A molecular receptor selective for zwitterioinic alanine

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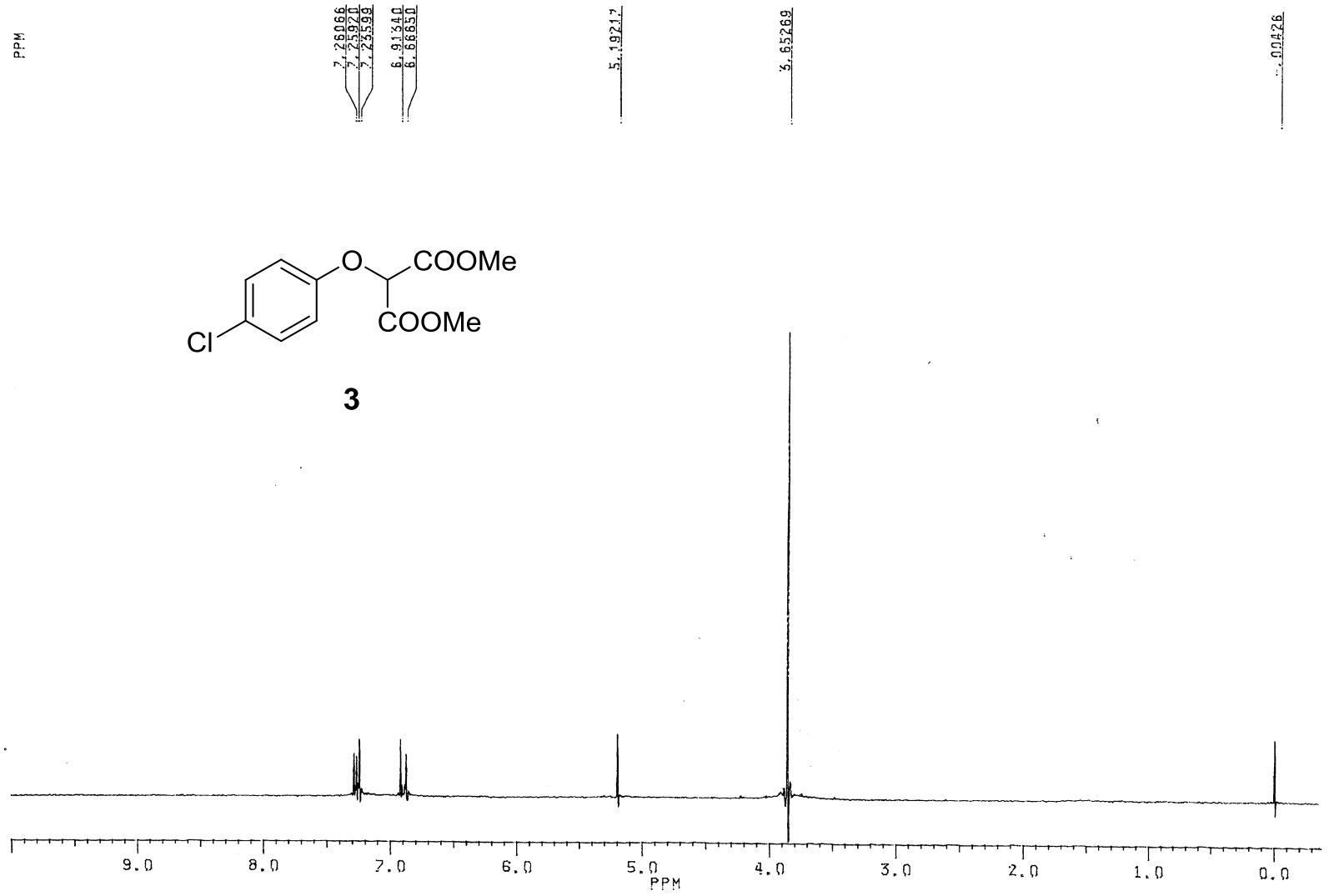


Figure S2. ^{13}C NMR spectrum of compound 3 (100 MHz, $CDCl_3$).

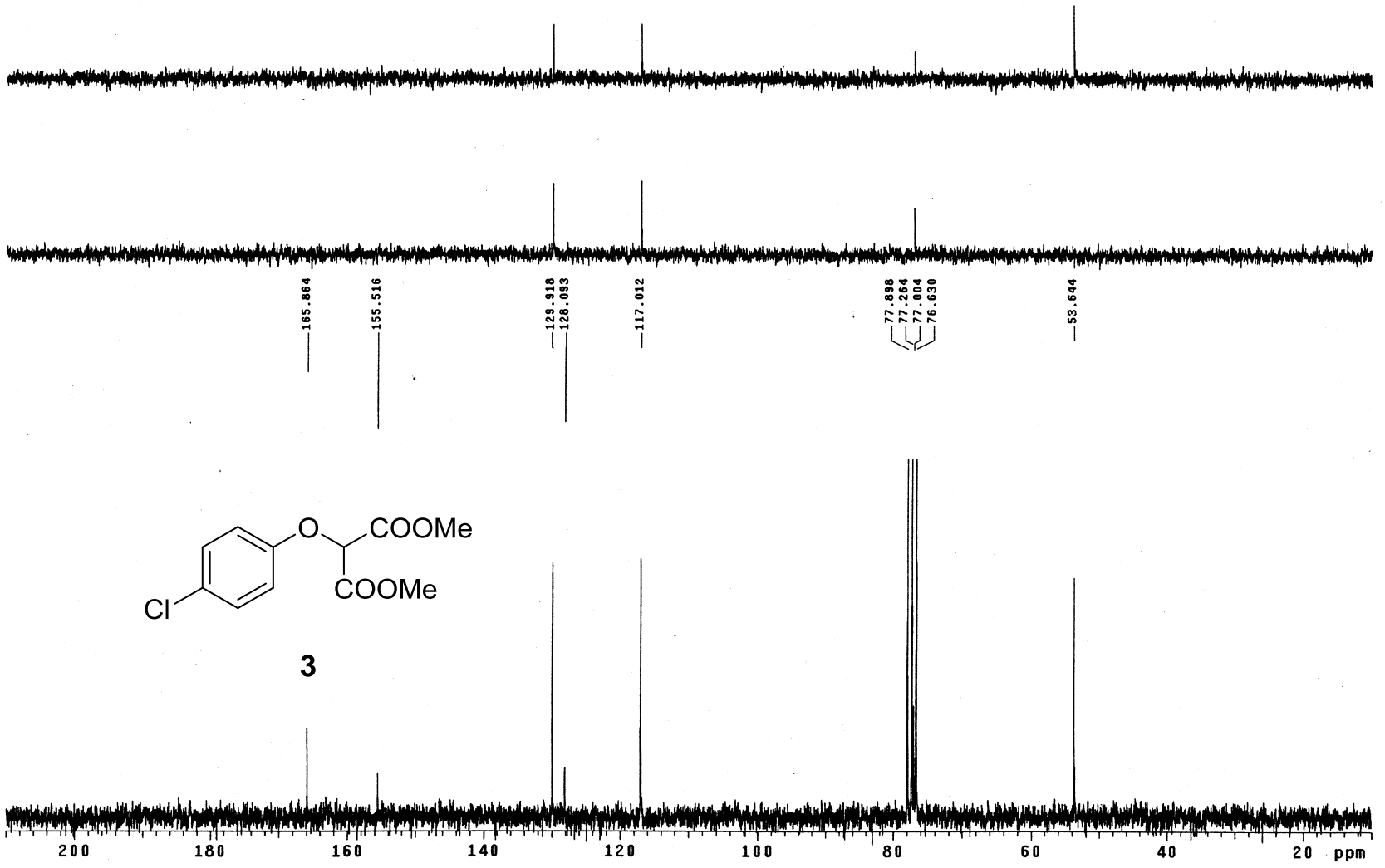


Figure S3. IR spectrum of compound 3.

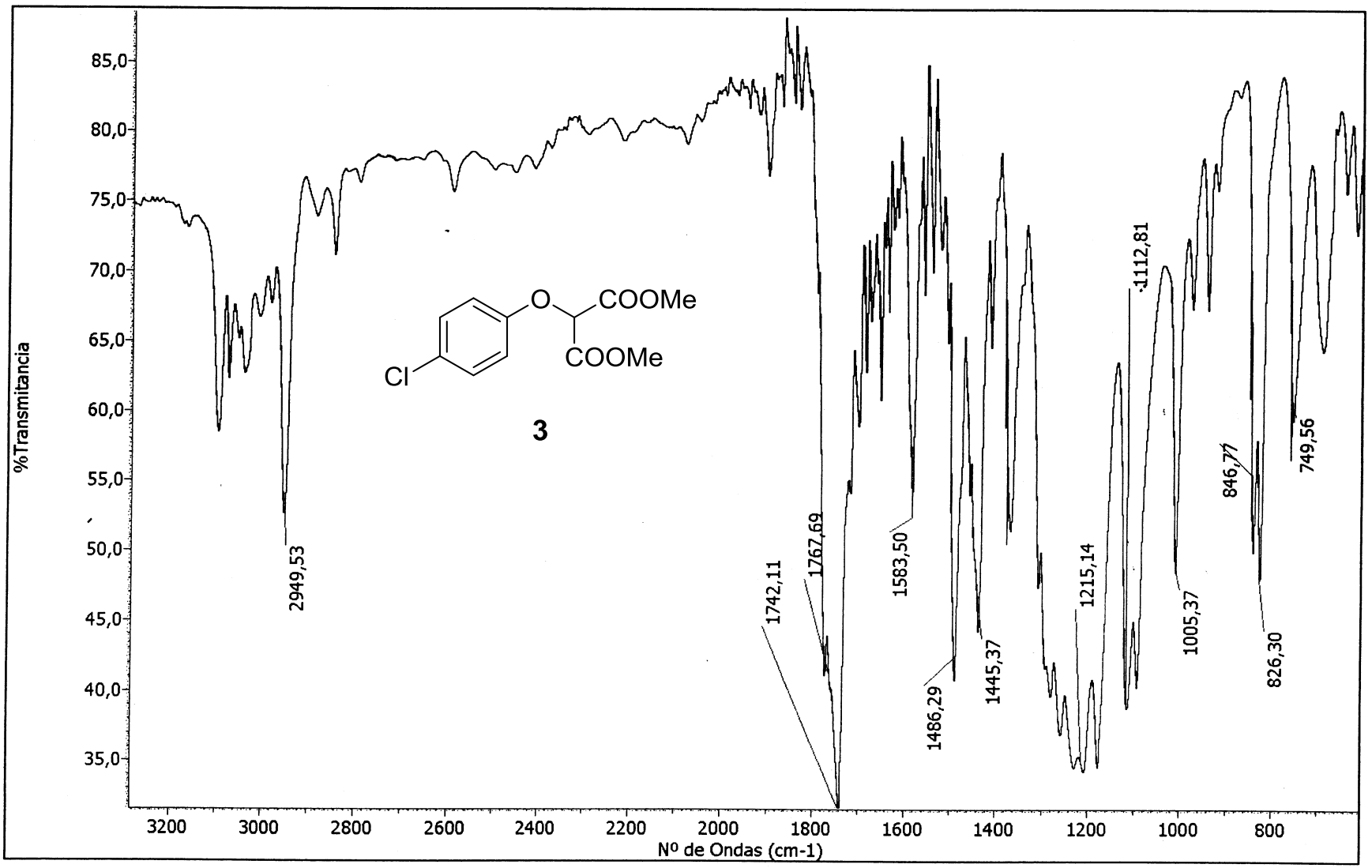


Figure S4. HRMS spectrum of compound 3 (ESI-QTOF).

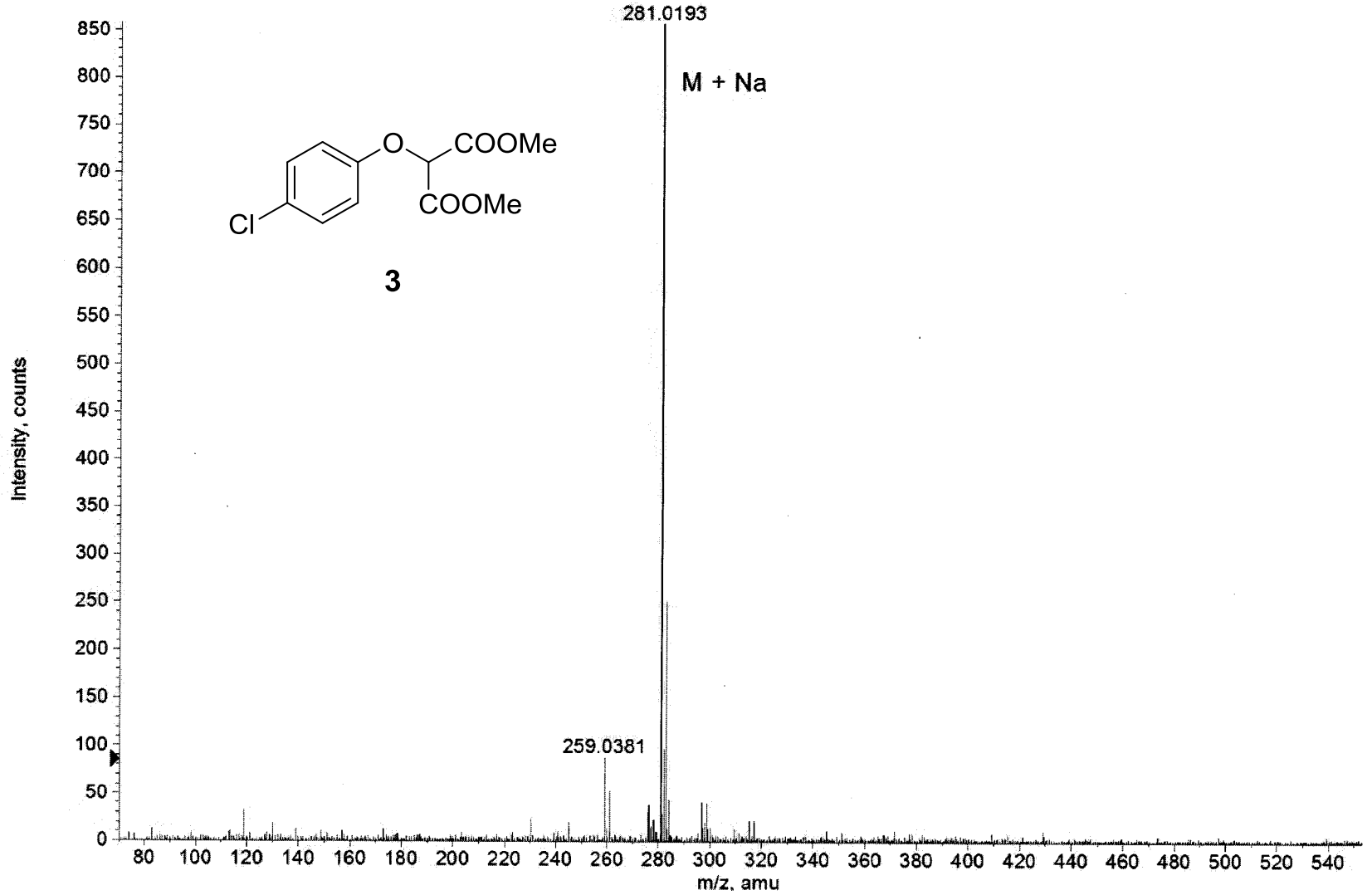


Figure S5. ^{1}H NMR spectrum of compound 4 (200 MHz, $CDCl_3$).

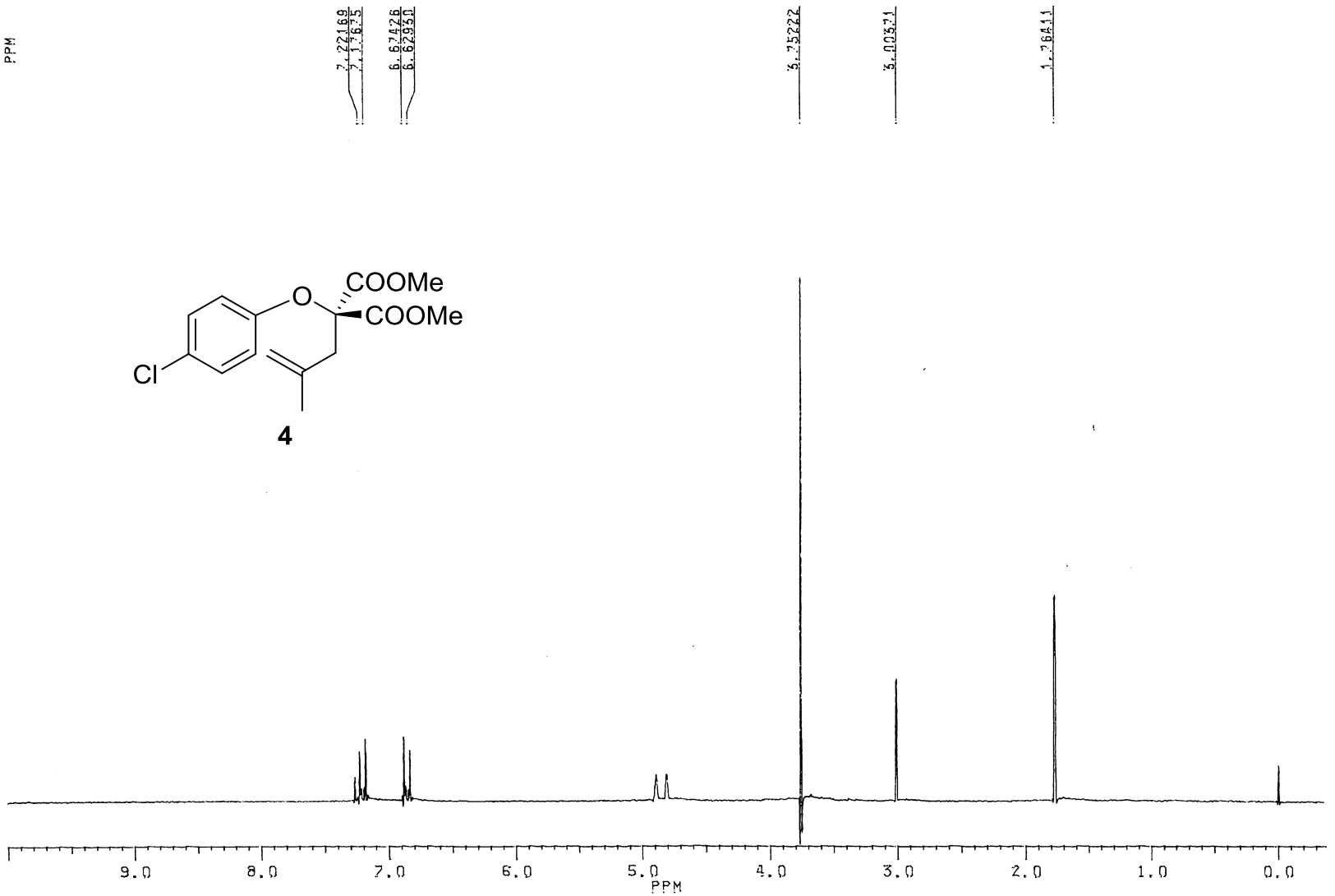


Figure S6. ^{13}C NMR spectrum of compound 4 (100 MHz, $CDCl_3$).

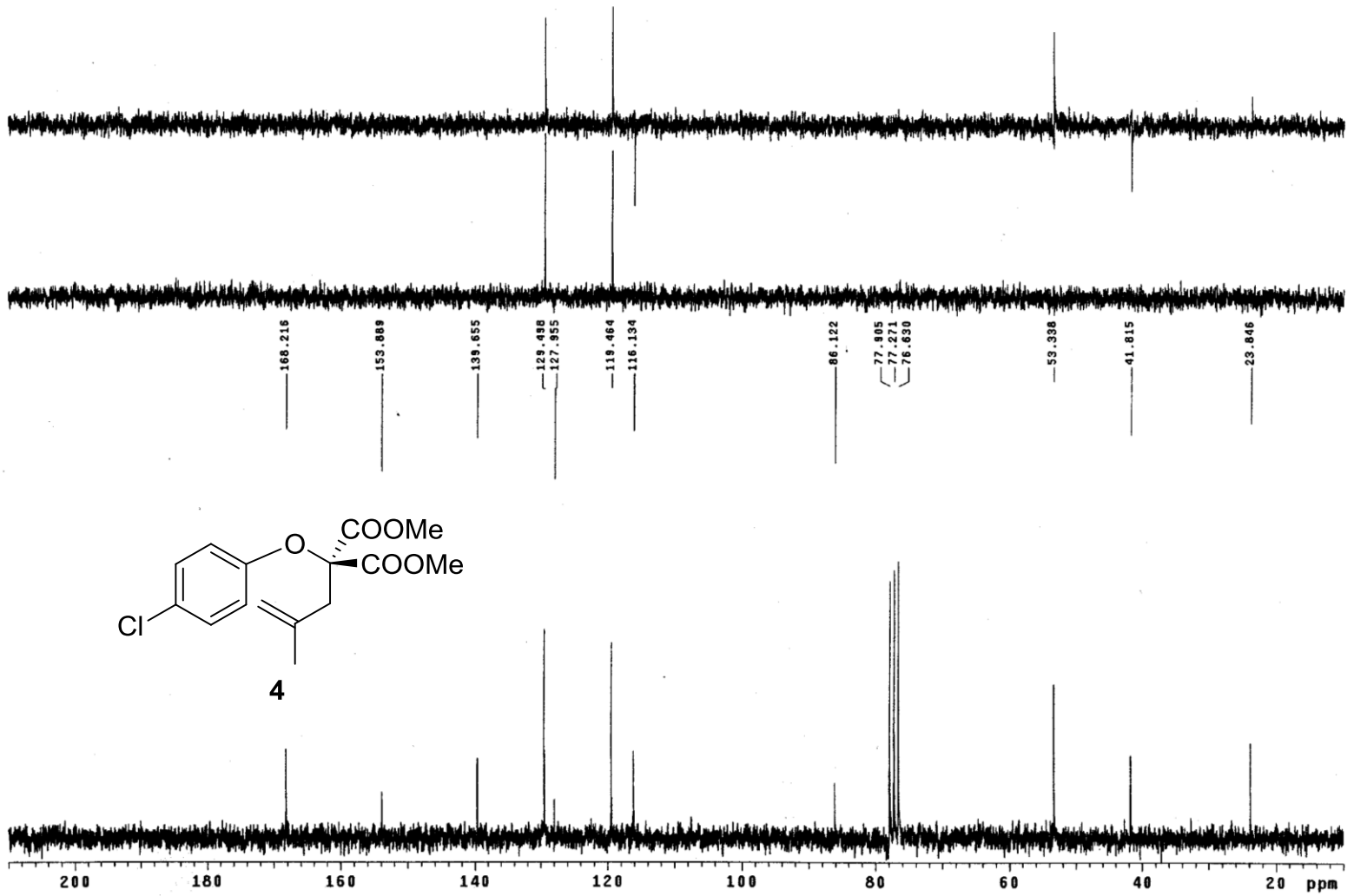


Figure S7. IR spectrum of compound 4.

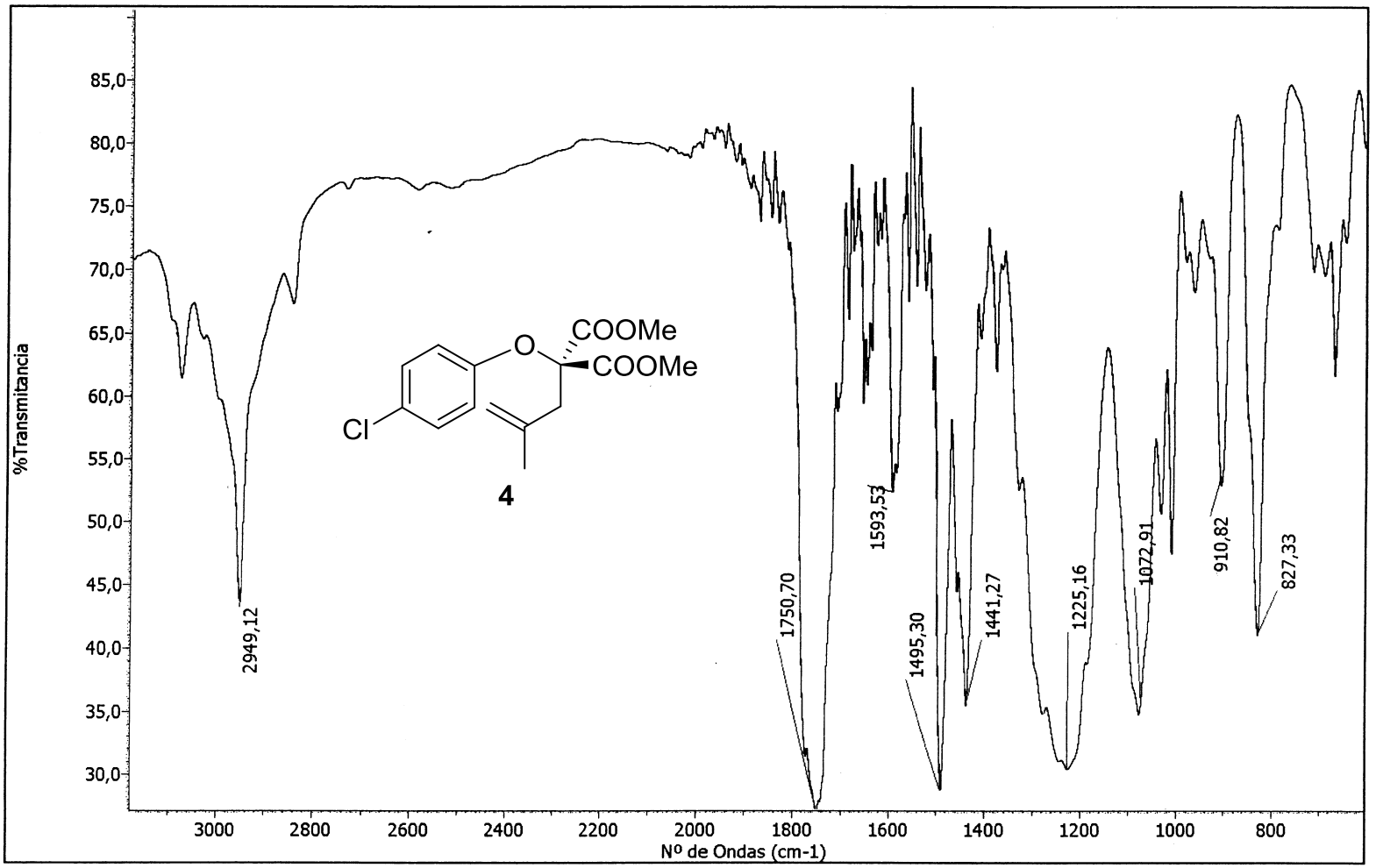


Figure S8. HRMS spectrum of compound 4 (ESI-QTOF).

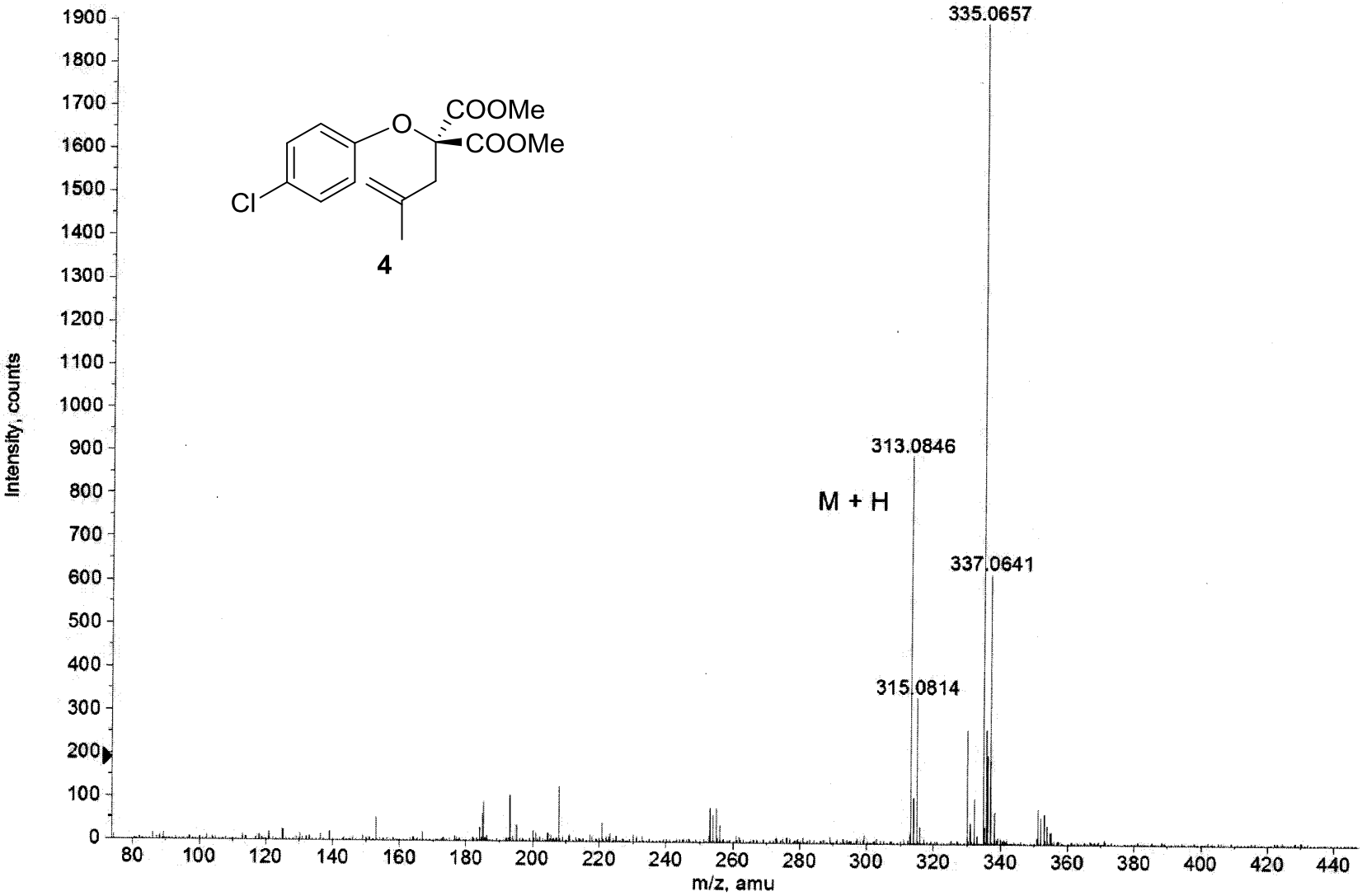


Figure S9. ^{1}H NMR spectrum of compound 5 (200 MHz, $CDCl_3$).

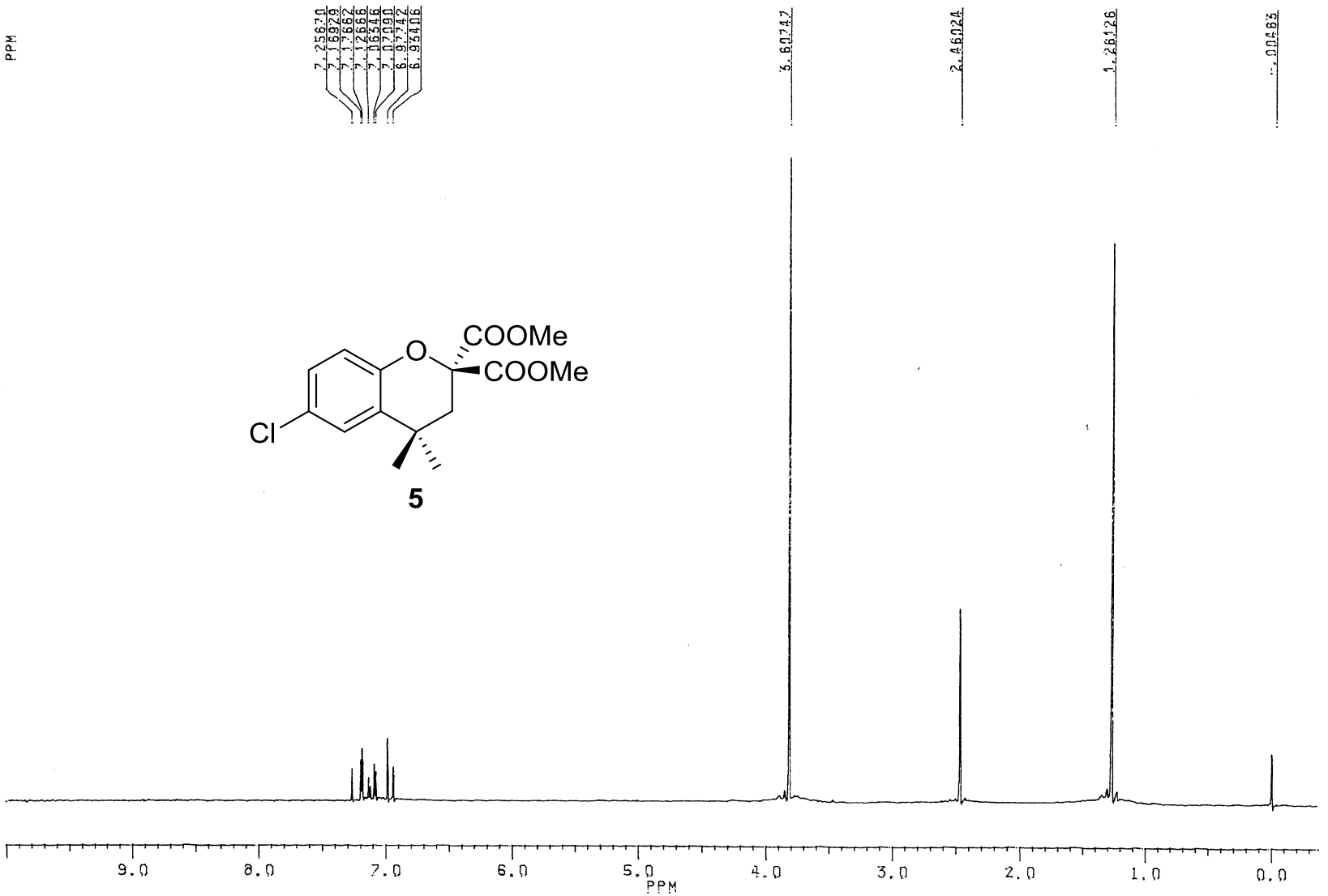


Figure S10. ^{13}C NMR spectrum of compound 5 (100 MHz, $CDCl_3$).

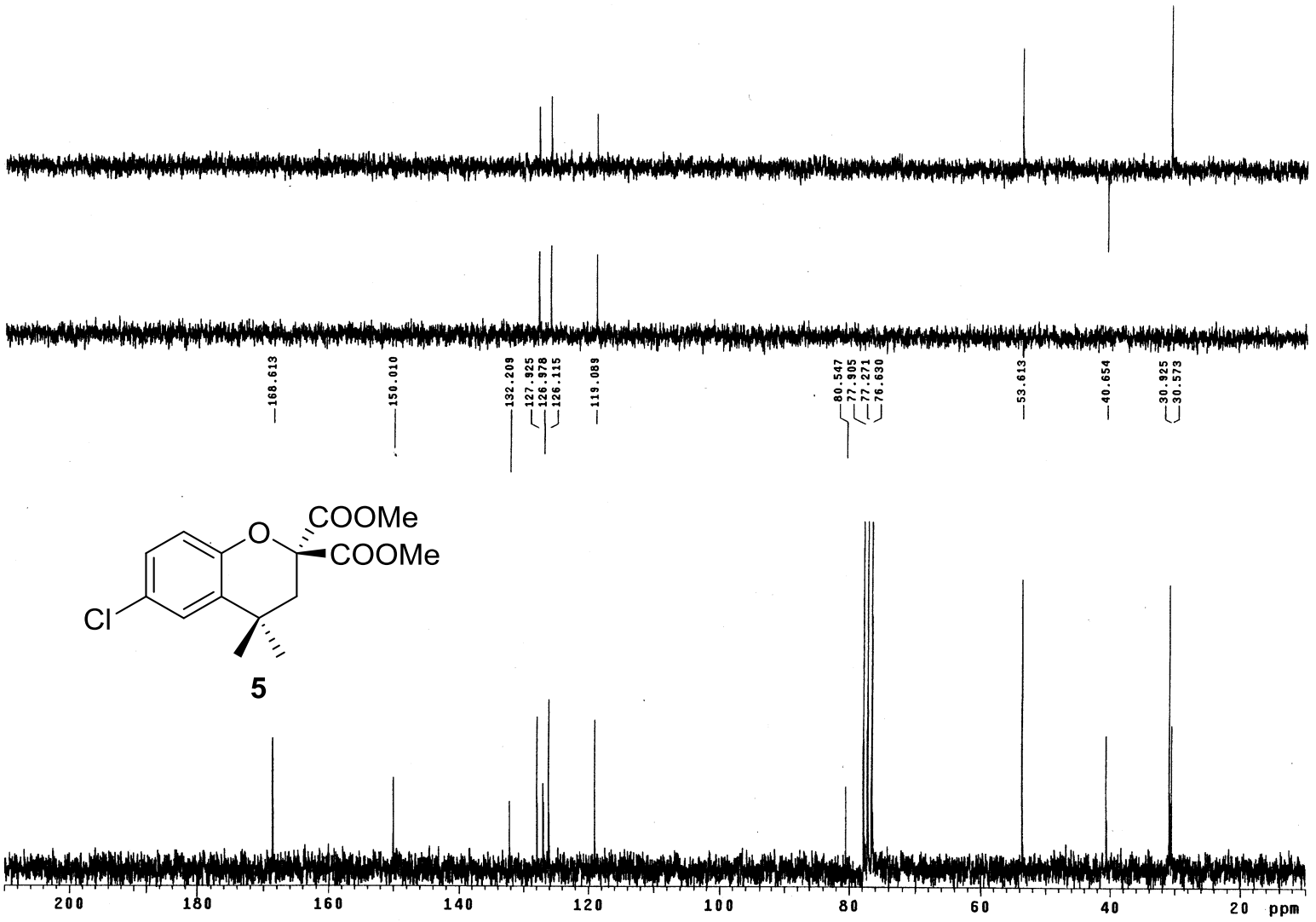


Figure S11. IR spectrum of compound 5.

