Electronic Supporting Information (ESI)

Catalytic enantioselective one-pot approach to *cis*- and *trans*-2,3-diaryl substituted 1,5-benzothiazepines

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Experimental Procedures and Compounds Characterization

General procedure for preparation of aminothiols 2

2-Aminobenzenethiol **2a** was purchased from TCI Europe N.V. and used as received. The substituted 2-aminobenzenethiols **2** were synthesized according to literature.[1] A solution of appropriate benzothiazole (2 mmol) in a mixture of 1:1 v/v aqueous 50% NaOH and ethylene glycol (C= 0.5 M) was re-fluxed under N_2 flux until the starting material disappeared (TLC eluent: petroleum ether/ethyl acetate 8/2). The mixture was then poured into ice-water, acidified to pH 3 with 2 N HCl and extracted several times with CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude aminothiophenol derivative was quickly filtered through a short pad of flash silica-gel (eluent $CHCl_3$), organic solvent was evaporated and a further purification was not necessary isolating the sufficiently pure aminothiophenols.

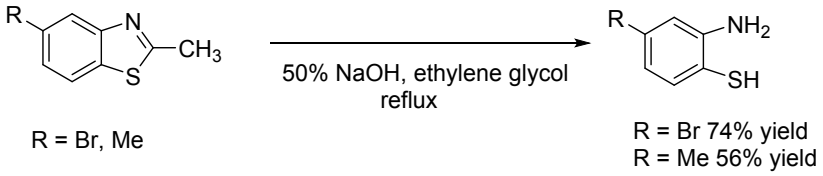
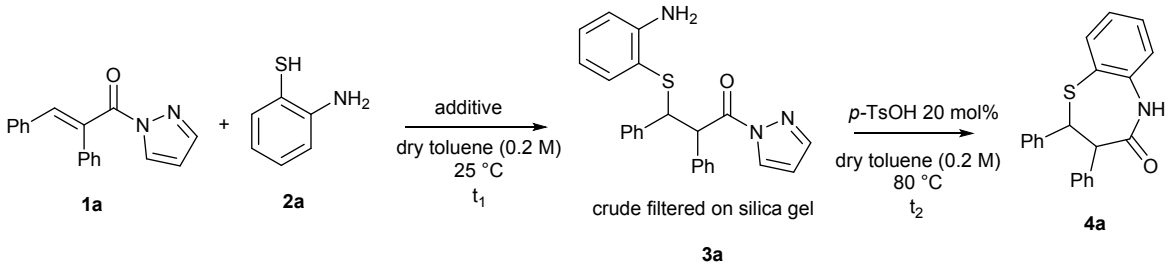


Table S1. Additive screening in the racemic synthesis of 1,5-benzothiazepine 4a.[a]

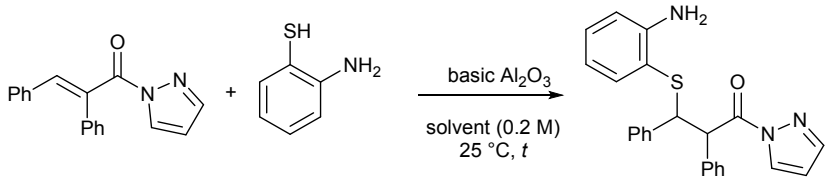


Entry	Additive (mg or eq.)	t_1 [h]	dr **3a**[b]	Yield **3a** [%][c]	t_2 [h]	Yield **4a** (*cis*) [%][d]
1	silica gel (113 mg)	21	100/0	21	-	-
2	NEt_3 (0.5 eq.)	48	75/25	28	-	-
3	neutral Al_2O_3 (10 eq.)	5	85/15	72	-	-
4	basic Al_2O_3 (10 eq.)	4	84/16	79	18	98
5[e]	basic Al_2O_3 (10 eq.)	6	83/17	89	-	-

[a] Unless otherwise noted reactions were conducted with **1a** (0.1mmol), **2a** (0.11 mmol) and additive in dry toluene (0.2 M). [b] Determined by ^{1}HNMR analysis of reaction crude mixture. [c] Determined by ^{1}HNMR spectroscopy using 1,3,5-$(MeO)_3C_6H_3$ as an internal standard. [d] Yield of product **4a** purified by flash chromatography. [e] **2a** added in two portions.

[1] (a) G. Manfroni, F. Meschini, M. L. Barreca, P. Leyssen, A. Samuele, N. Iraci, S. Sabatini, S. Massari, G. Maga, J. Neyts, V. Cecchetti *Bioorg. Med. Chem*. **2012**, *20*, 866; (b) Y. Fukata, K. Asano, S. Matsubara *J. Am. Chem. Soc.* **2015**, *137*, 5320.

Table S2. Solvent screening in the racemic synthesis of 3a.[a]

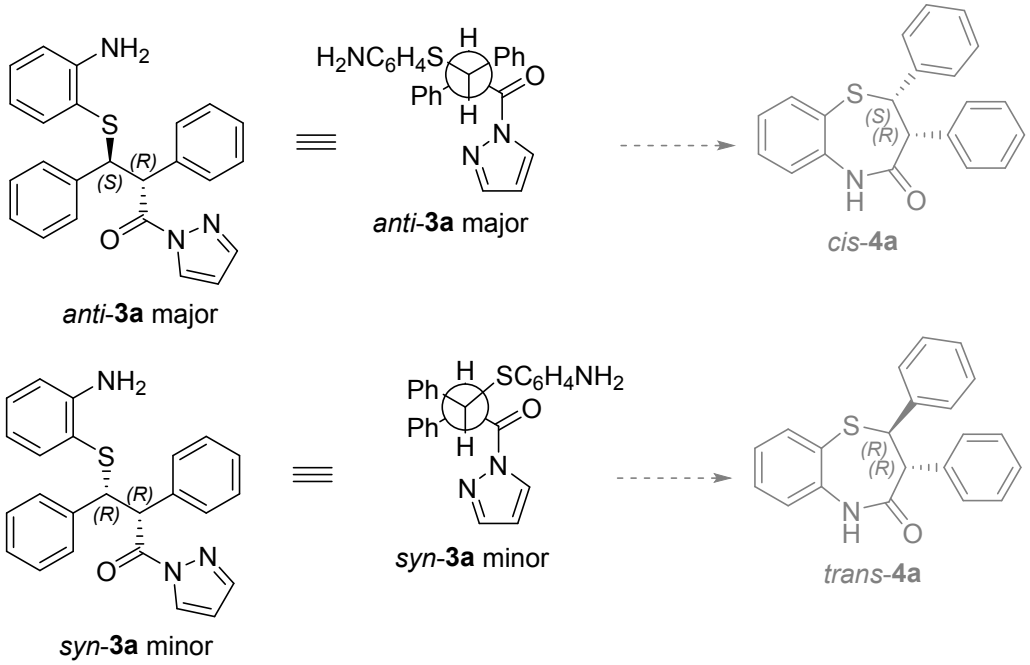


1a **2a** **3a**

Entry	Solvent	*t* [h]	dr **3a**[b]	Yield **3a** [%][c]
1	toluene	5	83/17	70
2	$CHCl_3$	24	85/15	27
3	acetonitrile	5	89/11	60
4	EtOAc	4	85/15	40
5	Et_2O	2	82/18	73

[a] Unless otherwise noted reactions were conducted with **1a** (0.1 mmol), **2a** (0.11 mmol) added in two portions and additive in dry solvent (0.2 M). [b] Determined by ^{1}HNMR analysis of reaction crude mixture. [c] Determined by ^{1}HNMR spectroscopy using 1,3,5-$(MeO)_3C_6H_3$ as an internal standard.

Characterization of 3-((2-aminophenyl)thio)-2,3-diphenyl-1-(1H-pyrazol-1-yl)propan-1-one (3a)



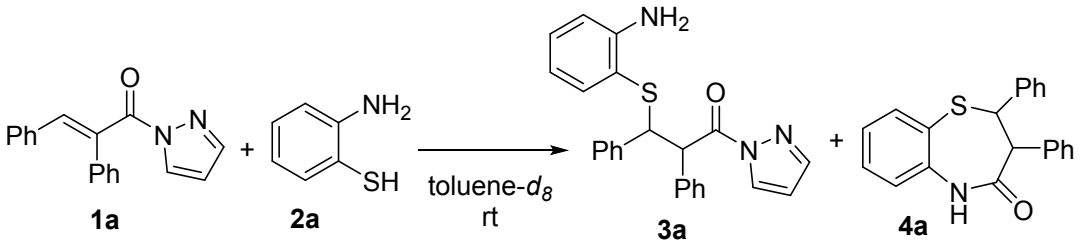
During the purification, we observed that the silica gel is able to promote the transformation of minor *syn*-**3a** diastereoisomer into *trans*-**4a**. In fact, the *syn*-**3a** minor diastereomer (90% ee) was recovered in small amount together with the major *anti*-**3a** (58% ee). Probably the silica gel during

the purification by the flash chromatography eroded the enantiomeric excess of the major *anti*-**3a** diastereomer, catalysing a retro-sulfa-Michael/sulfa-Michael process.

Mechanistic investigations

Experiment 1

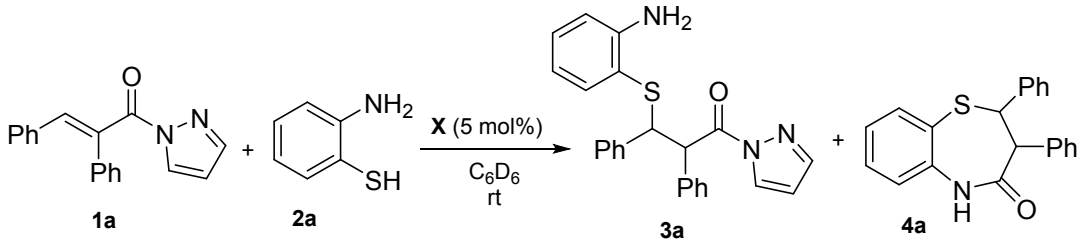
Table S3. Monitoring of model reaction over time in the presence of 1,2-dichloroethane as internal standard without catalyst in toluene-d_8 at rt (Figure 3 in the paper).



Entry	*t* (h)	**1a**	Conversion **3a**	dr **3a**	Conversion *cis*-**4a**	Conversion *trans*-**4a**	Pyrazole
1	0	100	0	0	0	0	0
2	0.47	100	0	0	0	0	0
3	2.02	88	3.8	87/13	2	0	6
4	3.05	85	5.9	86/14	3.4	0	9
5	4.08	79	8.6	86/14	5.8	0	13
6	5.1	72	10	83/17	8	1	18
7	5.8	68	10	84/16	8.3	1	22
8	7.2	61	12	83/17	10	1.3	27
9	8	54	14	81/19	11	1	32
10	9.5	44	17	81/19	12	2	40
11	14	29	20	81/19	15	2	51
12	16.5	26	20	80/20	16	1	54
13	19.7	14	23	83/17	14	2	63

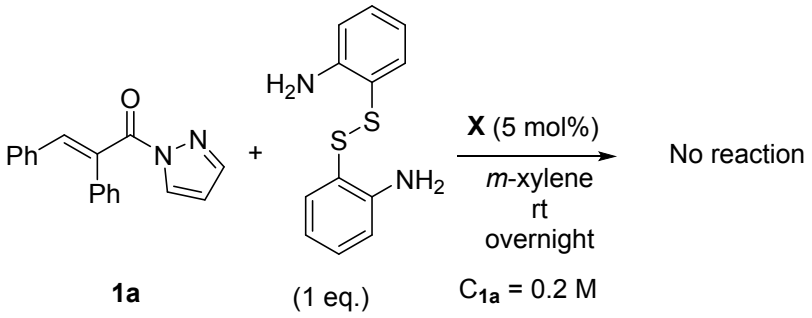
Experiment 2

Table S4. Monitoring of model reaction over time in the presence of 1,2-dichloroethane as internal standard with 5 mol% **X** in C_6D_6 at room temperature (Figure 4 in the paper).



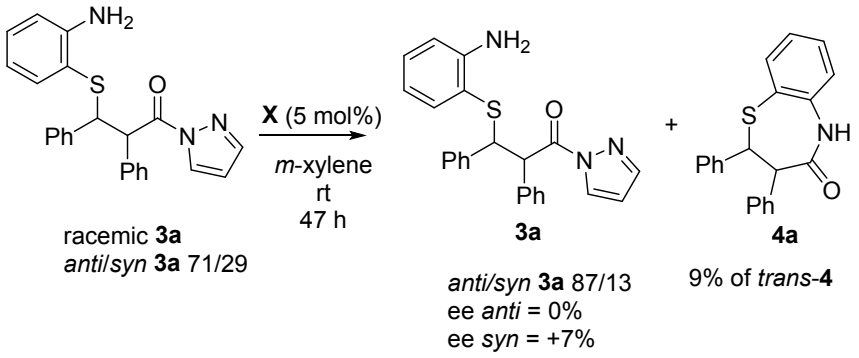
Entry	*t* (h)	**1a**	Conversion **3a**	dr **3a**	Conversion *cis*-**4a**	Conversion *trans*-**4a**	Pyrazole
1	0	100	0	0	0	0	0
2	0.23	82	14	65:35	0	0	4
3	0.77	58	30	63:37	0	0	12
4	1.3	43	39	66:34	0	0	18
5	2.4	26	45	67:37	0	0	27
6	3.4	17	50	64:36	0	0	31
7	4.5	13	55	65:35	0	0	32
8	5.6	10	57	64:36	0	0	32
9	6.6	7	61	65:35	0	0	32
10	7.7	5	63	65:35	0	0	32
11	8.8	4	64	65:35	0	0	32

Experiment 3



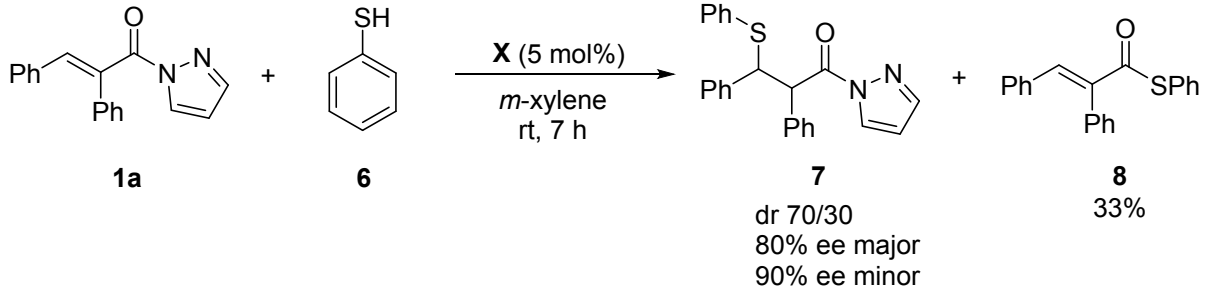
Experimental procedure: α,β-Unsaturated pyrazolamide **1a** (27.4 mg, 0.1 mmol) and catalyst **X** (3.3 mg, 0.005 mmol) were dissolved in *m*-xylene (0.5 mL) and 2-aminophenyl disulfide (24.8 mg, 0.10 mmol) was added. The reaction was stirred at room temperature for 15 h. ^{1}H NMR analysis of the crude reaction mixture showed only the presence of reagents. This experiment shows that even if the oxidation product of **2a** was formed in small amount, it would not react with **1a**.

Experiment 4



Experimental procedure: Racemic 3-((2-aminophenyl)thio)-2,3-diphenyl-1-(1H-pyrazol-1-yl)propan-1-one **3a** (31.9 mg, 0.08 mmol, *anti*/*syn* 71/29) and catalyst **X** (2.7 mg, 0.004 mmol) were dissolved in dry *m*-xylene (0.4 mL) and the mixture was stirred at room temperature for 47 h. After this time, the diastereoisomeric ratio of diastereomers of **3a** was determined by ^{1}HNMR analysis. 9% of *trans*-**4a** was detected respect to **3a**. Compound **3a** was recovered in racemic form for the major *anti* diastereomer and 7% ee for the minor *syn* diastereomer. By comparison of HPLC retention times, the *syn* (2*R*,3*R*)-adduct was preferentially recovered. This experiment confirmed that organocatalysed amidation reactions are negligible processes within the reaction times reported in Table 3 in the paper.

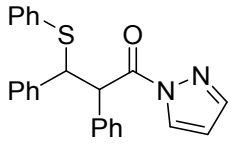
Asymmetric sulfa-Michael reaction of 1a with thiophenol



Experimental procedure: (*E*)-α,β-unsaturated *N*-acylpyrazole **1a** (41.1 mg, 0.15 mmol) and catalyst **X** (5.3 mg, 0.008 mmol) were dissolved in dry *m*-xylene (770 μL) and thiophenol **6** (18 μL, 0.165 mmol) was added under nitrogen atmosphere at room temperature. The reaction was stirred at room temperature for 7 hours (PE/EtOAc 8/2). The crude product was purified by flash chromatography (hexane/EtOAc 100/0.1-90/10) to afford adduct **7** as inseparable mixture of diastereoisomers in 32% yield and product **8**[2] in 33% yield.

[2] H. Yoshida, T. Ogata, *Nippon Kagaku Kaishi* **1982**, 534.

2,3-diphenyl-3-(phenylthio)-1-(1H-pyrazol-1-yl)propan-1-one (7)[3]



Mixture of diastereoisomers. White solid, 20.2 mg, 35% yield. 80 % ee major, 90% ee minor. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.30 (d, 0.6H, J = 2.8 Hz, minor), 7.93 (d, 1H, J = 2.8 Hz), 7.79 (s, 0.6H, minor), 7.67-7.65 (m, 3H), 7.38-7.34 (m, 2H), 7.32-7.28 (m, 4H), 7.24-7.17 (m, 3H, minor), 7.15-7.08 (m, 5H), 7.07-7.01 (m, 8H), 6.48-6.47 (m, 0.6H, minor), 6.28-6.27 (m, 1H), 5.86 (d, 1H, J = 12.1 Hz) major overlapped with 5.82 (d, 0.6H, J = 12.2 Hz) minor, 5.03 (d, 0.6H, J = 11.5 Hz) minor overlapped with 5.00 (d, 1H, J = 11.7 Hz) major. **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 171.0 (minor), 170.2, 144.1 (minor), 144.0, 140.4, 139.2 (minor), 135.7, 135.5 (minor), 134.0, 133.9 (minor), 133.6, 133.4 (minor), 129.5, 129.2 (minor), 128.8 (minor), 128.7, 128.64 (minor), 128.59 (minor), 128.44, 128.35 (minor), 128.21, 128.16, 128.07, 127.9 (minor), 127.6, 127.5 (minor), 127.2, 126.69 (minor), 110.30 (minor), 109.96, 57.1, 56.4 (minor), 53.7. HPLC analysis major diastereoisomer: with Chiralpak AD column, 95:5 *n*-hexane:2-propanol, 1 mL/min, 254 nm; minor enantiomer t_R = 14.8 min, major enantiomer t_R = 9.8 min; minor diasteroisomer: with Chiralpak IC column, 95:5 *n*-hexane:2-propanol, 1 mL/min, 254 nm; minor enantiomer t_R = 5.2 min, major enantiomer t_R = 5.7 min.

Relative and Absolute configuration of compound 4e

Unfortunately, it was not possible to obtain good crystals for compounds **4**. For this reason, a hybrid NMR/ECD approach supported by DFT conformational analysis and TD-DFT calculation of ECD spectra was employed to assign the relative and absolute configuration of compound **4e**. All the calculations were performed using the Gaussian 16 suite of programs.[4]

Conformational analysis

The conformational analysis of the *cis* (2*R**3*R**) and *trans* (2*R**3*R**) isomers of **4e** started by a molecular mechanics (MM) conformational search that explored the whole conformational space and selected the best conformations into a 10 kcal/mol window. MM search was run using the MMFF force field implemented in Titan software (1.0.5 release). The output geometries were then optimized using DFT and the B3LYP/3-21G level of theory. After this step, only four conformations were found to exist for the *trans* isomer, and three for the *syn* isomer. These were refined at the B3LYP/6-31G(d) level of theory, followed by further optimization at the PCM-

[3] S. Meninno, C. Volpe, A. Lattanzi *Chem. Eur. J.* **2017**, *23*, 4547.
[4] M. J. Frisch *et al* Gaussian 16 rev A.03; Gaussian inc., Wallingford, CT, 2016

B3LYP/6-311+G(d,p) level. At both levels of theory, all the conformations showed to be real energy minima, being absent any imaginary value in the frequency calculations step.

The four conformations of the *trans* isomer are due to the two available dihedral angles between the two CH of the thiazepine (H2 and H3), that can be close to 180 (*anti*) or close to 60 (*gauche*). An additional degree of freedom is the conformation of the cycle that is bent in two available directions (Figure S1), so the phenyl ring of thiazepine can be on the side of the H2 hydrogen (GS2 and GS3), or on the side of the H3 hydrogen (GS1 and GS4).

Despite the apparent similarity among the relative steric hindrance, GS1 is calculated to be much more stable that all the other conformation (as ZPE-corrected enthalpies), and it should be the only populated in solution. In order to check this result, the four conformations were optimized with a different model(ωB97XD/6-311+G(d,p)) that accounts for dispersive effect. The results were almost equivalent to that of B3LYP, the second conformation being 2.8 kcal/mol higher in energy with respect to GS1.

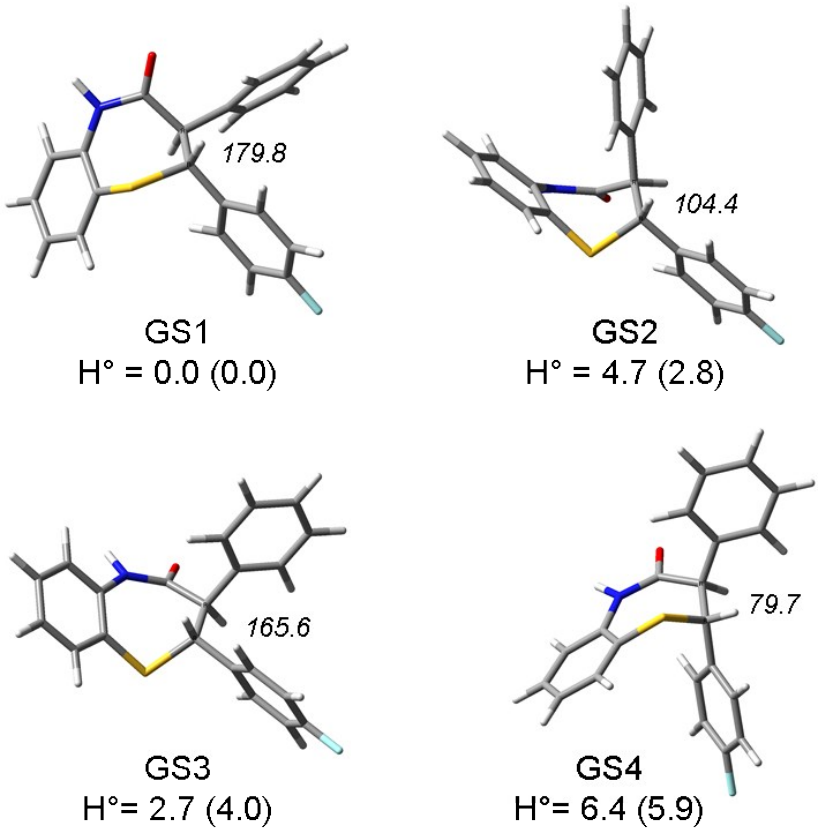


Figure S1. The four conformations of the trans isomer. Relative energies in kcal/mol at the PCM-B3LYP/6-311+G(d,p) level. The numers in parenthesis are relative to ωB97XD/6-311+G(d,p) optimization. The number in italics indicate the H2-C2-C3-H3 dihedral angle.

In the case of the *cis* isomer, only three conformations were found as true energy minima. The fourth one (GS4) converted into GS2 when optimized with DFT at the PCM-B3LYP/6-311+G(d,p) level. Also in this case one conformation (GS1) is much more stable than the others, and it should be the only populated one in solution. (Figure S2).

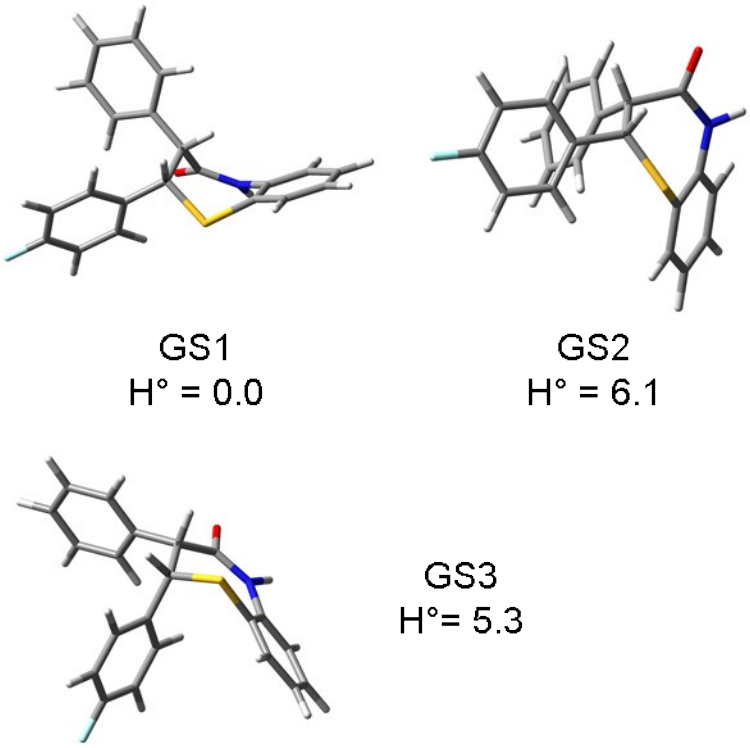


Figure S2. The three conformations of the *cis* isomer. Relative energies in kcal/mol at the PCM-B3LYP/6-311+G(d,p) level.

Relative configuration

Being only one conformation populated in both isomers, the relative disposition of the two CH should yield very different ^{3}J-coupling constants in the ^{1}H-NMR spectrum. ^{1}H-NMR spectra recorded in acetonitrile showed that the experimental coupling constant were 12.3 Hz and 6.7 Hz This is a clear indication of the *anti* conformation of the two hydrogens in the first case**,** and a gauche conformation in the second one. Coupling constant calculation were run for the GS1 conformation of *trans*-**4e** and *cis*-**4e** at the B3LYP/6-311++G(2d,p) including the Fermi contact. In the case of the *trans* isomer the calculated value was 12.6 Hz, and 6.9 Hz in the case of the *cis*, in perfect agreement with the experimental values. In addition to the assignment, this very good match confirms the presence of a single populated conformation in solution.

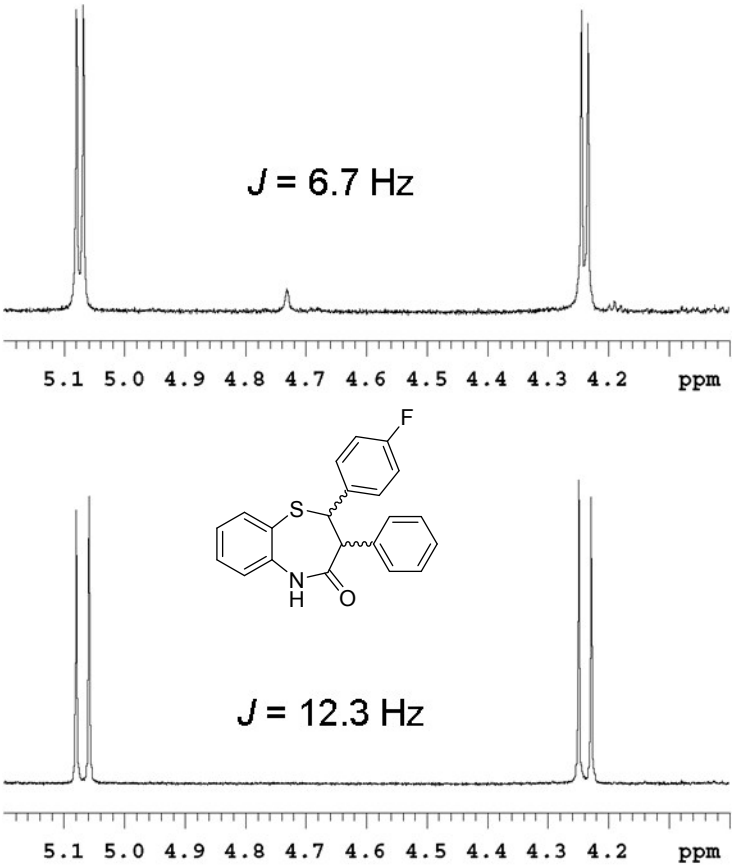


Figure S3: ^{1}H region of H2 and H3 of thiazepine (600 MHz in CD_3CN) of compound *trans*-**4e** (bottom) and compound *cis*-**4e** (top).

Absolute configuration

The determination of the absolute configuration (AC) of chiral molecules using chiro-optical techniques such as circular dichroism (Electronic CD and Vibrational CD) has become very reliability because of the development of theoretical methods for the prediction of these properties based on DFT (for VCD) and on Time-Dependent DFT (for ECD).[5] In the present case the theoretical calculation of the electronic circular dichroism spectra (ECD) was selected for the absolute configuration assignment because of the presence of strong UV chromophores. The ECD spectra of compounds *trans*-**4e** and *cis*-**4e** were acquired in HPLC-grade acetonitrile solution (about $1 \cdot 10^{-4}$ M) with a cell path of 0.2 cm in the 190-400 nm region by the sum of 16 scans at 50 nm/min scan rate (Figure S4).

[5] For reviews see: a) G. Bringmann, T. Bruhn, K. Maksimenka, Y. Hemberger *Eur. J. Org. Chem*. **2009**, 2717; b) T. D. Crawford, M. C. Tam, M. L. Abrams *J. Chem. Phys. A* **2007**, *111*, 12057; c) G. Pescitelli, L. Di Bari, N. Berova *Chem. Soc. Rev.* **2011**, *40*, 4603; c) A. Mazzanti, D. Casarini D. *WIRES Comput. Mol. Sc.* **2012**, *2*, 613; d) G. Pescitelli, T. Bruhn *Chirality* **2016**, *28*, 466.

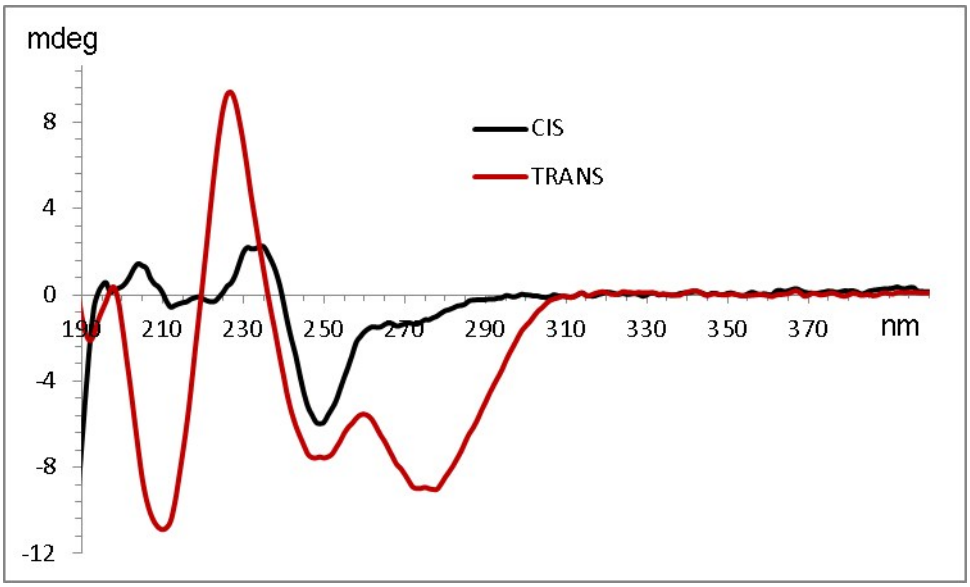


Figure S4. ECD spectra of compounds *trans*-**4e** and *cis*-**4e** in acetonitrile.

Trans-4e

The TD-DFT simulations of the ECD spectrum of compound*trans*-**4e** were performed using the geometries of the four conformations optimized including the solvent. For data redundancy, calculations were performed with the hybrid functionals BH&HLYP[6] and M06-2X,[7] with ωB97XD that includes empirical dispersion,[8] and with CAM-B3LYP[9] that includes long range correction. The calculations employed the 6-311++G(2d,p), that is known to yield good performances at a reasonable computational cost.[10] The rotational strengths were calculated in both length and velocity representation, obtaining similar results (RMS difference < 5%) that ruled out large basis set incompleteness errors (BSSE).[11] The shapes of the spectra of the four conformations of *trans*-**4e** are quite different (Figure S5), but the four different functionals provide similar results (Figure S6), so the reliability should be high.

[6] In Gaussian 09 the BH&HLYP functional has the form: $0.5*E_X^{HF} + 0.5*E_X^{LSDA} + 0.5*\Delta E_X^{Becke88} + E_C^{LYP}$
[7] Y. Zhao and D.G. Truhlar *Theor. Chem. Acc*. **2008**, *120*, 215.
[8] J-D. Chai and M. Head-Gordon *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615.
[9] T. Yanai, D. Tewand, and N.Handy *Chem. Phys. Lett.* **2004**, *393*, 51.
[10] a) M. Mancinelli, S. Perticarari, L. Prati, A. Mazzanti. *J. Org. Chem.* **2017**, *82*, 6874. b) M. Meazza, M. E. Light, A. Mazzanti, R. Rios. *Chem. Sci.* **2016**, *7*, 984. c) P. Gunasekaran, S. Perumal, J. Carlos Menéndez, M. Mancinelli, S. Ranieri, A. Mazzanti *J. Org. Chem.* **2014**, *79,* 11039. d) L. Caruana, M. Fochi, M. Comes Franchini, S. Ranieri, A. Mazzanti, L. Bernardi *Chem. Commun.* **2014**, *50*, 445. e) M. Ambrogi, A. Ciogli, M. Mancinelli, S. Ranieri, A. Mazzanti, *J. Org. Chem.* **2013**, *78*, 3709.
[11] P.J. Stephens, D.M. McCann, F.J. Devlin, J.R. Cheeseman, M.J. Frisch, *J. Am. Chem.Soc.* **2004**, *126*, 7514.

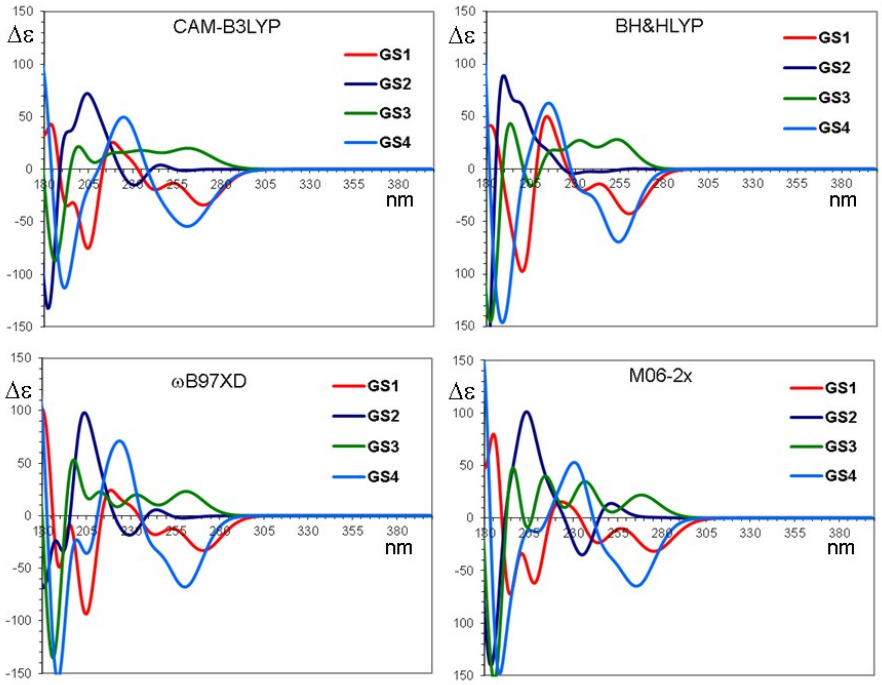


Figure S5. TD-DFT simulated spectra calculated for the four conformations of *trans*-**4e** assuming 2*R*,3*R* absolute configuration, with CAM-B3LYP, BH&HLYP, M06-2X, ωB97XD and the 6-311++G(2d,p) basis set. For each conformation, the first 70 excited states were calculated, and the spectra were obtained using a 0.20 eV line width at half height.

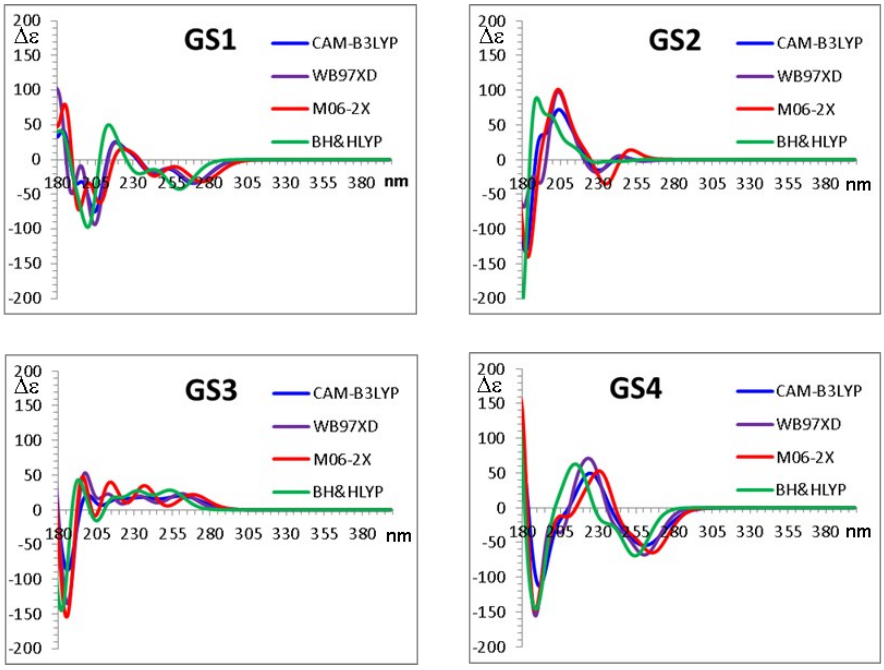
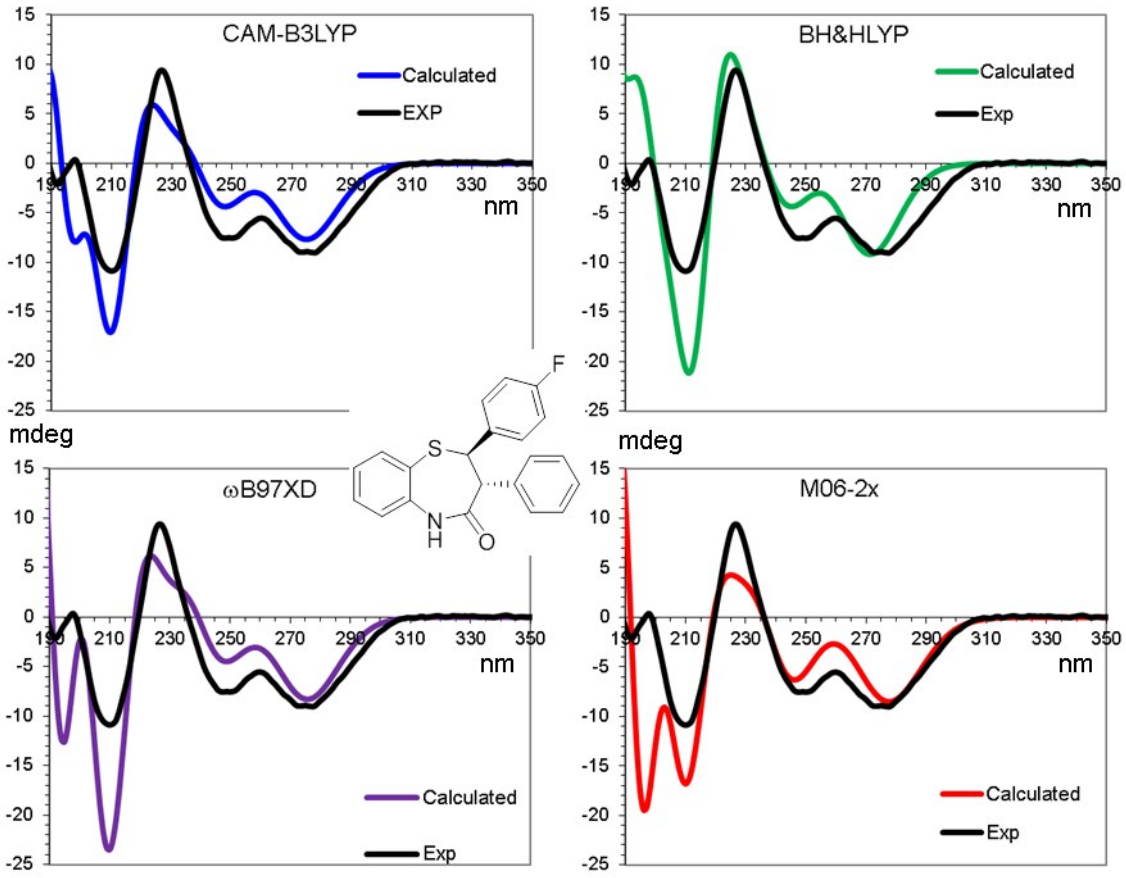


Figure S6. TD-DFT simulated spectra calculated for the same conformation of *trans*-**4e** assuming 2*R*,3*R* absolute configuration, with CAM-B3LYP, BH&HLYP, M06-2X, ωB97XD and the 6-311++G(2d,p) basis set. For each conformation, the first 70 excited states were calculated, and the spectrum was obtained using a 0.20 eV line width at half height.

The simulation of the weighted spectrum was obtained by using the populations obtained from Boltzmann distribution and the relative free energies obtained from the DFT-optimization (Figure S1). Since the GS1 conformation is much more stable than the others, the resulting spectrum is identical to that of GS1. Attempts were done by reducing to 1 kcal/mol the energy difference of the GS2-GS4 conformations, but the resulting spectrum was in worse agreement with the experimental one. The simulated spectra were vertically scaled to get the best match with the intensity experimental spectrum. Red-shifts were applied by comparison of the experimental with the simulated UV spectrum of GS1 (Figure S7; scaling factors: 0.23, 0.22, 0.30, 0.55; red shifts: 5, 11, 7, 2 nm for CAM-B3LYP, BH&HLYP, ωB97XD, and M06-2X, respectively). In all the cases the simulated spectra for the 2*R*,3*R* absolute configuration match very well the experimental spectrum.



FigureS7. Simulations of the experimental ECD spectrum of *trans*-**4e**. For each quadrant, the black line corresponds to the experimental spectrum. The colored lines correspond to the simulations obtained using the populations derived from PCM-B3LYP/6-311+G(d,p) optimization. Simulated spectra were scaled and red-shifted for the best fit to the experimental spectrum. Calculated spectra are for the 2*R*,3*R* enantiomer.

As a cross-check of the results obtained from ECD simulation, the optical rotation $[\alpha]_D$ of compound *trans*-**4e** (exp. value -322.3°) was calculated as -431° at the B3LYP/6-311++G(2d,p) level.

Cis-4e

The same approach was used in the case of compound *cis*-**4e**, where only three conformations are present. The simulations obtained for the 2*S*,3*R* enantiomer were in good agreement with the experimental ECD spectrum (Figures S8-S10). Also in this case the calculation of the optical rotation (B3LYP/6-311++G(2d,p) level) confirmed the assignment obtained with TD-DFT, being +83° the calculated value *vs* the experimental value of +37.9°.

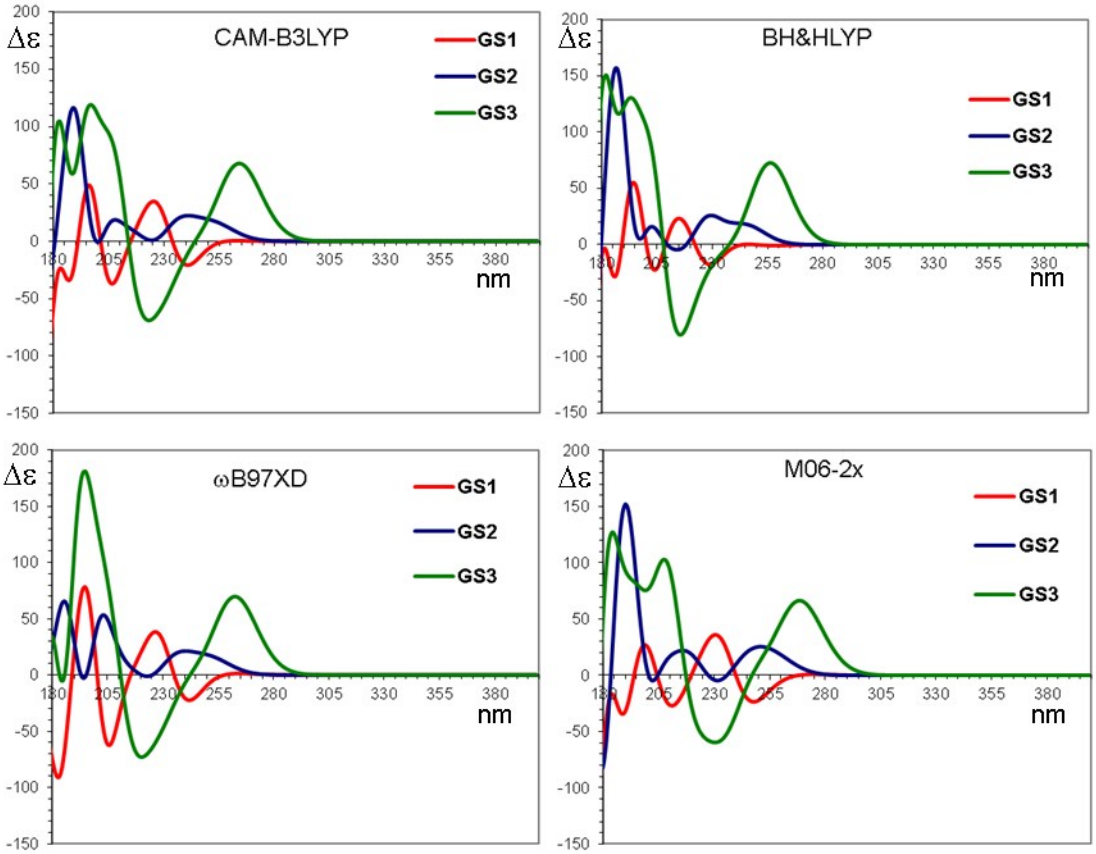


Figure S8. TD-DFT simulated spectra calculated for the three conformations of *cis*-**4e** assuming 2*S*,3*R* absolute configuration, with CAM-B3LYP, BH&HLYP, M06-2X, ωB97XD and the 6-311++G(2d,p) basis set. For each conformation, the first 70 excited states were calculated, and the spectrum was obtained using a 0.20 eV line width at half height.

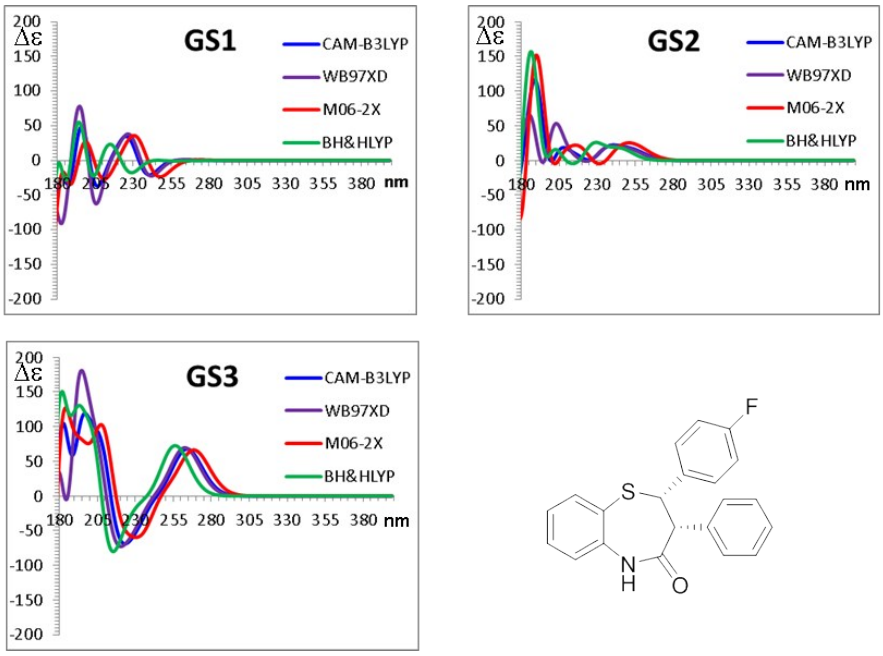


Figure S9. TD-DFT simulated spectra calculated for the same conformation of *cis*-**4e** assuming 2*S*,3*R* absolute configuration, with CAM-B3LYP, BH&HLYP, M06-2X, ωB97XD and the 6-311++G(2d,p) basis set. For each conformation, the first 70 excited states were calculated, and the spectrum was obtained using a 0.20 eV line width at half height.

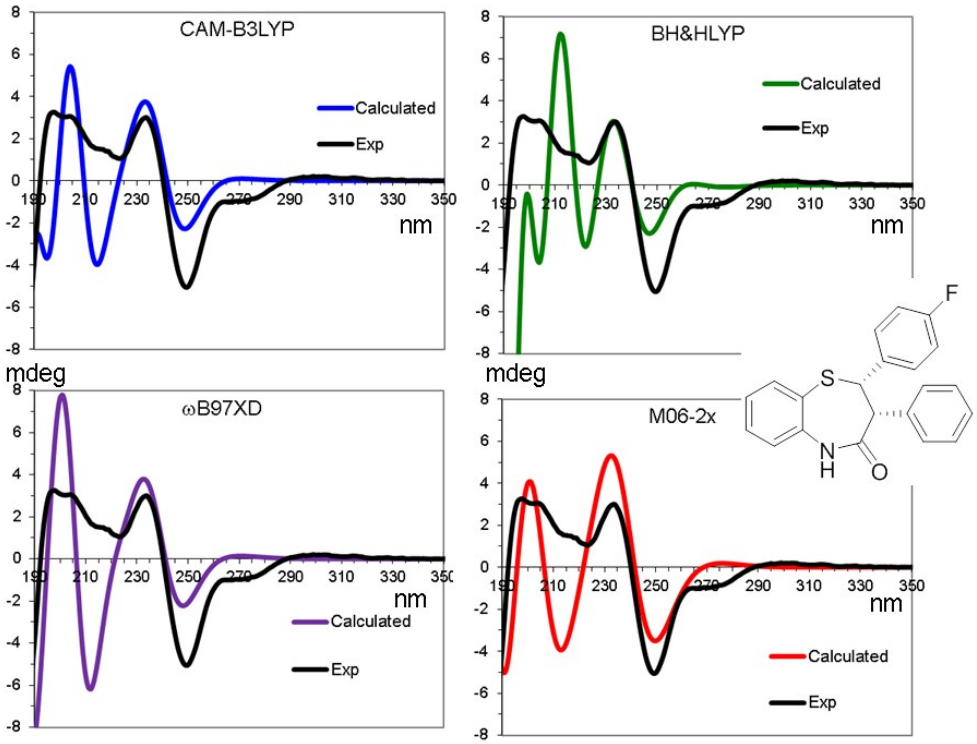


Figure S10. Simulations of the experimental ECD spectrum of *cis*-**4e**. For each quadrant, the black line corresponds to the experimental spectrum. The colored lines correspond to the simulations obtained using the populations derived from PCM-B3LYP/6-311+G(d,p) optimization. Simulated spectra were scaled and red-shifted for the best fit to the experimental spectrum (scaling factors: 0.11, 0.13, 0.10, 0.15; red shift: 8, 18, 8, 2 nm for CAM-B3LYP, BH&HLYP, ωB97XD, and M06-2X, respectively). Calculated spectra are for the 2*S*,3*R* enantiomer.

Computational data for compound 4e

Compound RR-4e (trans) - GS1

Method: b3lyp/6-311+g(d,p) scrf(solvent=acetonitrile)
SCF Done: E(RB3LYP) = -1438.20448219 A.U. after 1 cycles
Lowest frequency = 23.2021

Zero-point correction= 0.316831 (Hartree/Particle)
Thermal correction to Energy= 0.337007
Thermal correction to Enthalpy= 0.337951
Thermal correction to Gibbs Free Energy= 0.266080
Sum of electronic and zero-point Energies= -1437.887651
Sum of electronic and thermal Energies= -1437.867475
Sum of electronic and thermal Enthalpies= -1437.866531
Sum of electronic and thermal Free Energies= -1437.938402

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.463514	0.867455	-1.763044
2	6	0	-0.121298	0.071312	-1.141329
3	6	0	0.184449	-1.077416	-0.147556
4	6	0	1.272163	-2.018333	-0.704128
5	7	0	2.565449	-1.685785	-0.403722
6	6	0	4.045411	-0.488305	1.095326
7	6	0	4.578374	0.697271	1.591765
8	6	0	4.101698	1.924540	1.131407
9	6	0	3.100691	1.959349	0.164199
10	6	0	2.576292	0.774855	-0.366918
11	6	0	3.047074	-0.461685	0.117206
12	8	0	1.016588	-3.041734	-1.325843
13	1	0	0.591604	-0.627195	0.760099
14	1	0	4.399240	-1.445871	1.460325
15	1	0	5.355702	0.660657	2.345792
16	1	0	4.504593	2.850779	1.523469
17	1	0	2.729329	2.908415	-0.202464
18	1	0	3.252001	-2.383132	-0.666504
19	6	0	-1.064422	-1.848964	0.252466
20	6	0	-1.359989	-2.015122	1.609462
21	6	0	-1.929932	-2.407573	-0.695364
22	6	0	-2.492546	-2.721749	2.015005
23	1	0	-0.700686	-1.587927	2.357916
24	6	0	-3.062684	-3.112810	-0.293362
25	1	0	-1.720614	-2.302367	-1.752689
26	6	0	-3.348568	-3.272588	1.063186
27	1	0	-2.704389	-2.837878	3.071967
28	1	0	-3.722239	-3.539125	-1.041004
29	1	0	-4.230989	-3.820456	1.373890
30	6	0	-1.092174	1.103599	-0.612228

31	6	0	-2.207954	1.456213	-1.378997
32	6	0	-0.898811	1.742005	0.620121
33	6	0	-3.115690	2.418512	-0.937385
34	1	0	-2.377229	0.975281	-2.335978
35	6	0	-1.793047	2.704953	1.078906
36	1	0	-0.040624	1.499821	1.235333
37	6	0	-2.885411	3.021781	0.286254
38	1	0	-3.981652	2.692191	-1.527075
39	1	0	-1.649164	3.201763	2.030271
40	1	0	-0.527388	-0.352062	-2.060509
41	9	0	-3.765147	3.962569	0.731161

Compound RR-4e (trans) – GS2

Method: b3lyp/6-311+g(d,p) scrf(solvent=acetonitrile)
SCF Done: E(RB3LYP) = -1438.19721578 A.U. after 1 cycles
Lowest frequency = 13.0713

Zero-point correction= 0.316942 (Hartree/Particle)
Thermal correction to Energy= 0.337175
Thermal correction to Enthalpy= 0.338119
Thermal correction to Gibbs Free Energy= 0.265451
Sum of electronic and zero-point Energies= -1437.880274
Sum of electronic and thermal Energies= -1437.860041
Sum of electronic and thermal Enthalpies= -1437.859097
Sum of electronic and thermal Free Energies= -1437.931765

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.333540	-1.930760	-0.232488
2	6	0	0.059583	0.838342	0.539890
3	6	0	-0.417935	0.223867	1.873786
4	7	0	-1.487619	-0.626852	1.896674
5	6	0	-3.548442	-1.395317	0.894454
6	6	0	-3.548598	-2.689348	-1.143586
7	6	0	-2.162279	-2.579066	-1.207694
8	6	0	-1.452249	-1.895569	-0.214174
9	6	0	-2.155162	-1.287395	0.840086
10	8	0	0.100939	0.576613	2.930037
11	1	0	-4.082601	-0.923945	1.711703
12	1	0	-4.083565	-3.230533	-1.914831
13	1	0	-1.615163	-3.036004	-2.023423
14	1	0	-1.822187	-0.822626	2.832894
15	1	0	0.822110	1.540543	0.877223
16	6	0	-1.049255	1.699761	-0.078092
17	6	0	-1.354778	2.911705	0.559025

18	6	0	-1.761909	1.361004	-1.232112
19	6	0	-2.346034	3.755047	0.064423
20	1	0	-0.805507	3.200242	1.449283
21	6	0	-2.751891	2.208295	-1.734025
22	1	0	-1.560627	0.436032	-1.756443
23	6	0	-3.050657	3.405309	-1.088128
24	1	0	-2.561038	4.687787	0.573592
25	1	0	-3.288782	1.925981	-2.632659
26	1	0	-3.819158	4.061728	-1.480030
27	6	0	2.297337	-0.075464	-0.357664
28	6	0	2.973976	-0.179735	0.865125
29	6	0	3.046961	0.061478	-1.531053
30	6	0	4.364841	-0.138125	0.919567
31	1	0	2.418388	-0.286023	1.789225
32	6	0	4.440101	0.104257	-1.496614
33	1	0	2.541266	0.140354	-2.486950
34	6	0	5.067216	0.002760	-0.266894
35	1	0	4.895643	-0.212935	1.860405
36	1	0	5.025446	0.215774	-2.400654
37	9	0	6.427813	0.045082	-0.219667
38	6	0	-4.240361	-2.098928	-0.085806
39	1	0	-5.319593	-2.176589	-0.027358
40	6	0	0.784613	-0.131422	-0.442601
41	1	0	0.503755	0.132960	-1.459645

Compound RR-4e (trans) – GS3

Method: b3lyp/6-311+g(d,p) scrf(solvent=acetonitrile)
SCF Done: E(RB3LYP) = -1438.20019089 A.U. after 2 cycles
Lowest frequency = 17.2127

Zero-point correction= 0.316847 (Hartree/Particle)
Thermal correction to Energy= 0.337111
Thermal correction to Enthalpy= 0.338055
Thermal correction to Gibbs Free Energy= 0.265318
Sum of electronic and zero-point Energies= -1437.883344
Sum of electronic and thermal Energies= -1437.863080
Sum of electronic and thermal Enthalpies= -1437.862136
Sum of electronic and thermal Free Energies= -1437.934873

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.957897	-1.877071	-0.888957
2	6	0	-0.097089	-0.525727	-0.149456
3	6	0	0.005743	0.785993	-0.958001

4	6	0	1.355237	1.192827	-1.574452
5	7	0	2.578770	0.815663	-1.078618
6	6	0	4.256871	0.094122	0.476379
7	6	0	4.878406	-0.874403	1.254461
8	6	0	4.307085	-2.140900	1.382375
9	6	0	3.107938	-2.418809	0.735334
10	6	0	2.481410	-1.457641	-0.067123
11	6	0	3.062345	-0.185814	-0.203398
12	8	0	1.332524	1.990140	-2.510090
13	1	0	-0.630420	0.682432	-1.838024
14	1	0	4.699647	1.078947	0.377228
15	1	0	5.804482	-0.636606	1.764259
16	1	0	4.782440	-2.900694	1.990949
17	1	0	2.642350	-3.391129	0.842557
18	1	0	3.313764	1.357485	-1.519892
19	6	0	-0.526639	1.968600	-0.146882
20	6	0	0.125367	2.396455	1.016404
21	6	0	-1.682815	2.639731	-0.555902
22	6	0	-0.369681	3.470747	1.753364
23	1	0	1.027620	1.896740	1.352793
24	6	0	-2.181419	3.713665	0.181807
25	1	0	-2.196945	2.321808	-1.456232
26	6	0	-1.526129	4.132247	1.338748
27	1	0	0.148518	3.791096	2.650156
28	1	0	-3.080203	4.221708	-0.149176
29	1	0	-1.911671	4.967176	1.912663
30	6	0	-1.522562	-1.019860	-0.022711
31	6	0	-2.083122	-1.207616	1.245324
32	6	0	-2.299359	-1.316079	-1.150411
33	6	0	-3.389178	-1.670782	1.395567
34	1	0	-1.497714	-0.987612	2.130760
35	6	0	-3.604172	-1.785600	-1.020977
36	1	0	-1.891586	-1.190416	-2.147142
37	6	0	-4.120908	-1.950046	0.254113
38	1	0	-3.829914	-1.812008	2.374461
39	1	0	-4.208925	-2.019632	-1.888103
40	1	0	0.307807	-0.385442	0.851398
41	9	0	-5.397907	-2.404238	0.388701

Compound RR-4e (trans) – GS4

Method: b3lyp/6-311+g(d,p) scrf(solvent=acetonitrile)
SCF Done: E(RB3LYP) = -1438.19445932 A.U. after 1 cycles
Lowest frequency = 17.6091

Zero-point correction= 0.317007 (Hartree/Particle)
Thermal correction to Energy= 0.337142
Thermal correction to Enthalpy= 0.338086

Thermal correction to Gibbs Free Energy= 0.266151
Sum of electronic and zero-point Energies= -1437.877452
Sum of electronic and thermal Energies= -1437.857317
Sum of electronic and thermal Enthalpies= -1437.856373
Sum of electronic and thermal Free Energies= -1437.928308

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.278917	0.693053	-1.678911
2	6	0	0.388094	-0.755810	-0.517885
3	6	0	1.322763	-0.474172	0.681064
4	6	0	1.091643	0.736433	1.593278
5	7	0	0.218353	1.773498	1.350367
6	6	0	-1.823225	2.953099	0.994203
7	6	0	-2.871350	3.416185	0.211170
8	6	0	-2.972356	3.019193	-1.122210
9	6	0	-2.018453	2.156204	-1.647278
10	6	0	-0.942071	1.699211	-0.874440
11	6	0	-0.839840	2.099064	0.467073
12	8	0	1.747222	0.790392	2.632660
13	1	0	1.195225	-1.317827	1.367498
14	1	0	-1.752261	3.258981	2.032424
15	1	0	-3.609743	4.079346	0.645827
16	1	0	-3.789883	3.366640	-1.742201
17	1	0	-2.091695	1.825471	-2.676406
18	1	0	0.253632	2.401451	2.146684
19	6	0	2.788530	-0.509372	0.241111
20	6	0	3.460805	-1.736811	0.232507
21	6	0	3.471826	0.632642	-0.189315
22	6	0	4.781991	-1.825214	-0.204202
23	1	0	2.949761	-2.631556	0.573386
24	6	0	4.794474	0.547257	-0.623381
25	1	0	2.977335	1.596592	-0.184450
26	6	0	5.453481	-0.681610	-0.635150
27	1	0	5.286244	-2.785028	-0.200245
28	1	0	5.309383	1.443494	-0.950888
29	1	0	6.482090	-0.746281	-0.971314
30	6	0	-0.966176	-1.361598	-0.204407
31	6	0	-1.619132	-1.190947	1.020055
32	6	0	-1.590075	-2.145567	-1.186301
33	6	0	-2.861145	-1.779716	1.265475
34	1	0	-1.173163	-0.606488	1.814188
35	6	0	-2.827504	-2.739019	-0.963038
36	1	0	-1.100783	-2.295213	-2.142352
37	6	0	-3.438991	-2.539135	0.265554
38	1	0	-3.366251	-1.651027	2.214477
39	1	0	-3.307365	-3.348350	-1.718664
40	1	0	0.921376	-1.473301	-1.144034

41	9	0	-4.650284	-3.118364	0.495722

Compound RR-4e (trans) – GS1 WB97XD optimization

Method: wb97xd/6-311+g(d,p)
SCF Done: E(RwB97XD) = -1437.82744820 A.U. after 2 cycles
Lowest frequency = 23.1088

Zero-point correction= 0.321125 (Hartree/Particle)
Thermal correction to Energy= 0.340950
Thermal correction to Enthalpy= 0.341894
Thermal correction to Gibbs Free Energy= 0.271086
Sum of electronic and zero-point Energies= -1437.506323
Sum of electronic and thermal Energies= -1437.486499
Sum of electronic and thermal Enthalpies= -1437.485554
Sum of electronic and thermal Free Energies= -1437.556362

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.582681	0.569438	-1.859098
2	6	0	-0.015742	-0.070092	-1.186239
3	6	0	0.199763	-1.106777	-0.057960
4	6	0	1.254764	-2.140271	-0.464181
5	7	0	2.548593	-1.810073	-0.140820
6	6	0	3.956877	-0.459079	1.282378
7	6	0	4.489249	0.765483	1.658312
8	6	0	4.081566	1.927661	1.014252
9	6	0	3.149761	1.855490	-0.012083
10	6	0	2.629030	0.627566	-0.421229
11	6	0	3.033224	-0.541683	0.242320
12	8	0	0.997205	-3.199715	-0.991282
13	1	0	0.587625	-0.563366	0.808225
14	1	0	4.249492	-1.368764	1.795079
15	1	0	5.212071	0.811968	2.464512
16	1	0	4.485052	2.888691	1.310641
17	1	0	2.824021	2.754352	-0.522580
18	1	0	3.224125	-2.528569	-0.359380
19	6	0	-1.123645	-1.720458	0.346685
20	6	0	-1.673092	-1.393790	1.583990
21	6	0	-1.849068	-2.540667	-0.517619
22	6	0	-2.922190	-1.874654	1.958130
23	1	0	-1.124686	-0.743555	2.258457
24	6	0	-3.095830	-3.024224	-0.143984
25	1	0	-1.427052	-2.818441	-1.475241
26	6	0	-3.637820	-2.691580	1.092857

27	1	0	-3.336045	-1.606247	2.923580
28	1	0	-3.646245	-3.666710	-0.822273
29	1	0	-4.613187	-3.068198	1.379866
30	6	0	-0.964235	1.020674	-0.749517
31	6	0	-2.237983	1.096856	-1.304532
32	6	0	-0.616537	1.921939	0.257223
33	6	0	-3.154269	2.049325	-0.874170
34	1	0	-2.530469	0.391585	-2.074993
35	6	0	-1.515374	2.880376	0.700040
36	1	0	0.371000	1.881153	0.704231
37	6	0	-2.772848	2.924030	0.123359
38	1	0	-4.148900	2.112316	-1.297238
39	1	0	-1.255842	3.585909	1.479516
40	1	0	-0.442738	-0.590610	-2.046754
41	9	0	-3.651390	3.849883	0.551967

Compound RR-4e (trans) – GS2 WB97XD optimization

Method: wb97xd/6-311+g(d,p)
SCF Done: E(RwB97XD) = -1437.82325103 A.U. after 1 cycles
Lowest frequency = 25.3482

Zero-point correction= 0.321405 (Hartree/Particle)
Thermal correction to Energy= 0.341181
Thermal correction to Enthalpy= 0.342125
Thermal correction to Gibbs Free Energy= 0.271477
Sum of electronic and zero-point Energies= -1437.501846
Sum of electronic and thermal Energies= -1437.482070
Sum of electronic and thermal Enthalpies= -1437.481126
Sum of electronic and thermal Free Energies= -1437.551774

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.425794	-1.878260	-0.115841
2	6	0	0.069549	0.918236	0.367942
3	6	0	-0.236824	0.456198	1.802567
4	7	0	-1.261753	-0.427962	1.989807
5	6	0	-3.383636	-1.150414	1.094335
6	6	0	-3.498533	-2.544189	-0.862142
7	6	0	-2.114196	-2.518949	-0.955605
8	6	0	-1.348914	-1.825649	-0.019339
9	6	0	-1.993727	-1.133399	1.012708
10	8	0	0.357168	0.922597	2.755684
11	1	0	-3.870283	-0.586900	1.882545
12	1	0	-4.079830	-3.092188	-1.594365

