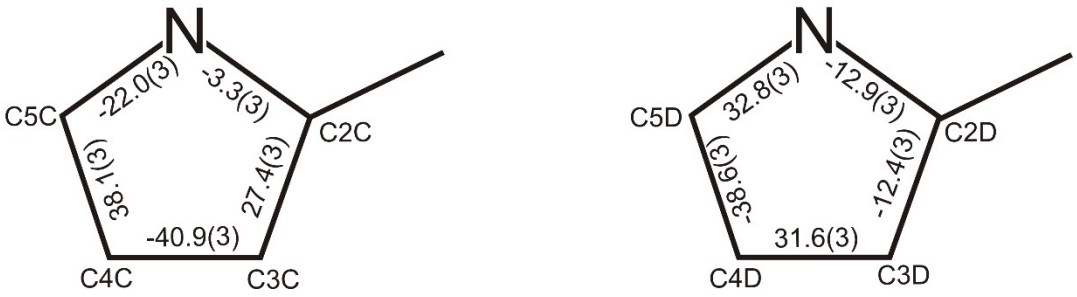
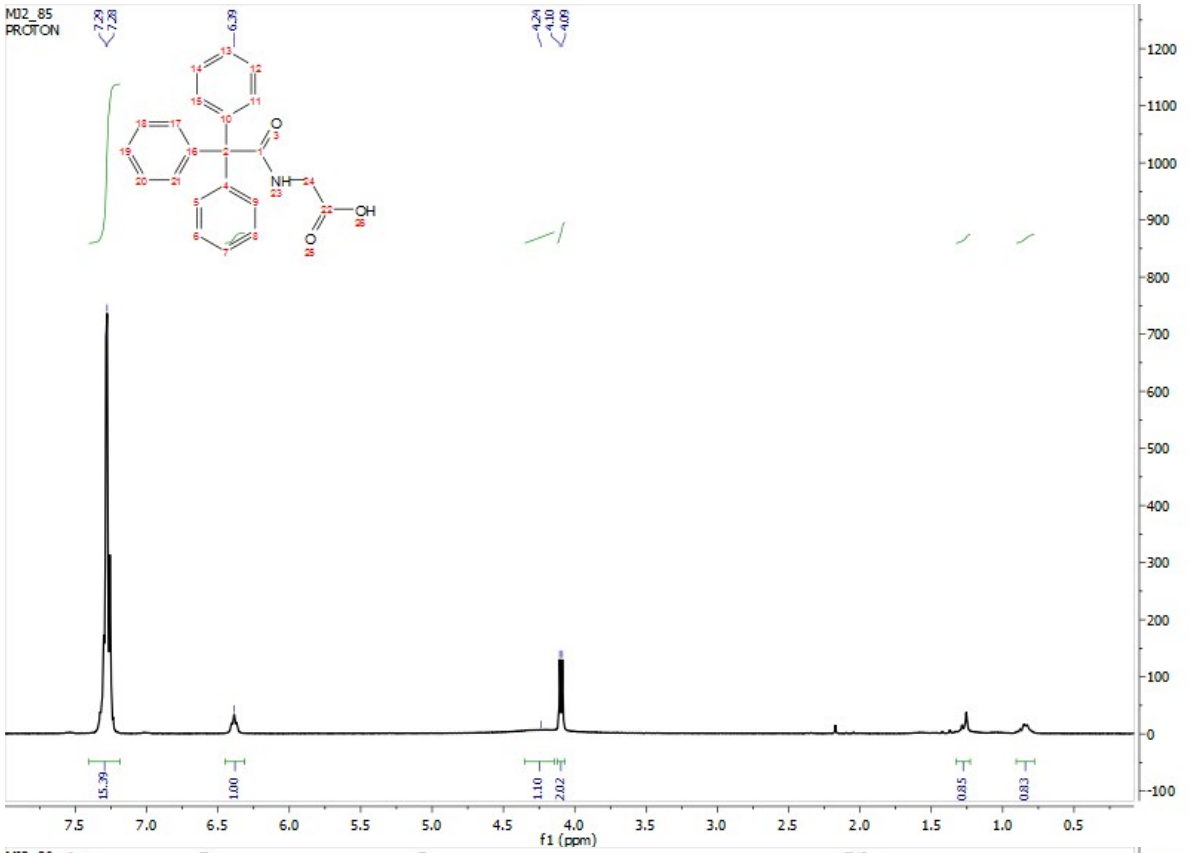
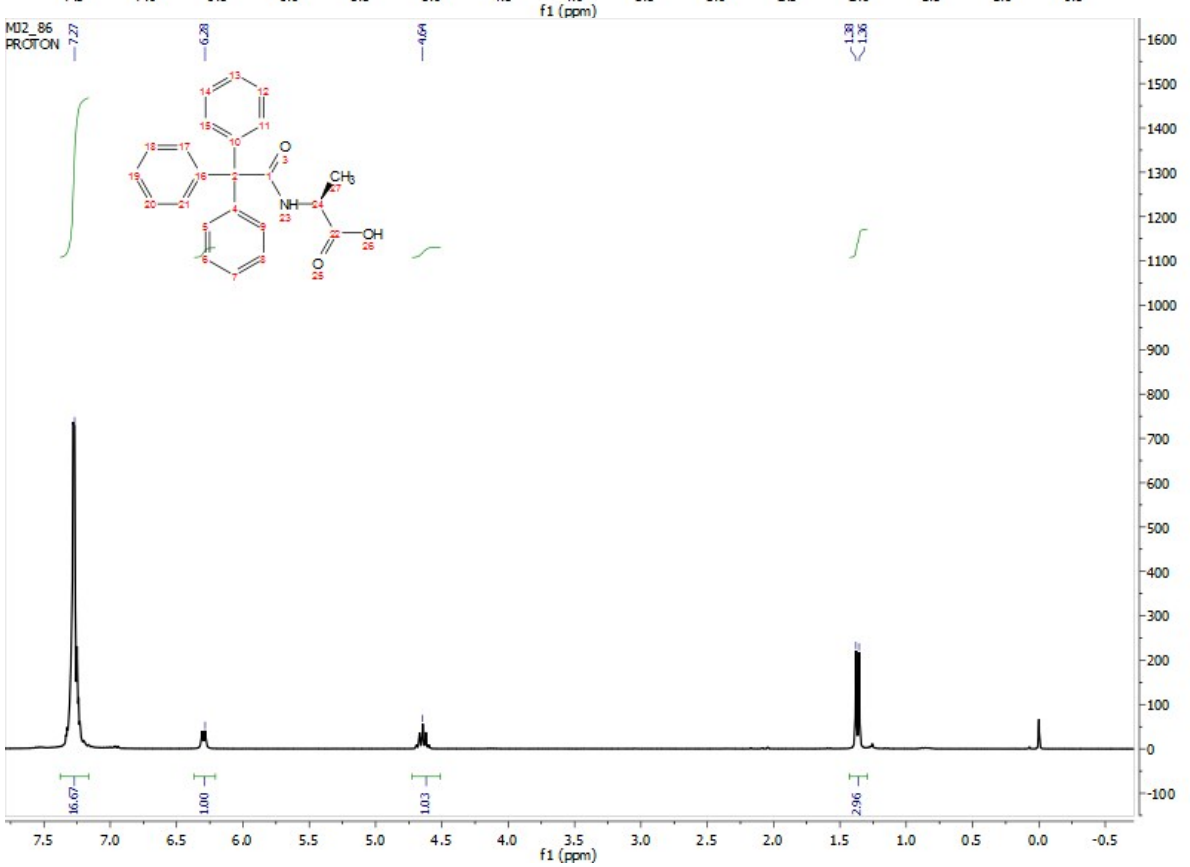
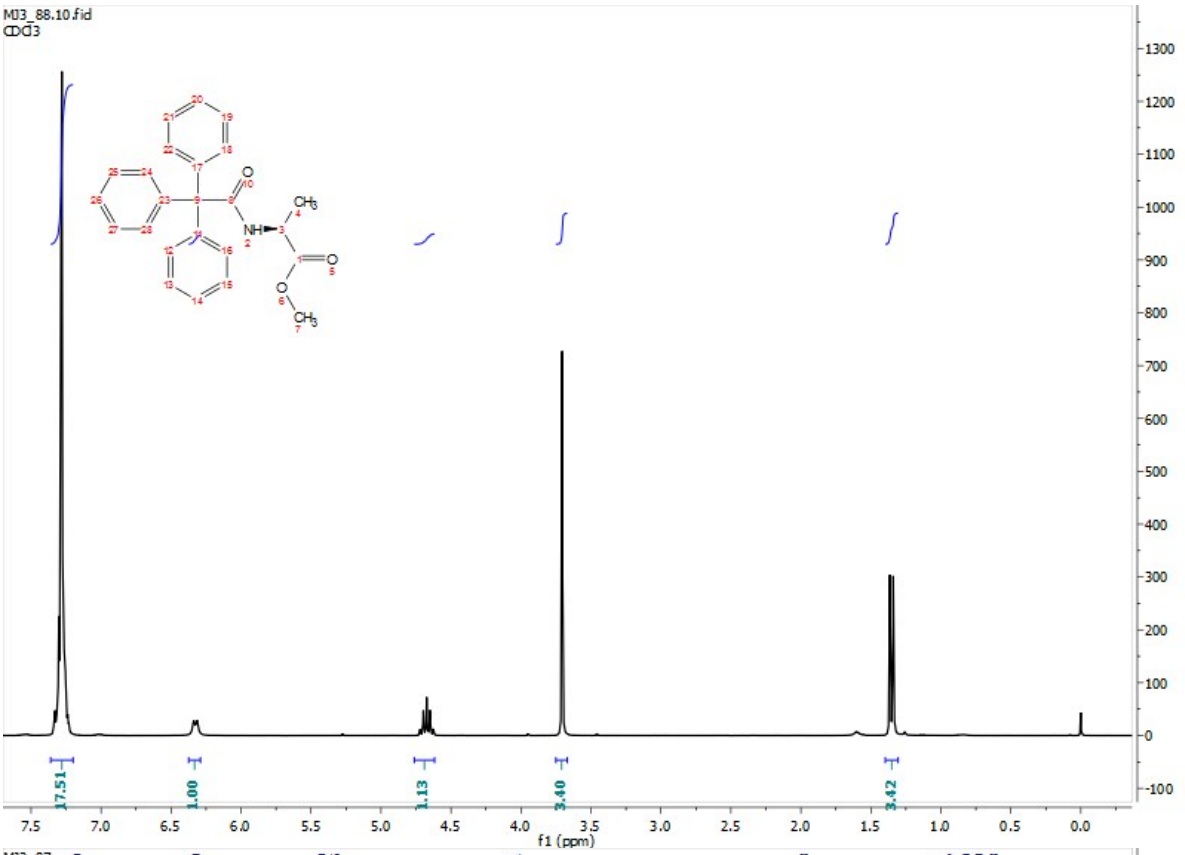


Fig. S30. Endocyclic torsion angles (°) in five-membered rings for proline derivatives **13a** and **13b**.

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



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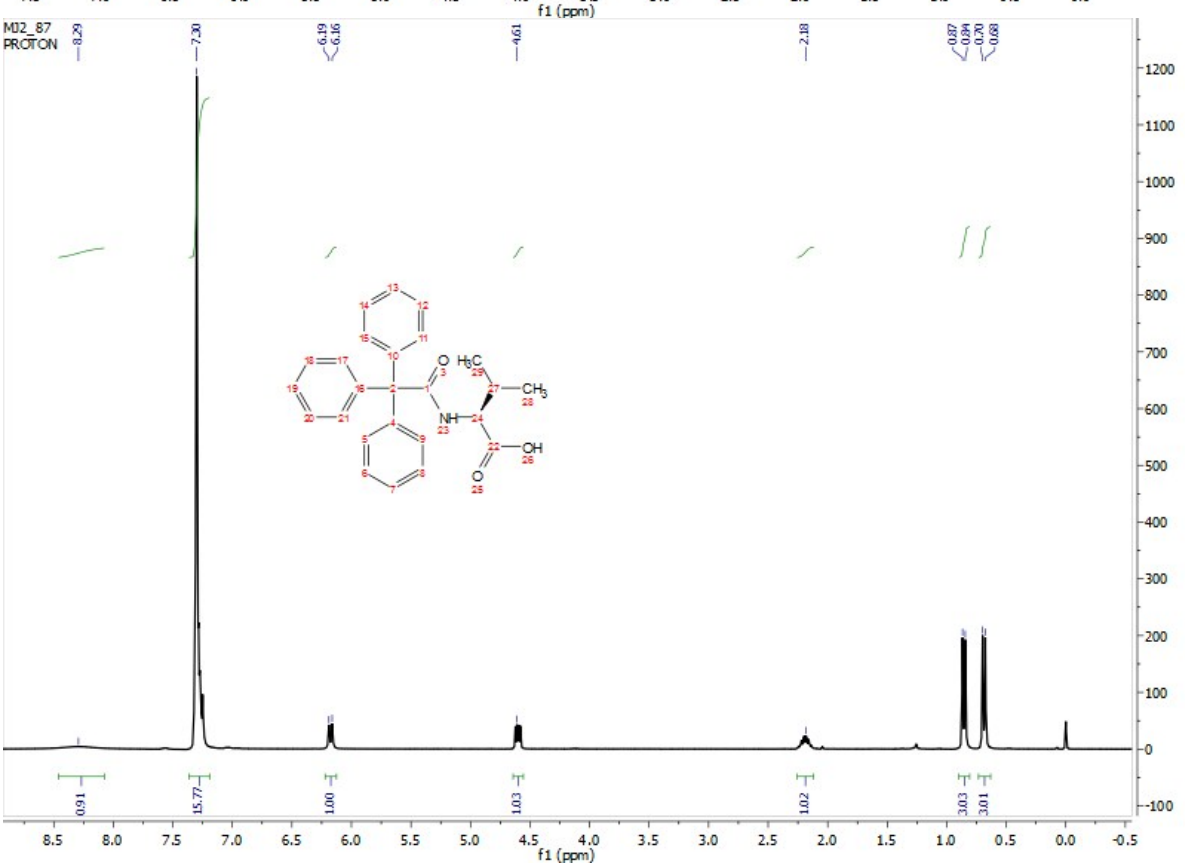
1.13
3.40
3.42
f1 (ppm)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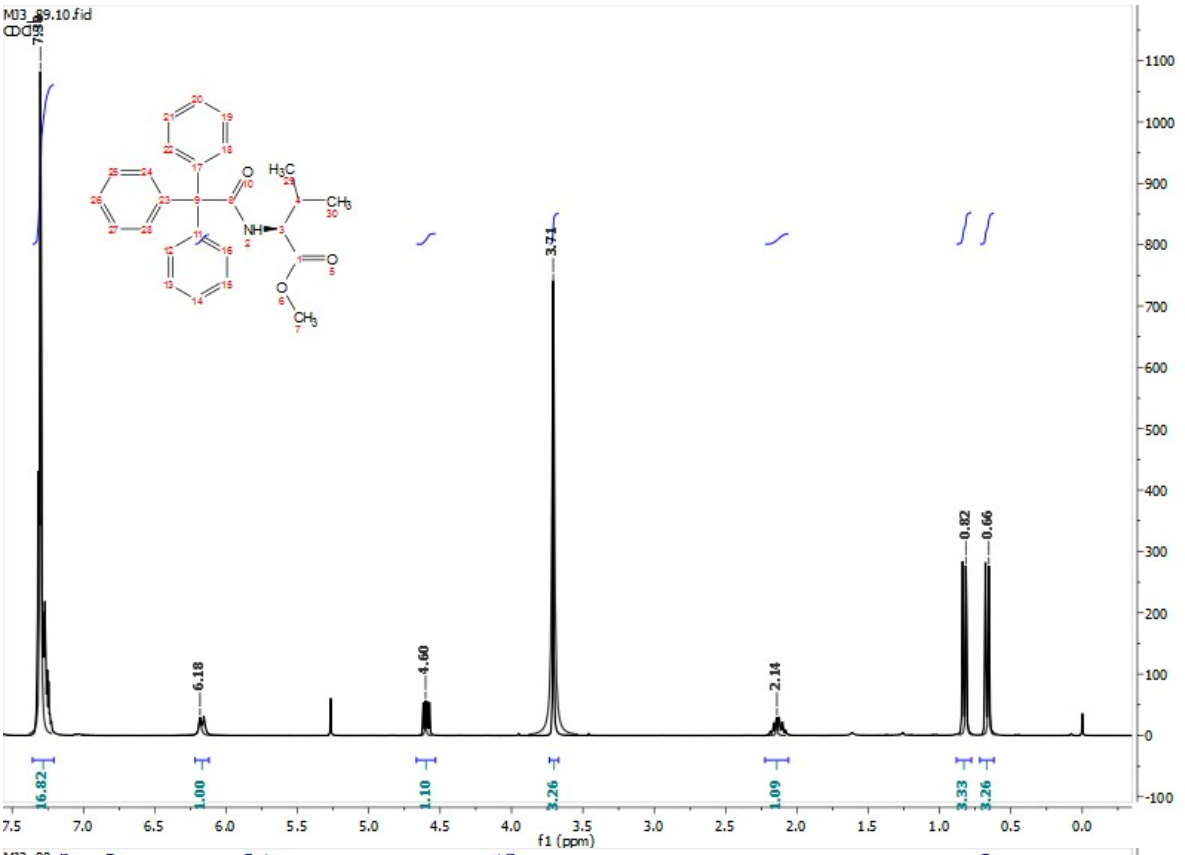
7.30
6.19
6.16
4.61
2.18
0.87
0.84
0.70
0.68
0.91
15.77
1.00
1.03
1.02
3.03
3.01
f1 (ppm)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6.18
4.60
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0.82
0.66
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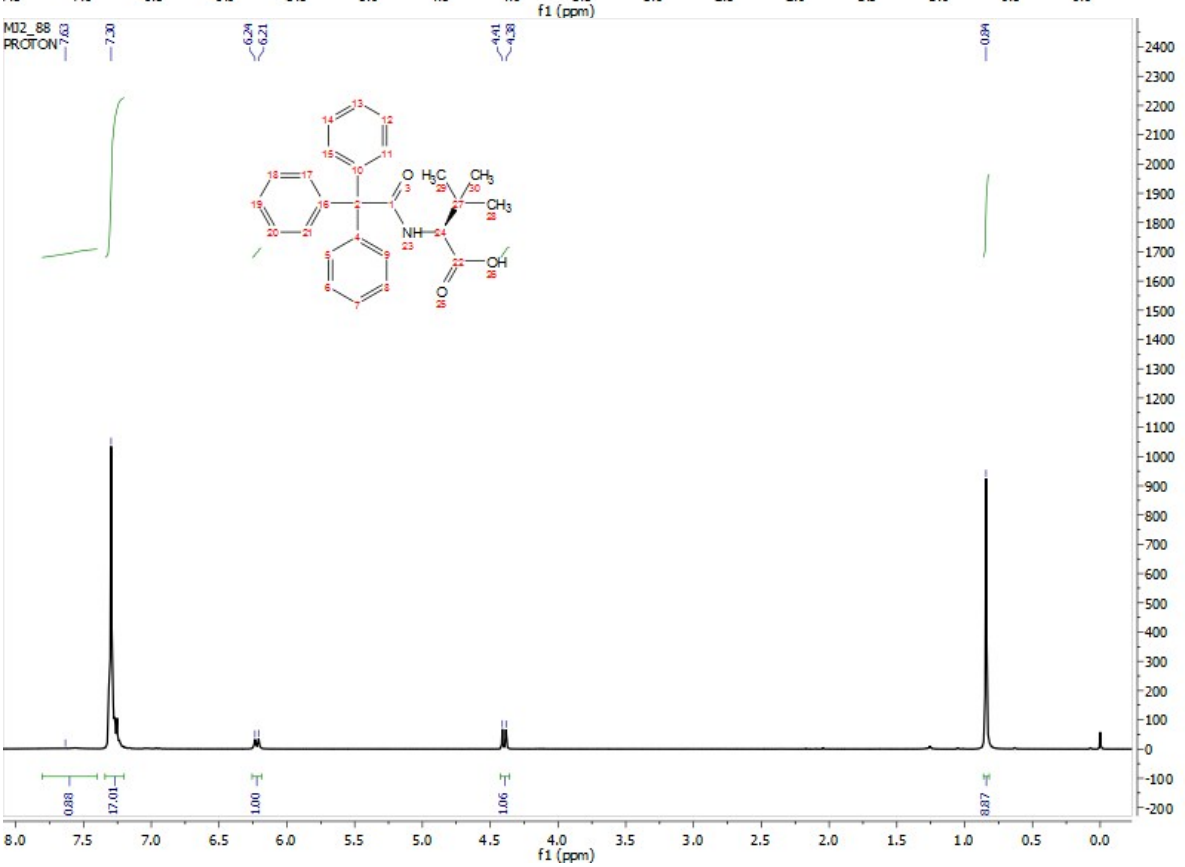
1.10
3.26
1.09
3.33
3.26
f1 (ppm)


M02_88
PROTON
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7.30
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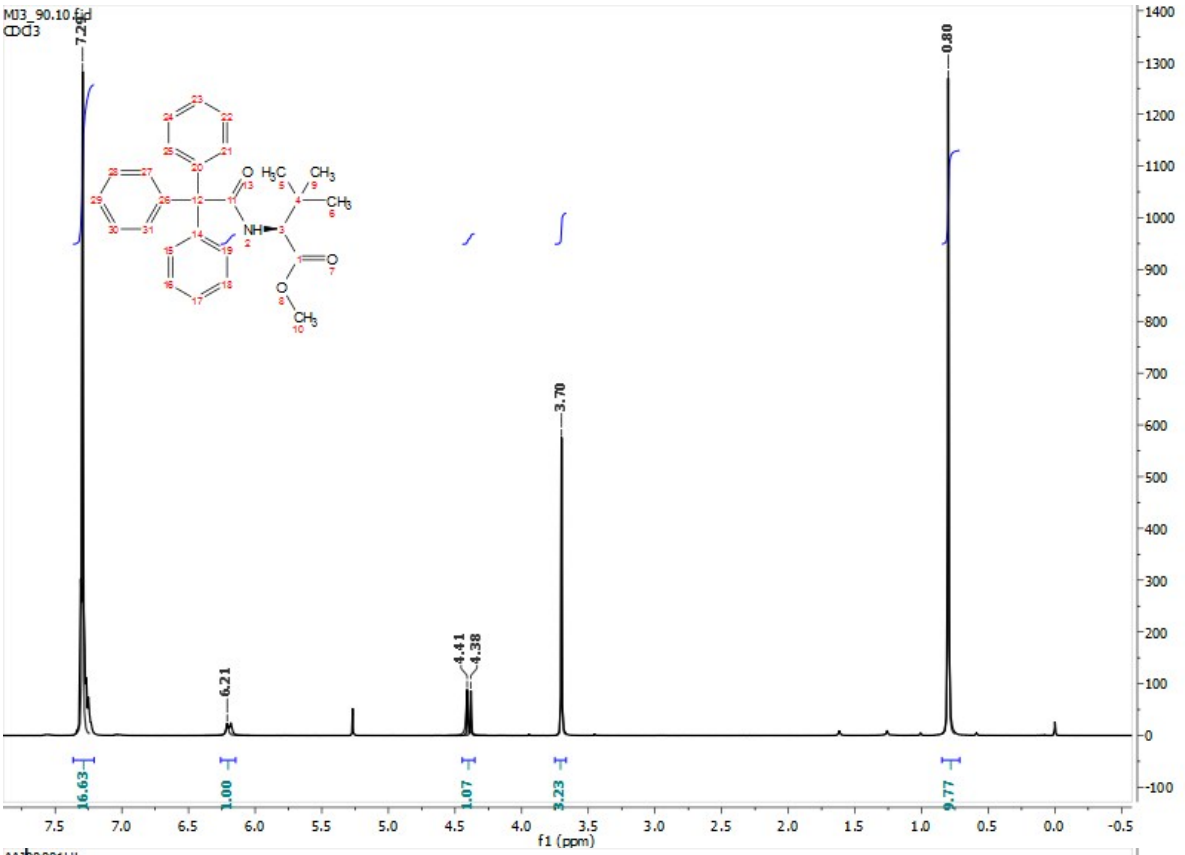
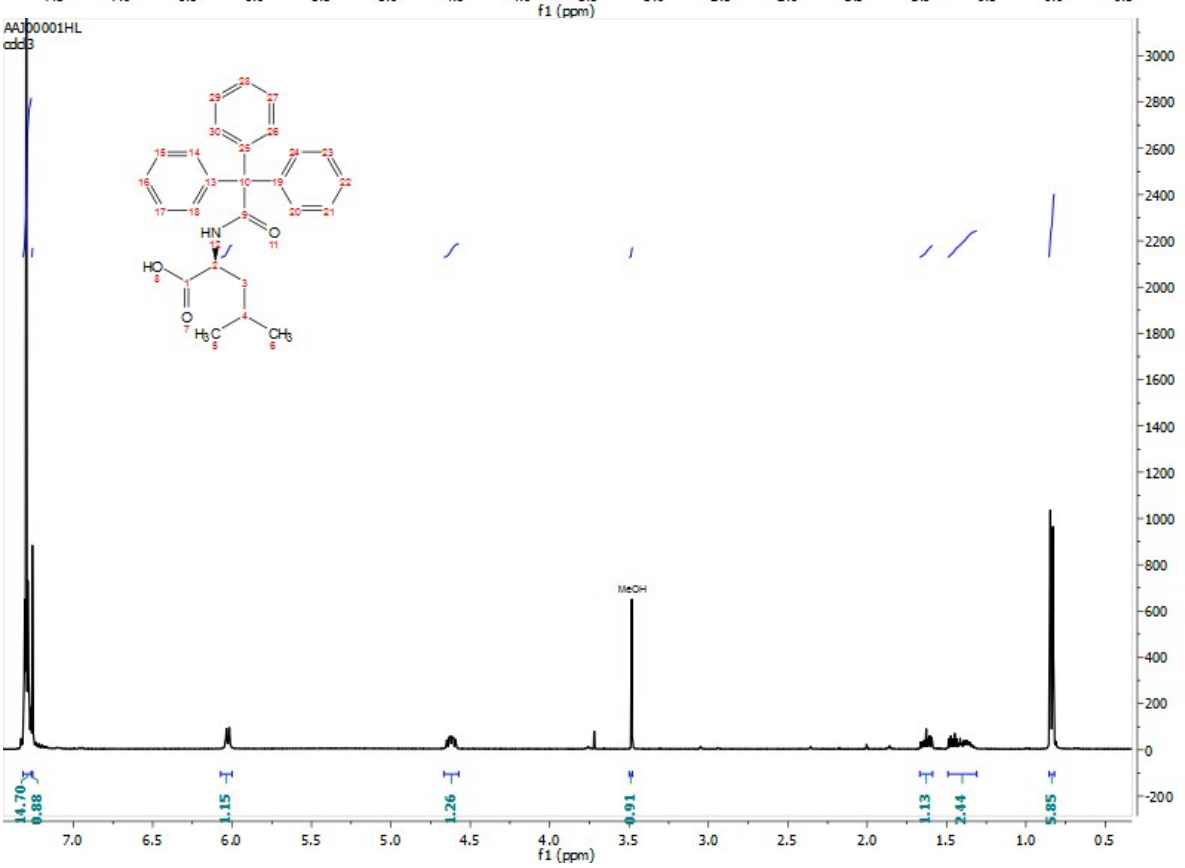
6.21
4.41
4.38
0.84
0.88
17.01
1.00
1.06
8.87
f1 (ppm)


