Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Diastereodivergent Aminocatalyzed Spirocyclization Strategies using 4-Alkylideneisoxazol-5-ones and Methyl Vinyl Ketones

Amanda F. da Silva,[a] Ives A. Leonarczyk,[b] Marco A. B. Ferreira*[b] and Igor D. Jurberg*[a]

[a]Institute of Chemistry, State University of Campinas, 13083-862, C.P. 6154, Campinas, SP, Brazil.
[b]Centre of Excellence for Research in Sustainable Chemistry (CERSusChem), Department of Chemistry, Federal University of São Carlos, 13565-905, São Carlos, SP, Brazil.

Table of Contents

1. General Information

All reactions were carried out under air, in oven dried glassware with magnetic stirring, unless otherwise noted. All reagents employed in this work were purchased from Sigma-Aldrich and used without further purification. All solvents employed in the reactions were distilled from appropriate drying agents prior to use. Organic solutions were concentrated under reduced pressure on an IKA rotary evaporator RV-10 Control. Reactions were monitored by thin-layer chromatography (TLC) on Silica gel 60 F_{254} aluminium plates (Merck). Chromatograms were visualized by fluorescence quenching with UV light at 254 nm or by staining using anisaldehyde solution. Flash column chromatography was performed using Merck silica gel 60 (particle size 35-70μm). ^{1}H and ^{13}C NMR spectra were recorded on either Bruker DPX-250, AV-400, AV-500 or AV-600 MHz spectrometers. Chemical shifts (δ) are given in parts per million, referenced to the residual peak of $CDCl_3$, δ = 7.24 (^{1}H NMR) and δ = 77.23 (^{13}C NMR) as internal references. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quint. = quintuplet, sext. = sextuplet, sept. = septuplet, m = multiplet, br s = broad singlet. High-resolution mass spectra were recorded on Thermo Scientific LTQ FT Ultra and Q Exactive Orbitrap spectrometers working with an electrospray ionization (ESI).

1.1. Preparation of Methyl Vinyl Ketones 3. Starting ketones 4-phenylbut-3-en-2-one (**3a**), 4-(4-chlorophenyl)but-3-en-2-one (**3b**), 4-methylpent-3-en-2-one (**3c**) were purchased from Sigma Aldrich. All other ketones employed in this work are also known compounds and have been prepared according to the literature:[1] (E)-4-(4-methoxyphenyl)but-3-en-2-one (**3d**),[2] (E)-4-(4-nitrophenyl)but-3-en-2-one (**3e**),[1,2] (E)-3-Hepten-2-one (**3f**),[3] (E)-4-(3-methoxyphenyl)but-3-en-2-one (**3g**),[4] (E)-4-(2-methoxyphenyl)but-3-en-2-one (**3h**),[5] (E)-4-(3-chlorophenyl)but-3-en-2-one (**3i**),[6] (E)-

[1] K. Zumbansen, A. Döhring, B. List, Morpholinium Trifluoroacetate-Catalyzed Aldol Condensation of Acetone with both Aromatic and Aliphatic Aldehydes, *Adv. Synth. Catal.,* 2010, **352**, 1135-1138.
[2] N. Solin, L. Han, S. Che, O. Terasaki, An Amphoteric Mesoporous Silica Catalyzed Aldol Reaction. *Catal. Commun.,* 2009, **10**, 1386-1389.
[3] W.-B. Yi, C. Cai, Aldol Condensations of Aldehydes and Ketones Catalyzed by Rare Eart(III) Perfluorooctane Sulfonates in Fluorous Solvents, *J. Fluorine Chem.,* 2005, **126**, 1553-1558.
[4] A. Bhowmik, R. A. Fernandes, Iron(III)/O_2-Mediated Regioselective Oxidative Cleavage of 1-Arylbutadienes to Cinnamaldehydes. *Org. Lett.*, 2019, **21**, 9203-9207.
[5] M. McConville, O. Saidi, J. Blacker, J. Xiao, Regioselective Hck Vinylation of Electron-Rich Olefins with Vinyl Halides: Is the Neutral Pathway in Operation?, *J. Org. Chem.* **2009**, *74*, 2692-2698.
[6] M. Bakos, Z. Dobi, D. Fegyverneki, Á. Gyömöre, I. Fernández, T. Soós, Janus Face of the Steric

4-(4-fluorophenyl)but-3-en-2-one (**3j**),[5] (E)-4-(4-(tert-butyl)phenyl)but-3-en-2-one (**3k**),[7] (E)-4-(naphthalen-2-yl)but-3-en-2-one (**3l**).[1,2]

1.2. Preparation of 4-Alkylideneisoxazol-5-ones 9. The following compounds are known and they were prepared according to methods previously described:[8,9] *(Z)*-4-benzylidene-3-phenylisoxazol-5(4H)-one (**9b**),[9] *(Z)*-4-benzylidene-3-methylisoxazol-5(4H)-one (**9c**),[10,11] *(Z)*-4-(4-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one (**9d**),[9] *(Z)*-4-(4-fluorobenzylidene)-3-phenylisoxazol-5(4H)-one (**9e**),[12] *(Z)*-4-benzylidene-3-ethylisoxazol-5(4H)-one (**9f**),[12] *(Z)*-4-(cyclopropylmethylene)-3-isopropylisoxazol-5(4H)-one (**9g**),[9] *(Z)*-4-(cyclopropylmethylene)-3-phenylisoxazol-5(4H)-one (**9h**),[9] *(Z)*-4-benzylidene-3-(4-methoxyphenyl)isoxazol-5(4H)-one (**9i**),[9] *(Z)*-4-(4-(tert-butyl)benzylidene)-3-phenylisoxazol-5(4H)-one (**9j**),[9] *(Z)*-4-benzylidene-3-(4-bromophenyl)isoxazol-5(4H)-one (**9k**),[9] *(Z)*-4-(4-methoxybenzylidene)-3-methylisoxazol-5(4H)-one (**9l**),[11] *(Z)*-4-(4-chlorobenzylidene)-3-methylisoxazol-5(4H)-one (**9o**),[13] *(Z)*-4-(3-chlorobenzylidene)-3-methylisoxazol-5(4H)-one (**9p**),[13] *(Z)*-4-(4-fluorobenzylidene)-3-methylisoxazol-5(4H)-one (**9q**),[14] *(Z)*-3-methyl-4-(naphthalen-2-ylmethylene)isoxazol-5(4H)-one (**9s**).[15]

Effect in a Lewis Acid Catalyst with Size-Exclusion Design: Steric Repulsion and Steric Attraction in the Catalytic Exo-Selective Diels-Alder Reaction, *ACS Sustainable Chem. Eng.* 2018, **6**, 10869-10875.

[7] J.-L. Shih, T. S. Nguyen, J. A. May, Organocatalyzed Asymmetric Conjugate Addition of Heteroaryl and Aryl Trifluoroborates: a Synthetic Strategy for Discoipyrrole D, *Angew. Chem. Int. Ed.* 2015, **54**, 9931-9935.

[8] N. M. R. Capreti, I. D. Jurberg, Michael Addition of Soft Carbon Nucleophiles to Alkylidene Isoxazol-5-ones: a Divergent Entry to α-Branched Carbonyl Compounds. *Org. Lett.* 2015, **17**, 2490-2493.

[9] I. D. Jurberg, An Aminocatalyzed Stereoselective Strategy for the Formal α-Propargylation of Ketones, *Chem. Eur. J.* 2017, **23**, 9716-9720.

[10] A. A. G. Fernandes, M. L. Stivanin, I. D. Jurberg, $RuCl_3$/ PPh_3-Catalyzed Direct Conversion of Isoxazol-5-ones to 2,3-Disubstituted Pyridines, *ChemistrySelect,* 2019, **4**, 3360-3365.

[11] M. S. Patil, C. Mudaliar, G. U. Chaturbhuj, Sulfated Polyborate Catalyzed Expeditious and Efficient Three-Component Synthesis of 3-Methyl-4-(Hetero)arylmethylene Isoxazol-5(4H)-ones,*Tetrahedron Lett.,* 2017, **58**, 3256-3261.

[12] M. L. Stivanin, M. Duarte, C. Sartori, N. M. R. Capreti, C. F. F. Angolini, I. D. Jurberg, An Aminocatalyzed Michael Addition/ Iron-Mediated Decarboxylative Cyclization Sequence for the Preparation of 2,3,4,6-Tetrasubstituted Pyridines: Scope and Mechanistic Insights, *J. Org. Chem.* 2017, **82**, 10319-10330.

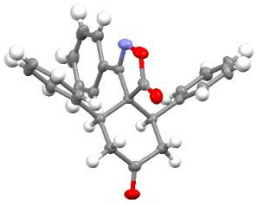
[13] F. Risitano, G. Grassi, F. Foti, R. Romeo, MIRC Reactions of (E)-Chalcones with Azol-5-ones - Diastereoselective Entry to Novel Spiro Tetrahydropyridine Derivatives, *Synthesis*, 2002, **1**, 116-120.

[14] ^{1}H NMR reported in d_6-DMSO: S. Fozooni, N. G. Hosseinzadeh, H. Hamidian, M. R. Akhgar, Nano Fe_2O_3, Clinoptilolite and $H_3PW_{12}O_{40}$ as Efficient Catalysts for Solvent-free Synthesis of 5(4H)-Isoxazolone under Microwave Irradiation Conditions, *J. Braz. Chem. Soc.,* 2013, **24**, 1649-1655.

[15] ^{1}H NMR reported in 1:1 d_6-DMSO:CCl_4: C. Wentrup, J. Becker, H.-W. Winter, Falling-Solid Flash Vacuum Pyrolysis: an Efficient Preparation of Arylacetylenes, *Angew. Chem. Int. Ed.,* 2015, **54**, 5702-5704.

2. X-rays

2.1. 1b (CCDC 2003785)



Bond precision: C-C = 0.0025 A Wavelength = 1.54178

Cell: a = 14.9898(11) b = 20.3897(14) c = 6.6198(5)

alpha = 90 beta = 90 gamma = 90

Temperature: 150 K

	Calculated	Reported
Volume	2023.3(3)	2023.3(3)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C26H21NO3	C26H21NO3
Sum formula	C26 H21 N O3	C26 H21 N O3
Mr	395.44	395.44
Dx,g cm^{-3}	1.298	1.298
Z	4	4
Mu (mm^{-1})	0.679	0.679
F000	832.0	832.0
F000’	834.48	
h,k,lmax	18,24,8	18,24,7
Nref	3740[2046]	3097
Tmin,Tmax	0.828, 0.895	0.690, 0.753
Tmin’	0.746	

Correction method= # Reported T Limits: Tmin = 0.690 Tmax = 0.753

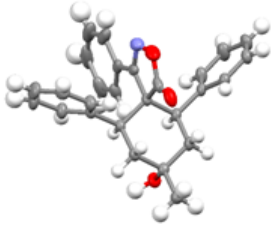
AbsCorr = MULTI-SCAN

Data completeness = 1.51/0.83 Theta(max) = 68.906

R(reflections) = 0.0285 (3078) wR2(reflections) = 0.0706 (3097)

S = 1.061 Npar = 272

1.2. 12 (CCDC 2003786)



Bond precision: C-C = 0.0021 A Wavelength = 1.54178

Cell: a = 33.6684 (18) b = 6.8422 (3) c = 19.7199 (11)

alpha = 90 beta = 103.309 (3) gamma = 90

Temperature: 150 K

	Calculated	Reported
Volume	4420.8 (4)	4420.8 (4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C27 H25 N O3	C27 H25 N O3
Sum formula	C27 H25 N O3	C27 H25 N O3
Mr	411.48	411.48
Dx, g cm^{-3}	1.237	1.236
Z	8	8
Mu (mm^{-1})	0.639	0.639
F000	1744.0	1744.0
F000’	1749.10	
h,k,lmax	40, 8, 23	40, 8, 23
Nref	8203	7992
Tmin,Tmax	0.914, 0.965	0.659, 0.753
Tmin’	0.885	

Correction method = # Reported T Limits: Tmin = 0.659 Tmax = 0.753

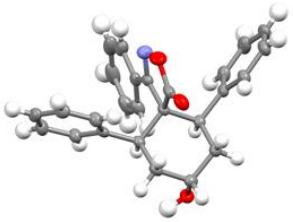
AbsCorr = MULTI-SCAN

Data completeness = 0.974 Theta(max) = 68.908

R(reflections) = 0.0394 (6879) wR2 (reflections) = 0.1071 (7992)

S = 1.023 Npar = 567

1.3. 13 (CCDC 2003787)



Bond precision: C-C = 0.0020 A Wavelength = 1.54178

Cell: a = 11.0366 (4) b = 6.8796 (2) c = 26.6895 (10)

alpha = 90 beta = 93.432 (2) gamma = 90

Temperature: 150 K

	Calculated	Reported
Volume	2022.83 (12)	2022.83 (12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H23 N O3	C26 H23 N O3
Sum formula	C26 H23 N O3	C26 H23 N O3
Mr	397.45	397.45
Dx, g cm^{-3}	1.305	1.305
Z	4	4
Mu (mm^{-1})	0.680	0.680
F000	840.0	840.0
F000’	842.48	
H, k, l max	13, 8, 32	13, 8, 32
Nref	3769	3673
Tmin, Tmax	0.955, 0.967	0.534, 0.753
Tmin’	0.723	

Correction method = # Reported T Limits: Tmin = 0.534 Tmax = 0.753

AbsCorr = MULTI-SCAN

Data completeness = 0.975 Theta(max) = 68.975

R(reflections) = 0.0386 (3286) wR2 (reflections) = 0.1041 (3673)

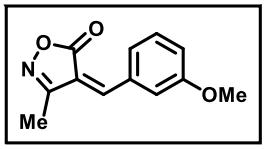
S = 1.039 Npar = 274

3. Characterization of Compounds

3.1. 4-Alkylideneisoxazole-5-ones

***(Z)*-4-(3-methoxybenzylidene)-3-methylisoxazol-5(4H)-one (9m)**

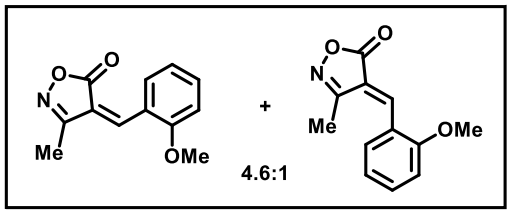
Prepared following general strategies previously described.[9] Yellow solid, 1.1g, 50% for 2 steps (10:1 Z:E, only major Z diastereoisomer is described).



^{1}H (250 MHz, $CDCl_3$) δ: 8.34-8.33 (m, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.38 (s, 1H), 7.13 (ddd, *J* = 8.0 Hz, *J* = 2.6 Hz, *J* = 0.9 Hz, 1H), 3.89 (s, 3H), 2.29 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 168.2, 161.3, 160.1, 150.2, 133.8, 130.0, 127.6, 121.8, 120.0, 116.7, 55.8, 11.9. IR (ATR, cm^{-1}): 1751, 1734, 1620, 1571, 1440, 1413, 1320, 1272, 1193, 1170, 1097. M. P.: 112 - 114 ^{o}C. HRMS (ESI+): Calcd. for $[C_{12}H_{11}NO_3 + H]^+$: 218.0812, found: 218.0813.

(Z)-4-(2-methoxybenzylidene)-3-methylisoxazol-5(4H)-one and **(E)-4-(2-methoxybenzylidene)-3-methylisoxazol-5(4H)-one (9n)**[16]

Prepared following general strategies previously described.[9] Yellow solid: 1.5 g, 70% for two steps (4.6:1 Z:E).

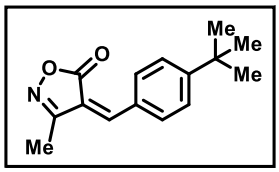


^{1}H (250 MHz, $CDCl_3$) δ: **Major Z diastereoisomer:** 8.87 (dd, *J* = 8.9 Hz, *J* = 1.5 Hz, 1H), 8.01 (s, 1H), 7.56-6.46 (m, 1H), 7.06-6.91 (m, 2H), 3.91 (s, 3H), 2.26 (s, 3H). **Minor E diastereoisomer:** 8.18 (s, 1H), 7.56-6.46 (m, 1H), 7.32 (dd, *J* = 7.4 Hz, *J* = 1.5 Hz, 1H), 7.06-6.91 (m, 2H), 3.87 (s, 3H), 2.14 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: **Major Z diastereoisomer:** 168.5, 161.7, 160.0, 144.2, 136.5, 133.6, 121.4, 121.1, 118.5, 110.9, 56.1, 11.9. **Minor E diastereoisomer:** 170.5, 159.1, 158.3, 147.2, 134.4, 131.6, 121.5, 120.5, 120.4, 111.3, 55.9, 15.2. IR (ATR, cm^{-1}): 1747, 1730, 1608, 1590, 1575, 1487, 1476, 1442, 1405, 1374, 1349, 1258, 1170, 1133, 1103. M. P.: 157 - 159 ^{o}C. HRMS (ESI+): Calcd. for $[C_{12}H_{11}NO_3 + H]^+$: 218.0812, found: 218.0813.

[16] For NMR data of previously reported Z isomer, see: D. Setamdideh, One-Pot Green Synthesis of Isoxazol-5(4H)-one Derivatives by Dowex1-x8OH in Water, *J. Serb. Chem. Soc.* 2016, **81**, 971-978.

***(Z)*-4-(4-(tert-butyl)benzylidene)-3-methylisoxazol-5(4H)-one (9r)**

Prepared following general strategies previously described.[9] Yellow solid, 713 mg, 49% for 2 steps.



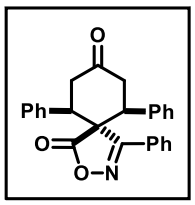
^{1}H (250 MHz, $CDCl_3$) δ: 8.30 (d, *J* = 8.6 Hz, 2H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.39 (s, 1H), 2.28 (s, 3H), 1.33 (s, 9H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 168.4, 161.4, 158.7, 149.9, 134.2, 130.1, 126.4, 118.8, 35.7, 31.1, 11.9. IR (ATR, cm^{-1}): 2363, 1749, 1733, 1622, 1597, 1556, 1425, 1411, 1396, 1352, 1229, 1134, 1109. M. P.: 103 - 105 ^{o}C. HRMS (ESI+): Calcd. for $[C_{15}H_{17}NO_2 + H]^+$: 244.1332, found: 244.1332.

3.2. 6,10-*cis*-Spiroisoxazol-5-ones

General Procedure A. *Racemic Aminocatalyzed cis-Spirocyclization of 4-Alkylideneisoxazol-5-ones **9** with Methyl Vinyl Ketones **3**.* A round bottom flask is charged with the 4-alkylideneisoxazol-5-one **9** (0.2 mmol, 1 equiv.), MeCN (1 mL, 0.2 M in relation to **9**), methyl vinyl ketone **3** (1 mmol, 5 equiv.), morpholine (7 µL, 0.08 mmol, 0.4 equiv.) and 4-chlorobenzoic acid (8 mg, 0.04 mmol, 0.2 equiv.). The reaction is allowed to stir at rt for 5 days (~120h). Upon completion, the reaction mixture is concentrated under reduced pressure. The crude reaction mixture is purified by flash column chromatography to afford the corresponding 6,10-*cis*-spiroisoxazol-5-one **1**.

4,6,10-triphenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1b)[13]

Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a light pink solid: 73 mg, 93%.

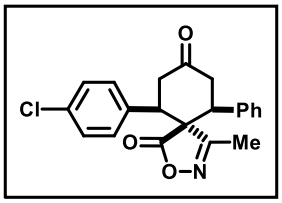


^{1}H (500 MHz, $CDCl_3$) δ: 7.47-7.32 (m, 2H), 7.58-7.55 (m, 1H), 7.50-7.47 (m, 2H), 7.21-7.13 (m, 6H), 6.95-6.94 (m, 4H), 4.05 (dd, *J* = 13.4 Hz, *J* = 3.5Hz, 2H), 3.92 (t, *J* = 14.5 Hz, 2H), 2.62 (dd, *J* = 14.5 Hz, *J* = 3.5 Hz, 2H). ^{13}C (125 MHz, $CDCl_3$) δ: 207.3, 178.2, 165.5, 136.4, 132.1, 129.4, 129.2, 128.9, 128.5, 127.5, 127.3, 60.5, 48.0, 41.9. IR (ATR, cm^{-1}): 2928, 2855, 2365, 1777, 1716, 1550, 1497, 1456, 1442, 1408, 1362, 1316, 1286,

1244, 1178, 1119, 1073, 1035, 1000. M. P.: 220 - 222 ^{o}C. HRMS (ESI+): Calcd. for $[C_{26}H_{21}NO_3 + H]^+$: 396.1594, found: 396.1589.

6-(4-chlorophenyl)-4-methyl-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1c)

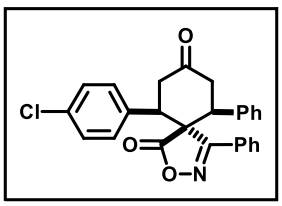
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a light yellow solid: 54 mg, 73%.