13	1	0	-1.608360	-3.043399	-1.758001
14	1	0	-1.493163	-0.585821	2.959849
15	1	0	0.758338	1.751199	0.524210
16	6	0	-1.188845	1.515139	-0.262971
17	6	0	-1.767820	2.608778	0.386203
18	6	0	-1.794857	1.039188	-1.421981
19	6	0	-2.924153	3.200150	-0.100600
20	1	0	-1.305563	2.996666	1.289229
21	6	0	-2.953308	1.631245	-1.914192
22	1	0	-1.392448	0.182267	-1.947018
23	6	0	-3.524709	2.710397	-1.255711
24	1	0	-3.355207	4.047226	0.421202
25	1	0	-3.411470	1.237025	-2.814266
26	1	0	-4.429009	3.169291	-1.638912
27	6	0	2.344907	-0.012460	-0.389381
28	6	0	2.998614	0.159315	0.832141
29	6	0	3.108827	-0.123535	-1.550114
30	6	0	4.383438	0.230728	0.891022
31	1	0	2.428685	0.253771	1.749343
32	6	0	4.495560	-0.058572	-1.508896
33	1	0	2.614863	-0.263238	-2.506278
34	6	0	5.106562	0.118548	-0.282450
35	1	0	4.900913	0.371172	1.831720
36	1	0	5.096052	-0.139758	-2.406166
37	9	0	6.449440	0.187275	-0.228920
38	6	0	-4.132837	-1.858323	0.167340
39	1	0	-5.214091	-1.861194	0.240790
40	6	0	0.838161	-0.114172	-0.490745
41	1	0	0.578255	0.055959	-1.535053

Compound RR-4e (trans) – GS3 WB97XD optimization

Method: wb97xd/6-311+g(d,p)
SCF Done: E(RwB97XD) = -1437.82113993 A.U. after 2 cycles
Lowest frequency = 17.1452

Zero-point correction= 0.321024 (Hartree/Particle)
Thermal correction to Energy= 0.341016
Thermal correction to Enthalpy= 0.341960
Thermal correction to Gibbs Free Energy= 0.269719
Sum of electronic and zero-point Energies= -1437.500116
Sum of electronic and thermal Energies= -1437.480124
Sum of electronic and thermal Enthalpies= -1437.479180
Sum of electronic and thermal Free Energies= -1437.551421

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	16	0	0.937540	-1.985027	-0.773723
2	6	0	-0.091260	-0.592316	-0.145728
3	6	0	0.006949	0.661054	-1.037701
4	6	0	1.319987	0.983054	-1.753391
5	7	0	2.555282	0.662679	-1.233483
6	6	0	4.183514	0.139293	0.438446
7	6	0	4.782036	-0.725713	1.339788
8	6	0	4.212752	-1.968093	1.594088
9	6	0	3.040125	-2.325519	0.946110
10	6	0	2.440944	-1.473798	0.017953
11	6	0	3.019952	-0.225551	-0.244867
12	8	0	1.274357	1.643695	-2.770357
13	1	0	-0.685024	0.531000	-1.871885
14	1	0	4.620208	1.113345	0.244262
15	1	0	5.689388	-0.423757	1.849791
16	1	0	4.669717	-2.648647	2.302408
17	1	0	2.570181	-3.280571	1.149915
18	1	0	3.283447	1.118804	-1.766289
19	6	0	-0.438231	1.878258	-0.244105
20	6	0	0.344645	2.364839	0.803375
21	6	0	-1.656679	2.491541	-0.517850
22	6	0	-0.083164	3.447821	1.559505
23	1	0	1.299309	1.897812	1.028755
24	6	0	-2.088794	3.573491	0.240511
25	1	0	-2.272521	2.117115	-1.328401
26	6	0	-1.303470	4.054214	1.280489
27	1	0	0.537025	3.819822	2.367372
28	1	0	-3.040942	4.041073	0.016593
29	1	0	-1.638893	4.899109	1.871186
30	6	0	-1.531273	-1.013114	0.015815
31	6	0	-2.169116	-0.856245	1.243224
32	6	0	-2.261046	-1.517320	-1.061287
33	6	0	-3.507195	-1.193984	1.404212
34	1	0	-1.618654	-0.451552	2.085580
35	6	0	-3.596016	-1.866988	-0.918931
36	1	0	-1.784413	-1.645045	-2.028350
37	6	0	-4.195009	-1.695610	0.316473
38	1	0	-4.013762	-1.069923	2.353044
39	1	0	-4.170217	-2.265183	-1.746056
40	1	0	0.314580	-0.373605	0.842417
41	9	0	-5.491088	-2.027063	0.461077

Compound RR-4e (trans) – GS4 WB97XD optimization

Method: wb97xd/6-311+g(d,p)
SCF Done: E(RwB97XD) = -1437.81820593 A.U. after 1 cycles
Lowest frequency = 24.0513

Zero-point correction= 0.321241 (Hartree/Particle)
Thermal correction to Energy= 0.341040
Thermal correction to Enthalpy= 0.341984
Thermal correction to Gibbs Free Energy= 0.270992
Sum of electronic and zero-point Energies= -1437.496965
Sum of electronic and thermal Energies= -1437.477166
Sum of electronic and thermal Enthalpies= -1437.476222
Sum of electronic and thermal Free Energies= -1437.547214

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.378514	0.621263	-1.681757
2	6	0	0.446222	-0.791607	-0.498963
3	6	0	1.361554	-0.497167	0.700872
4	6	0	1.103340	0.717877	1.591961
5	7	0	0.288505	1.784352	1.251924
6	6	0	-1.877778	2.738932	0.941842
7	6	0	-2.988552	3.059013	0.180013
8	6	0	-3.079025	2.618527	-1.134787
9	6	0	-2.048995	1.859793	-1.666733
10	6	0	-0.912064	1.555871	-0.918016
11	6	0	-0.823582	1.992239	0.406456
12	8	0	1.689195	0.779233	2.654396
13	1	0	1.251258	-1.337516	1.394420
14	1	0	-1.819168	3.068474	1.974354
15	1	0	-3.788728	3.642320	0.620388
16	1	0	-3.949768	2.850769	-1.735881
17	1	0	-2.110574	1.487417	-2.682530
18	1	0	0.315482	2.439104	2.023344
19	6	0	2.819689	-0.492355	0.261359
20	6	0	3.513088	-1.700450	0.219889
21	6	0	3.468432	0.670527	-0.146590
22	6	0	4.827050	-1.750544	-0.227957
23	1	0	3.022348	-2.611954	0.548486
24	6	0	4.783671	0.623495	-0.591462
25	1	0	2.946035	1.619835	-0.117000
26	6	0	5.466175	-0.586100	-0.636174
27	1	0	5.353682	-2.698042	-0.248818
28	1	0	5.276752	1.537437	-0.902837
29	1	0	6.493206	-0.620326	-0.981610
30	6	0	-0.934326	-1.319413	-0.175944
31	6	0	-1.538267	-1.150833	1.067016
32	6	0	-1.648787	-1.983692	-1.175818
33	6	0	-2.823621	-1.622834	1.312840
34	1	0	-1.019366	-0.648952	1.875001
35	6	0	-2.928932	-2.462576	-0.951458
36	1	0	-1.197038	-2.114892	-2.153598
37	6	0	-3.496596	-2.267523	0.296214

38	1	0	-3.297849	-1.491430	2.277183
39	1	0	-3.486073	-2.978907	-1.723146
40	1	0	0.963924	-1.554129	-1.086325
41	9	0	-4.741734	-2.724535	0.522299

Compound SR-4e (cis) – GS1

Method: b3lyp/6-311+g(d,p) scrf(solvent=acetonitrile)
SCF Done: E(RB3LYP) = -1438.20124497 A.U. after 2 cycles
Lowest frequency = 28.7576

Zero-point correction= 0.317118 (Hartree/Particle)
Thermal correction to Energy= 0.337208
Thermal correction to Enthalpy= 0.338152
Thermal correction to Gibbs Free Energy= 0.266989
Sum of electronic and zero-point Energies= -1437.884127
Sum of electronic and thermal Energies= -1437.864037
Sum of electronic and thermal Enthalpies= -1437.863093
Sum of electronic and thermal Free Energies= -1437.934256

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.211225	-1.853465	-0.616967
2	6	0	-0.037141	-0.462696	-0.750982
3	6	0	0.420323	0.792884	0.059299
4	6	0	0.810075	0.477401	1.509416
5	7	0	2.090911	0.024673	1.695209
6	6	0	4.378760	0.213092	0.922853
7	6	0	5.384931	-0.075463	0.006073
8	6	0	5.095051	-0.817042	-1.138882
9	6	0	3.799661	-1.280825	-1.352326
10	6	0	2.785014	-1.027952	-0.421522
11	6	0	3.077583	-0.256782	0.720259
12	6	0	-1.397719	-1.053820	-0.445049
13	6	0	-2.957891	-2.210061	1.018676
14	6	0	-1.693435	-1.682131	0.772374
15	6	0	-3.919973	-2.110321	0.025961
16	6	0	-3.668992	-1.511632	-1.196162
17	6	0	-2.397616	-0.986593	-1.422144
18	8	0	0.070474	0.647351	2.470979
19	1	0	-0.038240	-0.150689	-1.795613
20	1	0	1.341591	1.108172	-0.434930
21	1	0	4.592874	0.807097	1.804126
22	1	0	6.389365	0.291767	0.180301
23	1	0	5.871162	-1.032566	-1.863530
24	1	0	3.567309	-1.862178	-2.236308
25	1	0	-3.194450	-2.692949	1.958592
26	1	0	-0.936527	-1.764441	1.541261
27	1	0	-4.445117	-1.459995	-1.949355
28	1	0	-2.186422	-0.514377	-2.374915
29	1	0	2.367730	-0.045383	2.667398
30	6	0	-0.549339	1.956848	-0.081439
31	6	0	-0.190968	3.019342	-0.921056

32	6	0	-1.791070	2.007349	0.565746
33	6	0	-1.043894	4.106214	-1.111692
34	1	0	0.767688	2.999481	-1.429564
35	6	0	-2.642973	3.095117	0.379101
36	1	0	-2.087337	1.204638	1.225387
37	6	0	-2.275128	4.147228	-0.459950
38	1	0	-0.743652	4.917907	-1.764804
39	1	0	-3.598135	3.119511	0.892004
40	1	0	-2.941093	4.990900	-0.602232
41	9	0	-5.157563	-2.628214	0.260892

Compound SR-4e (cis) – GS2

Method: b3lyp/6-311+g(d,p) scrf(solvent=acetonitrile)
SCF Done: E(RB3LYP) = -1438.20124497 A.U. after 2 cycles
Lowest frequency = 16.8423

Zero-point correction= 0.317118 (Hartree/Particle)
Thermal correction to Energy= 0.337208
Thermal correction to Enthalpy= 0.338152
Thermal correction to Gibbs Free Energy= 0.266989
Sum of electronic and zero-point Energies= -1437.884127
Sum of electronic and thermal Energies= -1437.864037
Sum of electronic and thermal Enthalpies= -1437.863093
Sum of electronic and thermal Free Energies= -1437.934256

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.381242	-2.238780	0.625076
2	6	0	0.647949	-0.813511	1.244051
3	6	0	-0.113143	0.531826	1.418209
4	6	0	-1.397636	0.328972	2.244143
5	7	0	-2.516347	-0.164042	1.635850
6	6	0	-3.851596	-0.315195	-0.367817
7	6	0	-4.110381	-0.837839	-1.629852
8	6	0	-3.195805	-1.707430	-2.223971
9	6	0	-2.031018	-2.051398	-1.545189
10	6	0	-1.770032	-1.552108	-0.262935
11	6	0	-2.689495	-0.667929	0.326745
12	8	0	-1.429087	0.648310	3.429593
13	1	0	-4.551645	0.370931	0.095571
14	1	0	-5.018476	-0.557877	-2.150444
15	1	0	-3.383802	-2.112062	-3.211307
16	1	0	-1.314957	-2.724608	-2.000894
17	1	0	-3.346039	-0.118461	2.215703
18	1	0	0.848641	-1.142144	2.266439

19	6	0	2.012178	-0.666542	0.568267
20	6	0	2.338180	-1.230231	-0.666822
21	6	0	3.002459	0.054286	1.251538
22	6	0	3.605694	-1.065076	-1.225951
23	1	0	1.603308	-1.818550	-1.200872
24	6	0	4.272658	0.233498	0.710680
25	1	0	2.790379	0.481306	2.225642
26	6	0	4.544959	-0.330598	-0.525222
27	1	0	3.858864	-1.501924	-2.183939
28	1	0	5.037666	0.789579	1.238017
29	1	0	0.512069	1.093700	2.115766
30	6	0	-0.324395	1.468565	0.225725
31	6	0	-0.667561	2.796275	0.524994
32	6	0	-0.172783	1.114712	-1.117007
33	6	0	-0.866910	3.735349	-0.483227
34	1	0	-0.775356	3.100406	1.561358
35	6	0	-0.362484	2.055927	-2.130579
36	1	0	0.094078	0.105498	-1.391518
37	6	0	-0.713521	3.367326	-1.820330
38	1	0	-1.132754	4.753986	-0.223981
39	1	0	-0.235047	1.756834	-3.164959
40	1	0	-0.861605	4.095983	-2.609205
41	9	0	5.786422	-0.164839	-1.062556

Compound SR-4e (cis) – GS3

Method: b3lyp/6-311+g(d,p) scrf(solvent=acetonitrile)
SCF Done: E(RB3LYP) = -1438.19277317 A.U. after 2 cycles
Lowest frequency = 19.6029

Zero-point correction= 0.317215 (Hartree/Particle)
Thermal correction to Energy= 0.337276
Thermal correction to Enthalpy= 0.338220
Thermal correction to Gibbs Free Energy= 0.266831
Sum of electronic and zero-point Energies= -1437.875558
Sum of electronic and thermal Energies= -1437.855497
Sum of electronic and thermal Enthalpies= -1437.854553
Sum of electronic and thermal Free Energies= -1437.925942

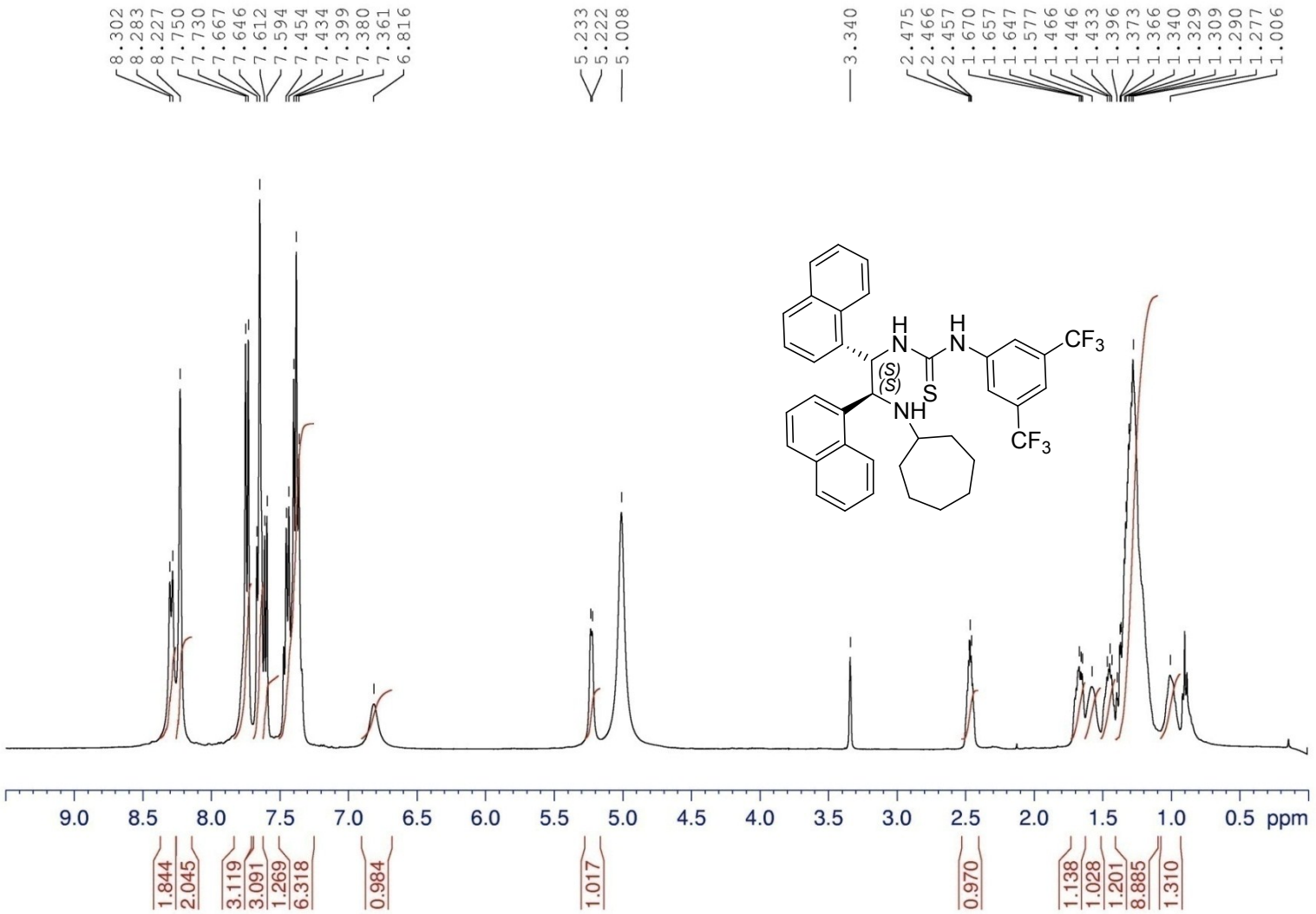
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.262688	-0.952612	2.064999
2	6	0	-0.296348	-0.303981	1.277044
3	6	0	-1.023580	-1.431601	0.502651
4	6	0	-0.328128	-2.215553	-0.618750
5	7	0	1.022453	-2.186675	-0.895728

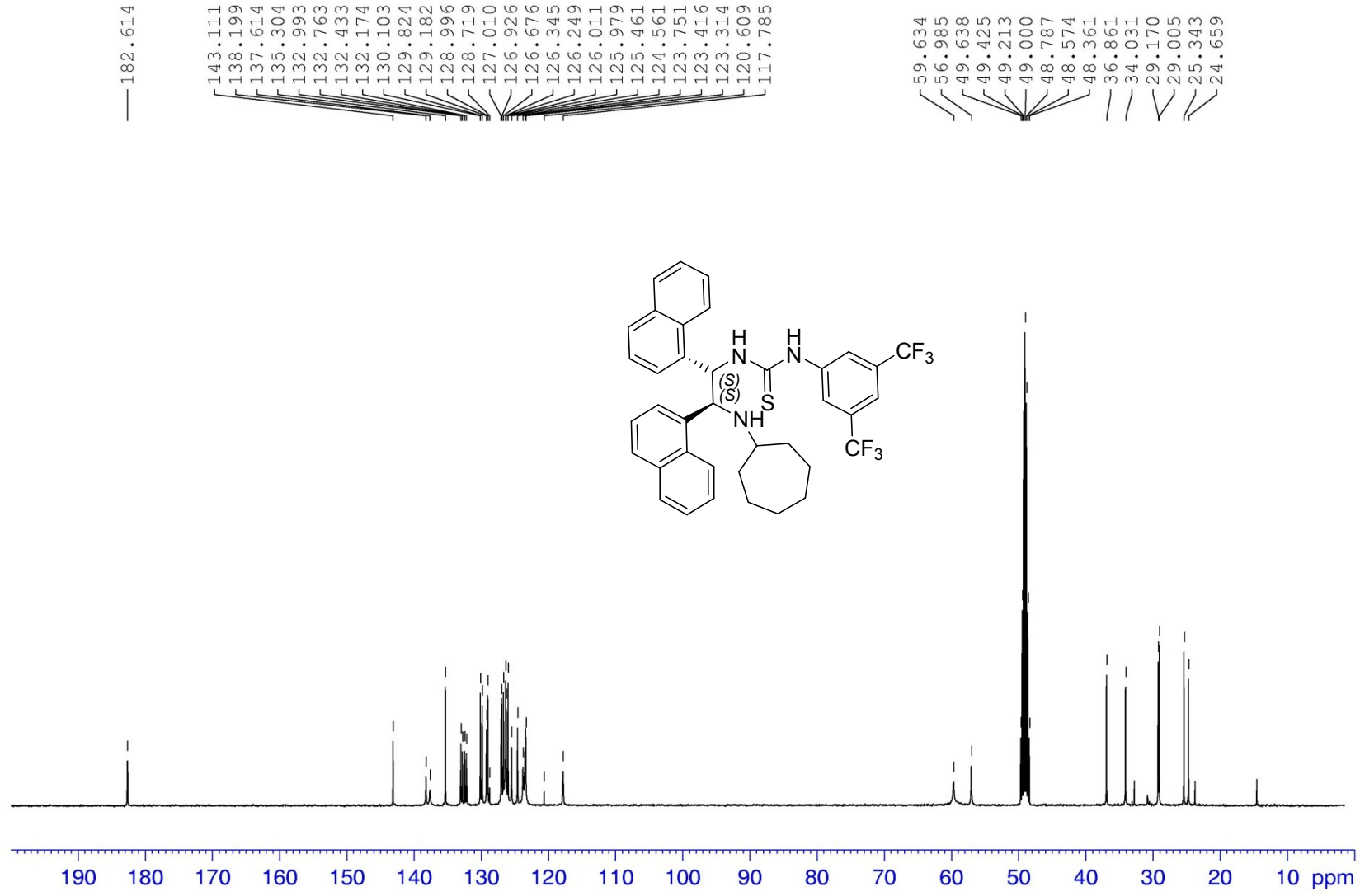
6	6	0	3.194594	-1.414129	-1.502967
7	6	0	4.415592	-0.807247	-1.243759
8	6	0	4.650510	-0.217885	-0.001450
9	6	0	3.650052	-0.244568	0.962288
10	6	0	2.421389	-0.875534	0.722947
11	6	0	2.184826	-1.467855	-0.527456
12	6	0	-0.110433	1.050370	0.628485
13	6	0	0.433127	2.500481	-1.250488
14	6	0	0.255480	1.226726	-0.710830
15	6	0	0.241421	3.597266	-0.429615
16	6	0	-0.123965	3.473663	0.901186
17	6	0	-0.297801	2.193637	1.418671
18	8	0	-1.011337	-2.993169	-1.280793
19	1	0	-0.907606	-0.145393	2.167454
20	1	0	-1.156096	-2.218043	1.253832
21	1	0	3.011878	-1.863193	-2.473348
22	1	0	5.176719	-0.788834	-2.014695
23	1	0	5.595853	0.266614	0.210810
24	1	0	3.811210	0.222091	1.926710
25	1	0	0.711834	2.637764	-2.287721
26	1	0	0.401377	0.377151	-1.363450
27	1	0	-0.272570	4.355759	1.511330
28	1	0	-0.585043	2.084441	2.458661
29	1	0	1.192703	-2.811209	-1.676703
30	6	0	-2.431118	-0.989582	0.102449
31	6	0	-2.725173	-0.409396	-1.136199
32	6	0	-3.462926	-1.121573	1.038257
33	6	0	-4.015199	0.029491	-1.428487
34	1	0	-1.953031	-0.307713	-1.888521
35	6	0	-4.754707	-0.680589	0.750988
36	1	0	-3.258575	-1.579250	2.001026
37	6	0	-5.034870	-0.101327	-0.485219
38	1	0	-4.223569	0.472342	-2.396038
39	1	0	-5.539423	-0.796986	1.490028
40	1	0	-6.038051	0.239657	-0.714641
41	9	0	0.411828	4.844868	-0.949640

NMR Spectra

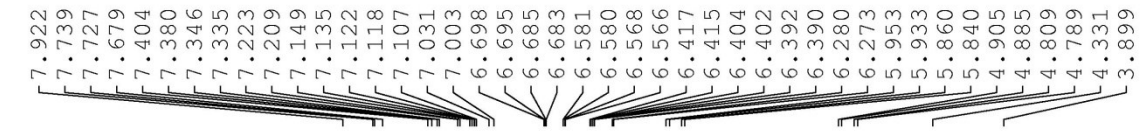
^{1}H NMR in MeOD (400 MHz)

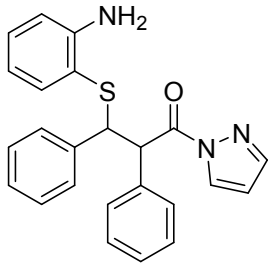


^{13}C NMR in MeOD (100 MHz)

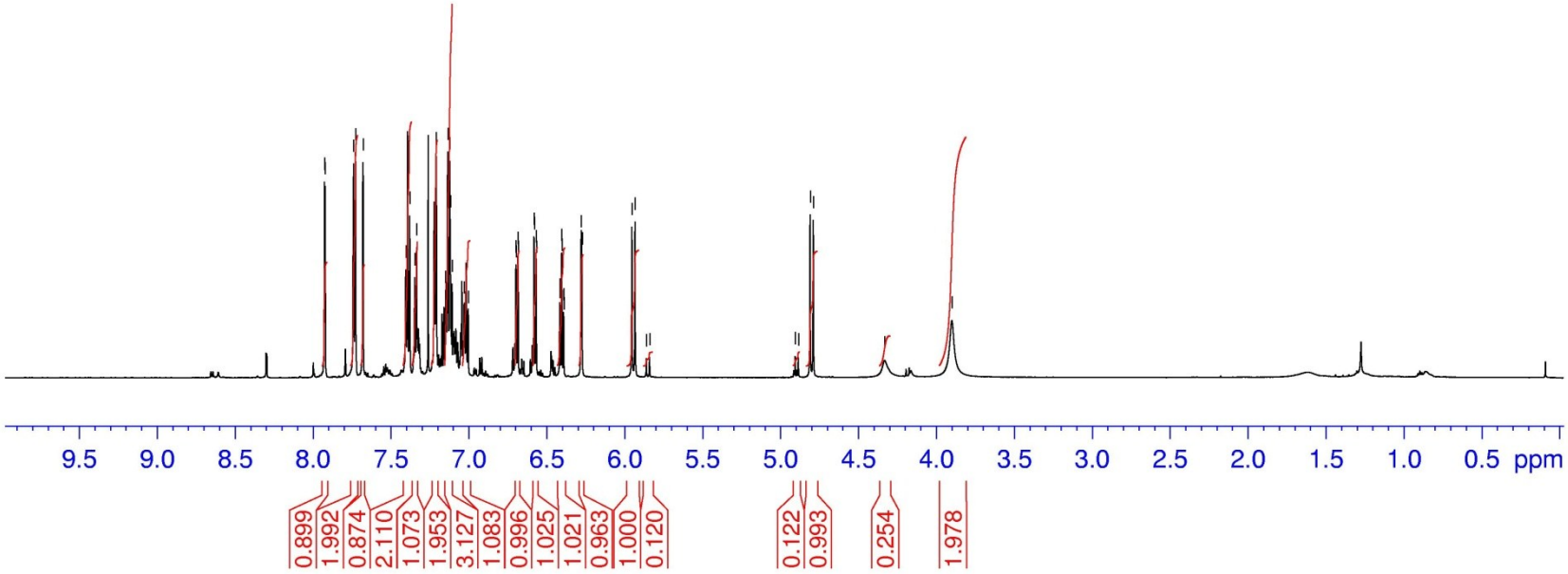


^{1}H NMR in $CDCl_3$ (600 MHz)

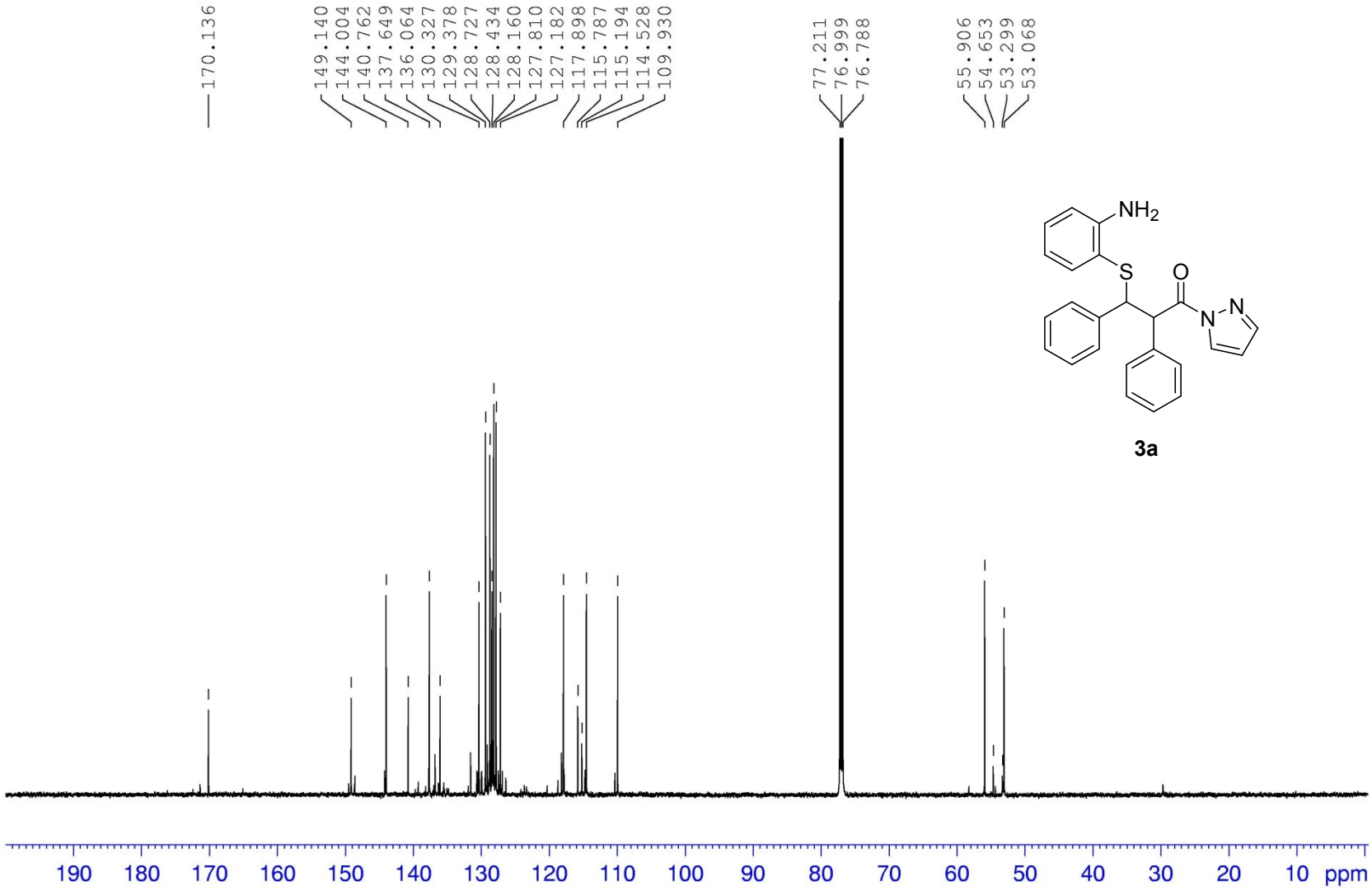




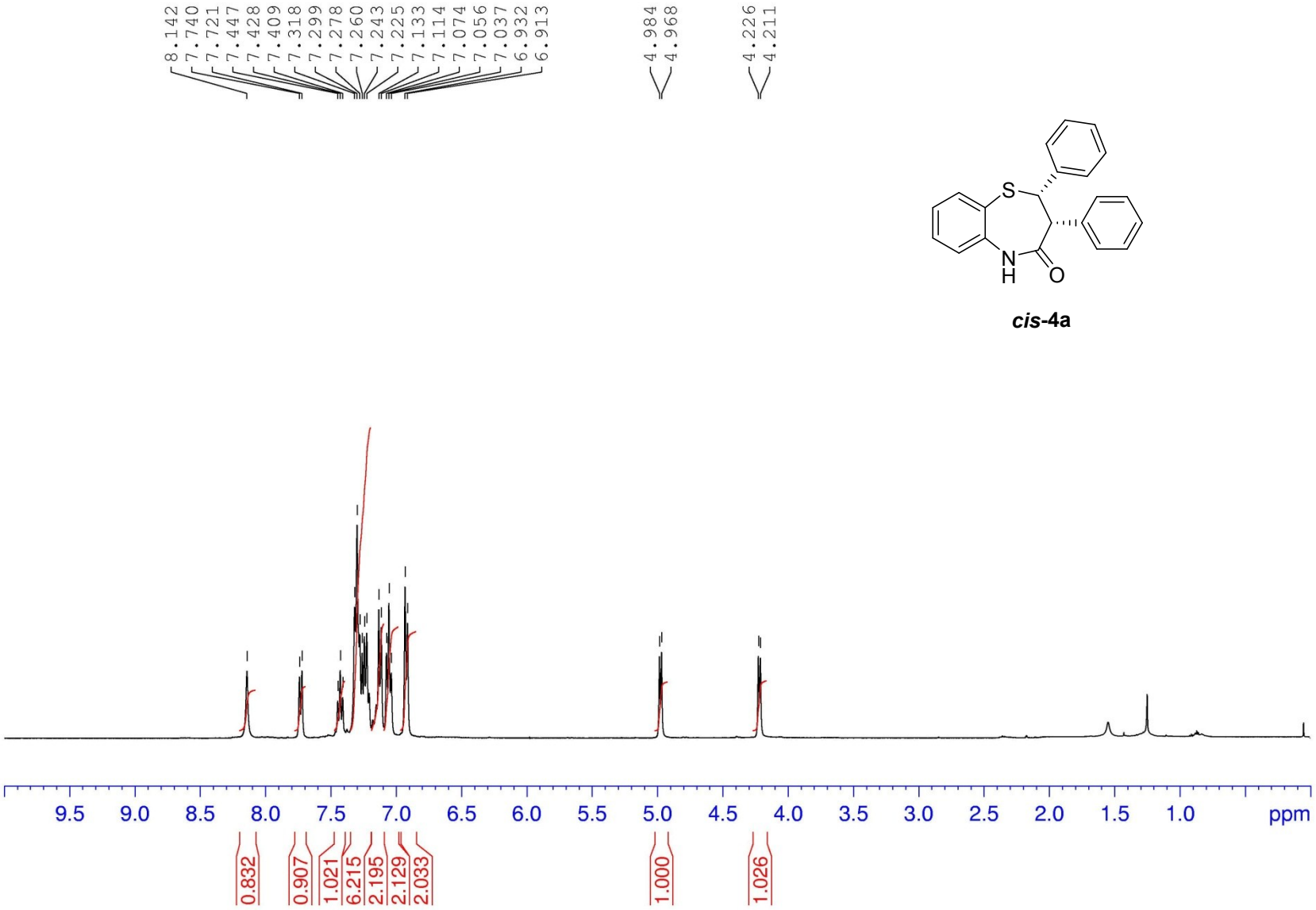
3a



^{13}C NMR in $CDCl_3$ (150 MHz)

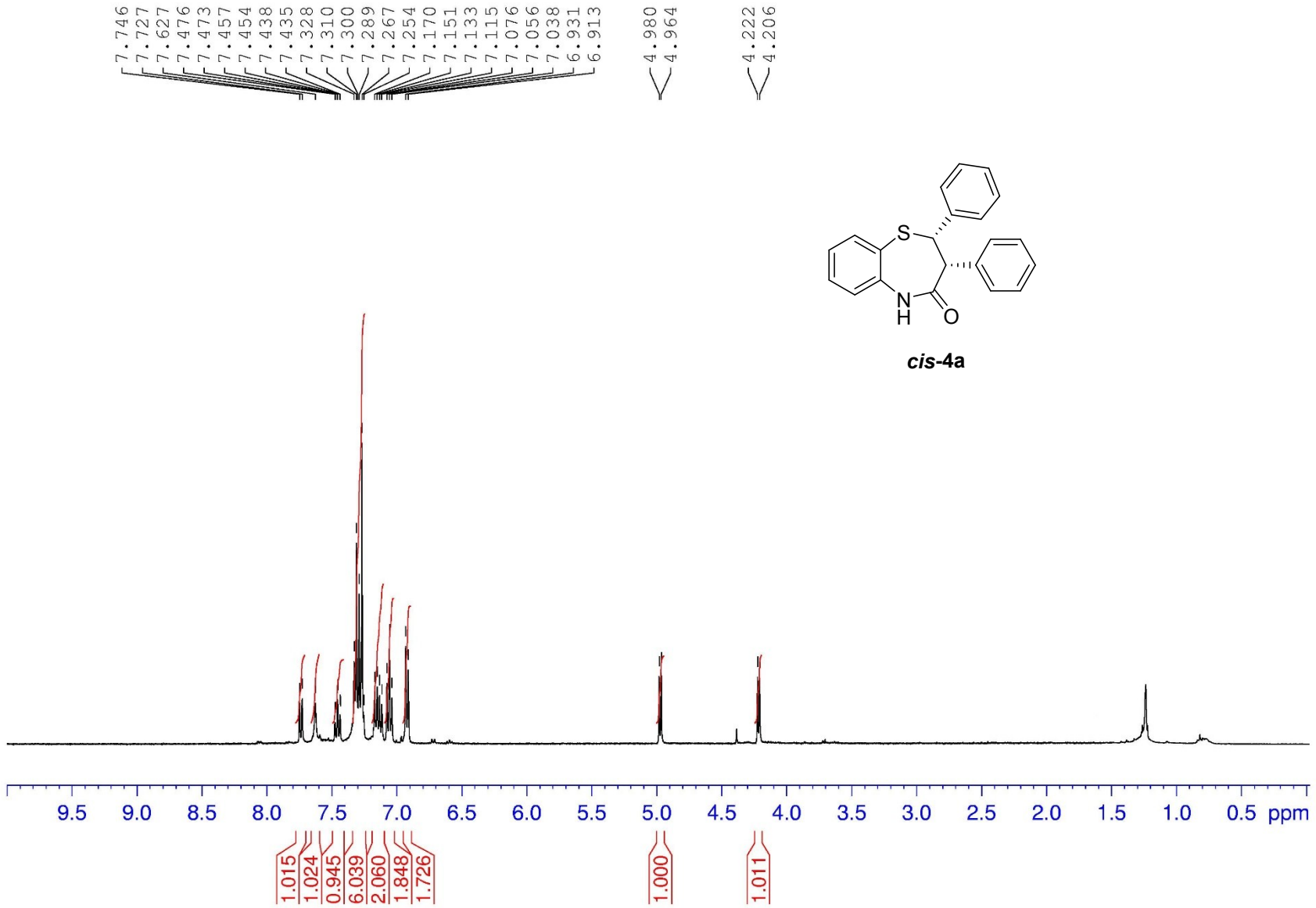


^{1}H NMR in $CDCl_3$ (400 MHz), reaction performed with catalyst **X**



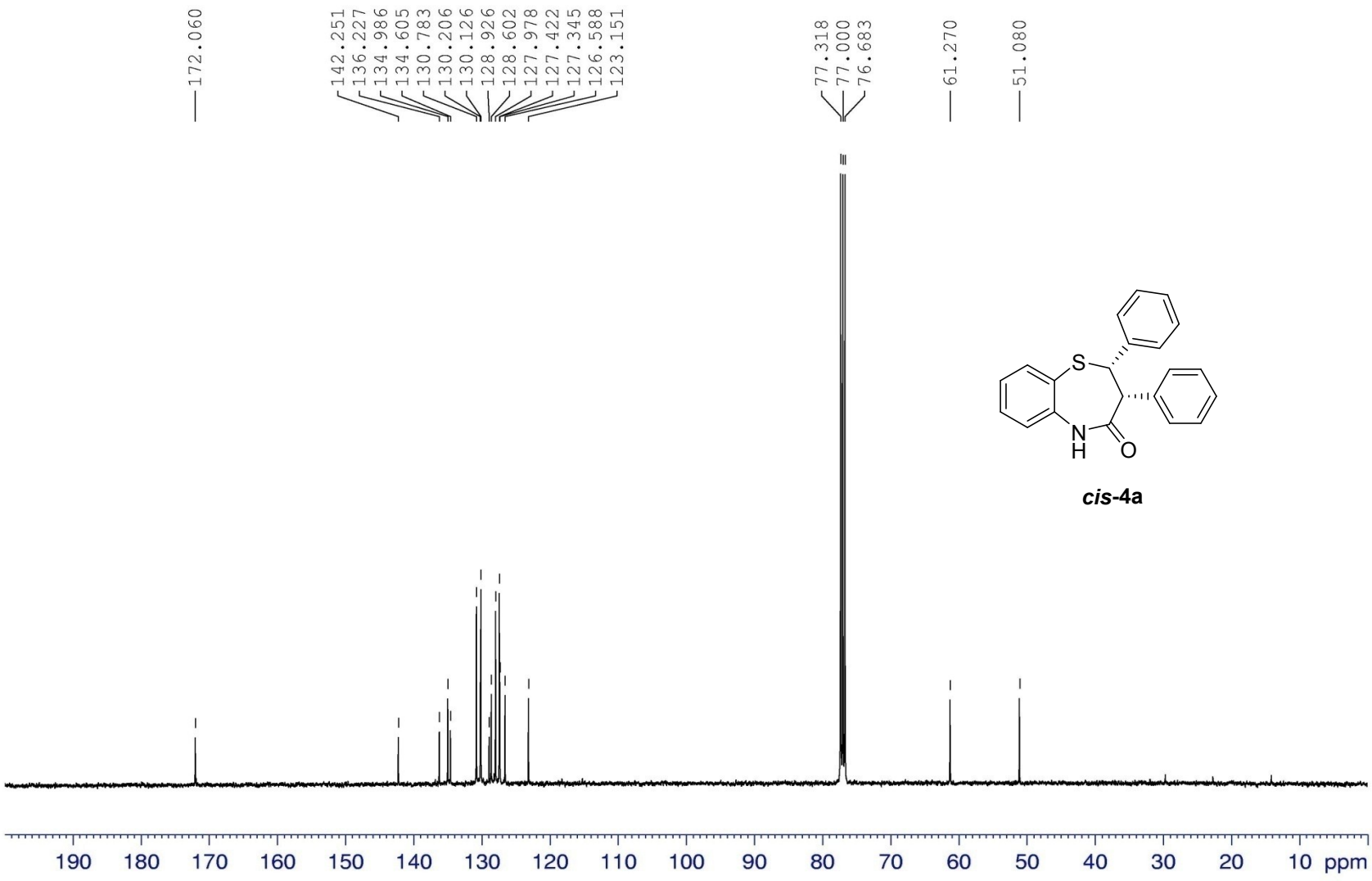
***cis*-4a**

^{1}H NMR in $CDCl_3$ (400 MHz), reaction performed with catalyst **VIII**



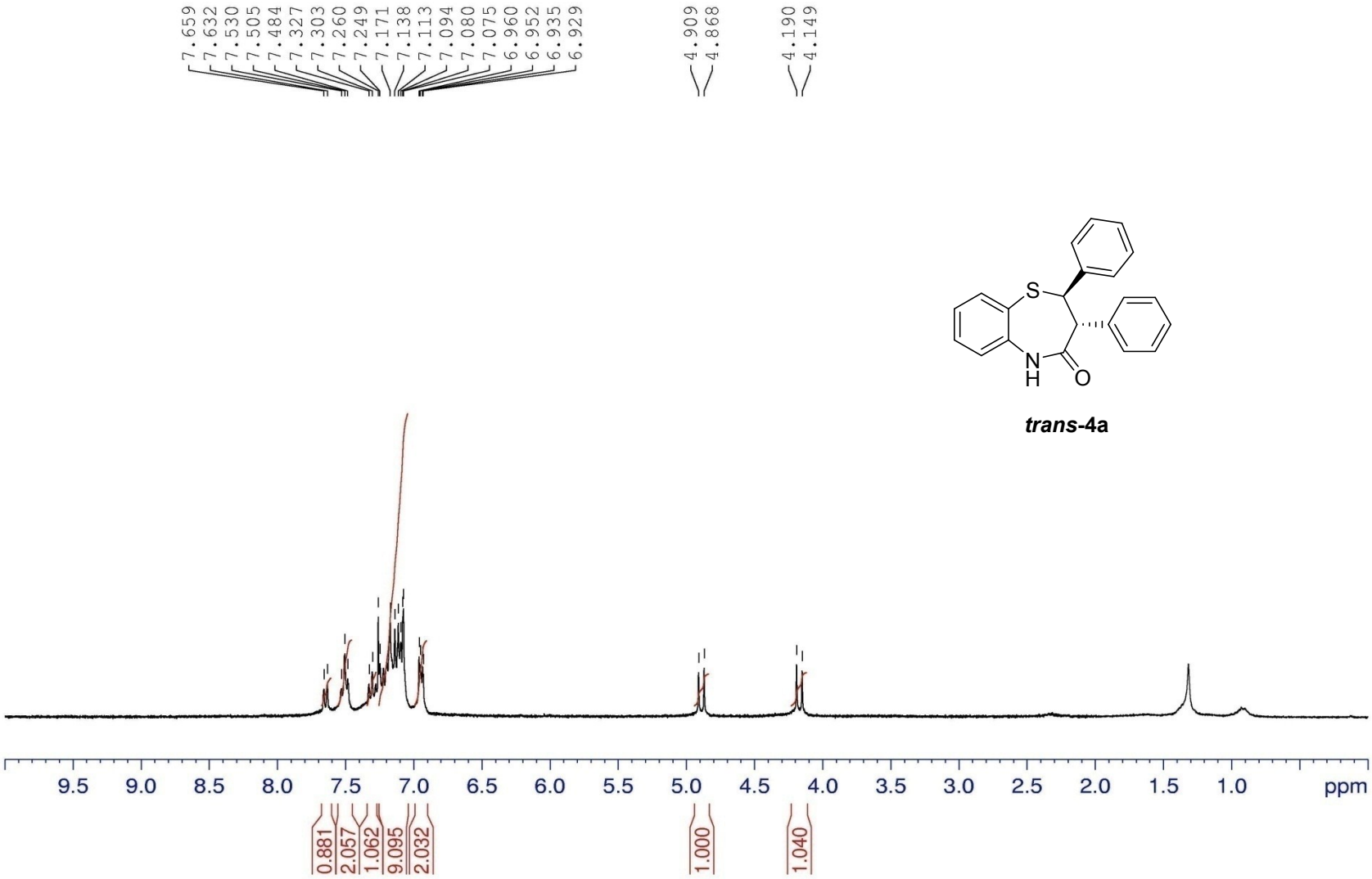
***cis*-4a**

^{13}C NMR in $CDCl_3$ (100 MHz)



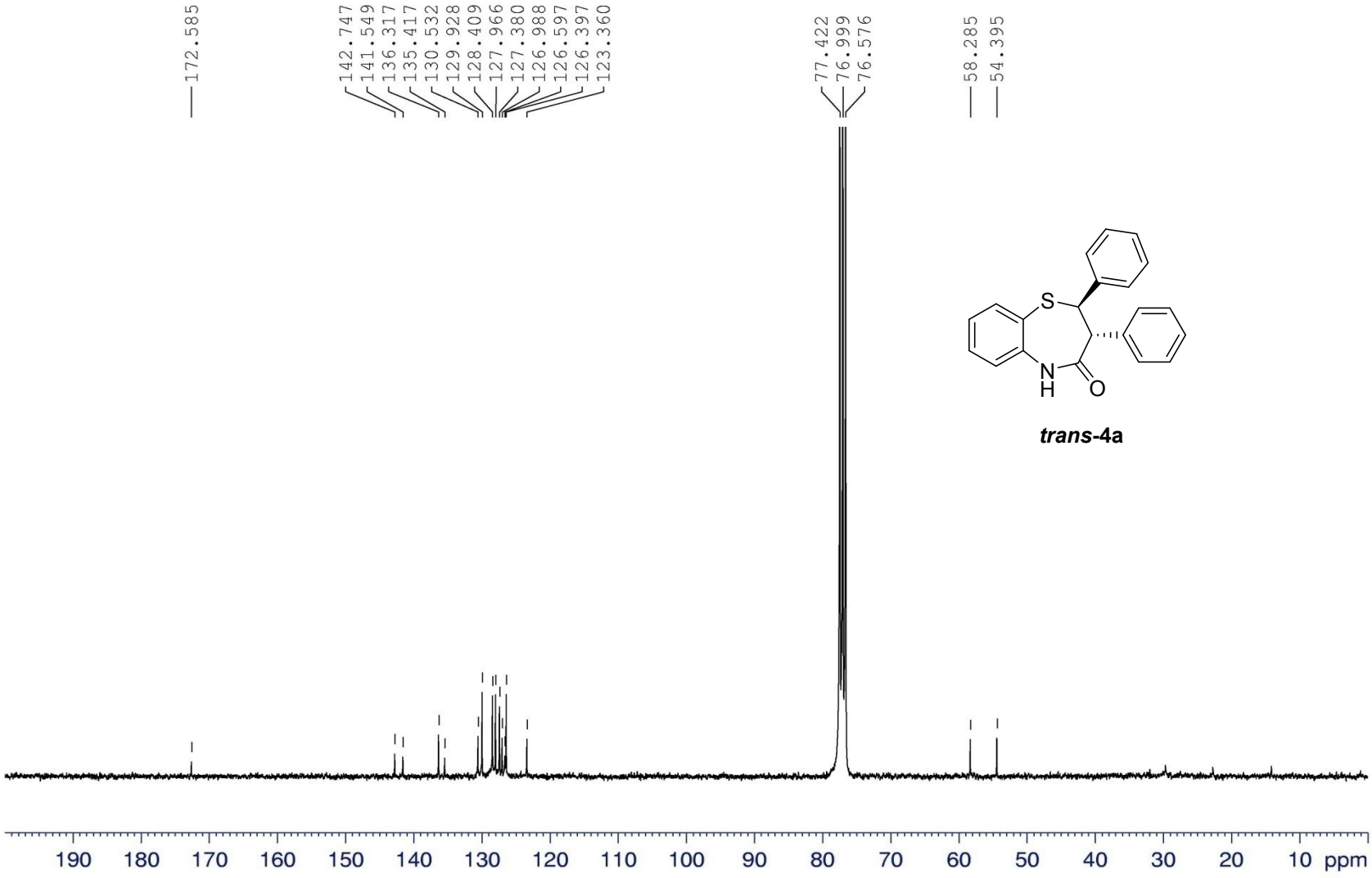
***cis*-4a**

^{1}H NMR in $CDCl_3$ (300 MHz)



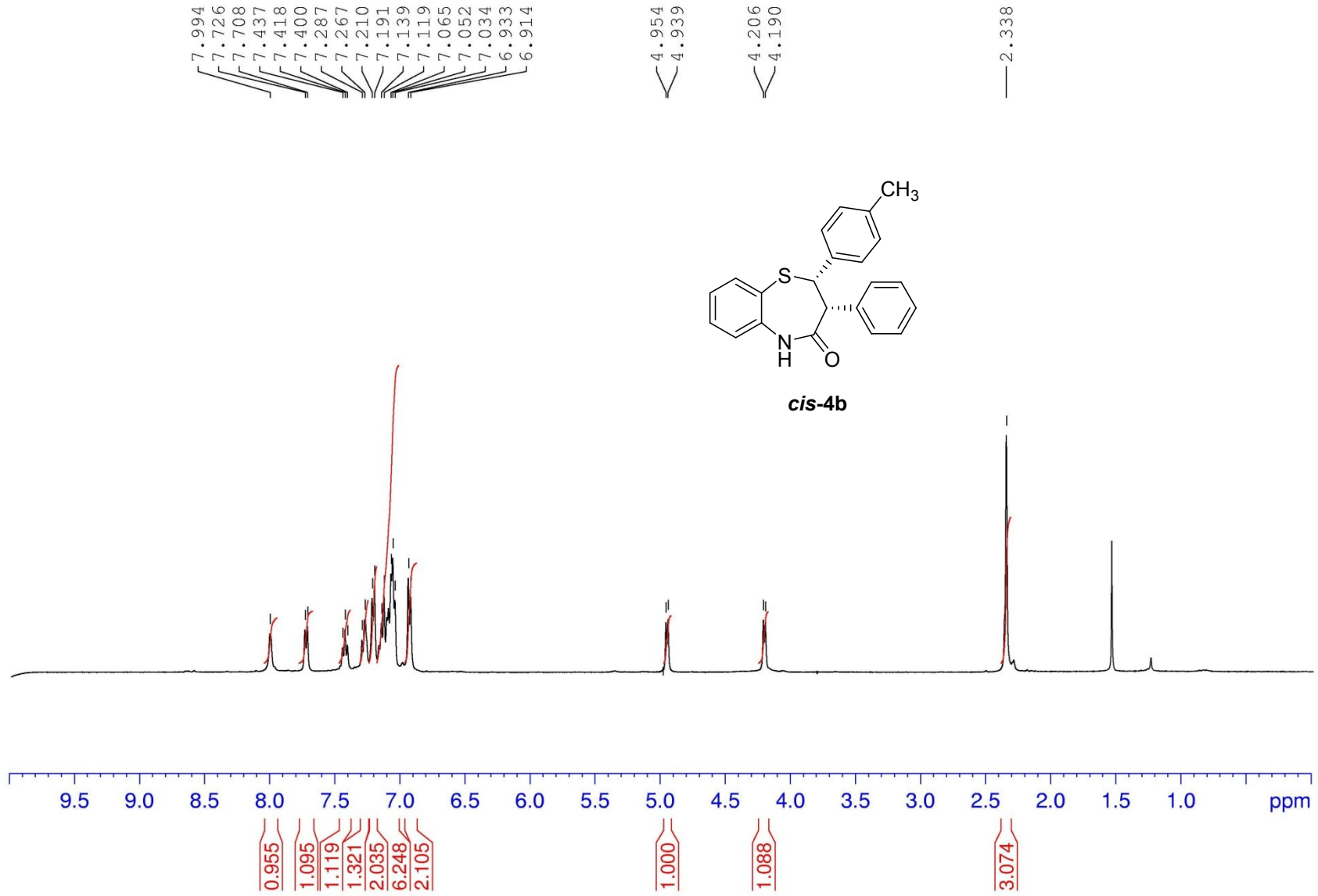
***trans*-4a**

^{13}C NMR in $CDCl_3$ (75 MHz)

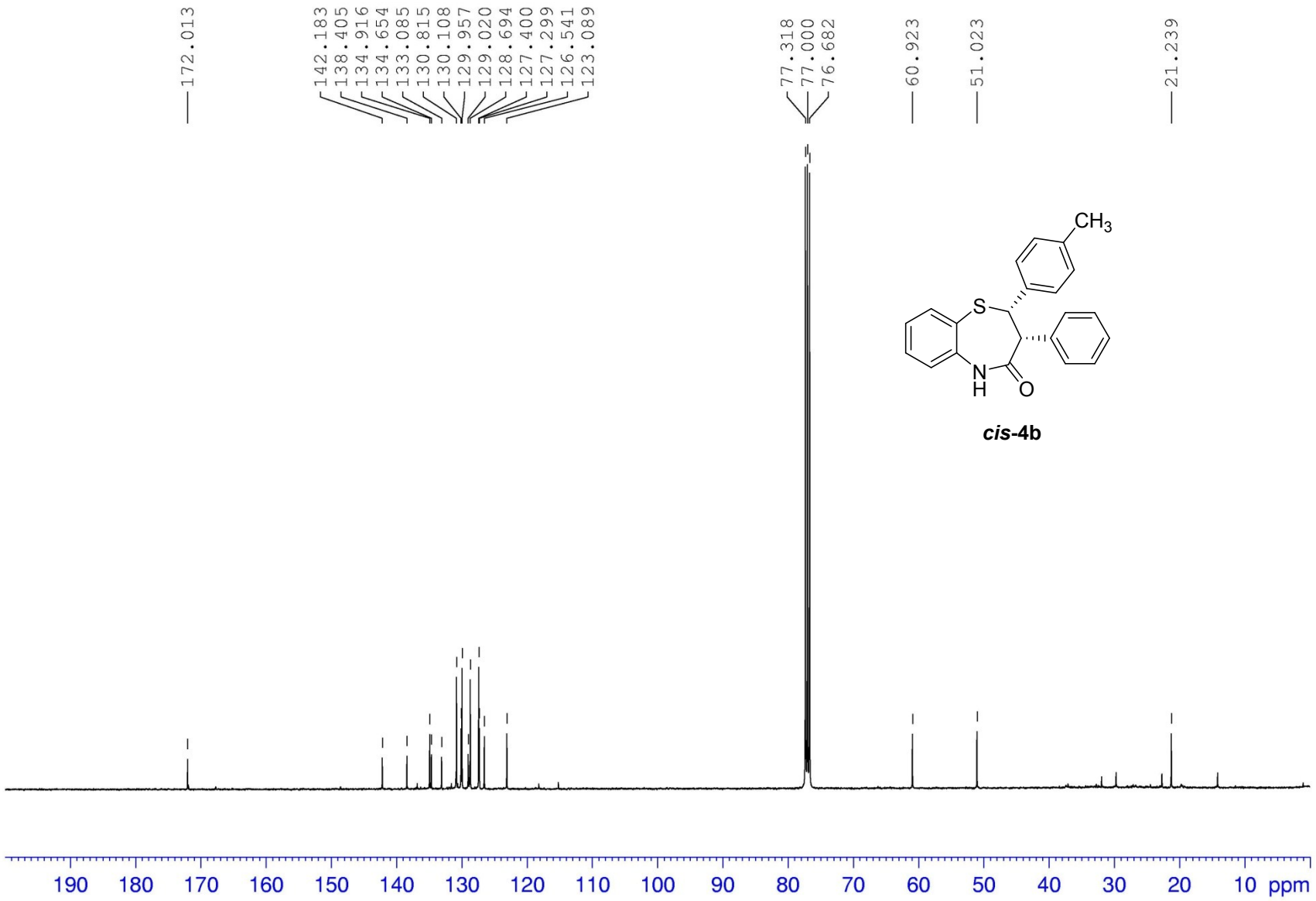


***trans*-4a**

^{1}H NMR in $CDCl_3$ (400 MHz)

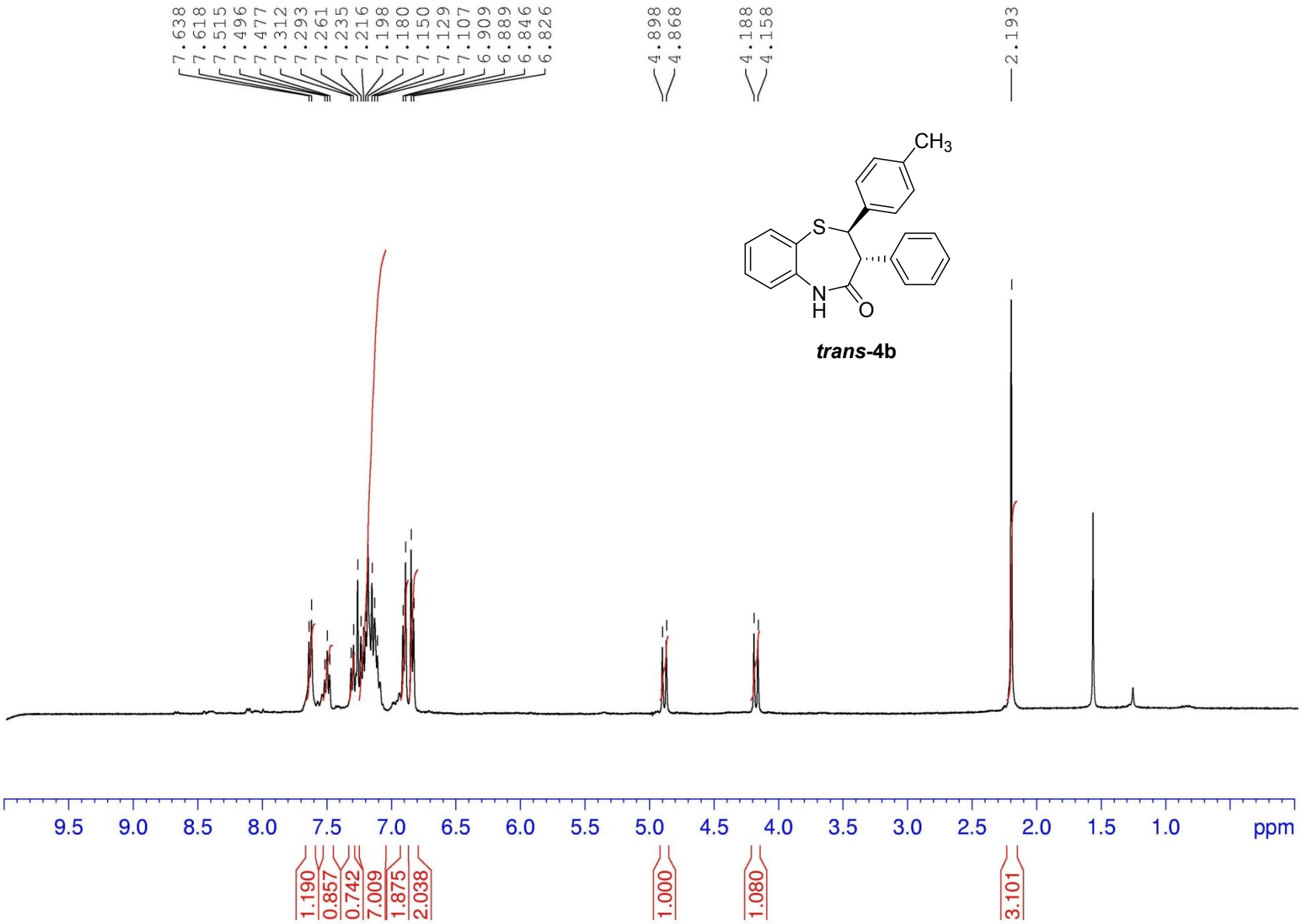


^{13}C NMR in $CDCl_3$ (100 MHz)

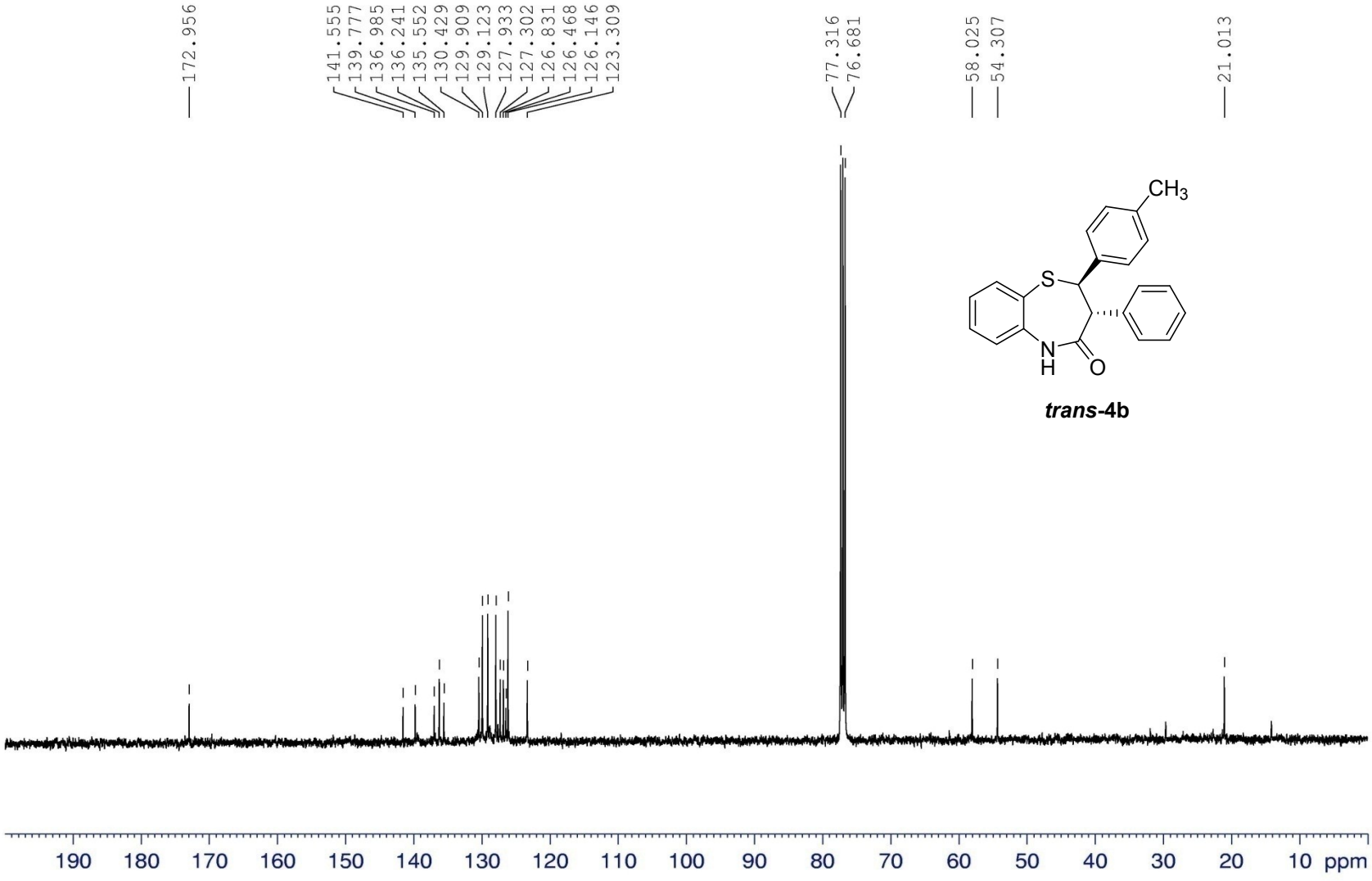


***cis*-4b**

^{1}H NMR in $CDCl_3$ (400 MHz)



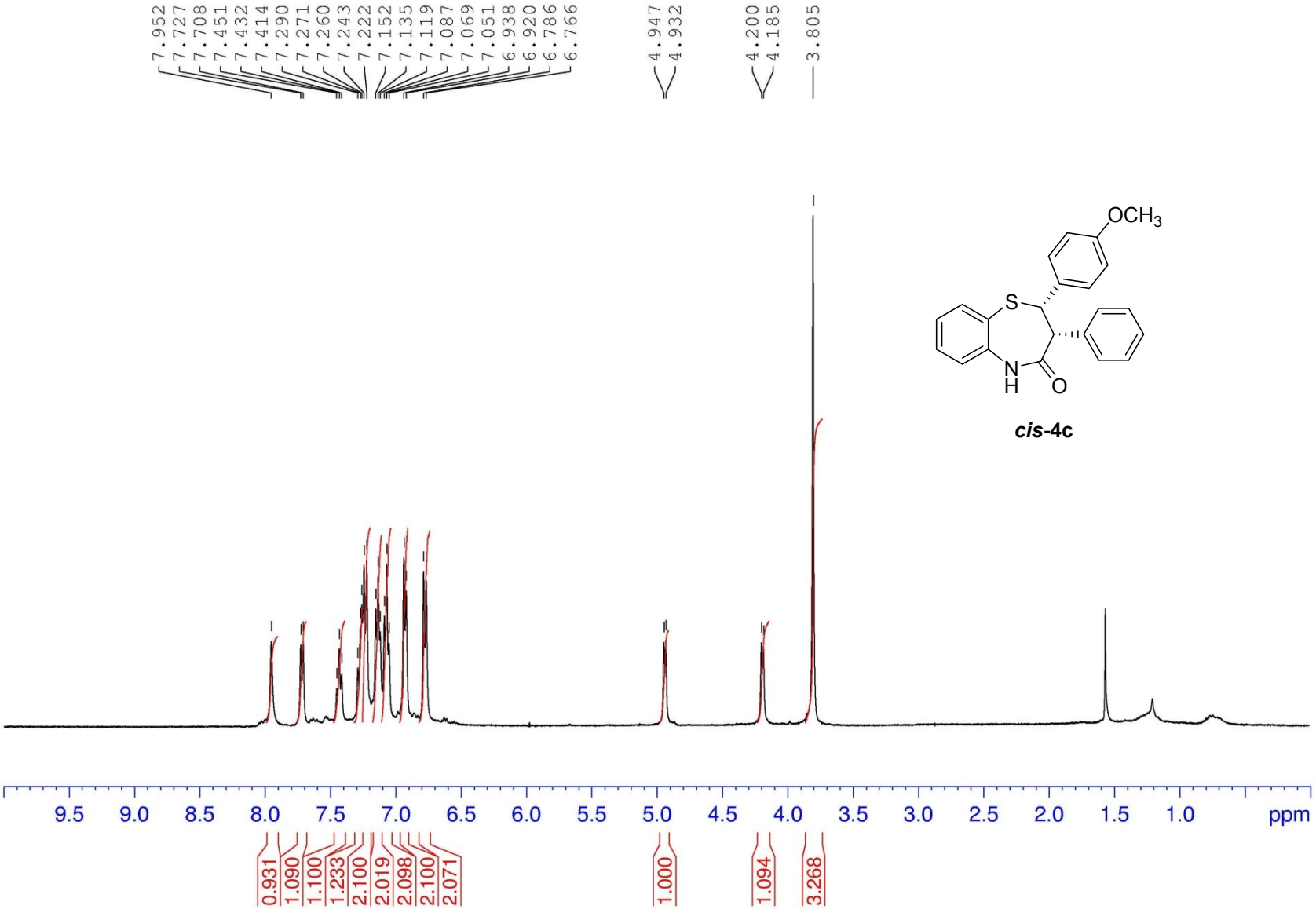
^{13}C NMR in $CDCl_3$ (100 MHz)