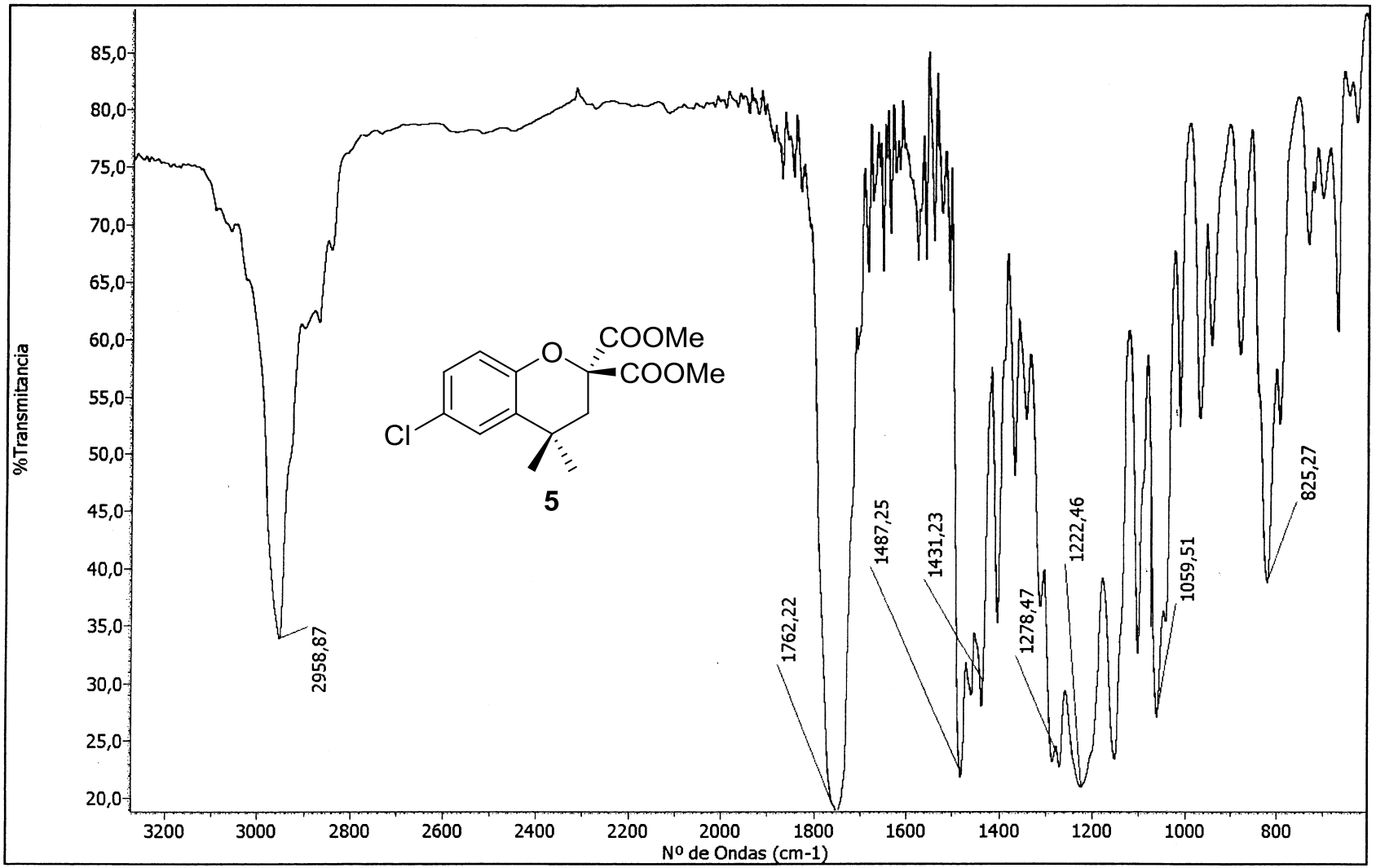


Figure S12. HRMS spectrum of compound 5 (ESI-QTOF).

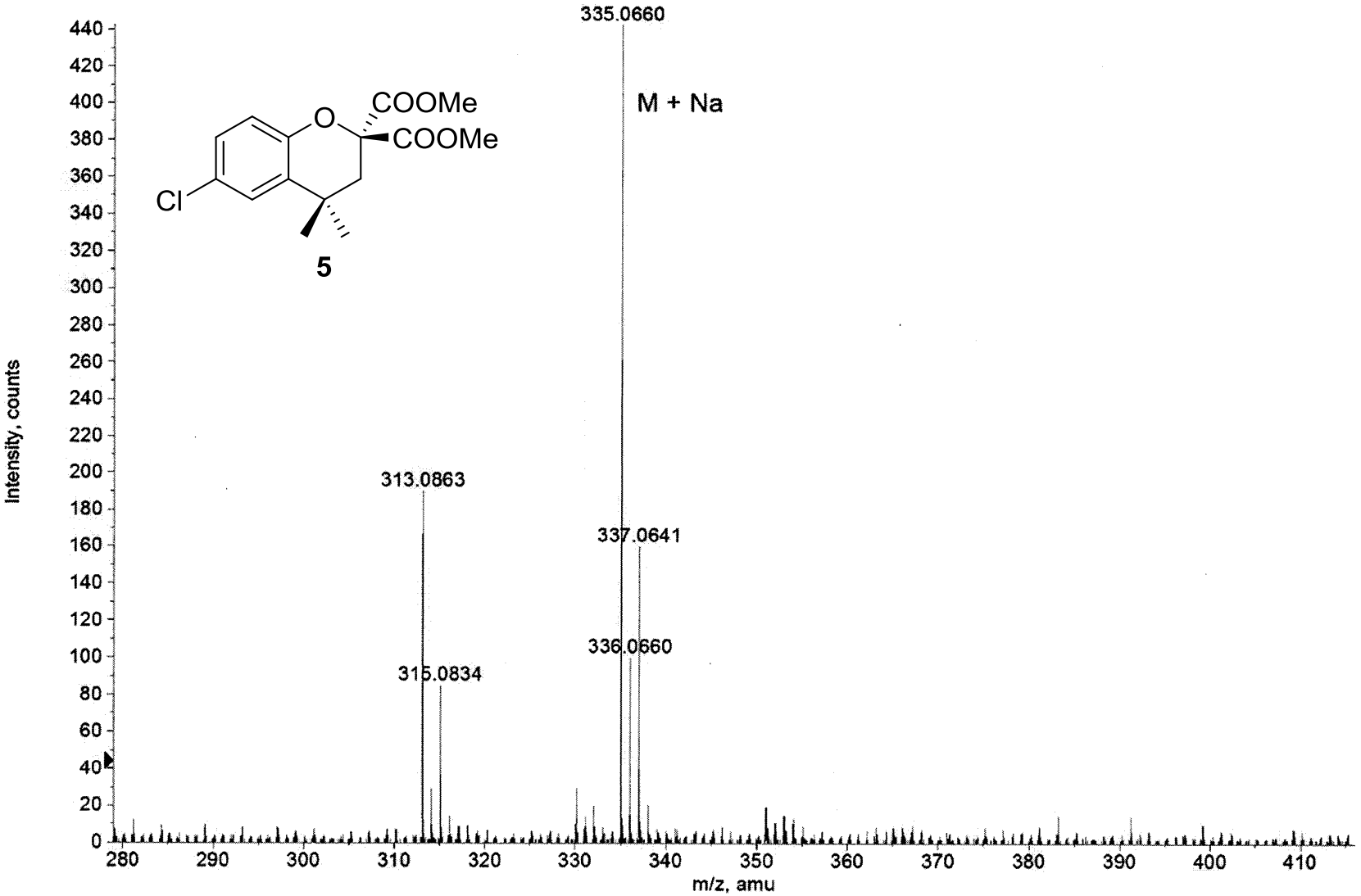


Figure S13. ^{1}H NMR spectrum of compound 6 (200 MHz, $CDCl_3$).

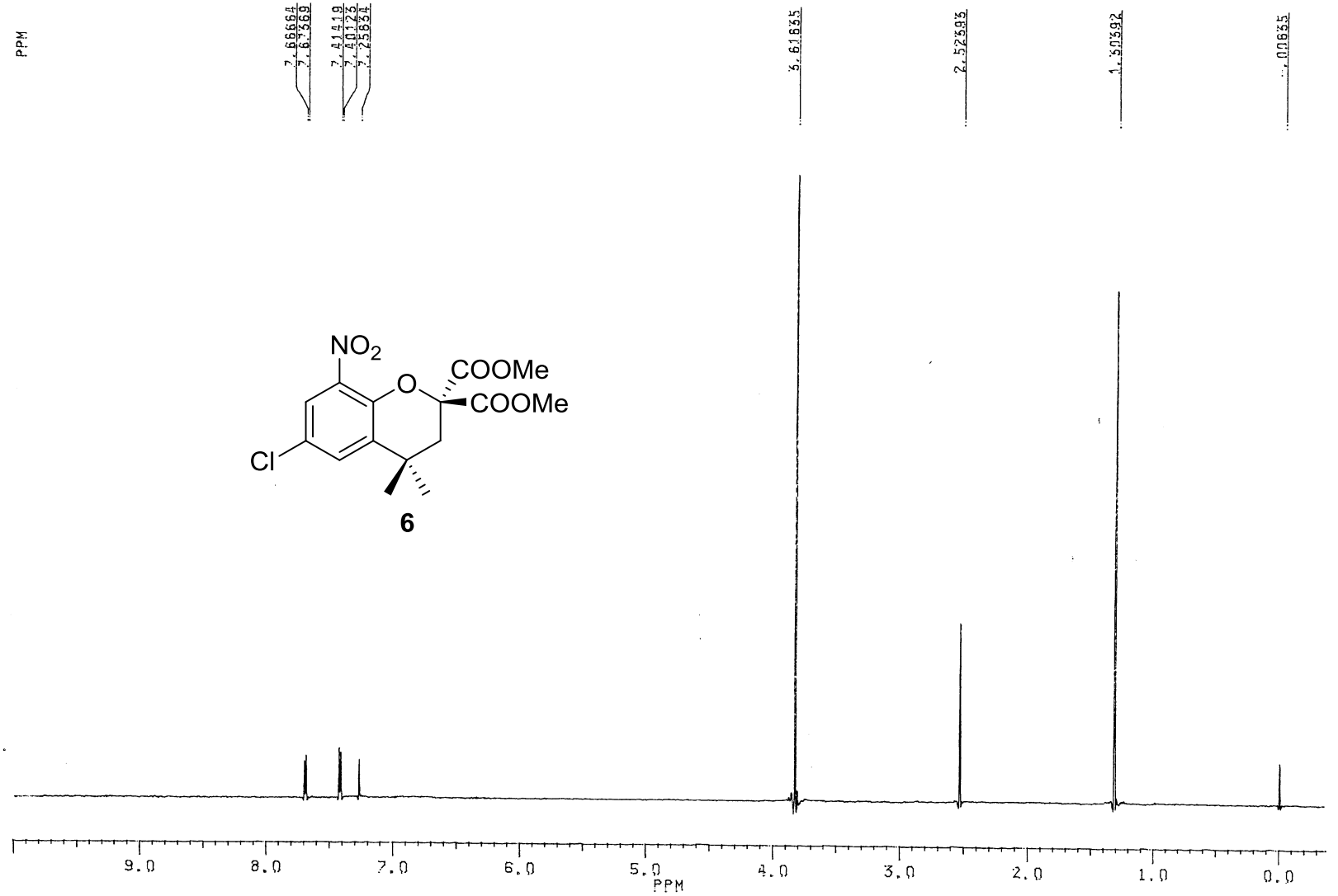


Figure S14. ^{13}C NMR spectrum of compound 6 (100 MHz, $CDCl_3$).

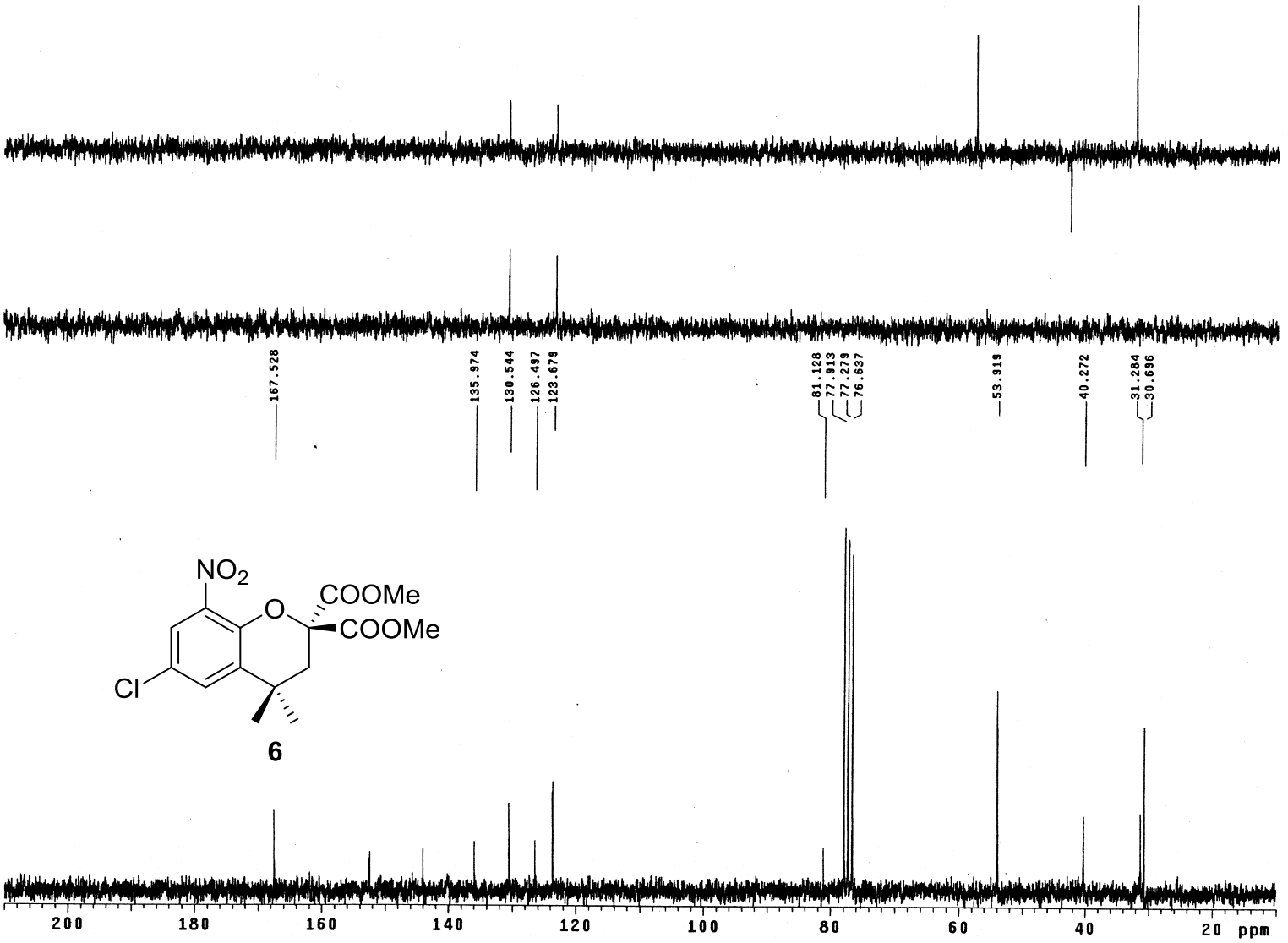


Figure S15. IR spectrum of compound 6.

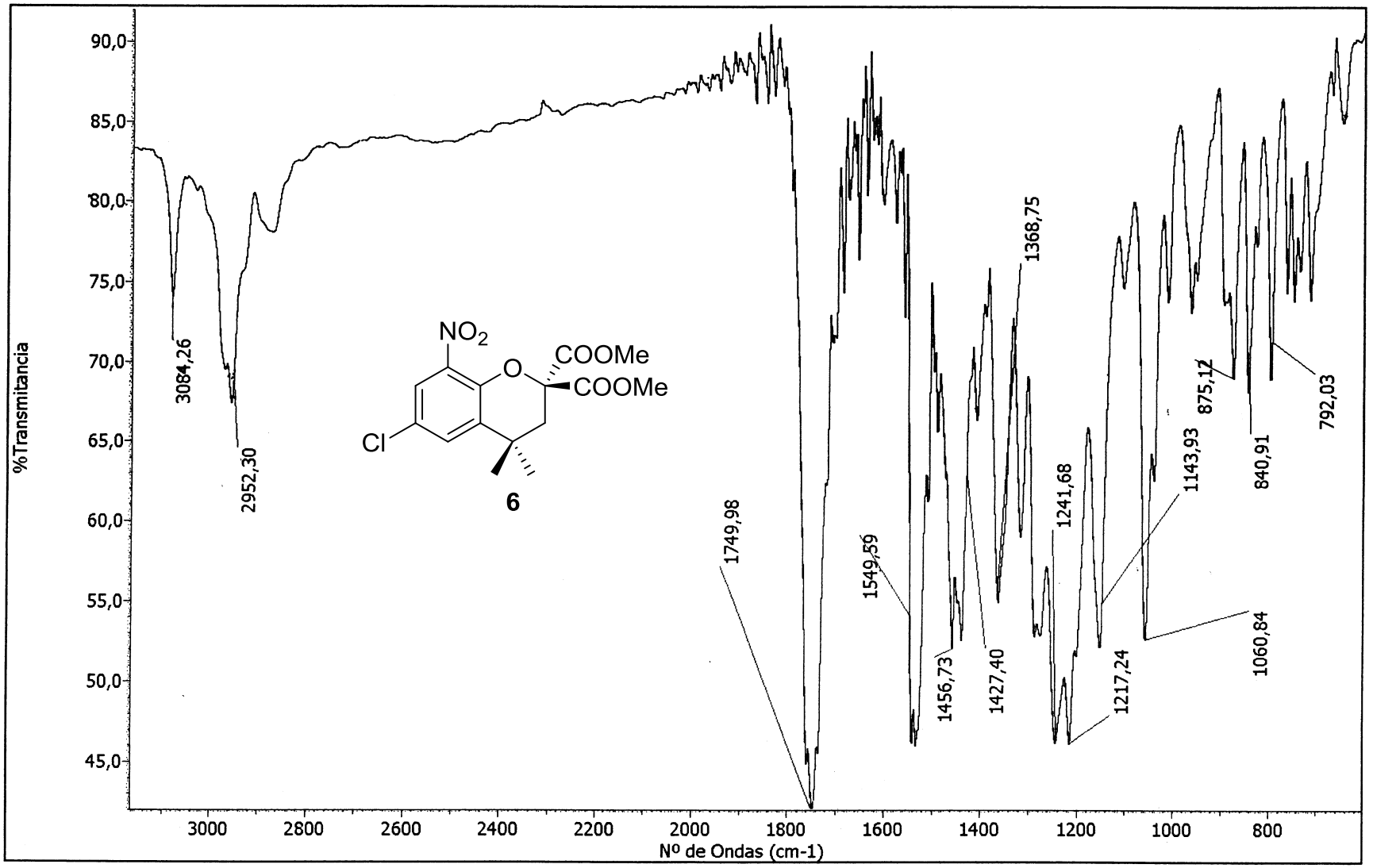


Figure S16. HRMS spectrum of compound 6 (ESI-QTOF).

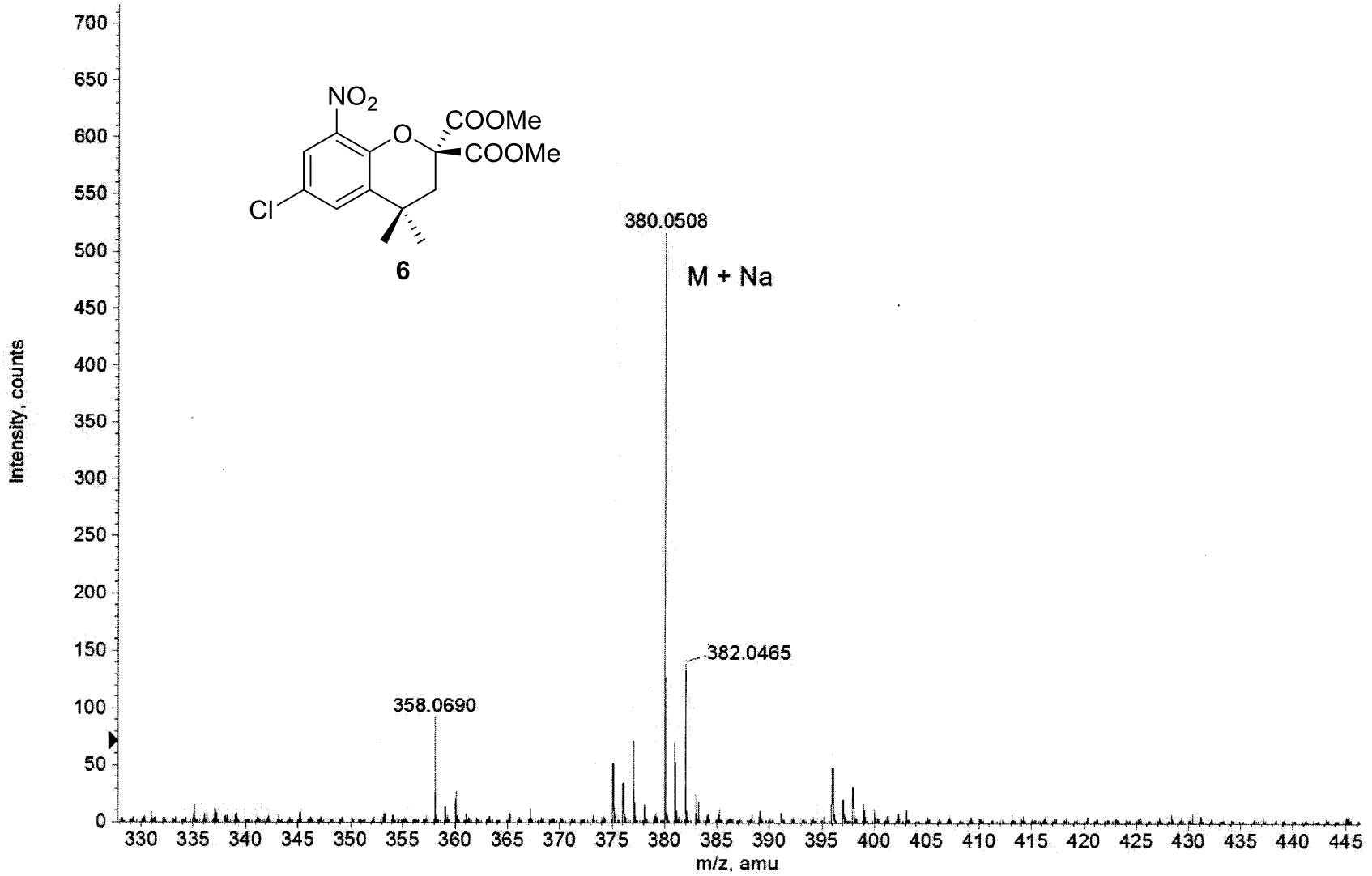


Figure S17. ^{1}H NMR spectrum of compound 7 (200 MHz, $CDCl_3$).

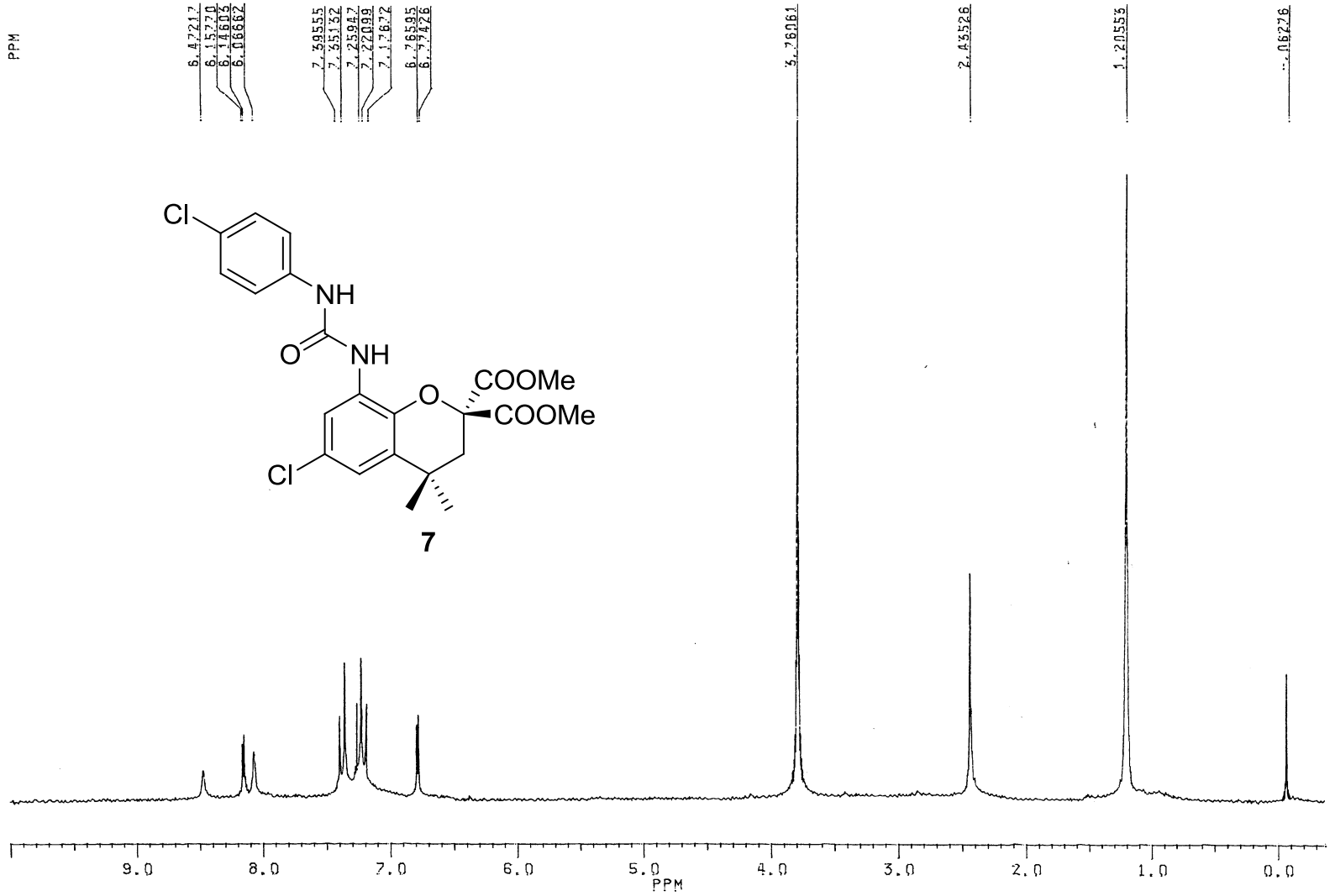


Figure S18. ^{13}C NMR spectrum of compound 7 (100 MHz, $CDCl_3$).

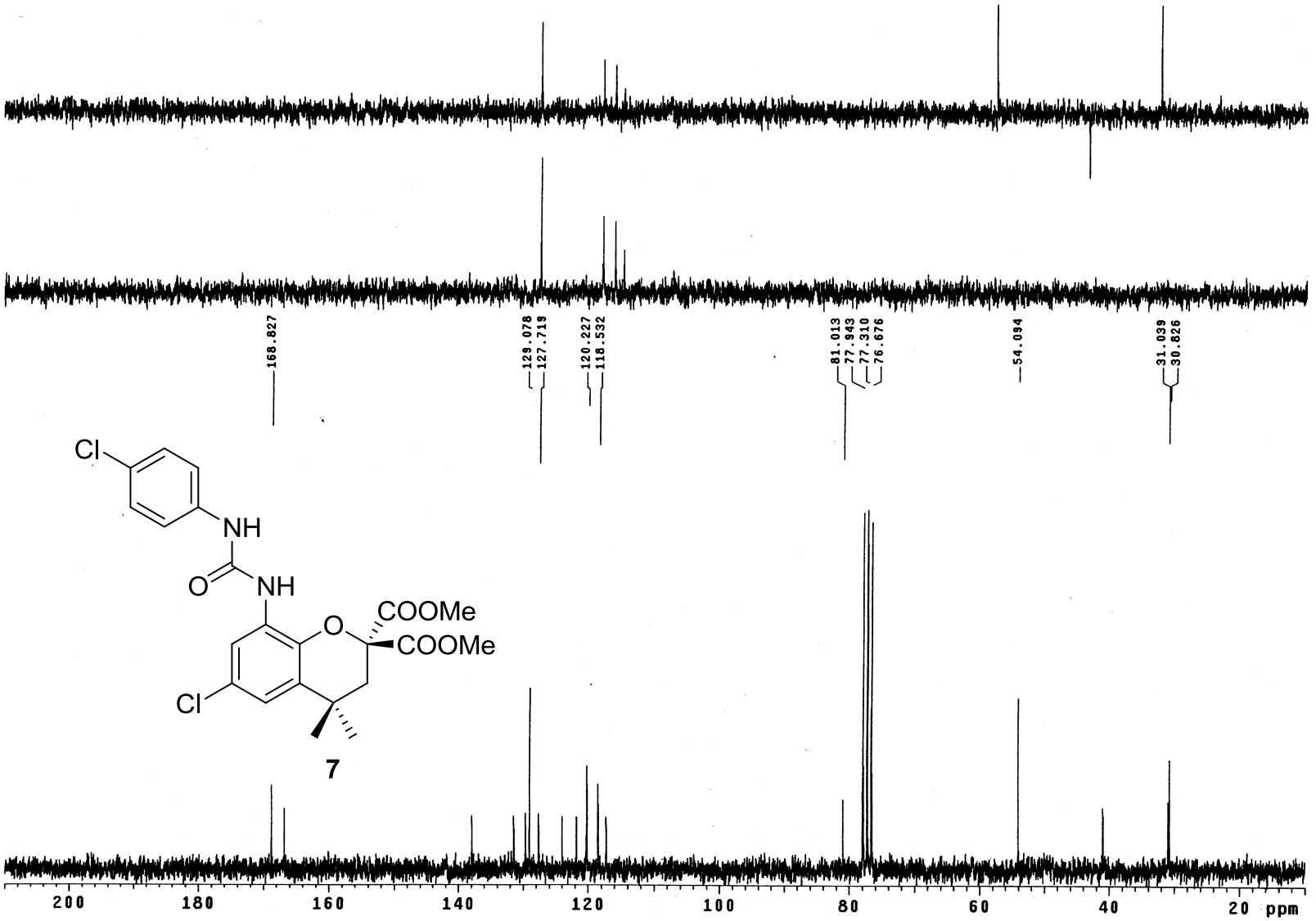


Figure S19. IR spectrum of compound 7.

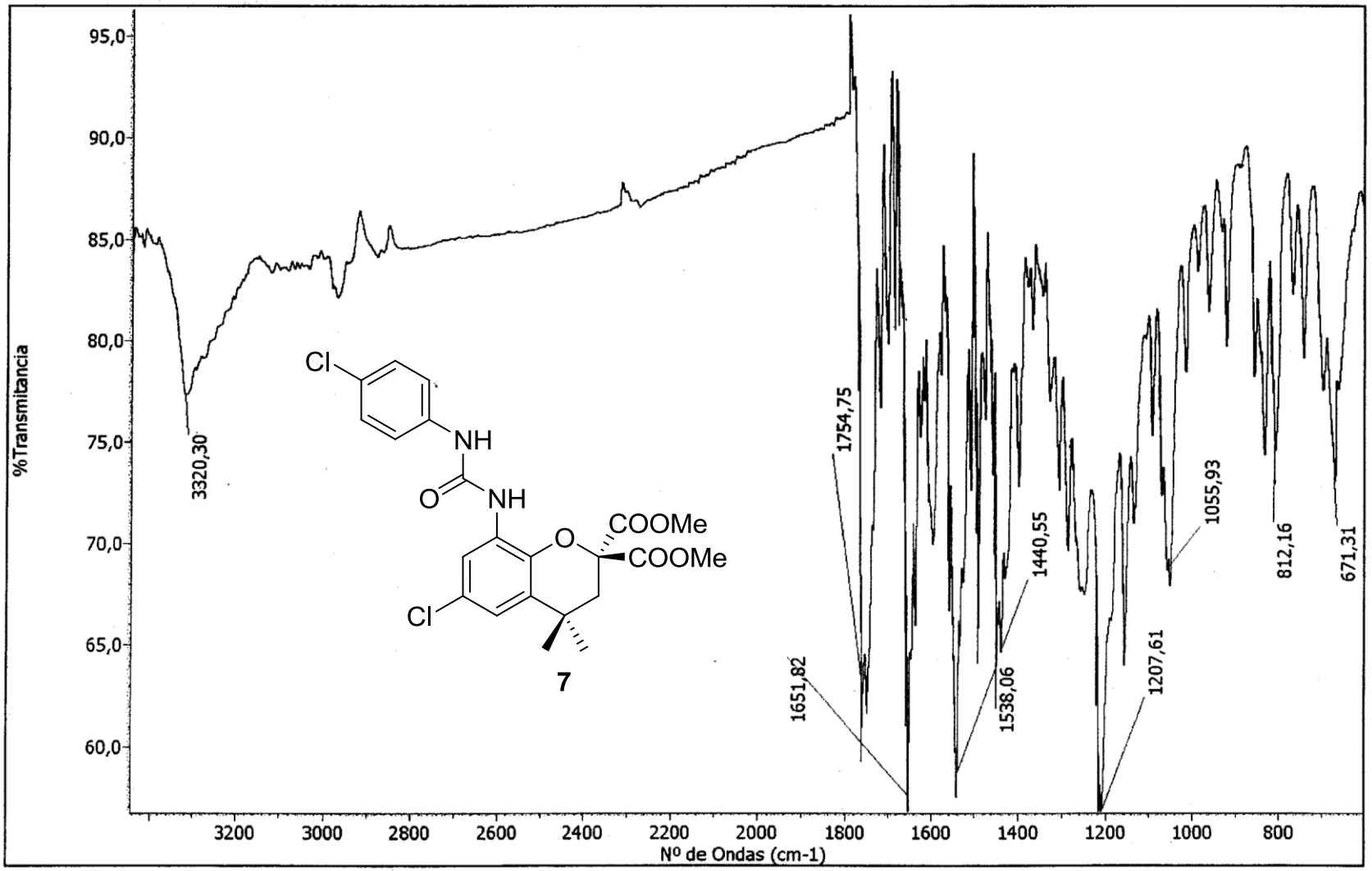


Figure S20. HRMS spectrum of compound 7 (ESI-QTOF).

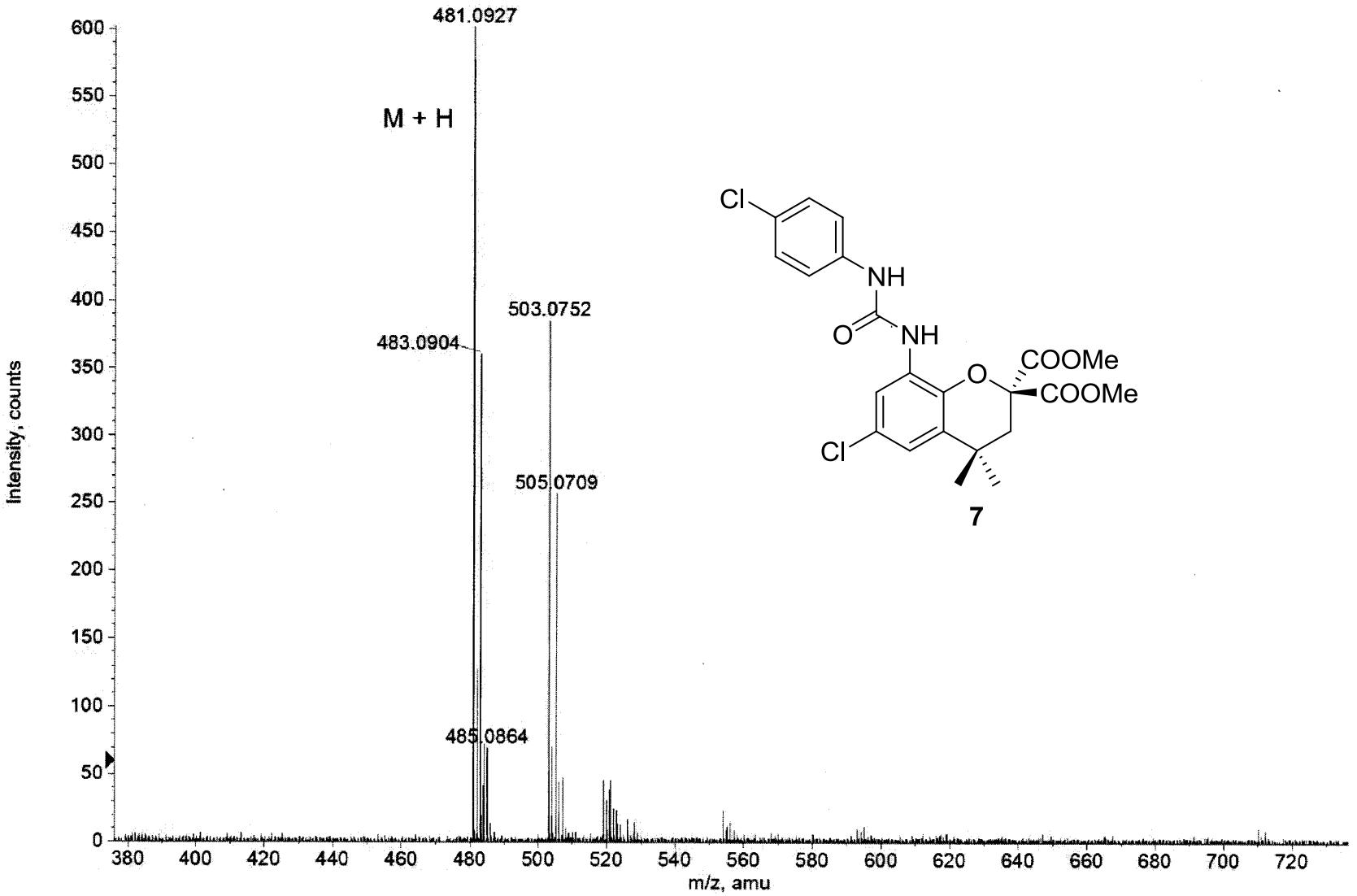


Figure S21. ^{1}H NMR spectrum of compound 8 (200 MHz, $CDCl_3$).

