A cleft type receptor which combines an oxyanion hole with electrostatic interactions

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

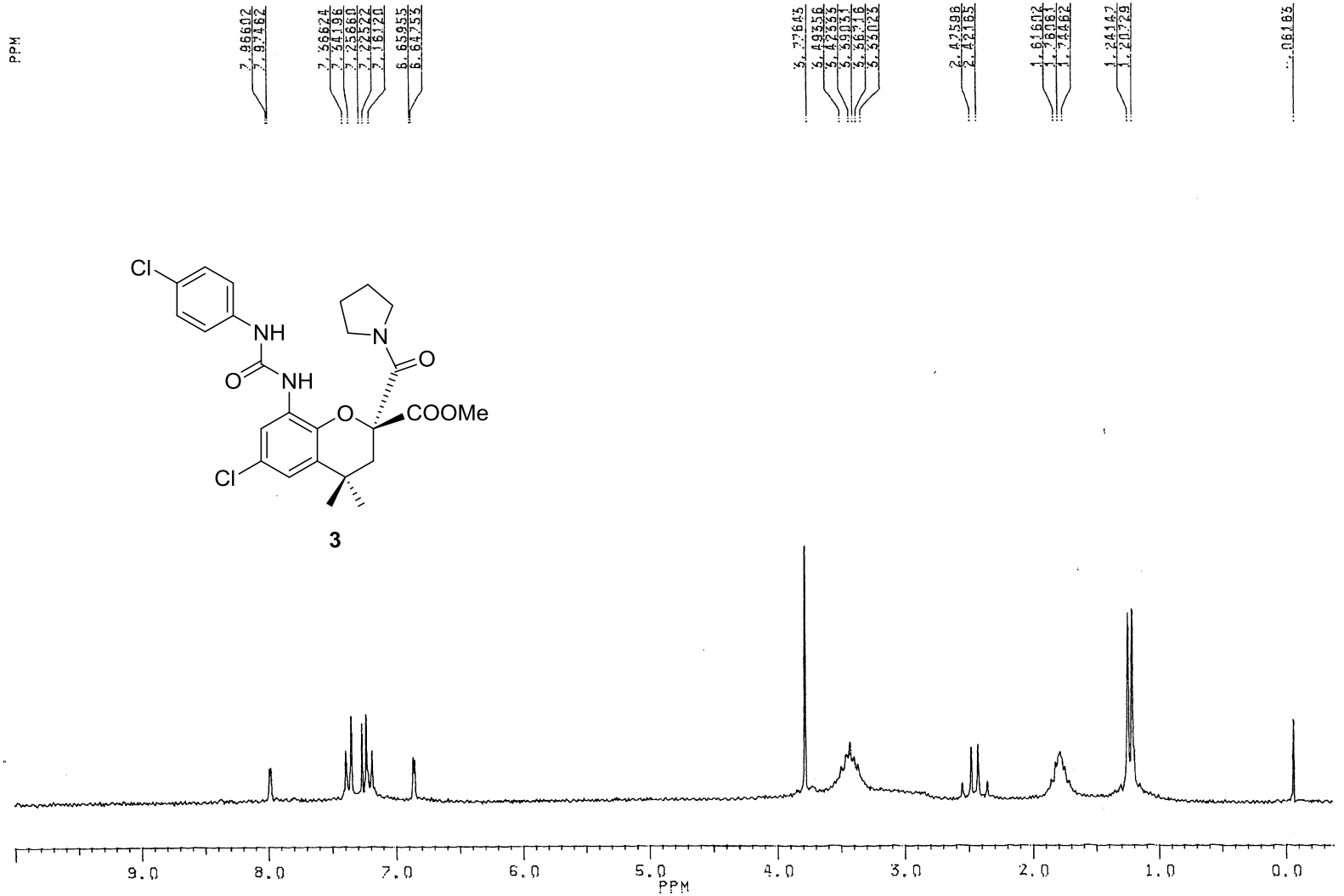


Figure S2. ^{13}C NMR spectrum of compound 3 (100 MHz, $CDCl_3$).

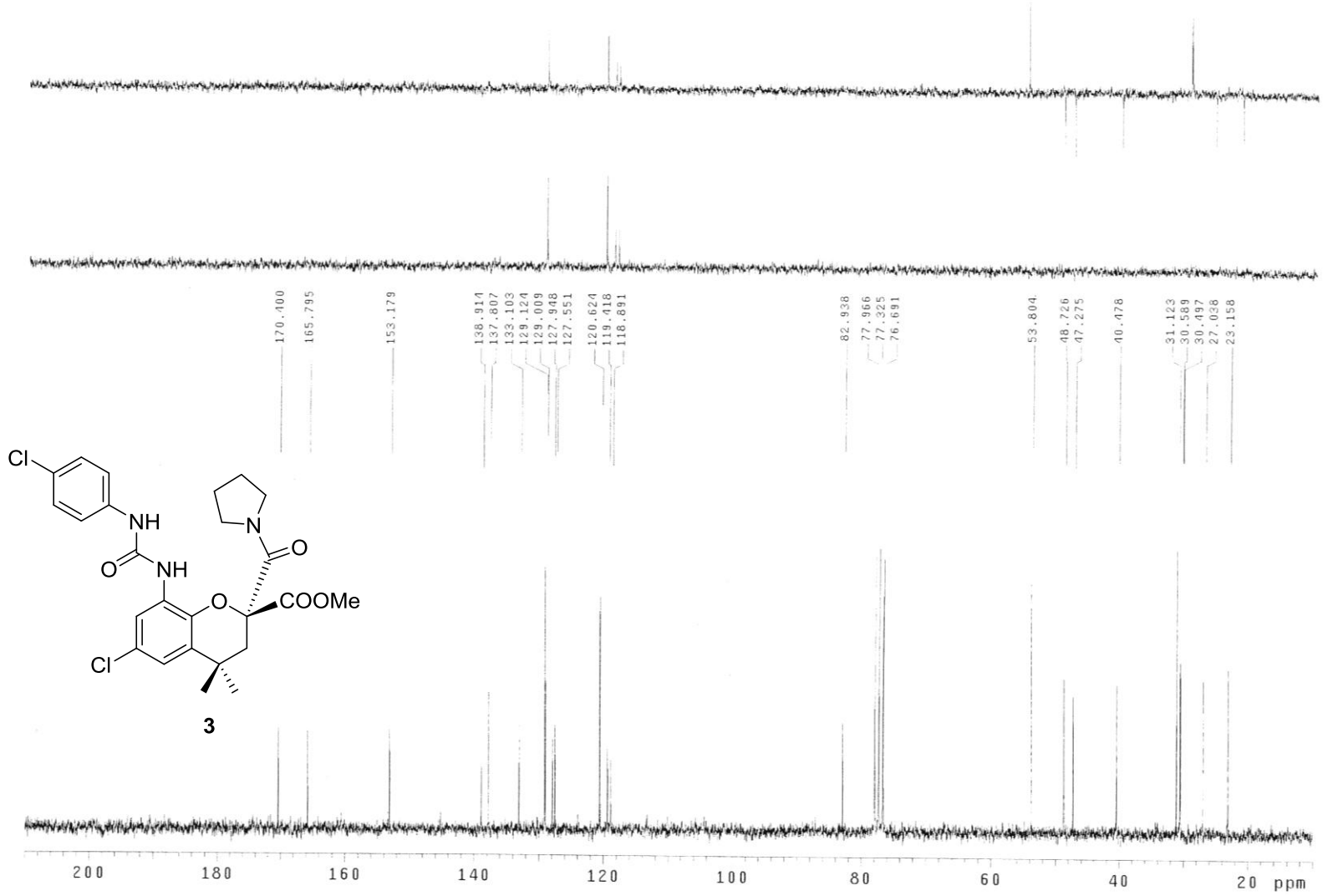


Figure S3. IR spectrum of compound 3.

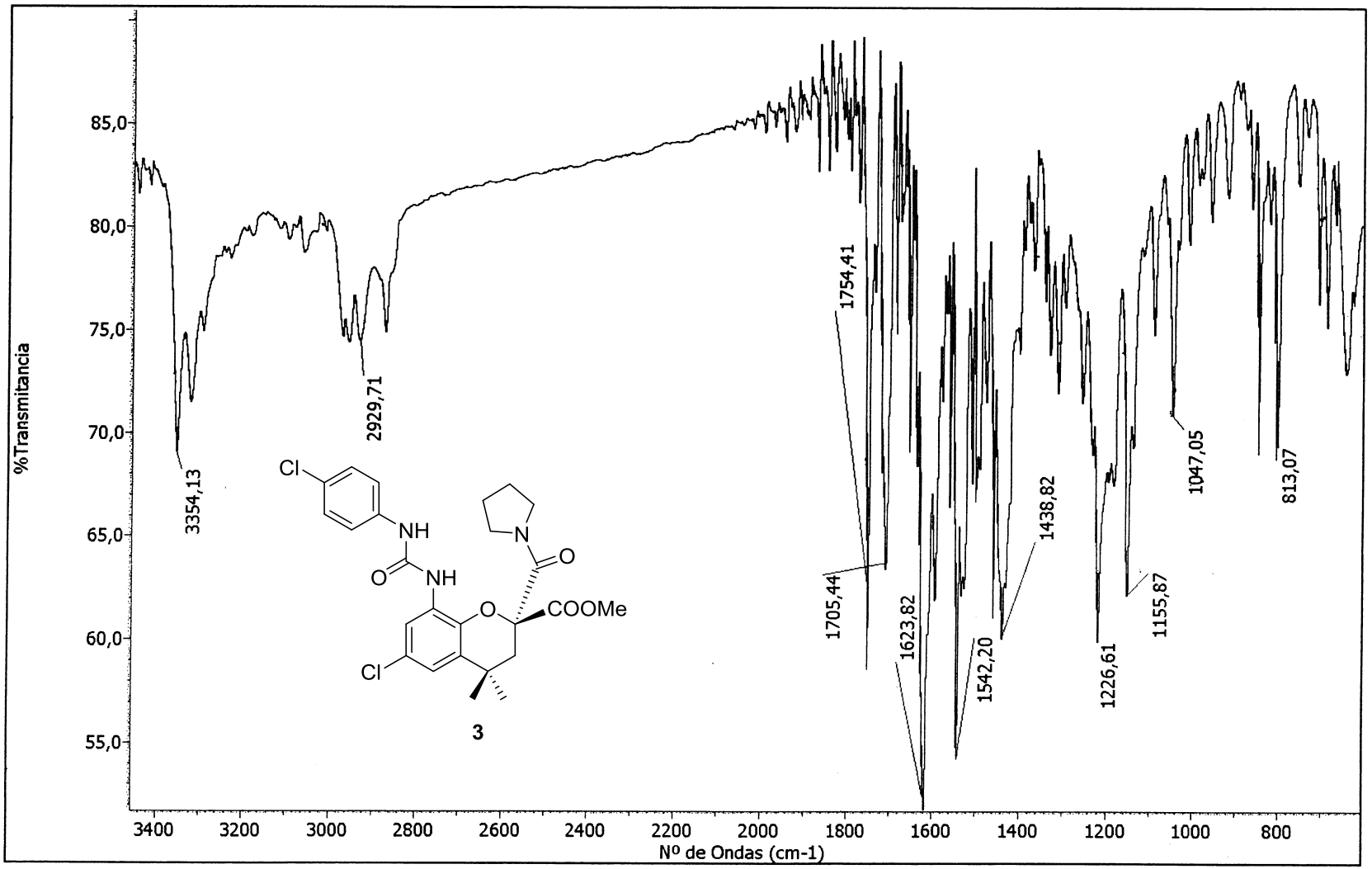


Figure S4. HRMS spectrum of compound 3 (ESI-QTOF).

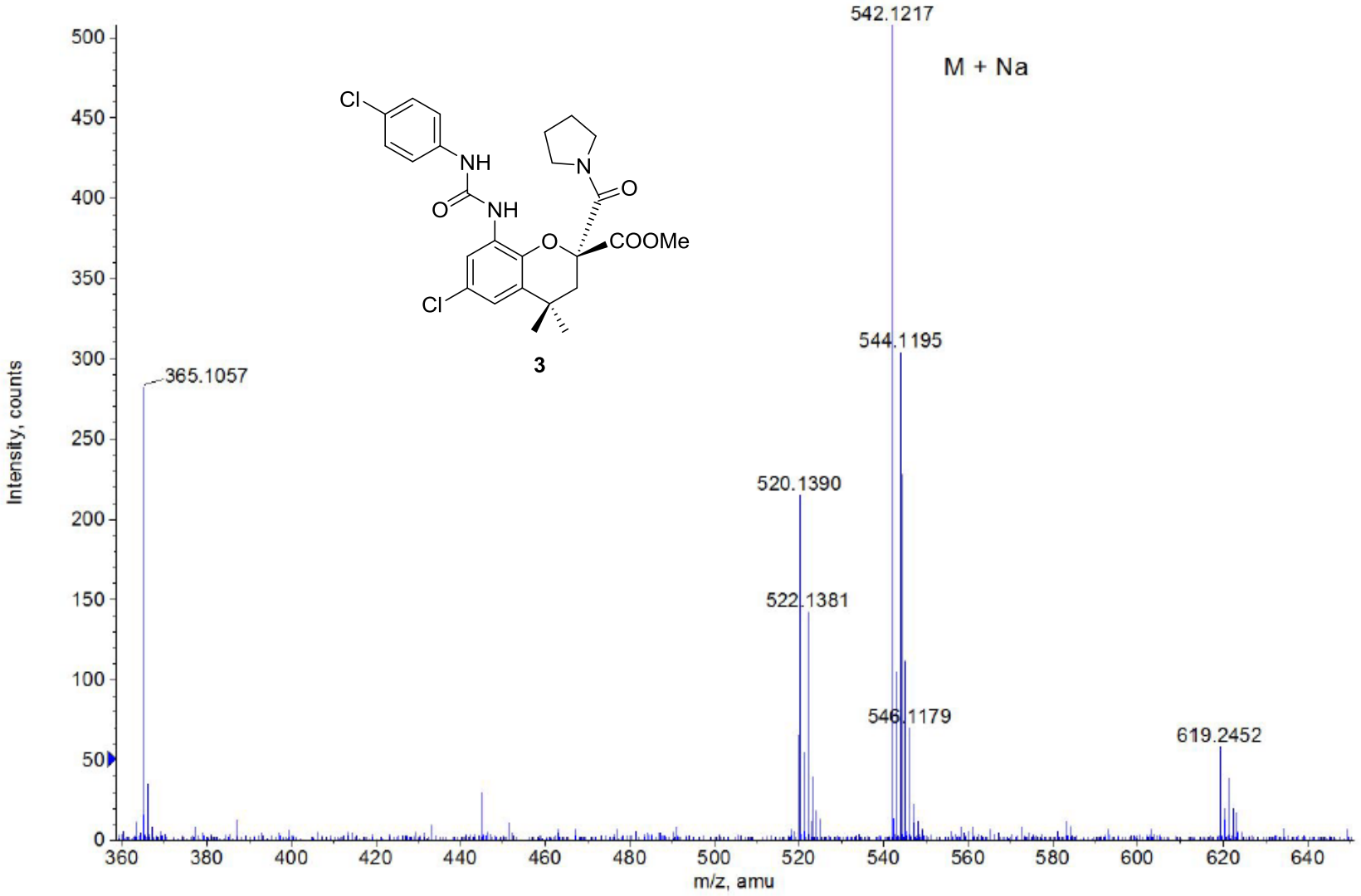


Figure S5. ^{1}H NMR spectrum of receptor 1 (200 MHz, $CDCl_3$).

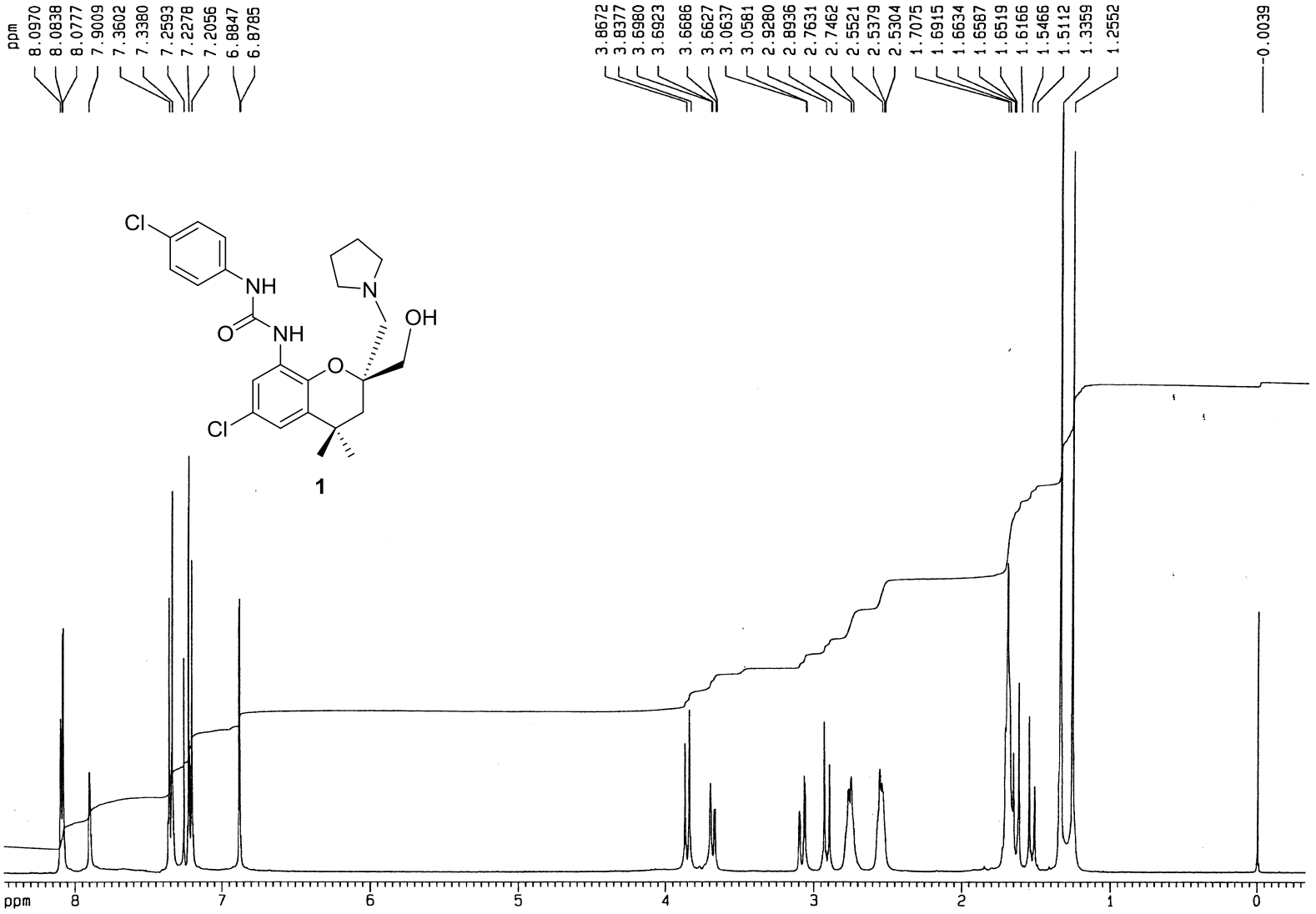


Figure S6. ^{13}C NMR spectrum of receptor 1 (100 MHz, $CDCl_3$).