^{1}H (250 MHz, $CDCl_3$) δ: 7.33-7.26 (m, 5H), 7.18-7.10 (m, 4H), 3.79-3.64 (m, 2H), 3.42 (dd, *J* = 14.3 Hz, *J* = 3.8 Hz, 2H), 2.62-2.51 (m, 2H), 1.97 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 205.8, 178.4, 166.8, 136.5, 135.2, 135.1, 129.9, 129.7, 129.2, 128.6, 127.2, 59.4, 48.3, 47.6, 42.2, 42.1, 12.4. IR (ATR, cm^{-1}): 2921, 1770, 1721, 1492, 1454, 1416, 1388, 1284, 1223, 1181, 1093, 1060. M. P.: 187 - 189 ^{o}C. HRMS (ESI+): Calcd. for $[C_{21}H_{18}ClNO_3 + H]^+$: 368.1048, found: 368.1049.

6-(4-chlorophenyl)-4,10-diphenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1d)

Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as an yellow solid: 64 mg, 75%.

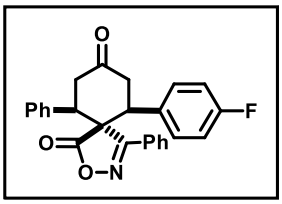


^{1}H (500 MHz, $CDCl_3$) δ: 7.75-7.74 (m, 2H), 7.59- 7.56 (m, 1H), 7.51-7.48 (m, 2H), 7.20-7.11 (m, 5H), 6.94 (d, *J* = 3.5 Hz, 2H), 6.87 (d, *J* = 4.3 Hz, 2H), 4.08-4.02 (m, 2H), 3.93-3.83 (m, 2H), 2.65-2.57 (m, 2H). ^{13}C (125 MHz, $CDCl_3$) δ: 206.8, 178.0, 165.3, 136.2, 134.9, 134.8, 132.3, 129.6, 129.4, 129.2, 129.0, 128.9, 128.3, 127.5, 127.2, 60.4, 47.9, 47.2, 41.8, 41.7. IR (ATR, cm^{-1}): 2361, 2342, 1765, 1716, 1492, 1284, 1261, 1241, 1228, 1180, 1091, 1040, 1012. M. P.: degradation at 210 ^{o}C. HRMS (ESI+): Calcd. for $[C_{26}H_{20}ClNO_3 + H]^+$: 430.1204, found: 430.1200.

6-(4-fluorophenyl)-4,10-diphenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1e)

Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt -

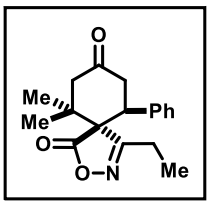
8:2 Hex:AcOEt) affords the title compound as an orange solid: 79 mg, 96%.



^{1}H (500 MHz, $CDCl_3$) δ: 7.75-7.73 (m, 2H), 7.59- 7.56 (m, 1H), 7.51-7.48 (m, 2H), 7.21-7.18 (m, 1H), 7.17-7.13 (m, 2H), 6.95-6.90 (m, 4H), 6.86-6.81 (m, 2H), 4.07-4.02 (m, 2H), 3.93-3.87 (m, 2H), 2.65-2.58 (m, 2H). ^{13}C (125 MHz, $CDCl_3$) δ: 207.0, 178.1, 165.3, 162.7 (d, *J* = 247.0 Hz), 136.2, 132.2, 132.2 (d, *J* = 3.0Hz), 129.5, 129.3 (d, *J* = 8.0Hz), 129.2, 128.9, 128.3, 127.5, 127.2, 116.2 (d, *J* = 21.5 Hz), 60.6, 47.9, 47.2, 41.9, 41.8. ^{19}F (235 MHz, $CDCl_3$) δ: -112.6. IR (ATR, cm^{-1}): 2923, 2853, 1778, 1718, 1511, 1244, 1178, 1161, 1072. M. P.: Degradation at 141 ^{o}C. HRMS (ESI+): Calcd. for $[C_{26}H_{20}FNO_3 + H]^+$: 414.1500, found: 414.1494.

4-ethyl-6,6-dimethyl-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1f)

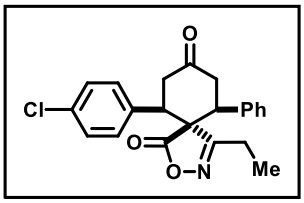
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a light yellow solid: 27 mg, 45%.



^{1}H (500 MHz, $CDCl_3$) δ: 7.30-7.28 (m, 3H), 7.16- 7.14 (m, 2H), 3.60-3.46 (m, 3H), 2.48-2.45 (m, 1H), 2.43-2.31 (m, 2H), 2.01 (dd, *J* = 14.0 Hz, *J* = 1.0 Hz, 1H), 1.25 (s, 3H), 1.03 (t, *J* = 7.5 Hz, 3H), 1.01 (s, 3H). ^{13}C (125 MHz, $CDCl_3$) δ: 207.6, 179.3, 170.6, 137.0, 129.5, 129.0, 127.4, 62.1, 50.1, 44.3, 42.6, 40.6, 26.4, 25.0, 23.7, 9.8. IR (ATR, cm^{-1}): 2978, 1778, 1719, 1496, 1450, 1381, 1239, 1186, 1172, 1087, 1065, 1036. M. P.: Degradation at 176 ^{o}C. HRMS (ESI+): Calcd. for $[C_{18}H_{21}NO_3 + H]^+$: 300.1594, found: 300.1587.

6-(4-chlorophenyl)-4-ethyl-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1g)

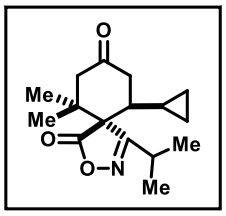
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as an yellow solid: 46 mg, 61%.



^{1}H (500 MHz, $CDCl_3$) δ: 7.31-7.27 (m, 5H), 7.16- 7.14 (m, 2H), 7.10 (d, *J* = 8.5 Hz, 2H), 3.75-3.66 (m, 2H), 3.41 (dd, *J* =15.0 Hz, *J* = 4.0 Hz, 2H), 2.59-2.52 (m, 2H), 2.41-2.29 (m, 2H), 0.94 (t, *J* = 7.0 Hz, 3H). ^{13}C (125 MHz, $CDCl_3$) δ: 205.9, 178.9, 170.3, 136.7, 135.4, 135.0, 129.9, 129.7, 129.2, 128.6, 127.2, 59.5, 48.5, 47.8, 42.4, 42.3, 20.6, 8.1. IR (ATR, cm^{-1}): 1764, 1719, 1494, 1456, 1417, 1285, 1243, 1227, 1190, 1094, 1068, 1014. M. P.: Degradation at 205 ºC. HRMS (ESI+): Calcd. for $[C_{22}H_{20}ClNO_3 + H]^+$: 382.1204, found: 382.1200.

10-cyclopropyl-4-isopropyl-6,6-dimethyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1h)

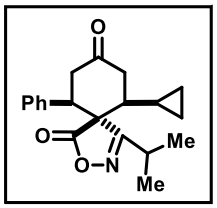
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a white solid: 46 mg, 83%.



^{1}H (500 MHz, $CDCl_3$) δ: 3.4 (d, *J* = 14.2Hz, 1H), 2.73 (t, *J* = 13.0Hz, 1H), 2.62-2.57 (m, 1H), 2.31-2.26 (m, 1H), 2.17- 2.13 (m, 1H), 1.89 (d, *J* = 14.2Hz, 1H), 1.44 (d, *J* = 7.5 Hz, 3H), 1.42 (d, *J* = 7.5Hz, 3H), 1.14 (s, 3H), 1.01 (s, 3H), 0.63-0.58 (m, 1H), 0.52-0.45 (m, 2H), 0.29-0.26 (m, 1H), 0.21-0.18 (m, 1H). ^{13}C (125 MHz, $CDCl_3$) δ: 208.5, 178.8, 175.3, 62.5, 50.5, 40.4, 39.1, 38.6, 28.7, 26.1, 24.4, 23.2, 23.1, 12.6, 4.3, 1.6. IR (ATR, cm^{-1}): 2927, 1760, 1714, 1469, 1423,1392, 1377, 1305, 1283, 1254, 1238, 1207,1182, 1162, 1145, 1098, 1079, 1032. M. P.: 132 - 134 ºC. HRMS (ESI+): Calcd. for $[C_{16}H_{23}NO_3 + H]^+$: 278.1751, found: 278.1746.

6-cyclopropyl-4-isopropyl-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1i)

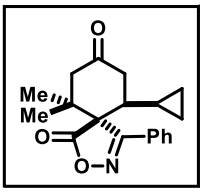
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as an yellow solid: 60 mg, 91%.



^{1}H (400 MHz, $CDCl_3$) δ: 7.32-7.27 (m, 3H), 7.14- 7.12 (m, 2H), 3.55 (t, *J* = 14.0 Hz, 1H), 3.37 (dd, *J* = 14.0 Hz, *J* = 3.6Hz, 1H), 2.91 (t, *J* = 14.0 Hz, 1H), 2.64-2.57 (m, 1H), 2.46-2.41 (m, 2H), 2.20- 2.15 (m, 1H), 1.31 (d, *J* = 6.8 Hz, 3H), 0.94 (d, *J* = 6.8 Hz, 3H), 0.74-0.69 (m, 1H), 0.52-0.42 (m, 2H), 0.40-0.34 (m, 1H), 0.26-0.20 (m, 1H). ^{13}C (100 MHz, $CDCl_3$) δ: 207.2, 178.7, 174.2, 137.6, 129.4, 128.5, 127.1, 59.0, 47.8, 43.4, 42.2, 37.4, 27.8, 21.8, 20.3, 11.6, 2.0, 1.0. IR (ATR, cm^{-1}): 2980, 1760, 1723, 1497, 1470, 1457, 1425, 1288, 1254, 1219, 1188, 1148, 1121, 1075, 1050, 1018. M. P.: 150 - 152 ^{o}C. HRMS (ESI+): Calcd. for $[C_{20}H_{23}NO_3 + H]^+$: 326.1751, found: 326.1745.

10-cyclopropyl-6,6-dimethyl-4-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1j)

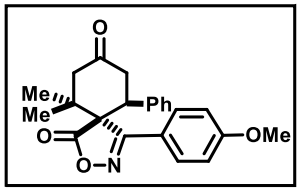
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a white solid: 52 mg, 83%.



^{1}H (400 MHz, $CDCl_3$) δ: 7.58-7.56 (m, 2H), 7.53- 7.43 (m, 3H), 3.39 (d, *J* = 14.0 Hz, 1H), 2.98-2.91 (m, 1H), 2.79- 2.73 (m, 1H), 2.34-2.29 (m, 1H), 1.87 (dd, *J* = 14.0Hz, *J* = 2.0 Hz, 1H), 0.95 (s, 3H), 0.88-0.82 (m, 1H), 0.70 (s, 3H), 0.57-0.52 (m, 1H), 0.48-0.36 (m, 2H), 0.35-0.30 (m, 1H). ^{13}C (100 MHz, $CDCl_3$) δ: 208.3, 178.7, 168.1, 131.5, 131.1, 129.4, 128.7, 62.7, 50.2, 40.5, 40.0, 39.5, 26.2, 25.7, 13.3, 3.0, 1.9. IR (ATR, cm^{-1}): 2359, 2340, 1771, 1719, 1198, 1161, 1104, 1066, 1031. M. P.: 156 - 158 ^{o}C. HRMS (ESI+): Calcd. for $[C_{19}H_{21}NO_3 + H]^+$: 312.1594, found: 312.1589.

4-(4-methoxyphenyl)-6,6-dimethyl-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1k)

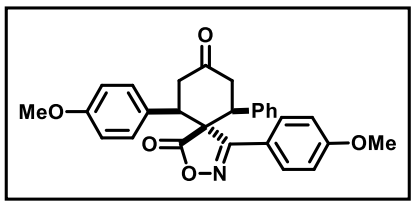
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a light yellow solid: 52 mg, 68%.



^{1}H (500 MHz, $CDCl_3$) δ: 7.51 (d, *J* = 9.0 Hz, 2H), 7.24- 7.15 (m, 5H), 6.83 (d, *J* = 9.0 Hz, 2H), 4.08 (dd, *J* = 13.5 Hz, *J* = 4.5 Hz, 1H), 3.74 (s, 3H), 3.54 (t , *J* = 14.2 Hz, 1H), 3.47 (d, *J* = 14.2 Hz, 1H), 2.44 (dd, *J* = 14.2 Hz, *J* = 3.0 Hz, 1H), 1.90 (dd, *J* = 14.2 Hz, *J* = 1.0 Hz, 1H), 0.91 (s, 3H), 0.85 (s, 3H). ^{13}C (125 MHz, $CDCl_3$) δ: 207.8, 179.3, 167.0, 162.1, 137.5, 130.5, 129.6, 128.7, 127.4, 122.6, 114.6, 62.2, 55.6, 50.2, 44.0, 43.7, 41.3, 26.2, 25.8. IR (ATR, cm^{-1}): 1771, 1710, 1582, 1537, 1513, 1450, 1417, 13877, 1341, 1320, 1299, 1181, 1156, 1120, 1098, 1025. M. P.: degradation at 210 °C. HRMS (ESI+): Calcd. for $[C_{23}H_{23}NO_4 + H]^+$: 378.1700, found: 378.1695.

4,6-bis(4-methoxyphenyl)-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1l)

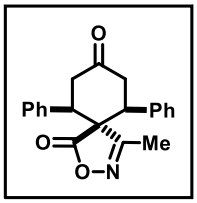
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a light yellow solid: 62 mg, 68%.



^{1}H (400 MHz, $CDCl_3$) δ: 7.71 (d, *J* = 8.8 Hz, 2H), 7.19-7.12 (m, 3H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.95-6.93 (m, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.67 (d, *J* = 8.8 Hz, 2H), 4.02-3.97 (m, 2H), 3.93-3.84 (m, 2H), 3.90 (s, 3H), 3.69 (s, 3H), 2.62-2.56 (m, 2H). ^{13}C (100 MHz, $CDCl_3$) δ: 207.7, 178.4, 165.0, 162.4, 159.7, 136.6, 129.1, 128.9, 128.8, 128.7, 128.4, 127.5, 120.8, 114.8, 114. 4, 60.8, 55.7, 55.3, 47.7, 47.3, 42.1, 41.9. IR (ATR, cm^{-1}): 2358, 2342, 1770, 1771, 1608, 1515, 1455, 1419, 1335, 1305, 1182, 1039, 1027. M. P.: degradation at 220 °C. HRMS (ESI+): Calcd. for $[C_{28}H_{25}NO_5 + H]^+$: 456.1805, found: 456.1799.

4-methyl-6,10-diphenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1m)

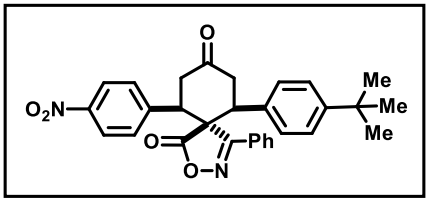
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a light yellow solid: 66 mg, 99%.



^{1}H (250 MHz, $CDCl_3$) δ: 7.33-7.27 (m, 6H), 7.19-7.15 (m, 4H), 3.75 (t, *J* = 14.2 Hz, 2H), 3.44 (dd, *J* = 14.2 Hz, *J* = 3.6 Hz, 2H), 2.58 (dd, *J* = 14.2 Hz, *J* = 3.6 Hz, 2H), 1.98 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 206.3, 178.6, 167.0, 136.7, 129.6, 129.1, 127.2, 59.5, 48.4, 42.3, 12.4. IR (ATR, cm^{-1}): 2355, 1771, 1720,1496, 1455, 1397, 1371, 1285, 1260, 1232, 1189, 1189, 1099, 1056. M. P.: degradation at 210 ºC. HRMS (ESI+): Calcd. for $[C_{21}H_{19}NO_3 + H]^+$: 334.1438, found: 334.1437.

6-(4-(tert-butyl)phenyl)-10-(4-nitrophenyl)-4-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1n)

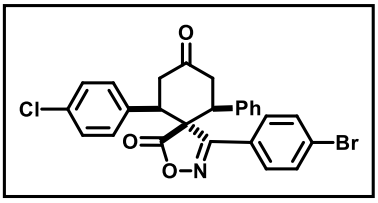
Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2Hex:AcOEt) affords the title compound as a light yellow solid: 66 mg, 66%.



^{1}H (500 MHz, $CDCl_3$) δ: 7.99 (d, *J* = 8.5 Hz, 2H), 7.77-7.75 (m, 2H), 7.61-7.58 (m, 1H), 7.53-7.50 (m, 2H), 7.16 (d, *J* = 8.5 Hz, 2H), 7.10 (d, *J* = 8.5 Hz, 2H), 6.89 (d, *J* = 8.5 Hz, 2H), 4.18-4.11 (m, 2H), 3.94-3.85 (m, 2H), 2.66-2.59 (m, 2H), 1.20 (s, 9H). ^{13}C (125 MHz, $CDCl_3$) δ: 206.1, 177.8, 165.1, 152.0, 148.1, 143.6, 132.7, 132.5, 129.7, 128.7, 128.0, 127.1 (x2), 126.2, 124.3, 60.0, 47.5, 47.4, 41.8, 41.3, 34.7, 31.3. IR (ATR, cm^{-1}): 2964, 1772, 1719, 1607, 1523, 1411, 1352, 1286, 1233, 1181, 1055, 1110, 1013. M. P.: Degradation at 205 ºC. HRMS (ESI+): Calcd. for $[C_{30}H_{28}N_2O_5 + H]^+$: 497.2071, found: 497.2067.

4-(4-bromophenyl)-6-(4-chlorophenyl)-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1o)

Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a light yellow solid: 35 mg, 70%.



^{1}H (500 MHz, $CDCl_3$) δ: 7.65-7.62 (m, 4H), 7.21-7.13 (m, 5H), 6.93 (d, *J* = 7.5Hz, 2H), 6.86 (d, *J* = 9.0 Hz, 2H), 4.01-3.96 (m, 2H), 3.93-3.80 (m, 2H), 2.64-2.58 (m, 2H). ^{13}C (125 MHz, $CDCl_3$) δ: 206.5, 177.8, 164.5, 136.0, 135.0, 134.7, 132.9, 129.5, 129.4, 129.1, 128.8, 128.5, 127.4, 127.2, 127.1, 60.2, 48.0, 47.3, 41.8, 41.7. IR (ATR, cm^{-1}): 1784, 1715, 1588, 1492, 1409, 1176, 1195, 1076, 1008. M. P.: Degradation at 211 ^{o}C. HRMS (ESI+): Calcd. for [$C_{26}H_{19}BrClNO_3$ + H]$^{+}$: 508.0310, found: 508.0300.

3.3. 6,10-*trans*-Spiroisoxazol-5-ones

General Procedure B:[17] *Enantioselective Aminocatalyzed trans-Spirocyclization of 4-Alkylideneisoxazol-5-ones **9** with Methyl Vinyl Ketones **3**.* A round bottom flask is charged with 4-alkylideneisoxazol-5-one **9** (0.1 mmol, 1 equiv.), toluene (1 mL, 0.1 M in respect to **9**), methyl vinyl ketone **3** (0.2 mmol, 2 equiv.), benzoic acid (5 mg, 0.04 mmol, 0.2 equiv.) and 9-amino(9-deoxy)*epi*-Quinidine **14** (6.5 mg, 0.02 mmol, 0.2 equiv.). The reaction is heated at 40 ^{o}C, while stirring, for 3h. Then, the reaction mixture is concentrated under reduced pressure. The residue is purified by flash column chromatography to afford the corresponding 6,10-*trans*-spiroisoxazol-5-one **1**.

Near-racemic mixtures of *trans*-spiroisoxazol-5-ones **1** are obtained by simultaneously running independent reactions with 9-amino(9-deoxy)*epi*-Quinidine **14** (0.2 equiv) and 9-amino(9-deoxy)*epi*-Quinine (0.2 equiv.), then mixing both reaction mixtures and purifying the resulting combination by flash column chromatography.[18]

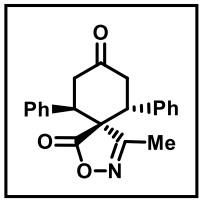
[17] J. Liang, Q. Chen, L. Liu, X. Jiang, R. Wang, An Organocatalytic Asymmetric Double Michael Cascade Reaction of Unsaturated Ketones and Unsaturated Pyrazolones: Highly Efficient Synthesis of Spiropyrazolones Derivatives, *Org. Biomol. Chem.* 2013, **11**, 1441-1445.

[18] Attempts to run racemic reactions with morpholine or other achiral primary amines as aminocatalysts generally led to mixtures containing the 6,10-*cis*-spiroisoxazol-5-one **1** as the major compound. Attempts to run racemic reactions with a mixture of aminocatalysts 9-amino(9-deoxy)*epi*-Quinidine **14** (0.1 equiv) + 9-amino(9-deoxy)*epi*-Quinine (0.1 equiv.) also often led to the formation of 6,10-*cis*-spiroisoxazol-5-one **1** as the (largely) major compound.

(6R,10R)-4-methyl-6,10-diphenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1q)

^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals only the formation of the *trans* diastereoisomer. Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a white solid: 23 mg, 70%, 99:1 er. The enantiomeric ratio is determined by HPLC analysis using a Daycel Chiralpak IC column, eluent: 90:10 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{major} = 22.9 min, τ_{minor}= 32.4 min.