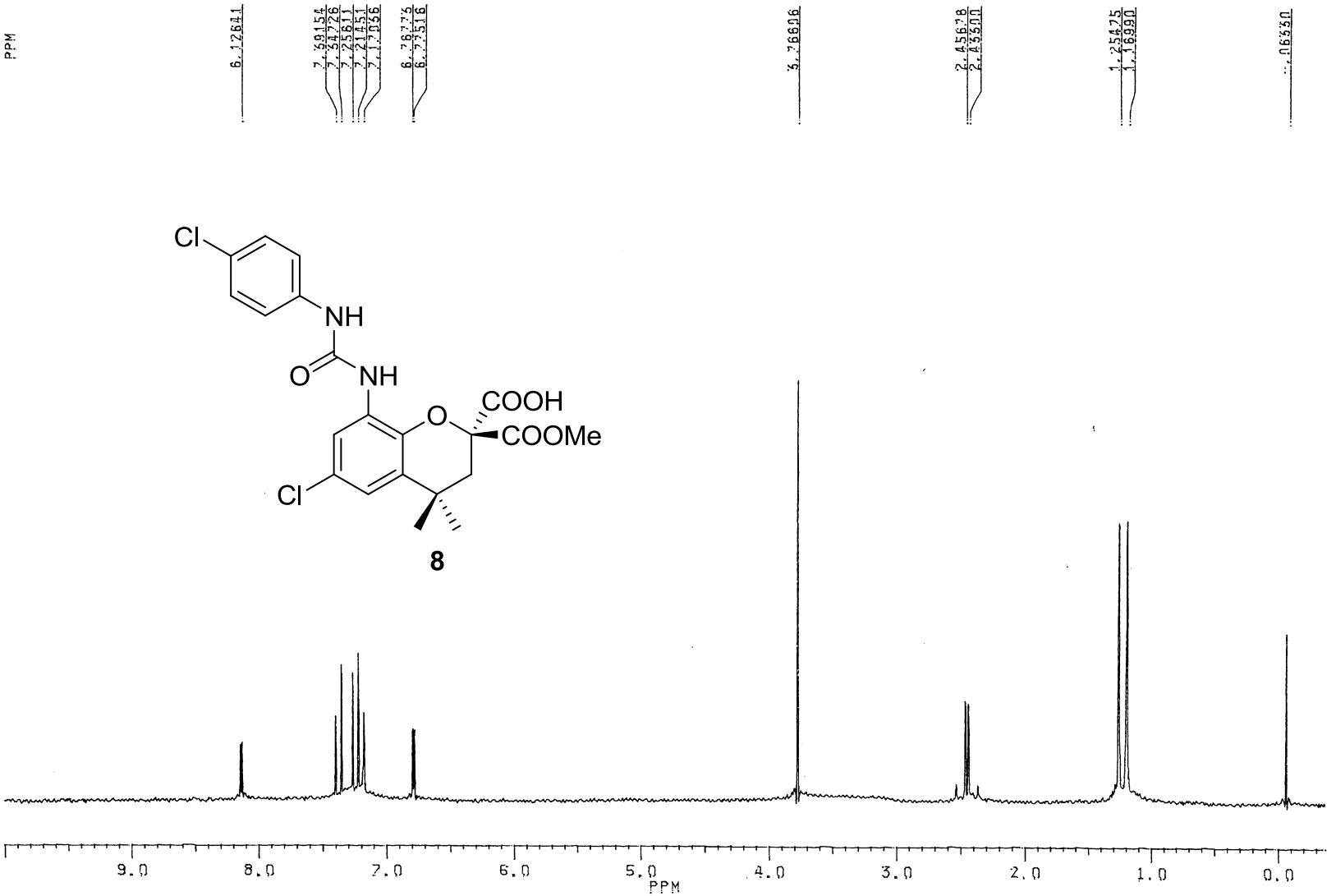


Figure S22. ^{13}C NMR spectrum of compound 8 (100 MHz, $CDCl_3$).

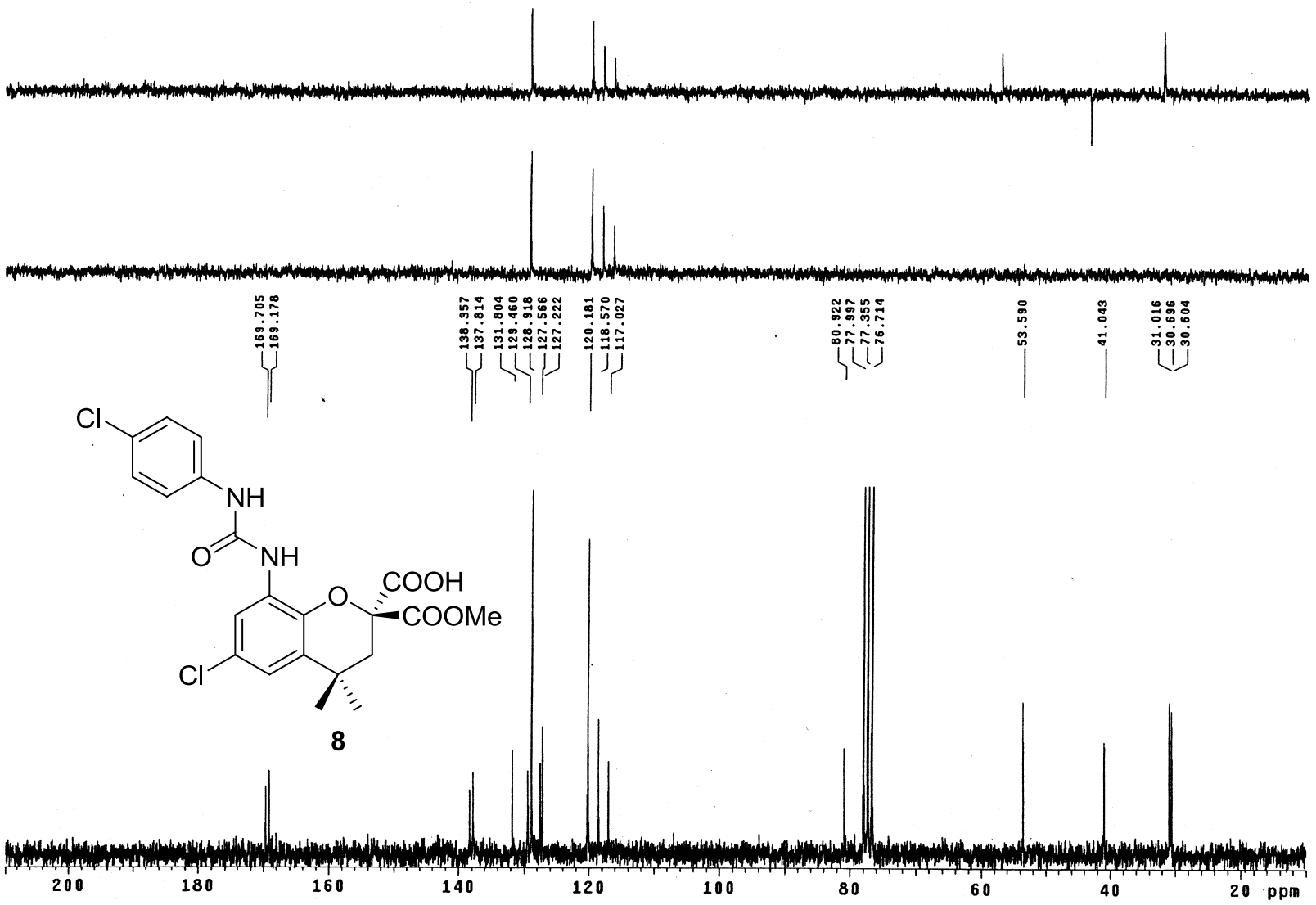


Figure S23. IR spectrum of compound 8.

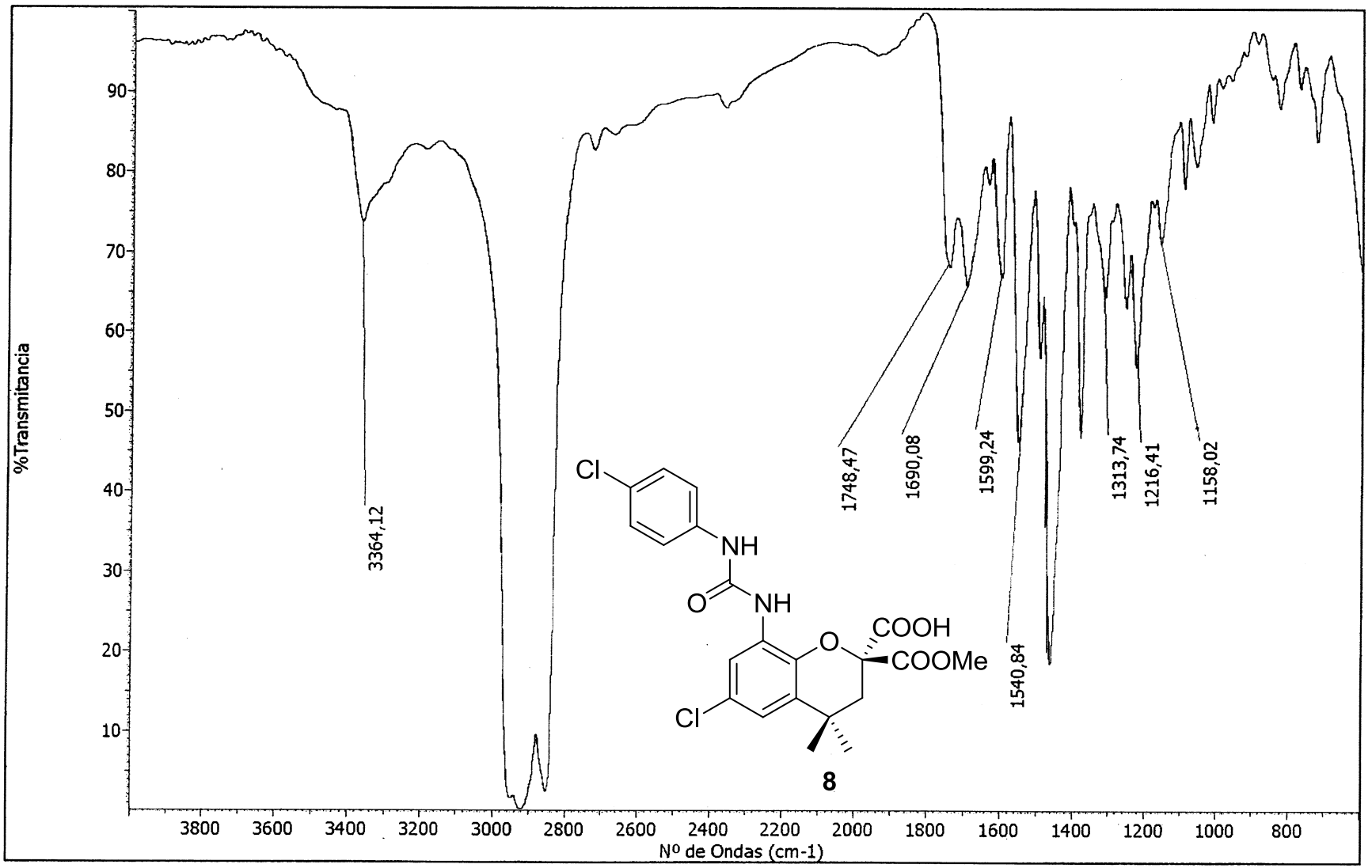


Figure S24. HRMS spectrum of compound 8 (ESI-QTOF).

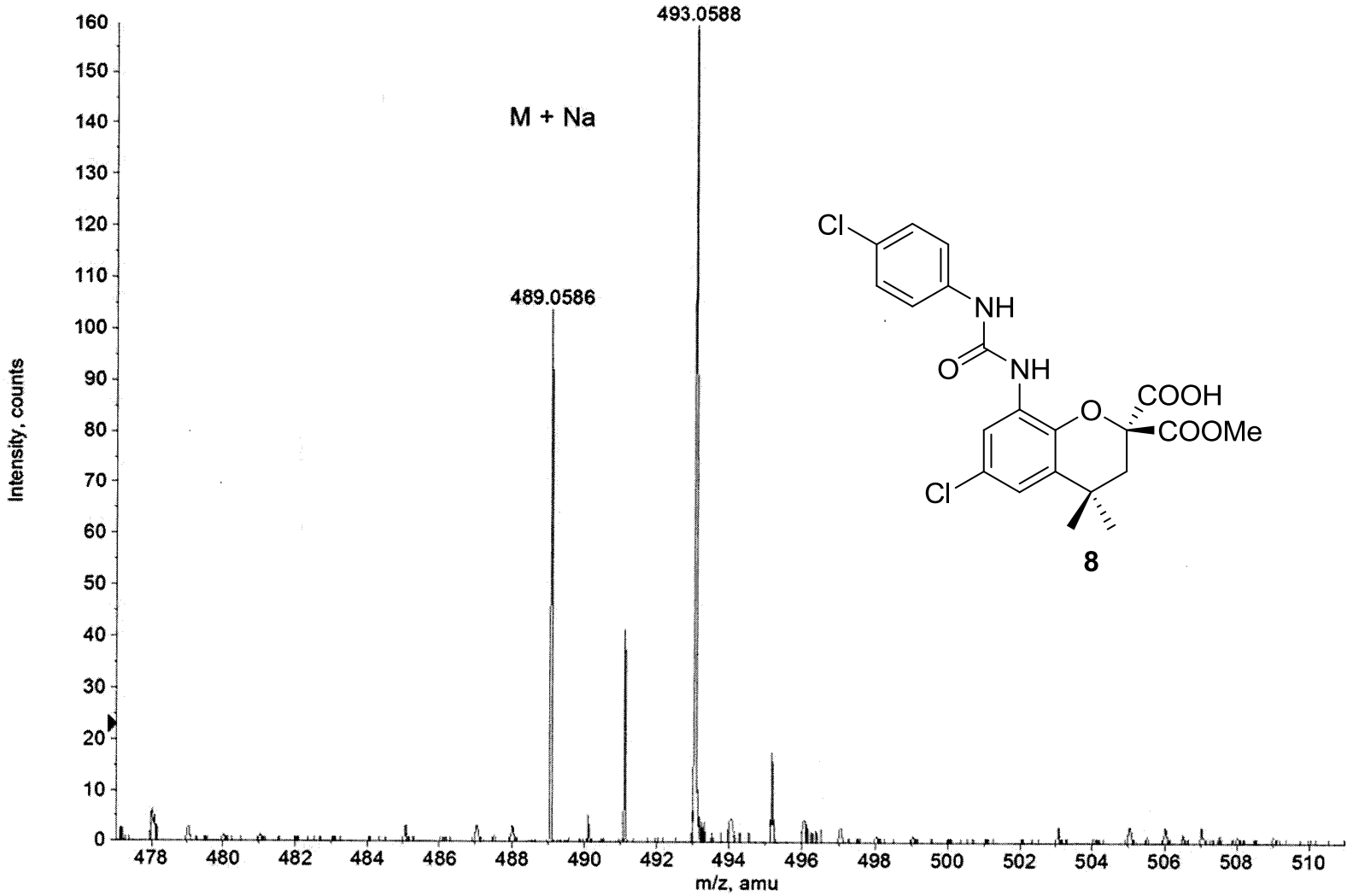


Figure S25. ^{1}H NMR spectrum of compound 9 (200 MHz, $CDCl_3$).

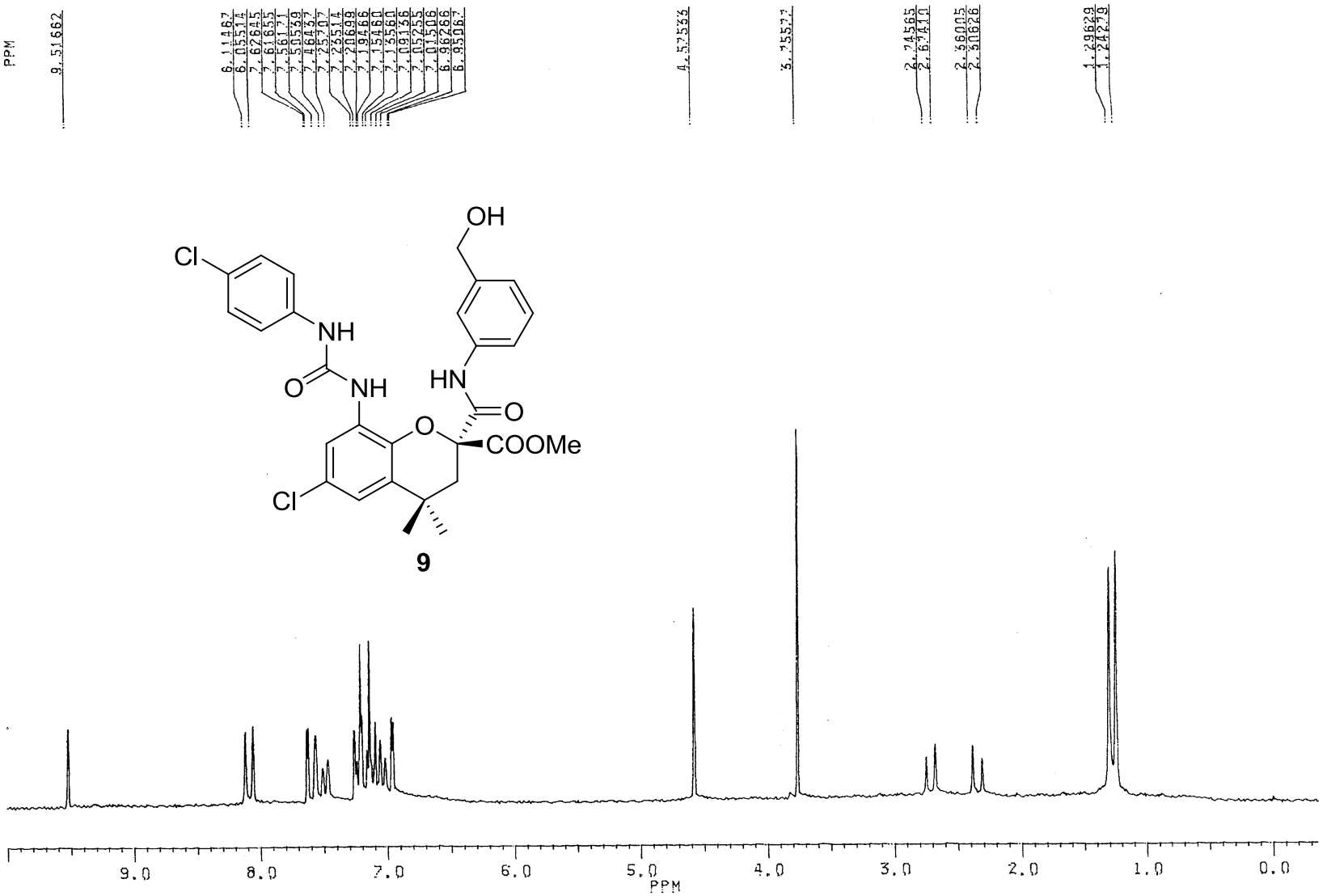


Figure S26. ^{13}C NMR spectrum of compound 9 (100 MHz, $CDCl_3$).

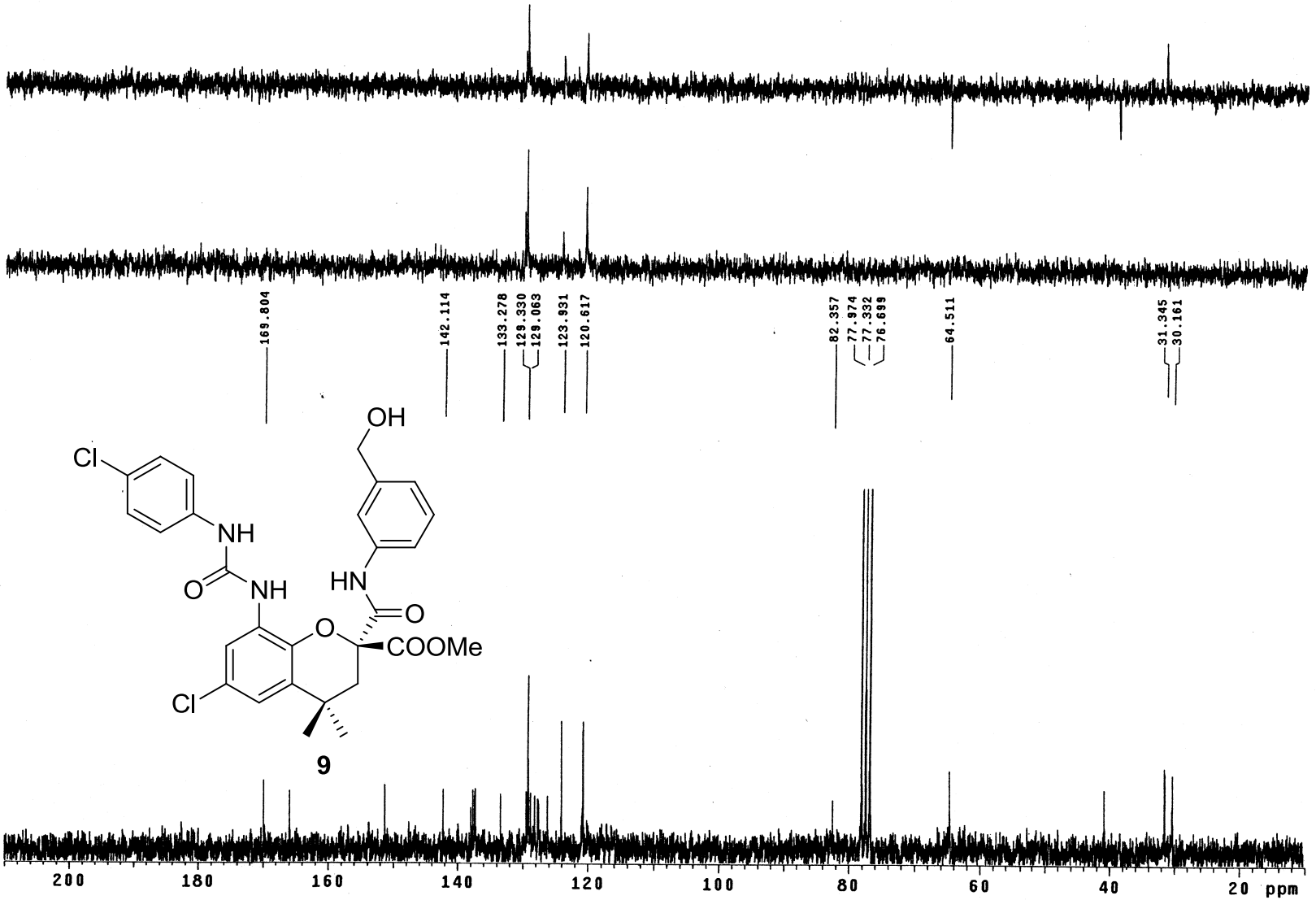


Figure S27. IR spectrum of compound 9.

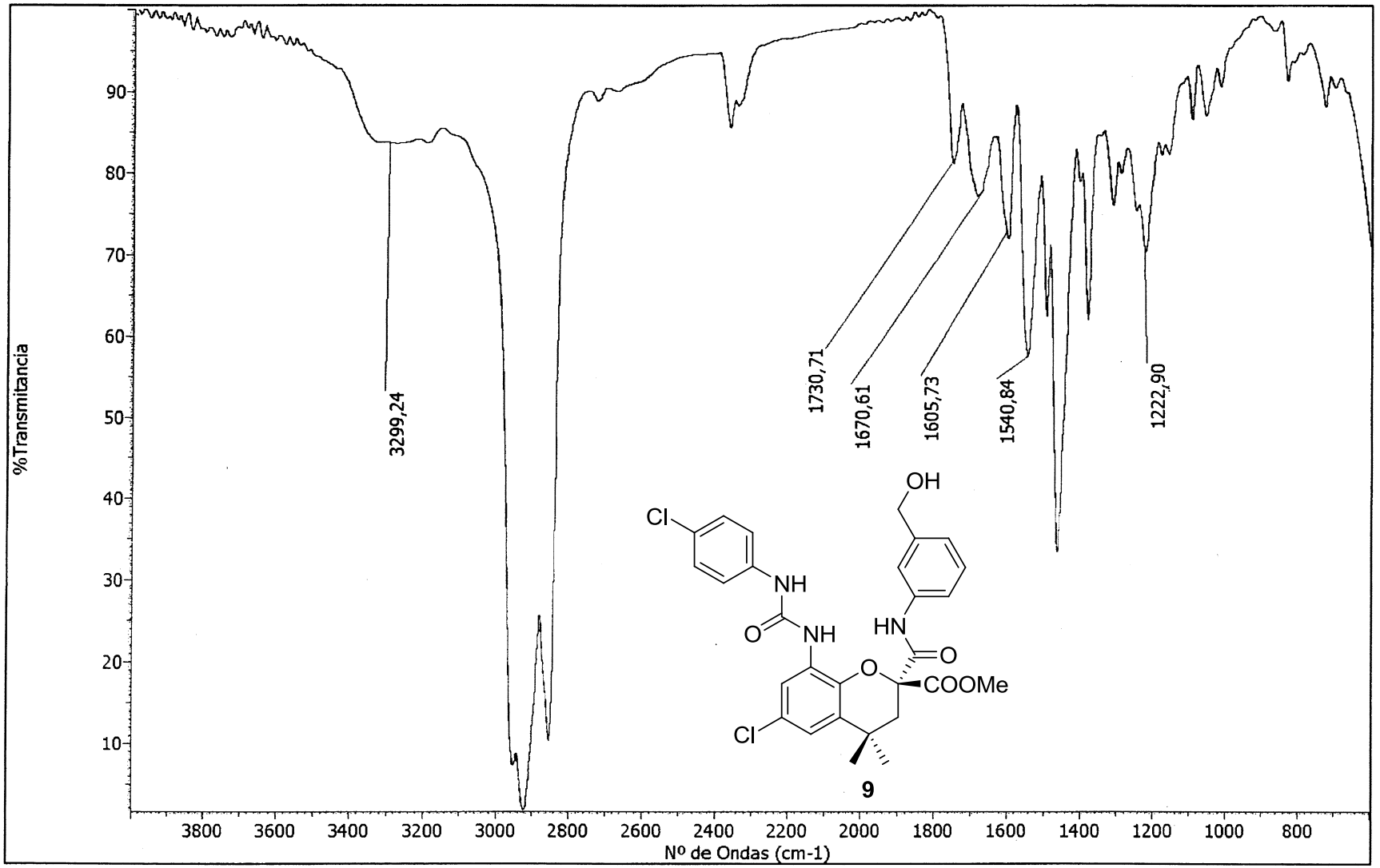


Figure S28. HRMS spectrum of compound 9 (ESI-QTOF).

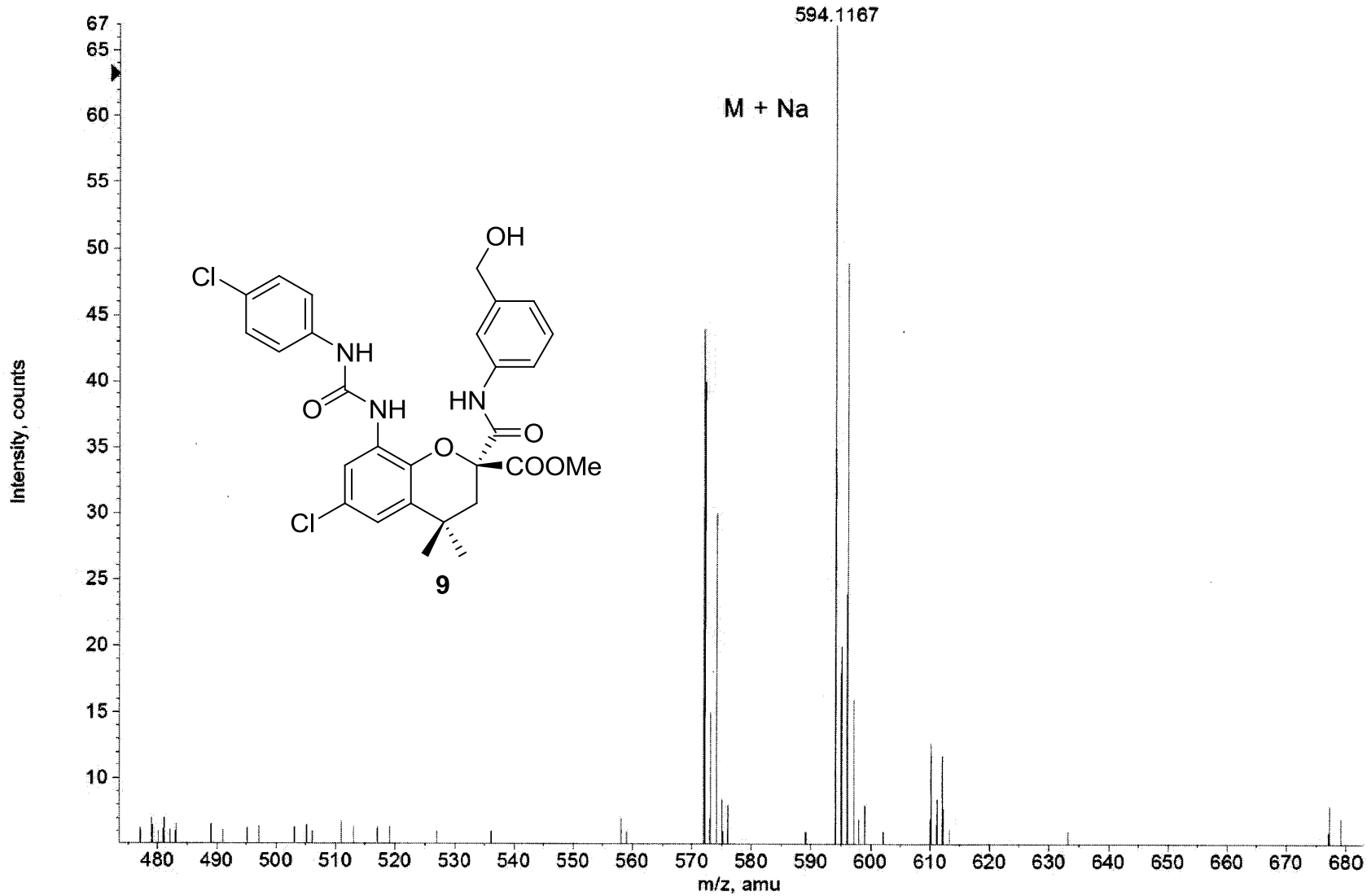


Figure S29. ^{1}H NMR spectrum of compound 10 (200 MHz, $CDCl_3$).

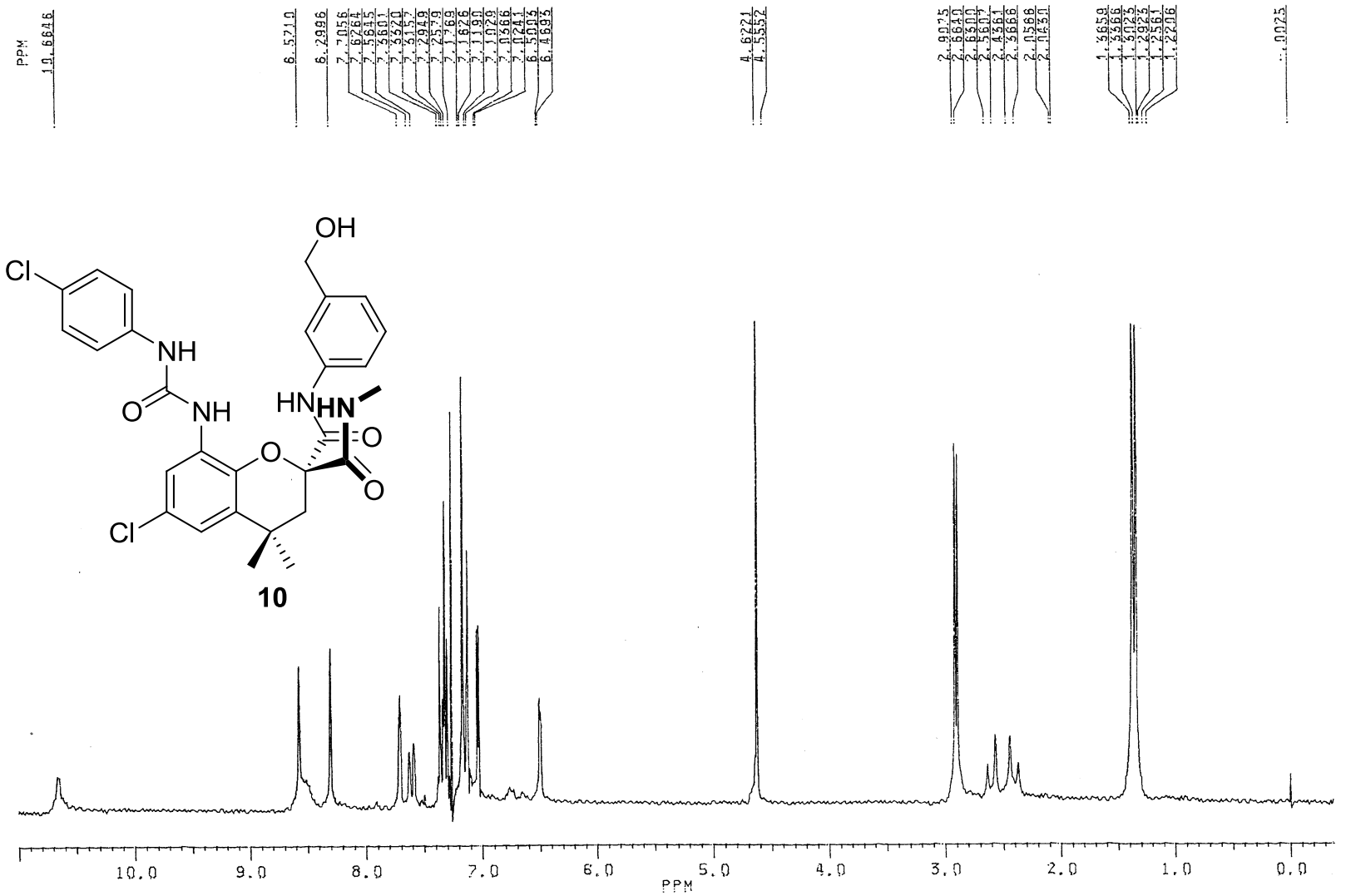


Figure S30. ^{13}C NMR spectrum of compound 10 (100 MHz, $CDCl_3$).

