Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.


# A HIGHLY SELECTIVE RECEPTOR FOR ZWITTERIONIC PROLINE

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**Figure S1. $^{1}$H NMR spectrum of compound 3 (200 MHz, $CDCl_3$).**

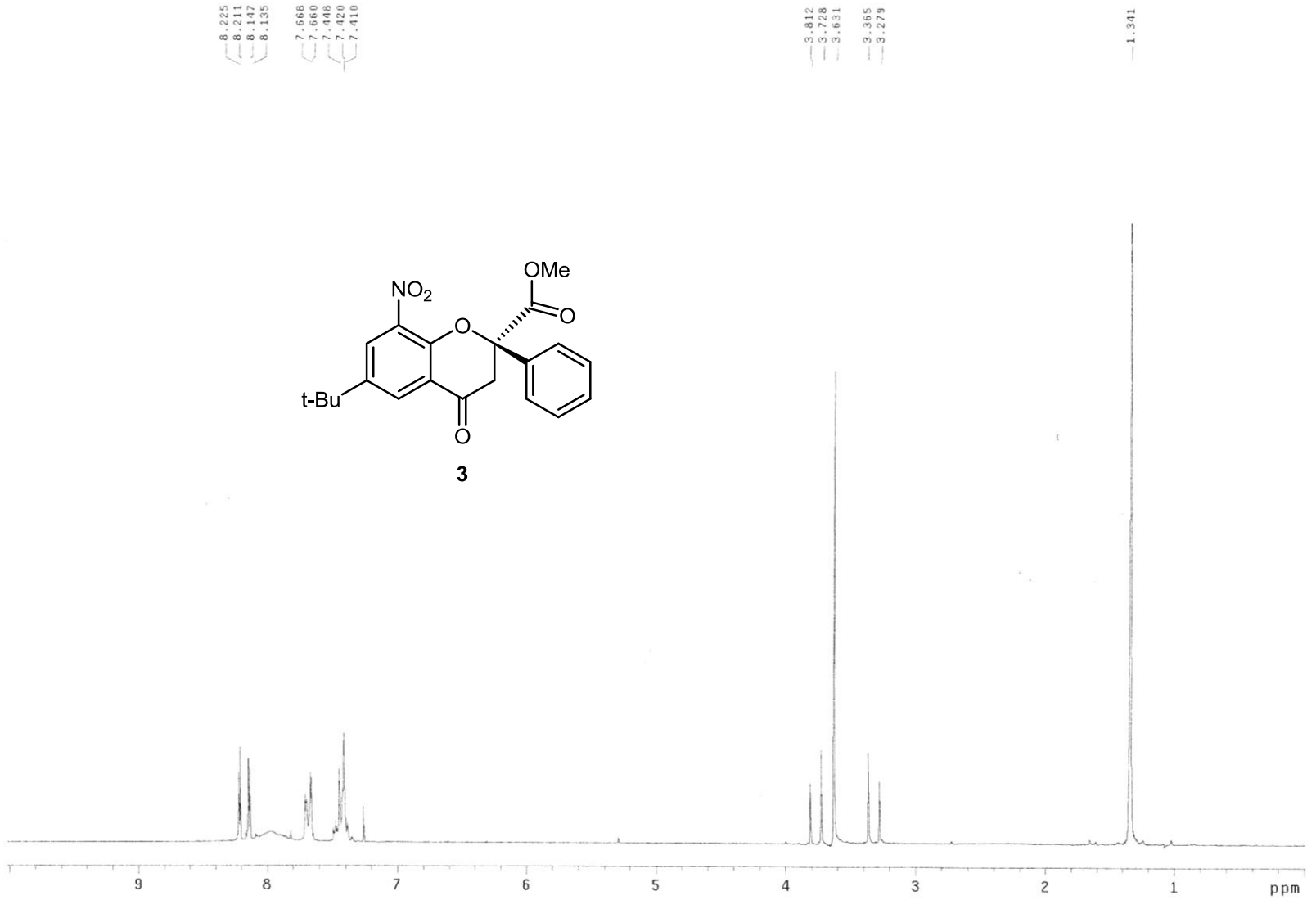


**Figure S2. $^{13}C$ NMR spectrum of compound 3 (50 MHz, $CDCl_3$).**

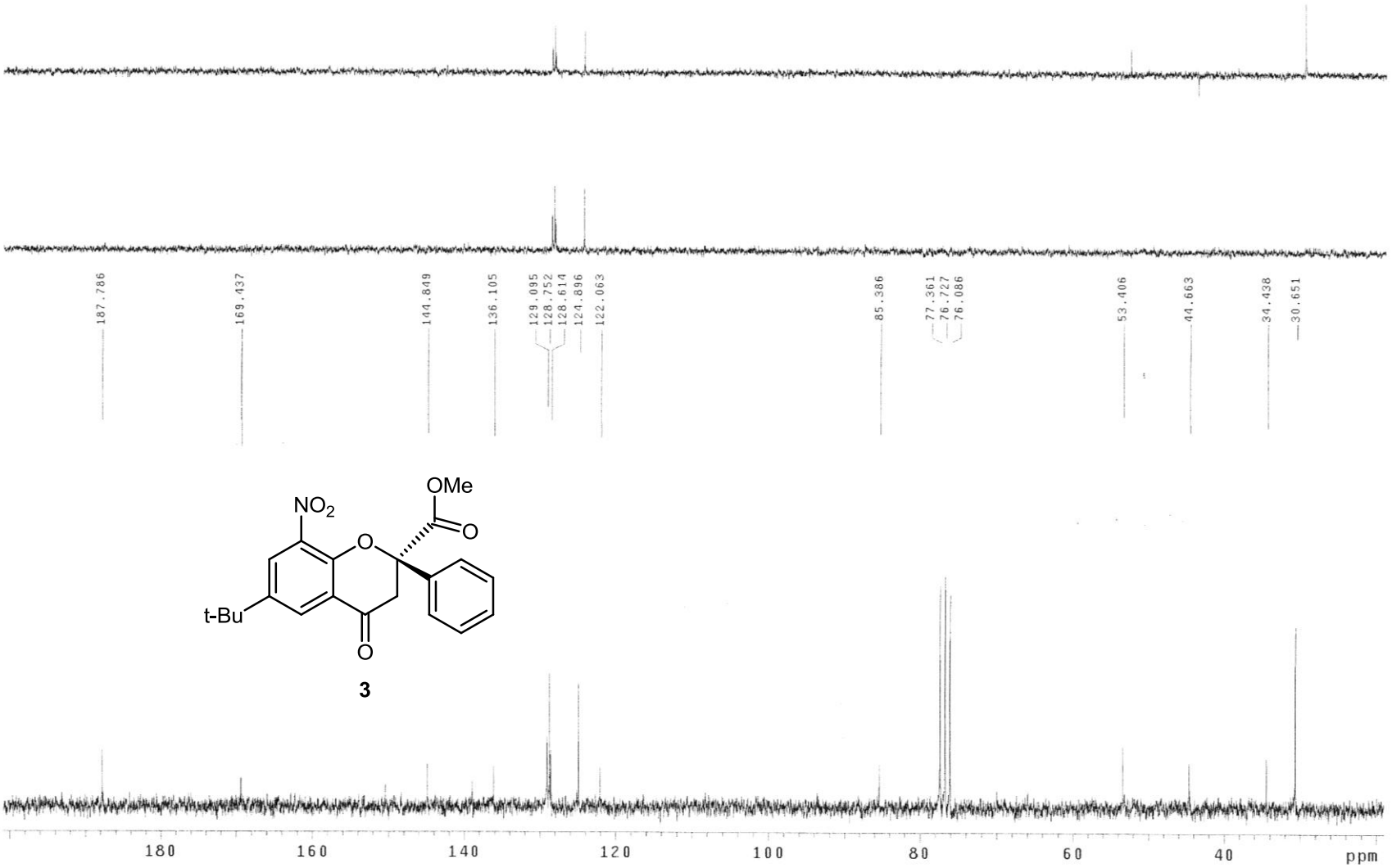


**Figure S3. IR spectrum of compound 3 (nujol).**

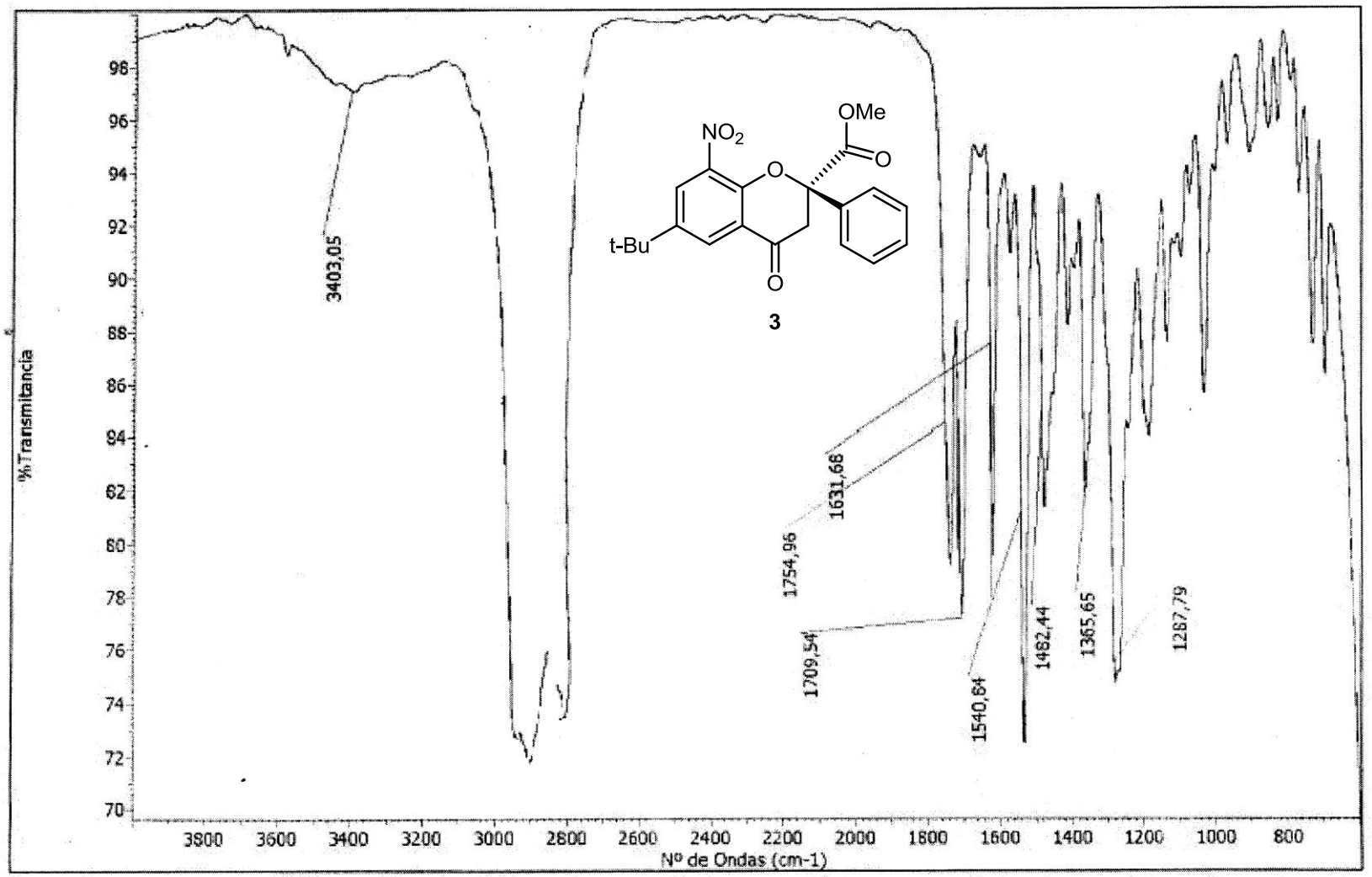


**Figure S4. HRM spectrum of compound 3 (ESI-QTOF).**

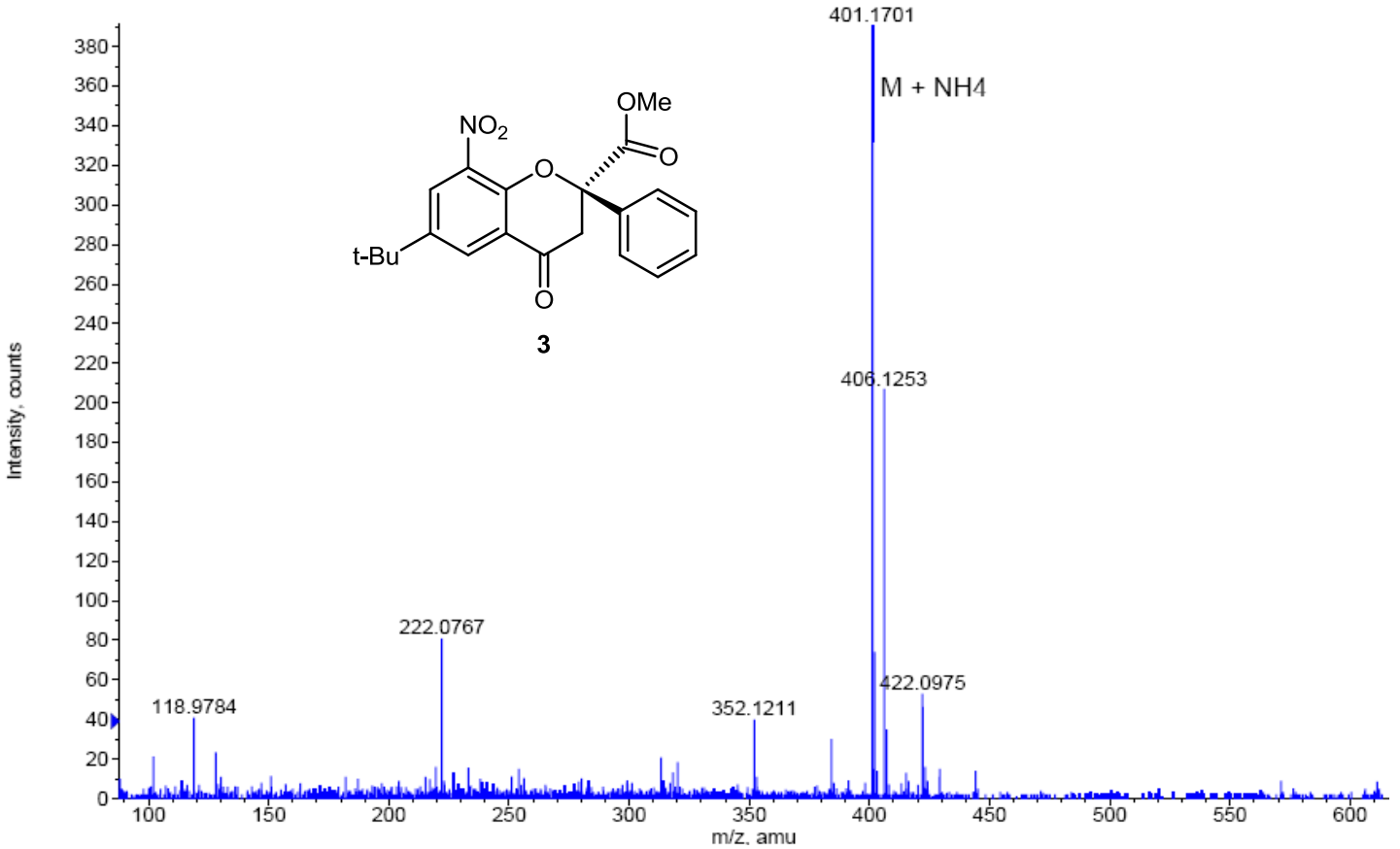


**Figure S5. $^{1}$H NMR spectrum of compound 4 (200 MHz, $CDCl_3$).**

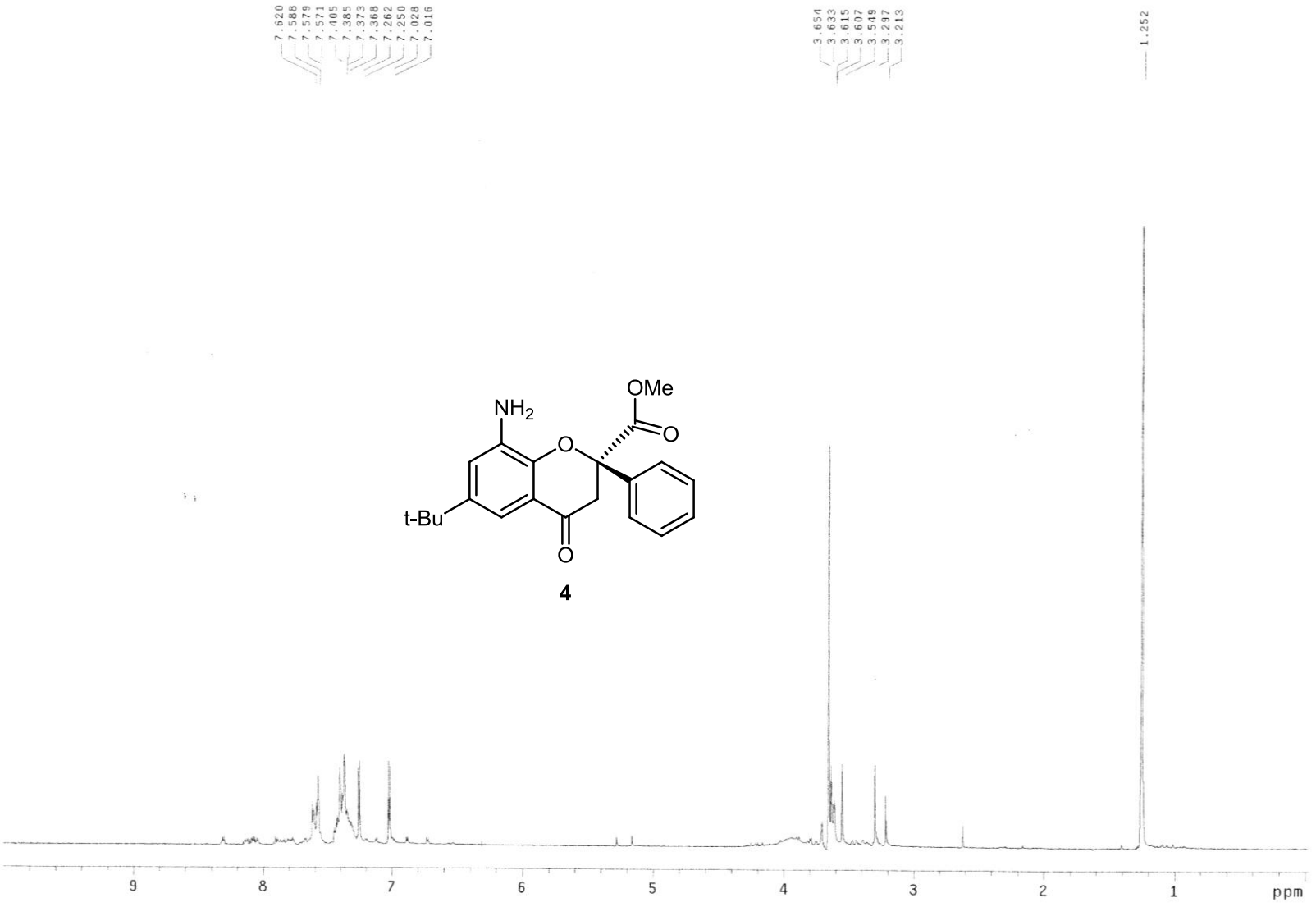


**Figure S6. $^{13}C$ NMR spectrum of compound 4 (50 MHz, $CDCl_3$).**

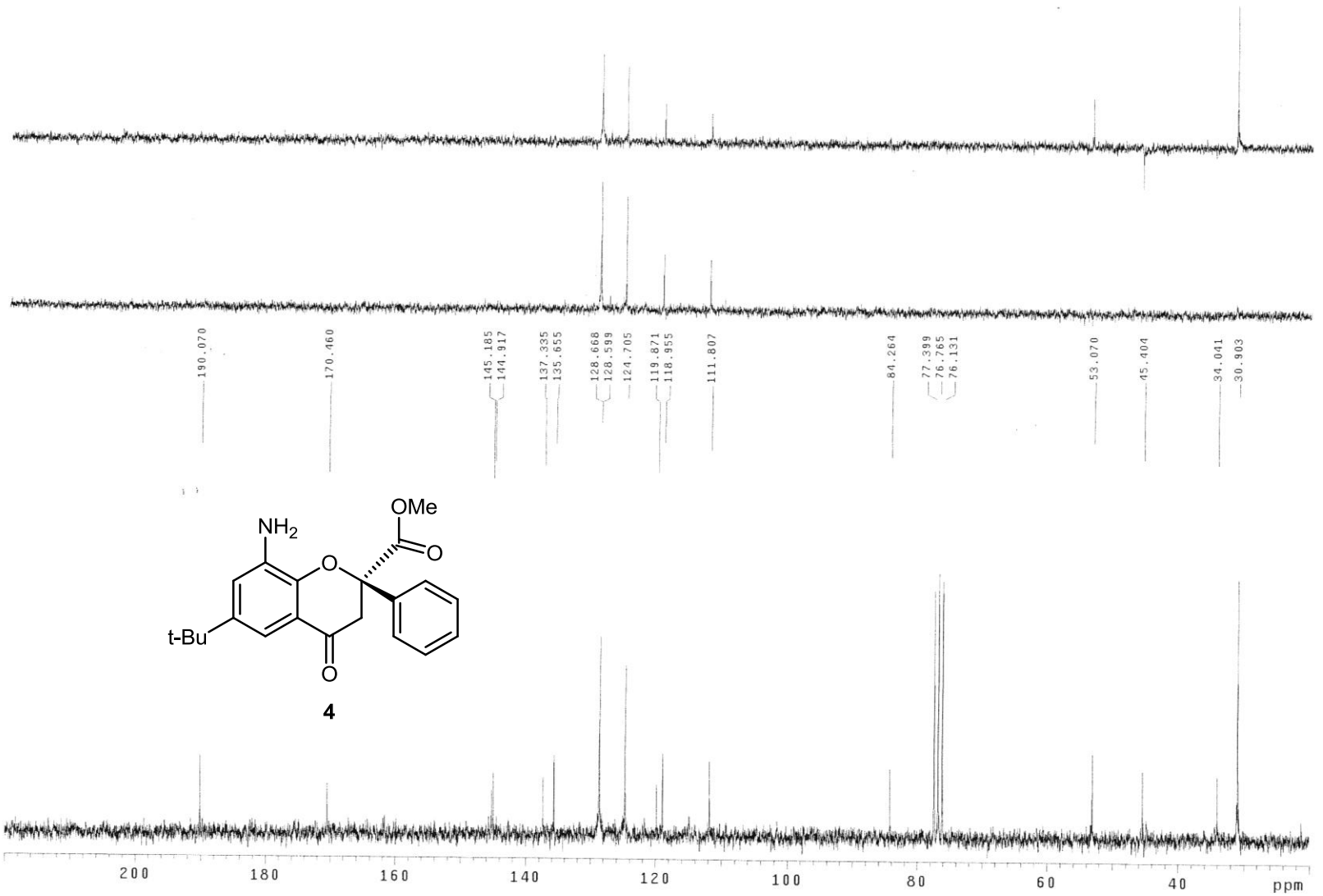


**Figure S7. IR spectrum of compound 4 (nujol).**

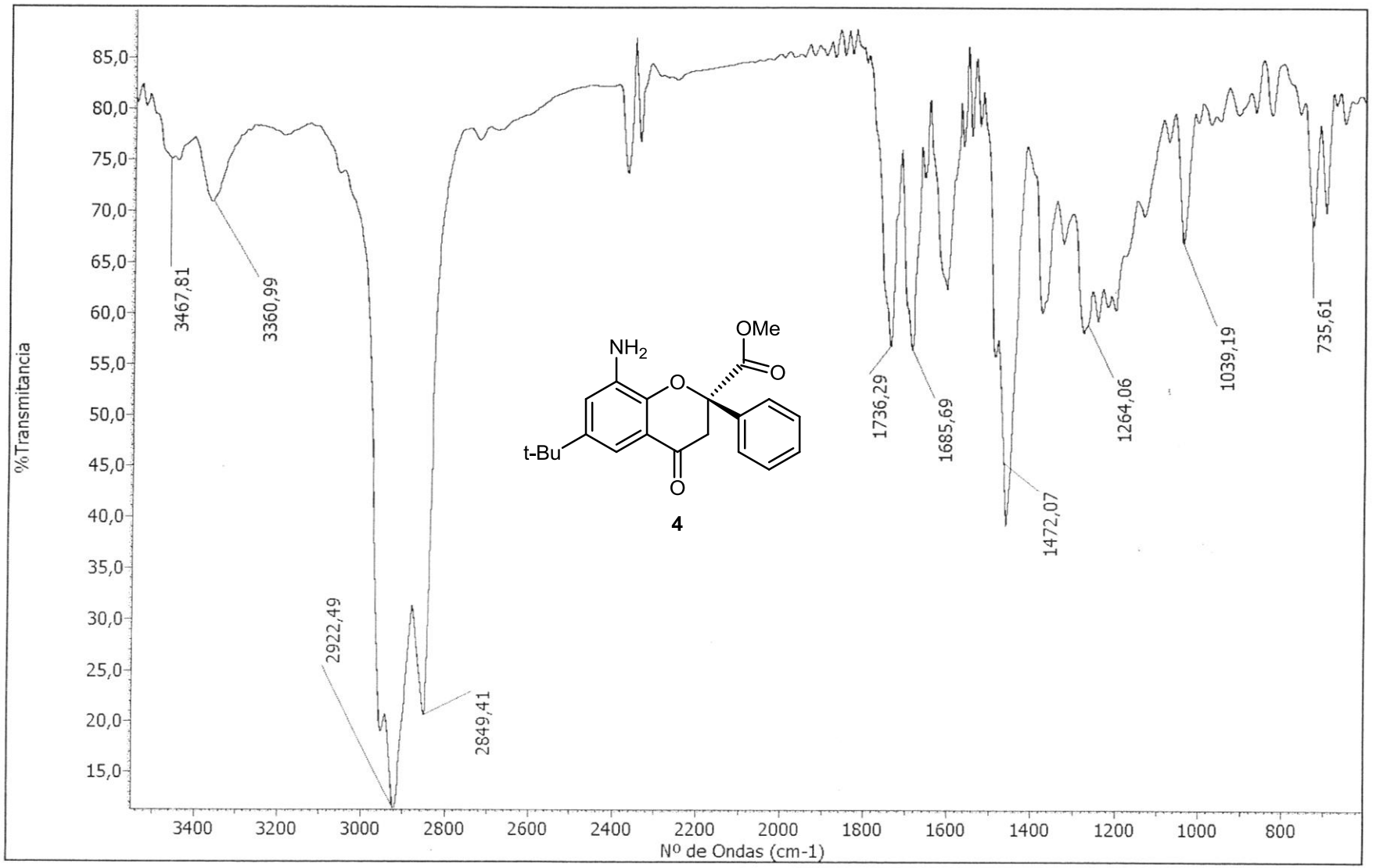


**Figure S8. HRM spectrum of compound 4 (ESI-QTOF).**

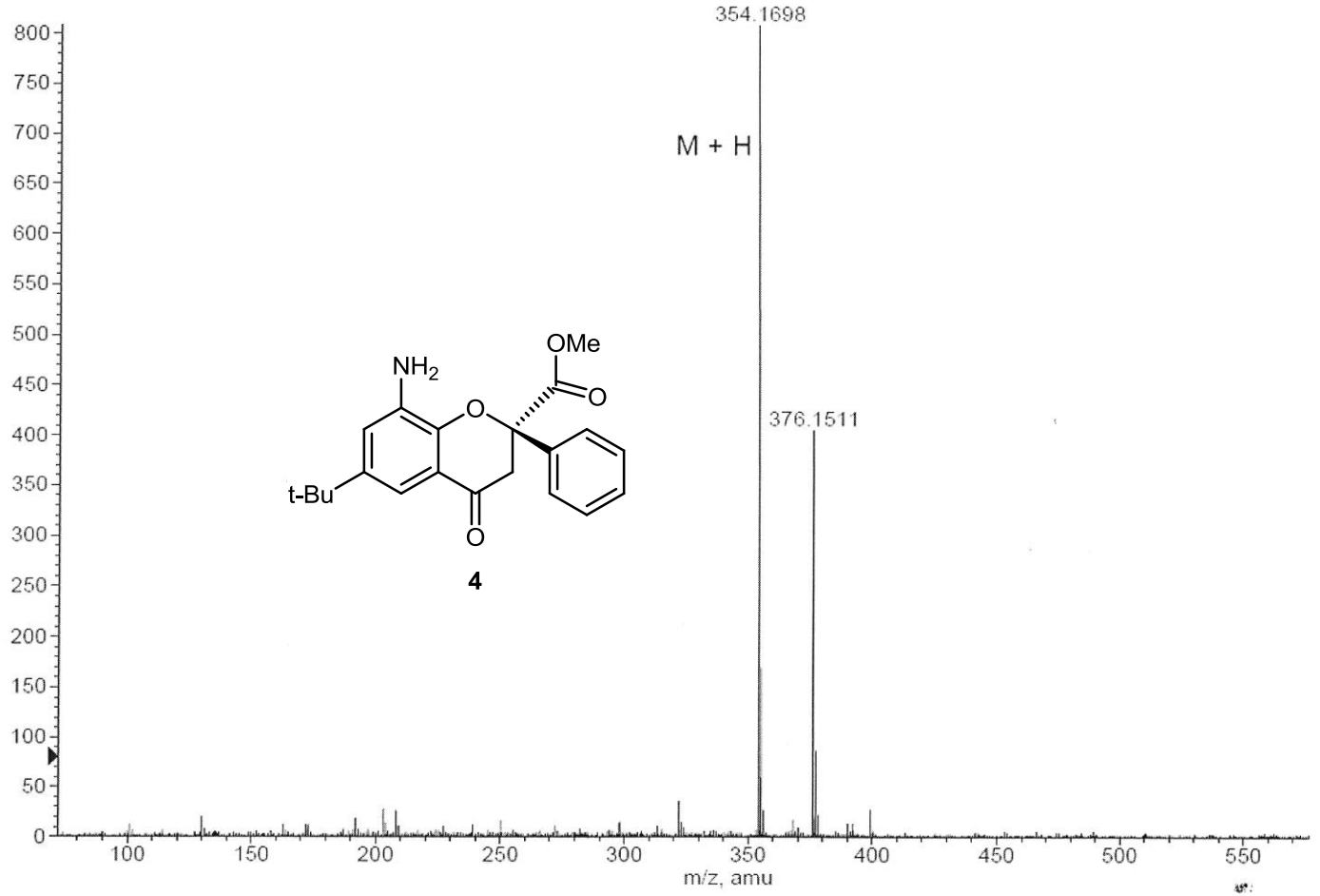