MJ3_90.10.fid
CDCl3
7.26
0.80
3.70
4.41
4.38
6.21
16.63
1.00
1.07
3.23
9.77
f1 (ppm)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cdcl3
MeOH
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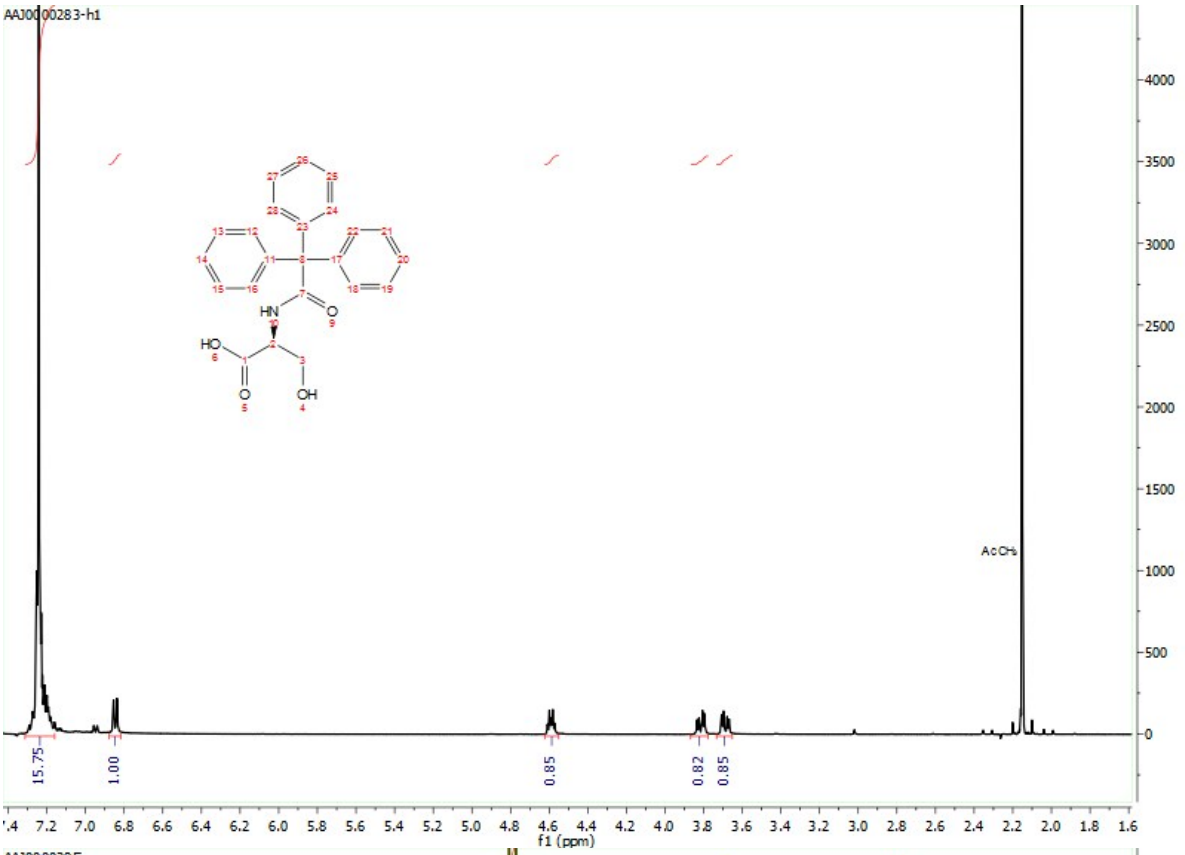
0.88
1.15
1.26
0.91
1.13
2.44
5.85
f1 (ppm)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AcCH3
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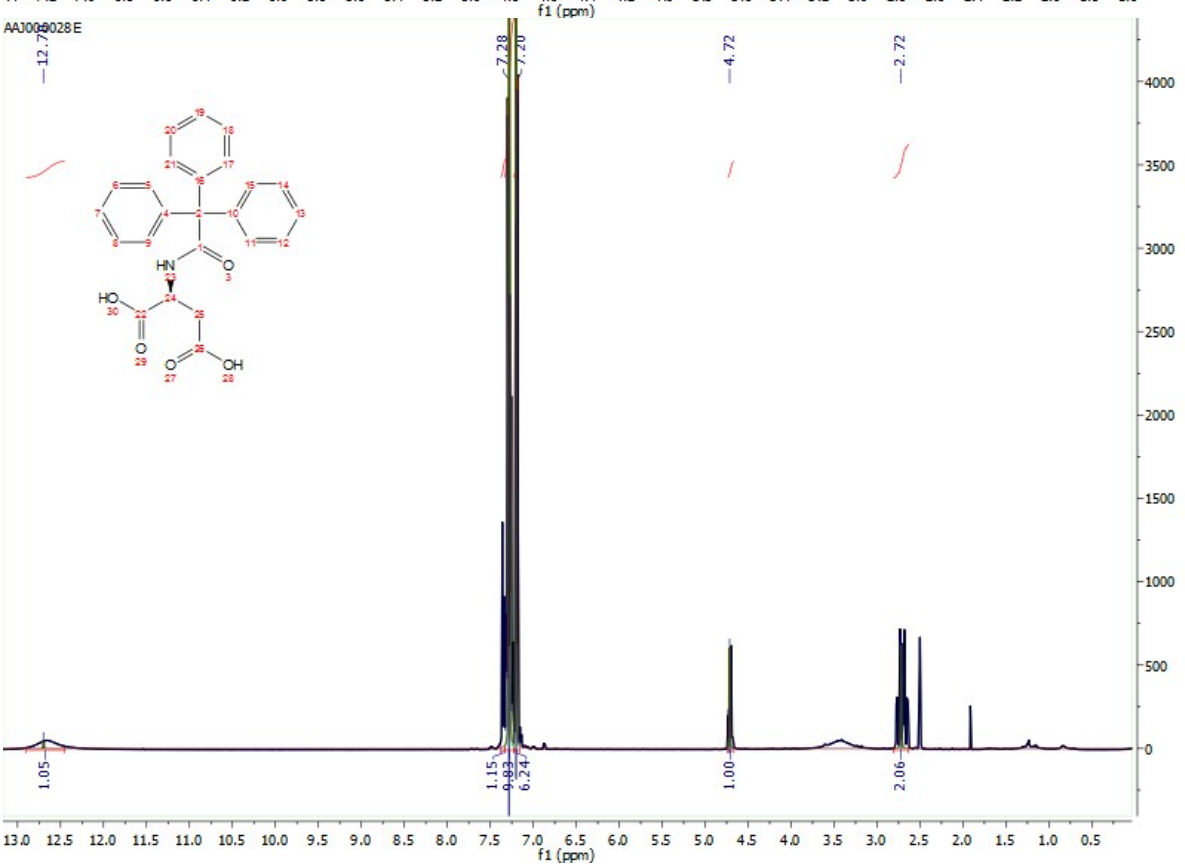
1.00
0.85
0.82
0.85
f1 (ppm)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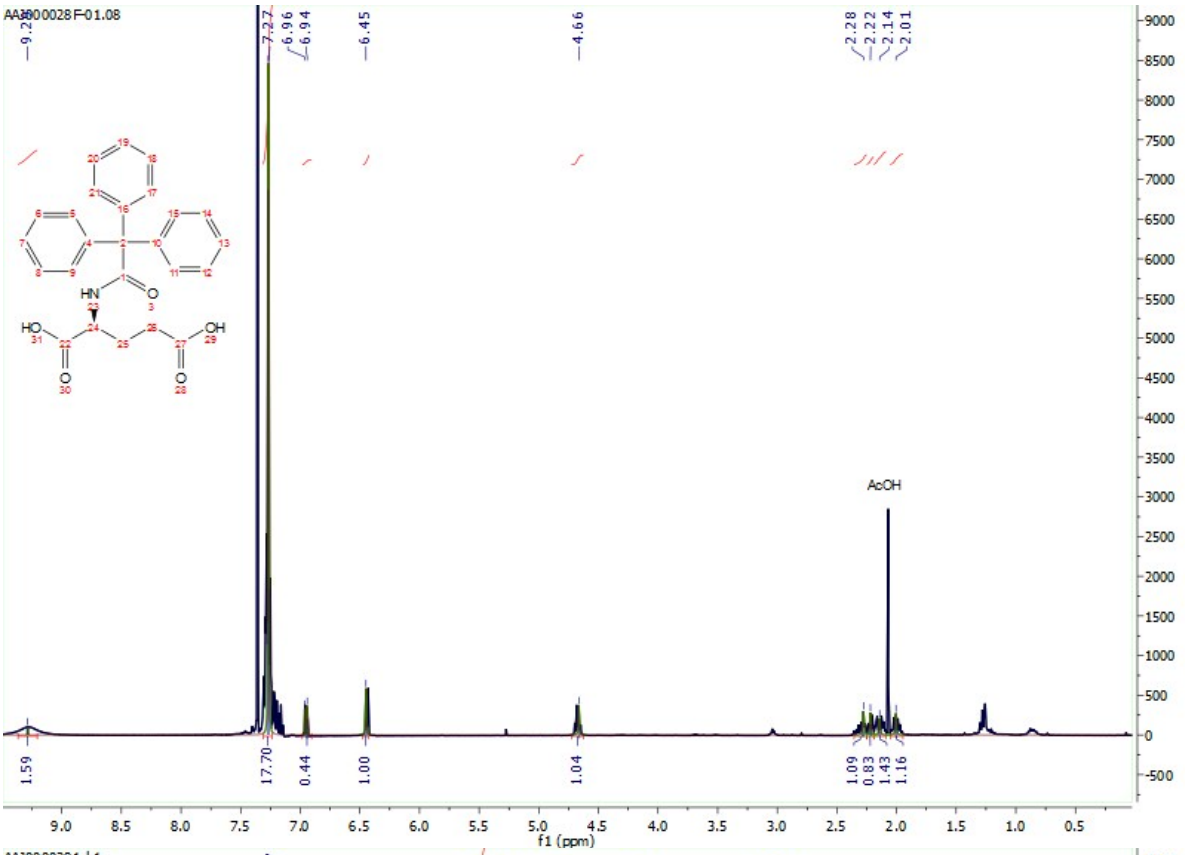
7.20
4.72
2.72
1.05
1.15
0.83
6.24
1.00
2.06
f1 (ppm)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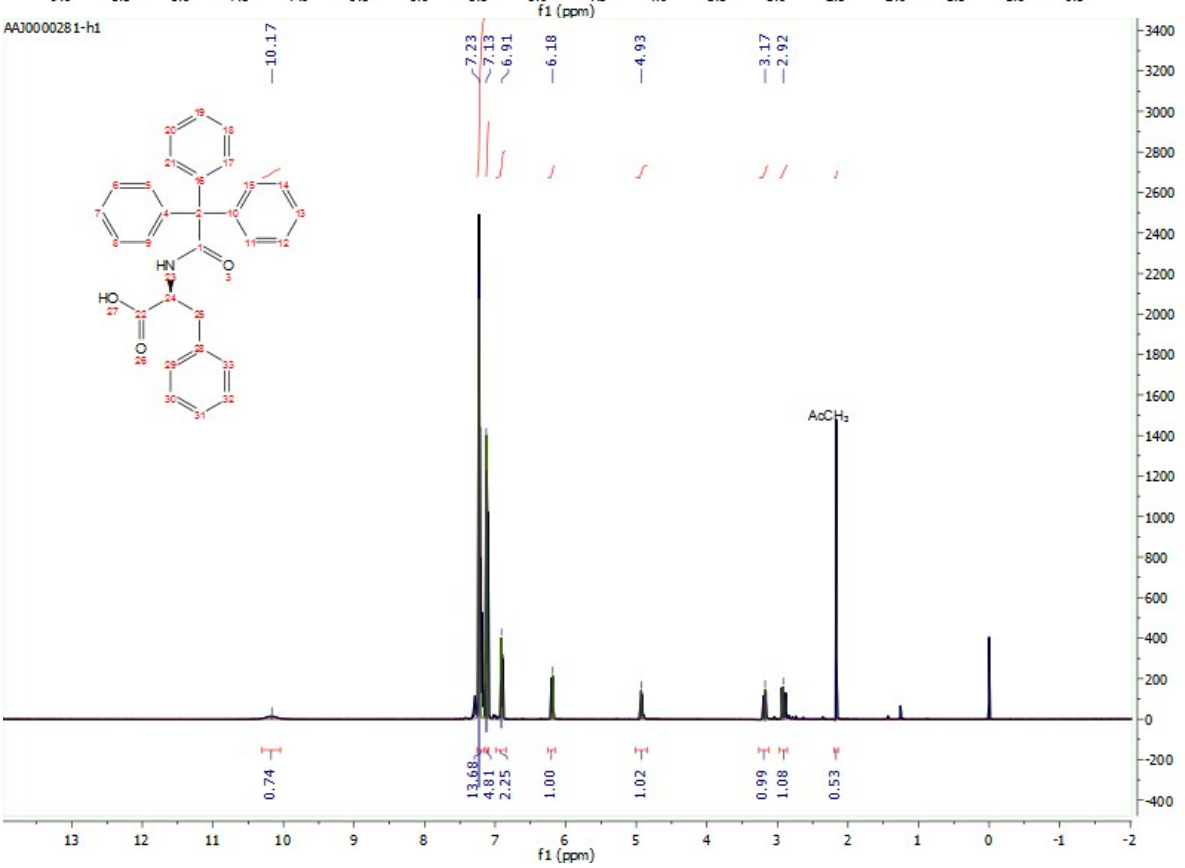
AcOH
f1 (ppm)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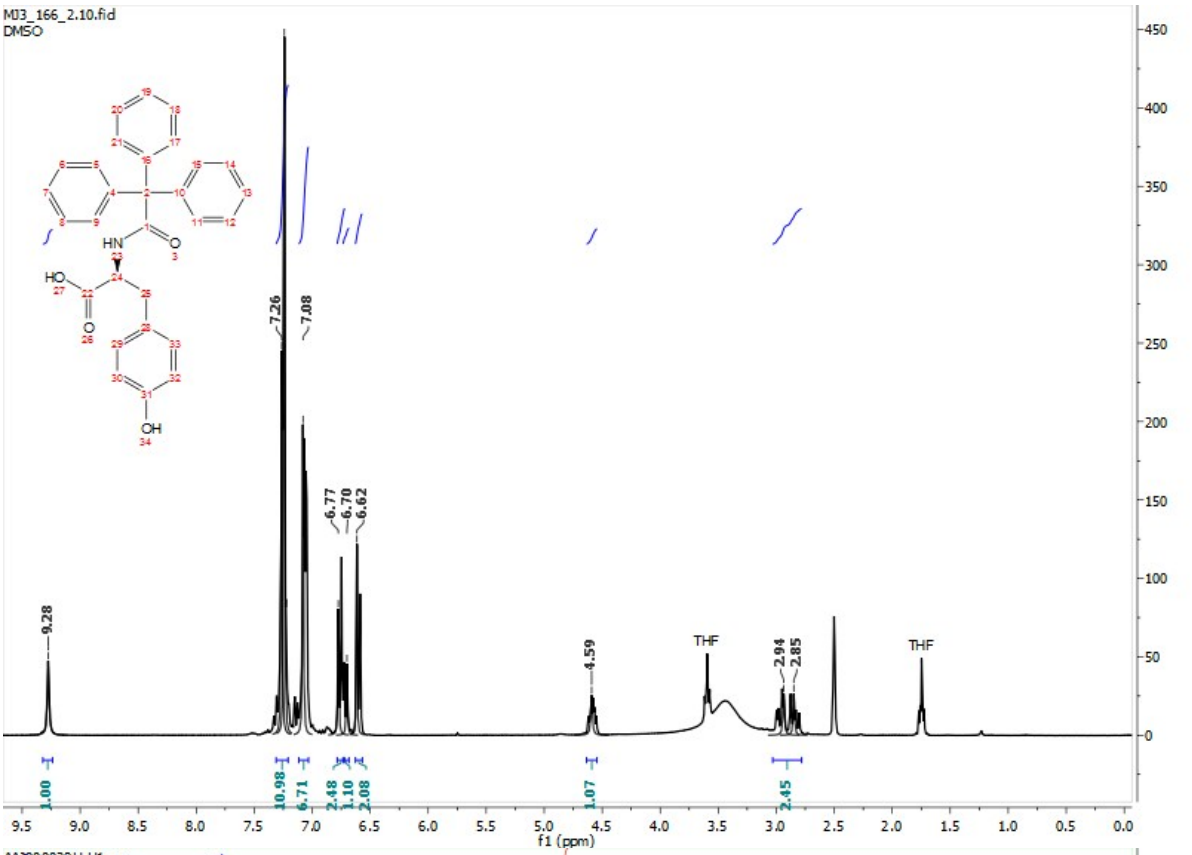
f1 (ppm)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7.08
6.77
6.70
6.62
4.59
THF
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THF
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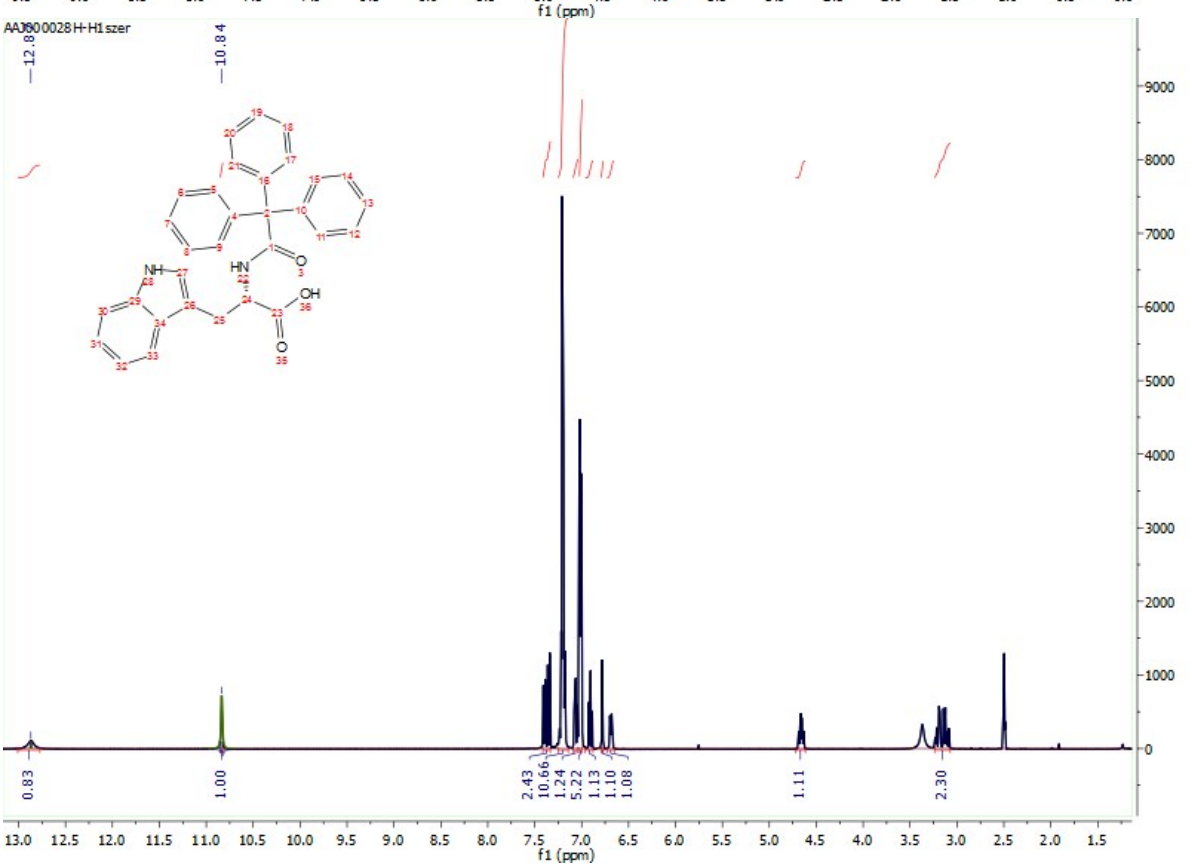
1.10
2.08
1.07
2.45
f1 (ppm)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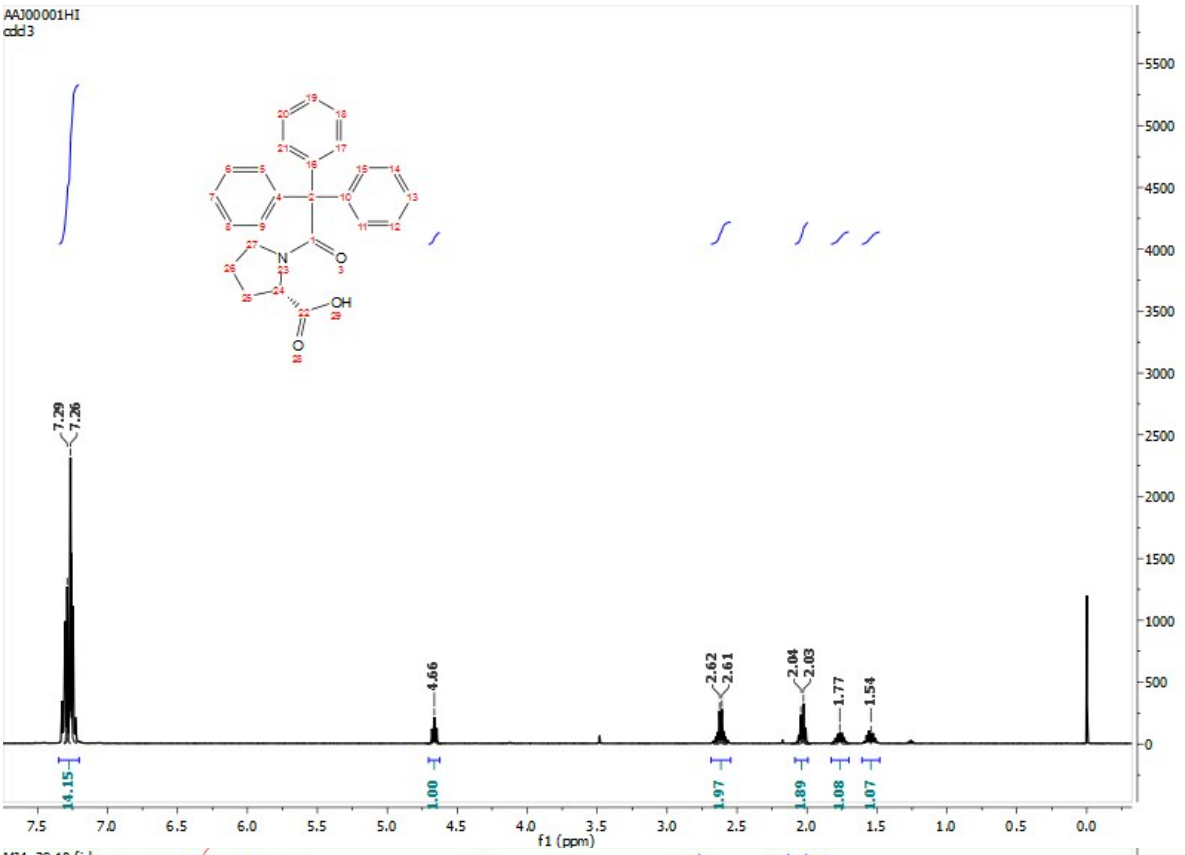
5.22
1.13
1.10
1.08
1.11
2.30
f1 (ppm)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7.26
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2.62
2.61
2.04
2.03
1.77
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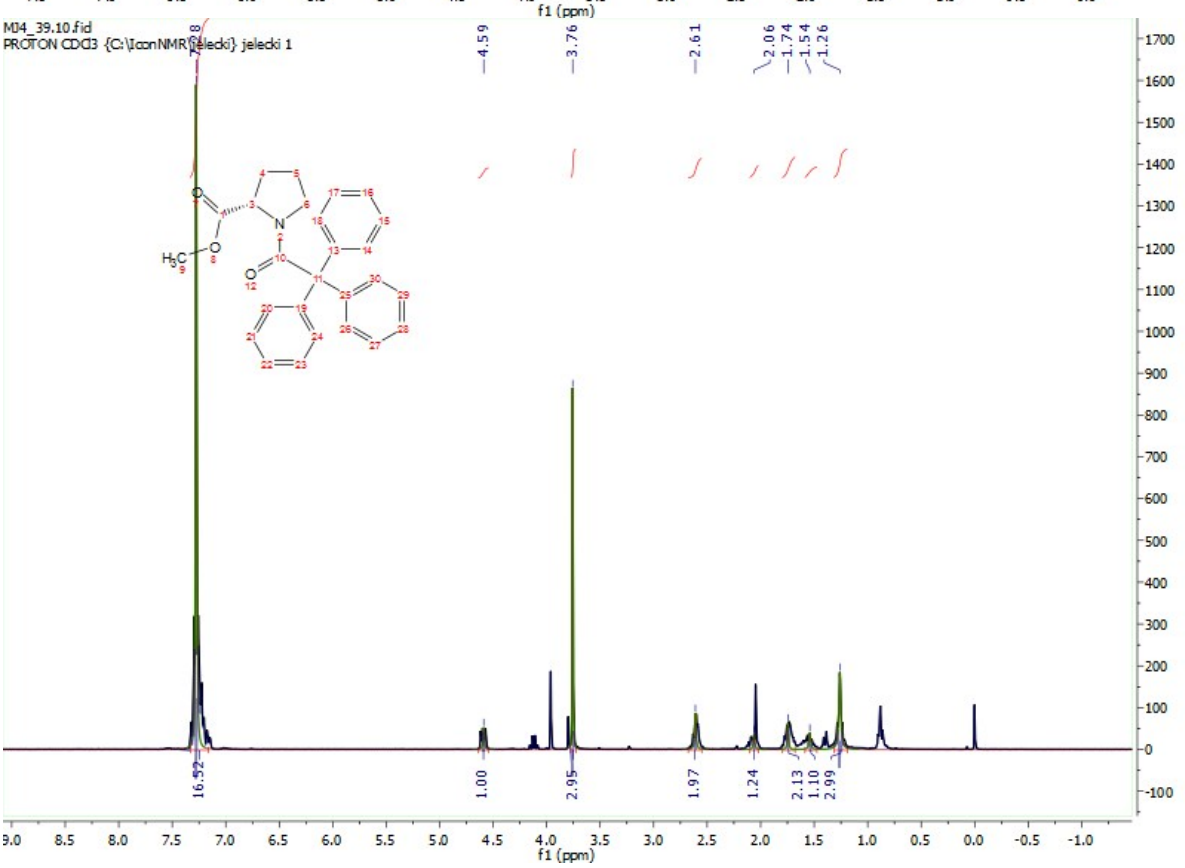
1.97
1.89
1.08
1.07
f1 (ppm)


M04_39.10.fid
PROTON CDCl3 {C:\IconNMR\jelecki} jelecki 1
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3.76
2.61
2.06
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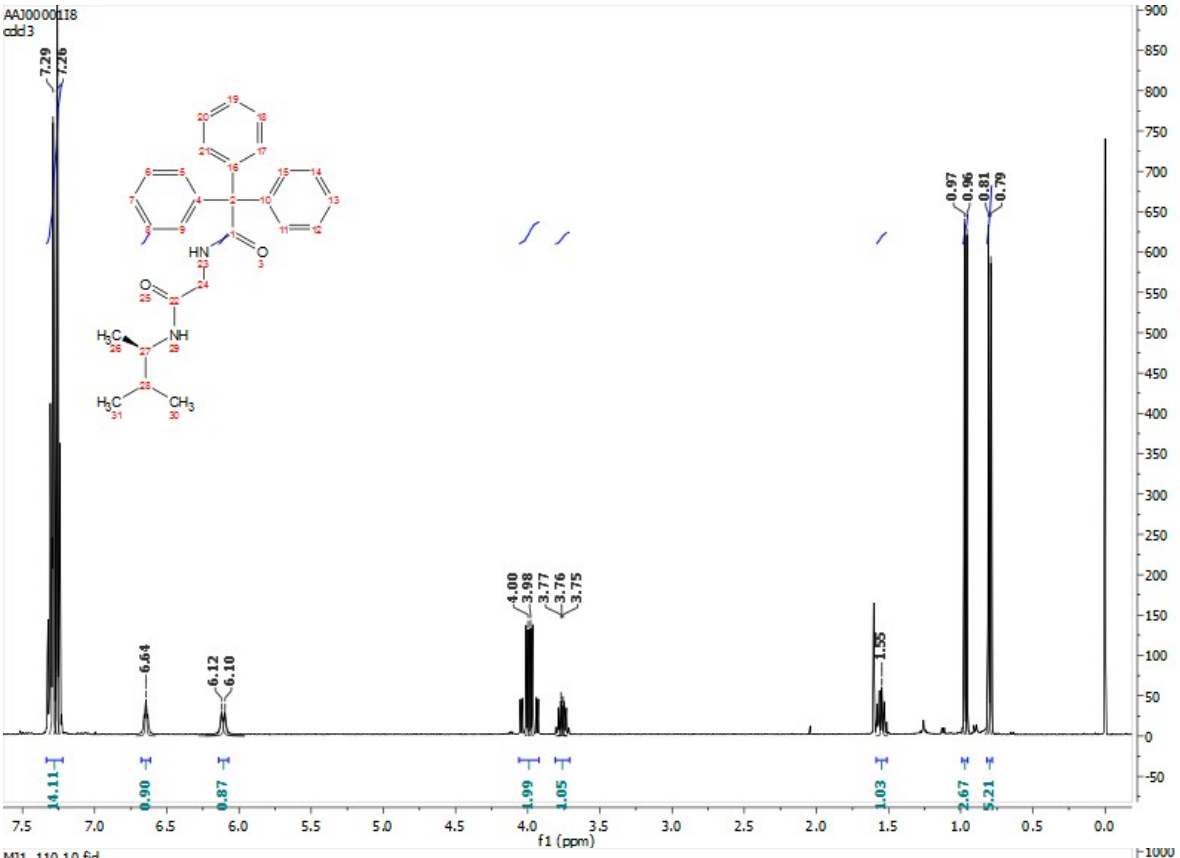
1.24
2.13
1.10
2.99
f1 (ppm)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4.00
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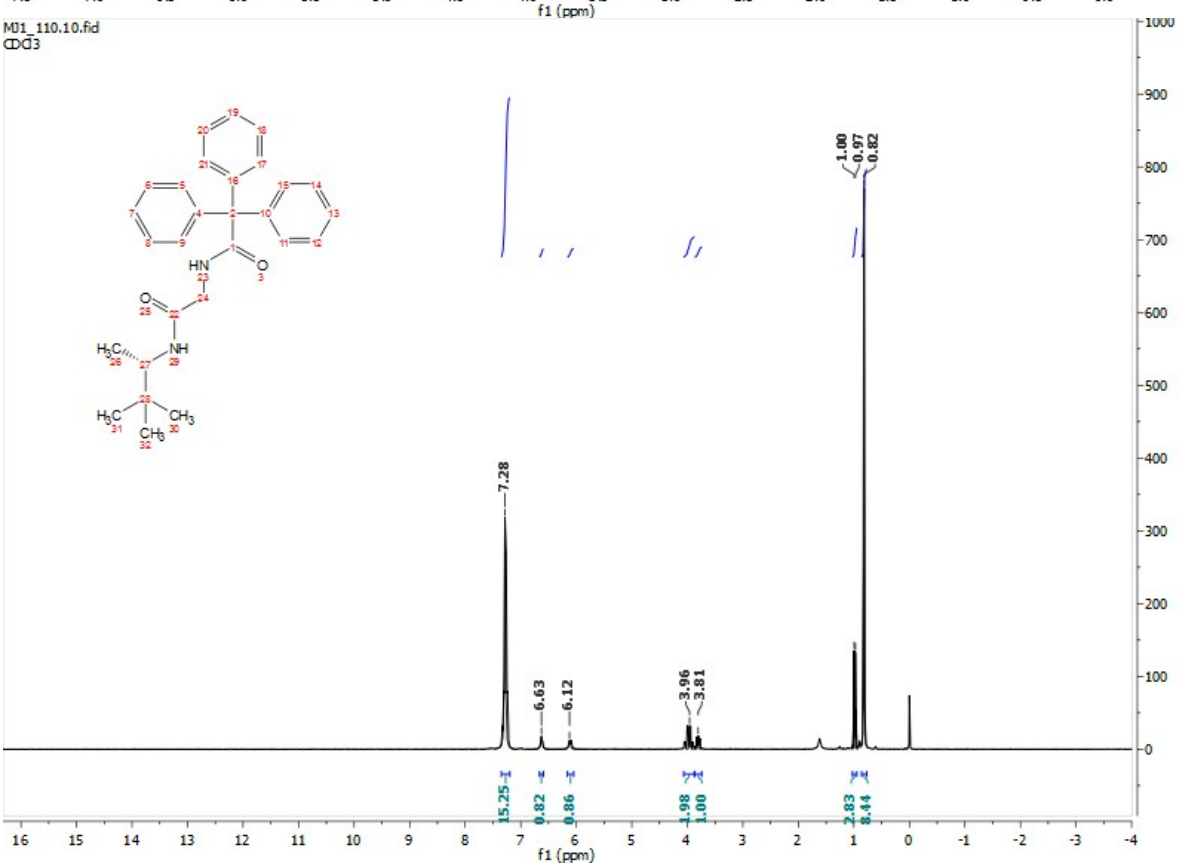
3.77
3.76
3.75
1.55
0.97
0.96
0.81
0.79
14.11
0.90
0.87
1.99
1.05
1.03
2.67
5.21
f1 (ppm)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6.63
6.12
3.96
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1.00
0.97
0.82
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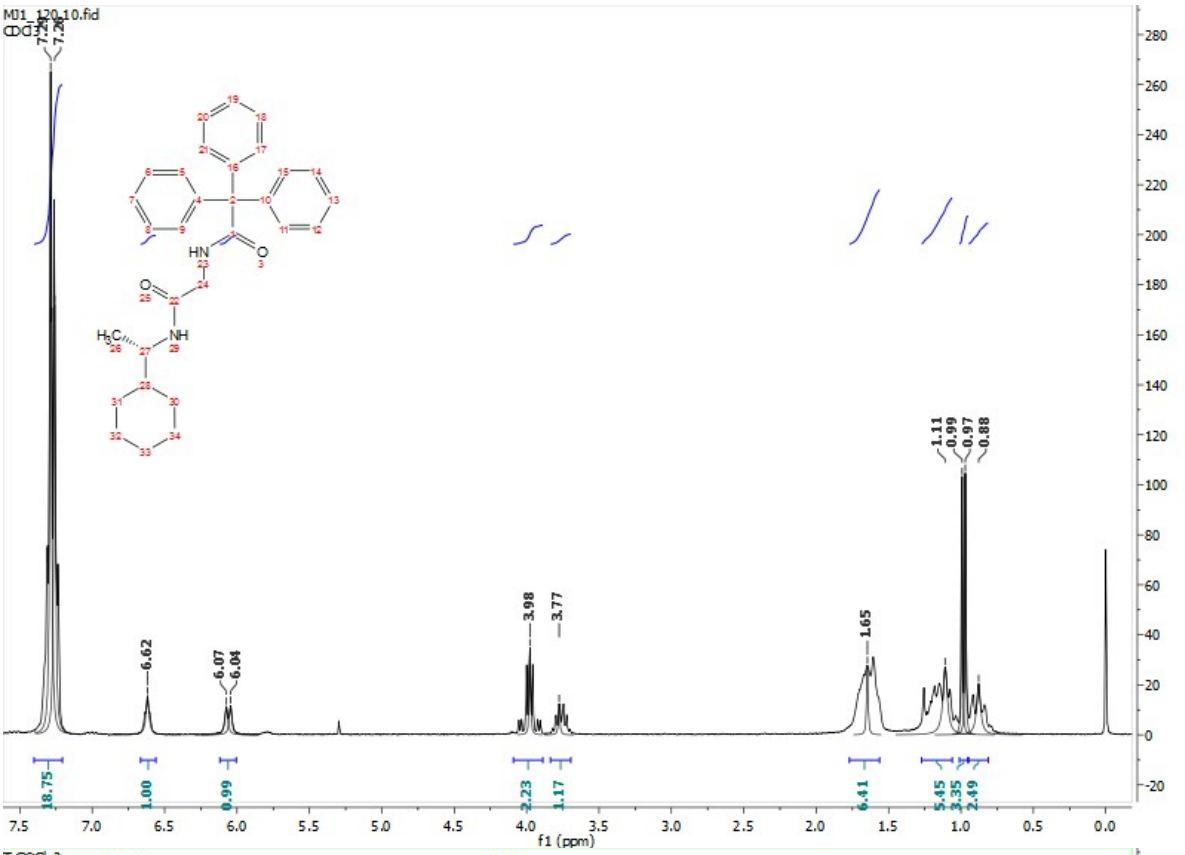
0.86
1.98
1.00
2.83
8.44
f1 (ppm)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6.62
6.07
6.04
3.98
3.77
1.65
1.11
0.99
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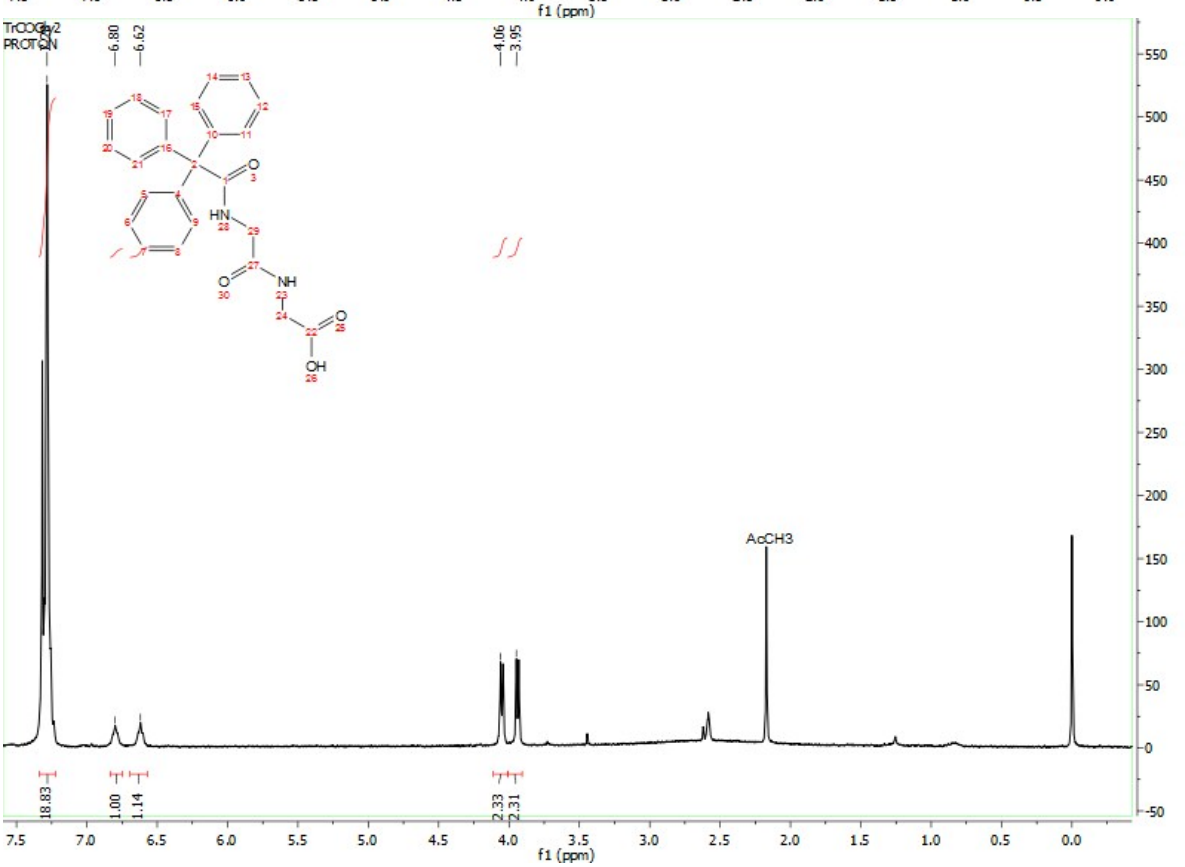
18.75
1.00
0.99
2.23
1.17
6.41
5.45
3.35
2.49
f1 (ppm)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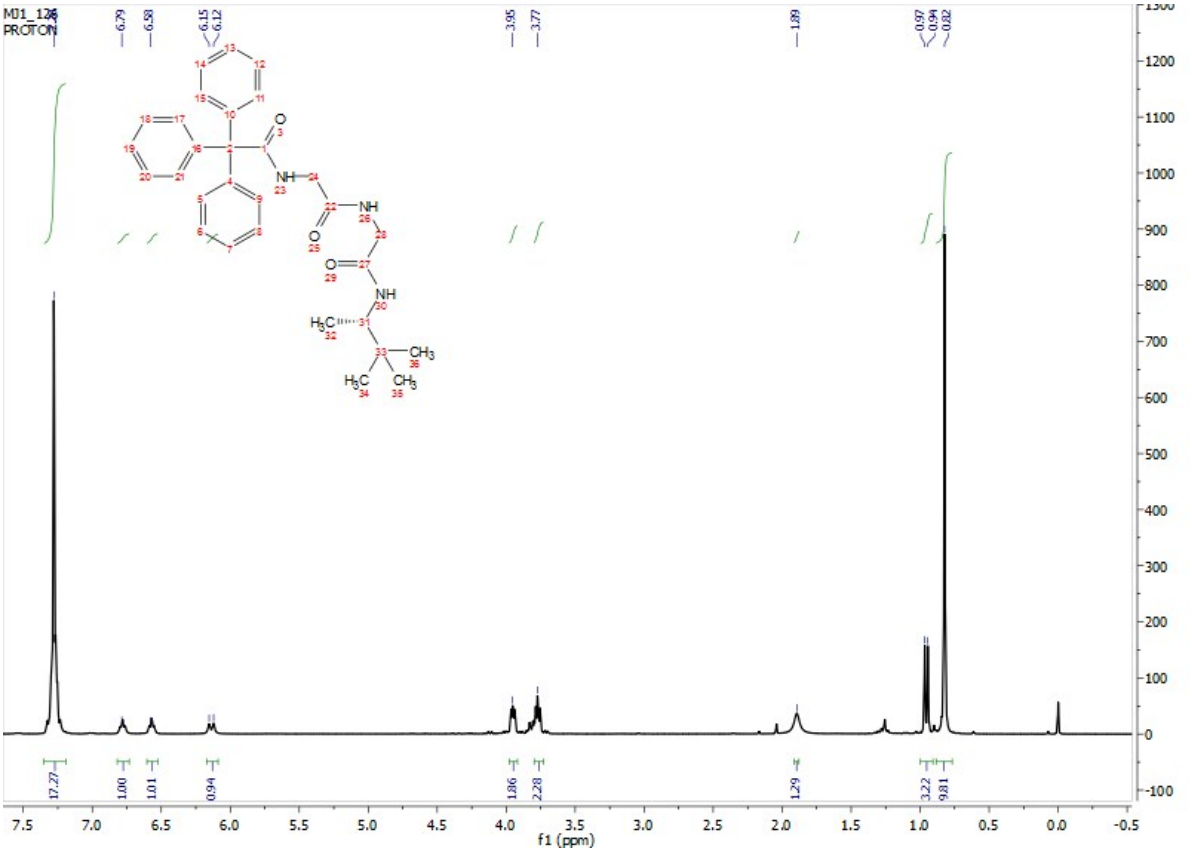
6.62
4.06
3.95
AcCH3
18.83
1.00
1.14
2.33
2.31
f1 (ppm)