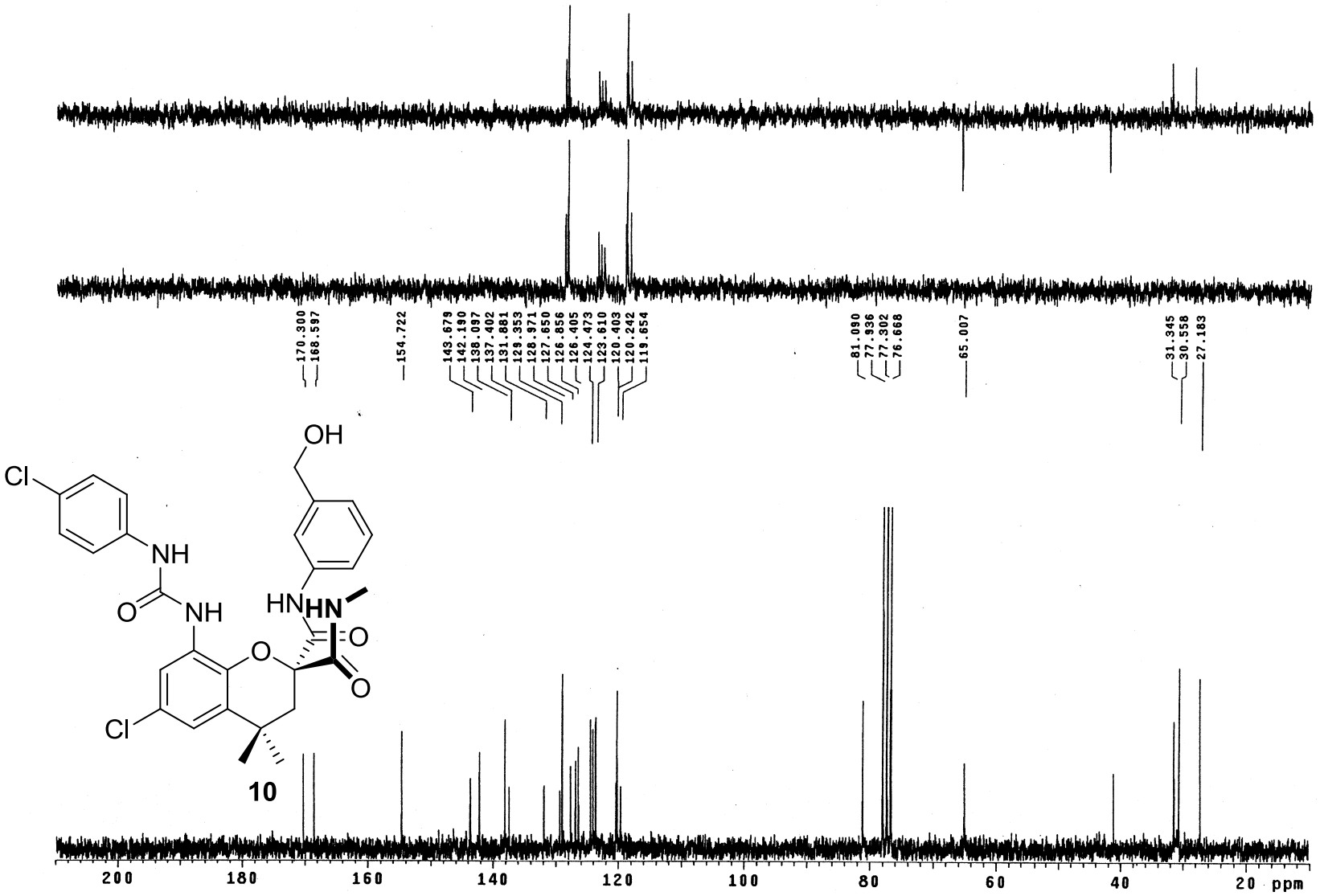


Figure S31. IR spectrum of compound 10.

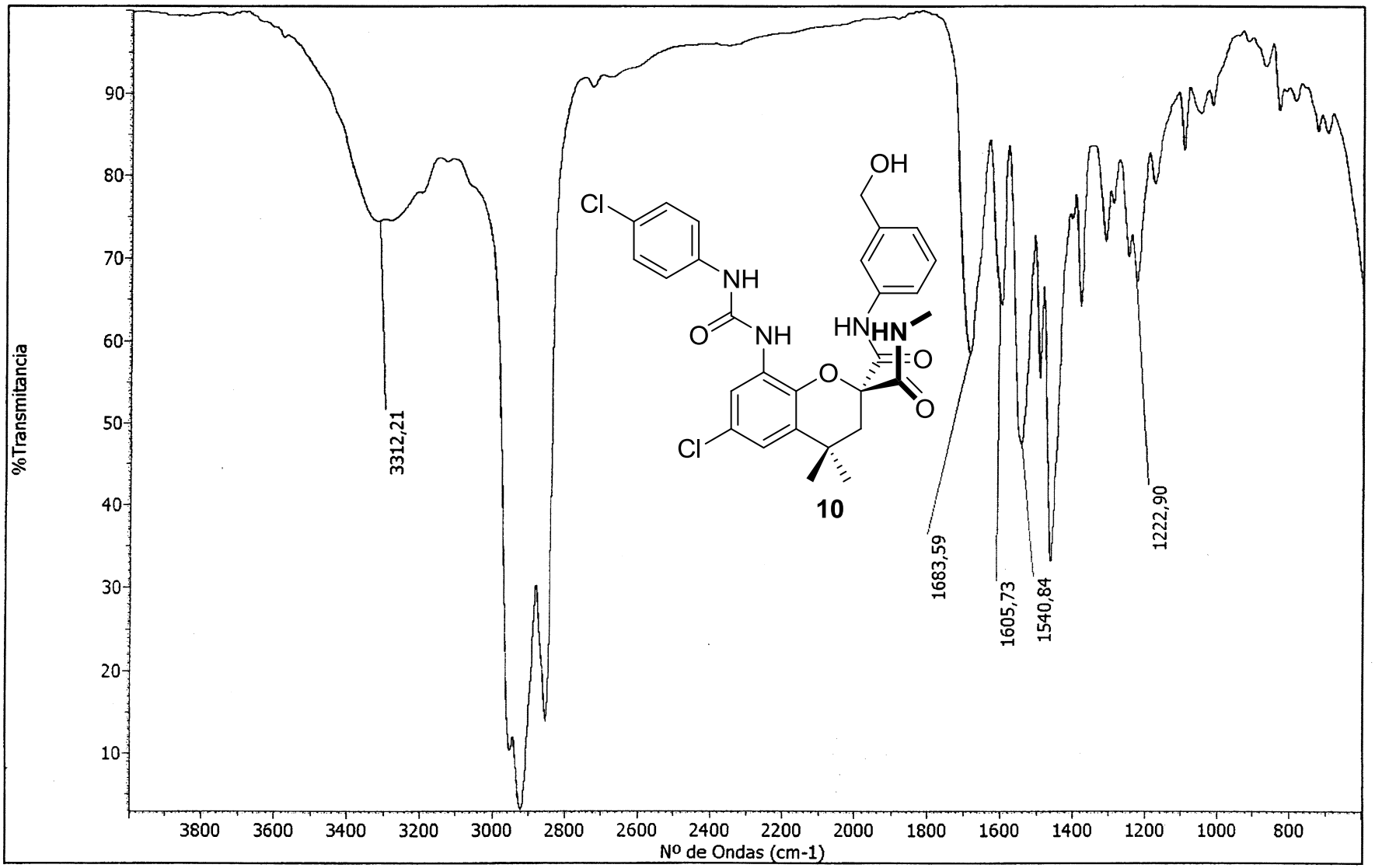


Figure S32. HRMS spectrum of compound 10 (ESI-QTOF).

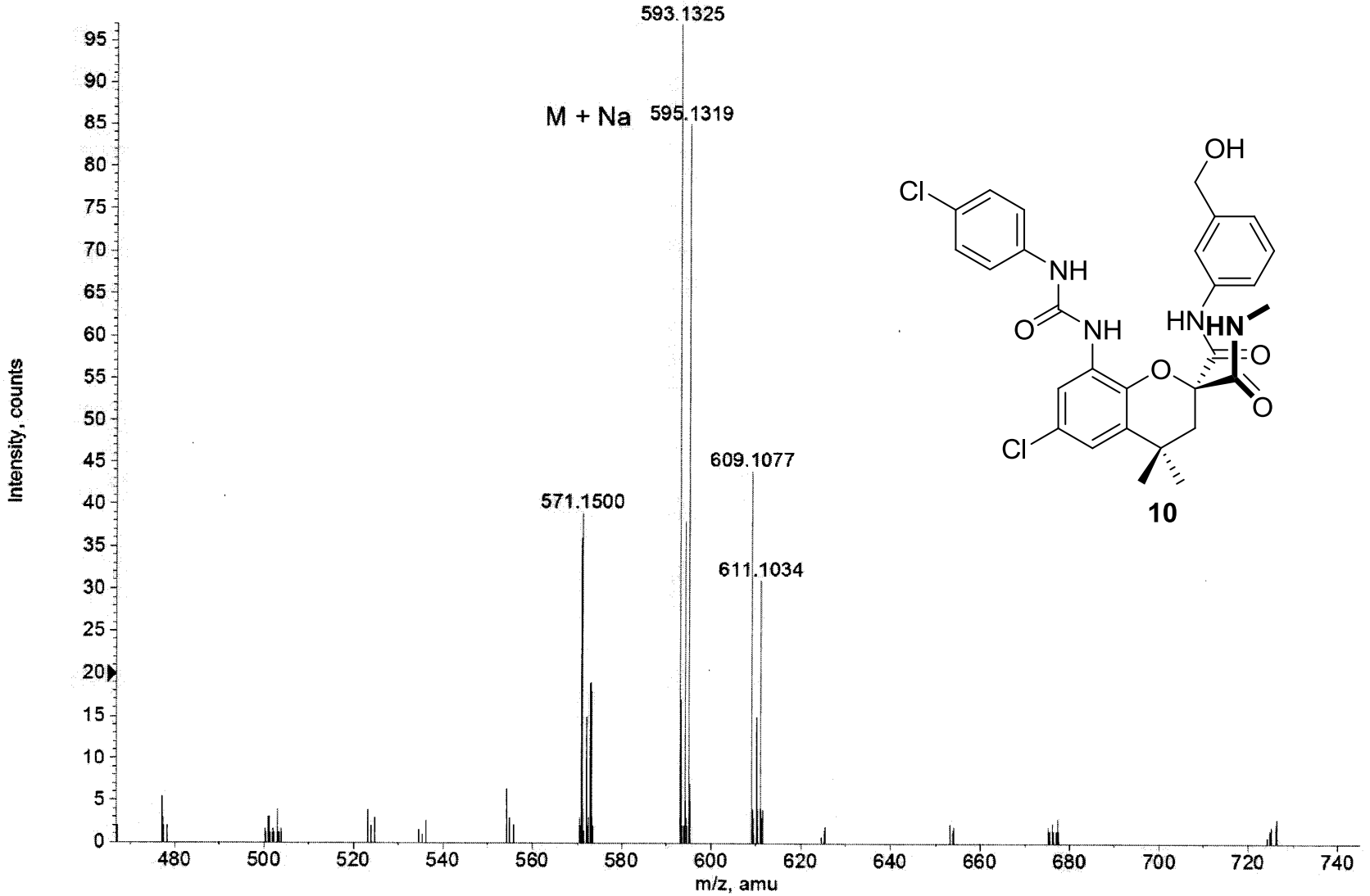


Figure S33. ^{1}H NMR spectrum of compound 11 (200 MHz, $CDCl_3$).

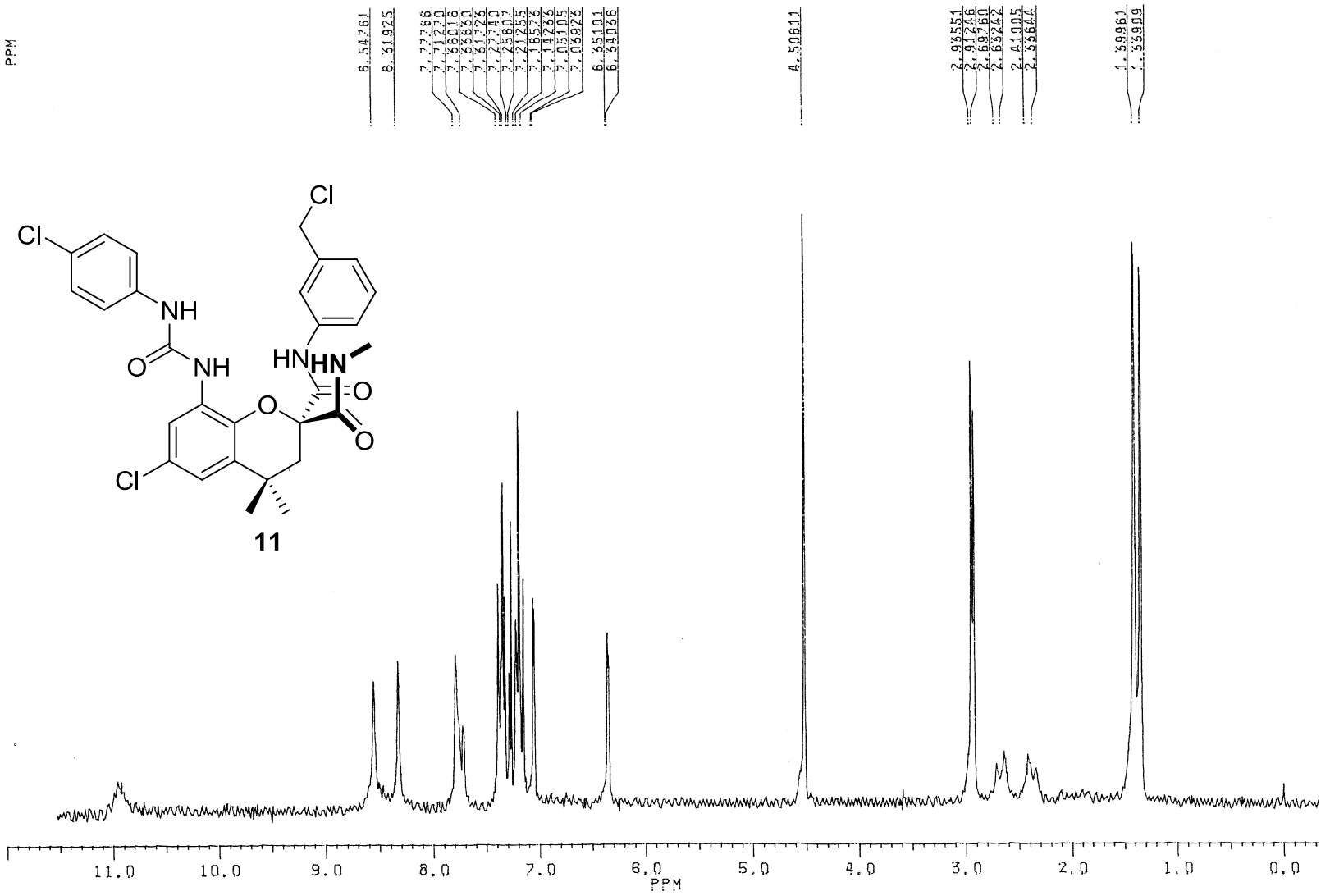


Figure S34. ^{13}C NMR spectrum of compound 11 (100 MHz, $CDCl_3$).

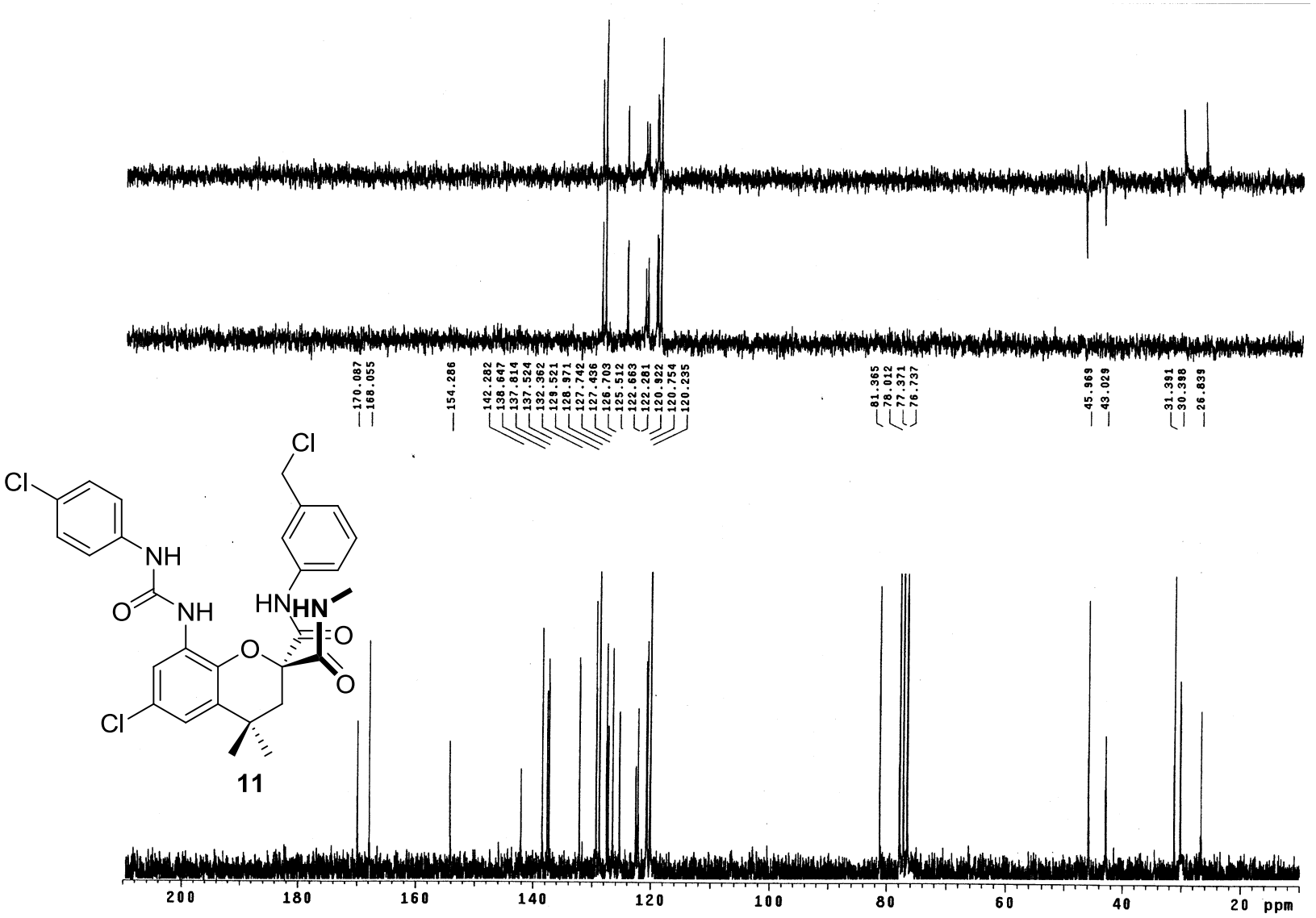


Figure S35. IR spectrum of compound 11.

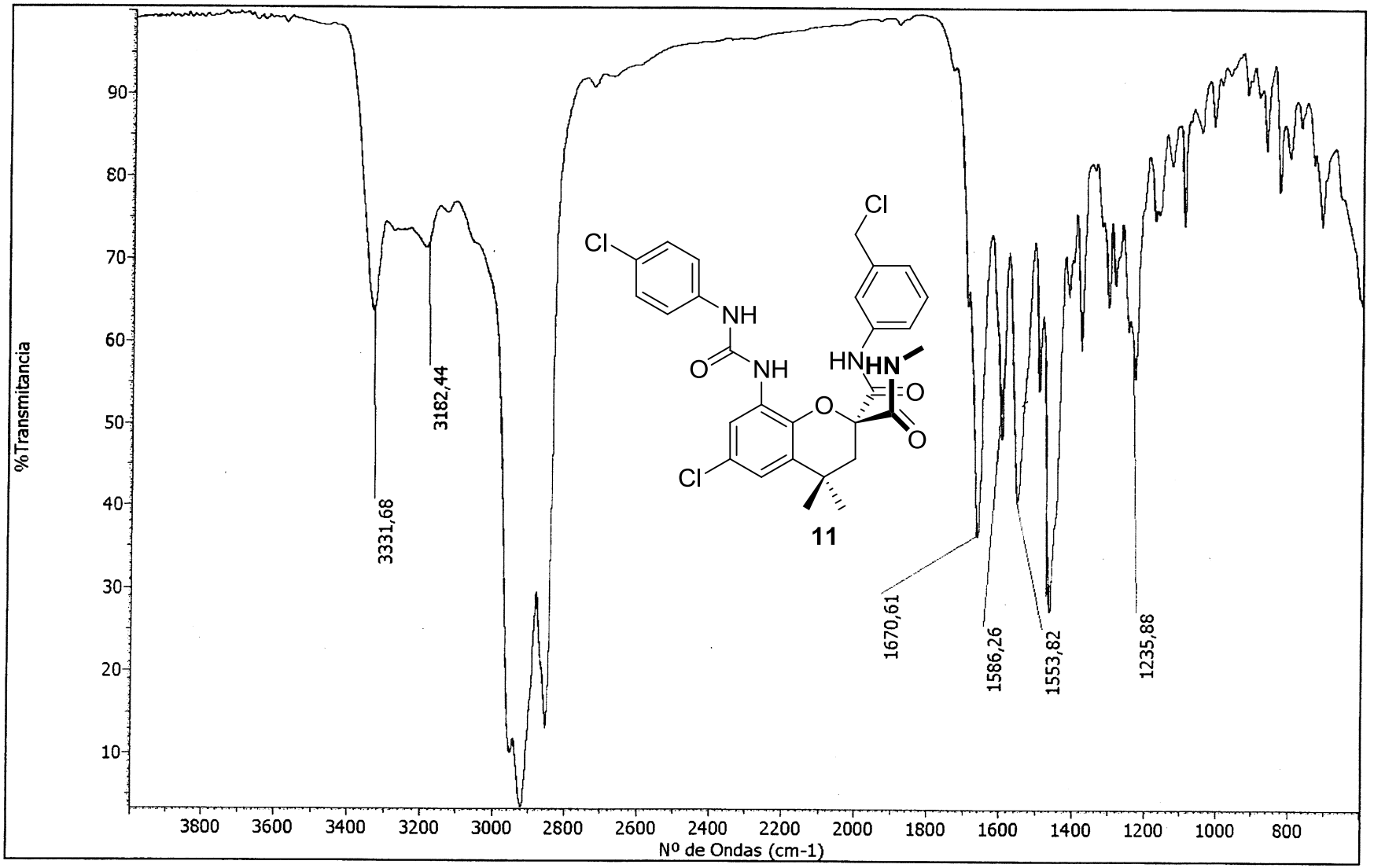


Figure S36. HRMS spectrum of compound 11 (ESI-QTOF).

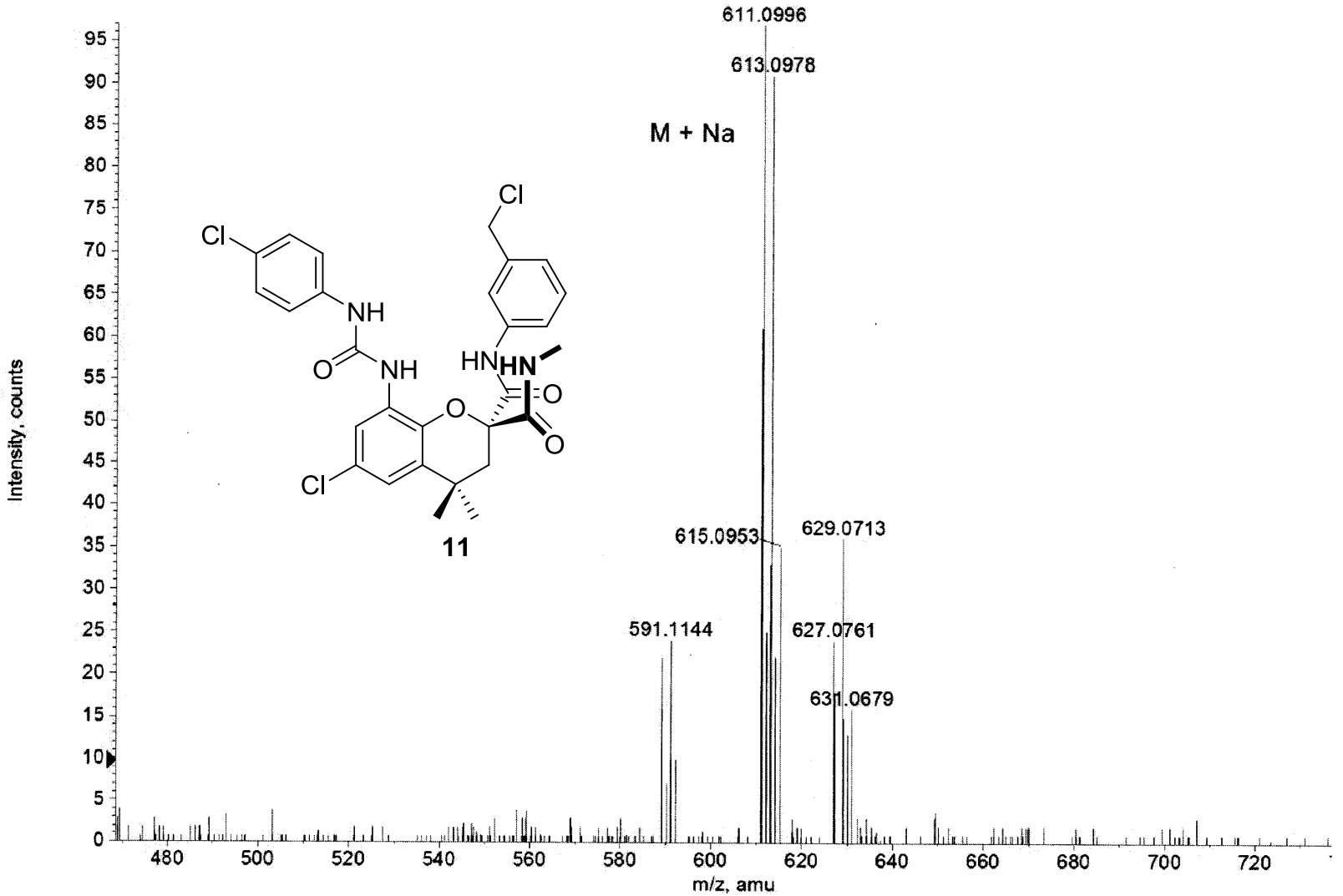


Figure S37. ^{1}H NMR spectrum of receptor 1 (400 MHz, $CDCl_3$).

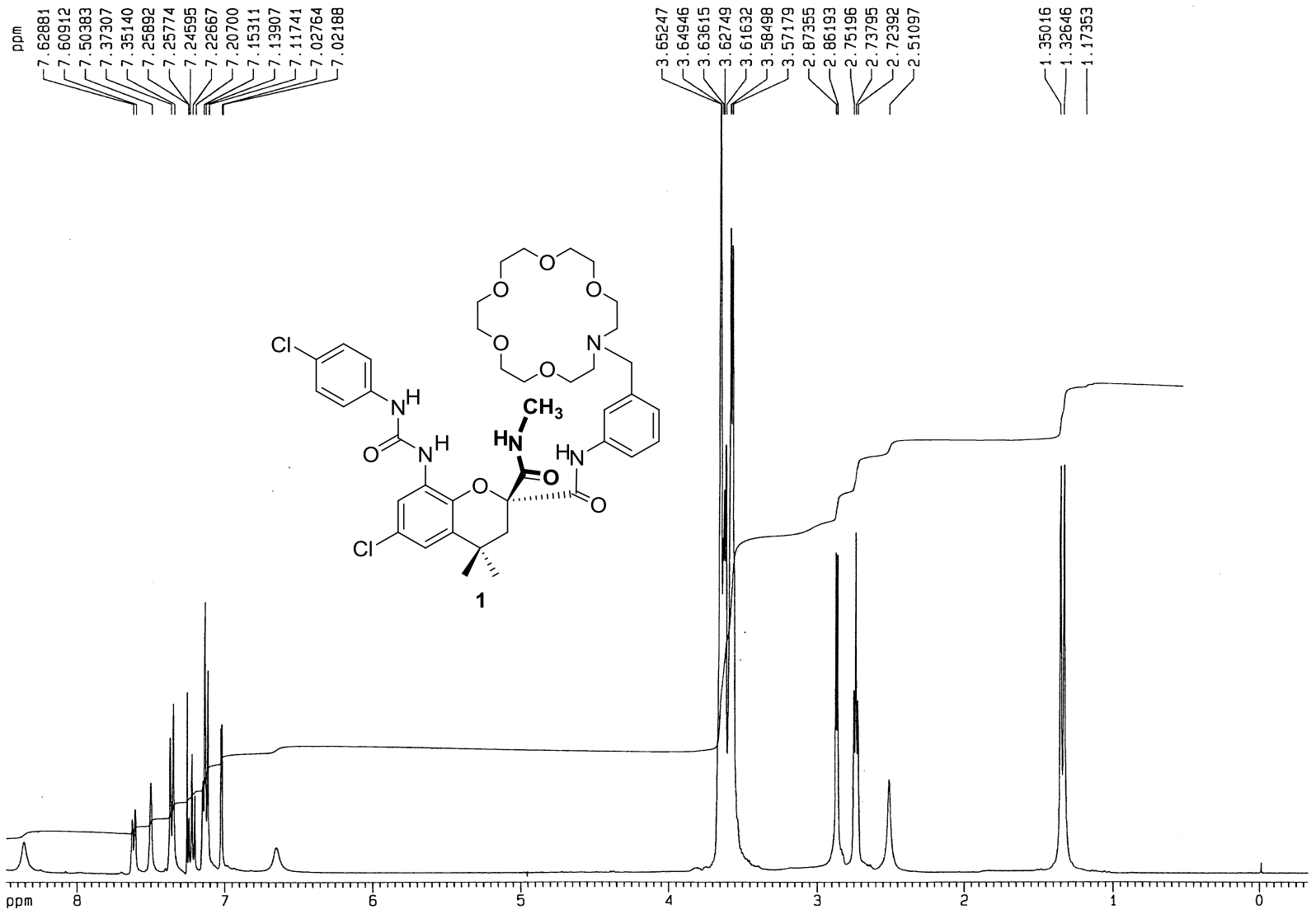


Figure S38. ^{13}C NMR spectrum of receptor 1 (100 MHz, $CDCl_3$).

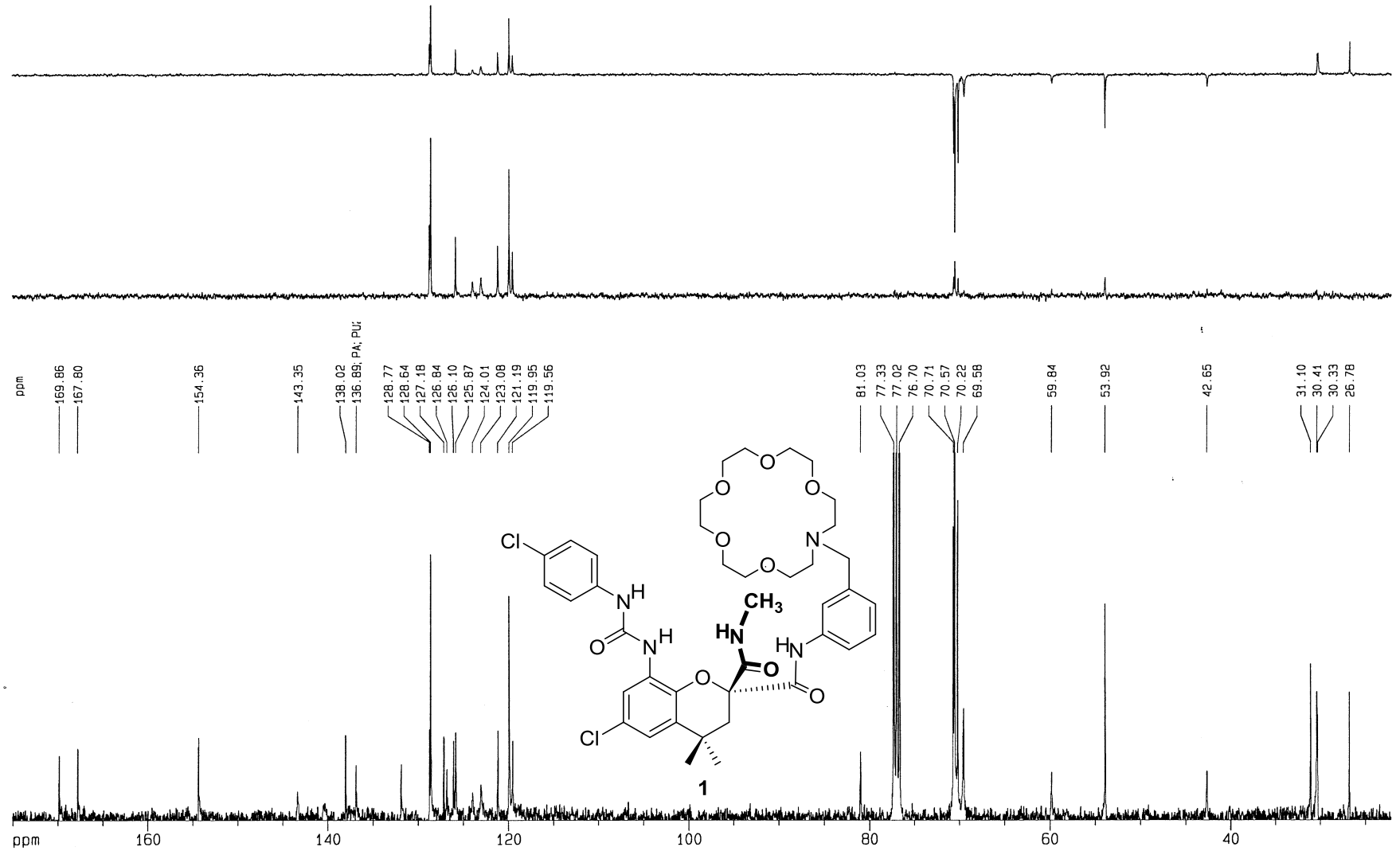


Figure S39. IR spectrum of receptor 1.

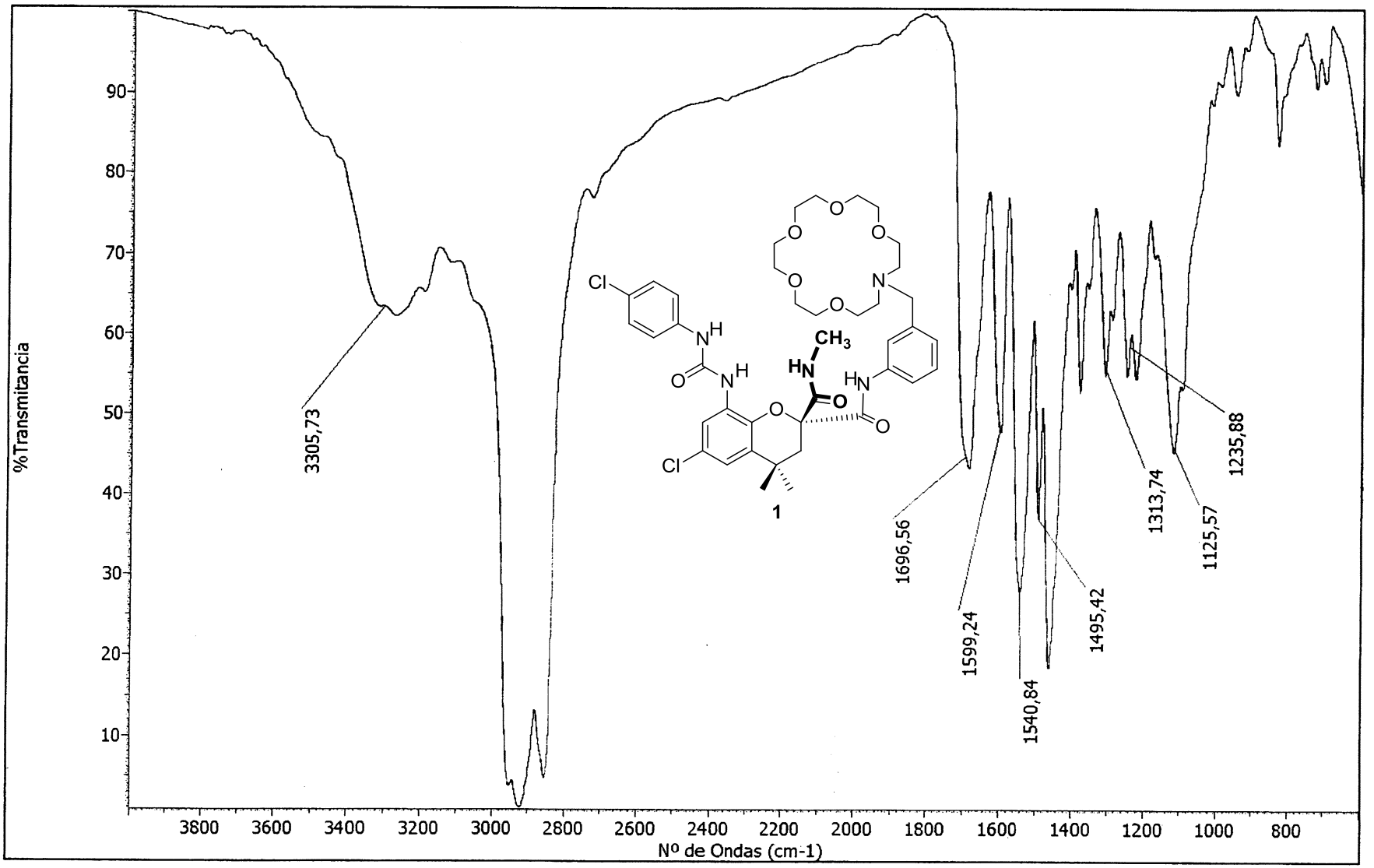


Figure S40. HRMS spectrum of receptor 1 (ESI-QTOF).