**Figure S9. $^{1}$H NMR spectrum of compound 5 (200 MHz, $CDCl_3$).**

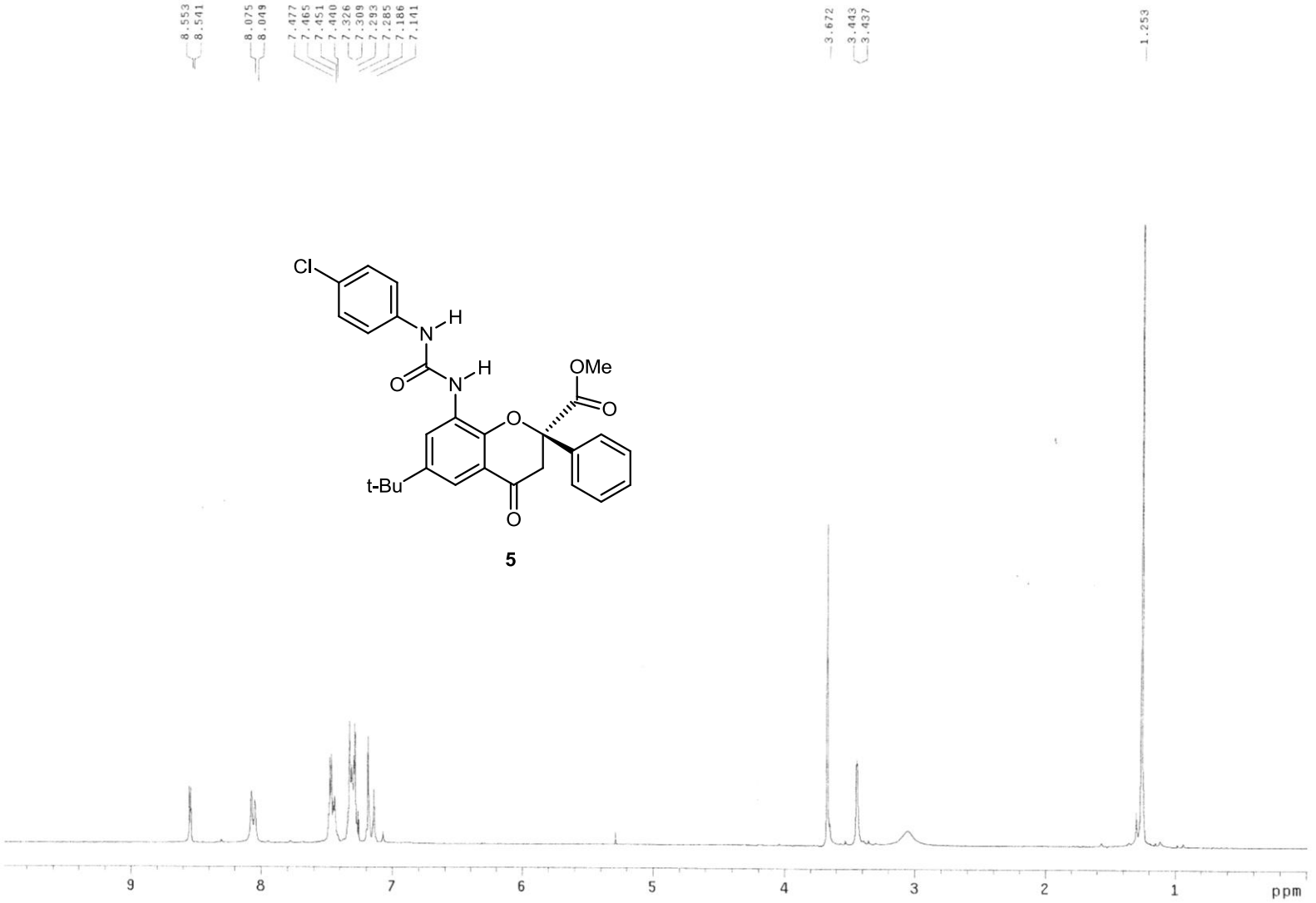


**Figure S10. $^{13}C$ NMR spectrum of compound 5 (50 MHz, $CDCl_3$).**

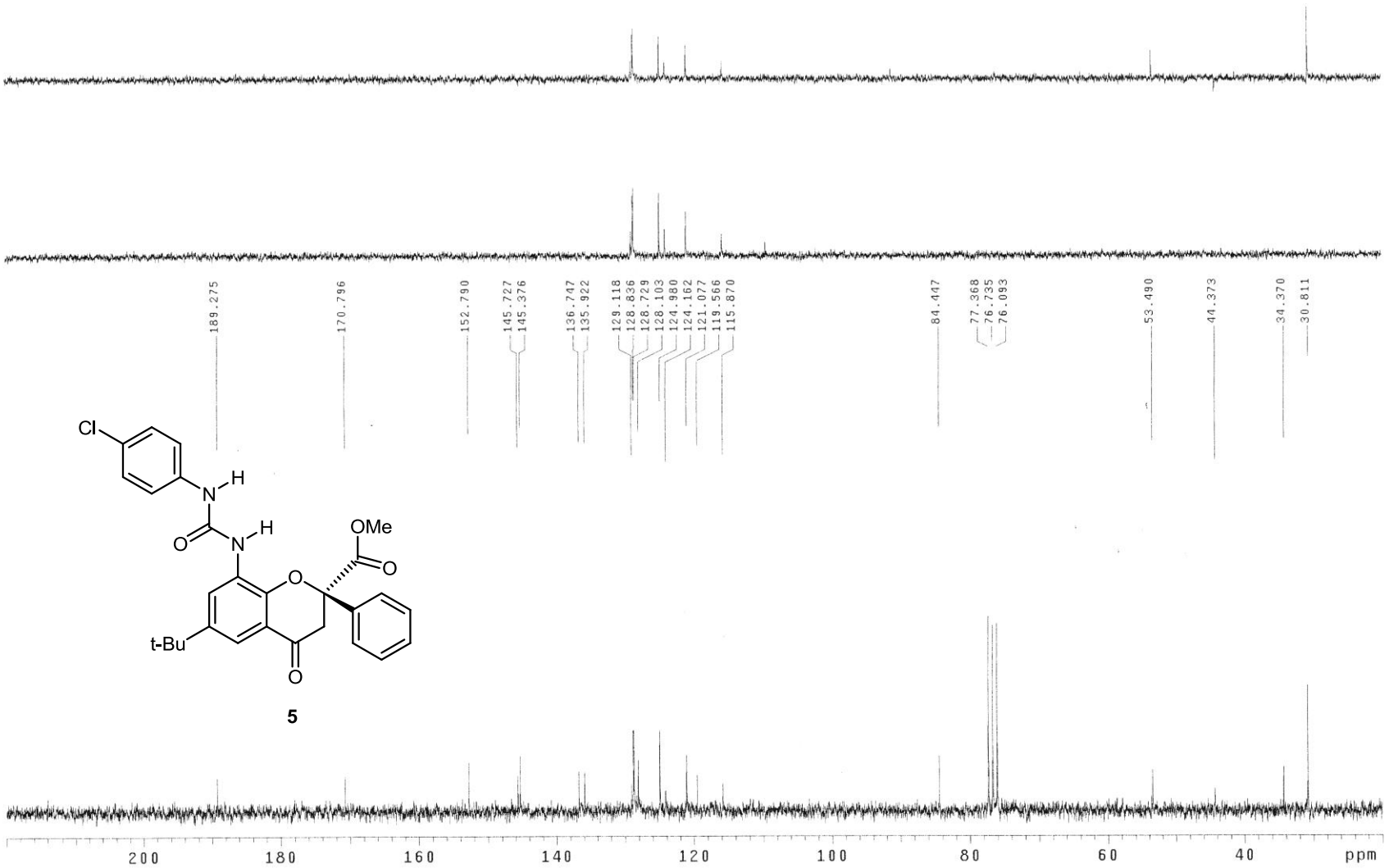


**Figure S11. IR spectrum of compound 5 (nujol).**

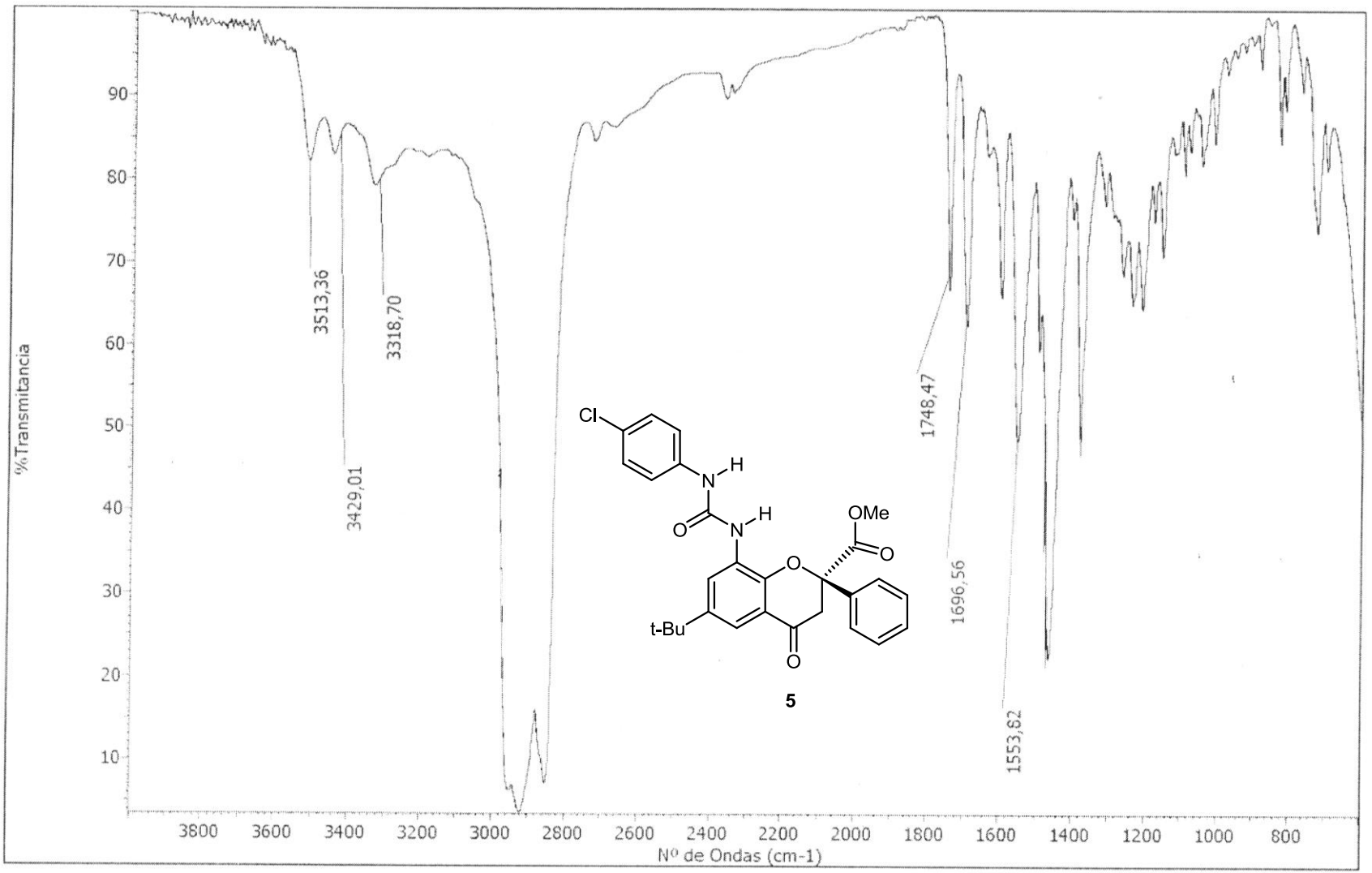


**Figure S12. HRM spectrum of compound 5 (ESI-QTOF).**

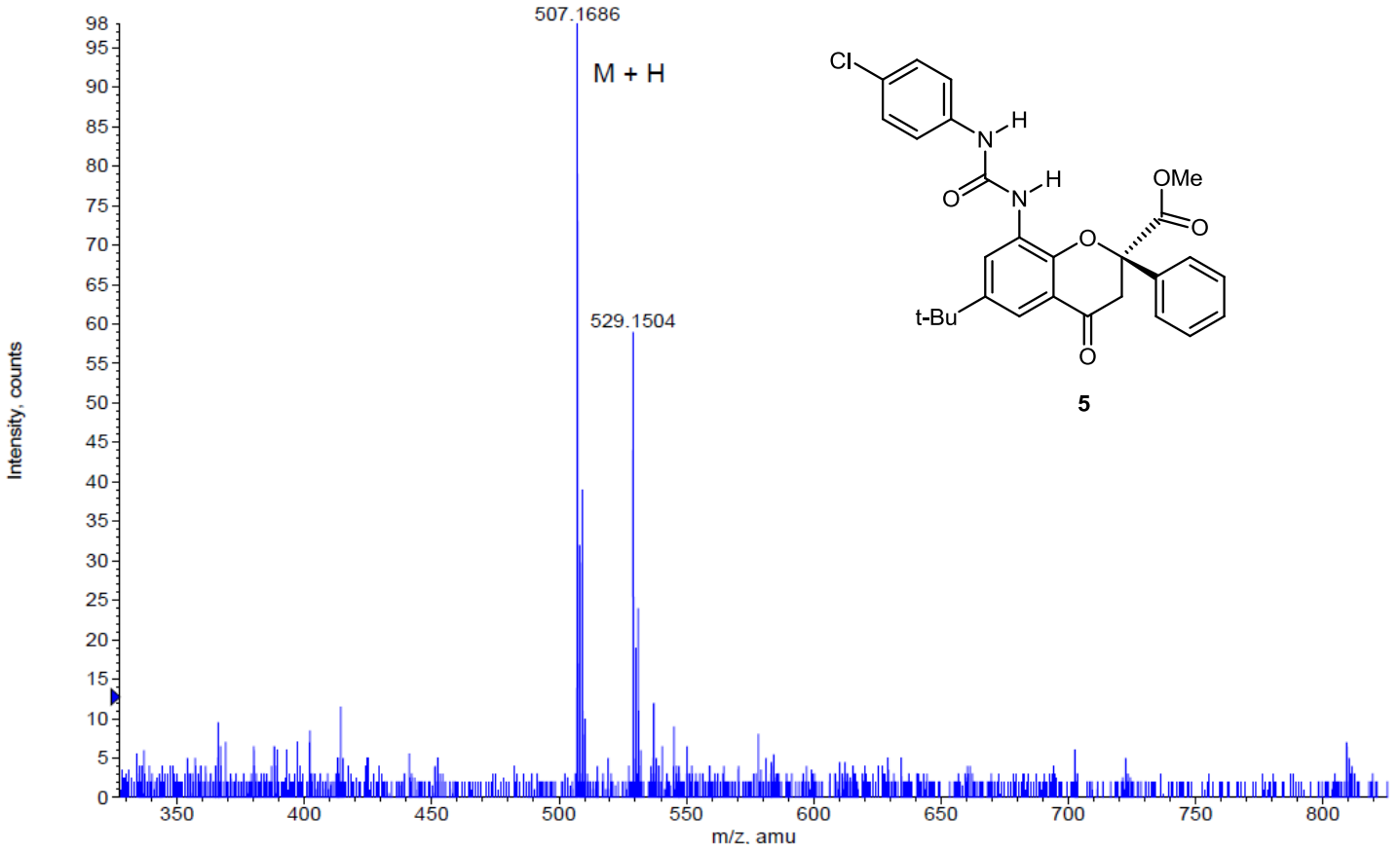


**Figure S13. $^{1}$H NMR spectrum of compound 6 (200 MHz, $CDCl_3$).**

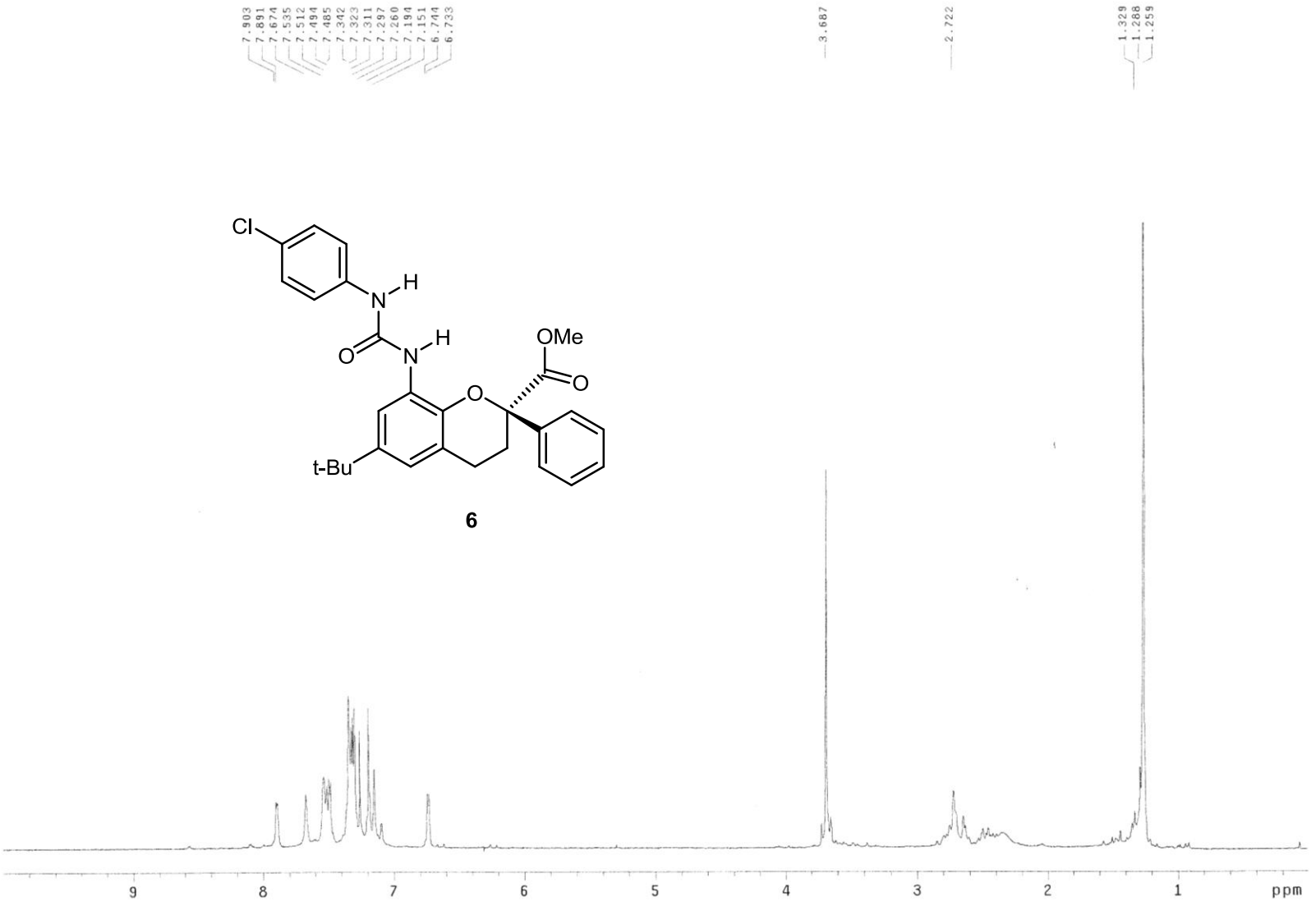


**Figure S14. $^{13}$C NMR spectrum of compound 6 (50 MHz, $CDCl_3$).**

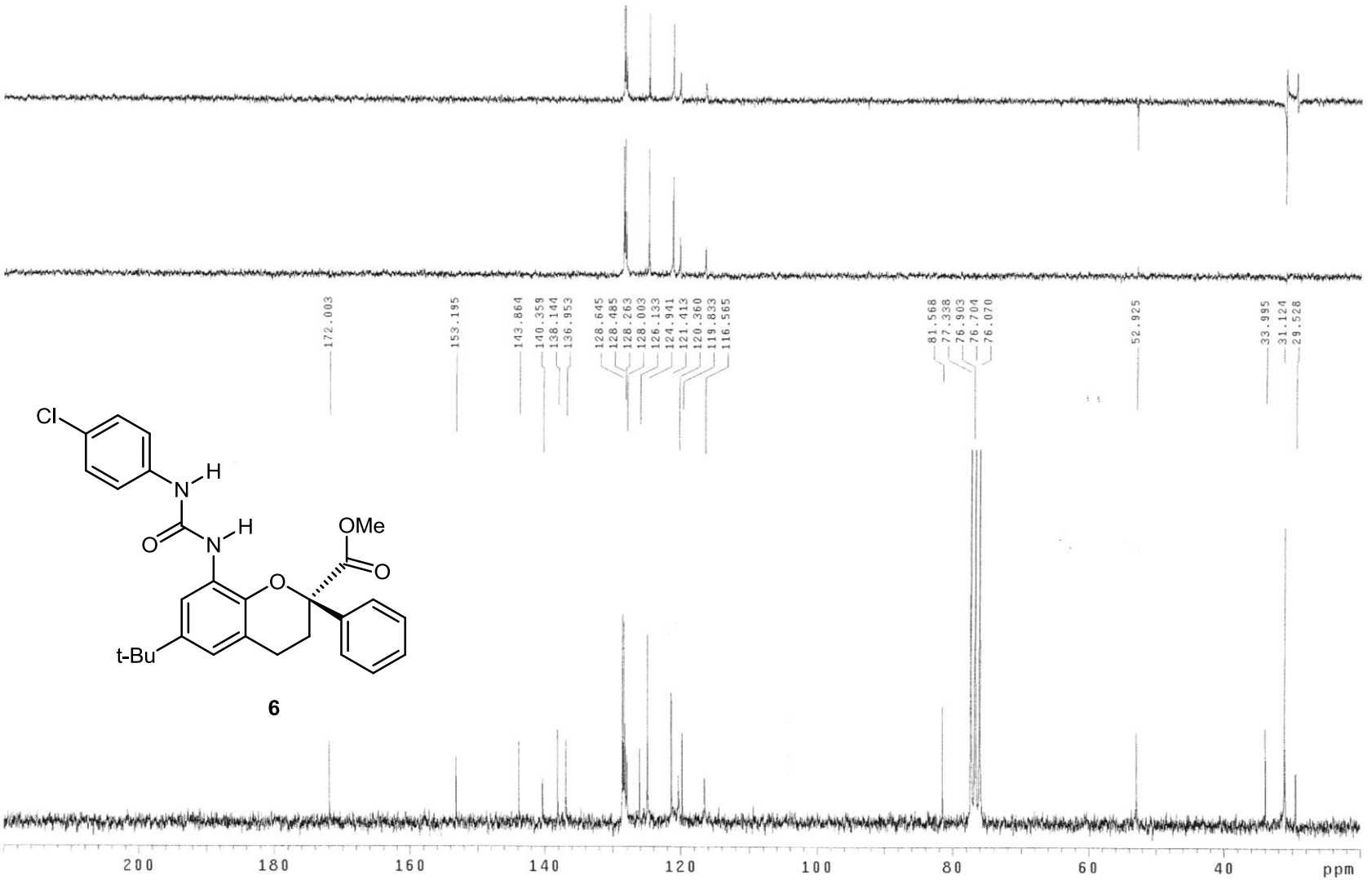


**Figure S15. IR spectrum of compound 6 (nujol).**

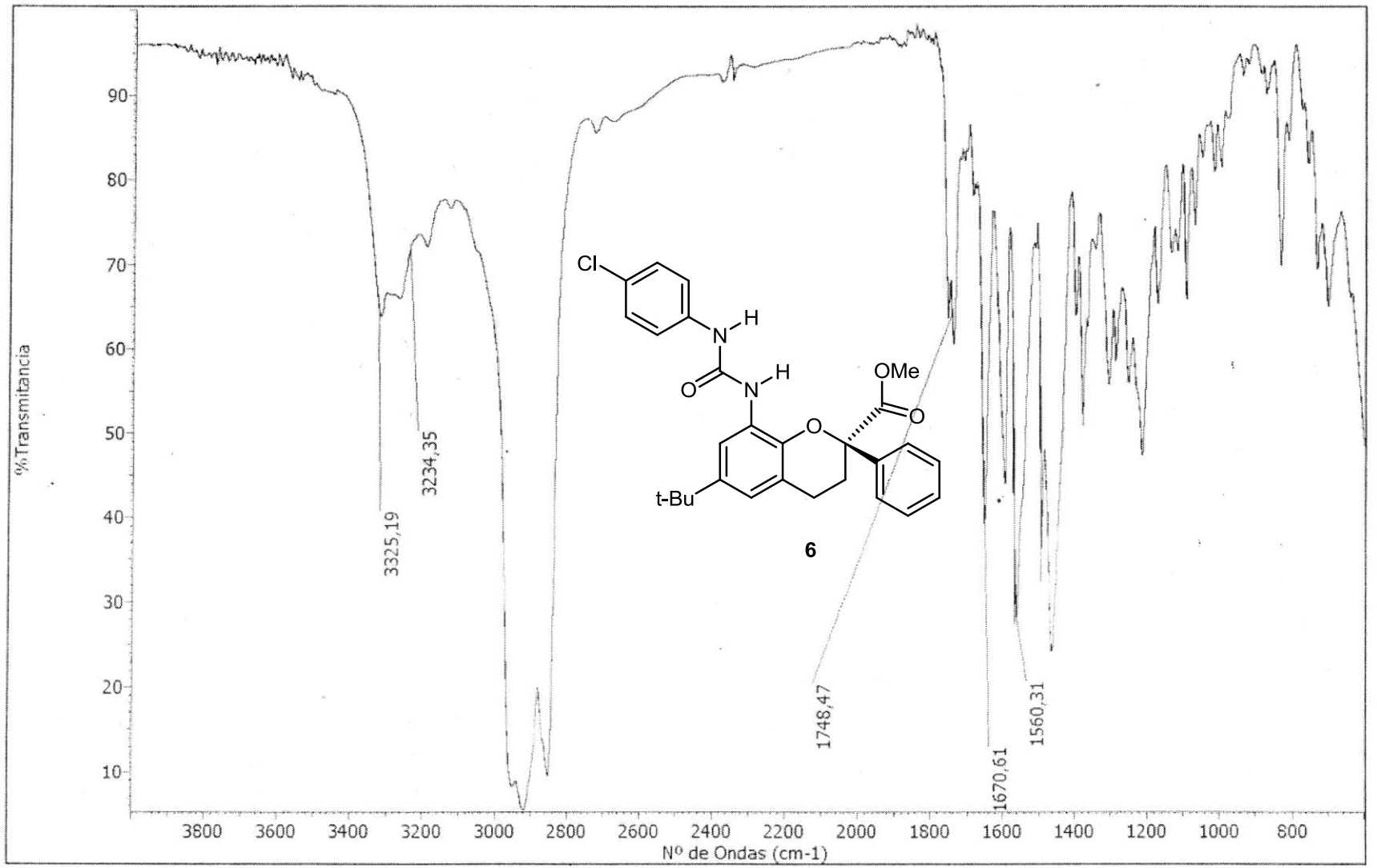


**Figure S16. HRM spectrum of compound 6 (ESI-QTOF).**

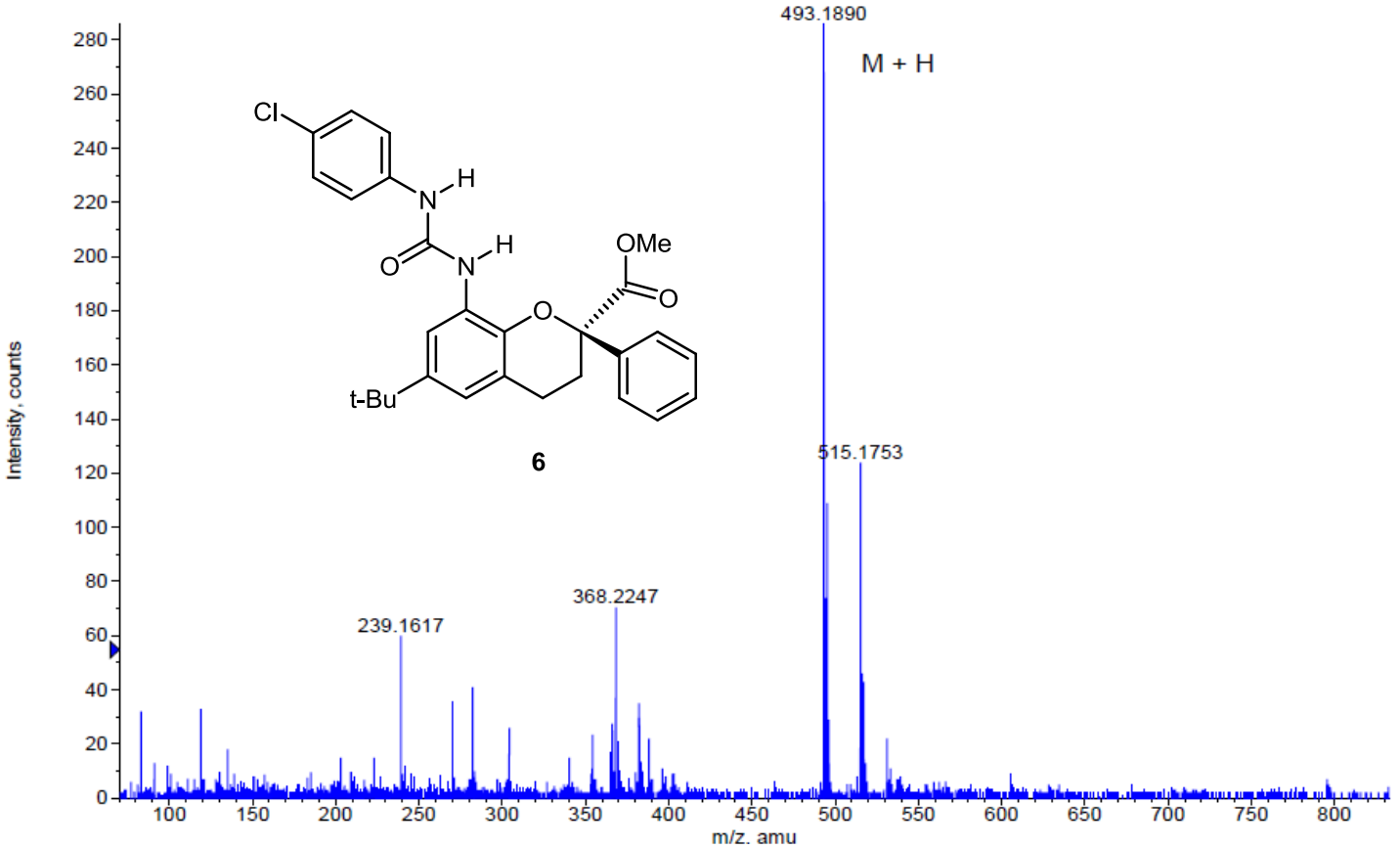


**Figure S17. $^{1}$H NMR spectrum of receptor 1. (200 MHz, $CDCl_3$).**

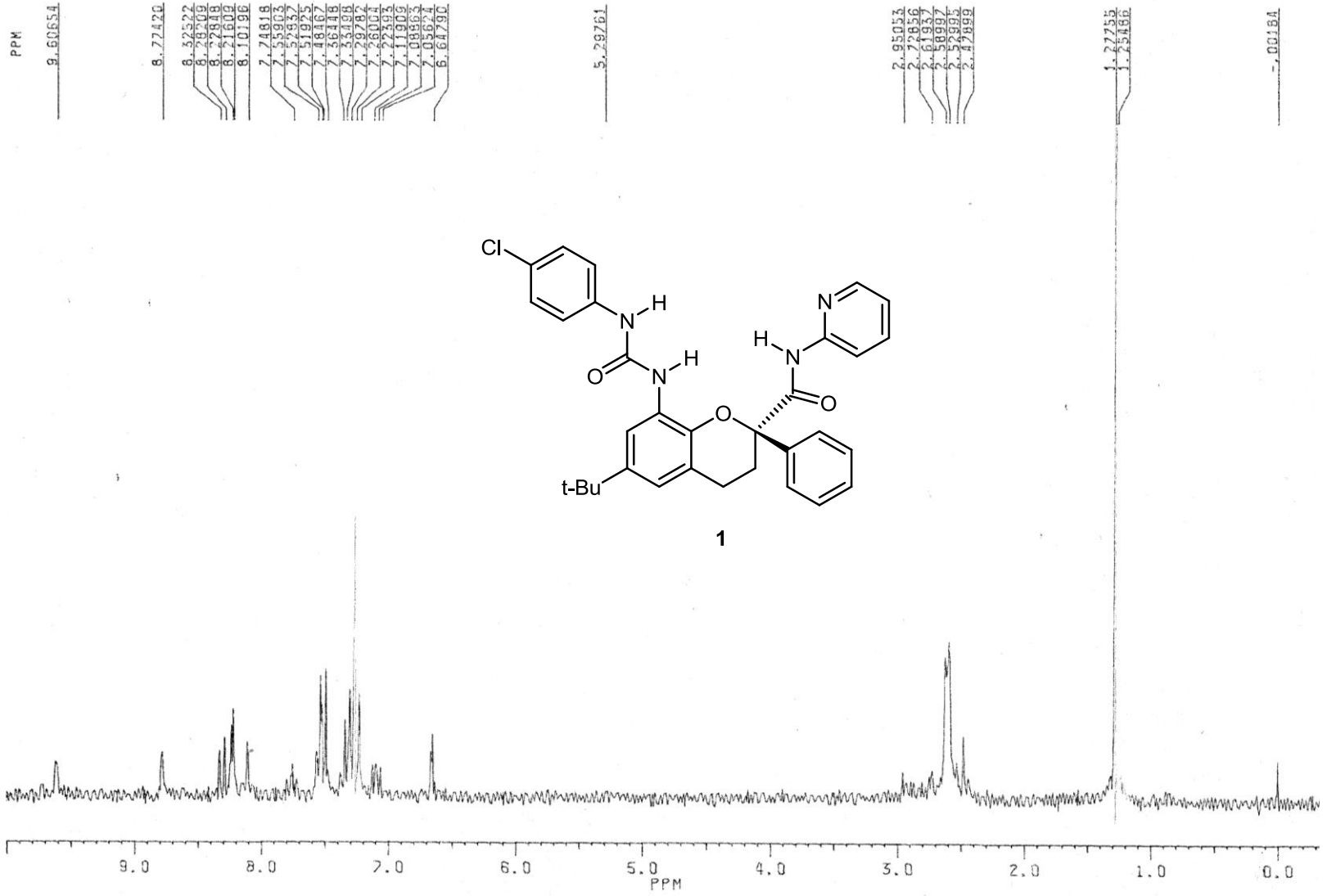
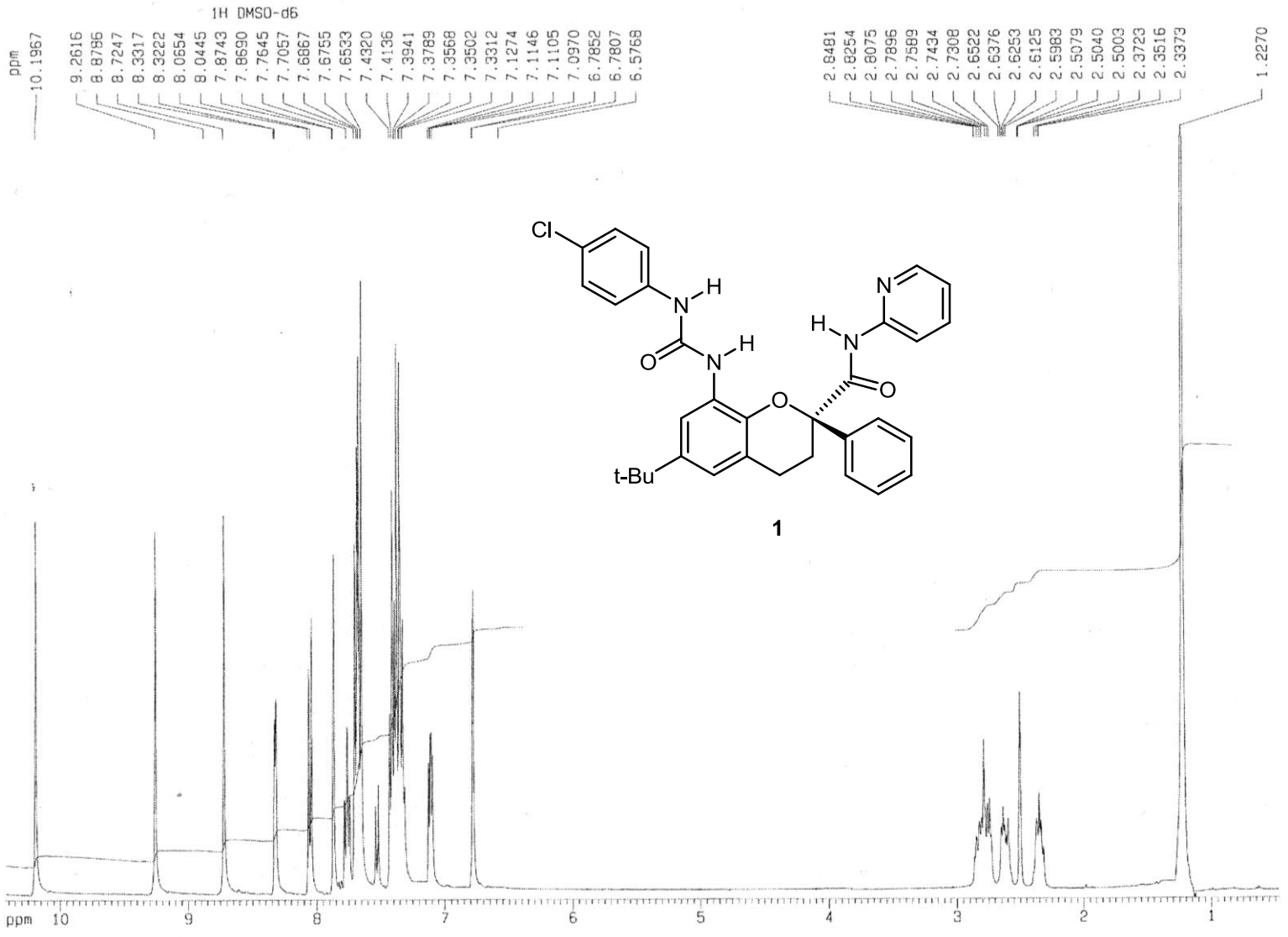