Alternatively, a one-pot protocol leads to a similar result: 3-methylisoxazol-5(4H)-one (10 mg, 0.1 mmol), benzaldehyde (12 µL, 0.12 mmol), *(E)*-4-phenylbut-3-en-2-one **3a** (29 mg, 0.2 mmol), 9-amino(9-deoxy)*epi*-Quinidine **14** (6.5 mg, 0.02 mmol), benzoic acid (5 mg, 0.04 mmol) and toluene (1 mL). ^{1}H NMR analysis of the crude mixture reveals only the formation of the 6,10-*trans* diastereoisomer. Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a white solid: 23 mg, 70%, 99:1 er. $[\alpha]^{20}_D$: +67 (c = 1, CH_2Cl_2).

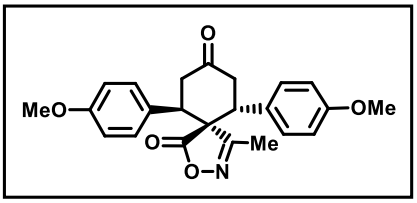


^{1}H (250 MHz, $CDCl_3$) δ: 7.37-7.34 (m, 3H), 7.29-7.26 (m, 3H), 7.14-7.08 (m, 4H), 3.79-3.74 (m, 1H), 3.70-3.59 (m, 2H), 3.40 (dd, *J* = 16.3 Hz, *J* = 6.0 Hz, 1H), 2.81 (dd, *J* = 16.3 Hz, *J* = 6.7 Hz, 1H), 2.67 (d, *J* = 12.4 Hz, 1H), 1.39 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) 1C cannot be unambiguously assigned, δ: 207.9, 179.9, 167.6, 138.0, 136.4, 129.6, 129.5, 128.9, 128.4, 127.7, 58.4, 46.2, 42.2, 41.9, 40.8, 13.7. IR (ATR, cm^{-1}): 1778, 1716, 1497, 1454, 1411, 1388, 1239, 1214, 1198, 1171, 1061, 1005. M. P.: 121 - 123 ^{o}C. HRMS (ESI+): Calcd. for $[C_{21}H_{19}NO_3 + H]^+$: 334.1438, found: 334.1437.

(6R,10R)-6,10-bis(4-methoxyphenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1r)

^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of **1r**$_{\_trans}$ (44%) and **1r**$_{\_cis}$ (30%). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt - 8:2 Hex:AcOEt – 7:3 Hex:AcOEt) affords the trans diastereoisomer as a pale yellow solid: 16 mg,

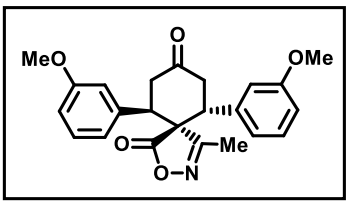
44%. 97:3 er. The enantiomeric ratio is determined by HPLC analysis using a Daycel Chiralpak IA column, eluent: 80:20 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{minor}= 18.1 min, τ_{major} = 20.6 min. $[\alpha]^{20}_{D}$: +92 (c = 1, CH_2Cl_2).



^{1}H (250 MHz, $CDCl_3$) δ: 7.05-6.99 (m, 4H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.78 (d, *J* = 8.7 Hz, 2H), 3.78 (s, 3H), 3.74 (s, 3H), 3.70-3.52 (m, 3H), 3.35 (dd, *J* = 16.2 Hz, *J* = 6.0 Hz, 1H), 2.75 (dd, *J* = 16.2 Hz, *J* = 9.1 Hz, 1H), 2.61 (d, *J* = 13.4 Hz, 1H), 1.44 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 208.2, 180.1, 167.9, 159.8 (x2), 129.9, 129.4, 128.8, 128.4, 114.8, 114.7, 58.8, 55.5, 55.4, 45.3, 42.1, 41.5, 41.0, 13.8. IR (ATR, cm^{-1}): 2923, 2866, 2359, 2341, 1767, 1729, 1610, 1514, 1456, 1298, 1260, 1212, 1181, 1054, 1032, 1005, 863, 837, 825, 812, 753. M. P.: 185 - 187 ^{o}C. HRMS (ESI+): Calcd. for $[C_{23}H_{23}NO_5 + H]^{+}$: 394.1649, found: 394.1649.

(6R,10R)-6,10-bis(3-methoxyphenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1s)

^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of **1s**$_{\_trans}$ (60%), and **1s**$_{\_cis}$ (9%). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt - 8:2 Hex:AcOEt – 7:3 Hex:AcOEt) affords the trans diastereoisomer as a pale yellow solid: 23 mg, 60%, 97:3 er. The enantiomeric excess is determined by HPLC analysis using a Daycel Chiralpak IA column, eluent: 80:20 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{major} = 13.7 min, τ_{minor} = 16.5 min. $[\alpha]^{20}_{D}$: +68 (c = 1, CH_2Cl_2).

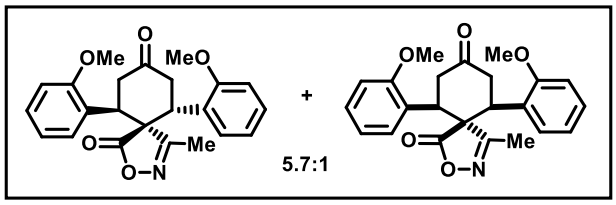


^{1}H (250 MHz, $CDCl_3$) δ: 7-30-7.15 (m, 2H), 6.82 (ddd, *J* = 18.1 Hz, *J* = 8.2 Hz, *J* = 2.1 Hz, 2H), 6.71-6.64 (m, 4H), 3.77 (s, 3H), 3.74 (s, 3H), 3.70-3.56 (m, 3H), 3.39 (dd, *J* =16.3 Hz, *J* = 6.1 Hz, 1H), 2.77 (dd, *J* =16.3 Hz, *J* = 6.7 Hz, 1H), 2.65 (d, *J* =11.2 Hz, 1H), 1.43 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 207.8, 180.0, 167.7, 160.3, 160.2, 139.5, 138.0, 130.6, 130.5, 120.5, 119.9, 114.7, 114.0, 113.8, 113.7, 58.2, 55.5, 55.4, 46.2, 42.3, 41.9, 40.8, 13.8. IR (ATR, cm^{-1}): 1763, 1719, 1608, 1583, 1491, 1454, 1437, 1402, 1316, 1295, 1261, 1232, 1223, 1204,

1151, 1045, 1029, 1007. M. P.: 245 - 247 ^{o}C. HRMS (ESI+): Calcd. for [$C_{23}H_{23}NO_5$ + H]$^{+}$: 394.1649, found: 394.1649.

(6R,10R)-6,10-bis(2-methoxyphenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1t_trans) and **6,10-bis(2-methoxyphenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1t_cis)**

^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of **1t_trans** (88%) and **1t_cis** (12%). Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt – 7:3 Hex:AcOEt) affords the mixture of **1t_trans** + **1t_cis** as a pale yellow solid: 33 mg, 85%, >99:1 er (**1t_trans**). The enantiomeric ratio of **1t_trans** is determined by HPLC analysis using a Daycel Chiralpak IA column, eluent: 80:20 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{major} = 10.4 min, τ_{minor}= 14.9 min. $[\alpha]^{20}_{D}$: +5 (c = 1, CH_2Cl_2).

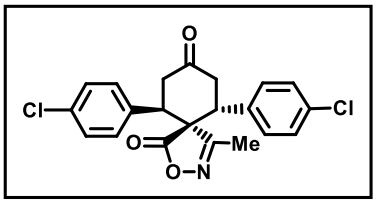


^{1}H (250 MHz, $CDCl_3$) 5.7:1 **1t_trans**:**1t_cis**, δ: 7.32- 7.14 (m, 4H), 7.00-6.88 (m, 2H), 6.85-6.76 (m, 2H), 4.37-4.24 (m, 1H), 4.08 (dd, *J* = 9.5 Hz, *J* = 5.8 Hz, 1H), 3.80 (s, 0.90H), 3.70 (s, 2.55H), 3.69 (s, 2.55H), 3.64-3.58 (m, 1H), 3.18-2.95 (m, 2H), 2.51-2.43 (m, 1H), 1.88 (s, 0.45H), 1.31 (s, 2.55H). ^{13}C (62.5 MHz, $CDCl_3$) **1t_trans** only, **δ:** 209.0, 180.4, 168.2, 157.3, 156.4, 129.7, 129.5, 128.7, 128.6, 126.6, 124.8, 121.5, 120.8, 110.6 (x2), 57.1, 55.1, 54.5, 42.3, 40.8, 40.7, 38.4, 13.2. IR (ATR, cm^{-1}): 2924, 1777, 1723, 1600, 1587, 1493, 1446, 1438, 1372, 1293, 1284, 1207, 1122, 1052, 1025. M. P.: 61 - 63 ^{o}C. HRMS (ESI+): Calcd. for [$C_{23}H_{23}NO_5$ + H]$^{+}$: 394.1649, found: 394.1648.

(6R,10R)-6,10-bis(4-chlorophenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1u)

^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of **1u_trans** (76%), and **1u_cis** (23%). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt – 8:2 Hex:AcOEt) affords the trans diastereoisomer **1u_trans** as a pale yellow solid: 33 mg,

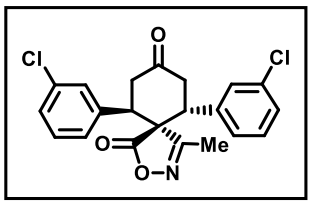
75%, >99:1 er. The enantiomeric ratio is determined by HPLC analysis using a Daycel Chiralpak IC column, eluent: 90:10 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{major} = 50.6 min, τ_{minor} = 53.8 min. $[\alpha]^{20}_{D}$: +102 (c = 1, CH_2Cl_2).



^{1}H (250 MHz, $CDCl_3$) δ: 7.34 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 7.03 (t, *J* = 8.5 Hz, 4H), 3.77 (dd, *J* = 8.0 Hz, *J* = 5.8 Hz, 1H), 3.70-3.51 (m, 2H), 3.30 (dd, *J* = 16.4 Hz, *J* = 5.6 Hz, 1H), 2.80 (dd, *J* = 16.4 *J* = 8.0, 1H), 2.63 (dd, *J* = 14.1, 1H), 1.52 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 206.9, 179.6, 166.9, 136.0, 135.1, 135.1, 134.4, 129.8 (x2), 129.4, 129.1, 58.5, 45.0, 41.6, 41.4, 40.5, 13.9. IR (ATR, cm^{-1}): 2919, 2852, 1766, 1727, 1439, 1412, 1389, 1285, 1234, 1211, 1193, 1165, 1091, 1014, 1091, 1014. M. P.: degradation at 213 ^{o}C. HRMS (ESI+): Calcd. for $[C_{21}H_{17}Cl_2NO_3 + H]^{+}$: 402.0658, found: 402.0658.

(6R,10R)-6,10-bis(3-chlorophenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1v)

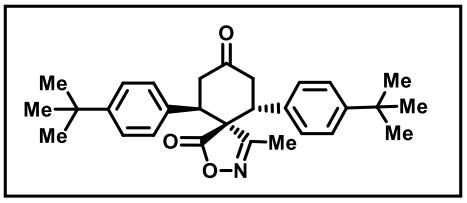
^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of **1v**$_{\_trans}$ (56%) and **1v**$_{\_cis}$ (10%). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt – 8:2 Hex:AcOEt) affords the trans diastereoisomer **1v**$_{\_trans}$ as a pale yellow solid: 33 mg, 52%, 99:1 er. The enantiomeric ratio is determined by HPLC analysis using a Daycel Chiralpak IC column, eluent: 90:10 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{major} = 22.2 min, τ_{minor} = 31.1 min. $[\alpha]^{20}_{D}$: +73 (c = 1, CH_2Cl_2).



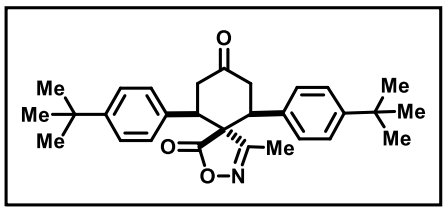
^{1}H (250 MHz, $CDCl_3$) δ: 7.33-7.25 (m, 4H), 7.11-7.00 (m, 4H), 3.78-3.70 (m, 1H), 3.64-3.51 (m, 2H), 3.33 (dd, *J* =16.4 Hz, *J* = 5.7 Hz, 1H), 2.81 (dd, *J* =16.4 Hz, *J* = 7.6 Hz, 1H), 2.65 (d, *J* = 14.1 Hz, 1H), 1.52 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 206.6, 179.4, 166.8, 139.5, 138.0, 135.6, 135.3, 130.9 (x2), 129.4, 129.3, 128.4, 128.2, 126.4, 125.8, 58.2, 45.4, 41.8, 41.4, 40.4, 13.9. IR (ATR, cm^{-1}): 2917, 2849, 1771, 1725, 1595, 1573, 1480, 1421, 1287, 1238, 1214, 1197, 1144, 1086, 1005. M. P.: 149 - 151 ^{o}C. HRMS (ESI+): Calcd. for $[C_{21}H_{17}Cl_2NO_3 + H]^{+}$: 402.0658, found: 402.0657.

(6R,10R)-6,10-bis(4-(tert-butyl)phenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1w$_{_trans}$) and **6,10-bis(4-(tert-butyl)phenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1w$_{_cis}$)**

^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of **1w$_{_trans}$** (75%) and **1w$_{_cis}$** (11%). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt - 8:2 Hex:AcOEt – 7:3 Hex:AcOEt) affords **1w$_{_trans}$** as a pale yellow solid: 34 mg, 75%, >99:1 er and **1w$_{_cis}$** as a pale yellow solid: 5 mg, 10%. **1w$_{_trans}$:** The enantiomeric ratio is determined by HPLC analysis using a Daycel Chiralpak IA column, eluent: 80:20 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{minor} = 6.3 min, τ_{major} = 7.2 min. $[\alpha]^{20}_D$: +84 (c = 1, CH_2Cl_2).



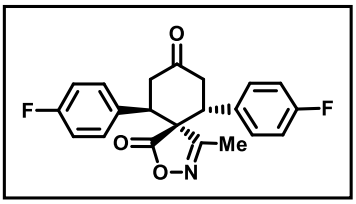
1w$_{_trans}$:^{1}H (250 MHz, $CDCl_3$) δ: 7.36 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.2 Hz, 2H), 7.03 (dd, *J* = 8.2 Hz, *J* = 6.4 Hz, 4H), 3.73-3.57 (m, 3H), 3.41 (dd, *J* = 16.0 Hz, *J* = 6.4 Hz, 1H), 2.76 (dd, *J* =16.0 Hz, *J* = 6.4 Hz, 1H), 2.64 (d, *J* = 11.6 Hz, 1H), 1.35 (s, 3H), 1.29 (s, 9H), 1.25 (s, 9H). ^{13}C (62.5 MHz, $CDCl_3$) 1C cannot be unambiguously assigned, δ: 208.3, 180.0, 152.1, 151.7, 135.0, 133.5, 128.1, 127.4, 126.4, 126.3, 58.2, 46.0, 42.3, 41.8, 40.9, 34.8, 34.7, 31.4 (x2), 13.7. IR (ATR, cm^{-1}): 2963, 2917, 2869, 2359, 2342, 1777, 1733, 1508, 1464, 1418, 1363, 1271, 1235, 1219, 1204, 1191, 1144, 1111, 1017, 1004. M. P.: 151 – 153 ^{o}C. HRMS (ESI+): Calcd. for $[C_{29}H_{35}NO_3 + H]^+$: 446.2690, found: 446.2689.



1w$_{_cis}$: ^{1}H (250 MHz, $CDCl_3$) δ: 7.29 (d, *J* = 8.2 Hz, 4H), 7.08 (d, *J* = 8.2 Hz, 4H), 3.72 (t, *J* = 14.2 Hz, 2H), 3.39 (dd, *J* = 14.2 Hz, *J* = 3.6 Hz, 2H), 2.54 (dd, *J* = 14.2 Hz, *J* = 3.6 Hz, 2H), 1.99 (s, 3H), 1.26 (s, 18H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 206.8, 178.7, 167.1, 151,9, 133.8, 126.9, 126.5, 59.4, 48.0, 42.5, 34.8, 31.4, 12.5. IR (ATR, cm^{-1}): 2960, 2917, 2884, 1765, 1715, 1511, 1422, 1362, 1289, 1271, 1233, 1188, 1010,1064, 1017, 915, 870, 837, 146, 675, 667. M. P.: degradation at 233 ^{o}C. HRMS (ESI+): Calcd. for $[C_{29}H_{35}NO_3 + H]^+$: 446.2690, found: 446.2690.

(6R,10R)-6,10-bis(4-fluorophenyl)-4-methyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1x)

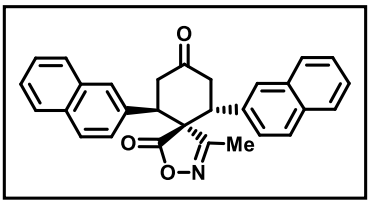
^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of **1x**$_{\text{trans}}$ (80%) and **1x**$_{\text{cis}}$ (8%). Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt - 8:2 Hex:AcOEt – 7:3 Hex:AcOEt) affords the trans diastereoisomer **1x**$_{\text{trans}}$ as a pale yellow solid: 25 mg, 78%, 99:1 er. The enantiomeric ratio is determined by HPLC analysis using a Daycel Chiralpak IA column, eluent: 80:20 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{minor} = 13.6 min, τ_{major} = 14.6 min. $[\alpha]^{20}_{D}$: +64 (c = 1, CH_2Cl_2).



^{1}H (250 MHz, $CDCl_3$) δ: 7.14-6.94 (m, 8H), 3.78 (dd, *J* = 7.7 Hz, *J* = 5.8 Hz, 1H), 3.70-3.53 (m, 2H), 3.32 (dd, *J* = 16.4 Hz, *J* = 5.6 Hz, 1H), 2.82 (dd, *J* = 16.4 Hz, *J* = 7.9 Hz, 1H), 2.63 (d, *J* = 13.4 Hz, 1H), 1.51 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 207.2, 179.7, 167.1, 162.8 (d, *J* = 249.7 Hz), 160.8, 133.4 (d, *J* = 3.4 Hz), 131.8 (d, *J* = 3.4 Hz), 129.8 (d, *J* = 8.1 Hz), 129.5 (d, *J* =8.3 Hz), 116.8 (d, *J* = 5.8 Hz), 116.4 (d, *J* = 5.8 Hz), 58.7, 44.9, 41.6, 41.5, 40.7, 13.8. ^{19}F (235 MHz, $CDCl_3$) δ: -112.1, -112.3. IR (ATR, cm^{-1}): 2923, 2850, 1768, 1729, 1607, 1510, 1460, 1417, 1338, 1293, 1223, 1210, 1194, 1161, 1105. M. P.: 168 - 170 ^{o}C. HRMS (ESI+): Calcd. for $[C_{21}H_{17}F_2NO_3 + H]^+$: 370.1249, found: 370.1251.

(6R,10R)-4-methyl-6,10-di(naphthalen-2-yl)-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1y)

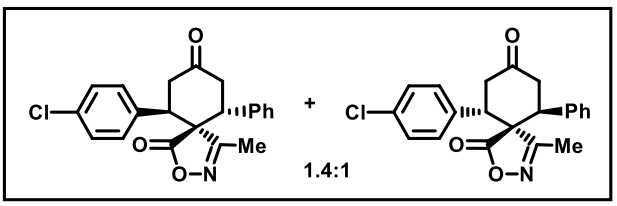
^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals only the formation of the *trans* diastereoisomer. Purification by flash column chromatography (SiO_2, gradient: Hex – 9:1 Hex:AcOEt - 8:2 Hex:AcOEt – 7:3 Hex:AcOEt) affords the title compound as a pale yellow solid: 39 mg, 90%, 90:10 er. The enantiomeric excess is determined by HPLC analysis using a Daycel Chiralpak IA column, eluent: 80:20 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm, τ_{minor} = 17.3 min, τ_{minor}= 19.1 min. $[\alpha]^{20}_{D}$: +152 (c = 1, CH_2Cl_2).



^{1}H (250 MHz, $CDCl_3$) δ: 7.87-7.71 (m, 6H), 7.63 (s, 1H), 7.55-7.51 (m, 3H), 7.48-7.44 (m,2H), 7.26-7.21 (m, 2H), 3.98 (t, *J* = 6.2 Hz, 1H), 3.93-3.79 (m, 2H), 3.56 (dd, *J* = 16.3 Hz, *J* = 6.2 Hz, 1H), 2.96 (dd, *J* = 16.3 Hz, *J* = 6.2 Hz, 1H), 2.88-2.73 (m, 1H), 1.38 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 207.9, 180.1, 167.7, 135.4, 133.9, 133.5, 133.4, 133.3, 133.1, 129.5 (2x), 128.3, 128.1, 128.0, 127.9, 127.5, 127.3, 127.2 (x2), 126.9 (2x), 126.0, 124.8, 58.4, 46.5, 42.5, 42.2, 41.0, 14.0. IR (ATR, cm^{-1}): 2922, 1777, 1721, 1599, 1409, 1393, 1237, 1210, 1194, 1159, 1143, 1097, 1032, 1001. M. P.: degradation at 232 ^{o}C. HRMS (ESI+): Calcd. for $[C_{29}H_{23}NO_3 + H]^+$: 434.1751, found: 434.1750.