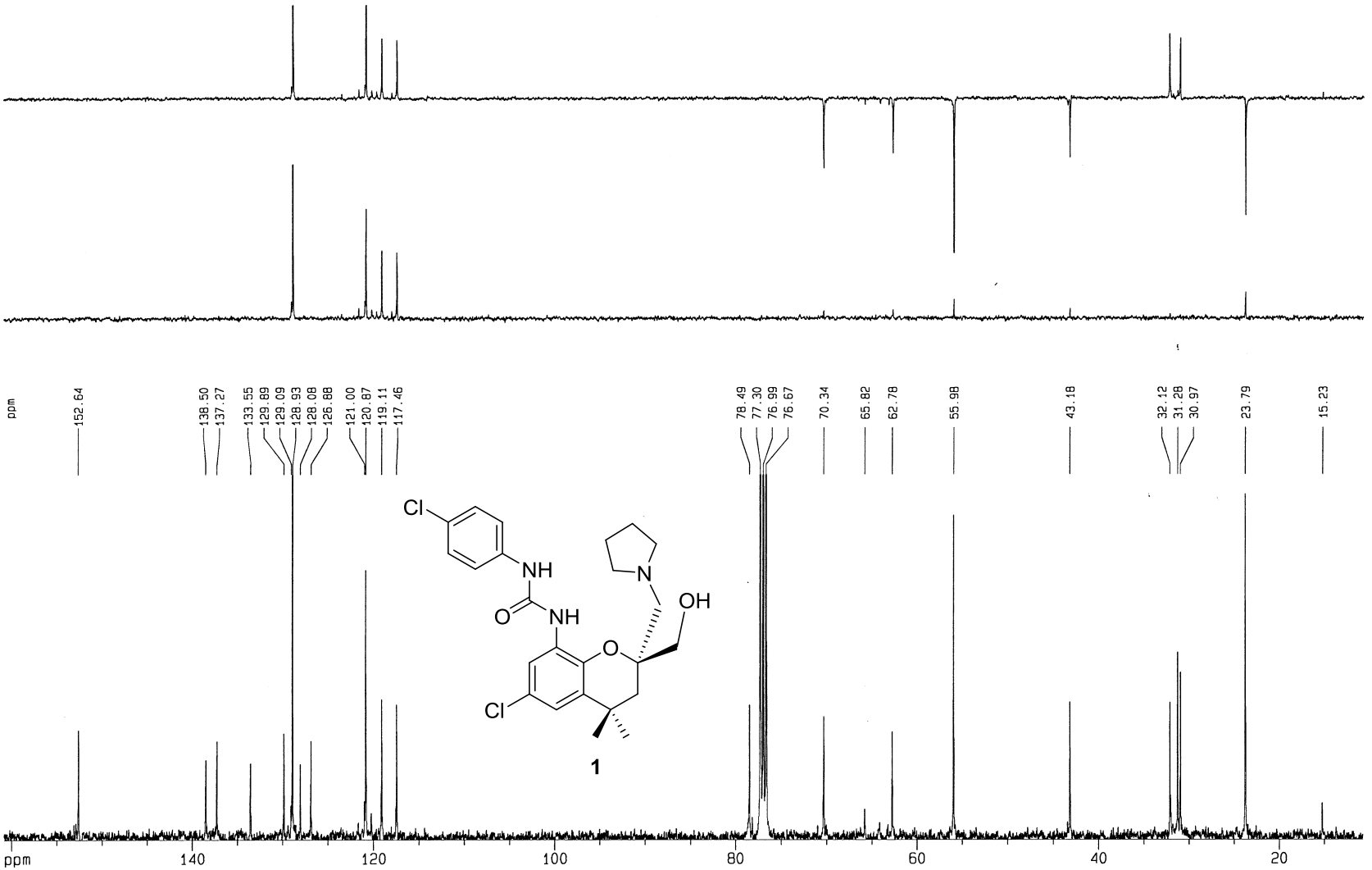


Figure S7. IR spectrum of receptor 1.

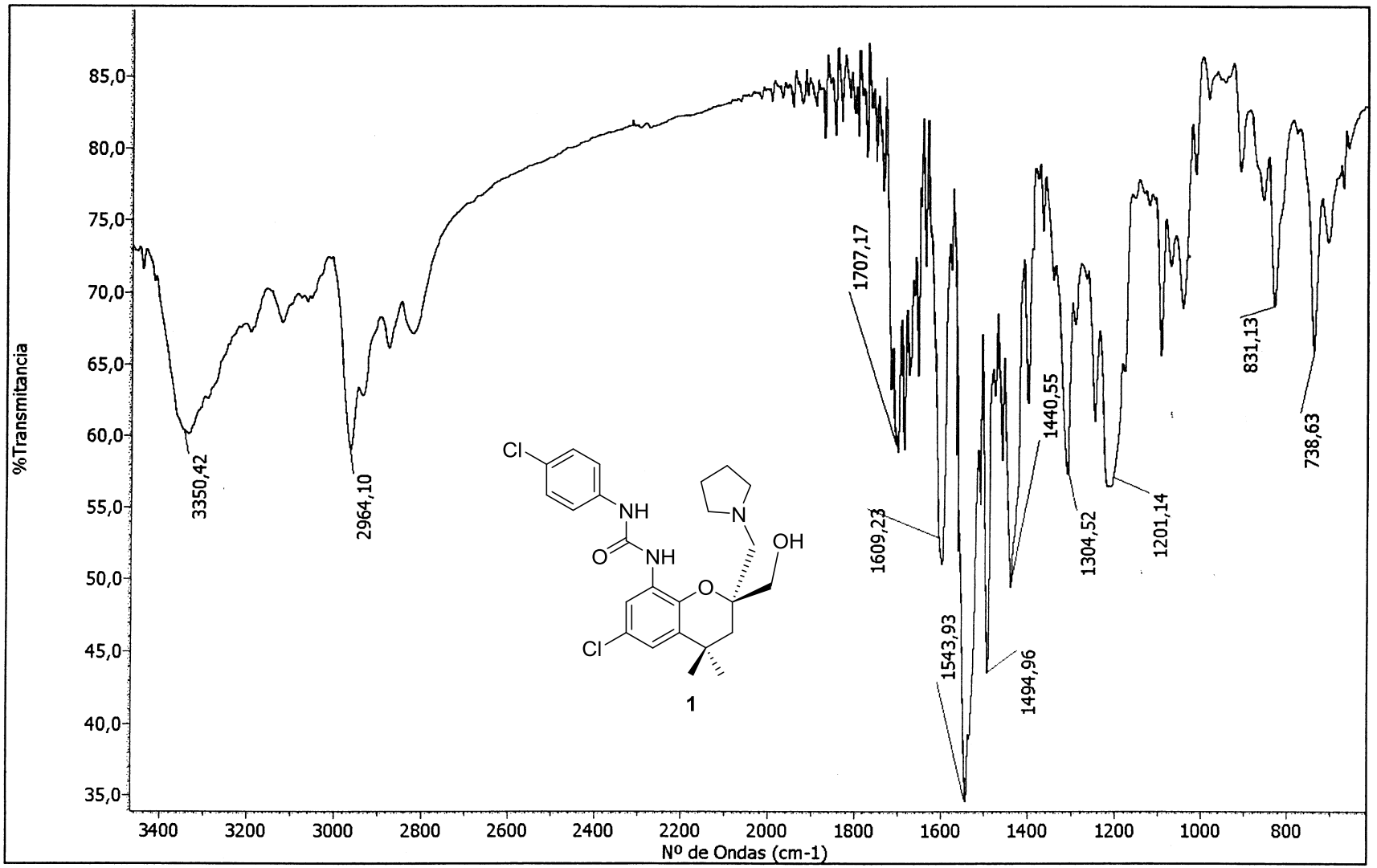


Figure S8. HRMS spectrum of receptor 1 (ESI-QTOF).

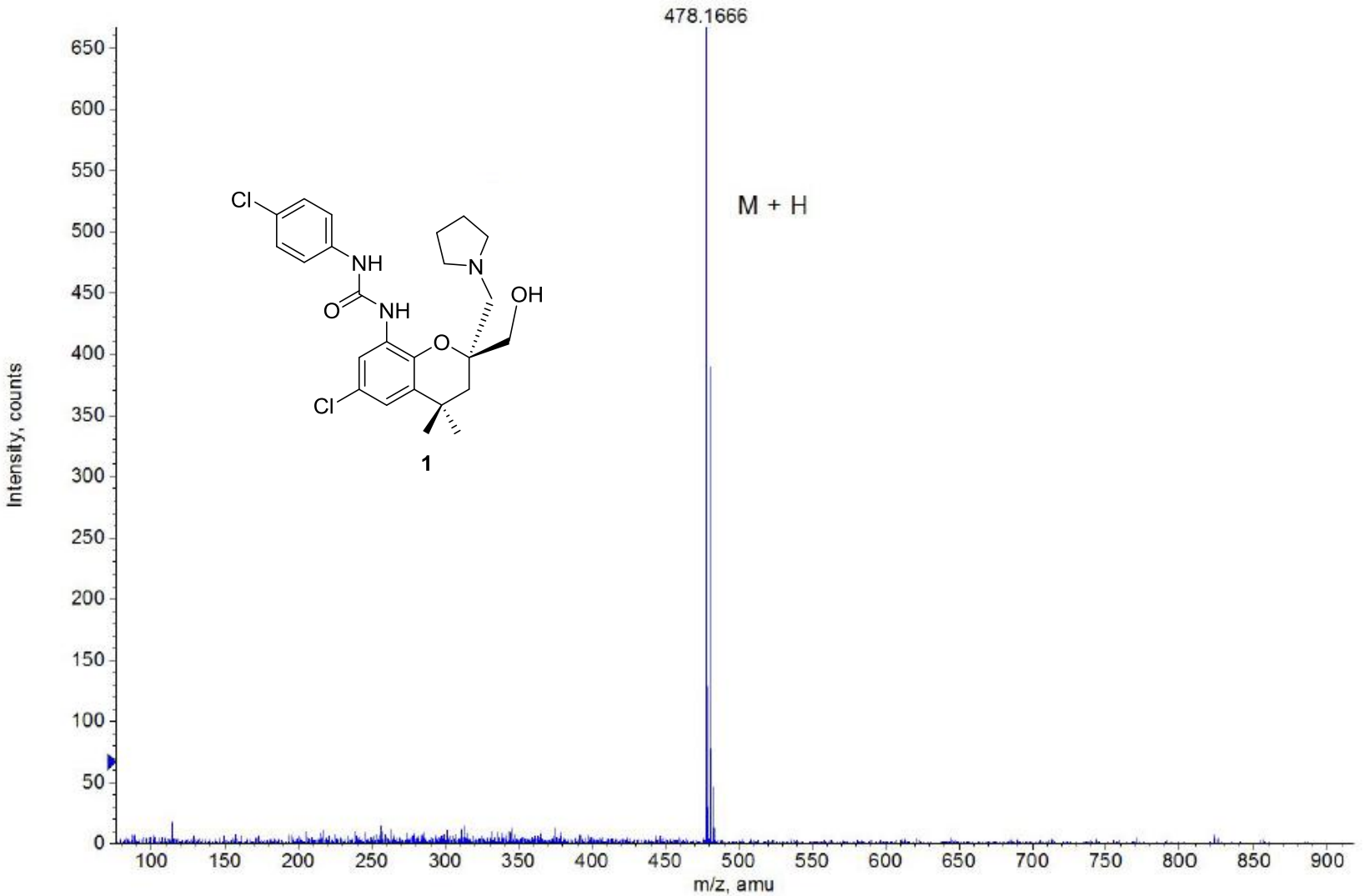


Figure S9. COSY spectrum of receptor 1 ($CDCl_3$).

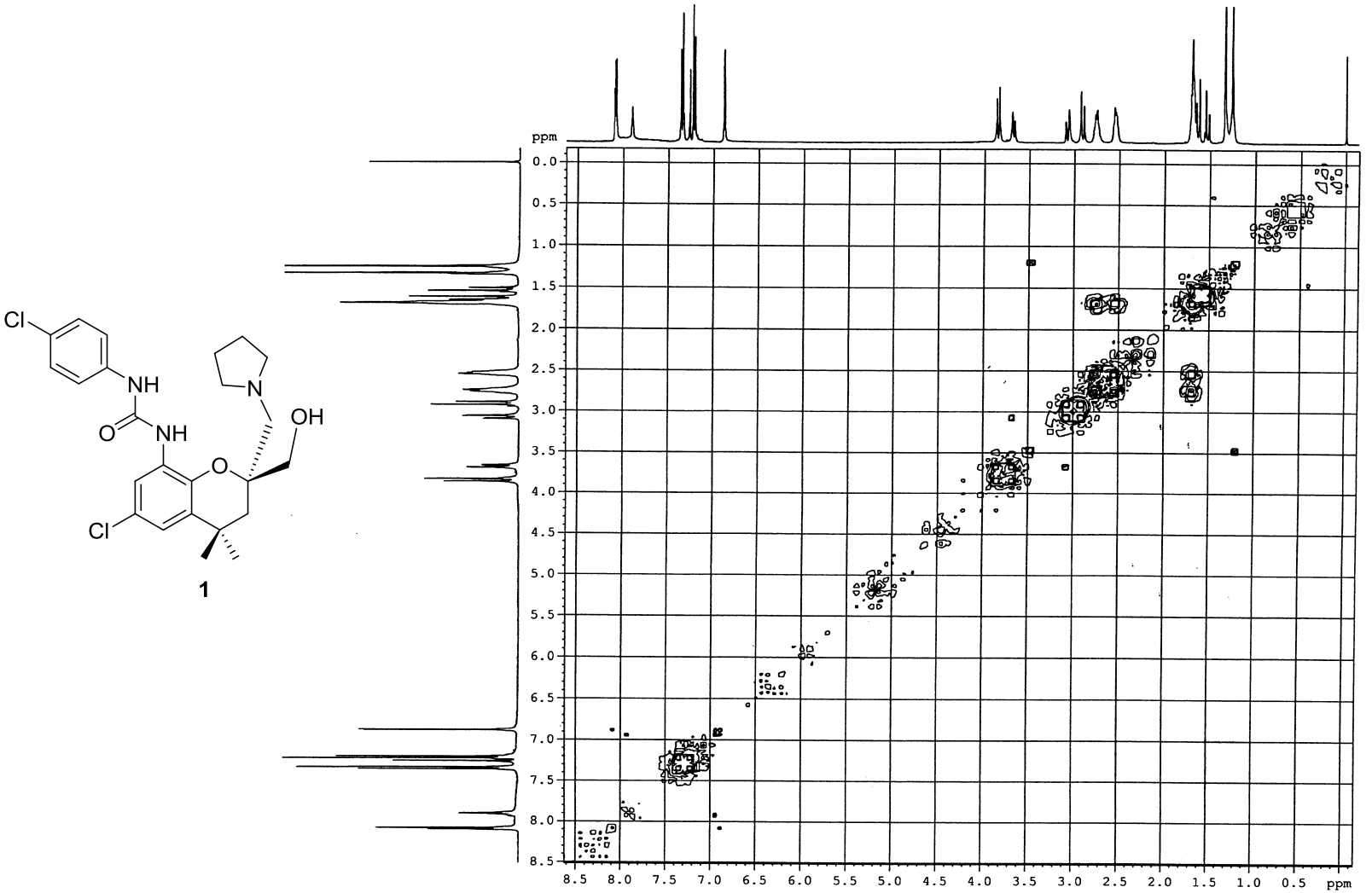


Figure S10. ROESY spectrum of receptor 1 ($CDCl_3$).

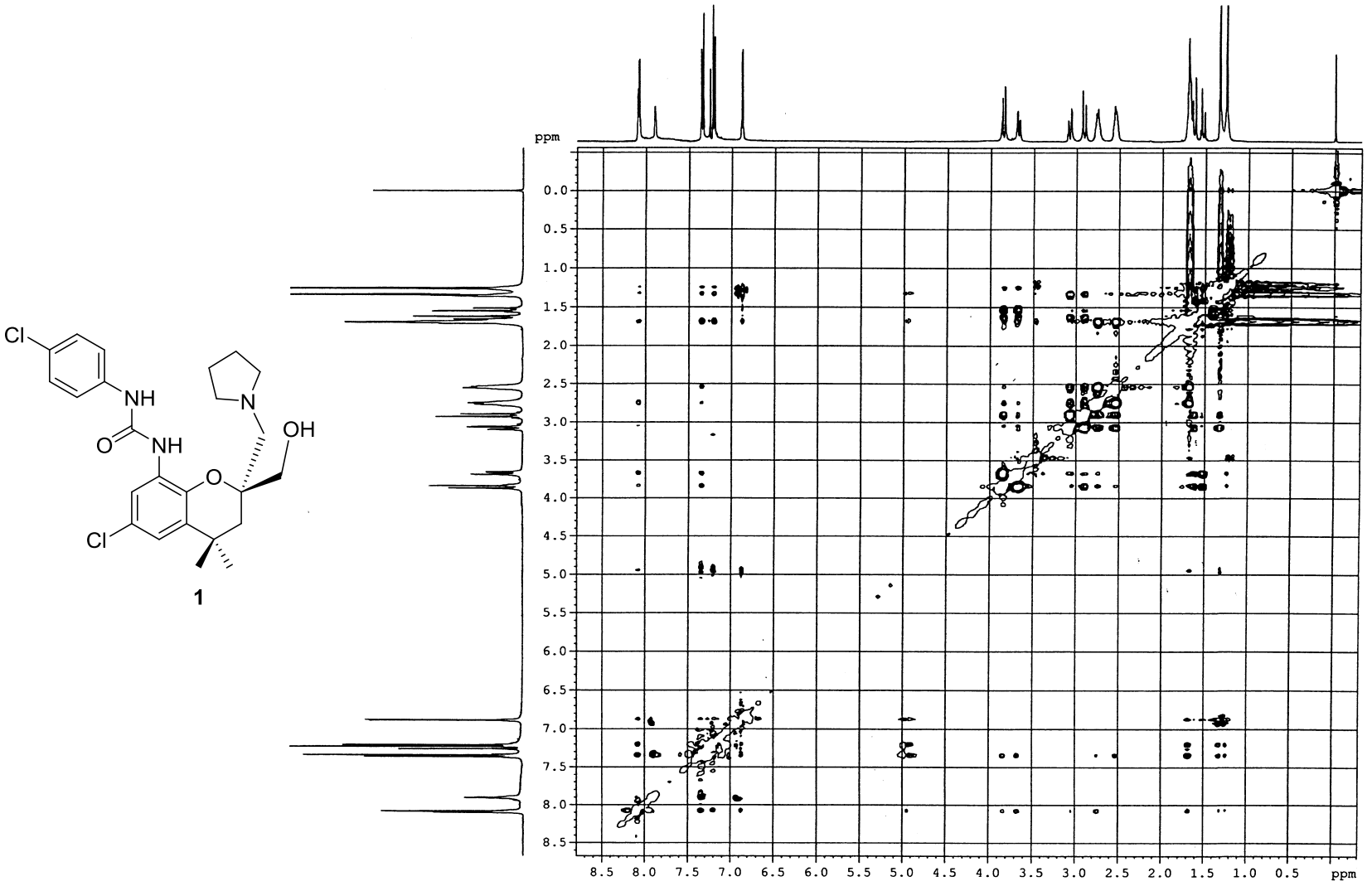


Figure S11. HMBC spectrum of receptor 1 ($CDCl_3$).