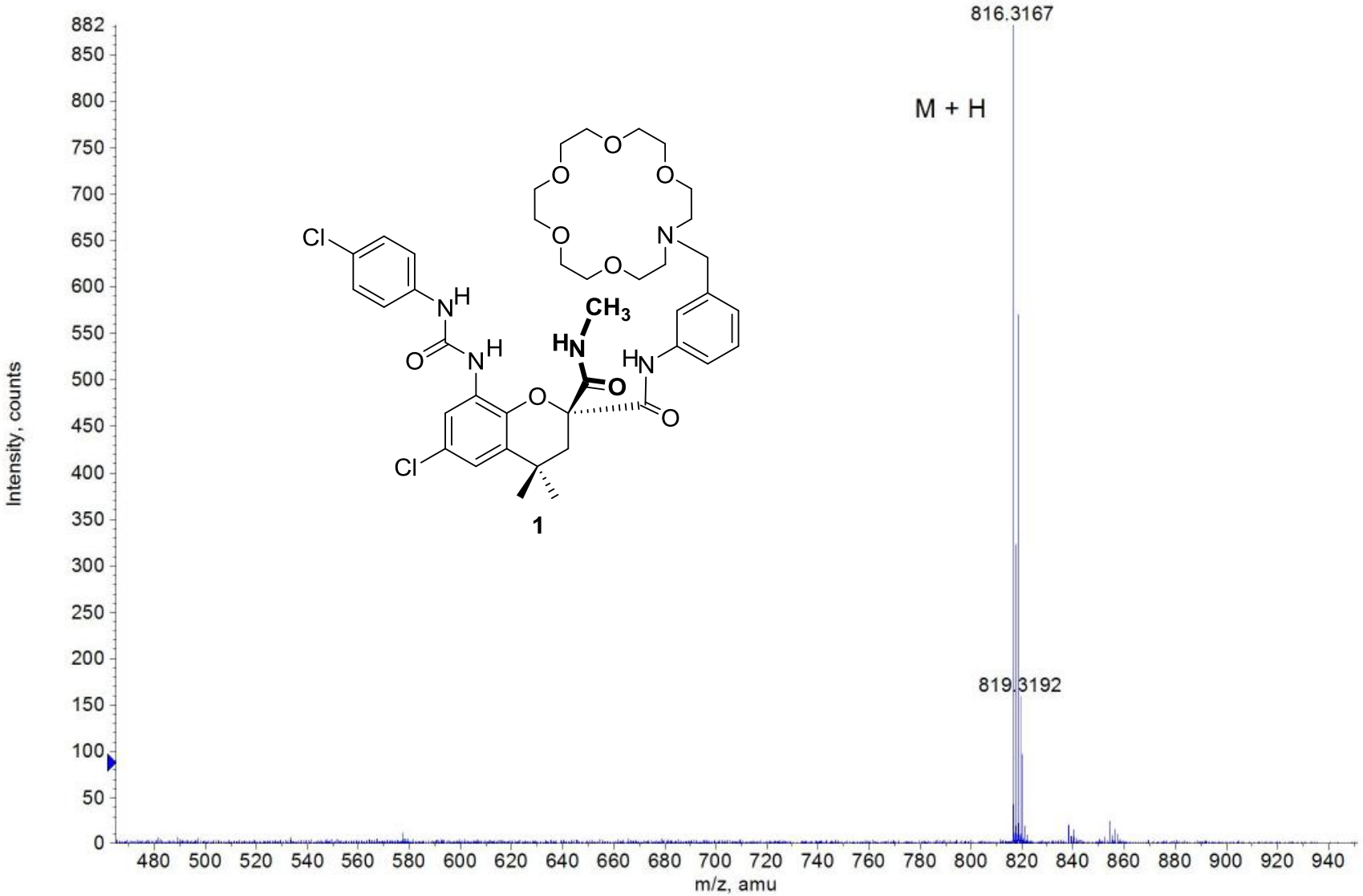


Figure S41. ^{1}H NMR spectrum of receptor 2 (400 MHz, $CDCl_3$).

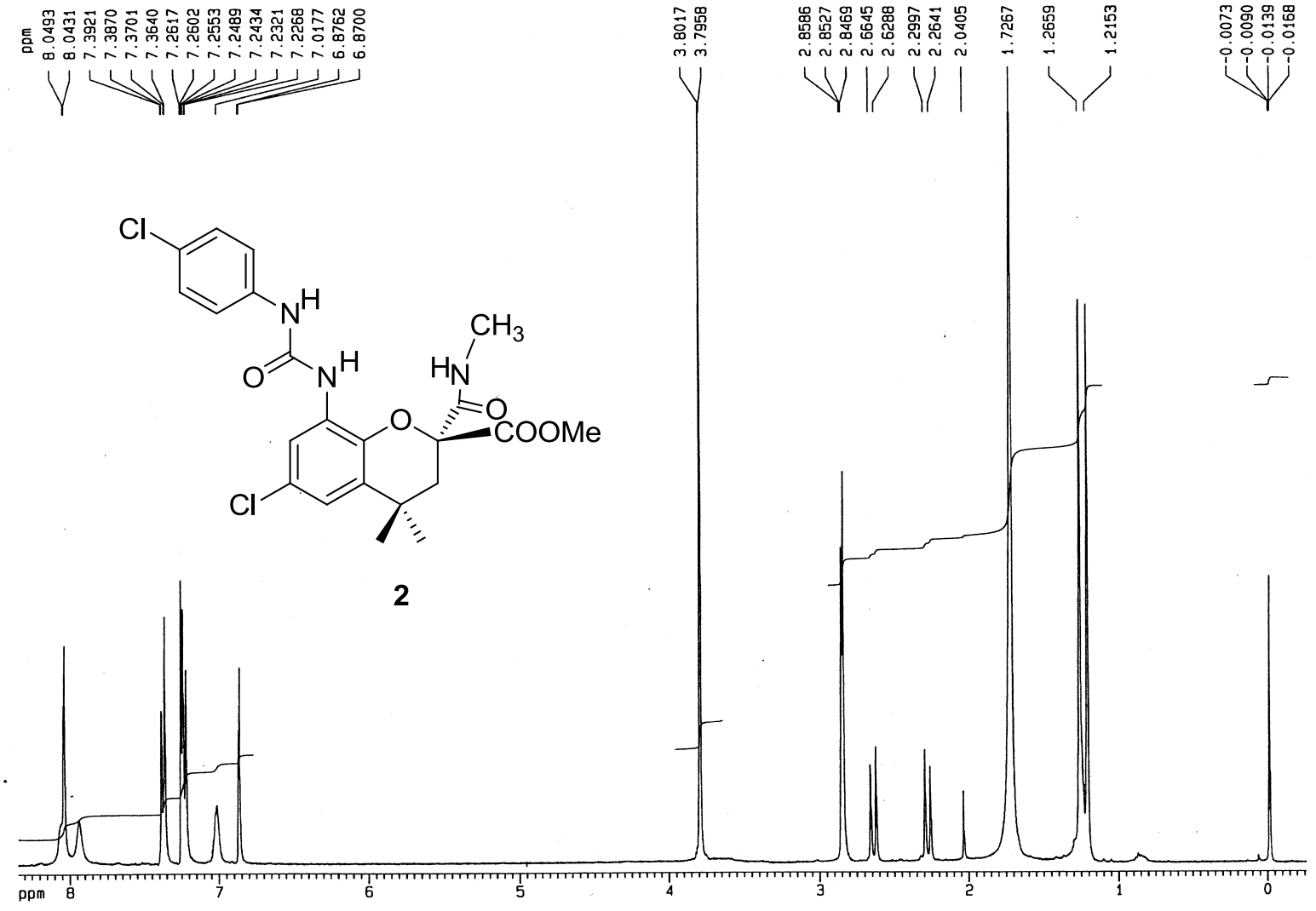


Figure S42. ^{13}C NMR spectrum of receptor 2 (100 MHz, $CDCl_3$).

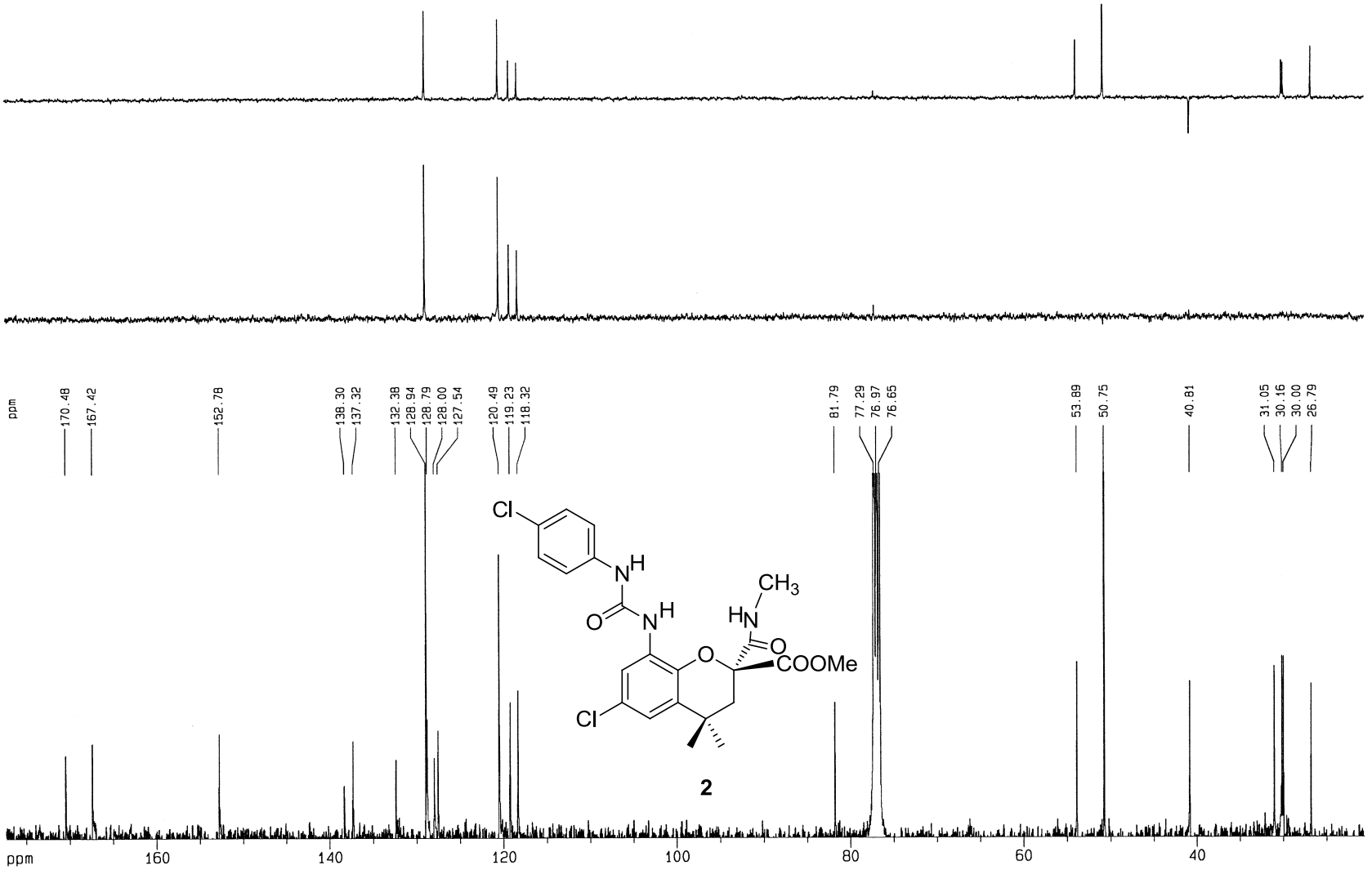


Figure S43. IR spectrum of receptor 2.

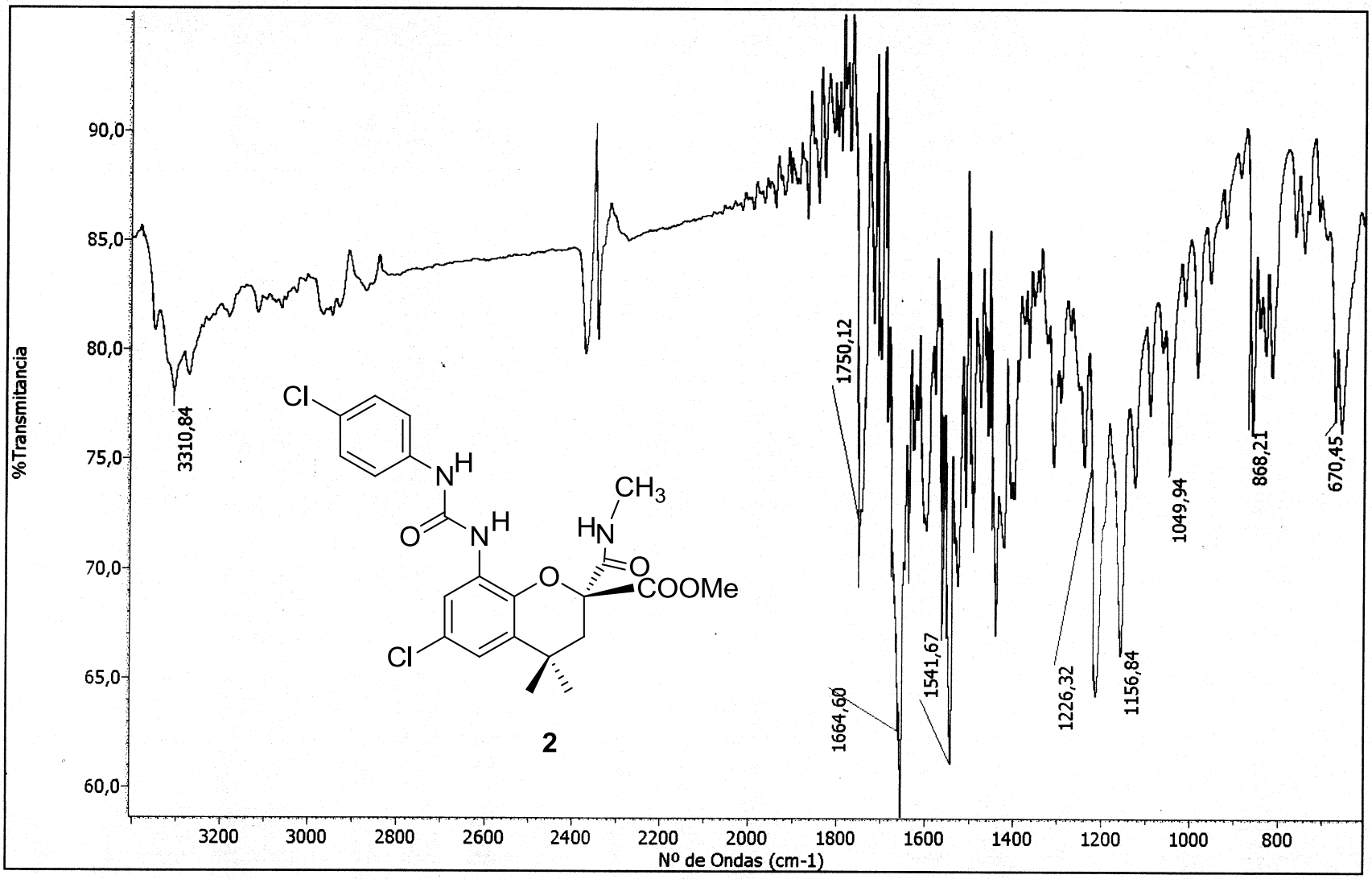


Figure S44. HRMS spectrum of receptor 2 (ESI-QTOF).

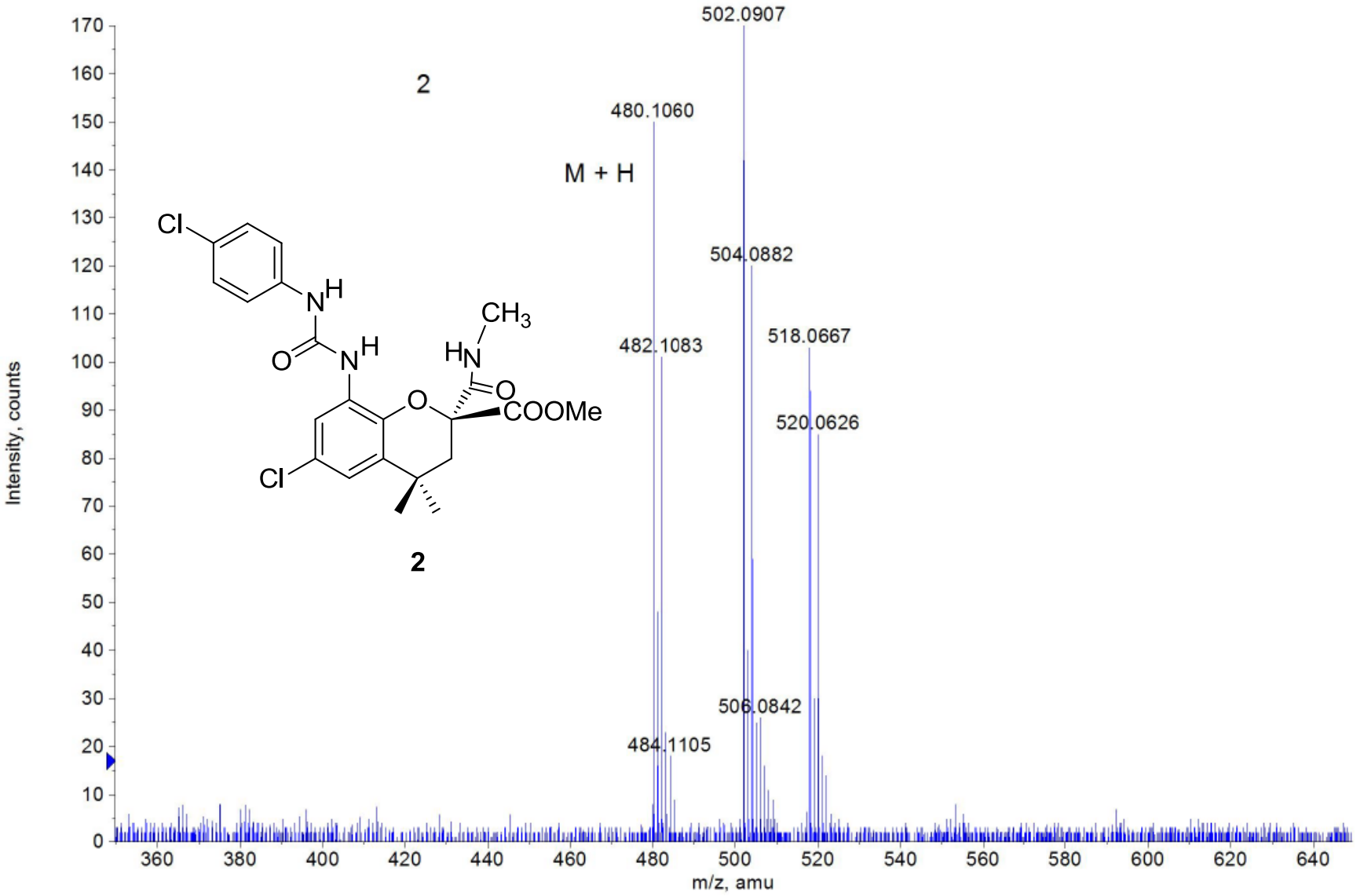
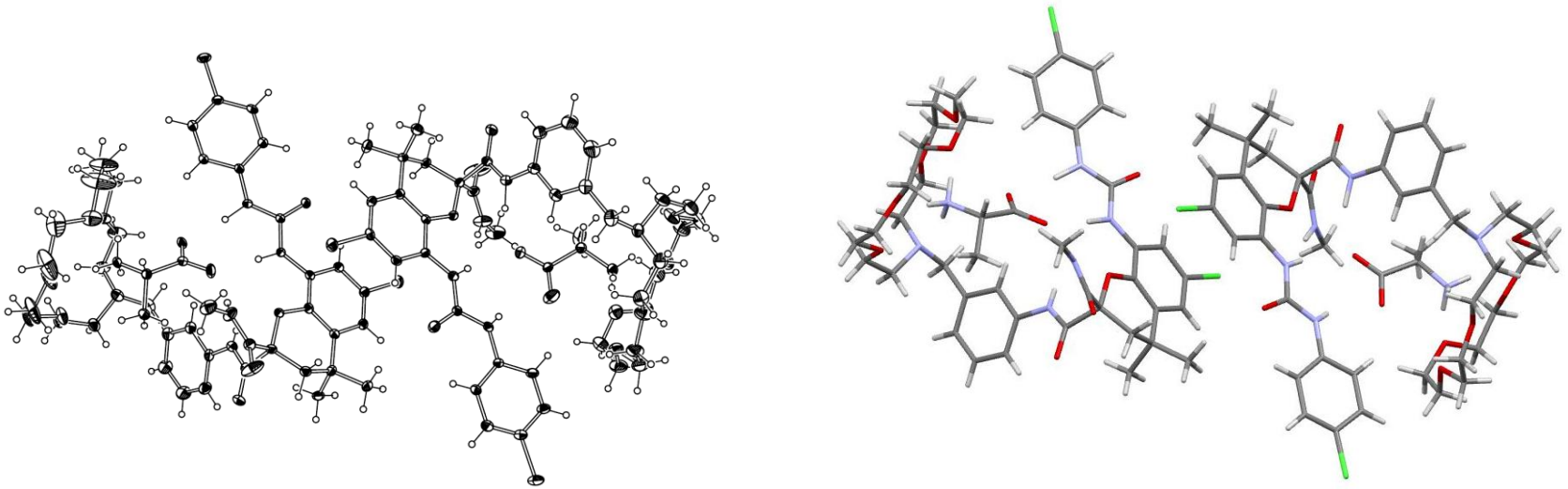


Figure S45. ORTEP diagram and X-ray crystal structure data of receptor 1 with *L*-alanine ($CHCl_3$ / MeOH).



Crystal data: $C_{43}H_{58}Cl_2N_6O_{11}$, M_w = 905.85, triclinic, space group P1, a = 13.2663(6) Å, b = 14.2260(7) Å, c = 15.0088(7) Å, α = 68.446(3)°, β = 63.857(3)°, γ = 73.509(3)°, V = 2339.59(19) $Å^3$, Z = 2, D_C = 1.286 Mg/m^3, m = (Cu-K_α) = 1.775 mm^{-1}, F(000) = 960. 14207 reflections were collected at $3.38 \leq \theta \leq 66.54$ and merged to give 8223 unique reflections (R_{int} = 0.0433). Final values are R_1 = 0.0593, wR_2 = 0.1638.

Figure S46. ^{1}H NMR spectrum of receptor 1 with *L*-alanine (200 MHz, $CDCl_3$).

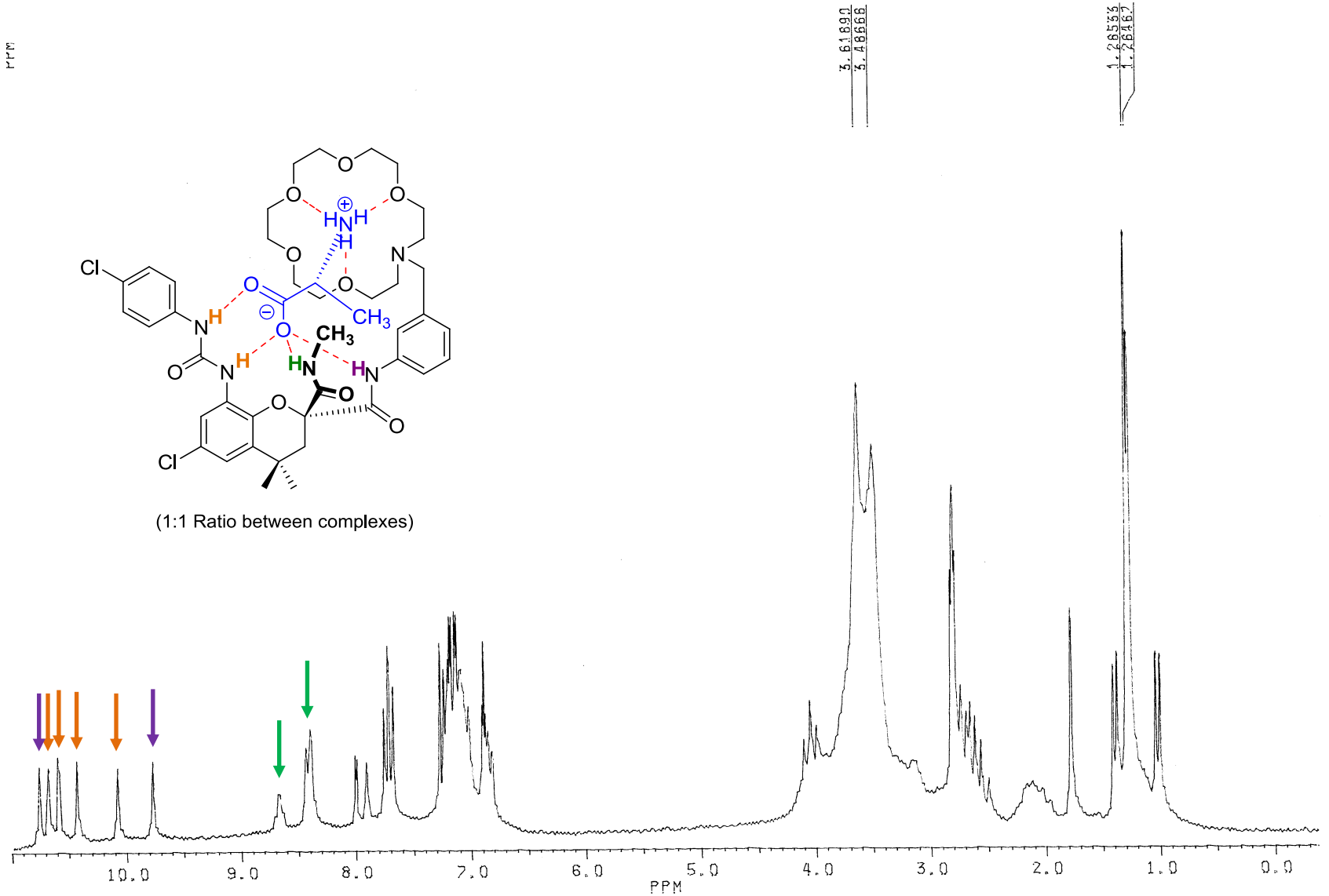


Figure S47. COSY spectrum of receptor 1 with *L*-alanine (400 MHz, $CDCl_3$).

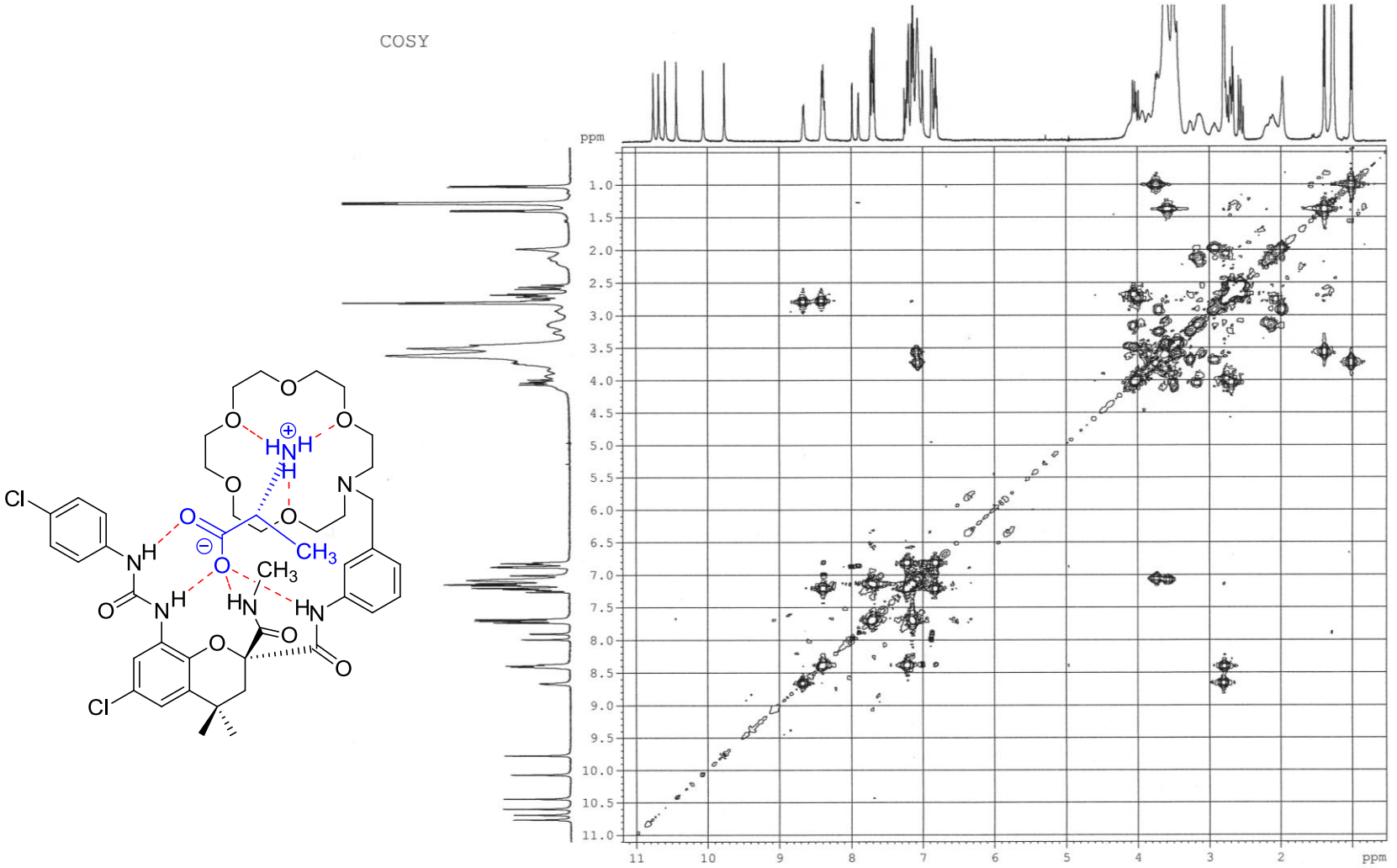


Figure S48. ROESY spectrum of receptor 1 with *L*-alanine (400 MHz, $CDCl_3$).

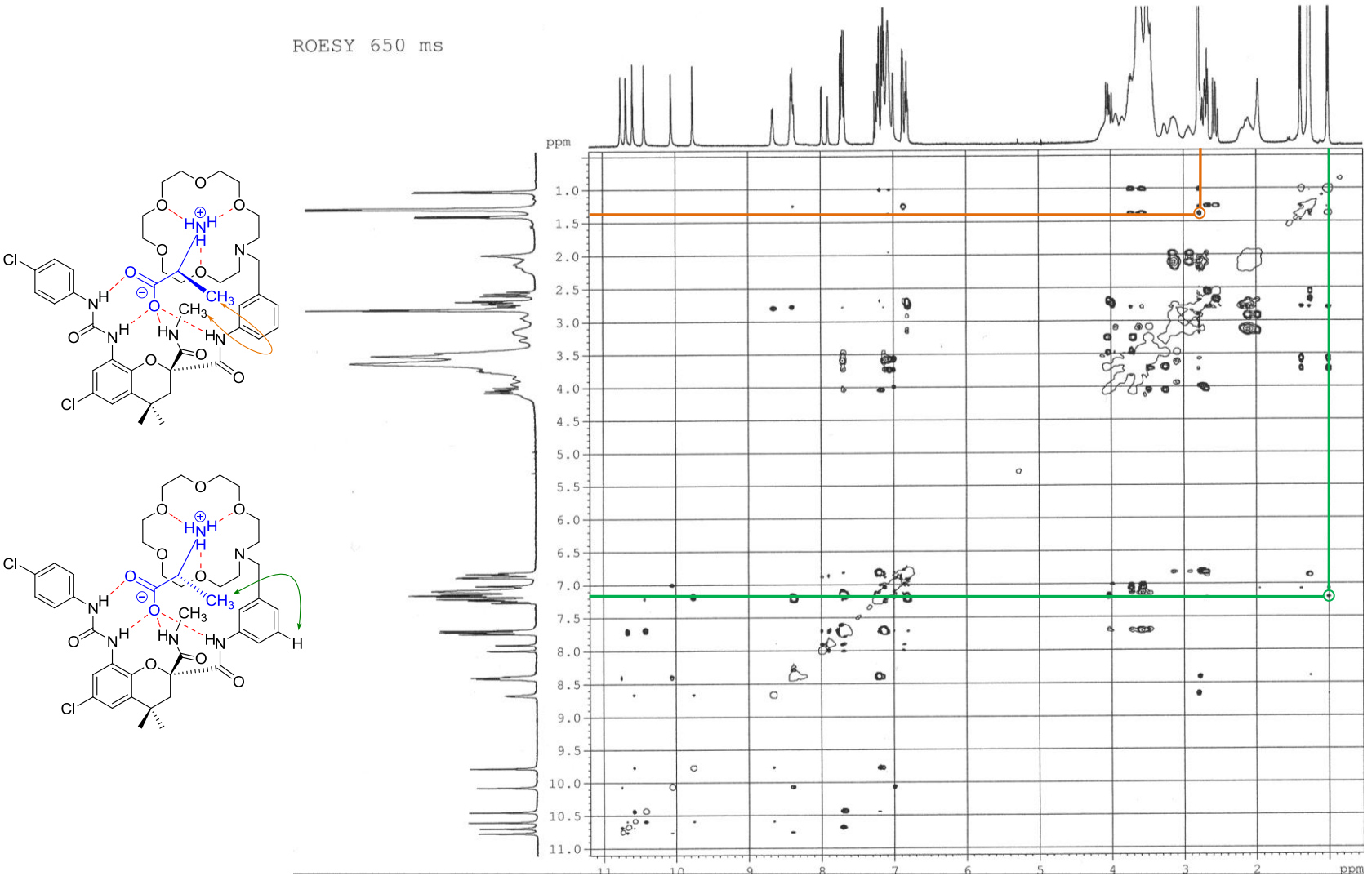


Figure S49. ^{1}H NMR spectrum of receptor 1 with *L*-alanine (200 MHz, MeOD).

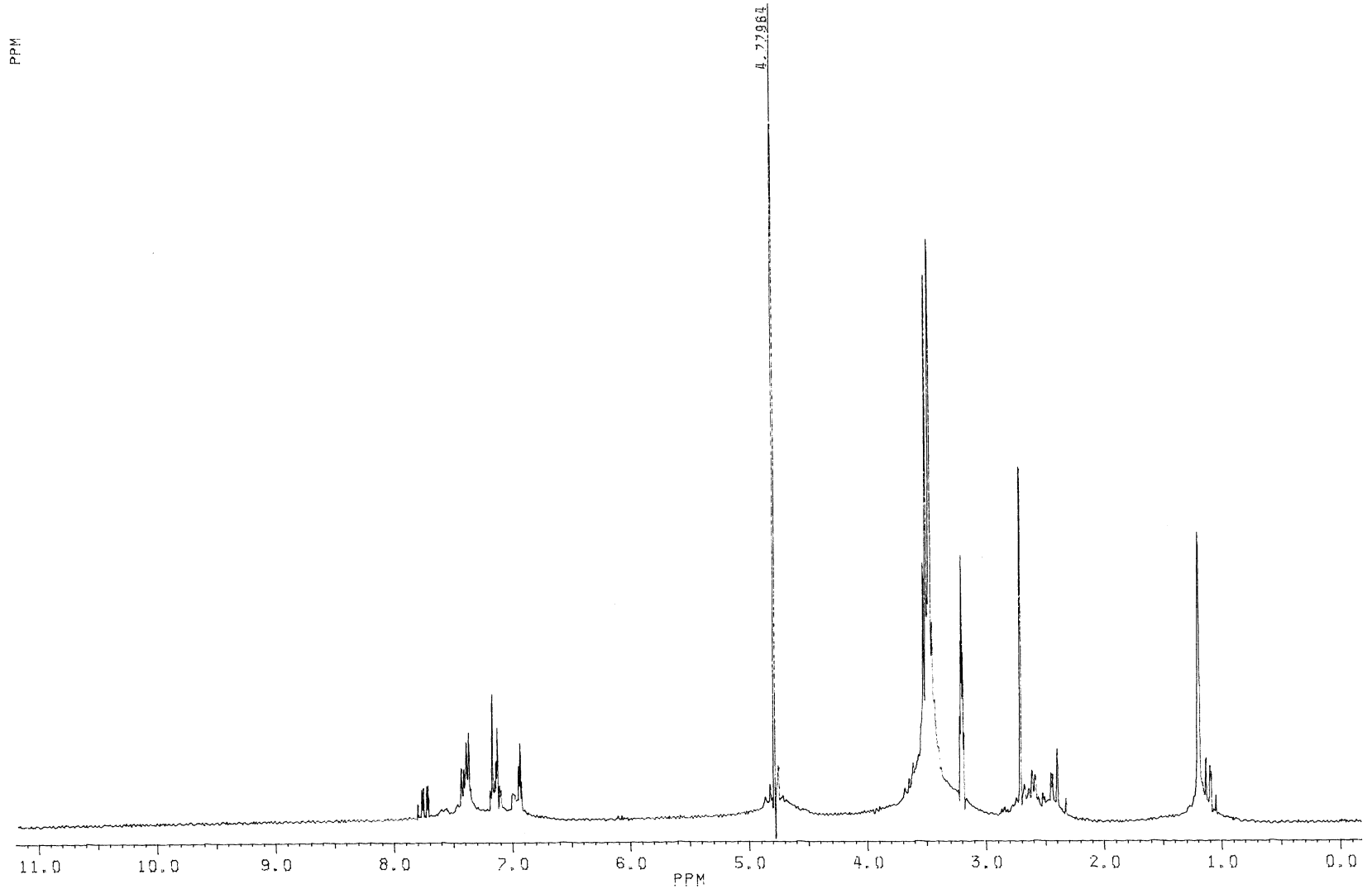
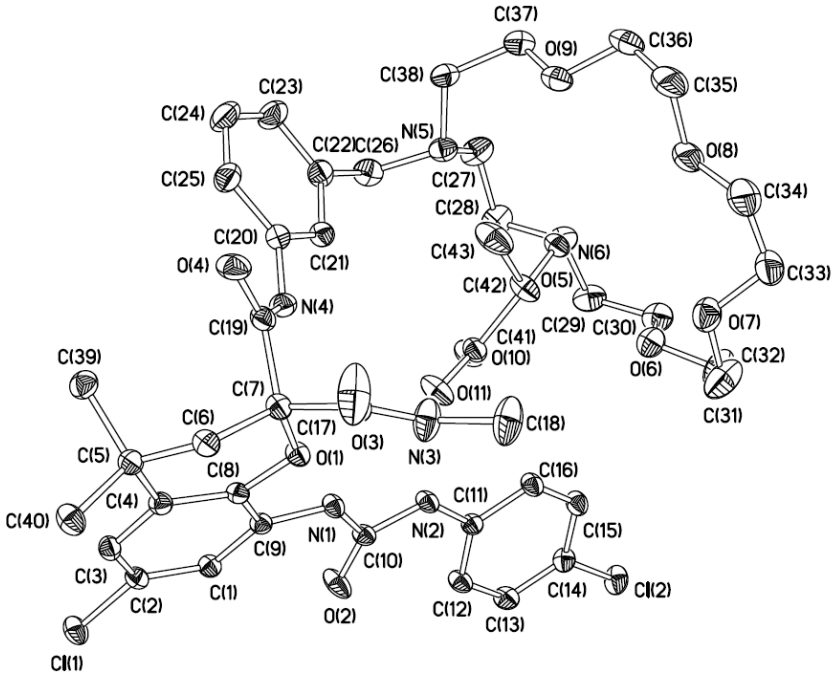
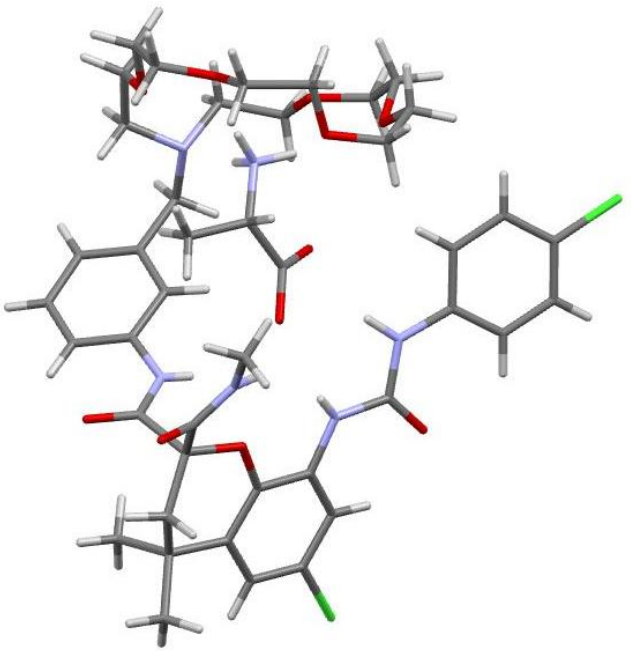


Figure S50. ORTEP diagram and X-ray crystal structure data of receptor 1 with *D,L*-alanine ($CDCl_3$).