MD1_126
PROTON
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6.58
6.15
6.12
3.95
3.77
1.89
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1.00
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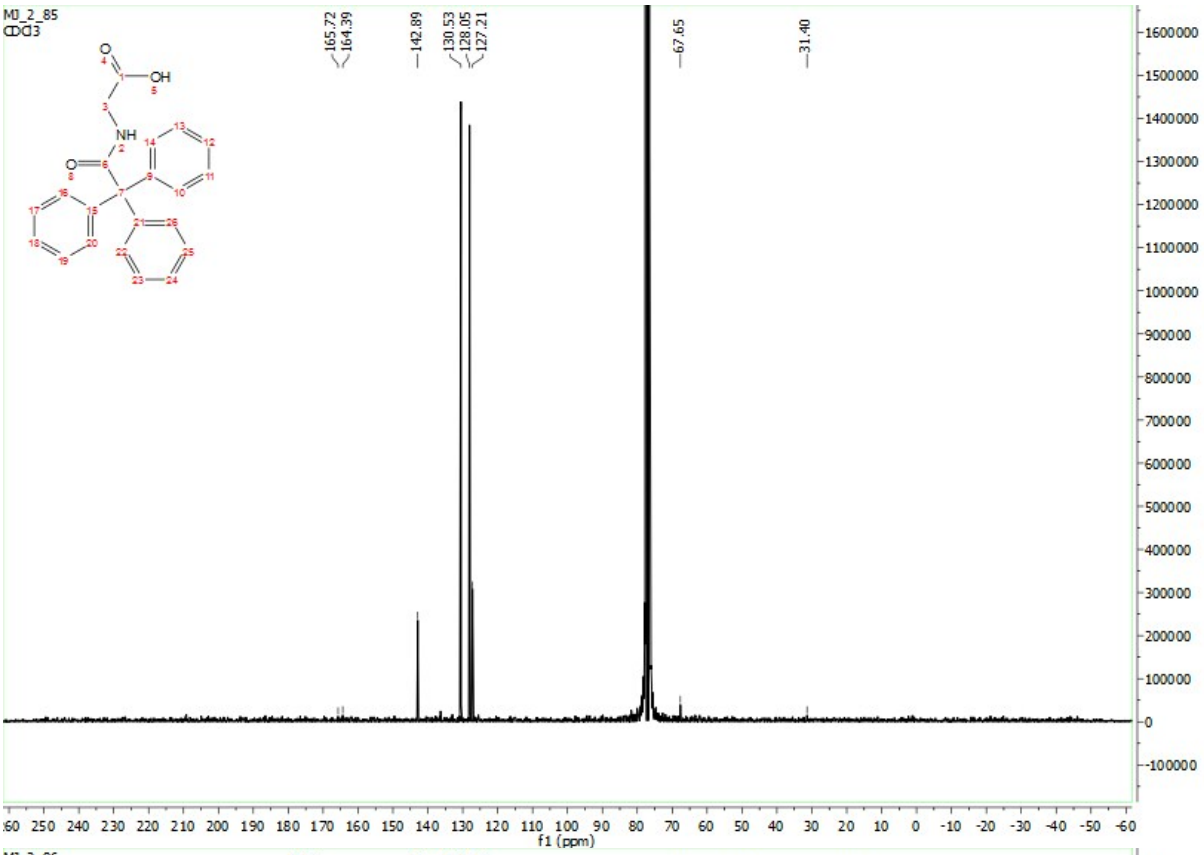
0.94
1.86
2.28
1.29
3.22
9.81
f1 (ppm)


MD_2_85
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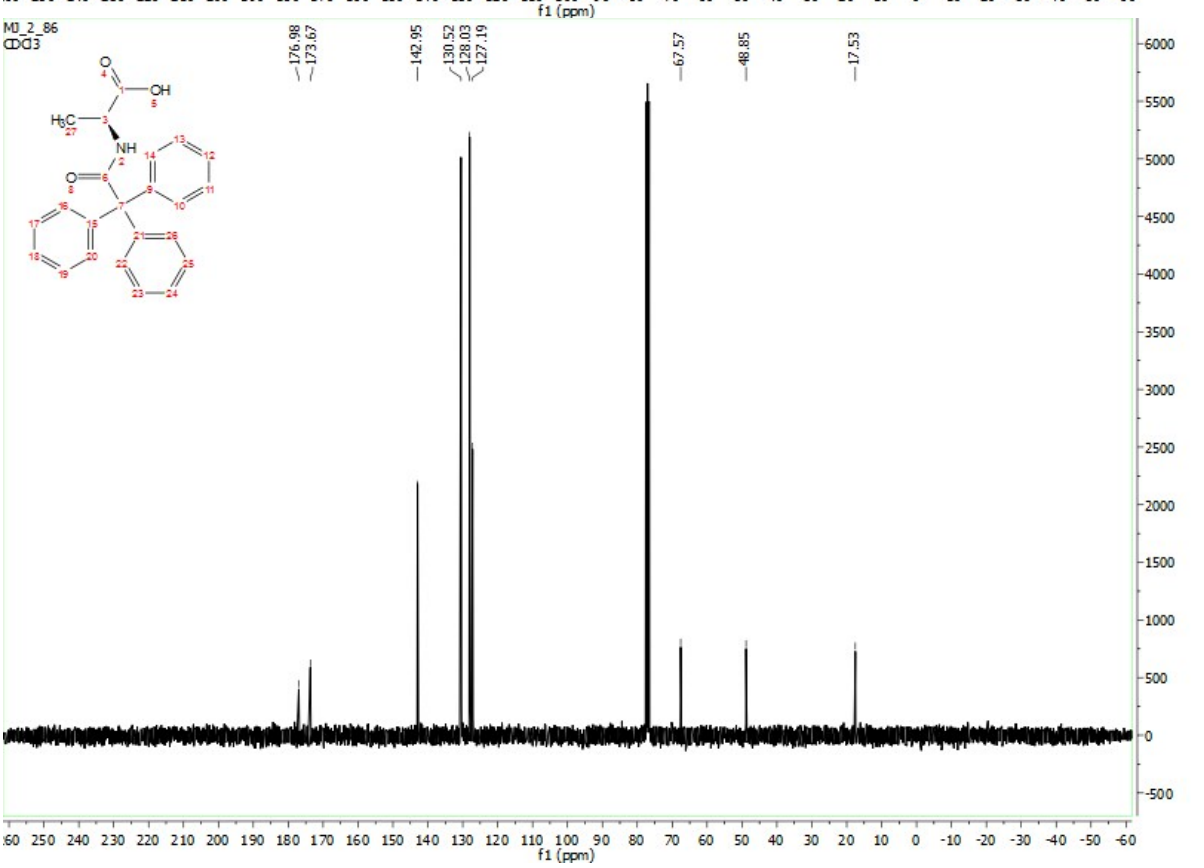
164.39
142.89
130.53
128.05
127.21
67.65
31.40
f1 (ppm)


MD_2_86
CDCl3
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173.67
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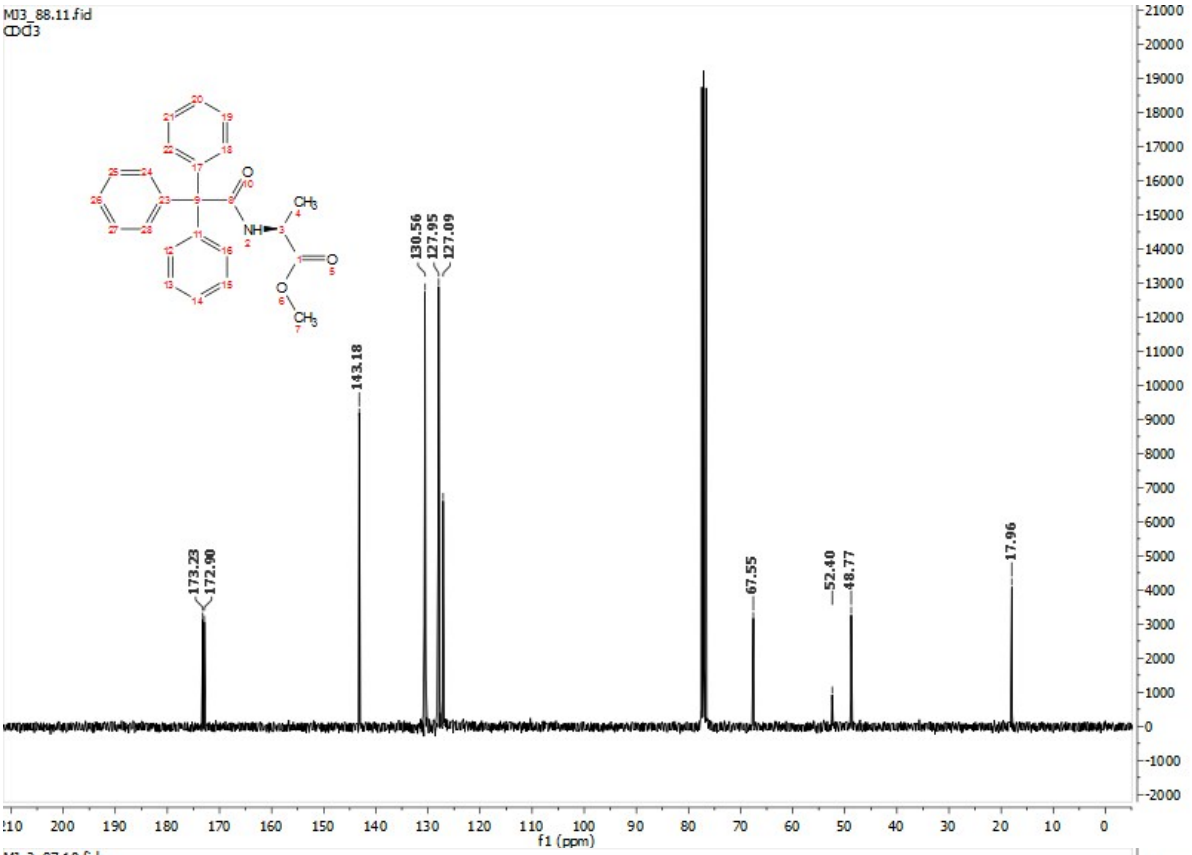
130.52
128.03
127.19
67.57
48.85
17.53
f1 (ppm)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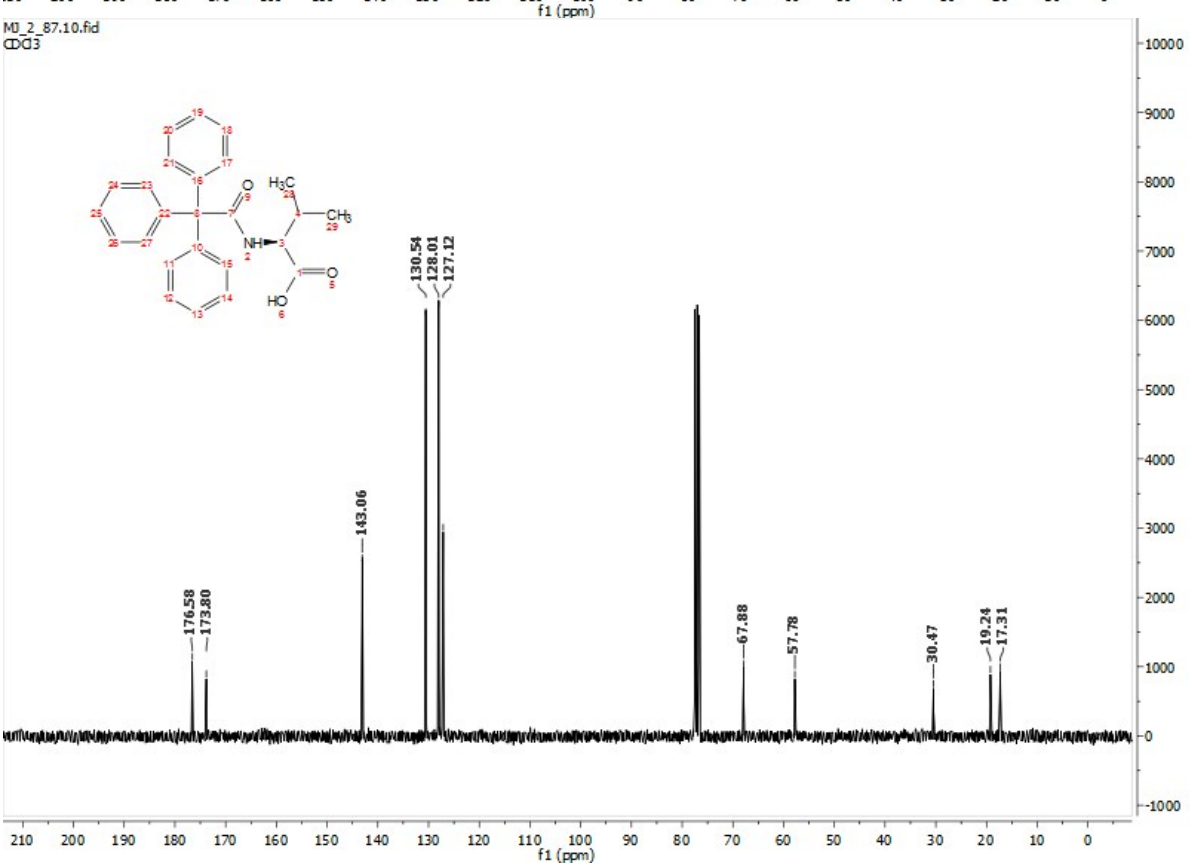
172.90
143.18
130.56
127.95
127.09
67.55
52.40
48.77
17.96
f1 (ppm)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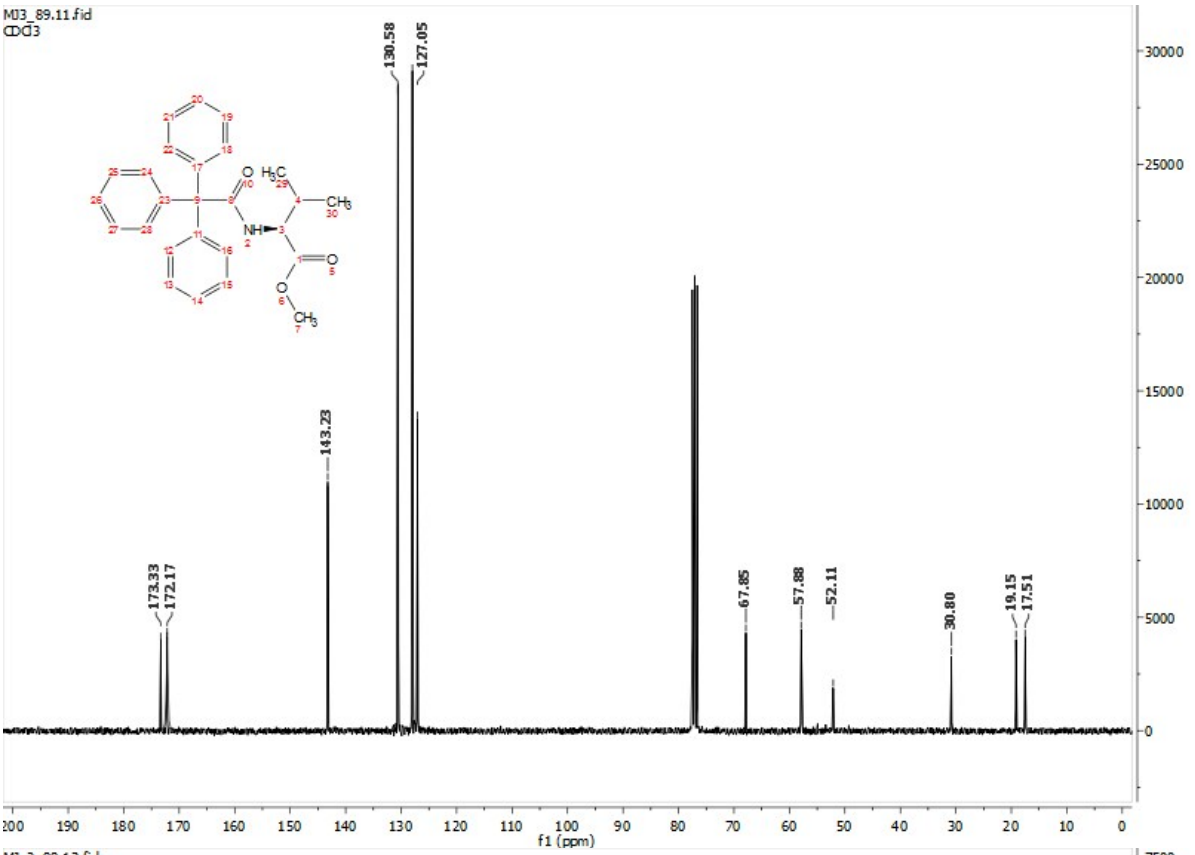
CDCl3
176.58
173.80
143.06
130.54
128.01
127.12
67.88
57.78
30.47
19.24
17.31
f1 (ppm)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127.05
143.23
173.33
172.17
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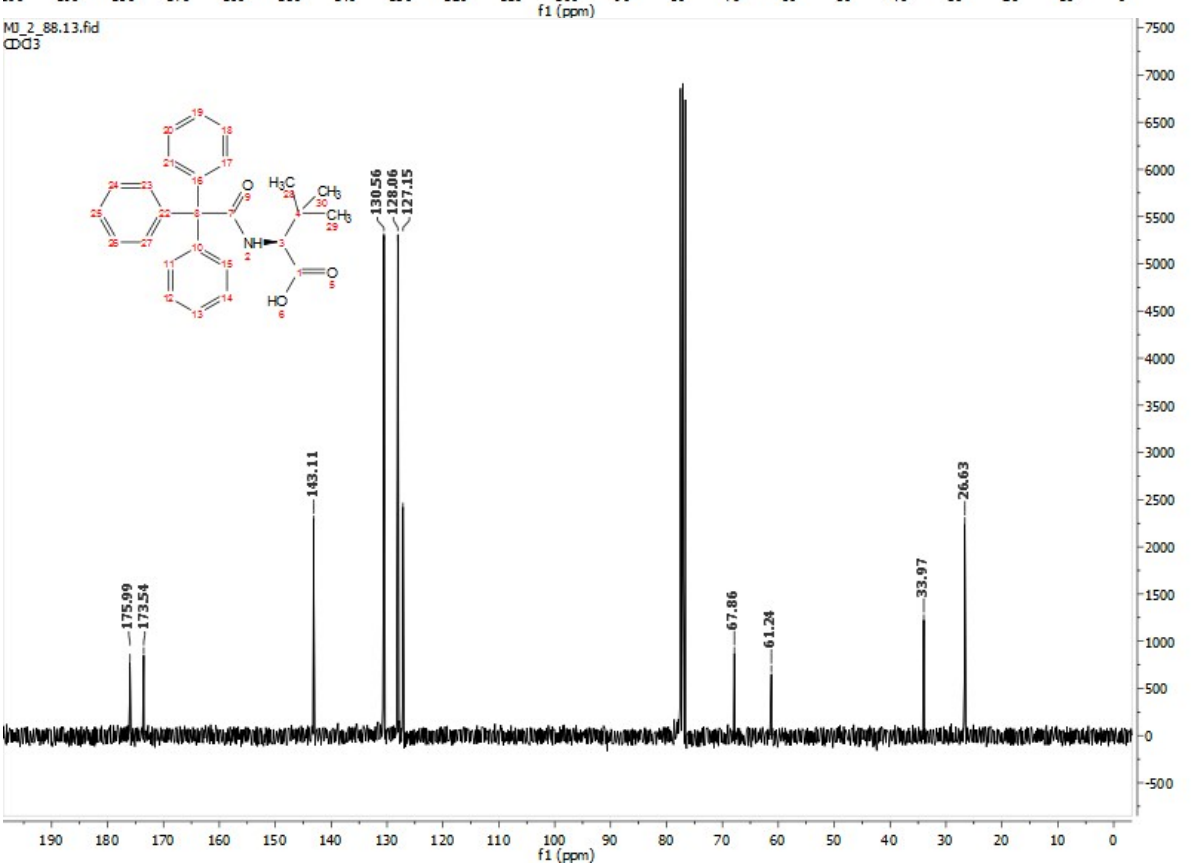
57.88
52.11
30.80
19.15
17.51
f1 (ppm)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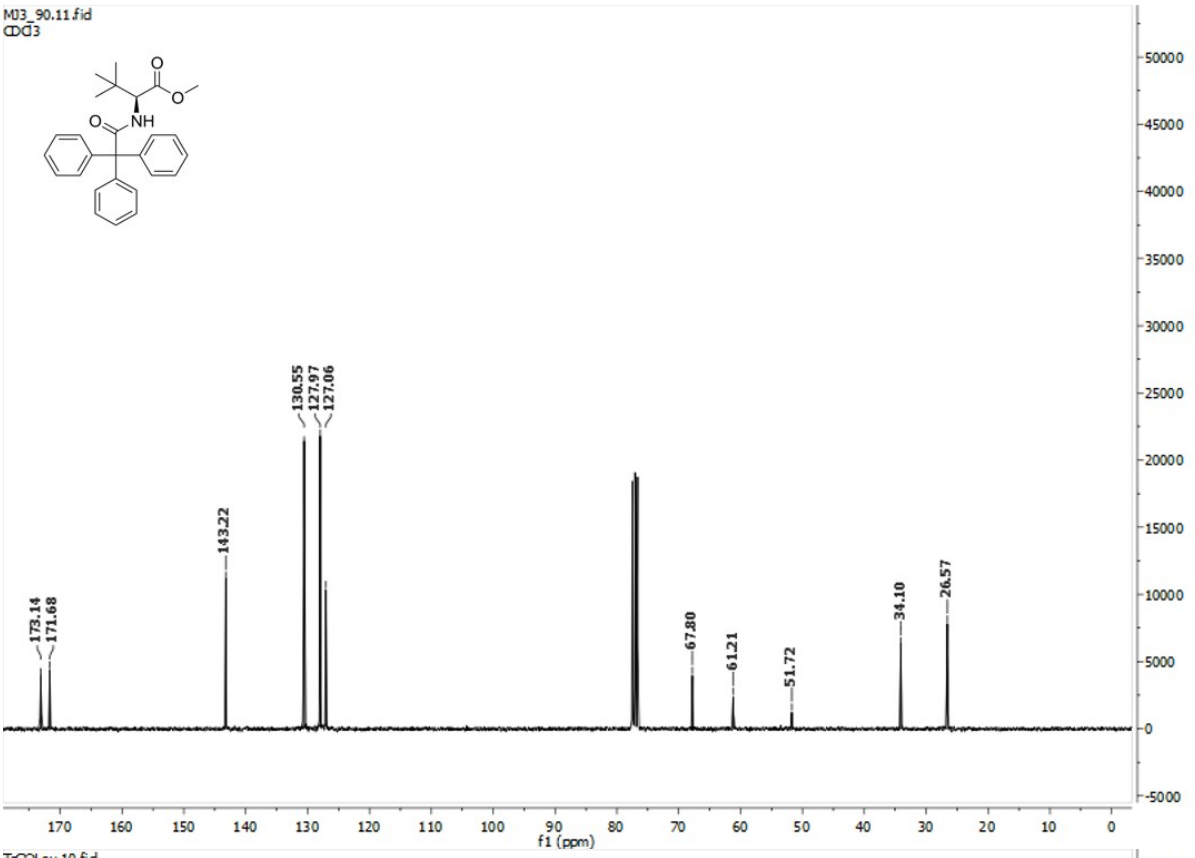
26.63
f1 (ppm)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O
O
NH
O
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130.55
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61.21
51.72
34.10
26.57
50000
45000
40000
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30000
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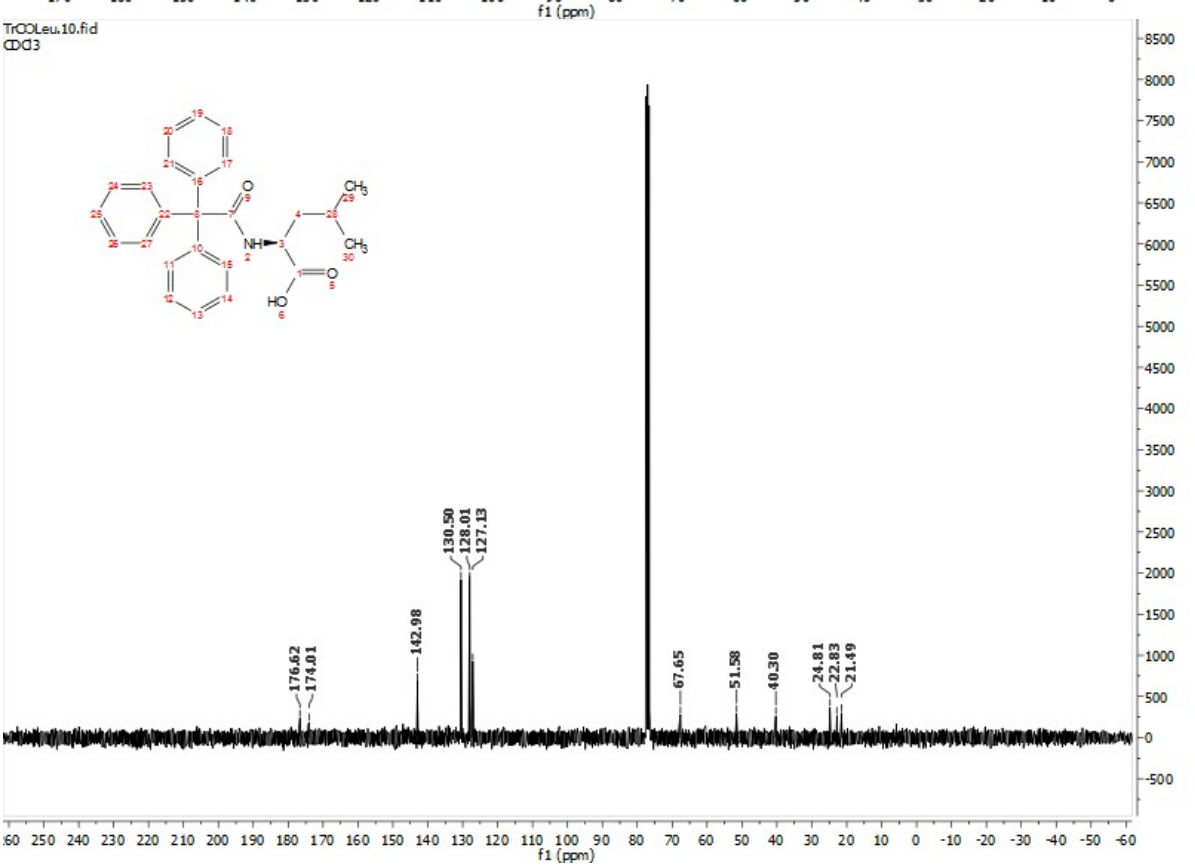
20000
15000
10000
5000
0
-5000
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