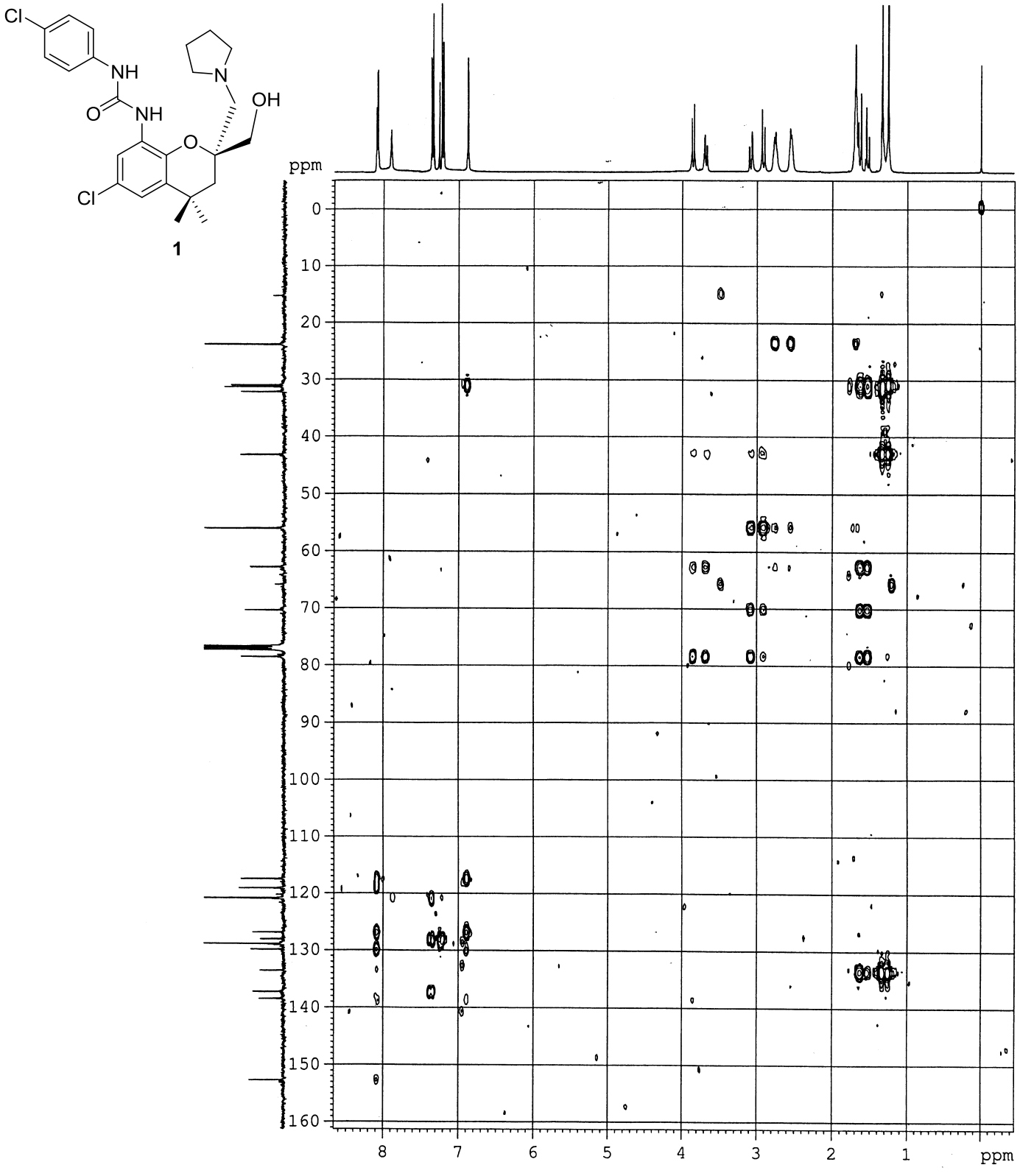
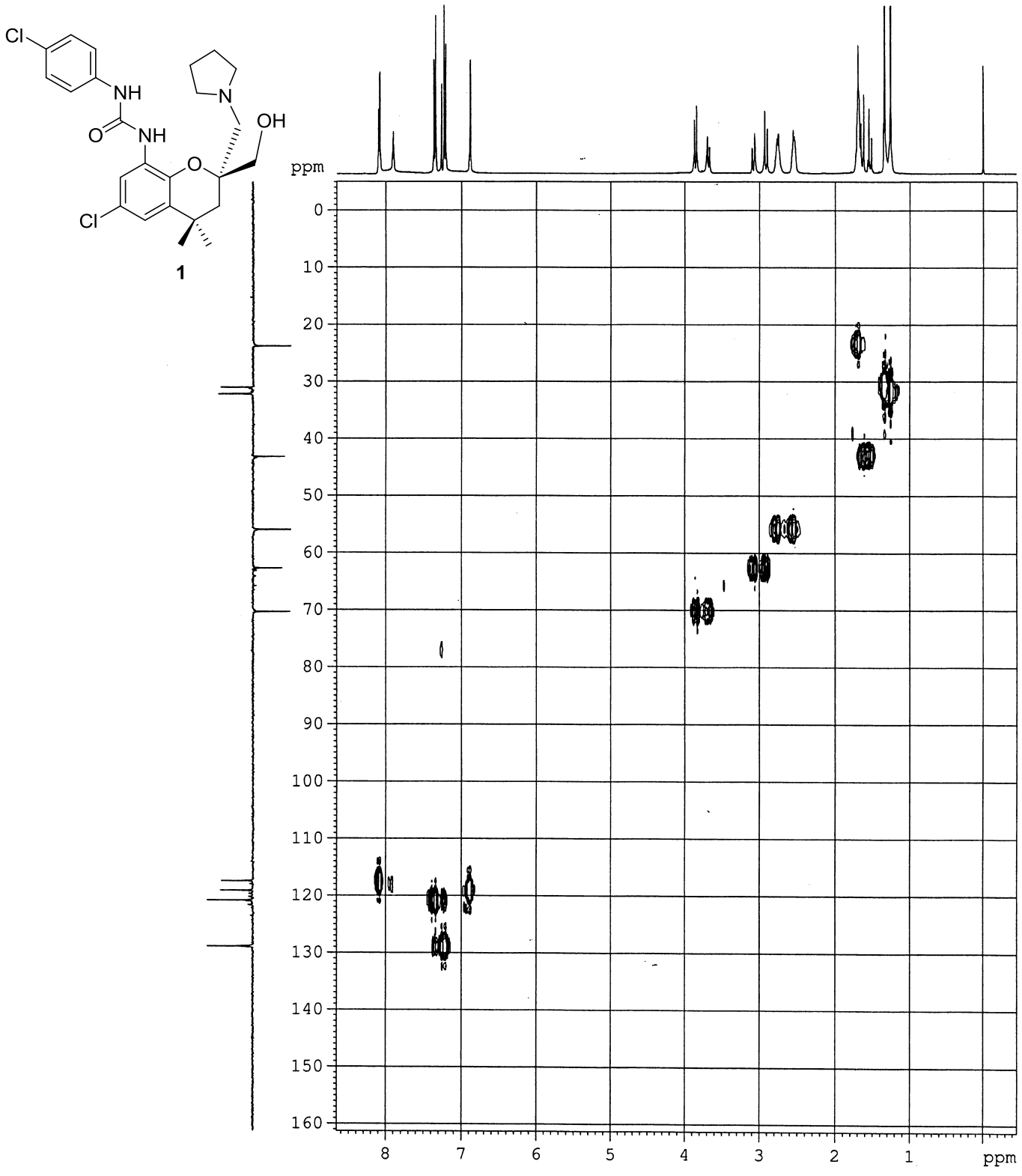


Figure S12. HMQC spectrum of receptor 1 ($CDCl_3$).



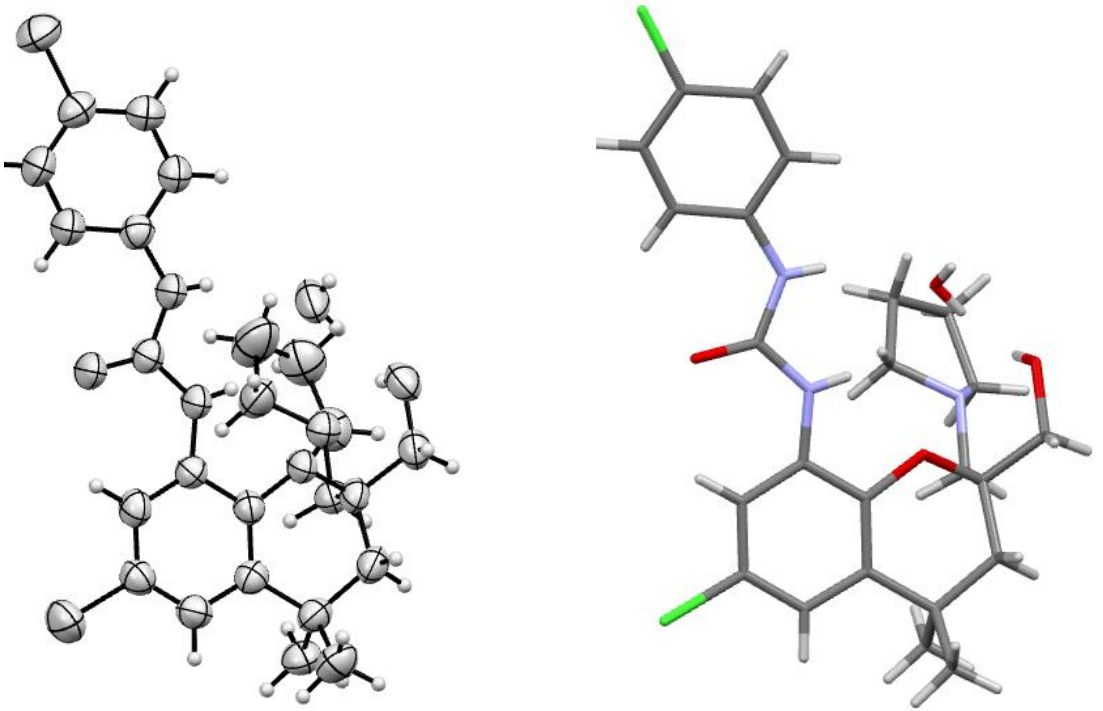
Chiral resolution experimental procedure.

By ^{1}H-NMR we were able to screen carboxylic acids which lead to a strong splitting of the receptor signals, corresponding to associates with well-defined, highly populated and different geometries, that could be easily separable. The best results were obtained with hydroxy acids, probably because the hydroxyl moiety constitutes new binding points that collaborates with the expected oxyanion hole interactions in a more rigid structure. Since the substituents cannot average their chemical shifts, very different signals for the two diastereomeric complexes showed up.

Therefore, an equimolecular mixture of racemic compound **1** and the corresponding chiral guest was dissolved in chloroform and methanol or water was slowly added through diffusion from a container with this solvent. This procedure yielded a first crop of crystals, whose ^{1}H-NMR spectrum showed a single diastereomeric complex in the case of using (*L*)-mandelic acid as guest and a 1:1 mixture of complexes in the rest of the cases. The free compound **1** can be obtained by extraction with CH_2Cl_2 from a 4% aqueous Na_2CO_3 solution of the complex, and their enantiomer can be isolated from the mother liquor following a similar procedure.

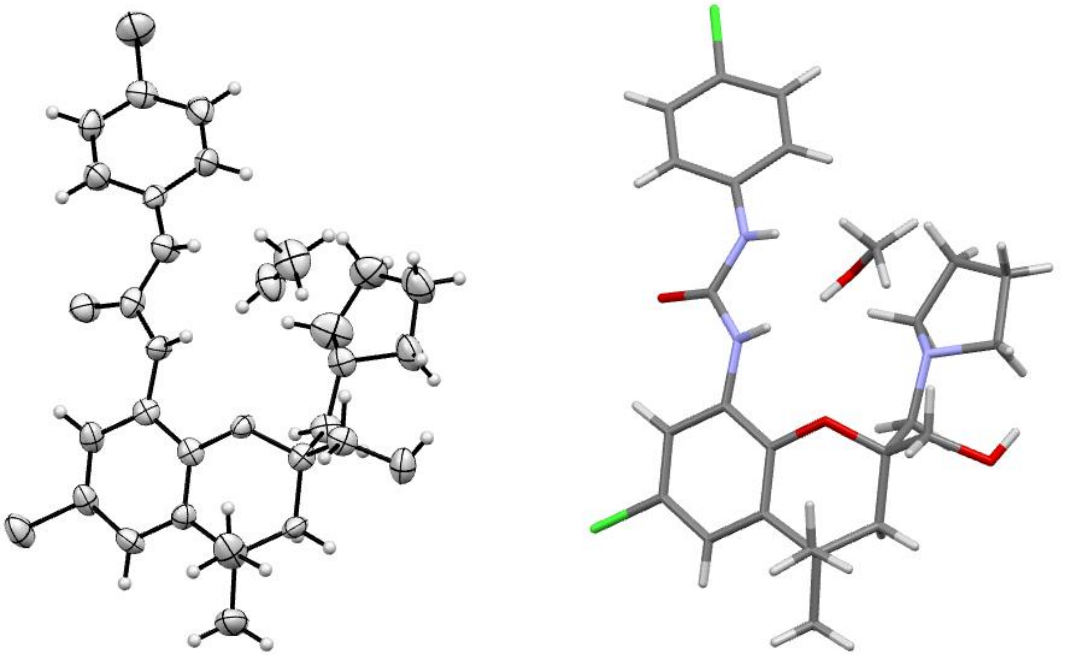
Crystals suitable for X-ray diffraction analysis of the corresponding complexes of receptor **1** could be obtained in some cases after slow evaporation of the complexes in MeOH solutions.

Figure S13. ORTEP diagram and X-ray crystal structure data of receptor 1 (DCM).



Crystal data: $C_{24}H_{31}Cl_2N_3O_4$, M_w = 496.42, triclinic, space group P1, a = 9.7883(3) Å, b = 10.7161(4) Å, c = 12.5654(4) Å, α = 83.489(2)°, β = 71.694(2)°, γ = 81.618(2)°, V = 1234.74(7) $Å^3$, Z = 2, D_C = 1.335 Mg/m^3, m = (Cu-K_α) = 2.655 mm^{-1}, F(000) = 524. 7511 reflections were collected at 3.71 ≤ θ ≤ 66.97 and merged to give 3749 unique reflections (R_{int} = 0.0287). Final values are R_1 = 0.0499, wR_2 = 0.1431.

Figure S14. ORTEP diagram and X-ray crystal structure data of (-)receptor 1 (MeOH:DCM).



Crystal data: $C_{25}H_{33}Cl_2N_3O_4$, M_w = 514.44, orthorhombic, space group $P2_12_12_1$, a = 9.0157(9) Å, b = 14.4040(2) Å, c = 19.6135(2) Å, α = 90°, β = 90°, γ = 90°, V = 2547.1(4) $Å^3$, Z = 4, D_C = 1.331 Mg/m^3, m = (Cu-K_α) = 2.589 mm^{-1}, F(000) = 1080. 14000 reflections were collected at $4.51 \leq \theta \leq 67.36$ and merged to give 3963 unique reflections (R_{int} = 0.0674). Final values are R_1 = 0.0843, wR_2 = 0.2116.

Figure S15. ^{1}H NMR spectrum of receptor 1 with (*L*)-mandelic acid (200 MHz, $CDCl_3$).

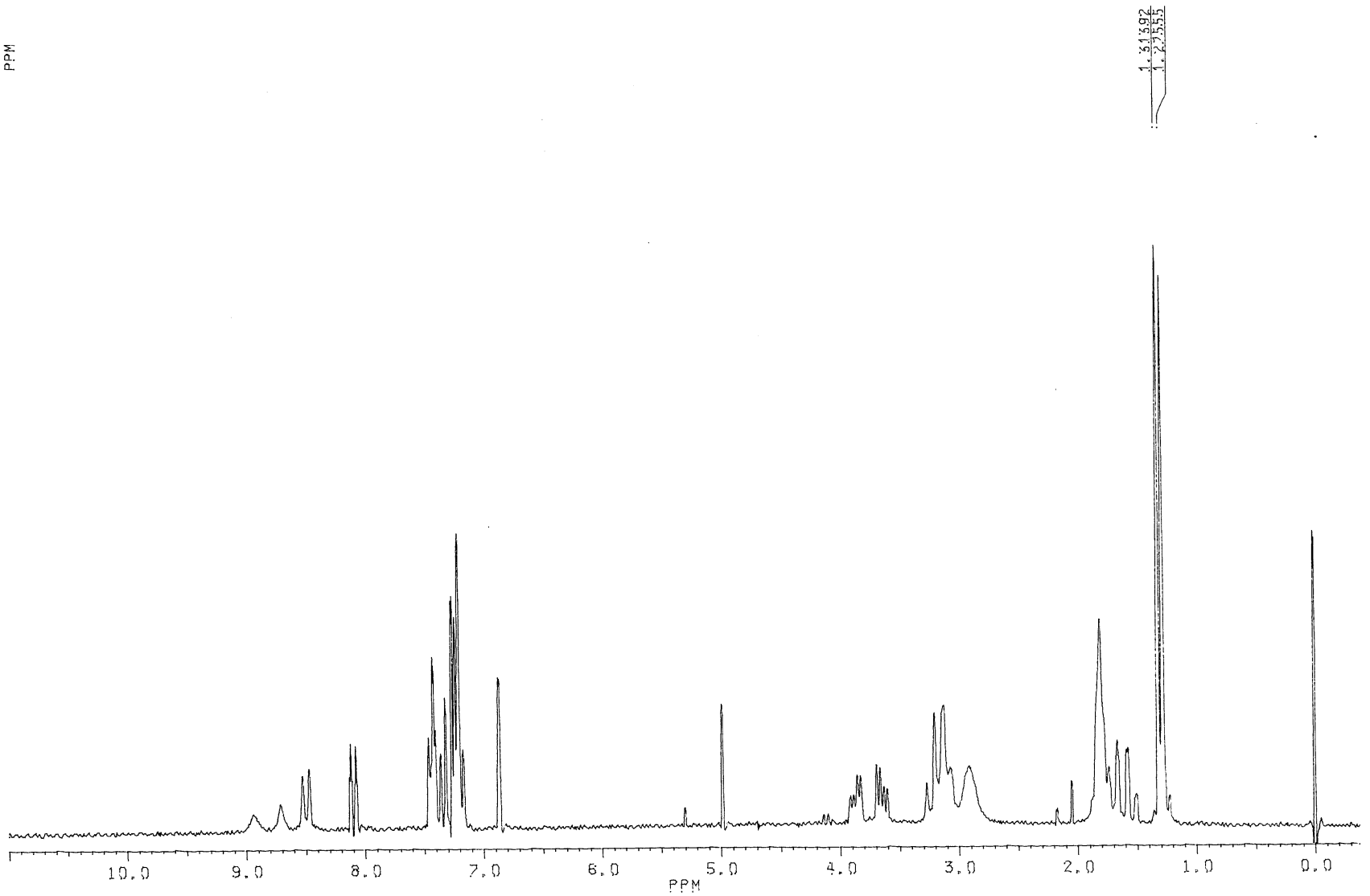


Figure S16. ^{1}H NMR spectrum of (-)receptor 1 with (*L*)-mandelic acid (200 MHz, $CDCl_3$).