(5R,6S,10S)-6-(4-chlorophenyl)-4-methyl-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione and (5R,6R,10R)-6-(4-chlorophenyl)-4-methyl-10-phenyl-2-oxa-3-azaspiro[4.5]dec-3-ene-1,8-dione (1z and 1z')

^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals the formation of three isomers in 35% (trans), 31% (trans) and 10% (cis, **1c**) yields, respectively. Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt - 7:3 Hex:AcOEt) affords a 1.4:1 mixture of *trans* diastereoisomers as an yellow solid: 25 mg, 66%, >99:1 er/ >99:1 er. The enantiomeric ratios are determined by HPLC analysis using a Daycel Chiralpak IC column, eluent: 90:10 Hex: ^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 220 nm. **1c**$_{cis}$: τ_1 = 14.6 min and τ_2 = 16.0 min; **1z**$_{trans}$: τ_{major} = 26.8 min and τ_{minor} = 31.3 min; **1z'**$_{trans}$:. τ_{major} = 28.8 min and τ_{minor} = 38.3 min. $[\alpha]^{20}_D$: +76 (c = 1, CH_2Cl_2).



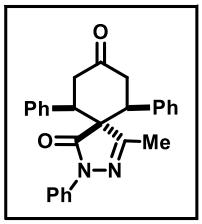
^{1}H (250 MHz, $CDCl_3$) 1.4:1 **1z**:**1z'**, δ: 7.37-7.24 (m, 10H), 7.13-7.02 (m, 8H), 3.79-3.74 (m, 2H), 3.71-3.53 (m, 4H), 3.42-3.28 (m, 2H), 2.86-2.77 (m, 2H), 2.70-2.61 (m, 2H), 1.51(s, 2.5 H), 1.40 (s, 3.5 H). ^{13}C (62.5 MHz, $CDCl_3$) 1.4:1 **1z**:**1z'**, 3C cannot be unambiguously assigned, δ: 207.5, 207.4, 179.7, 167.4, 167.1, 137.7, 136.2, 136.0, 135.0, 134.9 (x2), 129.7 (2x), 129.6, 129.5, 129.1, 129.0, 128.3, 127.7, 58.5, 58.3, 45.9, 45.2, 42.2, 41.7, 41.6 (2x), 40.7, 40.6, 13.9, 13.7. IR (ATR, cm^{-1}):

2924, 2853, 1775, 1724, 1494, 1455, 1412, 1388, 1287, 1236, 1211, 1192, 1140, 1093, 1037, 1013. M. P.: 160 - 162 ºC. HRMS (ESI+): Calcd. for $[C_{21}H_{18}ClNO_3 + H]^+$: 368.1048, found: 368.1047.

3.4. Spiropyrazol-5-ones

4-methyl-2,6,10-triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (7m)[19]

General procedure E is employed. Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as an yellow solid: 70 mg, 81%.

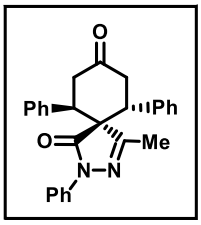


^{1}H (250 MHz, $CDCl_3$) δ: 7.41-7.27 (m, 4H), 7.24- 7.15 (m, 11H), 3.99 (t, *J* = 14.3 Hz, 2H), 3.49 (dd, *J* = 14.3 Hz, *J* = 3.8 Hz, 2H), 2.56 (dd, *J* = 14.3 Hz, *J* = 3.8 Hz, 2H), 2.06 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 208.0, 173.3, 160.4, 137.7, 137.2, 129.1, 128.9, 128.5, 127.4, 126.1, 120.6, 61.8, 48.7, 42.5, 14.4. IR (ATR, cm^{-1}): 2922, 2853, 2357, 1734, 1701, 1595, 1494, 1456, 1399, 1373, 1338, 1317, 1300, 1261, 1245, 1131, 1054, 1032. M. P.: 159 - 161 ºC. HRMS (ESI+): Calcd. for $[C_{27}H_{24}N_2O_2 + H]^+$: 409.1911, found: 409.1918.

(6R, 10R)-4-methyl-2,6,10-triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (7q)[17]

General procedure F is employed. ^{1}H NMR analysis of the crude mixture using 1,3,5-trimethoxybenzene as internal reference reveals only the formation of the *trans* diastereoisomer. Purification by flash column chromatography (SiO_2, gradient: Hex - 9:1 Hex:AcOEt - 8:2 Hex:AcOEt) affords the title compound as a white solid: 30 mg, 73%. >99:1 er. The enantiomeric excess is determined by HPLC analysis using a Daycel Chiralpak AD-H column, eluent: 70:30 Hex:^{i}PrOH, flow rate: 1 mL.min^{-1}, λ = 225 nm, τ_{major} = 9.9 min, τ_{minor}= 12.2 min. $[\alpha]^{20}_D$: +51.0 (c = 1, $CHCl_3$)/ +58.0 (c = 1, CH_2Cl_2).

[19] This 6,10-*cis*-spiroisoxazol-5-one has been mentioned by only one previous publication, but NMR data was not provided. See: B. Wu, J. Chen, M.-Q. Li, J.-X. Zhang, X.-P. Xu, S.-J. Ji, X.-W. Wang, Highly Enantioselective Synthesis of Spiro[cyclohexanone-oxindoles] and Spiro[cyclohexanone-pyrazolones] by Asymmetric Cascade [5+1] Double Michael Reactions, *Eur. J. Org. Chem.,* 2012, **2012**, 1318-1327.

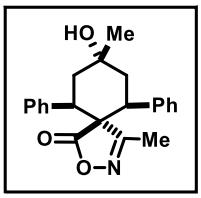


^{1}H (250 MHz, $CDCl_3$) δ: 7.47-7.44 (m, 2H), 7.33- 7.28 (m, 5H), 7.20-7.12 (m, 8H), 3.93-3.81 (m, 2H), 3.64 (dd, *J* = 14.3 Hz, *J* = 2.4 Hz, 1H), 3.36 (dd, *J* = 16.4 Hz, *J* = 5.1 Hz, 1H), 2.96 (dd, *J* = 16.4 Hz, *J* = 9.5 Hz, 1H), 2.64 (dd, *J* = 16.4 Hz, *J* = 2.4 Hz, 1H), 1.65 (s, 3H). ^{13}C (62.5 MHz, $CDCl_3$) δ: 209.5, 175.0, 160.8, 138.7, 137.3, 136.8, 129.2, 128.9, 128.8, 128.3 (x2), 127.9 (x2), 125.8, 120.0, 62.0, 44.4, 42.6, 41.5, 40.8, 15.9. HRMS (ESI+): Calcd. for $[C_{27}H_{24}N_2O_2 + H]^+$: 409.1911, found: 409.1917.

3.5. Applications

8-hydroxy-8-methyl-4,6,10-triphenyl-2-oxa-3-azaspiro[4.5]dec-3-en-1-one (12)

Under N_2, at room temperature, a round bottom flask is charged with spiroisoxazol-5-one **1b** (28 mg, 0.07 mmol) and dry THF (500 µL). Then, the reaction mixture is cooled down to -78 °C and MeMgCl (117 µL, 3M in THF, 3.5 mmol) is added. The reaction is stirred for 5 hours at -78 °C. Then, the temperature is allowed to warm up to room temperature. The reaction mixture is quenched with an aqueous saturated solution of NH_4Cl, extracted with AcOEt (3x), dried ($MgSO_4$) and concentrated under reduced pressure. The resulting residue is purified by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) to afford the title compound as a white solid: 27 mg, 94%.

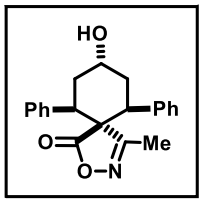


^{1}H (500 MHz, $CDCl_3$) δ: 7.96-7.94 (m, 2H), 7.57-7.53 (m, 1H), 7.51-7.48 (m, 2H), 7.15- 7.08 (m, 6H), 6.94-6.93 (m, 4H), 4.27 (dd, *J* = 13.5 Hz, *J* = 4.0 Hz, 2H), 2.94 (t, *J* = 13.5 Hz, 2H), 1.79-1.76 (m, 2H), 1.51 (s, 3H). ^{13}C (125 MHz, $CDCl_3$) δ: 178.5, 166.3, 138.5, 131.6, 129.3, 129.0, 128.8, 128.2 (x2), 127.4, 70.2, 60.7, 43.4, 38.3, 31.7. IR (ATR, cm^{-1}): 3377, 3263, 1781, 1496, 1454, 1172, 1131, 1084, 1046. M. P.: Degradation at 185 °C. HRMS (ESI+): Calcd. for $[C_{27}H_{25}NO_3 + H]^+$: 412.1907, found: 412.1902.

8-hydroxy-4,6,10-triphenyl-2-oxa-3-azaspiro[4.5]dec-3-en-1-one (13)

Under N_2, at room temperature, a round bottom flask is charged with spiroisoxazol-5-one **1b** (20 mg, 0.05 mmol) and dry THF (500 µL). Then, the reaction mixture is

cooled down to -78°C, and DiBAl-H (500 µL, 1M in THF, 0.25 mmol) is slowly added. The reaction is stirred at -78 ºC for 5 hours. Then, the temperature is allowed to warm up to room temperature. The reaction mixture is quenched with MeOH and H_2O; and the aqueous phase is extracted with DCM (3x). The combined organic layers are dried ($MgSO_4$) and concentrated under reduced pressure. The resulting residue is purified by flash column chromatography (SiO_2, gradient: Hex - 95:5 Hex:AcOEt - 9:1 Hex:AcOEt) to afford the title compound as a white solid: 18 mg, 91%.

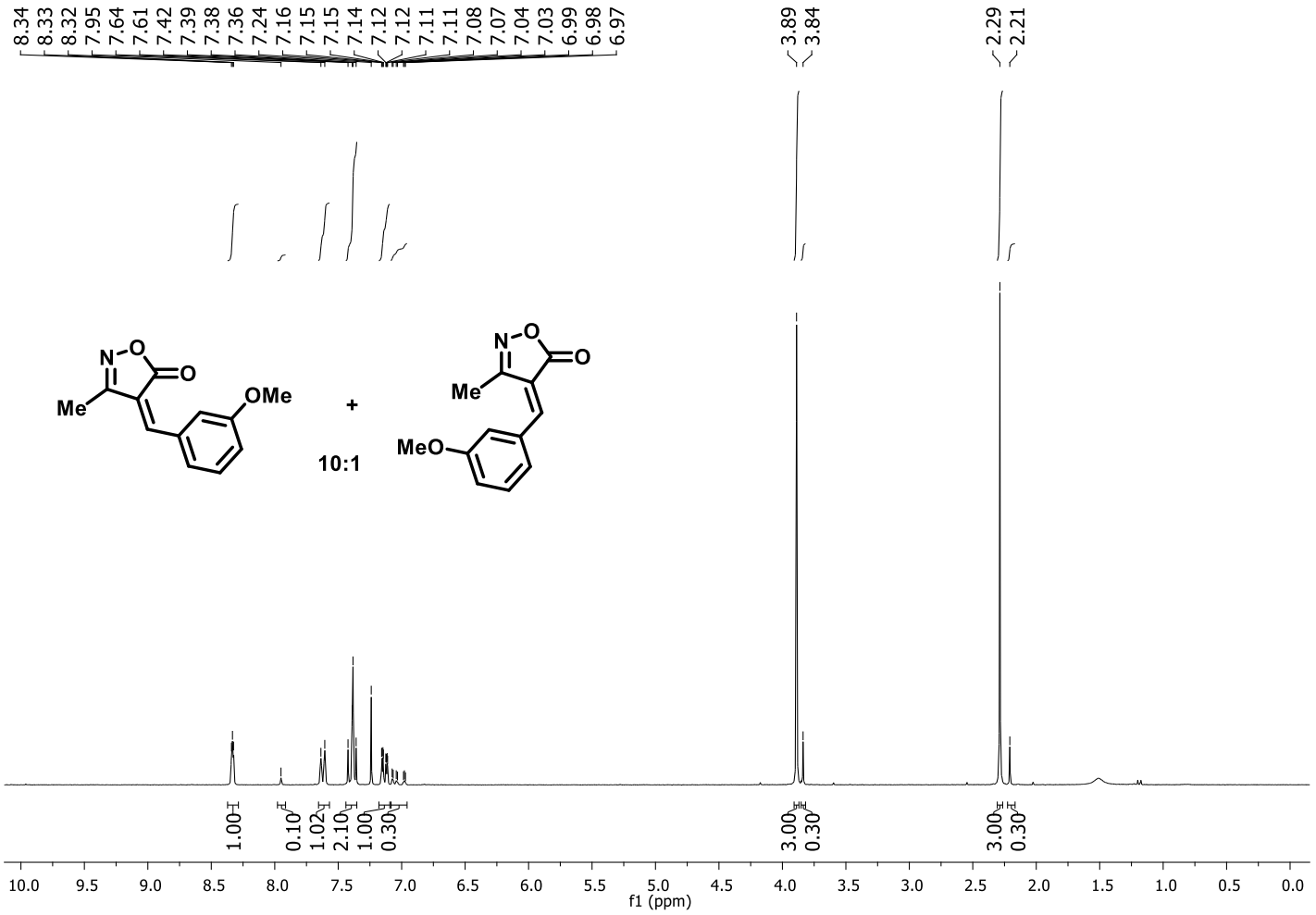


^{1}H (400 MHz, $CDCl_3$) δ: 7.81-7.79 (m, 2H), 7.59-7.55 (m, 1H), 7.52-7.48 (m, 2H), 7.16-7.09 (m, 6H), 6.94-6.92 (m, 4H), 4.16-4.09 (m, 1H), 3.73 (dd, *J* = 16.4 Hz, *J* = 4.0 Hz, 2H), 2.96-2.88 (m, 2H), 2.16-2.11 (dt, *J* = 12.4 Hz, *J* = 3.6 Hz, 2H). ^{13}C (100 MHz, $CDCl_3$) δ: 178.0, 165.9, 137.9, 131.8, 129.4, 129.1, 128.9, 128.3, 127.9, 127.4, 70.1, 60.4, 47.0, 34.8. IR (ATR, cm^{-1}): 1752, 1493, 1453, 1371, 1279, 1265, 1180, 1144, 1098, 1070, 1021. M. P.: Degradation at 242 ºC. HRMS (ESI+): Calcd. for $[C_{26}H_{23}NO_3 + H]^+$: 398.1751, found: 398.1757.

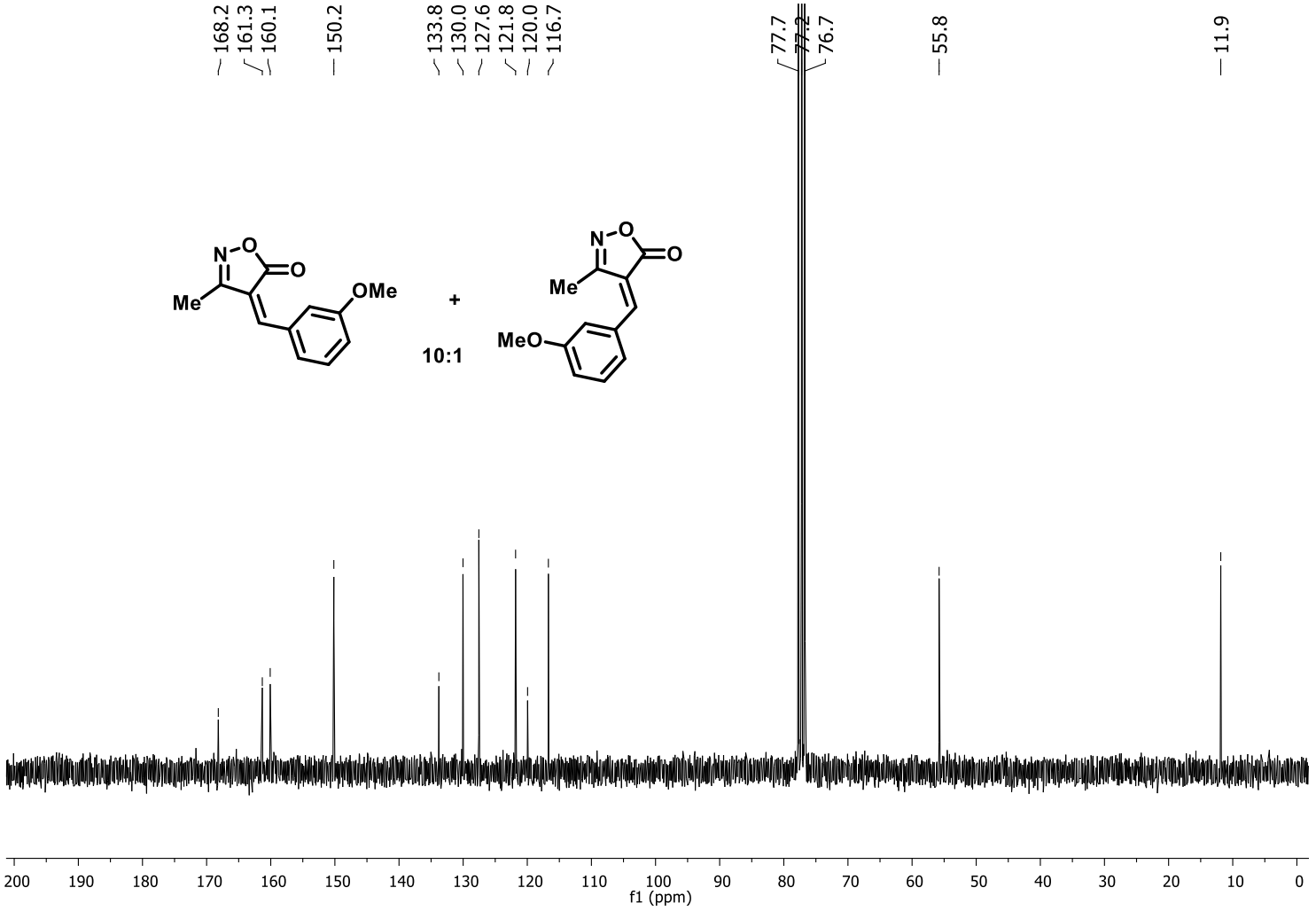
4. NMR spectra

4.1. Molecule 9m

^{1}H (250 MHz, $CDCl_3$)

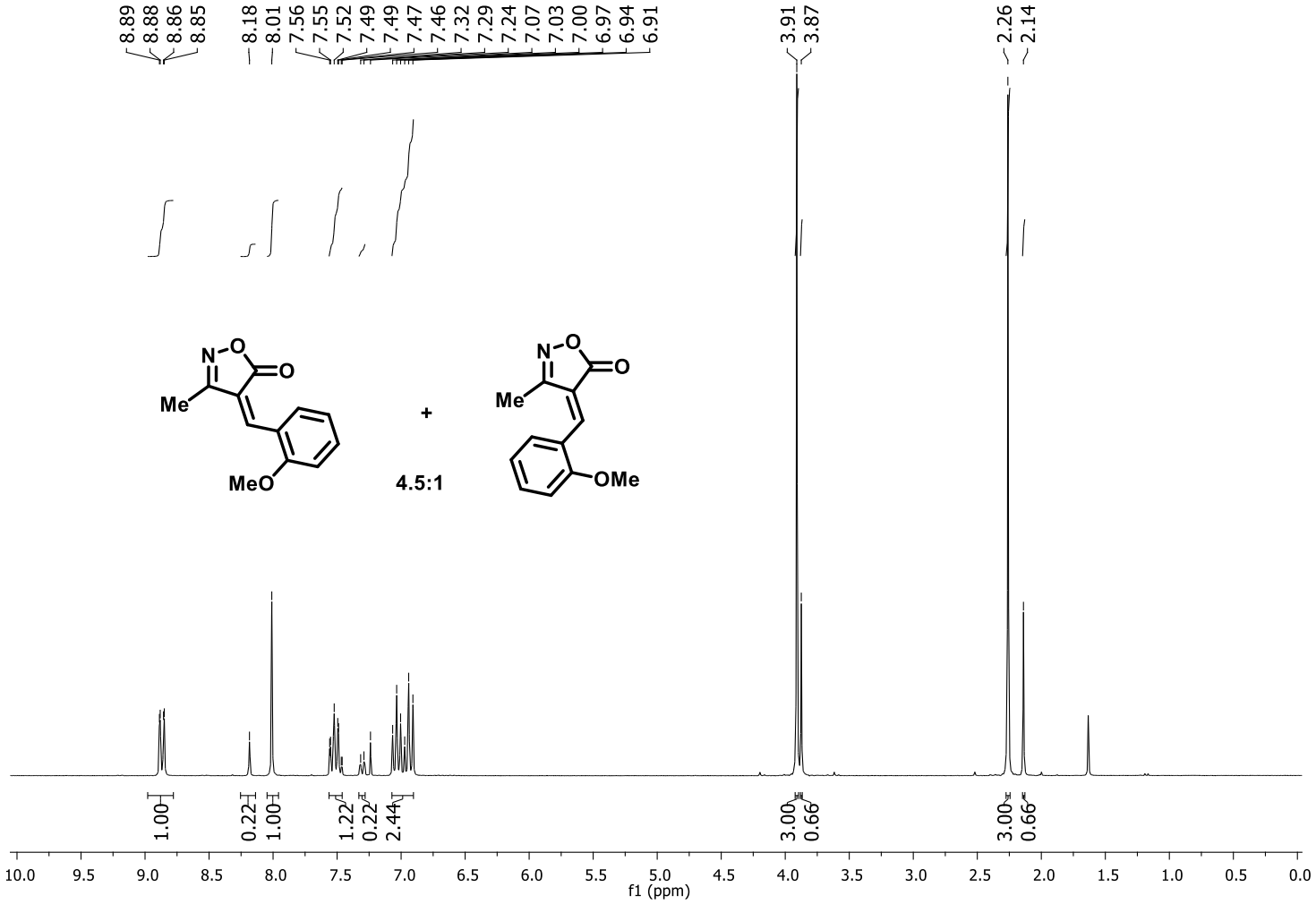


^{13}C (62.5 MHz, $CDCl_3$)