***trans*-4b**

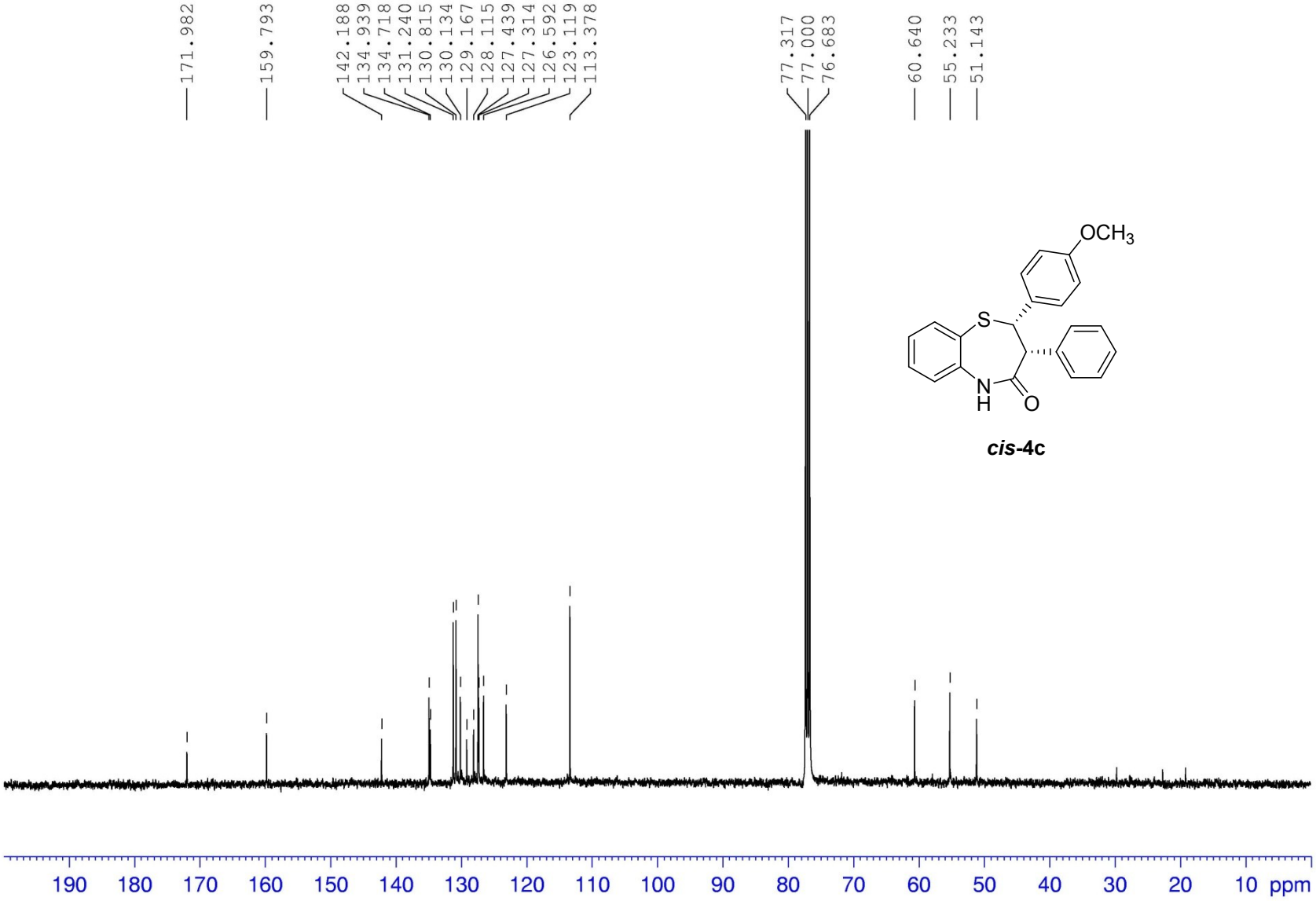
v

^{1}H NMR in $CDCl_3$ (400 MHz)



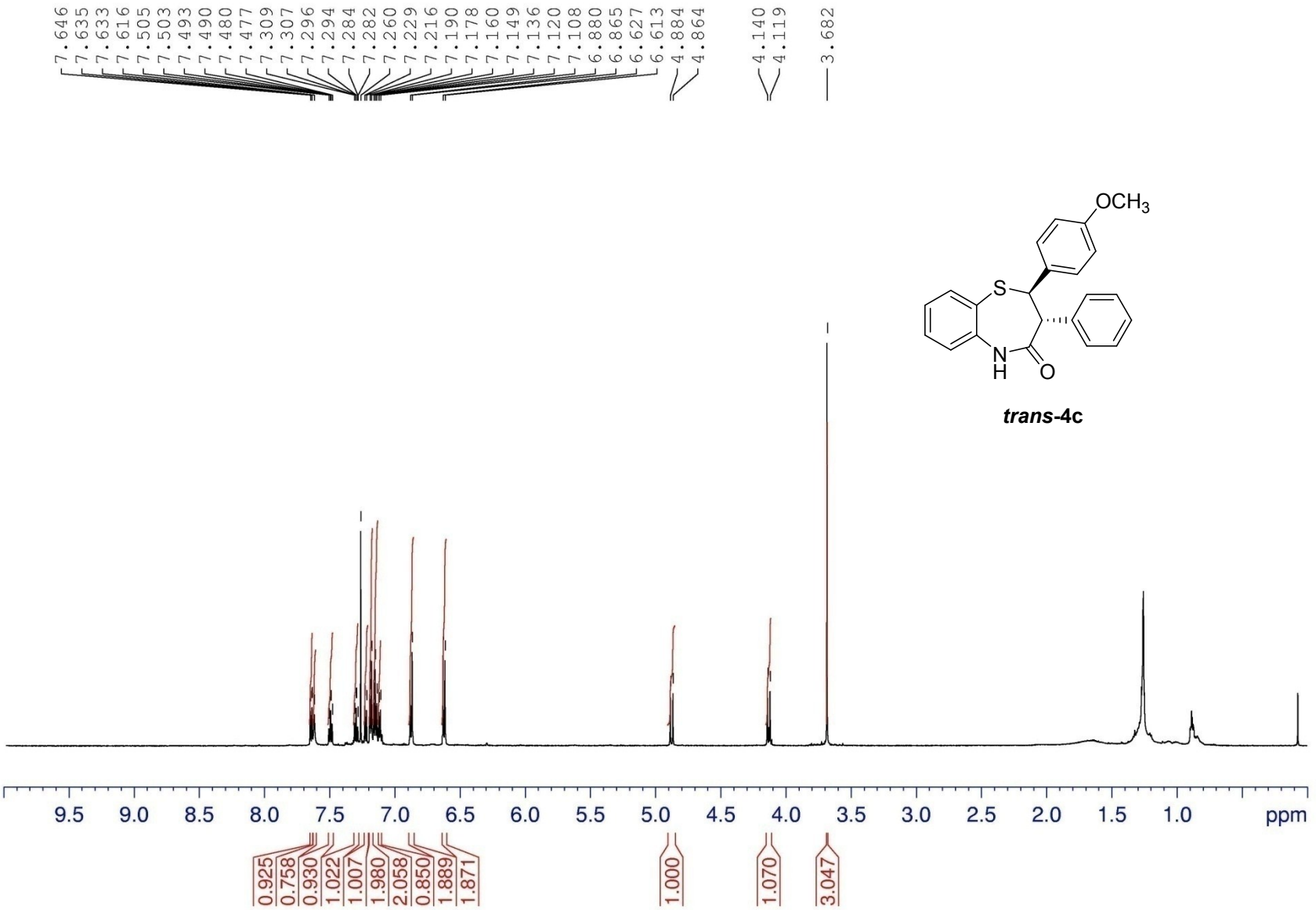
***cis*-4c**

^{13}C NMR in $CDCl_3$ (100 MHz)

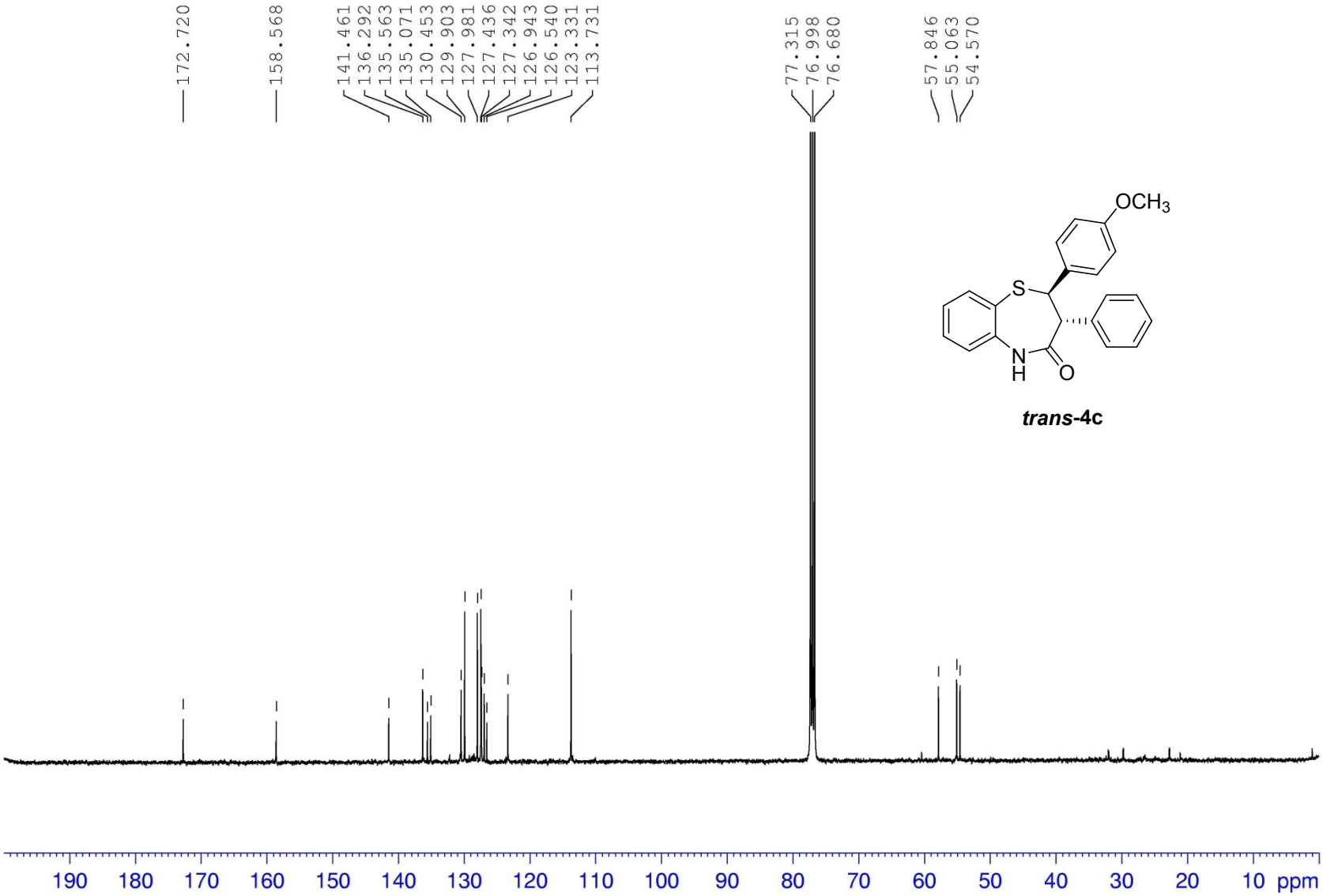


***cis*-4c**

^{1}H NMR in $CDCl_3$ (600 MHz)

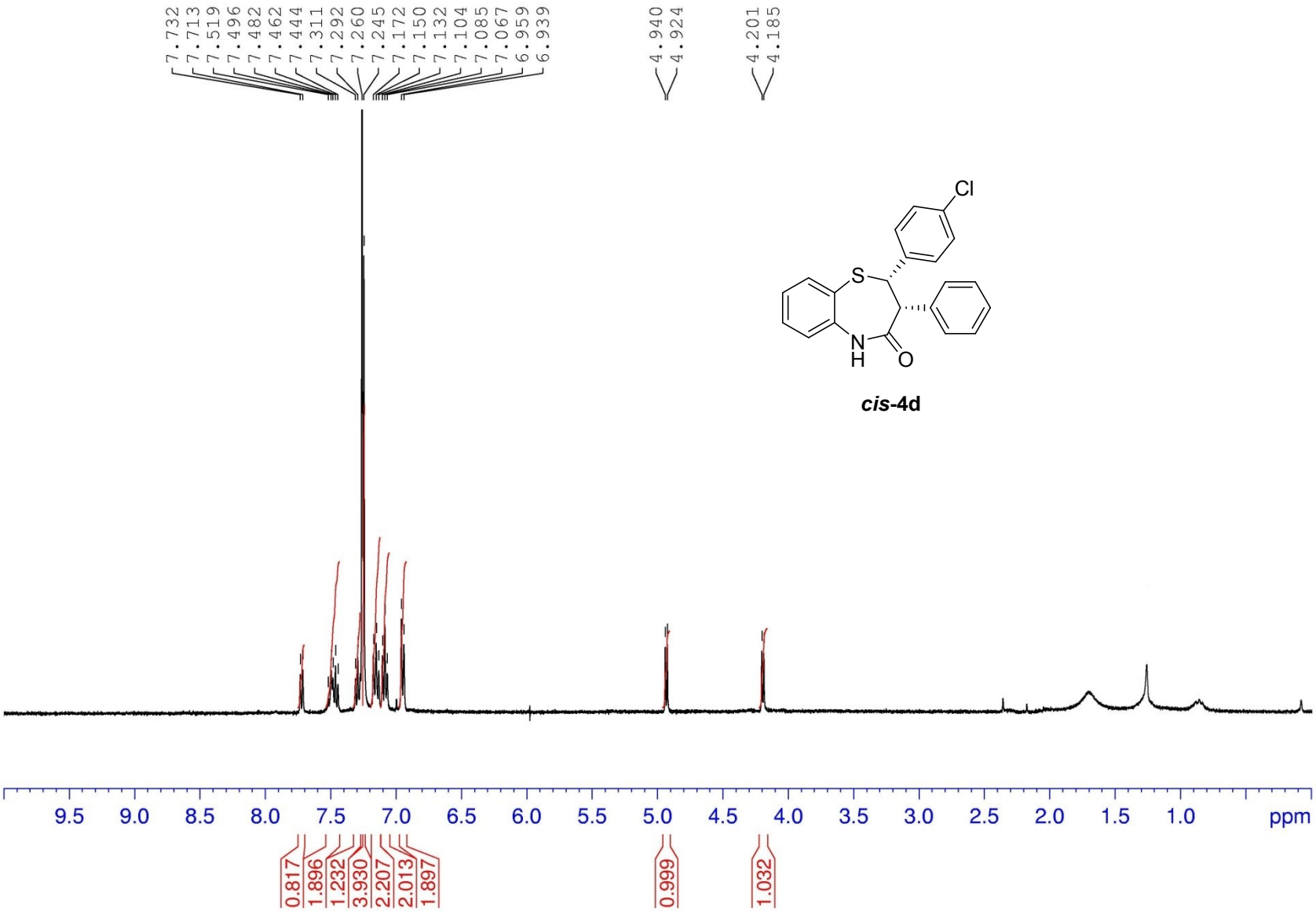


^{13}C NMR in $CDCl_3$ (100 MHz)



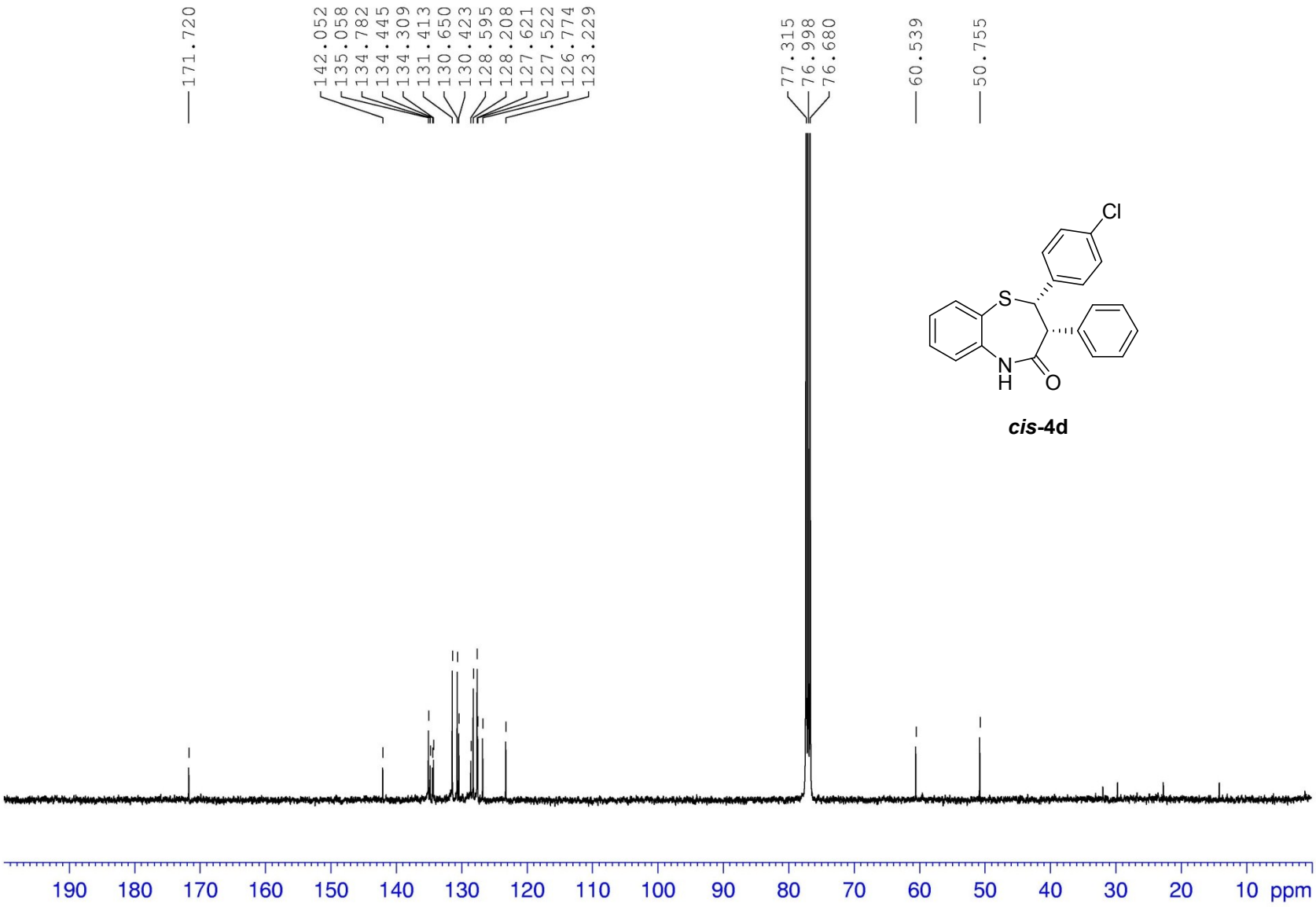
***trans*-4c**

^{1}H NMR in $CDCl_3$ (400 MHz)



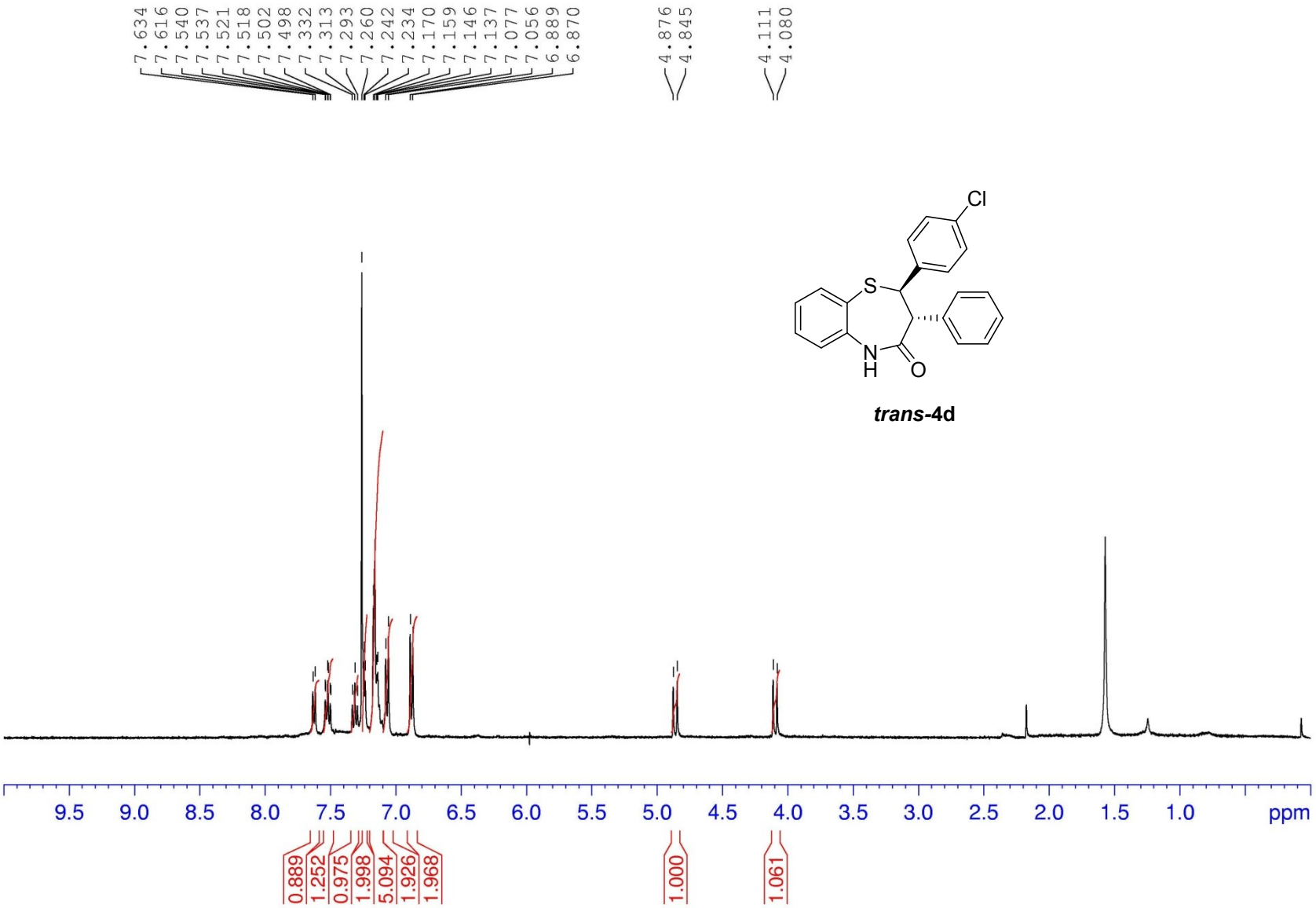
***cis*-4d**

^{13}C NMR in $CDCl_3$ (100 MHz)



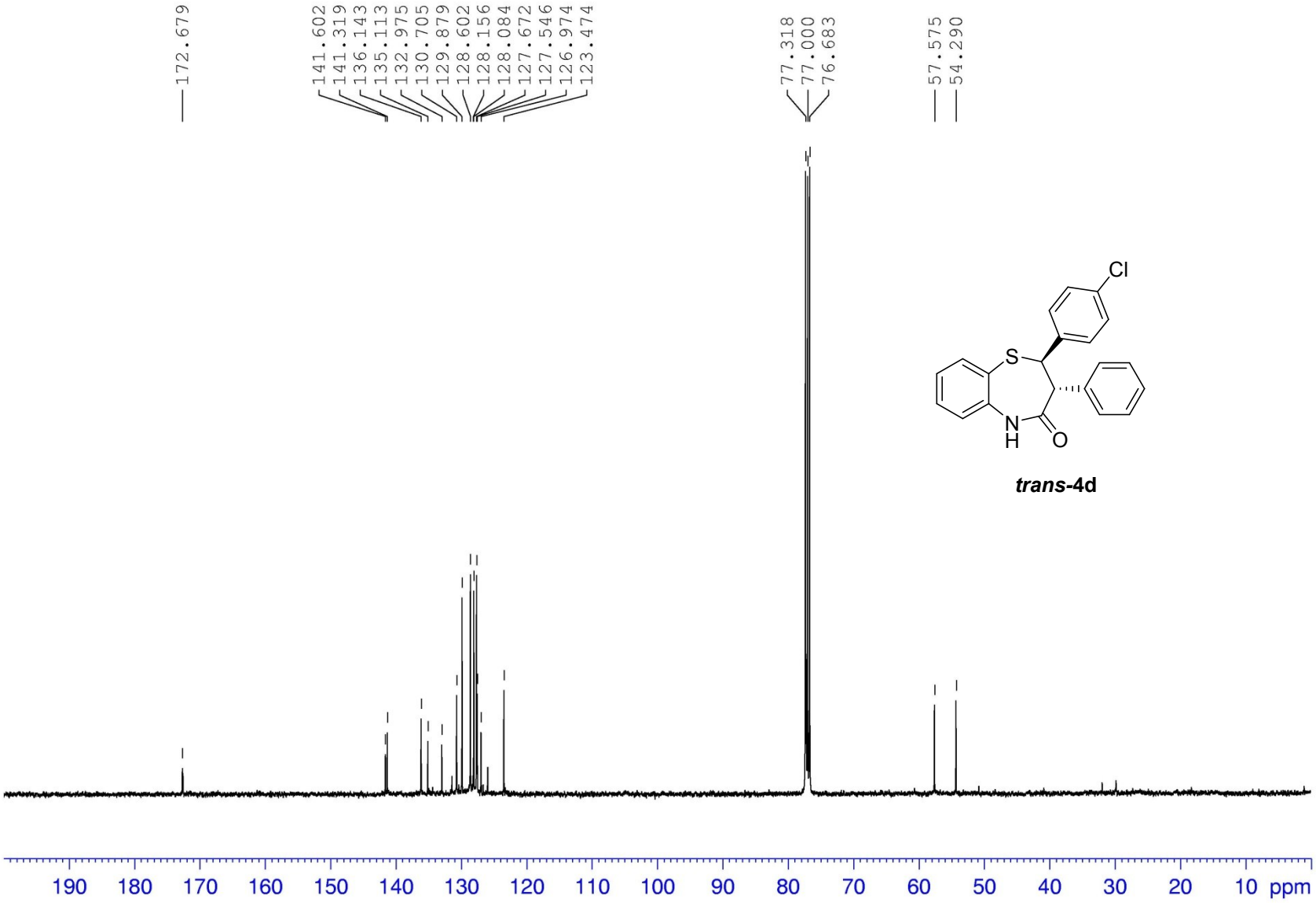
***cis*-4d**

^{1}H NMR in $CDCl_3$ (400 MHz)



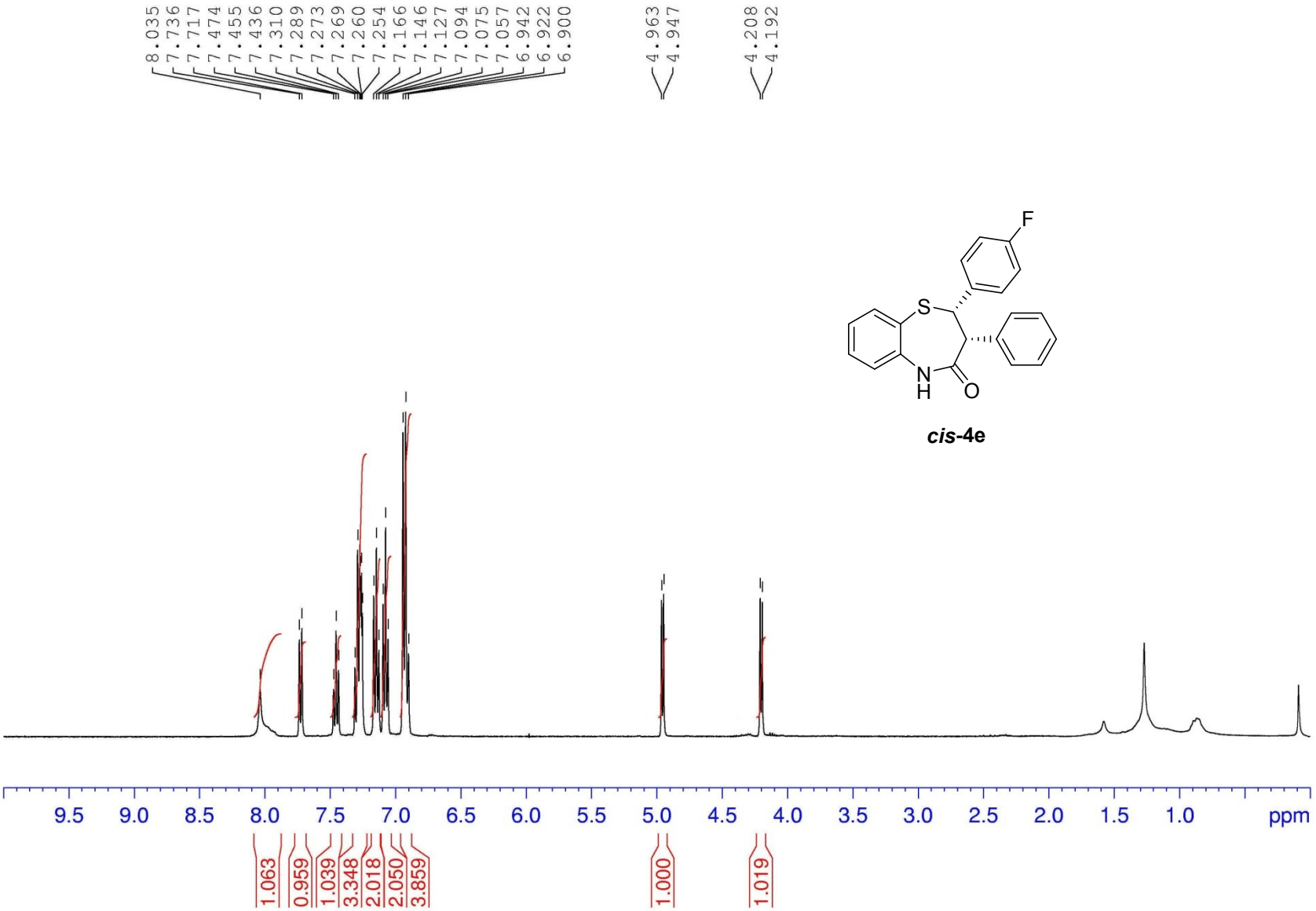
***trans*-4d**

^{13}C NMR in $CDCl_3$ (100 MHz)



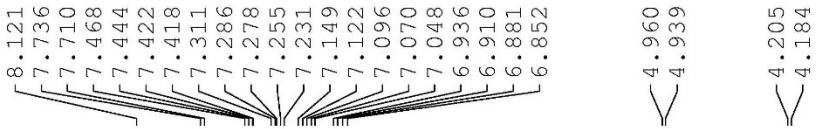
***trans*-4d**

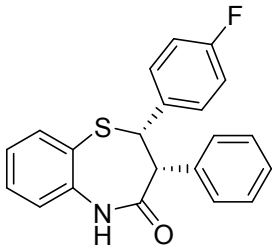
^{1}H NMR in $CDCl_3$ (400 MHz), reaction performed with catalyst **X**



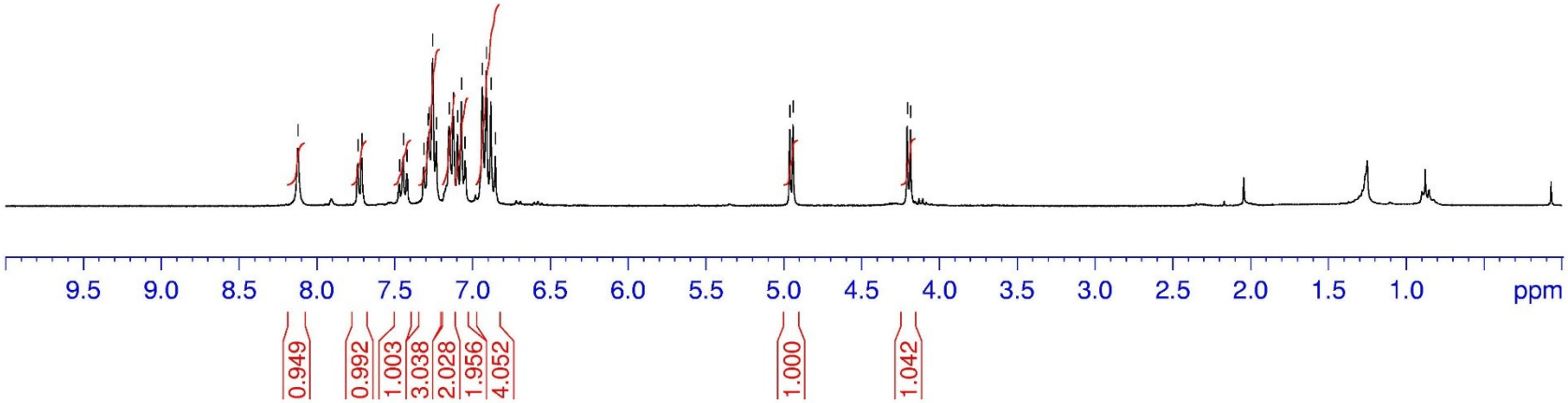
***cis*-4e**

^{1}H NMR in $CDCl_3$ (300 MHz), reaction performed with catalyst **VIII**

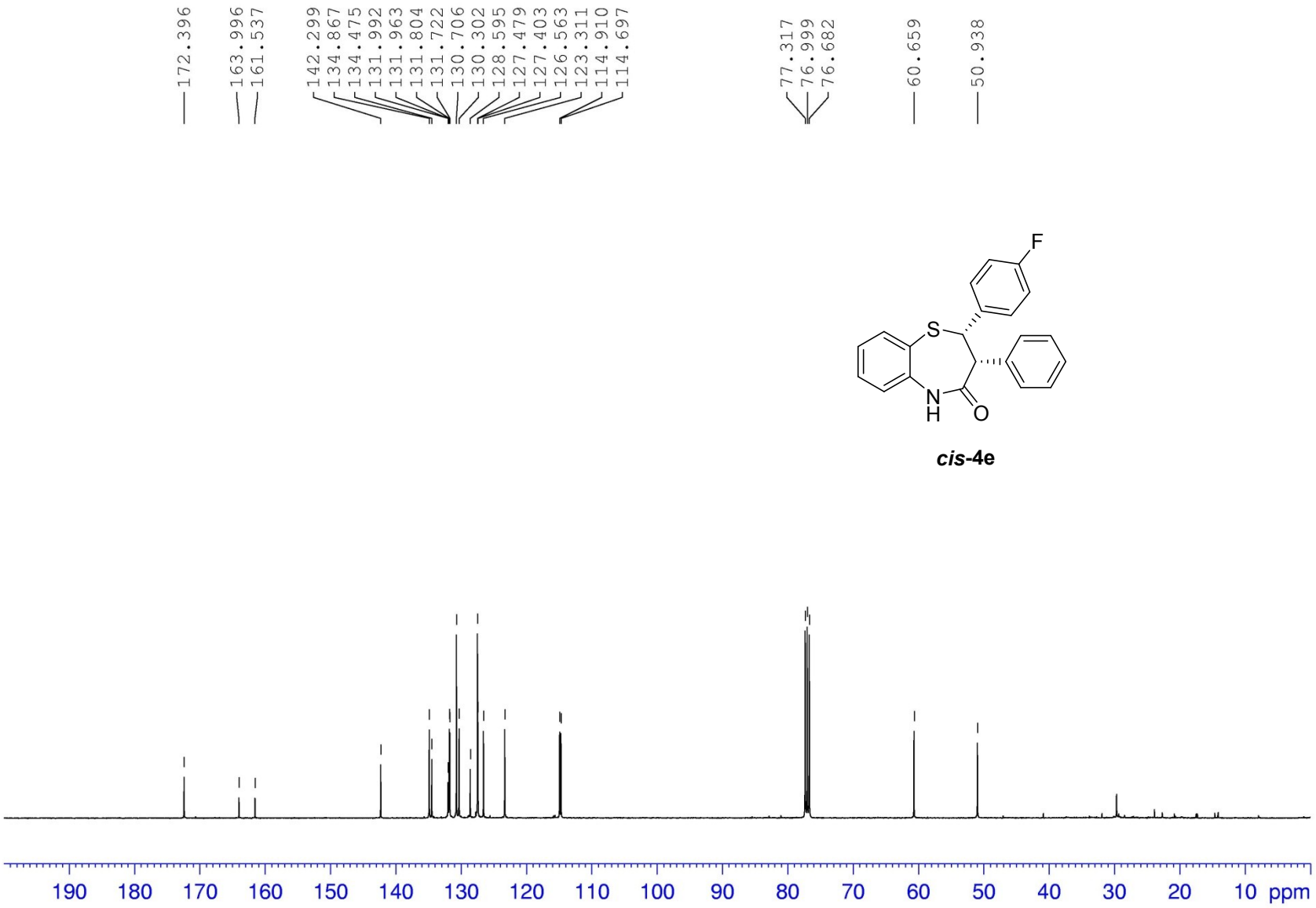




***cis*-4e**

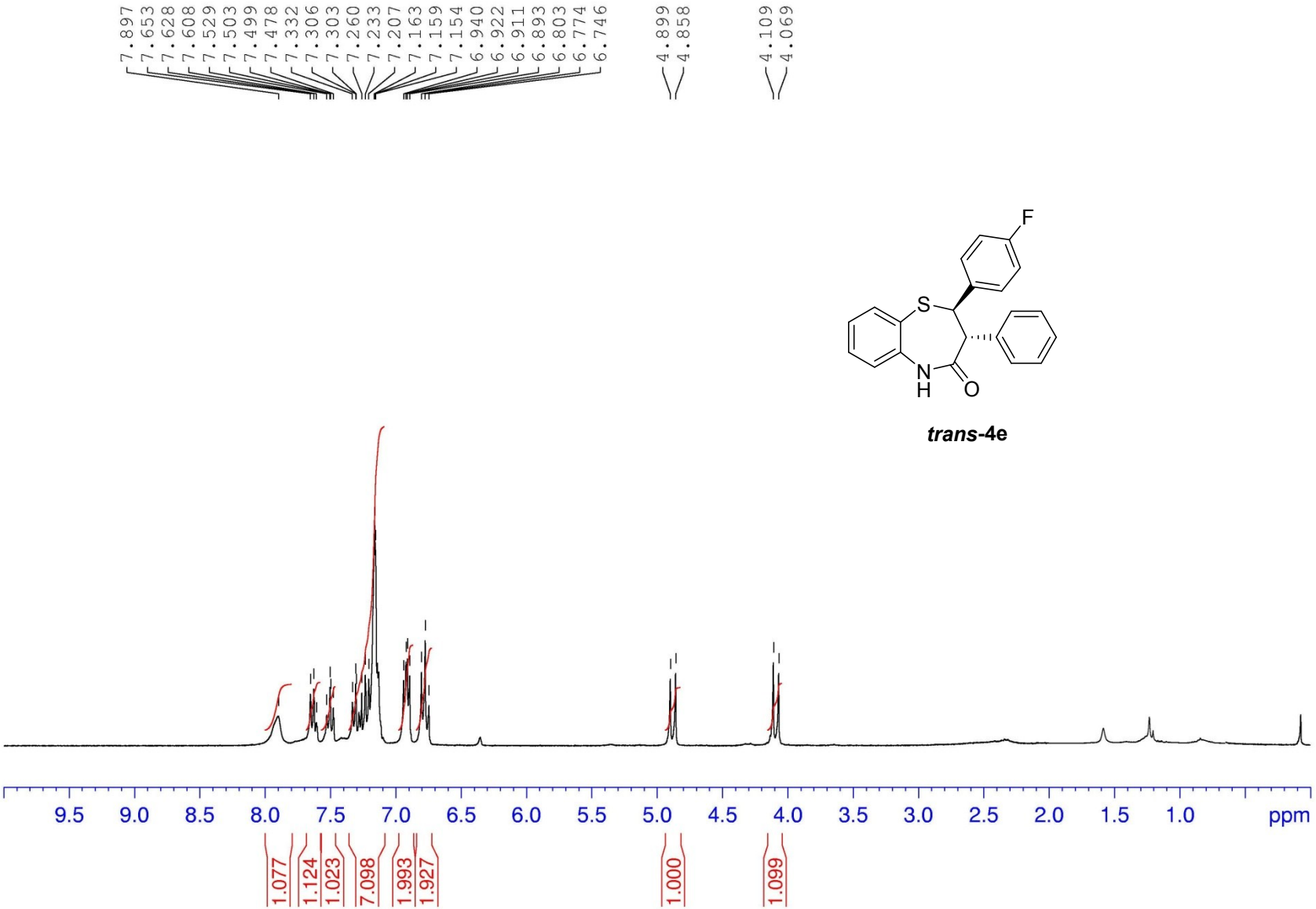


^{13}C NMR in $CDCl_3$ (100 MHz)



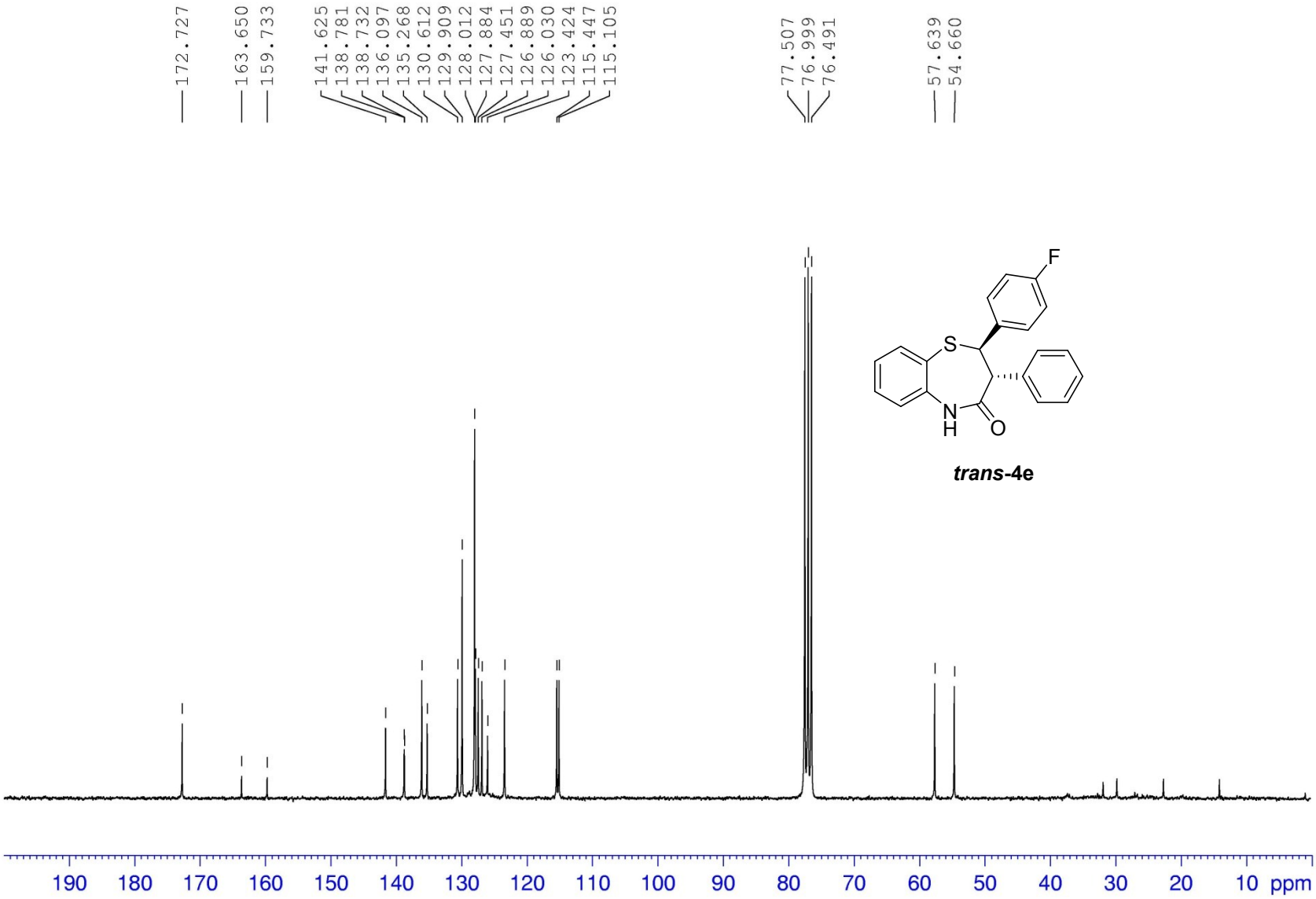
***cis*-4e**

^{1}H NMR in $CDCl_3$ (300 MHz)

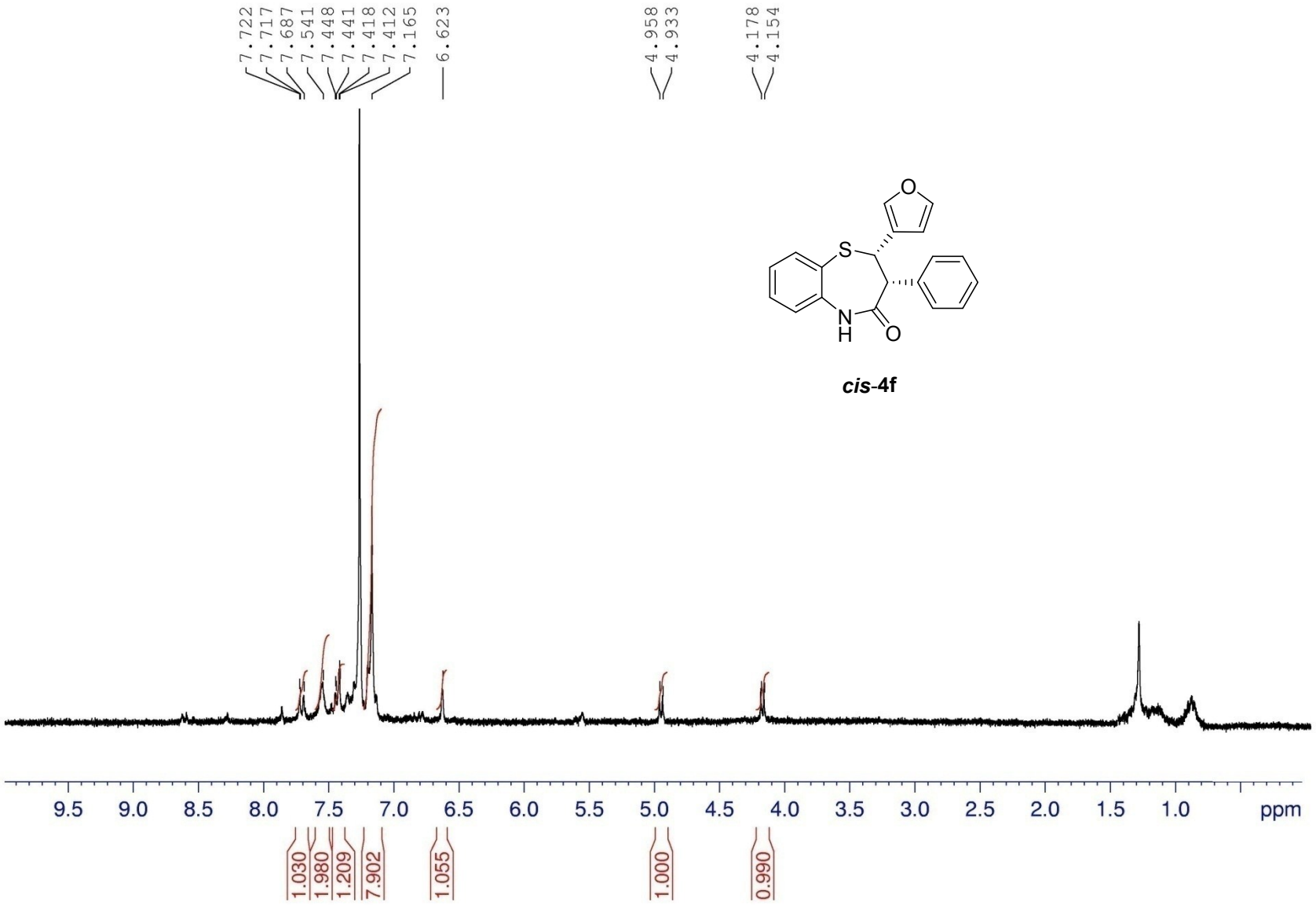


***trans*-4e**

^{13}C NMR in $CDCl_3$ (62.5 MHz)

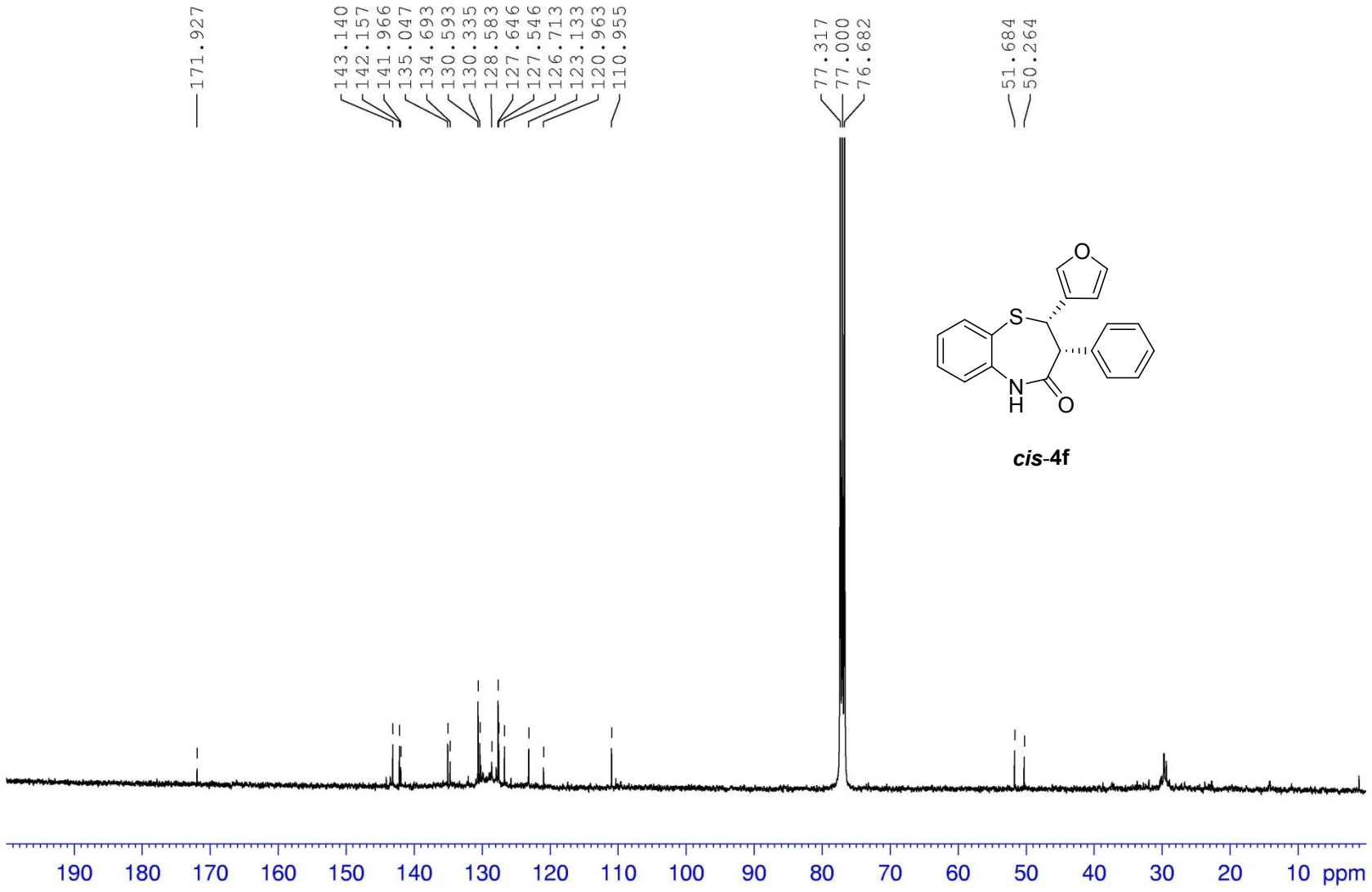


^{1}H NMR in $CDCl_3$ (250 MHz)



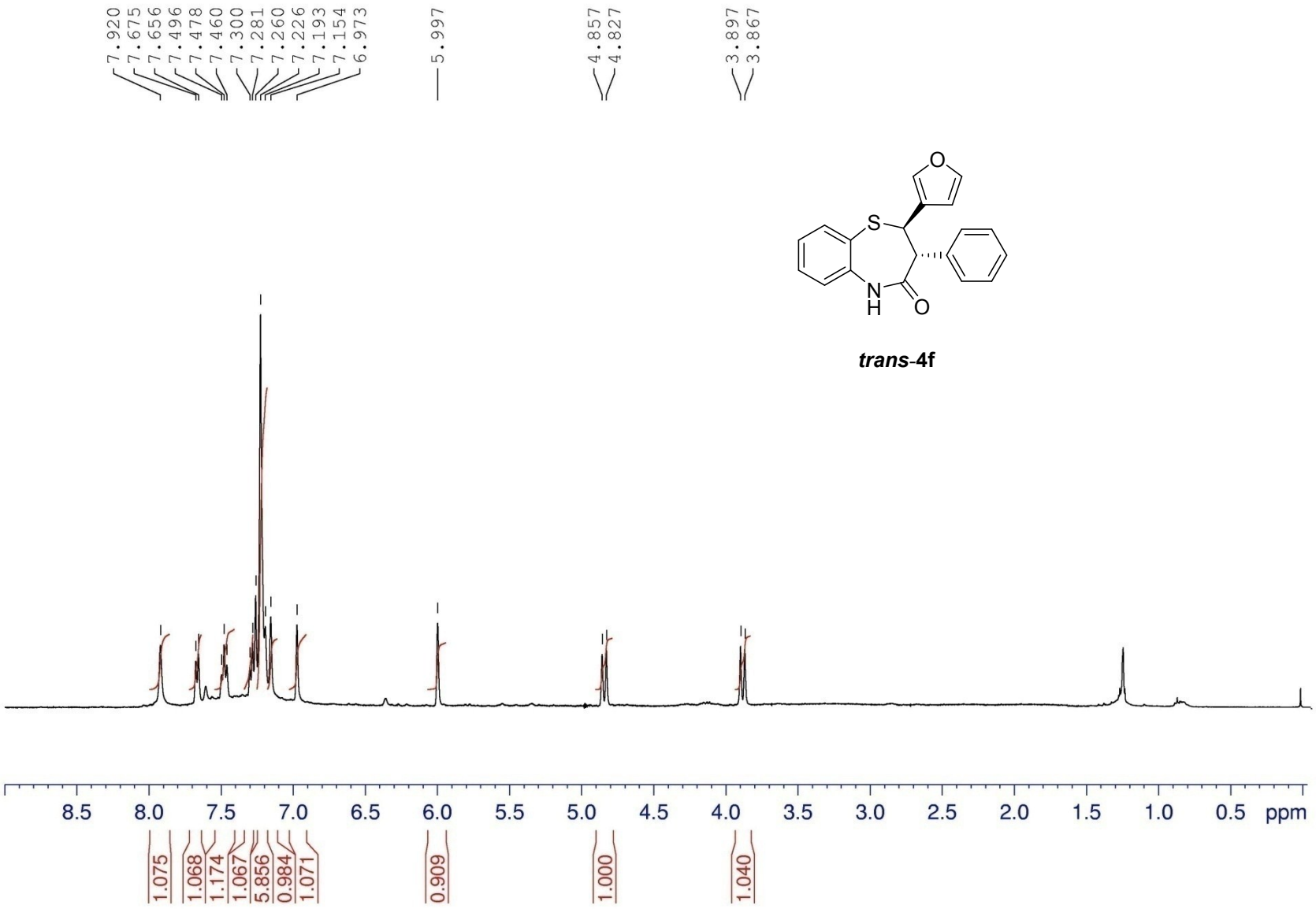
***cis*-4f**

^{13}C NMR in $CDCl_3$ (100 MHz)



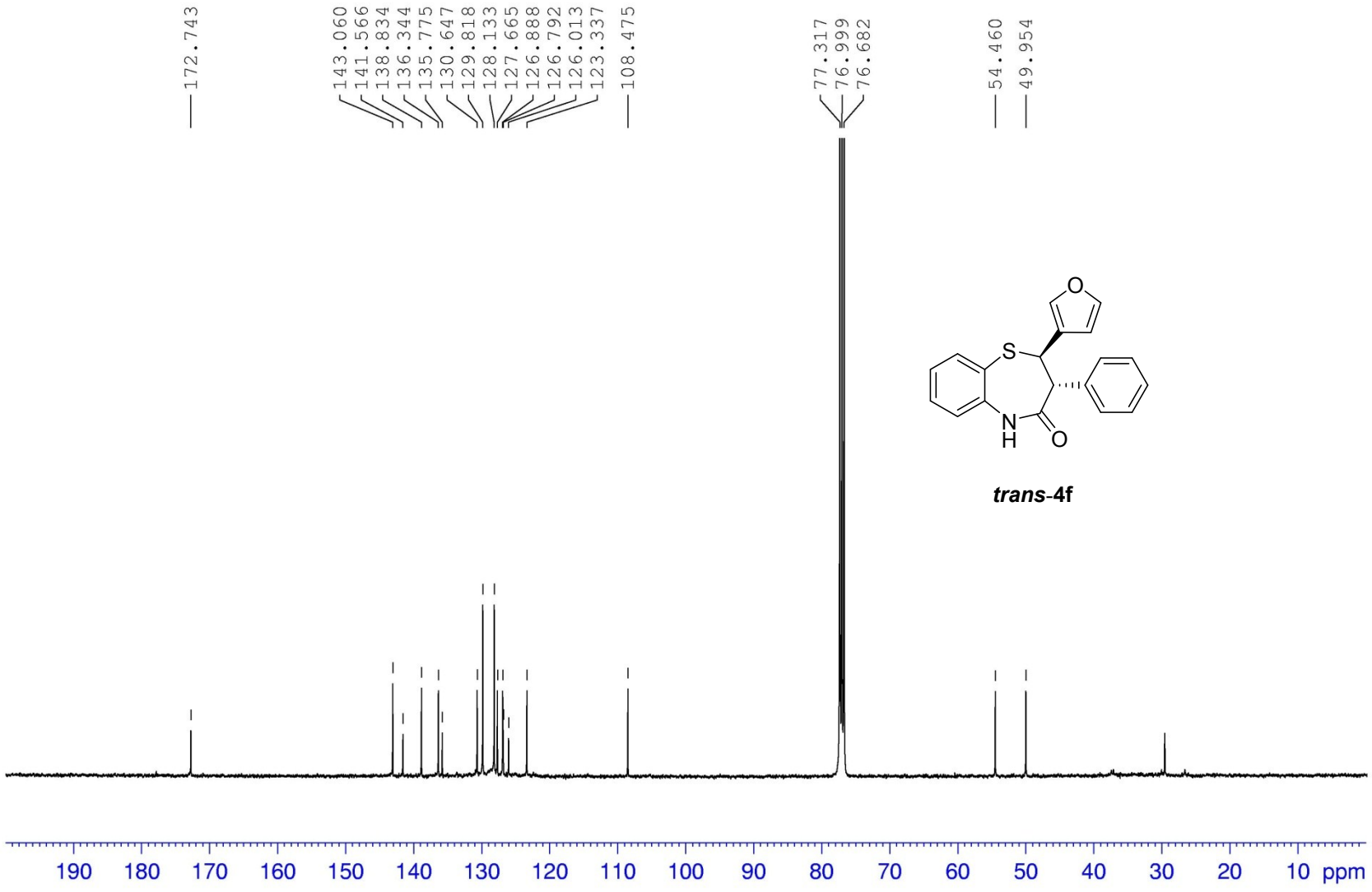
***cis*-4f**

^{1}H NMR in $CDCl_3$ (400 MHz)



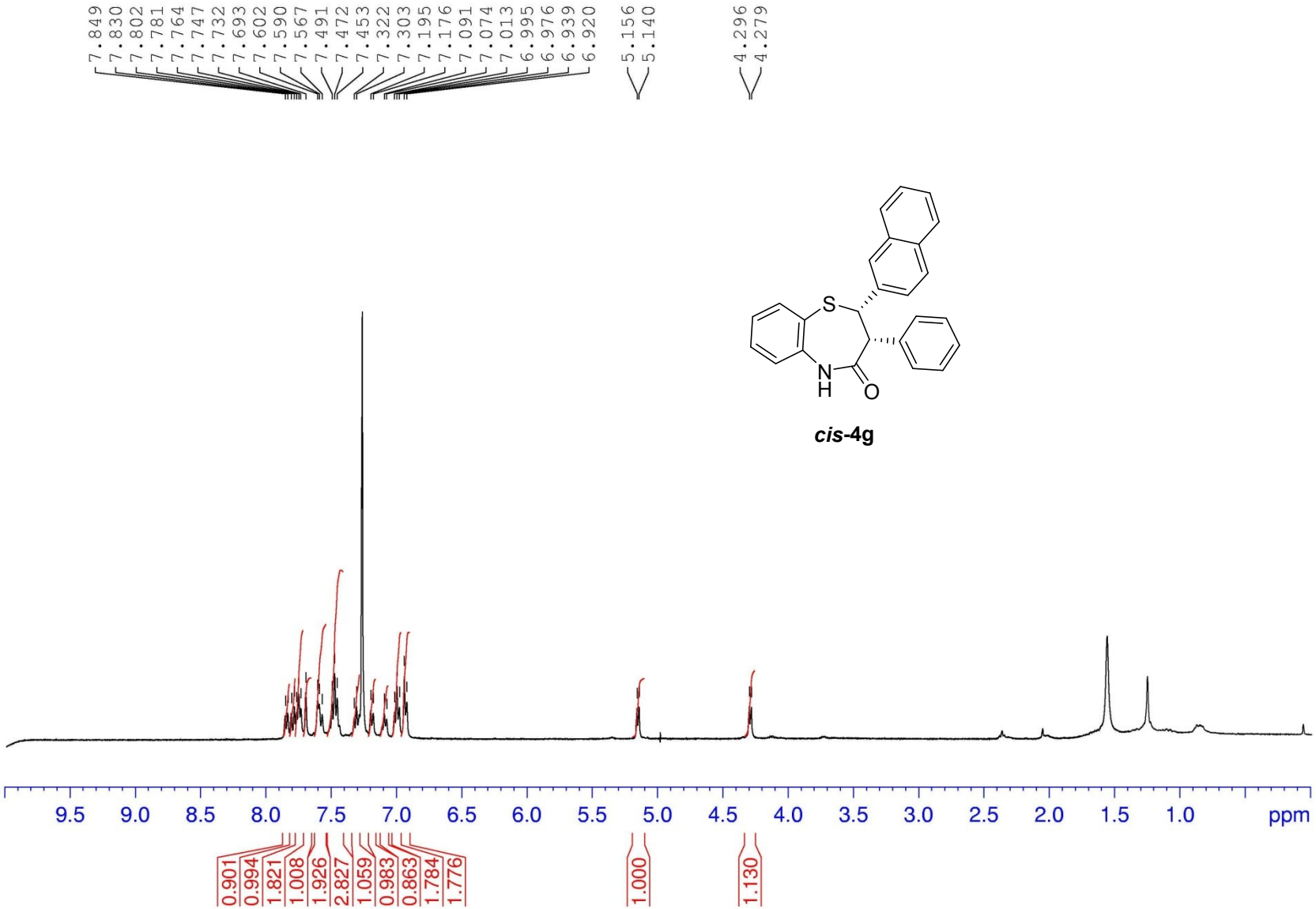
***trans*-4f**

^{13}C NMR in $CDCl_3$ (100 MHz)



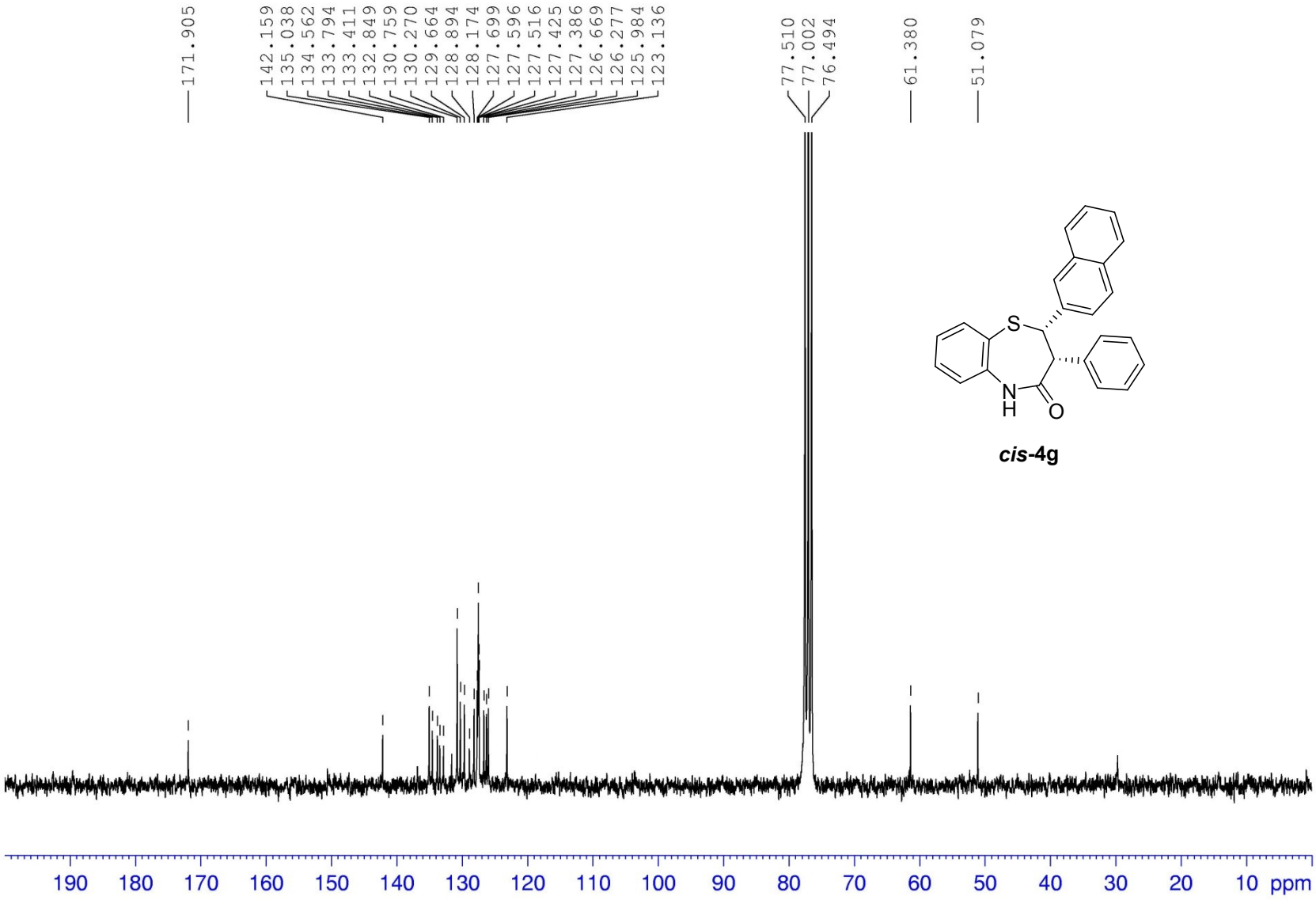
***trans*-4f**

^{1}H NMR in $CDCl_3$ (400 MHz)