Crystal data: $C_{40}H_{51}Cl_2N_5O_9$, M_w = 905.85, triclinic, space group P1, a = 13.2100(6) Å, b = 14.3452(6) Å, c = 14.9727(10) Å, α = 96.364(4)°, β = 116.168(3)°, γ = 107.161(3)°, V = 2334.7(2) $Å^3$, Z = 2, D_C = 1.289 Mg/m^3, m = (Cu-K_α) = 1.779 mm^{-1}, F(000) = 960. 12403 reflections were collected at 3.36 ≤ θ ≤ 67.57 and merged to give 6912 unique reflections (R_{int} = 0.0283). Final values are R_1 = 0.0649, wR_2 = 0.1879.

Figure S51. ^{1}H NMR spectrum of the solution of receptor 1 with *D,L*-alanine (200 MHz, $CDCl_3$).

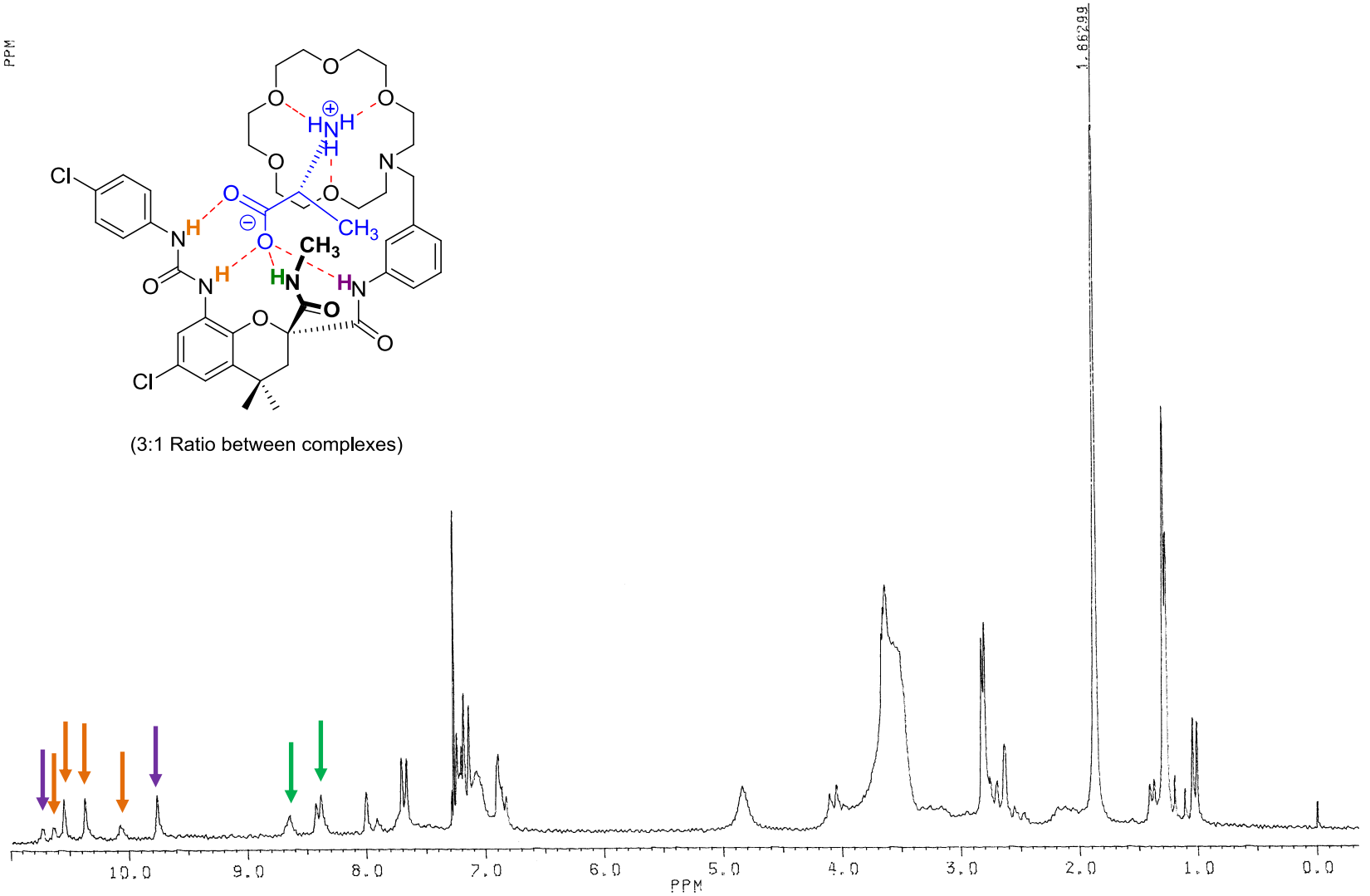
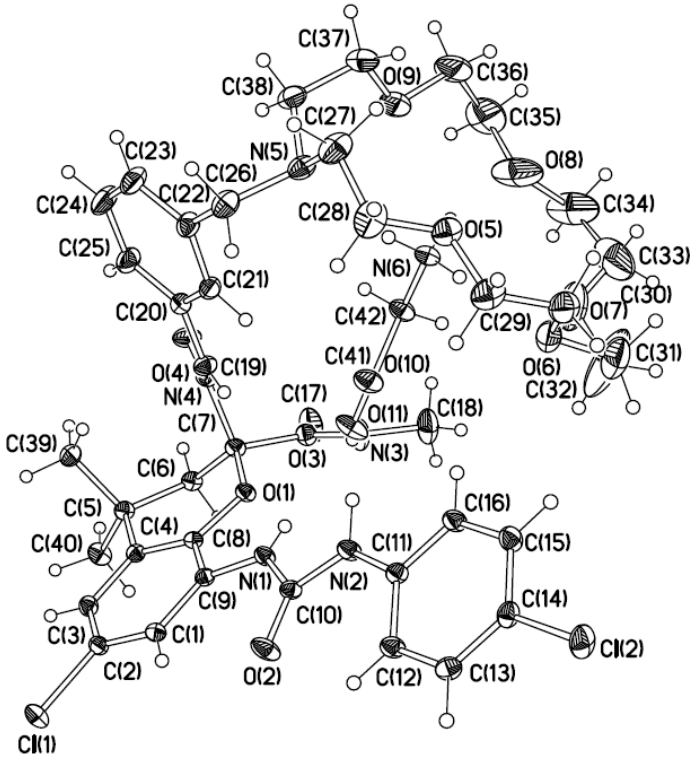
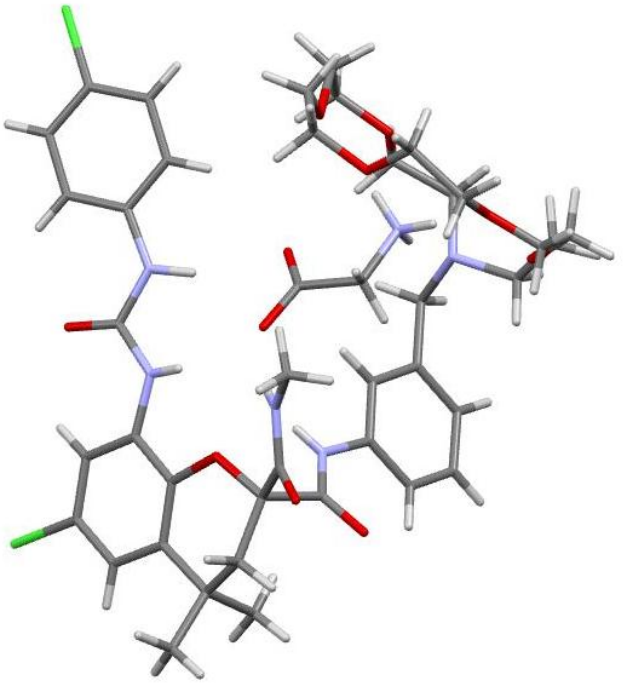


Figure S52. ORTEP diagram and X-ray crystal structure data of receptor 1 with glycine ($CDCl_3$).





Crystal data: $C_{42}H_{56}Cl_2N_6O_{11}$, M_w = 891.83, triclinic, space group P1, a = 12.8657(4) Å, b = 14.2553(4) Å, c = 14.8313(4) Å, α = 95.487(2)°, β = 114.669(2)°, γ = 107.436(2)°, V = 2280.61(11) $Å^3$, Z = 2, D_C = 1.299 Mg/m^3, m = (Cu-K_α) = 1.813 mm^{-1}, F(000) = 944. 12496 reflections were collected at $3.36 \leq \theta \leq 66.69$ and merged to give 6905 unique reflections (R_{int} = 0.0205). Final values are R_1 = 0.0577, wR_2 = 0.1616.

Figure S53. ^{1}H NMR spectrum of receptor 1 with glycine (200 MHz, $CDCl_3$).

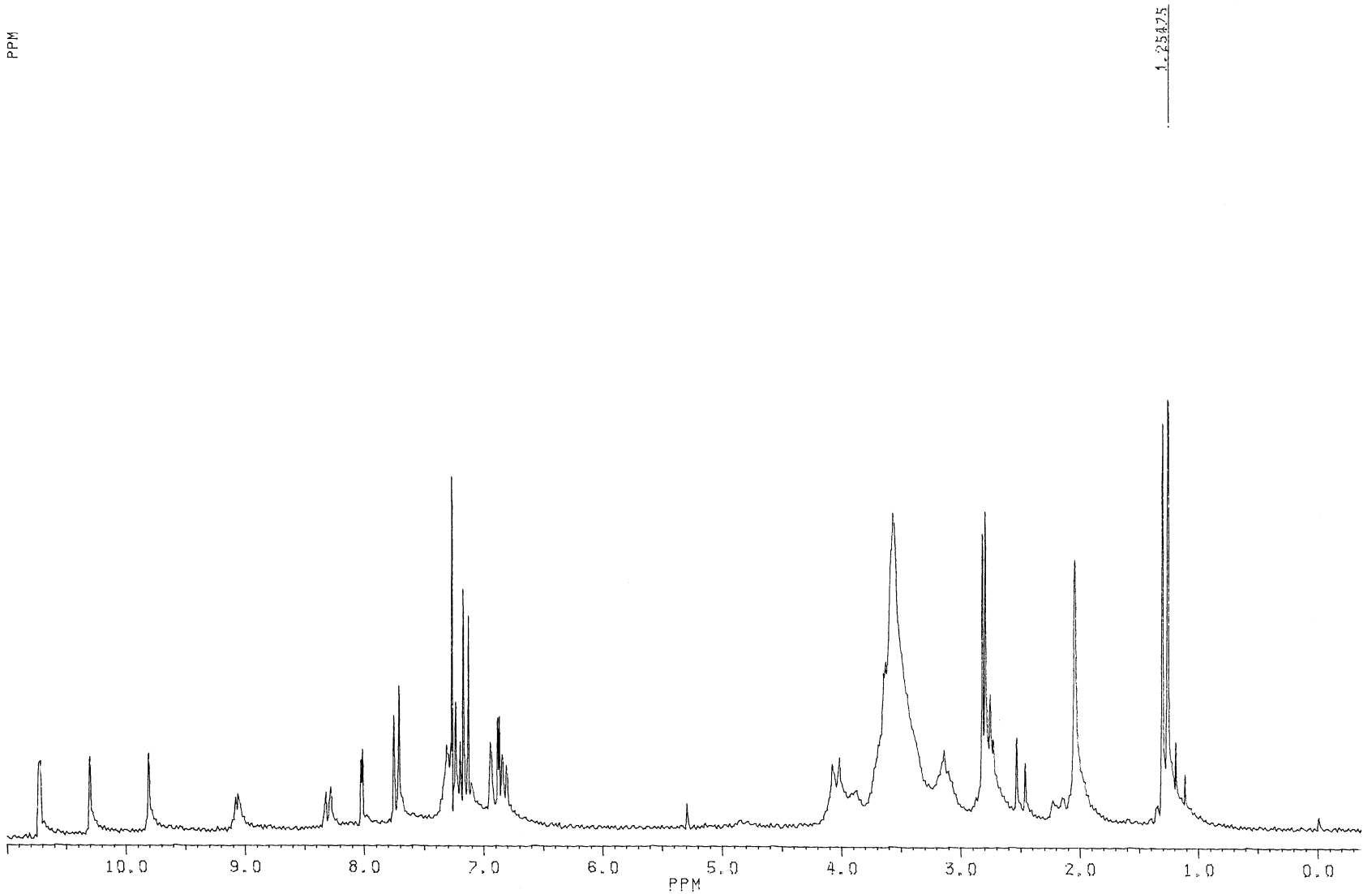


Figure S54. ^{1}H NMR spectrum of strong complex of (+)-*S*-receptor 1 with *L*-alanine (200 MHz, $CDCl_3$).

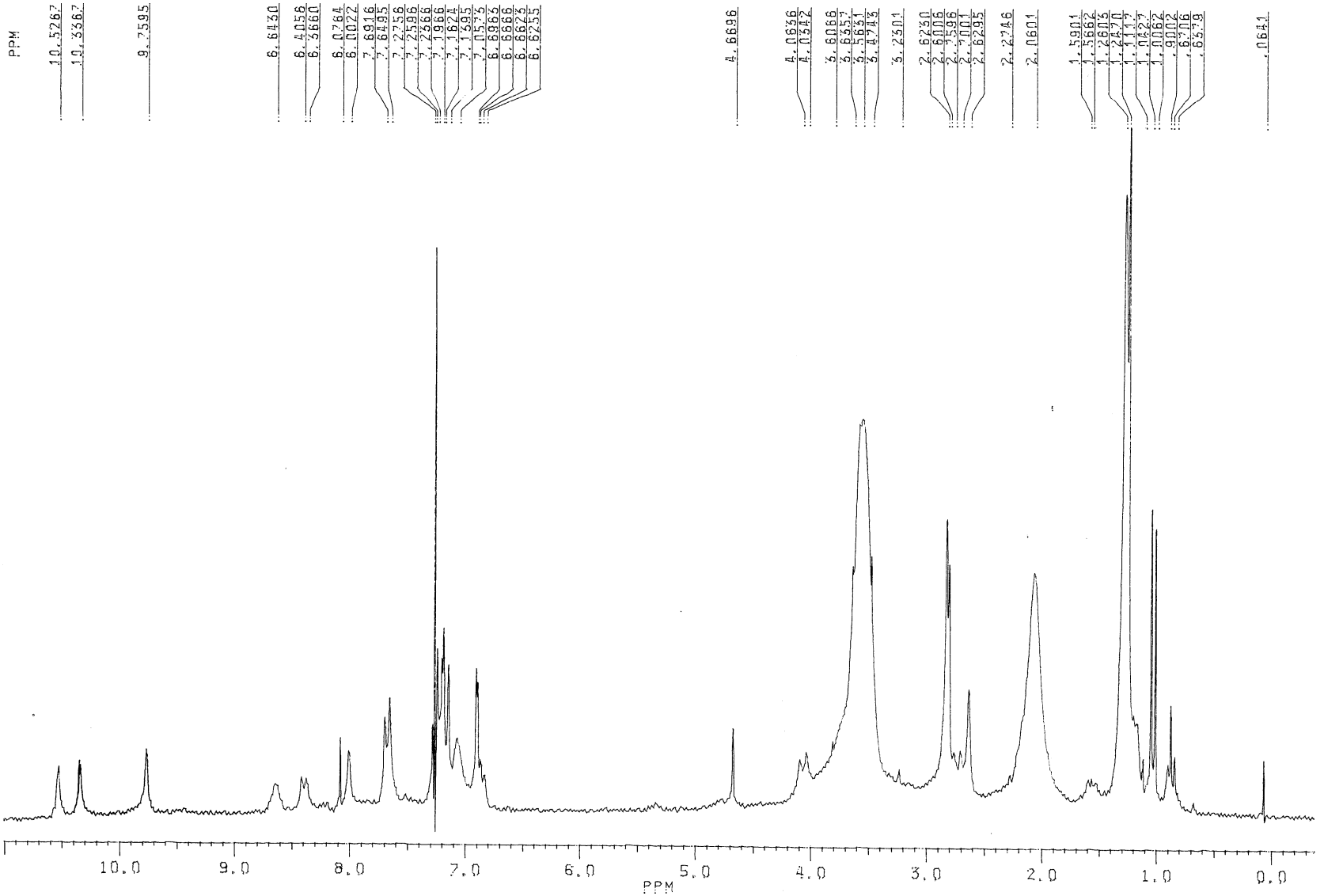


Figure S55. ^{1}H NMR spectrum of weak complex of (–)-*R*-receptor 1 with *L*-alanine (200 MHz, $CDCl_3$).

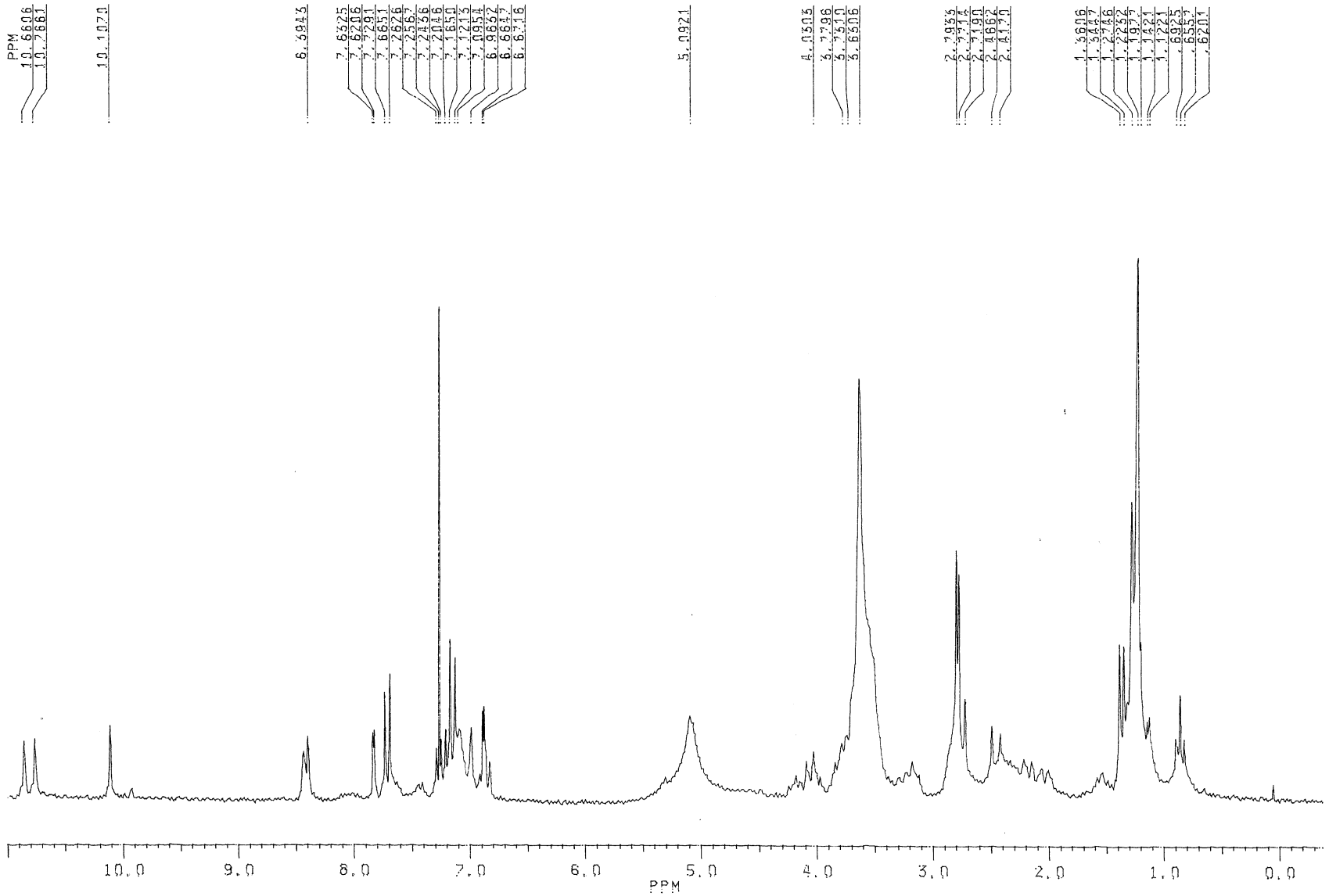


Figure S56. ^{1}H NMR spectrum of (+)-receptor 1 (200 MHz, $CDCl_3$).

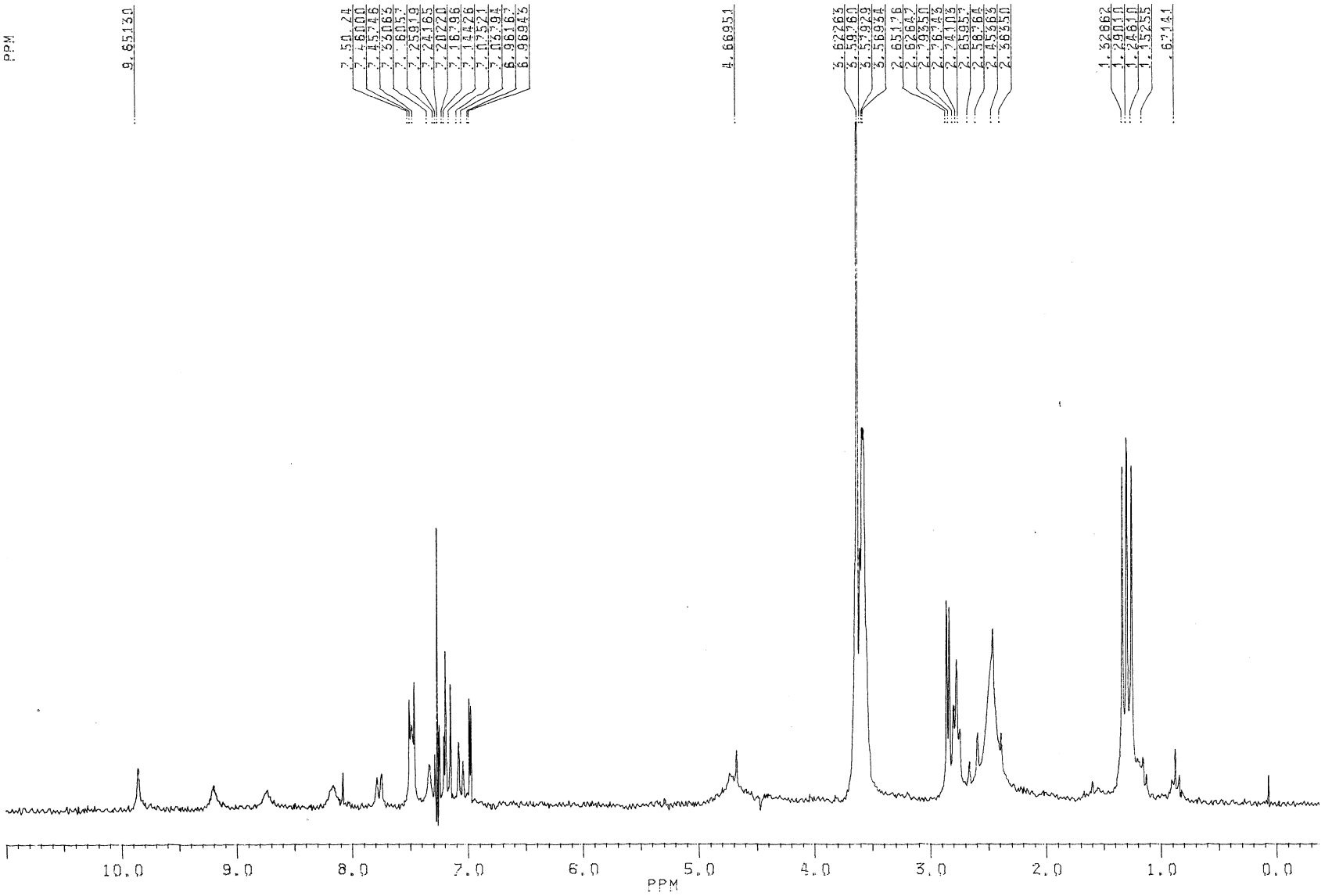


Figure S57. ^{1}H NMR spectrum of (-)-receptor 1 (200 MHz, $CDCl_3$).

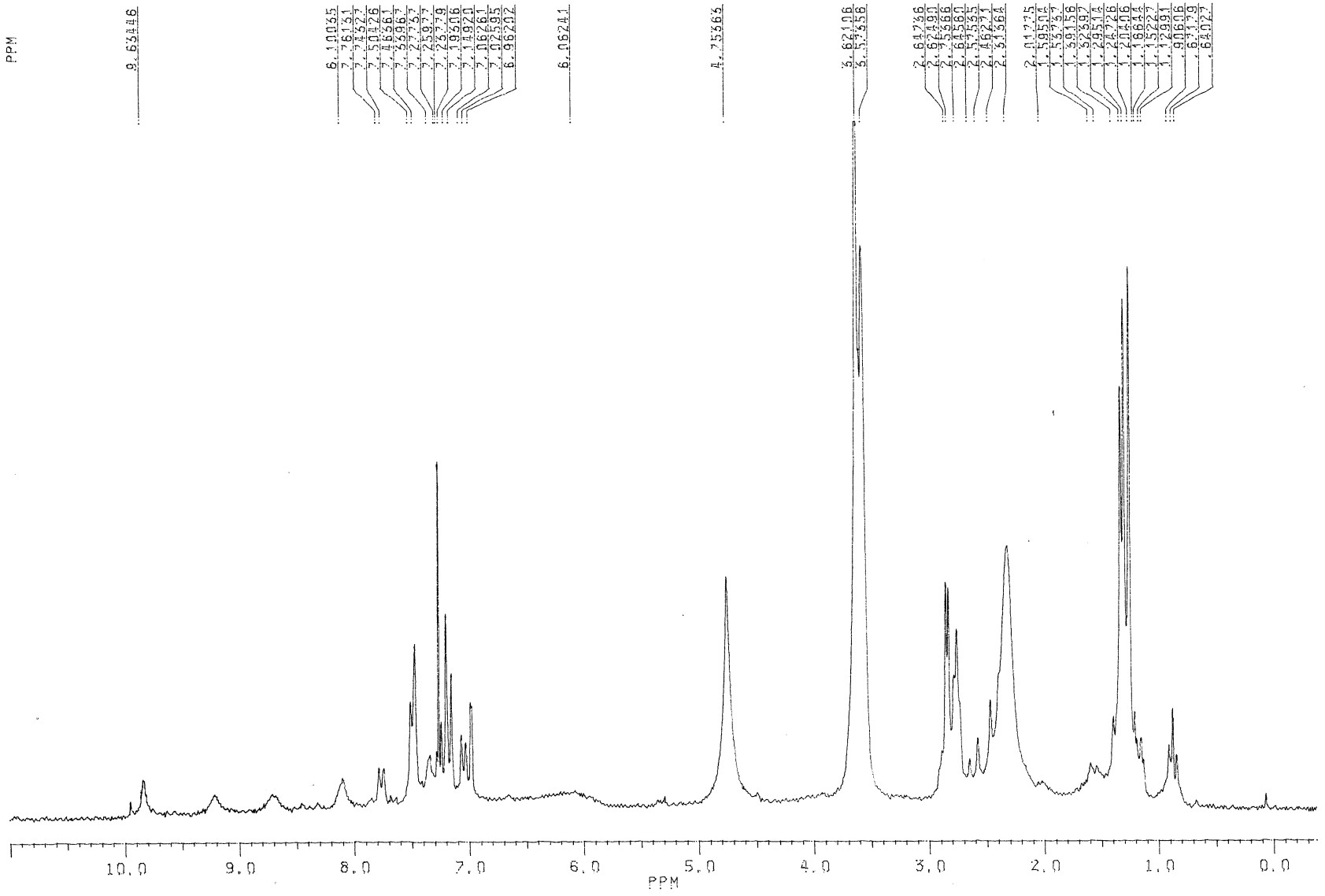


Figure S58. ^{1}H NMR spectrum of racemic receptor 1 and a saturated aqueous solution of *L*-Leucine (200 MHz, $CDCl_3$).

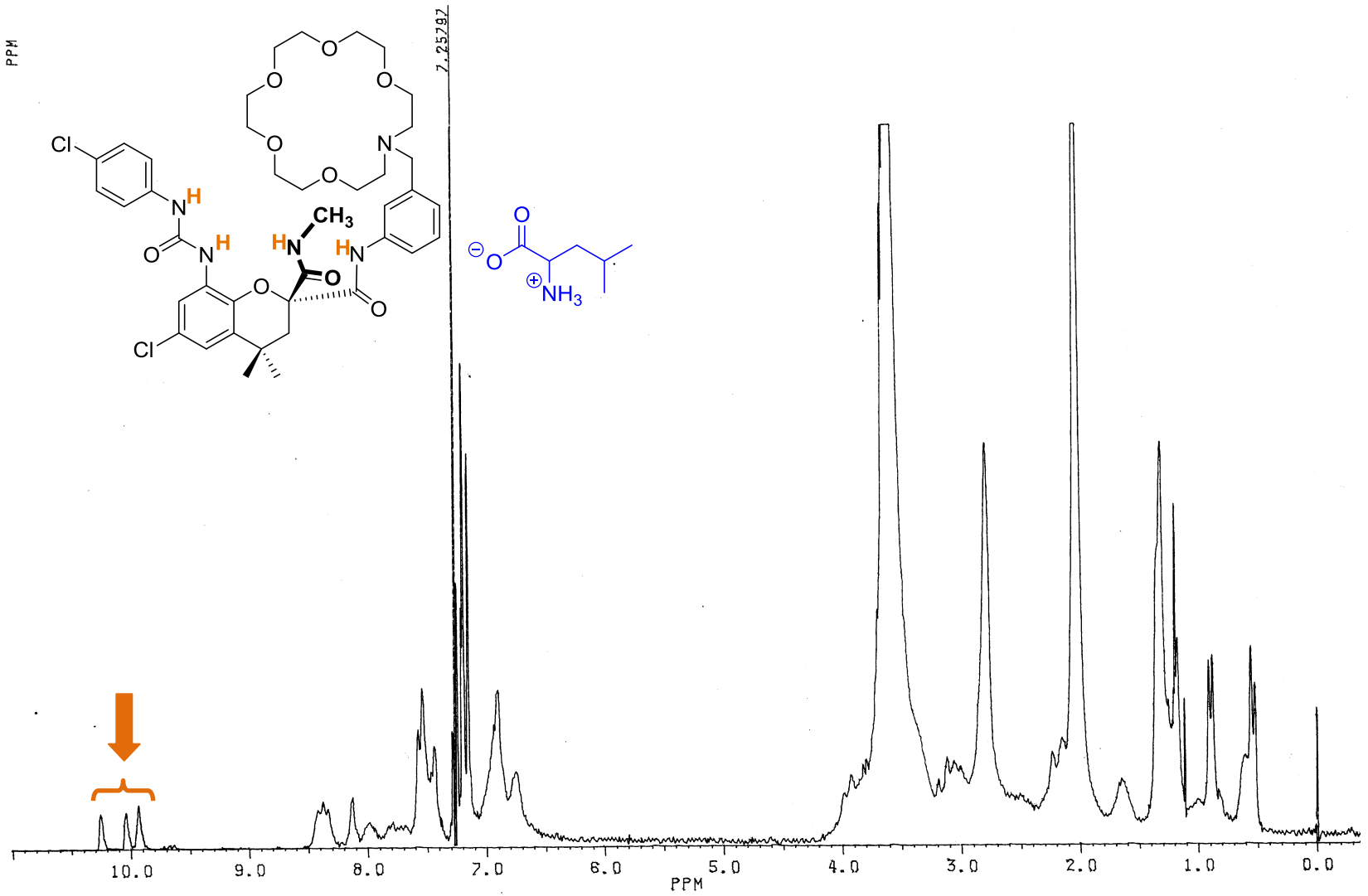


Figure S59. ^{1}**H NMR spectrum of racemic receptor 1 and a saturated aqueous solution of *L*-Leucine and *L*-Alanine (200 MHz, $CDCl_3$).**

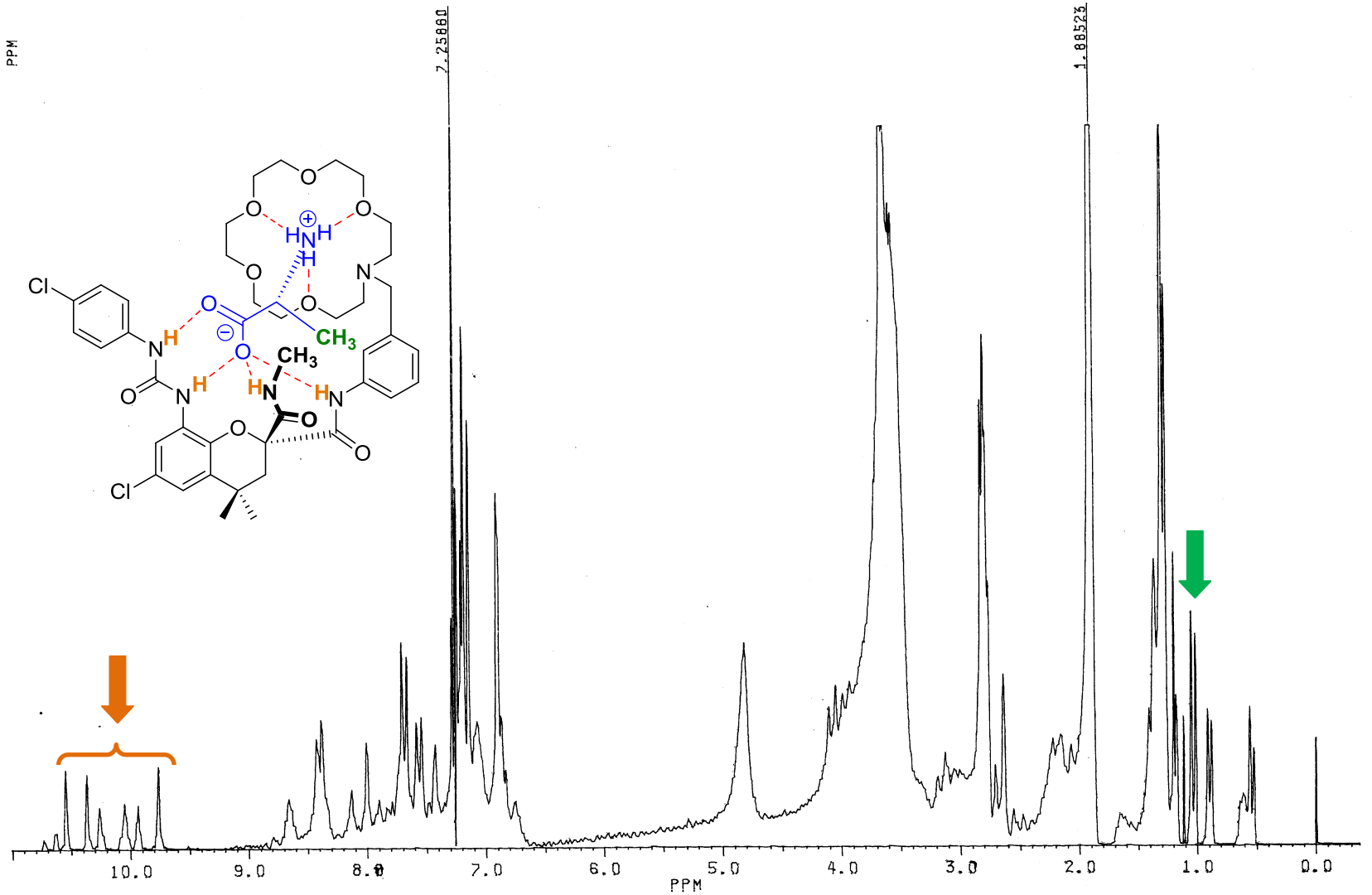


Figure S60. ^{1}H NMR spectrum of racemic receptor 2 and a saturated aqueous solution of *L*-Leucine in the presence of 18-crown-6 ether (200 MHz, $CDCl_3$).