**Figure S18. $^{1}$H NMR spectrum of receptor 1. (400 MHz, DMSO- $d_6$).**




**1**

**Figure S19. $^{13}$C NMR spectrum of receptor 1. (100 MHz, DMSO-$d_6$).**

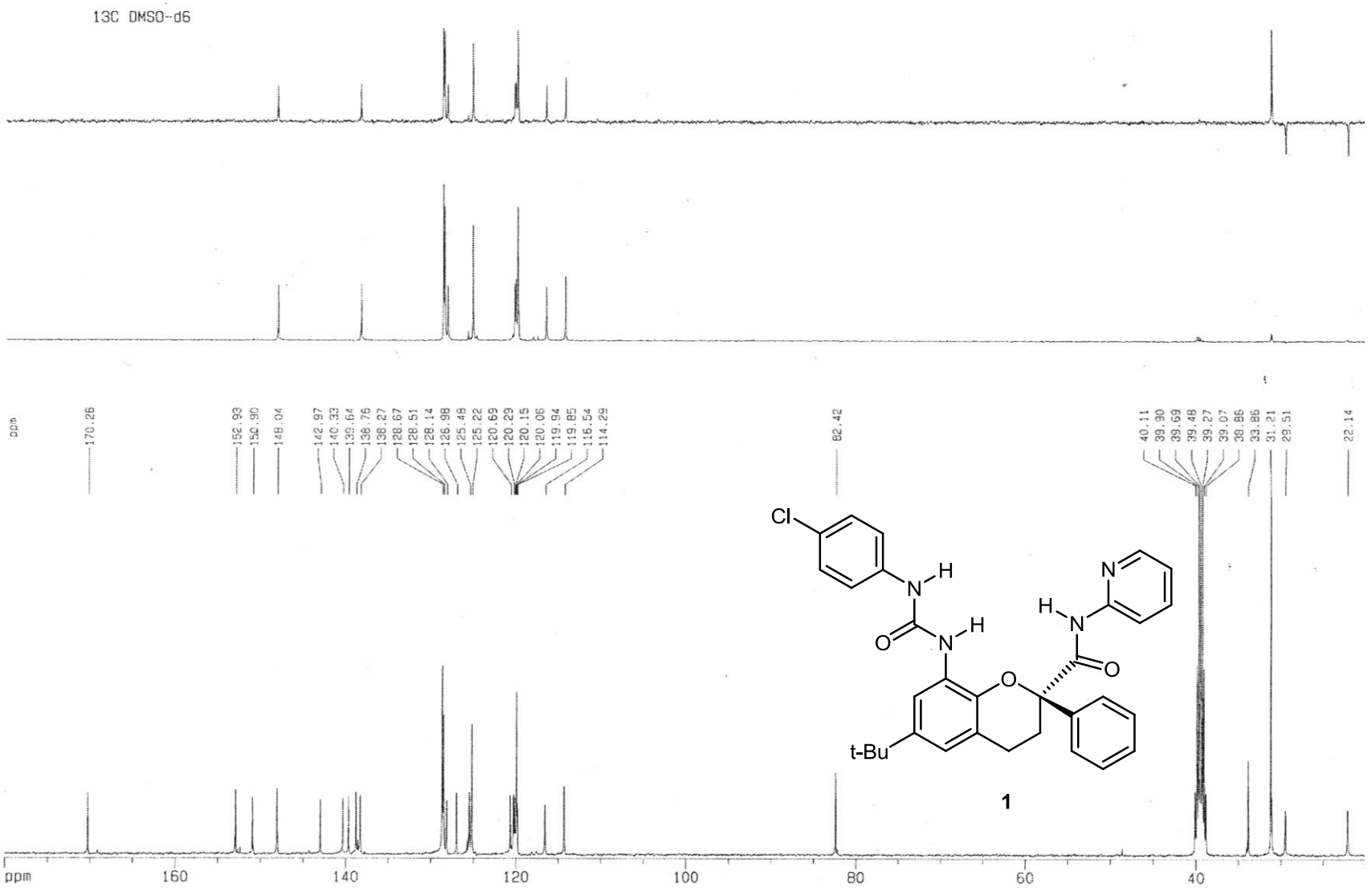


**Figure S20. ROESY spectrum of receptor 1 (DMSO-$d_6$).**

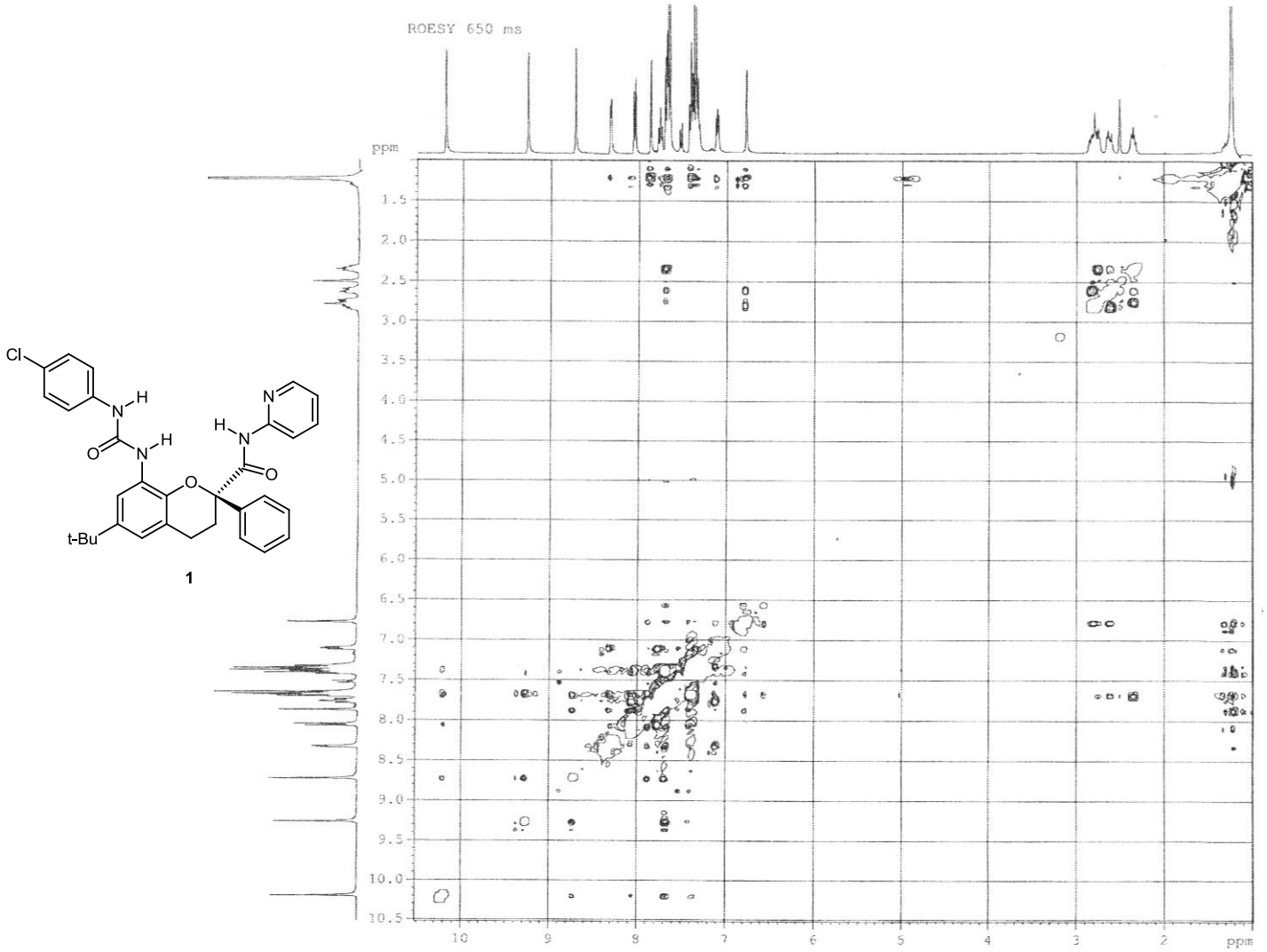


**Figure S21. COSY spectrum of receptor 1 (DMSO-$d_6$).**

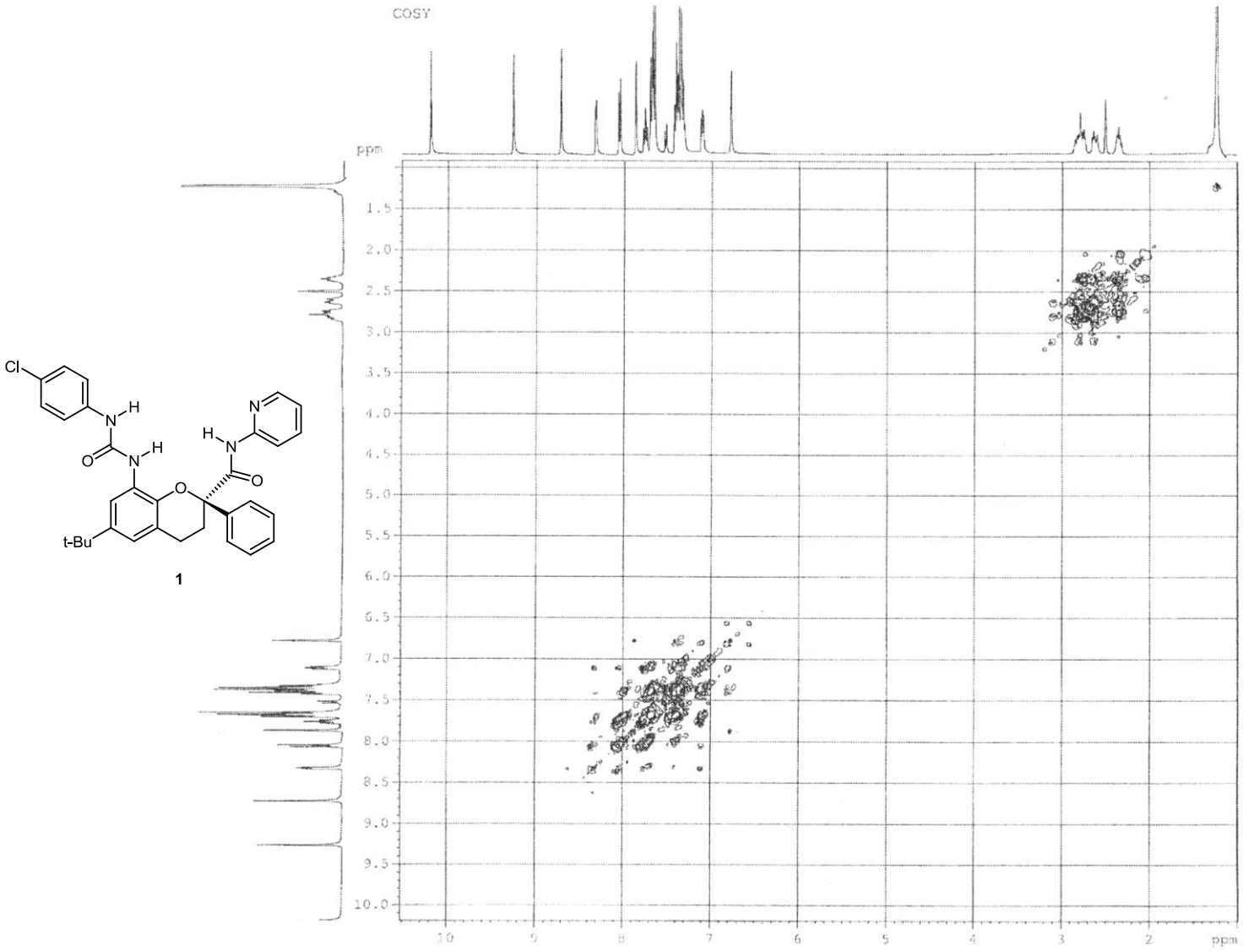


**Figure S22. HMQC spectrum of receptor 1 (DMSO-$d_6$).**

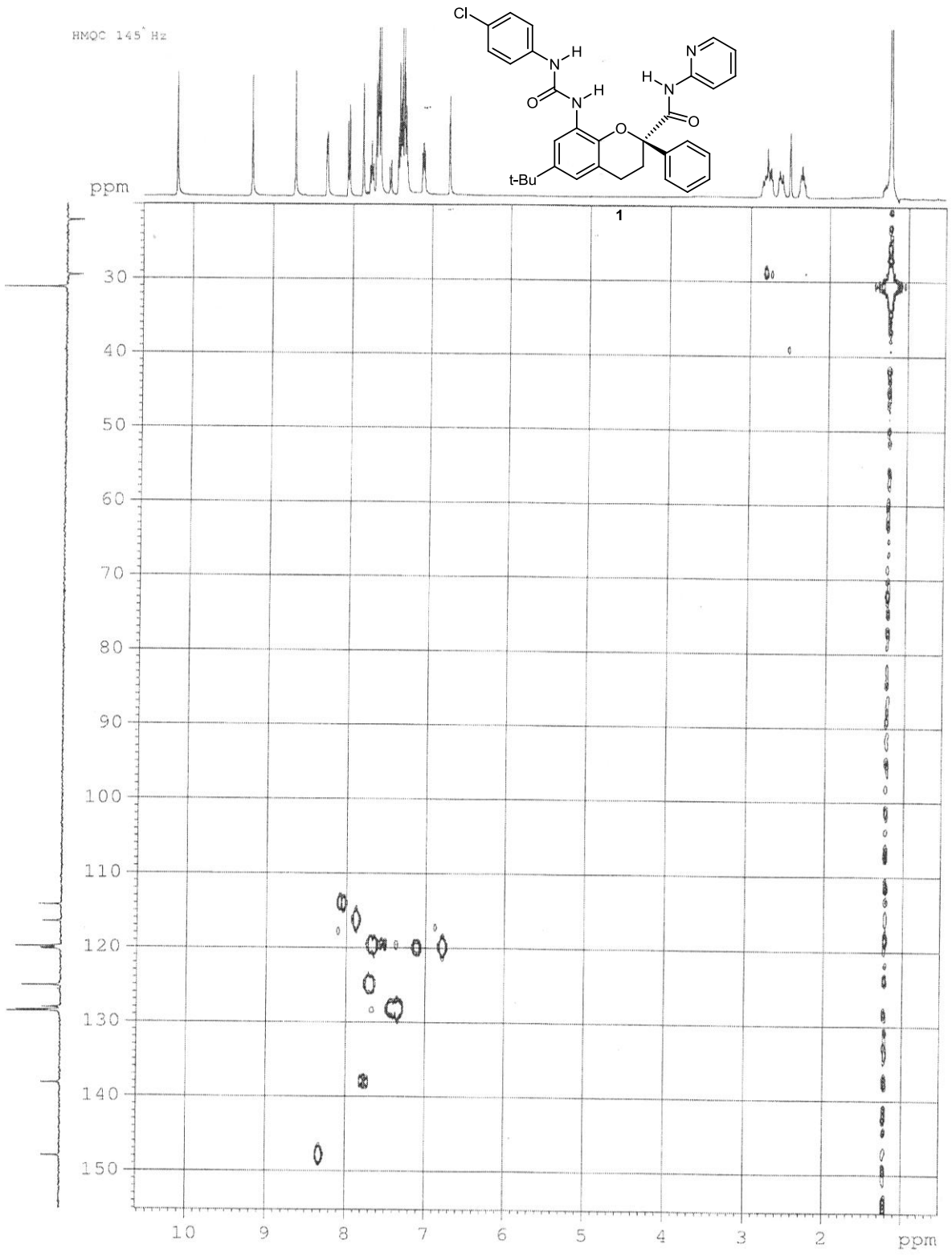


**Figure S23. HMBC spectrum of receptor 1 (DMSO-$d_6$).**

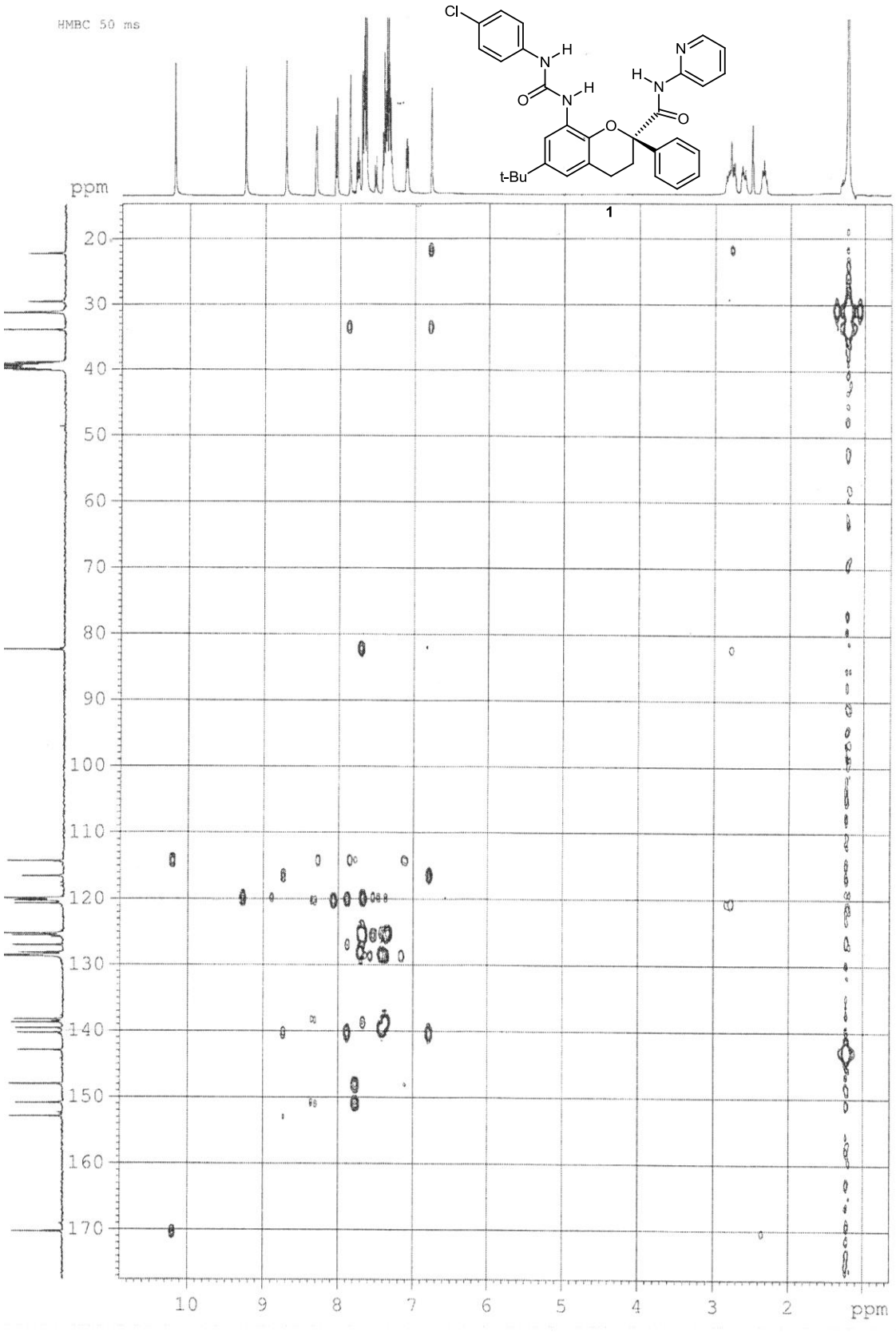


**Figure S24. IR spectrum of receptor 1 (nujol).**

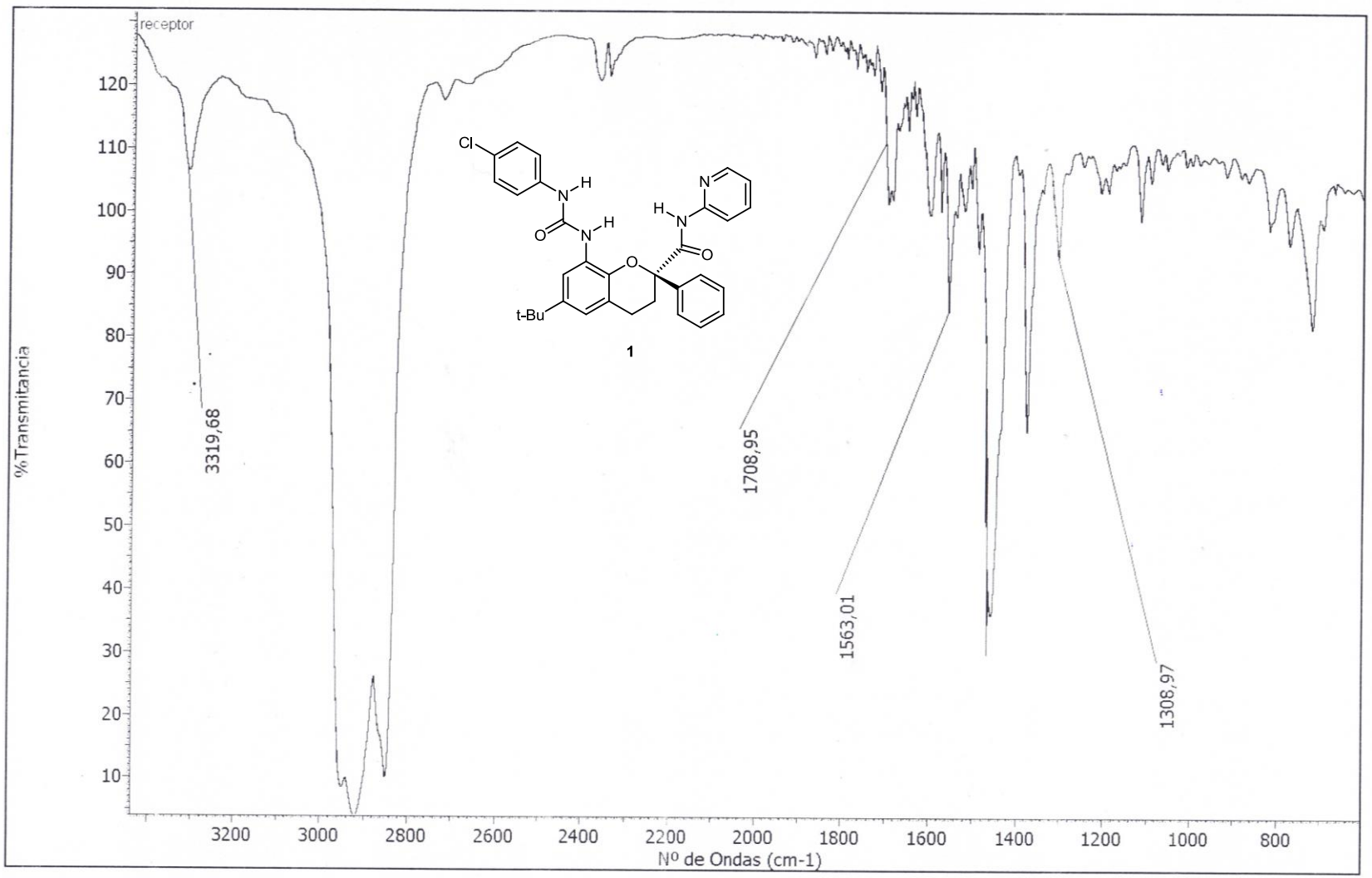


**Figure S25. HRM spectrum receptor 1 (ESI-QTOF).**

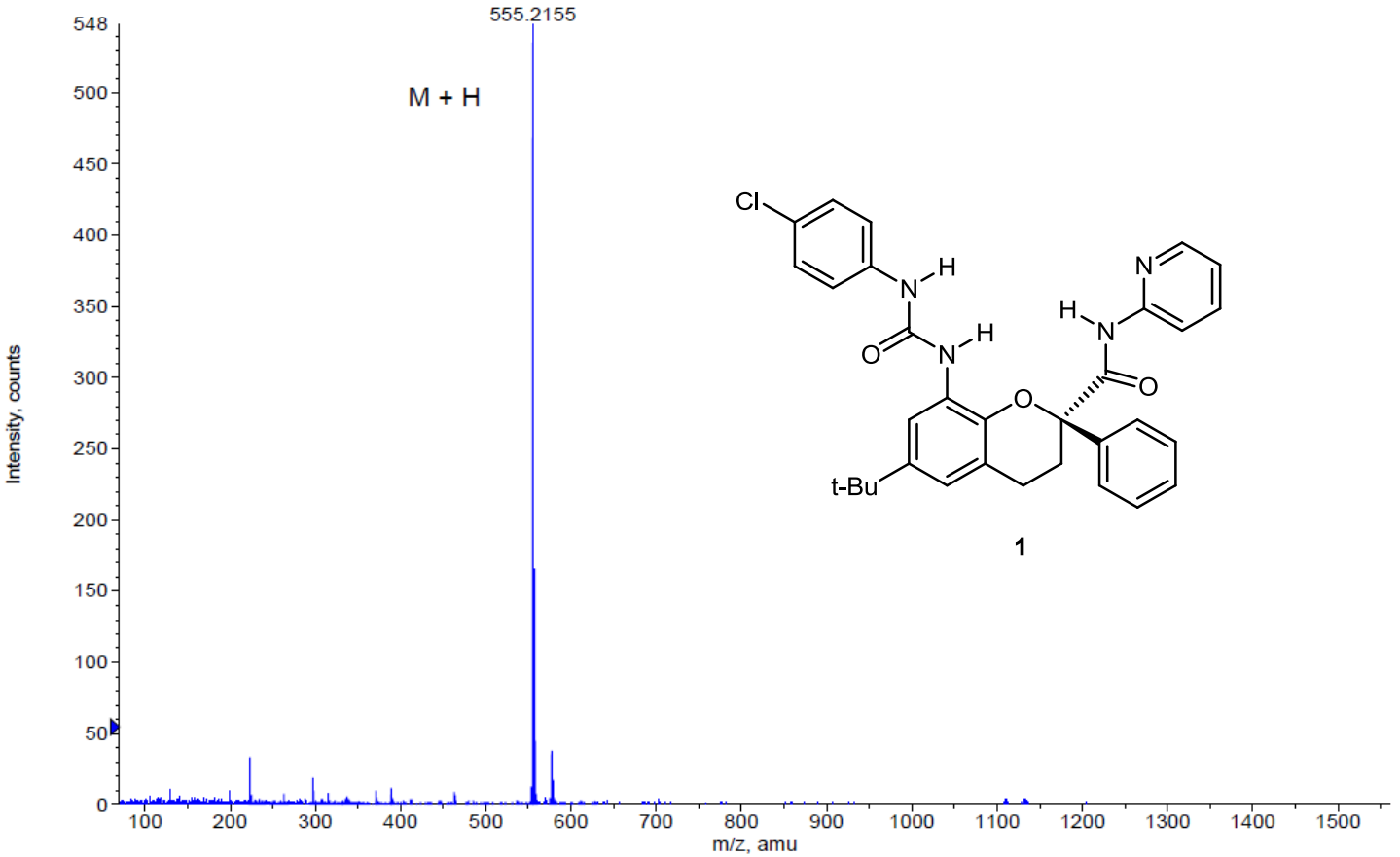
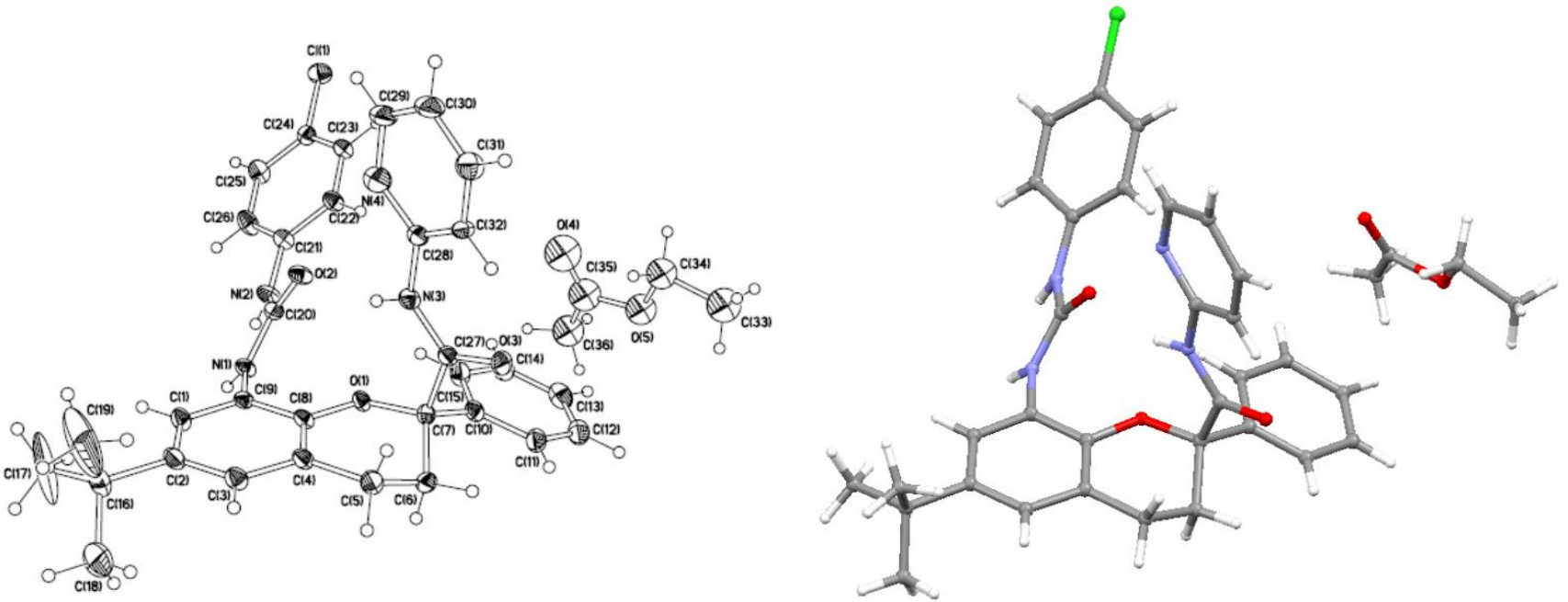
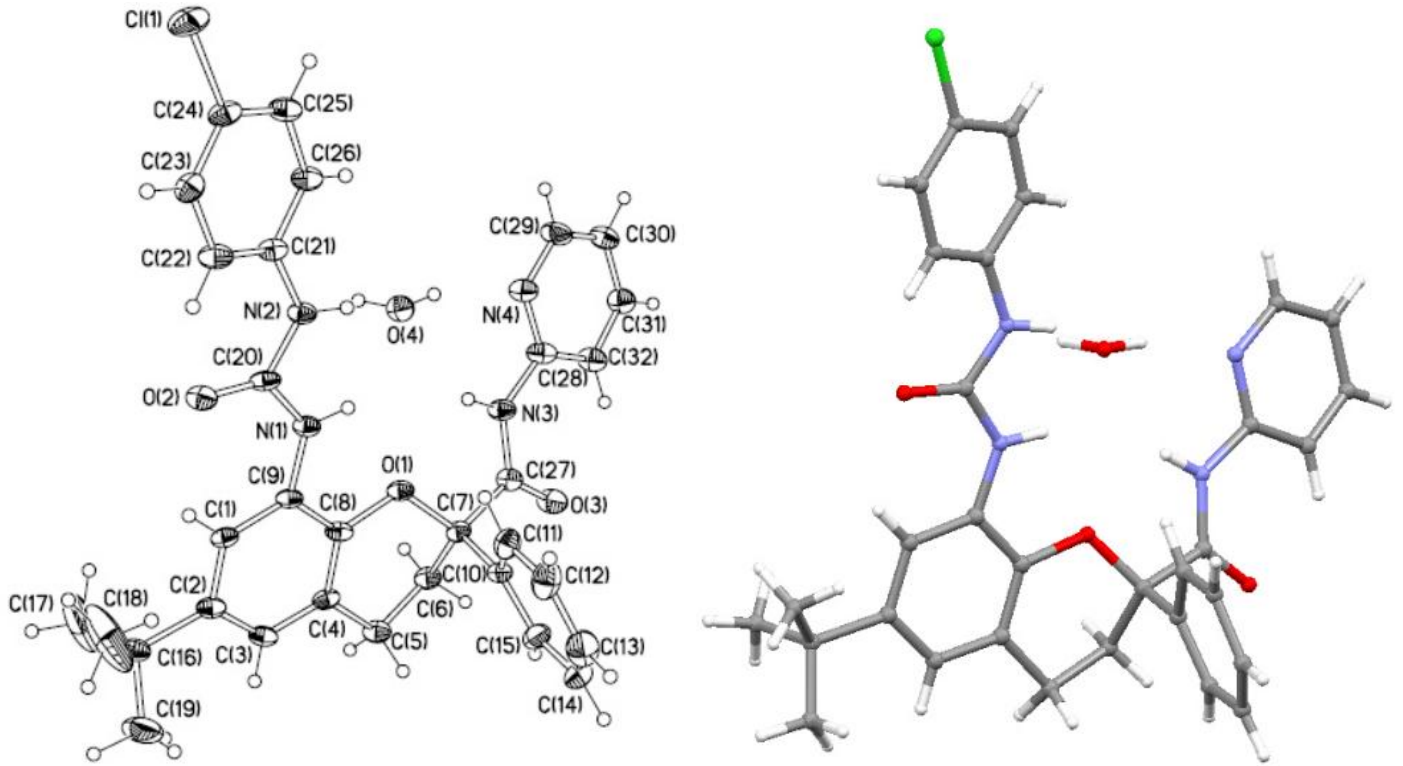


**Figure S26. ORTEP diagram and X-ray crystal structure data of receptor 1 with ethyl acetate.**




**Crystal data:** $C_{32}H_{31}ClN_4O_3$, $C_4H_8O_2M$ = 643.16, monoclinic， space group P21/n, a = 11.6441(4) Å, b = 19.0040(11) Å, c = 15.7545(8)Å, $\alpha = \gamma = 90°$, $\beta$ = 104.803(3), V = 3370.5(3) $Å^3$, Z = 4, $D_C$ = 1.267Mg/$m^3$, m = (Cu-$K_\alpha$) = 1.390 $mm^{-1}$, F(000) = 1360. 14091 reflections were collected at $3.72 \leq 2\theta \leq 67.20$ and merged to give 5575 unique reflections ($R_{int}$ = 0.0636). Final values are R = 0.1032, *w*R = 0.2658, GOF = 1.104, max/min residual electron density 0.409and -0.447e. $Å^{-3}$.