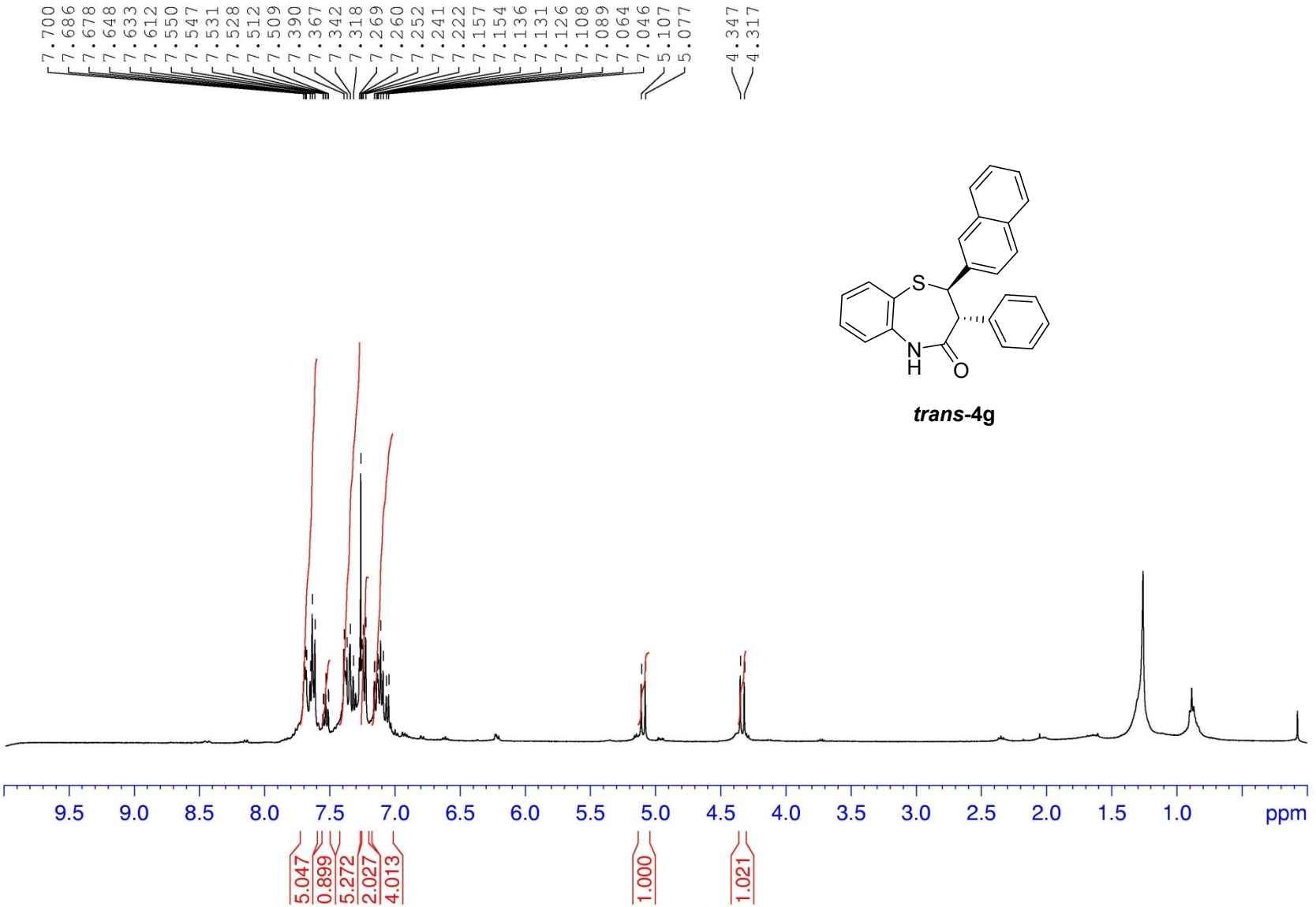
***cis*-4g**

^{13}C NMR in $CDCl_3$ (62.5 MHz)



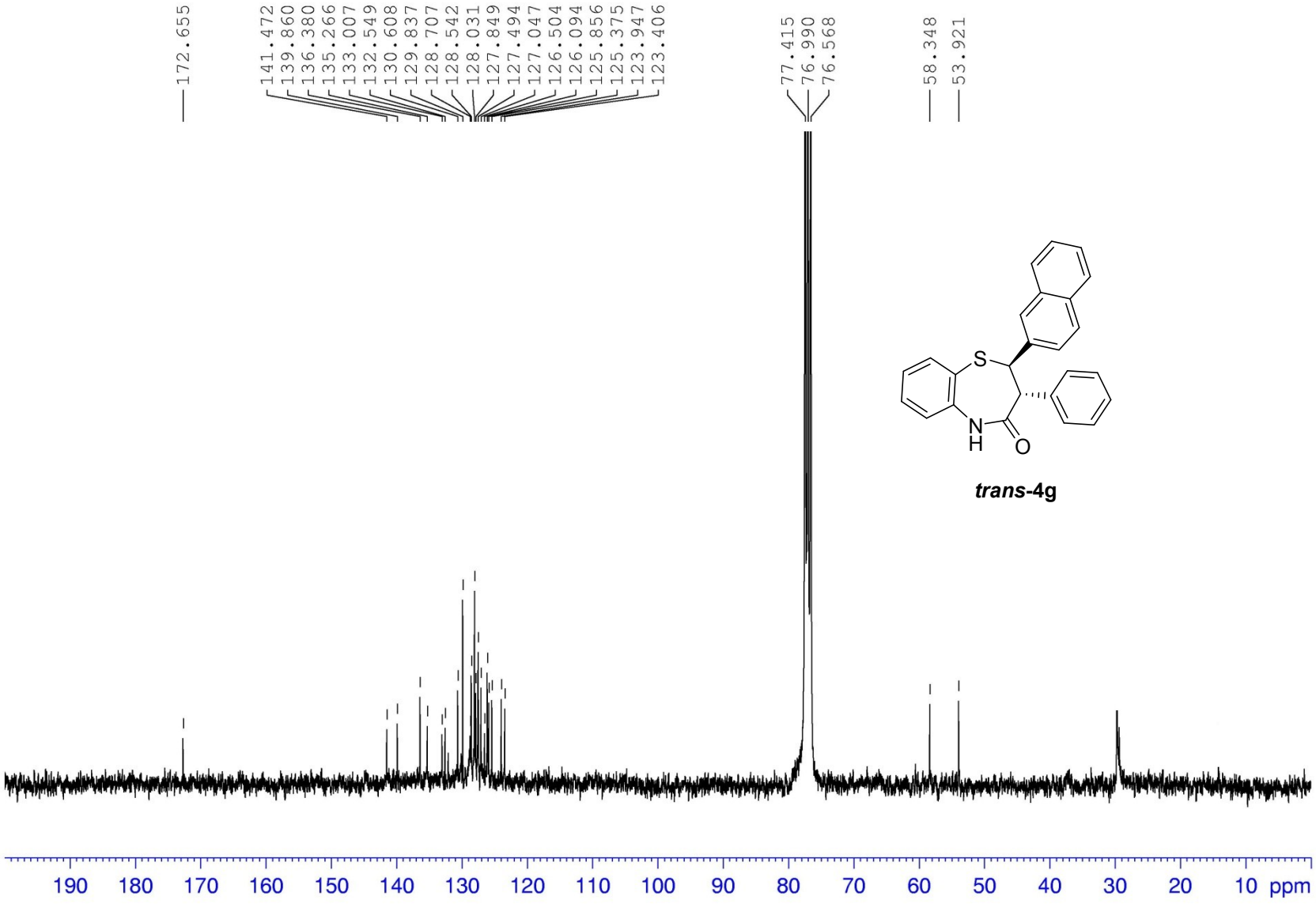
***cis*-4g**

^{1}H NMR in $CDCl_3$ (400 MHz)



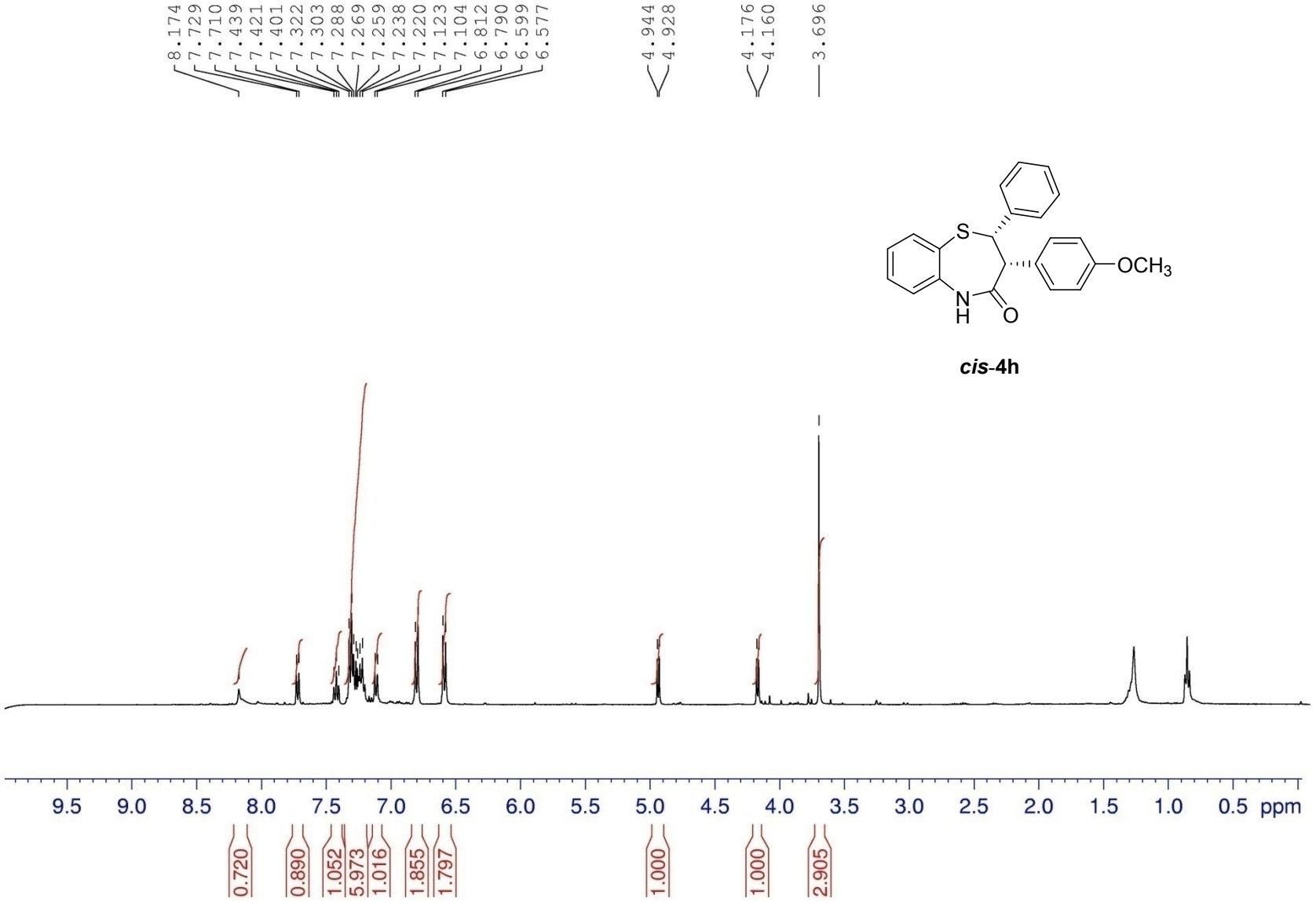
***trans*-4g**

^{13}C NMR in $CDCl_3$ (75 MHz)



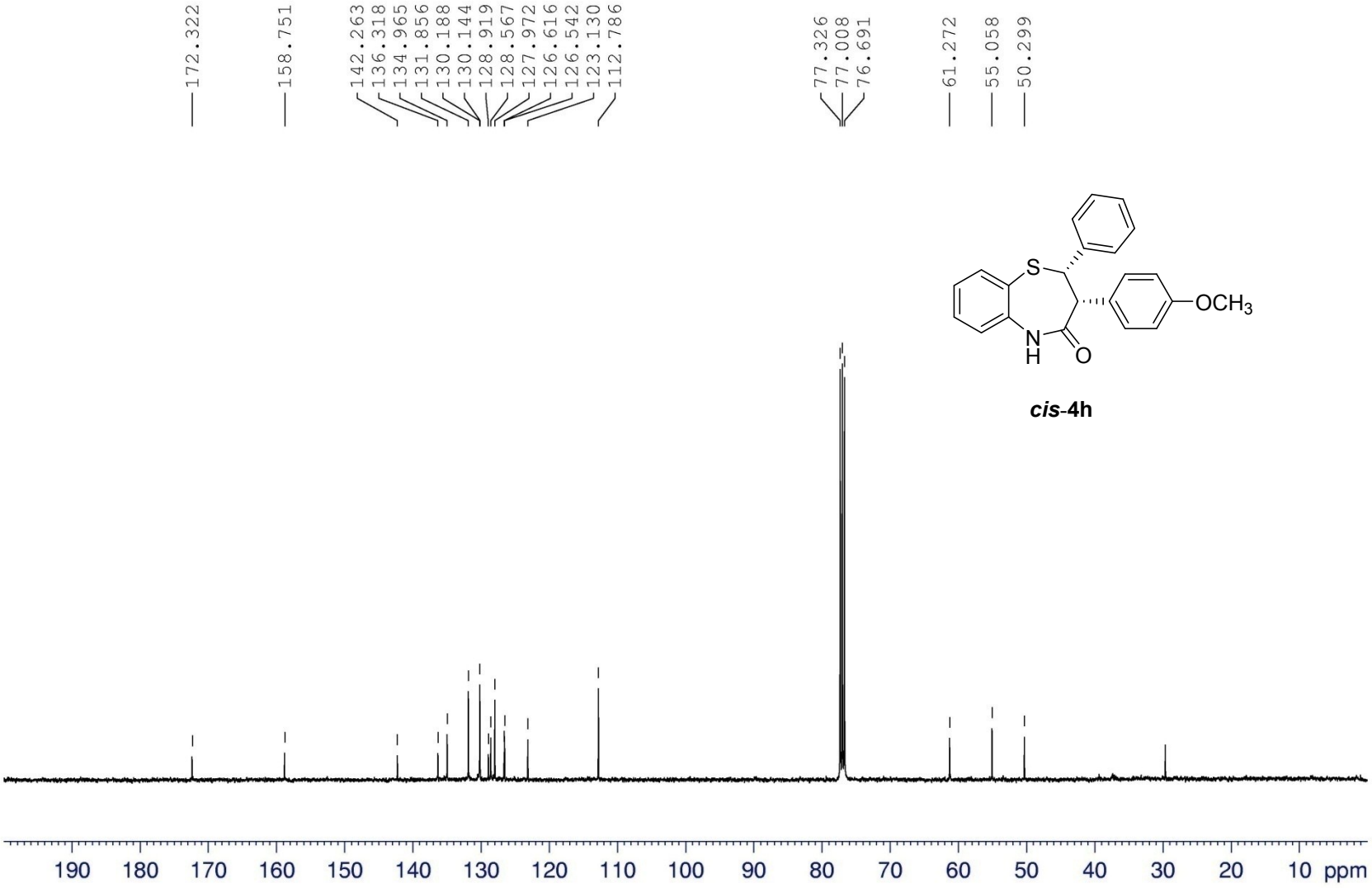
***trans*-4g**

^{1}H NMR in $CDCl_3$ (400 MHz)



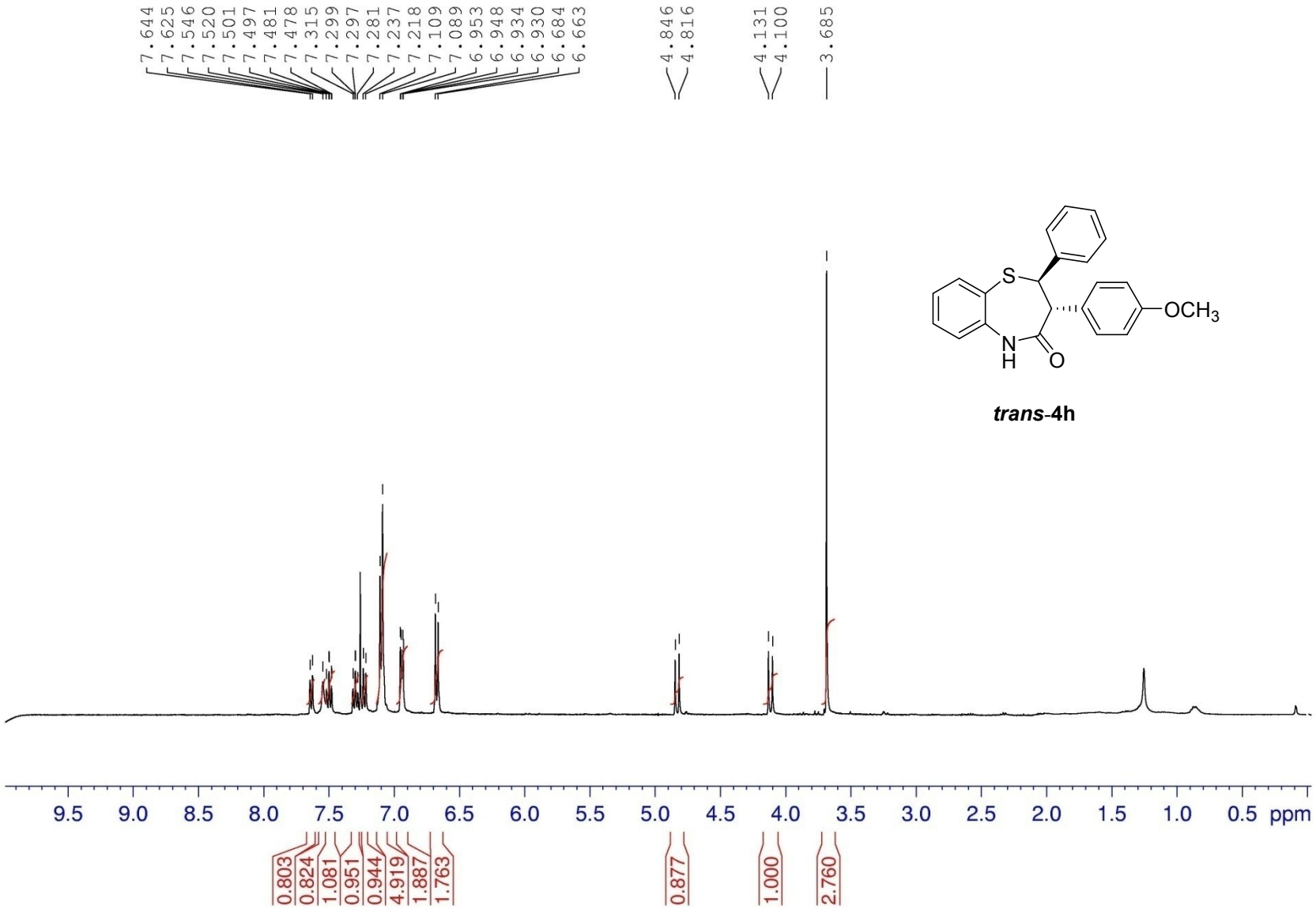
***cis*-4h**

^{13}C NMR in $CDCl_3$ (100 MHz)



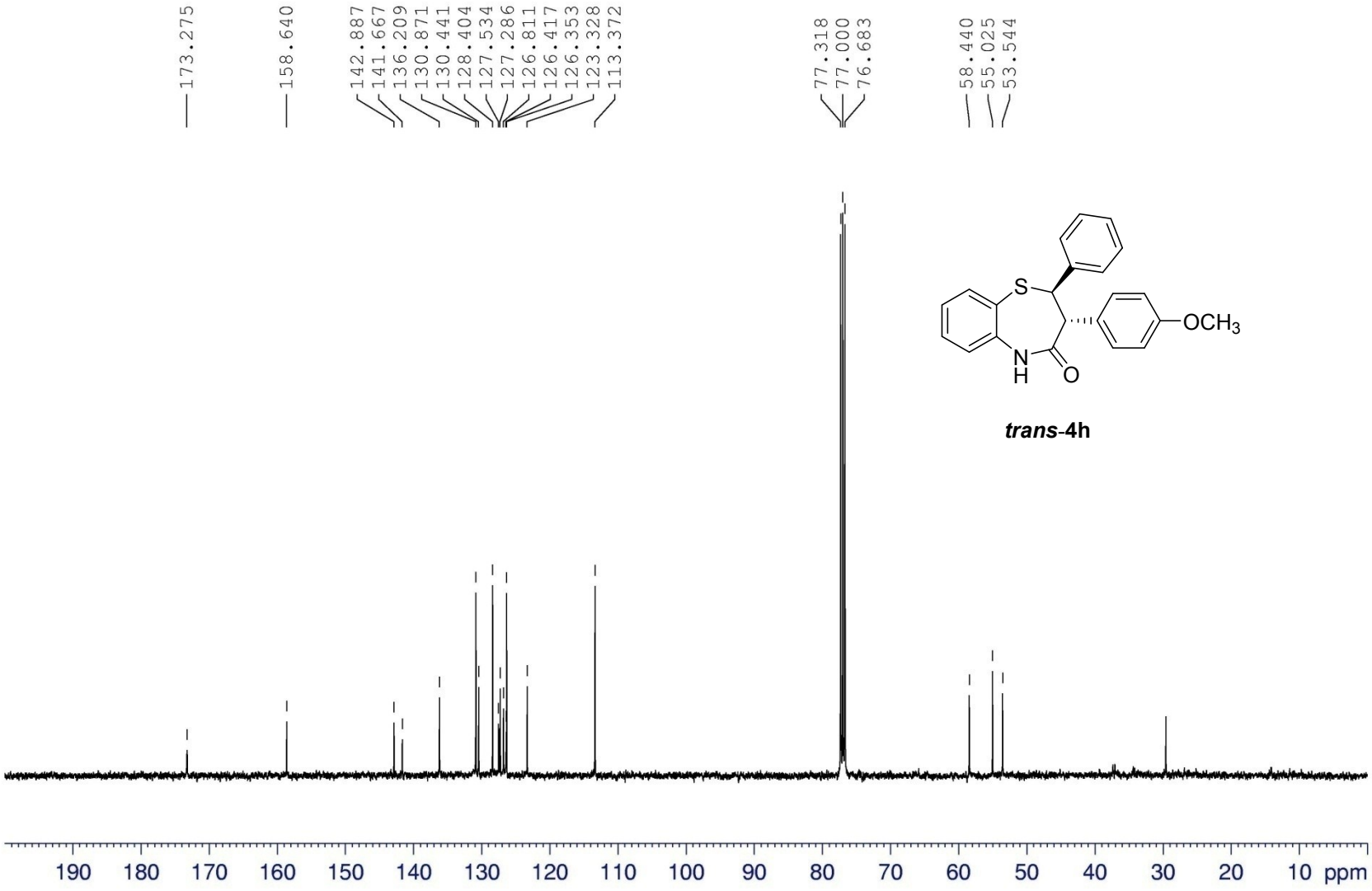
***cis*-4h**

^{1}H NMR in $CDCl_3$ (400 MHz)



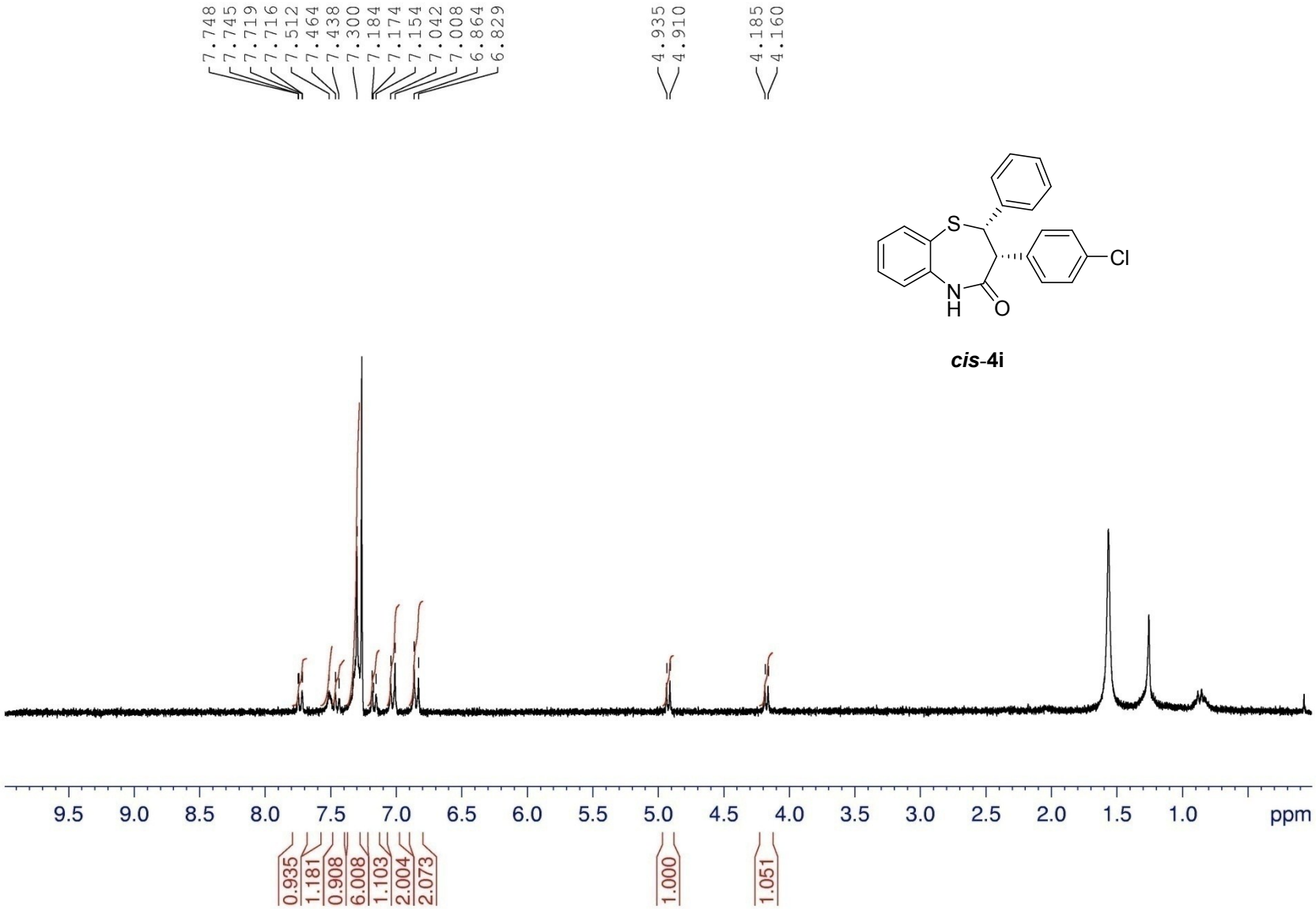
***trans*-4h**

^{13}C NMR in $CDCl_3$ (100 MHz)



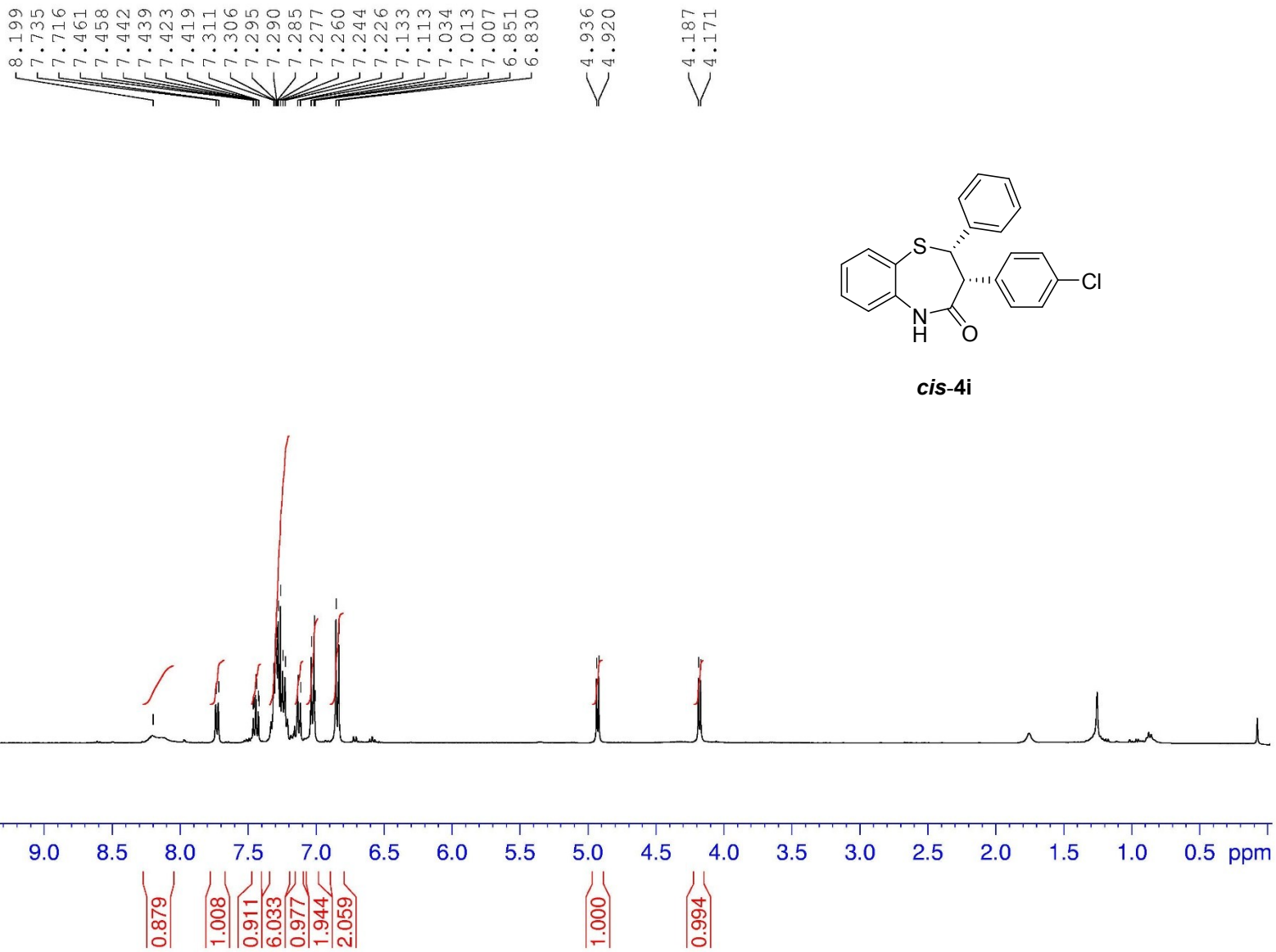
***trans*-4h**

^{1}H NMR in $CDCl_3$ (250 MHz), reaction performed with catalyst **X**



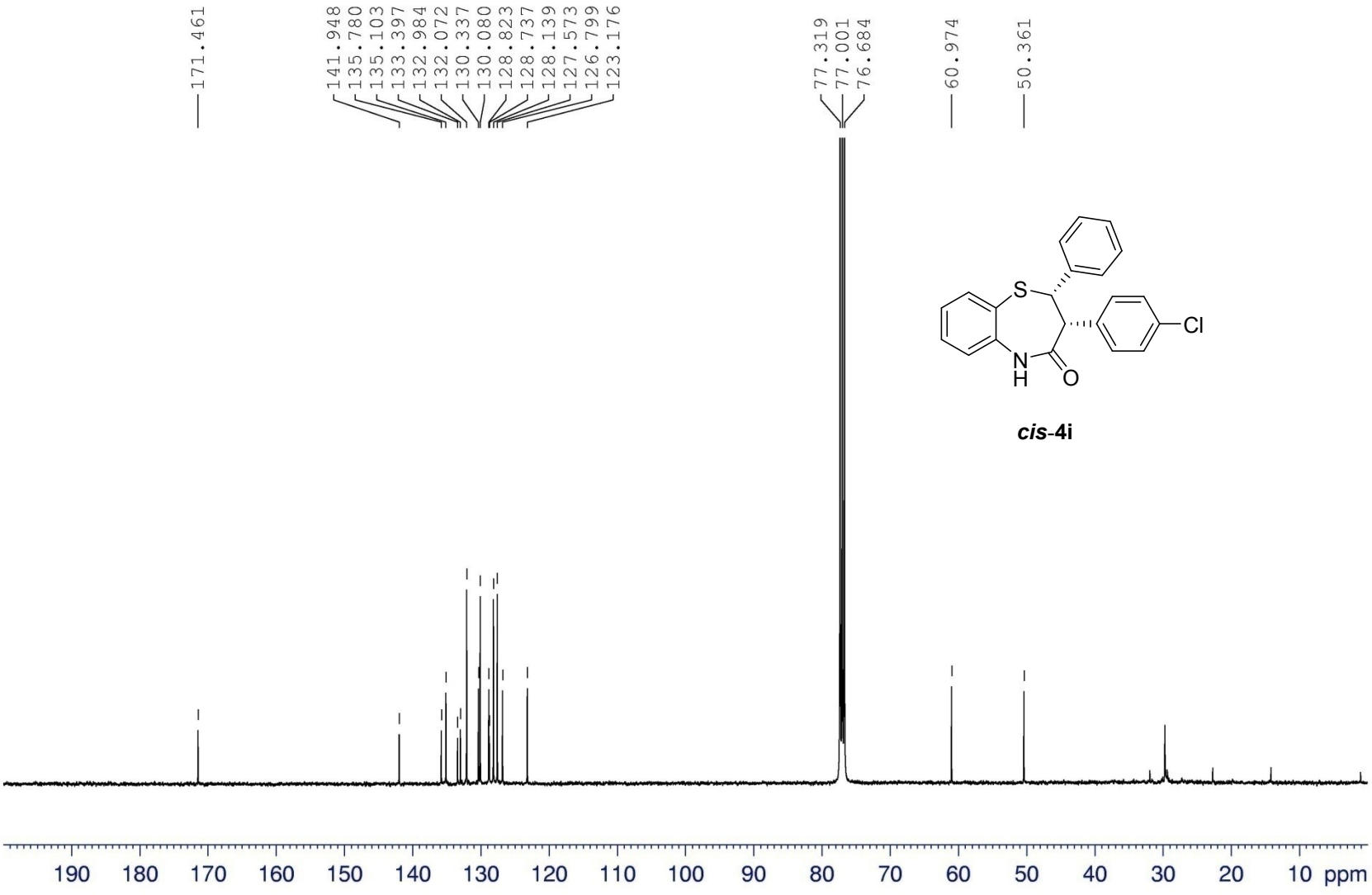
***cis*-4i**

^{1}H NMR in $CDCl_3$ (400 MHz), reaction performed with catalyst **VIII**



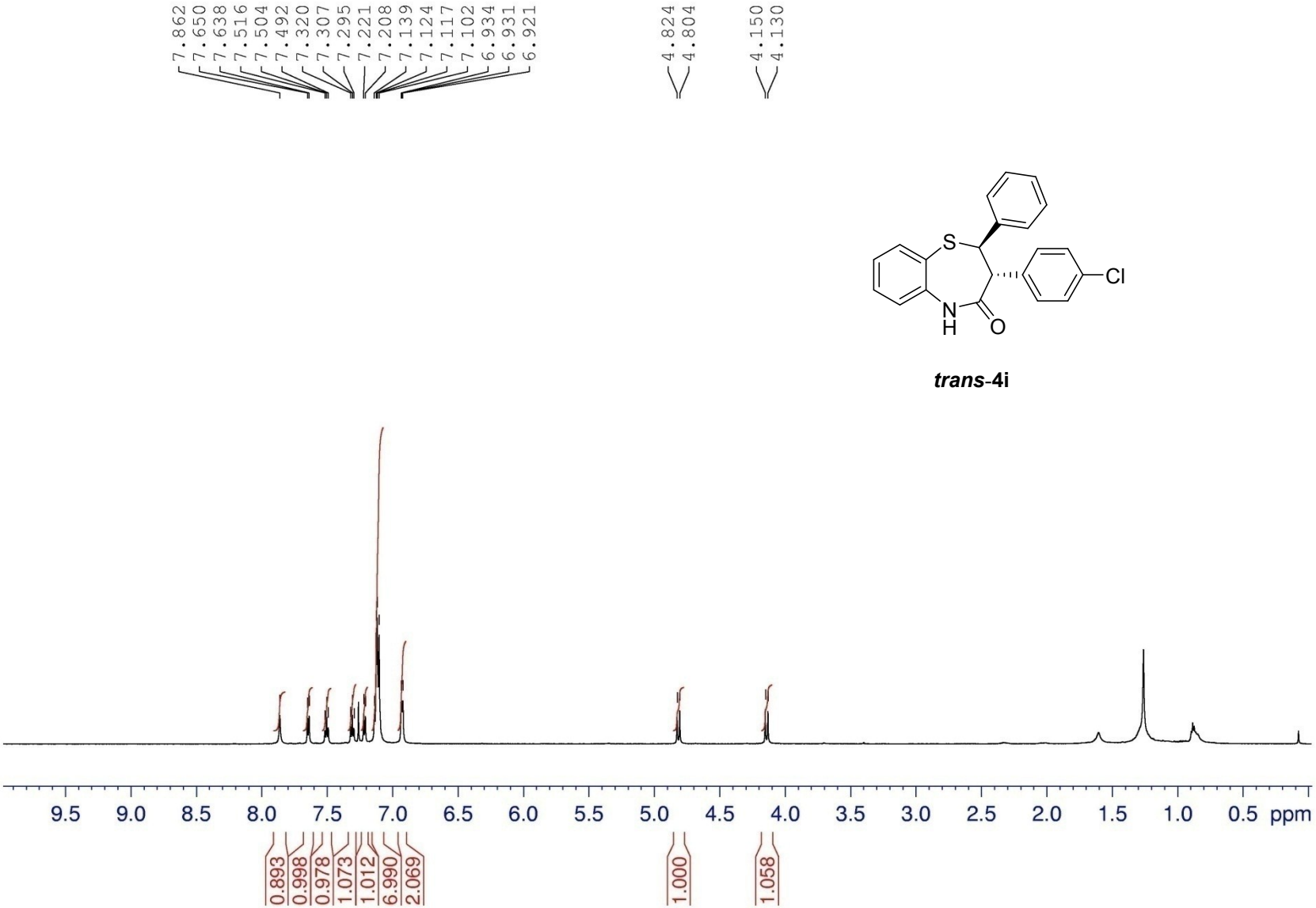
***cis*-4i**

^{13}C NMR in $CDCl_3$ (100 MHz)



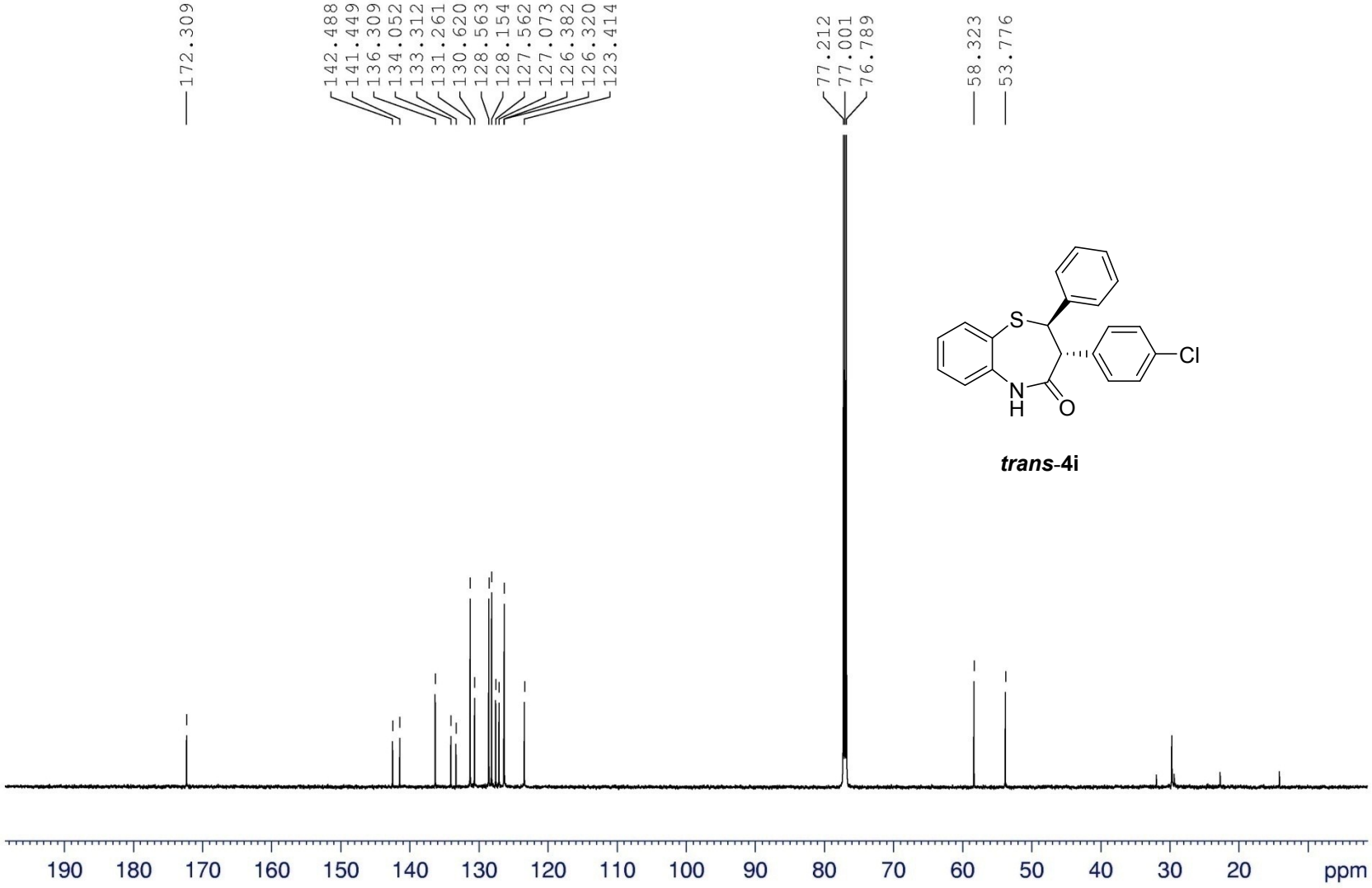
***cis*-4i**

^{1}H NMR in $CDCl_3$ (600 MHz)

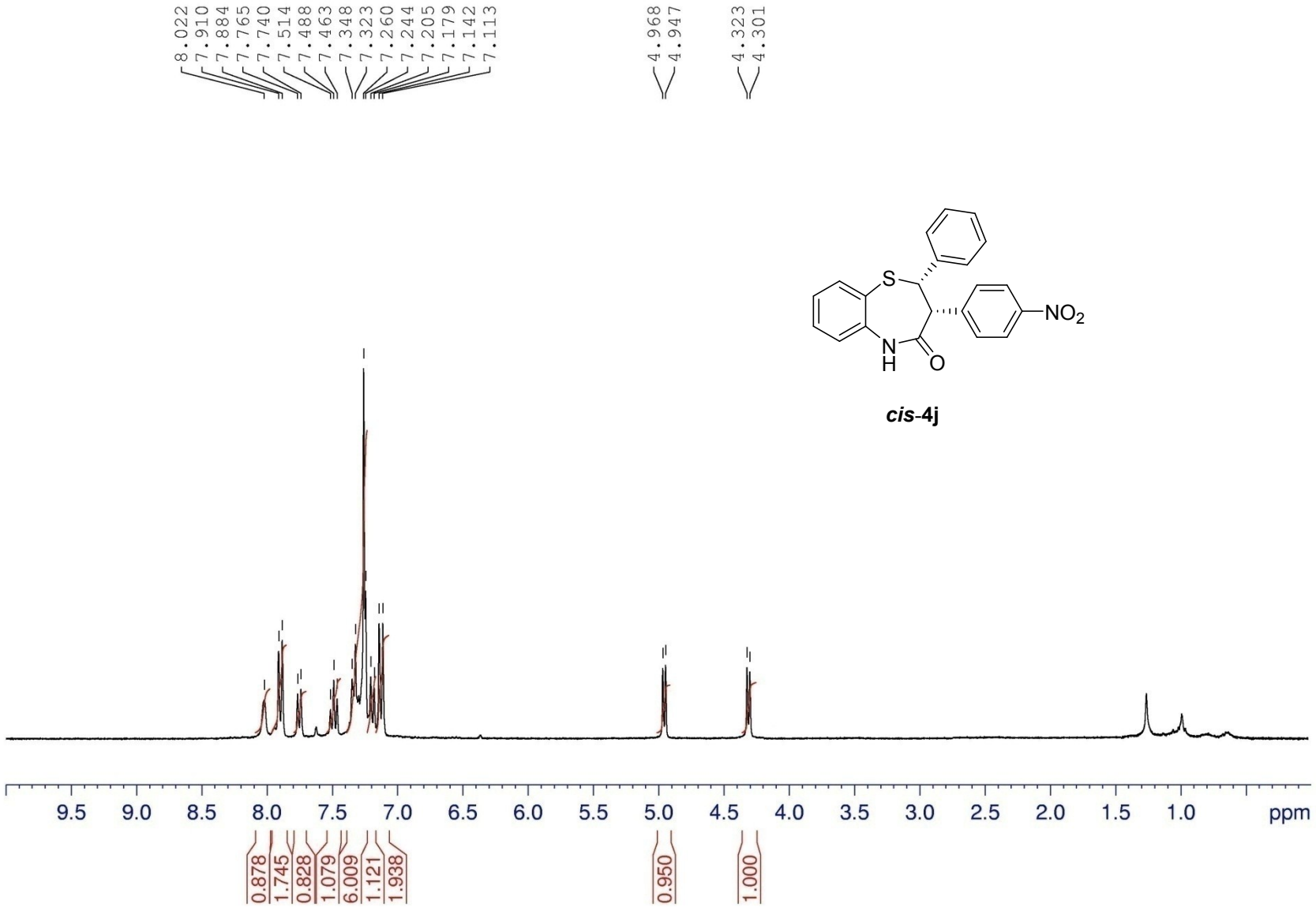


***trans*-4i**

^{13}C NMR in $CDCl_3$ (150 MHz)

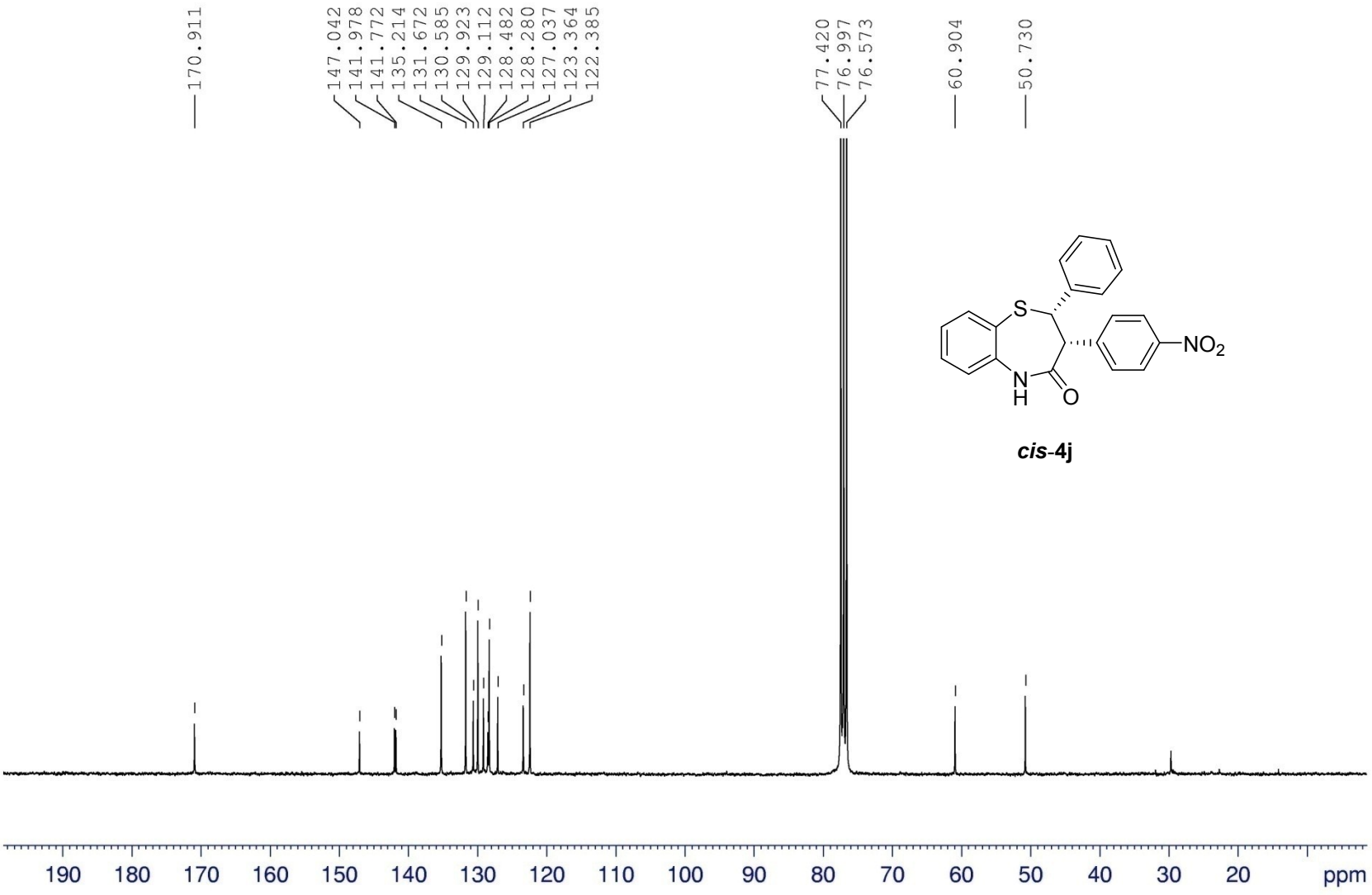


^{1}H NMR in $CDCl_3$ (300 MHz)

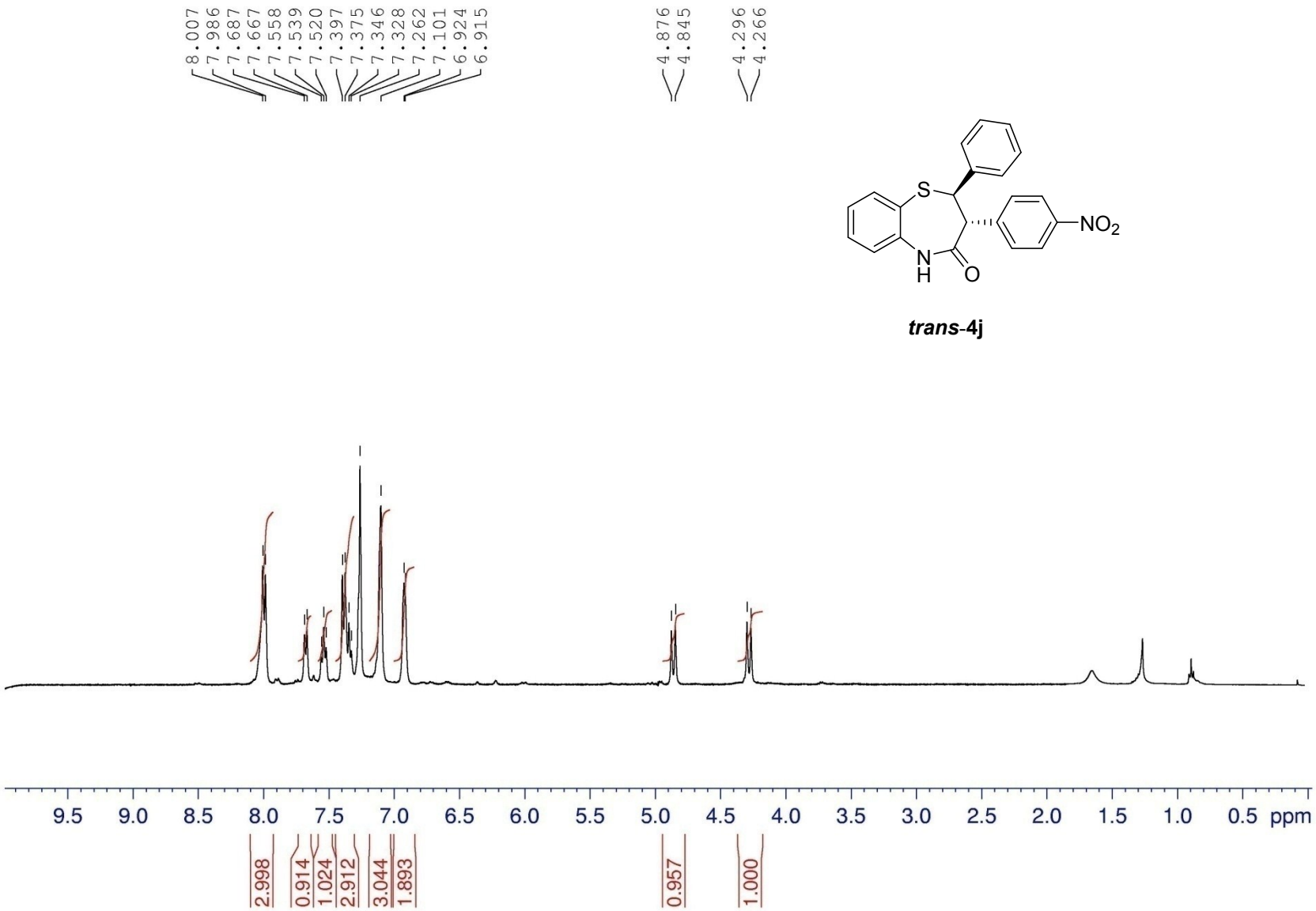


***cis*-4j**

^{13}C NMR in $CDCl_3$ (75 MHz)



***cis*-4j**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7.687
7.667
7.558
7.539
7.520
7.397
7.375
7.346
7.328
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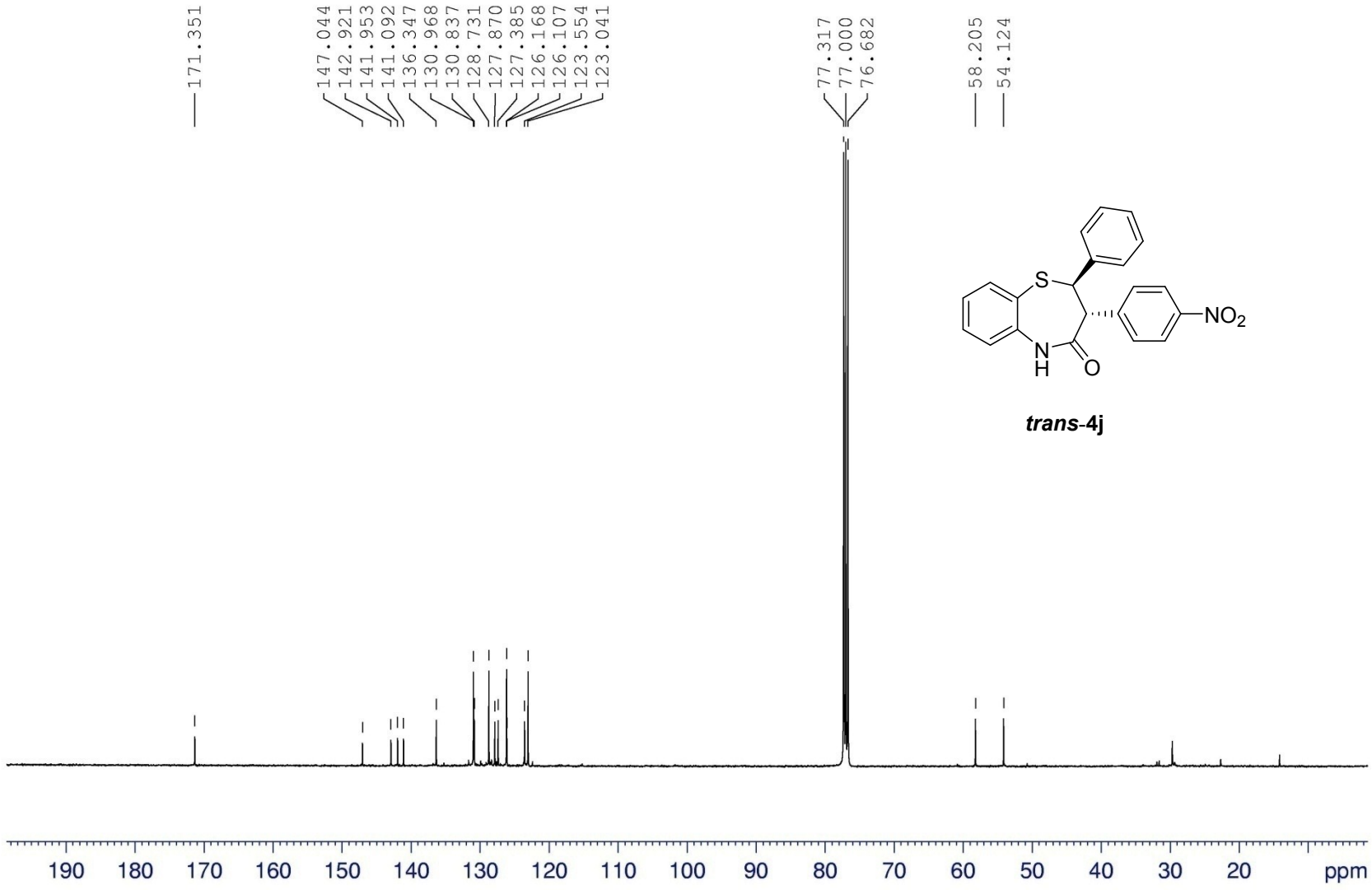
7.101
6.924
6.915
4.876
4.845
4.296
4.266
S
N
H
O
NO2
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.998
0.914
1.024
2.912
3.044
1.893
0.957
1.000

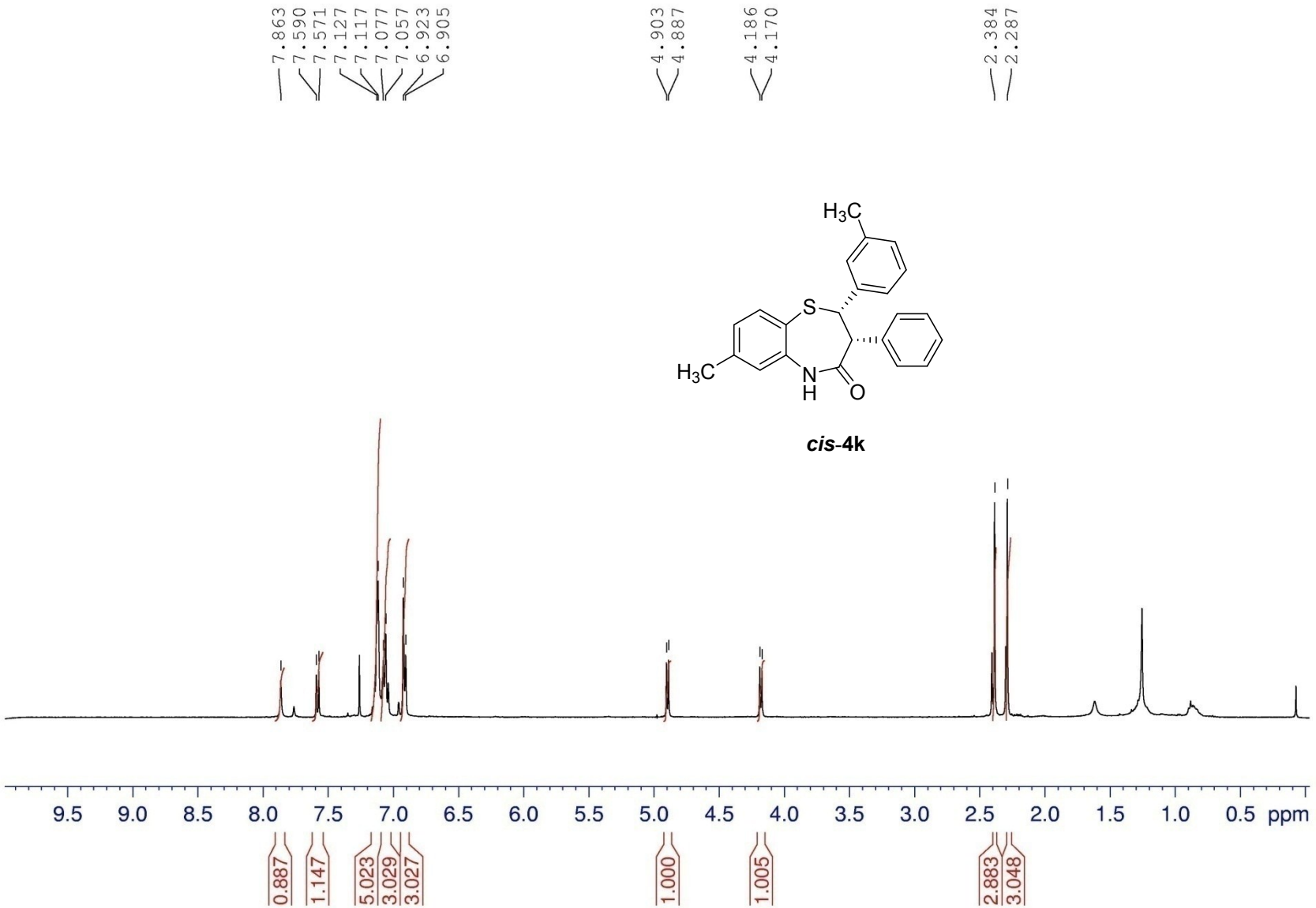
***trans*-4j**

^{13}C NMR in $CDCl_3$ (100 MHz)



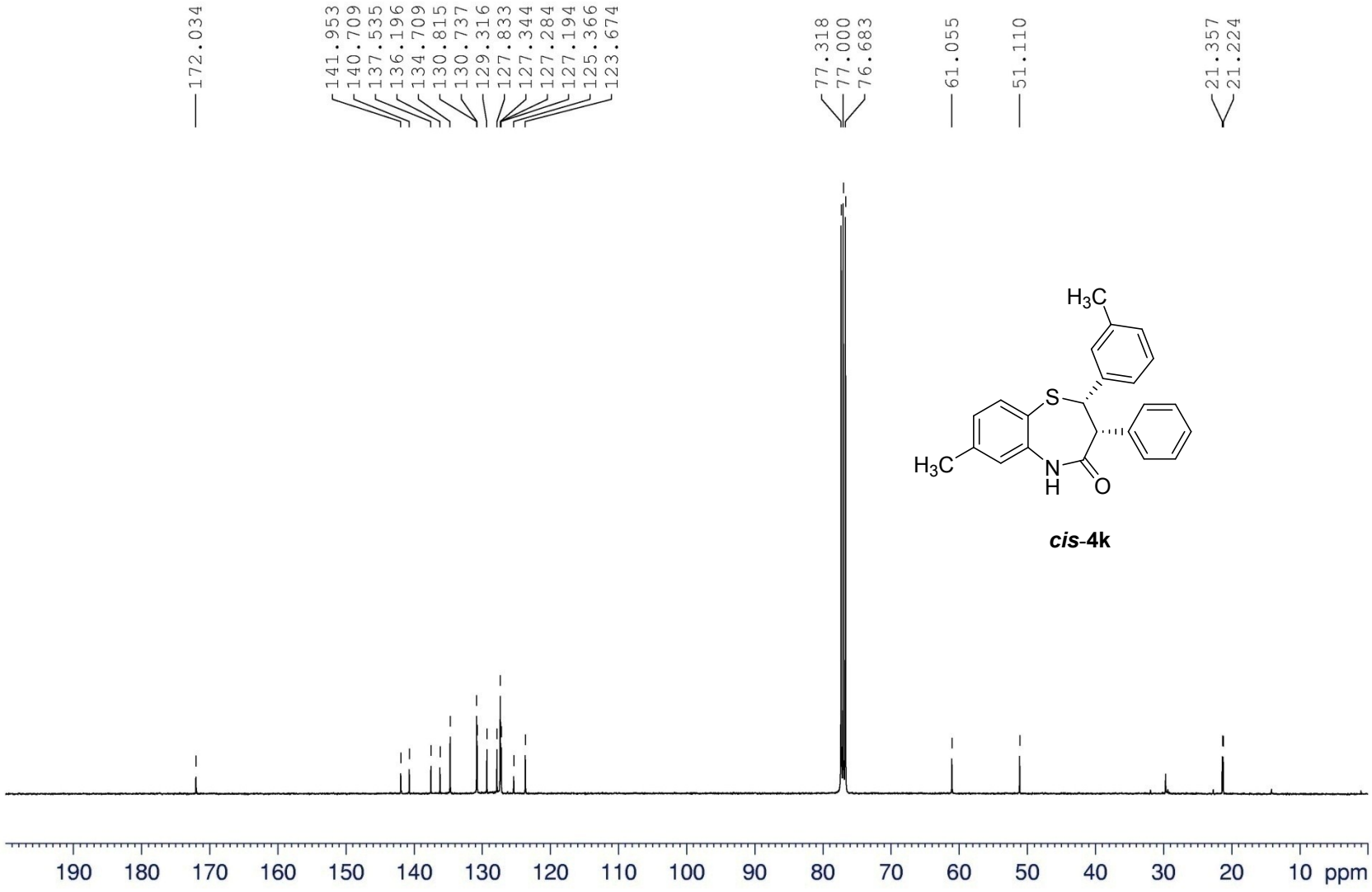
***trans*-4j**

^{1}H NMR in $CDCl_3$ (400 MHz)



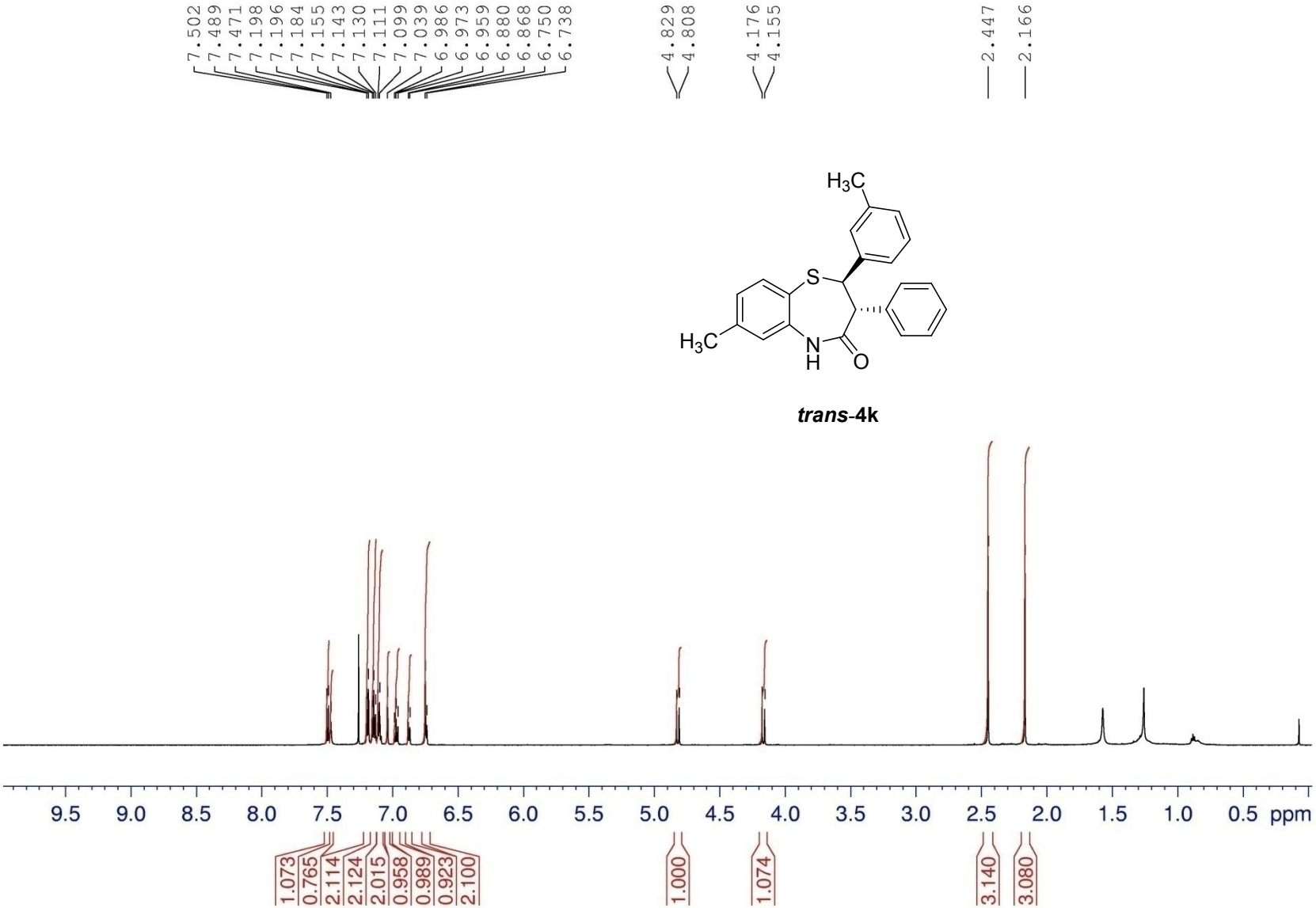
***cis*-4k**

^{13}C NMR in $CDCl_3$ (100 MHz)