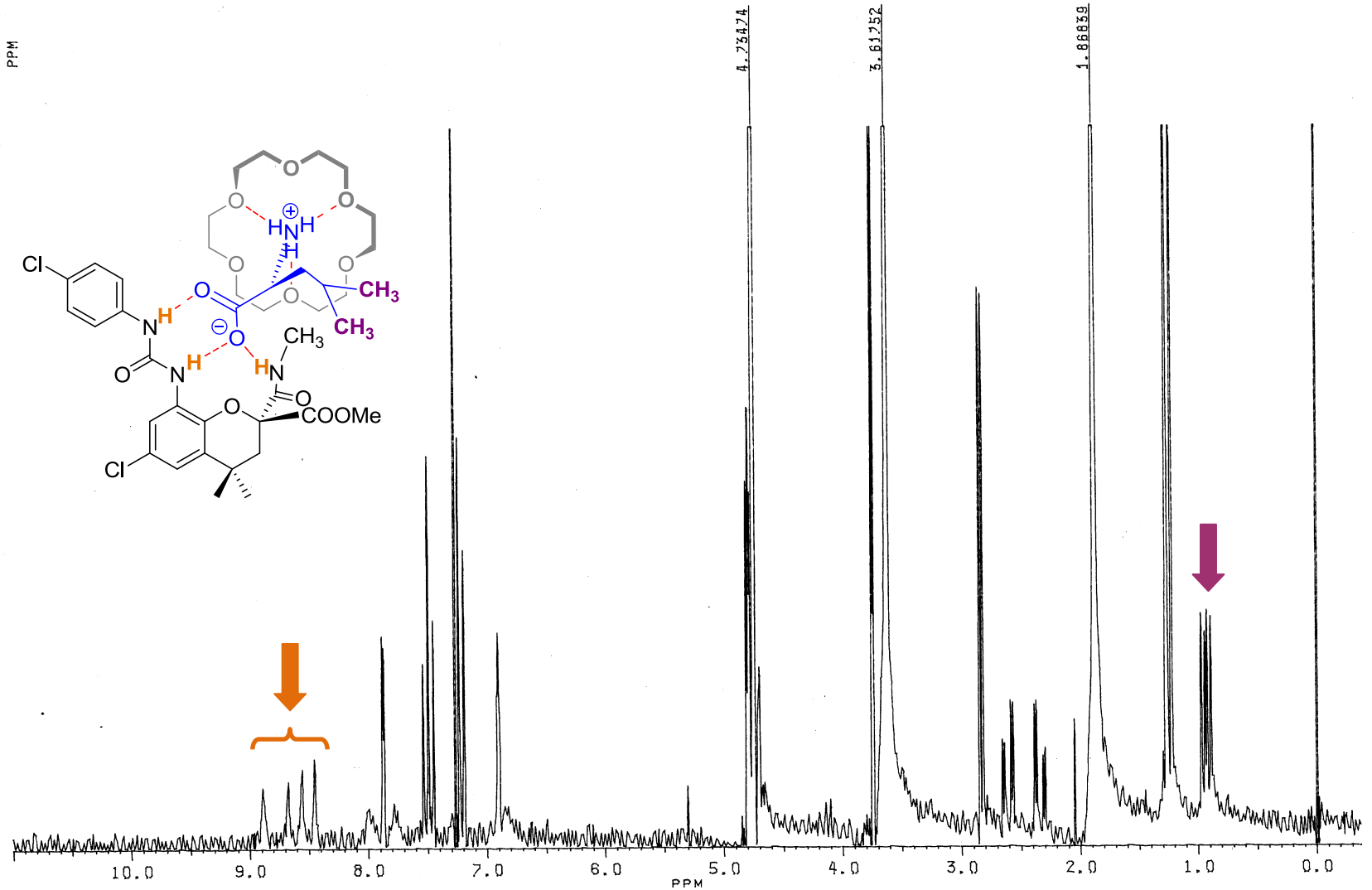


Figure S61. ^{1}**H NMR spectrum of racemic receptor 2 and a saturated aqueous solution of *L*-Leucine and *L*-Alanine in the presence of 18-crown-6 ether (200 MHz, $CDCl_3$).**

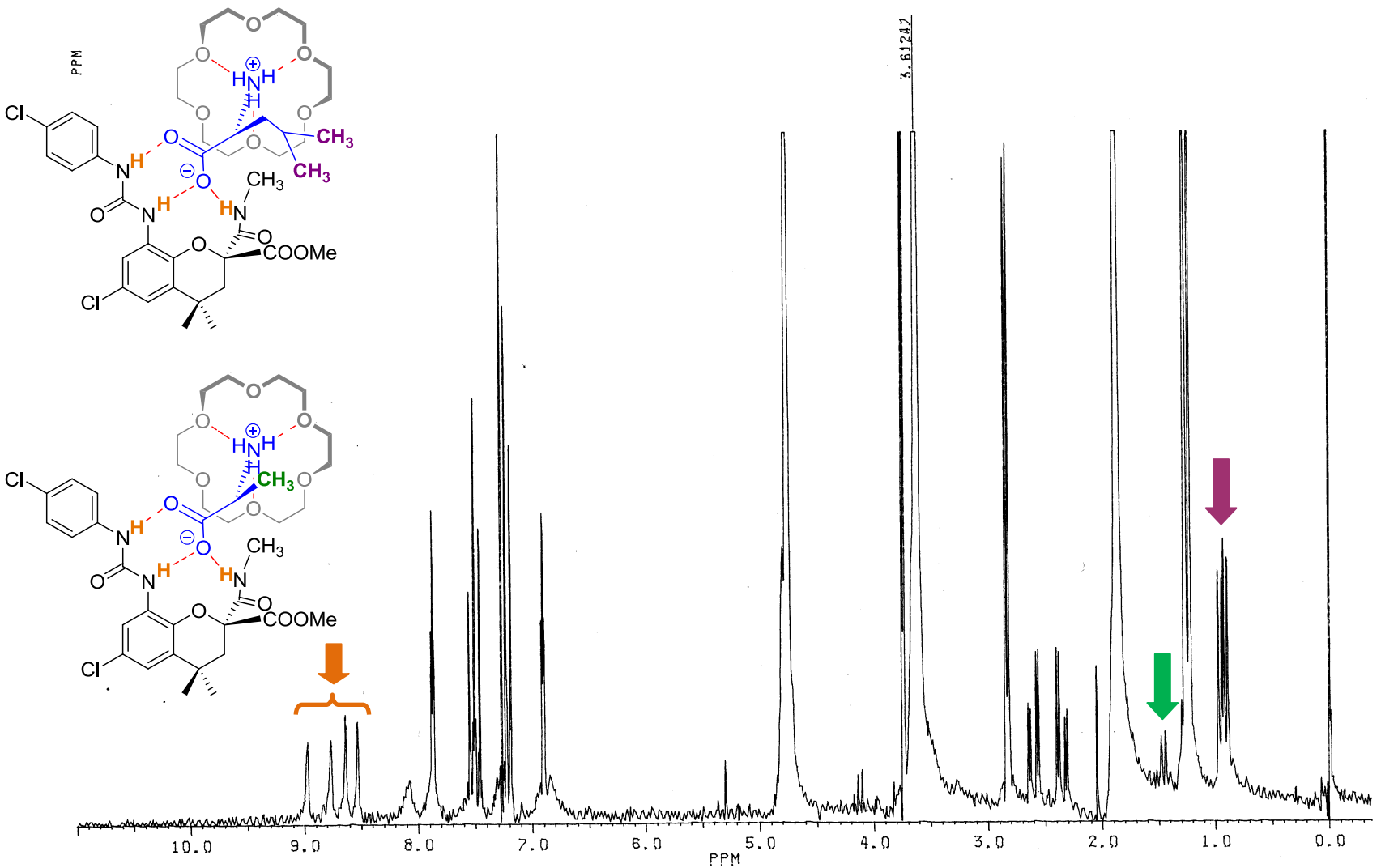


Figure S62. Circular dichroism spectrum for (+)-receptor 1 (DCM).

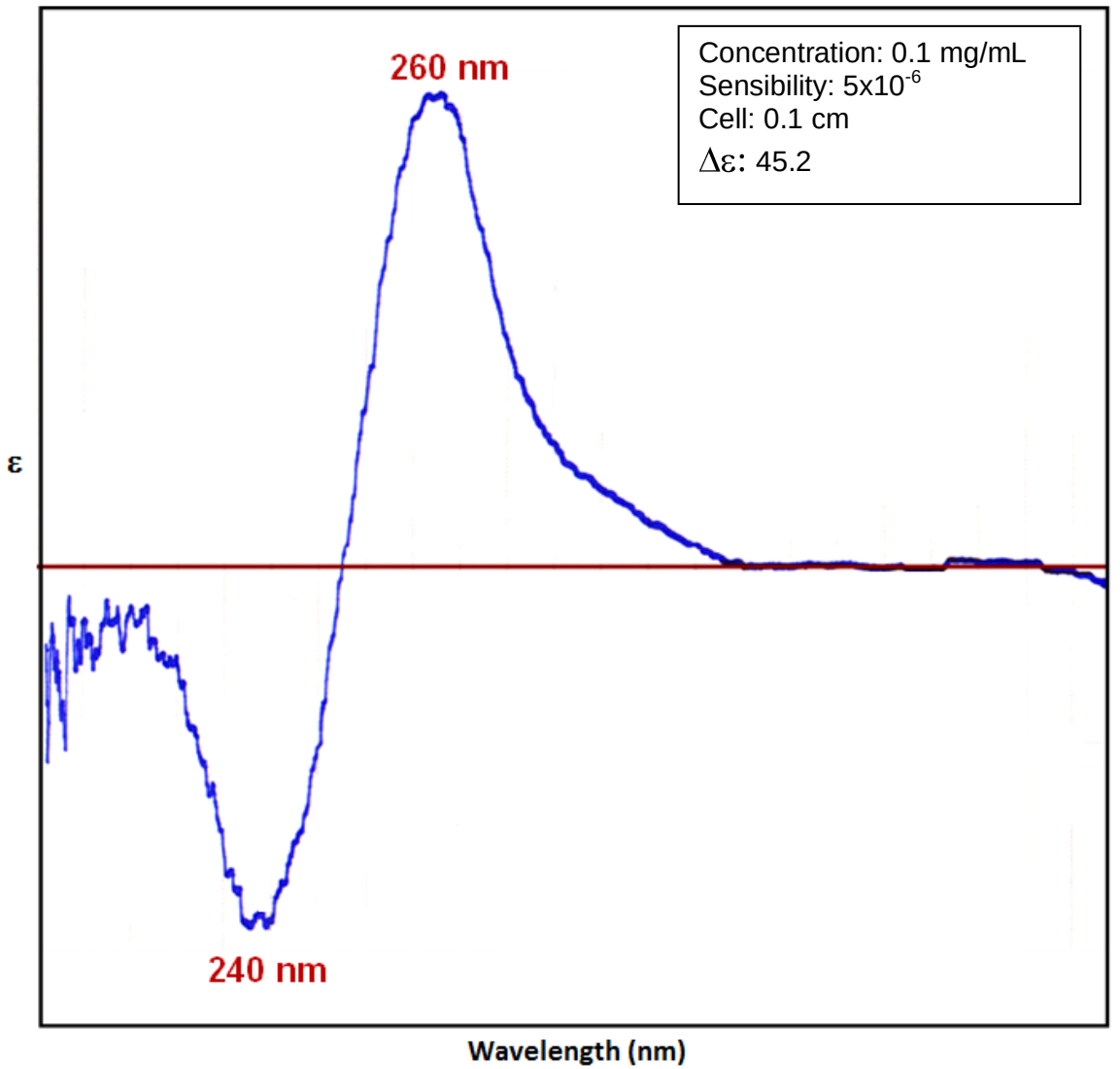


Figure S63. Circular dichroism spectrum for (-)-receptor 1 (DCM).

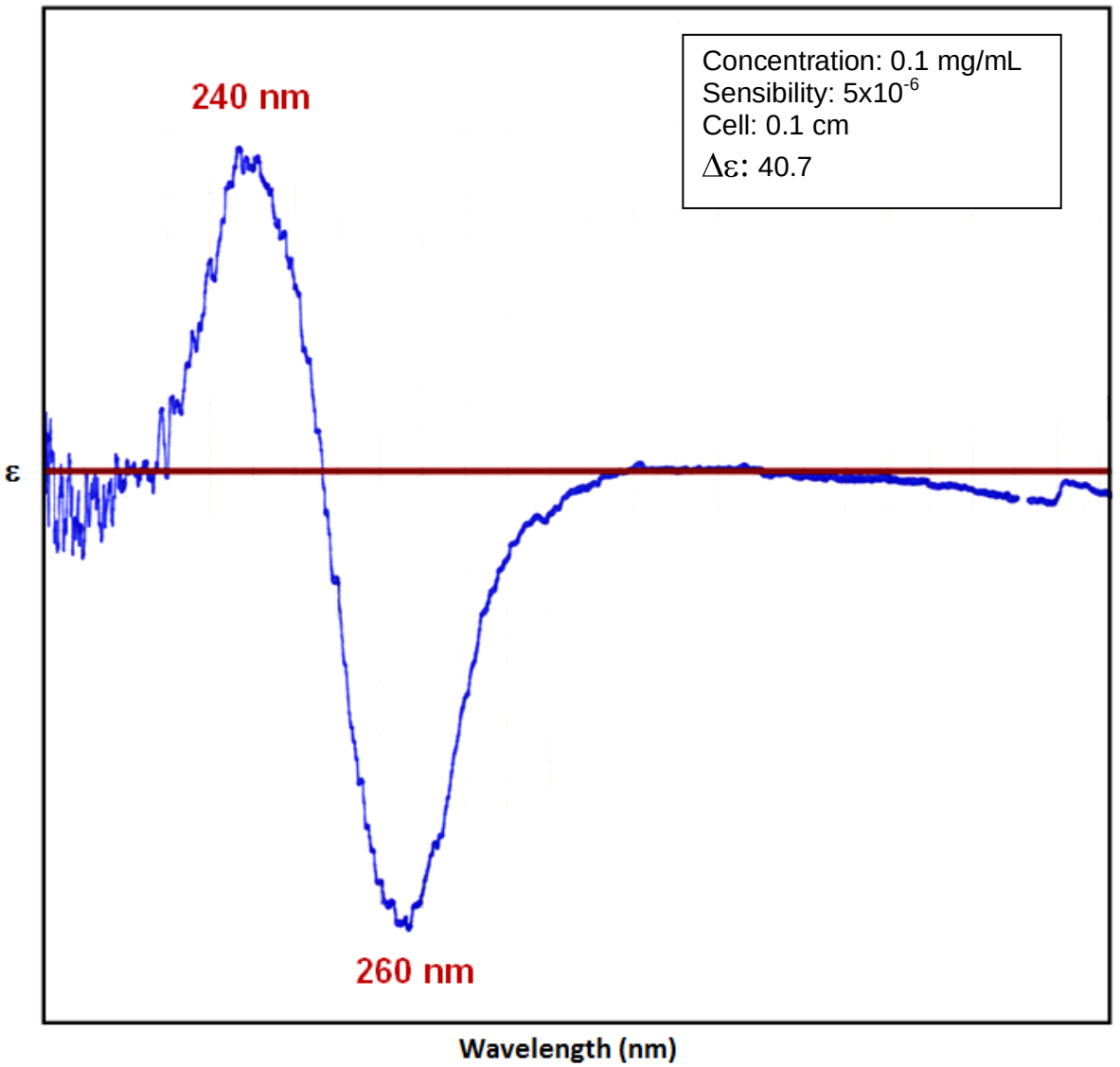


Figure S64. Circular dichroism spectrum for (-)-receptor 1 with glycine (DCM).

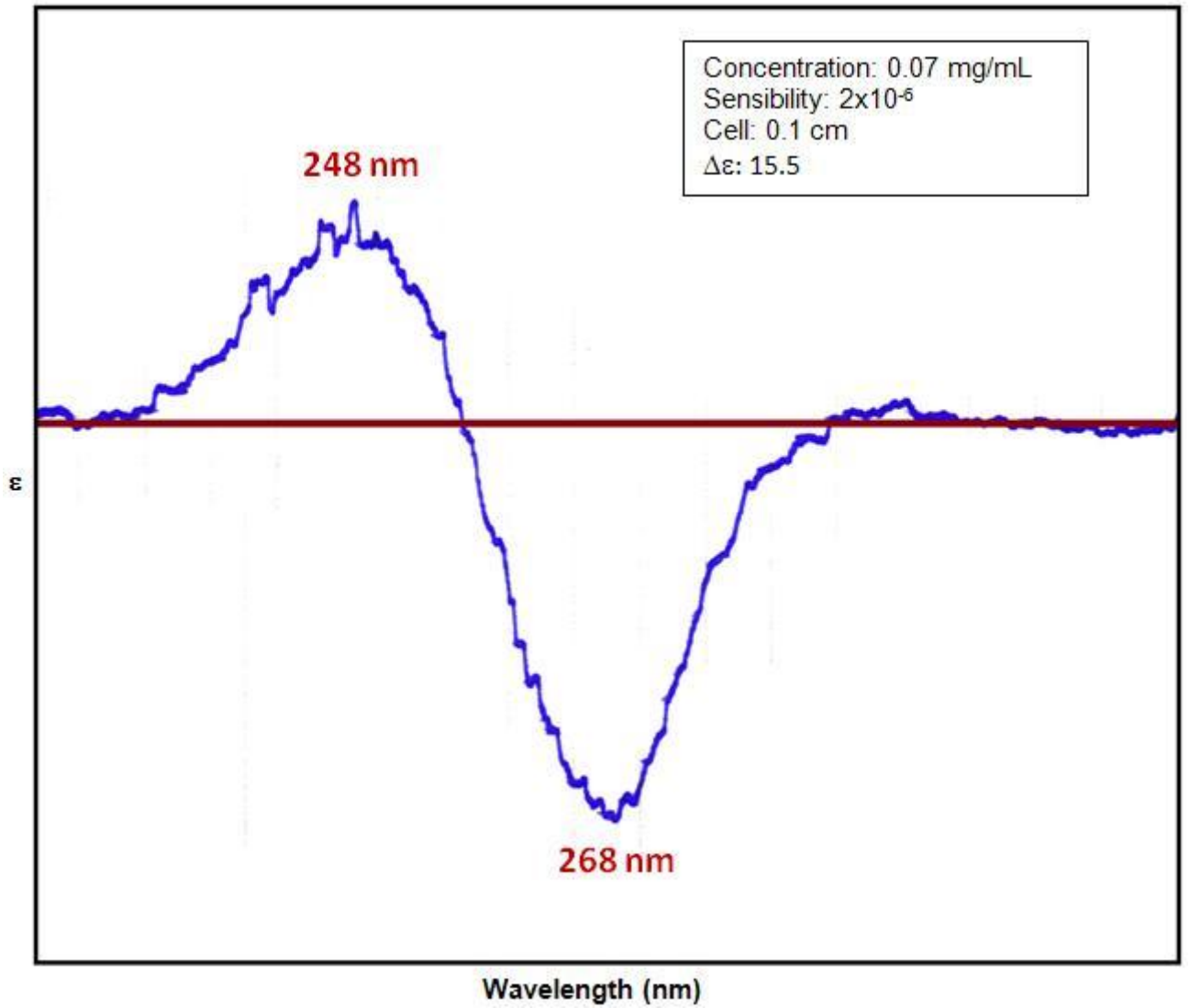


Figure S65. Determination of the absolute configuration of receptor 1 by simulation of ECD spectra.

All calculations were performed using Gaussian09 software.[1] 11 different conformations corresponding for the structure of the *R*-receptor **1** shown were optimized using B3LYP[2] DFT functional 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, 5] The results show a large energy difference for one of the conformations, so time-dependent DFT calculation was performed for this conformation using B98 functional[6] and 6-31G**, including the 50 more stable singlet excited states. This functional was chosen after considering its performance in the Truhlar benchmark database VES21 for electronic excitation energies involving valence excited states.[7] The ECD spectrum of this conformation was simulated using a value of σ=0.4 using Gaussum software.[8]

Conformation 1: ΔG: 0.0 kcal/mol

Cl	-6.04911	-4.01009	-2.34933
Cl	-5.32291	7.34293	0.63475
O	-0.99695	-2.24437	0.09628
O	-4.76889	0.68029	-1.13183
O	-1.61741	-0.96200	2.30707
O	1.69748	-3.53999	2.03910
O	1.93379	2.12576	-2.56651
O	-0.13225	1.84430	-0.33726
O	1.45921	0.24110	1.73814
O	3.65284	2.11651	2.73621
O	5.36542	2.47381	0.33918
N	-2.80096	-0.37419	-0.52359
N	-3.09420	1.85187	-0.05354
N	-0.30524	-2.25542	3.66060
N	1.61269	-2.31980	0.09266
N	4.73911	1.18380	-2.42972
C	-4.32193	-2.12423	-1.42758
H	-5.03811	-1.39203	-1.76804
C	-4.56207	-3.48890	-1.55626
C	-3.69519	-4.45790	-1.05874
H	-3.95511	-5.50617	-1.13760
C	-2.50076	-4.05202	-0.45545
C	-1.50007	-4.99038	0.21579
C	-1.06171	-4.26650	1.51940
H	-1.94072	-4.18283	2.16724
H	-0.31294	-4.85367	2.05838
C	-0.47586	-2.84968	1.28042
C	-2.22271	-2.68763	-0.38198
C	-3.14141	-1.70441	-0.79616
C	-3.66046	0.71562	-0.61037
C	-3.67855	3.12203	0.07798
C	-4.98271	3.43771	-0.34007
H	-5.59277	2.67436	-0.80098
C	-5.47801	4.72899	-0.16493
H	-6.48550	4.96666	-0.49034
C	-4.68643	5.71293	0.42222
C	-3.39207	5.41712	0.84459
H	-2.77811	6.18332	1.30632
C	-2.89692	4.12850	0.67293
H	-1.89117	3.89565	1.01307
C	-0.84178	-1.89813	2.47118
C	-0.53548	-1.48722	4.87307
H	-1.49474	-0.97640	4.77932
H	0.24642	-0.73425	5.03502
H	-0.56336	-2.15985	5.73522
C	1.06661	-2.93754	1.16495
C	2.97513	-2.24911	-0.28056
C	3.33289	-1.27866	-1.22214
H	2.59645	-0.55050	-1.55368
C	4.63582	-1.21235	-1.72605
C	5.59463	-2.10827	-1.24645
H	6.61063	-2.07009	-1.63225
C	5.24716	-3.05382	-0.27863
H	5.99833	-3.74363	0.09687
C	3.94489	-3.14186	0.20647
H	3.67341	-3.88220	0.94590
C	4.95757	-0.21561	-2.82432
H	5.98947	-0.37668	-3.18243
H	4.31069	-0.43470	-3.68115
C	4.14803	1.98930	-3.49664
H	4.66961	1.85386	-4.46564
H	4.25143	3.04602	-3.23293
C	2.66314	1.72123	-3.71136
H	2.32631	2.28839	-4.59632
H	2.47690	0.65586	-3.92606
C	0.53830	1.93519	-2.71948
H	0.29180	0.86251	-2.77821
H	0.18897	2.40760	-3.65462
C	-0.21821	2.56819	-1.56512
H	0.12129	3.60367	-1.42449
H	-1.27958	2.59215	-1.83397
C	0.88628	2.30299	0.56379
H	1.87676	2.19808	0.10788
H	0.71362	3.37001	0.78195
C	0.81046	1.50817	1.85897
H	-0.24064	1.32792	2.12022
H	1.27595	2.09975	2.65169
C	2.51720	0.00119	2.65852
H	2.71771	-1.07287	2.60025
H	2.19883	0.23548	3.68656
C	3.80767	0.74750	2.35708
H	4.62266	0.29323	2.94643
H	4.06114	0.65800	1.29586
C	4.82539	2.90417	2.63848
H	5.71014	2.32034	2.93638
H	4.70471	3.72765	3.35312
C	5.05495	3.50245	1.25858
H	4.15353	4.05017	0.93729
H	5.88407	4.23081	1.32179
C	5.72149	2.96141	-0.94103
H	6.64971	3.55488	-0.86878
H	4.93735	3.63190	-1.32633
C	5.95751	1.78115	-1.87880
H	6.64966	2.09903	-2.68399
H	6.47922	1.01554	-1.29560
C	-0.30408	-5.27651	-0.72136
H	-0.64310	-5.83808	-1.59864
H	0.45646	-5.87646	-0.20681

H	0.16910	-4.35905	-1.07963
C	-2.14070	-6.33031	0.62111
H	-3.02493	-6.18183	1.25056
H	-1.41924	-6.93528	1.18230
H	-2.44116	-6.91235	-0.25652
H	-2.03051	-0.30620	0.13802
H	-2.10702	1.79672	0.19227
H	0.96259	-1.75975	-0.44702
H	0.45454	-2.92859	3.62980

Conformation 2: ΔG: +1.9 kcal/mol

Cl	-6.89648	-3.94274	-3.26633
Cl	-7.82329	7.21904	0.53938
O	-2.53673	-1.85623	0.06895
O	-6.11382	0.90896	-1.76295
O	-3.55966	-0.81468	2.24933
O	0.03185	-2.90879	2.30177
O	7.99879	-0.69419	0.19712
O	7.30347	0.02130	-2.55039
O	5.01768	1.86604	-3.08233
O	5.27930	3.65696	-0.84045
O	5.16812	2.40616	1.80144
N	-4.52343	-0.20721	-0.51836
N	-5.25054	1.85334	0.16583
N	-2.33290	-2.10586	3.67761
N	0.00379	-1.53156	0.45004
N	5.80256	-0.55195	2.12272
C	-5.61122	-1.97737	-1.89756
H	-6.36118	-1.30074	-2.28140
C	-5.62919	-3.33670	-2.20104
C	-4.71519	-4.24454	-1.66750
H	-4.81466	-5.29992	-1.88970
C	-3.68409	-3.76925	-0.85021
C	-2.65632	-4.63406	-0.12151
C	-2.49033	-3.99987	1.29190
H	-3.44253	-4.10871	1.82219
H	-1.73204	-4.53705	1.86908
C	-2.09590	-2.50060	1.26175
C	-3.61598	-2.39884	-0.61339
C	-4.60500	-1.49897	-1.04745
C	-5.37066	0.85258	-0.79134
C	-5.89201	3.10294	0.19957
C	-6.74124	3.57214	-0.81591
H	-6.93869	2.94826	-1.67584
C	-7.32743	4.83193	-0.70409
H	-7.98364	5.19096	-1.49006
C	-7.07598	5.62868	0.41029
C	-6.23676	5.17669	1.42657
H	-6.04258	5.79812	2.29428
C	-5.65032	3.92007	1.31655
H	-4.99430	3.56928	2.11059
C	-2.73449	-1.70646	2.45315
C	-2.78405	-1.44882	4.89509
H	-3.78364	-1.04751	4.72324
H	-2.11983	-0.62417	5.18327
H	-2.81936	-2.17692	5.70996
C	-0.55446	-2.34151	1.37542
C	1.35925	-1.14521	0.28378
C	2.37985	-1.52978	1.16320
H	2.14373	-2.15965	2.01121
C	3.69182	-1.10289	0.93506
C	3.98431	-0.28190	-0.16133
H	4.99998	0.06362	-0.32321
C	2.96302	0.09606	-1.03276
H	3.20005	0.72704	-1.88392
C	1.65478	-0.33187	-0.81753
H	0.85995	-0.03326	-1.49892
C	4.80693	-1.58492	1.84918
H	4.37394	-2.00607	2.77734
H	5.31347	-2.42092	1.35339
C	7.13687	-1.06364	2.40938
H	7.13830	-1.81879	3.22369
H	7.74912	-0.22634	2.76001
C	7.84809	-1.67181	1.20393
H	8.83248	-2.04846	1.53634
H	7.29655	-2.54107	0.80910
C	8.61986	-1.19877	-0.96607
H	8.09154	-2.09275	-1.33612
H	9.66428	-1.49092	-0.75483
C	8.61533	-0.13829	-2.04909
H	8.99550	0.81110	-1.63873
H	9.30081	-0.45585	-2.85508
C	7.23624	0.93596	-3.62399
H	7.69331	1.89916	-3.34345
H	7.79821	0.55170	-4.49539
C	5.77895	1.13054	-4.02582
H	5.30328	0.14776	-4.10286
H	5.73811	1.61140	-5.01715
C	5.16164	3.27138	-3.18567
H	4.68608	3.63764	-4.11207
H	6.22079	3.56638	-3.21134
C	4.50691	3.93083	-1.98822
H	4.44491	5.01865	-2.17298
H	3.47845	3.55296	-1.86958
C	4.76001	4.24144	0.33655
H	3.69852	3.97964	0.47099
H	4.83315	5.34268	0.28671
C	5.54728	3.73759	1.53077
H	6.62567	3.80744	1.31314
H	5.33753	4.38639	2.40056
C	5.86627	1.83393	2.88767
H	5.70066	2.42841	3.80485
H	6.95104	1.83266	2.69127
C	5.34336	0.41840	3.11536
H	5.60203	0.10157	4.14501
H	4.25155	0.47191	3.06334
C	-1.32033	-4.66611	-0.89937
H	-1.45978	-5.16966	-1.86201
H	-0.55675	-5.21504	-0.33530
H	-0.93650	-3.66388	-1.10514
C	-3.15094	-6.07870	0.07278
H	-4.12301	-6.10886	0.57704
H	-2.43337	-6.64288	0.67938
H	-3.24806	-6.59953	-0.88557
H	-3.97709	-0.18888	0.34336
H	-4.69166	1.63685	0.98135
H	-0.65015	-1.17598	-0.23913
H	-1.49958	-2.68804	3.70391

Conformation 3: ΔG: +2.3 kcal/mol

Cl	-6.60233	-4.28683	-3.03887
Cl	-8.49711	6.89968	0.34587
O	-2.49503	-1.72559	0.28560
O	-6.26413	0.65942	-1.67732
O	-3.63298	-0.72475	2.42599
O	0.13348	-2.49245	2.56410
O	6.26461	3.44204	-1.28063
O	7.06341	2.68700	1.42509
O	6.82133	-0.15535	2.30535
O	7.50125	-1.52064	-0.13796
O	5.81887	-0.87430	-2.43894
N	-4.61180	-0.27956	-0.37001
N	-5.51861	1.73579	0.23098
N	-2.30833	-1.85688	3.90105
N	-0.00335	-1.14732	0.69370
N	4.24368	1.72651	-2.51825
C	-5.51884	-2.17732	-1.71028
H	-6.32186	-1.58221	-2.12105
C	-5.40959	-3.54023	-1.97667
C	-4.42403	-4.34684	-1.40912
H	-4.42339	-5.41222	-1.60394
C	-3.45122	-3.75871	-0.59381
C	-2.35919	-4.50719	0.16964
C	-2.27185	-3.82371	1.56694
H	-3.21859	-4.00307	2.08789
H	-1.47717	-4.27473	2.16850
C	-2.01190	-2.29720	1.49940
C	-3.51077	-2.38213	-0.39354

C	-4.57089	-1.58736	-0.86326
C	-5.53752	0.69697	-0.69233
C	-6.25426	2.93264	0.20458
C	-7.11161	3.29869	-0.84593
H	-7.24086	2.63111	-1.68583
C	-7.79337	4.51343	-0.79461
H	-8.45536	4.79288	-1.60757
C	-7.62968	5.36699	0.29378
C	-6.78402	5.01709	1.34440
H	-6.65815	5.68239	2.19191
C	-6.10234	3.80547	1.29490
H	-5.44164	3.53432	2.11580
C	-2.73232	-1.53134	2.66246
C	-2.82849	-1.20757	5.09502
H	-3.85976	-0.90679	4.90580
H	-2.24621	-0.31601	5.36023
H	-2.80201	-1.91033	5.93210
C	-0.49289	-1.99584	1.62400
C	1.30602	-0.61781	0.55506
C	1.51678	0.26736	-0.51232
H	0.68967	0.51024	-1.17897
C	2.76799	0.84485	-0.72790
C	3.82839	0.51885	0.12878
H	4.81084	0.94637	-0.04245
C	3.61399	-0.36138	1.18773
H	4.44410	-0.59988	1.84597
C	2.36187	-0.93670	1.41651
H	2.19959	-1.62050	2.23817
C	2.95898	1.86410	-1.83881
H	2.10499	1.81744	-2.54340
H	2.91793	2.86397	-1.39164
C	4.75688	2.96508	-3.09040
H	4.02276	3.46225	-3.75884
H	5.62293	2.71361	-3.71129
C	5.22087	3.98876	-2.05825
H	5.56320	4.89138	-2.59613
H	4.39011	4.30816	-1.40699
C	6.72486	4.32898	-0.28326
H	5.88825	4.68817	0.33824
H	7.20625	5.21270	-0.73934
C	7.73151	3.62260	0.60280
H	8.48861	3.12289	-0.02271
H	8.24935	4.37852	1.21985
C	7.92811	2.04716	2.33982
H	8.79057	1.60433	1.81500
H	8.33050	2.77652	3.06713
C	7.15200	0.97466	3.09495
H	6.20161	1.40195	3.42997
H	7.72644	0.67167	3.98608
C	7.86596	-1.10269	2.17583
H	8.04684	-1.60768	3.14073
H	8.80646	-0.62513	1.86427
C	7.47955	-2.13221	1.13264
H	8.19718	-2.97149	1.18017
H	6.47885	-2.53486	1.35841
C	7.15521	-2.40022	-1.18833
H	6.19986	-2.90674	-0.97857
H	7.93020	-3.17765	-1.31391
C	7.02217	-1.60934	-2.47532
H	7.89296	-0.94242	-2.58605
H	7.02475	-2.30933	-3.33055
C	5.61290	-0.07963	-3.58825
H	5.61093	-0.71156	-4.49520
H	6.42966	0.65199	-3.70235
C	4.25946	0.61506	-3.46857
H	3.93059	0.93663	-4.47626
H	3.54515	-0.14005	-3.12627
C	-1.01469	-4.43572	-0.59054
H	-1.09383	-4.97030	-1.54335
H	-0.21317	-4.90119	-0.00451
H	-0.71987	-3.40735	-0.81357
C	-2.72254	-5.98554	0.39692
H	-3.69377	-6.09170	0.89259
H	-1.96357	-6.46581	1.02507
H	-2.75990	-6.53717	-0.54836
H	-4.08122	-0.18858	0.49686
H	-4.95930	1.59479	1.06258
H	-0.68069	-0.86163	-0.00518
H	-1.42696	-2.36156	3.95158

Conformation 4: ΔG: +5.2 kcal/mol

Cl	5.70792	5.69154	-1.36052
Cl	10.29766	-5.15348	-0.19071
O	2.00619	1.30896	-0.10523
O	6.68372	0.65061	-1.32042
O	2.89195	-0.00119	1.98596
O	-1.16866	0.67493	1.37818
O	-5.75603	-3.55200	1.31143
O	-4.94869	-1.15601	2.75711
O	-4.88946	1.51777	1.34177
O	-7.09883	1.71551	-0.56830
O	-7.26055	-0.28657	-2.60670
N	4.56482	0.69895	-0.40893
N	5.90947	-1.11955	-0.04673
N	0.98776	0.27457	3.21411
N	-0.19765	0.05680	-0.62197
N	-5.77630	-2.65864	-1.43487
C	5.08969	3.07849	-0.93955
H	6.11049	2.85382	-1.21346
C	4.61256	4.38677	-0.90793
C	3.32092	4.71261	-0.49600
H	3.02331	5.75210	-0.43357
C	2.43223	3.68290	-0.16952
C	1.01793	3.86896	0.37880
C	0.84904	2.79197	1.49206
H	1.55150	3.02908	2.29841
H	-0.15926	2.82876	1.91474
C	1.10923	1.34483	1.00173
C	2.88319	2.37015	-0.27944
C	4.21768	2.04318	-0.57611
C	5.80359	0.12905	-0.64761
C	6.97997	-2.02758	-0.11612
C	8.13507	-1.81498	-0.88607
H	8.23461	-0.90295	-1.45702
C	9.14452	-2.77612	-0.90347
H	10.03589	-2.60853	-1.49897
C	9.01429	-3.94704	-0.16050
C	7.87457	-4.17187	0.60887
H	7.77475	-5.08410	1.18734
C	6.86579	-3.21419	0.62714
H	5.97614	-3.39187	1.22788
C	1.75592	0.45513	2.11960
C	1.40582	-0.57006	4.32321
H	2.49349	-0.53423	4.39699
H	1.09852	-1.61360	4.17906
H	0.96580	-0.19545	5.25124
C	-0.22406	0.66256	0.58535
C	-1.19449	-0.71813	-1.27062
C	-2.52433	-0.77414	-0.84228
H	-2.84048	-0.20043	0.01987
C	-3.45824	-1.56189	-1.53358
C	-3.03519	-2.29098	-2.65143
H	-3.74076	-2.90979	-3.19421
C	-1.70757	-2.22712	-3.08009
H	-1.38959	-2.79368	-3.95133
C	-0.78346	-1.44478	-2.39800
H	0.25276	-1.40237	-2.72659
C	-4.90552	-1.55937	-1.03568
H	-4.89795	-1.50399	0.05834
H	-5.39084	-0.63504	-1.36045
C	-5.41685	-4.00981	-1.03019
H	-4.66791	-4.49240	-1.69064
H	-6.32269	-4.62855	-1.08021
C	-4.84877	-4.11211	0.38046
H	-4.66642	-5.17934	0.59450
H	-3.87826	-3.59719	0.44291
C	-5.27899	-3.51372	2.64320
H	-4.18092	-3.56863	2.67239
H	-5.67464	-4.36796	3.21715
C	-5.71062	-2.21630	3.30265