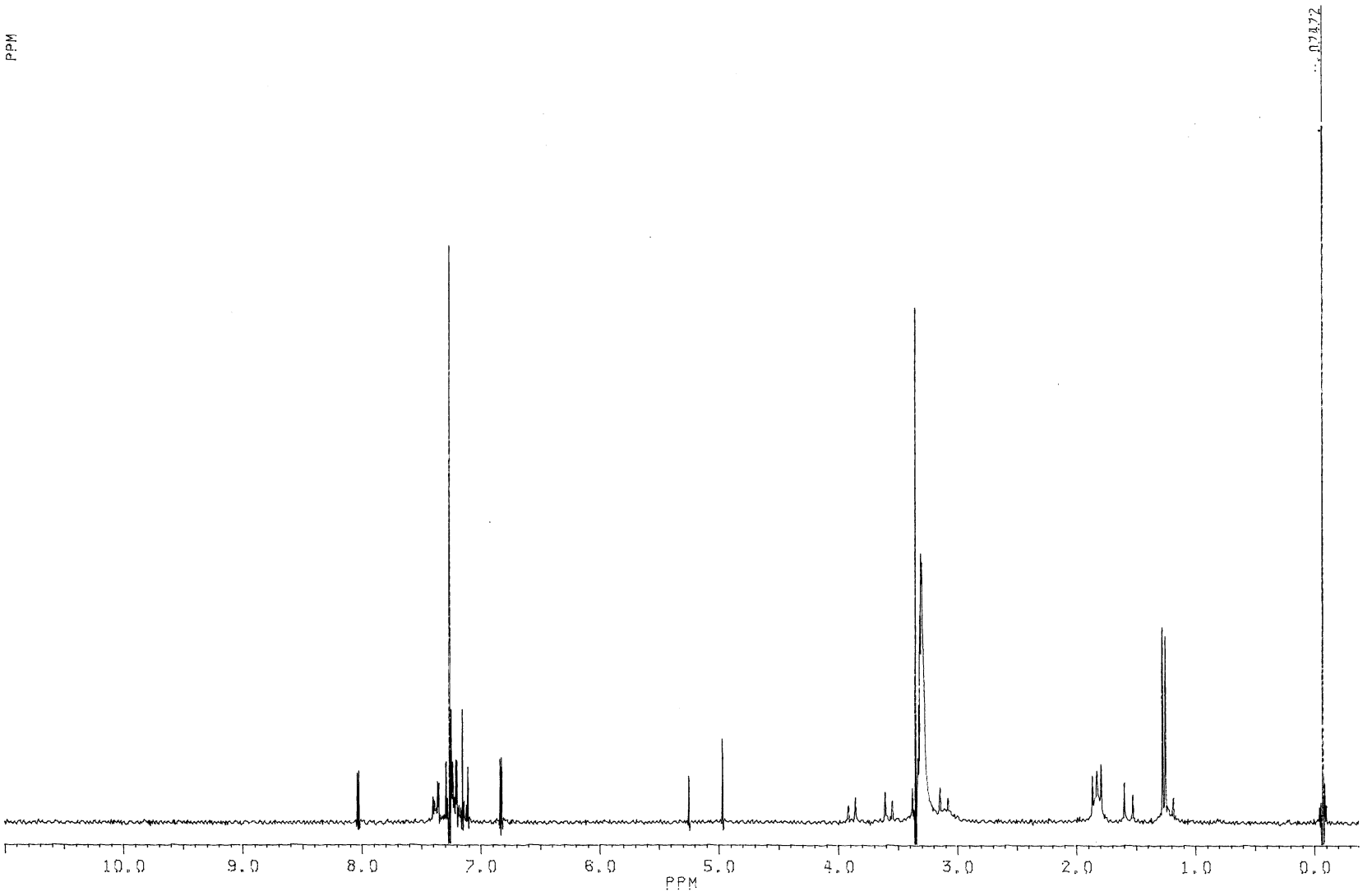
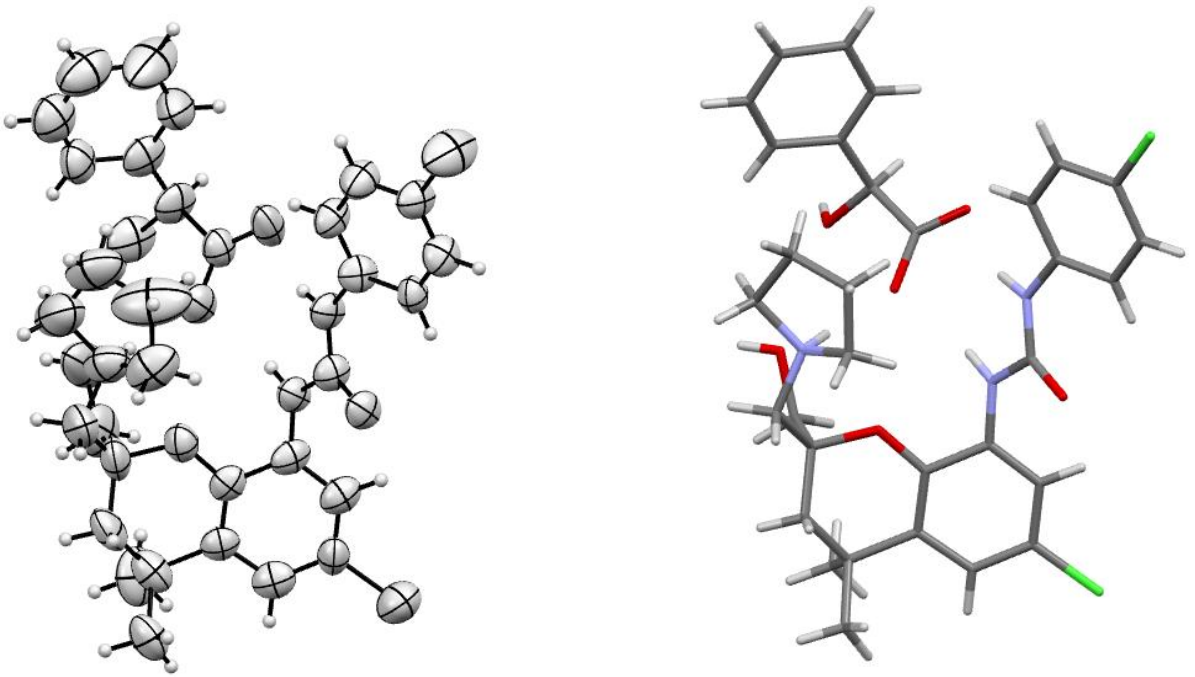


Figure S17. ORTEP diagram and X-ray crystal structure data of (-)receptor 1 with (*L*)-mandelic acid (MeOH:H_2O).



Crystal data: $C_{32}H_{37}Cl_2N_3O_6$, M_w = 630.55, orthorhombic, space group $P2_12_12_1$, a = 8.4007(6) Å, b = 14.3494(1) Å, c = 26.2774 (2) Å, α = 90°, β = 90°, γ = 90°, V = 3167.6(4) $Å^3$, Z = 4, D_C = 1.322 Mg/m^3, m = (Cu-K_α) = 2.238 mm^{-1}, F(000) = 1328. 16604 reflections were collected at $3.36 \leq \theta \leq 66.46$ and merged to give 5179 unique reflections (R_{int} = 0.0896). Final values are R_1 = 0.0961, wR_2 = 0.2332.

Figure S18. ^{1}H NMR spectrum of receptor 1 with (*L*)-lactic acid (200 MHz, $CDCl_3$).

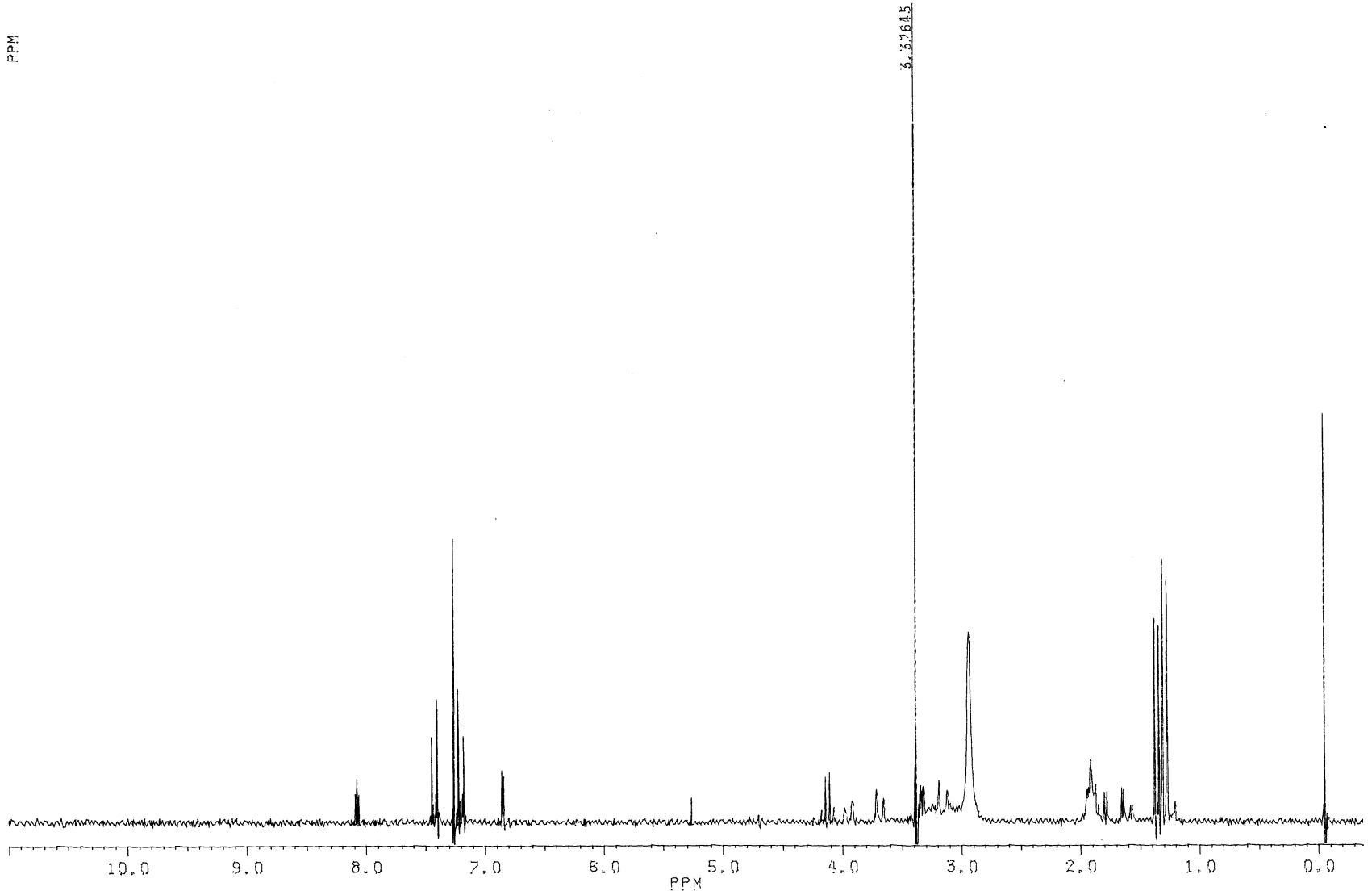
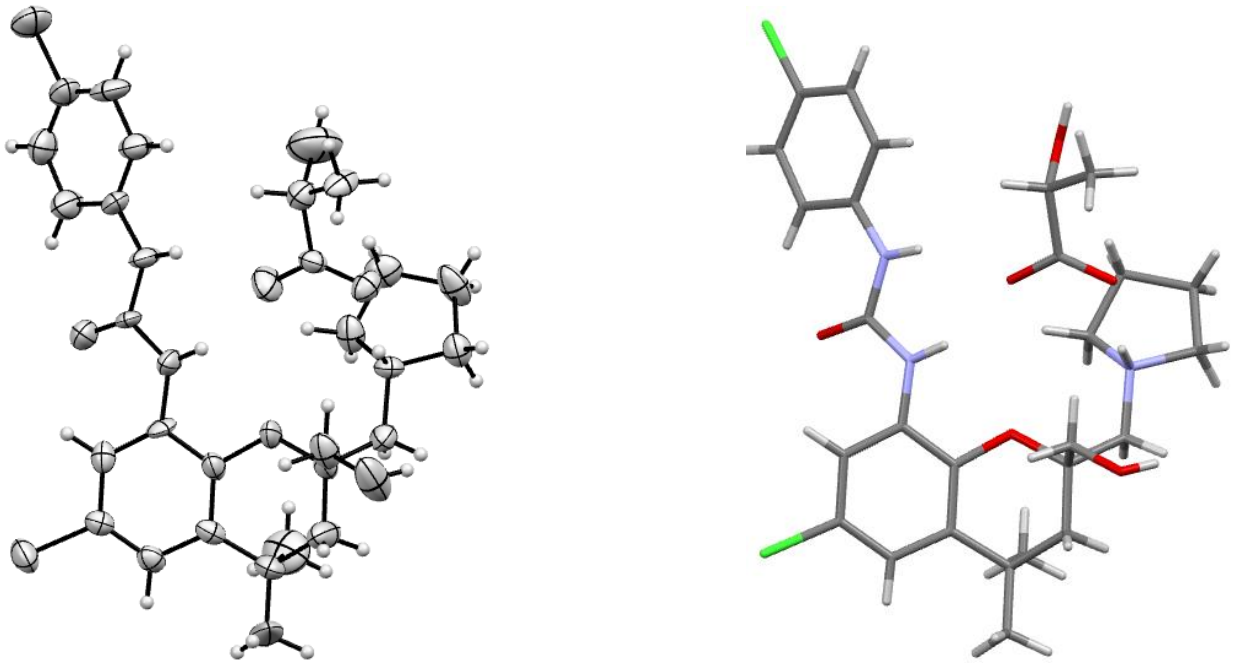


Figure S19. ORTEP diagram and X-ray crystal structure data of receptor 1 with (*L*)-lactic acid (MeOH).



Crystal data: $C_{27}H_{35}Cl_2N_3O_6$, M_w = 568.48, monoclinic, space group P2(1), a = 15.3308(4) Å, b = 11.5720(3) Å, c = 15.6536(5) Å, α = 90°, β = 97.625(2)°, γ = 90°, V = 2752.52(13) $Å^3$, Z = 4, D_C = 1.372 Mg/m^3, m = (Cu-K_α) = 2.510 mm^{-1}, F(000) = 1200. 11331 reflections were collected at $2.85 \leq \theta \leq 67.08$ and merged to give 5426 unique reflections (R_{int} = 0.0534). Final values are R_1 = 0.0596, wR_2 = 0.1650.

Figure S20. ^{1}H NMR spectrum of receptor 1 with (*L*)-tartaric acid (200 MHz, $CDCl_3$).

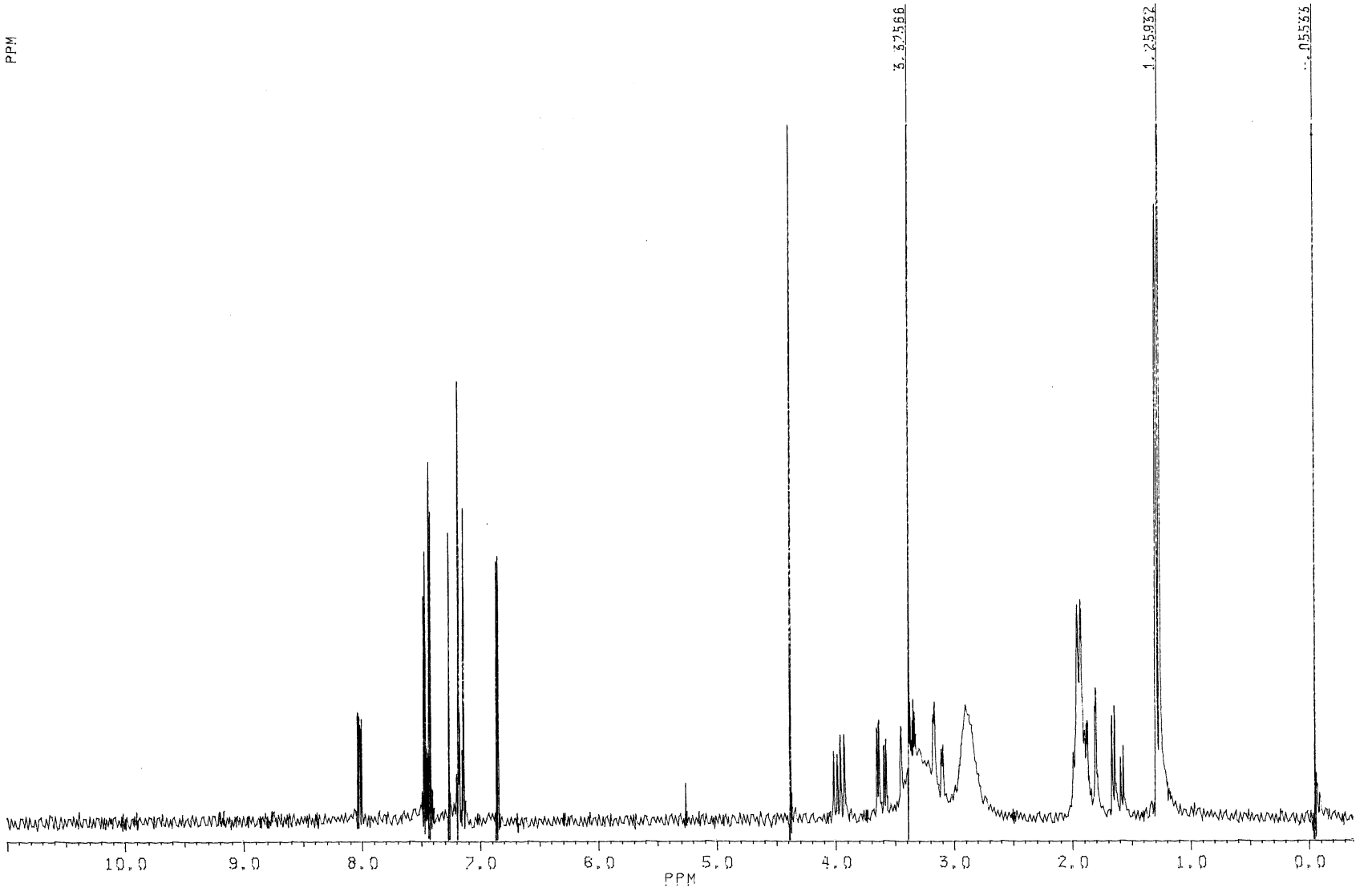
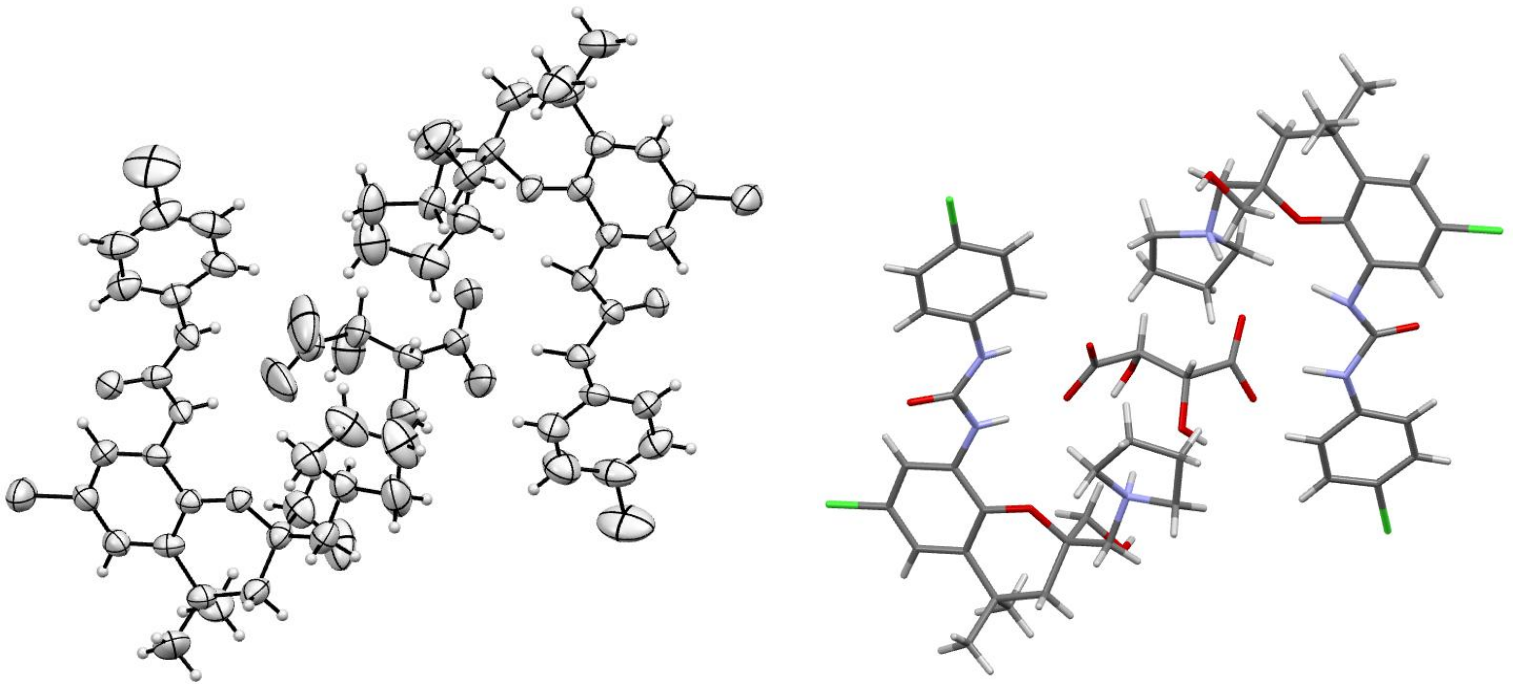


Figure S21. ORTEP diagram and X-ray crystal structure data of receptor 1 with (*L*)-tartaric acid (MeOH).



Crystal data: $C_{52}H_{64}Cl_4N_6O_{13}$, M_w = 1122.89, monoclinic, space group C2, a = 17.4116(8) Å, b = 19.0364(9) Å, c = 17.3720(7) Å, α = 90°, β = 97.836(3)°, γ = 90°, V = 5704.3(4) $Å^3$, Z = 4, D_C = 1.308 Mg/m^3, m = (Cu-K_α) = 2.431 mm^{-1}, F(000) = 2360. 15518 reflections were collected at $2.57 \leq \theta \leq 67.12$ and merged to give 8225 unique reflections (R_{int} = 0.0569). Final values are R_1 = 0.0724, wR_2 = 0.1928.

Figure S22. ^{1}H NMR spectrum of receptor 1 with N-tosyl-(*L*)-alanine (200 MHz, $CDCl_3$).