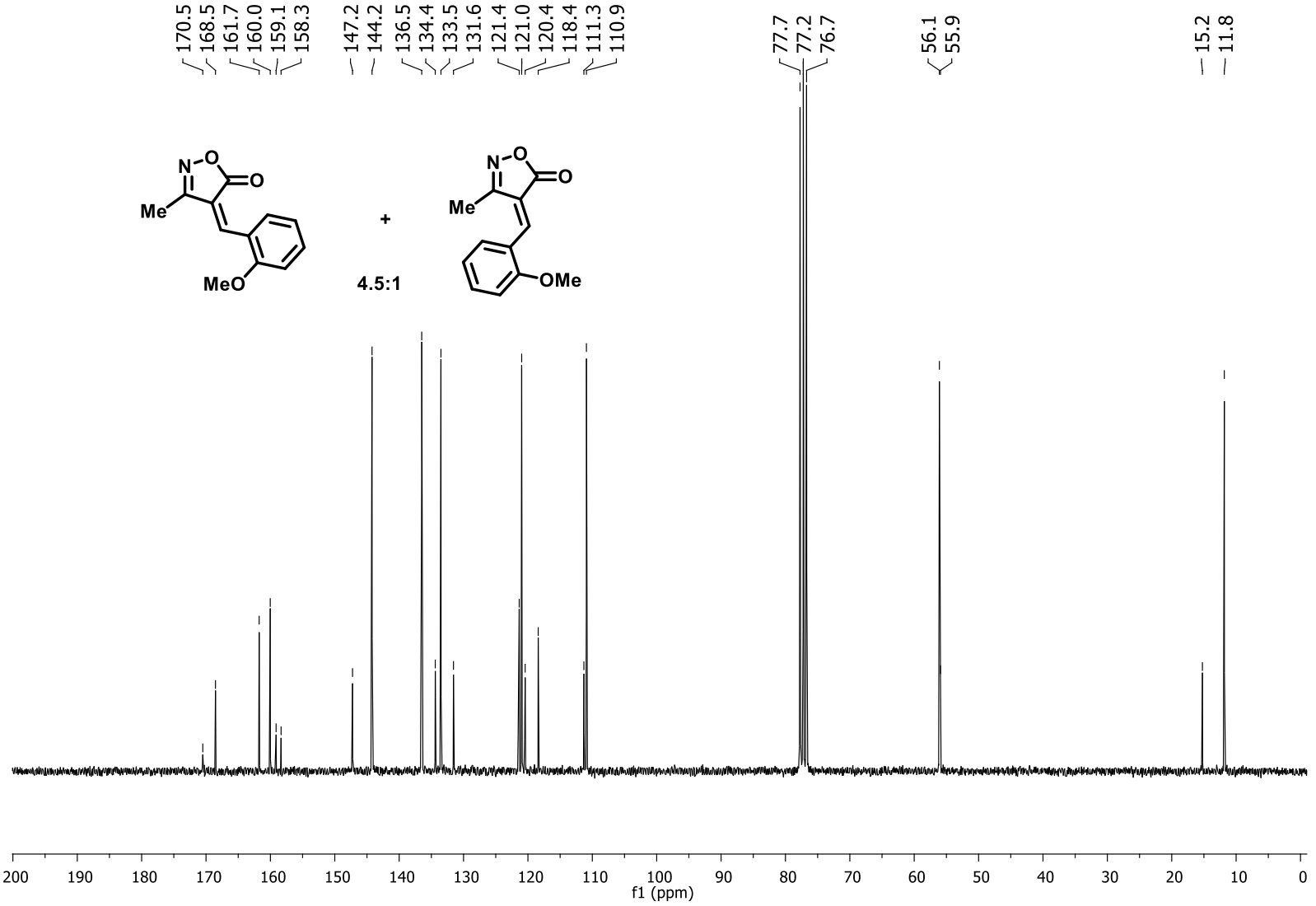


4.2. Molecule 9n

^{1}H (250 MHz, $CDCl_3$)

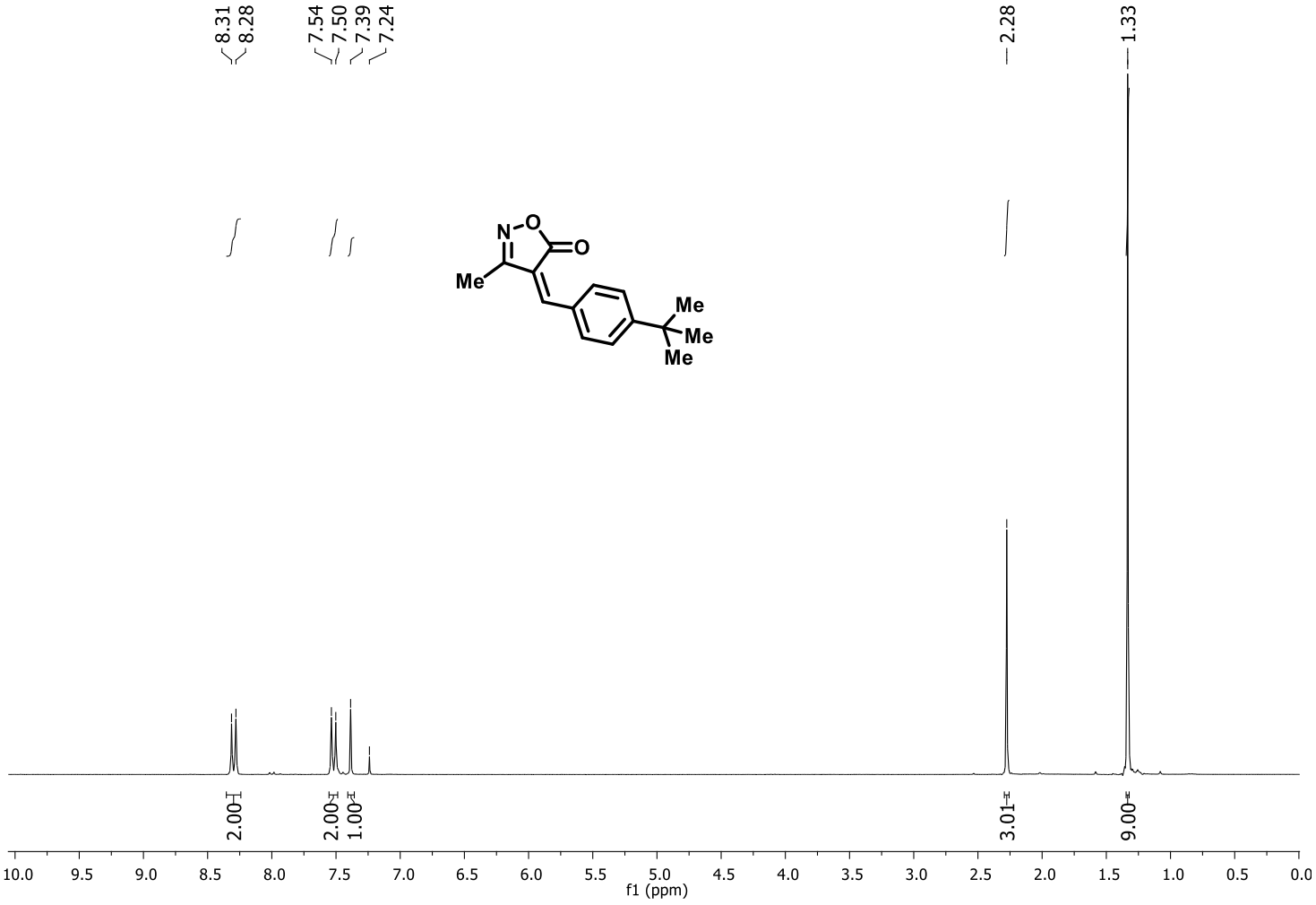


^{13}C (62.5 MHz, $CDCl_3$)

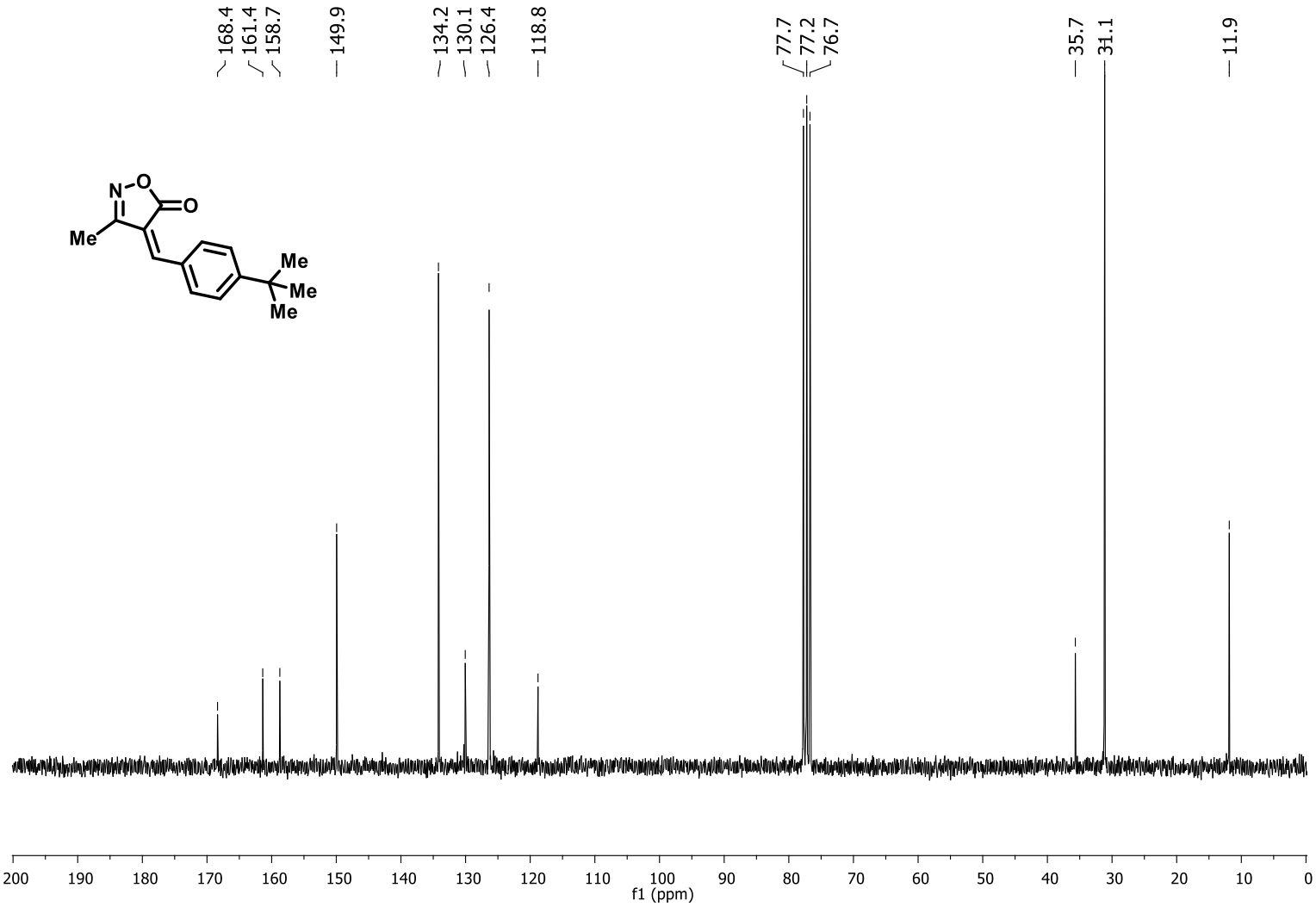


4.3. Molecule 9r

^{1}H (250 MHz, $CDCl_3$)

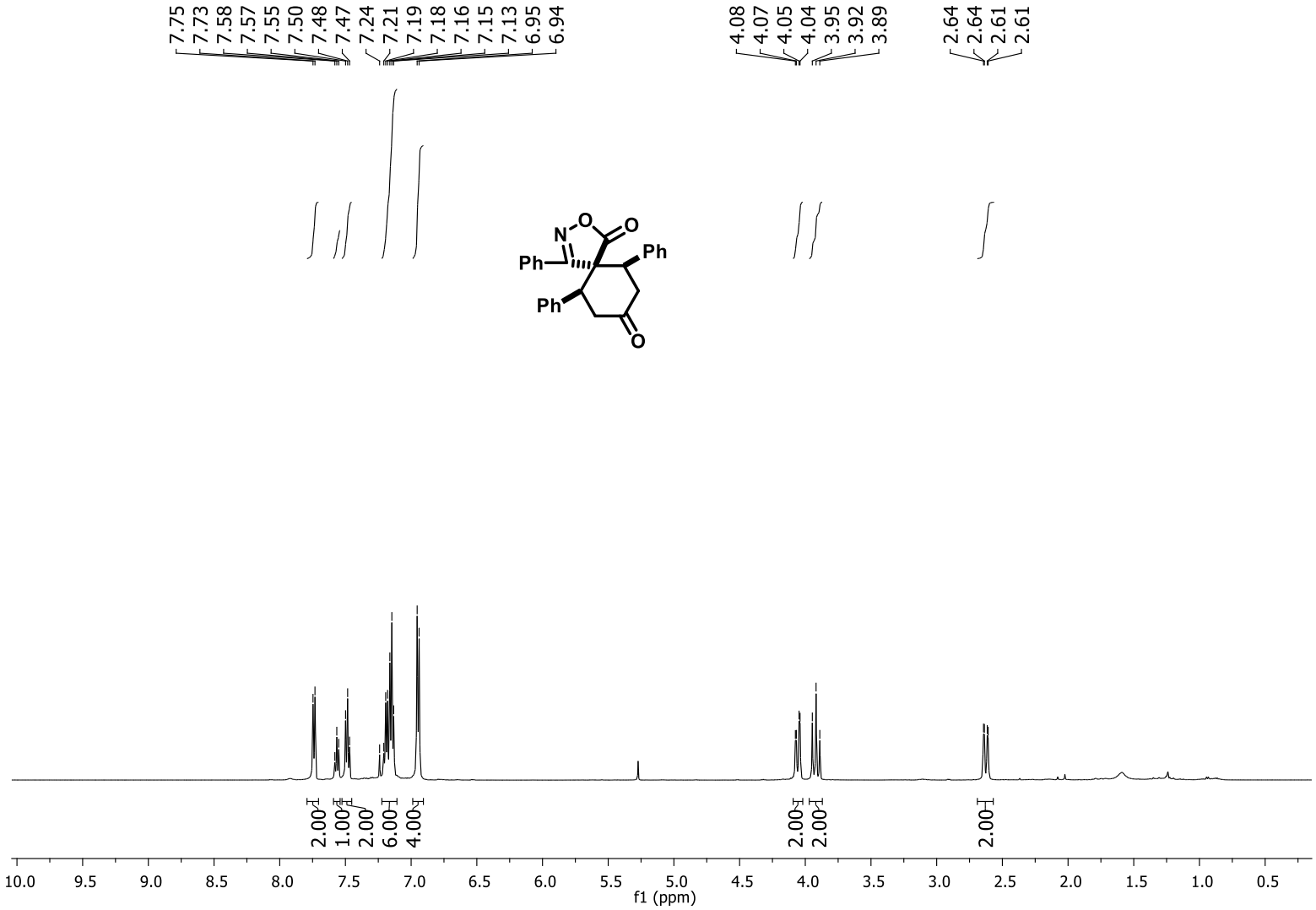


^{13}C (62.5 MHz, $CDCl_3$)

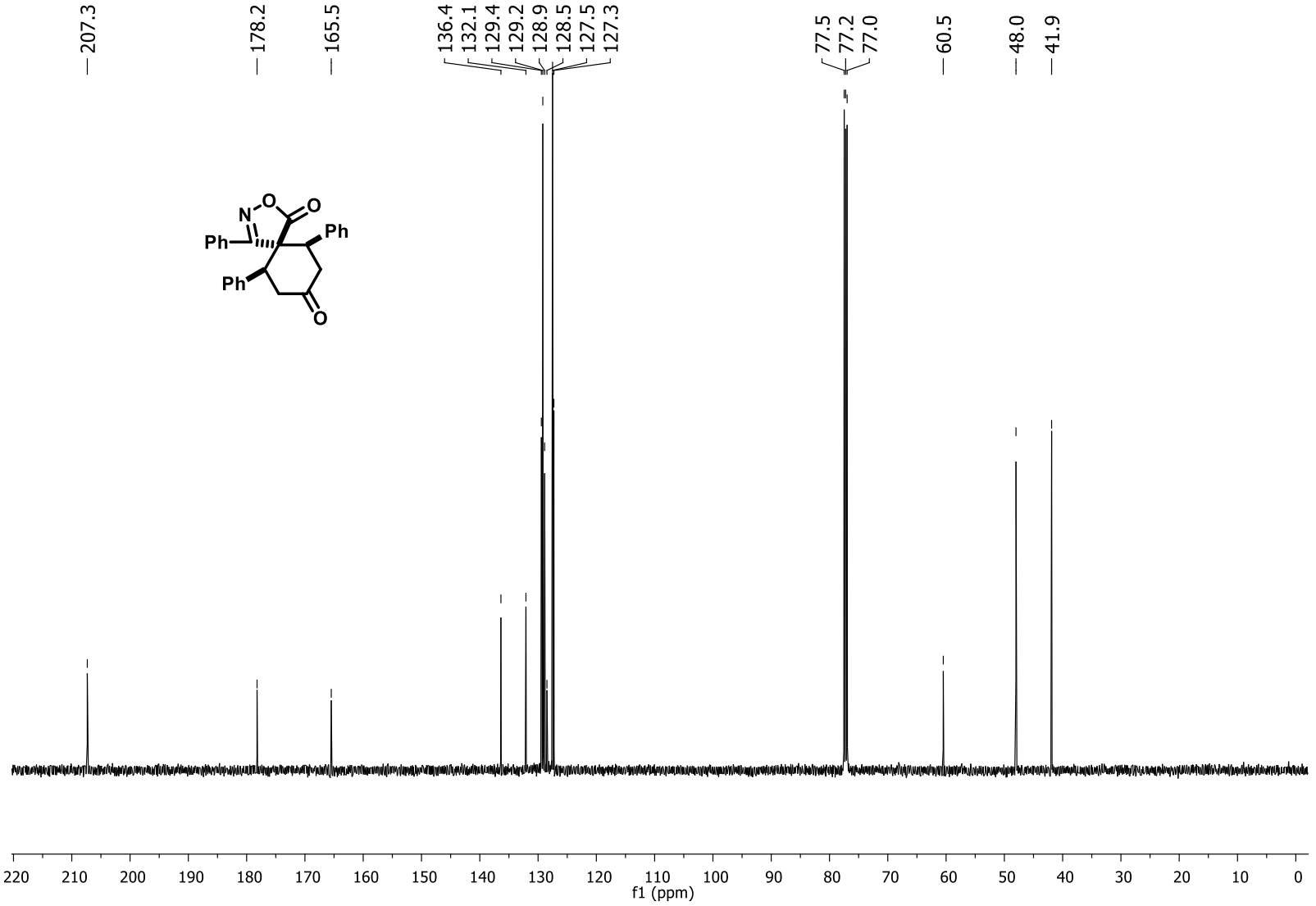


4.4. Molecule 1b

^{1}H (500 MHz, $CDCl_3$)