**Figure S27. ORTEP diagram and X-ray crystal structure data of receptor 1 with water.**




**Crystal data:** $C_{32}H_{31}ClN_4O_3$, $H_2OM$ = 573.07, Triclínico, space group P-1, a = 8.4156(5) Å, b = 11.6638(8) Å, c = 14.9936(8)Å, $\alpha$ = 87.286(5), $\beta$ = 83.220(4), $\gamma$ = 82.716(5), V = 1448.87(15) $Å^3$, Z = 2, $D_C$ = 1314 $Mg/m^3$, m = (Cu-$K_\alpha$) = 1.525 $mm^{-1}$, F(000) = 604. 8298 reflections were collected at $2.97 \leq 2\theta \leq 67.29$ and merged to give 4419 unique reflections ($R_{int}$ = 0.0755). Final values are R = 0.1298, *w*R = 0.3206, GOF = 2.257, max/min residual electron density 0.843 -0.797 e. $Å^{-3}$.

**Figure S28. $^{1}$H NMR spectrum of receptor 1with tetrabutylammonium acetate (200MHz, $CDCl_3$).**

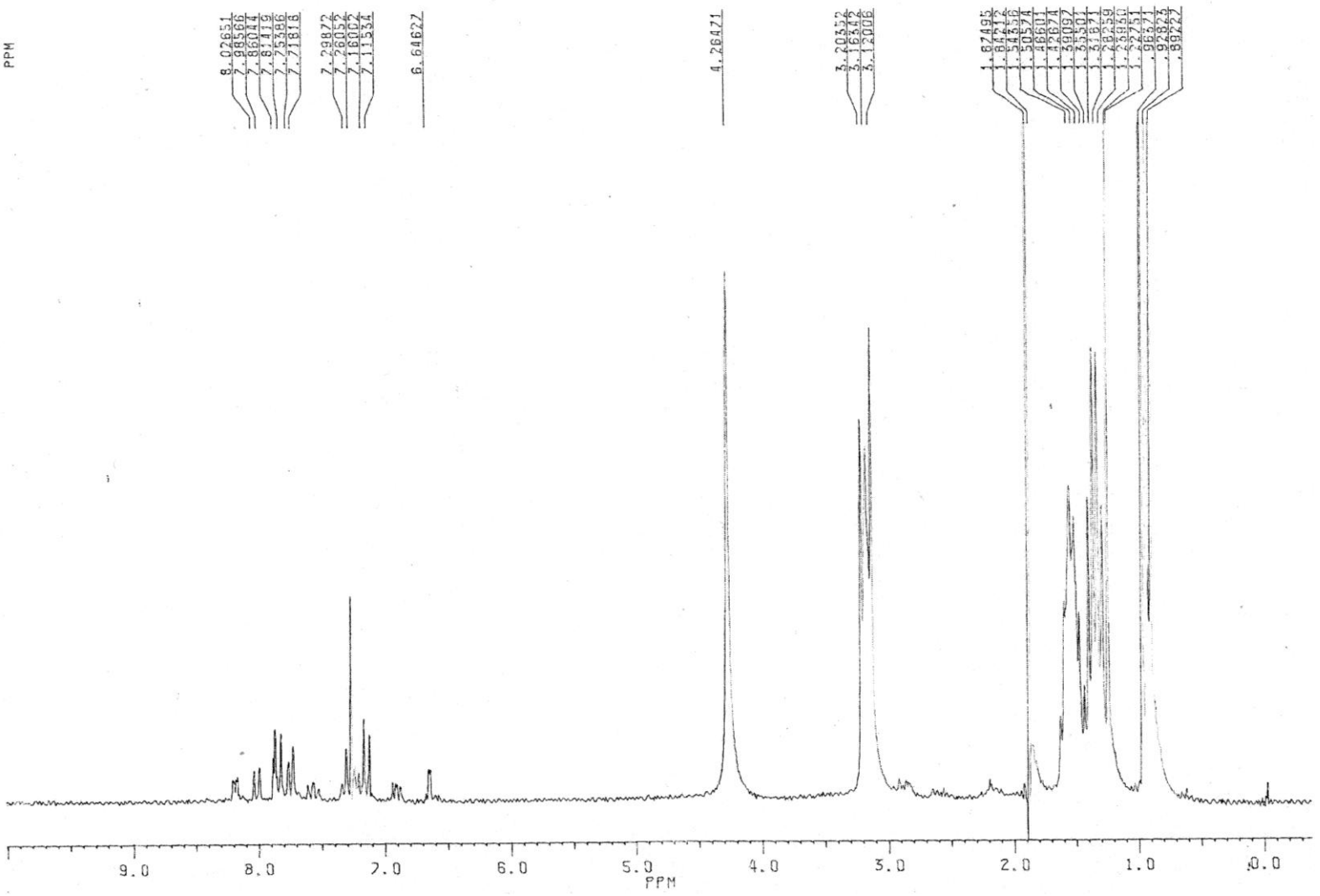


**Figure S29. $^{1}$H NMR spectrum of receptor 1with *L*-proline (400MHz, DMSO-$d_6$).**

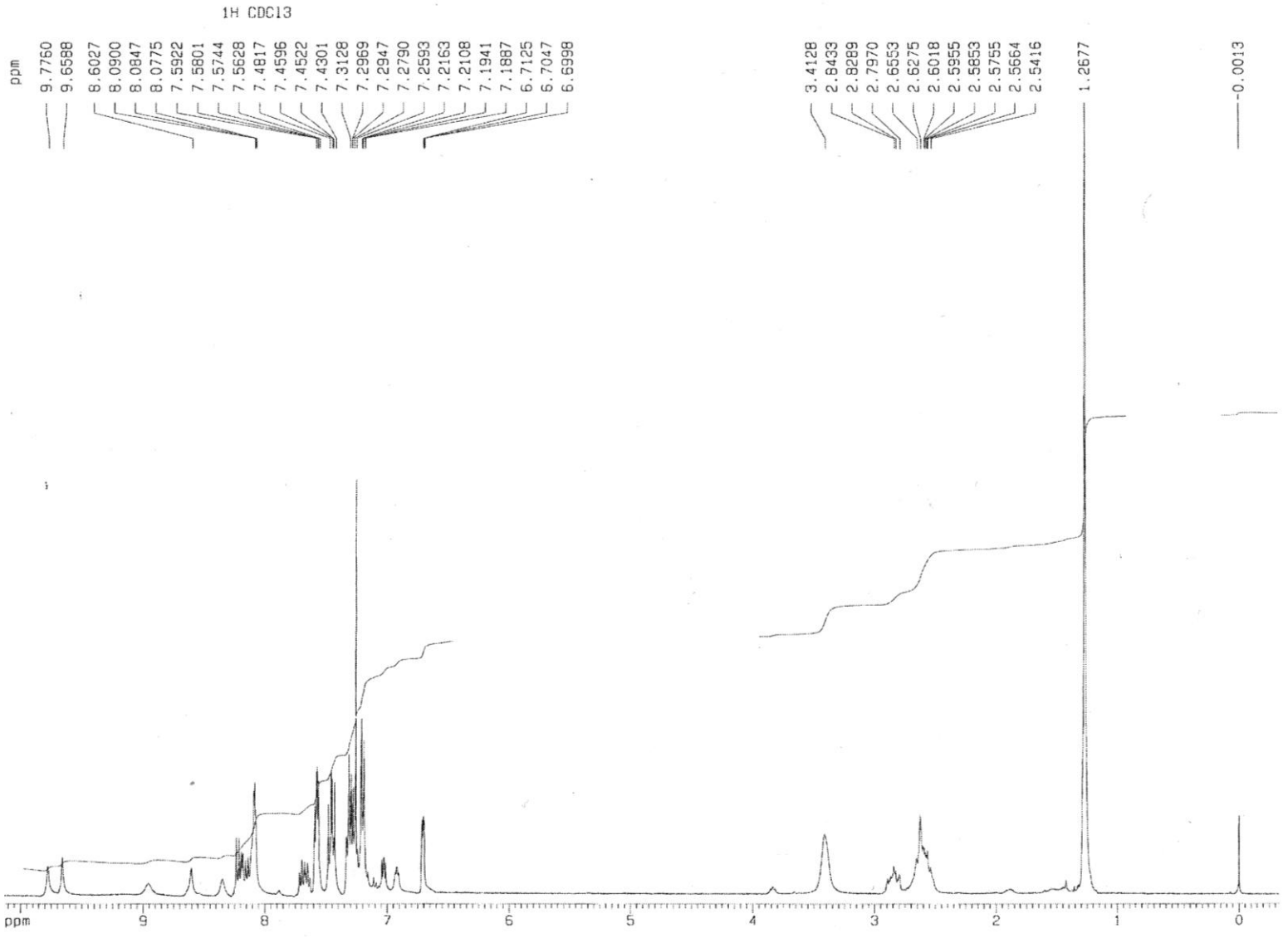


**Figure S30. COSY spectrum of receptor 1with *L*-proline (DMSO-$d_6$).**

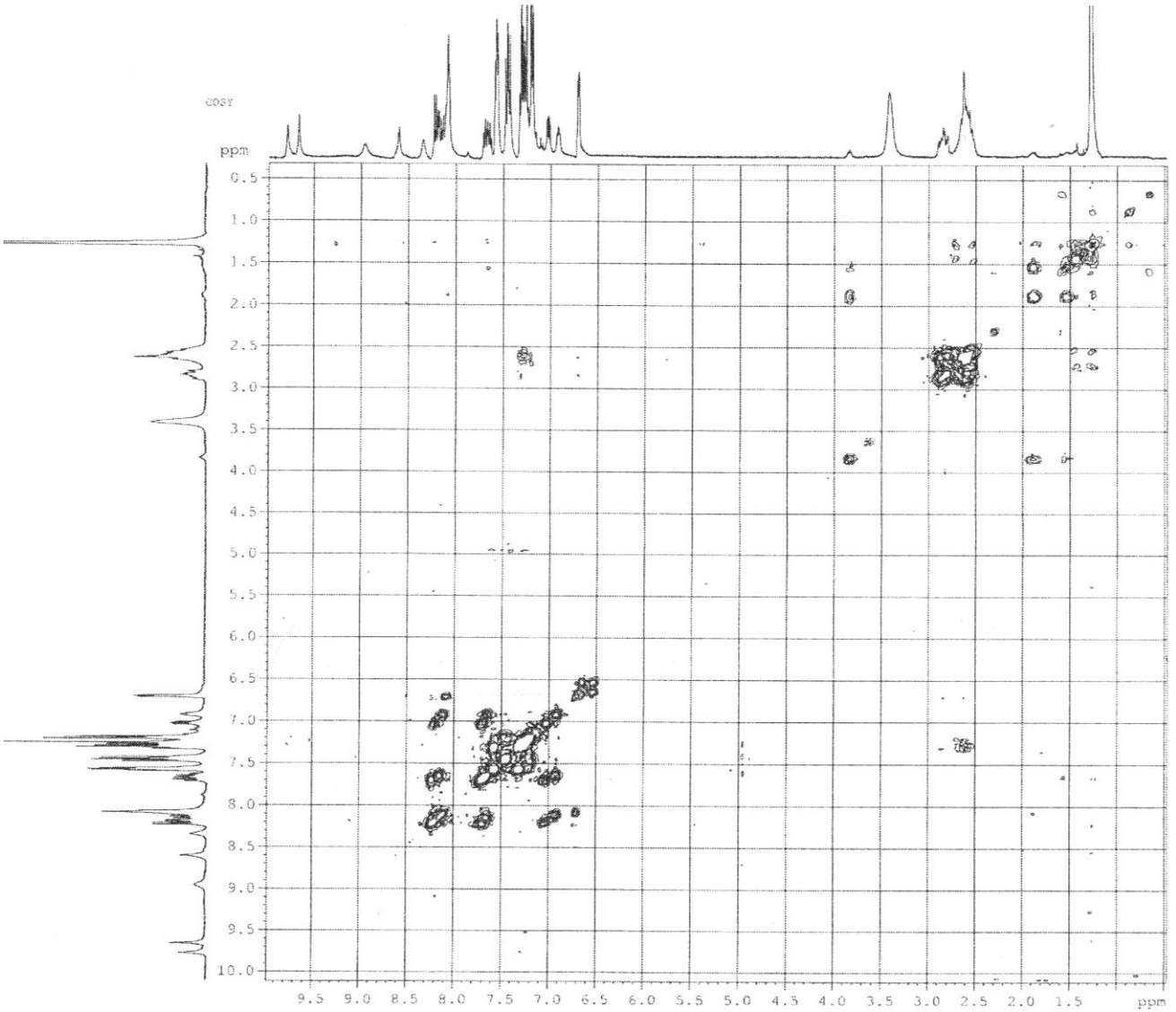


**Figure S31. ROESY spectrum of receptor 1with *L*-proline (DMSO-$d_6$).**

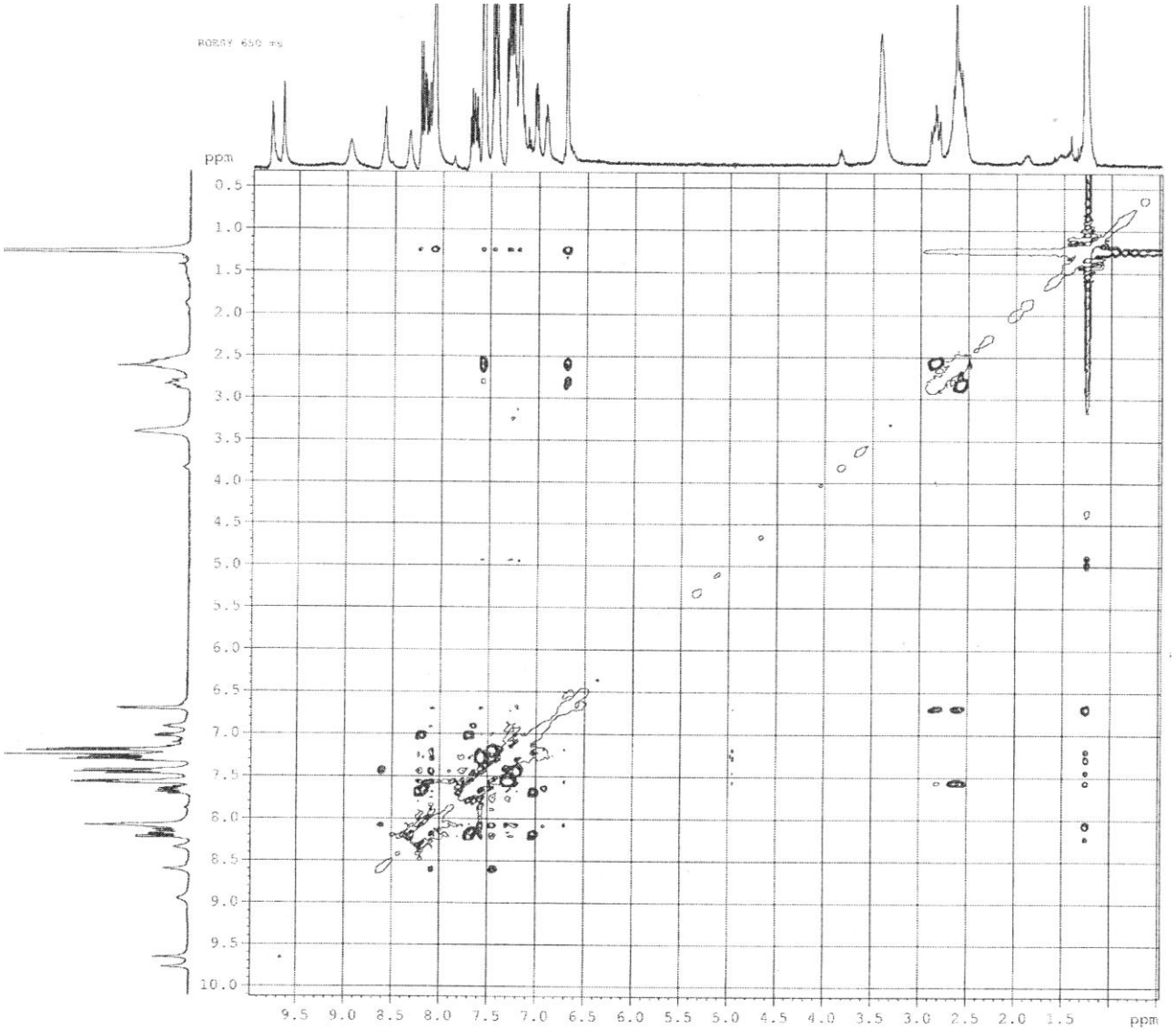


**Figure S32. $^{1}$H NMR spectrum of strong complex of receptor 1 with *L*-proline (200 MHz, $CDCl_3$).**

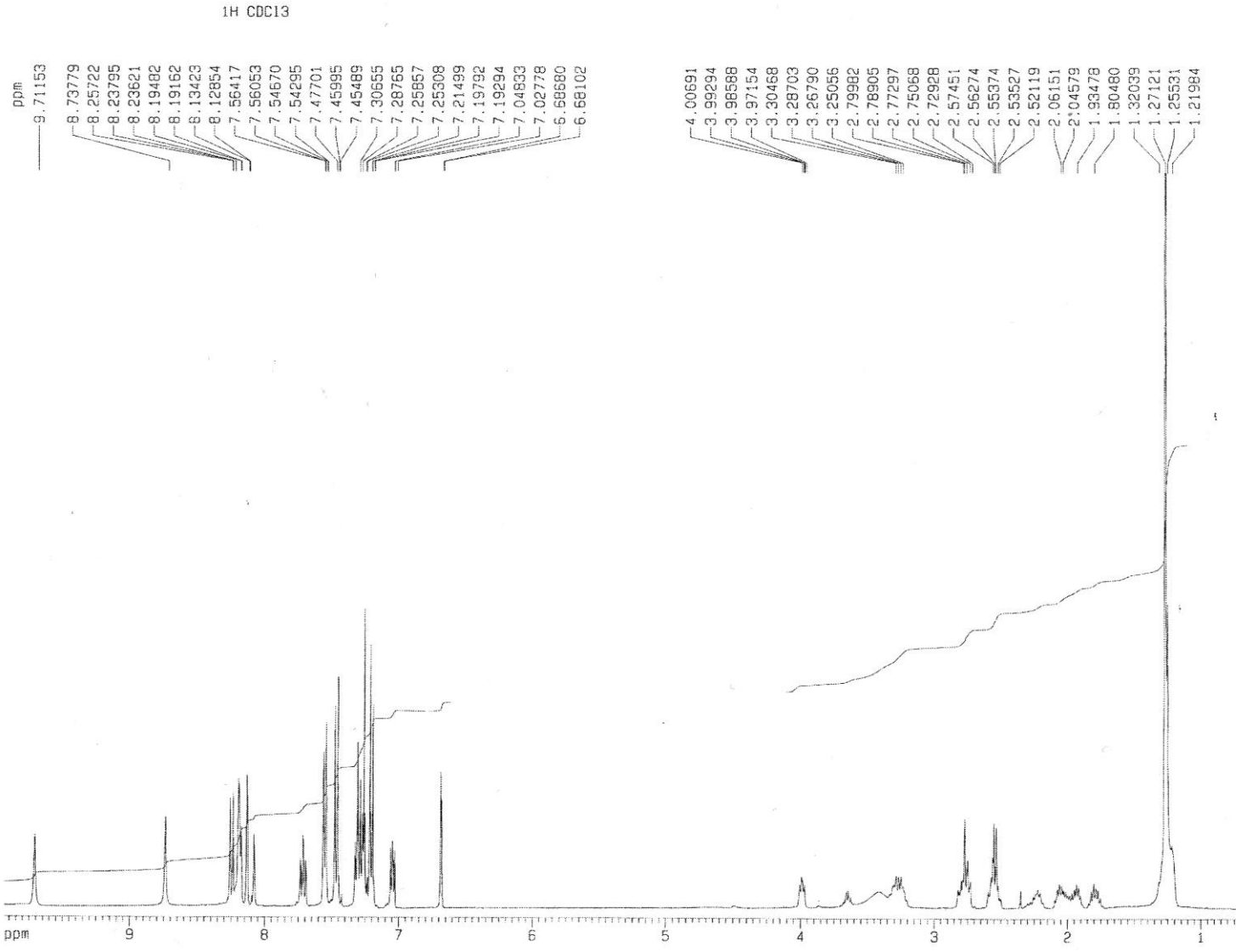


**Figure S33. COSY spectrum of strong complex of receptor 1 with *L*-proline ($CDCl_3$).**

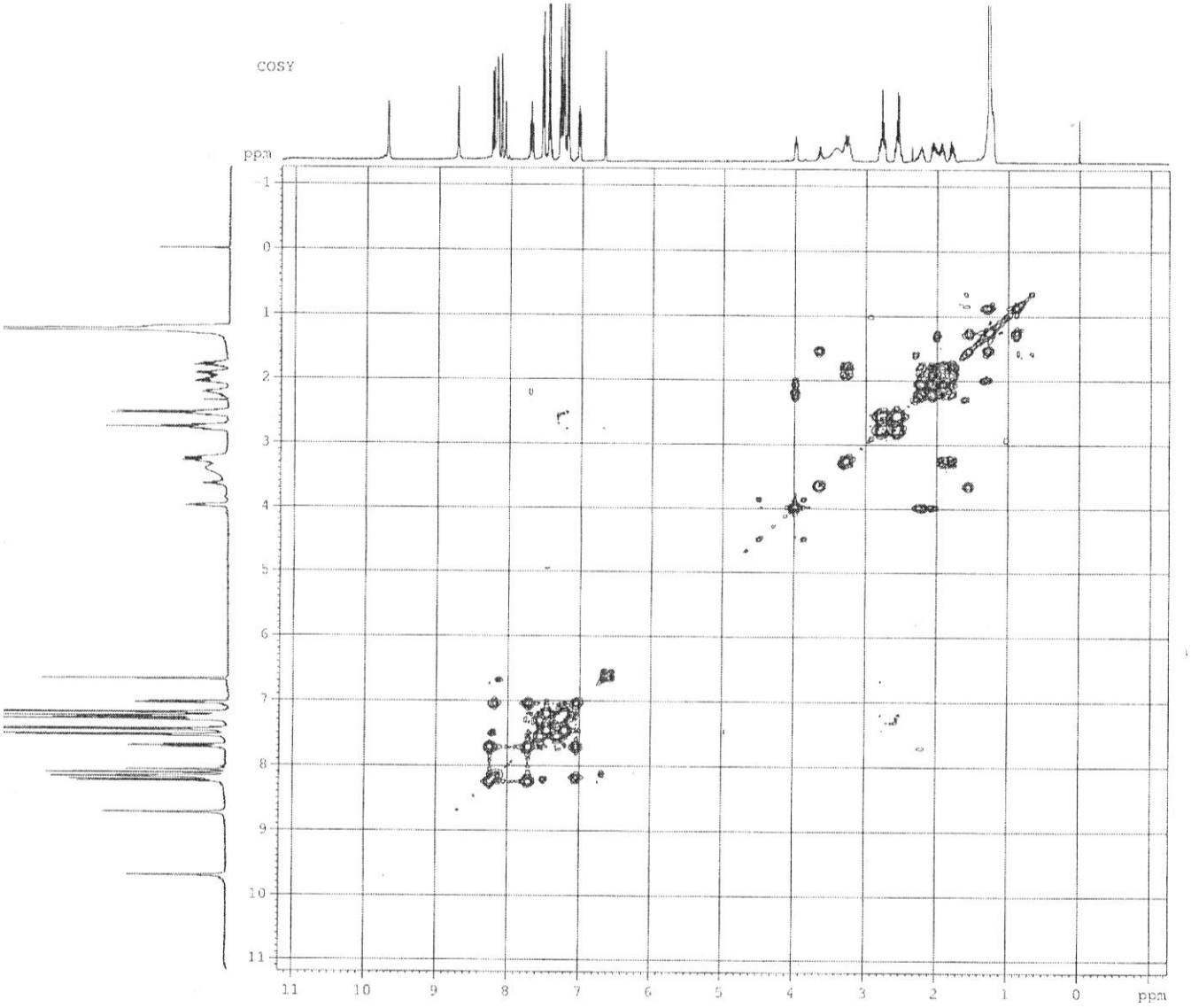


**Figure S34. ROESY spectrum of strong complex of receptor 1 with *L*-proline ($CDCl_3$).**

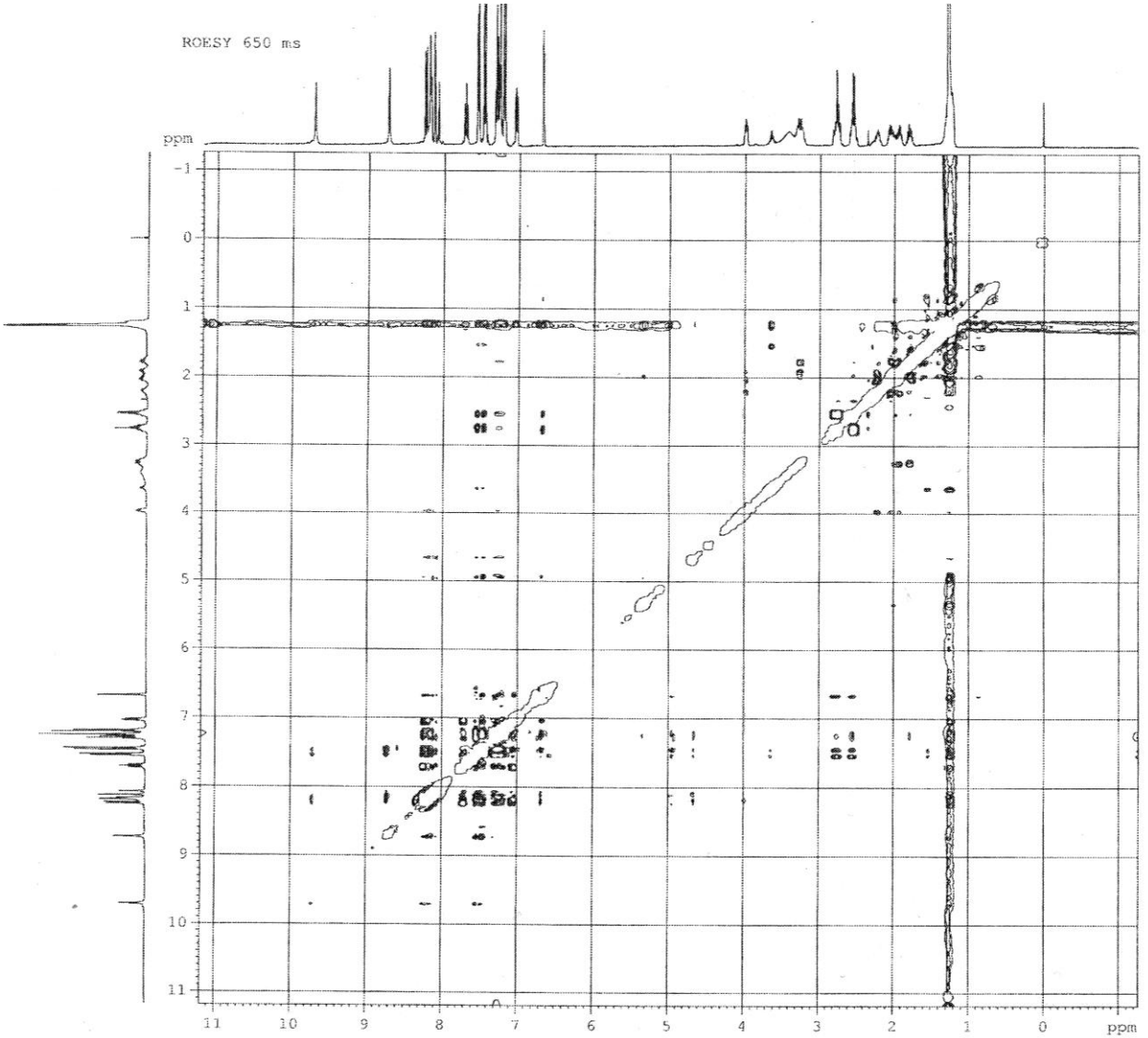


**Figure S35. $^{1}$H NMR spectrum of weak complex of receptor 1 with *L*-proline (400 MHz, $CDCl_3$).**

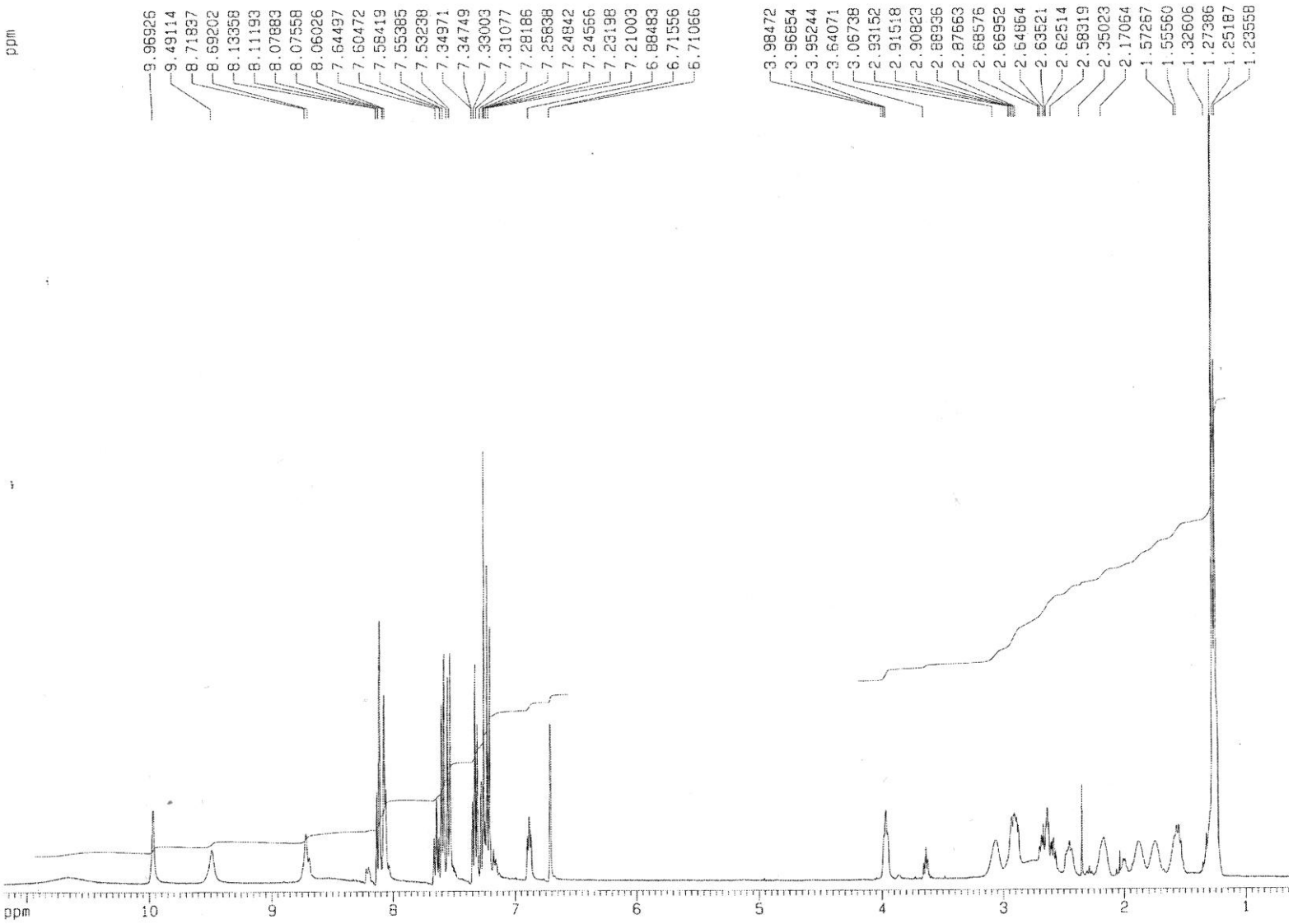


**Figure S36. COSY spectrum of the weak complex of receptor 1 with *L*-proline ($CDCl_3$).**

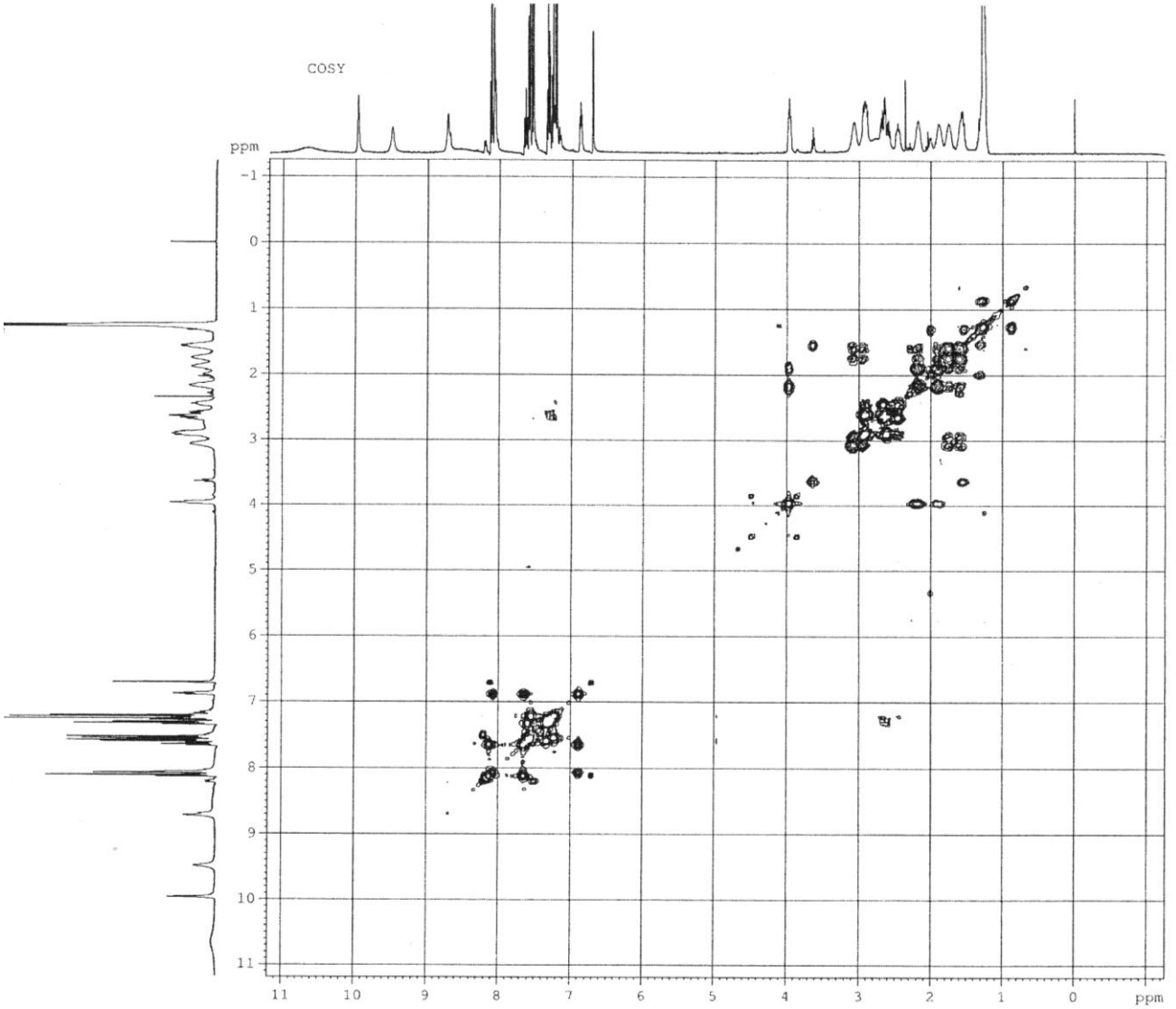


**Figure S37. ROESY spectrum of the weak complex of receptor 1 with *L*-proline ($CDCl_3$).**

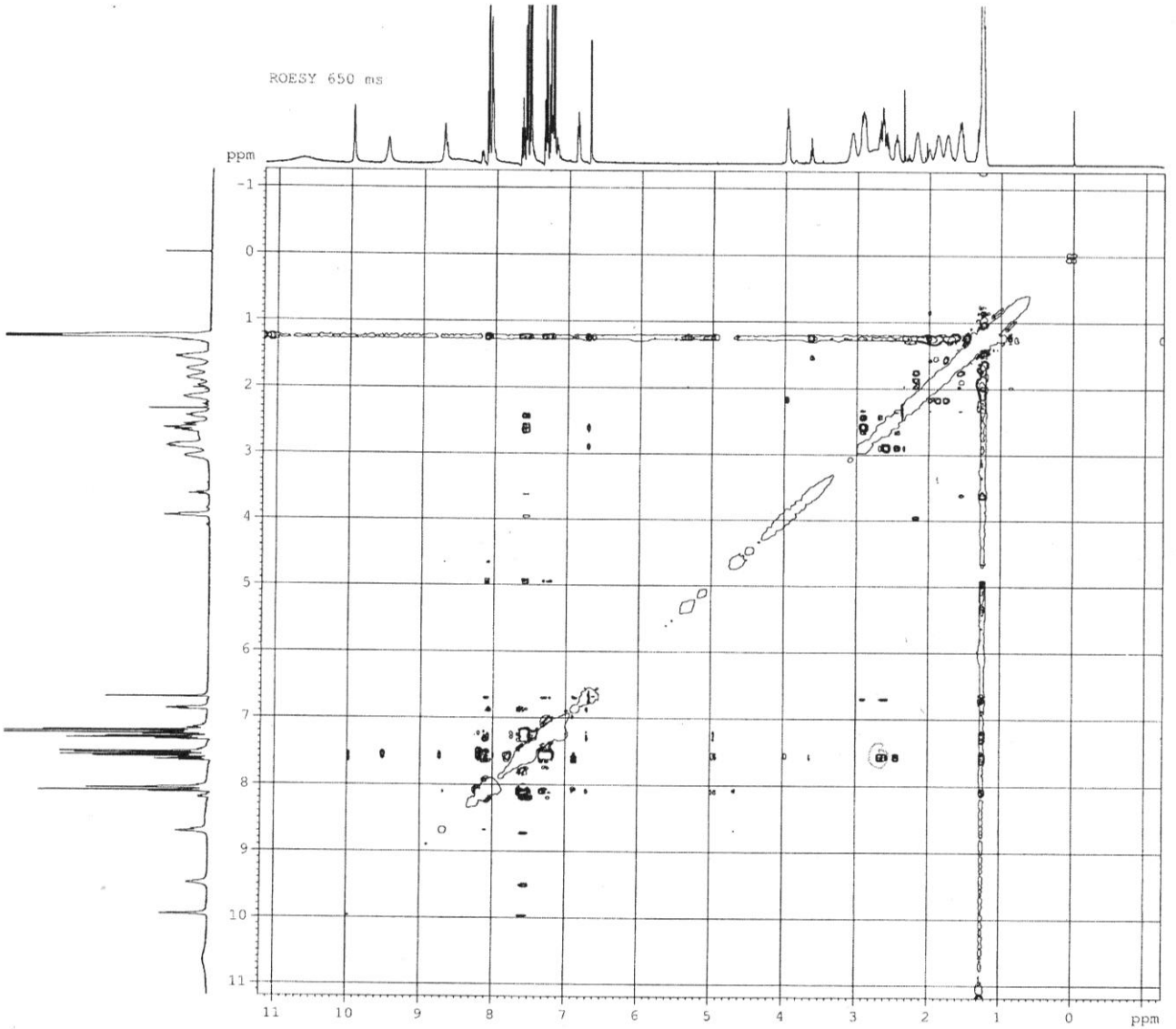


**Figure S38. $^{1}$H NMR spectrum of receptor 1 with *L*+ *D* proline.**

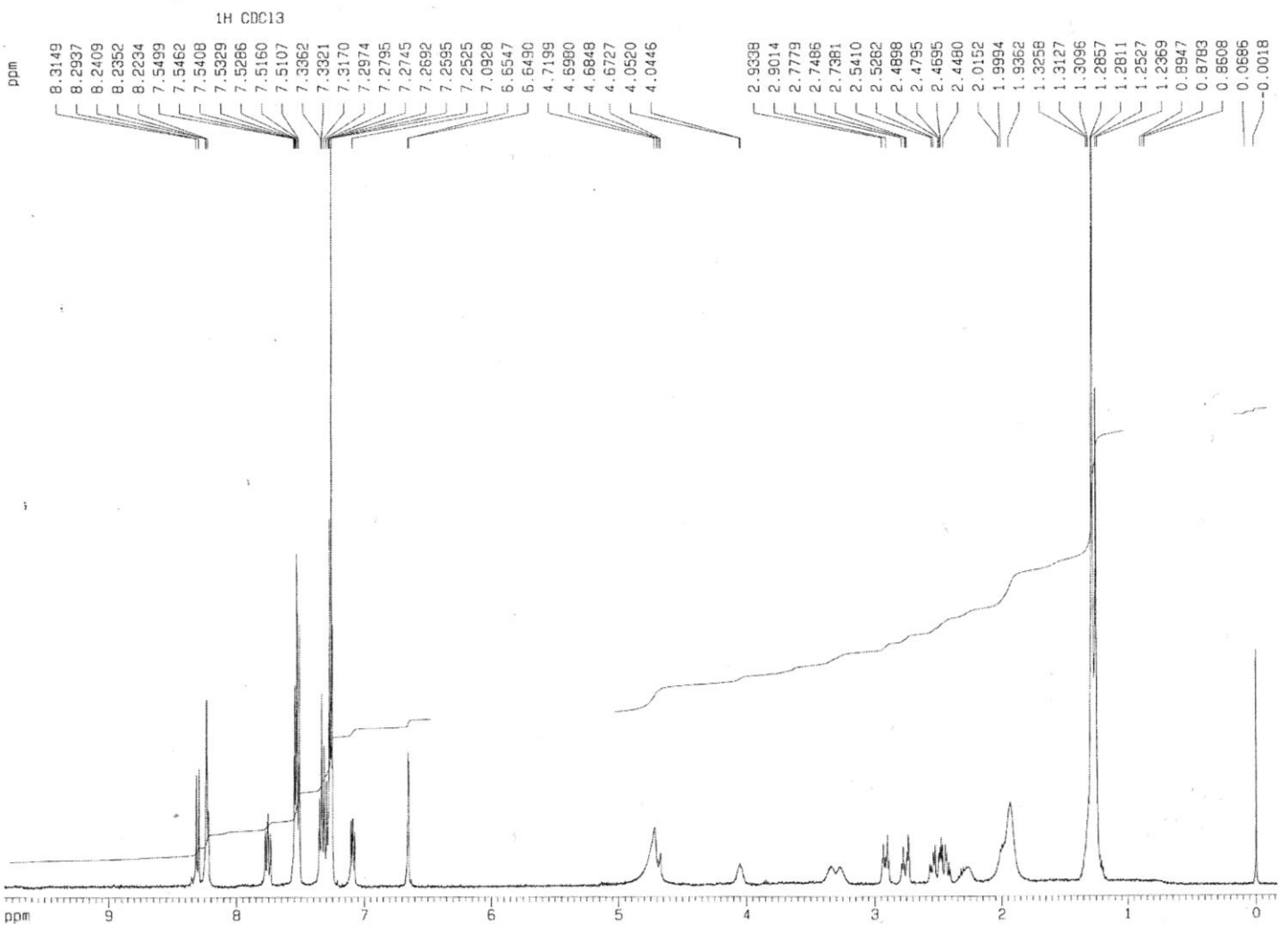


**Figure S39. Movement for the urea and the amide NHs of the receptor 1 by formation of diastereomeric associates with *L*-proline.**

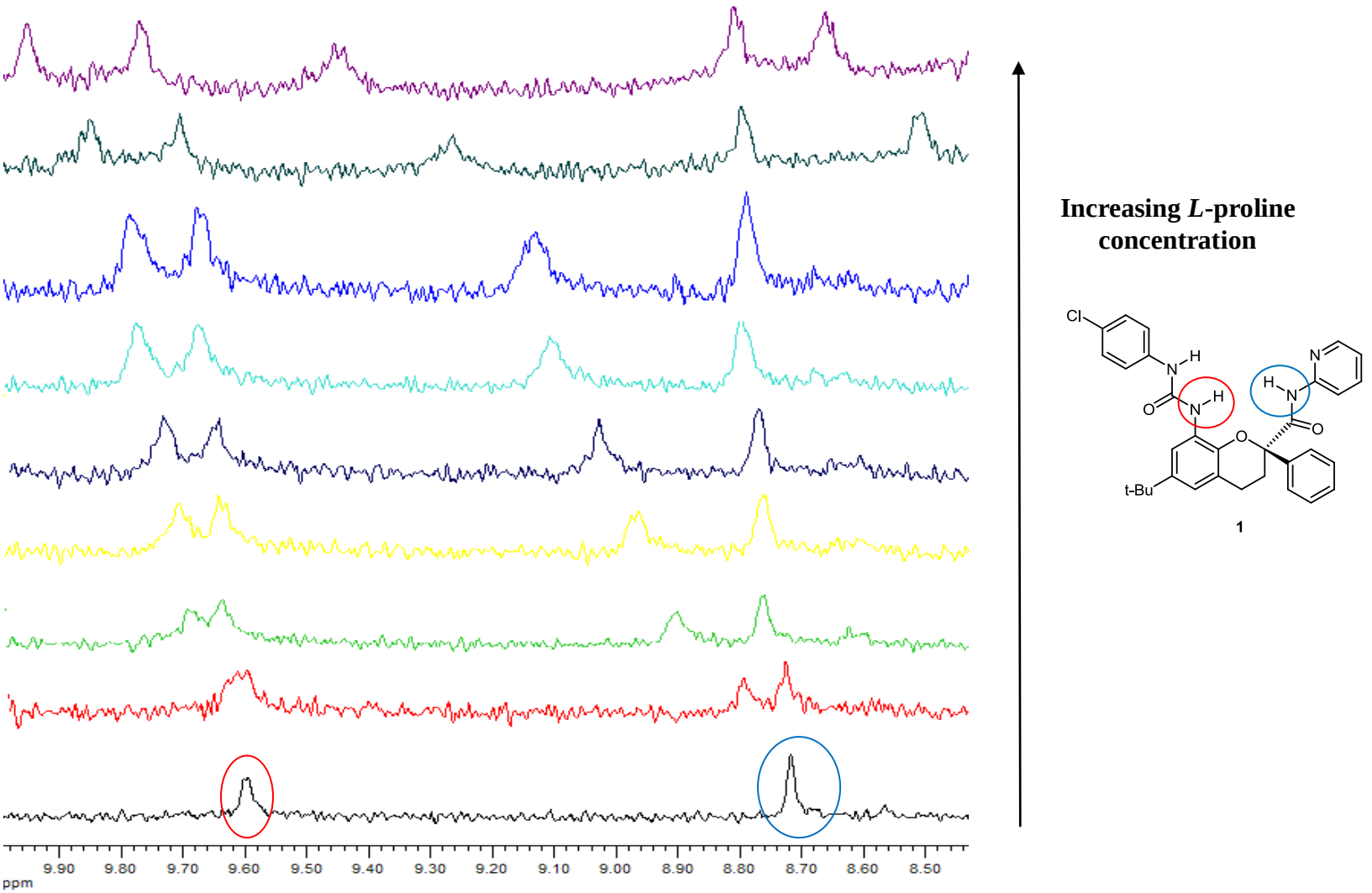
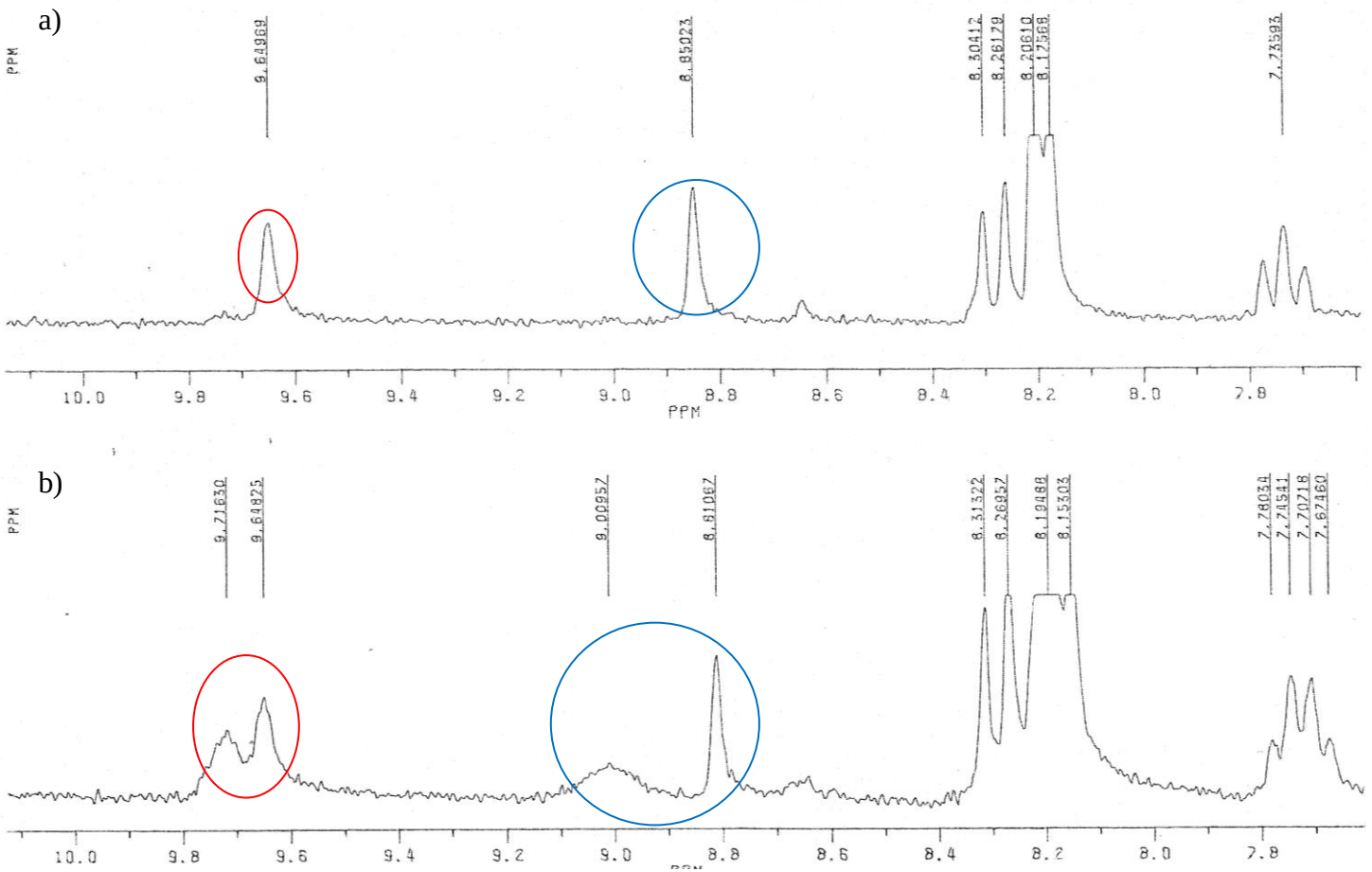


**Figure S40. RMN spectrum of racemic receptor 1 and a saturated aqueous solution *D,L*-proline (a) and *L*-proline (b) (200 MHz, $CDCl_3$).**



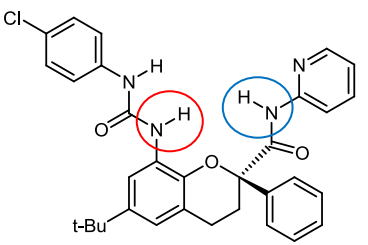




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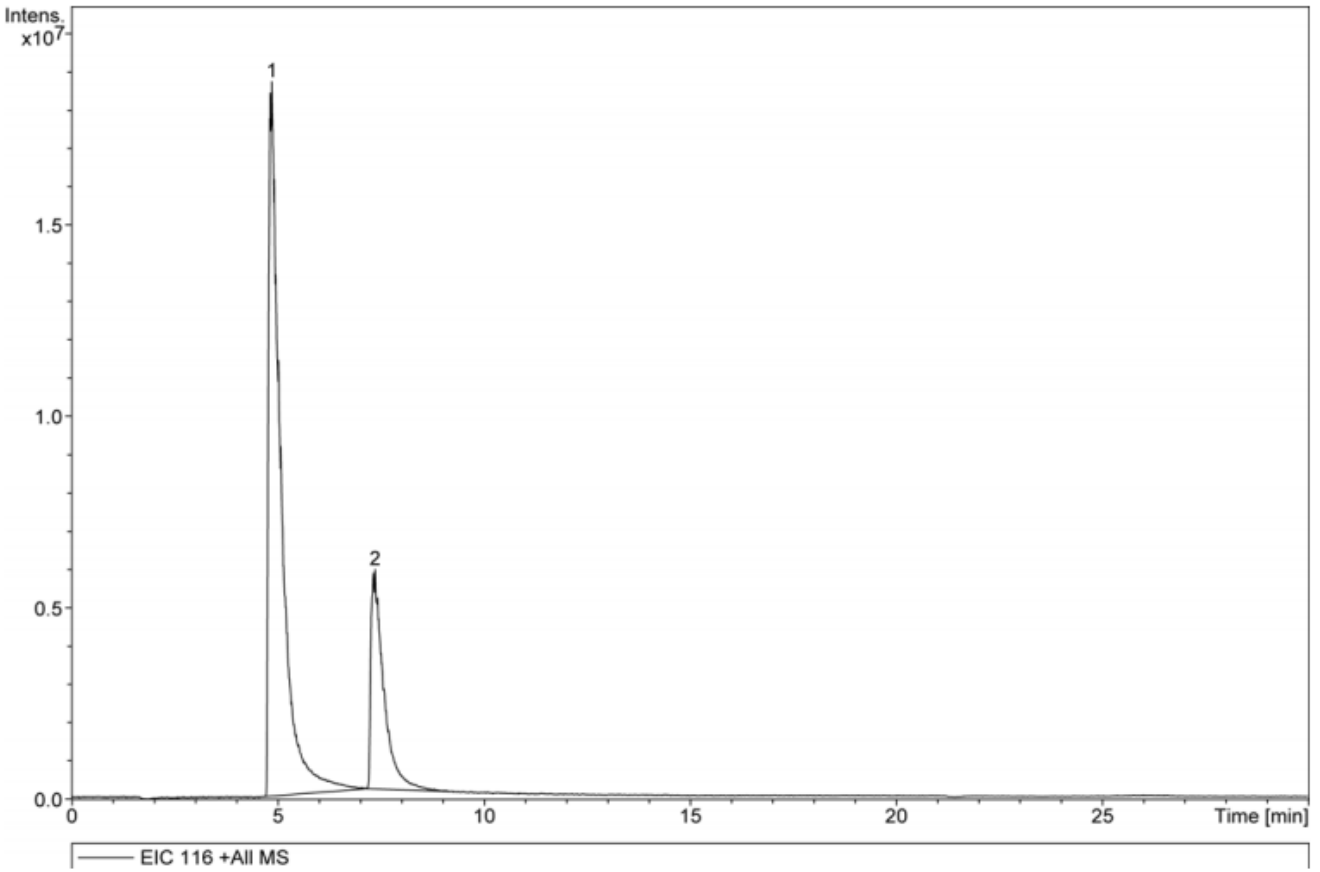
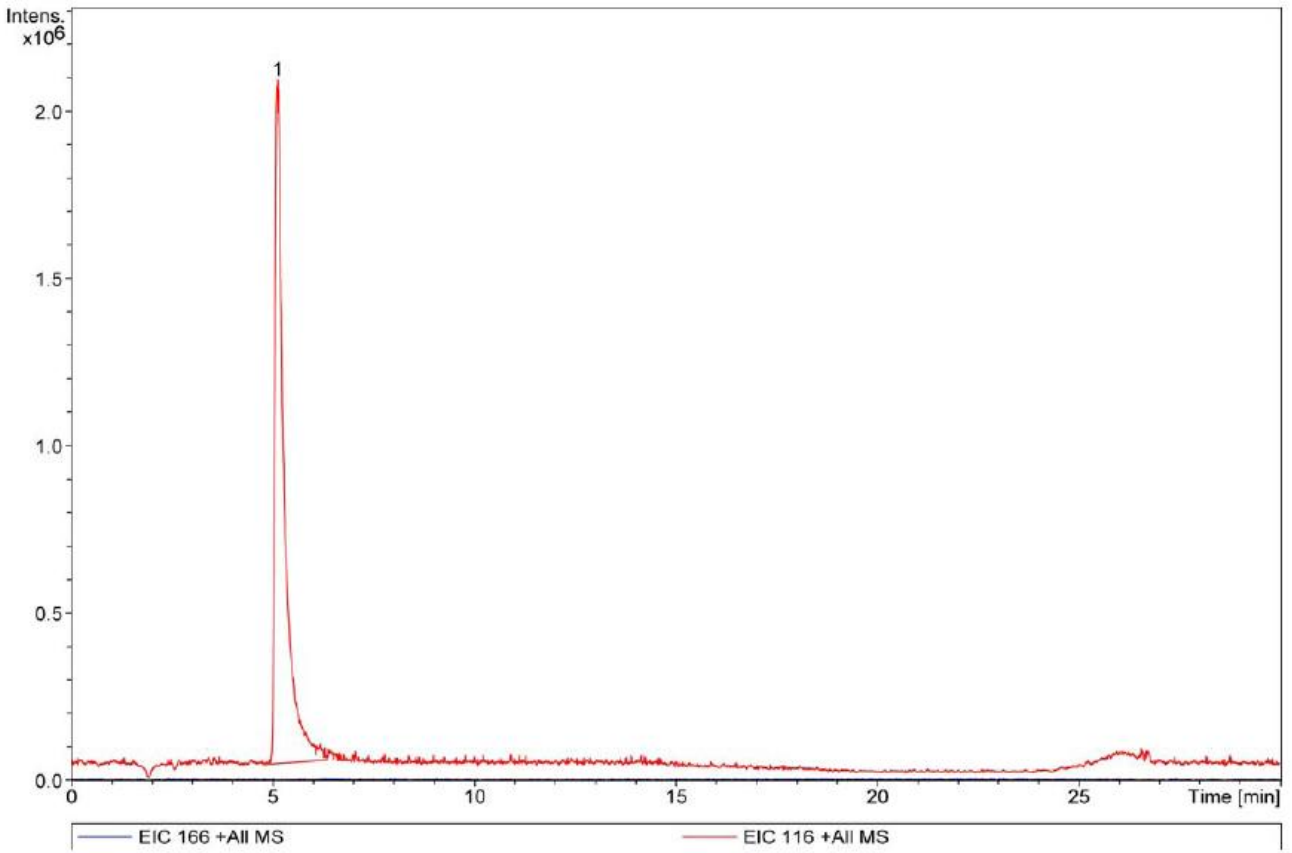
**Figure S41. HPLC of extraction of *L*-proline with the receptor 1.**




**Compound List:**

| # | RT [min] | Range [min] | Height | Area | Area Frac % |
|---|---|---|---|---|---|
| 1 | 4.9 | 4.7 - 7.1 | 18659609 | 389976045 | 76.0 |
| 2 | 7.4 | 7.1 - 9.2 | 5739521 | 123230053 | 24.0 |

**Figure S.42. HPLC of extraction of a mixture of amino acids (*L*-proline, *L*-alanine, *L*-isoleucine, *L*-leucine, *L*-valine) with the receptor 1.**



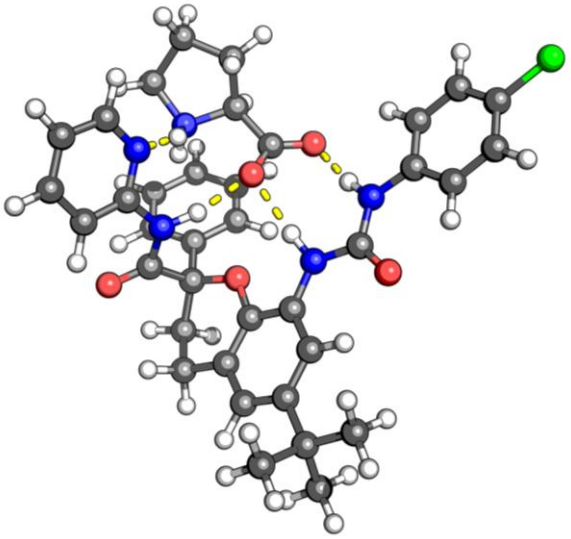

**Compound List:**

| # | RT [min] | Range [min] | Height | Area | Area Frac % |
|---|---|---|---|---|---|
| 1 | 5.1 | 4.9 - 6.3 | 2042436 | 33307528 | 100.0 |

**Figure S43. Modelling studies of the associates between receptor and *L*-proline.**

All calculations were performed using Gaussian09 software[1]. Geometry optimization were performed using M06-2X DFT functional [2] and 6-31G** basis set[3] in the gas phase. Gibbs free energy correction at 298.15 K was calculated with this method and corrected according to the so-called "quasi-harmonic approach" using a free rotor approximation for vibrational modes below 100 $cm^{-1}$ and a rigid rotor approximation above this cutoff[4]. Single point energy was calculated on the optimized structures using M06-2X DFT functional [2] and 6-311+G** basis set. Solvent (chloroform) was modeled in this single-point calculation using SMD solvation model.[5] The Gibbs free energy of each structure is calculated adding to this single point energy the ΔG correction term calculated as described above.