TrCOLeu.10.fid
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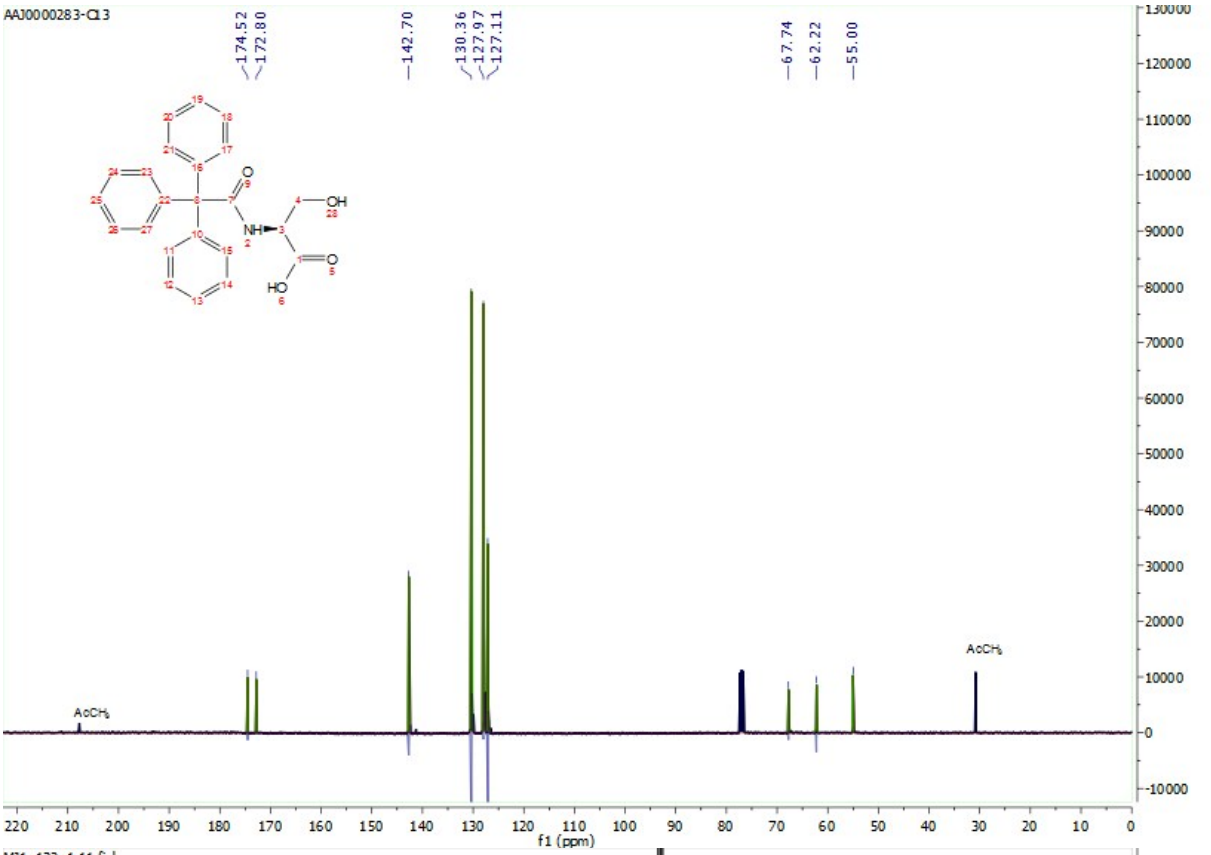
CH3
CH3
NH
HO
O
O
176.62
174.01
142.98
130.50
128.01
127.13
67.65
51.58
40.30
24.81
22.83
21.49
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
60 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)


AAJ0000283-C13
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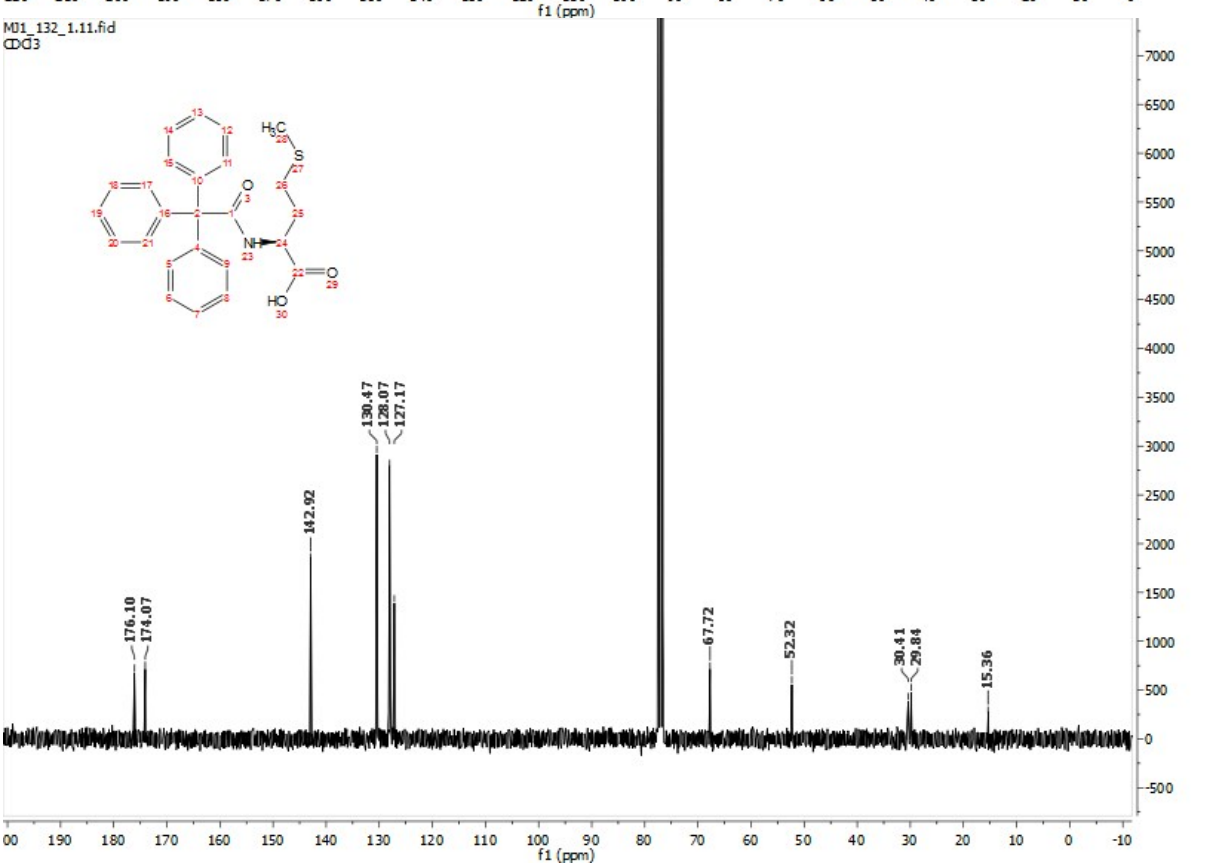
62.22
55.00
AcCH3
AcCH3
f1 (ppm)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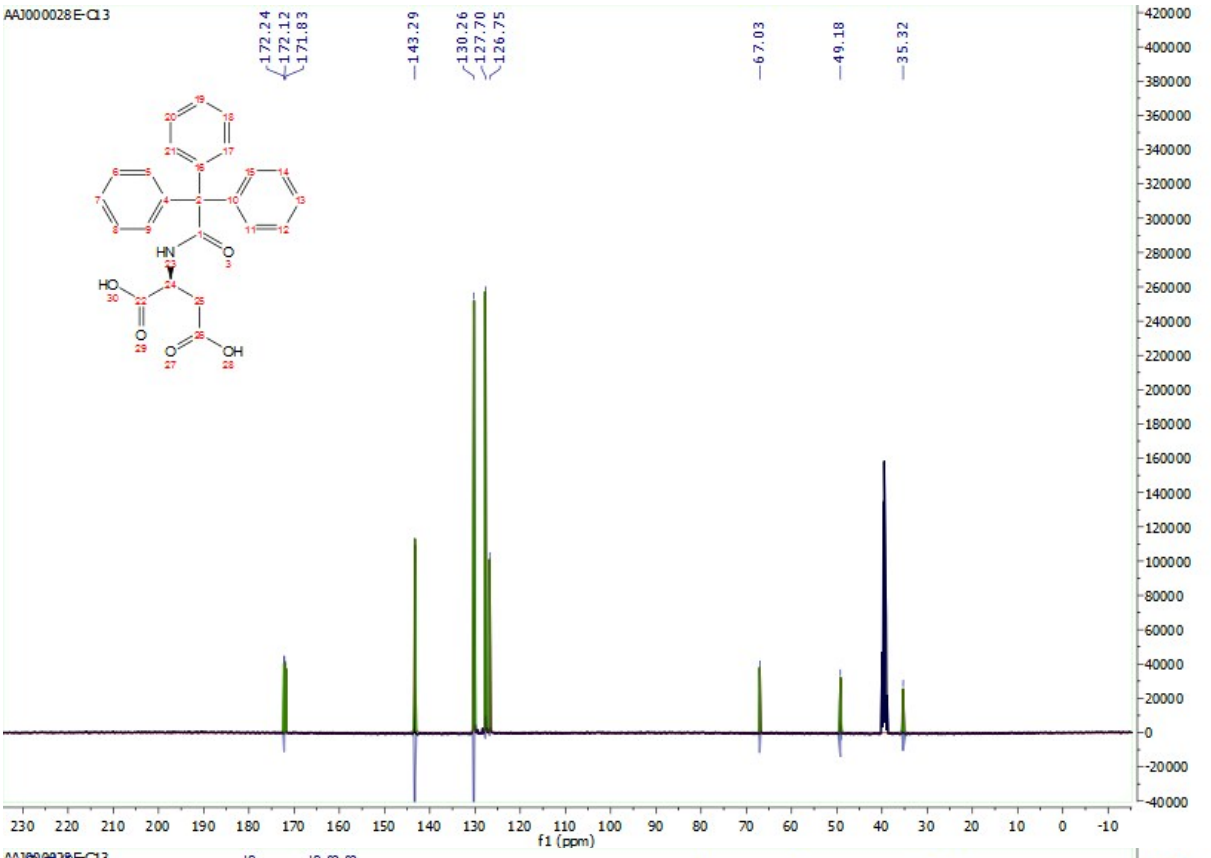
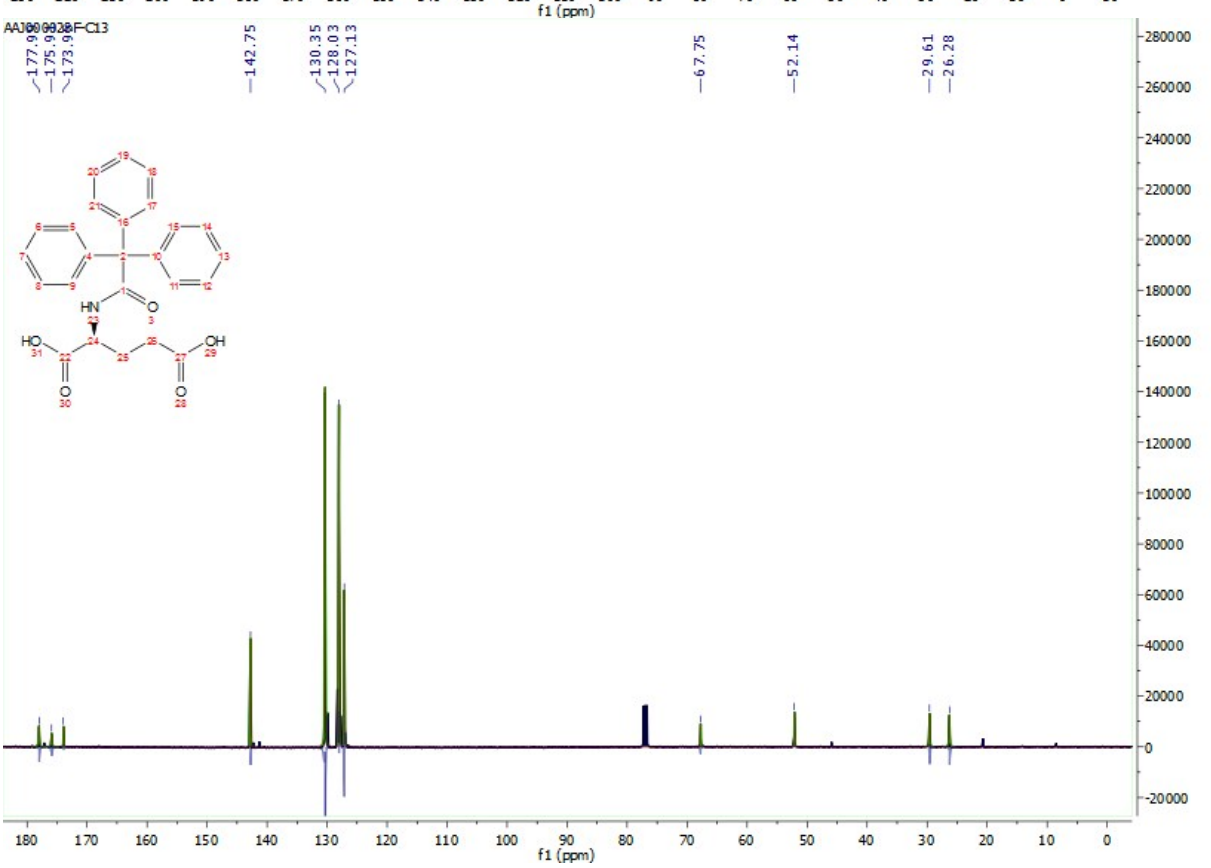
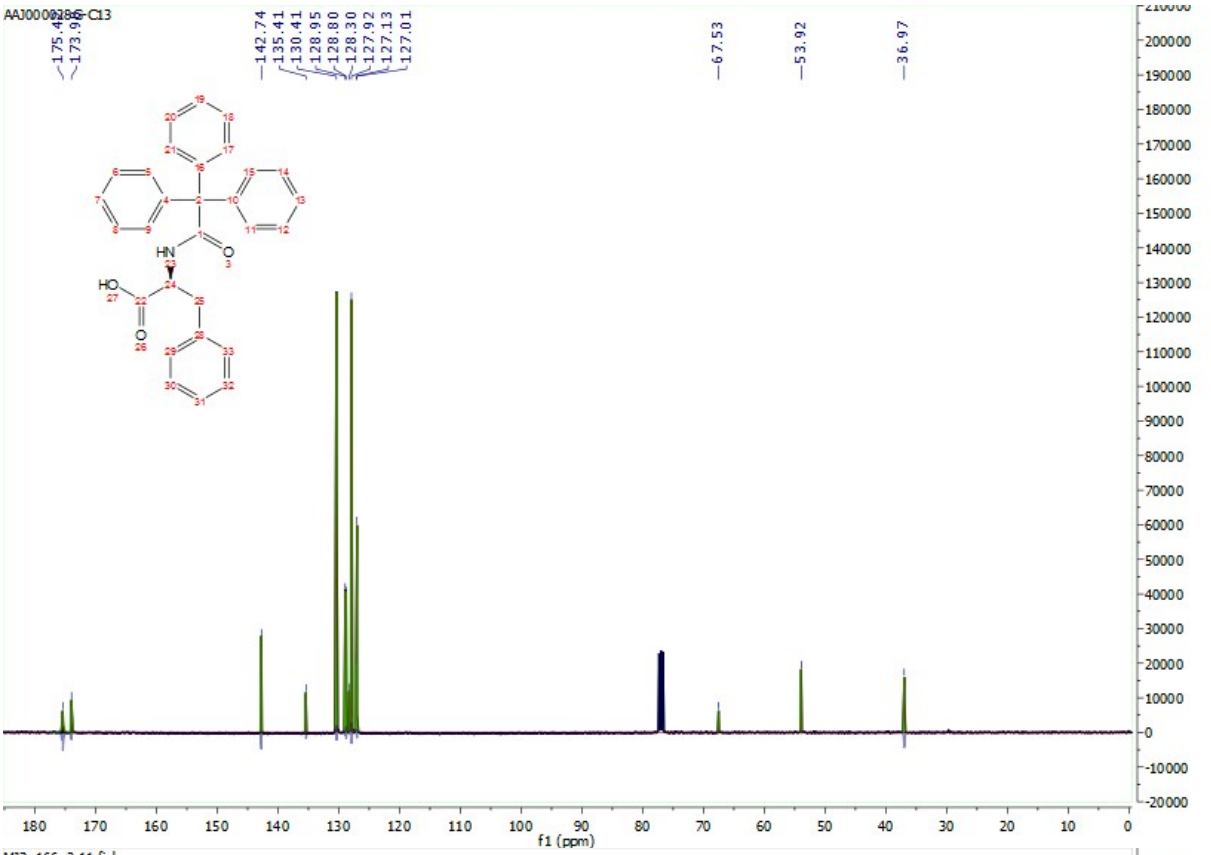
127.17
142.92
176.10
174.07
67.72
52.32
30.41
29.84
15.36
f1 (ppm)


AAJ000028E-C13
172.24
172.12
171.83
143.29
130.26
127.70
126.75
67.03
49.18
35.32
f1 (ppm)


142.75
130.35
128.03
127.13
67.75
52.14
29.61
26.28
f1 (ppm)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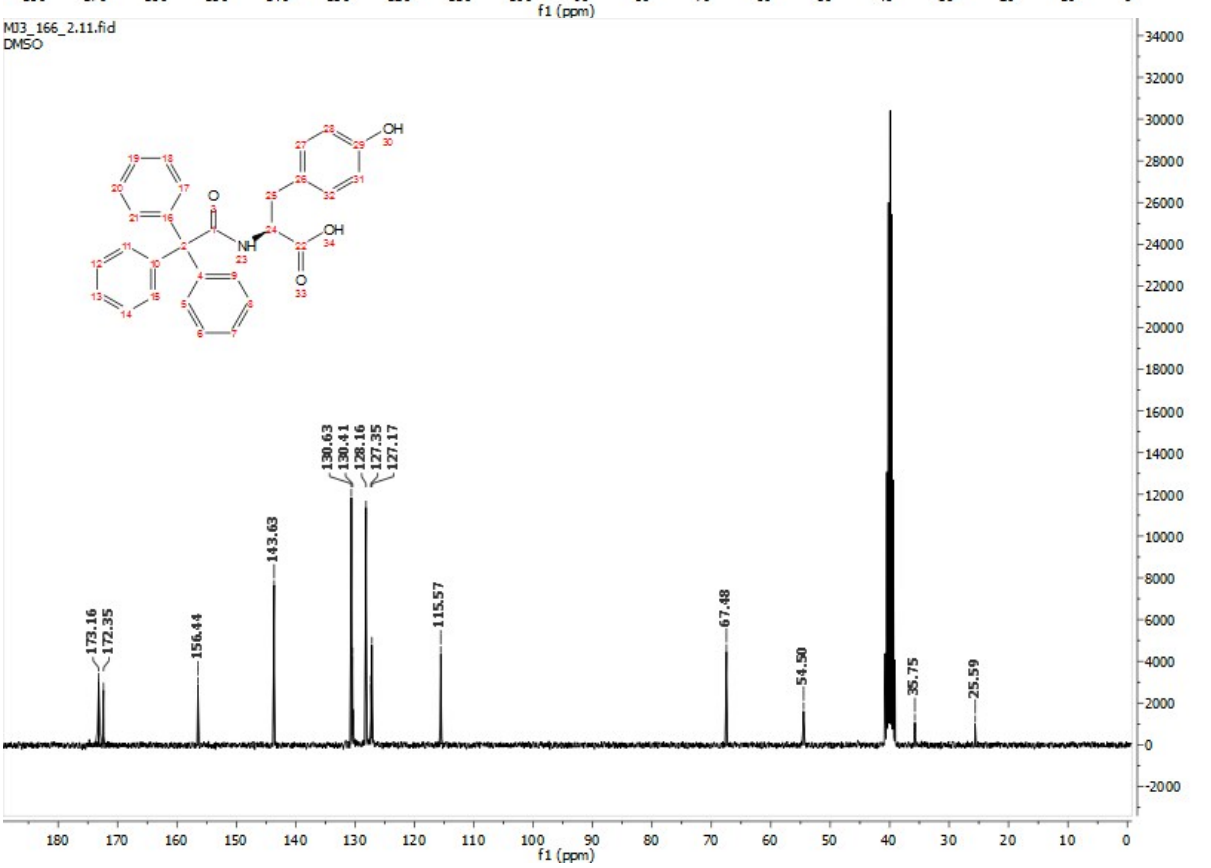
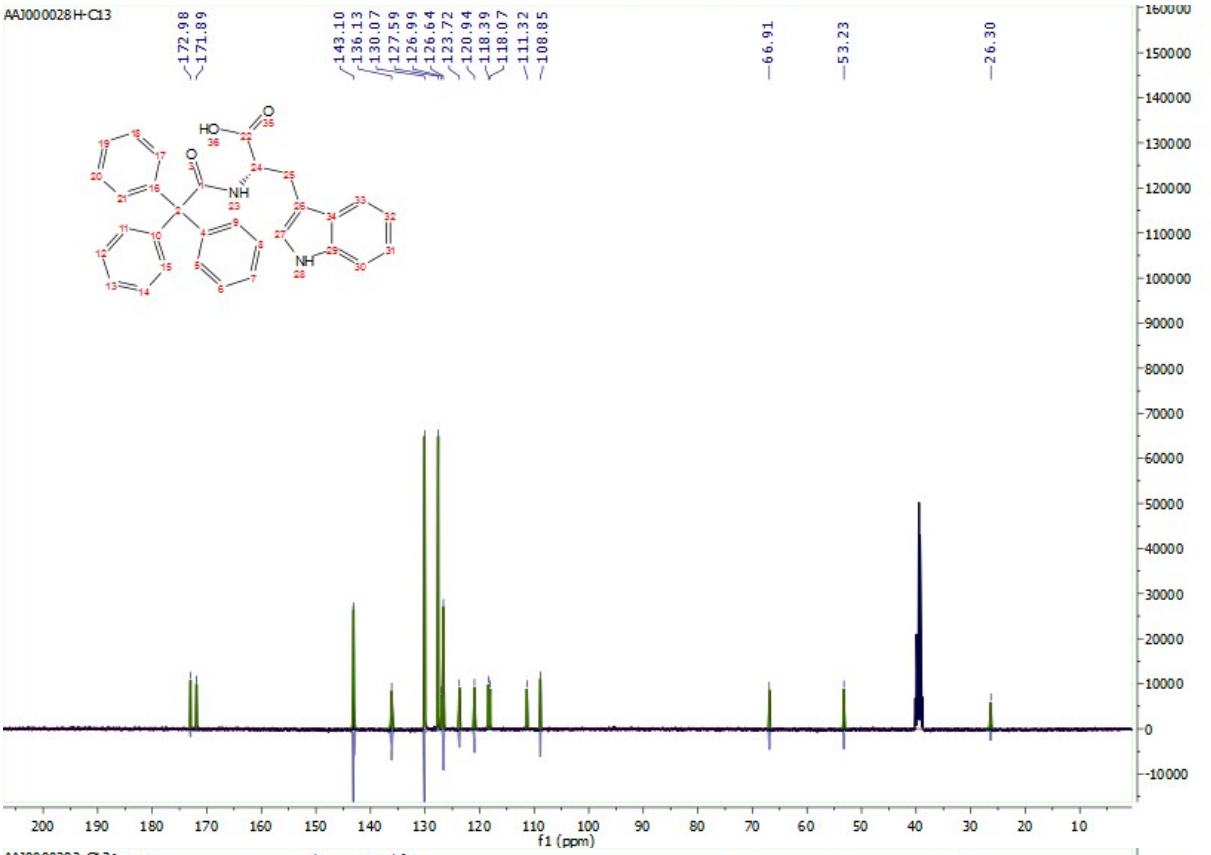
175.48
173.96
142.74
135.41
130.41
128.95
128.80
128.30
127.92
127.13
127.01
67.53
53.92
36.97
f1 (ppm)


M03_166_2.11.fid
DMSO
173.16
172.35
156.44
143.63
130.63
130.41
128.16
127.35
127.17
115.57
67.48
54.50
35.75
25.59
f1 (ppm)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171.89
143.10
136.13
130.07
127.59
126.99
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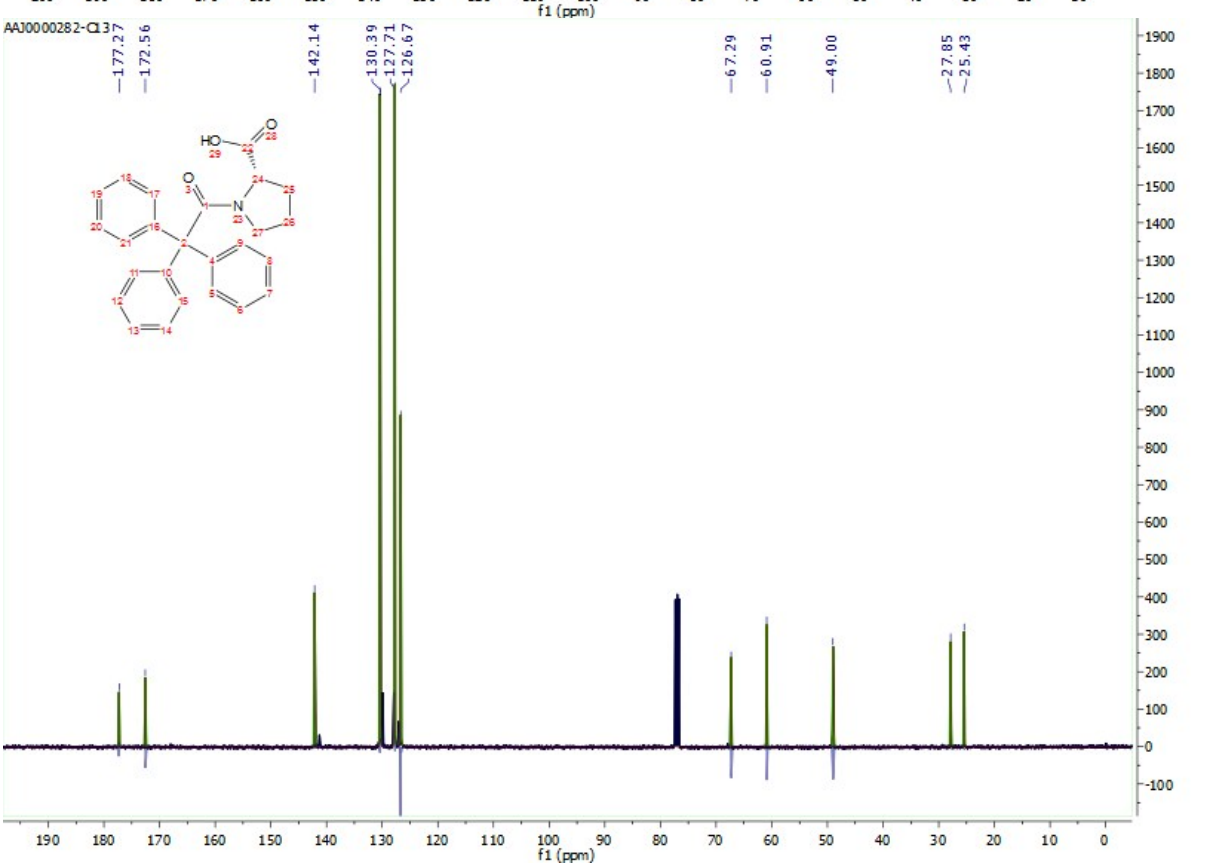
120.94
118.39
118.07
111.32
108.85
66.91
53.23
26.30
f1 (ppm)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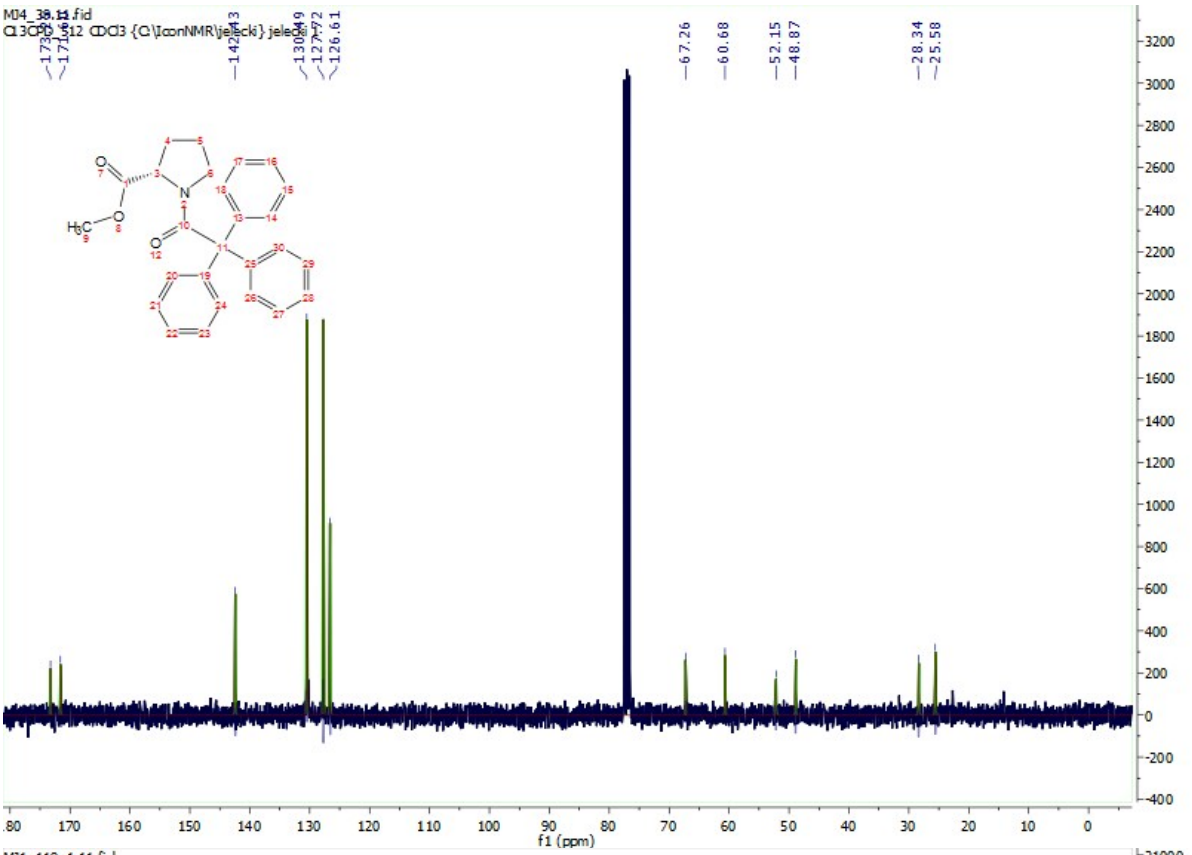
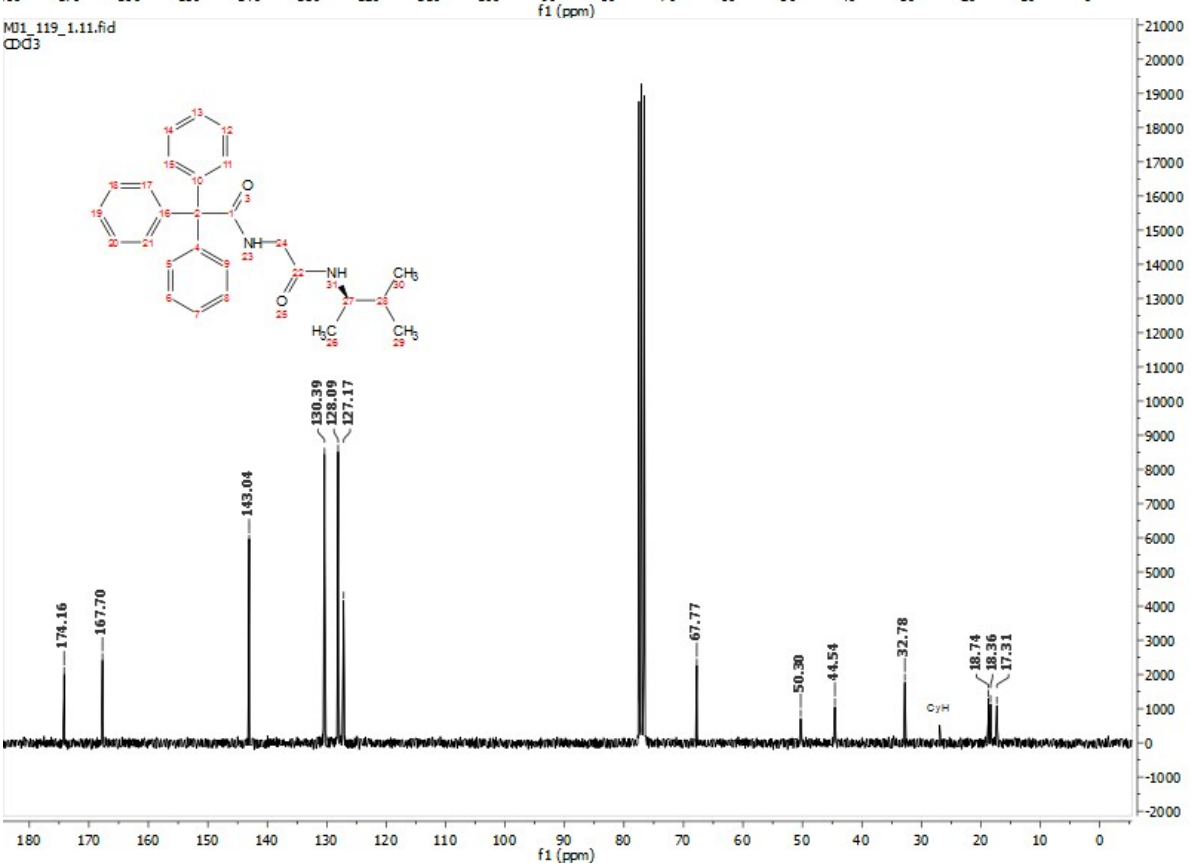
60.91
49.00
27.85
25.43
f1 (ppm)