H	-6.78702	-2.05271	3.13456
H	-5.54518	-2.29011	4.39249
C	-5.23882	0.10094	3.33502
H	-6.31548	0.32521	3.25920
H	-4.98147	0.09421	4.41028
C	-4.41261	1.17408	2.63398
H	-3.39309	0.80415	2.49499
H	-4.37132	2.07033	3.27579
C	-5.91554	2.49183	1.35457
H	-5.54979	3.42162	1.82553
H	-6.79351	2.15127	1.92510
C	-6.35116	2.80146	-0.06447
H	-6.96265	3.72154	-0.05080
H	-5.46516	2.99534	-0.69038
C	-7.62176	1.93873	-1.86266
H	-6.82384	2.22524	-2.56641
H	-8.36794	2.75285	-1.84729
C	-8.27628	0.65567	-2.33783
H	-8.95496	0.28782	-1.55265
H	-8.87895	0.85645	-3.24070
C	-7.69717	-1.63392	-2.66991
H	-8.30955	-1.79317	-3.57603
H	-8.31096	-1.87993	-1.79002
C	-6.47546	-2.55199	-2.70861
H	-6.83471	-3.55150	-2.98212
H	-5.82908	-2.21550	-3.53698
C	-0.03094	3.70300	-0.74491
H	0.07534	4.50910	-1.47893
H	-1.04746	3.74647	-0.33573
H	0.08090	2.75602	-1.27847
C	0.82885	5.24908	1.03350
H	1.58033	5.43649	1.80829
H	-0.16274	5.31205	1.49620
H	0.89452	6.05368	0.29355
H	3.91298	0.21621	0.20976
H	5.15774	-1.39112	0.57400
H	0.68424	0.15499	-1.11371
H	0.00434	0.50961	3.11016

Conformation 5: ΔG: +6.7 kcal/mol

Cl	-7.44128	-5.01130	-1.23083
Cl	-10.20204	6.33964	0.47718
O	-3.01608	-1.32224	-0.09526
O	-7.57298	0.12095	-1.08605
O	-3.60480	0.08510	2.03917
O	0.26925	-1.23410	1.27126
O	7.45976	0.96188	-2.55616
O	9.11666	2.69912	-0.88150
O	8.98846	2.32387	2.07685
O	8.62905	-0.55304	2.29878
O	6.32053	-1.76368	0.92276
N	-5.44709	-0.29166	-0.28955
N	-6.47411	1.69458	0.20706
N	-1.72457	-0.50510	3.19110
N	-0.66132	-0.43597	-0.68365
N	5.05368	-0.25523	-1.35262
C	-6.38077	-2.54326	-0.81862
H	-7.35969	-2.14892	-1.05072
C	-6.12782	-3.91309	-0.81268
C	-4.89471	-4.45467	-0.45121
H	-4.77325	-5.52988	-0.40403
C	-3.83512	-3.59135	-0.15328
C	-2.45402	-4.01701	0.34471
C	-2.06641	-2.99306	1.45337
H	-2.76834	-3.11718	2.28489
H	-1.06393	-3.20180	1.83854
C	-2.10021	-1.51788	0.97916
C	-4.06421	-2.22093	-0.24074
C	-5.33558	-1.67209	-0.48249
C	-6.59271	0.47204	-0.44217
C	-7.39690	2.75455	0.23477
C	-8.59171	2.76880	-0.50298
H	-8.84639	1.92141	-1.12337
C	-9.44362	3.86931	-0.42315
H	-10.36667	3.87693	-0.99338
C	-9.11617	4.95565	0.38469
C	-7.93439	4.95596	1.12277
H	-7.68116	5.80248	1.75205
C	-7.08275	3.85883	1.04421
H	-6.15997	3.86056	1.62083
C	-2.55185	-0.54775	2.12667
C	-1.96389	0.37319	4.32707
H	-3.03931	0.52356	4.42941
H	-1.48355	1.35056	4.19336
H	-1.57328	-0.09287	5.23554
C	-0.69079	-1.05825	0.51859
C	0.43056	0.15449	-1.36509
C	1.72464	0.21455	-0.83262
H	1.91279	-0.20801	0.14524
C	2.75875	0.83021	-1.55060
C	2.47517	1.39712	-2.80050
H	3.26021	1.90608	-3.35340
C	1.18660	1.33355	-3.33242
H	0.97319	1.77694	-4.30118
C	0.16375	0.71219	-2.62360
H	-0.84182	0.66853	-3.03633
C	4.17454	0.85581	-0.97669
H	4.66805	1.78917	-1.26725
H	4.12445	0.86301	0.11705
C	5.43887	-0.33245	-2.75499
H	4.57021	-0.46401	-3.43180
H	6.06268	-1.22508	-2.87466
C	6.24928	0.85233	-3.27165
H	6.44352	0.68586	-4.34708
H	5.67956	1.79422	-3.19950
C	8.26936	2.02408	-3.01364
H	7.71400	2.97662	-2.99978
H	8.59642	1.84392	-4.05383
C	9.49292	2.15146	-2.12718
H	9.95530	1.15968	-1.99613
H	10.23011	2.80227	-2.63160
C	10.20606	2.86211	0.00131
H	10.76621	1.91815	0.10555
H	10.91293	3.61810	-0.38921
C	9.68268	3.32563	1.35645
H	8.96733	4.13843	1.19291
H	10.52285	3.72372	1.95054
C	9.82850	1.44581	2.79952
H	10.31737	1.98114	3.63316
H	10.62098	1.02290	2.16362
C	8.99898	0.30497	3.35602
H	9.59998	-0.23732	4.10873
H	8.10911	0.70971	3.86494
C	7.88541	-1.67564	2.72373
H	7.01132	-1.36899	3.32078
H	8.50816	-2.33582	3.35443
C	7.40813	-2.44645	1.50728
H	8.24258	-2.54747	0.79449
H	7.10675	-3.46377	1.81715
C	5.87488	-2.35183	-0.28271
H	5.56272	-3.39815	-0.10751
H	6.68964	-2.37192	-1.02500
C	4.67915	-1.55508	-0.80030
H	4.12377	-2.17519	-1.52787
H	4.00884	-1.40240	0.05064
C	-1.43194	-4.02422	-0.81536
H	-1.70003	-4.79549	-1.54534
H	-0.42428	-4.24380	-0.44246
H	-1.39876	-3.06873	-1.34511
C	-2.47861	-5.41391	0.99103
H	-3.22206	-5.47548	1.79327
H	-1.49602	-5.64852	1.41608
H	-2.70847	-6.19023	0.25373
H	-4.69951	0.06448	0.30649
H	-5.67038	1.81177	0.81095
H	-1.55818	-0.41004	-1.15735
H	-0.79893	-0.90262	3.05639

Conformation 6: ΔG: +7.5 kcal/mol

Cl	7.29878	-4.47813	-0.63285
Cl	6.95138	7.20541	1.13461
O	2.01295	-2.01115	0.03606
O	6.21658	0.32116	0.85811
O	1.82944	0.02088	-1.60637
O	-1.41455	-2.50183	-0.78595
O	-4.78774	1.96821	2.05393
O	-3.39941	3.42494	-0.22240
O	-3.10253	2.40326	-3.00949
O	-5.83253	1.46775	-2.92160
O	-6.94498	-0.17011	-0.62018
N	4.12859	-0.43437	0.23073
N	4.54327	1.81659	0.29102
N	-0.09196	-0.71026	-2.60745
N	-0.30138	-2.03590	1.17962
N	-5.68019	-0.97188	2.11373
C	5.64140	-2.38945	-0.10383
H	6.53048	-1.81595	0.11585
C	5.71203	-3.71923	-0.51275
C	4.58803	-4.46293	-0.87018
H	4.70830	-5.47297	-1.24196
C	3.32112	-3.88347	-0.74186
C	2.00181	-4.52400	-1.17182
C	1.16972	-3.38395	-1.83245
H	1.69524	-3.06929	-2.74047
H	0.18461	-3.75095	-2.13498
C	0.96134	-2.15017	-0.91744
C	3.24387	-2.58307	-0.25043
C	4.37873	-1.78873	-0.01080
C	5.07162	0.54576	0.48622
C	5.16708	3.05692	0.50611
C	6.45458	3.19882	1.04914
H	7.02214	2.31726	1.31077
C	6.99250	4.47075	1.23843
H	7.98769	4.57652	1.65748
C	6.25967	5.60324	0.89155
C	4.98131	5.47884	0.35144
H	4.41215	6.36194	0.08123
C	4.44247	4.21036	0.16220
H	3.44386	4.11524	-0.25918
C	0.93561	-0.81718	-1.74506
C	-0.29925	0.45344	-3.46028
H	0.52124	1.14991	-3.28357
H	-1.25273	0.94016	-3.23096
H	-0.29134	0.15696	-4.51576
C	-0.38550	-2.26260	-0.15490
C	-1.31889	-2.10325	2.16064
C	-2.68318	-2.11919	1.84995
H	-3.00240	-2.06409	0.81761
C	-3.63252	-2.21311	2.87657
C	-3.20761	-2.28529	4.20670
H	-3.94221	-2.37523	5.00284
C	-1.84628	-2.24567	4.51602
H	-1.51895	-2.29501	5.55080
C	-0.90208	-2.15570	3.50049
H	0.15927	-2.14027	3.73861
C	-5.10972	-2.26054	2.53006
H	-5.24764	-2.95799	1.69648
H	-5.65863	-2.68358	3.39600
C	-5.64808	0.02871	3.19094
H	-5.58972	-0.46251	4.17777
H	-6.58671	0.59361	3.18918
C	-4.51920	1.05049	3.10037
H	-4.46625	1.58690	4.06567
H	-3.55015	0.55912	2.93950
C	-3.92035	3.08371	2.09243
H	-2.86579	2.76662	2.12527
H	-4.11598	3.68190	3.00056
C	-4.12666	3.95587	0.86797
H	-5.20254	4.01574	0.63789
H	-3.77473	4.97857	1.09343
C	-3.51176	4.21064	-1.38888
H	-4.55832	4.25276	-1.73329
H	-3.18769	5.24916	-1.18833
C	-2.61480	3.62343	-2.47138
H	-1.63869	3.39785	-2.03004
H	-2.46469	4.36954	-3.26773
C	-4.04948	2.55615	-4.05486
H	-3.53489	2.62003	-5.02834
H	-4.63865	3.47410	-3.92409
C	-5.00346	1.37777	-4.05849
H	-5.60138	1.41253	-4.98733
H	-4.43831	0.43125	-4.06088
C	-6.87945	0.51628	-2.91510
H	-6.49038	-0.50582	-3.04520
H	-7.57925	0.71927	-3.74519
C	-7.62108	0.59815	-1.59357
H	-7.69307	1.65604	-1.29379
H	-8.65057	0.21927	-1.72736
C	-7.51901	-0.03152	0.66793
H	-8.61877	-0.10808	0.59735
H	-7.27886	0.95801	1.08531
C	-7.03062	-1.15797	1.57475
H	-7.77477	-1.30044	2.38415
H	-7.04118	-2.07336	0.97400
C	1.27140	-5.14218	0.04268
H	1.85130	-5.98235	0.43963
H	0.28339	-5.51756	-0.24952
H	1.13630	-4.42425	0.85560
C	2.21063	-5.61997	-2.23263
H	2.76521	-5.24329	-3.09899
H	1.24116	-5.99280	-2.58237
H	2.75976	-6.47382	-1.82207
H	3.21610	-0.15376	-0.13138
H	3.62477	1.86586	-0.13141
H	0.64586	-1.90305	1.51722
H	-0.84831	-1.37866	-2.49157

Conformation 7: ΔG: +10.0 kcal/mol

Cl	6.77983	-3.44646	3.57488
Cl	6.76362	7.68796	-0.50456
O	2.77802	-1.98545	-0.48963
O	5.96367	1.10943	1.49705
O	3.52294	-3.02927	-3.44591
O	-0.08061	-3.55737	-1.97967
O	-7.72867	-0.80130	0.59726
O	-6.66681	0.62069	2.91447
O	-4.40520	2.53770	2.57997
O	-5.03670	3.65091	-0.00336
O	-5.23719	1.72094	-2.18949
N	4.50378	-0.16313	0.24583
N	4.89255	2.02885	-0.32974
N	2.07466	-1.28165	-3.25940
N	0.18154	-1.72104	-0.60350
N	-5.82609	-1.19808	-1.59315
C	5.56476	-1.73699	1.84699
H	6.24434	-0.98048	2.20967
C	5.59707	-3.04132	2.33377
C	4.74202	-4.03526	1.86963
H	4.82272	-5.03914	2.26741
C	3.78458	-3.72799	0.89511
C	2.79979	-4.74244	0.31680
C	2.59779	-4.37090	-1.17277
H	3.53480	-4.52787	-1.71407
H	1.84191	-5.01336	-1.63370
C	2.16449	-2.92617	-1.41548
C	3.73285	-2.41788	0.41985
C	4.62514	-1.41922	0.86102
C	5.19243	0.99923	0.55443
C	5.37541	3.35160	-0.31784
C	6.23306	3.86187	0.66947
H	6.56590	3.22014	1.47241
C	6.65294	5.18956	0.60412
H	7.31654	5.58067	1.36816
C	6.22634	6.01339	-0.43486
C	5.37584	5.52025	-1.42226

H	5.04525	6.16196	-2.23190
C	4.95577	4.19566	-1.35880
H	4.29151	3.81377	-2.13180
C	2.64333	-2.44596	-2.83230
C	2.36185	-0.73517	-4.57785
H	3.36948	-1.04075	-4.86181
H	2.30450	0.35696	-4.54644
H	1.65905	-1.10633	-5.33436
C	0.62026	-2.78465	-1.33785
C	-1.14814	-1.29701	-0.33810
C	-2.27244	-1.89802	-0.91965
H	-2.14011	-2.73784	-1.58959
C	-3.55108	-1.41615	-0.62152
C	-3.70910	-0.32469	0.24173
H	-4.70147	0.05955	0.45294
C	-2.58558	0.26758	0.81783
H	-2.71771	1.10777	1.49279
C	-1.30862	-0.21328	0.53489
H	-0.43434	0.25181	0.98801
C	-4.76990	-2.12396	-1.19096
H	-4.46226	-2.79352	-2.01730
H	-5.17295	-2.78119	-0.41219
C	-7.17091	-1.75802	-1.53666
H	-7.26221	-2.70495	-2.10951
H	-7.85204	-1.04191	-2.00826
C	-7.68807	-2.01395	-0.12427
H	-8.69673	-2.45894	-0.20121
H	-7.06078	-2.74944	0.40613
C	-8.15709	-0.97446	1.93126
H	-7.55057	-1.74079	2.44124
H	-9.21051	-1.30631	1.96303
C	-8.03189	0.33607	2.68223
H	-8.50596	1.14296	2.10044
H	-8.57592	0.24638	3.63944
C	-6.47643	1.78576	3.68886
H	-7.01232	2.64030	3.24393
H	-6.88205	1.64430	4.70778
C	-4.98497	2.08152	3.79116
H	-4.46163	1.15563	4.04953
H	-4.81555	2.81044	4.60103
C	-4.60300	3.91604	2.32178
H	-4.03191	4.52653	3.04280
H	-5.66326	4.19421	2.41043
C	-4.13797	4.23286	0.91442
H	-4.10249	5.33058	0.79128
H	-3.11657	3.84687	0.76368
C	-4.68946	3.88499	-1.35250
H	-3.64688	3.58682	-1.54708
H	-4.78582	4.95810	-1.59726
C	-5.60942	3.07998	-2.24995
H	-6.65282	3.22158	-1.92370
H	-5.52701	3.46073	-3.28429
C	-6.05937	0.88102	-2.97372
H	-6.02982	1.19745	-4.03255
H	-7.10867	0.95093	-2.64275
C	-5.54018	-0.55020	-2.87255
H	-5.93848	-1.13622	-3.72406
H	-4.45421	-0.50431	-2.99988
C	1.47434	-4.69997	1.11420
H	1.64211	-5.03420	2.14400
H	0.72704	-5.35824	0.65627
H	1.05147	-3.69226	1.16393
C	3.35518	-6.17868	0.35927
H	4.33054	-6.24696	-0.13435
H	2.66518	-6.85737	-0.15462
H	3.46299	-6.54206	1.38662
H	3.84789	-0.16248	-0.52438
H	4.30094	1.80662	-1.11850
H	0.91118	-1.24730	-0.08305
H	1.24871	-0.94952	-2.77908

Conformation 8: ΔG: +10.2 kcal/mol

Cl	-6.07843	-3.87677	-3.61049
Cl	-7.79568	7.17610	0.31131
O	-2.66174	-1.92505	0.77015
O	-6.01473	0.74387	-1.52130
O	-3.44819	-3.06670	3.67015
O	0.28589	-3.10385	2.44069
O	5.85957	3.59010	-1.02132
O	6.99099	2.50918	1.44650
O	6.82006	-0.41410	1.99894
O	7.15344	-1.45731	-0.67201
O	5.21165	-0.54041	-2.65855
N	-4.53759	-0.34080	-0.12268
N	-5.25079	1.78405	0.39269
N	-2.22012	-1.15133	3.58052
N	-0.13213	-1.32661	1.02600
N	3.68569	2.04503	-2.21177
C	-5.24644	-2.03200	-1.79643
H	-5.98463	-1.36839	-2.22128
C	-5.06804	-3.32719	-2.27603
C	-4.13385	-4.20343	-1.73486
H	-4.04941	-5.20722	-2.13196
C	-3.31025	-3.77999	-0.68412
C	-2.25593	-4.66505	-0.02171
C	-2.20873	-4.26793	1.47372
H	-3.15278	-4.54451	1.95101
H	-1.41004	-4.80659	1.99192
C	-1.98441	-2.77909	1.73432
C	-3.46896	-2.47631	-0.21456
C	-4.44254	-1.59971	-0.73696
C	-5.33180	0.72799	-0.50697
C	-5.88550	3.03899	0.31732
C	-6.70075	3.43905	-0.75326
H	-6.87647	2.75958	-1.57466
C	-7.28130	4.70642	-0.74643
H	-7.91159	5.01250	-1.57472
C	-7.05737	5.57838	0.31641
C	-6.25170	5.19424	1.38638
H	-6.07892	5.87340	2.21431
C	-5.67123	3.93003	1.38133
H	-5.04210	3.63336	2.21843
C	-2.60972	-2.37329	3.11610
C	-2.66129	-0.65677	4.87700
H	-3.64264	-1.08269	5.08874
H	-2.73204	0.43470	4.85188
H	-1.97364	-0.94999	5.68020
C	-0.47053	-2.43461	1.74817
C	1.14836	-0.74661	0.82135
C	1.23011	0.29014	-0.12033
H	0.33385	0.59828	-0.65889
C	2.44252	0.92864	-0.38075
C	3.59367	0.51588	0.30444
H	4.54668	0.98995	0.09278
C	3.50689	-0.51169	1.24168
H	4.40656	-0.81736	1.76727
C	2.29502	-1.15187	1.51367
H	2.23248	-1.95659	2.23329
C	2.50368	2.09169	-1.35680
H	1.56366	2.14138	-1.94182
H	2.54172	3.02136	-0.77765
C	4.14194	3.34638	-2.68356
H	3.33906	3.92281	-3.19007
H	4.92197	3.17504	-3.43253
C	4.74372	4.23398	-1.59774
H	5.03936	5.19305	-2.06035
H	4.00137	4.47808	-0.81936
C	6.45598	4.34818	0.00983
H	5.71085	4.62597	0.77332
H	6.88697	5.28242	-0.39285
C	7.55890	3.54071	0.66474
H	8.22181	3.12424	-0.11066
H	8.16223	4.21672	1.29669
C	7.95906	1.76578	2.15690
H	8.74114	1.39350	1.47483
H	8.46072	2.40278	2.90874
C	7.27441	0.60660	2.87100
H	6.38588	0.98789	3.38412
H	7.95950	0.19384	3.63002
C	7.82034	-1.33859	1.60992
H	8.11771	-1.96400	2.46957

H	8.71984	-0.82595	1.23891
C	7.28109	-2.22469	0.50470
H	7.98107	-3.06642	0.35339
H	6.30919	-2.64781	0.80581
C	6.67394	-2.20105	-1.77385
H	5.74549	-2.73398	-1.51477
H	7.42011	-2.95329	-2.08694
C	6.39565	-1.25787	-2.92834
H	7.25245	-0.57654	-3.05864
H	6.29074	-1.84691	-3.85751
C	4.87366	0.38670	-3.66849
H	4.74187	-0.13131	-4.63611
H	5.68170	1.12496	-3.80213
C	3.56005	1.06484	-3.28989
H	3.11269	1.51399	-4.19820
H	2.88073	0.27391	-2.95758
C	-0.89002	-4.47155	-0.72206
H	-0.94250	-4.82658	-1.75712
H	-0.10747	-5.03715	-0.20327
H	-0.58226	-3.42233	-0.75403
C	-2.63295	-6.15799	-0.08476
H	-3.62601	-6.33990	0.33980
H	-1.90561	-6.74719	0.48505
H	-2.62421	-6.53648	-1.11224
H	-3.95881	-0.25866	0.70305
H	-4.71694	1.63466	1.23780
H	-0.88494	-0.95760	0.45626
H	-1.41164	-0.71393	3.15810

Conformation 9: ΔG: +11.3 kcal/mol

Cl	-6.47603	-3.82044	-3.46822
Cl	-7.30349	7.31765	0.48805
O	-2.62206	-2.03320	0.60964
O	-5.97186	0.81127	-1.45853
O	-3.13935	-3.07720	3.60609
O	0.41480	-3.37741	1.97050
O	4.41123	3.10508	0.58769
O	5.68319	1.15566	2.46019
O	6.88112	-1.35258	1.48537
O	7.85891	-0.33267	-1.07725
O	6.26837	1.27079	-3.01343
N	-4.46154	-0.35065	-0.16055
N	-5.01985	1.81020	0.39277
N	-1.82102	-1.24101	3.32602
N	-0.04258	-1.59721	0.57053
N	3.64196	2.42242	-2.24494
C	-5.39645	-2.01162	-1.75096
H	-6.12212	-1.30727	-2.12919
C	-5.33563	-3.32086	-2.22185
C	-4.41962	-4.24771	-1.73729
H	-4.42831	-5.25957	-2.12276
C	-3.49327	-3.86532	-0.75842
C	-2.44948	-4.81081	-0.16598
C	-2.23974	-4.38798	1.30841
H	-3.15266	-4.58921	1.87573
H	-1.43501	-4.96998	1.76679
C	-1.89365	-2.91436	1.50884
C	-3.53287	-2.54824	-0.30148
C	-4.48901	-1.61905	-0.76252
C	-5.22189	0.75890	-0.49405
C	-5.59758	3.09420	0.36181
C	-6.43810	3.54754	-0.66717
H	-6.68309	2.88777	-1.48686
C	-6.95603	4.84087	-0.61994
H	-7.60652	5.18797	-1.41583
C	-6.64377	5.68656	0.44188
C	-5.81149	5.24988	1.47054
H	-5.57049	5.90864	2.29795
C	-5.29387	3.95944	1.42533
H	-4.64454	3.62125	2.23068
C	-2.33244	-2.44582	2.94205
C	-2.07913	-0.69121	4.64876
H	-3.03729	-1.07866	4.99676
H	-2.12259	0.40087	4.59531
H	-1.30322	-0.98111	5.36838
C	-0.36829	-2.66976	1.34985
C	1.24070	-1.10504	0.20972
C	1.27826	-0.08148	-0.74667
H	0.34619	0.28126	-1.18145
C	2.49263	0.47208	-1.15879
C	3.68316	0.00239	-0.59316
H	4.62934	0.43651	-0.89728
C	3.64079	-1.01296	0.36280
H	4.57310	-1.36827	0.79009
C	2.43248	-1.57914	0.77277
H	2.40251	-2.37136	1.50814
C	2.50087	1.51615	-2.27047
H	2.51134	0.97996	-3.22775
H	1.54418	2.07243	-2.25397
C	3.41000	3.66696	-1.52511
H	2.52798	4.20817	-1.92875
H	4.27821	4.31789	-1.67358
C	3.20710	3.52506	-0.02054
H	2.90198	4.51143	0.37435
H	2.39320	2.81868	0.20580
C	4.32144	3.07080	1.99744
H	3.49912	2.41530	2.32587
H	4.12278	4.08389	2.39145
C	5.62390	2.56156	2.58516
H	6.46924	3.04174	2.06621
H	5.67460	2.85271	3.64985
C	6.87644	0.60492	2.97389
H	7.75338	1.01302	2.44400
H	6.99379	0.85715	4.04430
C	6.81715	-0.91061	2.83148
H	5.85744	-1.26024	3.22549
H	7.62049	-1.36744	3.43164
C	8.19689	-1.49277	0.98110
H	8.66933	-2.39794	1.40022
H	8.82406	-0.62999	1.24913
C	8.15728	-1.60105	-0.53046
H	9.14506	-1.95028	-0.88066
H	7.40937	-2.35065	-0.83471
C	8.00755	-0.28558	-2.48257
H	7.34860	-1.01619	-2.97821
H	9.04847	-0.52614	-2.76349
C	7.67089	1.10882	-2.97541
H	8.13792	1.84783	-2.30476
H	8.09984	1.25127	-3.98334
C	5.87080	2.58684	-3.34642
H	6.33563	2.89931	-4.29916
H	6.20039	3.29591	-2.56937
C	4.35329	2.61554	-3.50506
H	4.07173	3.56300	-4.00174
H	4.08676	1.80784	-4.19363
C	-1.14226	-4.73251	-0.99047
H	-1.31413	-5.10670	-2.00582
H	-0.35678	-5.34098	-0.52780
H	-0.76657	-3.70908	-1.08075
C	-2.93640	-6.27305	-0.15472
H	-3.89989	-6.37147	0.35673
H	-2.20703	-6.90142	0.36870
H	-3.04226	-6.67403	-1.16814
H	-3.81796	-0.29578	0.61809
H	-4.45472	1.62529	1.21011
H	-0.82976	-1.18855	0.07966
H	-1.04681	-0.86093	2.79753

Conformation 10: ΔG: +12.3 kcal/mol

Cl	-7.47373	1.12231	-2.14807
Cl	1.37135	8.63139	-0.20803
O	-2.74579	-0.97398	0.67988
O	-3.26064	3.58594	-0.96945
O	-2.90001	-1.34855	3.88105
O	-1.78716	-4.32894	1.51981
O	3.81529	0.81758	-2.17181
O	3.10541	2.14854	0.44645
O	2.83783	0.53683	2.96151

O	4.90355	-1.42677	2.36468
O	5.09121	-2.81399	-0.27273
N	-2.67154	1.49367	-0.19125
N	-1.17048	3.23767	-0.06283
N	-0.85092	-1.28863	2.90605
N	-1.00073	-2.79933	-0.01643
N	3.61579	-2.11908	-2.89197
C	-4.96358	1.29148	-1.11935
H	-4.93791	2.29809	-1.50743
C	-6.08518	0.48139	-1.27297
C	-6.15156	-0.80511	-0.75356
H	-7.05408	-1.38895	-0.88359
C	-5.05328	-1.33657	-0.06529
C	-5.04640	-2.74132	0.53435
C	-4.15396	-2.69235	1.79538
H	-4.63469	-2.07460	2.55870
H	-4.02755	-3.69314	2.21764
C	-2.75508	-2.12602	1.56939
C	-3.91681	-0.53793	0.07440
C	-3.86216	0.78205	-0.42400
C	-2.44311	2.83867	-0.45160
C	-0.62382	4.53514	-0.13648
C	-1.38464	5.68652	-0.39421
H	-2.44449	5.59949	-0.58452
C	-0.76680	6.93611	-0.41658
H	-1.35719	7.82399	-0.61683
C	0.60113	7.04785	-0.18060
C	1.36729	5.91273	0.07519
H	2.43328	6.00421	0.25585
C	0.75550	4.66233	0.09391
H	1.35841	3.77524	0.27763
C	-2.17793	-1.57486	2.92139
C	-0.17948	-0.76313	4.08755
H	-0.79591	0.02306	4.52987
H	0.78832	-0.35549	3.78769
H	-0.03334	-1.54342	4.84530
C	-1.80547	-3.21809	1.00789
C	-0.10192	-3.56029	-0.80594
C	0.71357	-2.85526	-1.69752
H	0.68426	-1.76739	-1.70936
C	1.57471	-3.52317	-2.57051
C	1.61265	-4.92122	-2.53795
H	2.26079	-5.45834	-3.22616
C	0.82315	-5.62484	-1.62662
H	0.86724	-6.71025	-1.59921
C	-0.03584	-4.96064	-0.75381
H	-0.65038	-5.50264	-0.04862
C	2.43570	-2.72451	-3.52916
H	2.72595	-3.36304	-4.38722
H	1.83147	-1.91035	-3.94326
C	4.13279	-1.00821	-3.69512
H	4.08584	-1.23284	-4.77900
H	5.18917	-0.85779	-3.45526
C	3.43269	0.32298	-3.44090
H	3.73260	1.03311	-4.23208
H	2.33601	0.21956	-3.50141
C	3.39589	2.14776	-1.95156
H	2.29667	2.23331	-1.97488
H	3.79181	2.80908	-2.74252
C	3.91783	2.63467	-0.61260
H	4.95636	2.29259	-0.48904
H	3.92027	3.73800	-0.60722
C	3.61325	2.51292	1.71867
H	4.64318	2.14150	1.83725
H	3.64390	3.61269	1.81963
C	2.71496	1.94254	2.80858
H	1.66885	2.13924	2.55016
H	2.92577	2.45890	3.75815
C	3.88934	0.14492	3.83331
H	3.58539	0.29149	4.88314
H	4.79399	0.74341	3.65604
C	4.23043	-1.31269	3.59808
H	4.87027	-1.66176	4.42857
H	3.31224	-1.92295	3.60846
C	5.37162	-2.73633	2.10507
H	4.54294	-3.46193	2.10632
H	6.09145	-3.04387	2.88426
C	6.05902	-2.76258	0.75386
H	6.69486	-1.86691	0.66058
H	6.71942	-3.64693	0.70135
C	5.67033	-2.74403	-1.56089
H	6.50983	-3.45825	-1.63765
H	6.08550	-1.73863	-1.73736
C	4.63909	-3.12989	-2.61608
H	5.17879	-3.41870	-3.54142
H	4.13850	-4.02927	-2.24683
C	-4.53451	-3.75542	-0.51655
H	-5.23989	-3.81818	-1.35265
H	-4.43315	-4.75319	-0.07495
H	-3.56459	-3.46968	-0.93443
C	-6.45185	-3.18014	0.99275
H	-6.89458	-2.45320	1.68191
H	-6.38685	-4.14422	1.50976
H	-7.13410	-3.31115	0.14647
H	-2.02692	1.00177	0.41419
H	-0.51019	2.51574	0.19417
H	-1.19367	-1.85853	-0.34031
H	-0.28120	-1.60783	2.13428

Conformation 11: ΔG: +17.1 kcal/mol

Cl	8.33133	-1.49061	1.96222
Cl	0.02847	7.86964	0.31431
O	2.97415	-0.95511	-0.43823
O	3.16061	1.72518	1.05522
O	2.30754	-2.80648	-3.42865
O	0.42608	-1.24873	0.07684
O	-4.89471	-2.06368	2.96702
O	-2.60007	-0.26289	2.92675
O	-2.11334	1.54525	0.56864
O	-4.65543	2.55009	-0.48394
O	-6.58978	0.61120	-1.34105
N	4.69585	1.16490	-0.59254
N	3.50309	3.14115	-0.74022
N	3.25629	-0.76474	-3.03168
N	0.06570	-2.63300	-1.72930
N	-5.81293	-1.87468	0.23375
C	6.35304	-0.14063	0.66390
H	7.03675	0.70218	0.65359
C	6.72614	-1.34331	1.25501
C	5.85172	-2.42683	1.30586
H	6.17281	-3.34562	1.78127
C	4.57506	-2.32246	0.74801
C	3.53397	-3.43577	0.75253
C	2.89437	-3.44485	-0.66013
H	3.63797	-3.80763	-1.37690
H	2.06682	-4.16047	-0.68545
C	2.37468	-2.05618	-1.13575
C	4.21043	-1.12181	0.12396
C	5.08803	-0.02838	0.08495
C	3.72325	2.00264	0.01588
C	2.65746	4.22848	-0.44136
C	1.95209	4.35008	0.76566
H	2.02862	3.57120	1.51116
C	1.15106	5.46918	0.98977
H	0.60893	5.56382	1.92478
C	1.04548	6.46450	0.02032
C	1.73953	6.35476	-1.18296
H	1.65633	7.13048	-1.93654
C	2.54193	5.24025	-1.40682
H	3.08566	5.15881	-2.34595
C	2.64988	-1.90774	-2.65295
C	3.56053	-0.46519	-4.41929
H	3.24484	-1.31650	-5.02365
H	4.63606	-0.30484	-4.55740
H	3.02224	0.42952	-4.75362
C	0.83105	-1.91313	-0.86277
C	-1.34054	-2.81029	-1.73298
C	-2.21636	-2.04656	-0.95313
H	-1.82485	-1.27044	-0.30926
C	-3.60041	-2.26936	-1.00951
C	-4.09222	-3.27528	-1.85051

H	-5.15801	-3.46847	-1.90251	H	-2.92075	2.62440	-1.62602
C	-3.21746	-4.03375	-2.63156	C	-5.58678	2.75683	-1.52545
H	-3.60746	-4.81026	-3.28491	H	-5.18814	2.40058	-2.48908
C	-1.84651	-3.80821	-2.58055	H	-5.82130	3.83107	-1.63343
H	-1.16607	-4.40466	-3.18436	C	-6.85217	1.98996	-1.19012
C	-4.50210	-1.36733	-0.16315	H	-7.14582	2.22224	-0.15487
H	-3.95517	-1.07830	0.74063	H	-7.67209	2.31129	-1.85608
H	-4.67334	-0.43022	-0.69914	C	-7.49043	-0.24872	-0.66314
C	-5.86015	-3.10017	1.01671	H	-8.47746	-0.23344	-1.16063
H	-5.74631	-4.02351	0.41281	H	-7.62283	0.07926	0.37895
H	-6.84768	-3.15659	1.49357	C	-6.93173	-1.67192	-0.67649
C	-4.79979	-3.18540	2.10876	H	-7.74583	-2.33650	-0.36235
H	-4.96325	-4.12582	2.66353	H	-6.70375	-1.93287	-1.72442
H	-3.79425	-3.23948	1.66620	C	2.48127	-3.15317	1.85247
C	-3.88071	-1.99168	3.95305	H	2.95810	-3.16602	2.83878
H	-3.03163	-2.64111	3.69663	H	1.70690	-3.93011	1.83941
H	-4.27580	-2.32161	4.92803	H	1.99190	-2.18649	1.71592
C	-3.37157	-0.56593	4.07140	C	4.15395	-4.82283	0.99527
H	-4.22263	0.12780	4.16661	H	4.95087	-5.04578	0.27663
H	-2.75880	-0.47731	4.98672	H	3.38384	-5.59617	0.89805
C	-1.99930	1.01736	2.97531	H	4.56916	-4.90477	2.00564
H	-2.76091	1.79531	3.15116	H	5.48007	1.67111	-0.99153
H	-1.28053	1.06718	3.81344	H	3.90533	3.15245	-1.66776
C	-1.25565	1.27147	1.66947	H	0.57725	-3.08428	-2.48635
H	-0.68119	0.38150	1.40166	H	3.48151	-0.09357	-2.30500
H	-0.54590	2.10223	1.81496				
C	-2.48934	2.90384	0.46490				
H	-1.59338	3.53936	0.35219				
H	-3.03224	3.24770	1.35970				
C	-3.38097	3.10117	-0.74570				
H	-3.46197	4.18384	-0.94997				

1. Gaussian 09, Revision B.01, R. B. Gaussian 09, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, J. A., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
2. A. D. Becke, *J. Chem. Phys.*, 1983, **98**, 5648-5652.
3. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650-654.
4. S. Grimme, *Chem.--Eur. J.*, 2012, **18**, 9955-9964.
5. R. Paton, http://paton.chem.ox.ac.uk/software/software.html, 2016).
6. H. L. Schmider and A. D. Becke, *J. Chem. Phys.*, 1998, **109**, 8188-8199.
7. H. Zhao and D. G. Truhlar, *Theor Chem Acta*, 2007, **120**, 215-241.
8. N. M. O'Boyle, A. L. Tenderholt and K. M. Langner, *J. Comput. Chem.*, 2008, **29**, 839-845.