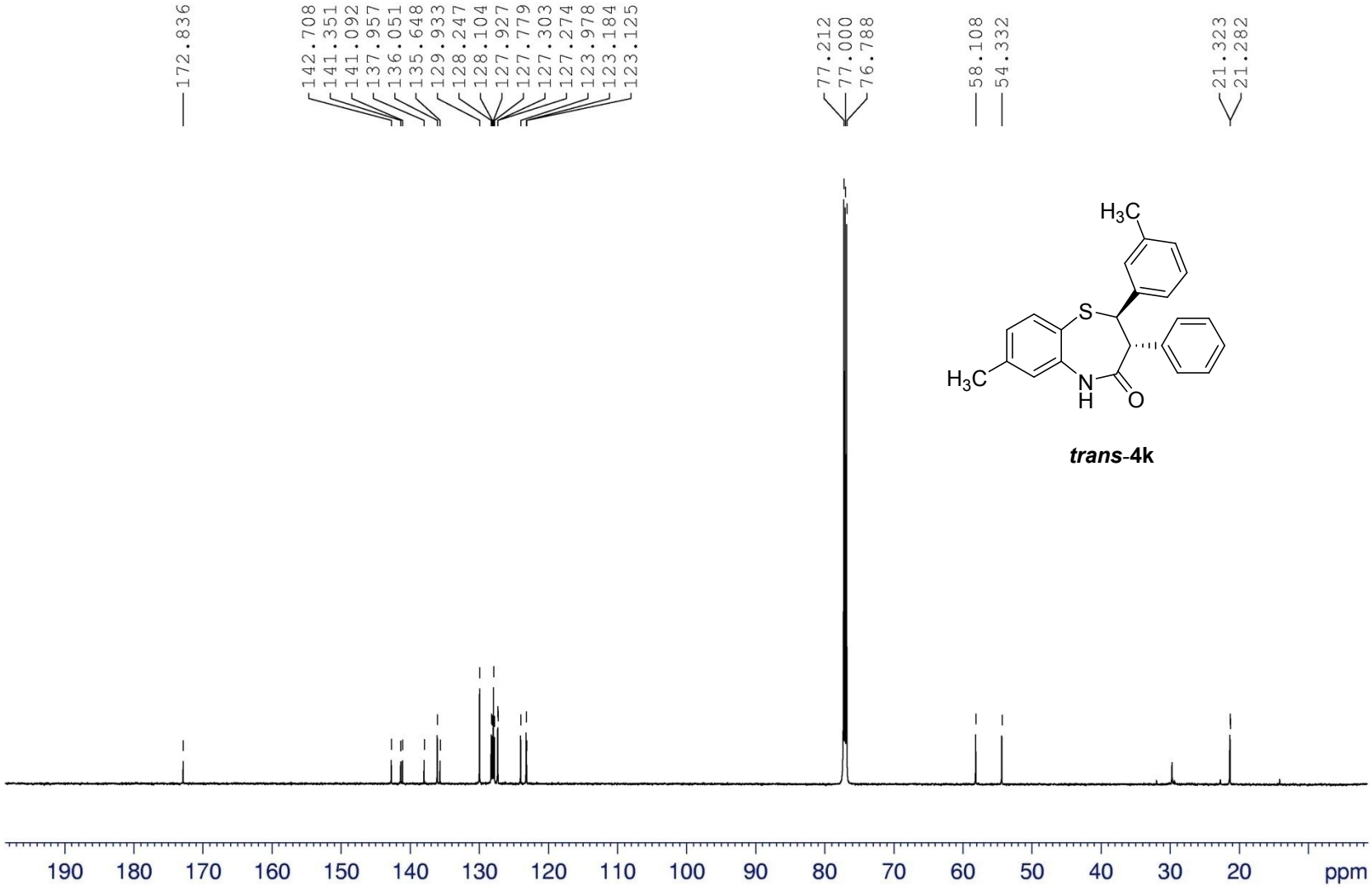
***cis*-4k**

^{1}H NMR in $CDCl_3$ (600 MHz)



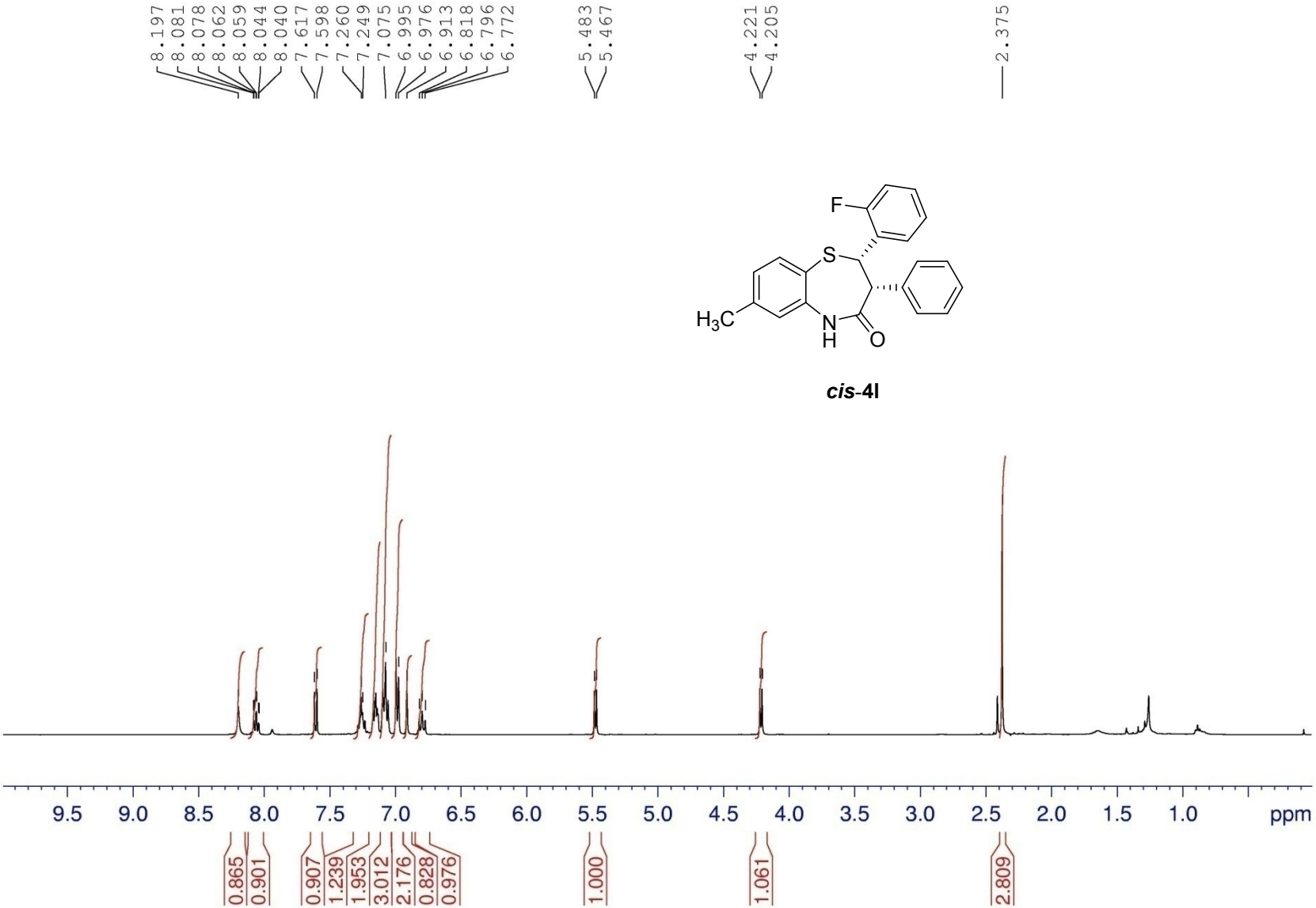
***trans*-4k**

^{13}C NMR in $CDCl_3$ (150 MHz)



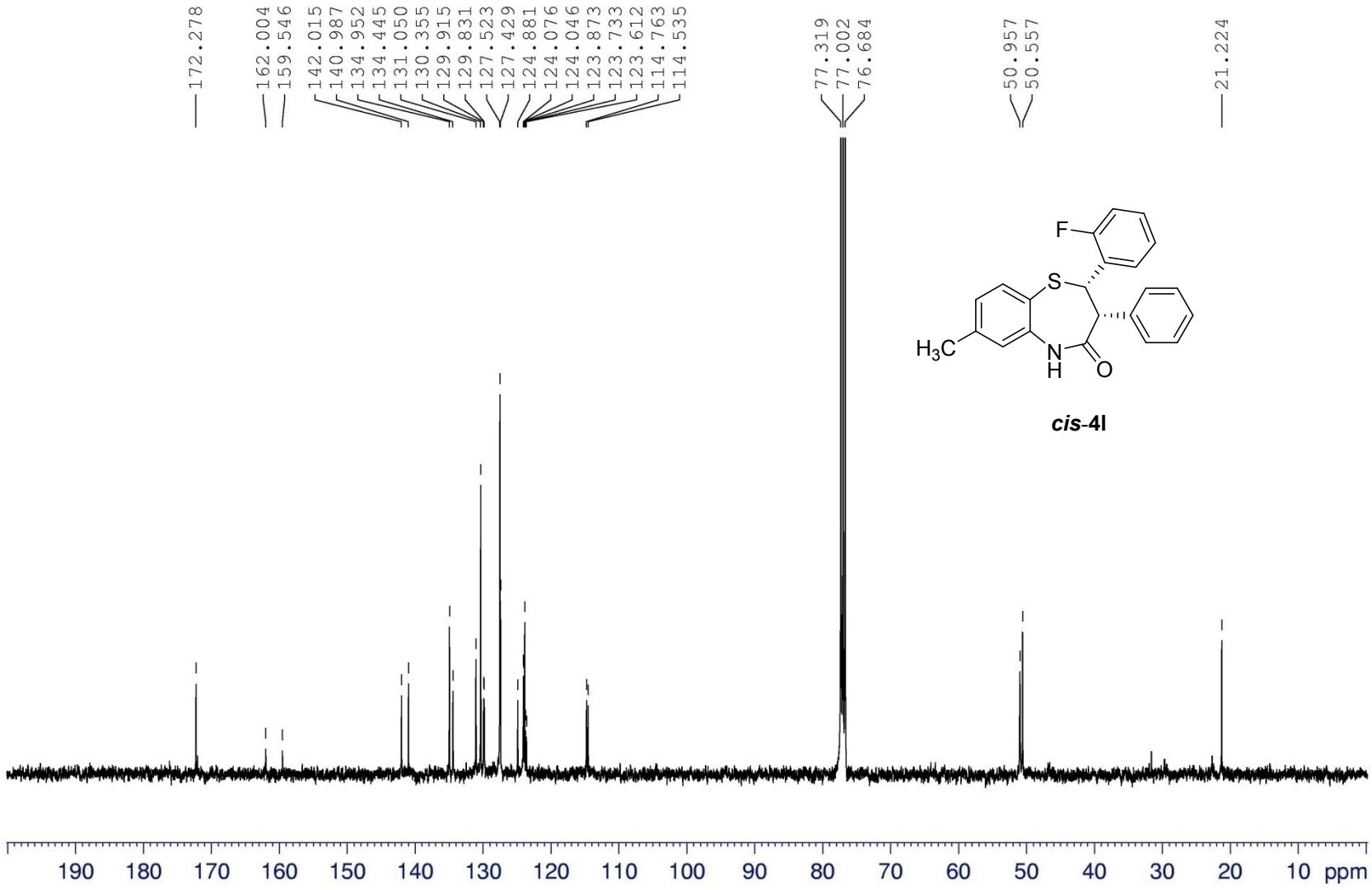
***trans*-4k**

^{1}H NMR in $CDCl_3$ (400 MHz)



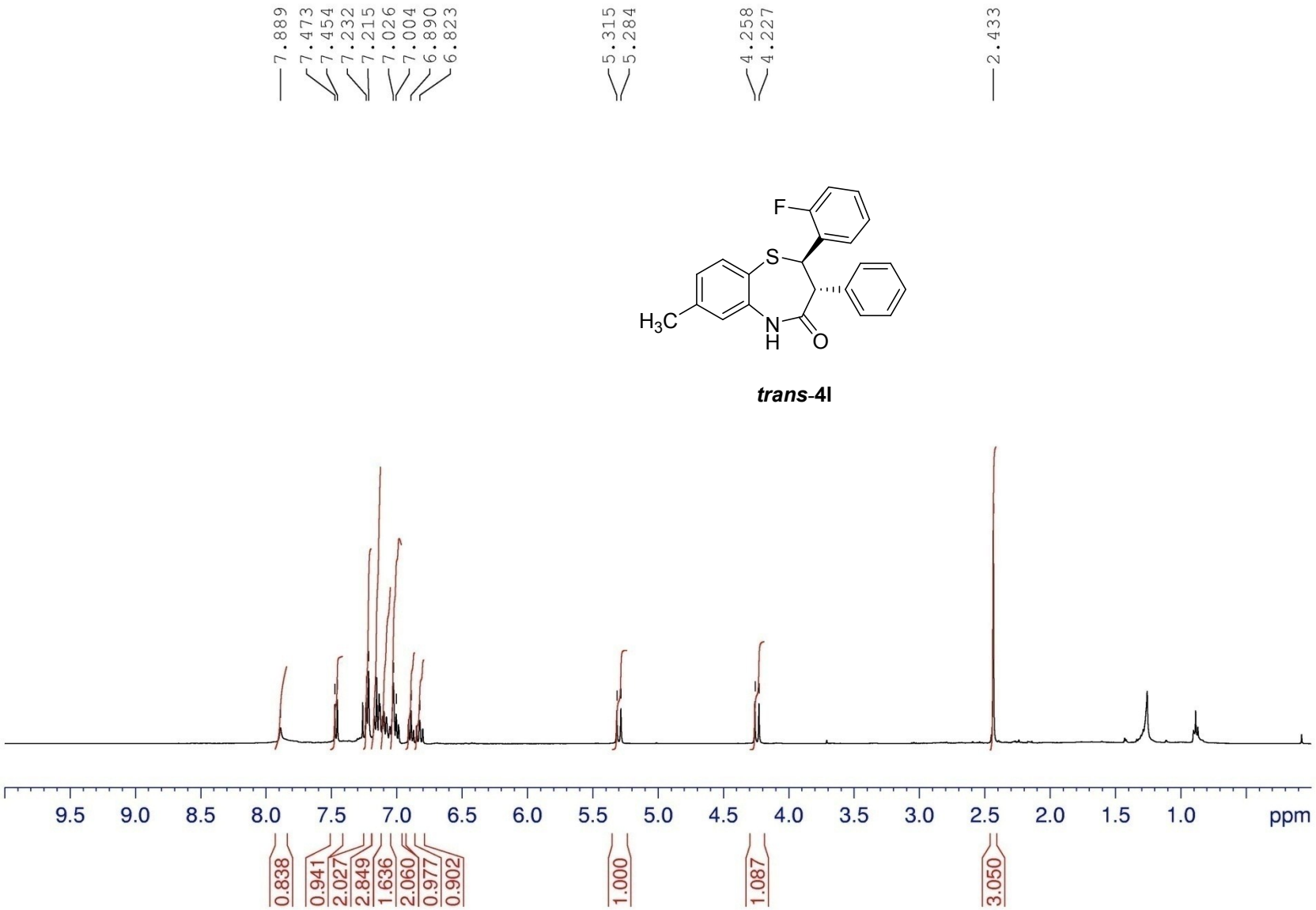
***cis*-4l**

^{13}C NMR in $CDCl_3$ (100 MHz)



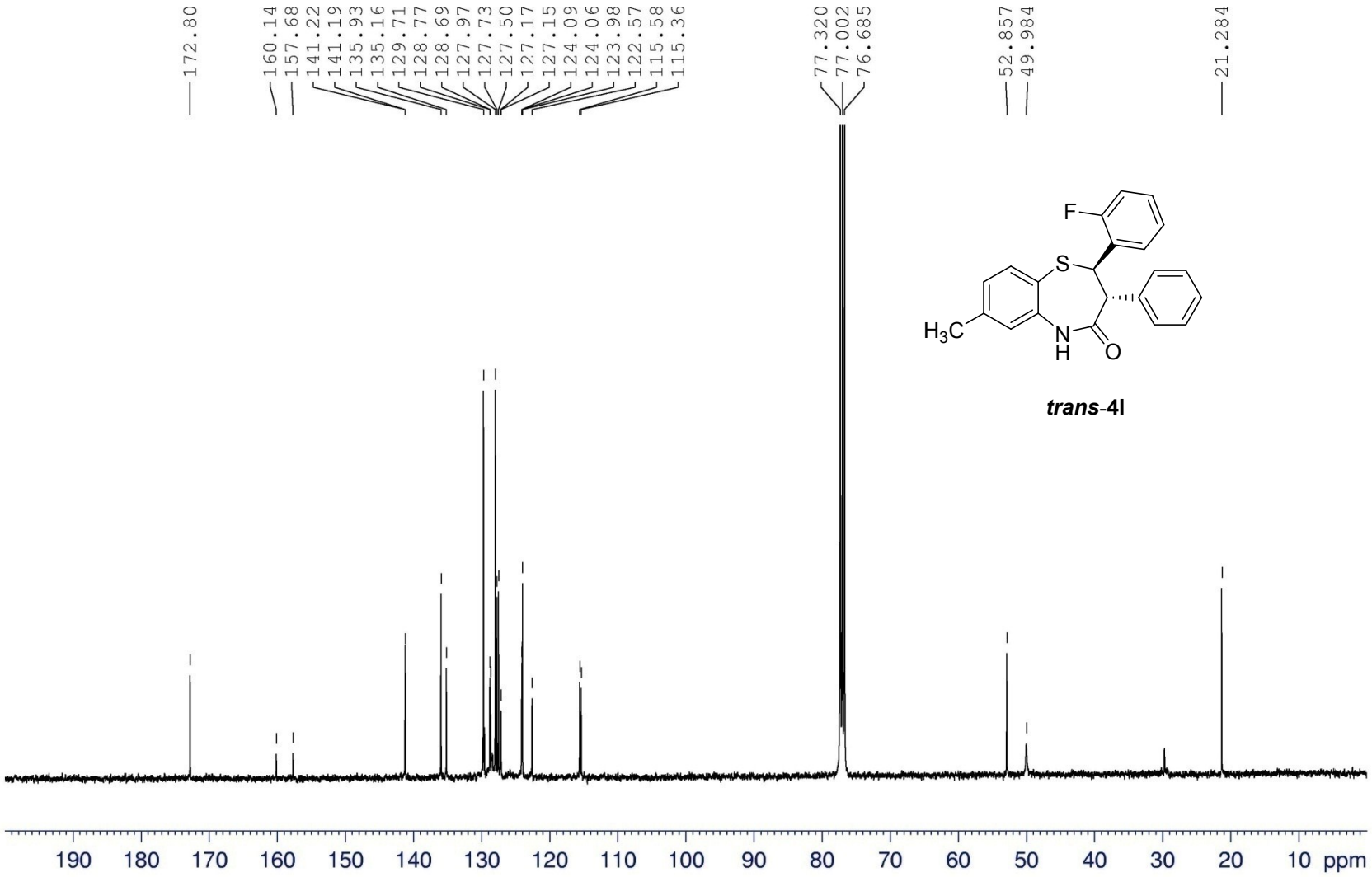
***cis*-4l**

^{1}H NMR in $CDCl_3$ (400 MHz)



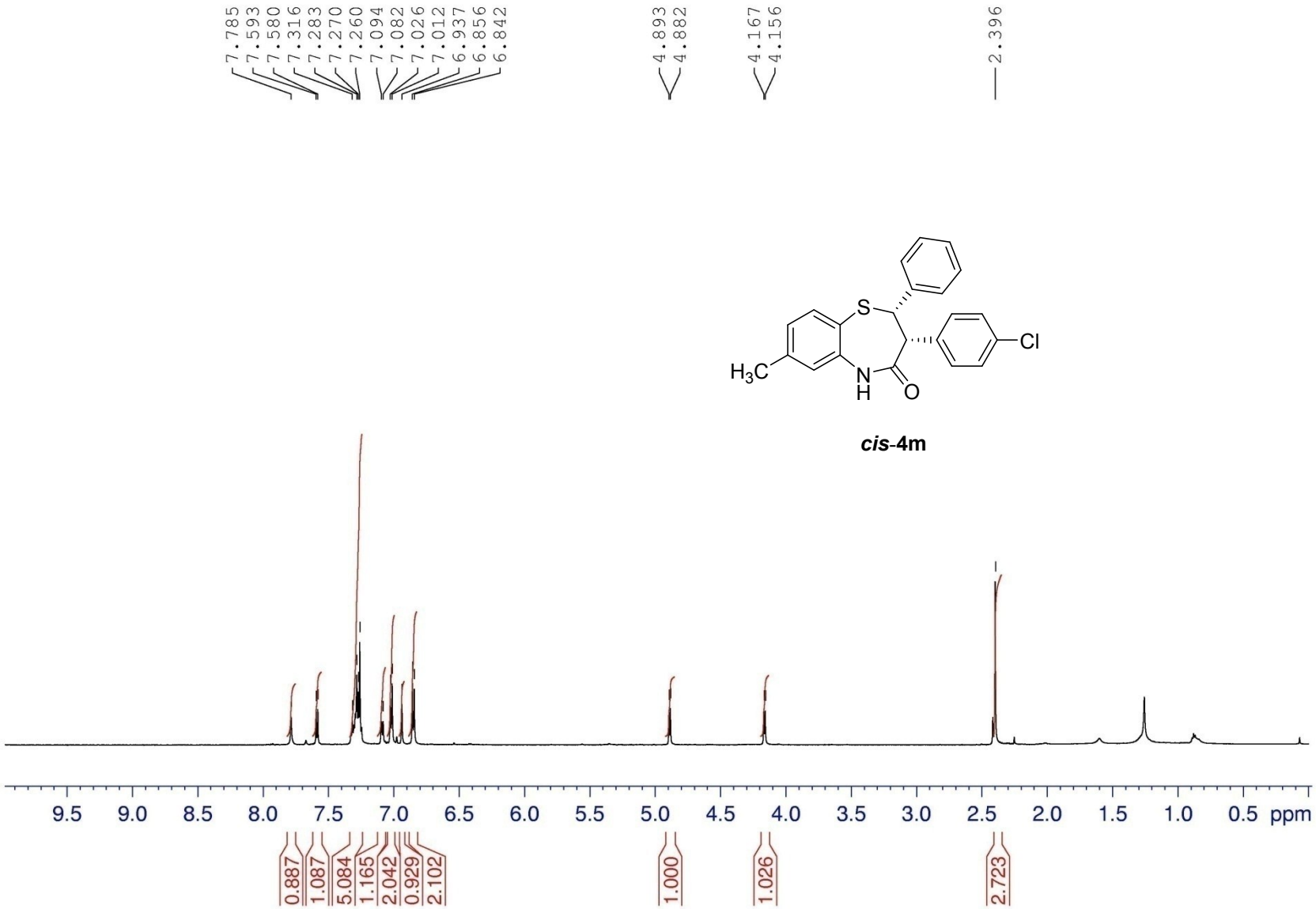
***trans*-4l**

^{13}C NMR in $CDCl_3$ (100 MHz)



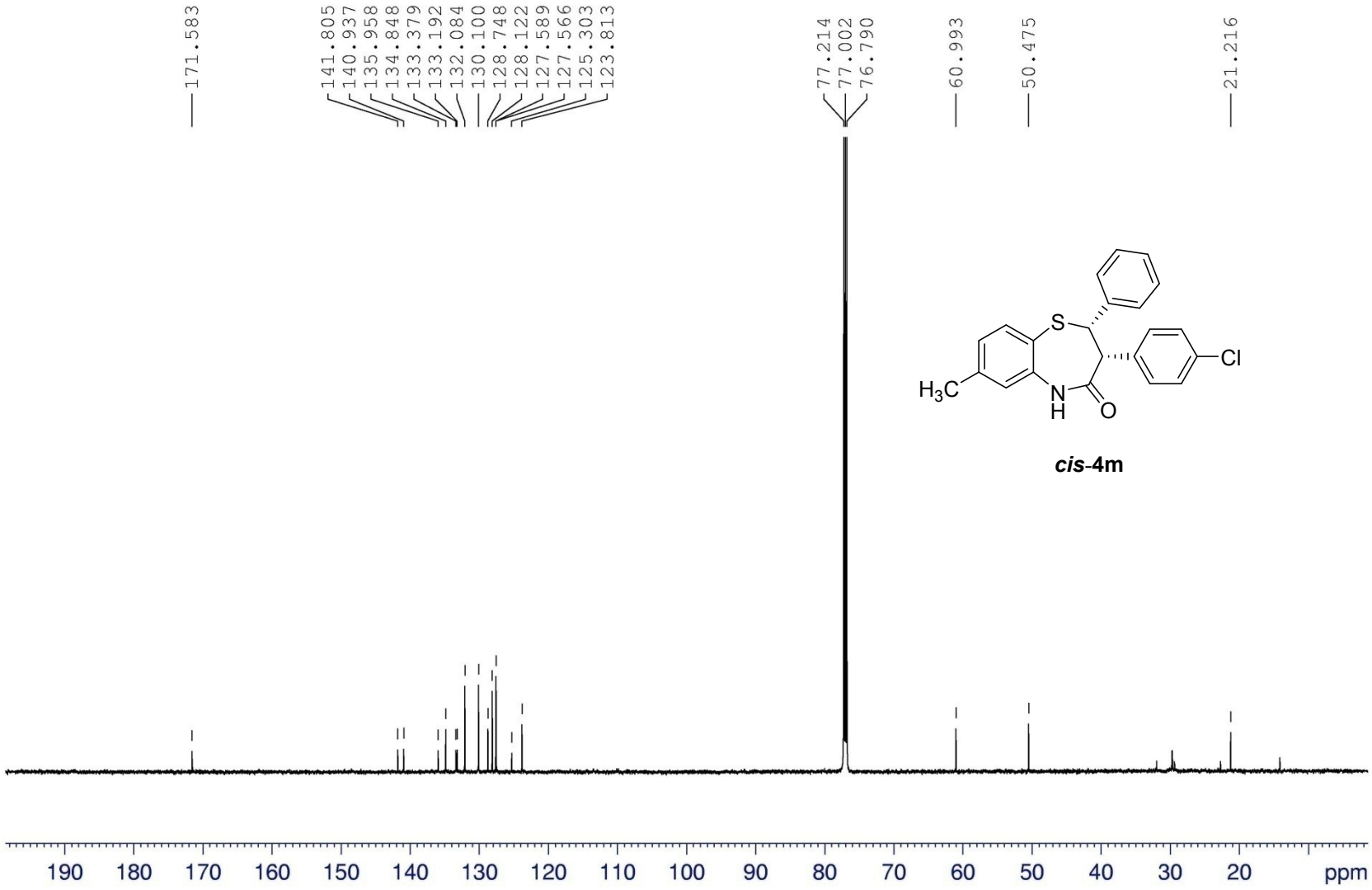
***trans*-4l**

^{1}H NMR in $CDCl_3$ (600 MHz)



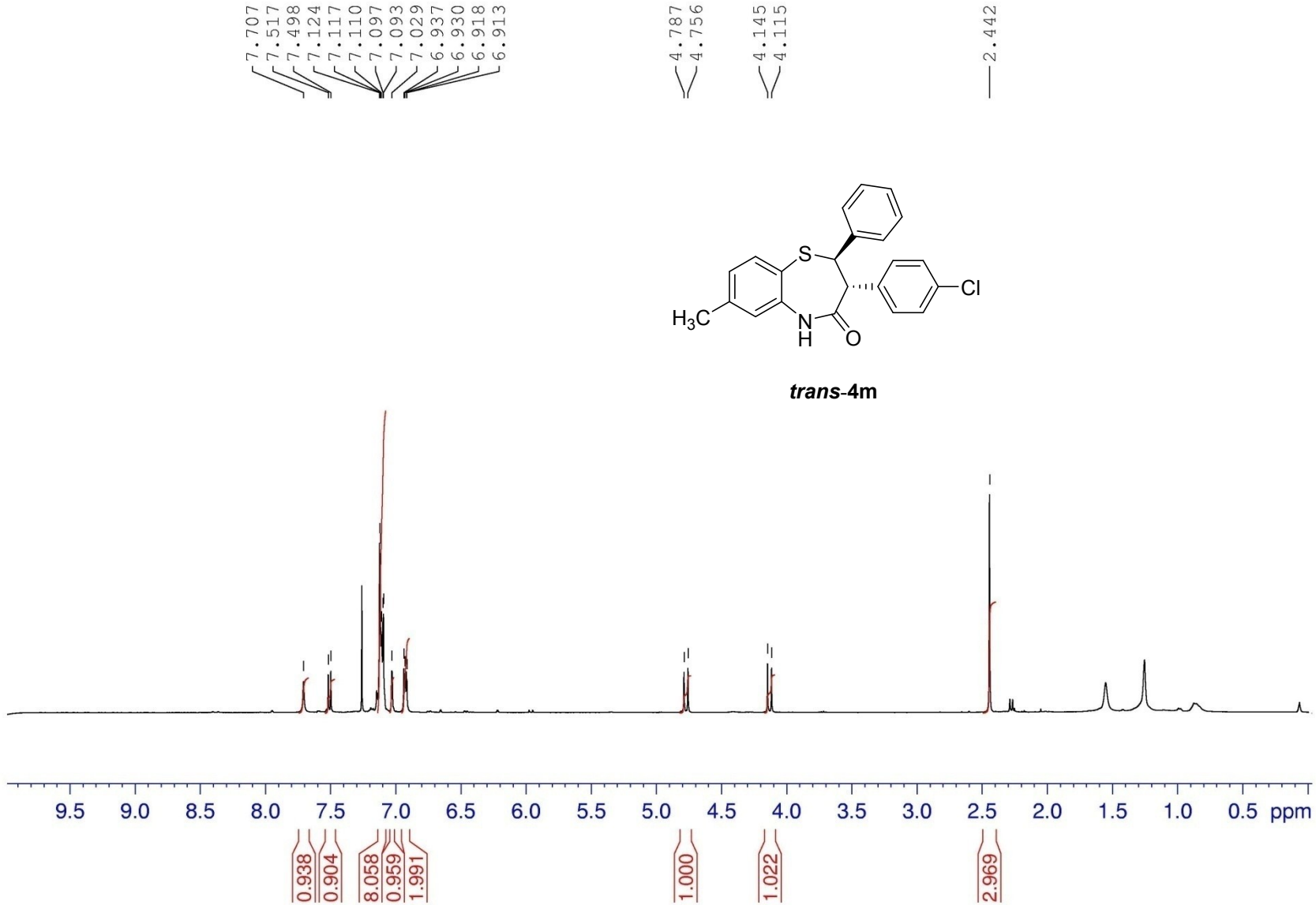
***cis*-4m**

^{13}C NMR in $CDCl_3$ (150 MHz)



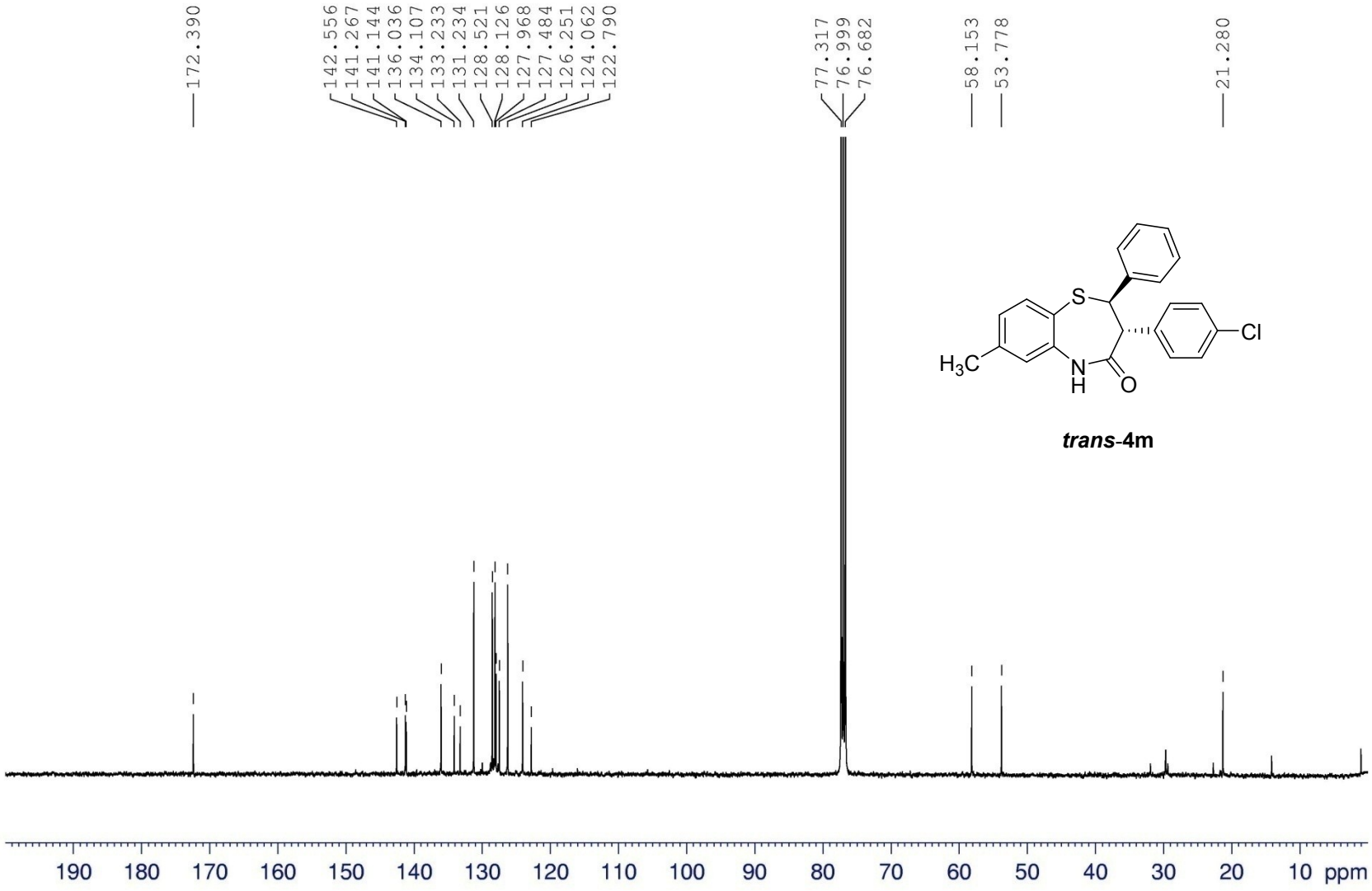
***cis*-4m**

^{1}H NMR in $CDCl_3$ (400 MHz)



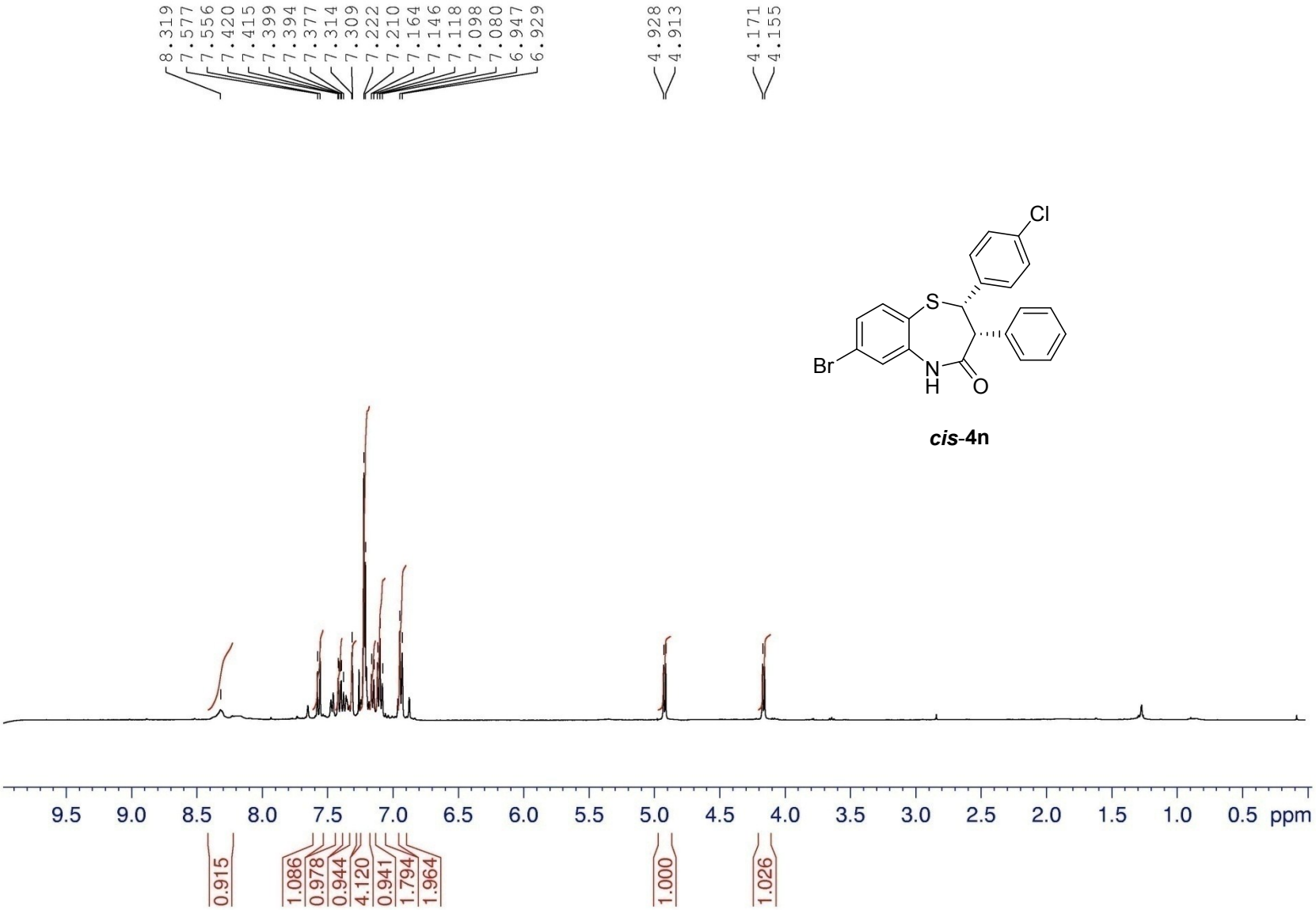
***trans*-4m**

^{13}C NMR in $CDCl_3$ (100 MHz)



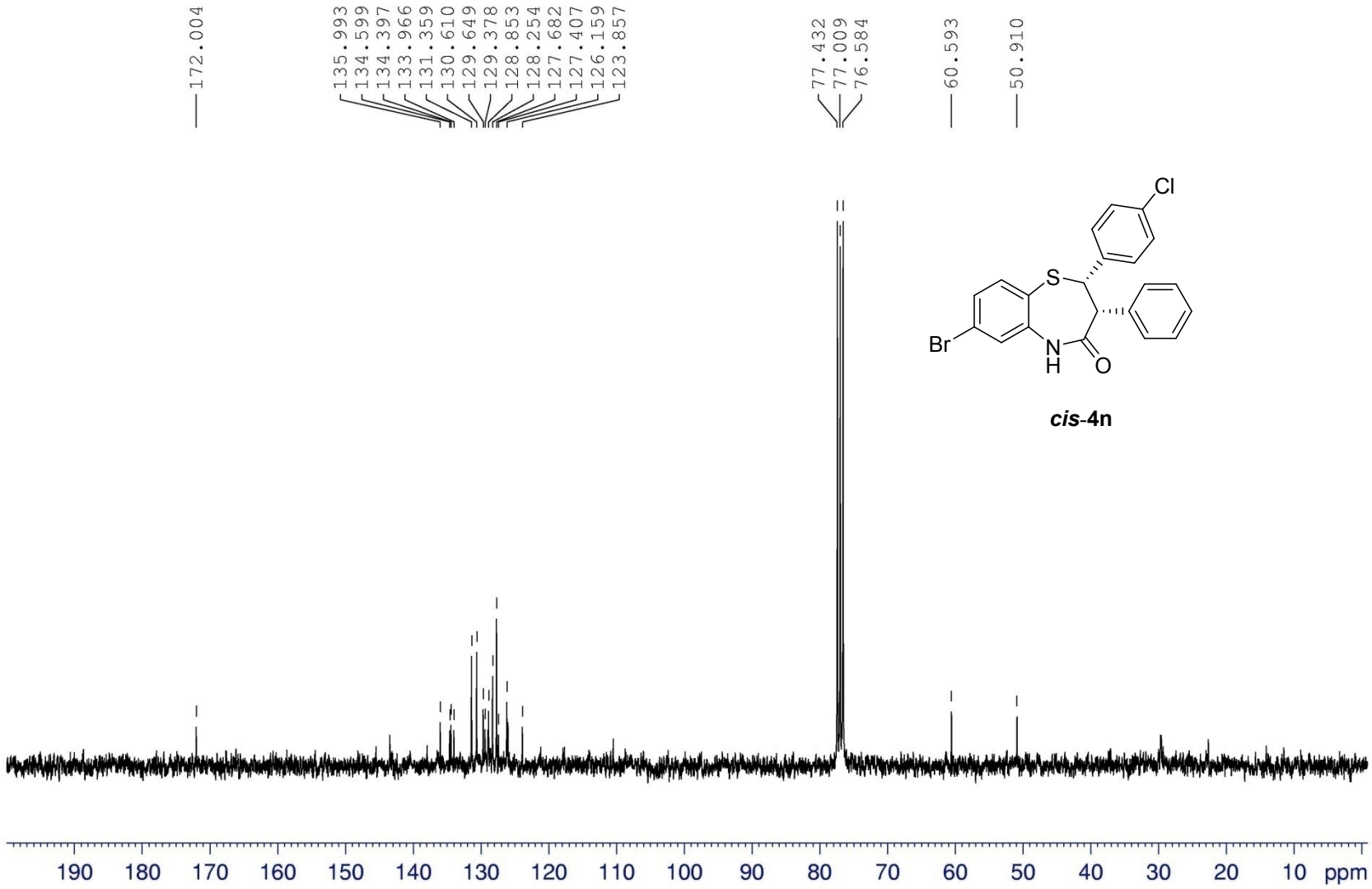
***trans*-4m**

^{1}H NMR in $CDCl_3$ (400 MHz)



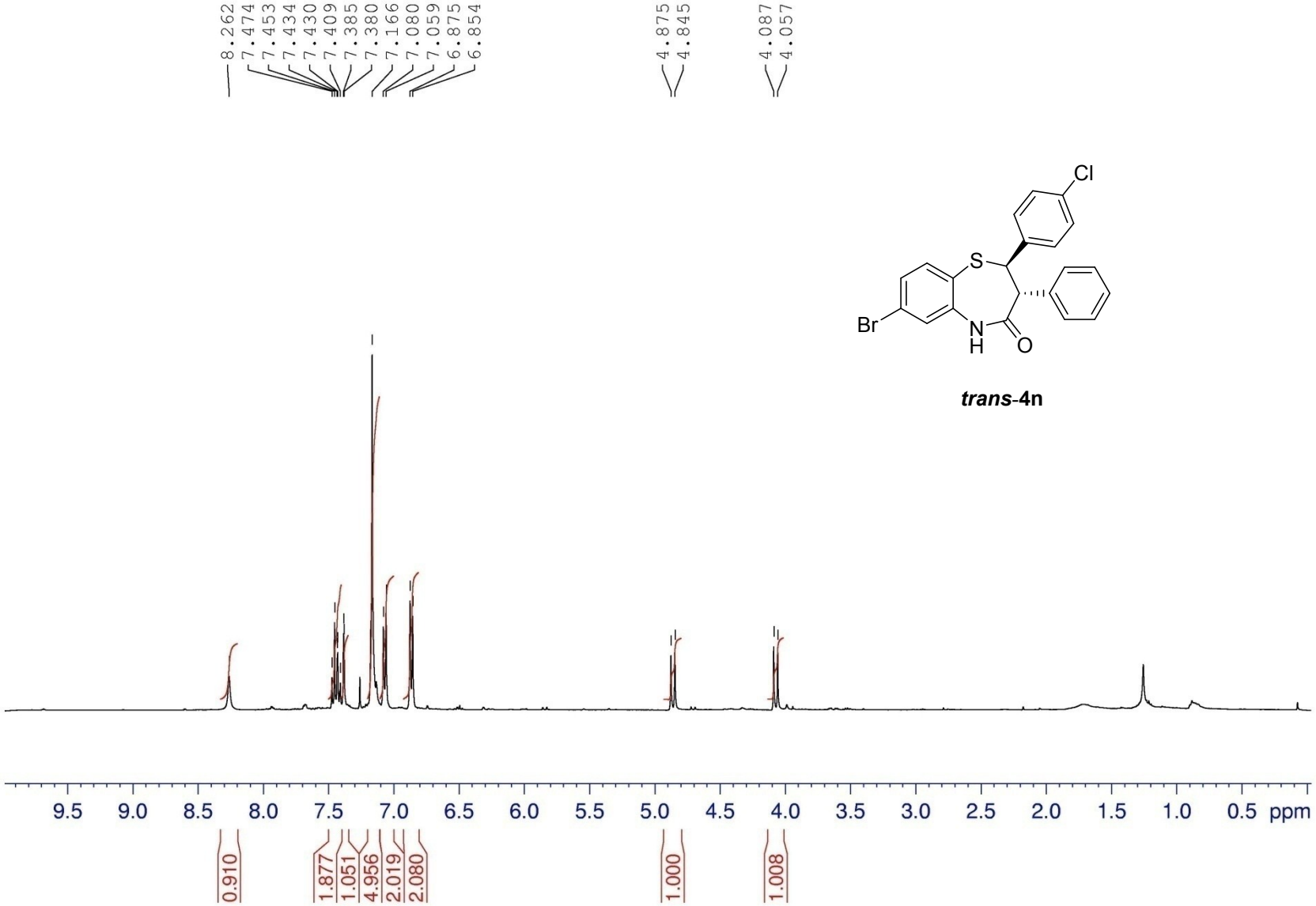
***cis*-4n**

^{13}C NMR in $CDCl_3$ (75 MHz)



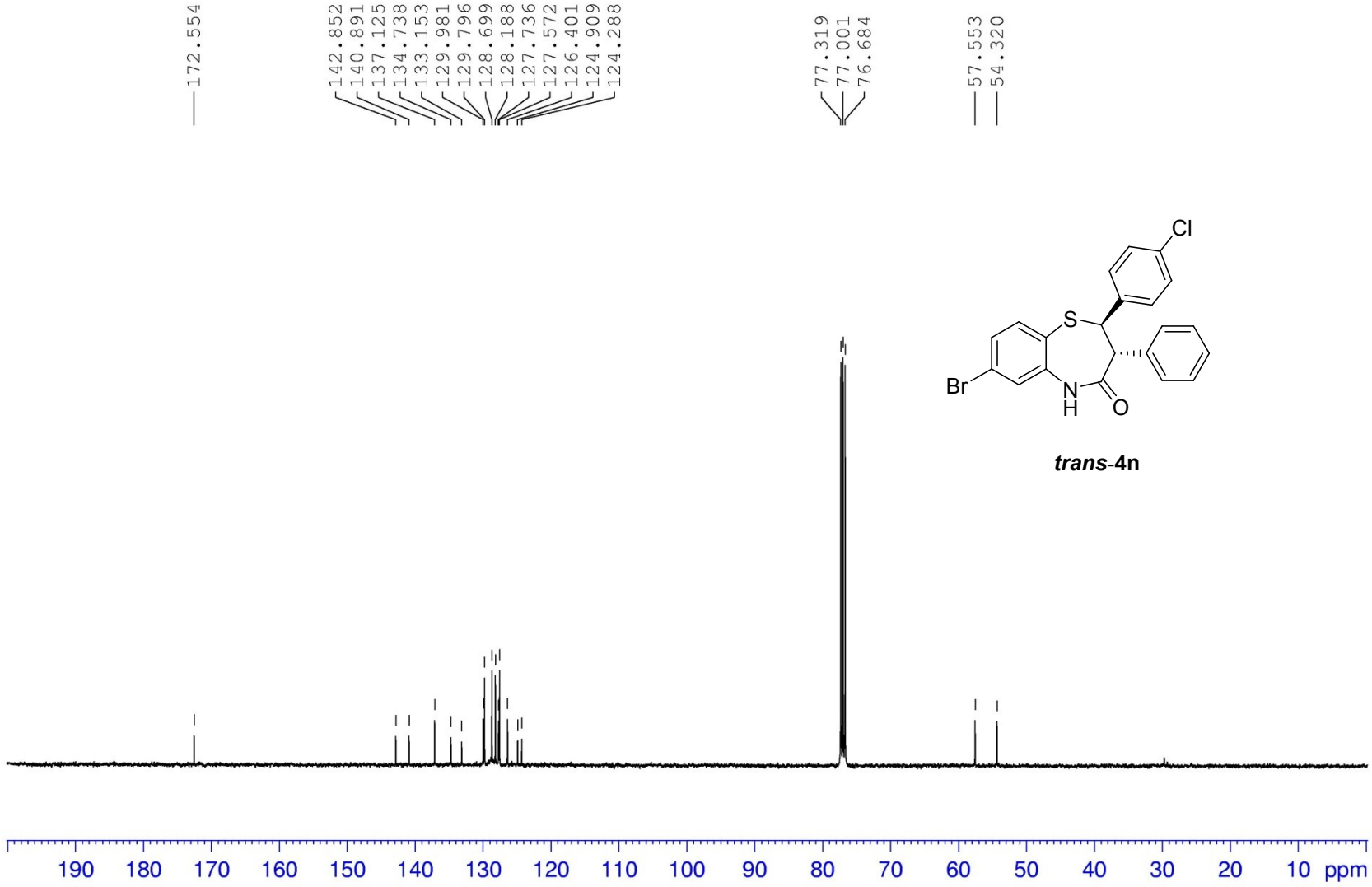
***cis*-4n**

^{1}H NMR in $CDCl_3$ (400 MHz)



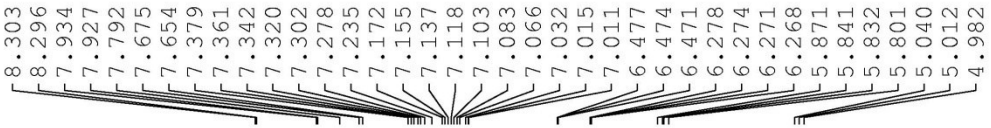
***trans*-4n**

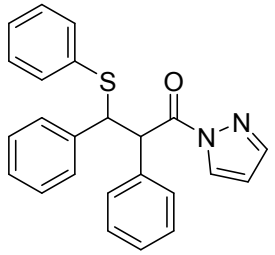
^{13}C NMR in $CDCl_3$ (100 MHz)



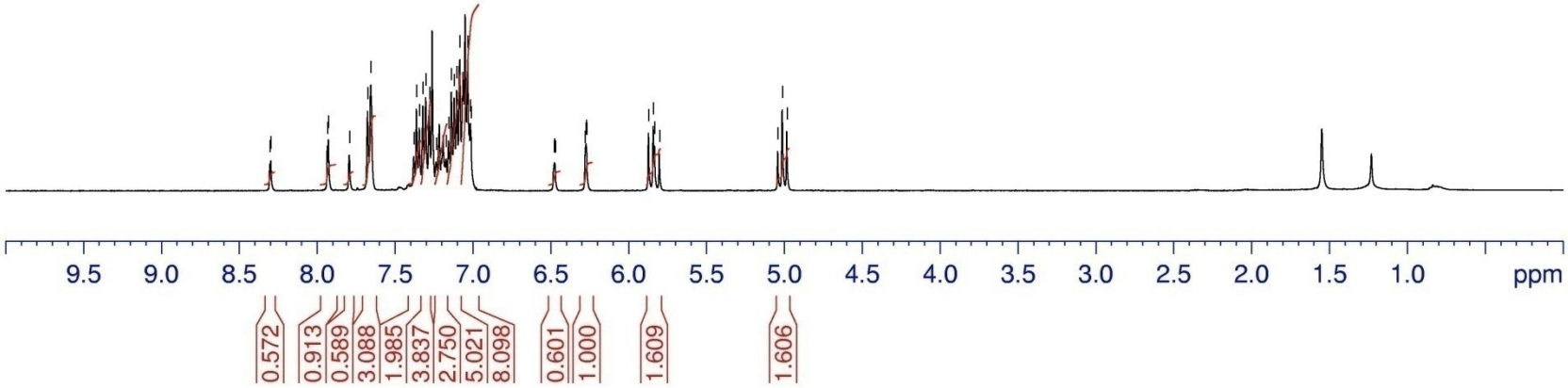
***trans*-4n**

^{1}H NMR in $CDCl_3$ (400 MHz)

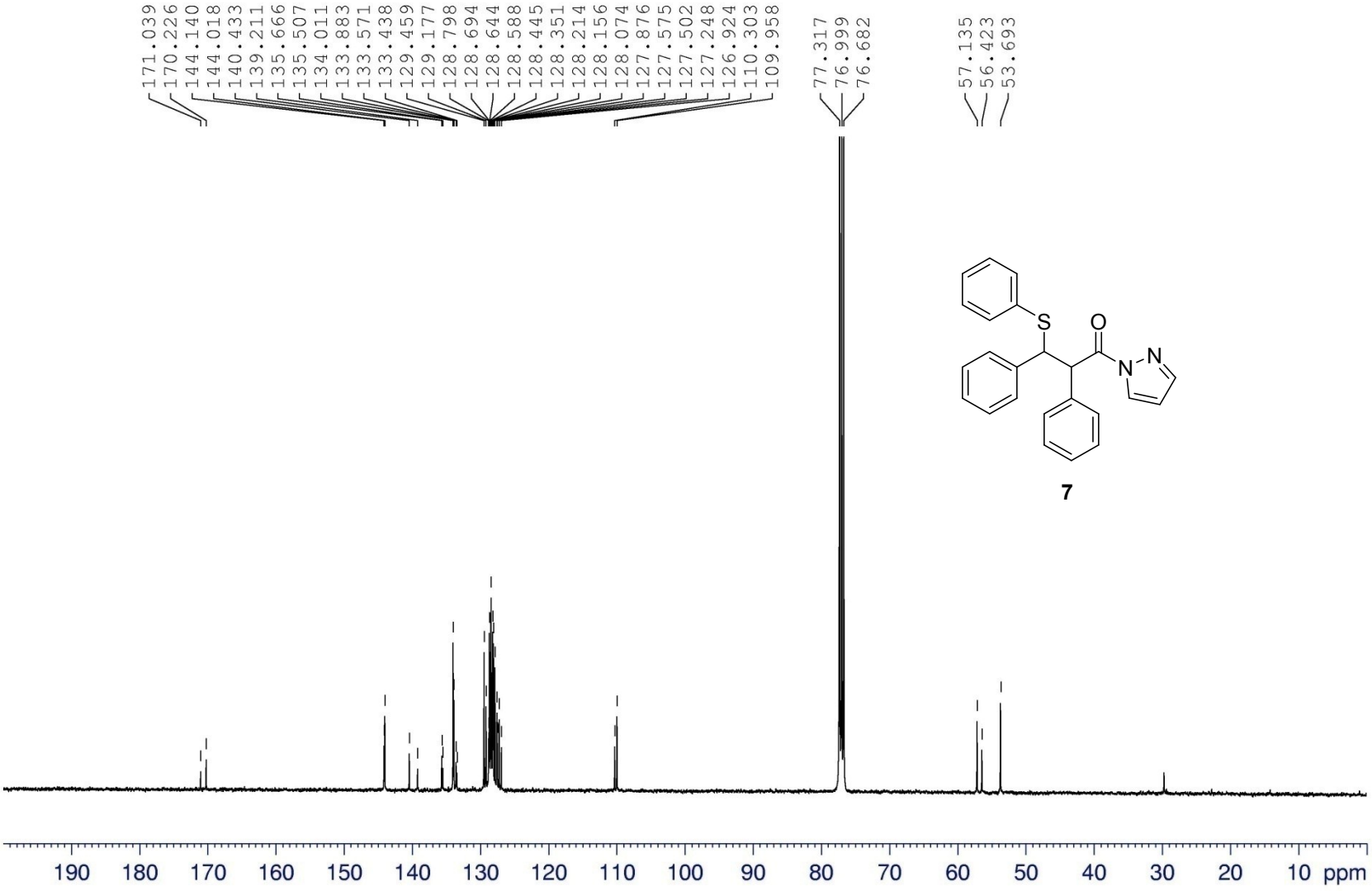




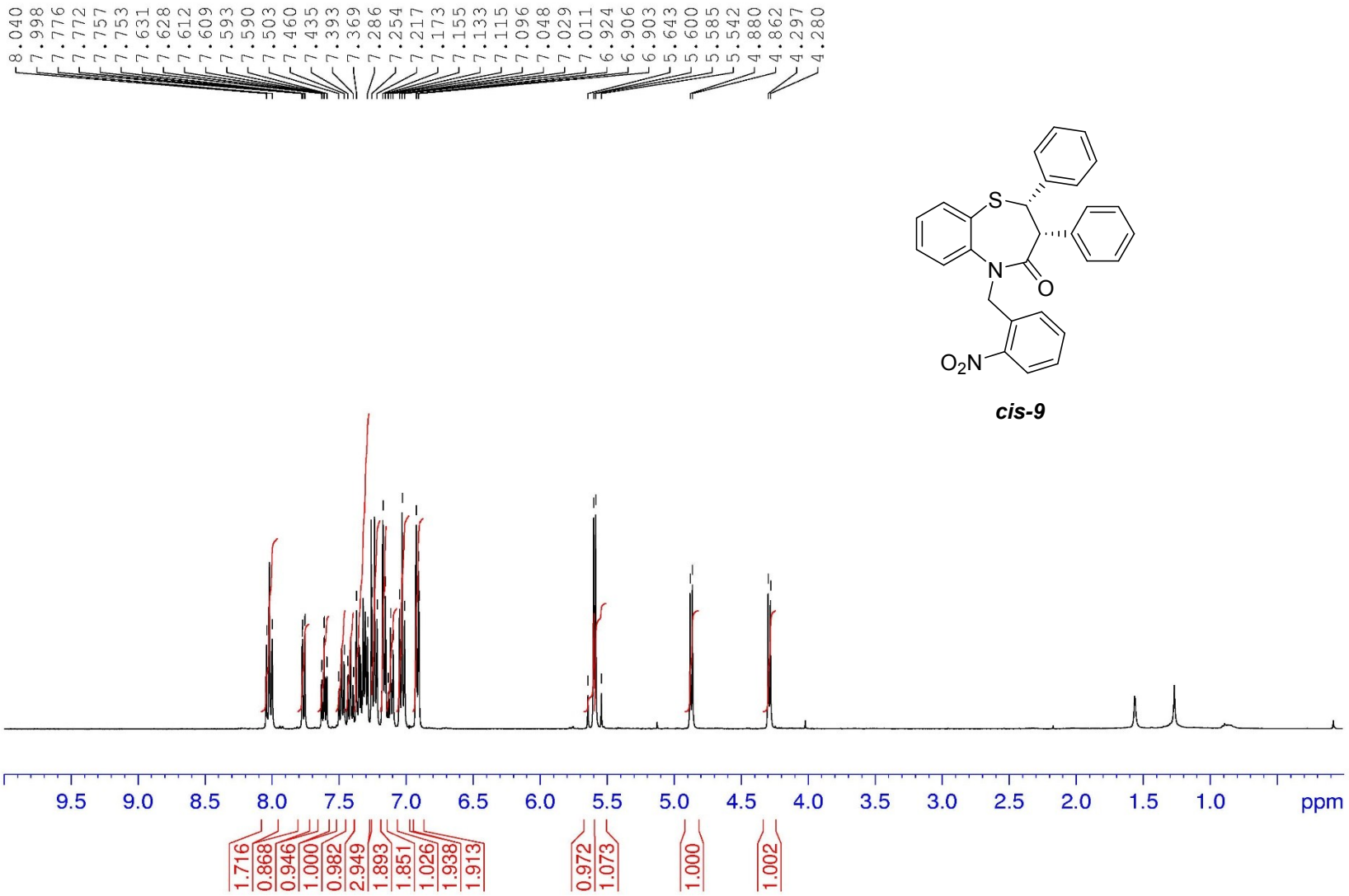
7



^{13}C NMR in $CDCl_3$ (100 MHz)

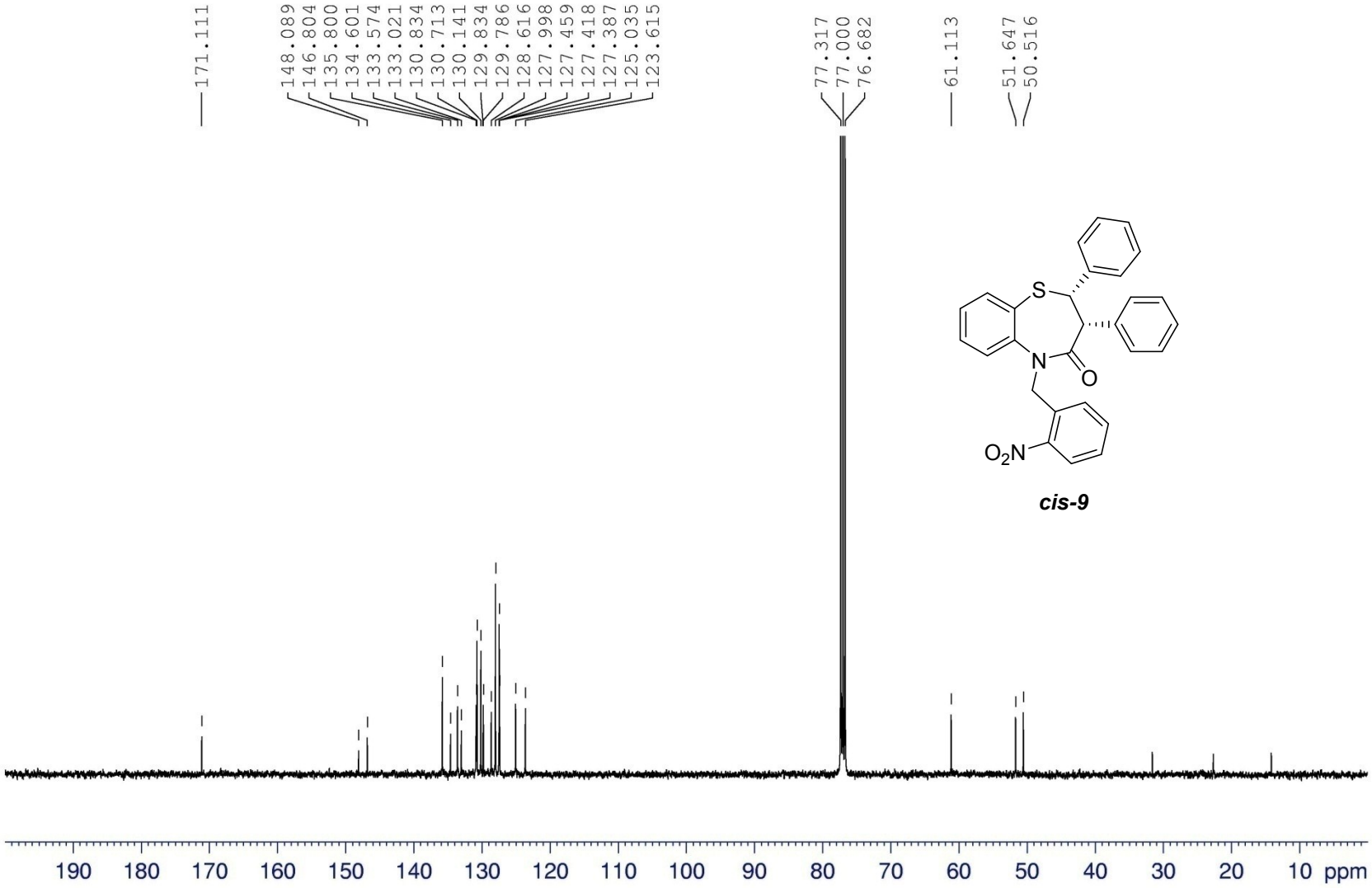


^{1}H NMR in $CDCl_3$ (400 MHz)



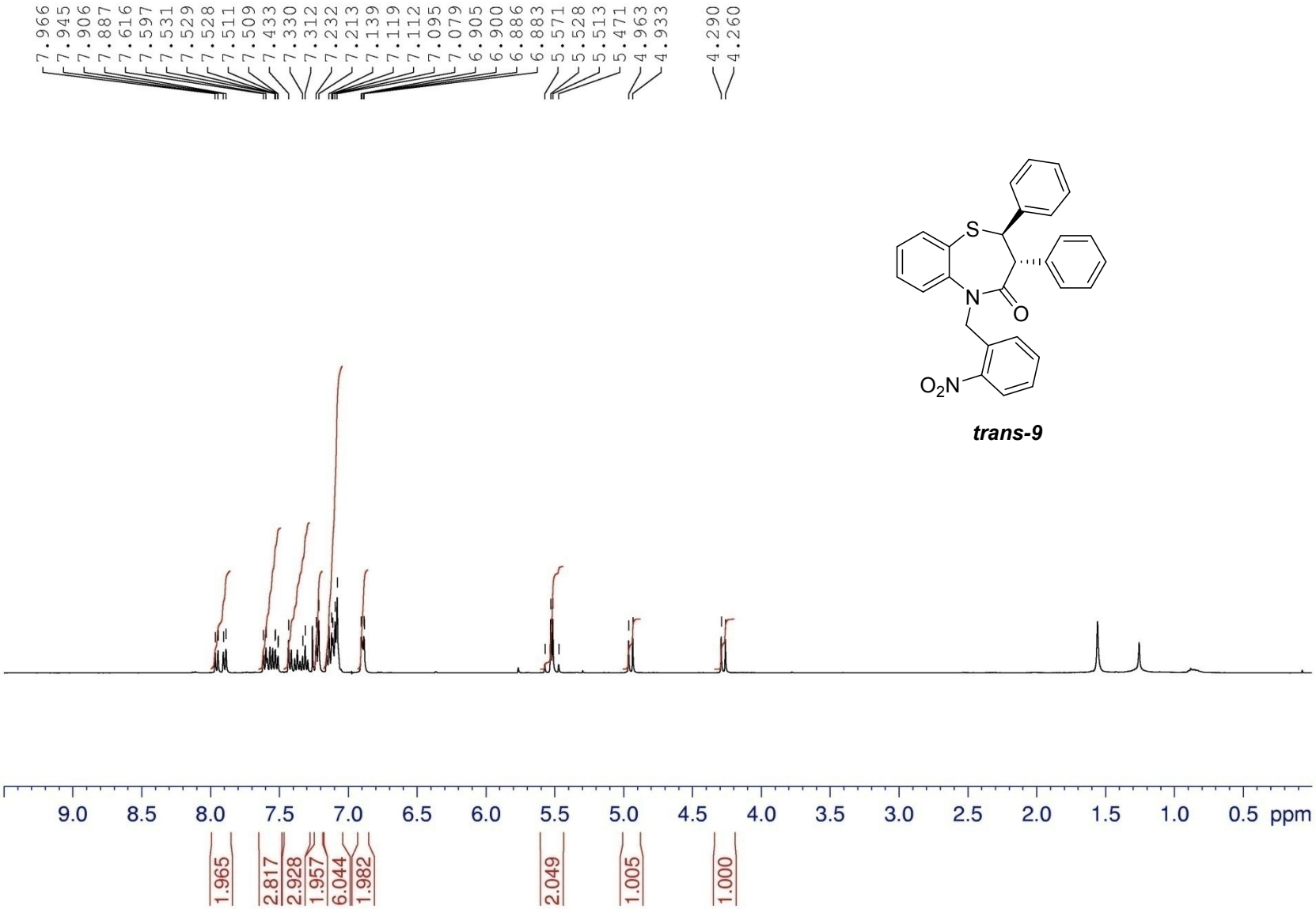
cis-9

^{13}C NMR in $CDCl_3$ (100 MHz)