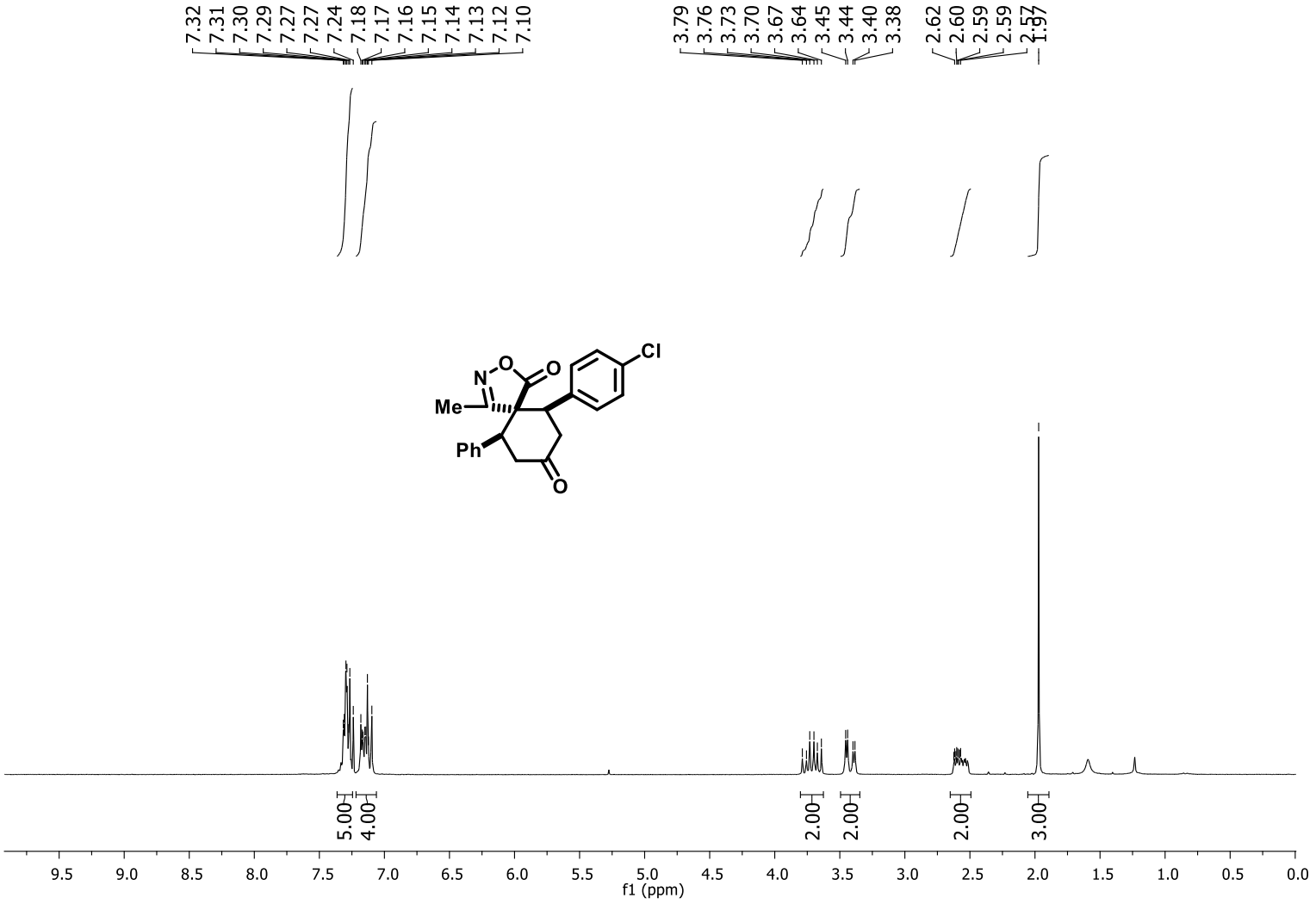


^{13}C (125 MHz, $CDCl_3$)

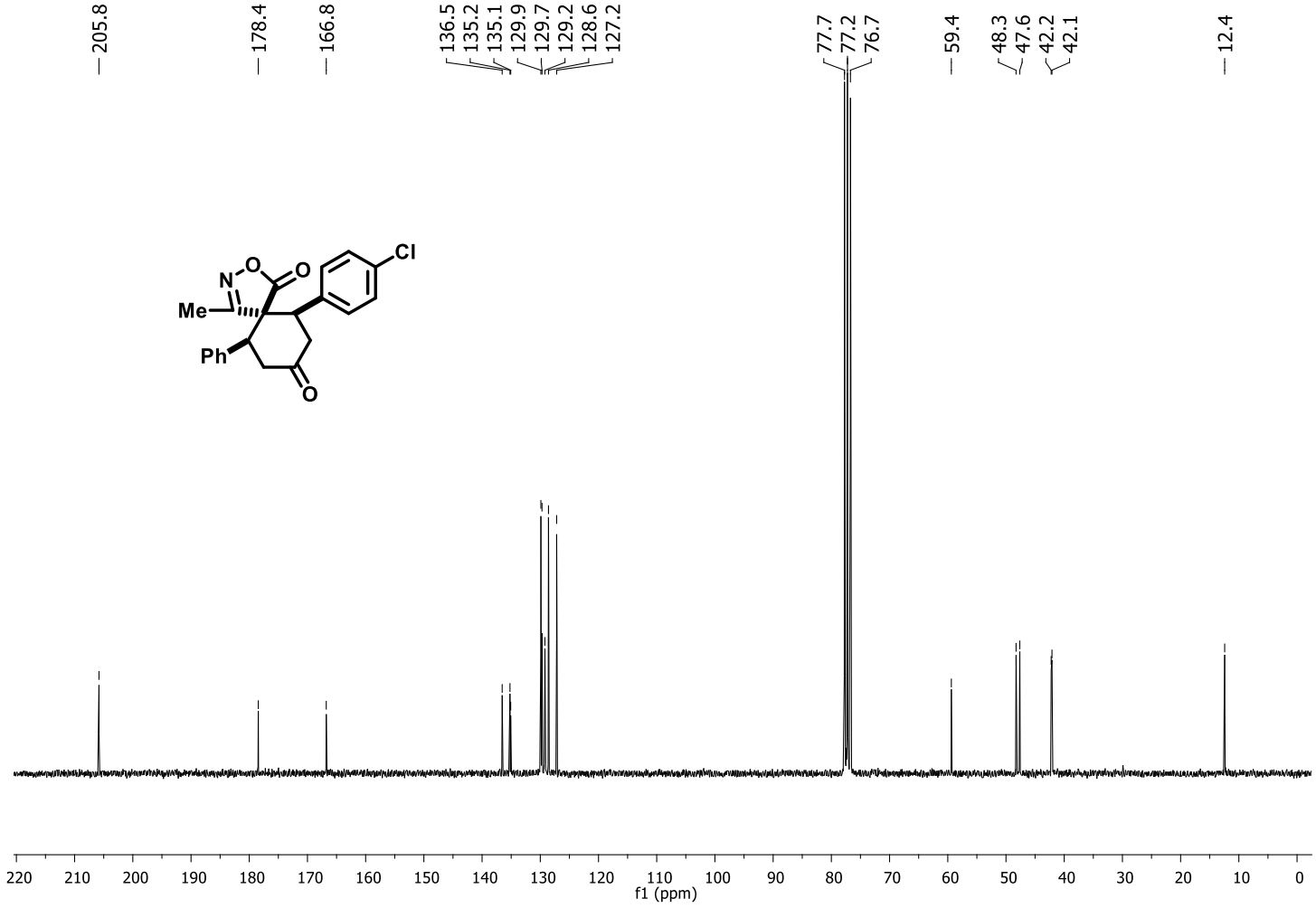


4.5. Molecule 1c

^{1}H (250 MHz, $CDCl_3$)

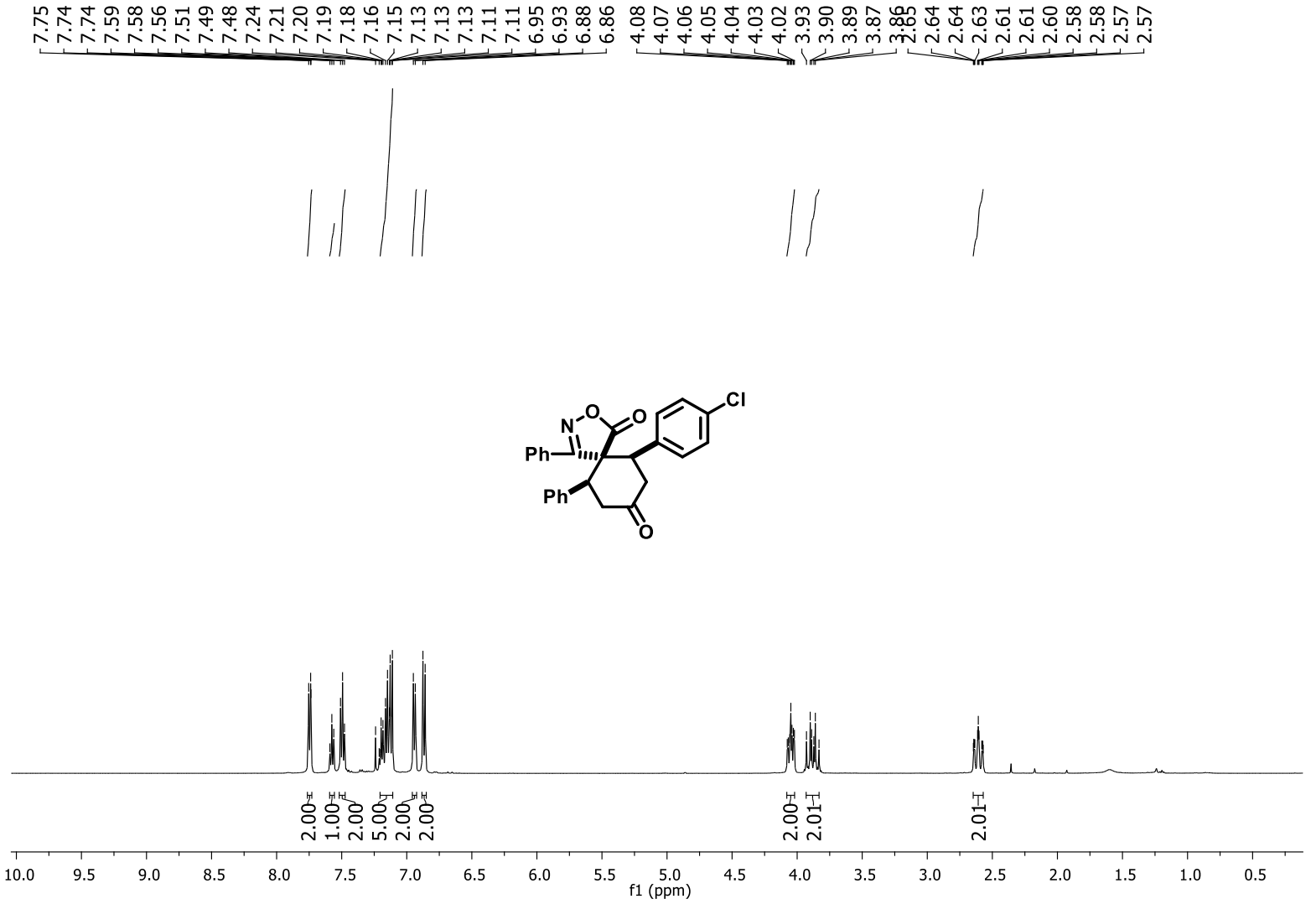


^{13}C (62.5 MHz, $CDCl_3$)

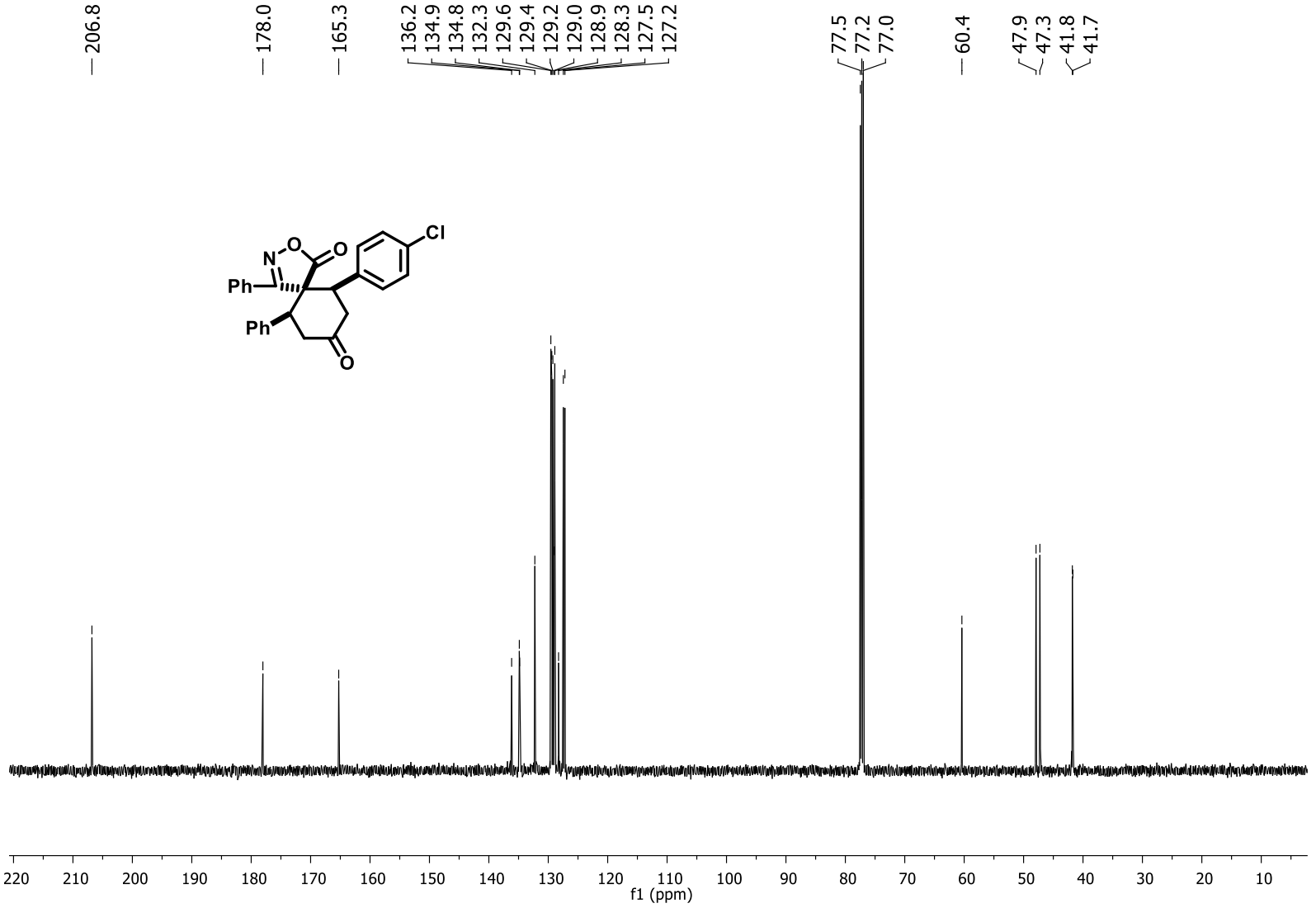


4.6. Molecule 1d

^{1}H (500 MHz, $CDCl_3$)

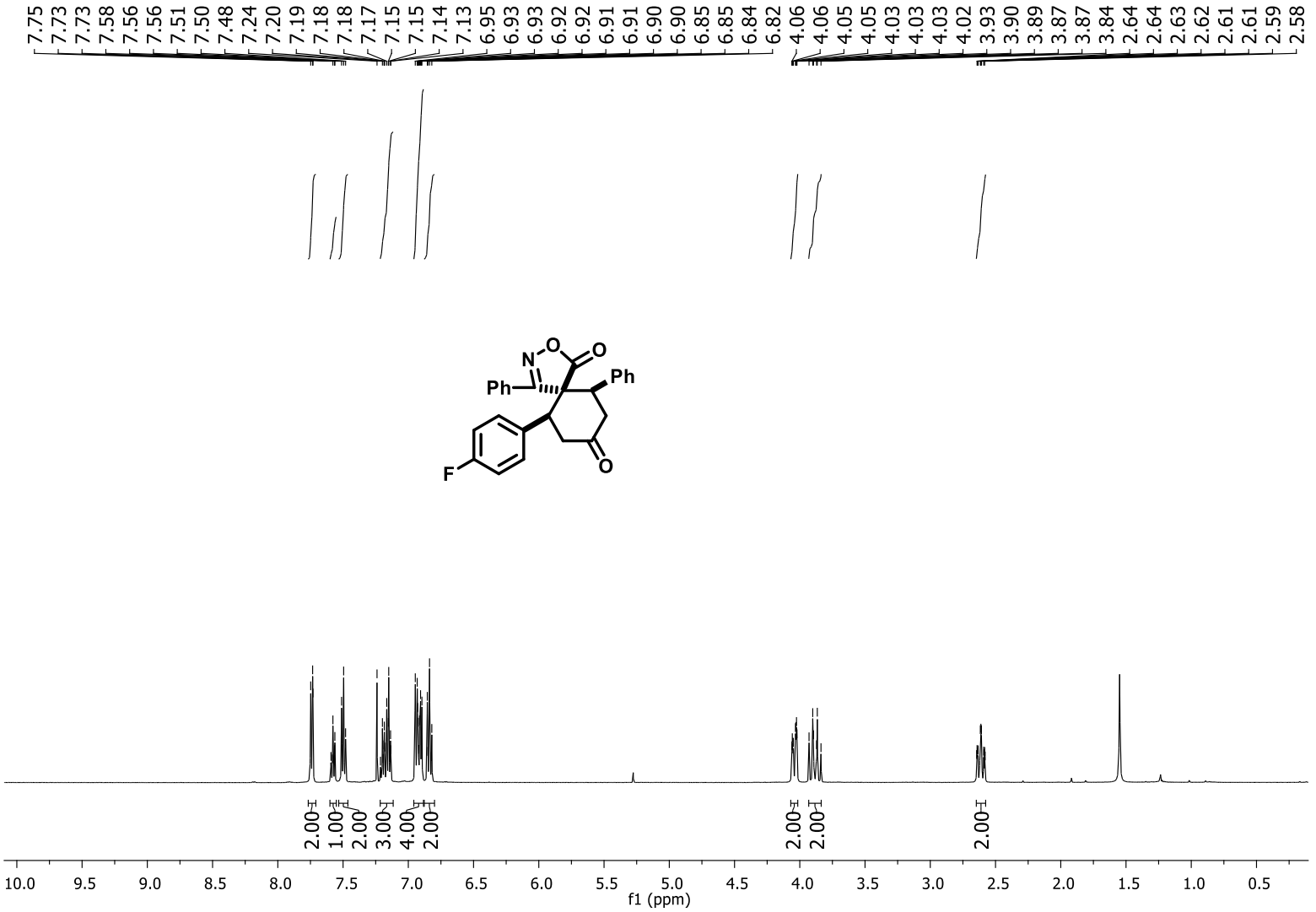


^{13}C (125 MHz, $CDCl_3$)