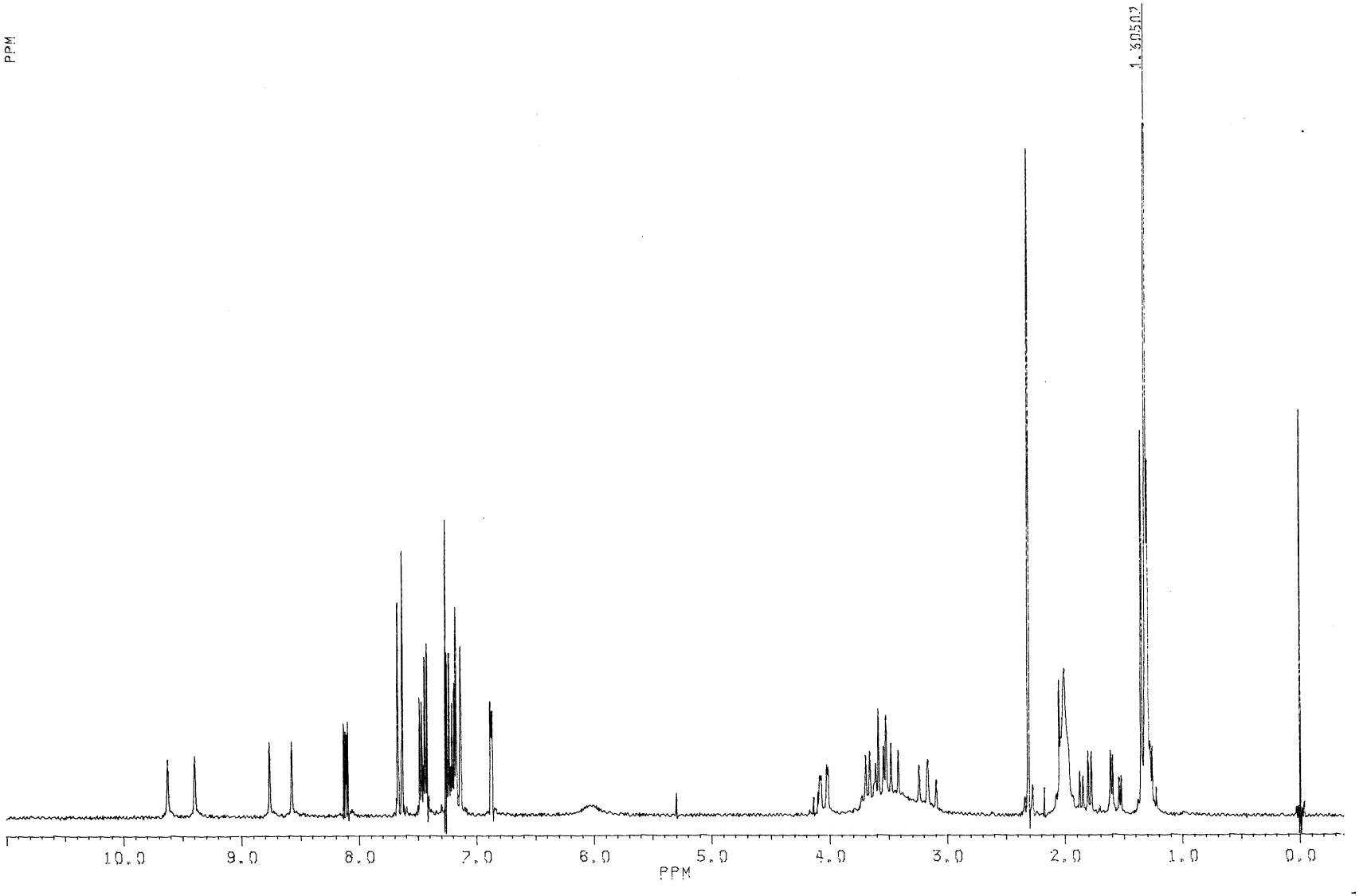
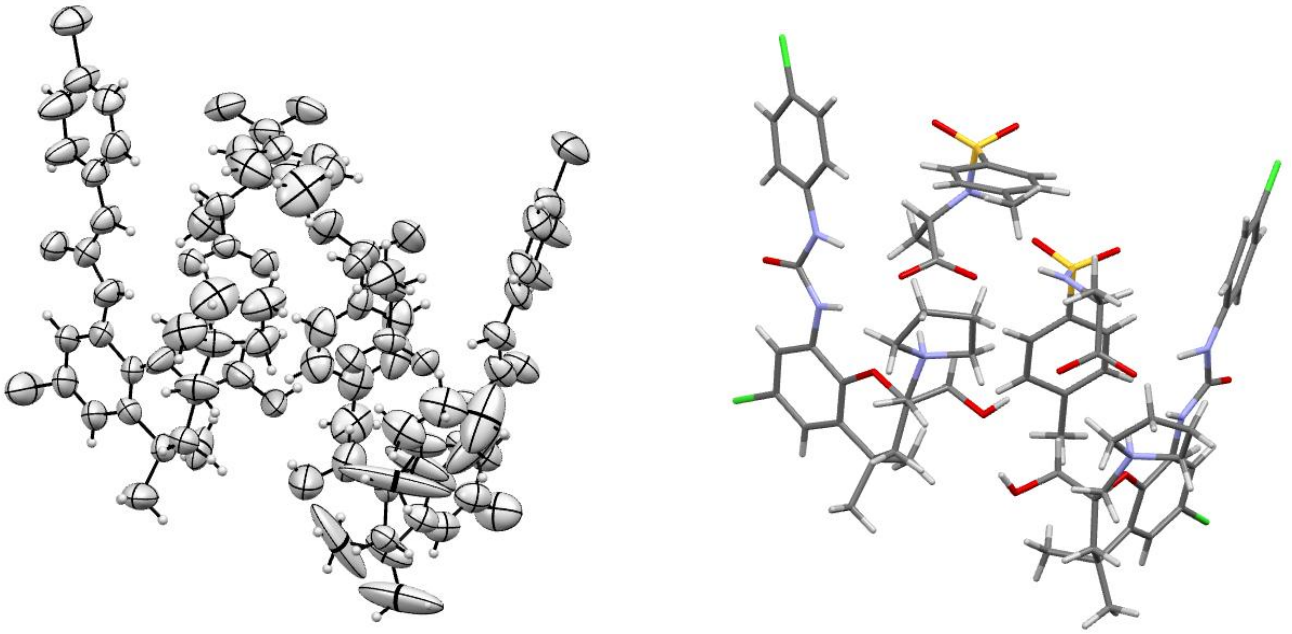


Figure S23. ORTEP diagram and X-ray crystal structure data of receptor 1 with N-tosyl-(*L*)-alanine (MeOH:DCM).



Crystal data: $C_{68}H_{84}Cl_4N_8O_{14}S_2$, M_w = 1443.35, monoclinic, space group $P2_12_12_1$, a = 10.7729(6) Å, b = 23.4747(1) Å, c = 28.9321(2) Å, α = 90°, β = 90°, γ = 90°, V = 7316.7(7) Å^3, Z = 4, D_C = 1.310 Mg/m^3, m = (Cu-K_α) = 2.554 mm^{-1}, F(000) = 2554. 43084 reflections were collected at $2.42 \leq \theta \leq 67.35$ and merged to give 12237 unique reflections (R_{int} = 0.1354). Final values are R_1 = 0.1055, wR_2 = 0.2699.

Figure S24. ^{1}H NMR spectrum of receptor 1 with 3,5-dinitrobenzoic acid (200 MHz, $CDCl_3$).

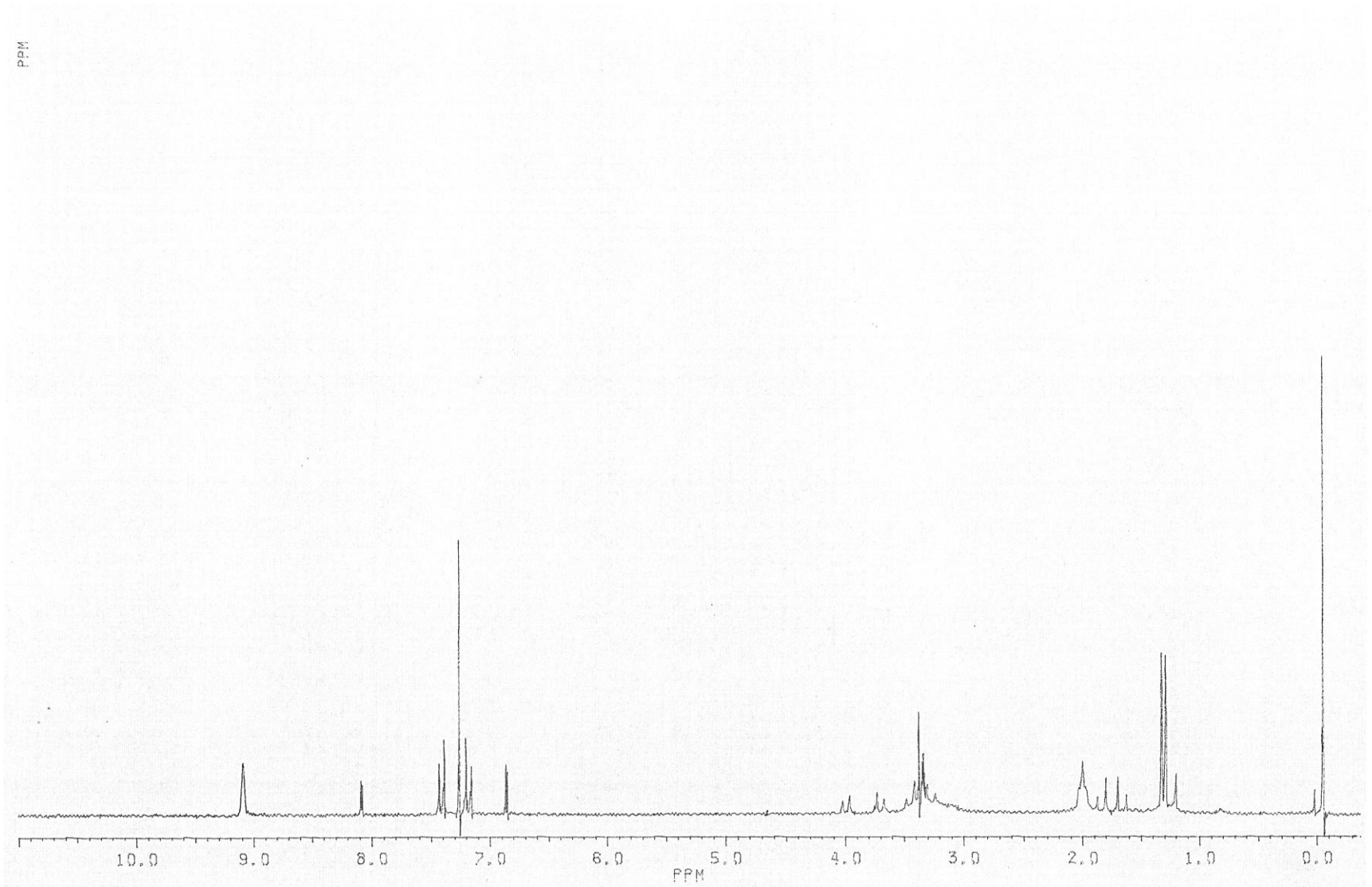
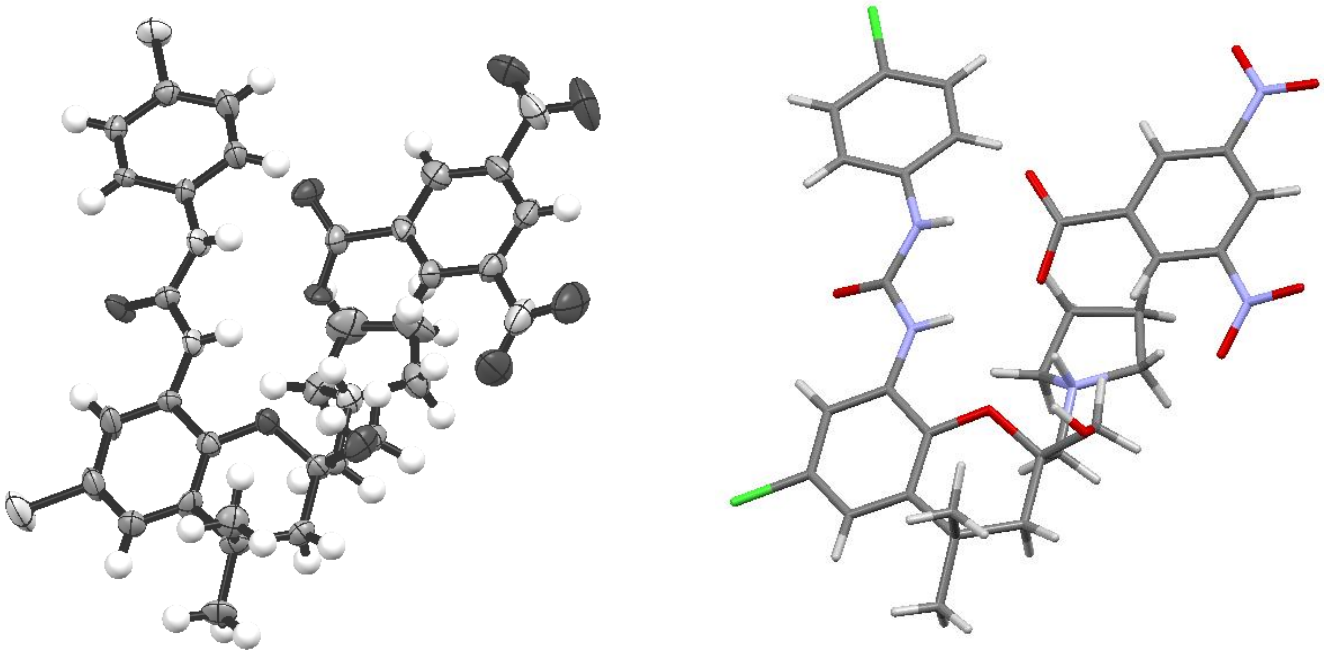


Figure S25. ORTEP diagram and X-ray crystal structure data of receptor 1 with 3,5-dinitrobenzoic acid (MeOH:$CHCl_3$).



Crystal data: $C_{31}H_{33}Cl_2N_5O_9$, M_w = 690.52, monoclinic, space group $P2_1/c$, a = 12.2705(5) Å, b = 15.0706(6) Å, c = 17.1904(7) Å, α = 90.00°, β = 91.145(3)°, γ = 90.00°, V = 3178.3(2) $Å^3$, Z = 4, D_C = 1.443 Mg/m^3, m = (Cu-K_α) = 2.377 mm^{-1}, F(000) = 1440. 5091 reflections were collected at $3.60 \leq \theta \leq 67.36$ and merged to give 3305 unique reflections (R_{int} = 0.0740). Final values are R_1 = 0.1294, wR_2 = 0.3075.

Figure S26. ^{1}H NMR spectrum of receptor 1 with the chlorophenyl urea of (*L*)-isoleucine (200 MHz, $CDCl_3$).

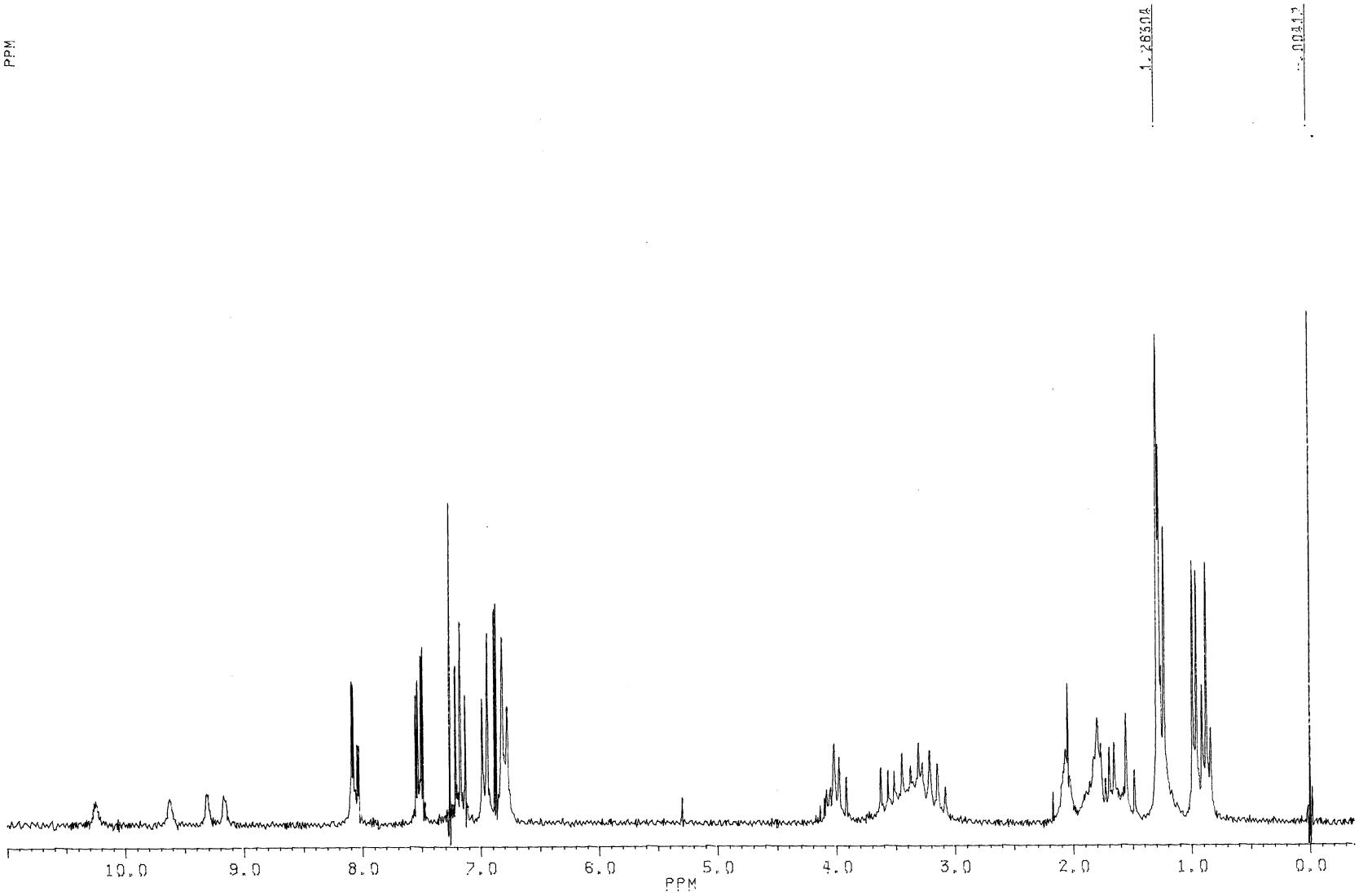


Figure S27. ^{1}H NMR spectrum of (+)receptor 1 with the chlorophenyl urea of (*L*)-isoleucine (200 MHz, $CDCl_3$).