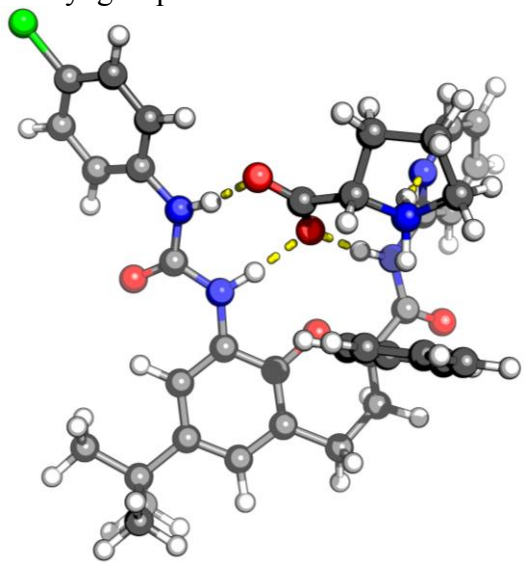
Complex between (*R)*-receptor and *L*-proline
Phenyl group ecuatorial: ΔG: 0.00 kcal/mol



| | | | |
|---|---|---|---|
| C | 1.69822 | 4.45794 | -0.37370 |
| C | 2.07251 | 3.17246 | -0.76706 |
| C | 1.11538 | 2.16838 | -0.72067 |
| C | -0.20250 | 2.41468 | -0.29776 |
| C | -0.54190 | 3.71410 | 0.08716 |
| C | 0.40192 | 4.74597 | 0.05085 |
| H | 2.44910 | 5.24369 | -0.41859 |
| H | -1.55640 | 3.88949 | 0.40865 |
| C | 2.70853 | 0.47817 | -1.28779 |
| C | 3.50829 | 1.55019 | -2.02793 |
| H | 3.04719 | 1.66510 | -3.01448 |
| H | 4.53460 | 1.20228 | -2.16367 |
| C | 3.47047 | 2.86566 | -1.25154 |
| C | 3.33717 | 0.18029 | 0.09591 |
| O | 4.50853 | 0.40721 | 0.33993 |
| N | 2.47701 | -0.47170 | 0.93464 |
| H | 1.52266 | -0.67329 | 0.60118 |
| C | 2.84701 | -1.07384 | 2.13918 |
| C | 3.82108 | -0.53928 | 2.99081 |
| C | 2.44250 | -2.82807 | 3.56866 |
| C | 4.08381 | -1.21151 | 4.17310 |
| H | 4.33887 | 0.36755 | 2.71168 |
| C | 3.37895 | -2.37457 | 4.48387 |
| H | 4.82838 | -0.82178 | 4.85960 |
| H | 3.55287 | -2.91433 | 5.40675 |
| N | 2.18767 | -2.20605 | 2.41212 |
| N | -1.06998 | 1.32081 | -0.30381 |
| C | -2.44000 | 1.35885 | -0.12373 |
| H | -0.63441 | 0.39768 | -0.33457 |
| O | -3.06925 | 2.36789 | 0.15828 |
| N | -3.00371 | 0.11606 | -0.31265 |
| H | -2.41637 | -0.62614 | -0.69935 |
| C | -4.34368 | -0.23377 | -0.12570 |
| C | -5.33011 | 0.63661 | 0.35765 |
| C | -4.69483 | -1.55744 | -0.43578 |
| C | -6.63373 | 0.18061 | 0.52598 |
| H | -5.07378 | 1.65951 | 0.59050 |
| C | -5.99624 | -2.00517 | -0.26872 |
| H | -3.92770 | -2.22799 | -0.81317 |
| C | -6.96284 | -1.13110 | 0.21522 |
| C | 0.04330 | 6.17879 | 0.46081 |
| C | 0.28351 | 7.12395 | -0.72811 |
| H | 1.33006 | 7.11398 | -1.04609 |
| H | -0.33254 | 6.83097 | -1.58346 |
| H | 0.02539 | 8.15237 | -0.45269 |
| C | -1.42201 | 6.30855 | 0.88762 |
| H | -2.10303 | 6.02926 | 0.07825 |
| H | -1.64647 | 5.67980 | 1.75429 |
| H | -1.63069 | 7.34733 | 1.16182 |
| C | 0.93120 | 6.60913 | 1.64015 |
| H | 0.77663 | 5.94932 | 2.49934 |
| H | 1.99248 | 6.57782 | 1.37679 |
| H | 0.68871 | 7.63348 | 1.94354 |
| C | 2.67645 | -0.84698 | -2.04396 |
| C | 3.81903 | -1.65568 | -2.08232 |
| C | 1.50654 | -1.27899 | -2.67309 |
| C | 3.78636 | -2.88741 | -2.73437 |
| H | 4.72682 | -1.32369 | -1.58398 |
| C | 1.48014 | -2.50852 | -3.33116 |
| H | 0.61228 | -0.66861 | -2.62067 |
| C | 2.61437 | -3.31912 | -3.35898 |
| H | 4.67743 | -3.50695 | -2.75726 |
| H | 0.55792 | -2.83273 | -3.80402 |
| H | 2.59024 | -4.27589 | -3.87147 |
| H | -7.39766 | 0.85325 | 0.90042 |
| H | -6.26308 | -3.02760 | -0.51284 |
| Cl | -8.60753 | -1.69428 | 0.43162 |
| O | -0.06190 | -1.39487 | 0.13971 |
| C | -0.55706 | -2.29045 | -0.59365 |
| O | -1.54580 | -2.23170 | -1.33535 |
| C | 0.15683 | -3.65466 | -0.52267 |
| H | 0.17438 | -4.13166 | -1.50581 |
| C | 0.81533 | -5.57113 | 0.80268 |
| C | 2.07763 | -4.81245 | 0.33003 |
| H | 1.54980 | -2.85233 | 0.78031 |
| H | 2.15164 | -3.00659 | -0.78169 |

| | | | |
|---|---|---|---|
| H | 0.89240 | -5.86033 | 1.85208 |
| H | 0.69387 | -6.48549 | 0.21850 |
| H | 2.83575 | -4.67633 | 1.10266 |
| H | 2.53648 | -5.27209 | -0.54708 |
| O | 1.36251 | 0.86834 | -1.12455 |
| H | 1.86909 | -3.73287 | 3.75834 |
| N | 1.56940 | -3.46849 | -0.07288 |
| C | -0.36006 | -4.59995 | 0.55950 |
| H | -0.57427 | -4.01178 | 1.45848 |
| H | -1.27813 | -5.09912 | 0.25056 |
| H | 4.15859 | 2.79961 | -0.40205 |
| H | 3.82383 | 3.68297 | -1.88750 |