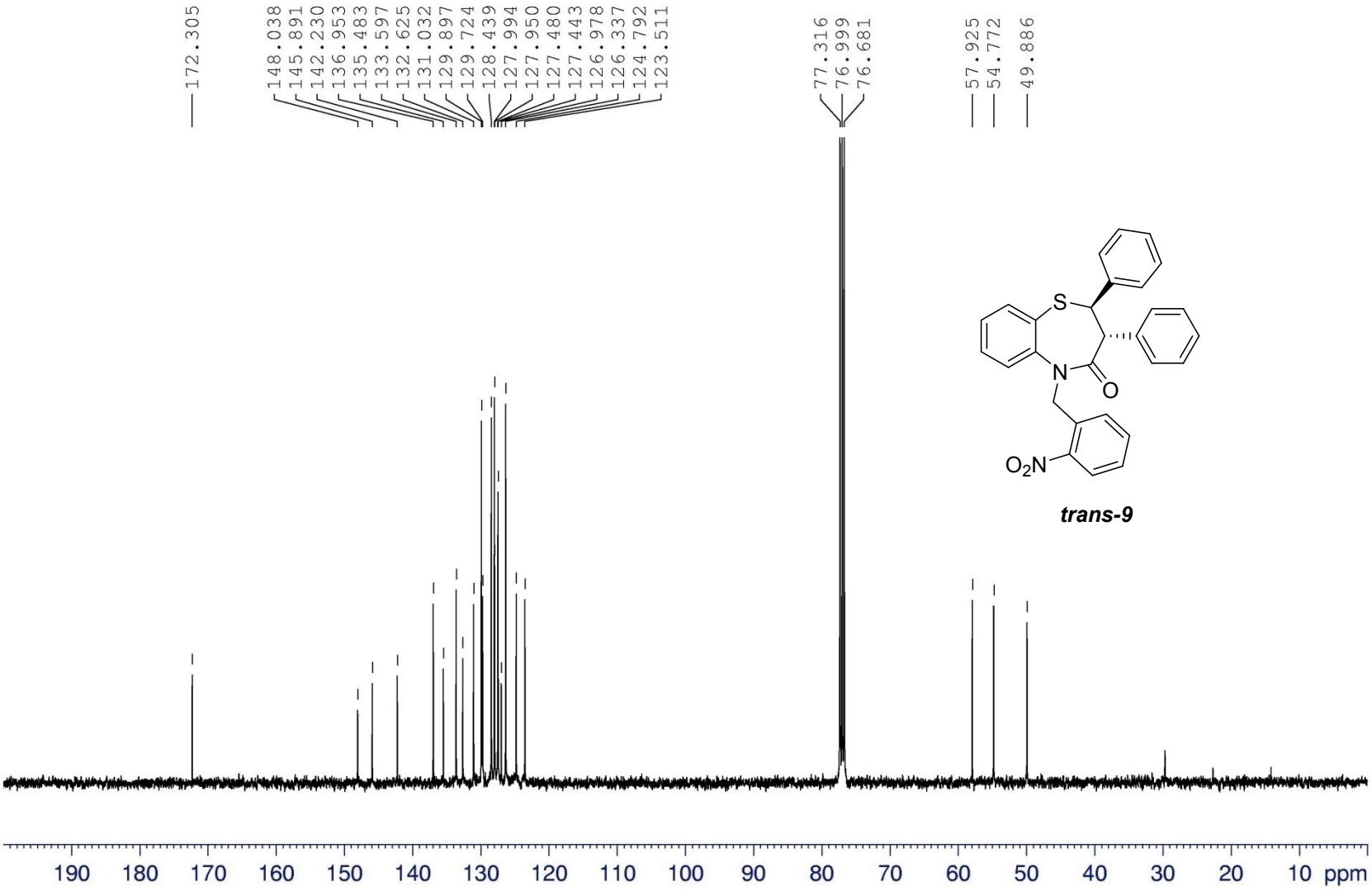
cis-9

^{1}H NMR in $CDCl_3$ (400 MHz)



trans-9

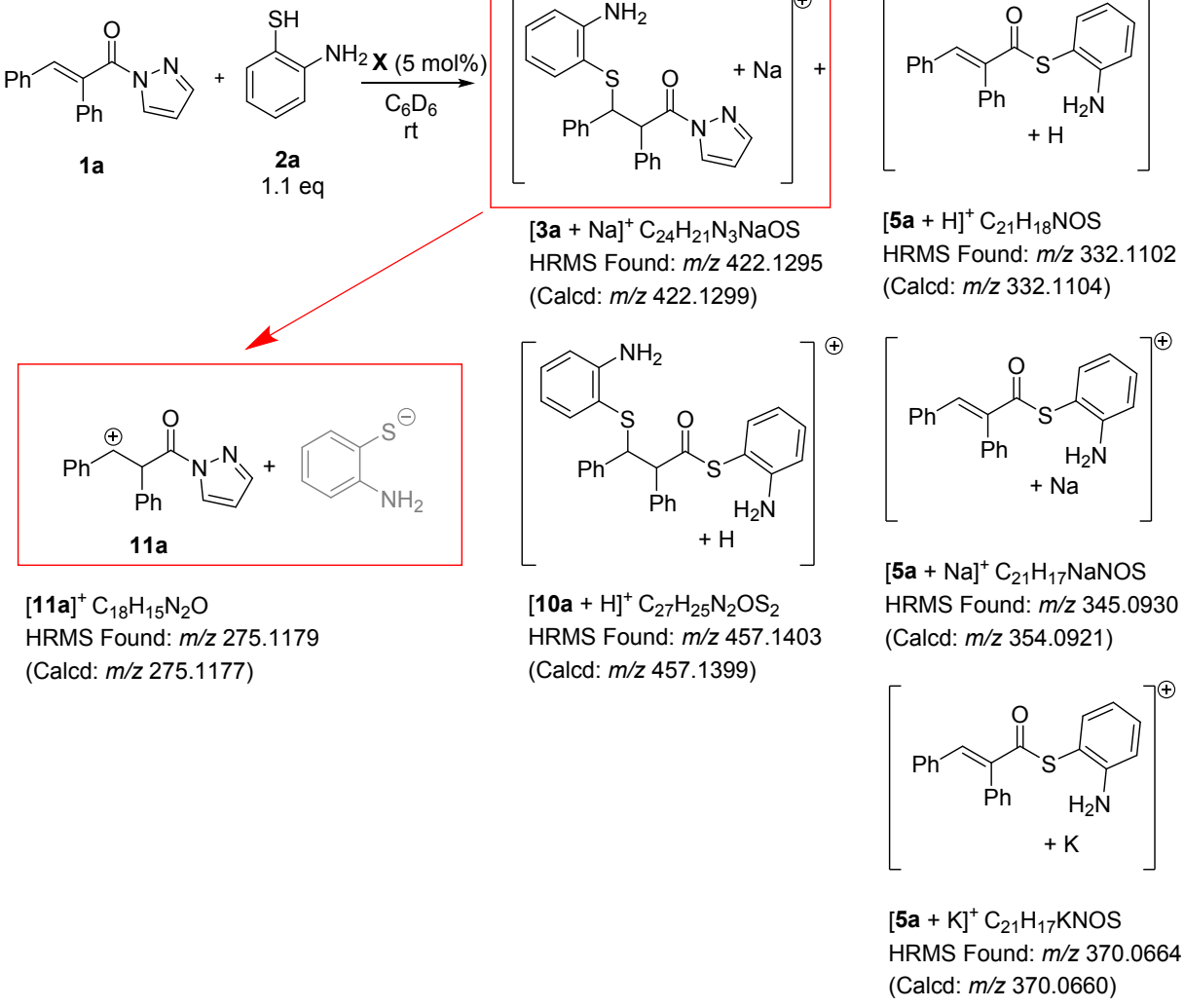
^{13}C NMR in $CDCl_3$ (100 MHz)

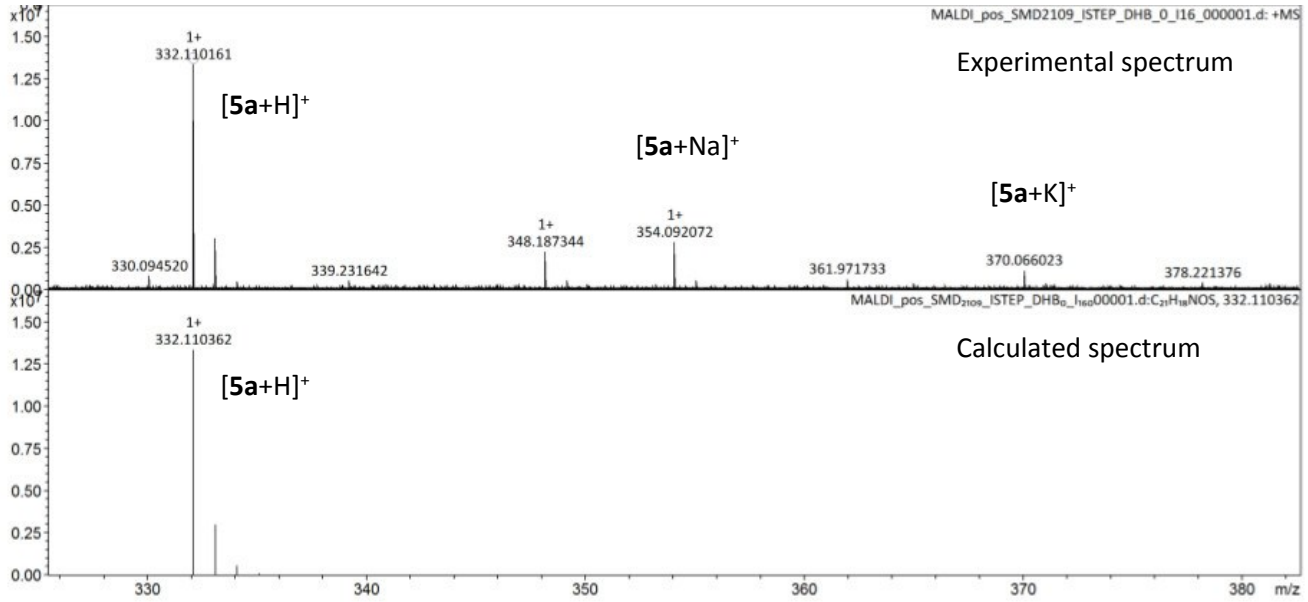


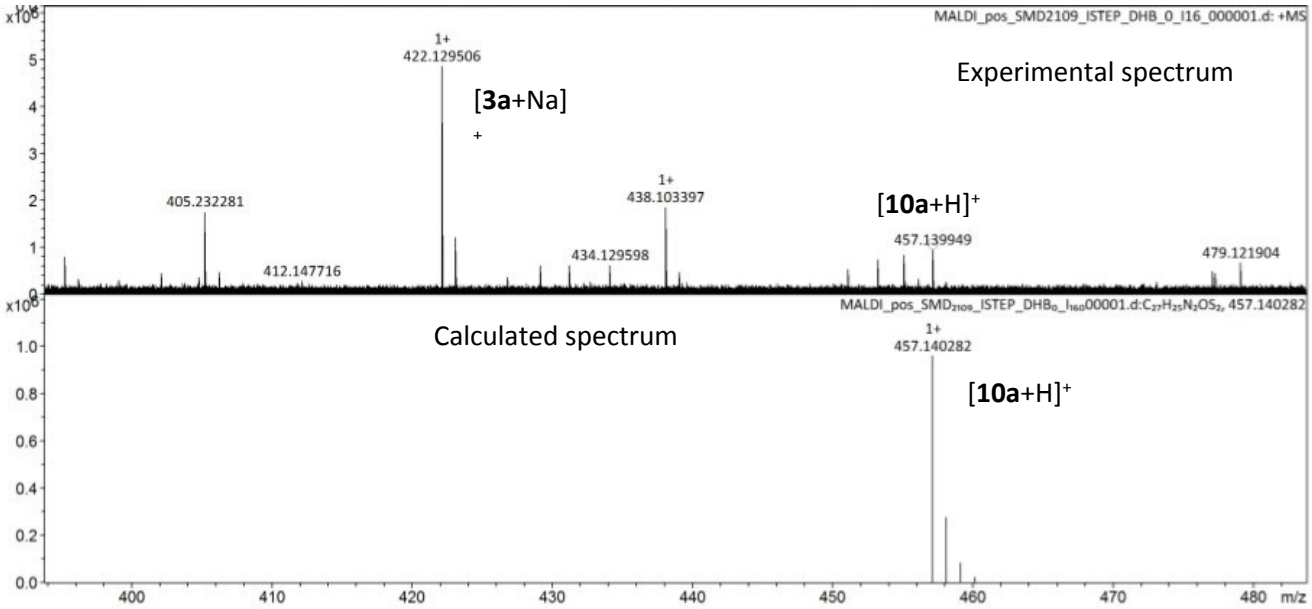
trans-9

HRMS Spectra

Figure S11. High resolution mass spectrometry analysis of the crude reaction mixture of model reaction with 5 mol% of catalyst **X** in C_6D_6 at room temperature




MALDI_pos_SMD2109_ISTEP_DHB_0_I16_000001.d: +MS
Experimental spectrum
1+
332.110161
[5a+H]+
[5a+Na]+
[5a+K]+
1+
348.187344
1+
354.092072
330.094520
339.231642
361.971733
370.066023
378.221376
MALDI_pos_SMD2109_ISTEP_DHB_0_I16_000001.d:C21H18NOS, 332.110362
Calculated spectrum
1+
332.110362
[5a+H]+
330
340
350
360
370
380
m/z


MALDI_pos_SMD2109_ISTEP_DHB_0_I16_000001.d: +MS
Experimental spectrum
1+
422.129506
[3a+Na]+
405.232281
412.147716
434.129598
1+
438.103397
[10a+H]+
457.139949
479.121904
MALDI_pos_SMD2109_ISTEP_DHB_0_I16_000001.d:C27H25N2OS2, 457.140282
Calculated spectrum
1+
457.140282
[10a+H]+
400
410
420
430
440
450
460
470
480
m/z

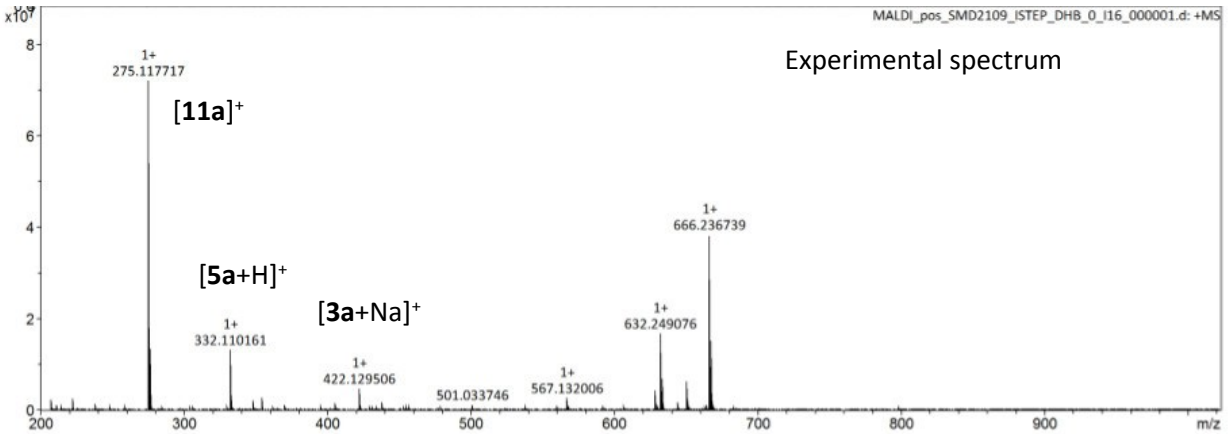
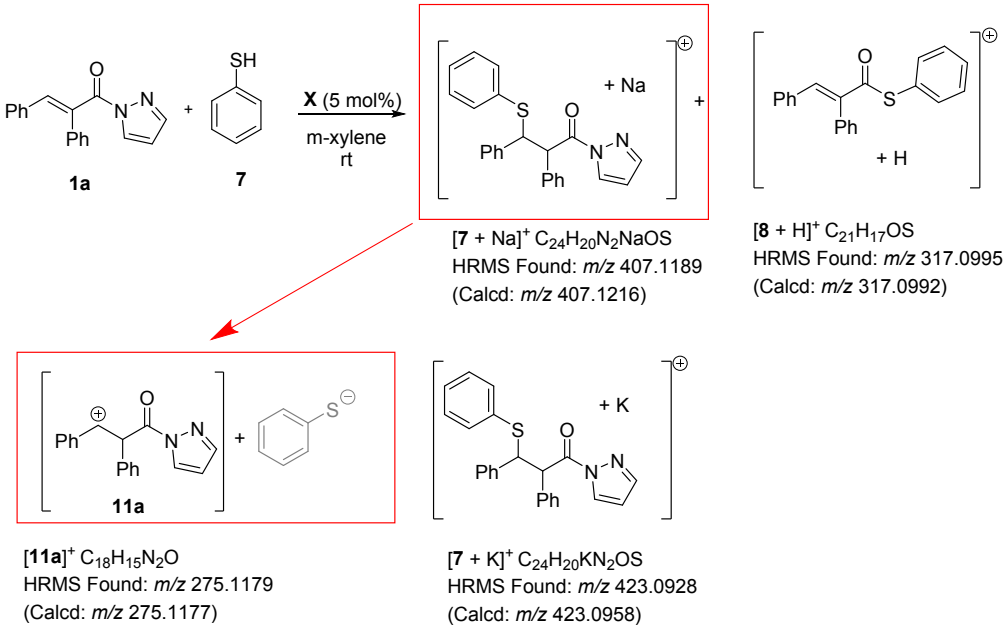
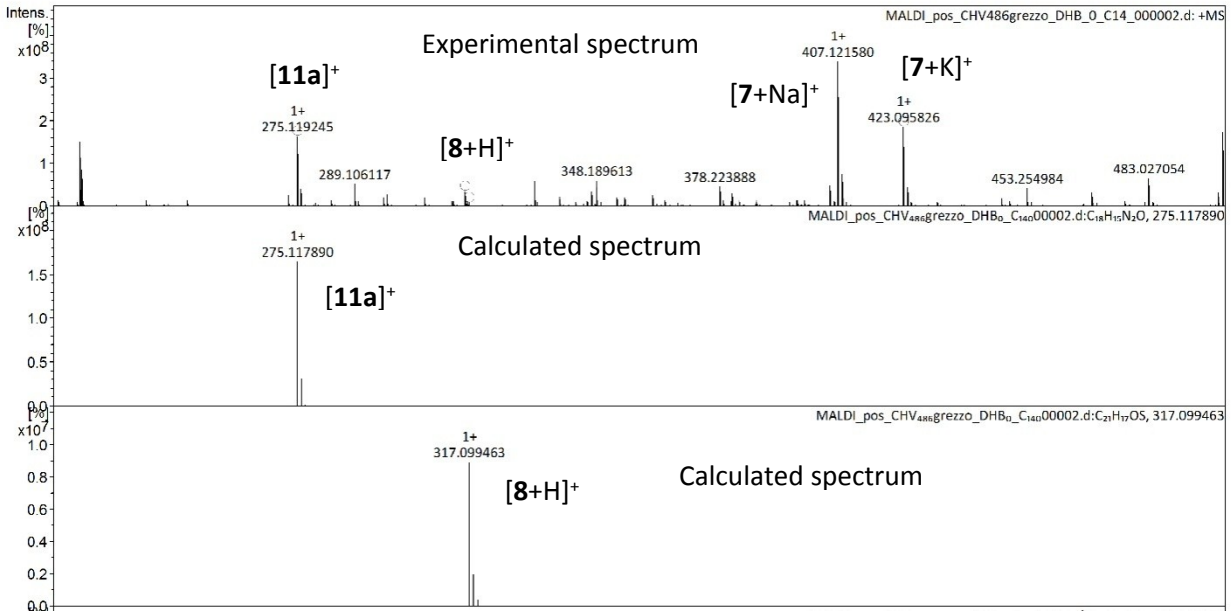
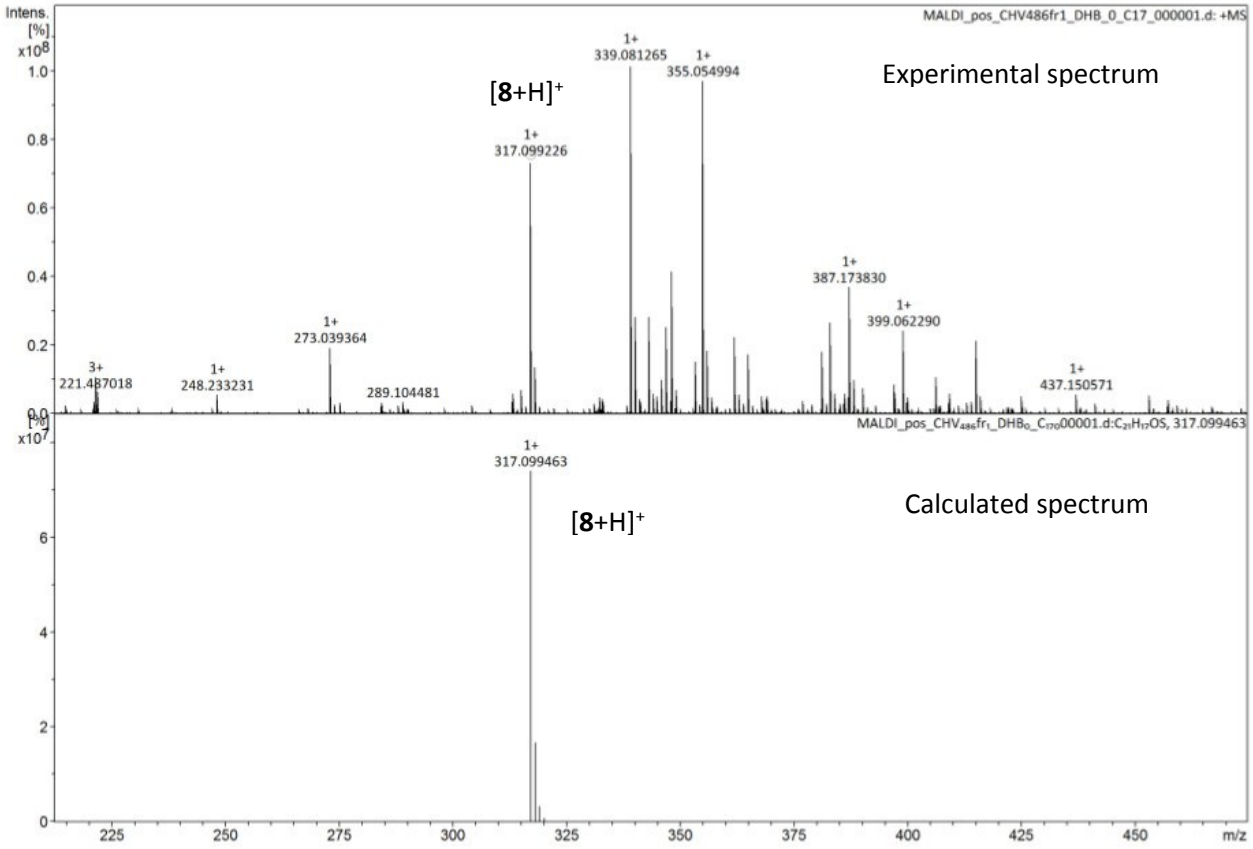

MALDI_pos_SMD2109_ISTEP_DHB_0_I16_000001.d: +MS
Experimental spectrum
1+
275.117717
[11a]+
[5a+H]+
[3a+Na]+
1+
666.236739
1+
632.249076
1+
332.110161
1+
422.129506
501.033746
1+
567.132006
200
300
400
500
600
700
800
900
m/z

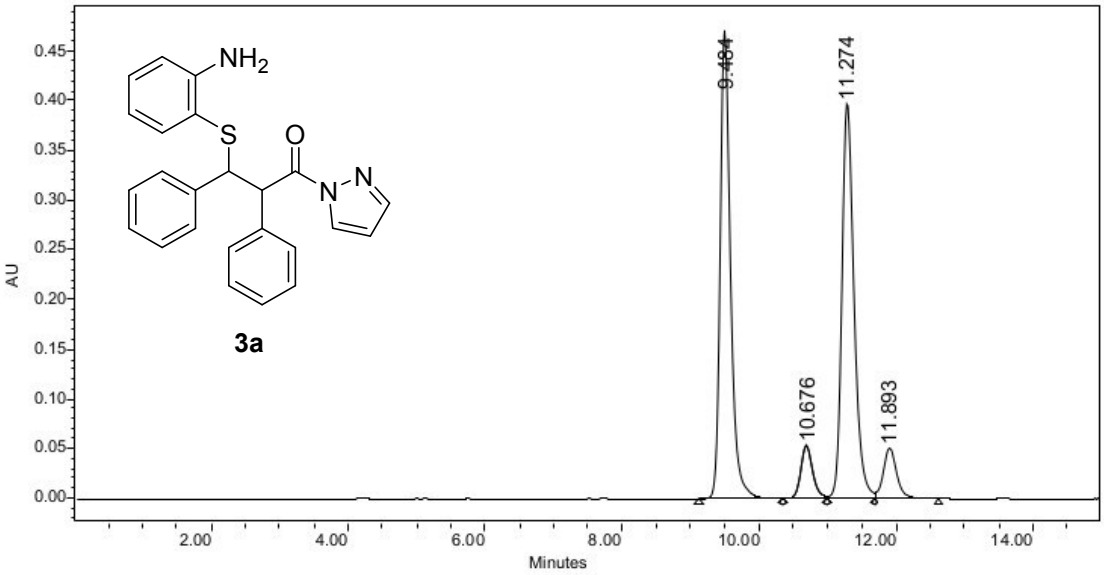
Figure S12. High resolution mass spectrometry analysis of the crude reaction mixture of asymmetric sulfa-Michael reaction of **1a** with thiophenol with 5 mol% of catalyst **X** in C_6D_6 at room temperature (Scheme 3 in the paper).



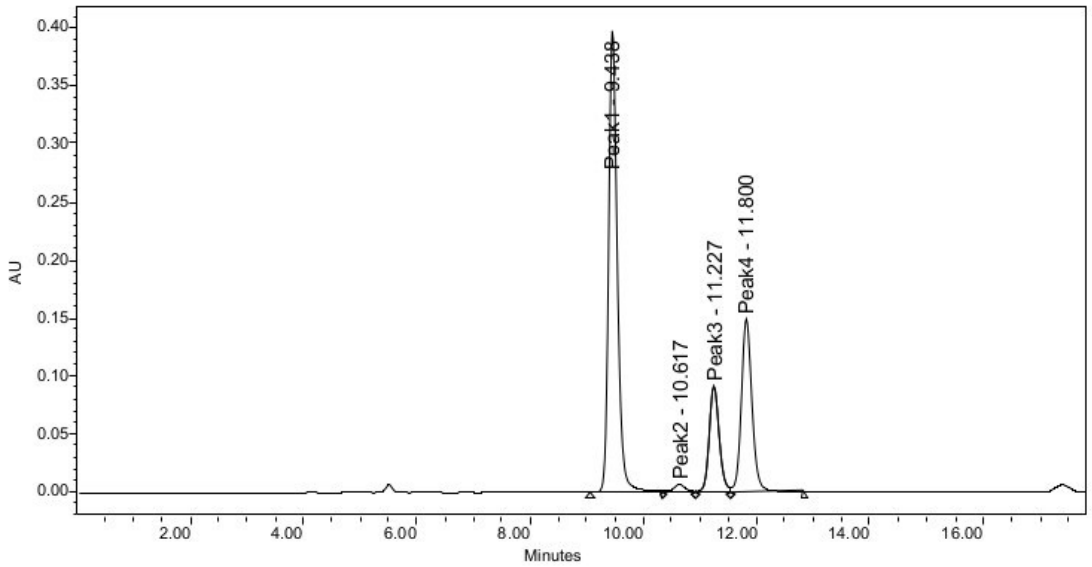



MALDI_pos_CHV486fr1_DHB_0_C17_000001.d: +MS
Intens.
[%]
x10^8
1.0
0.8
0.6
0.4
0.2
0.0
1+
339.081265
1+
355.054994
[8+H]+
1+
317.099226
Experimental spectrum
1+
387.173830
1+
399.062290
1+
273.039364
3+
221.487018
1+
248.233231
289.104481
1+
437.150571
MALDI_pos_CHV486fr1_DHB0_C17000001.d:C21H17OS, 317.099463
x10^7
6
4
2
0
1+
317.099463
[8+H]+
Calculated spectrum
225
250
275
300
325
350
375
400
425
450
m/z

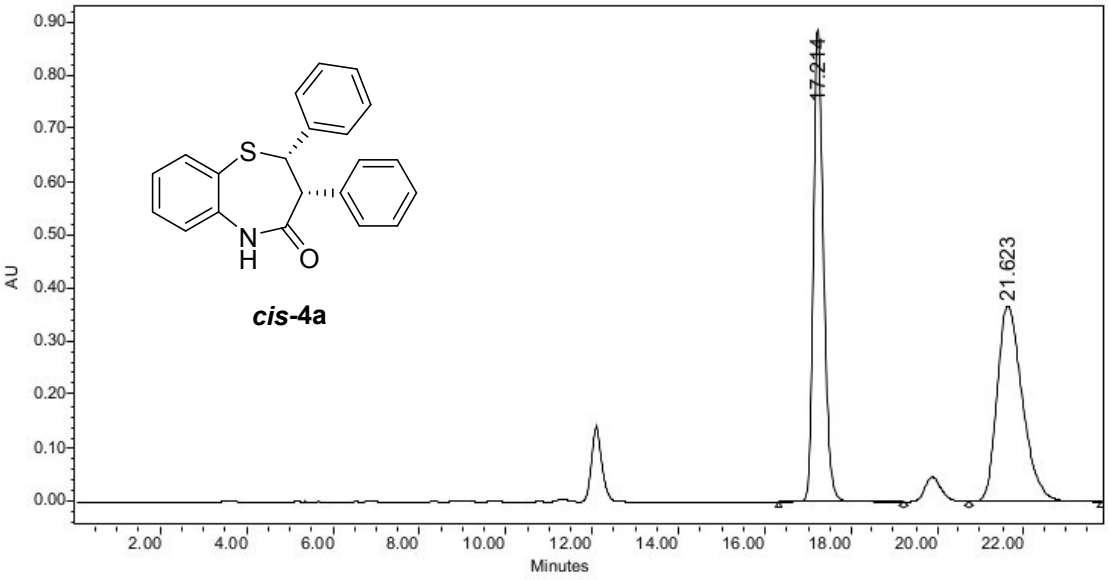
HPLC Chromatograms



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.484	4929943	44.08	471367	48.31
2	10.676	657361	5.88	53774	5.51
3	11.274	4900658	43.82	398995	40.89
4	11.893	696904	6.23	51597	5.29

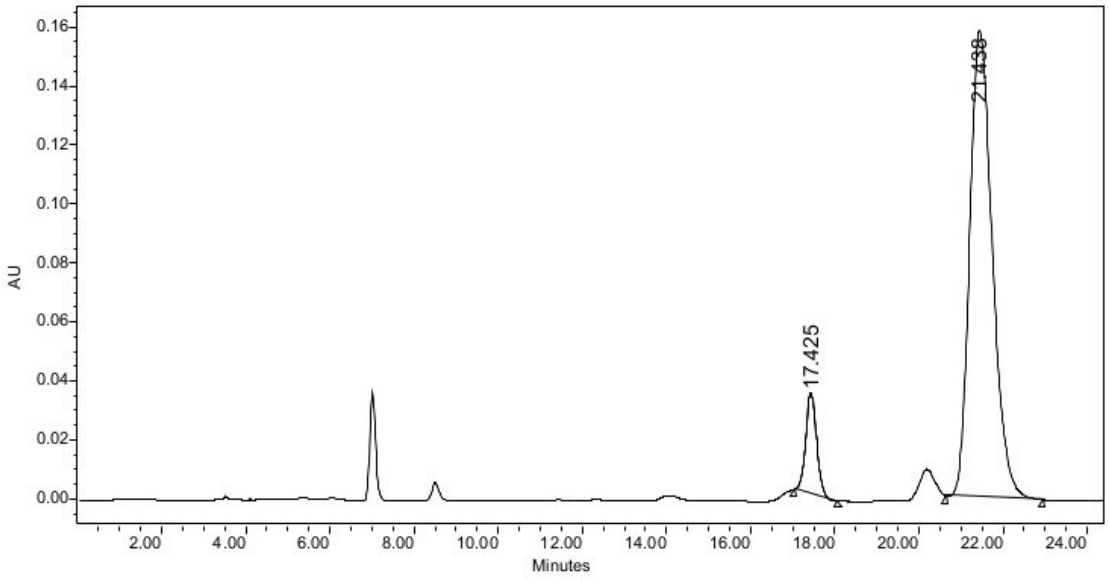


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	9.438	4252111	57.10	398399	61.64
2	Peak2	10.617	101942	1.37	6777	1.05
3	Peak3	11.227	1138027	15.28	92135	14.25
4	Peak4	11.800	1954739	26.25	149030	23.06

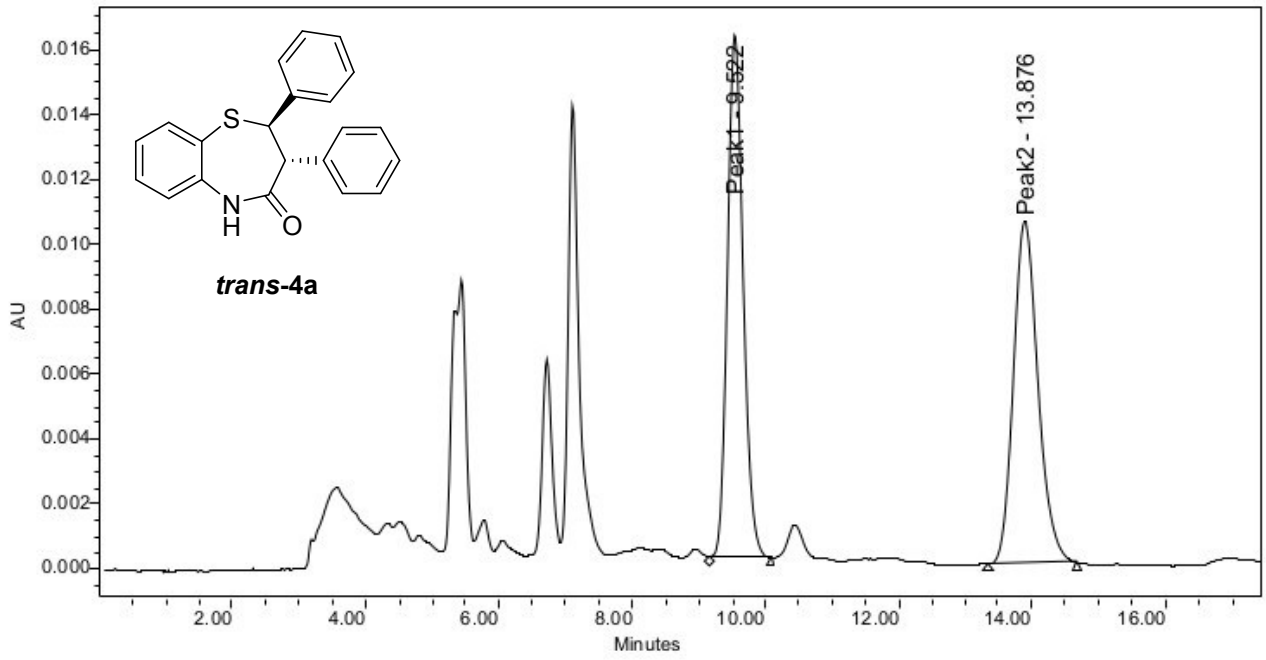


***cis*-4a**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	17.214	14709921	49.49	886466	70.66
2	21.623	15011600	50.51	368116	29.34

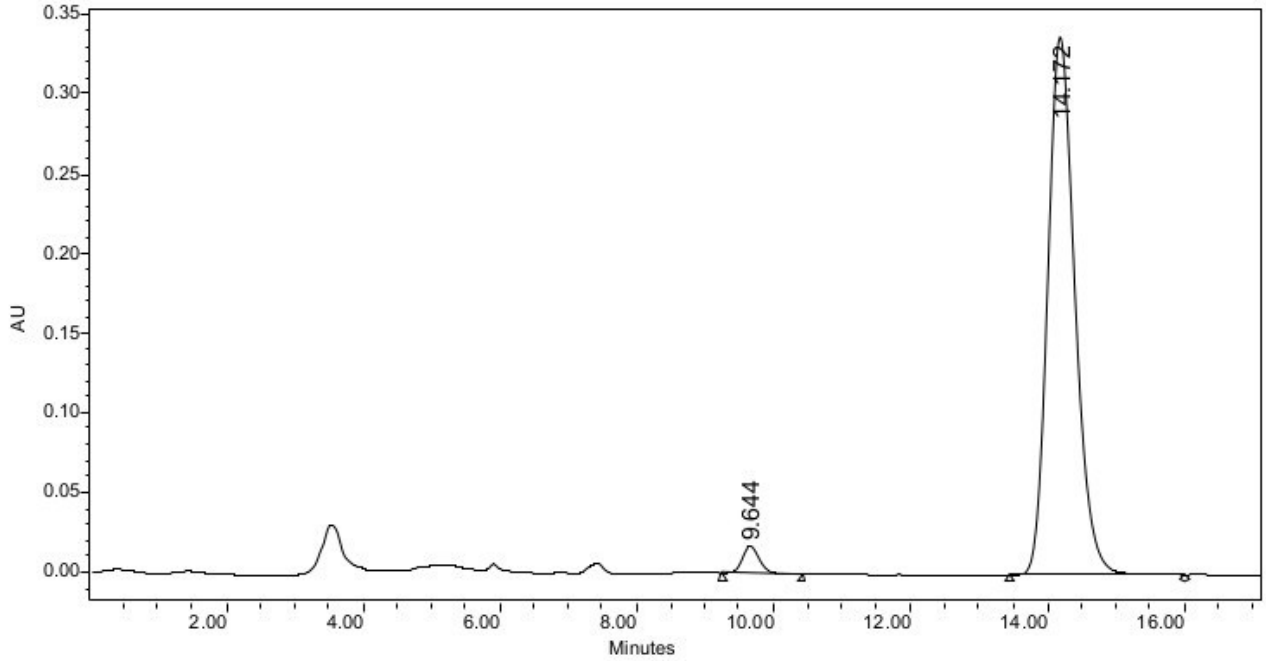


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	17.425	611531	9.39	33912	17.67
2	21.438	5898347	90.61	158020	82.33

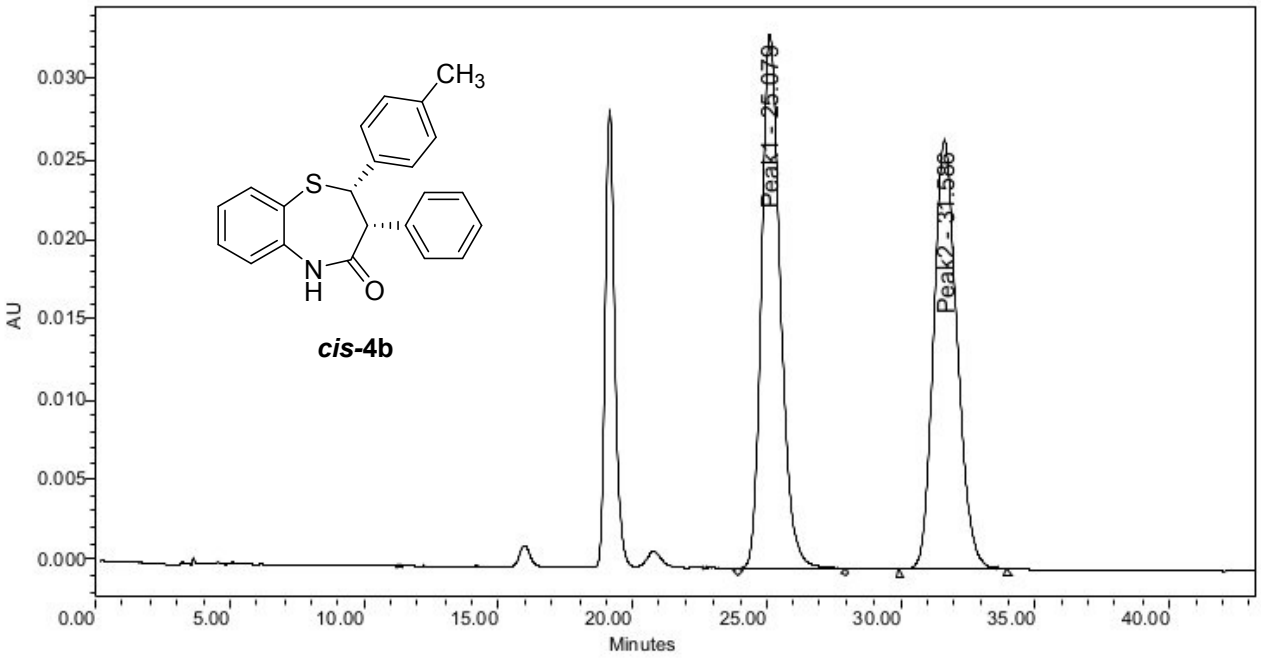


***trans*-4a**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	9.522	264929	49.46	16100	60.48
2	Peak2	13.876	270718	50.54	10521	39.52

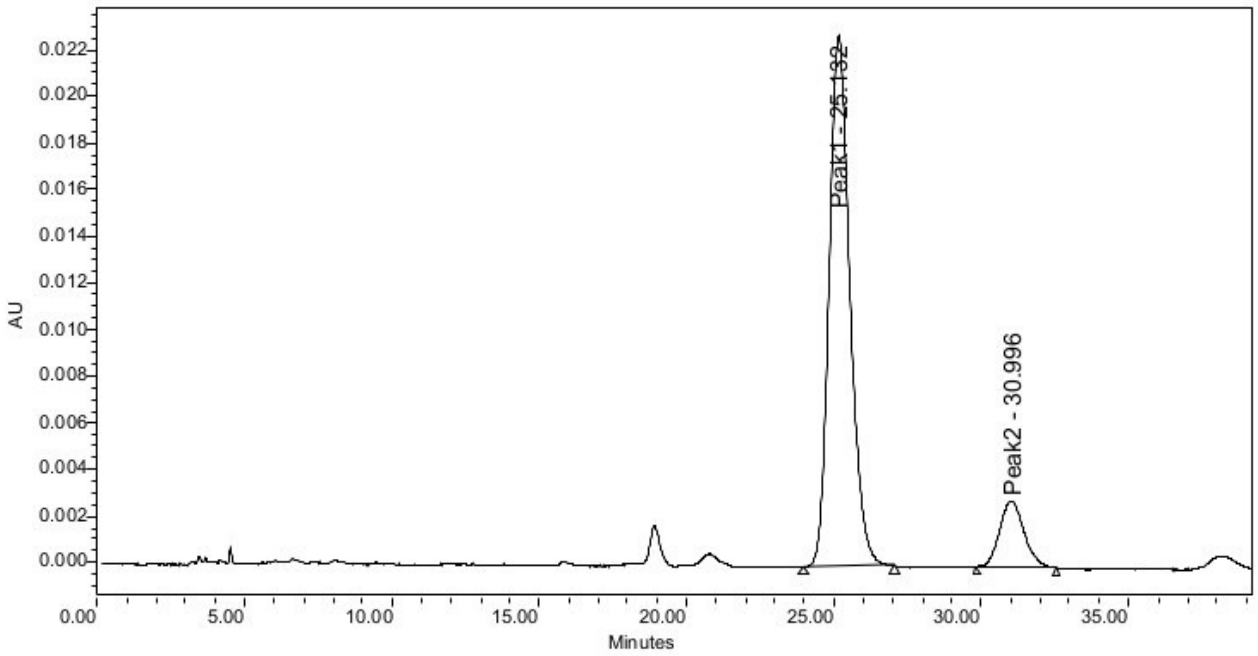


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.644	298864	3.11	17220	4.85
2	14.172	9314870	96.89	338079	95.15

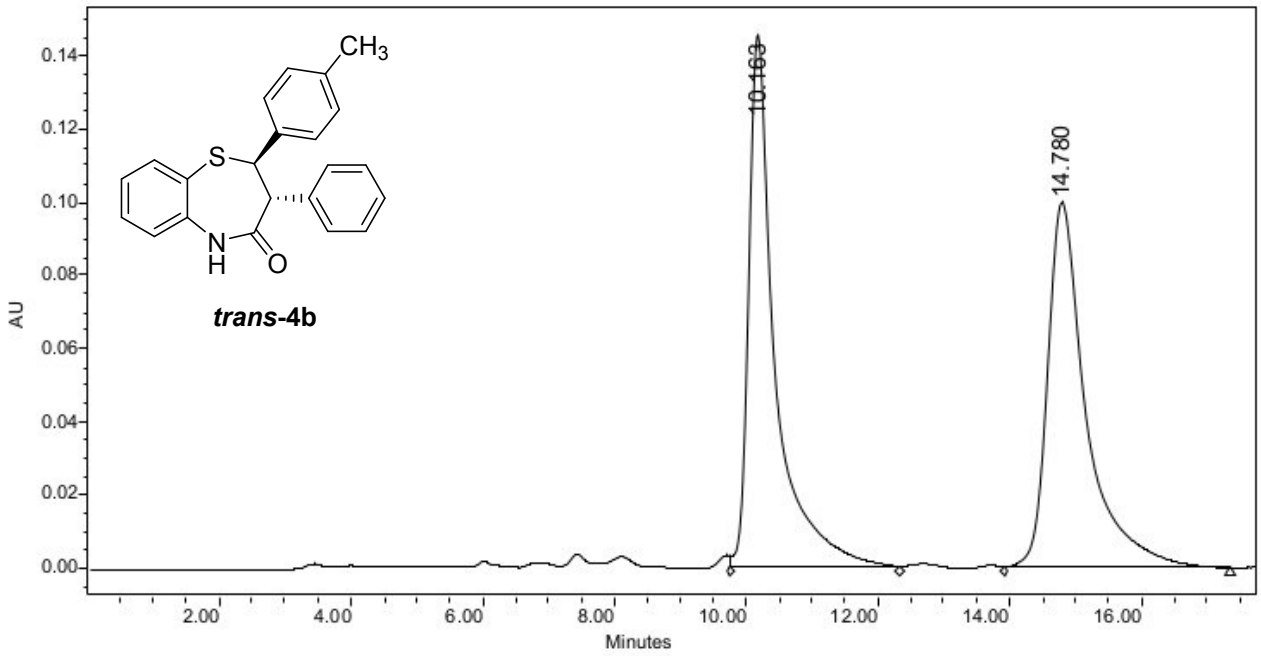


***cis*-4b**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	25.079	1649074	50.23	33351	55.43
2	Peak2	31.586	1634151	49.77	26819	44.57

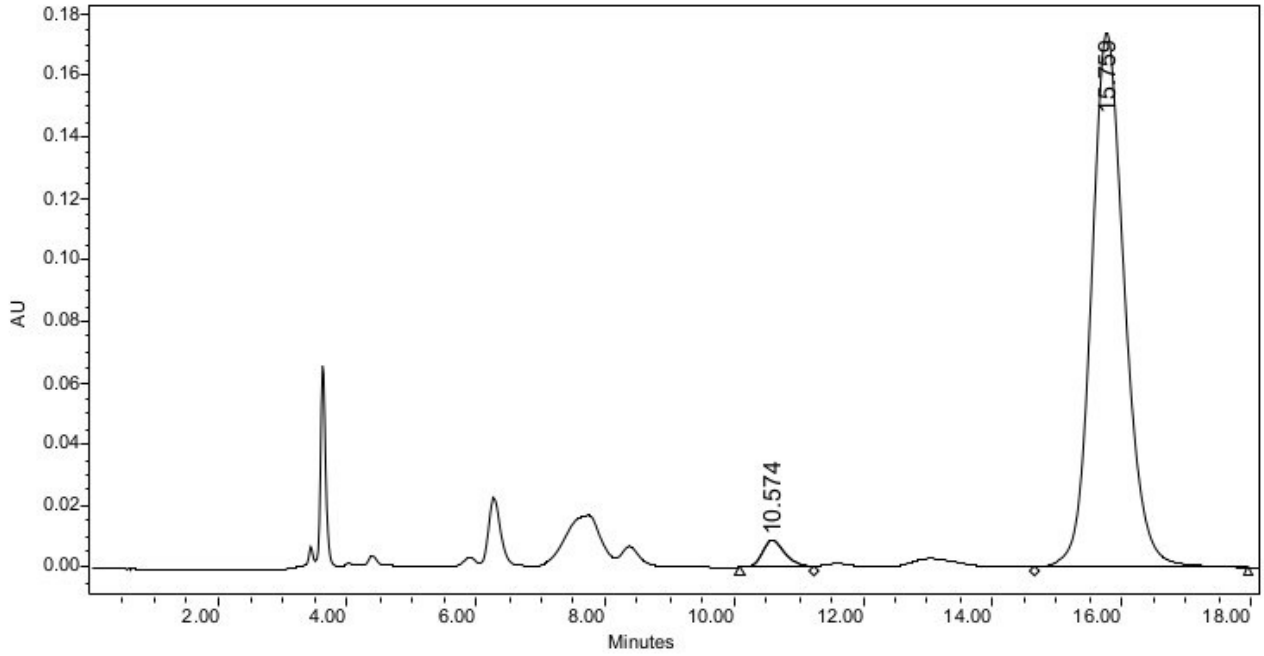


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	25.132	1115729	87.09	22791	88.88
2	Peak2	30.996	165396	12.91	2852	11.12

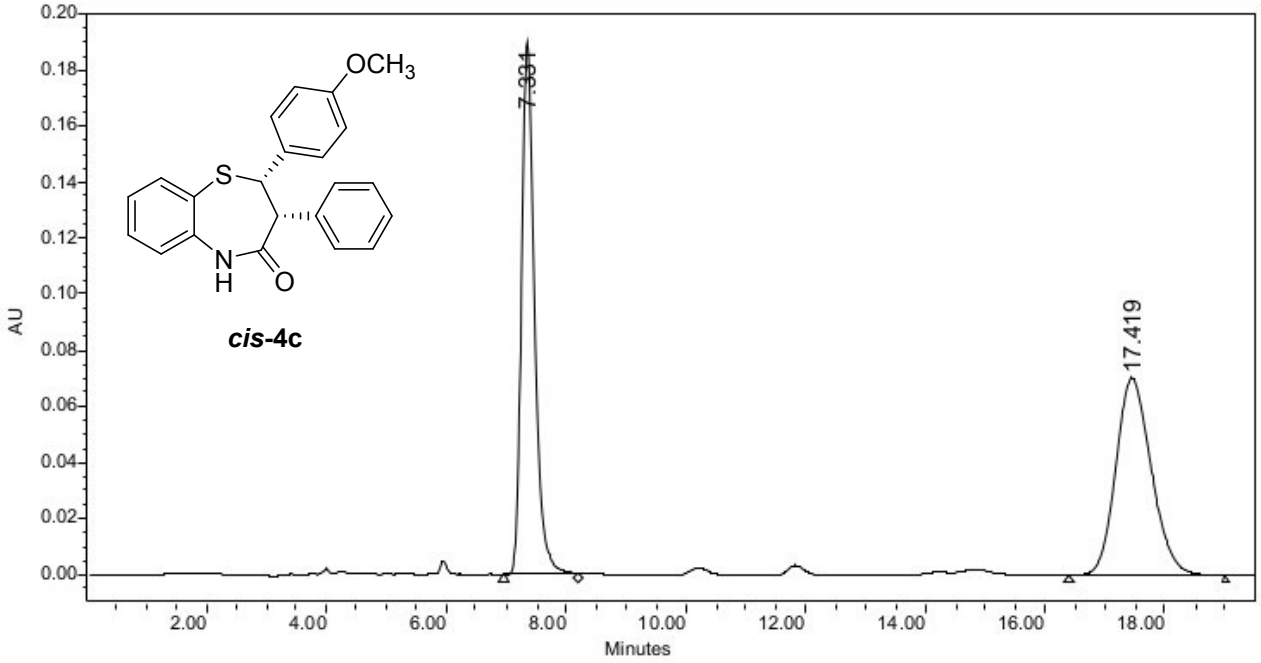


***trans*-4b**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.163	4093067	50.09	145747	59.32
2	14.780	4078671	49.91	99966	40.68

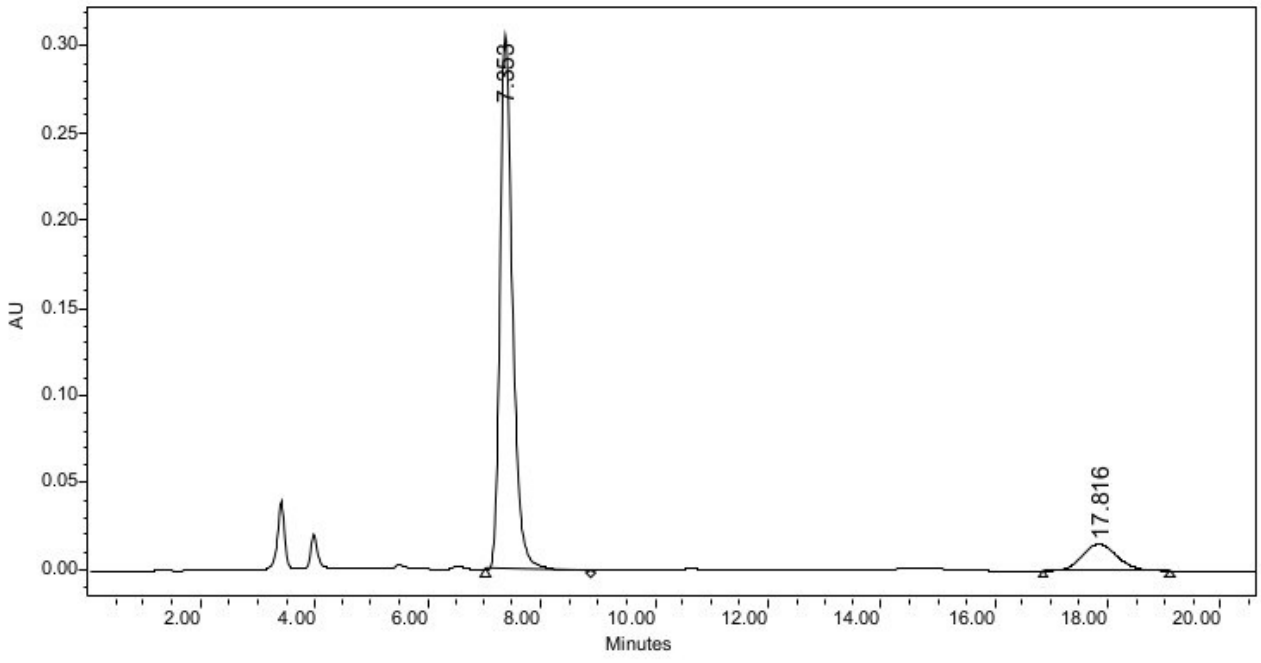


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.574	218561	3.39	8792	4.81
2	15.759	6229702	96.61	173953	95.19

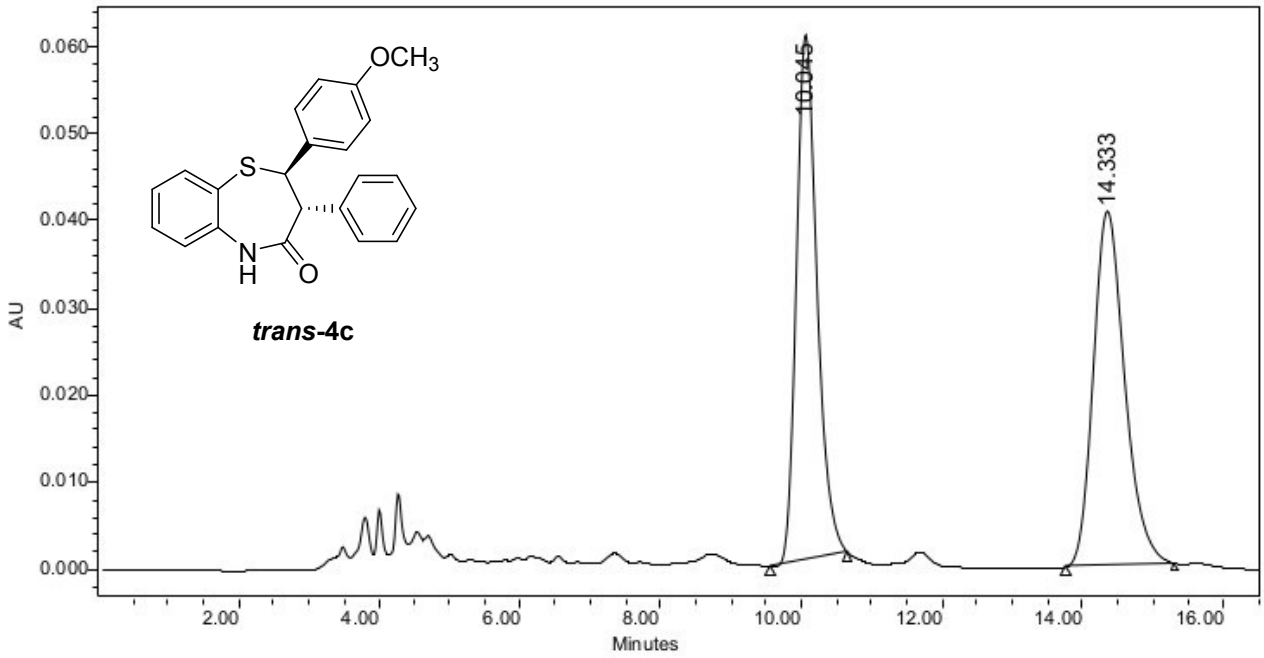


***cis*-4c**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.331	2889635	49.89	190448	72.98
2	17.419	2902357	50.11	70523	27.02

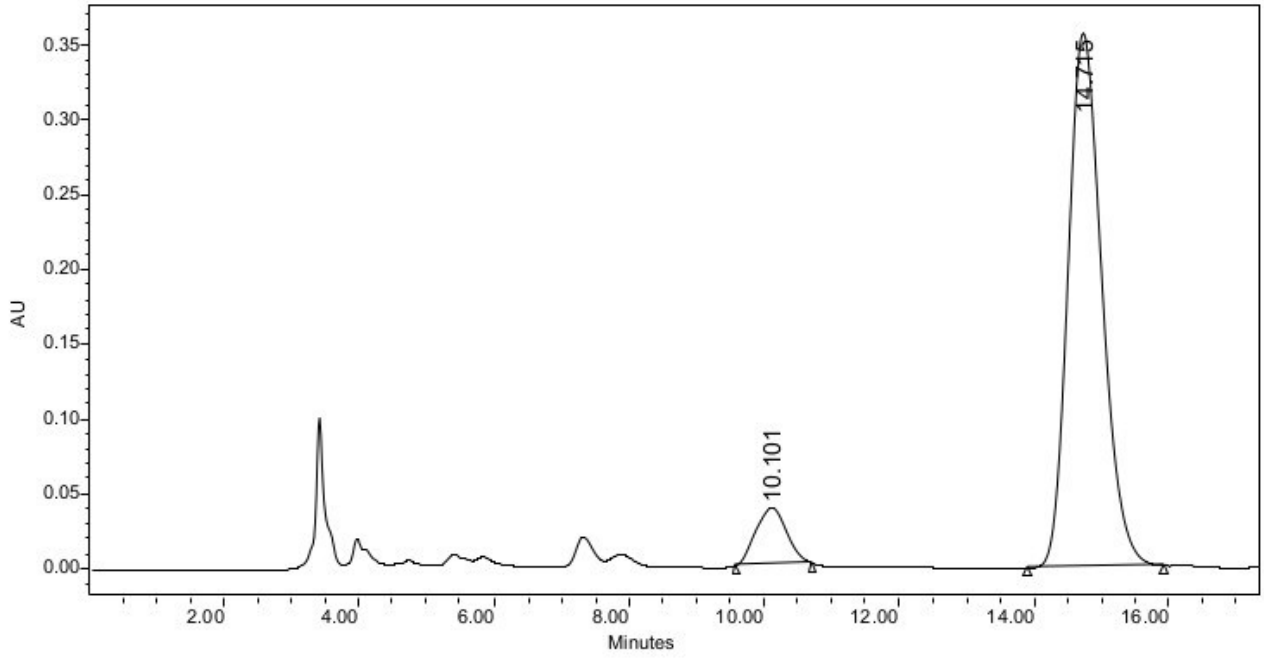


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.353	4755086	87.67	306268	95.22
2	17.816	668559	12.33	15388	4.78

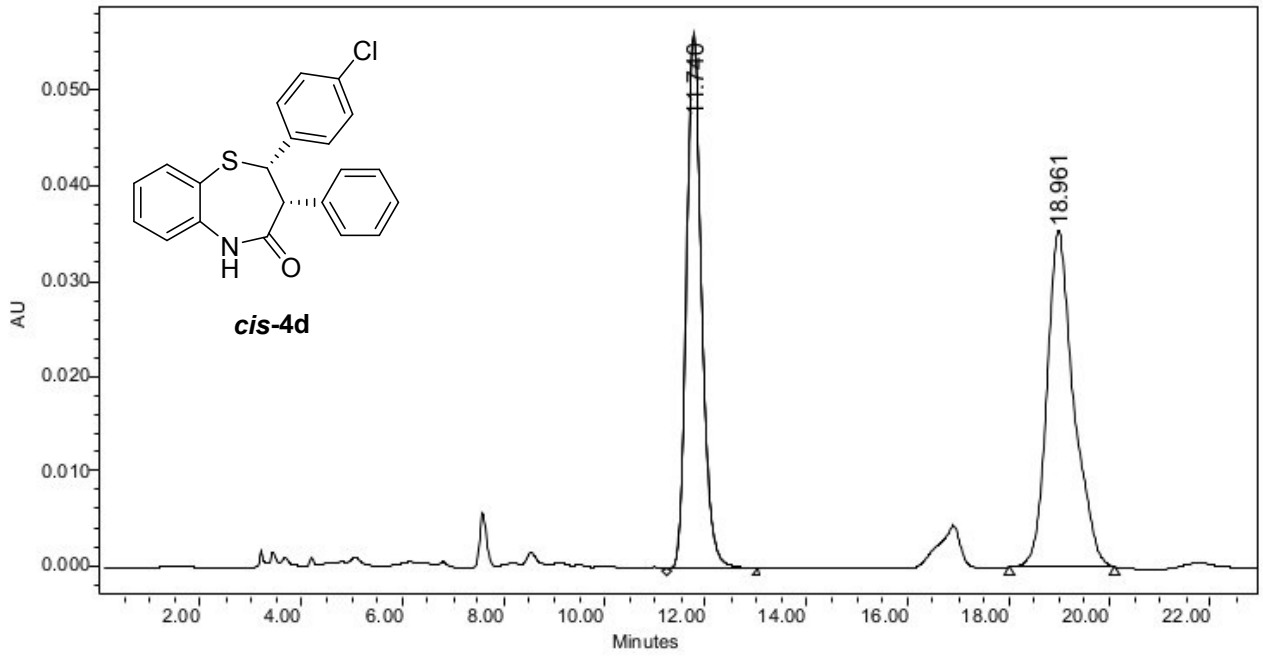


***trans*-4c**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.045	1231840	49.40	60400	59.73
2	14.333	1261656	50.60	40720	40.27

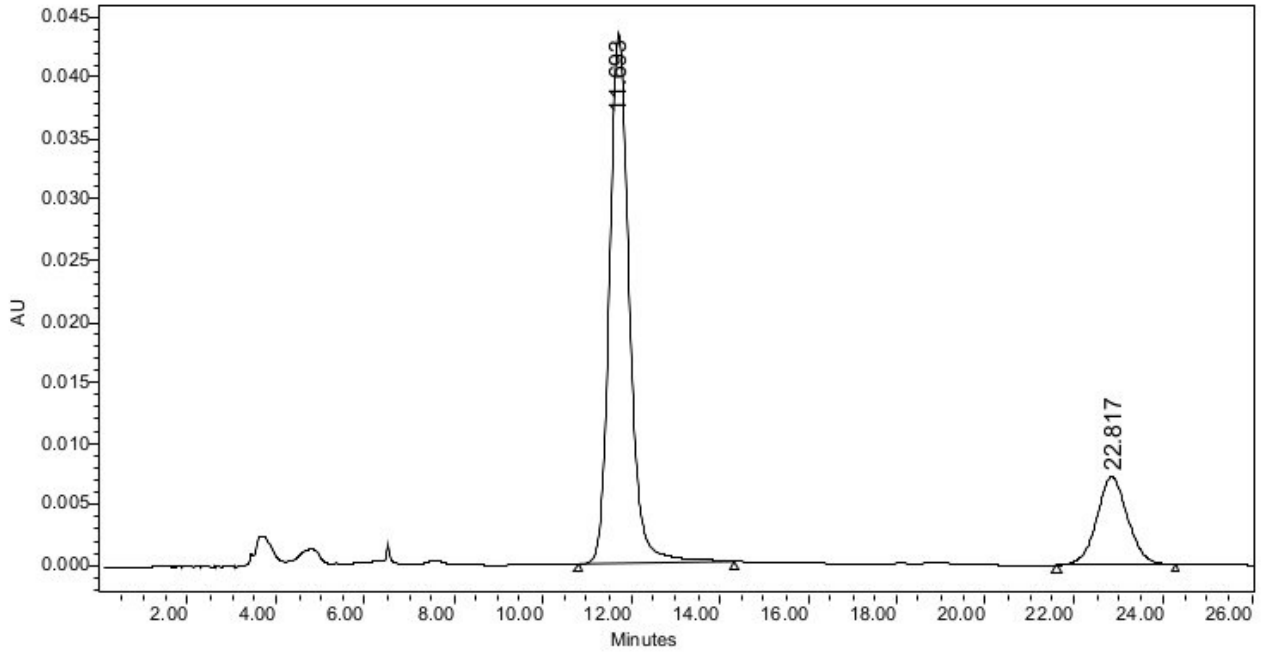


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.101	1219907	8.93	38042	9.63
2	14.715	12445312	91.07	357185	90.37