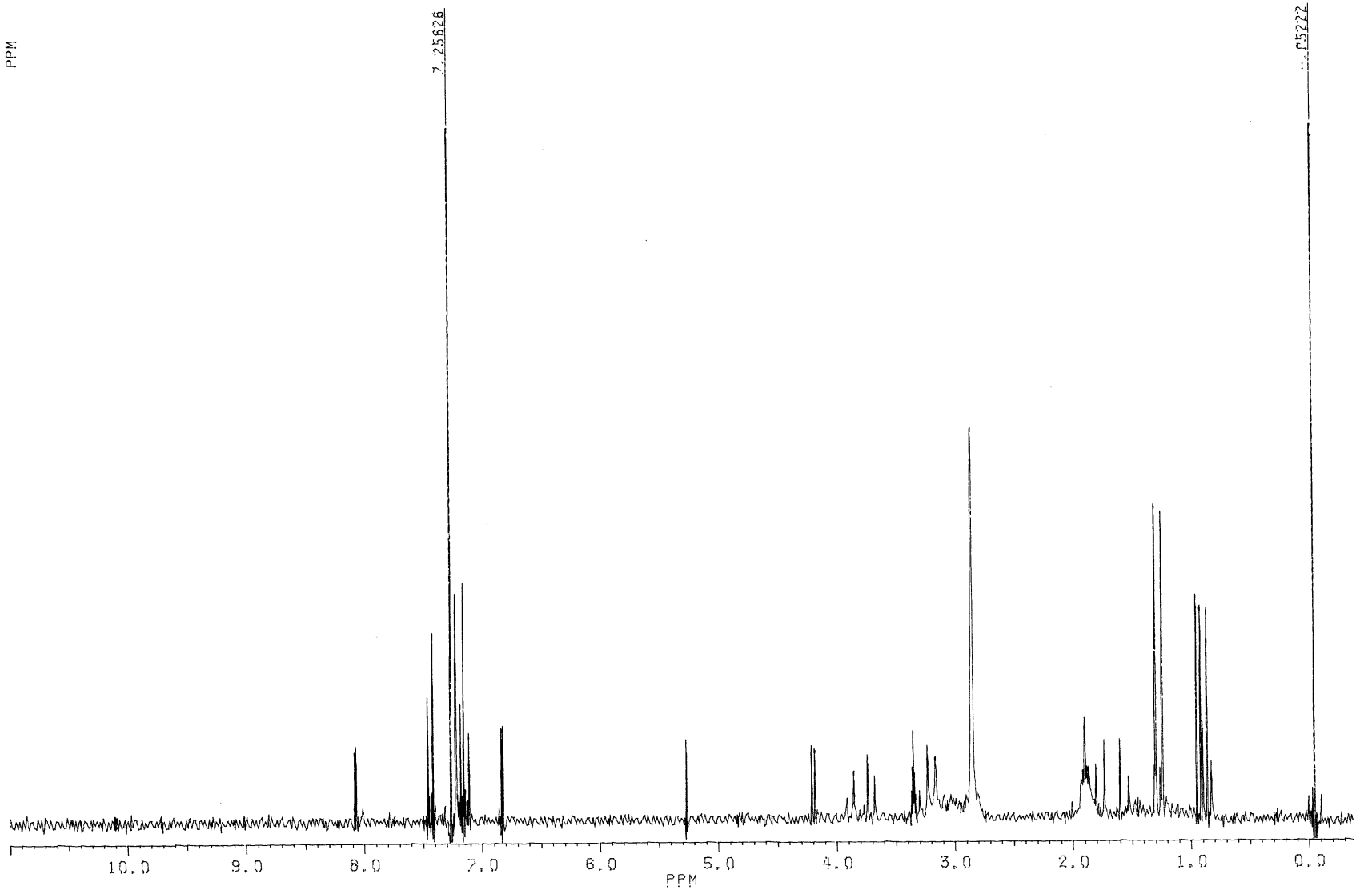


Figure S28. ^{1}H NMR spectrum of receptor 1 hydroiodide (200 MHz, $CDCl_3$).

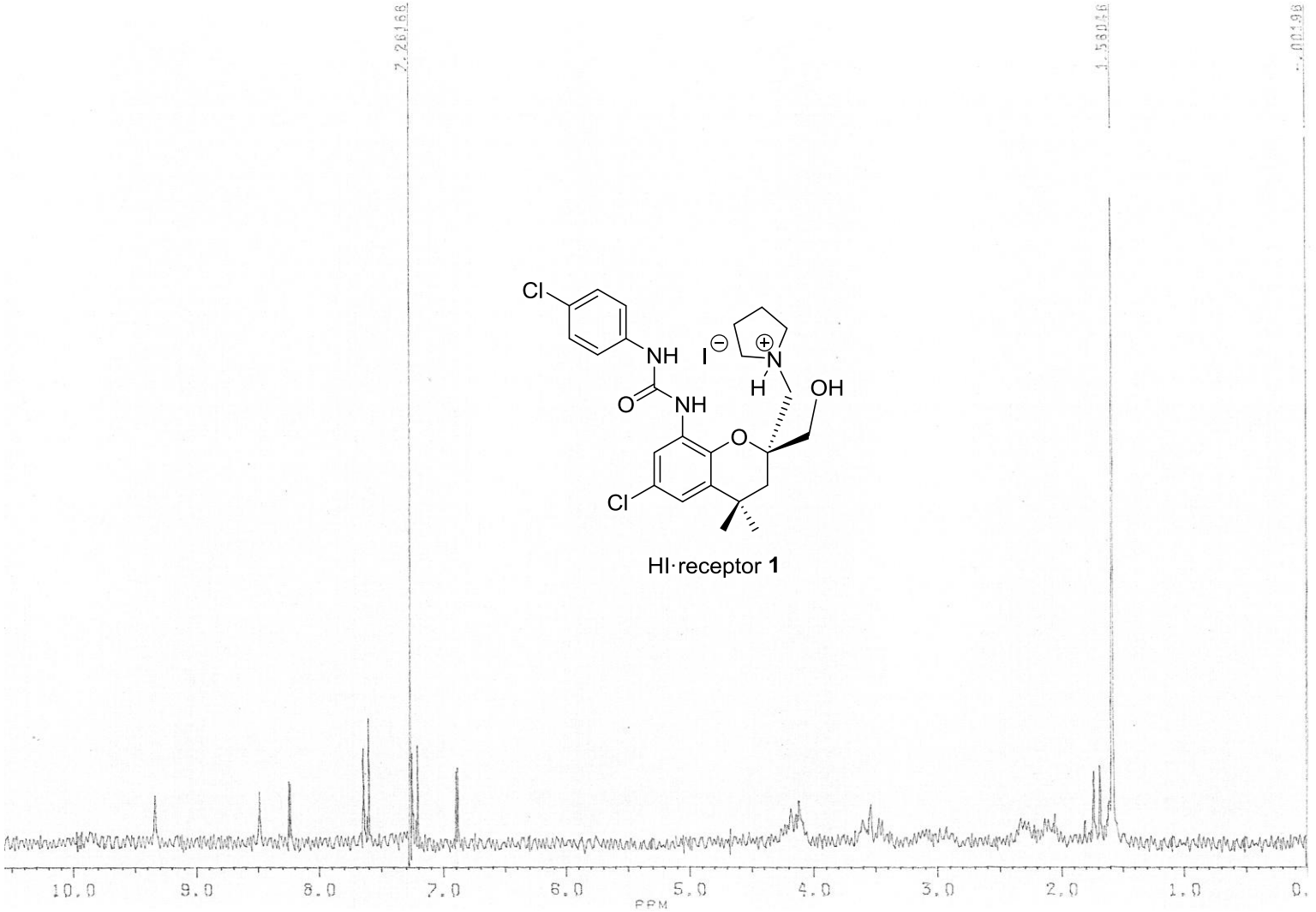


Figure S29. ^{13}C NMR spectrum of receptor 1 hydroiodide (100 MHz, $CDCl_3$).

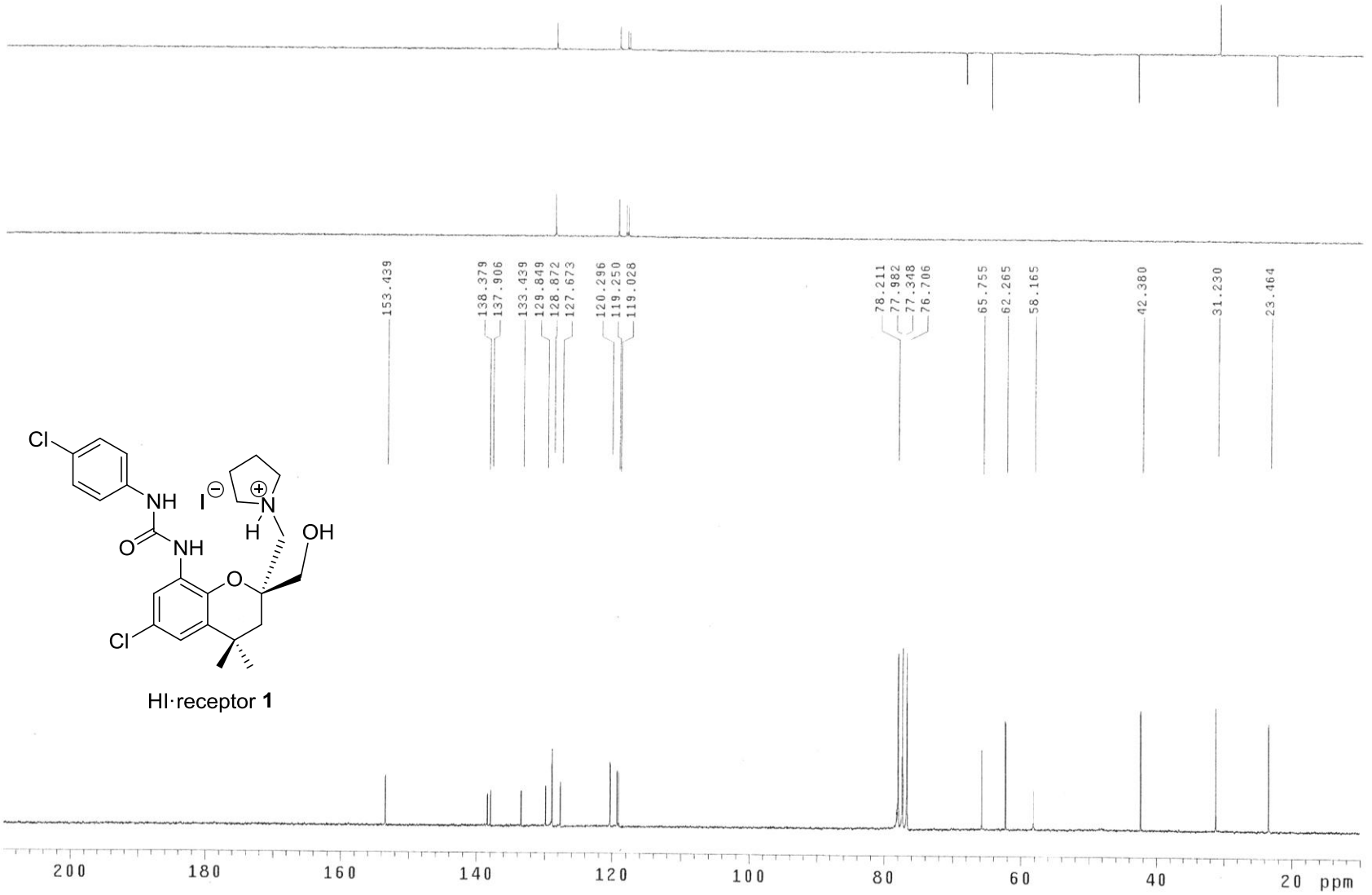


Figure S30. ^{1}H NMR spectrum of receptor 1 hydroiodide with tetraethylammonioum acetate (400 MHz, $CDCl_3$).

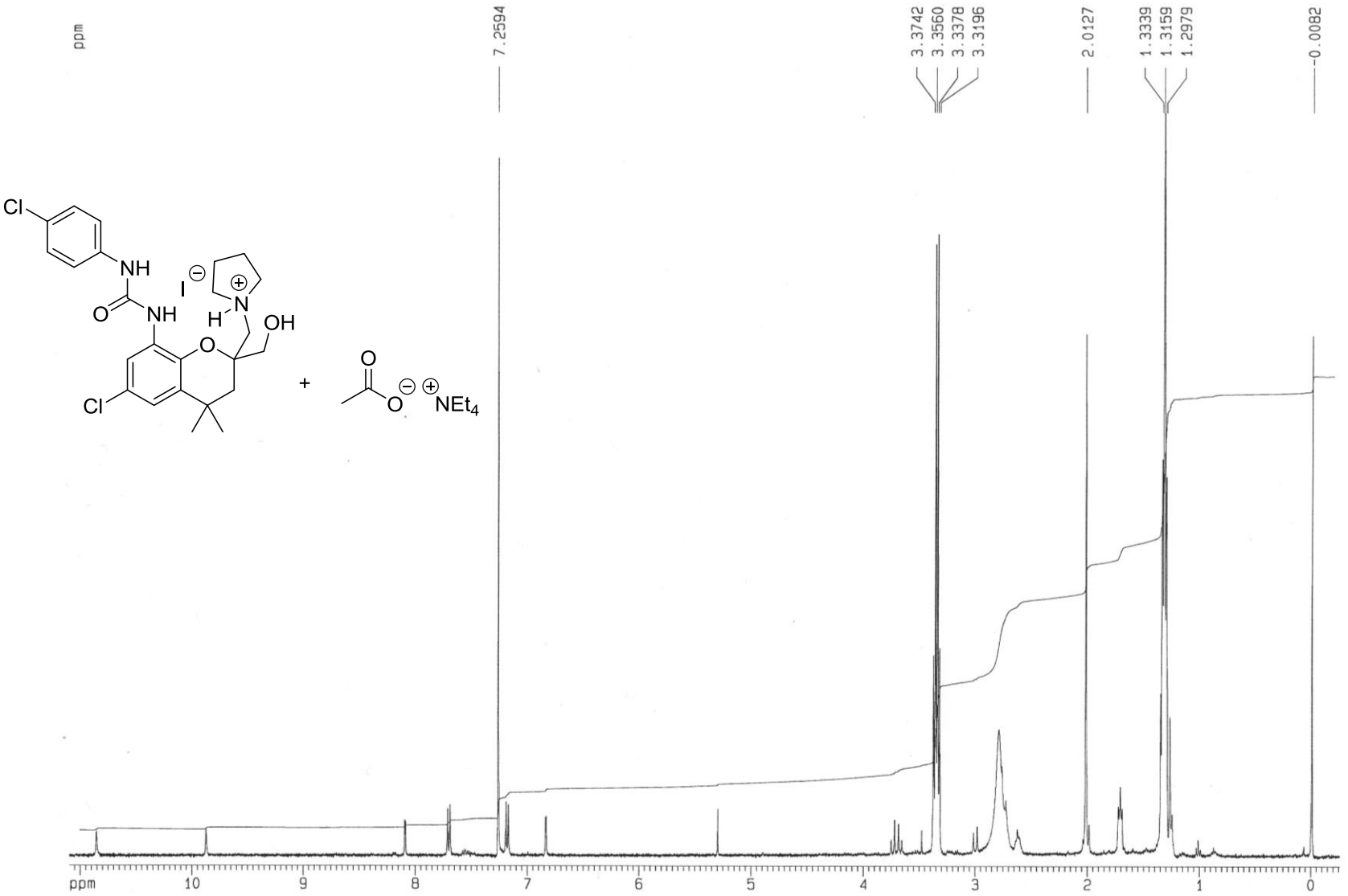


Figure S31. ROESY spectrum of receptor 1 hydroiodide with tetraethylammonioum acetate ($CDCl_3$).

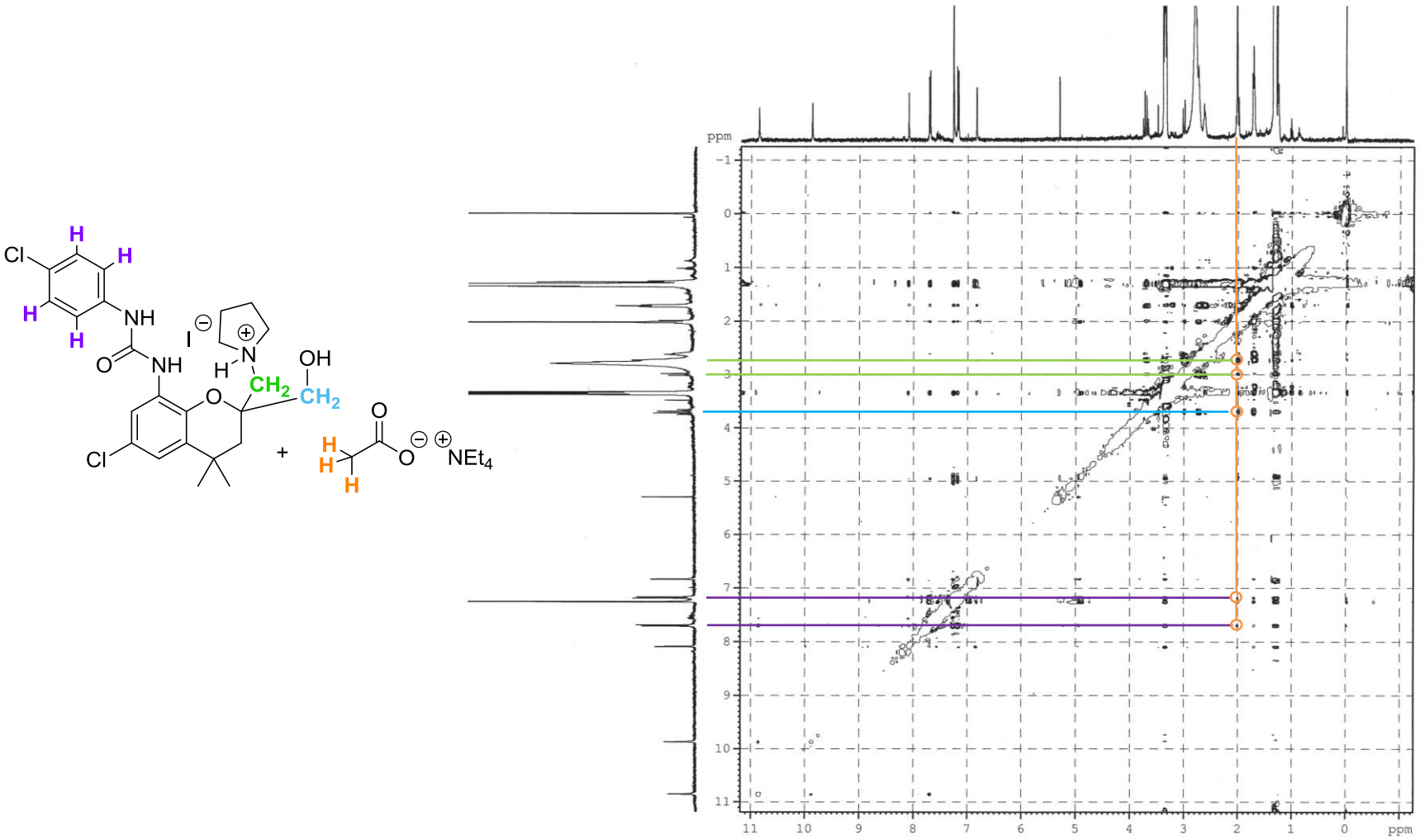


Figure S32. ^{1}H NMR spectrum of receptor 1 hydroiodide with mandelic acid tetraethylammonium salt (400 MHz, $CDCl_3$).

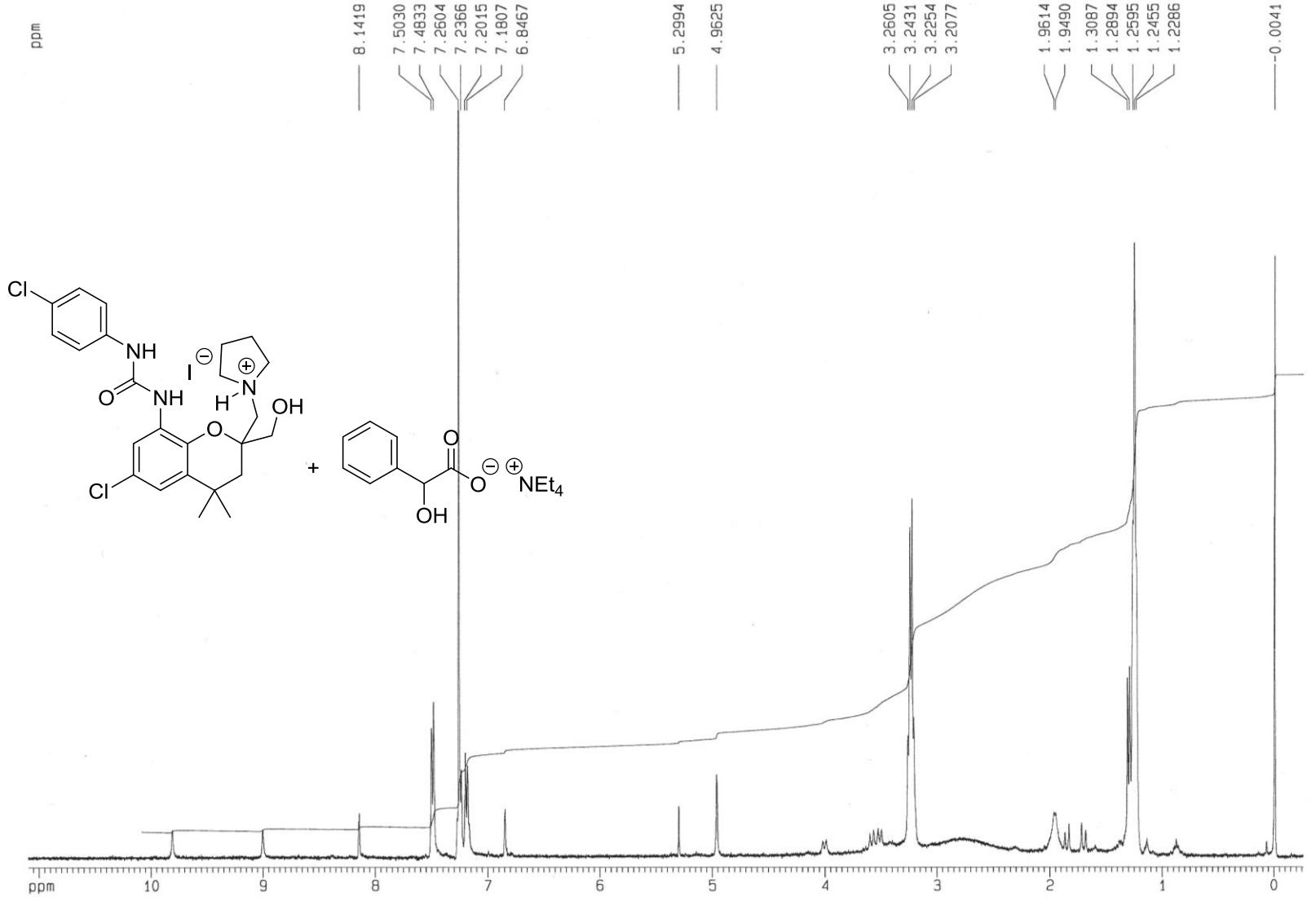


Figure S33. ROESY spectrum of receptor 1 hydroiodide with mandelic acid tetraethylammonium salt ($CDCl_3$).