MD4_38.11.fid
C13CPD_512 CDCl3 {C:\IconNMR\jeleck} jeleck
173.29
171.16
142.43
130.49
127.92
126.61
67.26
60.68
52.15
48.87
28.34
25.58
f1 (ppm)


MD1_119_1.11.fid
CDCl3
174.16
167.70
143.04
130.39
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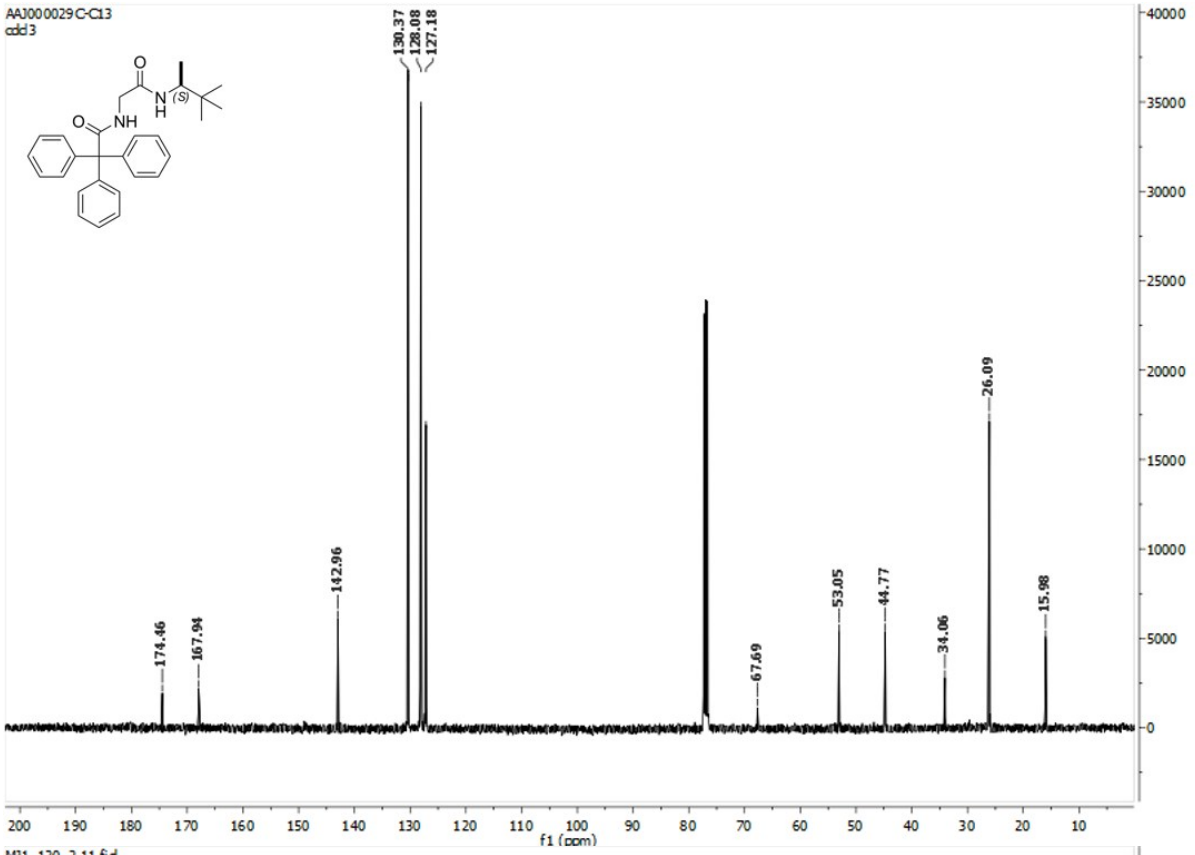
127.17
67.77
50.30
44.54
32.78
18.74
18.36
17.31
CyH
f1 (ppm)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cdcl3
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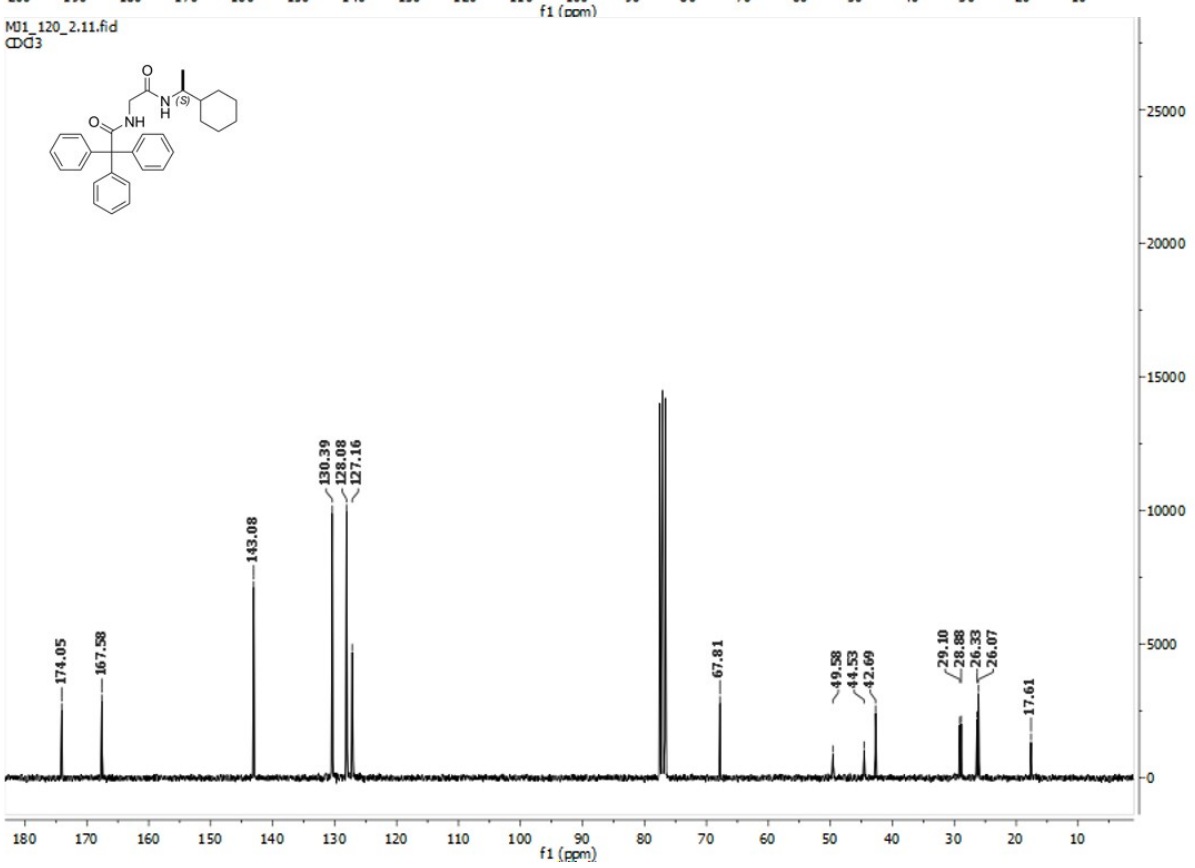
142.96
174.46
167.94
67.69
53.05
44.77
34.06
26.09
15.98
f1 (ppm)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130.39
128.08
127.16
174.05
167.58
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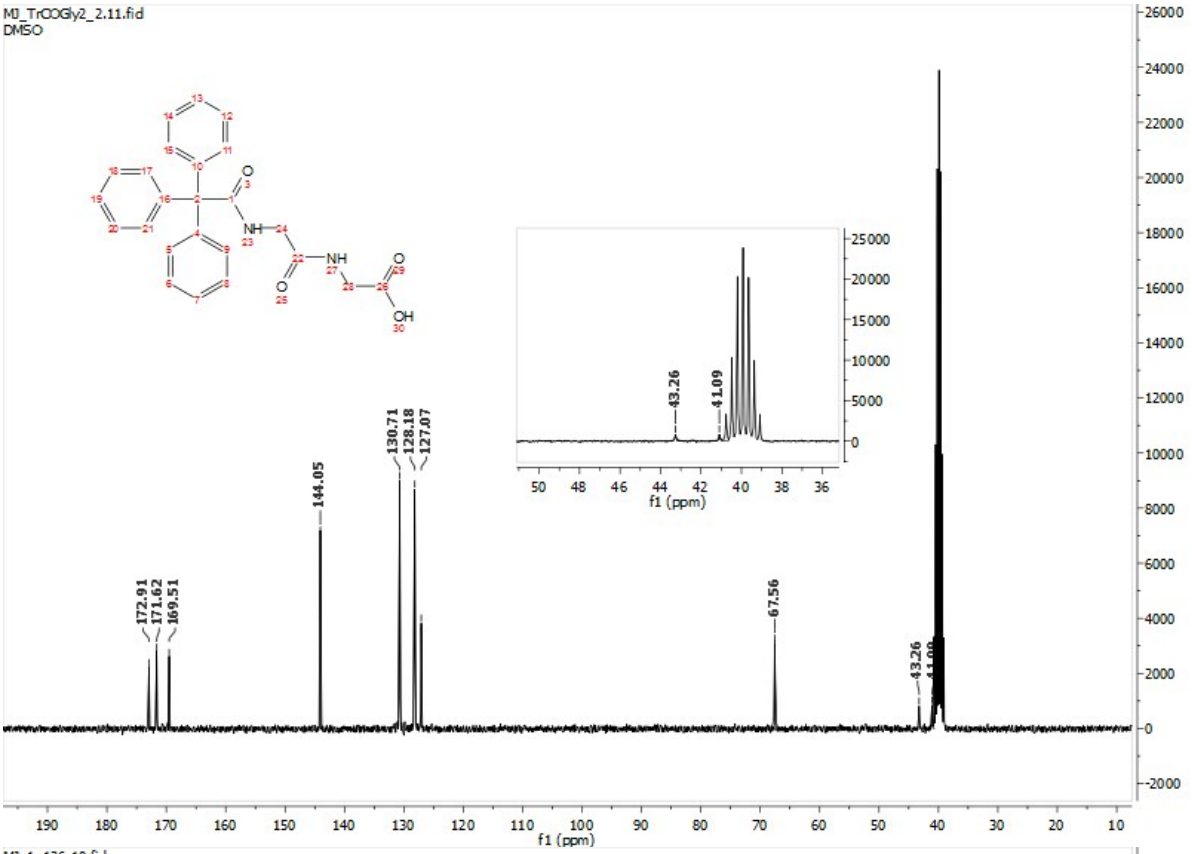
49.58
44.53
42.69
29.10
28.88
26.33
26.07
17.61
f1 (ppm)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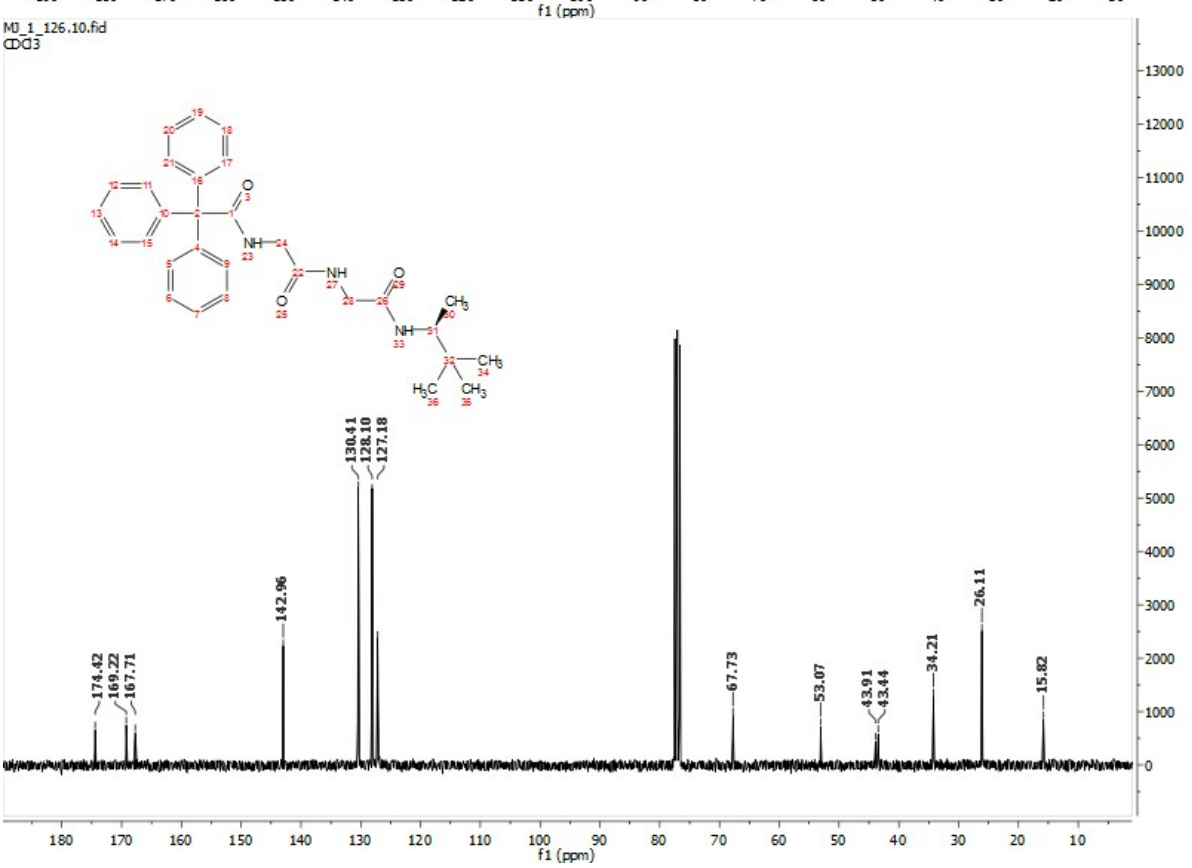
128.18
127.07
67.56
43.26
41.09
f1 (ppm)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CDCl3
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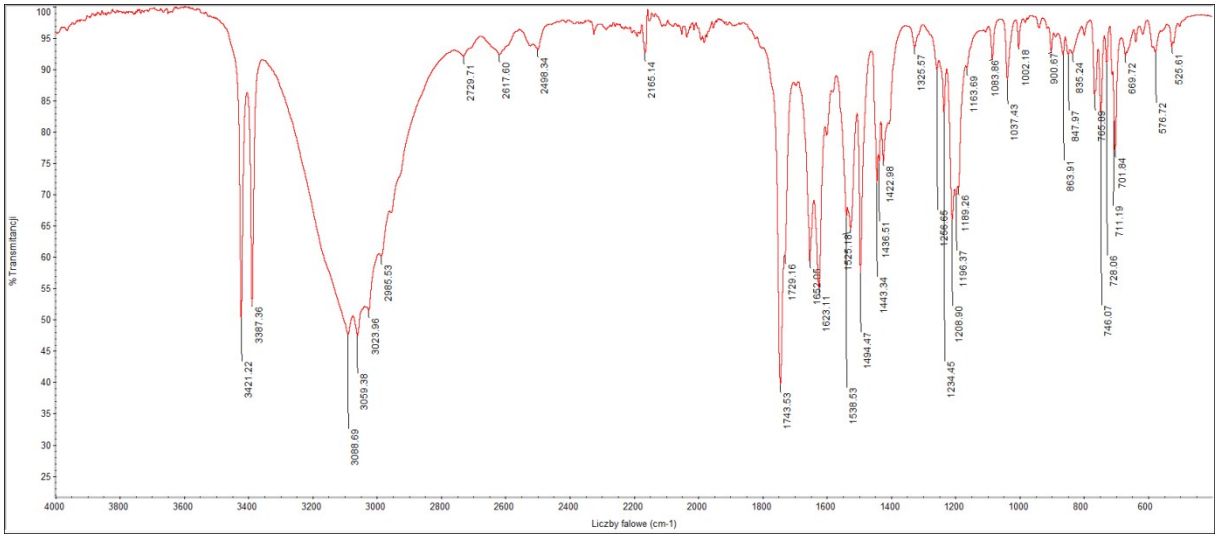
169.22
167.71
142.96
130.41
128.10
127.18
67.73
53.07
43.91
43.44
34.21
26.11
15.82
f1 (ppm)

Copies of IR spectra

1



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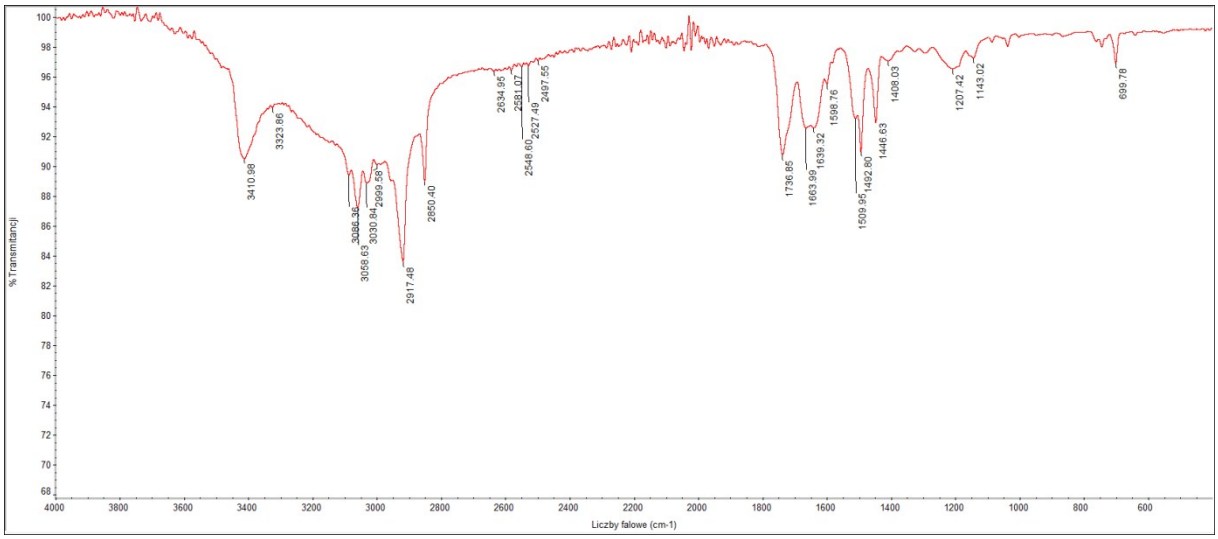
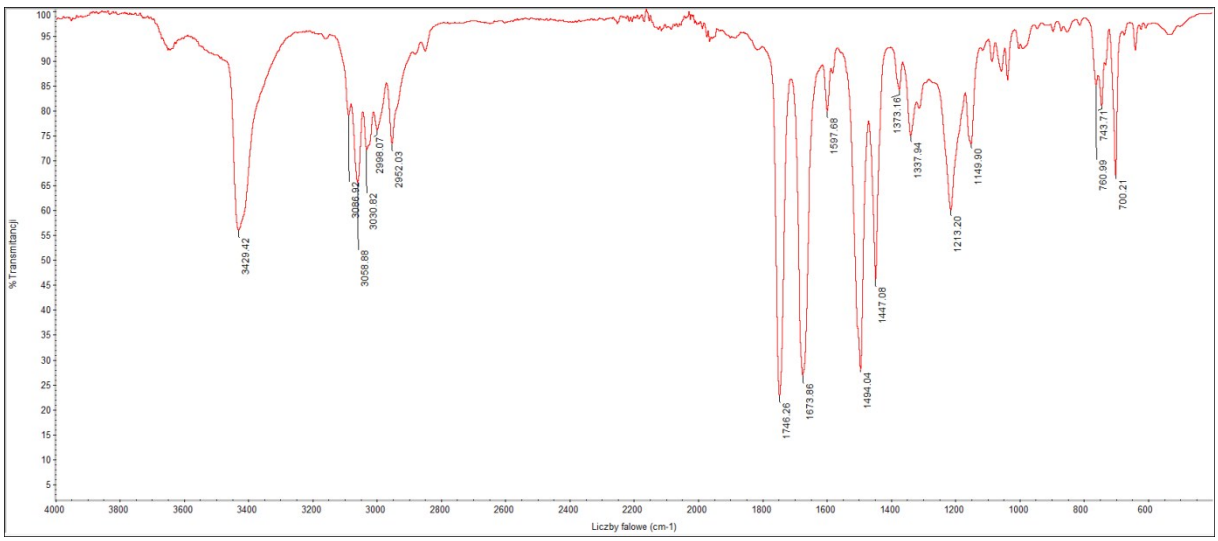


2b



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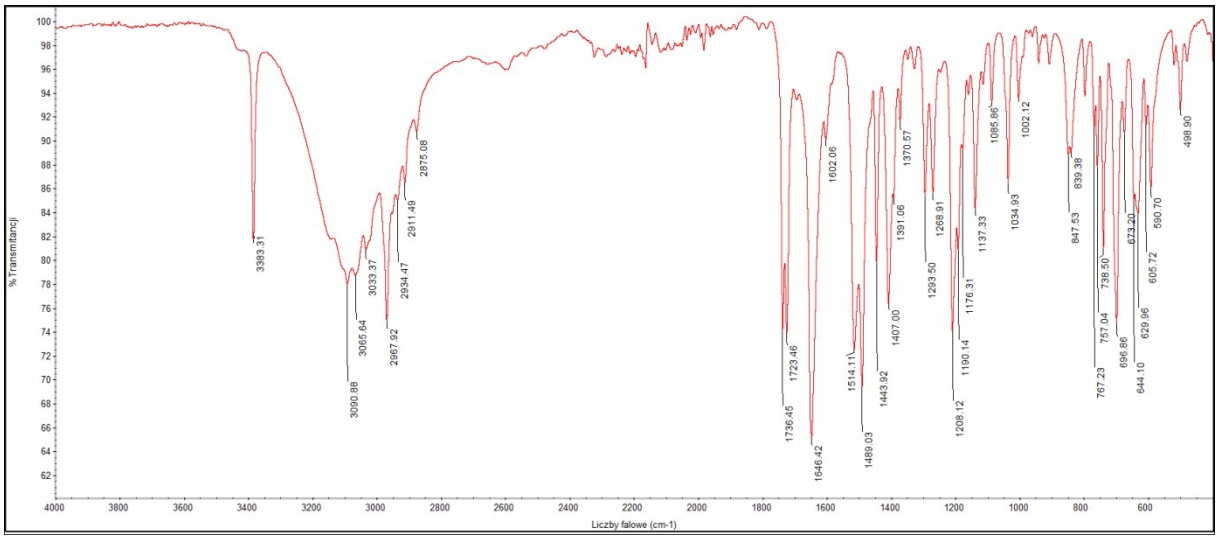
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Liczby falowe (cm-1)
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3033.37
2967.92
2934.47
2911.49
2875.08
1736.45
1723.46
1646.42
1602.06
1514.11
1489.03
1443.92
1407.00
1391.06
1370.57
1293.50
1268.91
1208.12
1190.14
1176.31
1137.33
1085.86
1034.93
1002.12
847.53
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767.23
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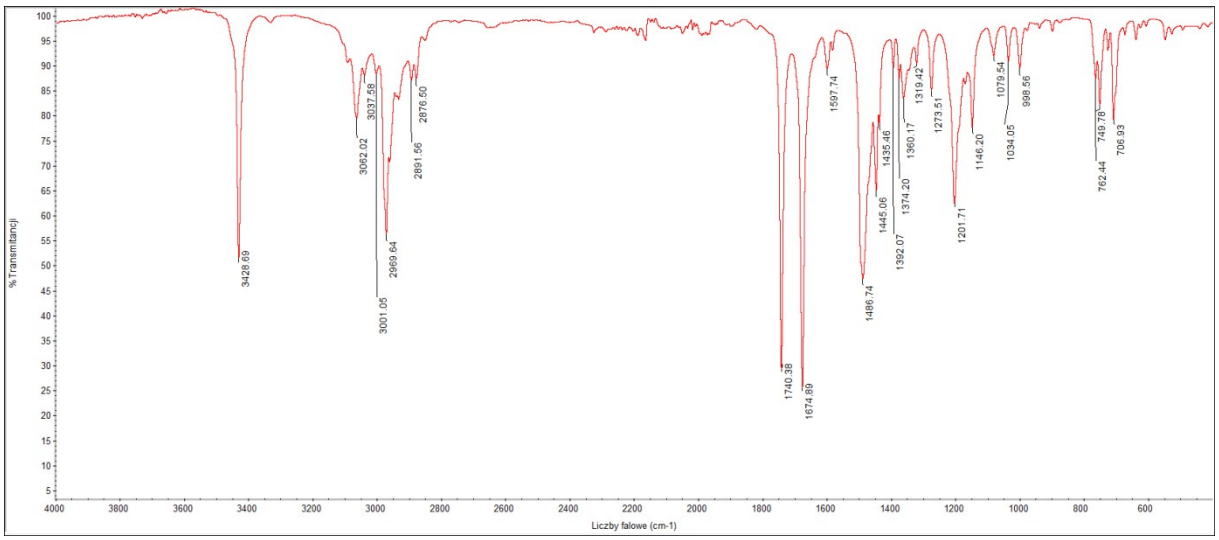
738.50
696.86
673.20
644.10
629.96
605.72
590.70
498.90

3b


%Transmitancji
Liczby falowe (cm-1)
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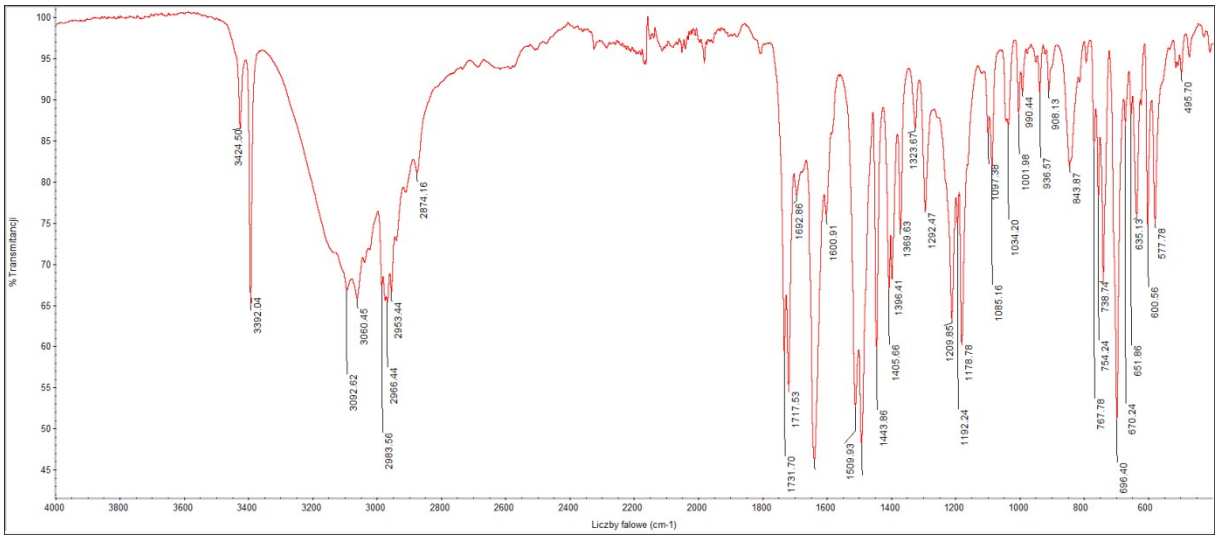
3001.05
2969.64
2891.56
2876.50
1740.38
1674.89
1597.74
1486.74
1445.46
1435.46
1392.07
1374.20
1360.17
1319.42
1273.51
1201.71
1146.20
1079.54
1034.05
998.56
762.44
749.78
706.93