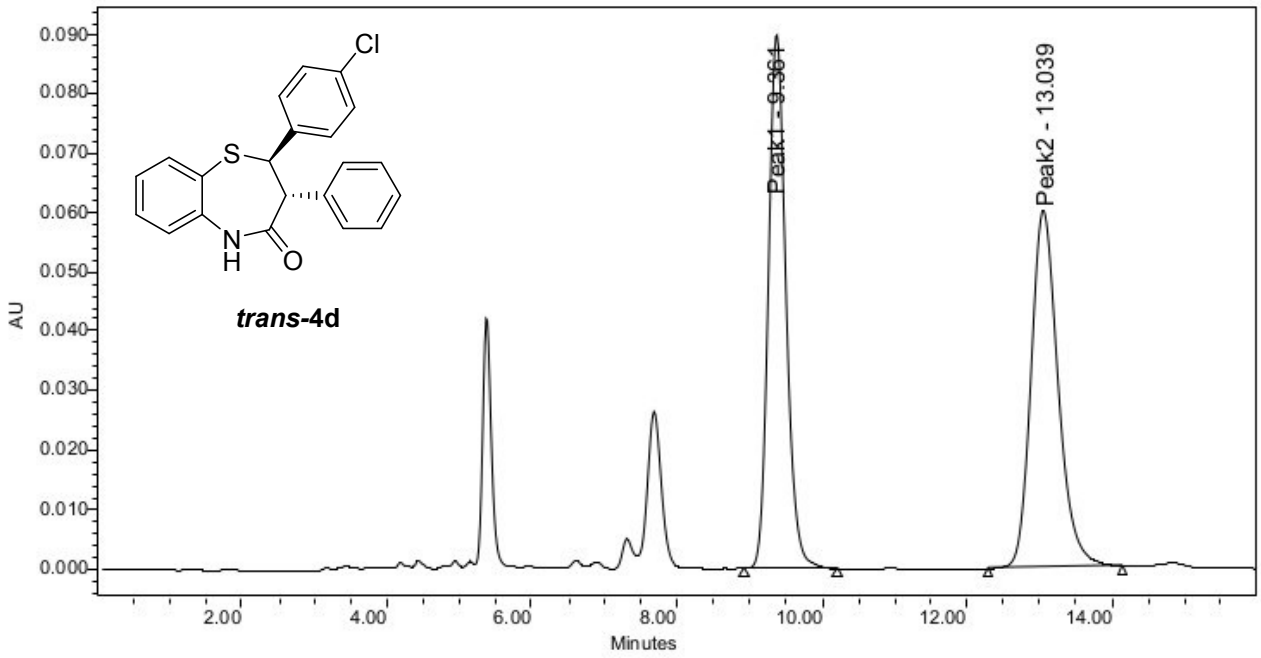


***cis*-4d**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.740	1191740	47.77	56059	61.37
2	18.961	1303144	52.23	35294	38.63

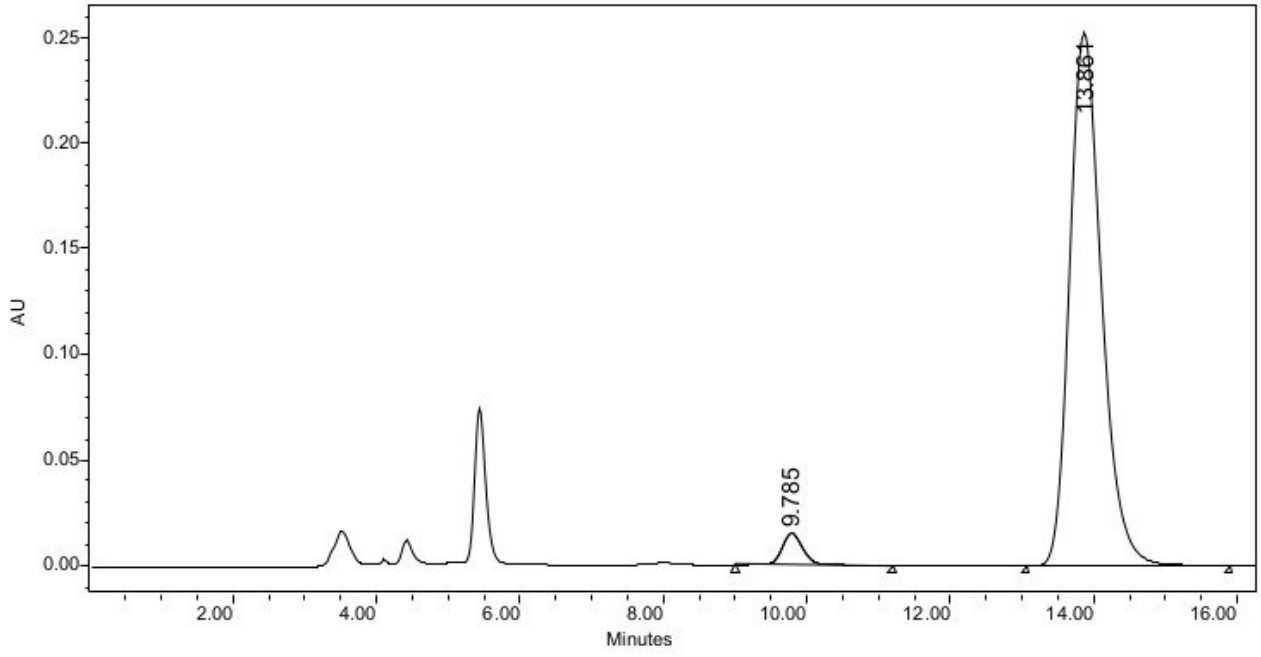


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.693	1362403	79.55	43509	85.73
2	22.817	350195	20.45	7244	14.27

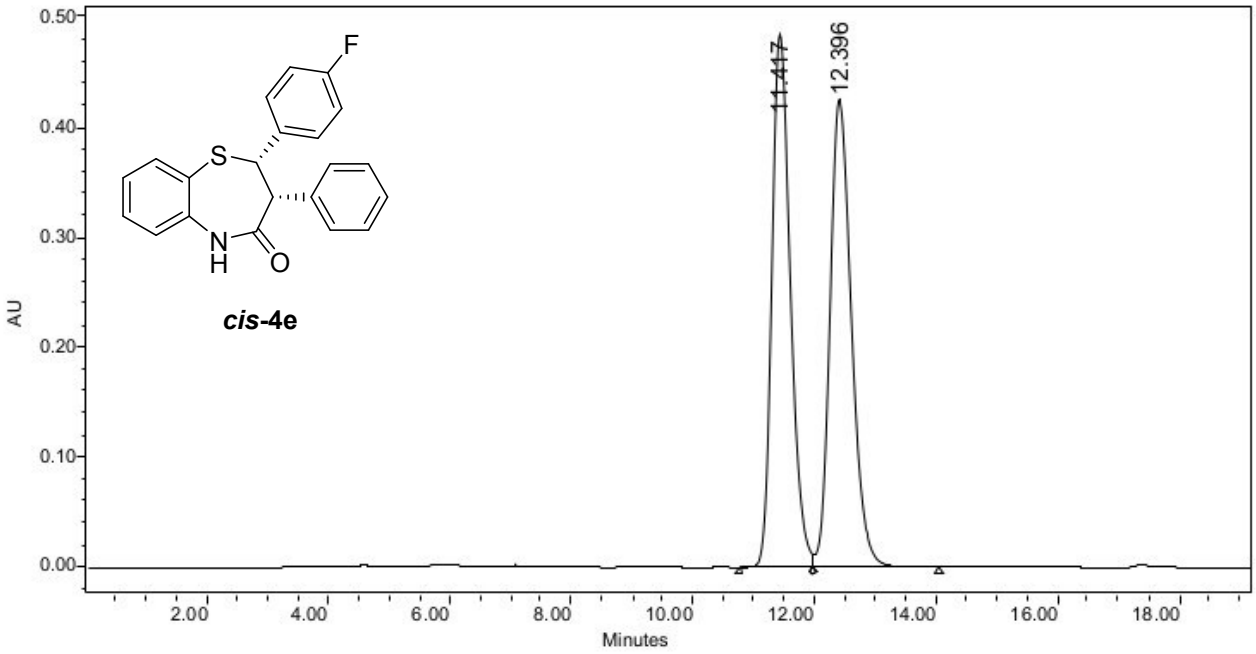


***trans*-4d**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	9.361	1513823	49.09	90008	59.94
2	Peak2	13.039	1569933	50.91	60160	40.06

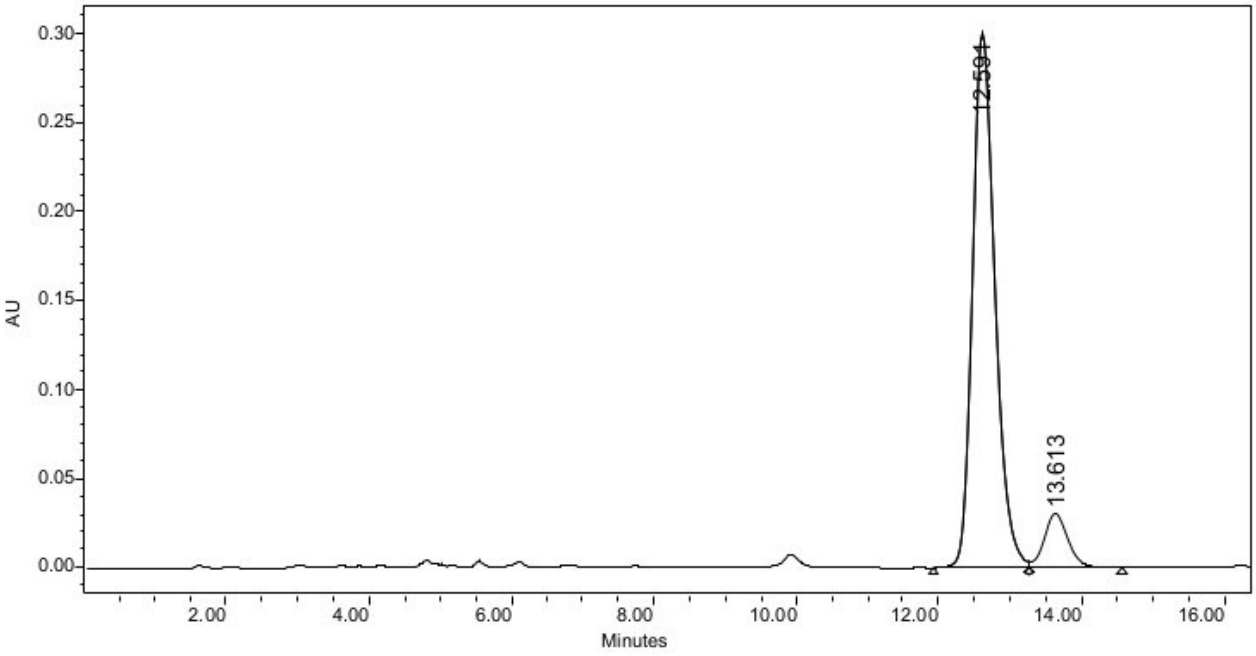


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.785	338830	4.14	15213	5.68
2	13.861	7841965	95.86	252794	94.32

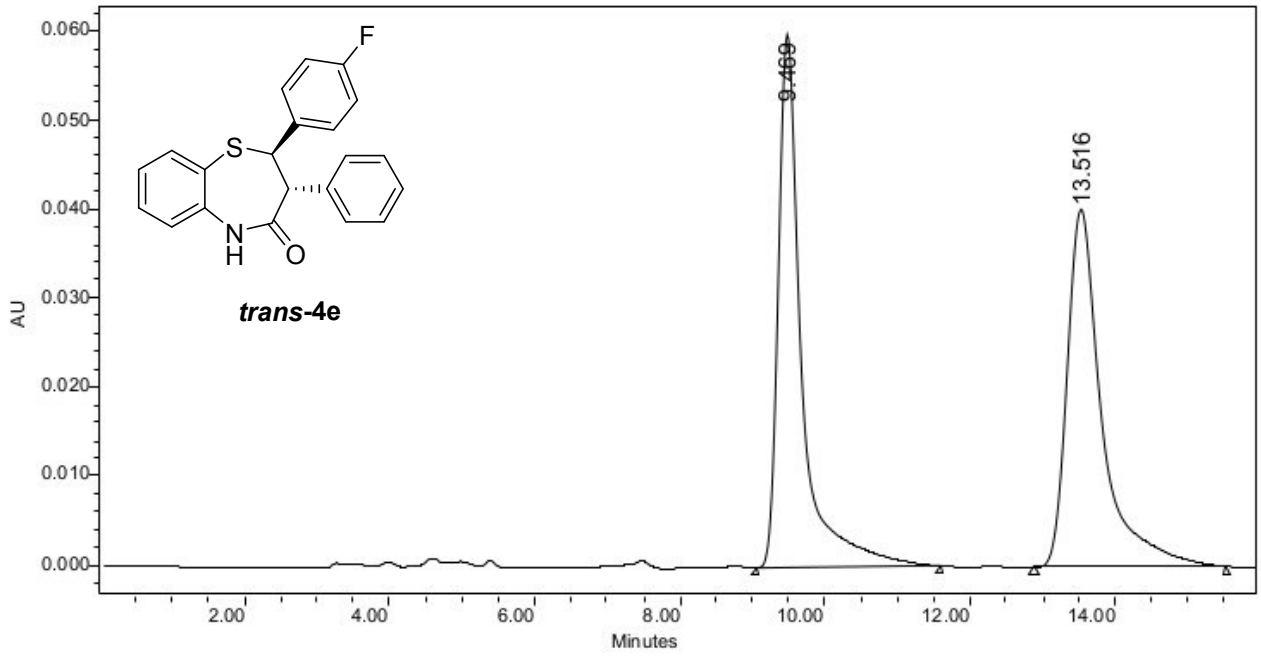


***cis*-4e**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.417	10270068	49.61	484964	53.22
2	12.396	10432317	50.39	426198	46.78

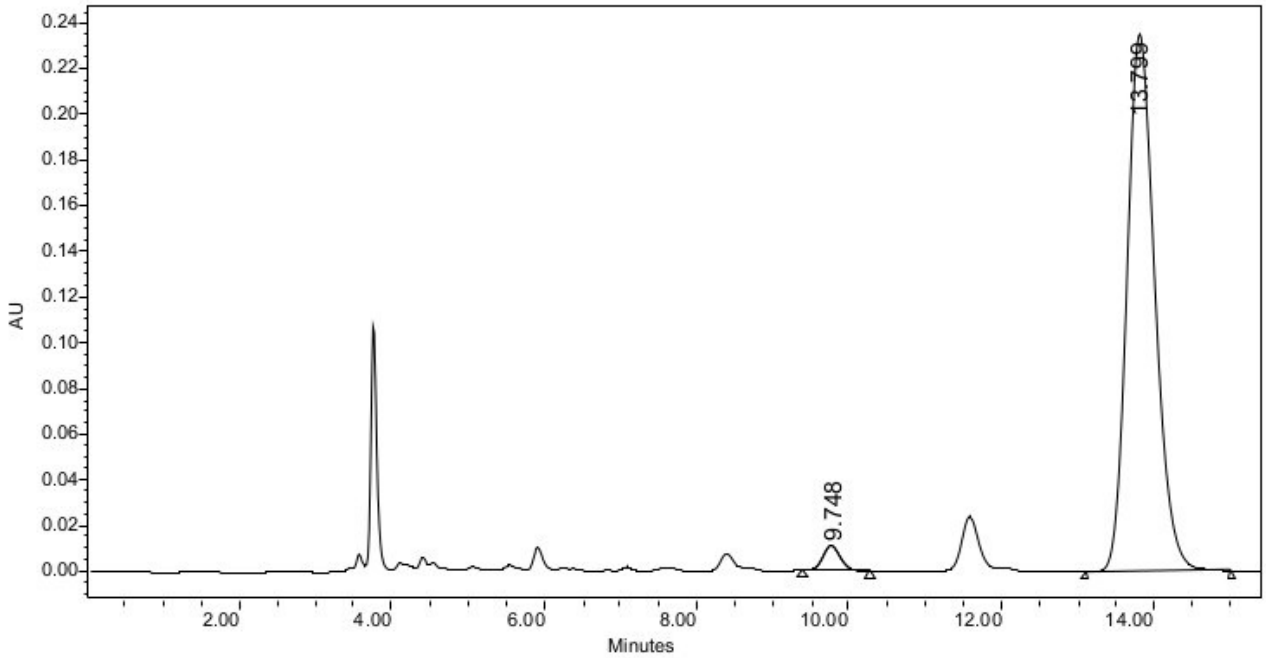


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	12.591	6576454	90.35	300995	90.79
2	13.613	702777	9.65	30544	9.21

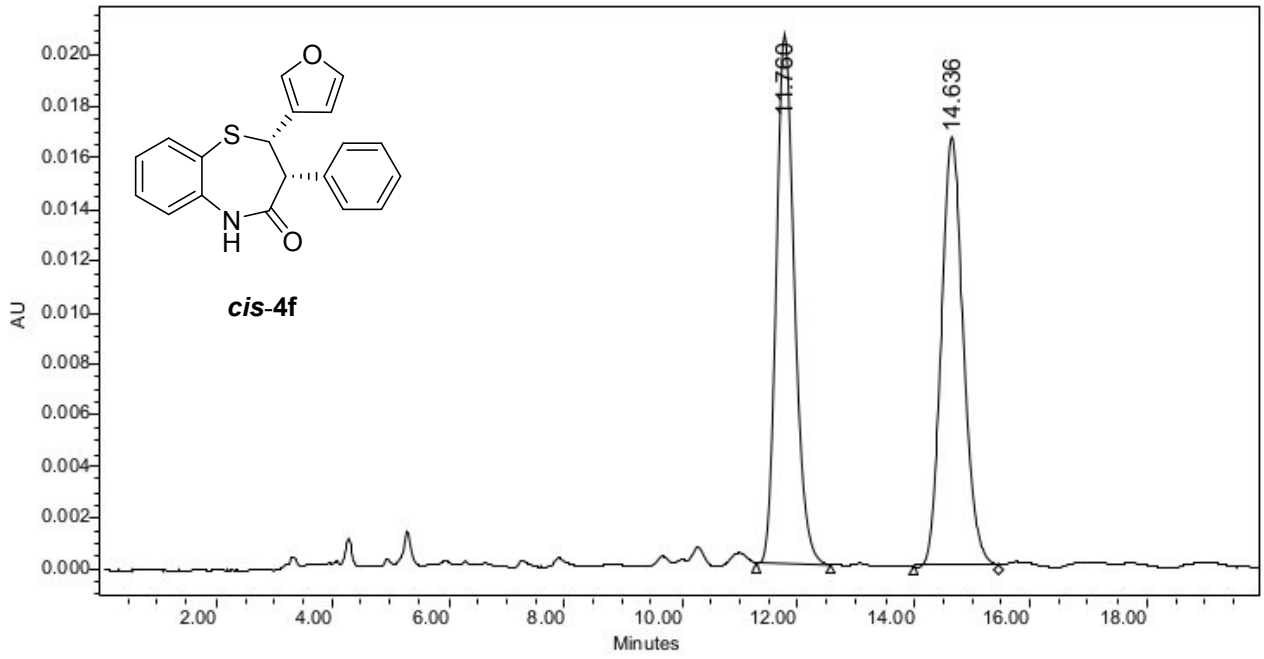


***trans*-4e**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.469	1347534	50.26	59979	59.85
2	13.516	1333826	49.74	40235	40.15

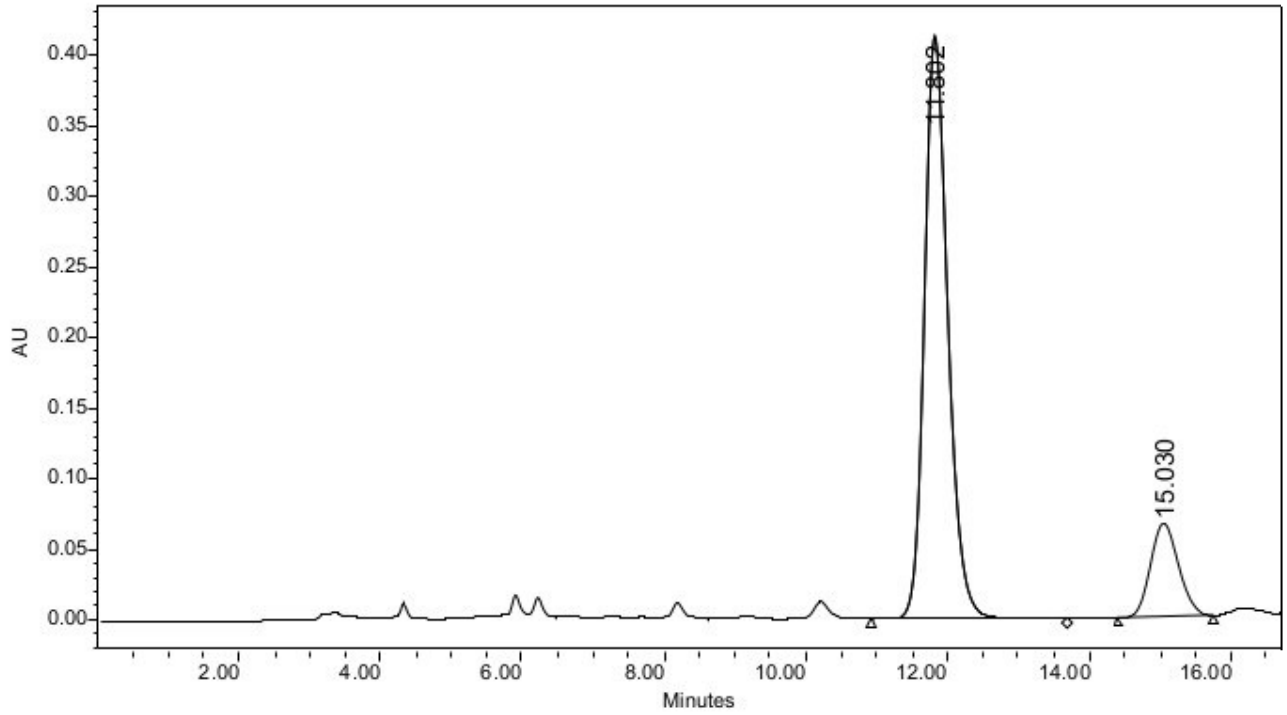


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.748	175970	2.84	10980	4.45
2	13.799	6015954	97.16	235779	95.55

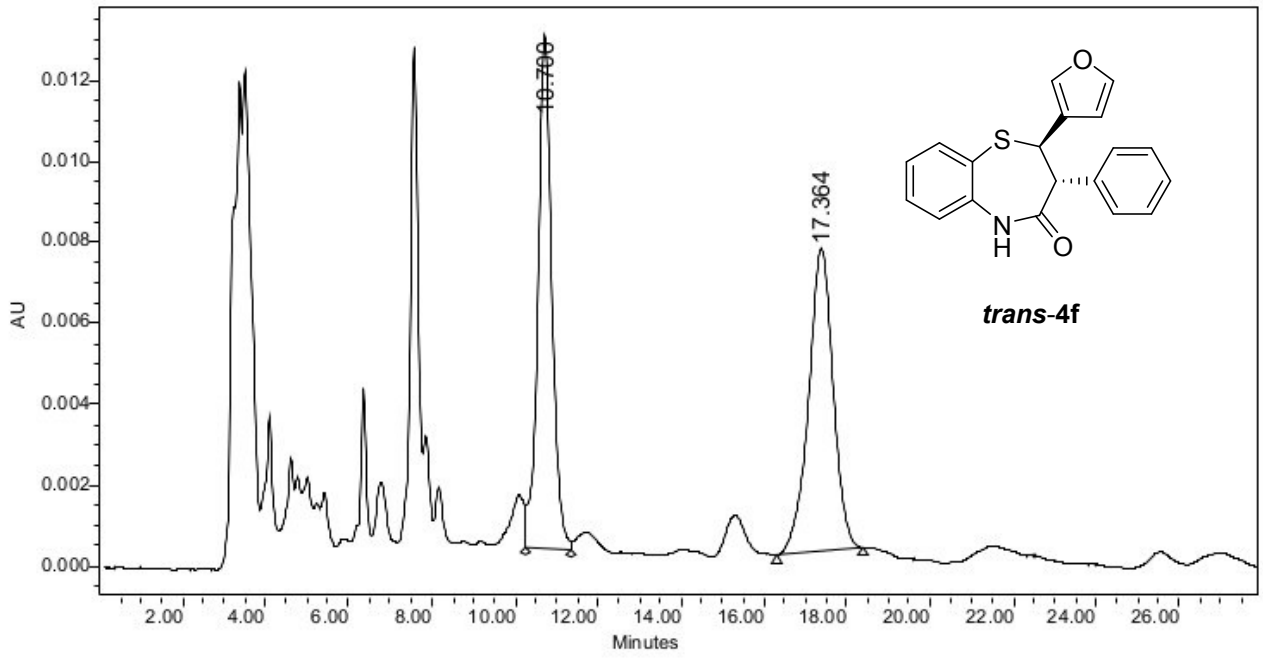


***cis*-4f**

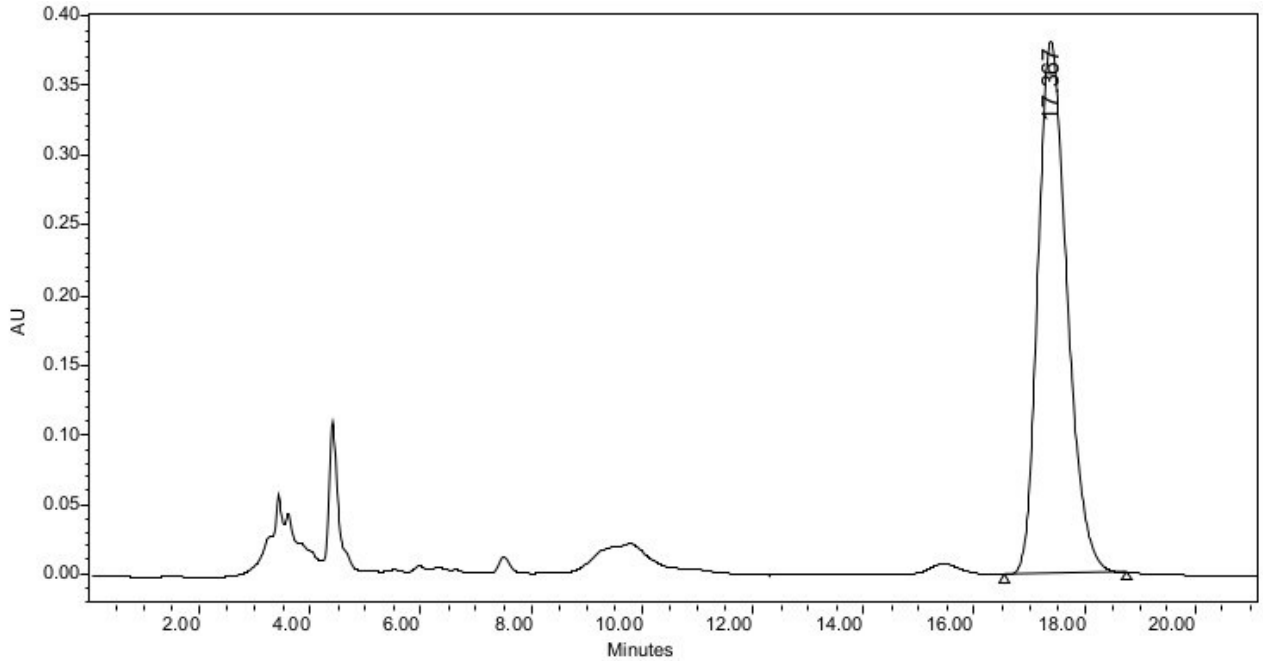
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.760	448414	50.26	20629	55.21
2	14.636	443792	49.74	16736	44.79



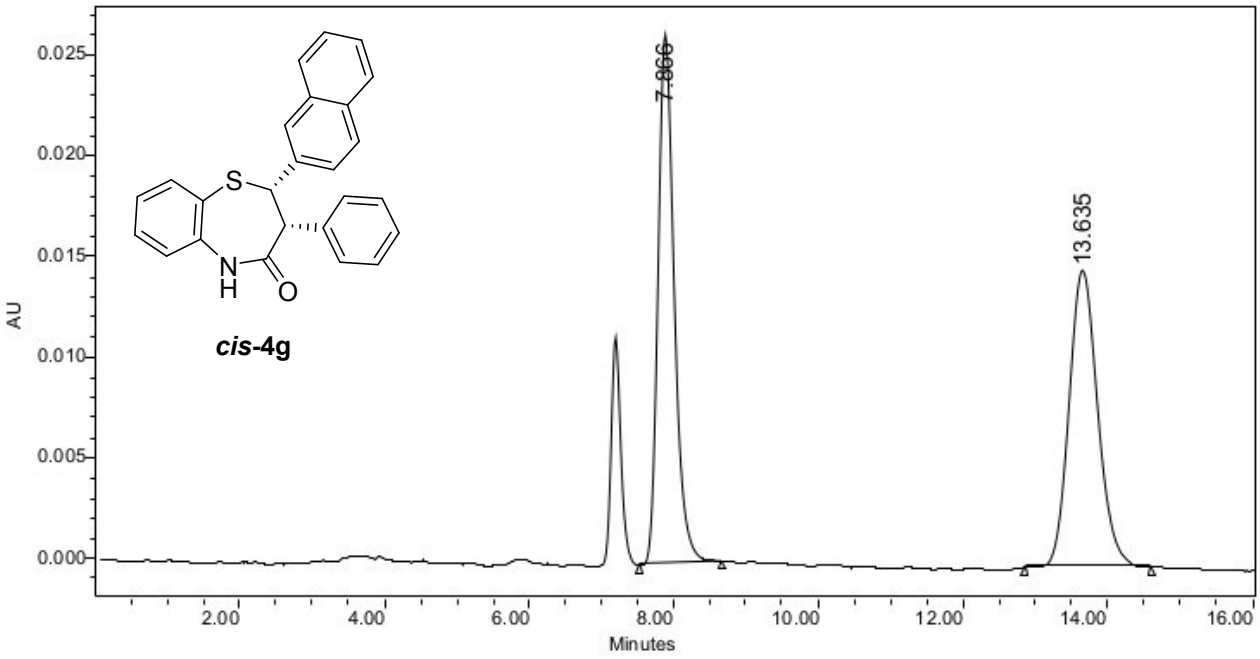
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.802	9480125	83.71	411603	86.08
2	15.030	1844457	16.29	66553	13.92



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.700	292052	48.51	12699	62.90
2	17.364	309945	51.49	7489	37.10

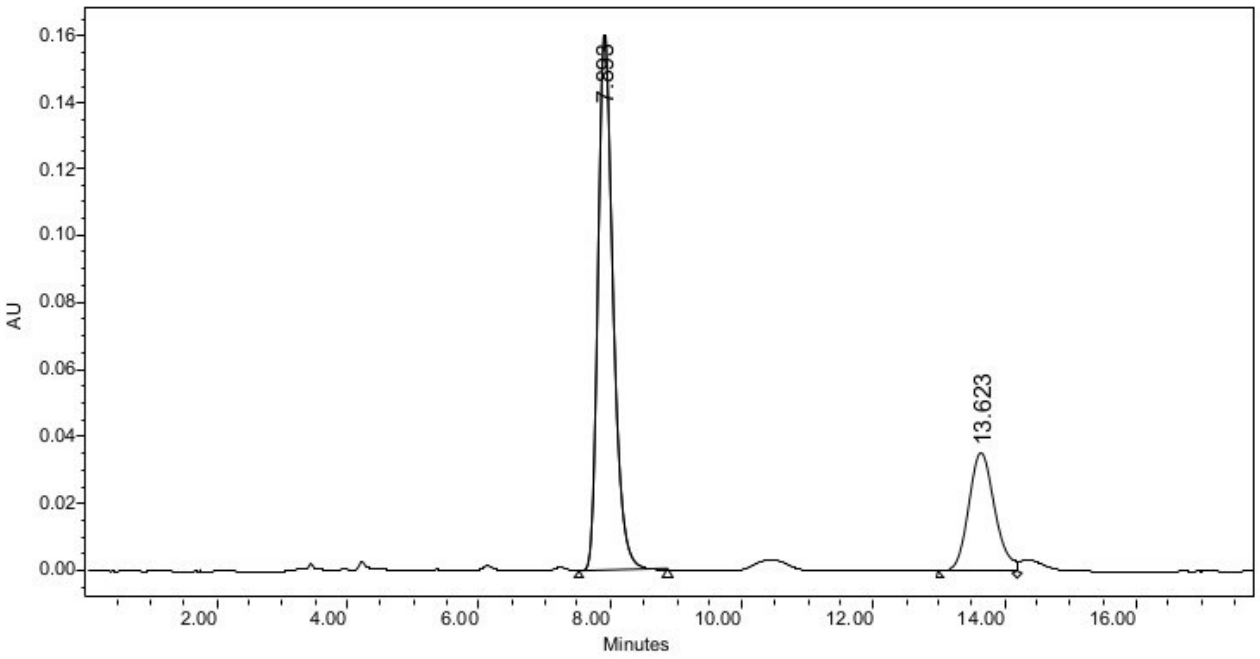


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	17.367	13962576	100.00	380864	100.00

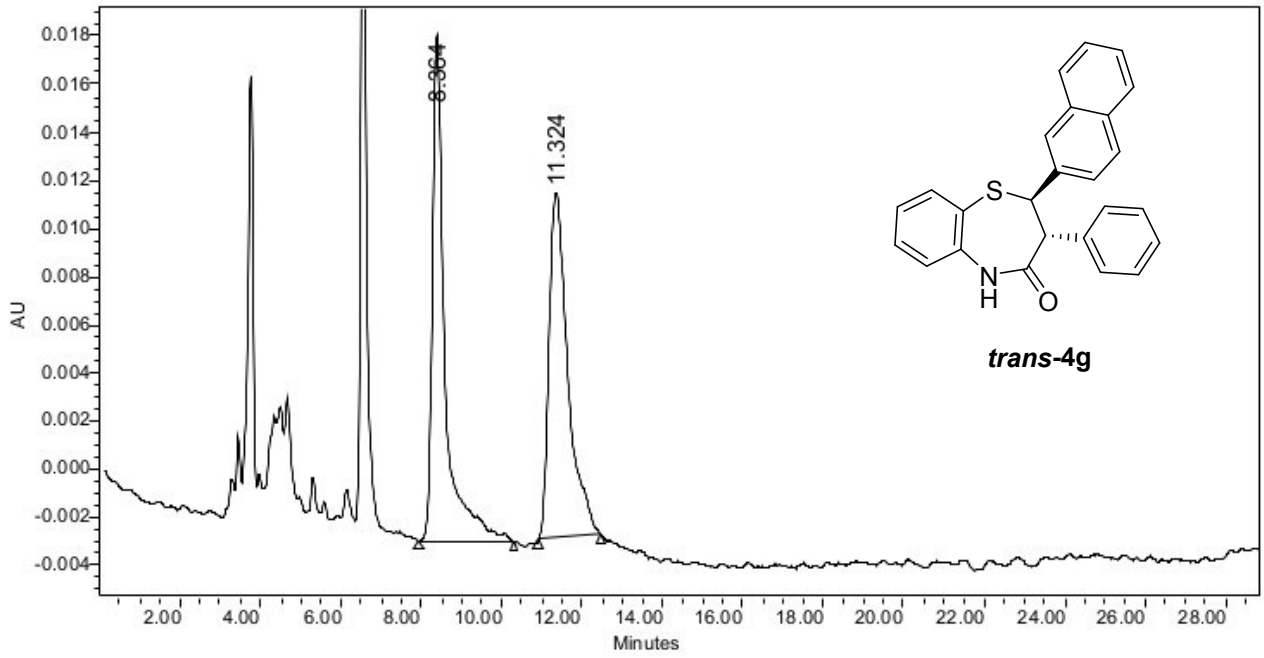


***cis*-4g**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.866	408770	50.21	26295	64.07
2	13.635	405312	49.79	14743	35.93

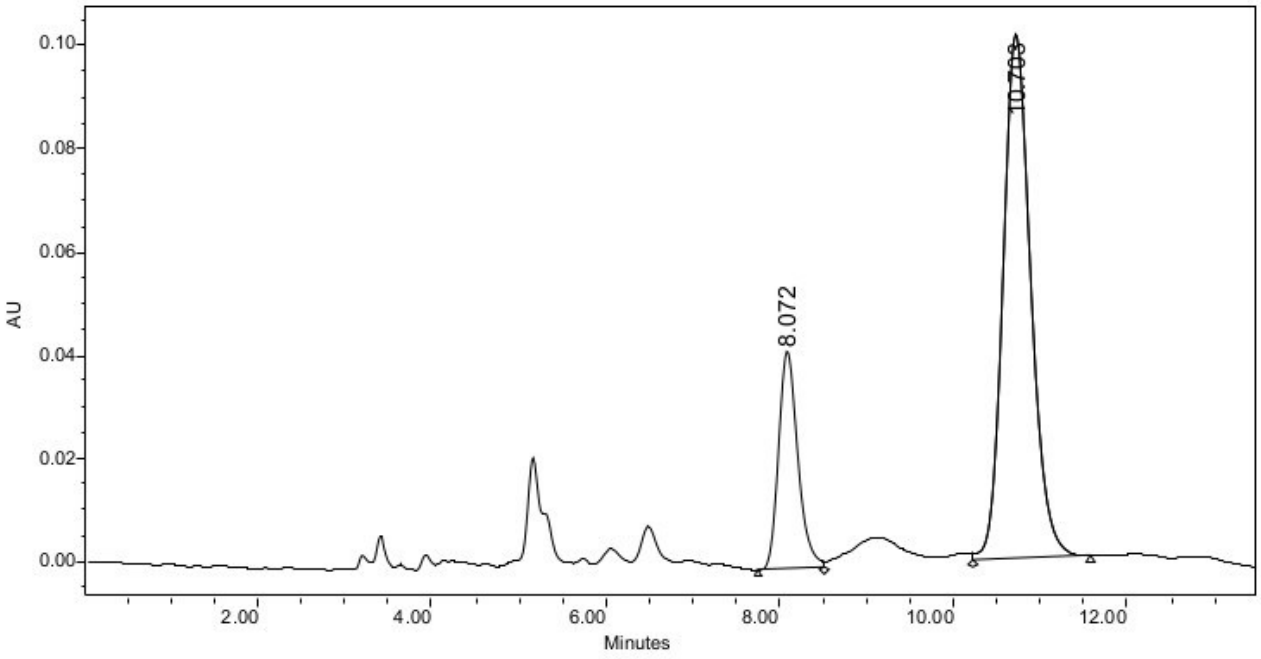


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.893	2587351	72.59	160559	81.91
2	13.623	976867	27.41	35466	18.09

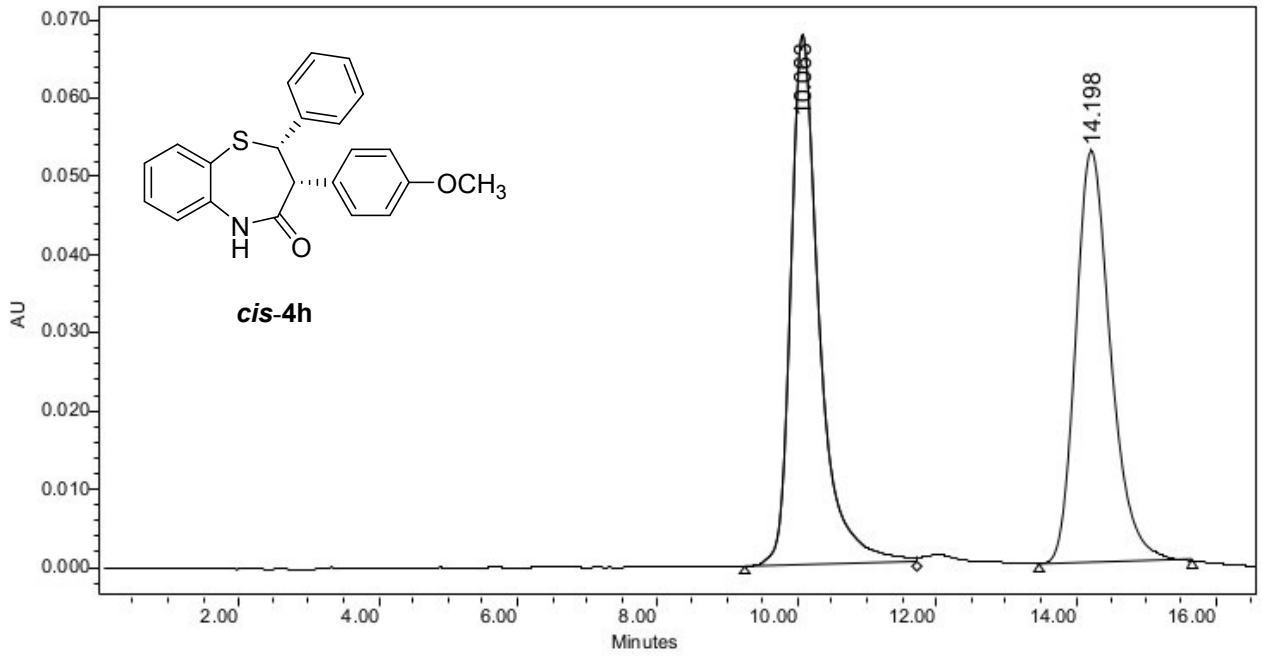


***trans*-4g**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.364	461676	49.44	21066	59.35
2	11.324	472064	50.56	14427	40.65

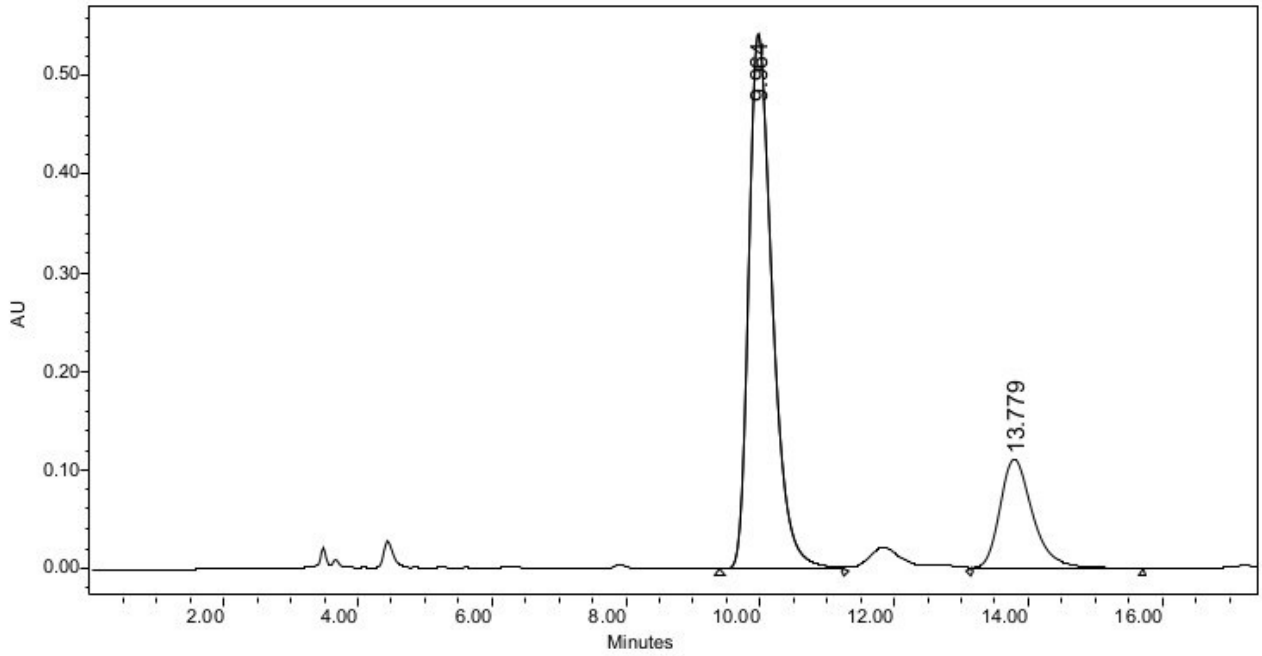


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.072	652728	22.41	42224	29.34
2	10.703	2260070	77.59	101673	70.66

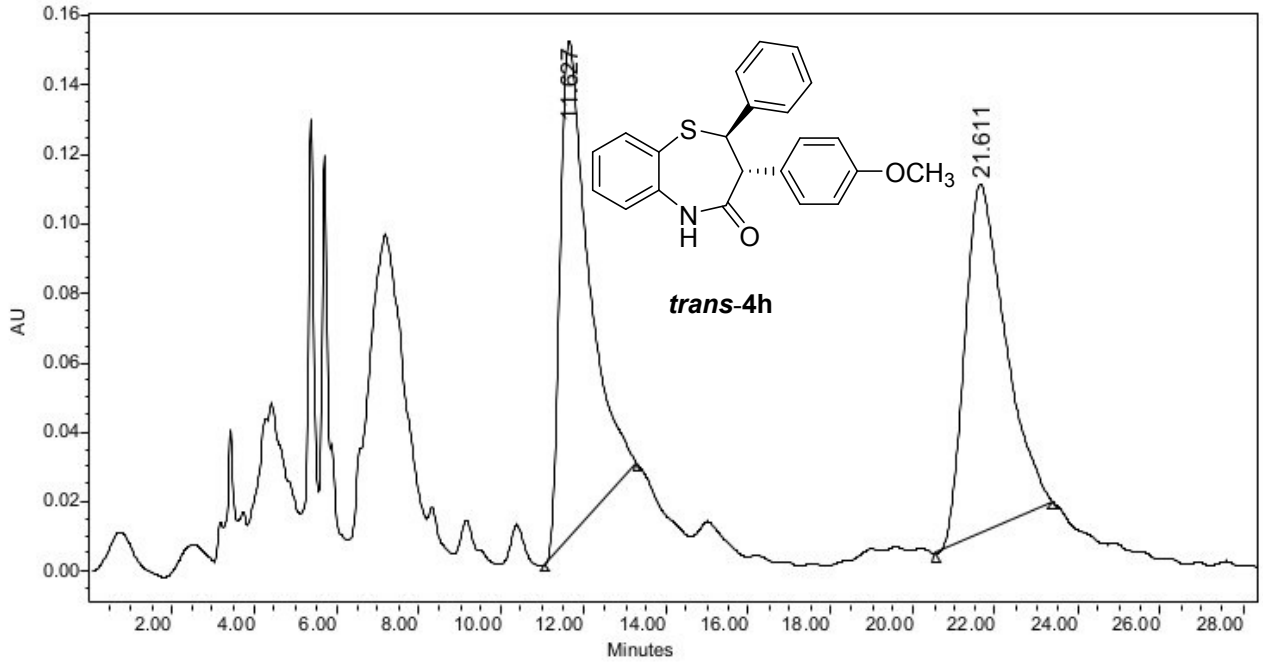


***cis*-4h**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.063	1937311	51.26	67835	56.25
2	14.198	1842197	48.74	52763	43.75

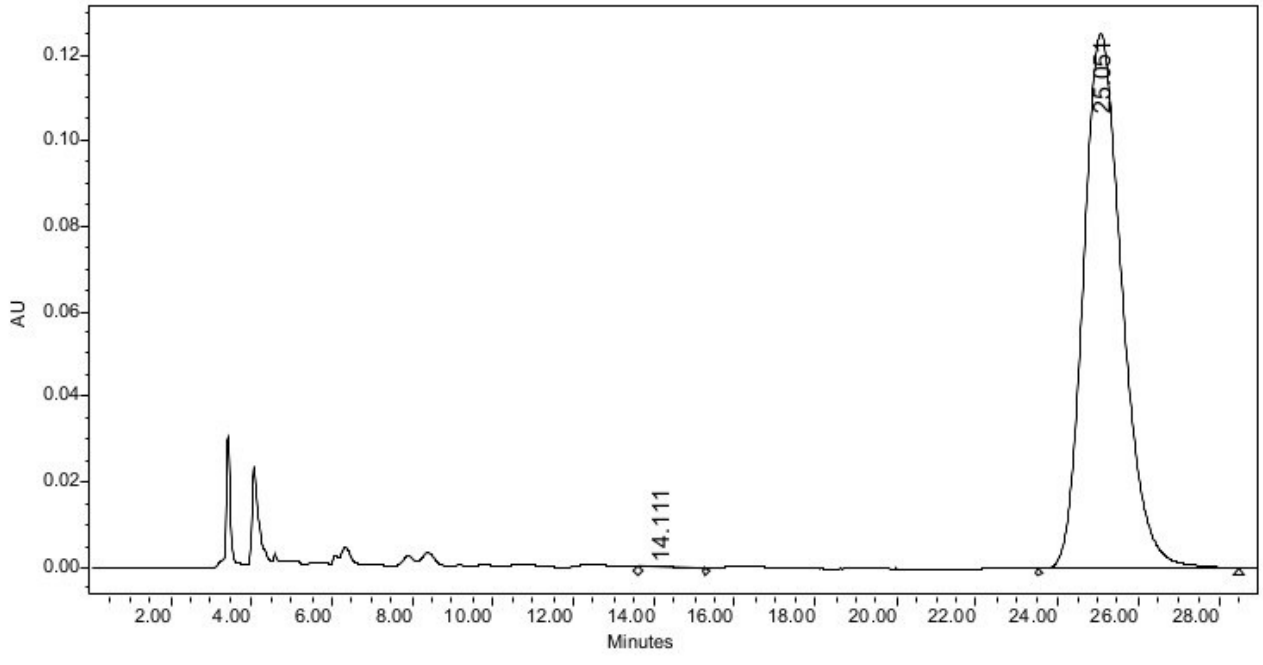


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.964	13310334	77.55	543225	82.98
2	13.779	3852876	22.45	111455	17.02

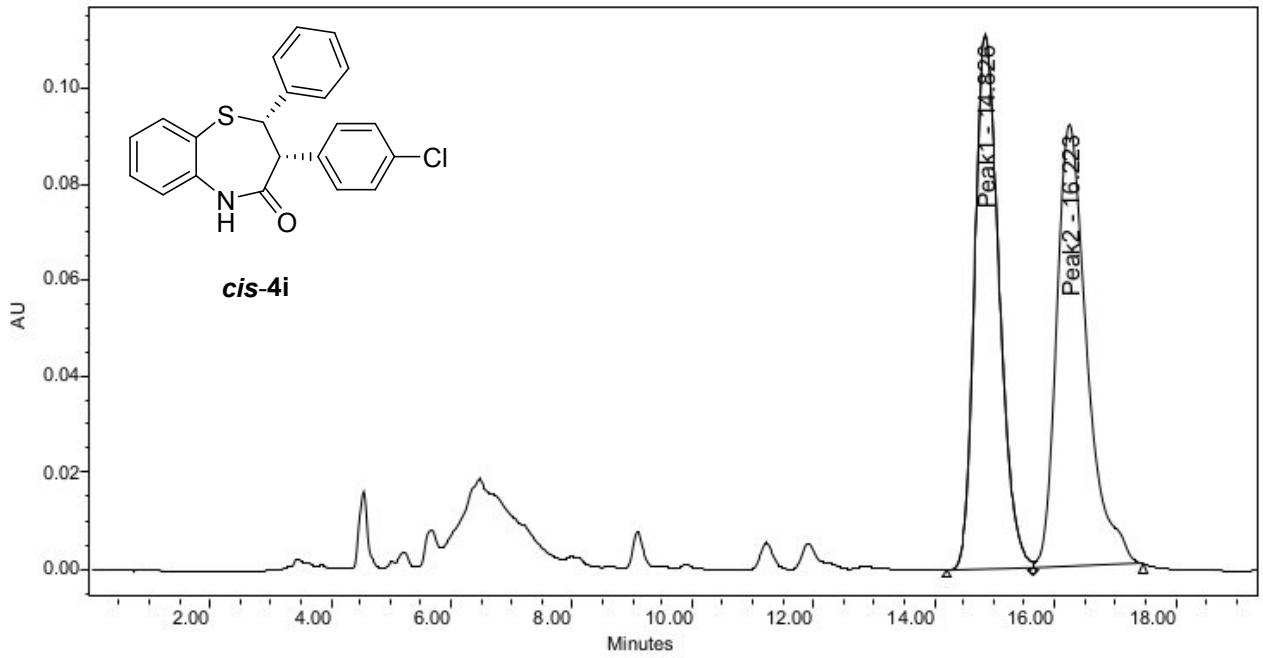


***trans*-4h**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	11.627	7058396	50.34	143618	58.69
2	21.611	6961691	49.66	101093	41.31

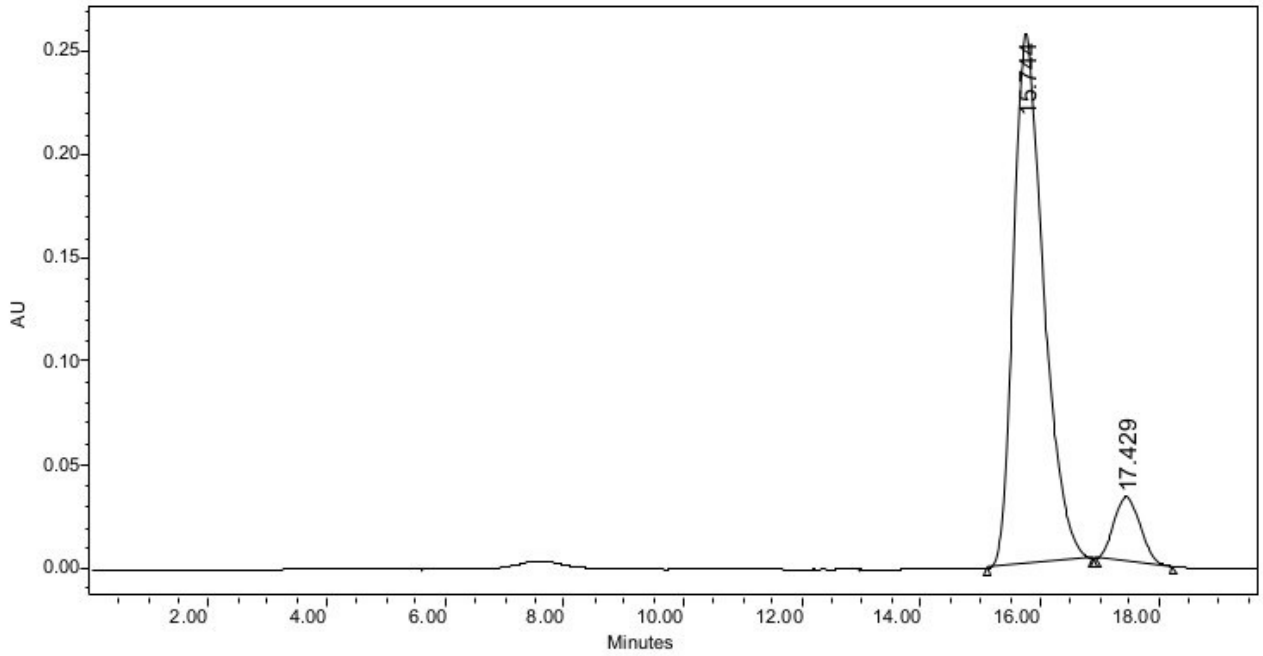


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	14.111	21088	0.25	475	0.38
2	25.051	8339827	99.75	125253	99.62

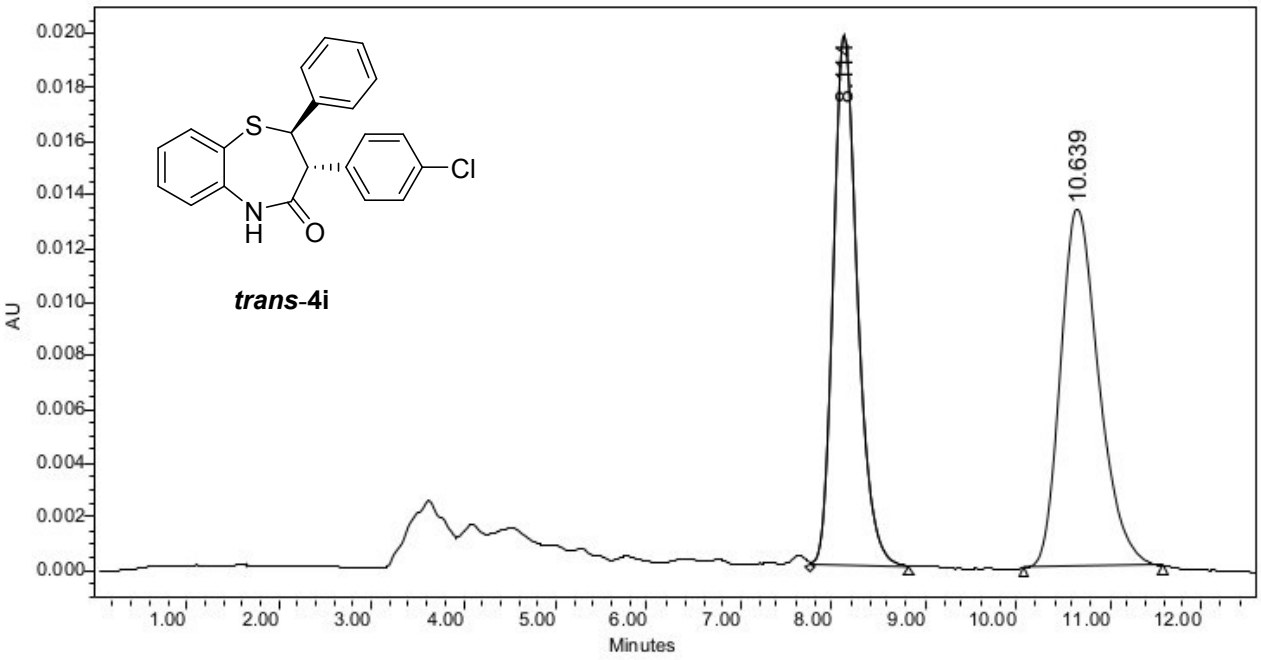


***cis*-4i**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	14.826	3152680	49.53	111125	54.68
2	Peak2	16.223	3213101	50.47	92087	45.32

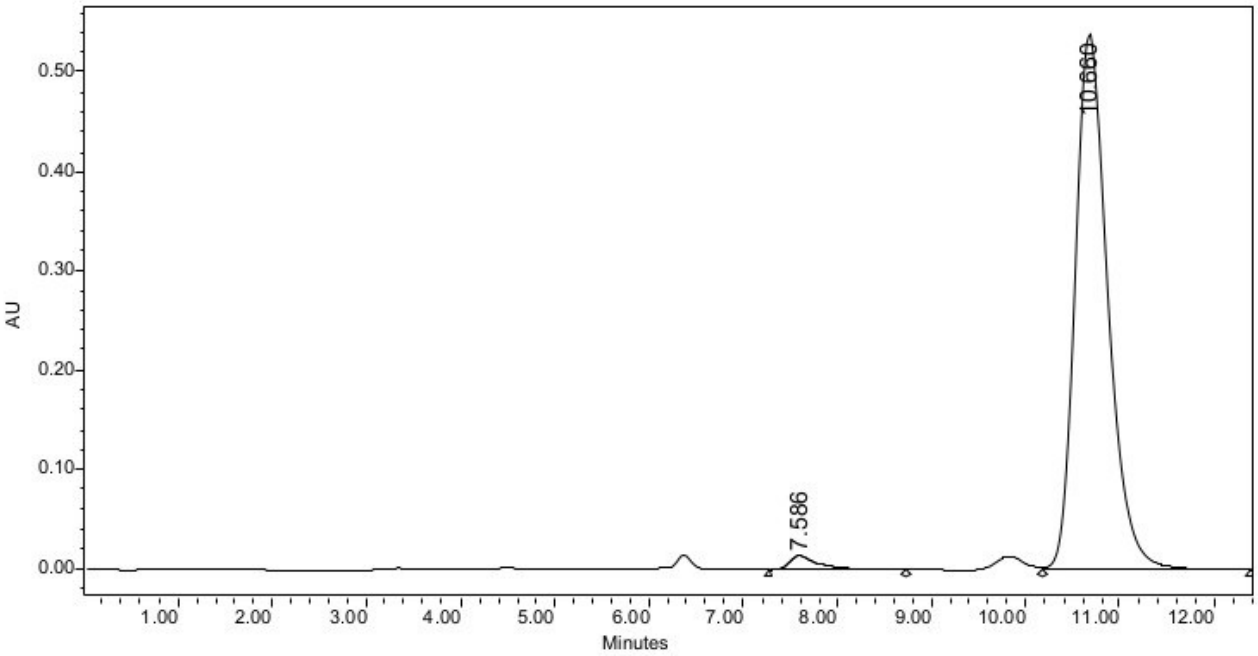


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	15.744	9105315	90.26	256935	89.03
2	17.429	982679	9.74	31655	10.97

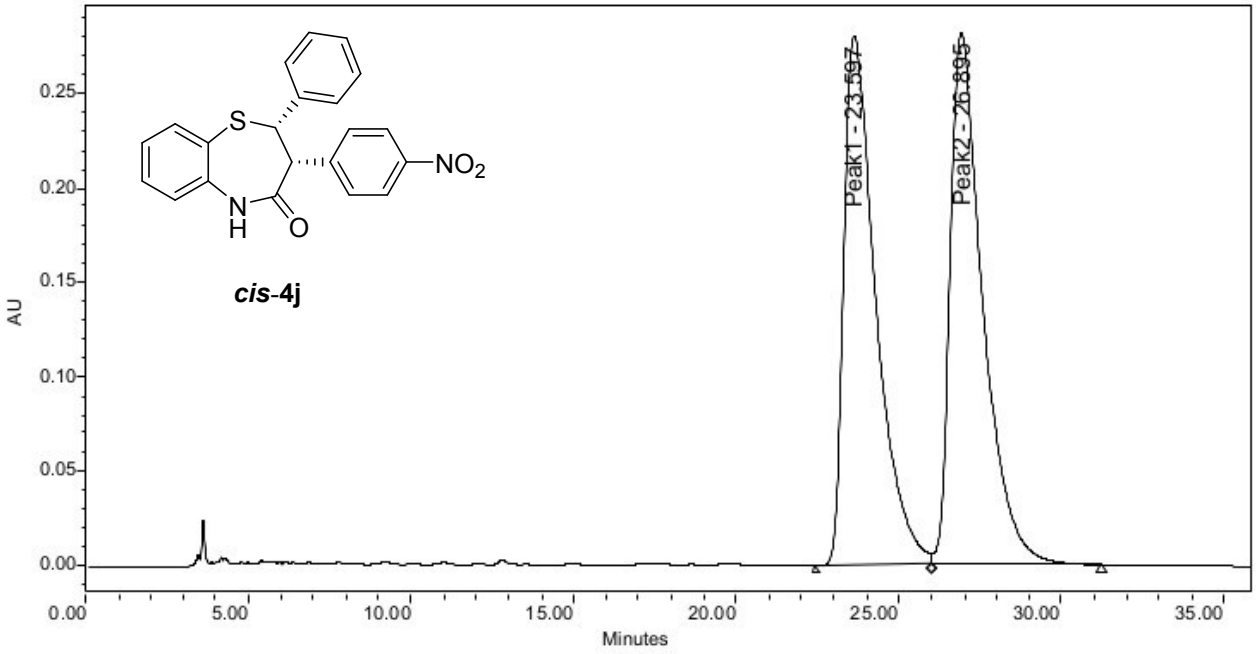


***trans*-4i**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.114	360254	48.08	19750	59.63
2	10.639	388952	51.92	13372	40.37

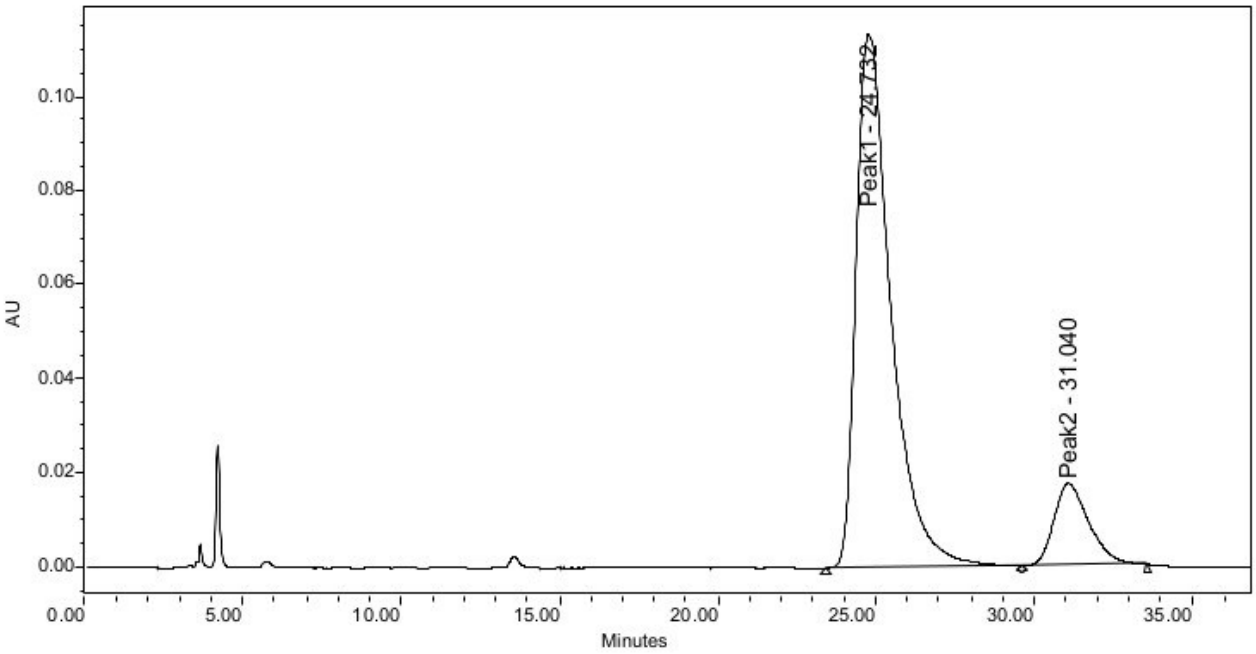


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	7.586	329240	2.46	14406	2.60
2	10.660	13044134	97.54	539983	97.40

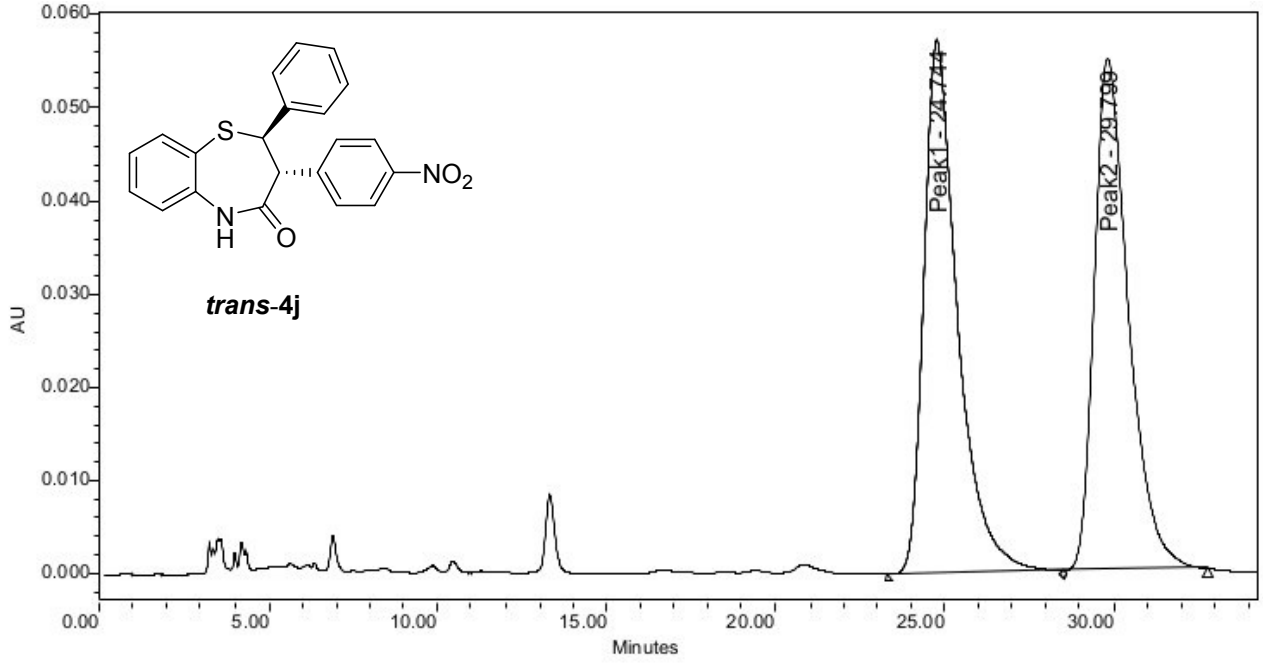


***cis*-4j**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	23.597	19286590	49.50	280676	49.89
2	Peak2	26.895	19678490	50.50	281882	50.11