Complex between *(R)*-receptor and *L*-proline
Phenyl group axial: ΔG: 1.2 kcal/mol



| | | | |
|---|---|---|---|
| C | -0.18328 | 4.85405 | -0.19531 |
| C | -1.02262 | 3.76943 | -0.44130 |
| C | -0.45563 | 2.50676 | -0.57926 |
| C | 0.92183 | 2.30023 | -0.39343 |
| C | 1.73503 | 3.41286 | -0.15562 |
| C | 1.19724 | 4.69861 | -0.06775 |
| H | -0.63543 | 5.83922 | -0.10745 |
| H | 2.79475 | 3.23997 | -0.04587 |
| C | -2.60017 | 1.44483 | -0.78121 |
| C | -3.13627 | 2.77585 | -1.30932 |
| H | -4.22635 | 2.77246 | -1.24799 |
| H | -2.87136 | 2.83554 | -2.36951 |
| C | -2.51929 | 3.93173 | -0.53518 |
| C | -3.15687 | 0.29595 | -1.64976 |
| O | -4.14830 | 0.44036 | -2.34007 |
| N | -2.50040 | -0.88764 | -1.46808 |
| H | -1.68322 | -0.91681 | -0.83234 |
| C | -2.91365 | -2.11127 | -1.99363 |
| C | -3.55121 | -2.24206 | -3.23377 |
| C | -2.95408 | -4.38887 | -1.64653 |
| C | -3.88132 | -3.51783 | -3.65973 |
| H | -3.77030 | -1.36000 | -3.81858 |
| C | -3.57174 | -4.62189 | -2.86370 |
| H | -4.36884 | -3.65430 | -4.61960 |
| H | -3.80727 | -5.63199 | -3.17575 |
| N | -2.64205 | -3.16314 | -1.21032 |
| N | 1.37674 | 0.98074 | -0.38697 |
| C | 2.70256 | 0.58726 | -0.45965 |
| H | 0.67189 | 0.24759 | -0.29667 |
| O | 3.61532 | 1.32961 | -0.78669 |
| N | 2.85637 | -0.74059 | -0.12597 |
| H | 2.09455 | -1.19588 | 0.37906 |
| C | 4.05343 | -1.46541 | -0.15047 |
| C | 5.21824 | -1.03876 | -0.80130 |
| C | 4.04856 | -2.70958 | 0.49720 |
| C | 6.34980 | -1.84847 | -0.79496 |
| H | 5.23683 | -0.07829 | -1.29534 |
| C | 5.17872 | -3.51358 | 0.49852 |
| H | 3.14521 | -3.03003 | 1.00780 |
| C | 6.32784 | -3.07690 | -0.14983 |
| C | 2.07798 | 5.92854 | 0.17539 |
| C | 1.64676 | 6.61827 | 1.48013 |
| H | 0.60435 | 6.94737 | 1.43707 |
| H | 1.75100 | 5.93605 | 2.32933 |
| H | 2.27011 | 7.49936 | 1.66760 |
| C | 3.56094 | 5.56272 | 0.29027 |
| H | 3.74578 | 4.89214 | 1.13489 |
| H | 3.92667 | 5.07535 | -0.61835 |
| H | 4.14986 | 6.47158 | 0.44827 |
| C | 1.91132 | 6.90969 | -0.99694 |
| H | 2.20986 | 6.43922 | -1.93846 |
| H | 0.87392 | 7.24167 | -1.09875 |
| H | 2.53540 | 7.79638 | -0.84055 |
| C | -3.03160 | 1.15183 | 0.65942 |
| C | -4.37976 | 0.89185 | 0.93432 |
| C | -2.09377 | 1.06893 | 1.69262 |
| C | -4.78521 | 0.54872 | 2.22203 |
| H | -5.10525 | 0.93351 | 0.12504 |
| C | -2.50676 | 0.74498 | 2.98613 |
| H | -1.04284 | 1.22875 | 1.48134 |
| C | -3.84846 | 0.47738 | 3.25410 |
| H | -5.83240 | 0.34305 | 2.42057 |
| H | -1.77160 | 0.69918 | 3.78401 |
| H | -4.16411 | 0.22390 | 4.26143 |
| H | 7.25370 | -1.52037 | -1.29652 |
| H | 5.17161 | -4.47325 | 1.00345 |
| Cl | 7.75919 | -4.08439 | -0.14988 |
| O | -0.42498 | -1.20027 | 0.30823 |
| C | -0.10880 | -1.91275 | 1.30129 |
| O | 1.01523 | -2.21573 | 1.70901 |
| C | -1.28616 | -2.45628 | 2.13211 |
| H | -1.34190 | -1.91728 | 3.08477 |
| C | -2.77137 | -4.24980 | 2.74700 |
| C | -3.59898 | -3.12013 | 2.08706 |
| H | -2.45770 | -2.57483 | 0.42141 |
| H | -2.84775 | -1.25384 | 1.39231 |
| H | -3.10342 | -5.23550 | 2.41745 |
| H | -2.89303 | -4.20747 | 3.83163 |
| H | -4.29681 | -3.46978 | 1.32395 |
| H | -4.14291 | -2.51658 | 2.81526 |
| O | -1.19040 | 1.37309 | -0.88862 |
| H | -2.69912 | -5.20963 | -0.98032 |
| N | -2.58513 | -2.24523 | 1.42382 |
| C | -1.30915 | -3.96250 | 2.35650 |
| H | -1.04227 | -4.46504 | 1.42007 |
| H | -0.58437 | -4.26246 | 3.11223 |
| H | -2.76292 | 4.88242 | -1.01858 |
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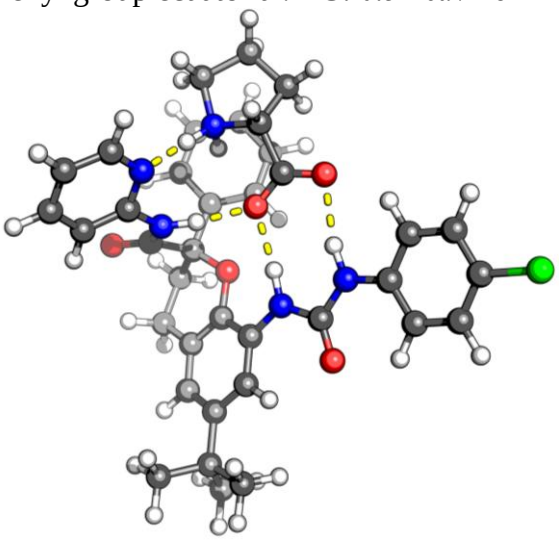
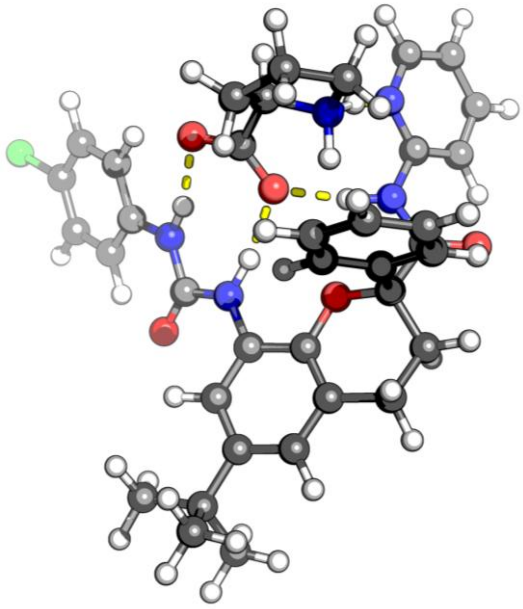
Complex between *(S)*-receptor and *L*-proline
Phenyl group ecuatorial: ΔG: 0.5 kcal/mol



| | | | |
|---|---|---|---|
| C | 1.20116 | 4.49175 | -0.64261 |
| C | 1.69882 | 3.23941 | -1.00252 |
| C | 0.86028 | 2.13764 | -0.88679 |
| C | -0.46559 | 2.26060 | -0.43480 |
| C | -0.92673 | 3.53123 | -0.07901 |
| C | -0.10252 | 4.65569 | -0.17802 |
| H | 1.86183 | 5.35053 | -0.74045 |
| H | -1.94454 | 3.61251 | 0.26710 |
| C | 2.64209 | 0.62079 | -1.31794 |
| C | 3.32531 | 1.70651 | -2.15147 |
| H | 2.87452 | 1.66145 | -3.14846 |
| H | 4.38927 | 1.47777 | -2.24401 |
| C | 3.11199 | 3.07837 | -1.51375 |
| C | 3.25055 | 0.55855 | 0.10408 |
| O | 4.35941 | 0.99350 | 0.35541 |
| N | 2.47155 | -0.13751 | 0.98896 |
| H | 1.57734 | -0.53531 | 0.65701 |
| C | 2.88610 | -0.49298 | 2.27371 |
| C | 3.65001 | 0.35668 | 3.08269 |
| C | 2.80719 | -2.10745 | 3.91443 |
| C | 3.98263 | -0.08242 | 4.35258 |
| H | 3.96019 | 1.32007 | 2.70284 |
| C | 3.54781 | -1.33399 | 4.79166 |
| H | 4.57023 | 0.55438 | 5.00580 |
| H | 3.78103 | -1.70083 | 5.78374 |
| N | 2.49242 | -1.70788 | 2.67573 |
| N | -1.22147 | 1.08754 | -0.35352 |
| C | -2.59672 | 1.02753 | -0.22544 |
| H | -0.70146 | 0.20786 | -0.36788 |
| O | -3.31671 | 2.01438 | -0.17538 |
| N | -3.06195 | -0.26824 | -0.16753 |
| H | -2.39669 | -1.04027 | -0.23199 |
| C | -4.39979 | -0.66508 | -0.03044 |
| C | -5.48848 | 0.21697 | 0.01784 |
| C | -4.63877 | -2.04559 | 0.06011 |
| C | -6.78024 | -0.28278 | 0.15493 |
| H | -5.32049 | 1.28092 | -0.05151 |
| C | -5.92838 | -2.53675 | 0.19559 |
| H | -3.79643 | -2.72846 | 0.02249 |
| C | -6.99705 | -1.64994 | 0.24303 |
| C | -0.59735 | 6.05447 | 0.20470 |
| C | -0.53680 | 6.96955 | -1.02966 |
| H | 0.48232 | 7.05301 | -1.41846 |
| H | -1.17272 | 6.57895 | -1.82967 |
| H | -0.88426 | 7.97615 | -0.77243 |
| C | -2.03933 | 6.03617 | 0.72161 |
| H | -2.73373 | 5.65113 | -0.03074 |
| H | -2.13468 | 5.41954 | 1.62062 |
| H | -2.34796 | 7.05456 | 0.97772 |
| C | 0.30379 | 6.63101 | 1.30919 |
| H | 0.28091 | 5.99269 | 2.19772 |
| H | 1.34328 | 6.71331 | 0.97890 |
| H | -0.03948 | 7.63143 | 1.59431 |
| C | 2.81955 | -0.76052 | -1.93970 |
| C | 4.06169 | -1.39998 | -1.85958 |
| C | 1.75910 | -1.39395 | -2.59237 |
| C | 4.24372 | -2.65811 | -2.42934 |
| H | 4.88499 | -0.90676 | -1.34816 |
| C | 1.94679 | -2.65415 | -3.16158 |
| H | 0.79300 | -0.90469 | -2.62861 |
| C | 3.18466 | -3.29022 | -3.08148 |
| H | 5.21530 | -3.13968 | -2.37103 |
| H | 1.12105 | -3.13360 | -3.67862 |
| H | 3.32880 | -4.26393 | -3.54000 |
| H | -7.62252 | 0.39959 | 0.19110 |
| H | -6.10569 | -3.60435 | 0.26504 |
| Cl | -8.62761 | -2.26686 | 0.41338 |
| O | 0.16371 | -1.41969 | 0.06022 |
| C | -0.38235 | -2.55821 | 0.05366 |
| O | -1.55081 | -2.85319 | -0.20702 |
| C | 0.55217 | -3.73484 | 0.39100 |
| H | 0.32358 | -4.11286 | 1.39339 |
| C | 2.82772 | -4.48369 | 0.28911 |
| H | 2.15769 | -2.70352 | 1.29743 |
| H | 2.09576 | -2.62392 | -0.37714 |
| C | 1.97916 | -5.49434 | -0.51395 |
| H | 0.43211 | -4.42984 | -1.63441 |
| H | -0.23696 | -5.56541 | -0.46836 |
| H | 3.76652 | -4.20643 | -0.19028 |
| H | 3.03459 | -4.83702 | 1.30173 |
| H | 2.41901 | -5.67415 | -1.49664 |
| H | 1.94404 | -6.45016 | 0.01228 |
| N | 1.97297 | -3.26910 | 0.41586 |
| C | 0.57574 | -4.86055 | -0.64013 |
| O | 1.25292 | 0.85605 | -1.23398 |
| H | 2.45191 | -3.09373 | 4.20119 |
| H | 3.82207 | 3.20530 | -0.69028 |
| H | 3.32531 | 3.86402 | -2.24525 |

Complex between *(S)*-receptor and *L*-proline
Phenyl group axial: ΔG: 1.8 kcal/mol

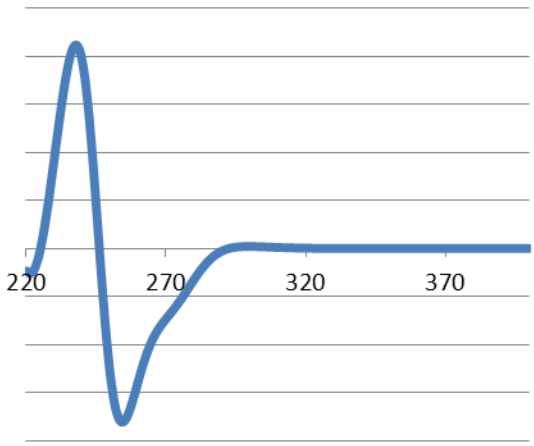


| | | | |
|---|---|---|---|
| C | -0.93296 | 4.62593 | -0.46795 |
| C | -1.55852 | 3.40367 | -0.70498 |
| C | -0.79299 | 2.24148 | -0.66556 |
| C | 0.57445 | 2.28457 | -0.34504 |
| C | 1.16803 | 3.52906 | -0.11351 |
| C | 0.42974 | 4.71142 | -0.18212 |
| H | -1.54024 | 5.52666 | -0.52066 |
| H | 2.22375 | 3.54072 | 0.11093 |
| C | -2.71398 | 0.84618 | -1.01553 |
| C | -3.34374 | 2.02981 | -1.75352 |
| H | -4.41593 | 1.85973 | -1.86176 |
| H | -2.91370 | 2.05389 | -2.76014 |
| C | -3.03352 | 3.31948 | -1.00840 |
| C | -2.99980 | -0.44719 | -1.80409 |
| O | -3.96002 | -0.53190 | -2.54668 |
| N | -2.16504 | -1.48776 | -1.50363 |
| H | -1.37841 | -1.33291 | -0.85375 |
| C | -2.34295 | -2.78522 | -1.99815 |
| C | -2.77412 | -3.04028 | -3.30491 |
| C | -2.15370 | -5.03493 | -1.54323 |
| C | -2.88336 | -4.36065 | -3.70755 |
| H | -3.01114 | -2.21375 | -3.95999 |
| C | -2.55730 | -5.38653 | -2.81981 |
| H | -3.20866 | -4.59094 | -4.71685 |
| H | -2.61904 | -6.42883 | -3.10800 |
| N | -2.06186 | -3.76447 | -1.13051 |
| N | 1.25166 | 1.07077 | -0.21801 |
| C | 2.62336 | 0.91180 | -0.29857 |
| H | 0.68171 | 0.23153 | -0.09528 |
| O | 3.39040 | 1.79499 | -0.65024 |
| N | 3.01077 | -0.36224 | 0.05833 |
| H | 2.33458 | -0.95717 | 0.53976 |
| C | 4.31048 | -0.87882 | 0.00493 |
| C | 5.38497 | -0.24020 | -0.62863 |
| C | 4.51755 | -2.13080 | 0.60429 |
| C | 6.63496 | -0.84975 | -0.65467 |
| H | 5.23938 | 0.72729 | -1.08564 |
| C | 5.76591 | -2.73396 | 0.57472 |
| H | 3.68343 | -2.62100 | 1.09733 |
| C | 6.82221 | -2.08813 | -0.05697 |
| C | 1.07436 | 6.08259 | 0.04428 |
| C | 0.37100 | 6.79694 | 1.21004 |
| H | -0.69169 | 6.95564 | 1.00480 |
| H | 0.45368 | 6.20944 | 2.12953 |
| H | 0.82904 | 7.77656 | 1.38457 |
| C | 2.56566 | 5.96995 | 0.37611 |
| H | 2.73067 | 5.40346 | 1.29776 |
| H | 3.12150 | 5.48106 | -0.42942 |
| H | 2.98460 | 6.97105 | 0.51731 |
| C | 0.92669 | 6.92636 | -1.23281 |
| H | 1.41941 | 6.43519 | -2.07706 |
| H | -0.12464 | 7.07650 | -1.49525 |
| H | 1.38387 | 7.91180 | -1.09121 |
| C | -3.31059 | 0.65002 | 0.38284 |
| C | -4.67519 | 0.37013 | 0.51788 |
| C | -2.51140 | 0.73395 | 1.52665 |
| C | -5.23939 | 0.20034 | 1.77892 |
| H | -5.29043 | 0.27630 | -0.37353 |
| C | -3.08315 | 0.56451 | 2.78983 |
| H | -1.44664 | 0.91551 | 1.42493 |
| C | -4.44549 | 0.30544 | 2.92092 |
| H | -6.30094 | -0.00729 | 1.87008 |
| H | -2.46075 | 0.65892 | 3.67523 |
| H | -4.88775 | 0.19051 | 3.90593 |
| H | 7.46740 | -0.35686 | -1.14496 |
| H | 5.92140 | -3.70088 | 1.04049 |
| Cl | 8.40135 | -2.84563 | -0.09781 |
| O | -0.22594 | -1.26422 | 0.51143 |
| C | 0.23577 | -2.09331 | 1.35084 |
| O | 1.40282 | -2.28503 | 1.69088 |
| C | -0.84143 | -2.91248 | 2.08957 |
| H | -0.61897 | -3.98211 | 2.03870 |
| C | -3.22478 | -3.03807 | 2.43212 |
| H | -2.20256 | -3.18352 | 0.51106 |
| H | -2.18286 | -1.67522 | 1.21396 |
| C | -2.55591 | -2.85727 | 3.81460 |
| H | -0.98964 | -1.35831 | 3.55897 |
| H | -0.37534 | -2.87686 | 4.21636 |
| H | -4.08595 | -2.38898 | 2.26945 |
| H | -3.51556 | -4.07371 | 2.24760 |
| H | -3.07514 | -2.09629 | 4.40058 |
| H | -2.59718 | -3.79431 | 4.37350 |
| N | -2.16659 | -2.68048 | 1.44374 |
| C | -1.09768 | -2.44741 | 3.52289 |
| O | -1.30671 | 0.98173 | -0.93901 |
| H | -1.89981 | -5.79358 | -0.80757 |
| H | -3.34039 | 4.18452 | -1.60344 |
| H | -3.61011 | 3.35482 | -0.07459 |

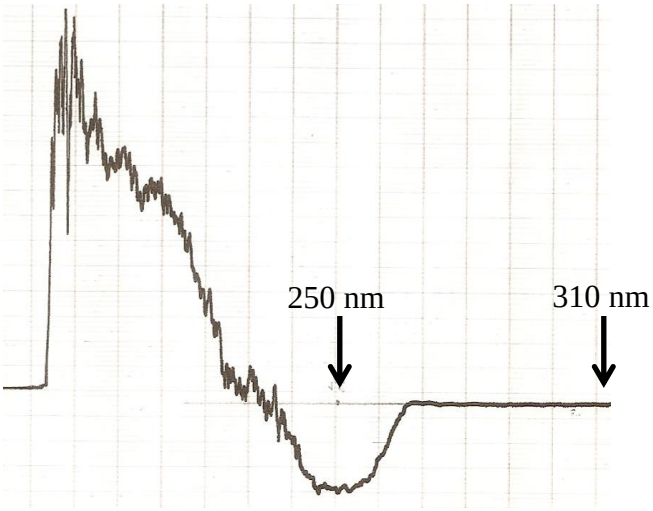
**Determination of the absolute configuration of the receptor by simulation of ECD spectra.**

All calculations were performed using Gaussian09 software[1]. 16 different conformations corresponding for the structure of the R receptor shown were optimized using M06-2X DFT functional [2] and 6-31G** basis set.[3] Gibbs free energy at 298.15 K was calculated for each structure from the Gaussian output files, corrected according to the so-called "quasi-harmonic approach" using a free- rotor approximation for vibrational modes below 100 cm−1 and a rigid rotor approximation above this cutoff[4]. For the optimized structures a time-dependent DFT calculation, including the 50 more stable singlet excited states, was performed using B98 functional [6] and 6-31G**. This functional was chosen after considering its performance in the Truhlar benchmark database VES21 for electronic excitation energies involving valence excited states.[2] For each structure, the ECD spectra was simulated using a value of □=0.4 using Gaussum software[7], and the absorbance was averaged considering the Maxwell-Boltzman relative population of each structure from the Gibbs free energy calculated as described above at 298.15 K.

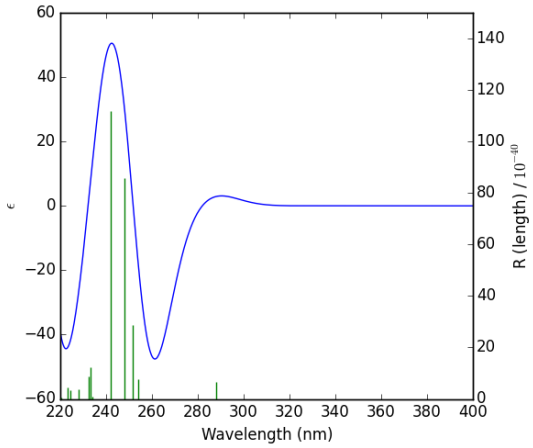
Simmulated ECD:




Experimental ECD:

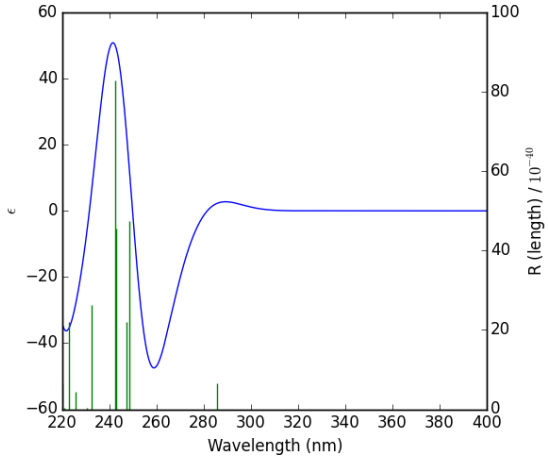


## Conformation 1: ΔG: 0.559606697




| | | | |
|---|---|---|---|
| C | 3.54157 | 2.22544 | 0.28559 |
| C | 3.40780 | 0.85243 | 0.08120 |
| C | 2.34034 | 0.41105 | -0.69152 |
| C | 1.37912 | 1.30504 | -1.17515 |
| C | 1.54987 | 2.67148 | -0.97489 |
| C | 2.64078 | 3.15121 | -0.24479 |
| H | 4.37774 | 2.56740 | 0.89159 |
| H | 0.79493 | 3.33722 | -1.36590 |
| C | 2.60287 | -1.84076 | -0.00254 |
| C | 4.08453 | -1.57313 | 0.27191 |
| H | 4.44637 | -2.29995 | 1.00199 |
| H | 4.60520 | -1.75262 | -0.67435 |
| C | 4.31447 | -0.14450 | 0.76599 |
| C | 1.74737 | -1.66934 | 1.27788 |
| O | 2.19378 | -1.91877 | 2.38406 |
| N | 0.47237 | -1.28381 | 1.00095 |
| H | 0.26251 | -1.06328 | 0.03590 |
| C | -0.58924 | -0.98842 | 1.86456 |
| C | -0.52259 | -1.13868 | 3.25231 |
| C | -2.73869 | -0.21780 | 1.92823 |
| C | -1.65576 | -0.79129 | 3.97558 |
| H | 0.38202 | -1.50535 | 3.71693 |
| C | -2.78659 | -0.31958 | 3.31443 |
| H | -1.65176 | -0.88875 | 5.05672 |
| H | -3.68311 | -0.03872 | 3.85397 |
| N | -1.66519 | -0.54816 | 1.20910 |
| N | 0.24344 | 0.75553 | -1.81133 |
| C | -1.04610 | 1.18379 | -1.51798 |
| H | 0.37232 | -0.18772 | -2.14938 |
| O | -1.29537 | 2.25891 | -1.01647 |
| N | -2.01248 | 0.26319 | -1.90448 |
| H | -1.67963 | -0.67504 | -2.07542 |
| C | -3.34024 | 0.29969 | -1.43970 |
| C | -4.02335 | 1.49424 | -1.18886 |
| C | -3.99635 | -0.91924 | -1.24132 |
| C | -5.33356 | 1.45517 | -0.72303 |
| H | -3.52345 | 2.44066 | -1.33582 |
| C | -5.30786 | -0.95822 | -0.78952 |
| H | -3.46589 | -1.85102 | -1.41735 |
| C | -5.96939 | 0.23546 | -0.52485 |
| C | 2.85230 | 4.64640 | 0.01064 |
| C | 2.81828 | 4.91177 | 1.52510 |
| H | 3.61105 | 4.36834 | 2.04720 |
| H | 1.85899 | 4.60123 | 1.94951 |
| H | 2.95563 | 5.97989 | 1.72418 |
| C | 1.76784 | 5.50078 | -0.65310 |
| H | 0.77224 | 5.25774 | -0.26943 |
| H | 1.76146 | 5.36706 | -1.73939 |
| H | 1.95998 | 6.55796 | -0.44683 |
| C | 4.21831 | 5.07198 | -0.55183 |
| H | 4.26741 | 4.89089 | -1.62982 |
| H | 5.03710 | 4.52201 | -0.07916 |
| H | 4.38342 | 6.13986 | -0.37353 |
| H | -5.86458 | 2.37824 | -0.51883 |
| H | -5.80925 | -1.90607 | -0.63091 |
| Cl | -7.61474 | 0.19856 | 0.05951 |
| C | 2.39632 | -3.24470 | -0.55130 |
| C | 2.22322 | -3.45582 | -1.91898 |
| C | 2.43364 | -4.33951 | 0.31602 |
| C | 2.07668 | -4.75007 | -2.41241 |
| H | 2.21252 | -2.60732 | -2.59347 |
| C | 2.28789 | -5.62981 | -0.18209 |
| H | 2.56949 | -4.17464 | 1.38132 |
| C | 2.10617 | -5.83885 | -1.54707 |
| H | 1.94209 | -4.90592 | -3.47819 |
| H | 2.31345 | -6.47389 | 0.49940 |
| H | 1.99070 | -6.84597 | -1.93422 |
| H | -3.59520 | 0.14208 | 1.36086 |
| O | 2.12961 | -0.92370 | -0.98965 |
| H | 5.36229 | 0.13771 | 0.62340 |
| H | 4.11573 | -0.10387 | 1.84290 |

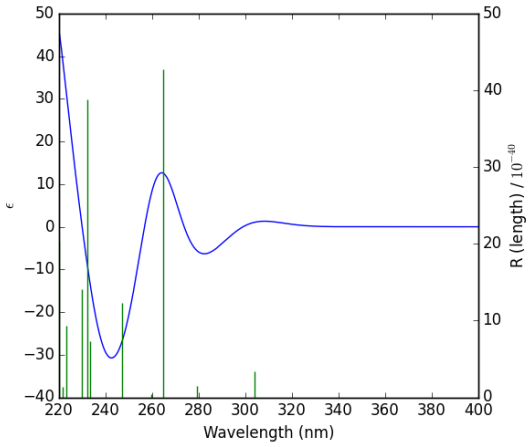
## Conformation 2: ΔG: 0.502522158




| | | | |
|---|---|---|---|
| C | 3.49872 | 2.30268 | 0.30138 |
| C | 3.39952 | 0.92286 | 0.08273 |
| C | 2.34841 | 0.45735 | -0.69016 |
| C | 1.36004 | 1.32979 | -1.17203 |
| C | 1.49616 | 2.69265 | -0.96098 |
| C | 2.57400 | 3.20103 | -0.22068 |
| H | 4.32626 | 2.65420 | 0.90939 |
| H | 0.72585 | 3.34805 | -1.34510 |
| C | 2.66567 | -1.78670 | -0.00523 |
| C | 4.14131 | -1.48419 | 0.26494 |
| H | 4.52273 | -2.20228 | 0.99366 |
| H | 4.66298 | -1.65114 | -0.68303 |
| C | 4.33848 | -0.05017 | 0.75799 |
| C | 1.81020 | -1.63176 | 1.27751 |
| O | 2.26676 | -1.86166 | 2.38367 |
| N | 0.52399 | -1.28312 | 1.00233 |
| H | 0.30642 | -1.07441 | 0.03645 |
| C | -0.53936 | -0.99961 | 1.86766 |
| C | -0.46381 | -1.13469 | 3.25652 |
| C | -2.70219 | -0.26740 | 1.93369 |
| C | -1.59967 | -0.80009 | 3.98160 |
| H | 0.44939 | -1.48024 | 3.72064 |
| C | -2.74180 | -0.35538 | 3.32107 |
| H | -1.58895 | -0.88630 | 5.06365 |

| | | | |
|---|---|---|---|
| H | -3.64057 | -0.08462 | 3.86198 |
| N | -1.62625 | -0.58586 | 1.21282 |
| N | 0.23802 | 0.75167 | -1.80551 |
| C | -1.06082 | 1.15403 | -1.51671 |
| H | 0.38809 | -0.18918 | -2.14152 |
| O | -1.33402 | 2.22743 | -1.02371 |
| N | -2.00634 | 0.20987 | -1.89725 |
| H | -1.65243 | -0.72248 | -2.05798 |
| C | -3.33501 | 0.21990 | -1.43348 |
| C | -4.04524 | 1.40002 | -1.19026 |
| C | -3.96348 | -1.01250 | -1.22851 |
| C | -5.35492 | 1.33382 | -0.72575 |
| H | -3.56661 | 2.35663 | -1.34174 |
| C | -5.27440 | -1.07869 | -0.77821 |
| H | -3.41195 | -1.93299 | -1.39913 |
| C | -5.96325 | 0.10118 | -0.52139 |
| C | 2.65931 | 4.71245 | 0.00548 |
| C | 3.89508 | 5.10558 | 0.82029 |
| H | 4.82069 | 4.80628 | 0.31801 |
| H | 3.87986 | 4.65527 | 1.81787 |
| H | 3.91865 | 6.19209 | 0.94610 |
| C | 1.40538 | 5.17798 | 0.76477 |
| H | 1.34756 | 4.69490 | 1.74482 |
| H | 0.48950 | 4.93519 | 0.21884 |
| H | 1.43654 | 6.26240 | 0.91545 |
| C | 2.72895 | 5.42670 | -1.35447 |
| H | 1.84777 | 5.21258 | -1.96508 |
| H | 3.61425 | 5.10993 | -1.91442 |
| H | 2.78248 | 6.51079 | -1.20882 |
| H | -5.90669 | 2.24579 | -0.52661 |
| H | -5.75463 | -2.03668 | -0.61511 |
| Cl | -7.60767 | 0.03029 | 0.06161 |
| C | 2.48832 | -3.19556 | -0.55116 |
| C | 2.31622 | -3.41301 | -1.91798 |
| C | 2.54972 | -4.28756 | 0.31829 |
| C | 2.19385 | -4.71092 | -2.40835 |
| H | 2.28699 | -2.56625 | -2.59418 |
| C | 2.42815 | -5.58153 | -0.17672 |
| H | 2.68478 | -4.11774 | 1.38295 |
| C | 2.24689 | -5.79704 | -1.54078 |
| H | 2.05950 | -4.87167 | -3.47343 |
| H | 2.47194 | -6.42342 | 0.50659 |
| H | 2.14978 | -6.80709 | -1.92536 |
| H | -3.56761 | 0.07100 | 1.36671 |
| O | 2.16867 | -0.88128 | -0.99166 |
| H | 5.37712 | 0.25933 | 0.60424 |
| H | 4.15081 | -0.01416 | 1.83708 |

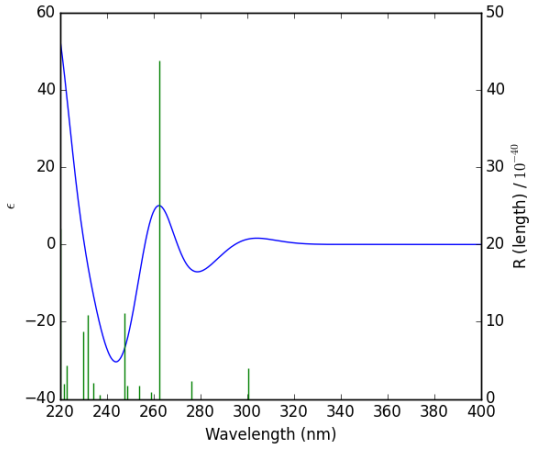
## Conformation 3: ΔG: 4.687703043




| | | | |
|---|---|---|---|
| C | -0.66960 | 3.98286 | -0.75135 |
| C | -1.34788 | 2.76427 | -0.73774 |
| C | -0.60817 | 1.60549 | -0.54989 |
| C | 0.78712 | 1.64261 | -0.41172 |
| C | 1.43994 | 2.87374 | -0.42793 |
| C | 0.71376 | 4.05940 | -0.59042 |
| H | -1.25186 | 4.88962 | -0.89845 |
| H | 2.51223 | 2.88202 | -0.31058 |
| C | -2.55329 | 0.26172 | -0.29018 |
| C | -3.26444 | 1.23666 | -1.24467 |
| H | -4.34918 | 1.11305 | -1.19020 |
| H | -2.95337 | 0.95614 | -2.25645 |
| C | -2.84291 | 2.67293 | -0.93221 |
| C | -2.89880 | -1.18953 | -0.72009 |
| O | -2.17380 | -1.80546 | -1.47378 |
| N | -4.09481 | -1.64655 | -0.24425 |
| H | -4.57674 | -1.11158 | 0.46800 |
| C | -4.73957 | -2.85686 | -0.54301 |
| C | -4.23259 | -3.80609 | -1.43886 |
| C | -6.59410 | -4.11115 | -0.09882 |
| C | -4.98828 | -4.95192 | -1.64150 |
| H | -3.29033 | -3.63706 | -1.93758 |
| C | -6.19328 | -5.12095 | -0.96534 |
| H | -4.63070 | -5.71236 | -2.32865 |
| H | -6.80416 | -6.00537 | -1.10212 |
| N | -5.89138 | -2.99926 | 0.11397 |
| N | 1.40552 | 0.38716 | -0.28950 |
| C | 2.74645 | 0.13947 | -0.10047 |
| H | 0.77187 | -0.38748 | -0.43547 |
| O | 3.58196 | 1.00345 | 0.09471 |
| N | 3.03459 | -1.21485 | -0.14727 |
| H | 2.28416 | -1.84265 | -0.39359 |
| C | 4.29031 | -1.82383 | 0.00077 |
| C | 5.45327 | -1.13346 | 0.36280 |
| C | 4.35764 | -3.20512 | -0.21928 |
| C | 6.65201 | -1.82591 | 0.49375 |
| H | 5.41505 | -0.06799 | 0.53276 |
| C | 5.55452 | -3.89309 | -0.08529 |
| H | 3.46064 | -3.75060 | -0.50093 |
| C | 6.70212 | -3.19538 | 0.27108 |
| C | 1.40209 | 5.42866 | -0.61264 |
| C | 0.82668 | 6.30721 | 0.51045 |
| H | -0.24914 | 6.46318 | 0.38904 |
| H | 0.99274 | 5.84377 | 1.48752 |
| H | 1.31109 | 7.28961 | 0.50766 |
| C | 2.91604 | 5.31717 | -0.40778 |
| H | 3.15878 | 4.85264 | 0.55277 |
| H | 3.38885 | 4.73079 | -1.20139 |
| H | 3.36043 | 6.31712 | -0.42029 |
| C | 1.14535 | 6.10466 | -1.96978 |