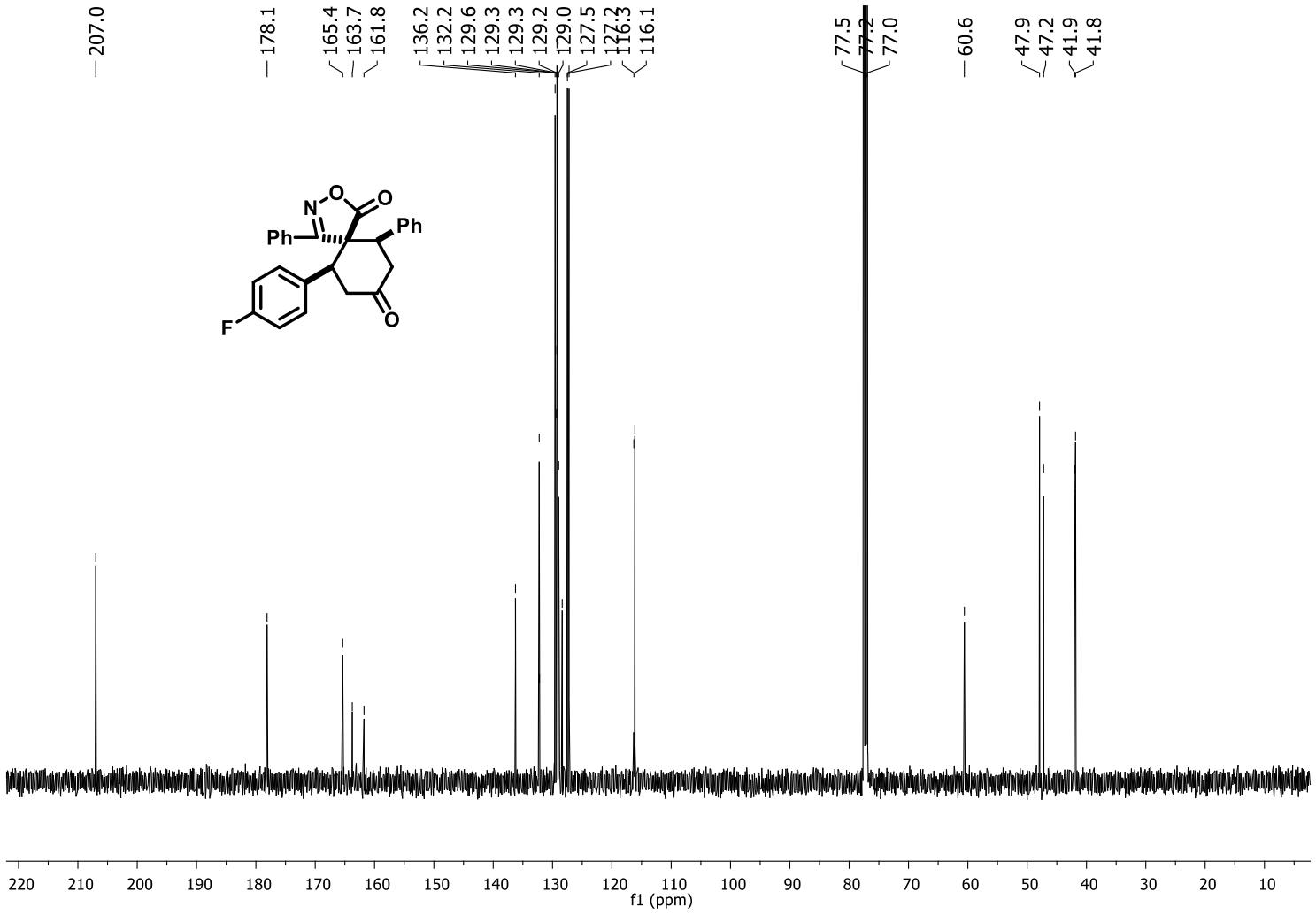


4.7. Molecule 1e

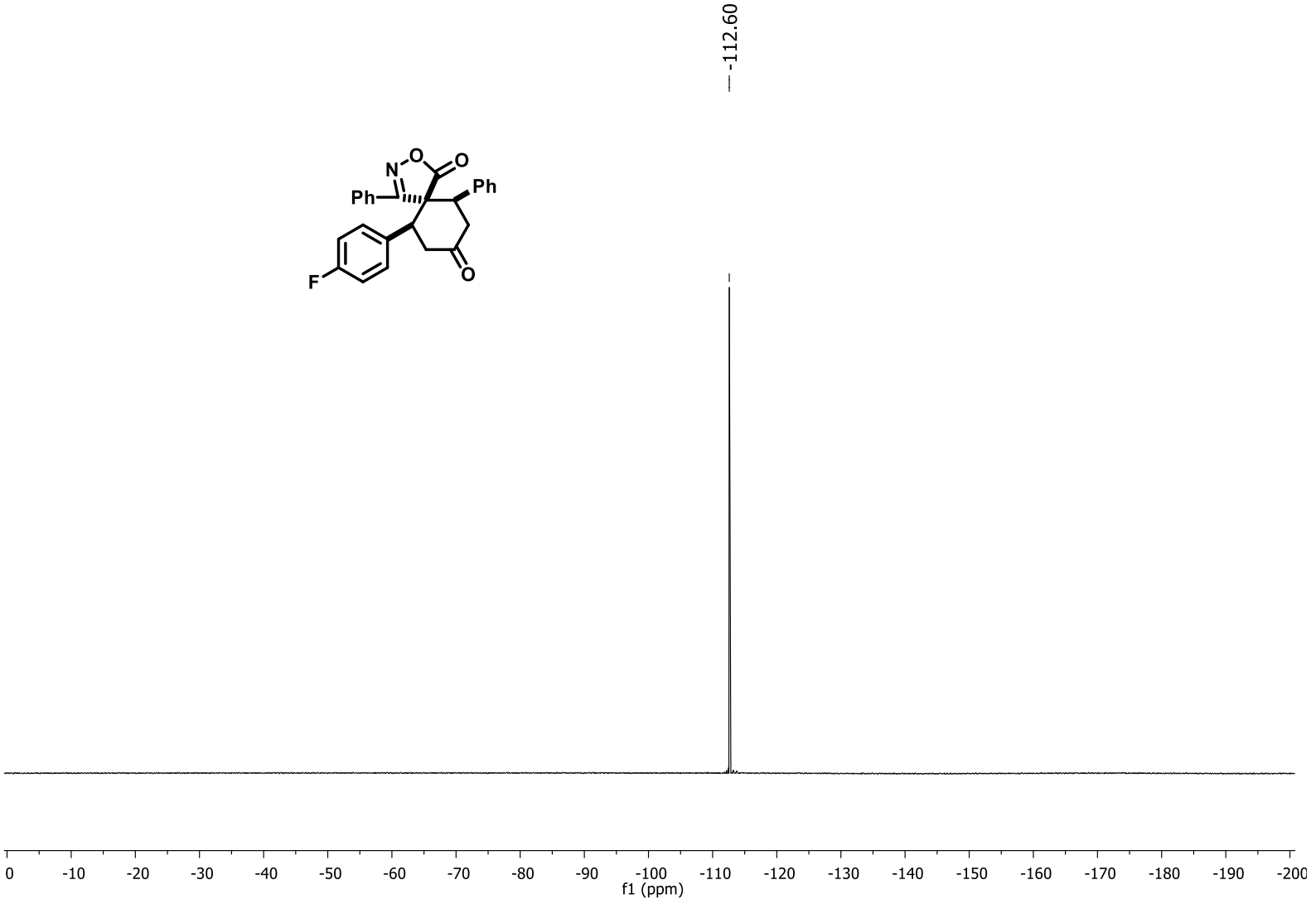
^{1}H (500 MHz, $CDCl_3$)



^{13}C (125 MHz, $CDCl_3$)

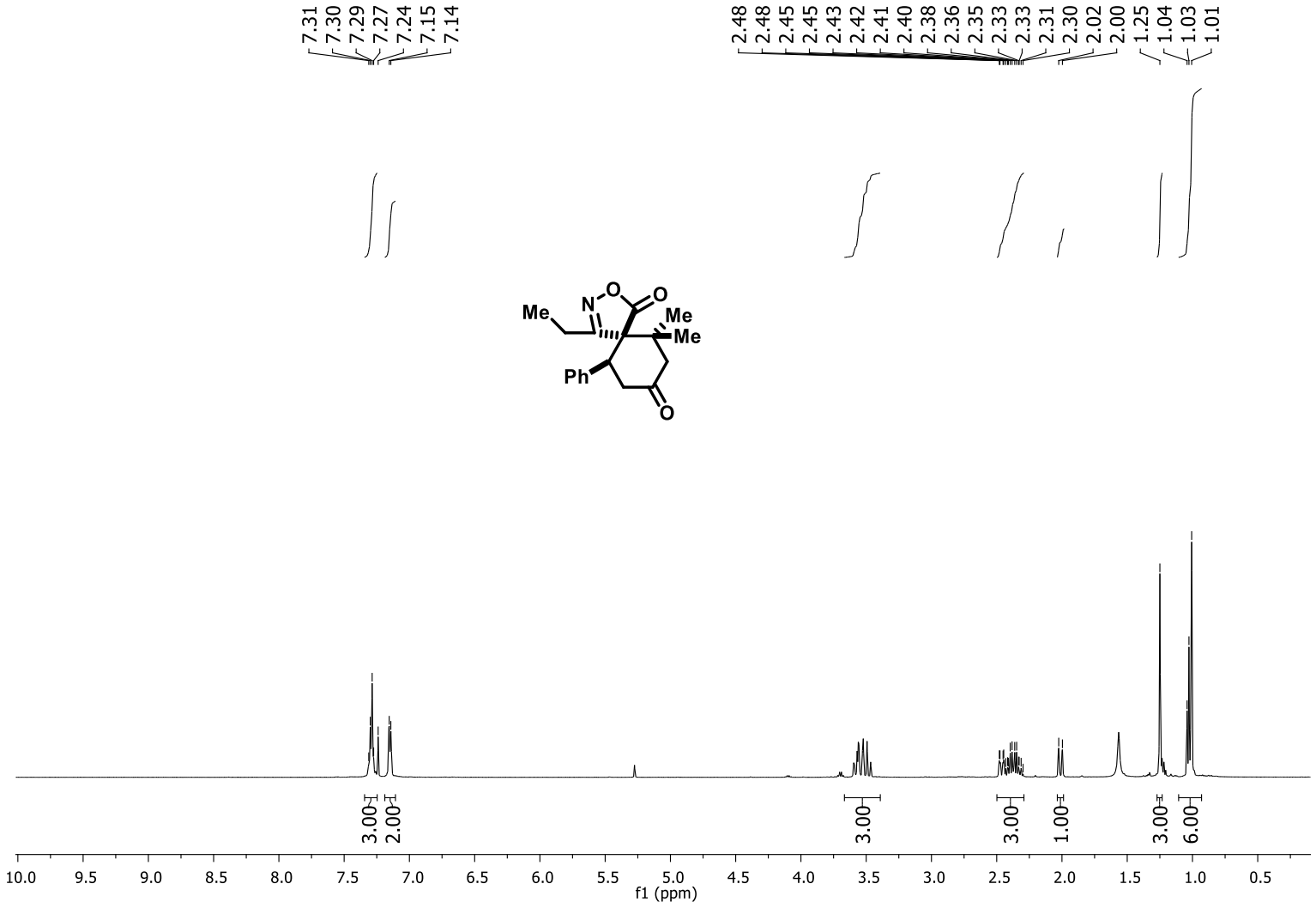


^{19}F (235 MHz, $CDCl_3$)

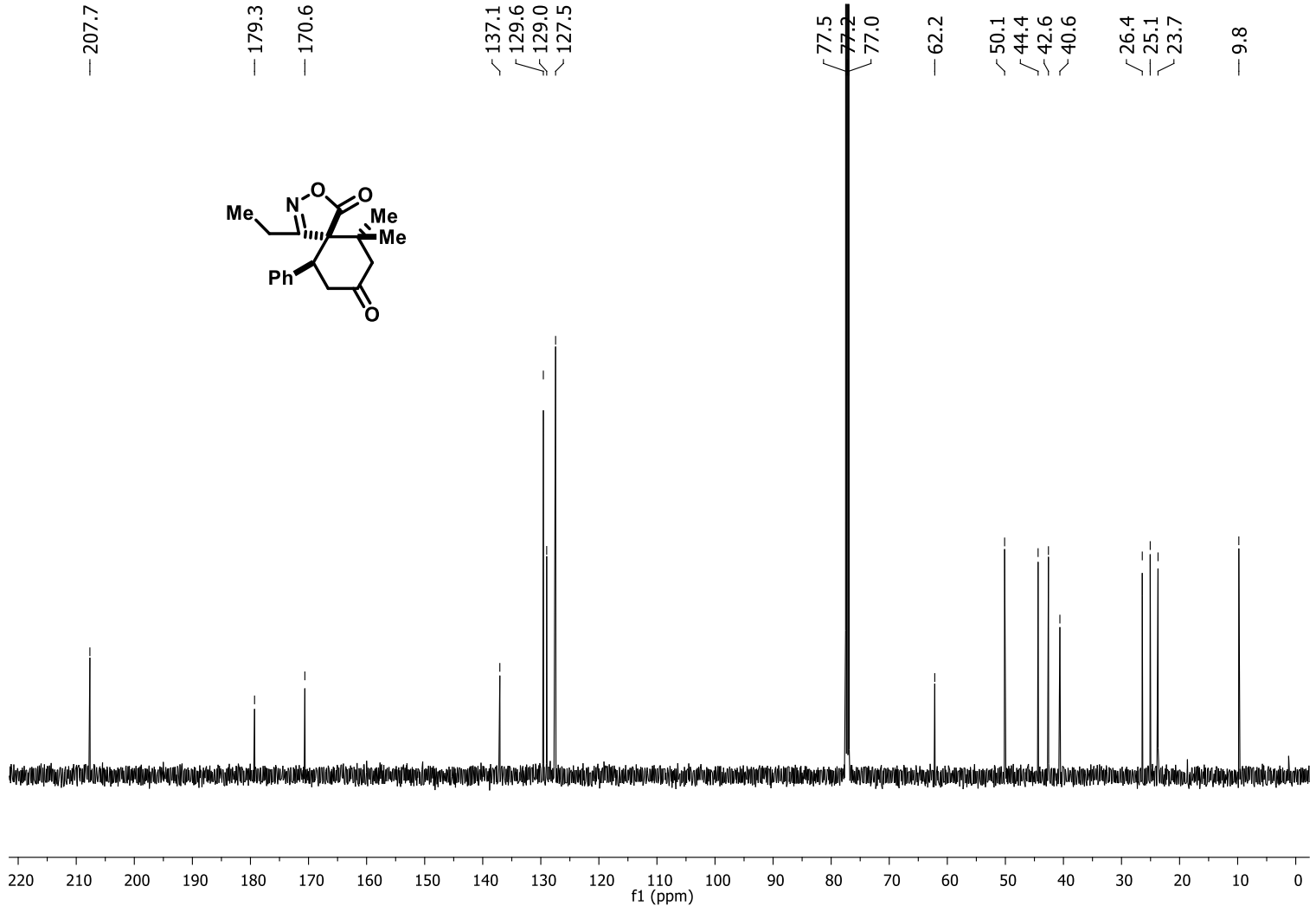


4.8. Molecule 1f

^{1}H (500 MHz, $CDCl_3$)

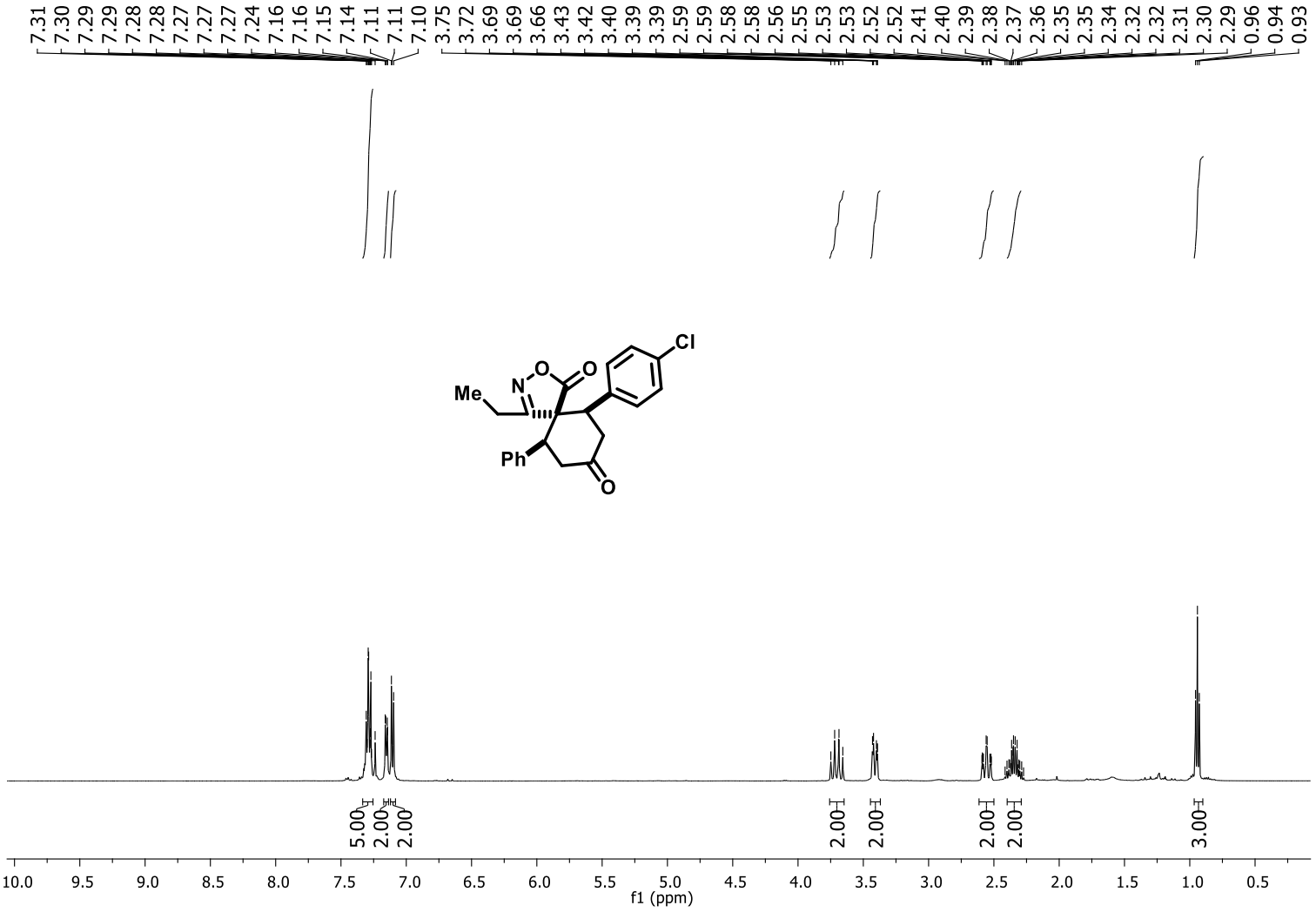


^{13}C (125 MHz, $CDCl_3$)

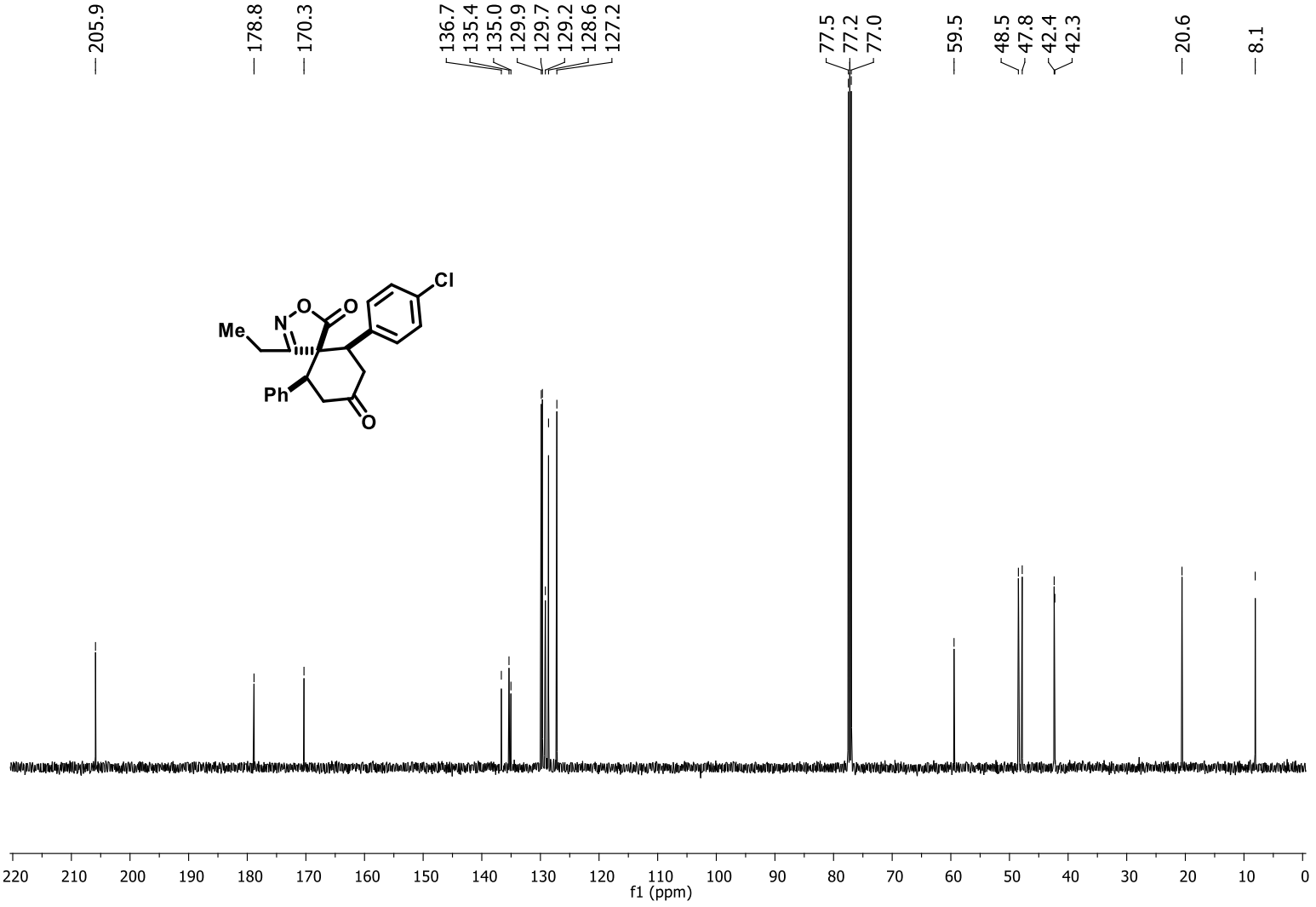


4.9. Molecule 1g

^{1}H (500 MHz, $CDCl_3$)