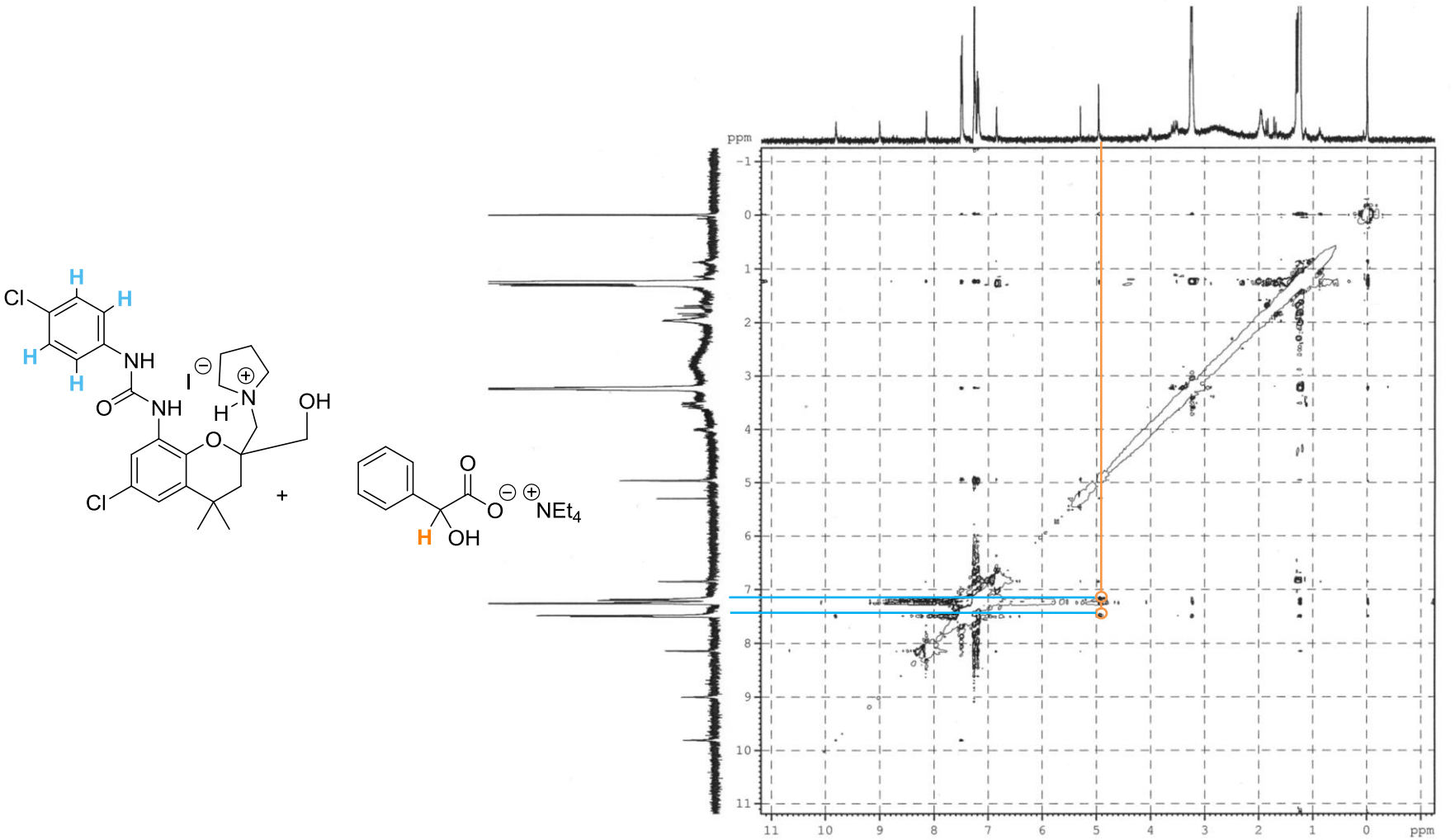
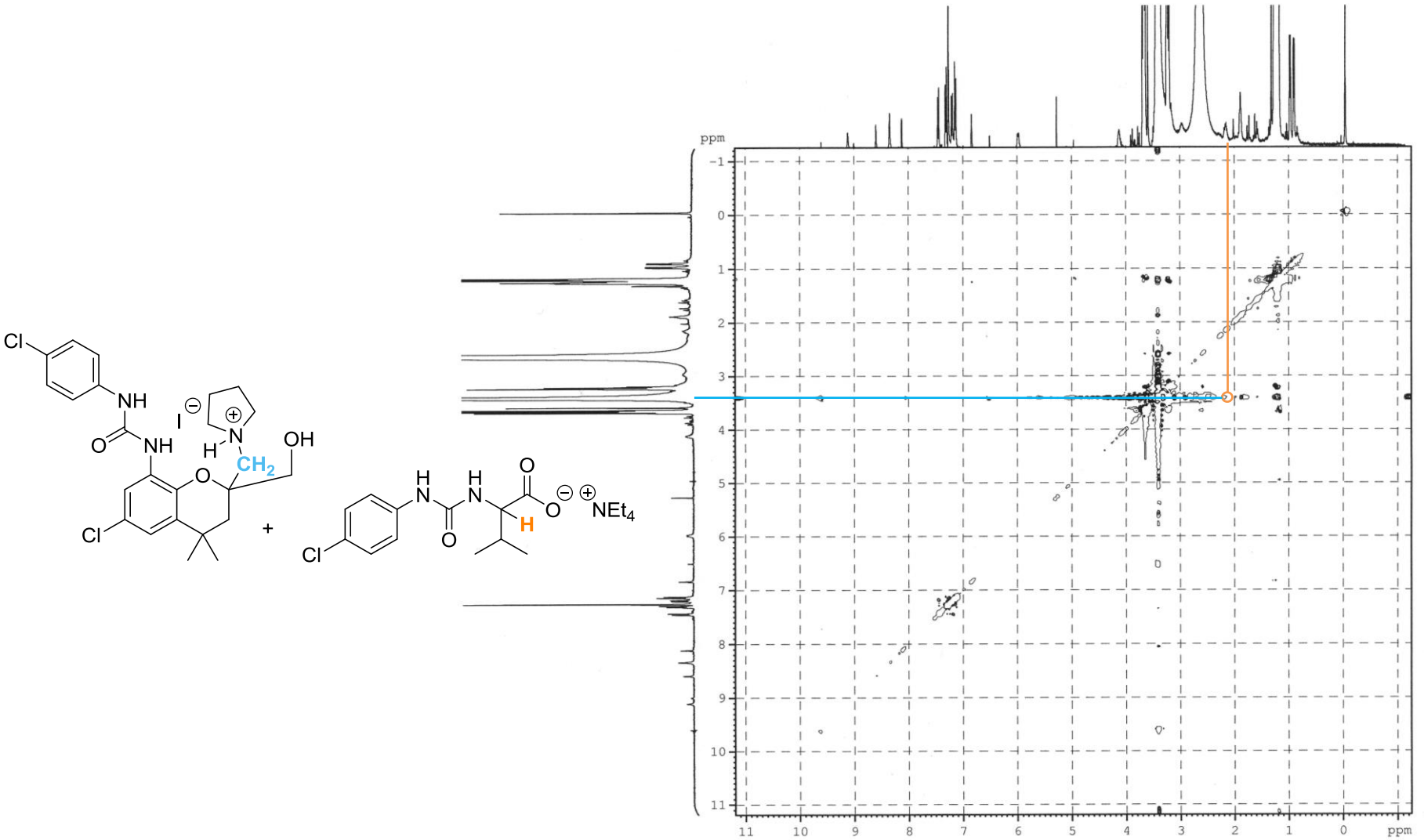


Figure S34. ^{1}H NMR spectrum of receptor 1 hydroiodide with chlorophenyl urea of valine tetraethylammonioum salt (400 MHz, $CDCl_3$).

Figure S35. ROESY spectrum of receptor 1 hydroiodide with chlorophenyl urea of valine tetraethylammonioum salt ($CDCl_3$).



Experimental procedure for the determination of association constants for receptor 1 hydroiodide.

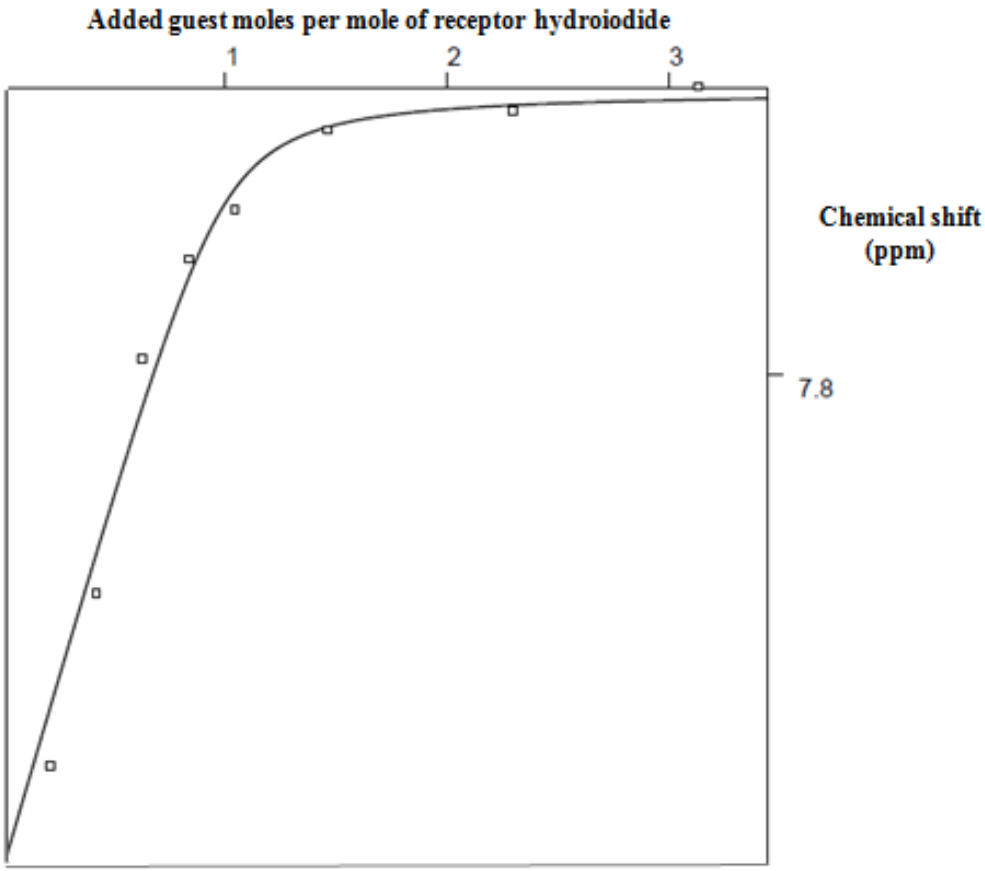
A solution of the racemic receptor **1** hydroiodide (4.9×10^{-3} M) was prepared in MeOD (0.4 mL) and transferred to a standard NMR tube. The ^{1}H-NMR spectrum was collected for this sample at 293 K. Aliquots of a solution of the corresponding tetraethylammonium carboxylate (2-3 eq) in MeOD (0.15 mL) were then added to the NMR tube. After each addition, the contents of the tube were mixed well and a spectrum collected at 293 K. The chemical shift of H-7 of the receptor after each addition were plotted and their movements were analyzed by a non-linear curve fitting a program based on Montecarlo Method to give K_{ass}[1] and the limiting chemical shift. Uncertainty of K determination is estimated around 20%.[2]

Figure S36. ^{1}H NMR titration of receptor 1 hydroiodide with tetraethylammonium acetate (MeOD, 20°C).

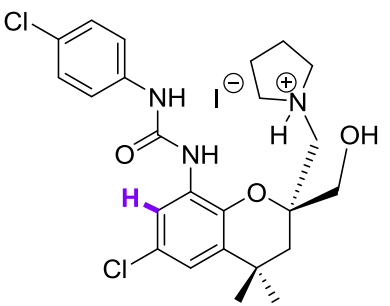
Absolute titration
Constant: 9×10^{3} 1/M
Max. shift (ppm): 7.8422

Host: Receptor **1** hydroiodide
Molecular weight: 606

Guest: Tetraethylammonium acetate
Molecular weight: 261

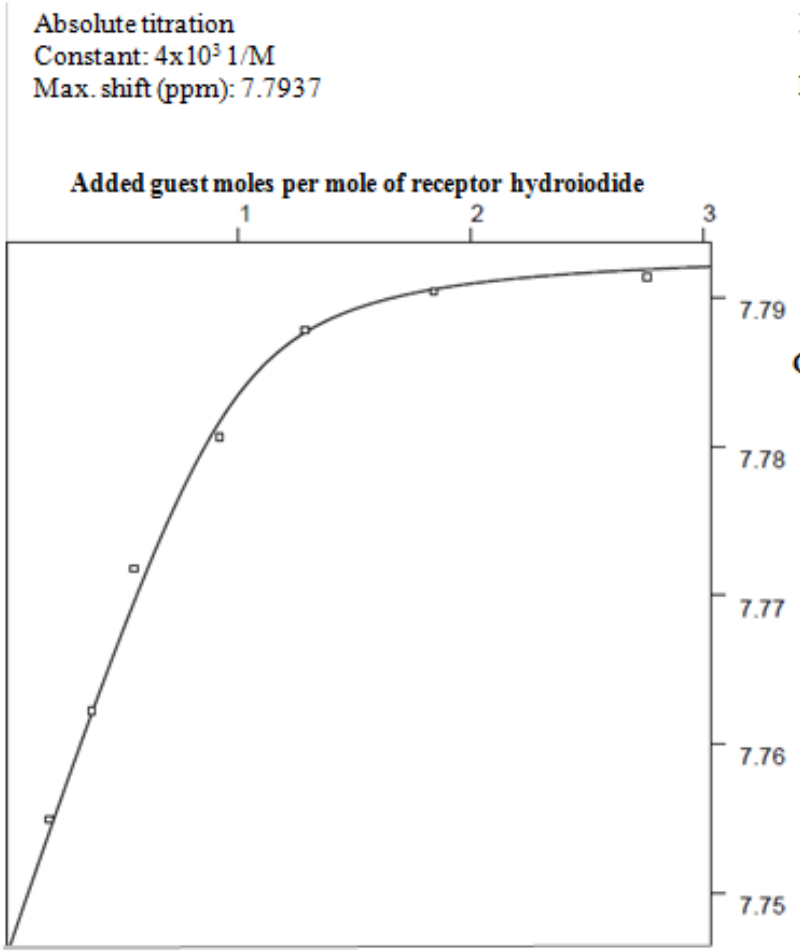


Chemical shift (ppm)	Added guest volume (mL)
7.7275	0
7.7422	0.01
7.7677	0.01
7.8024	0.01
7.817	0.01
7.8243	0.01
7.8361	0.02
7.8389	0.04
7.8425	0.04

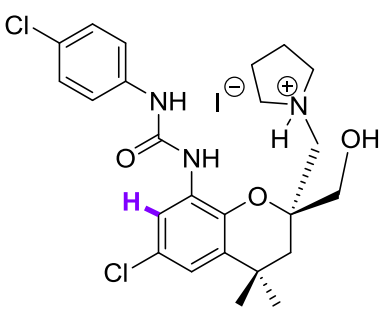


HI·receptor **1**

Figure S37. ^{1}H NMR titration of receptor 1 hydroiodide with mandelic acid tetraethylammonium salt (MeOD, 20ºC).



Chemical shift (ppm)	Added guest volume (mL)
7.7457	0
7.7549	0.01
7.7622	0.01
7.7718	0.01
7.7806	0.02
7.7878	0.02
7.7904	0.03
7.7914	0.05



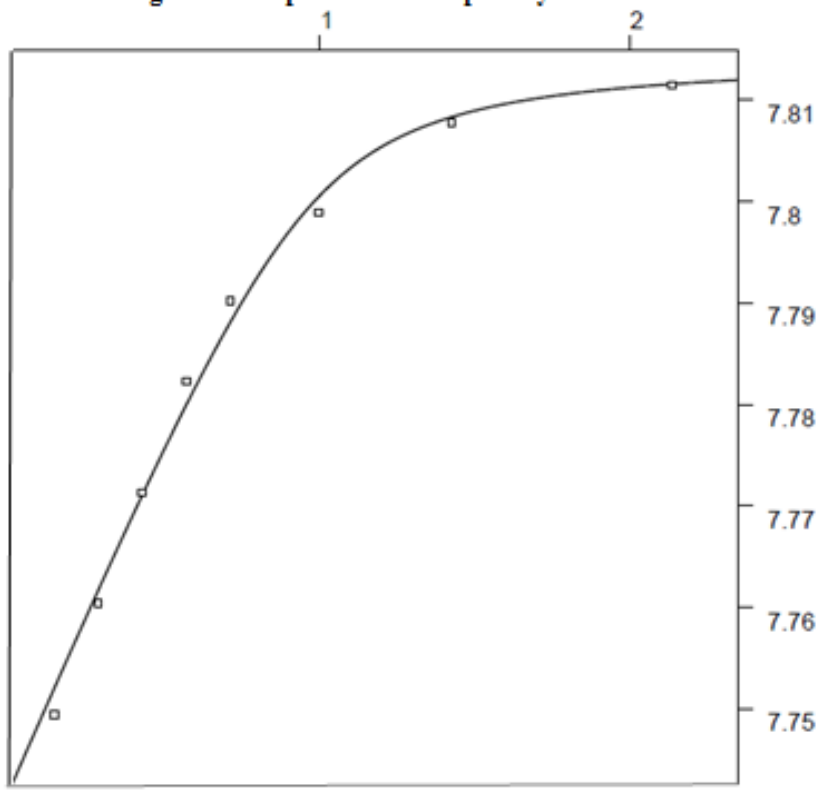
HI·receptor **1**

Figure S38. ^{1}H NMR titration of receptor 1 hydroiodide with chlorophenyl urea of valine tetraethylammonioum salt (MeOD, 20°C).

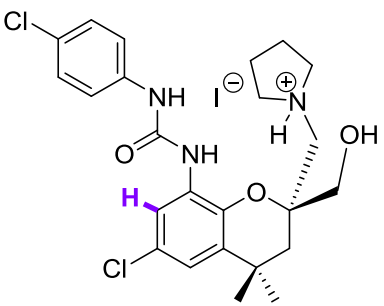
Absolute titration
Constant: 4.3×10^{3} 1/M
Max. shift (ppm): 7.8149

Host: Receptor **1** hydroiodide
Molecular weight: 606

Guest: Chlorophenyl urea of valine tetraethylammonioum salt
Molecular weight: 399



Chemical shift (ppm)	Added guest volume (mL)
7.7421	0
7.7494	0.01
7.7604	0.01
7.7713	0.01
7.7823	0.01
7.7902	0.01
7.7989	0.02
7.8078	0.03
7.8115	0.05



HI·receptor **1**

Experimental procedure for the determination of the relative constant for receptor 1 with (*L*)-mandelic acid.