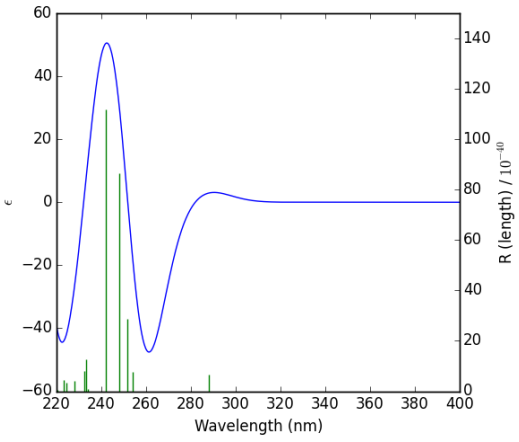
| | | | |
|---|---|---|---|
| H | 1.54098 | 5.49333 | -2.78643 |
| H | 0.07687 | 6.25640 | -2.14828 |
| H | 1.63471 | 7.08394 | -2.00359 |
| C | -2.85237 | 0.51963 | 1.18604 |
| C | -4.10781 | 0.95995 | 1.61751 |
| C | -1.85867 | 0.27965 | 2.13801 |
| C | -4.36874 | 1.14085 | 2.97358 |
| H | -4.89254 | 1.17723 | 0.89678 |
| C | -2.11765 | 0.46887 | 3.49129 |
| H | -0.87648 | -0.04286 | 1.80798 |
| C | -3.37380 | 0.89570 | 3.91403 |
| H | -5.34860 | 1.48206 | 3.29095 |
| H | -1.33312 | 0.28515 | 4.21811 |
| H | -3.57393 | 1.04259 | 4.97020 |
| H | 7.55455 | -1.29325 | 0.77182 |
| H | 5.59797 | -4.96248 | -0.25785 |
| Cl | 8.21648 | -4.04901 | 0.43882 |
| O | -1.15955 | 0.34526 | -0.52237 |
| H | -7.52654 | -4.19281 | 0.45471 |
| H | -3.35375 | 3.02584 | -0.02865 |
| H | -3.14870 | 3.33447 | -1.74877 |

## Conformation 4: ΔG: 4.258398694




| | | | |
|---|---|---|---|
| C | -0.64858 | 3.99461 | -0.76854 |
| C | -1.33501 | 2.77400 | -0.75283 |
| C | -0.60812 | 1.61351 | -0.55739 |
| C | 0.79148 | 1.63904 | -0.41266 |
| C | 1.44727 | 2.86227 | -0.43109 |
| C | 0.72975 | 4.05832 | -0.60230 |
| H | -1.22991 | 4.89818 | -0.92127 |
| H | 2.52121 | 2.87165 | -0.31002 |
| C | -2.56278 | 0.28594 | -0.29726 |
| C | -3.26142 | 1.26033 | -1.26164 |
| H | -4.34736 | 1.14563 | -1.21191 |
| H | -2.94753 | 0.97079 | -2.27001 |
| C | -2.82929 | 2.69499 | -0.95655 |
| C | -2.91815 | -1.16560 | -0.71759 |
| O | -2.19303 | -1.79575 | -1.45941 |
| N | -4.12233 | -1.60642 | -0.24729 |
| H | -4.60430 | -1.06022 | 0.45633 |
| C | -4.77802 | -2.81219 | -0.54005 |
| C | -4.27587 | -3.77486 | -1.42409 |
| C | -6.64966 | -4.04133 | -0.09720 |
| C | -5.04343 | -4.91370 | -1.62193 |
| H | -3.32823 | -3.62078 | -1.91758 |
| C | -6.25473 | -5.06307 | -0.95238 |
| H | -4.69026 | -5.68423 | -2.30007 |
| H | -6.87488 | -5.94156 | -1.08554 |
| N | -5.93571 | -2.93574 | 0.11044 |
| N | 1.39640 | 0.37844 | -0.28103 |
| C | 2.73637 | 0.12146 | -0.09700 |
| H | 0.75552 | -0.39120 | -0.42210 |
| O | 3.57877 | 0.98114 | 0.08754 |
| N | 3.01417 | -1.23504 | -0.13475 |
| H | 2.25811 | -1.85893 | -0.37379 |
| C | 4.26649 | -1.85189 | 0.01062 |
| C | 5.43432 | -1.16839 | 0.36979 |
| C | 4.32472 | -3.23375 | -0.20822 |
| C | 6.62906 | -1.86804 | 0.49884 |
| H | 5.40310 | -0.10256 | 0.53888 |
| C | 5.51759 | -3.92898 | -0.07588 |
| H | 3.42382 | -3.77387 | -0.48775 |
| C | 6.67020 | -3.23800 | 0.27732 |
| C | 1.50693 | 5.37807 | -0.61080 |
| C | 2.23713 | 5.54678 | 0.73205 |
| H | 1.52220 | 5.57040 | 1.56021 |
| H | 2.93819 | 4.72766 | 0.91383 |
| H | 2.80347 | 6.48427 | 0.73817 |
| C | 2.53855 | 5.35620 | -1.75106 |
| H | 3.25807 | 4.54219 | -1.62826 |
| H | 2.04368 | 5.22701 | -2.71843 |
| H | 3.09672 | 6.29838 | -1.77230 |
| C | 0.58882 | 6.58633 | -0.81628 |
| H | 0.06301 | 6.53320 | -1.77502 |
| H | -0.15452 | 6.66851 | -0.01687 |
| H | 1.18538 | 7.50340 | -0.81327 |
| C | -2.86687 | 0.55673 | 1.17579 |
| C | -4.12101 | 1.00945 | 1.59794 |
| C | -1.87984 | 0.31557 | 2.13436 |
| C | -4.38753 | 1.20082 | 2.95149 |
| H | -4.90037 | 1.22832 | 0.87187 |
| C | -2.14423 | 0.51538 | 3.48507 |
| H | -0.89837 | -0.01609 | 1.81133 |
| C | -3.39934 | 0.95410 | 3.89861 |
| H | -5.36647 | 1.55114 | 3.26170 |
| H | -1.36469 | 0.33069 | 4.21700 |
| H | -3.60380 | 1.10906 | 4.95280 |
| H | 7.53545 | -1.34076 | 0.77460 |
| H | 5.55410 | -4.99878 | -0.24753 |
| Cl | 8.17982 | -4.10063 | 0.44215 |
| O | -1.16718 | 0.35720 | -0.52295 |
| H | -7.58640 | -4.10766 | 0.45105 |
| H | -3.34366 | 3.06017 | -0.05982 |
| H | -3.12311 | 3.35263 | -1.78071 |

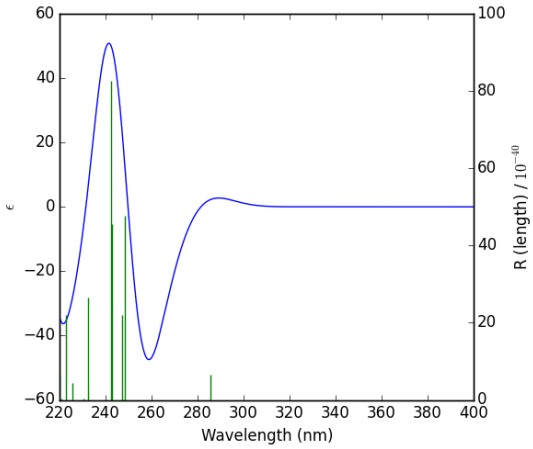
## Conformation 5: ΔG: 0.565442535




| | | | |
|---|---|---|---|
| C | 3.54126 | 2.22569 | 0.28626 |
| C | 3.40751 | 0.85271 | 0.08180 |
| C | 2.34019 | 0.41141 | -0.69120 |

| | | | |
|---|---|---|---|
| C | 1.37924 | 1.30548 | -1.17509 |
| C | 1.55001 | 2.67191 | -0.97483 |
| C | 2.64068 | 3.15157 | -0.24435 |
| H | 4.37728 | 2.56764 | 0.89247 |
| H | 0.79520 | 3.33764 | -1.36612 |
| C | 2.60281 | -1.84060 | -0.00270 |
| C | 4.08438 | -1.57278 | 0.27204 |
| H | 4.44635 | -2.29986 | 1.00177 |
| H | 4.60507 | -1.75180 | -0.67432 |
| C | 4.31402 | -0.14429 | 0.76667 |
| C | 1.74717 | -1.66962 | 1.27770 |
| O | 2.19363 | -1.91904 | 2.38386 |
| N | 0.47202 | -1.28463 | 1.00069 |
| H | 0.26220 | -1.06395 | 0.03565 |
| C | -0.58966 | -0.98957 | 1.86434 |
| C | -0.52303 | -1.14016 | 3.25205 |
| C | -2.73925 | -0.21936 | 1.92815 |
| C | -1.65627 | -0.79313 | 3.97539 |
| H | 0.38162 | -1.50683 | 3.71660 |
| C | -2.78717 | -0.32148 | 3.31432 |
| H | -1.65229 | -0.89087 | 5.05649 |
| H | -3.68375 | -0.04091 | 3.85392 |
| N | -1.66568 | -0.54936 | 1.20896 |
| N | 0.24358 | 0.75616 | -1.81158 |
| C | -1.04599 | 1.18402 | -1.51758 |
| H | 0.37247 | -0.18695 | -2.14998 |
| O | -1.29540 | 2.25882 | -1.01550 |
| N | -2.01230 | 0.26349 | -1.90439 |
| H | -1.67947 | -0.67467 | -2.07574 |
| C | -3.34005 | 0.29996 | -1.43965 |
| C | -4.02294 | 1.49455 | -1.18841 |
| C | -3.99638 | -0.91892 | -1.24170 |
| C | -5.33318 | 1.45556 | -0.72268 |
| H | -3.52283 | 2.44092 | -1.33499 |
| C | -5.30793 | -0.95781 | -0.79001 |
| H | -3.46606 | -1.85073 | -1.41797 |
| C | -5.96926 | 0.23591 | -0.52498 |
| C | 2.85235 | 4.64673 | 0.01102 |
| C | 2.81804 | 4.91236 | 1.52542 |
| H | 3.61057 | 4.36891 | 2.04787 |
| H | 1.85859 | 4.60212 | 1.94966 |
| H | 2.95559 | 5.98050 | 1.72430 |
| C | 1.76815 | 5.50120 | -0.65306 |
| H | 0.77239 | 5.25798 | -0.26991 |
| H | 1.76229 | 5.36769 | -1.73938 |
| H | 1.96012 | 6.55836 | -0.44654 |
| C | 4.21856 | 5.07197 | -0.55122 |
| H | 4.26781 | 4.89080 | -1.62919 |
| H | 5.03711 | 4.52180 | -0.07836 |
| H | 4.38390 | 6.13982 | -0.37294 |
| H | -5.86403 | 2.37867 | -0.51818 |
| H | -5.80948 | -1.90562 | -0.63170 |
| Cl | -7.61463 | 0.19911 | 0.05929 |
| C | 2.39653 | -3.24449 | -0.55172 |
| C | 2.43476 | -4.33944 | 0.31540 |
| C | 2.22277 | -3.45547 | -1.91933 |
| C | 2.28930 | -5.62972 | -0.18282 |
| H | 2.57102 | -4.17467 | 1.38067 |
| C | 2.07653 | -4.74971 | -2.41289 |
| H | 2.21143 | -2.60690 | -2.59372 |
| C | 2.10696 | -5.83862 | -1.54775 |
| H | 2.31562 | -6.47390 | 0.49852 |
| H | 1.94144 | -4.90546 | -3.47862 |
| H | 1.99174 | -6.84573 | -1.93501 |
| H | -3.59583 | 0.14048 | 1.36086 |
| O | 2.12952 | -0.92333 | -0.98953 |
| H | 5.36182 | 0.13810 | 0.62446 |
| H | 4.11491 | -0.10392 | 1.84349 |

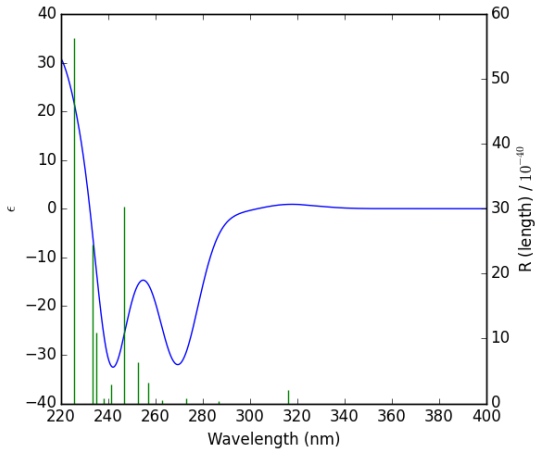
## Conformation 6: ΔG: 0.501605994




| | | | |
|---|---|---|---|
| C | 3.49855 | 2.30290 | 0.30131 |
| C | 3.39943 | 0.92308 | 0.08263 |
| C | 2.34830 | 0.45754 | -0.69023 |
| C | 1.35990 | 1.32995 | -1.17208 |
| C | 1.49598 | 2.69281 | -0.96104 |
| C | 2.57379 | 3.20122 | -0.22072 |
| H | 4.32610 | 2.65447 | 0.90928 |
| H | 0.72567 | 3.34819 | -1.34519 |
| C | 2.66581 | -1.78651 | -0.00545 |
| C | 4.14144 | -1.48387 | 0.26462 |
| H | 4.52306 | -2.20201 | 0.99319 |
| H | 4.66300 | -1.65067 | -0.68344 |
| C | 4.33855 | -0.04988 | 0.75778 |
| C | 1.81039 | -1.63176 | 1.27736 |
| O | 2.26705 | -1.86172 | 2.38345 |
| N | 0.52412 | -1.28325 | 1.00228 |
| H | 0.30650 | -1.07441 | 0.03644 |
| C | -0.53914 | -0.99982 | 1.86776 |
| C | -0.46338 | -1.13504 | 3.25659 |
| C | -2.70196 | -0.26764 | 1.93419 |
| C | -1.59914 | -0.80053 | 3.98188 |
| H | 0.44988 | -1.48064 | 3.72055 |
| C | -2.74136 | -0.35575 | 3.32155 |
| H | -1.58826 | -0.88685 | 5.06391 |
| H | -3.64006 | -0.08506 | 3.86262 |
| N | -1.62611 | -0.58601 | 1.21311 |
| N | 0.23789 | 0.75180 | -1.80559 |
| C | -1.06099 | 1.15402 | -1.51663 |
| H | 0.38799 | -0.18906 | -2.14155 |
| O | -1.33427 | 2.22741 | -1.02366 |
| N | -2.00641 | 0.20966 | -1.89684 |
| H | -1.65242 | -0.72269 | -2.05739 |
| C | -3.33511 | 0.21970 | -1.43320 |
| C | -4.04541 | 1.39981 | -1.19018 |
| C | -3.96356 | -1.01270 | -1.22818 |
| C | -5.35516 | 1.33360 | -0.72584 |
| H | -3.56683 | 2.35644 | -1.34171 |
| C | -5.27453 | -1.07890 | -0.77803 |
| H | -3.41196 | -1.93319 | -1.39862 |
| C | -5.96347 | 0.10096 | -0.52143 |
| C | 2.65899 | 4.71262 | 0.00552 |
| C | 3.89475 | 5.10580 | 0.82031 |
| H | 4.82036 | 4.80660 | 0.31796 |
| H | 3.87962 | 4.65543 | 1.81785 |
| H | 3.91823 | 6.19229 | 0.94620 |
| C | 1.40501 | 5.17795 | 0.76488 |
| H | 1.34728 | 4.69477 | 1.74489 |
| H | 0.48916 | 4.93507 | 0.21894 |
| H | 1.43604 | 6.26236 | 0.91565 |
| C | 2.72852 | 5.42703 | -1.35436 |

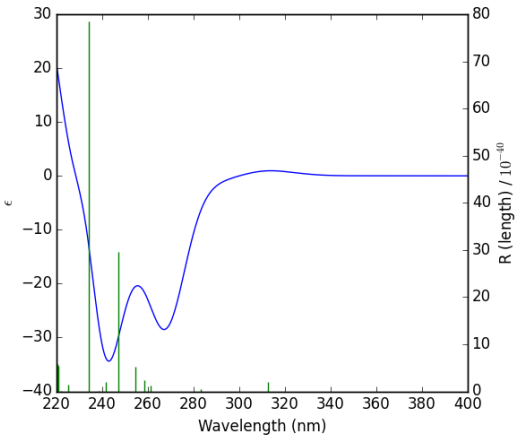
| | | | |
|---|---|---|---|
| H | 1.84737 | 5.21289 | -1.96502 |
| H | 3.61387 | 5.11044 | -1.91434 |
| H | 2.78192 | 6.51110 | -1.20859 |
| H | -5.90699 | 2.24558 | -0.52689 |
| H | -5.75473 | -2.03690 | -0.61487 |
| Cl | -7.60795 | 0.03006 | 0.06137 |
| C | 2.48856 | -3.19536 | -0.55140 |
| C | 2.55045 | -4.28734 | 0.31806 |
| C | 2.31602 | -3.41287 | -1.91815 |
| C | 2.42895 | -5.58134 | -0.17686 |
| H | 2.68578 | -4.11745 | 1.38267 |
| C | 2.19372 | -4.71083 | -2.40844 |
| H | 2.28640 | -2.56615 | -2.59437 |
| C | 2.24728 | -5.79692 | -1.54087 |
| H | 2.47313 | -6.42320 | 0.50646 |
| H | 2.05904 | -4.87163 | -3.47347 |
| H | 2.15025 | -6.80699 | -1.92540 |
| H | -3.56746 | 0.07084 | 1.36737 |
| O | 2.16865 | -0.88109 | -0.99179 |
| H | 5.37715 | 0.25969 | 0.60388 |
| H | 4.15101 | -0.01394 | 1.83689 |

## Conformation 7: ΔG: 5.358316171




| | | | |
|---|---|---|---|
| C | 1.35402 | 3.47617 | -0.78503 |
| C | 1.69520 | 2.14208 | -1.00023 |
| C | 0.72951 | 1.16819 | -0.78803 |
| C | -0.56312 | 1.51214 | -0.36826 |
| C | -0.87719 | 2.85332 | -0.15282 |
| C | 0.07991 | 3.85183 | -0.36083 |
| H | 2.11623 | 4.23183 | -0.96054 |
| H | -1.87777 | 3.09315 | 0.17098 |
| C | 2.28152 | -0.62075 | -1.14222 |
| C | 3.05011 | 0.33363 | -2.06416 |
| H | 4.06731 | -0.02934 | -2.23523 |
| H | 2.53047 | 0.34832 | -3.02838 |
| C | 3.07569 | 1.73194 | -1.45058 |
| C | 2.92325 | -0.62305 | 0.27364 |
| O | 2.32256 | -0.22247 | 1.24826 |
| N | 4.20586 | -1.10073 | 0.28443 |
| H | 4.56944 | -1.53020 | -0.55794 |
| C | 5.07901 | -1.23226 | 1.37545 |
| C | 4.78520 | -0.76496 | 2.66204 |
| C | 7.13091 | -2.00634 | 2.00565 |
| C | 5.75390 | -0.95369 | 3.63792 |
| H | 3.83946 | -0.28535 | 2.86743 |
| C | 6.95288 | -1.58468 | 3.31759 |
| H | 5.56792 | -0.60598 | 4.64928 |
| H | 7.72649 | -1.74540 | 4.05887 |
| N | 6.22030 | -1.83772 | 1.04714 |
| N | -1.44640 | 0.43601 | -0.18698 |
| C | -2.79968 | 0.50498 | 0.04526 |
| H | -1.00693 | -0.46508 | -0.30982 |
| O | -3.42578 | 1.54299 | 0.16087 |
| N | -3.37650 | -0.75280 | 0.13806 |
| H | -2.77651 | -1.55268 | 0.00643 |
| C | -4.72952 | -1.05794 | 0.34752 |
| C | -5.72129 | -0.09561 | 0.57410 |
| C | -5.08635 | -2.41224 | 0.32910 |
| C | -7.03761 | -0.49727 | 0.77268 |
| H | -5.45972 | 0.95165 | 0.59063 |
| C | -6.40003 | -2.80948 | 0.52933 |
| H | -4.32445 | -3.16776 | 0.15493 |
| C | -7.37447 | -1.84397 | 0.75043 |
| C | -0.24004 | 5.33486 | -0.14621 |
| C | 0.72546 | 5.92178 | 0.89680 |
| H | 1.76745 | 5.83898 | 0.57462 |
| H | 0.62502 | 5.39925 | 1.85275 |
| H | 0.50727 | 6.98286 | 1.05870 |
| C | -1.67316 | 5.55010 | 0.35050 |
| H | -1.84554 | 5.05233 | 1.30970 |
| H | -2.40937 | 5.17611 | -0.36721 |
| H | -1.85335 | 6.62036 | 0.49038 |
| C | -0.07120 | 6.08705 | -1.47674 |
| H | -0.75518 | 5.69024 | -2.23292 |
| H | 0.94837 | 5.99686 | -1.86284 |
| H | -0.28746 | 7.15219 | -1.34059 |
| H | -7.80732 | 0.24636 | 0.94635 |
| H | -6.66724 | -3.86009 | 0.51399 |
| Cl | -9.03236 | -2.33029 | 1.00568 |
| C | 2.19041 | -2.05886 | -1.63183 |
| C | 2.79865 | -2.50606 | -2.80187 |
| C | 1.46883 | -2.96412 | -0.84588 |
| C | 2.68292 | -3.84252 | -3.18529 |
| H | 3.35961 | -1.82109 | -3.42923 |
| C | 1.35015 | -4.29242 | -1.23030 |
| H | 1.01307 | -2.61197 | 0.07667 |
| C | 1.95926 | -4.73523 | -2.40444 |
| H | 3.15912 | -4.18096 | -4.09975 |
| H | 0.79057 | -4.98683 | -0.61186 |
| H | 1.87193 | -5.77419 | -2.70493 |
| O | 0.94126 | -0.17756 | -1.00727 |
| H | 8.04842 | -2.50494 | 1.70231 |
| H | 3.46186 | 2.45332 | -2.17659 |
| H | 3.76511 | 1.74615 | -0.59581 |

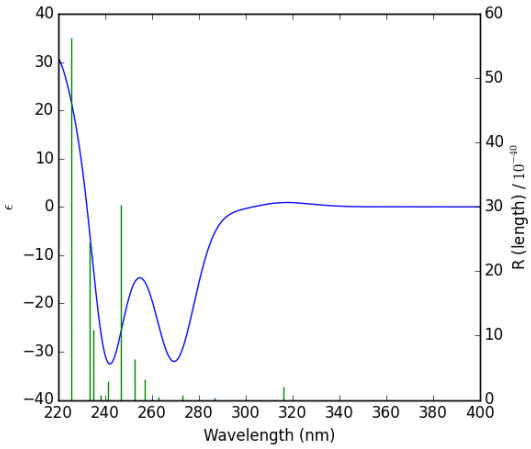
## Conformation 8: ΔG: 4.838681829




| | | | |
|---|---|---|---|
| C | 1.36155 | 3.49601 | -0.78533 |
| C | 1.70785 | 2.15849 | -1.00894 |
| C | 0.74640 | 1.18147 | -0.82146 |
| C | -0.55825 | 1.51579 | -0.41509 |
| C | -0.87561 | 2.84970 | -0.19549 |

| | | | |
|---|---|---|---|
| C | 0.08336 | 3.85867 | -0.37950 |
| H | 2.12821 | 4.24783 | -0.94206 |
| H | -1.88107 | 3.09265 | 0.11699 |
| C | 2.31023 | -0.59761 | -1.15814 |
| C | 3.09038 | 0.36459 | -2.06183 |
| H | 4.11237 | 0.00832 | -2.21777 |
| H | 2.58744 | 0.37999 | -3.03487 |
| C | 3.09694 | 1.76063 | -1.44320 |
| C | 2.92116 | -0.60605 | 0.27143 |
| O | 2.28930 | -0.23783 | 1.23915 |
| N | 4.21318 | -1.05639 | 0.30344 |
| H | 4.60628 | -1.45928 | -0.53873 |
| C | 5.06260 | -1.19431 | 1.41227 |
| C | 4.72715 | -0.76555 | 2.70211 |
| C | 7.11576 | -1.93790 | 2.07402 |
| C | 5.67581 | -0.95748 | 3.69693 |
| H | 3.76624 | -0.31145 | 2.89493 |
| C | 6.89628 | -1.55351 | 3.39105 |
| H | 5.45727 | -0.64014 | 4.71175 |
| H | 7.65538 | -1.71543 | 4.14695 |
| N | 6.22500 | -1.76584 | 1.09769 |
| N | -1.43665 | 0.43247 | -0.25920 |
| C | -2.78602 | 0.49207 | -0.00285 |
| H | -0.99326 | -0.46440 | -0.39776 |
| O | -3.41169 | 1.52605 | 0.14693 |
| N | -3.35910 | -0.76853 | 0.06775 |
| H | -2.75539 | -1.56455 | -0.07012 |
| C | -4.70496 | -1.08262 | 0.30788 |
| C | -5.70588 | -0.12518 | 0.51403 |
| C | -5.04582 | -2.44087 | 0.33597 |
| C | -7.01475 | -0.53576 | 0.74169 |
| H | -5.45655 | 0.92498 | 0.49531 |
| C | -6.35237 | -2.84687 | 0.56334 |
| H | -4.27690 | -3.19276 | 0.17768 |
| C | -7.33566 | -1.88630 | 0.76639 |
| C | -0.32771 | 5.31143 | -0.12434 |
| C | -1.49342 | 5.68390 | -1.05568 |
| H | -2.36200 | 5.04084 | -0.88933 |
| H | -1.19662 | 5.58574 | -2.10448 |
| H | -1.80108 | 6.72037 | -0.87965 |
| C | 0.82415 | 6.28846 | -0.37853 |
| H | 1.16977 | 6.24116 | -1.41620 |
| H | 1.67501 | 6.08723 | 0.28024 |
| H | 0.48606 | 7.31099 | -0.18510 |
| C | -0.77658 | 5.46292 | 1.33868 |
| H | 0.03697 | 5.19780 | 2.02082 |
| H | -1.63098 | 4.81958 | 1.56575 |
| H | -1.07092 | 6.49905 | 1.53783 |
| H | -7.79116 | 0.20417 | 0.90071 |
| H | -6.60708 | -3.90050 | 0.58360 |
| Cl | -8.98418 | -2.38345 | 1.05723 |
| C | 2.23708 | -2.03447 | -1.65477 |
| C | 2.87097 | -2.47301 | -2.81438 |
| C | 1.50510 | -2.94712 | -0.88720 |
| C | 2.77055 | -3.80831 | -3.20582 |
| H | 3.44030 | -1.78226 | -3.42763 |
| C | 1.40177 | -4.27439 | -1.27979 |
| H | 1.02907 | -2.60156 | 0.02758 |
| C | 2.03656 | -4.70857 | -2.44344 |
| H | 3.26724 | -4.13980 | -4.11189 |
| H | 0.83405 | -4.97471 | -0.67559 |
| H | 1.96127 | -5.74668 | -2.75006 |
| O | 0.96520 | -0.16167 | -1.04832 |
| H | 8.05170 | -2.40773 | 1.78119 |
| H | 3.48590 | 2.48726 | -2.16249 |
| H | 3.77628 | 1.77811 | -0.58049 |

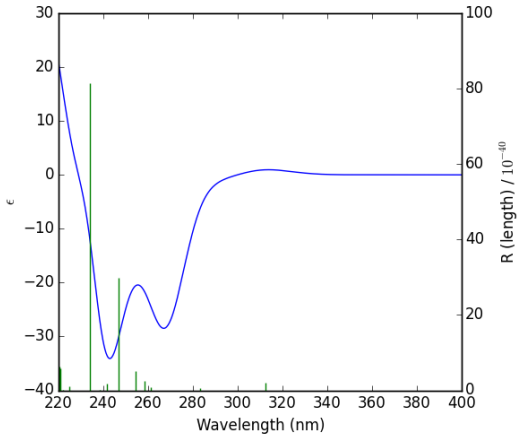
Conformation 9: ΔG: 5.382676089




| | | | |
|---|---|---|---|
| C | 1.35402 | 3.47617 | -0.78502 |
| C | 1.69520 | 2.14208 | -1.00024 |
| C | 0.72951 | 1.16819 | -0.78803 |
| C | -0.56312 | 1.51214 | -0.36826 |
| C | -0.87719 | 2.85332 | -0.15282 |
| C | 0.07990 | 3.85183 | -0.36082 |
| H | 2.11623 | 4.23183 | -0.96053 |
| H | -1.87777 | 3.09315 | 0.17098 |
| C | 2.28152 | -0.62074 | -1.14223 |
| C | 3.05012 | 0.33364 | -2.06416 |
| H | 4.06731 | -0.02933 | -2.23524 |
| H | 2.53047 | 0.34833 | -3.02839 |
| C | 3.07569 | 1.73195 | -1.45059 |
| C | 2.92325 | -0.62305 | 0.27364 |
| O | 2.32255 | -0.22247 | 1.24826 |
| N | 4.20587 | -1.10071 | 0.28443 |
| H | 4.56945 | -1.53018 | -0.55795 |
| C | 5.07901 | -1.23225 | 1.37546 |
| C | 4.78519 | -0.76496 | 2.66205 |
| C | 7.13090 | -2.00636 | 2.00566 |
| C | 5.75389 | -0.95370 | 3.63793 |
| H | 3.83945 | -0.28534 | 2.86743 |
| C | 6.95286 | -1.58471 | 3.31760 |
| H | 5.56791 | -0.60600 | 4.64928 |
| H | 7.72647 | -1.74543 | 4.05889 |
| N | 6.22029 | -1.83772 | 1.04714 |
| N | -1.44639 | 0.43601 | -0.18698 |
| C | -2.79968 | 0.50497 | 0.04526 |
| H | -1.00692 | -0.46508 | -0.30982 |
| O | -3.42578 | 1.54299 | 0.16087 |
| N | -3.37650 | -0.75281 | 0.13806 |
| H | -2.77650 | -1.55268 | 0.00642 |
| C | -4.72952 | -1.05795 | 0.34752 |
| C | -5.72129 | -0.09561 | 0.57410 |
| C | -5.08635 | -2.41224 | 0.32910 |
| C | -7.03761 | -0.49728 | 0.77268 |
| H | -5.45972 | 0.95164 | 0.59062 |
| C | -6.40002 | -2.80949 | 0.52933 |
| H | -4.32445 | -3.16777 | 0.15493 |
| C | -7.37446 | -1.84398 | 0.75043 |
| C | -0.24005 | 5.33486 | -0.14621 |
| C | 0.72545 | 5.92179 | 0.89680 |
| H | 1.76744 | 5.83899 | 0.57462 |
| H | 0.62502 | 5.39925 | 1.85276 |
| H | 0.50726 | 6.98286 | 1.05871 |
| C | -1.67317 | 5.55010 | 0.35051 |
| H | -1.84554 | 5.05233 | 1.30971 |
| H | -2.40938 | 5.17611 | -0.36720 |
| H | -1.85336 | 6.62035 | 0.49039 |
| C | -0.07121 | 6.08705 | -1.47673 |

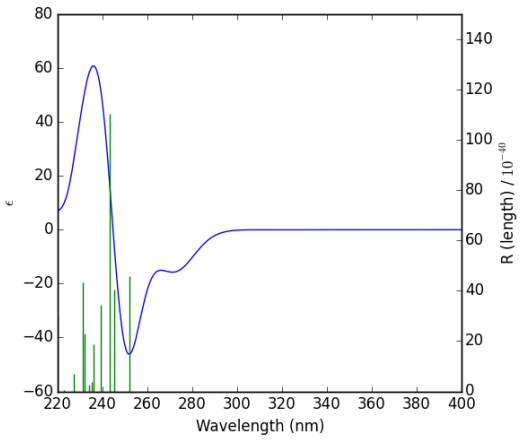
| | | | |
|---|---|---|---|
| H | -0.75519 | 5.69024 | -2.23291 |
| H | 0.94836 | 5.99687 | -1.86283 |
| H | -0.28747 | 7.15219 | -1.34058 |
| H | -7.80731 | 0.24635 | 0.94635 |
| H | -6.66723 | -3.86009 | 0.51398 |
| Cl | -9.03235 | -2.33030 | 1.00567 |
| C | 2.19042 | -2.05885 | -1.63184 |
| C | 2.79866 | -2.50606 | -2.80187 |
| C | 1.46883 | -2.96412 | -0.84589 |
| C | 2.68294 | -3.84251 | -3.18529 |
| H | 3.35962 | -1.82108 | -3.42923 |
| C | 1.35016 | -4.29241 | -1.23031 |
| H | 1.01307 | -2.61197 | 0.07666 |
| C | 1.95927 | -4.73522 | -2.40444 |
| H | 3.15913 | -4.18095 | -4.09975 |
| H | 0.79058 | -4.98682 | -0.61186 |
| H | 1.87195 | -5.77418 | -2.70493 |
| O | 0.94126 | -0.17755 | -1.00727 |
| H | 8.04840 | -2.50496 | 1.70232 |
| H | 3.46185 | 2.45333 | -2.17660 |
| H | 3.76511 | 1.74616 | -0.59582 |