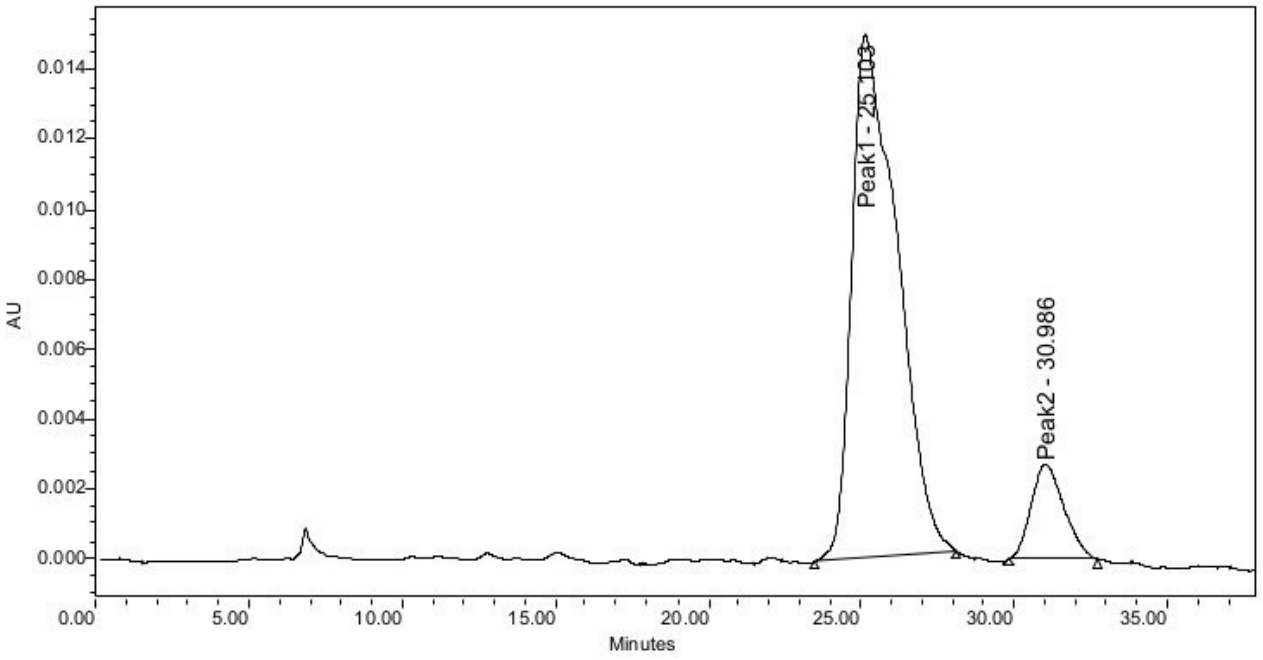


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	24.732	8707560	86.63	113305	86.69
2	Peak2	31.040	1343834	13.37	17402	13.31

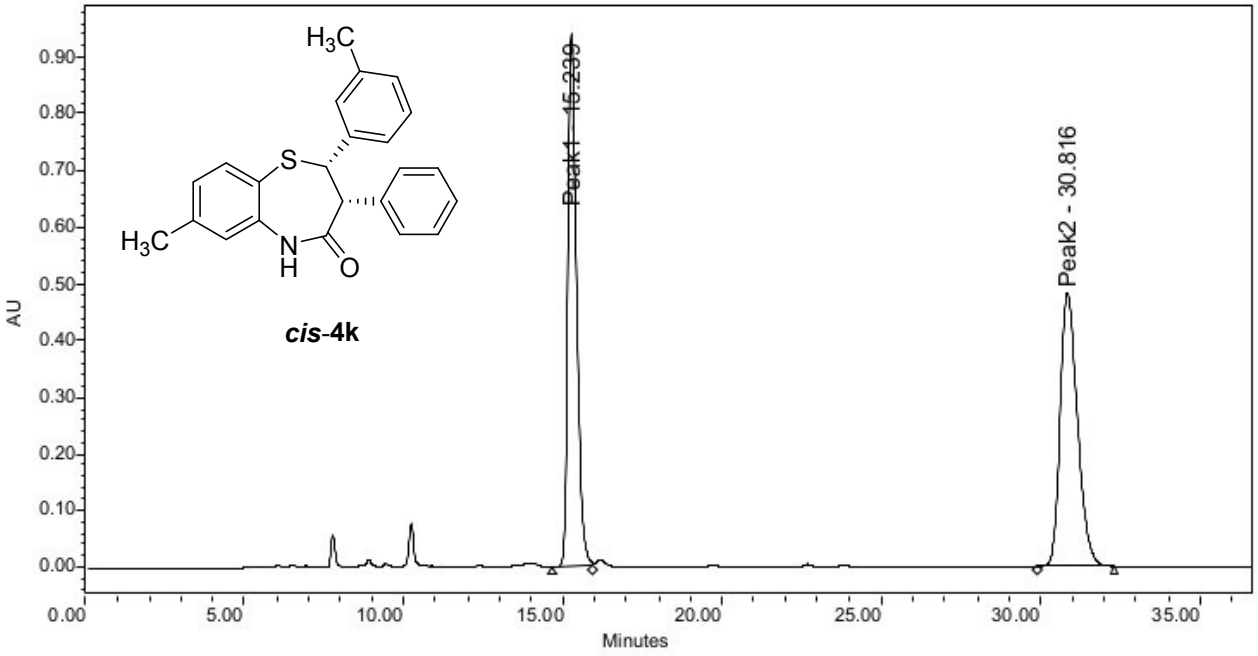


***trans*-4j**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	24.744	3976056	50.62	57300	51.03
2	Peak2	29.799	3878476	49.38	54976	48.97

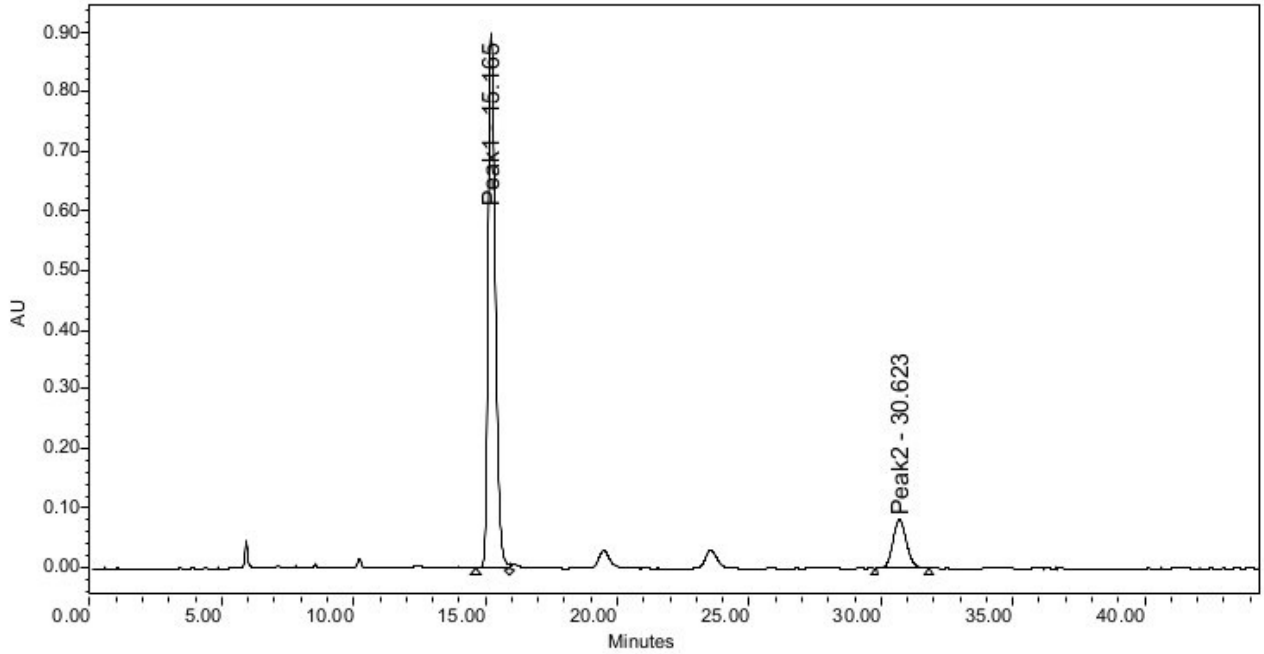


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	25.103	1547063	88.36	14992	84.66
2	Peak2	30.986	203782	11.64	2716	15.34

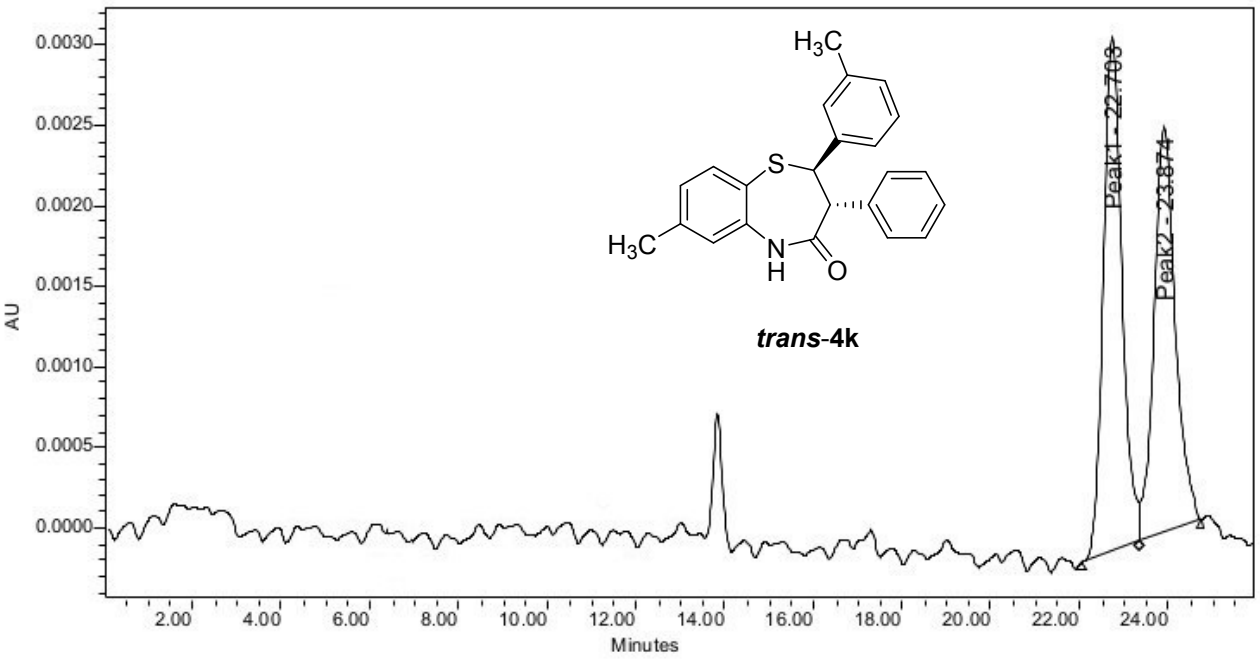


***cis*-4k**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	15.239	17964007	49.52	943352	66.09
2	Peak2	30.816	18308915	50.48	483927	33.91

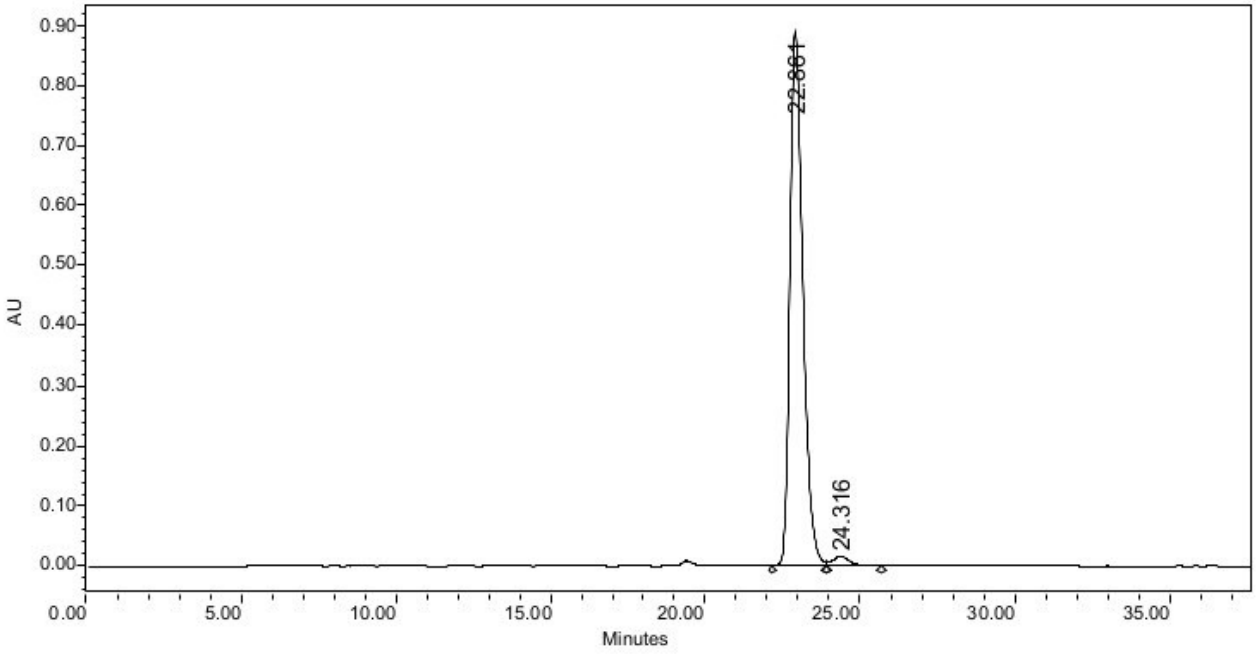


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	15.165	16678352	85.15	900912	91.67
2	Peak2	30.623	2907574	14.85	81898	8.33

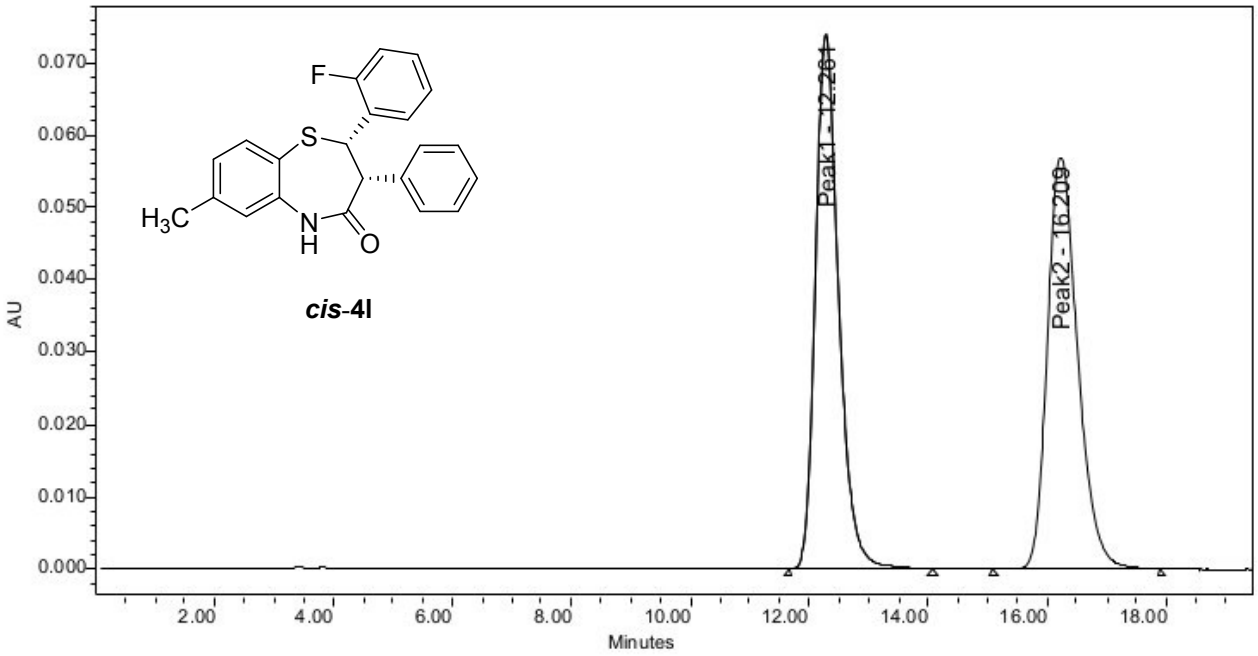


***trans*-4k**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	22.703	93127	52.50	3199	55.92
2	Peak2	23.874	84251	47.50	2522	44.08

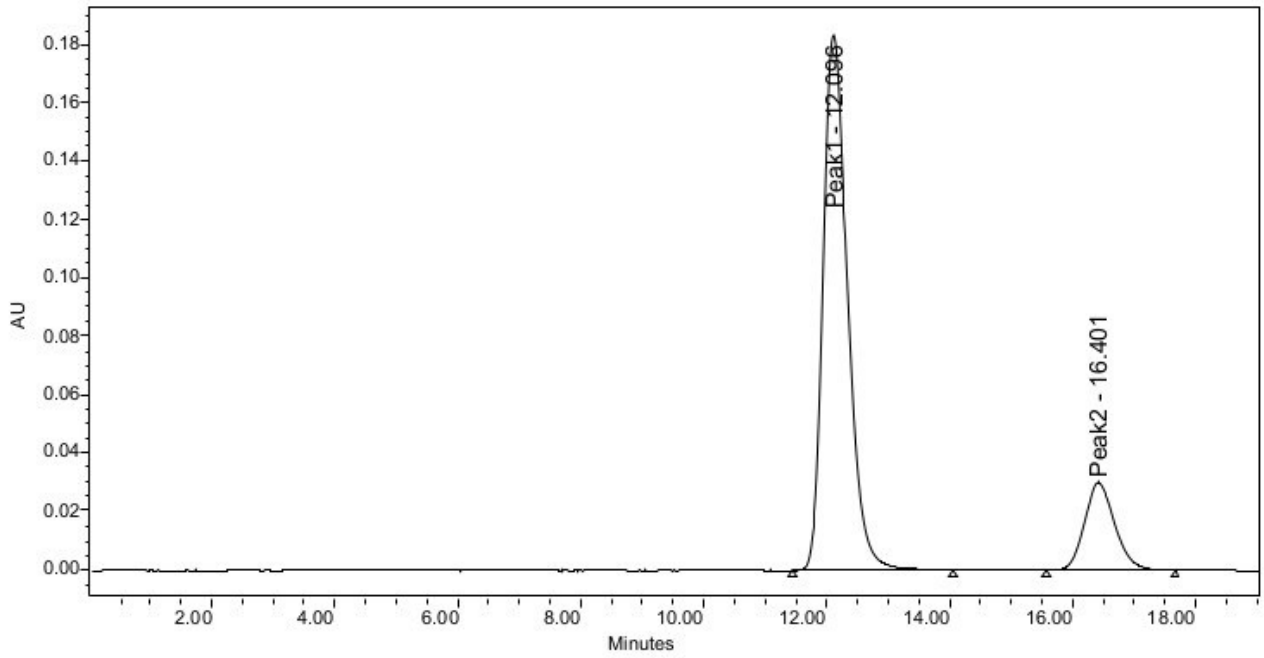


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	22.861	25984778	97.70	890257	98.18
2	24.316	612789	2.30	16466	1.82

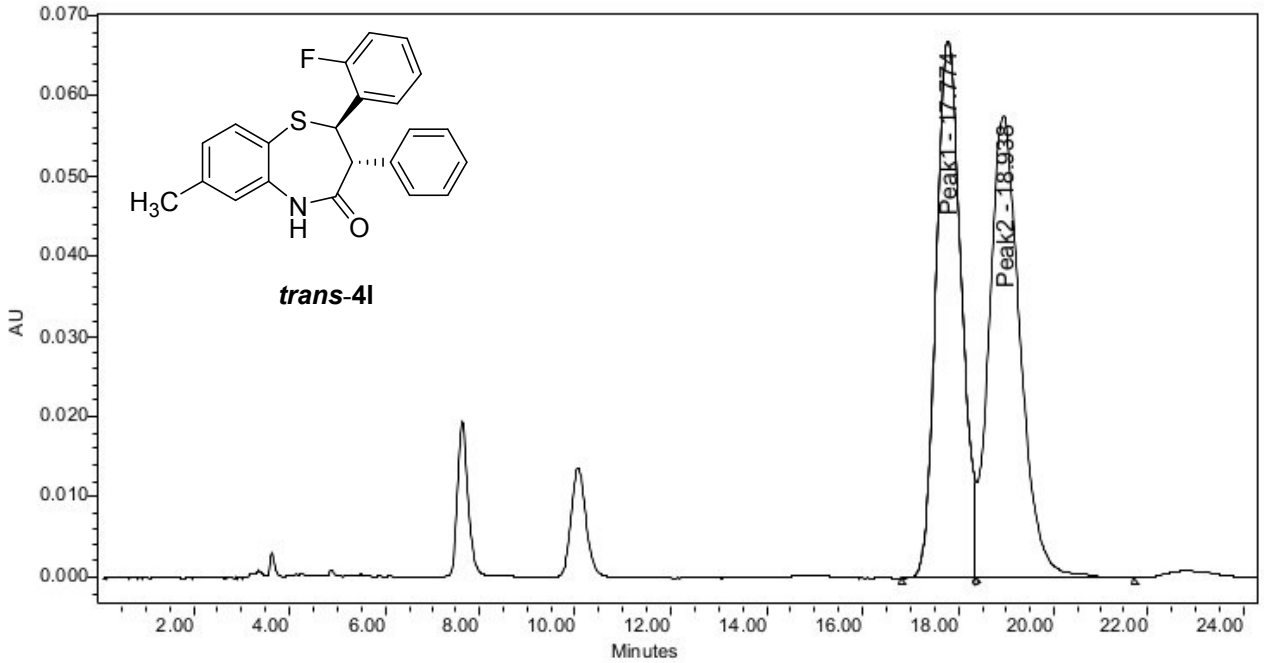


***cis*-4l**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	12.261	2019076	49.98	74300	56.50
2	Peak2	16.209	2020904	50.02	57200	43.50

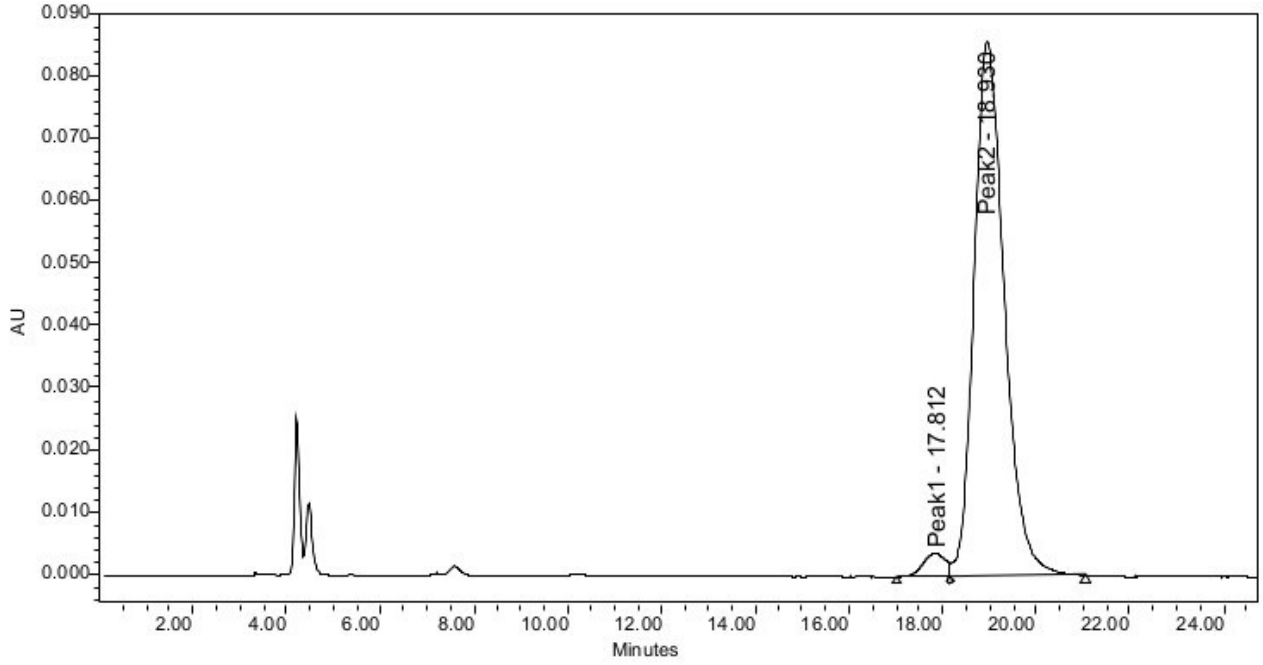


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	12.096	5088932	83.17	183703	85.88
2	Peak2	16.401	1029835	16.83	30212	14.12

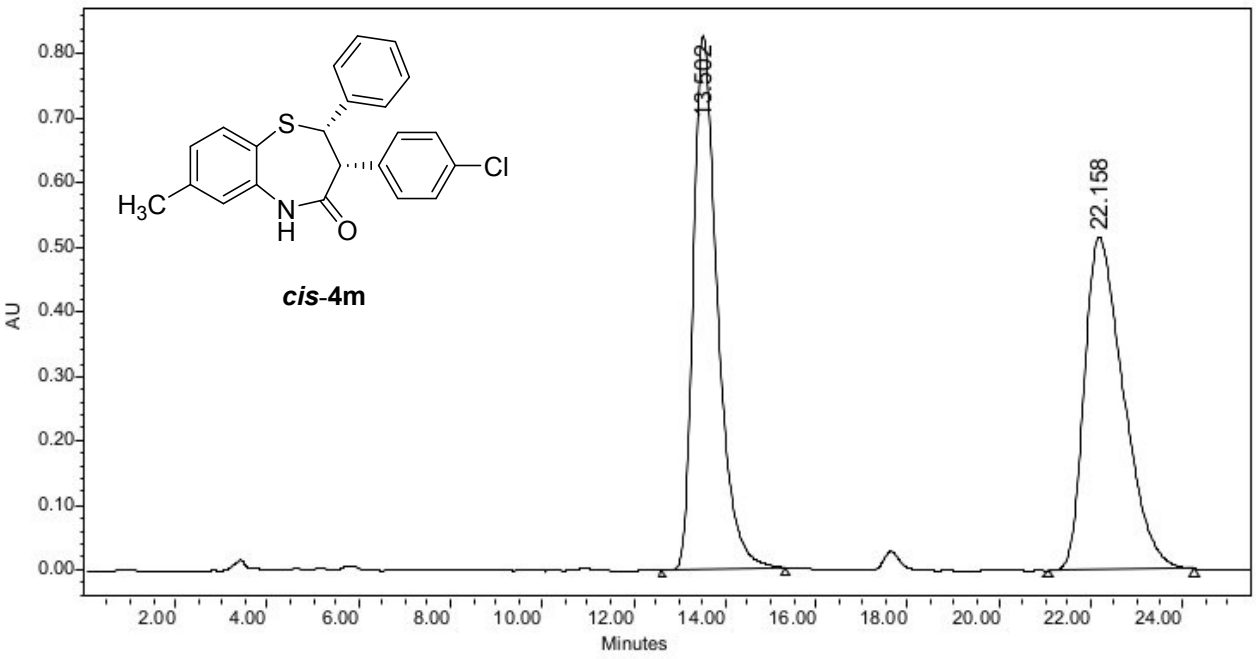


***trans*-4l**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	17.774	2473865	48.93	66918	53.68
2	Peak2	18.938	2582285	51.07	57747	46.32

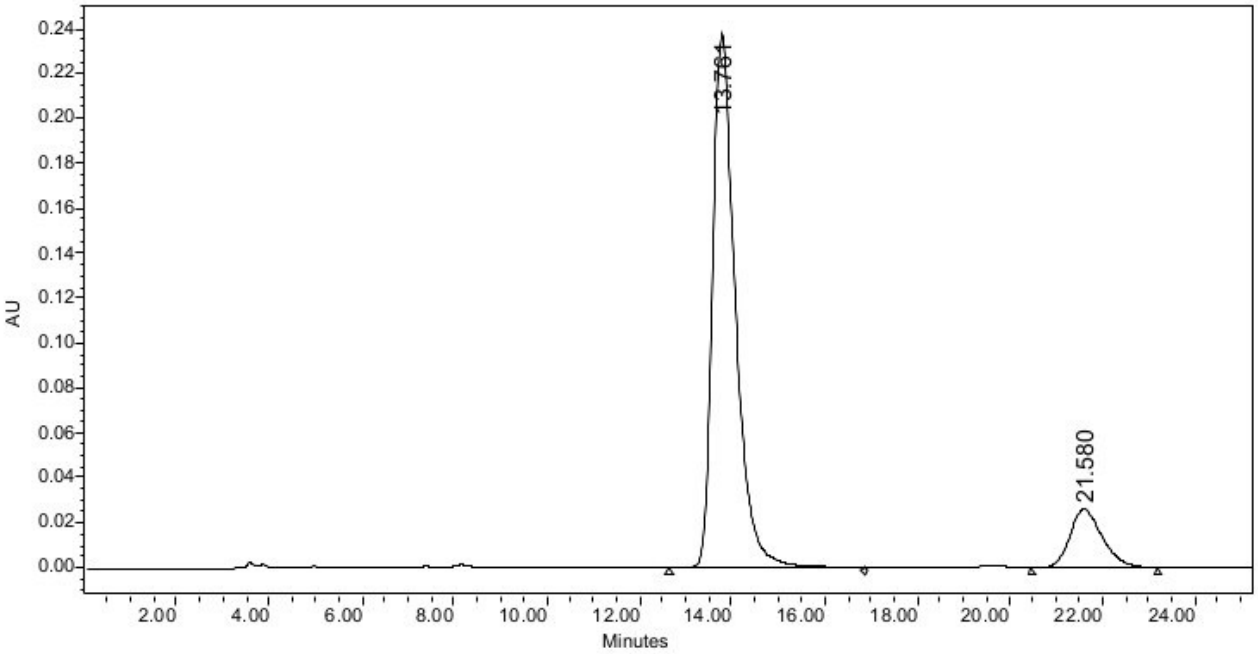


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	17.812	129582	3.25	3762	4.20
2	Peak2	18.930	3856682	96.75	85915	95.80

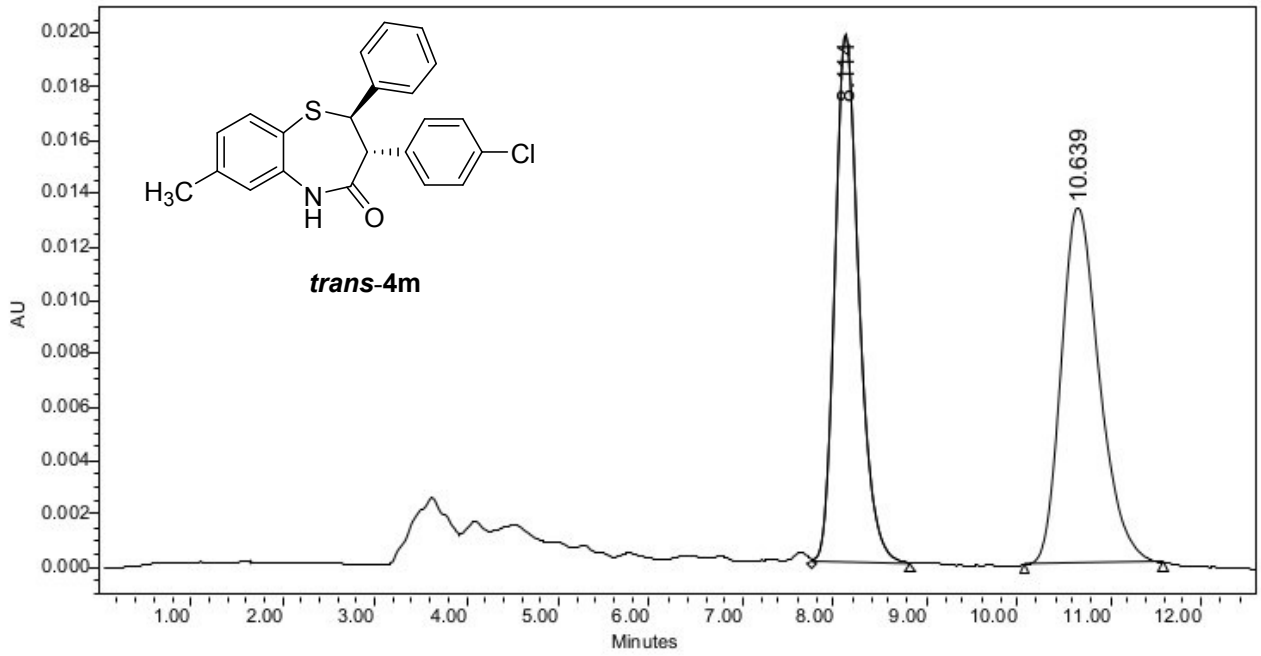


***cis*-4m**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	13.502	30418422	49.82	827916	61.54
2	22.158	30641672	50.18	517482	38.46

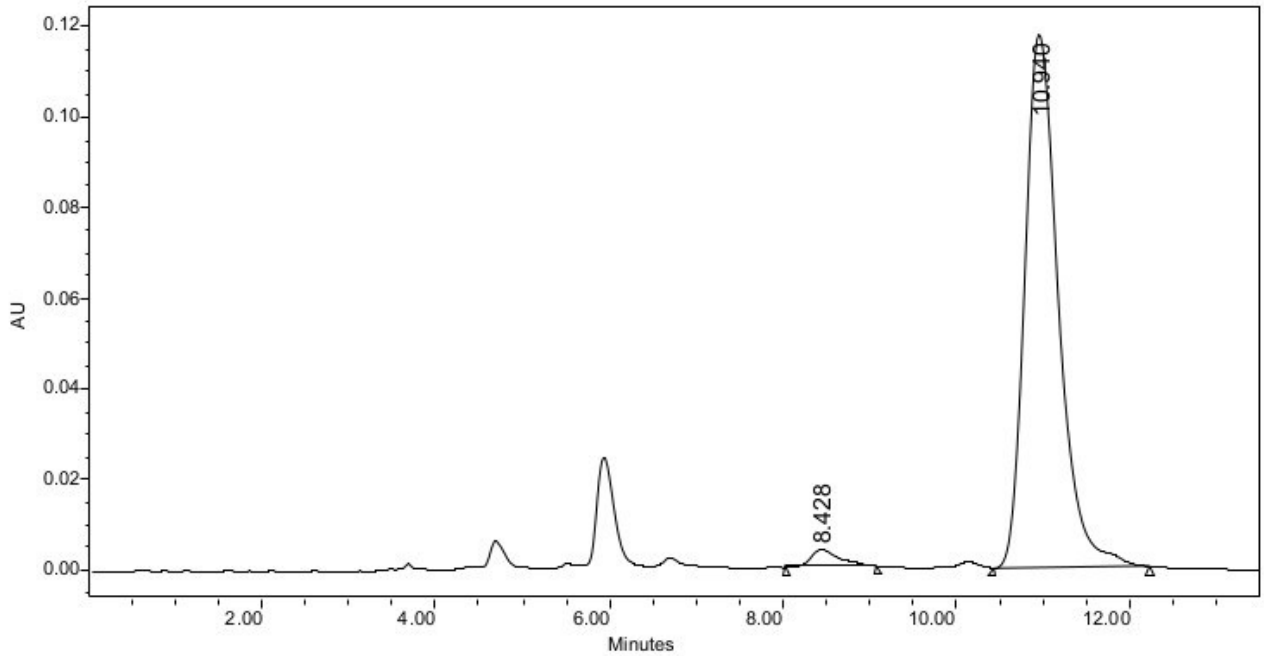


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	13.761	8158574	86.49	237900	89.98
2	21.580	1274861	13.51	26483	10.02

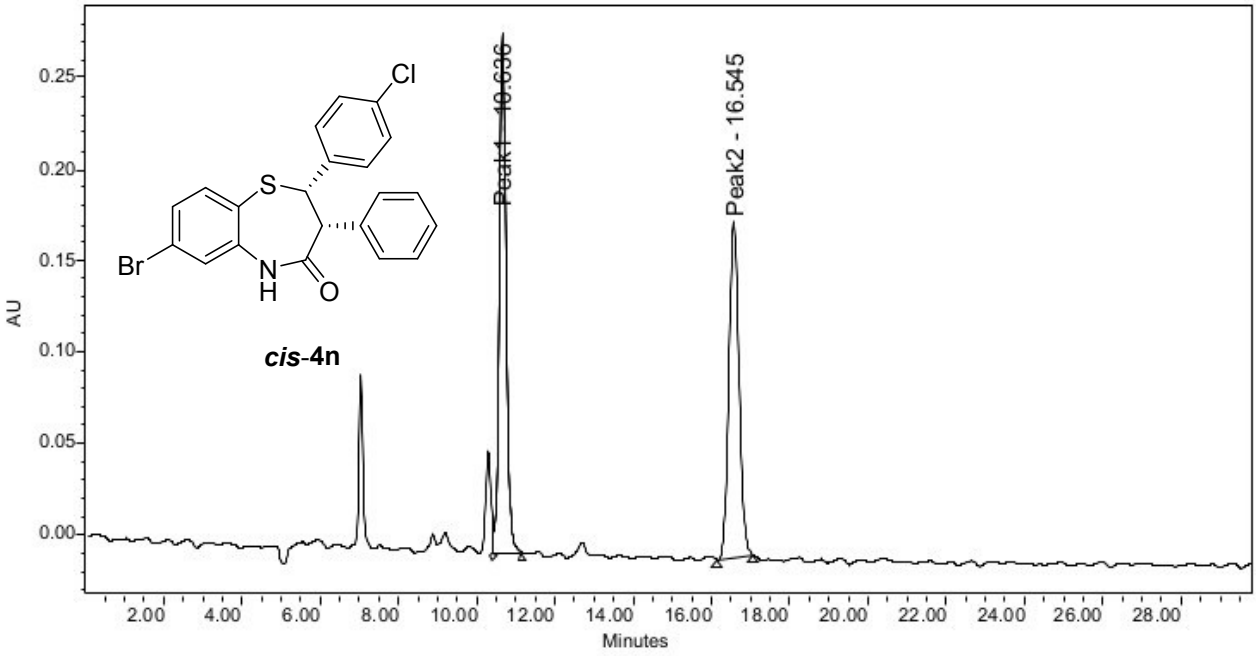


***trans*-4m**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.114	360254	48.08	19750	59.63
2	10.639	388952	51.92	13372	40.37

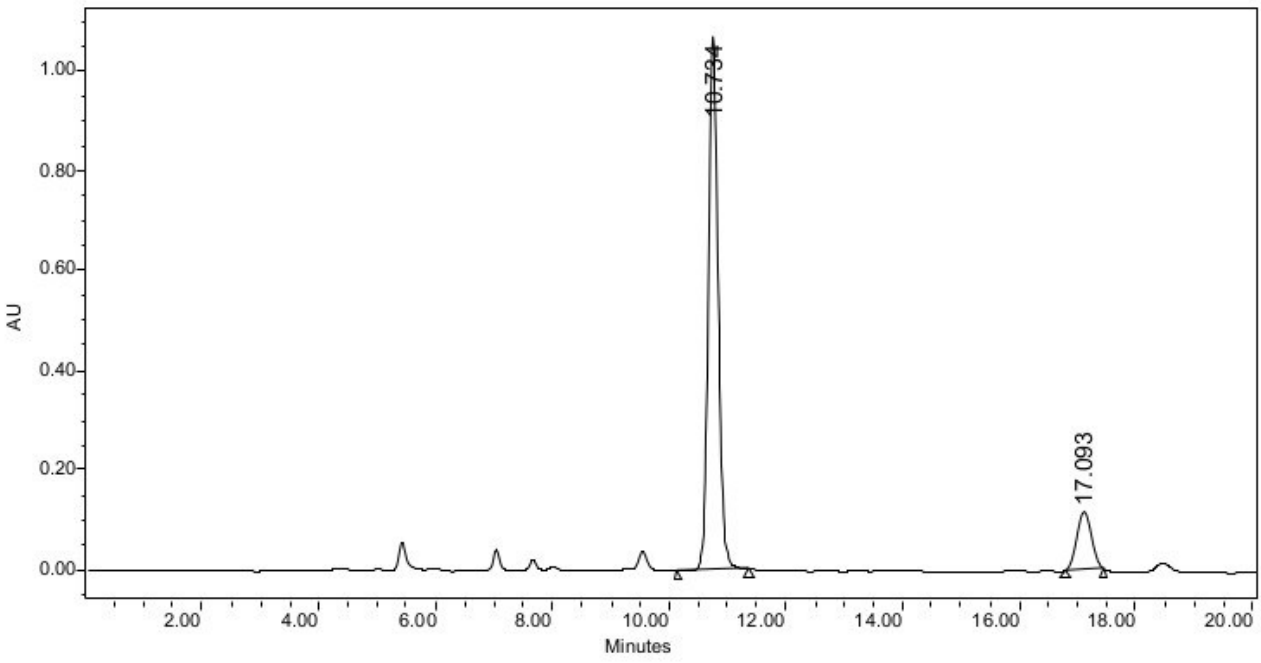


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.428	89430	2.74	3884	3.19
2	10.940	3169020	97.26	117739	96.81

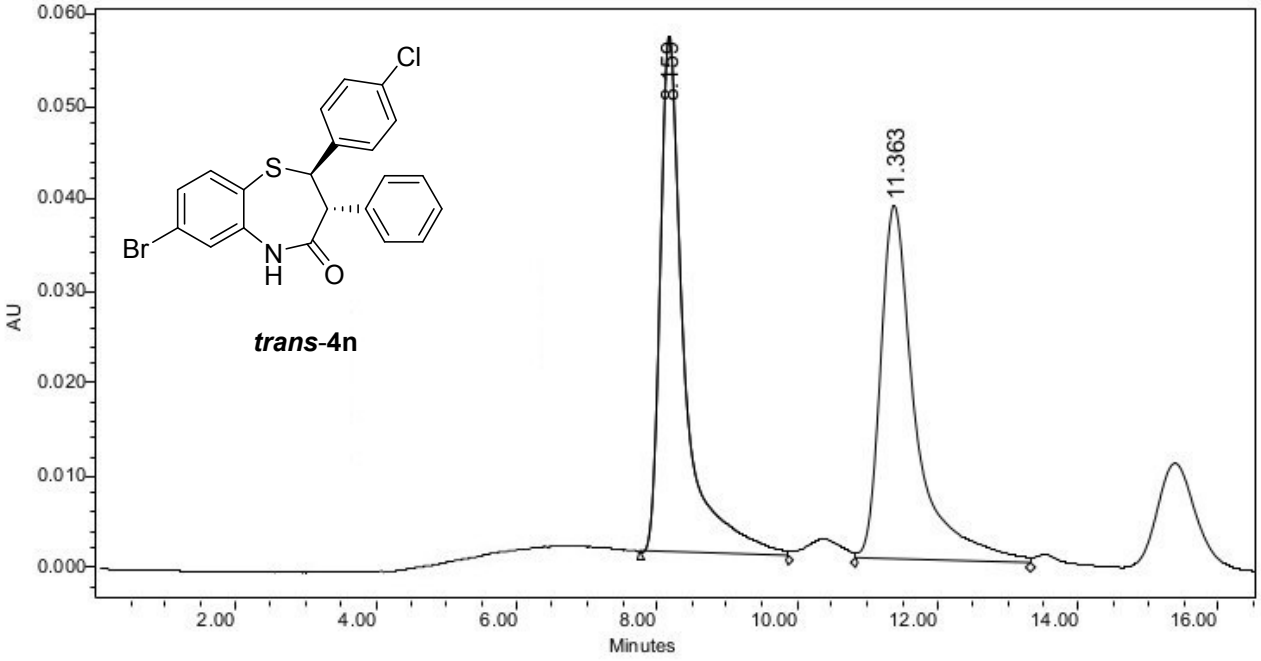


***cis*-4n**

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	10.636	3365568	50.32	284642	60.60
2	Peak2	16.545	3322808	49.68	185068	39.40

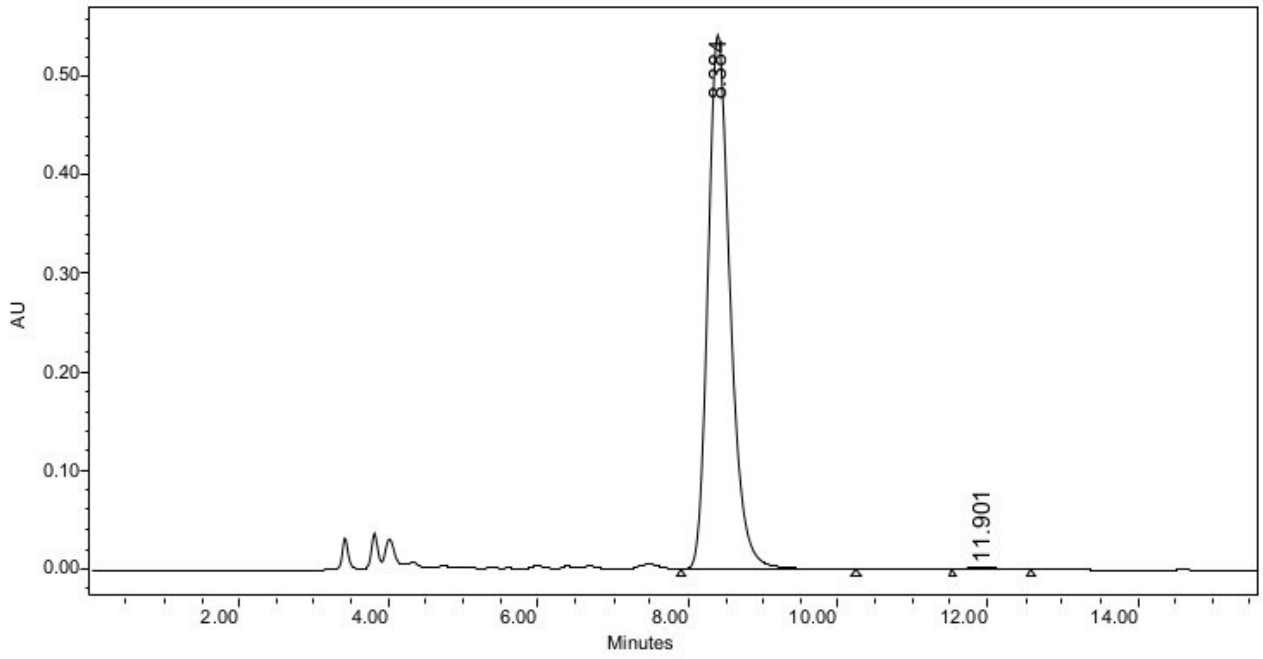


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.734	12499749	85.93	1072367	90.19
2	17.093	2046734	14.07	116585	9.81

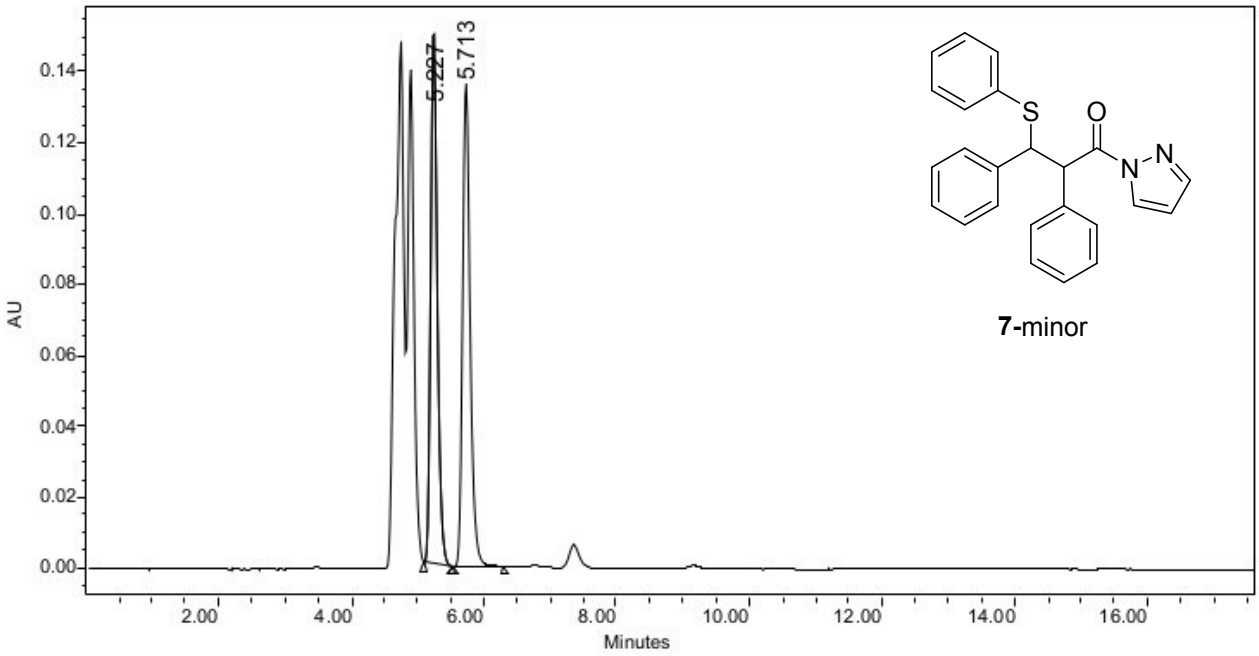


***trans*-4n**

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.159	1353964	49.93	56085	59.33
2	11.363	1358030	50.07	38447	40.67

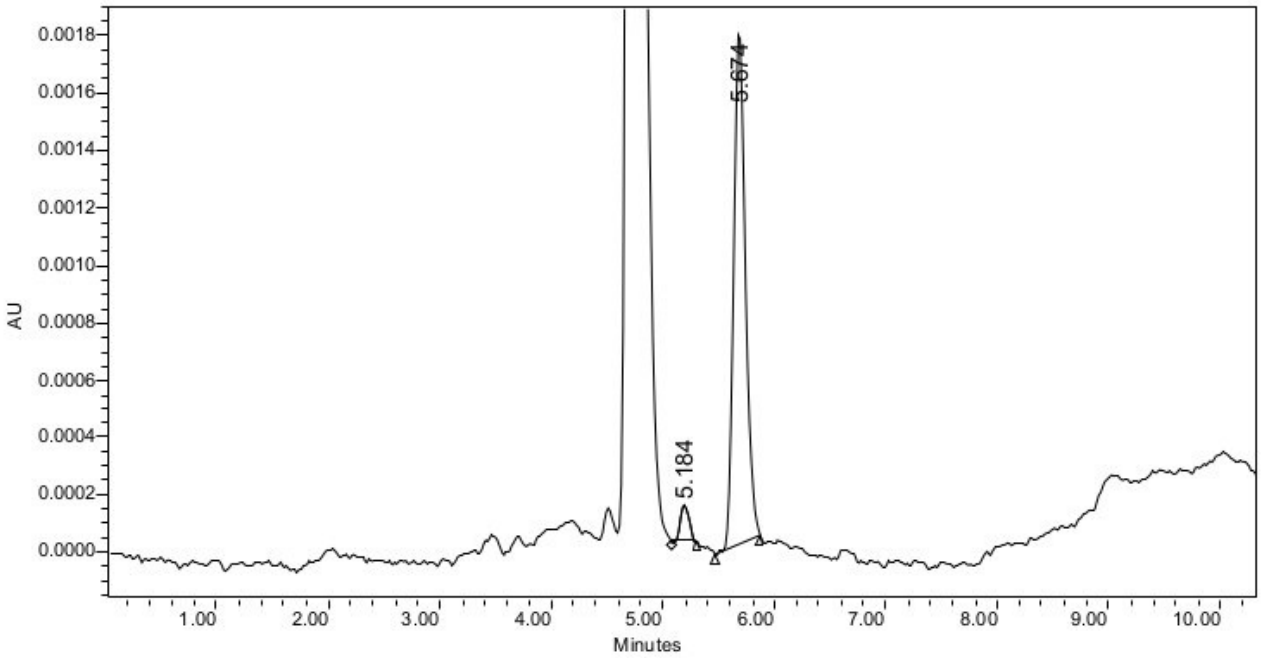


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	8.384	11217693	99.45	543006	99.63
2	11.901	61677	0.55	2009	0.37

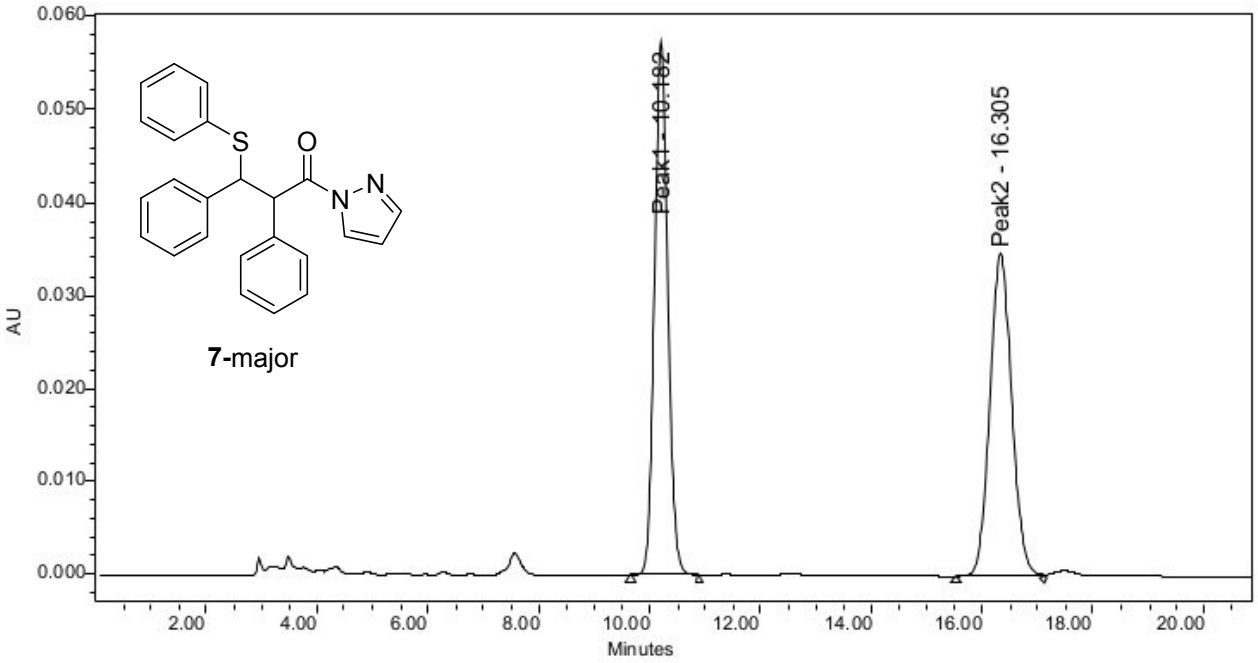


7-minor

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	5.227	1043440	49.25	150217	52.44
2	5.713	1075012	50.75	136215	47.56

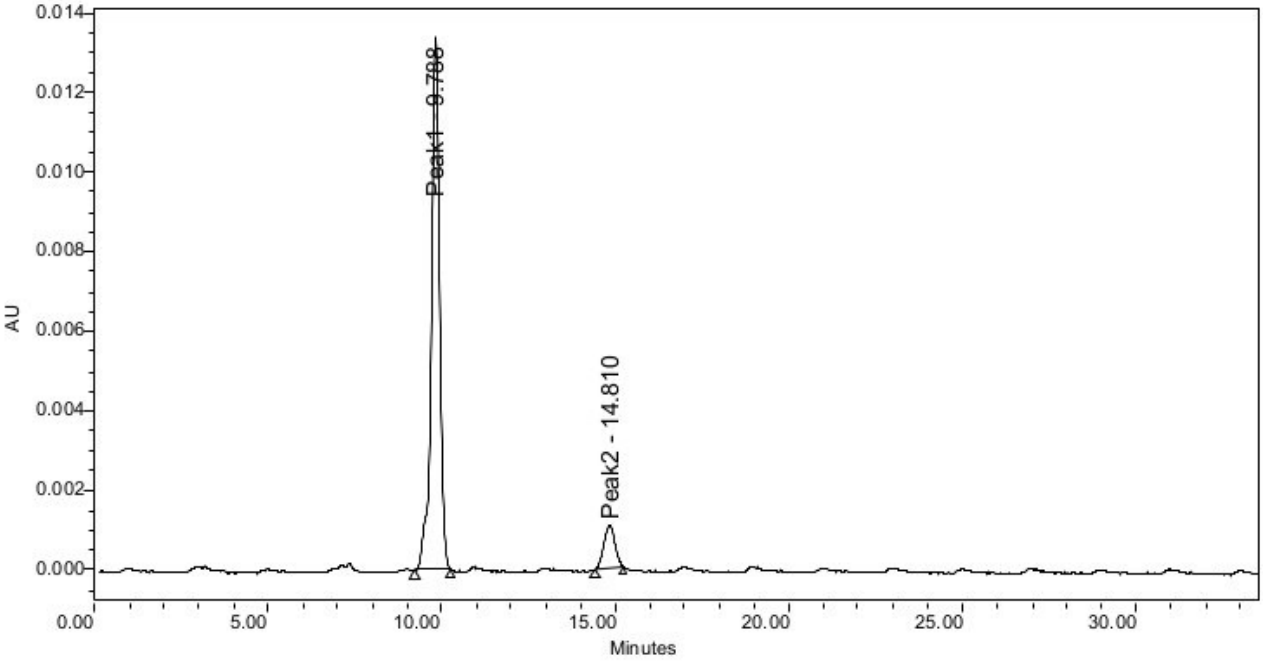


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	5.184	691	4.99	126	6.57
2	5.674	13163	95.01	1792	93.43

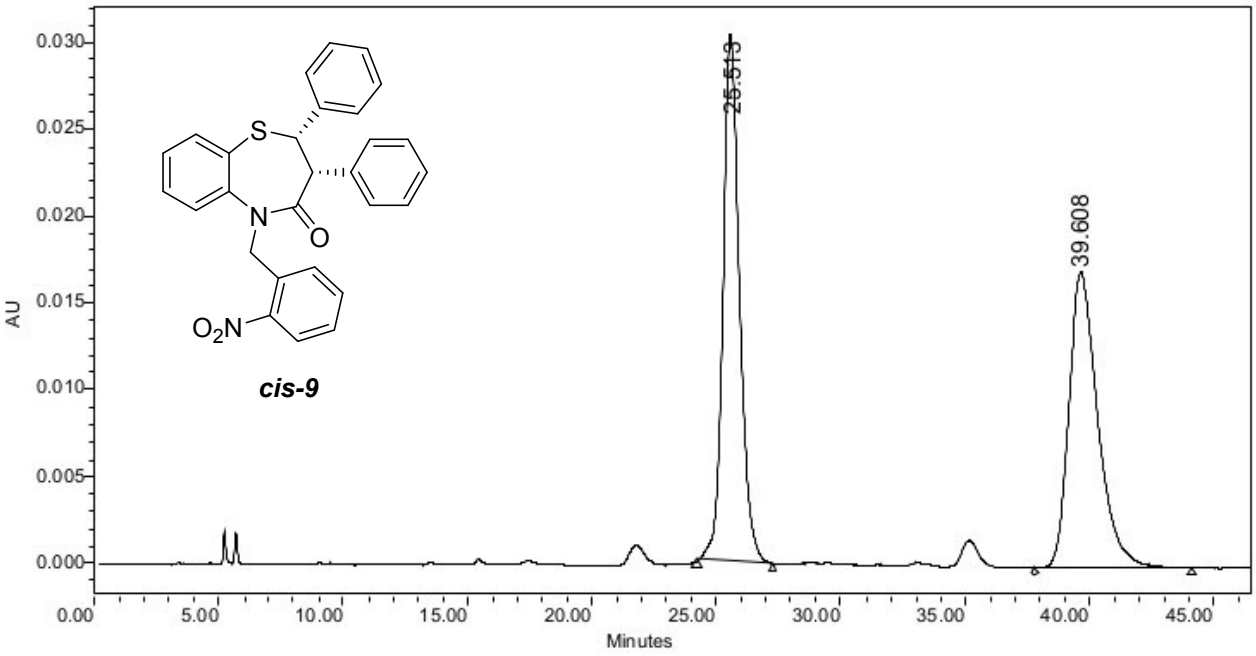


7-major

	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	10.182	956142	50.14	57409	62.29
2	Peak2	16.305	950975	49.86	34754	37.71

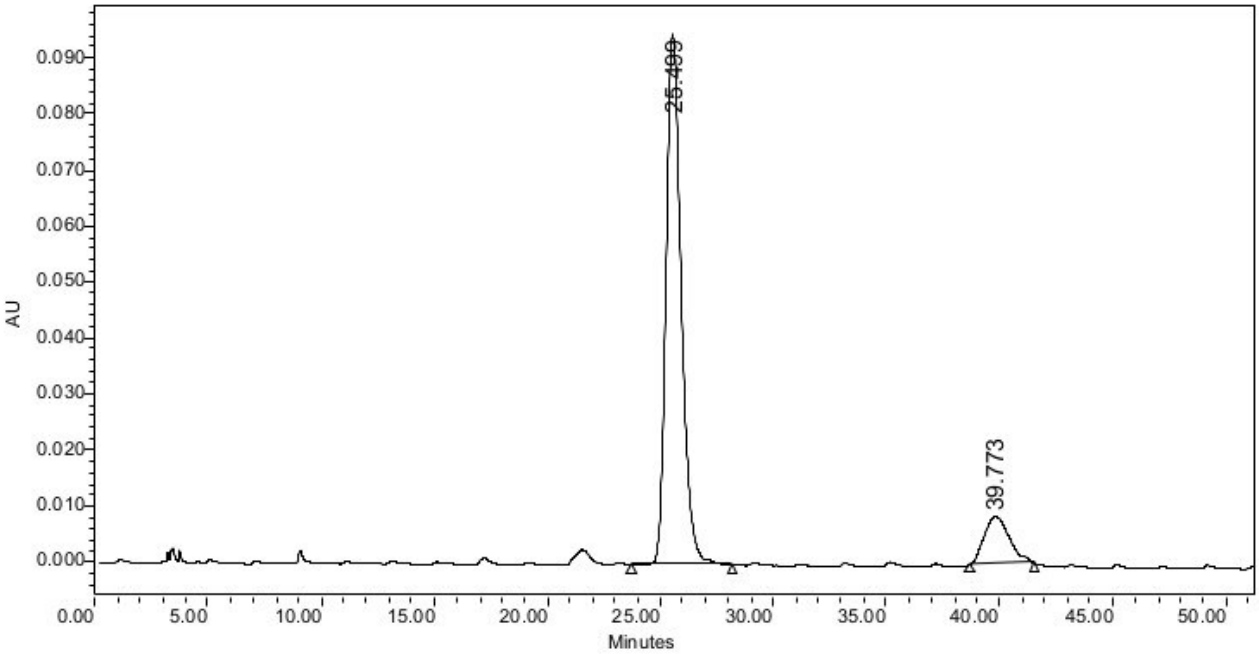


	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	9.788	221036	89.95	13409	92.46
2	Peak2	14.810	24687	10.05	1094	7.54

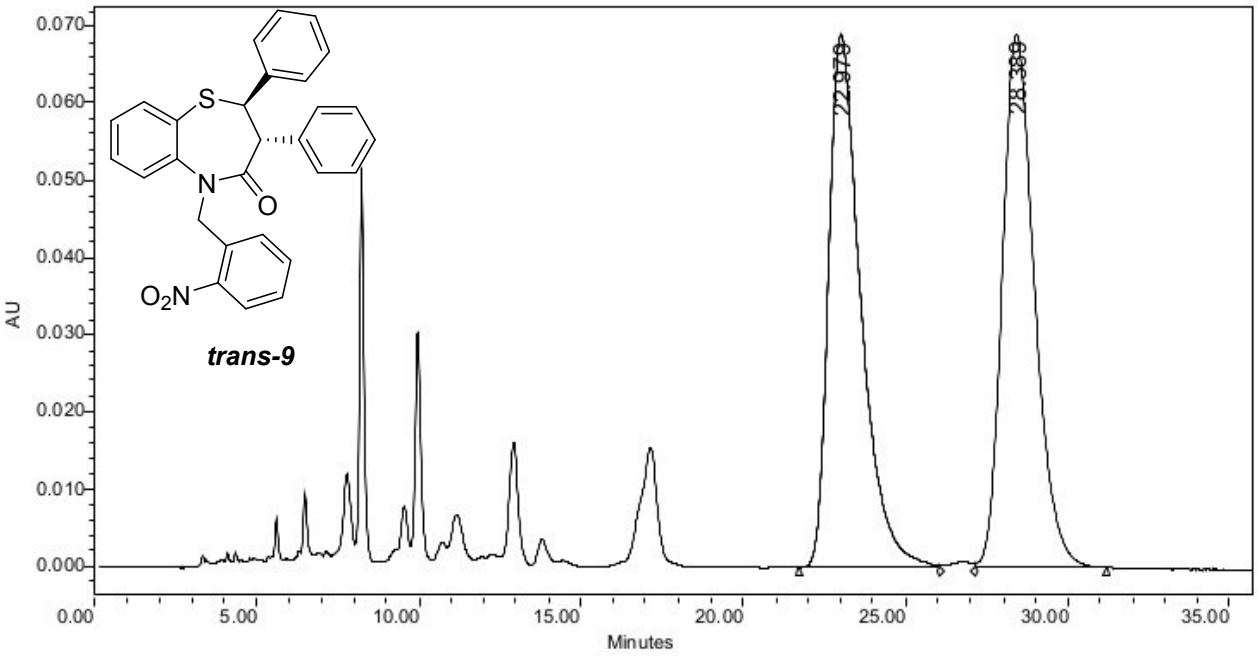


cis-9

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	25.513	1399142	50.42	30366	64.03
2	39.608	1375919	49.58	17060	35.97

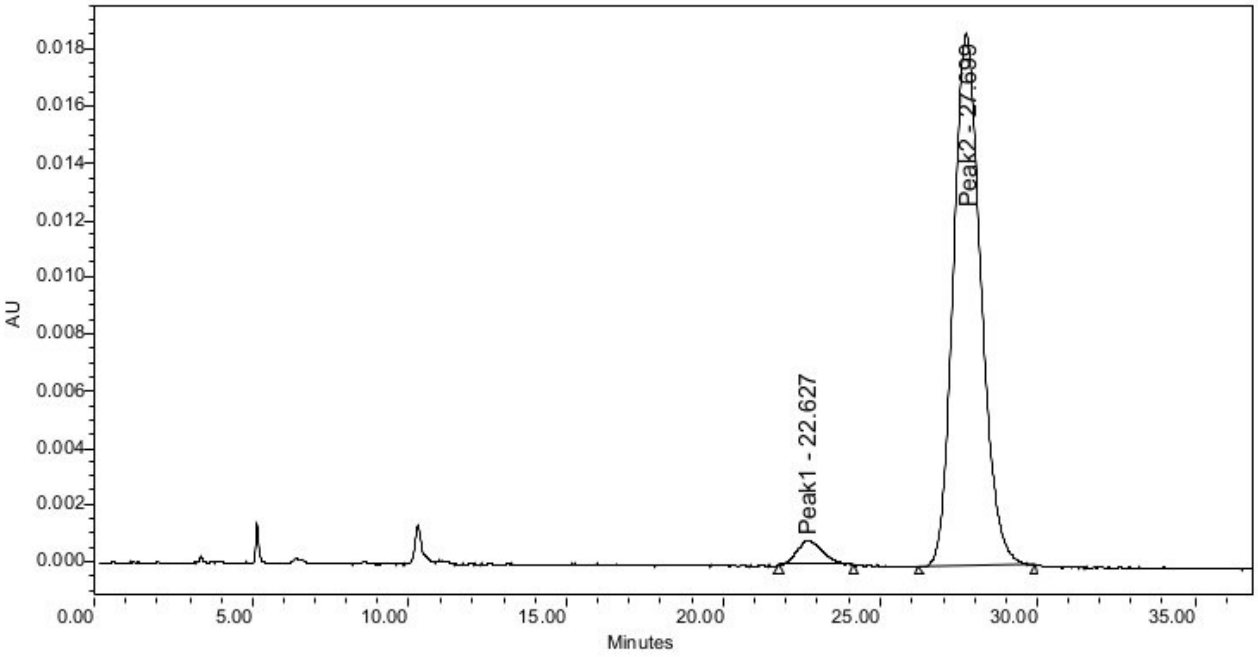


	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	25.499	4435144	87.20	94840	91.83
2	39.773	651016	12.80	8441	8.17



trans-9

	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	22.979	4773150	50.05	69060	49.99
2	28.389	4764509	49.95	69098	50.01



	Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	Peak1	22.627	52181	4.33	882	4.50
2	Peak2	27.699	1151974	95.67	18716	95.50