A solution of the racemic receptor **1** (7.8 x 10^{-3} M) was prepared in $CDCl_3$ (0.5 mL) and transferred to a standard NMR tube. The ^1H NMR spectrum was collected for this sample at 293 K. Aliquots of a solution of (*L*)-mandelic acid (>3 eq) in $CDCl_3$ (0.2 mL) were then added to the NMR tube. After each addition, the contents of the tube were mixed well and a spectrum collected at 293 K. The chemical shift of H-7 of both enantiomers of the receptor after each addition were plotted and their movements were analyzed by a non-linear curve fitting a program based on Montecarlo Method to give K_{rel} and the limiting chemical shift. Uncertainty of K determination is estimated around 20%.[2]

Figure S39. ^{1}H NMR titration of receptor 1 with (*L*)-mandelic acid (MeOD, 20ºC).

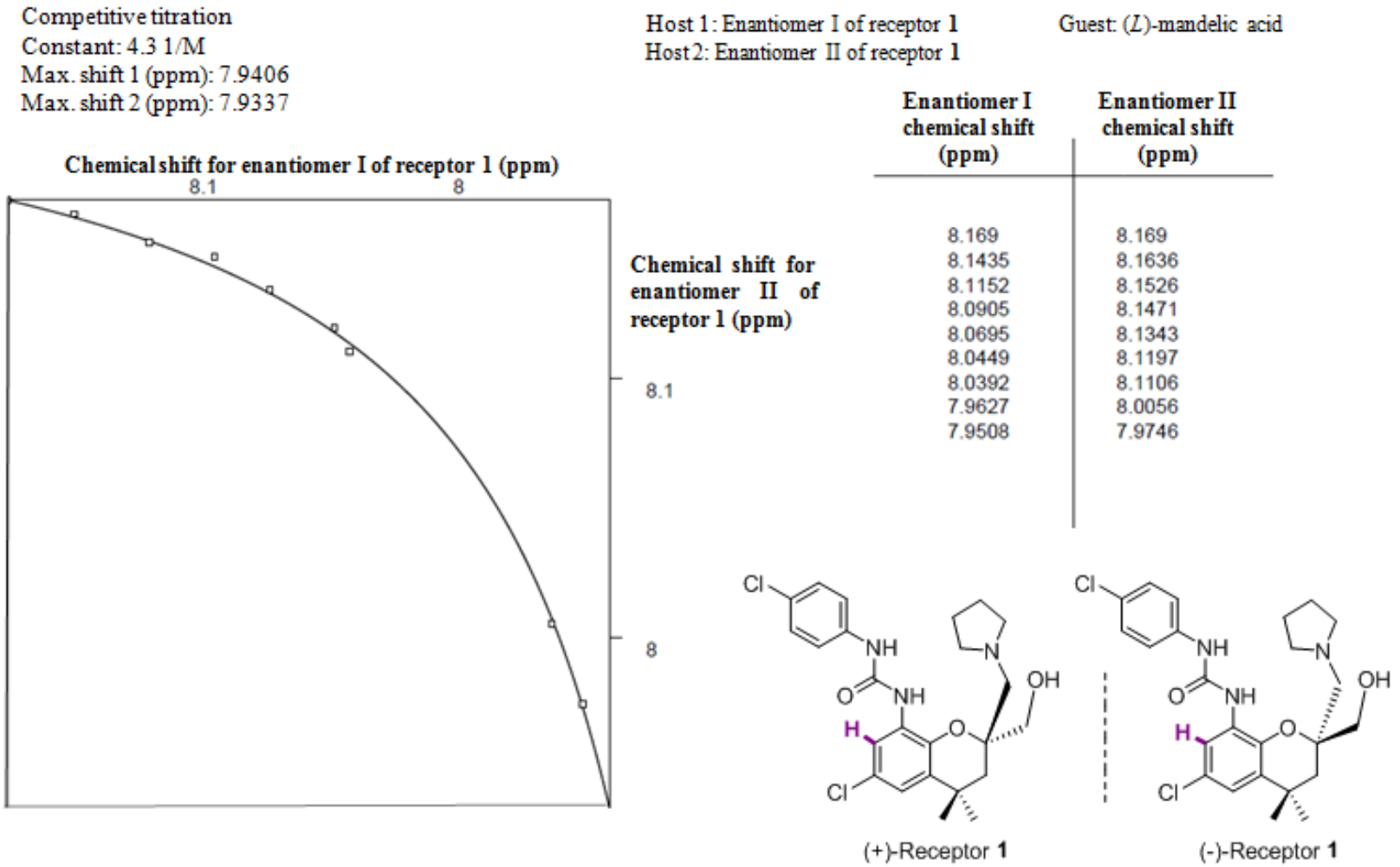
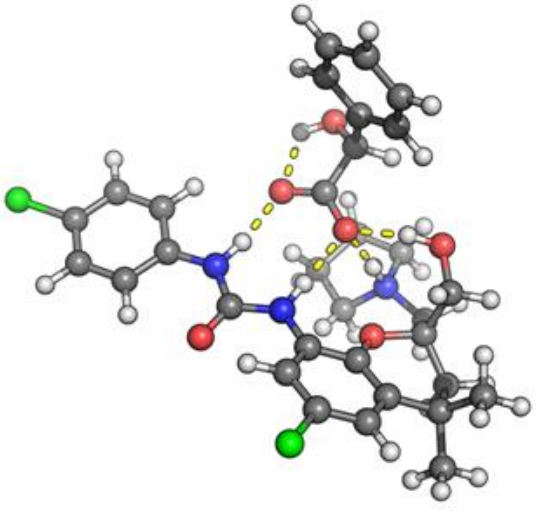


Figure S40. DFT methodology and cartesian coordinates of the structures found.

Calculations were performed using Gaussian09[3] program. The structures were optimized using the B3LYP[4] functional and 6-31G(d,p).[5] Single point energy was calculated by the M06-2X[6] DFT functional and 6-311G(d,p) basis set; solvent (chloroform) was included by means of an IEFPCM[7] method with the SMD universal solvation model[8] and SAS cavity. The energy from these single point calculations was added to the Gibbs free energy correction, that was obtained from the frequency calculations using using a free-rotor approximation for vibrational modes below 100 cm^{-1} and a rigid rotor approximation above this cut-off as described by Grimme[9] and implemented in the "goodvibes" program.[10] Figure 5 was prepared with *Pymol v0.*99.[11] Non-covalent interaction index (NCI)[12] were calculated using NCI-PLOT.[12b]

Cartesian coordinates for the complex shown in figure 4:

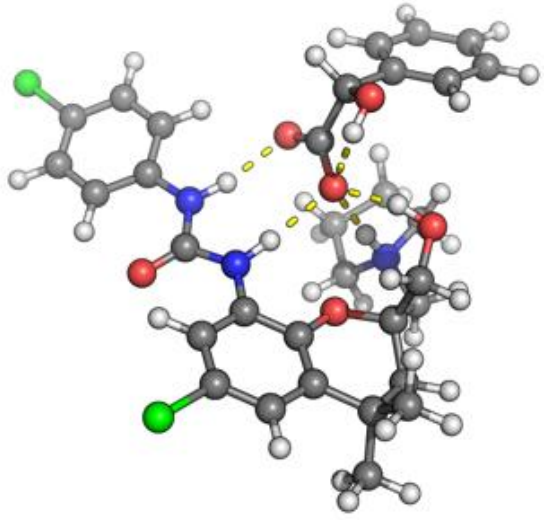


Single point energy: -2777.51961411 a.u.
ΔG correction: 0.590098 a.u.

Cl	3.06969	-4.89288	2.60160
Cl	-7.89633	-2.86612	-0.59324
O	2.29799	-0.23433	-0.93061
O	-1.07714	-3.34084	0.28507
O	2.47730	2.71876	0.04359
H	1.60006	2.32740	0.26800
N	0.14865	-1.39628	0.12551
H	0.11443	-0.38383	-0.01439
N	-2.14411	-1.33821	-0.14150
H	-2.01948	-0.32682	-0.22299
N	1.41220	1.71853	-2.48472
H	0.98935	1.66224	-1.52296
C	1.57476	-3.05516	1.26256
H	0.70878	-3.56956	1.65045
C	2.86348	-3.49215	1.55238
C	3.99025	-2.85650	1.05083
H	4.97371	-3.23299	1.30467
C	3.84860	-1.74383	0.20819
C	5.08846	-1.06600	-0.38899
C	4.65171	-0.02593	-1.45432
H	5.46385	0.68860	-1.63377
H	4.48632	-0.56067	-2.39689
C	3.34686	0.72413	-1.14300
C	2.55493	-1.29708	-0.08002
C	1.40390	-1.93462	0.44194
C	-1.04031	-2.12652	0.11197

C	-3.48199	-1.76723	-0.22956
C	-3.88429	-3.11314	-0.19278
H	-3.14167	-3.88783	-0.07269
C	-5.23520	-3.44084	-0.30248
H	-5.54092	-4.48101	-0.27203
C	-6.18991	-2.43930	-0.45120
C	-5.80840	-1.09980	-0.48832
H	-6.55559	-0.32178	-0.59984
C	-4.46216	-0.76861	-0.37716
H	-4.16000	0.27321	-0.39940
C	3.45230	1.69649	0.06266
H	3.40867	1.11374	0.99074
H	4.42886	2.19160	0.02324
C	2.90217	1.50806	-2.39883
H	3.37347	2.49116	-2.39119
H	3.19538	0.98199	-3.31006
C	0.65445	0.71488	-3.32189
H	1.20276	0.60564	-4.26263
H	0.64330	-0.23665	-2.79257
C	-0.71746	1.36873	-3.52134
H	-1.15591	1.05859	-4.47209
H	-1.39941	1.06952	-2.72280
C	-0.46054	2.90421	-3.45377
H	-1.11774	3.37510	-2.71851
H	-0.64181	3.39431	-4.41300
C	1.01925	3.05790	-3.05842
H	1.66031	3.23194	-3.92731
H	1.22813	3.81736	-2.30430
C	5.94404	-0.42068	0.72704
H	6.82559	0.06899	0.29723
H	6.29530	-1.18369	1.42723
H	5.39226	0.31997	1.30901
C	5.96849	-2.10956	-1.11878
H	5.39336	-2.65236	-1.87494
H	6.38290	-2.84333	-0.42283
H	6.81090	-1.61475	-1.61553
O	-2.13688	1.61193	-0.41748
O	0.07639	1.58200	-0.06048
O	-2.25759	4.22492	-0.42334
H	-2.84658	3.45933	-0.55813
C	-1.06600	2.16509	-0.09593
C	-1.13642	3.67416	0.24294
H	-0.23156	4.15508	-0.14925
C	-1.16942	3.87097	1.75654
C	-2.38993	4.01809	2.42190
H	-3.30773	4.03830	1.84436
C	-2.42340	4.16565	3.80876
H	-3.37757	4.28249	4.31466
C	-1.23725	4.16643	4.54408
H	-1.26391	4.28261	5.62363
C	-0.01547	4.02578	3.88345
H	0.91298	4.03588	4.44740
C	0.01938	3.88040	2.49655
H	0.97518	3.78127	1.98819

Cartesian coordinates for the arrangement found in the crystal structure:



Single point energy: -2777.520637 a.u.
ΔG correction: 0.590753 a.u.

Cl	-3.89811	-5.18912	-1.52441
Cl	7.51022	-3.86930	0.40419
O	-2.26127	0.01743	0.69999
O	0.62507	-3.71892	0.04700
O	-2.17998	2.77279	-0.87606
H	-1.35700	2.28758	-1.10307
N	-0.37463	-1.64868	-0.11570
H	-0.22271	-0.64305	-0.20083
N	1.92151	-1.80821	0.04581
H	1.90604	-0.78955	-0.02851
N	-0.99545	2.08728	1.71565
H	-0.66643	1.71981	0.78693
C	-2.07958	-3.31988	-0.74811
H	-1.31857	-4.03236	-1.02804
C	-3.43341	-3.62074	-0.86875
C	-4.42737	-2.72593	-0.49914

H	-5.46748	-3.00650	-0.61243	C	1.07414	3.16382	2.40680
C	-4.07957	-1.47477	0.03290	H	1.81274	3.40294	1.64037
C	-5.16783	-0.49377	0.48684	H	1.28840	3.78475	3.28007
C	-4.51728	0.68249	1.26201	C	-0.35605	3.44709	1.90548
H	-5.21172	1.52975	1.30312	H	-0.95426	3.97682	2.65130
H	-4.35599	0.35350	2.29520	H	-0.41601	3.97825	0.95554
C	-3.15183	1.14570	0.73016	C	-5.98752	-0.00018	-0.72928
C	-2.72151	-1.16568	0.15022	H	-6.75612	0.71303	-0.40950
C	-1.70557	-2.07087	-0.24123	H	-6.49402	-0.84051	-1.21234
C	0.72727	-2.49763	-0.00921	H	-5.36844	0.48218	-1.48802
C	3.21367	-2.36266	0.12696	C	-6.14226	-1.19008	1.46706
C	3.47425	-3.72632	0.34109	H	-5.60553	-1.62996	2.31296
H	2.65029	-4.41802	0.43563	H	-6.70470	-1.98765	0.97531
C	4.79038	-4.17998	0.42215	H	-6.86853	-0.46802	1.85745
H	4.98775	-5.23375	0.58627	O	2.23232	1.11261	-0.31354
C	5.84875	-3.28514	0.29560	O	0.03741	1.26109	-0.76872
C	5.60700	-1.92953	0.08230	O	0.47985	2.59492	-3.04809
H	6.43493	-1.23667	-0.02060	H	-0.08613	1.83543	-2.85134
C	4.29588	-1.47317	-0.00314	C	1.27743	1.55276	-0.97518
H	4.10055	-0.41991	-0.17861	C	1.56395	2.52994	-2.14101
C	-3.21832	1.84113	-0.66011	H	2.46512	2.15209	-2.64396
H	-3.24427	1.06811	-1.43820	C	1.86129	3.91065	-1.56651
H	-4.15636	2.40385	-0.71770	C	0.88906	4.91684	-1.59568
C	-2.50405	2.11320	1.74521	H	-0.06273	4.71096	-2.07262
H	-2.82133	3.13100	1.52113	C	1.15753	6.16929	-1.03703
H	-2.79922	1.86230	2.76632	H	0.40000	6.94750	-1.07456
C	-0.35197	1.21046	2.76512	C	2.39474	6.42704	-0.44480
H	-0.84265	1.44026	3.71619	H	2.60433	7.40375	-0.01809
H	-0.53291	0.16905	2.50241	C	3.36808	5.42478	-0.41596
C	1.11167	1.64840	2.74809	H	4.33747	5.61970	0.03410
H	1.59298	1.44173	3.70642	C	3.10375	4.17404	-0.97435
H	1.65388	1.11263	1.96614	H	3.85698	3.39223	-0.94669

Experimental procedure for the determination of the association constant for receptor 1 hexafluorophosphate with tetrabutylammonium iodide.

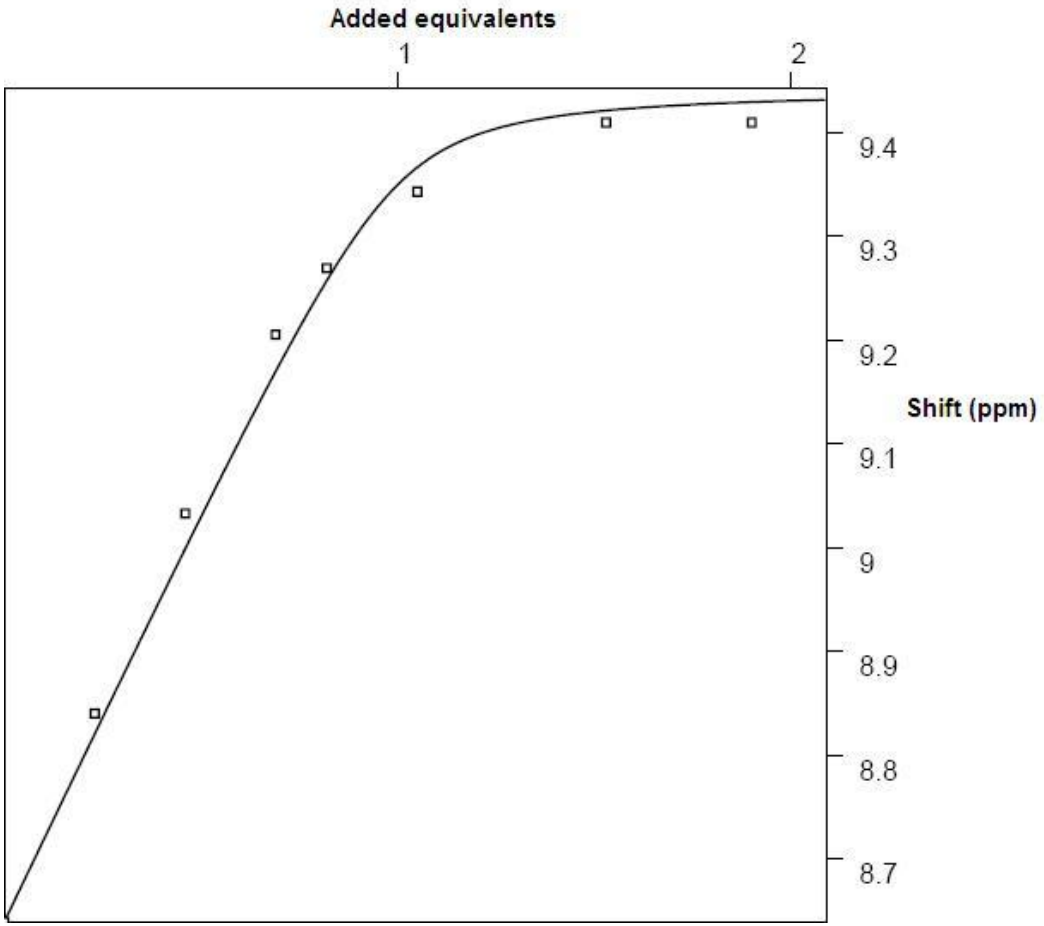
Receptor **1** hexafluorophosphate was prepared by treatment of receptor **1** with excess HPF_6 and successive washing with water.

A solution of the racemic receptor **1** hexafluorophosphate (4.0×10^{-2} M) was prepared in $CDCl_3$ (0.4 mL) and transferred to a standard NMR tube. The ^1H NMR spectrum was collected for this sample at 293 K. Aliquots of a solution of tetrabutylammonium iodide (2 eq) in $CDCl_3$ (0.2 mL) were then added to the NMR tube. After each addition, the contents of the tube were mixed well and a spectrum collected at 293 K. The chemical shift of one of the urea's NHs of the receptor after each addition were plotted and its movement was analyzed by a non-linear curve fitting a program based on Montecarlo Method to give K_{ass}[1] and the limiting chemical shift. Uncertainty of K determination is estimated around 20%.[2]

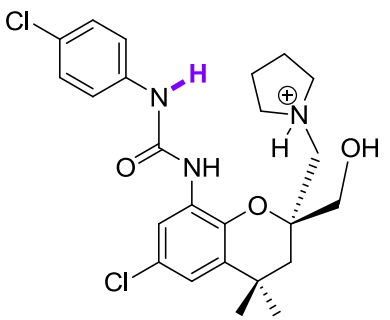
Figure S39. ^{1}H NMR titration of receptor 1 with (*L*)-mandelic acid (MeOD, 20ºC).

Association Constant
Constant: 1.7e+03 1/M
Max. shift (ppm): 9.4421

Host: Receptor 1 hexafluorophosphate Guest: NBu4I
Molecular weight: 624
Used weight (mg): 10
Total volume (ml): 0.4
Used volume (ml): 0.4



Shift (ppm)	Added equivalents
8.6388	0
8.8398	0.23
9.0326	0.46
9.2049	0.69
9.2688	0.82
9.3427	1.05
9.4093	1.53
9.4093	1.9



HPF_6·receptor **1**

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