## Conformation 10: ΔG: 4.456616395




| | | | |
|---|---|---|---|
| C | 1.36126 | 3.49309 | -0.79432 |
| C | 1.70636 | 2.15486 | -1.01543 |
| C | 0.74533 | 1.17865 | -0.82159 |
| C | -0.55759 | 1.51454 | -0.41122 |
| C | -0.87383 | 2.84917 | -0.19429 |
| C | 0.08464 | 3.85734 | -0.38482 |
| H | 2.12756 | 4.24427 | -0.95583 |
| H | -1.87806 | 3.09320 | 0.12125 |
| C | 2.30754 | -0.60181 | -1.15740 |
| C | 3.08517 | 0.35701 | -2.06695 |
| H | 4.10665 | 0.00008 | -2.22471 |
| H | 2.57924 | 0.36899 | -3.03846 |
| C | 3.09390 | 1.75534 | -1.45327 |
| C | 2.92256 | -0.60564 | 0.27037 |
| O | 2.29305 | -0.23583 | 1.23901 |
| N | 4.21513 | -1.05469 | 0.29977 |
| H | 4.60567 | -1.46012 | -0.54238 |
| C | 5.06746 | -1.19034 | 1.40663 |
| C | 4.73558 | -0.75849 | 2.69637 |
| C | 7.12211 | -1.93309 | 2.06466 |
| C | 5.68683 | -0.94842 | 3.68913 |
| H | 3.77519 | -0.30391 | 2.89078 |
| C | 6.90630 | -1.54551 | 3.38136 |
| H | 5.47103 | -0.62864 | 4.70376 |
| H | 7.66737 | -1.70594 | 4.13558 |
| N | 6.22881 | -1.76303 | 1.09031 |
| N | -1.43566 | 0.43192 | -0.24872 |
| C | -2.78464 | 0.49270 | 0.00939 |
| H | -0.99131 | -0.46572 | -0.37901 |
| O | -3.41031 | 1.52744 | 0.15378 |
| N | -3.35722 | -0.76754 | 0.08894 |
| H | -2.75629 | -1.56374 | -0.05967 |
| C | -4.70491 | -1.08015 | 0.32056 |
| C | -5.70173 | -0.12262 | 0.54547 |
| C | -5.05142 | -2.43735 | 0.32319 |
| C | -7.01254 | -0.53190 | 0.76409 |
| H | -5.44816 | 0.92671 | 0.54637 |
| C | -6.35973 | -2.84204 | 0.54247 |
| H | -4.28545 | -3.18934 | 0.15155 |
| C | -7.33920 | -1.88133 | 0.76257 |
| C | -0.32478 | 5.31091 | -0.13153 |
| C | -0.76511 | 5.46636 | 1.33370 |
| H | 0.05212 | 5.20215 | 2.01176 |
| H | -1.61875 | 4.82427 | 1.56710 |
| H | -1.05746 | 6.50320 | 1.53211 |
| C | -1.49586 | 5.68119 | -1.05700 |
| H | -2.36381 | 5.03918 | -0.88352 |
| H | -1.20548 | 5.57979 | -2.10729 |
| H | -1.80187 | 6.71834 | -0.88215 |
| C | 0.82572 | 6.28702 | -0.39511 |
| H | 1.16575 | 6.23626 | -1.43448 |
| H | 1.68015 | 6.08794 | 0.25967 |
| H | 0.48877 | 7.31022 | -0.20321 |
| H | -7.78607 | 0.20809 | 0.93634 |
| H | -6.61882 | -3.89481 | 0.54333 |
| Cl | -8.99014 | -2.37685 | 1.04246 |
| C | 2.23258 | -2.04048 | -1.64854 |
| C | 2.86239 | -2.48352 | -2.80867 |
| C | 1.50304 | -2.95011 | -0.87510 |
| C | 2.76038 | -3.82029 | -3.19471 |
| H | 3.42975 | -1.79515 | -3.42645 |
| C | 1.39814 | -4.27884 | -1.26226 |
| H | 1.03028 | -2.60115 | 0.04007 |
| C | 2.02891 | -4.71755 | -2.42639 |
| H | 3.25376 | -4.15532 | -4.10128 |
| H | 0.83234 | -4.97671 | -0.65343 |
| H | 1.95243 | -5.75681 | -2.72883 |
| O | 0.96291 | -0.16520 | -1.04551 |
| H | 8.05710 | -2.40394 | 1.77043 |
| H | 3.48053 | 2.47939 | -2.17652 |
| H | 3.77644 | 1.77587 | -0.59304 |

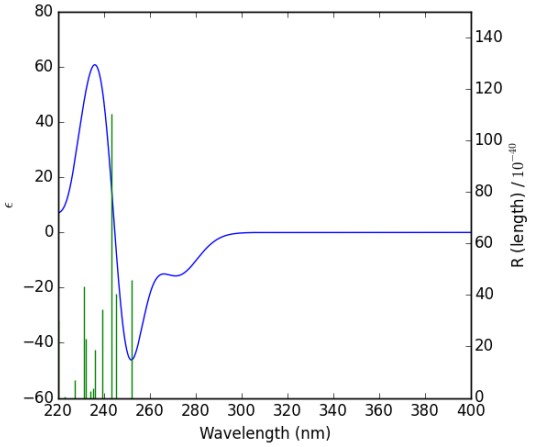
## Conformation 11: ΔG: 0.101499661




| | | | |
|---|---|---|---|
| C | -4.43393 | -0.34354 | 0.28655 |
| C | -3.38318 | 0.51175 | -0.03676 |
| C | -2.20049 | -0.03859 | -0.53413 |
| C | -2.08872 | -1.42496 | -0.69000 |
| C | -3.15492 | -2.25116 | -0.35053 |

| | | | |
|---|---|---|---|
| C | -4.35336 | -1.72999 | 0.13994 |
| H | -5.35228 | 0.10683 | 0.65707 |
| H | -3.02160 | -3.32119 | -0.47236 |
| C | -1.14831 | 2.11702 | -0.76846 |
| C | -2.56311 | 2.67596 | -0.92816 |
| H | -2.52356 | 3.75478 | -0.77364 |
| H | -2.88324 | 2.47978 | -1.95690 |
| C | -3.50474 | 2.01085 | 0.07081 |
| C | -0.59809 | 2.49864 | 0.62976 |
| O | -0.89840 | 3.57729 | 1.12124 |
| N | 0.25472 | 1.59281 | 1.16810 |
| H | 0.38181 | 0.69706 | 0.69365 |
| C | 1.01192 | 1.73111 | 2.33988 |
| C | 0.84168 | 2.78156 | 3.25187 |
| C | 2.67868 | 0.79280 | 3.59262 |
| C | 1.65891 | 2.79454 | 4.37260 |
| H | 0.09906 | 3.54385 | 3.07001 |
| C | 2.59932 | 1.78600 | 4.56088 |
| H | 1.55471 | 3.59281 | 5.10088 |
| H | 3.24942 | 1.76698 | 5.42752 |
| N | 1.91278 | 0.75873 | 2.50300 |
| N | -0.90254 | -1.96812 | -1.24349 |
| C | 0.31265 | -1.78574 | -0.60424 |
| H | -1.01553 | -2.78068 | -1.83187 |
| O | 0.41517 | -1.17850 | 0.44655 |
| N | 1.37284 | -2.33907 | -1.28142 |
| H | 1.18851 | -2.72248 | -2.19627 |
| C | 2.72709 | -2.32686 | -0.89129 |
| C | 3.21698 | -1.59123 | 0.19469 |
| C | 3.61077 | -3.08601 | -1.66565 |
| C | 4.57773 | -1.63136 | 0.48209 |
| H | 2.55837 | -0.98836 | 0.80812 |
| C | 4.96730 | -3.11781 | -1.37671 |
| H | 3.23311 | -3.66309 | -2.50603 |
| C | 5.44486 | -2.38671 | -0.29636 |
| C | -5.54769 | -2.61008 | 0.51767 |
| C | -5.88358 | -2.40238 | 2.00375 |
| H | -6.14178 | -1.36099 | 2.21540 |
| H | -5.03143 | -2.67272 | 2.63422 |
| H | -6.73777 | -3.02544 | 2.28922 |
| C | -5.25905 | -4.09750 | 0.29269 |
| H | -4.41551 | -4.43949 | 0.90079 |
| H | -5.03956 | -4.31064 | -0.75857 |
| H | -6.13551 | -4.68768 | 0.57570 |
| C | -6.76252 | -2.21778 | -0.33987 |
| H | -6.54821 | -2.35948 | -1.40352 |
| H | -7.03983 | -1.17095 | -0.18774 |
| H | -7.62722 | -2.83601 | -0.07647 |
| H | 4.96502 | -1.05638 | 1.31622 |
| H | 5.64718 | -3.70677 | -1.98159 |
| Cl | 7.14994 | -2.41660 | 0.07808 |
| C | -0.20504 | 2.69855 | -1.81800 |
| C | 0.32920 | 1.89728 | -2.82626 |
| C | 0.10293 | 4.06171 | -1.78529 |
| C | 1.15830 | 2.45732 | -3.79549 |
| H | 0.09442 | 0.83945 | -2.84701 |
| C | 0.93088 | 4.61457 | -2.75579 |
| H | -0.29423 | 4.68004 | -0.98552 |
| C | 1.46008 | 3.81450 | -3.76551 |
| H | 1.57129 | 1.82586 | -4.57594 |
| H | 1.16648 | 5.67340 | -2.71977 |
| H | 2.10852 | 4.24661 | -4.52092 |
| O | -1.12704 | 0.70283 | -0.93599 |
| H | 3.39399 | -0.02105 | 3.69181 |
| H | -4.53967 | 2.31099 | -0.11809 |
| H | -3.25156 | 2.34902 | 1.08266 |

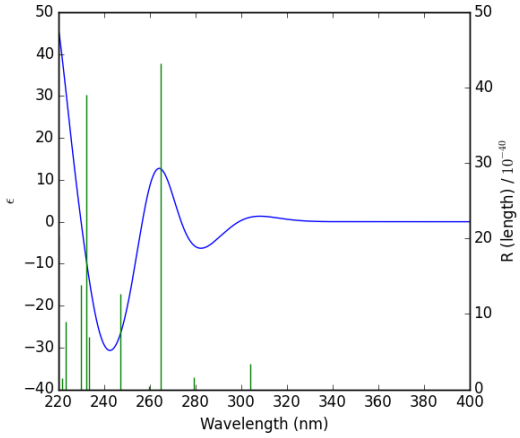
## Conformation 12: ΔG: 0.0




| | | | |
|---|---|---|---|
| C | -4.44709 | -0.30116 | 0.30332 |
| C | -3.38493 | 0.54632 | -0.02822 |
| C | -2.21086 | -0.01027 | -0.52614 |
| C | -2.10710 | -1.40204 | -0.68103 |
| C | -3.17635 | -2.21353 | -0.33821 |
| C | -4.37484 | -1.68305 | 0.15717 |
| H | -5.35518 | 0.16287 | 0.67534 |
| H | -3.05982 | -3.28816 | -0.45687 |
| C | -1.14289 | 2.13493 | -0.76750 |
| C | -2.55397 | 2.70351 | -0.92689 |
| H | -2.50665 | 3.78233 | -0.77445 |
| H | -2.87601 | 2.50770 | -1.95509 |
| C | -3.49986 | 2.04644 | 0.07342 |
| C | -0.58960 | 2.51401 | 0.63014 |
| O | -0.88249 | 3.59493 | 1.12089 |
| N | 0.25790 | 1.60321 | 1.16882 |
| H | 0.37947 | 0.70659 | 0.69485 |
| C | 1.01655 | 1.73788 | 2.34002 |
| C | 0.85155 | 2.78919 | 3.25202 |
| C | 2.67955 | 0.79219 | 3.59214 |
| C | 1.66940 | 2.79871 | 4.37228 |
| H | 0.11226 | 3.55476 | 3.07055 |
| C | 2.60533 | 1.78593 | 4.56021 |
| H | 1.56915 | 3.59759 | 5.10046 |
| H | 3.25589 | 1.76412 | 5.42644 |
| N | 1.91293 | 0.76134 | 2.50285 |
| N | -0.92621 | -1.95079 | -1.24002 |
| C | 0.29136 | -1.77536 | -0.60220 |
| H | -1.04584 | -2.76547 | -1.82415 |
| O | 0.39776 | -1.17188 | 0.45031 |
| N | 1.34748 | -2.33096 | -1.28326 |
| H | 1.15964 | -2.70880 | -2.19974 |
| C | 2.70210 | -2.32980 | -0.89388 |
| C | 3.19786 | -1.60068 | 0.19378 |
| C | 3.57960 | -3.09351 | -1.67074 |
| C | 4.55831 | -1.65218 | 0.48070 |
| H | 2.54423 | -0.99412 | 0.80887 |
| C | 4.93595 | -3.13645 | -1.38243 |
| H | 3.19708 | -3.66532 | -2.51253 |
| C | 5.41933 | -2.41213 | -0.30010 |
| C | -5.52445 | -2.62703 | 0.51730 |
| C | -6.75237 | -1.86638 | 1.02628 |
| H | -7.13970 | -1.17511 | 0.27115 |
| H | -6.52451 | -1.29755 | 1.93299 |
| H | -7.54798 | -2.57726 | 1.26830 |
| C | -5.06251 | -3.59322 | 1.62090 |
| H | -4.76138 | -3.04138 | 2.51613 |
| H | -4.21068 | -4.19860 | 1.29748 |

| | | | |
|---|---|---|---|
| H | -5.87620 | -4.27455 | 1.89122 |
| C | -5.93576 | -3.43251 | -0.72633 |
| H | -5.10660 | -4.03522 | -1.10836 |
| H | -6.26721 | -2.76583 | -1.52813 |
| H | -6.75802 | -4.11275 | -0.48074 |
| H | 4.95043 | -1.08251 | 1.31624 |
| H | 5.61113 | -3.72885 | -1.98918 |
| Cl | 7.12422 | -2.45601 | 0.07382 |
| C | -0.19584 | 2.70845 | -1.81790 |
| C | 0.33331 | 1.90203 | -2.82478 |
| C | 0.12140 | 4.06954 | -1.78723 |
| C | 1.16654 | 2.45491 | -3.79459 |
| H | 0.09128 | 0.84577 | -2.84398 |
| C | 0.95340 | 4.61525 | -2.75827 |
| H | -0.27177 | 4.69179 | -0.98855 |
| C | 1.47755 | 3.81004 | -3.76656 |
| H | 1.57548 | 1.81943 | -4.57391 |
| H | 1.19620 | 5.67251 | -2.72384 |
| H | 2.12928 | 4.23655 | -4.52231 |
| O | -1.13204 | 0.72050 | -0.93343 |
| H | 3.39111 | -0.02496 | 3.69116 |
| H | -4.53309 | 2.35020 | -0.11941 |
| H | -3.24811 | 2.38824 | 1.08439 |

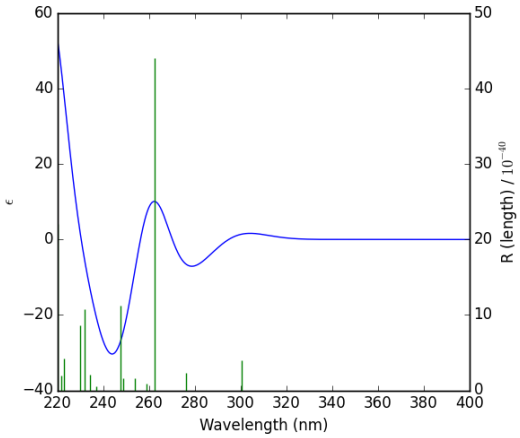
## Conformation 13: ΔG: 4.702731895




| | | | |
|---|---|---|---|
| C | -0.67008 | 3.98210 | -0.75258 |
| C | -1.34802 | 2.76332 | -0.73898 |
| C | -0.60811 | 1.60485 | -0.55005 |
| C | 0.78708 | 1.64242 | -0.41084 |
| C | 1.43955 | 2.87372 | -0.42701 |
| C | 0.71313 | 4.05910 | -0.59056 |
| H | -1.25244 | 4.88865 | -0.90051 |
| H | 2.51175 | 2.88235 | -0.30884 |
| C | -2.55296 | 0.26084 | -0.29059 |
| C | -3.26390 | 1.23481 | -1.24618 |
| H | -4.34864 | 1.11103 | -1.19220 |
| H | -2.95233 | 0.95362 | -2.25762 |
| C | -2.84284 | 2.67145 | -0.93471 |
| C | -2.89783 | -1.19106 | -0.71883 |
| O | -2.17123 | -1.80879 | -1.46949 |
| N | -4.09508 | -1.64679 | -0.24484 |
| H | -4.57836 | -1.11044 | 0.46545 |
| C | -4.73968 | -2.85733 | -0.54289 |
| C | -4.23145 | -3.80805 | -1.43643 |
| C | -6.59552 | -4.11024 | -0.10022 |
| C | -4.98727 | -4.95383 | -1.63885 |
| H | -3.28814 | -3.64017 | -1.93358 |
| C | -6.19355 | -5.12141 | -0.96462 |
| H | -4.62880 | -5.71538 | -2.32430 |
| H | -6.80456 | -6.00577 | -1.10126 |
| N | -5.89274 | -2.99833 | 0.11222 |

| | | | |
|---|---|---|---|
| N | 1.40561 | 0.38713 | -0.28737 |
| C | 2.74680 | 0.13980 | -0.09969 |
| H | 0.77217 | -0.38768 | -0.43340 |
| O | 3.58230 | 1.00402 | 0.09445 |
| N | 3.03518 | -1.21448 | -0.14633 |
| H | 2.28465 | -1.84252 | -0.39175 |
| C | 4.29106 | -1.82323 | 0.00130 |
| C | 5.45413 | -1.13257 | 0.36244 |
| C | 4.35846 | -3.20459 | -0.21825 |
| C | 6.65302 | -1.82482 | 0.49306 |
| H | 5.41589 | -0.06703 | 0.53195 |
| C | 5.55549 | -3.89236 | -0.08460 |
| H | 3.46137 | -3.75029 | -0.49923 |
| C | 6.70318 | -3.19438 | 0.27091 |
| C | 1.40102 | 5.42857 | -0.61265 |
| C | 0.82462 | 6.30717 | 0.50990 |
| H | -0.25118 | 6.46278 | 0.38776 |
| H | 0.99019 | 5.84396 | 1.48716 |
| H | 1.30873 | 7.28971 | 0.50724 |
| C | 2.91488 | 5.31763 | -0.40678 |
| H | 3.15715 | 4.85343 | 0.55405 |
| H | 3.38841 | 4.73118 | -1.19993 |
| H | 3.35897 | 6.31771 | -0.41925 |
| C | 1.14496 | 6.10423 | -1.97009 |
| H | 1.54134 | 5.49287 | -2.78637 |
| H | 0.07655 | 6.25561 | -2.14933 |
| H | 1.63403 | 7.08365 | -2.00376 |
| C | -2.85278 | 0.51994 | 1.18532 |
| C | -4.10833 | 0.96076 | 1.61583 |
| C | -1.85958 | 0.28042 | 2.13796 |
| C | -4.36996 | 1.14258 | 2.97167 |
| H | -4.89264 | 1.17790 | 0.89458 |
| C | -2.11924 | 0.47056 | 3.49096 |
| H | -0.87729 | -0.04244 | 1.80859 |
| C | -3.37556 | 0.89785 | 3.91277 |
| H | -5.34994 | 1.48414 | 3.28829 |
| H | -1.33514 | 0.28722 | 4.21833 |
| H | -3.57619 | 1.04542 | 4.96876 |
| Cl | 8.21772 | -4.04777 | 0.43826 |
| H | 7.55563 | -1.29195 | 0.77047 |
| H | 5.59898 | -4.96182 | -0.25676 |
| O | -1.15919 | 0.34452 | -0.52227 |
| H | -7.52895 | -4.19078 | 0.45178 |
| H | -3.35459 | 3.02522 | -0.03204 |
| H | -3.14794 | 3.33206 | -1.75227 |

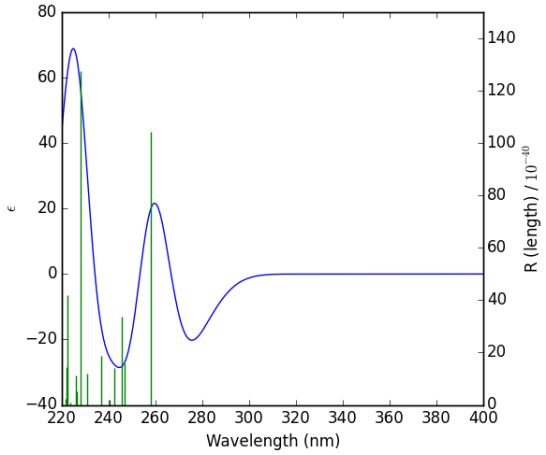
## Conformation 14: ΔG: 4.267190102




| | | | |
|---|---|---|---|
| C | -0.64890 | 3.99432 | -0.76907 |
| C | -1.33514 | 2.77363 | -0.75332 |

| | | | |
|---|---|---|---|
| C | -0.60813 | 1.61329 | -0.55737 |
| C | 0.79140 | 1.63906 | -0.41213 |
| C | 1.44702 | 2.86239 | -0.43058 |
| C | 0.72938 | 4.05828 | -0.60233 |
| H | -1.23026 | 4.89780 | -0.92223 |
| H | 2.52091 | 2.87195 | -0.30908 |
| C | -2.56263 | 0.28553 | -0.29739 |
| C | -3.26118 | 1.25944 | -1.26226 |
| H | -4.34712 | 1.14467 | -1.21273 |
| H | -2.94710 | 0.96964 | -2.27050 |
| C | -2.82933 | 2.69430 | -0.95762 |
| C | -2.91756 | -1.16637 | -0.71691 |
| O | -2.19167 | -1.79725 | -1.45733 |
| N | -4.12230 | -1.60668 | -0.24754 |
| H | -4.60501 | -1.05979 | 0.45502 |
| C | -4.77785 | -2.81257 | -0.54005 |
| C | -4.27500 | -3.77589 | -1.42298 |
| C | -6.65006 | -4.04119 | -0.09811 |
| C | -5.04254 | -4.91475 | -1.62080 |
| H | -3.32688 | -3.62228 | -1.91570 |
| C | -6.25447 | -5.06353 | -0.95227 |
| H | -4.68886 | -5.68575 | -2.29814 |
| H | -6.87461 | -5.94203 | -1.08544 |
| N | -5.93616 | -2.93555 | 0.10946 |
| N | 1.39639 | 0.37855 | -0.27979 |
| C | 2.73652 | 0.12172 | -0.09671 |
| H | 0.75563 | -0.39118 | -0.42102 |
| O | 3.57897 | 0.98150 | 0.08719 |
| N | 3.01442 | -1.23476 | -0.13445 |
| H | 2.25825 | -1.85877 | -0.37284 |
| C | 4.26679 | -1.85154 | 0.01078 |
| C | 5.43470 | -1.16792 | 0.36947 |
| C | 4.32499 | -3.23345 | -0.20770 |
| C | 6.62948 | -1.86752 | 0.49843 |
| H | 5.40352 | -0.10204 | 0.53825 |
| C | 5.51790 | -3.92863 | -0.07546 |
| H | 3.42404 | -3.77367 | -0.48688 |
| C | 6.67059 | -3.23754 | 0.27728 |
| C | 1.50633 | 5.37816 | -0.61087 |
| C | 2.23596 | 5.54734 | 0.73223 |
| H | 1.52070 | 5.57095 | 1.56011 |
| H | 2.93715 | 4.72842 | 0.91445 |
| H | 2.80209 | 6.48496 | 0.73838 |
| C | 2.53838 | 5.35618 | -1.75073 |
| H | 3.25796 | 4.54229 | -1.62747 |
| H | 2.04388 | 5.22670 | -2.71825 |
| H | 3.09643 | 6.29843 | -1.77198 |
| C | 0.58809 | 6.58622 | -0.81699 |
| H | 0.06262 | 6.53275 | -1.77589 |
| H | -0.15552 | 6.66853 | -0.01785 |
| H | 1.18452 | 7.50339 | -0.81404 |
| C | -2.86711 | 0.55684 | 1.17552 |
| C | -4.12129 | 1.00982 | 1.59720 |
| C | -1.88033 | 0.31583 | 2.13442 |
| C | -4.38813 | 1.20161 | 2.95065 |
| H | -4.90042 | 1.22863 | 0.87086 |
| C | -2.14505 | 0.51602 | 3.48498 |
| H | -0.89883 | -0.01602 | 1.81168 |
| C | -3.40023 | 0.95502 | 3.89808 |
| H | -5.36711 | 1.55215 | 3.26051 |
| H | -1.36575 | 0.33142 | 4.21718 |
| H | -3.60494 | 1.11031 | 4.95216 |
| Cl | 8.18026 | -4.10011 | 0.44199 |
| H | 7.53592 | -1.34016 | 0.77384 |
| H | 5.55439 | -4.99848 | -0.24683 |
| O | -1.16702 | 0.35692 | -0.52278 |
| H | -7.58730 | -4.10706 | 0.44933 |
| H | -3.34416 | 3.05988 | -0.06132 |
| H | -3.12285 | 3.35147 | -1.78227 |

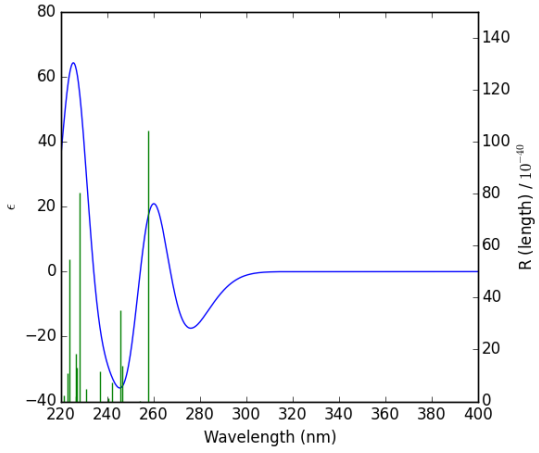
## Conformation 15: ΔG: 4.769003174




| | | | |
|---|---|---|---|
| C | -4.35680 | -0.55539 | 0.01425 |
| C | -3.36737 | 0.36991 | -0.30759 |
| C | -2.11494 | -0.10311 | -0.70913 |
| C | -1.88820 | -1.48143 | -0.79271 |
| C | -2.89861 | -2.37824 | -0.46079 |
| C | -4.15648 | -1.93629 | -0.04918 |
| H | -5.32656 | -0.16602 | 0.31666 |
| H | -2.67270 | -3.43735 | -0.52712 |
| C | -1.21395 | 2.11559 | -0.88337 |
| C | -2.63791 | 2.57190 | -1.20653 |
| H | -2.69347 | 3.65229 | -1.06875 |
| H | -2.83034 | 2.34090 | -2.25966 |
| C | -3.63069 | 1.85587 | -0.29548 |
| C | -0.87813 | 2.50288 | 0.58417 |
| O | -1.30846 | 3.54386 | 1.03863 |
| N | -0.07030 | 1.60503 | 1.21692 |
| H | 0.09892 | 0.72123 | 0.73985 |
| C | 0.49267 | 1.72701 | 2.49605 |
| C | 0.93272 | 0.55117 | 3.12666 |
| C | 1.16958 | 3.01818 | 4.23998 |
| C | 1.52257 | 0.66624 | 4.37368 |
| H | 0.80215 | -0.40708 | 2.63572 |
| C | 1.64446 | 1.92723 | 4.95613 |
| H | 1.87590 | -0.22049 | 4.89108 |
| H | 2.09468 | 2.06169 | 5.93276 |
| N | 0.61171 | 2.93666 | 3.03019 |
| N | -0.64657 | -1.96122 | -1.28685 |
| C | 0.54441 | -1.70699 | -0.64911 |
| H | -0.68848 | -2.70983 | -1.96189 |
| O | 0.61523 | -1.08089 | 0.39876 |
| N | 1.63875 | -2.21726 | -1.30744 |
| H | 1.47991 | -2.65668 | -2.20156 |
| C | 2.98128 | -2.19095 | -0.88171 |
| C | 3.44831 | -1.38738 | 0.16385 |
| C | 3.88187 | -3.00668 | -1.57432 |
| C | 4.79616 | -1.41925 | 0.50494 |
| H | 2.76786 | -0.74415 | 0.70222 |
| C | 5.22761 | -3.02949 | -1.23818 |
| H | 3.52573 | -3.63734 | -2.38478 |
| C | 5.67870 | -2.23399 | -0.19187 |
| C | -5.29050 | -2.89144 | 0.33066 |
| C | -5.67881 | -2.65747 | 1.80010 |
| H | -6.01539 | -1.63044 | 1.96737 |
| H | -4.82633 | -2.84415 | 2.45990 |
| H | -6.49338 | -3.33054 | 2.08809 |
| C | -4.88474 | -4.35933 | 0.16645 |
| H | -4.03909 | -4.61903 | 0.81115 |
| H | -4.61619 | -4.58836 | -0.87004 |
| H | -5.72440 | -5.00359 | 0.44291 |
| C | -6.50977 | -2.62457 | -0.56739 |

| | | | |
|---|---|---|---|
| H | -6.25850 | -2.78203 | -1.62066 |
| H | -6.87555 | -1.59999 | -0.45716 |
| H | -7.32828 | -3.30233 | -0.30307 |
| H | 5.16171 | -0.79653 | 1.31374 |
| H | 5.92080 | -3.66288 | -1.77975 |
| Cl | 7.36648 | -2.25935 | 0.24495 |
| C | -0.19364 | 2.78197 | -1.79794 |
| C | 0.51233 | 2.04928 | -2.75183 |
| C | 0.01762 | 4.16000 | -1.69373 |
| C | 1.41491 | 2.69152 | -3.59639 |
| H | 0.35382 | 0.97976 | -2.82738 |
| C | 0.91906 | 4.79495 | -2.53979 |
| H | -0.51048 | 4.72363 | -0.93038 |
| C | 1.62007 | 4.06324 | -3.49559 |
| H | 1.96166 | 2.11377 | -4.33523 |
| H | 1.07885 | 5.86440 | -2.44681 |
| H | 2.32563 | 4.55945 | -4.15435 |
| H | 1.24724 | 4.02175 | 4.65264 |
| O | -1.08066 | 0.70641 | -1.07546 |
| H | -4.65785 | 2.04649 | -0.62086 |
| H | -3.53484 | 2.25522 | 0.72038 |

## Conformation 16: ΔG: 4.785343521




| | | | |
|---|---|---|---|
| C | -4.36619 | -0.53523 | -0.02746 |
| C | -3.36784 | 0.38732 | -0.35461 |
| C | -2.11410 | -0.08663 | -0.73435 |
| C | -1.88355 | -1.46988 | -0.80034 |
| C | -2.89451 | -2.35673 | -0.46601 |
| C | -4.16159 | -1.91129 | -0.06902 |
| H | -5.33456 | -0.13567 | 0.25753 |
| H | -2.67458 | -3.42035 | -0.51409 |
| C | -1.20852 | 2.12684 | -0.90534 |
| C | -2.62507 | 2.58450 | -1.25806 |
| H | -2.68229 | 3.66539 | -1.12502 |
| H | -2.79570 | 2.35066 | -2.31433 |
| C | -3.63746 | 1.87230 | -0.36580 |
| C | -0.90361 | 2.51124 | 0.56975 |
| O | -1.34581 | 3.54958 | 1.01878 |
| N | -0.10621 | 1.61400 | 1.21628 |
| H | 0.07605 | 0.73223 | 0.74054 |
| C | 0.42405 | 1.73216 | 2.50977 |
| C | 0.83760 | 0.55338 | 3.15237 |
| C | 1.06266 | 3.01914 | 4.27105 |
| C | 1.39356 | 0.66451 | 4.41531 |
| H | 0.71303 | -0.40388 | 2.65798 |
| C | 1.50891 | 1.92480 | 5.00045 |
| H | 1.72558 | -0.22452 | 4.94277 |
| H | 1.93355 | 2.05625 | 5.98886 |
| N | 0.53795 | 2.94124 | 3.04630 |
| N | -0.63916 | -1.95257 | -1.28440 |
| C | 0.54867 | -1.69440 | -0.64201 |
| H | -0.67766 | -2.70502 | -1.95527 |
| O | 0.61370 | -1.06608 | 0.40483 |
| N | 1.64583 | -2.20497 | -1.29513 |
| H | 1.49080 | -2.63811 | -2.19300 |
| C | 2.98693 | -2.18070 | -0.86520 |
| C | 3.44731 | -1.40180 | 0.20175 |
| C | 3.89326 | -2.97521 | -1.57504 |
| C | 4.79443 | -1.43644 | 0.54567 |
| H | 2.76248 | -0.77527 | 0.75400 |
| C | 5.23796 | -3.00107 | -1.23531 |
| H | 3.54279 | -3.58638 | -2.40276 |
| C | 5.68271 | -2.22975 | -0.16838 |
| C | -5.24035 | -2.93190 | 0.30144 |
| C | -4.76049 | -3.76241 | 1.50355 |
| H | -4.57048 | -3.11825 | 2.36706 |
| H | -3.83653 | -4.30227 | 1.27647 |
| H | -5.52113 | -4.49952 | 1.78216 |
| C | -5.49734 | -3.86550 | -0.89270 |
| H | -4.59624 | -4.41857 | -1.17366 |
| H | -5.83127 | -3.29653 | -1.76560 |
| H | -6.27220 | -4.59689 | -0.64027 |
| C | -6.56182 | -2.25575 | 0.67790 |
| H | -6.96119 | -1.66396 | -0.15181 |
| H | -6.44464 | -1.60054 | 1.54655 |
| H | -7.30336 | -3.01880 | 0.93245 |
| H | 5.15470 | -0.83292 | 1.37122 |
| H | 5.93526 | -3.61790 | -1.79052 |
| Cl | 7.36929 | -2.25834 | 0.27273 |
| C | -0.16843 | 2.79353 | -1.79652 |
| C | 0.55825 | 2.06202 | -2.73558 |
| C | 0.04096 | 4.17130 | -1.68548 |
| C | 1.47949 | 2.70522 | -3.55899 |
| H | 0.40111 | 0.99264 | -2.81599 |
| C | 0.96115 | 4.80721 | -2.51028 |
| H | -0.50389 | 4.73409 | -0.93332 |
| C | 1.68282 | 4.07672 | -3.45155 |
| H | 2.04239 | 2.12823 | -4.28622 |
| H | 1.11932 | 5.87643 | -2.41203 |
| H | 2.40300 | 4.57377 | -4.09360 |
| H | 1.13705 | 4.02234 | 4.68523 |
| O | -1.07406 | 0.71769 | -1.09689 |
| H | -4.65641 | 2.05417 | -0.72099 |
| H | -3.57143 | 2.28255 | 0.64812 |

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