4a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Liczby falowe (cm-1)
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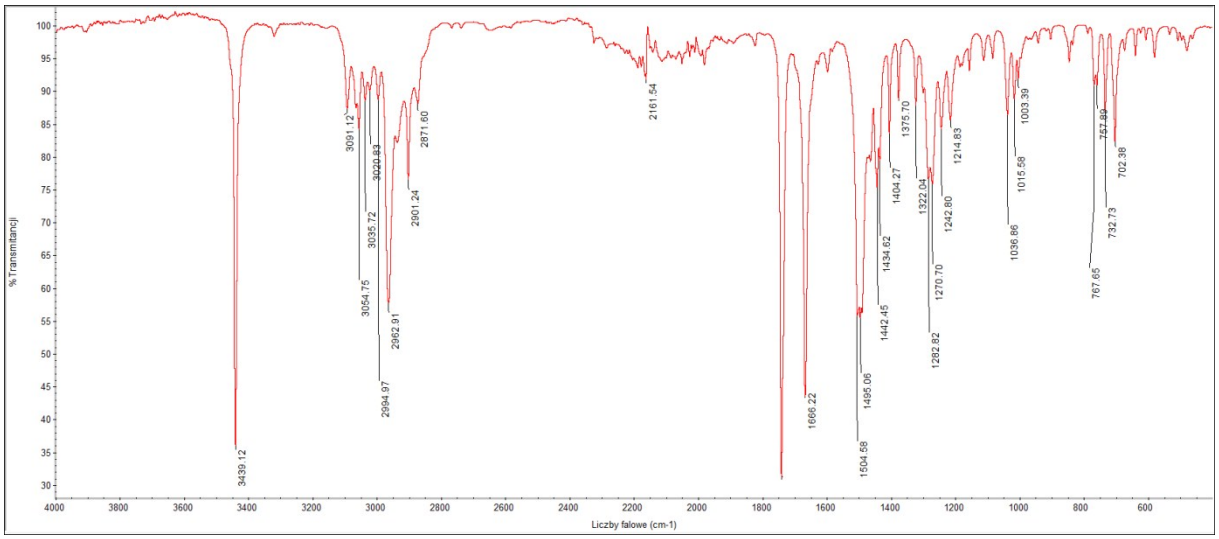
3392.04
3092.62
3060.45
2983.56
2966.44
2953.44
2874.16
1731.70
1717.53
1692.86
1600.91
1509.93
1443.86
1405.66
1396.41
1369.63
1323.67
1292.47
1209.86
1192.24
1178.78
1097.39
1085.16
1034.20
1001.98
990.44
936.57
908.13
843.87
767.78
754.24
738.74
696.40
670.24
651.86
635.13
600.56
577.78
495.70

4b


% Transmitancji
Liczby falowe (cm-1)
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3091.12
3054.75
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2994.97
2962.91
2901.24
2871.60
2161.54
1666.22
1504.58
1495.06
1442.45
1434.62
1404.27
1375.70
1322.04
1282.82
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767.65
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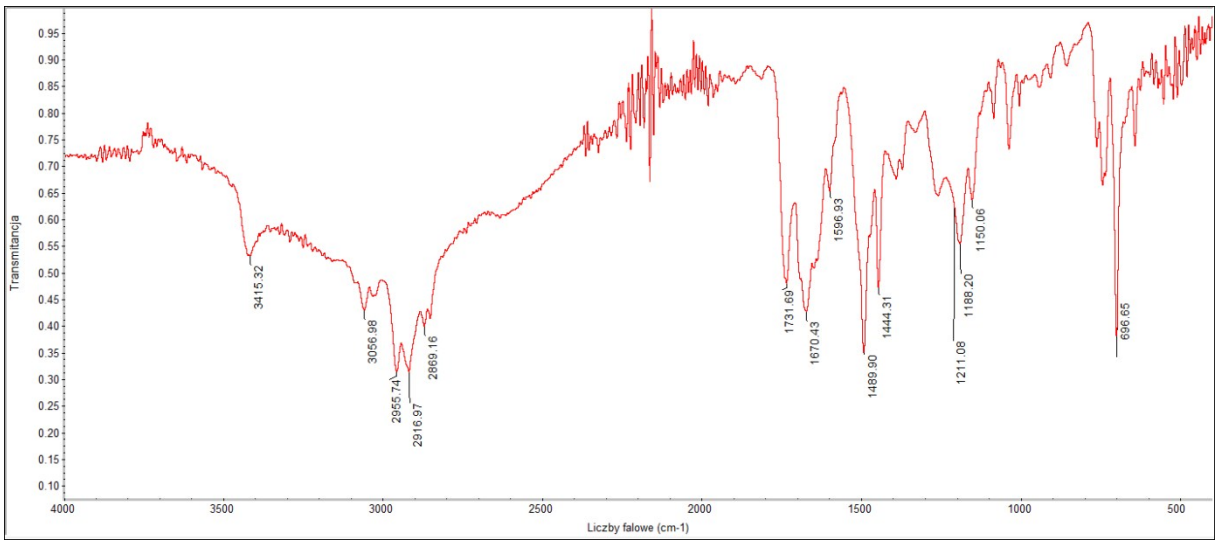
732.73
702.38

5


Transmitancja
Liczby falowe (cm-1)
3415.32
3056.98
2955.74
2916.97
2869.16
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1596.93
1489.90
1444.31
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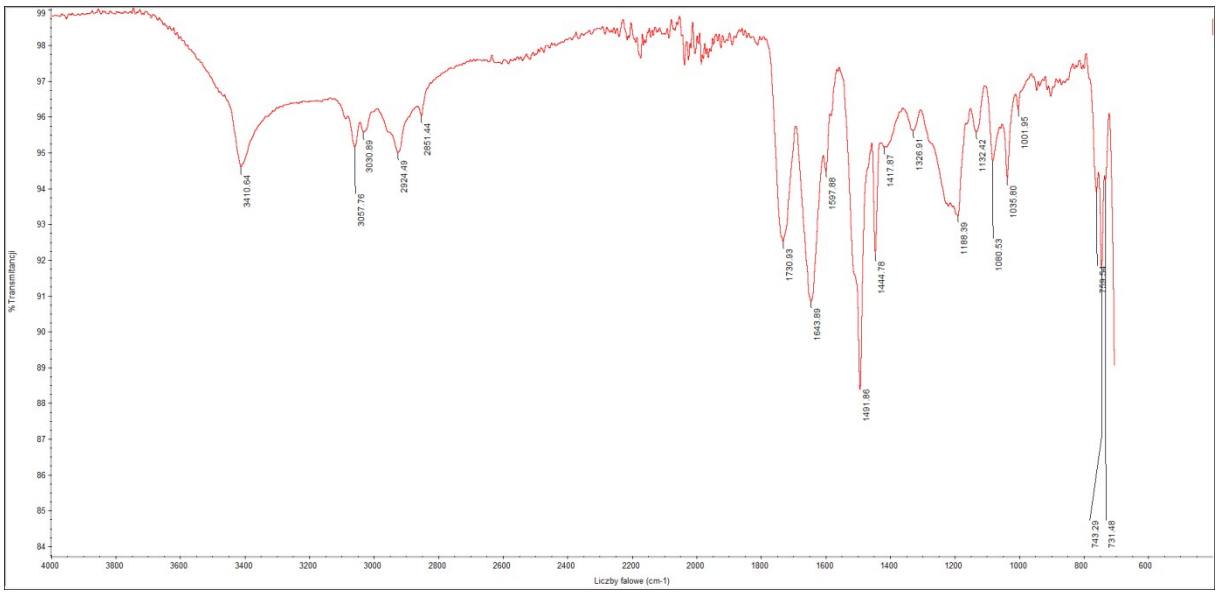
1150.06
696.65

6


% Transmitancji
Liczby falowe (cm-1)
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2924.49
2851.44
1730.93
1643.89
1597.88
1491.86
1444.76
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1326.91
1188.39
1132.42
1080.53
1035.80
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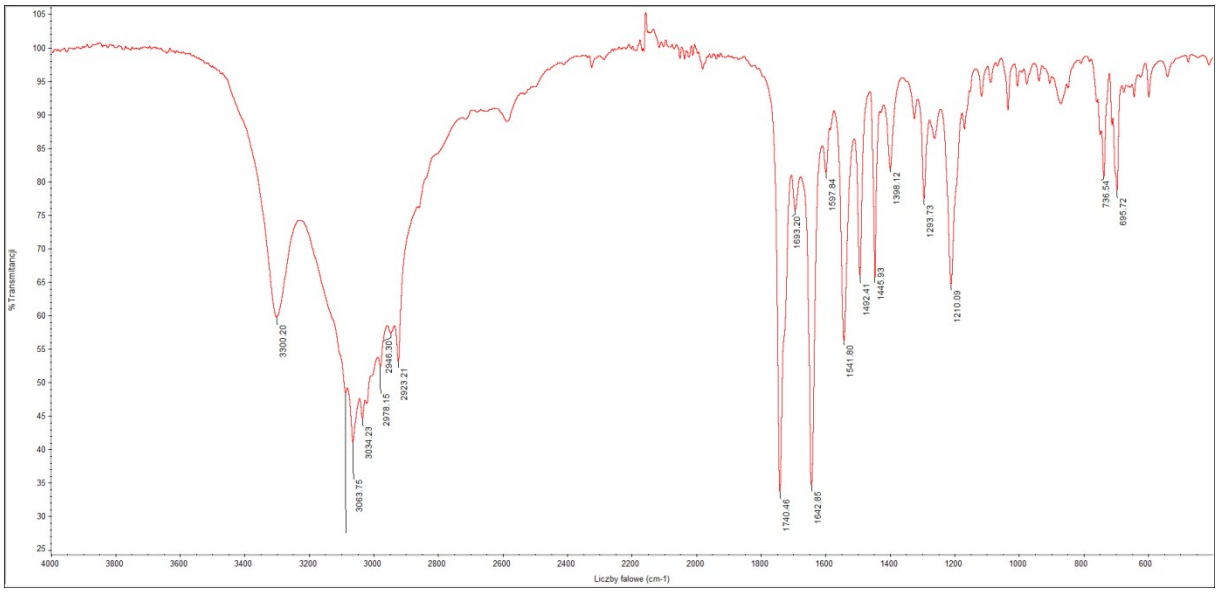
743.29
731.48

7


% Transmitancji
Liczby falowe (cm-1)
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3034.23
2978.15
2946.30
2923.21
1740.46
1693.20
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1541.80
1492.41
1445.93
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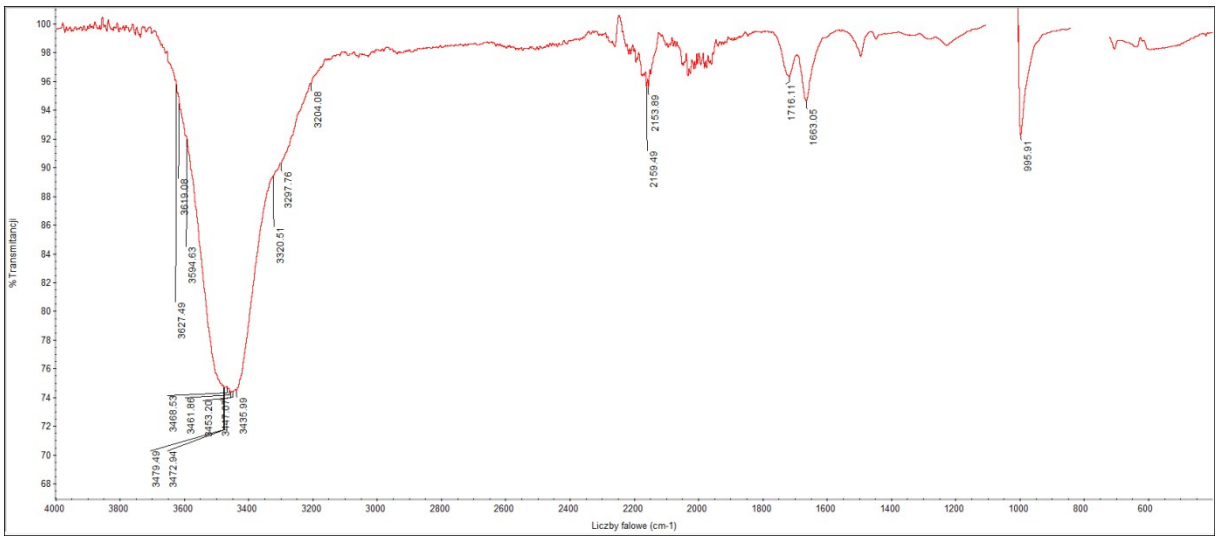
695.72

8


% Transmitancji
Liczby falowe (cm-1)
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3479.49
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3468.53
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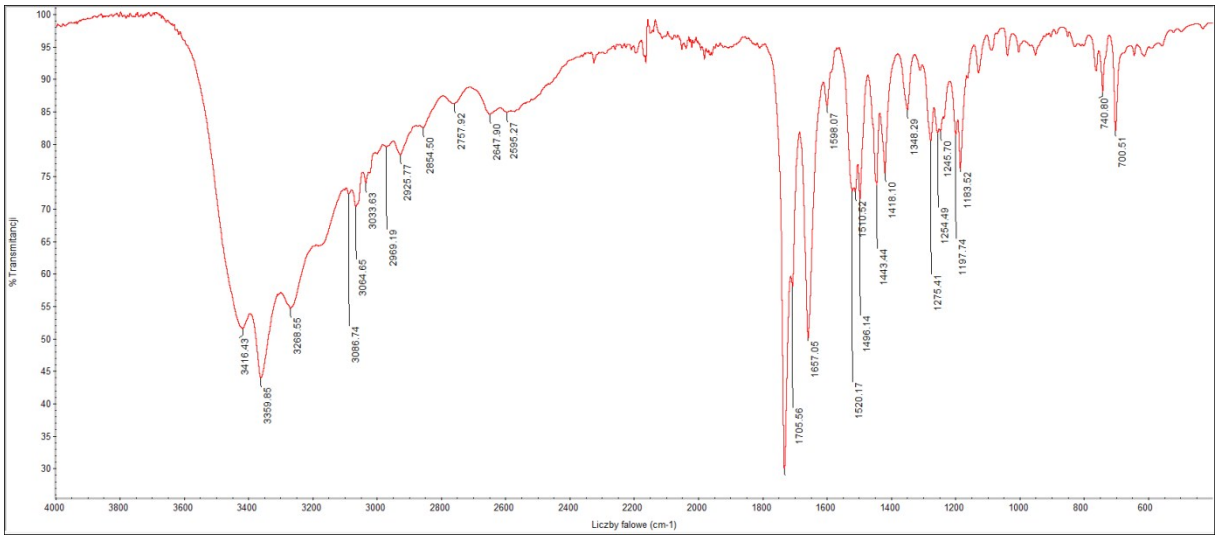
9


% Transmitancji
Liczby falowe (cm-1)
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3033.63
2969.19
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2757.92
2647.90
2596.27
1705.56
1657.05
1598.07
1520.17
1510.52
1496.14
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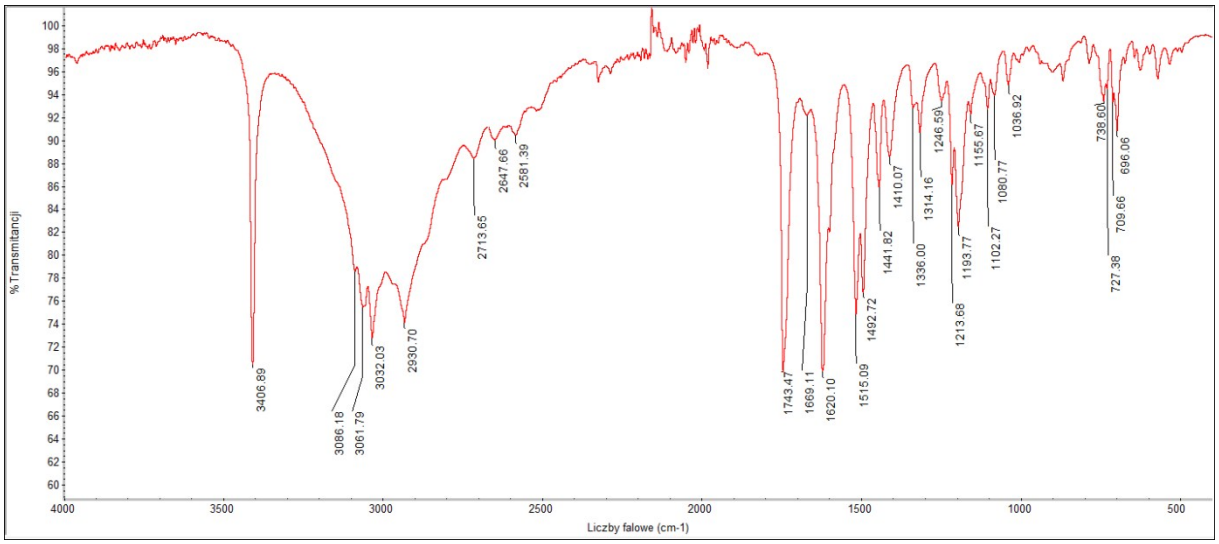
10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Liczby falowe (cm-1)
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1743.47
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1620.10
1515.09
1492.72
1441.82
1410.07
1336.00
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1246.59
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738.60
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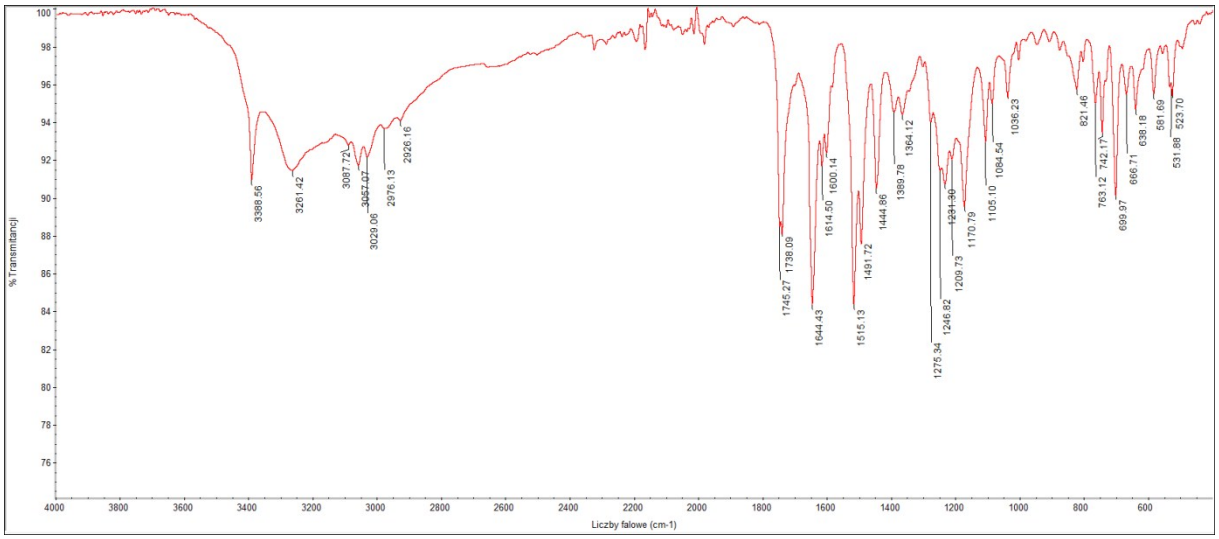
709.66
696.06

11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Liczby falowe (cm-1)
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3057.07
3029.06
2976.13
2926.16
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1738.09
1644.43
1614.50
1600.14
1515.13
1491.72
1444.86
1389.78
1364.12
1275.34
1246.82
1231.30
1209.73
1170.79
1105.10
1084.54
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763.12
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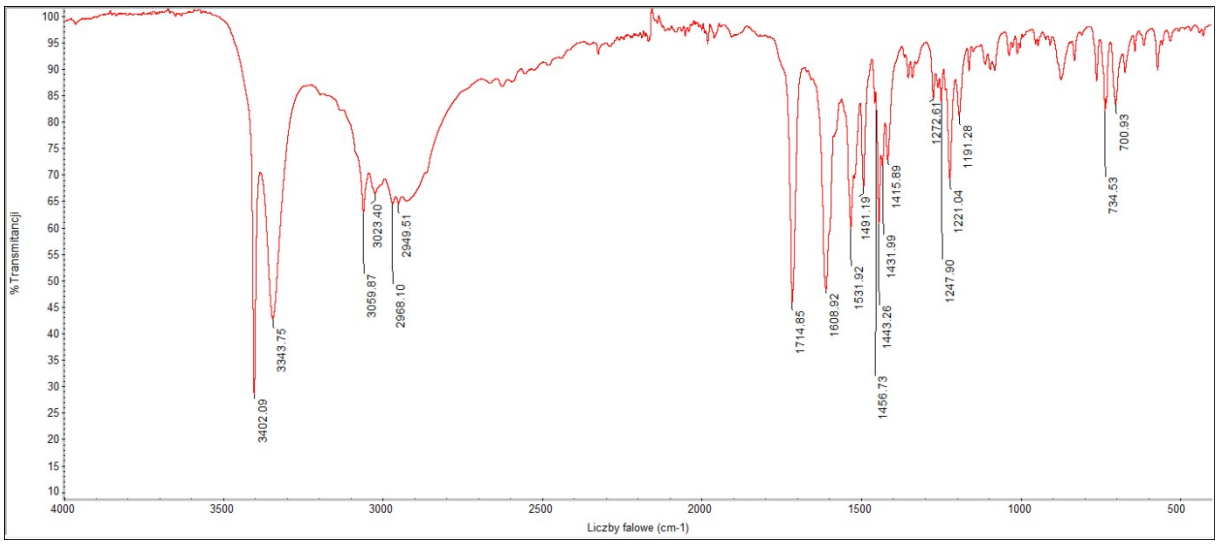
12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Liczby falowe (cm-1)
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2968.10
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1608.92
1531.92
1491.19
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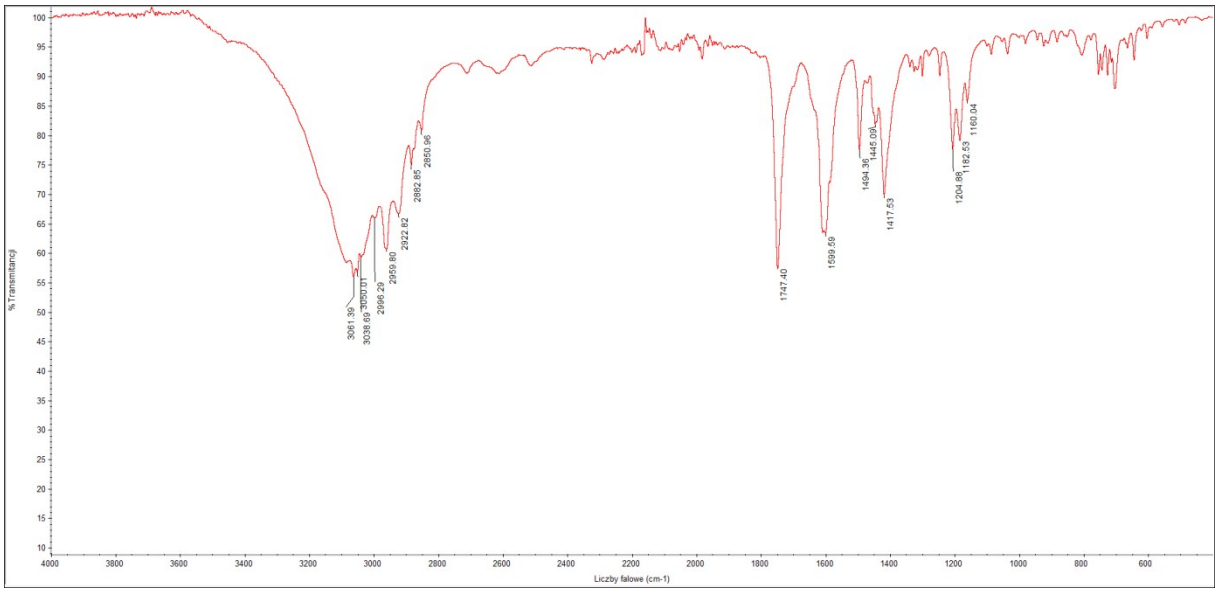
13a


% Transmitancj
Liczby falowe (cm-1)
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3000.01
2966.29
2959.80
2922.82
2882.85
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1599.58
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1445.09
1417.53
1204.98
1182.53
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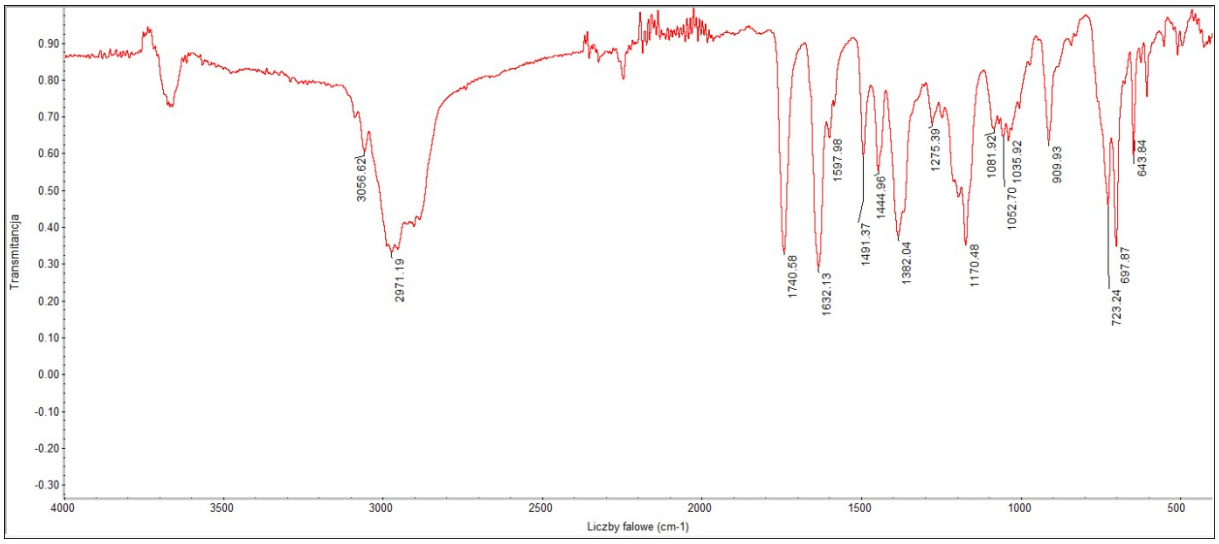
13b


Transmitancja
Liczby falowe (cm-1)
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1632.13
1597.98
1491.37
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1081.92
1052.70
1035.92
909.93
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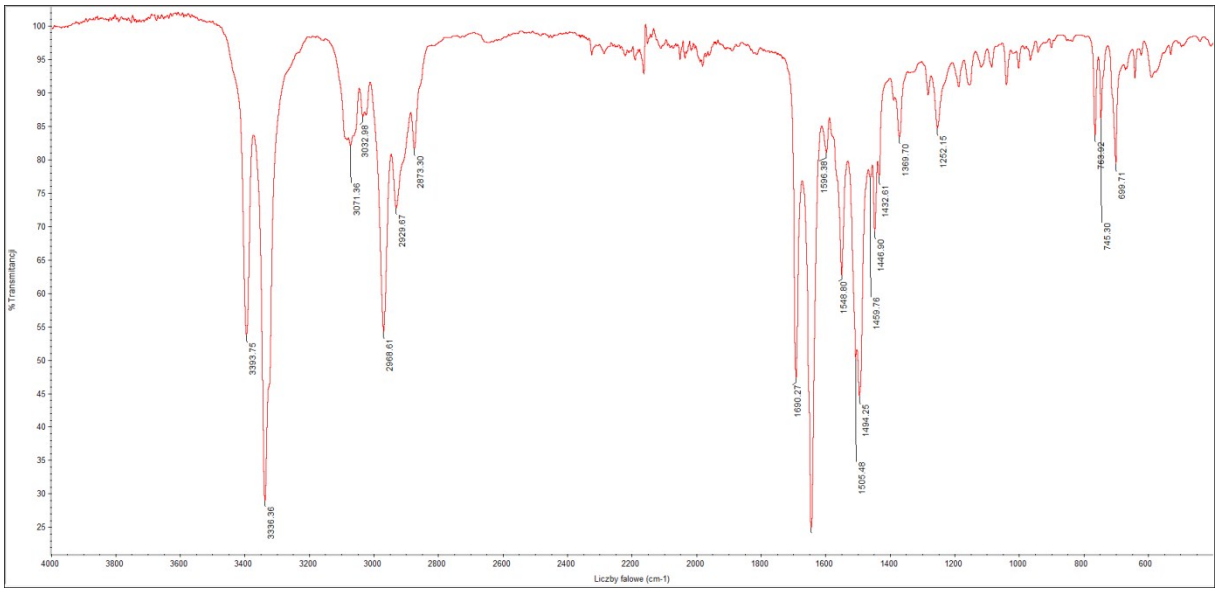
697.87
643.84

14


% Transmitancj
Liczby falowe (cm-1)
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3336.36
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3032.88
2929.67
2873.30
2668.61
1690.27
1596.38
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1432.61
1369.70
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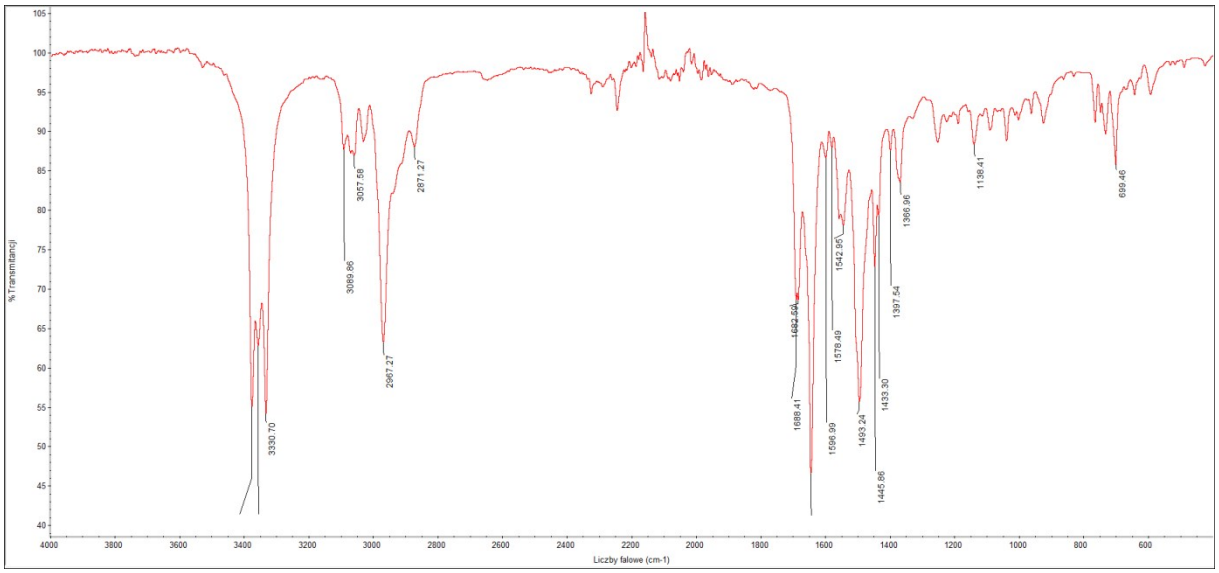
745.30
699.71

15


% Transmitancji
Liczby falowe (cm-1)
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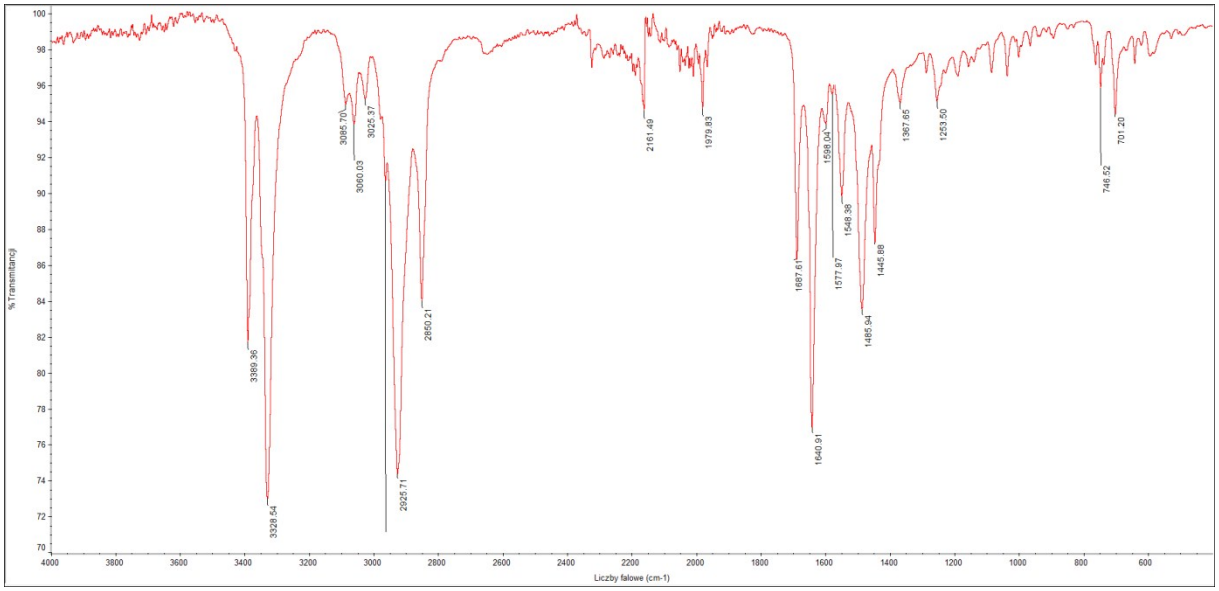
699.46

16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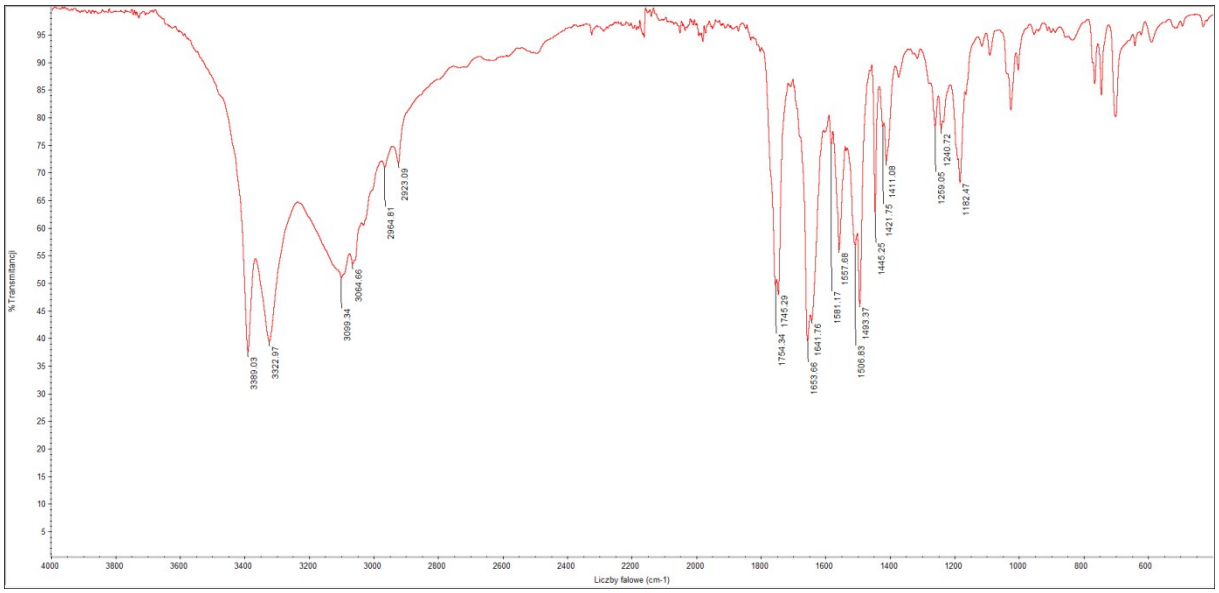
17


% Transmitancji
Liczby falowe (cm-1)
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1653.66
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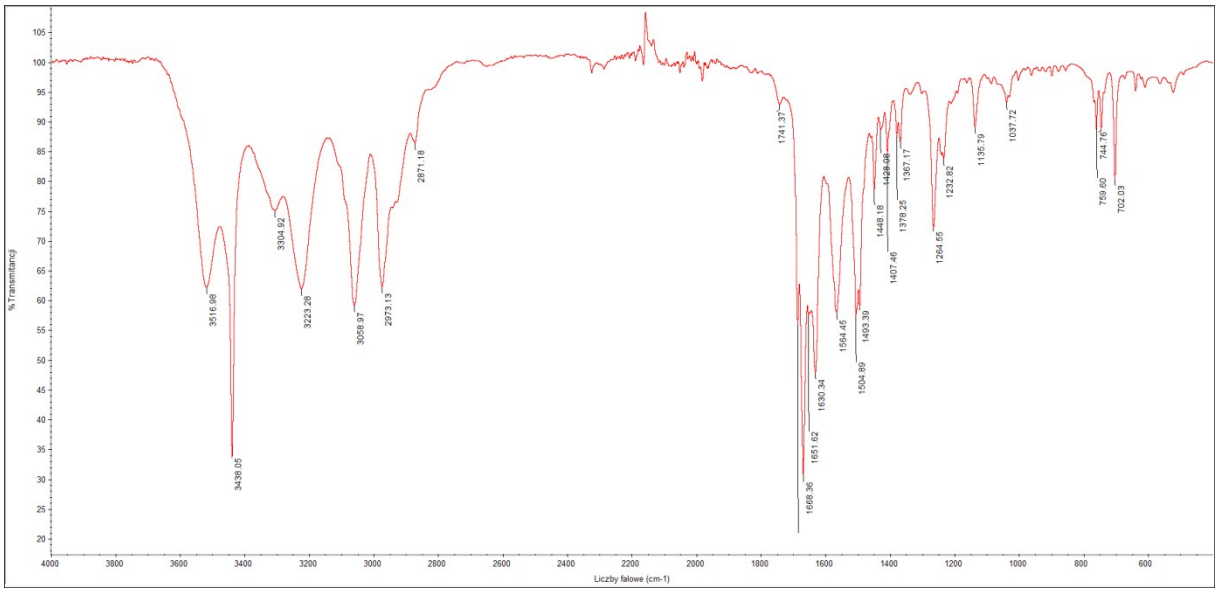
1182.47

18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1037.72
759.60
744.76
702.03

Cartesian coordinates for all calculated structures.

Compound **2b** conf. 2

C	0.73557000	0.01886500	-0.02589900
C	1.80604200	-0.92850200	-0.63422600
C	3.79056200	-2.66887900	-1.62896700
C	3.16661000	-0.61999400	-0.50824900
C	1.46206600	-2.12707500	-1.26896000
C	2.44217400	-2.98651600	-1.76461300
C	4.14775600	-1.48040400	-0.99532800
H	3.46498100	0.30422800	-0.02962700
H	0.42171500	-2.40300400	-1.38551100
H	2.14565000	-3.90380000	-2.26129400
H	5.19335500	-1.21493100	-0.88434900
H	4.55313300	-3.33494200	-2.01664700
C	1.21559700	1.48907400	-0.19247700
C	2.19489800	4.11571700	-0.54829000
C	1.41124100	2.02260200	-1.47681600
C	1.55448200	2.29125100	0.90308600
C	2.03620000	3.59054600	0.72888900
C	1.88335000	3.31996300	-1.64996900
H	1.18387700	1.42139700	-2.34379100
H	1.45684400	1.91153300	1.91049600
H	2.28927600	4.18471400	1.60027500
H	2.01346300	3.70705600	-2.65471600
H	2.56510600	5.12561400	-0.68607000
C	0.48524900	-0.31939800	1.46272300
C	-0.04517200	-0.88150500	4.17961200
C	1.21335700	-1.29242200	2.15363600
C	-0.52146100	0.36622700	2.16623600
C	-0.78495800	0.08999000	3.50402400
C	0.95254900	-1.56950400	3.49793400
H	1.99314800	-1.84481700	1.64689700
H	-1.10857900	1.12200100	1.65707400
H	-1.56760000	0.63568700	4.01952200
H	1.53565800	-2.32906100	4.00683300
H	-0.24738100	-1.09732400	5.22265400
C	-0.59238400	-0.19429700	-0.85823100
O	-0.75704700	0.28857700	-1.96505300
N	-1.52361000	-1.03313800	-0.31889000
C	-2.77567000	-1.29799500	-1.00473000
C	-3.75912400	-0.11967800	-1.01922500
O	-4.68947300	-0.06070700	-1.78426800
H	-1.44429900	-1.29527900	0.65135800
H	-2.55323300	-1.47795500	-2.05842000
C	-3.46026400	-2.53337400	-0.40564600
H	-4.39608900	-2.73055200	-0.92929300
H	-2.81215700	-3.40648900	-0.50574700
H	-3.68396000	-2.38708100	0.65550900
O	-3.50311400	0.80050100	-0.07415100
C	-4.38612800	1.94064100	-0.05783000
H	-4.33223100	2.46934900	-1.00976700
H	-4.02961000	2.57308700	0.75204200
H	-5.41396800	1.62357200	0.12247300

Compound **2b** conf. 25

C	0.90927800	-0.01179000	-0.07166100
C	0.57380600	-0.88280500	1.16120700
C	-0.06650200	-2.54302300	3.35289400
C	0.56543800	-0.38237300	2.46612300
C	0.24502800	-2.23741300	0.97783900
C	-0.06932300	-3.05758100	2.05538800
C	0.25024100	-1.20437500	3.55123400
H	0.80400700	0.65684300	2.64819600
H	0.23973900	-2.65487000	-0.02292200
H	-0.31770700	-4.09892800	1.88246200
H	0.25084400	-0.78712100	4.55207100
H	-0.31308600	-3.17990800	4.19489600
C	2.18583400	-0.52197600	-0.79773500
C	4.56373300	-1.31793100	-2.09856200
C	2.99436500	-1.53534100	-0.27185900
C	2.61211900	0.10693600	-1.97894200
C	3.77800700	-0.29251000	-2.62389100
C	4.16948100	-1.93102900	-0.91511000
H	2.72504600	-2.02493200	0.65357000
H	2.02458900	0.91006300	-2.39722200
H	4.07621200	0.20658300	-3.53947600
H	4.77383900	-2.71941600	-0.47970200
H	5.47427200	-1.62559000	-2.60078600
C	1.14347600	1.46825900	0.33851100
C	1.61777500	4.12042800	1.17781600
C	2.39681900	1.85943000	0.82938100
C	0.13464800	2.43499400	0.27927100
C	0.36929300	3.74777600	0.68986000
C	2.63145500	3.16620500	1.24792300
H	3.20063200	1.13572200	0.88122600
H	-0.84945300	2.17657000	-0.08937600
H	-0.43022700	4.47749700	0.62413800
H	3.61183800	3.43885600	1.62291500
H	1.80102800	5.14065200	1.49565400
C	-0.30926500	-0.03691000	-1.07933100
O	-0.18458300	0.19794800	-2.27103800
N	-1.53343400	-0.26963400	-0.53535500
C	-2.74074400	-0.21710700	-1.34409200
C	-3.91541300	0.06025400	-0.41618600
O	-3.87918200	-0.02691300	0.78830500
H	-1.64461900	-0.45529000	0.45183400
H	-2.65033600	0.61395900	-2.04864600
C	-2.97349500	-1.50944400	-2.15133400
H	-2.11478400	-1.67768400	-2.80159300
H	-3.08727800	-2.36674300	-1.48293800
H	-3.86942900	-1.41796300	-2.76772500
O	-5.01314100	0.39358800	-1.11244000
C	-6.20740200	0.63787100	-0.34057700
H	-6.48724500	-0.25594100	0.21802600
H	-6.97370300	0.89205000	-1.06891100
H	-6.04680200	1.46278200	0.35419800

Compound **3b** conf. 9

C	1.11472100	0.09691000	-0.06190600
C	1.50819500	1.56130300	-0.39981700
C	2.15225200	4.24488700	-0.97921700
C	2.80853100	1.92679200	-0.75283900
C	0.53265800	2.56842900	-0.34837400
C	0.84800000	3.89300300	-0.63286100
C	3.12808000	3.25591600	-1.03775500
H	3.58368500	1.17578600	-0.81956300
H	-0.48835200	2.32053900	-0.07959300
H	0.07249600	4.64970000	-0.58727000
H	4.14555300	3.51050200	-1.31361600
H	2.40026400	5.27580900	-1.20569100
C	0.85613000	-0.09069400	1.45606900
C	0.39884900	-0.54586300	4.20578500
C	0.54848000	-1.37403900	1.94215400
C	0.94133400	0.95139700	2.38352500
C	0.71559200	0.72621200	3.74385400
C	0.31641300	-1.59949700	3.29434400
H	0.50485500	-2.20902400	1.25240100
H	1.19280400	1.94991600	2.05355500
H	0.79161800	1.55494600	4.43901400

H	0.08026800	-2.60050400	3.63832600
H	0.22306200	-0.71953200	5.26140800
C	2.24186500	-0.88936600	-0.48829400
C	4.38983500	-2.59281800	-1.17944100
C	3.29379600	-1.13866900	0.40735600
C	2.30159700	-1.50127000	-1.74652100
C	3.35872100	-2.34921900	-2.08110600
C	4.35417700	-1.97522200	0.06887300
H	3.28929400	-0.67491200	1.38570300
H	1.52898800	-1.30476300	-2.47460200
H	3.37178600	-2.81463900	-3.06075600
H	5.15012600	-2.14467300	0.78587300
H	5.21029600	-3.25039800	-1.44452200
C	-0.19180900	-0.15273800	-0.90665100
O	-0.17388900	-0.07998700	-2.12614900
N	-1.34414100	-0.40057700	-0.22148200
C	-2.63333400	-0.43186300	-0.89222000
C	-3.57341000	0.54426000	-0.19061900
O	-3.34984500	1.08915600	0.86410600
H	-1.34776400	-0.29149100	0.78246500
H	-2.47123700	-0.06813000	-1.90979700
C	-3.25991800	-1.85495800	-0.98895000
H	-4.21807700	-1.71630000	-1.50013100
O	-4.70405800	0.71826500	-0.89643800
C	-2.38801900	-2.77566600	-1.85062600
H	-1.40801200	-2.93653900	-1.39364700
H	-2.86829400	-3.75175900	-1.96328100
H	-2.22552900	-2.35777700	-2.84681100
C	-3.53286100	-2.47141600	0.38952500
H	-4.01491900	-3.44622900	0.27793500
H	-4.19032800	-1.84679900	1.00147400
H	-2.60372300	-2.62608600	0.94611500
C	-5.68046100	1.61205200	-0.32400900
H	-6.00763600	1.24467200	0.64934200
H	-6.50849500	1.62435000	-1.02882000
H	-5.25789100	2.61073700	-0.20895800

Compound **3b** conf. 13

C	1.07600800	0.06761700	-0.02700900
C	0.80553400	-0.17252900	1.47724300
C	0.27240000	-0.53261200	4.22693500
C	1.36189400	-1.24226300	2.18615300
C	-0.03190300	0.71391400	2.17887800
C	-0.29684800	0.53565100	3.53334300
C	1.10049400	-1.41927600	3.54682900
H	2.00627600	-1.94908300	1.68126700
H	-0.49442200	1.54540800	1.65961100
H	-0.94955100	1.23420300	4.04489500
H	1.54823400	-2.25715900	4.06987500
H	0.06884400	-0.67109100	5.28291600
C	1.89136700	-1.10575600	-0.63613600
C	3.41630200	-3.25716100	-1.63868200
C	3.28855400	-1.11362800	-0.52897200
C	1.27638500	-2.19859600	-1.25555400
C	2.02955000	-3.26105600	-1.75560300
C	4.04239400	-2.17691200	-1.01943900
H	3.79441700	-0.27800800	-0.06170000
H	0.19937500	-2.23052800	-1.35735200
H	1.52590000	-4.09039500	-2.24009100
H	5.12232700	-2.15543300	-0.92231800
H	4.00259400	-4.08145600	-2.02898200
C	1.86446700	1.38908400	-0.25294900
C	3.38295400	3.72290100	-0.72932700
C	2.34739000	2.16674100	0.80458900
C	2.18384000	1.79302500	-1.55980600
C	2.92418500	2.94699200	-1.79342800
C	3.09646400	3.32227200	0.57022300
H	2.15467800	1.87911000	1.82853200
H	1.84479200	1.20310600	-2.39795100
H	3.14701900	3.23753400	-2.81435500
H	3.45591300	3.90232900	1.41322700
H	3.96229200	4.62099600	-0.91320300
C	-0.29009800	0.14709800	-0.82151000
O	-0.37303200	0.66441900	-1.92108000
N	-1.36407300	-0.48274500	-0.25288000
C	-2.68091000	-0.37123600	-0.85143200
C	-3.32932100	0.97079800	-0.48636500
O	-2.97607600	1.70237100	0.40480000
H	-1.30989600	-0.70962600	0.72809200
H	-2.54473700	-0.36101000	-1.93422700
C	-3.60585000	-1.56309200	-0.48285300
H	-4.55641200	-1.35102300	-0.98207500
O	-4.37432500	1.22530400	-1.29569100
C	-3.05726100	-2.87981200	-1.04781900
H	-3.76240800	-3.69497100	-0.86358300
H	-2.10788300	-3.14898600	-0.57742200
H	-2.89450800	-2.81419800	-2.12715700
C	-3.87817100	-1.67271200	1.02516300
H	-2.97474600	-1.93293900	1.58657100
H	-4.60922400	-2.46249900	1.21689100
H	-4.27479100	-0.74346200	1.44222700
C	-5.06983500	2.46668100	-1.06432100
H	-5.86188100	2.49805400	-1.80898600
H	-4.38899000	3.30899800	-1.19092000
H	-5.48713400	2.48779000	-0.05674600

Compound **3b** conf. 16

C	1.12093000	0.04177800	-0.04813000
C	2.34179900	-0.63974200	-0.72969100
C	4.62505800	-1.75600000	-1.96807800
C	3.21382100	-1.47750100	-0.02480800
C	2.65925300	-0.34733800	-2.06654200
C	3.77787700	-0.90560700	-2.67731500
C	4.34081700	-2.03181800	-0.63573700
H	3.03266100	-1.70317600	1.01667800
H	2.02372100	0.31637900	-2.63206800
H	3.99022900	-0.66704100	-3.71385600
H	4.99486300	-2.67641200	-0.05860400
H	5.49783700	-2.18733600	-2.44578200
C	1.35721100	1.57811000	-0.00076900
C	1.81095600	4.35569500	0.19981700
C	2.65507500	2.09199700	0.11024900
C	0.29083200	2.48567900	0.00088000
C	0.51470700	3.85841900	0.09502100
C	2.88041900	3.46353600	0.21163200
H	3.50166300	1.41784100	0.11544100
H	-0.73095400	2.13318500	-0.05736200
H	-0.33107400	4.53707500	0.08836700
H	3.89702900	3.83197400	0.29491400
H	1.98543500	5.42345900	0.27083600
C	0.89862300	-0.52008400	1.37573700
C	0.49555300	-1.62502200	3.94292900
C	1.01658400	0.26557800	2.52575200
C	0.57174700	-1.87747600	1.54231200
C	0.37247700	-2.42415700	2.80507300
C	0.81787400	-0.28088500	3.79623600
H	1.26514700	1.31468000	2.43943900
H	0.48036700	-2.51536500	0.67056200
H	0.12394100	-3.47537500	2.90155400
H	0.91604600	0.35442200	4.66944700

H	0.34082500	-2.04867000	4.92885500
C	-0.17182400	-0.18632900	-0.93375900
O	-0.14077300	-0.14385700	-2.15191400
N	-1.34255700	-0.37786400	-0.25809900
C	-2.62576400	-0.38121100	-0.94045000
C	-3.53607200	0.65539600	-0.28701000
O	-3.30267500	1.23296700	0.74816400
H	-1.34840300	-0.29234100	0.74763400
H	-2.43722000	-0.06018200	-1.96761000
C	-3.30868000	-1.78041100	-0.99786100
H	-4.25455200	-1.61996000	-1.52523000
O	-4.65212800	0.84432900	-1.01185200
C	-2.46637100	-2.76356000	-1.81896200
H	-2.98681400	-3.72122900	-1.90913700
H	-2.27212100	-2.38386800	-2.82464400
H	-1.50016100	-2.95247200	-1.34394600
C	-3.62215200	-2.33850300	0.39688800
H	-4.14563600	-3.29446200	0.31146900
H	-4.25832100	-1.66585800	0.97992100
H	-2.70696200	-2.51528300	0.96968800
C	-5.59874300	1.79752300	-0.48713100
H	-5.95184100	1.48163300	0.49518100
H	-6.41728900	1.81504000	-1.20281500
H	-5.13795800	2.78246500	-0.40511400

Compound **3b** conf. 17

C	1.14153300	-0.03818000	-0.03490800
C	1.59059300	1.33305900	-0.61016300
C	2.45669800	3.84623600	-1.55599000
C	0.73190900	2.16590000	-1.33439300
C	2.89564900	1.78597100	-0.37152200
C	3.32302400	3.02786300	-0.83248500
C	1.16054400	3.40732600	-1.80644500
H	-0.28294800	1.85464800	-1.54533300
H	3.58812500	1.15837000	0.17579100
H	4.33843000	3.35166700	-0.63202600
H	0.47542100	4.02659100	-2.37488000
H	2.79088400	4.80967400	-1.92414700
C	0.74833600	0.08744900	1.45584200
C	-0.01616000	0.22948300	4.17105700
C	0.84233100	1.28558300	2.16996100
C	0.25263700	-1.04018900	2.13435300
C	-0.12303600	-0.97356800	3.47142400
C	0.46566400	1.35575100	3.51399500
H	1.21241900	2.17745700	1.68254900
H	0.16604700	-1.98400400	1.60779900
H	-0.49767300	-1.86172400	3.96822800
H	0.55245700	2.29905200	4.04190900
H	-0.30717500	0.28397200	5.21405600
C	2.30497100	-1.04958900	-0.23428500
C	4.49363900	-2.78374500	-0.66163700
C	2.99726400	-1.62029600	0.83922600
C	2.75565600	-1.34270400	-1.53174200
C	3.82707000	-2.20479100	-1.74103400
C	4.07826000	-2.47965500	0.62939200
H	2.71085300	-1.39565200	1.85713600
H	2.26033200	-0.89802600	-2.38152800
H	4.14563000	-2.41918700	-2.75532500
H	4.59331200	-2.90434100	1.48420500
H	5.33078500	-3.45287500	-0.82705800
C	-0.11607400	-0.51156200	-0.87060800
O	-0.01501300	-1.06110100	-1.95555800
N	-1.33278900	-0.20141400	-0.34628300
C	-2.56370000	-0.47137400	-1.08126100
C	-3.65583000	0.52324700	-0.70773500
O	-4.62422700	0.74822900	-1.38979100
H	-1.40077700	0.24784600	0.55353600
H	-2.35464900	-0.32213800	-2.14278500
C	-3.04551500	-1.94966100	-0.91484100
H	-2.14063800	-2.53632200	-1.10057600
O	-3.44184500	1.10495700	0.49243700
C	-3.54122200	-2.25661300	0.50342600
H	-3.72317800	-3.32902700	0.61381800
H	-2.81178800	-1.96343100	1.26269500
H	-4.48370900	-1.74299000	0.72102000
C	-4.08079400	-2.33822400	-1.97668200
H	-3.69649500	-2.16521600	-2.98558600
H	-5.00679600	-1.76889400	-1.86923400
H	-4.32256400	-3.40121000	-1.88872000
C	-4.44367600	2.04403700	0.93375000
H	-4.53343700	2.86291200	0.21944800
H	-4.09433800	2.40849600	1.89684700
H	-5.40895800	1.54705900	1.03527500

Compound **3b** conf. 27

C	1.19302500	-0.00220500	-0.04595900
C	2.34334900	-0.87611900	-0.62000000
C	4.50596900	-2.34118000	-1.69630600
C	3.13580400	-1.69775200	0.18891800
C	2.67928000	-0.78001000	-1.98033400
C	3.73820800	-1.50955300	-2.51088100
C	4.20398900	-2.42437400	-0.34215100
H	2.93808800	-1.77551300	1.24888900
H	2.10483600	-0.13466700	-2.62740400
H	3.96702500	-1.42144100	-3.56739500
H	4.79835300	-3.05140100	0.31355100
H	5.33268700	-2.90689300	-2.11162500
C	1.58061000	1.49013400	-0.23636600
C	2.34173200	4.19578700	-0.48942600
C	2.90305900	1.89508600	-0.00690500
C	0.65060100	2.47091700	-0.59581500
C	1.02653100	3.80847900	-0.72515100
C	3.27913600	3.22995900	-0.12655100
H	3.64968900	1.15825100	0.26211900
H	-0.38147800	2.20399400	-0.78203900
H	0.28466500	4.54495100	-1.01363500
H	4.30981300	3.51292900	0.05716200
H	2.63514600	5.23453900	-0.59129500
C	0.92771300	-0.32306600	1.44355200
C	0.39637900	-0.99394700	4.13365000
C	1.07486900	0.62036800	2.46397200
C	0.49934800	-1.61332400	1.80198500
C	0.23901600	-1.94705900	3.12604200
C	0.81266500	0.28821200	3.79587400
H	1.39388400	1.62662800	2.22811300
H	0.37392000	-2.36661300	1.03222700
H	-0.08722900	-2.95154700	3.37227500
H	0.93387800	1.04231300	4.56555100
H	0.19219500	-1.25096800	5.16691500
C	-0.12824700	-0.25911000	-0.87679800
O	-0.11862700	-0.49679000	-2.07448800
N	-1.29771200	-0.13413600	-0.19407000
C	-2.58290400	-0.21611600	-0.87331200
C	-3.57599700	0.60354100	-0.05833700
O	-3.41343200	0.92909600	1.09427200
H	-1.30565600	0.09522000	0.78998900
H	-2.47814600	0.24231000	-1.85982800
C	-3.03705200	-1.69615100	-1.09439200
H	-2.13798800	-2.17932500	-1.48829900
O	-4.66708300	0.91863400	-0.77442600

C	-3.42994100	-2.39458100	0.21272800
H	-4.35776200	-1.98595800	0.62698500
H	-2.65224200	-2.29856300	0.97437200
H	-3.59325700	-3.46100200	0.03520100
C	-4.12994500	-1.82378000	-2.16222100
H	-5.07039900	-1.36975100	-1.84223500
H	-4.32013600	-2.87995900	-2.37278800
H	-3.82659400	-1.34682900	-3.09830500
C	-5.68350400	1.67509200	-0.08279900
H	-6.47364000	1.83052500	-0.81351500
H	-5.27886400	2.62906300	0.25657100
H	-6.05582600	1.11563900	0.77597800

Compound **3b** conf. 32

C	-1.10246800	0.00892700	-0.06154300
C	-1.18465700	1.46250100	0.46208700
C	-1.28283700	4.14591900	1.33607400
C	-0.95228200	2.52753400	-0.42629900
C	-1.45396600	1.77622300	1.79721800
C	-1.50356200	3.10470000	2.22999200
C	-1.00363000	3.84958100	0.00042100
H	-0.73250100	2.31570000	-1.46689100
H	-1.62736400	0.98366300	2.51255700
H	-1.71694400	3.31678200	3.27182900
H	-0.82585200	4.64983900	-0.70963400
H	-1.32403600	5.17618500	1.67128400
C	-2.16936300	-0.26765500	-1.15605100
C	-4.15394400	-0.88847300	-3.06728800
C	-2.20344900	-1.52300300	-1.78459200
C	-3.16858600	0.65309400	-1.48675200
C	-4.14977400	0.34835600	-2.43345300
C	-3.17551900	-1.82428700	-2.73229600
H	-1.46333400	-2.26749400	-1.53188300
H	-3.20462600	1.61922900	-1.00284100
H	-4.91130600	1.08489600	-2.66569900
H	-3.17050600	-2.79938200	-3.20708600
H	-4.91293300	-1.12670000	-3.80425300
C	-1.32088300	-1.01312900	1.08816700
C	-1.80872300	-2.79291700	3.22011200
C	-2.62822600	-1.29244500	1.51313200
C	-0.26402700	-1.64625500	1.74980700
C	-0.50814200	-2.53035100	2.80325800
C	-2.87065900	-2.16621900	2.56858100
H	-3.46665200	-0.82648500	1.01001100
H	0.76408300	-1.47259700	1.45972500
H	0.33114900	-3.01318600	3.29141000
H	-3.89199500	-2.36250500	2.87623000
H	-1.99594800	-3.48024400	4.03763100
C	0.33667500	-0.22793900	-0.67268500
O	0.56025800	-1.03150900	-1.56194600
N	1.35005100	0.49994600	-0.12462200
C	2.72564900	0.34094900	-0.57318400
C	3.24771400	-1.04904100	-0.18766500
O	3.05180100	-1.58513300	0.87681200
H	1.15734800	1.11820300	0.64773300
H	2.74838100	0.40223600	-1.66407400
C	3.61207100	1.46186500	0.02969200
H	3.46748800	1.42869800	1.11766000
O	3.98343500	-1.58435500	-1.17286200
C	5.10417600	1.23824000	-0.25256300
H	5.30118800	1.19365800	-1.32779200
H	5.68648300	2.06532800	0.16128200
H	5.47782500	0.31554800	0.19636200
C	3.17336400	2.84045700	-0.48719600
H	3.32609800	2.91176600	-1.56904800
H	3.76766400	3.62675400	-0.01417100
H	2.12158600	3.05064700	-0.28446800
C	4.52296200	-2.89638500	-0.91968900
H	5.06877900	-3.16375000	-1.82146800
H	3.71424000	-3.60407300	-0.73534800
H	5.18988300	-2.87584800	-0.05644200

Compound **4b** conf. 8

C	-1.23514000	0.01434500	-0.06934800
C	-1.22456600	1.48886500	0.39826000
C	-1.14872100	4.20540700	1.16589800
C	-0.95915500	2.50409500	-0.53787500
C	-1.43911100	1.86872700	1.72628200
C	-1.40199100	3.21374400	2.10632100
C	-0.92492400	3.84239200	-0.16372900
H	-0.78132200	2.24003700	-1.57453100
H	-1.63705300	1.11606100	2.47760300
H	-1.57394100	3.47787500	3.14393100
H	-0.72352200	4.60326600	-0.90984200
H	-1.12291600	5.24851100	1.46050100
C	-2.34211000	-0.24217200	-1.12820500
C	-4.40598500	-0.82019500	-2.96772700
C	-3.30357700	0.71709200	-1.46201400
C	-2.45506500	-1.51259200	-1.71599500
C	-3.46611500	-1.79324200	-2.62874500
C	-4.32396700	0.43329400	-2.37304000
H	-3.27867900	1.69834800	-1.00867600
H	-1.74564500	-2.28499500	-1.45936300
H	-3.52200200	-2.78129300	-3.07248200
H	-5.05450600	1.19954900	-2.60871500
H	-5.19553600	-1.04207900	-3.67718900
C	-1.48176300	-0.94970400	1.12412700
C	-2.01445100	-2.61981300	3.33278300
C	-0.44432800	-1.60785100	1.79216500
C	-2.79258100	-1.14712100	1.58276600
C	-3.05688400	-1.96655600	2.67596700
C	-0.71091700	-2.43813000	2.88323600
H	0.58522300	-1.49629000	1.47766200
H	-3.61696000	-0.66058900	1.07601000
H	-4.08044800	-2.10004100	3.00881100
H	0.11304100	-2.94313600	3.37511900
H	-2.21907200	-3.26560500	4.17949000
C	0.17463300	-0.32507000	-0.70164800
O	0.33220700	-1.17228200	-1.56440600
N	1.23850000	0.36527100	-0.20290700
C	2.58873600	0.11276300	-0.68332000
C	3.04446400	-1.28908400	-0.25254800
O	2.83212100	-1.78587900	0.82802100
H	1.09399100	1.01936900	0.54878500
H	2.56319200	0.10440800	-1.77512500
C	3.58132600	1.23722300	-0.22984400
C	3.13876800	2.56546600	-0.87606900
C	4.99807600	0.89916200	-0.73360200
H	5.40801000	0.01269800	-0.24420800
H	5.67063900	1.73445400	-0.52100500
H	5.00844600	0.72178300	-1.81210500
H	3.13934600	2.49015700	-1.96758300
H	3.83095100	3.36427200	-0.59495900
H	2.13761200	2.86719900	-0.56098800
C	3.61947300	1.38967400	1.30393900
H	2.66582900	1.72933400	1.71893800
H	4.36636400	2.14054200	1.57670000
H	3.88197900	0.45215300	1.79773100
O	3.73395600	-1.89734000	-1.23011400
C	4.19956100	-3.23014400	-0.94235900

H	4.88062600	-3.22178600	-0.09001900
H	4.71421700	-3.55743800	-1.84275800
H	3.35425100	-3.88311000	-0.72343100

Compound **4b** conf. 15

C	-1.23510200	0.01419600	-0.06940600
C	-1.48170300	-0.95010600	1.12386500
C	-2.01425900	-2.62039100	3.33242200
C	-2.79255800	-1.14814500	1.58209600
C	-0.44414400	-1.60764900	1.79232500
C	-0.71065900	-2.43802800	2.88333100
C	-3.05680100	-1.96768200	2.67524500
H	-3.61701200	-0.66200800	1.07508400
H	0.58545000	-1.49554300	1.47816200
H	0.11339200	-2.94257000	3.37553500
H	-4.08040400	-2.10165600	3.00776700
H	-2.21883000	-3.26626800	4.17907600
C	-1.22465800	1.48859200	0.39854500
C	-1.14940700	4.20498200	1.16680300
C	-1.43925700	1.86811300	1.72666900
C	-0.95954600	2.50409700	-0.53736300
C	-0.92558800	3.84232600	-0.16290500
C	-1.40242500	3.21303600	2.10701300
H	-1.63699900	1.11521800	2.47781800
H	-0.78182100	2.24035500	-1.57411800
H	-0.72444900	4.60341300	-0.90887100
H	-1.57440300	3.47689700	3.14468800
H	-1.12381200	5.24801900	1.46165900
C	-2.34198300	-0.24208900	-1.12843200
C	-4.40559700	-0.81968300	-2.96838400
C	-2.45466400	-1.51227600	-1.71678100
C	-3.30358600	0.71715400	-1.46191600
C	-4.32386200	0.43356000	-2.37313600
C	-3.46559000	-1.79271400	-2.62973300
H	-1.74512500	-2.28466600	-1.46041600
H	-3.27892000	1.69820700	-1.00812800
H	-5.05451500	1.19978700	-2.60855100
H	-3.52126300	-2.78058700	-3.07389300
H	-5.19505200	-1.04140400	-3.67800500
C	0.17469900	-0.32505800	-0.70172400
O	0.33235500	-1.17222400	-1.56451400
N	1.23848600	0.36540500	-0.20299100
C	2.58877100	0.11291900	-0.68329600
C	3.04461200	-1.28884000	-0.25235000
O	2.83220300	-1.78554900	0.82823400
H	1.09390800	1.01939700	0.54877400
H	2.56325800	0.10449300	-1.77510100
C	3.58120700	1.23753200	-0.22987900
C	3.13849700	2.56563200	-0.87628200
C	4.99803700	0.89957300	-0.73348000
H	5.40806000	0.01326600	-0.24387500
H	5.67044500	1.73501300	-0.52098800
H	5.00851400	0.72198600	-1.81194500
H	3.13930600	2.49024400	-1.96778900
H	3.83044900	3.36460900	-0.59508800
H	2.13722100	2.86715500	-0.56138800
C	3.61917600	1.39019700	1.30389300
H	2.66548700	1.72996300	1.71870500
H	4.36603400	2.14110700	1.57663400
H	3.88161800	0.45275400	1.79785900
O	3.73419100	-1.89714500	-1.22981600
C	4.19977700	-3.22991700	-0.94196700
H	4.88138500	-3.22140300	-0.09005400
H	4.71384800	-3.55754400	-1.84257800
H	3.35453000	-3.88271400	-0.72230900

Compound **15** conf. 15

C	-3.56807500	-0.56199500	3.33853100
C	-2.57017400	-0.58149400	2.36351300
C	-2.73192600	0.09753300	1.15146700
C	-3.93002000	0.79494100	0.94500500
C	-4.93088800	0.80858000	1.91272800
C	-4.75418300	0.13101000	3.11793200
C	-1.66173000	0.06232500	0.02512500
C	-1.95122200	2.94912000	-2.54453500
C	-1.60517200	4.05287400	-1.77422600
C	-1.27655300	3.86580500	-0.43183800
C	-1.28592500	2.59233800	0.12763600
C	-1.60735200	1.46417700	-0.64482800
C	-1.95426400	1.66954100	-1.98427800
C	-1.97987300	-1.04531500	-1.00820100
C	-3.14085600	-1.82243800	-0.95779500
C	-3.38399400	-2.81595300	-1.90990600
C	-2.46927400	-3.05568600	-2.92911900
C	-1.30285400	-2.29227700	-2.99170900
C	-1.06483800	-1.30200500	-2.04495900
C	-0.27344900	-0.24260400	0.70809700
O	0.40371000	0.62914900	1.24184500
N	0.11170300	-1.54315200	0.74716700
C	1.31363600	-1.98183600	1.45181500
C	2.61431300	-1.84462100	0.63375700
O	3.22741300	-2.83761500	0.26513400
C	4.15021100	-0.20144200	-0.42991800
C	5.23471300	0.56584000	0.39842900
C	3.65947000	0.52264900	-1.69262800
N	2.99306400	-0.56422800	0.39445100
C	4.70315400	1.90866300	0.93394100
C	6.46611900	0.82283000	-0.49287000
C	5.67255500	-0.31546300	1.58442700
H	-3.41053300	-1.08960000	4.27271300
H	-1.66113100	-1.13341900	2.56537100
H	-4.08134800	1.33824100	0.02058300
H	-5.84737300	1.35705600	1.72515900
H	-5.52905300	0.14803000	3.87593600
H	-2.22669900	3.07367100	-3.58605100
H	-1.60093900	5.04676700	-2.20779100
H	-1.01741800	4.71681900	0.18854100
H	-1.03939700	2.47202100	1.17189200
H	-2.24268700	0.83612900	-2.60930000
H	-3.86738000	-1.65914300	-0.17333100
H	-4.29366300	-3.40253100	-1.84540900
H	-2.65751900	-3.82868100	-3.66547200
H	-0.57699700	-2.46820200	-3.77761500
H	-0.15431000	-0.71708100	-2.11293000
H	-0.40606900	-2.22497800	0.21481000
H	1.20405000	-3.03787800	1.69211200
H	1.39709800	-1.40758200	2.37792400
H	4.59439800	-1.15369500	-0.72816700
H	3.13908200	1.45358300	-1.45179200
H	2.96146500	-0.12059300	-2.23366100
H	4.48397300	0.75874300	-2.36746700
H	2.36197400	0.16472600	0.71235700
H	3.83514300	1.77179000	1.58546400
H	4.41780600	2.58915100	0.12721700
H	5.47581600	2.40904200	1.52522300
H	6.83245700	-0.10647600	-0.94112200
H	7.27985700	1.24543800	0.10362900
H	6.25379900	1.52798400	-1.29993000
H	6.05154200	-1.28216700	1.24056500
H	6.46831900	0.17825300	2.15011700

H	4.84407300	-0.50663000	2.26971500

Compound **15** conf. 18

C	3.09184400	-1.92151600	3.16097900
C	2.18847500	-1.35135900	2.26279100
C	2.63804800	-0.70057000	1.10757500
C	4.02175900	-0.66473000	0.87517200
C	4.92213500	-1.24352800	1.76585000
C	4.46127600	-1.87171100	2.92082600
C	1.67823900	-0.08830500	0.04404300
C	-0.09141200	-1.82212800	-2.89826000
C	0.68330800	-2.96520600	-3.09279300
C	1.77568200	-3.19305700	-2.26268400
C	2.09623200	-2.28850100	-1.24846500
C	1.33293300	-1.13690800	-1.04658000
C	0.23124400	-0.92295300	-1.88706200
C	2.34910900	1.16965700	-0.57095600
C	2.85873500	2.16595200	0.28217400
C	3.45269100	3.31825200	-0.22290200
C	3.56845100	3.50171100	-1.60114800
C	3.08589600	2.51890700	-2.45781800
C	2.48277300	1.36621900	-1.94867600
C	0.30694700	0.27417200	0.72359000
O	-0.41550600	-0.60555500	1.18745200
N	-0.06655100	1.57447200	0.76129300
C	-1.25692000	2.02760000	1.47741300
C	-2.57226400	1.93295600	0.67716800
O	-3.17874000	2.94596600	0.35453300
C	-4.18378300	0.34892700	-0.36124000
C	-5.19288500	-0.50715500	0.47467800
C	-3.77693700	-0.25633800	-1.71321900
N	-2.97893800	0.66665300	0.41195100
C	-6.46137200	-0.76189800	-0.36379700
C	-5.59603500	0.28570000	1.73323700
C	-4.58552200	-1.85799300	0.89893400
H	2.71318000	-2.41195700	4.05107300
H	1.12929900	-1.42965600	2.45868500
H	4.40665200	-0.17968700	-0.01305400
H	5.98491200	-1.19909700	1.55450400
H	5.15983200	-2.31761800	3.61994600
H	-0.95106200	-1.63095200	-3.53096400
H	0.43269200	-3.67031800	-3.87730200
H	2.38324700	-4.08168400	-2.39372900
H	2.94364900	-2.49691800	-0.60986300
H	-0.38839200	-0.04326800	-1.75275100
H	2.80421200	2.02914500	1.35622800
H	3.83461700	4.06780200	0.46132600
H	4.03501600	4.39621700	-1.99771600
H	3.17679100	2.64013000	-3.53150400
H	2.12502900	0.61541400	-2.63948800
H	0.52162200	2.26728600	0.32512100
H	-1.12225000	3.07751700	1.73107900
H	-1.34678000	1.44472800	2.39760000
H	-4.66148600	1.31325200	-0.54803600
H	-4.64483400	-0.44061600	-2.34865700
H	-3.12284300	0.44258600	-2.24008000
H	-3.23538400	-1.19784800	-1.59009700
H	-2.35325600	-0.08184700	0.69475000
H	-7.22970800	-1.23650000	0.25341800
H	-6.27021900	-1.42377800	-1.21175500
H	-6.87835100	0.17390200	-0.74990300
H	-4.73511600	0.48621200	2.37454300
H	-6.32655300	-0.27902400	2.32021300
H	-6.04680800	1.24644900	1.46740500
H	-3.70373400	-1.72819300	1.53291700
H	-4.29728100	-2.46752300	0.03832800
H	-5.31617500	-2.43250200	1.47620000

Compound **15** conf. 21

C	0.19676100	-0.73511900	-3.41778200
C	0.36127600	-0.25180600	-2.11923300
C	1.46376600	-0.62677800	-1.34421600
C	2.40081900	-1.49896200	-1.91489600
C	2.24244100	-1.97643100	-3.21316300
C	1.13634500	-1.59852900	-3.97232700
C	1.70693800	-0.06383900	0.08350500
C	3.63046700	3.06761900	1.21269800
C	4.20498900	3.52256400	0.02459700
C	3.97704900	2.81932700	-1.15249200
C	3.18184100	1.66997200	-1.14912000
C	2.60087300	1.19919600	0.03174900
C	2.84092800	1.92318700	1.21343000
C	2.35178000	-1.17872300	0.95384200
C	1.66869000	-2.38951300	1.15236700
C	2.23844900	-3.42252900	1.88883200
C	3.51494200	-3.28472700	2.43353800
C	4.21466300	-2.10287400	2.22208700
C	3.63896300	-1.06290800	1.48833500
C	0.30168500	0.31704500	0.69574100
O	-0.42234300	-0.50311300	1.24858100
N	-0.10239300	1.60238800	0.53313000
C	-1.31840900	2.12495700	1.15370600
C	-2.61143000	1.89445100	0.34620500
O	-3.21430100	2.83858400	-0.14723600
C	-4.19995900	0.15506800	-0.45314500
C	-5.27722300	-0.44215900	0.51307100
C	-3.77755800	-0.76674700	-1.60635900
N	-3.00572300	0.59867500	0.27315200
C	-6.55148800	-0.77521700	-0.28914000
C	-5.63981400	0.61411900	1.57532700
C	-4.77165900	-1.71581300	1.21641600
H	-0.67153700	-0.43272900	-3.99261900
H	-0.38571800	0.42216900	-1.72000500
H	3.26220900	-1.81248100	-1.33870800
H	2.98423900	-2.64979600	-3.62826300
H	1.00830900	-1.97467200	-4.98101900
H	3.79820700	3.60411000	2.13997000
H	4.82027500	4.41510300	0.02089700
H	4.41378300	3.16066600	-2.08438300
H	3.01725200	1.14377200	-2.07967600
H	2.40624500	1.58313600	2.14700900
H	0.68414100	-2.52363900	0.73026300
H	1.68241600	-4.34252900	2.03220100
H	3.95860500	-4.09217800	3.00530300
H	5.21549700	-1.98047800	2.62143800
H	4.21811500	-0.16370500	1.33180600
H	0.52773900	2.26068100	0.10257200
H	-1.20830600	3.20245200	1.26112600
H	-1.42167700	1.67406000	2.14454400
H	-4.62539600	1.06674300	-0.87848500
H	-3.27175600	-1.66648500	-1.24604200
H	-4.63342800	-1.07568900	-2.20873800
H	-3.08420100	-0.23569500	-2.26199200
H	-2.38341200	-0.09093800	0.68353600
H	-7.35438000	-1.07450000	0.39085700
H	-6.39713100	-1.59750400	-0.99158100
H	-6.90353500	0.09405000	-0.85390200
H	-6.43168000	0.23723900	2.22958400
H	-5.99585000	1.53779000	1.11018700
H	-4.78164200	0.86542500	2.20249600

H	-3.87335200	-1.52434300	1.81068400
H	-4.54438900	-2.51391000	0.50464100
H	-5.53642900	-2.09630800	1.90013500

Compound **15** conf. 22

C	1.69397600	3.82220800	-0.93088600
C	2.05410300	2.59053700	-0.38091400
C	1.22529900	1.47463000	-0.51472200
C	0.01715300	1.63378300	-1.20788300
C	-0.34491900	2.85915200	-1.75786200
C	0.49589700	3.96314900	-1.62305800
C	1.61189800	0.07845800	0.03654700
C	5.10943300	0.39640100	1.61720100
C	4.83171700	0.51952600	2.97700700
C	3.50672300	0.49524800	3.39979400
C	2.46721700	0.34789500	2.48025700
C	2.73178800	0.20416300	1.11295800
C	4.07310900	0.23815800	0.70082200
C	2.10954300	-0.85908300	-1.09839500
C	2.03105800	-0.52338300	-2.45337100
C	2.47444300	-1.40456400	-3.44245500
C	3.00674800	-2.64232400	-3.10017000
C	3.10506400	-2.98975100	-1.75273200
C	2.67000700	-2.10738400	-0.76877600
C	0.31421900	-0.49319100	0.71917000
O	-0.30159300	0.16980300	1.55062400
N	-0.10076100	-1.73292100	0.36839600
C	-1.13607400	-2.45327300	1.10511500
C	-2.59631600	-2.16339300	0.70218700
O	-3.30139800	-3.06138400	0.26067700
C	-4.41856300	-0.48157000	0.81466800
C	-4.65077200	0.56803700	-0.32145800
C	-4.91564600	-0.05607500	2.20458900
N	-3.01335100	-0.89235200	0.92822300
C	-3.94580500	1.90327700	-0.01928500
C	-6.16483300	0.81594800	-0.47809600
C	-4.11881800	-0.00567100	-1.64880400
H	2.35507900	4.67294300	-0.80769900
H	2.98551800	2.51378600	0.16301500
H	-0.65410900	0.79012100	-1.32441100
H	-1.28659100	2.95121800	-2.28712000
H	0.21544500	4.92079300	-2.04696300
H	6.13464700	0.41976400	1.26432500
H	5.63678800	0.63541200	3.69392900
H	3.26983100	0.59587600	4.45331900
H	1.44649200	0.36110800	2.83340000
H	4.31696000	0.13859500	-0.34947600
H	1.63116000	0.43579100	-2.75098100
H	2.40182900	-1.11252600	-4.48417700
H	3.34893400	-3.32569900	-3.86893600
H	3.53098900	-3.94457900	-1.46501500
H	2.78383500	-2.38398800	0.27313200
H	0.40170400	-2.23035800	-0.35015600
H	-1.01530000	-2.23429300	2.16988300
H	-0.98386500	-3.51895100	0.94365500
H	-4.95096500	-1.38816300	0.51887700
H	-5.97394500	0.20973900	2.19119800
H	-4.78818600	-0.88280500	2.90719000
H	-4.35499400	0.80003600	2.59020900
H	-2.33672700	-0.25894200	1.34422800
H	-2.86734900	1.77772000	0.10918200
H	-4.34101500	2.37697300	0.88319800
H	-4.09637700	2.60432400	-0.84605400
H	-6.59639500	1.31097800	0.39502100
H	-6.70632800	-0.12167900	-0.63974100
H	-6.35195500	1.45948300	-1.34277800
H	-3.04157100	-0.17960400	-1.60743000
H	-4.31776300	0.68970100	-2.46998800
H	-4.59896300	-0.95866200	-1.88827100

Compound **15** conf. 30

C	2.98617200	-2.15684000	-2.80943400
C	2.86806300	-1.45464100	-1.60728500
C	1.70853500	-0.73485300	-1.30371600
C	0.66600800	-0.74561400	-2.24764900
C	0.77918500	-1.44743400	-3.44311700
C	1.94519700	-2.15786900	-3.73109100
C	1.52897600	0.04853500	0.01915800
C	1.00589800	3.81503300	0.63286200
C	1.15651300	4.36143000	-0.64119400
C	1.42422900	3.51507700	-1.71068900
C	1.52444100	2.13613400	-1.51235900
C	1.35414400	1.57156700	-0.24350700
C	1.11271200	2.44231800	0.83171500
C	2.75656700	-0.15399000	0.95094300
C	2.79822200	-1.15918900	1.92285200
C	3.93167000	-1.35000800	2.71331300
C	5.05247500	-0.54307500	2.54201900
C	5.02652600	0.45943500	1.57430800
C	3.89058500	0.65347200	0.79245100
C	0.26968300	-0.50149400	0.79499000
O	-0.28950700	0.13954600	1.67867000
N	-0.12716800	-1.76390600	0.49731600
C	-1.16662600	-2.45822000	1.25252300
C	-2.61314200	-2.14761900	0.81405600
O	-3.31914700	-3.02504200	0.33481100
C	-4.36399300	-0.37906800	0.77628500
C	-4.39524100	0.71335100	-0.34456200
C	-4.99748400	0.03865400	2.11182500
N	-3.00450400	-0.86759500	1.03056200
C	-3.79985700	0.11827400	-1.63512800
C	-3.59586400	1.96804100	0.05504000
C	-5.85840600	1.10938300	-0.62755000
H	3.89815800	-2.70534600	-3.01717100
H	3.69136100	-1.47328200	-0.90616700
H	-0.24612300	-0.19549600	-2.04546200
H	-0.04348000	-1.43882500	-4.14924500
H	2.03623200	-2.70584700	-4.66201500
H	0.81178100	4.46107300	1.48211300
H	1.07709900	5.43211800	-0.79328800
H	1.56225000	3.91973400	-2.70736800
H	1.74837400	1.50992700	-2.36452800
H	1.00591100	2.04165000	1.82832400
H	1.94473800	-1.80711400	2.07715400
H	3.93209000	-2.13120100	3.46535800
H	5.93308400	-0.68930600	3.15719800
H	5.88972800	1.09967500	1.42970300
H	3.88600500	1.44521300	0.05391900
H	0.29060700	-2.23833400	-0.28788600
H	-1.04741600	-2.20861400	2.31030000
H	-1.02614700	-3.52945700	1.11963300
H	-4.90807600	-1.24521200	0.39300700
H	-6.03388900	0.35519600	1.98400200
H	-4.98930900	-0.80948000	2.80018900
H	-4.44750800	0.85755500	2.58401800
H	-2.32640200	-0.25039000	1.46589800
H	-4.35343600	-0.77000400	-1.95281200
H	-2.75671400	-0.17269500	-1.49489900
H	-3.83972300	0.85199800	-2.44573500
H	-2.54465800	1.74053500	0.25208300

H	-4.01066900	2.45008500	0.94436100
H	-3.62110400	2.70308100	-0.75495200
H	-5.90728000	1.77021400	-1.49795200
H	-6.31207200	1.64223200	0.21120300
H	-6.47361000	0.23004400	-0.84434700

Compound **15** conf.35

C	0.36902800	-1.29318600	-3.02878000
C	0.02928900	-0.59290600	-1.87008500
C	-1.17671100	-0.83844500	-1.20593200
C	-2.03497400	-1.80895600	-1.74286000
C	-1.70174900	-2.50274400	-2.90249200
C	-0.49460600	-2.24948300	-3.55225800
C	-1.61718300	-0.04870500	0.05735700
C	-4.31585500	-1.81639100	2.20444800
C	-3.61586900	-2.91431600	2.68986500
C	-2.27965500	-3.08171300	2.32616600
C	-1.65346800	-2.15814900	1.49677500
C	-2.33972500	-1.03010800	1.01991400
C	-3.68374600	-0.88542500	1.37631000
C	-2.52598200	1.14545500	-0.32308500
C	-2.96586400	1.38285200	-1.62814100
C	-3.77912900	2.48028300	-1.92534400
C	-4.16599700	3.36283200	-0.92373300
C	-3.73180100	3.14252100	0.38469000
C	-2.92287500	2.05051800	0.67737000
C	-0.32801300	0.51148500	0.77873000
O	0.27480700	-0.11292500	1.64352600
N	0.11290000	1.72677000	0.36197100
C	1.15495800	2.47028000	1.06910100
C	2.61470800	2.13416500	0.70162300
O	3.35803800	3.00903200	0.27737200
C	4.37936600	0.39118200	0.86504700
C	4.62672400	-0.59610300	-0.32333000
C	4.78551000	-0.13956600	2.24779100
N	2.98575800	0.85019300	0.93565000
C	6.12372200	-0.96194600	-0.37871300
C	4.25714800	0.10974700	-1.64199100
C	3.79204100	-1.88240200	-0.18147300
H	1.31559500	-1.08684200	-3.51551400
H	0.72237600	0.14713600	-1.49234600
H	-2.97221000	-2.02886800	-1.24718100
H	-2.38598800	-3.24728300	-3.29427200
H	-0.23061100	-2.79435000	-4.45160100
H	-5.36014100	-1.67642700	2.46130800
H	-4.10411800	-3.63645700	3.33473700
H	-1.72125000	-3.93895400	2.68583400
H	-0.62207500	-2.31455700	1.21715200
H	-4.26216400	-0.05092700	1.00506200
H	-2.67678000	0.71319800	-2.42693700
H	-4.10486300	2.63911800	-2.94727000
H	-4.79561900	4.21445700	-1.15513200
H	-4.02340600	3.82225800	1.17759200
H	-2.59691800	1.89415300	1.70007300
H	-0.44523700	2.23472600	-0.30654500
H	1.02388800	2.31462200	2.14450100
H	1.02317200	3.52760600	0.84756900
H	4.96309200	1.29012700	0.65358500
H	4.63172100	0.63907900	2.99841900
H	4.19015900	-1.00884100	2.54141400
H	5.83799200	-0.42545200	2.27509200
H	2.28679300	0.24786200	1.36063100
H	6.33314600	-1.54826400	-1.27823400
H	6.43677700	-1.56058100	0.47990000
H	6.75094800	-0.06524600	-0.41545800
H	4.44855400	-0.55153800	-2.49253700
H	4.84451700	1.02147700	-1.78065700
H	3.20226300	0.39004100	-1.66375300
H	3.96854200	-2.54183200	-1.03651800
H	2.72037700	-1.66831300	-0.15167200
H	4.05234800	-2.44338100	0.72040100

Compound **15** conf. 36

C	1.49044700	3.54207200	-1.66291400
C	1.55954300	2.15822000	-1.48693000
C	1.39817700	1.57885700	-0.22363700
C	1.19804200	2.43874100	0.86866200
C	1.12189400	3.81651100	0.69218500
C	1.26331800	4.37834800	-0.57620000
C	1.54005600	0.04846400	0.01370000
C	3.95774100	-1.43820400	2.64762000
C	5.09605500	-0.66000800	2.46026600
C	5.07759600	0.35108500	1.50125100
C	3.93205400	0.58153400	0.74377100
C	2.78009000	-0.19681200	0.91851300
C	2.81423600	-1.21071800	1.88161300
C	1.67412400	-0.72016700	-1.32299200
C	0.61281700	-0.69225000	-2.24553200
C	0.68577400	-1.37849800	-3.45306500
C	1.82843100	-2.11216400	-3.77462200
C	2.88689500	-2.15034500	-2.87393700
C	2.80945000	-1.46336000	-1.65975400
C	0.28297300	-0.48223500	0.80516900
O	-0.25238000	0.16430100	1.69952400
N	-0.14046100	-1.73609800	0.50804900
C	-1.17012900	-2.42210400	1.28394600
C	-2.62637000	-2.09460200	0.89274400
O	-3.37208000	-2.97697300	0.48893200
C	-4.34675800	-0.29808600	0.86738400
C	-4.45894800	0.65046800	-0.37261400
C	-4.84556400	0.29928900	2.19134200
N	-2.98120100	-0.79699900	1.06443200
C	-5.93557100	1.04019000	-0.58408900
C	-3.97749100	-0.10732900	-1.62499800
C	-3.61504600	1.92699300	-0.19651800
H	1.62076400	3.95850300	-2.65576000
H	1.75226000	1.53958000	-2.35218800
H	1.09917600	2.02593300	1.86108900
H	0.95932300	4.45407800	1.55435500
H	1.20811100	5.45288000	-0.71085100
H	3.95210800	-2.22546800	3.39328700
H	5.98450000	-0.83484600	3.05641000
H	5.95448200	0.96948000	1.34450400
H	3.93363800	1.37966100	0.01208500
H	1.94702700	-1.83672800	2.04889900
H	-0.28204500	-0.12425200	-2.01700300
H	-0.14997900	-1.33962500	-4.14263300
H	1.88787100	-2.64776000	-4.71525600
H	3.78089300	-2.71765500	-3.10768200
H	3.64542800	-1.51258700	-0.97520100
H	0.25836400	-2.21412600	-0.28482400
H	-1.02174500	-2.18169800	2.34037400
H	-1.04656700	-3.49416400	1.14142500
H	-4.94244400	-1.18543700	0.64123400
H	-5.88428400	0.62552100	2.11891200
H	-4.78674300	-0.45562300	2.97867800
H	-4.24180900	1.15616500	2.50346300
H	-2.27872700	-0.18052500	1.46116700
H	-6.04557300	1.60207900	-1.51630900
H	-6.31708600	1.67076800	0.22224700

H	-6.57471900	0.15408000	-0.65480900
H	-2.92683900	-0.39303100	-1.53932000
H	-4.08419600	0.52277100	-2.51314200
H	-4.55739900	-1.02076800	-1.78366600
H	-3.95855500	2.53283000	0.64633800
H	-3.68399500	2.55007200	-1.09327400
H	-2.55694200	1.69959300	-0.03974700

Compound **15** conf.42

C	-4.11505900	-1.67017500	2.61041100
C	-3.28077200	-0.76087100	1.96923200
C	-2.62695900	-1.09811400	0.77424800
C	-2.87301200	-2.36273600	0.22945800
C	-3.71644500	-3.27357800	0.86895400
C	-4.33545100	-2.93530300	2.06666000
C	-1.76941700	-0.03257900	0.04180300
C	-3.56388300	3.37896900	-0.39642100
C	-4.63340400	3.02596800	-1.21080500
C	-4.77107900	1.69741100	-1.61440500
C	-3.84650300	0.74189200	-1.20841600
C	-2.75006100	1.08593700	-0.40258000
C	-2.63126300	2.41835700	0.00269000
C	-0.98062700	-0.63586100	-1.14417900
C	-0.08092000	-1.68536900	-0.88883100
C	0.68641600	-2.24102000	-1.90575400
C	0.58591300	-1.75160300	-3.20984100
C	-0.28546800	-0.70227600	-3.47500800
C	-1.06094600	-0.14846800	-2.45121900
C	-0.69857400	0.58494700	1.02244000
O	-0.76086300	0.49263200	2.23273700
N	0.31576600	1.27571100	0.40626600
C	1.21146800	2.14895600	1.14972200
C	2.67201100	1.70289100	1.30738200
O	3.45604900	2.45237400	1.87058800
C	4.31241700	-0.13622300	1.00158400
C	5.15901600	-0.18691000	-0.31348200
C	4.11039900	-1.48579500	1.70414900
N	2.99909300	0.48876900	0.79763000
C	6.56537700	-0.73052600	0.01011300
C	5.31082400	1.24223700	-0.86988800
C	4.50235400	-1.07759800	-1.38354400
H	-4.59860900	-1.38526600	3.53827500
H	-3.13444900	0.21662700	2.40481400
H	-2.41555600	-2.65355900	-0.70646700
H	-3.88666400	-4.24648500	0.42093900
H	-4.98799600	-3.64203200	2.56705900
H	-3.44939100	4.40321900	-0.05945400
H	-5.35772700	3.77097300	-1.51975300
H	-5.60720700	1.40145700	-2.23827400
H	-3.98493600	-0.28940800	-1.51055300
H	-1.82043300	2.72847900	0.64892800
H	0.00518600	-2.07897200	0.11840000
H	1.36410000	-3.05739600	-1.68226800
H	1.18324300	-2.18395200	-4.00438200
H	-0.37161200	-0.30628100	-4.48081500
H	-1.73294400	0.66648600	-2.68531400
H	0.28175100	1.36788200	-0.59834100
H	0.81385600	2.26217900	2.15921600
H	1.23694100	3.13897700	0.68718200
H	4.83520000	0.53624100	1.68574500
H	3.55759400	-1.33627000	2.63411800
H	3.54252500	-2.18735700	1.08543300
H	5.06328700	-1.95461700	1.95384300
H	2.24625500	-0.06765000	0.41711500
H	6.54697600	-1.78298000	0.30306100
H	7.03500800	-0.16037600	0.81803400
H	7.21065700	-0.64877500	-0.86933300
H	5.77002700	1.90772200	-0.13428500
H	4.34477200	1.67043600	-1.14648600
H	5.94157700	1.23443200	-1.76385200
H	5.10444900	-1.07334600	-2.29713000
H	3.50399700	-0.71986700	-1.65075000
H	4.41650900	-2.11729300	-1.05542700

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