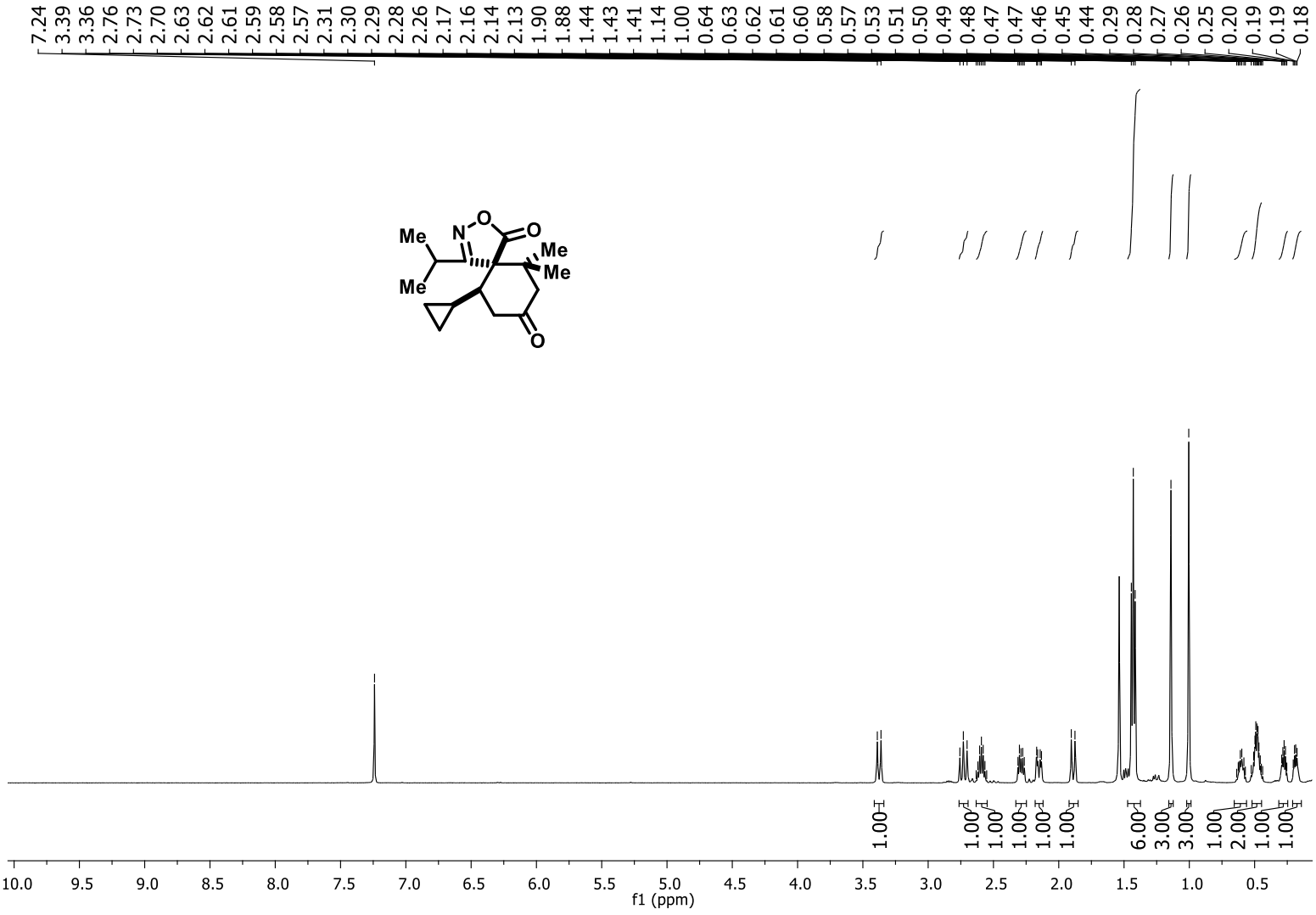


^{13}C (125 MHz, $CDCl_3$)

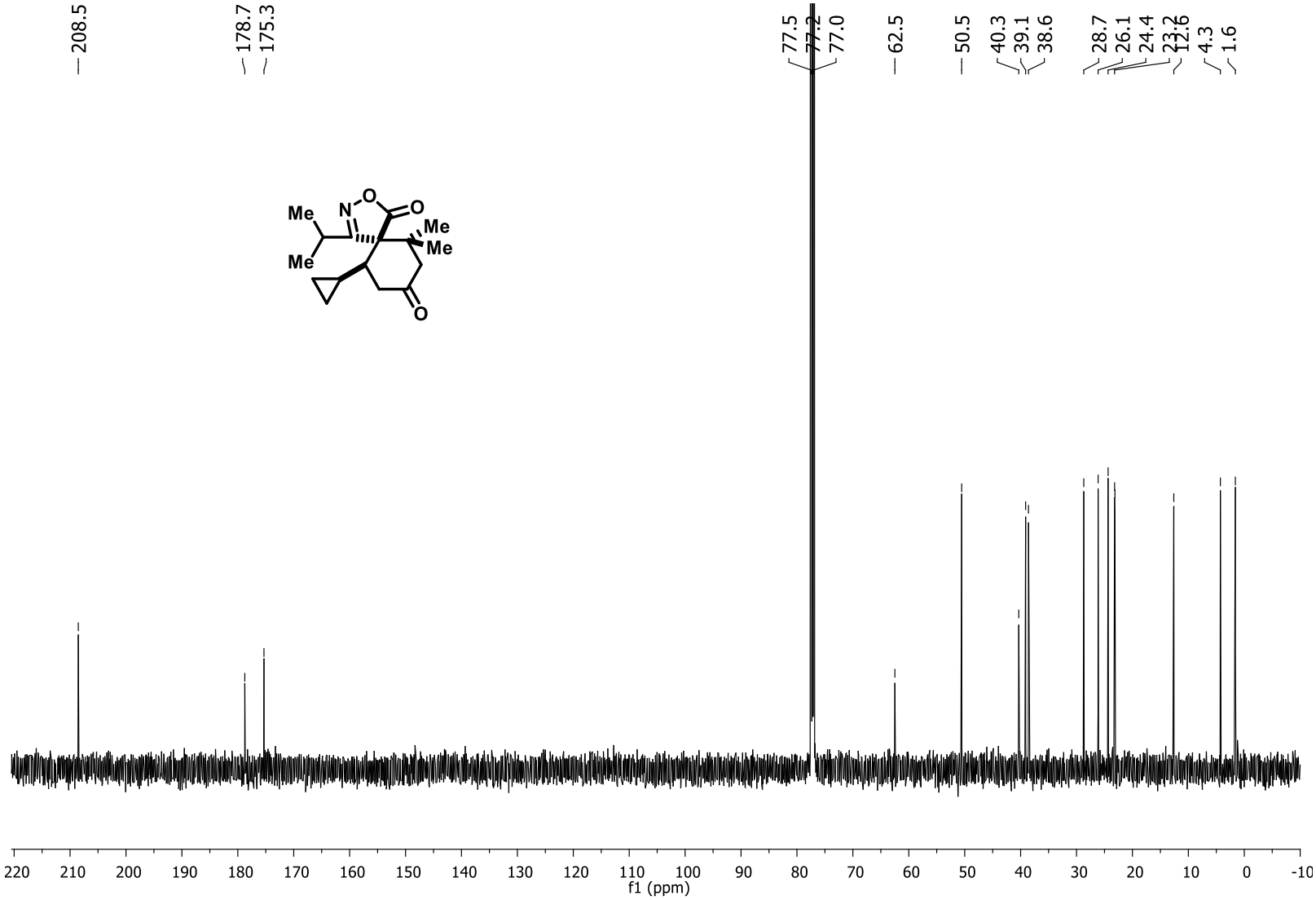


4.10. Molecule 1h

^{1}H (500 MHz, $CDCl_3$)

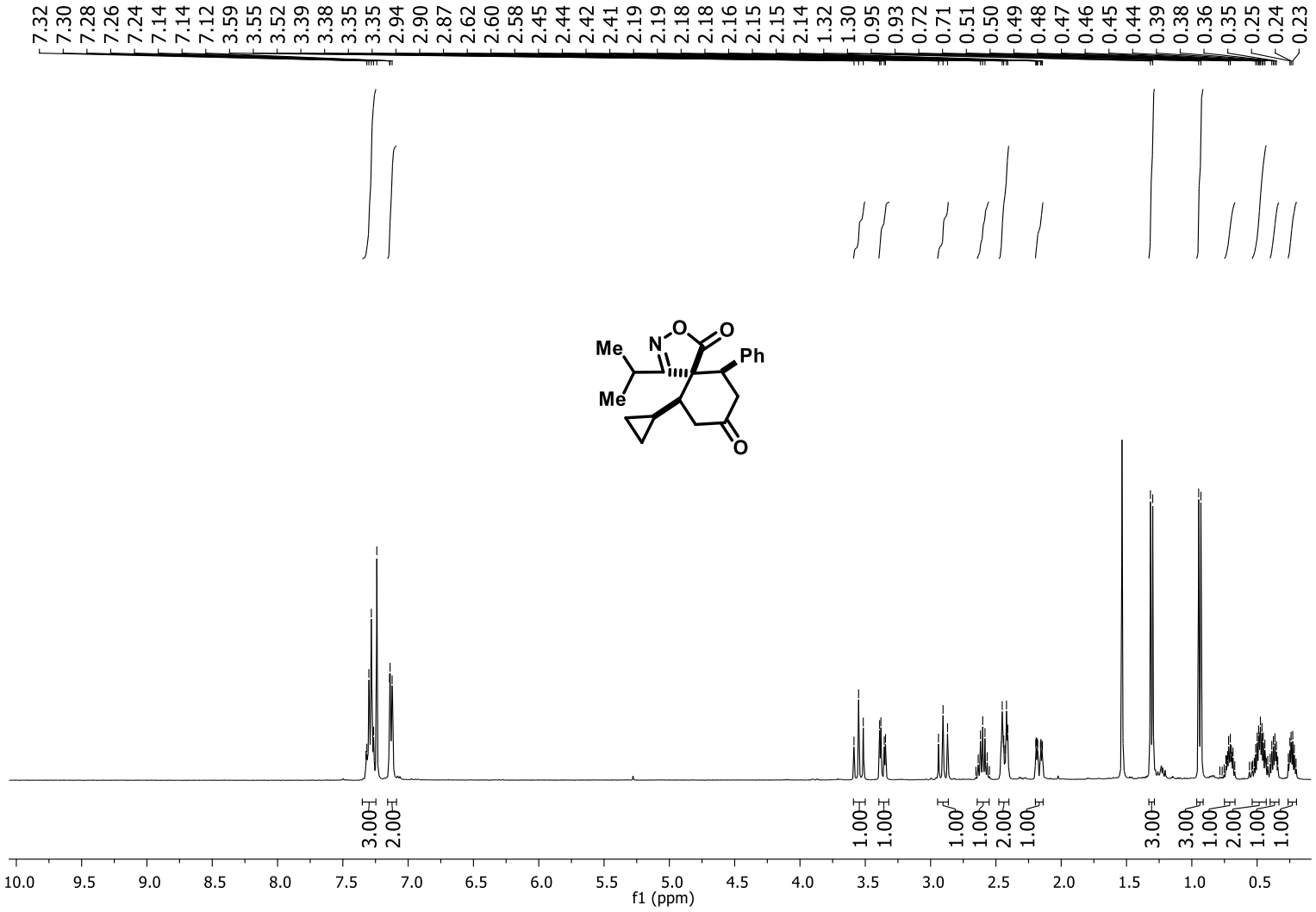


^{13}C (125 MHz, $CDCl_3$)

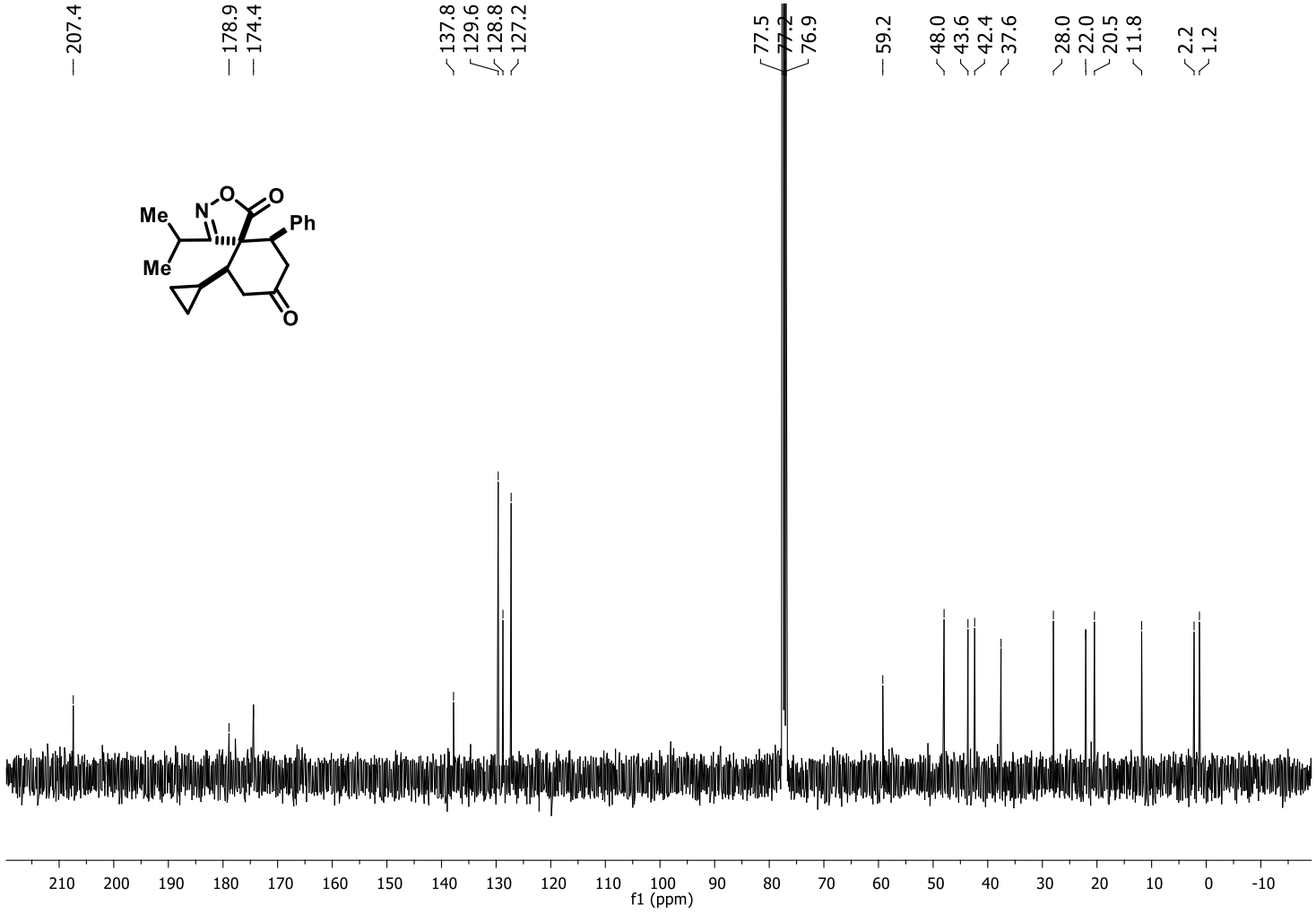


4.11. Molecule 1i

^{1}H (400 MHz, $CDCl_3$)

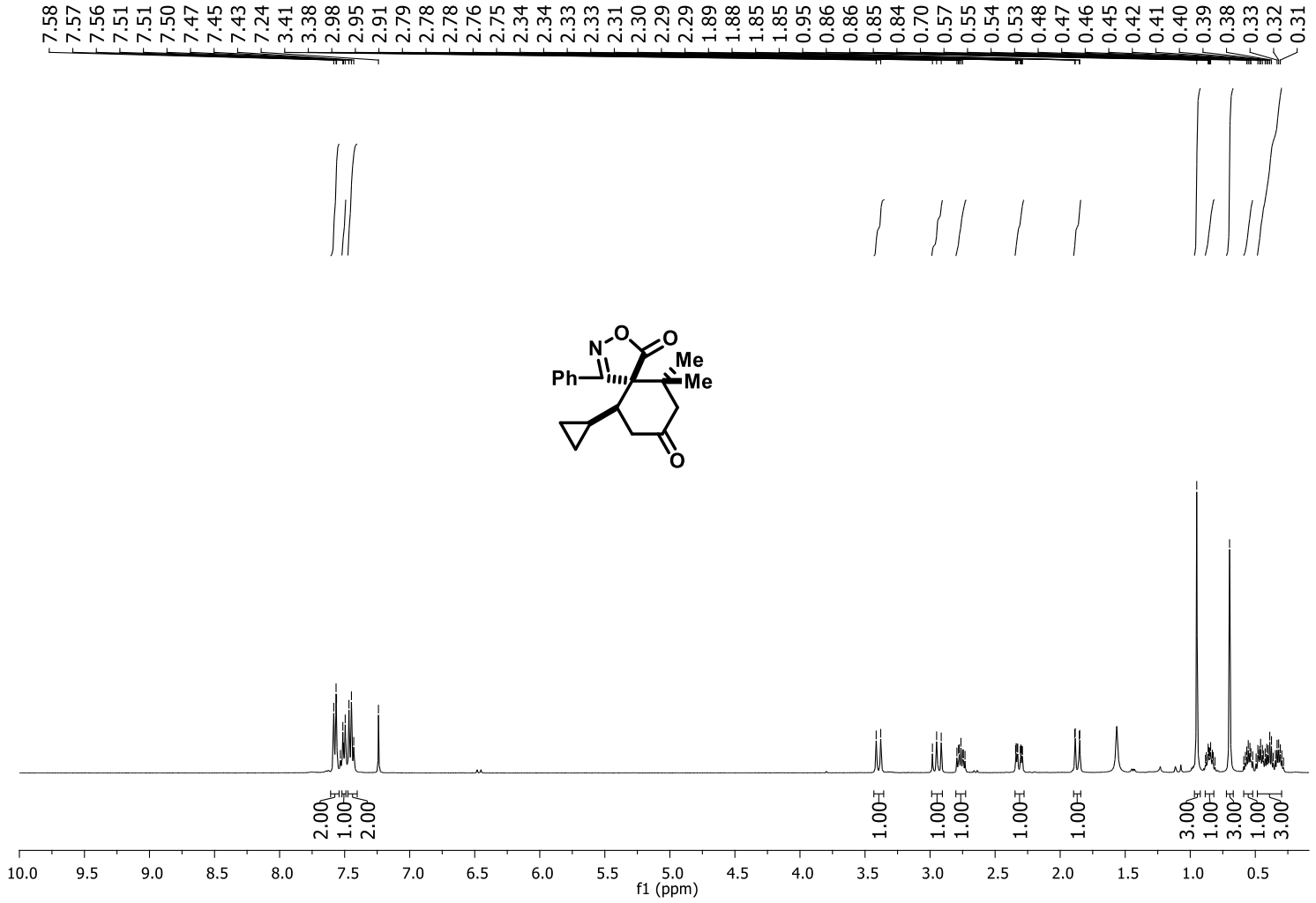


^{13}C (100 MHz, $CDCl_3$)

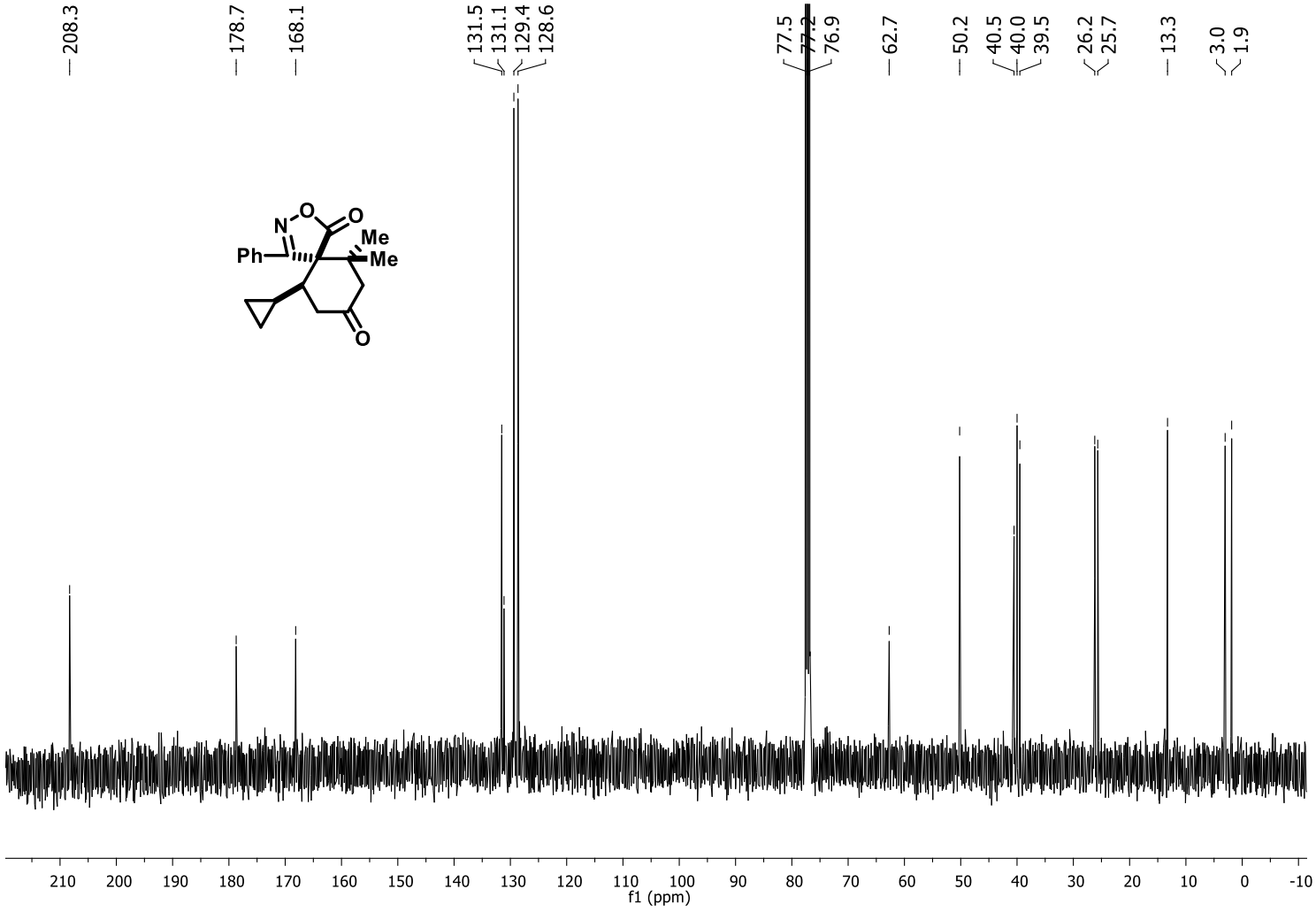


4.12. Molecule 1j

^{1}H (400 MHz, $CDCl_3$)

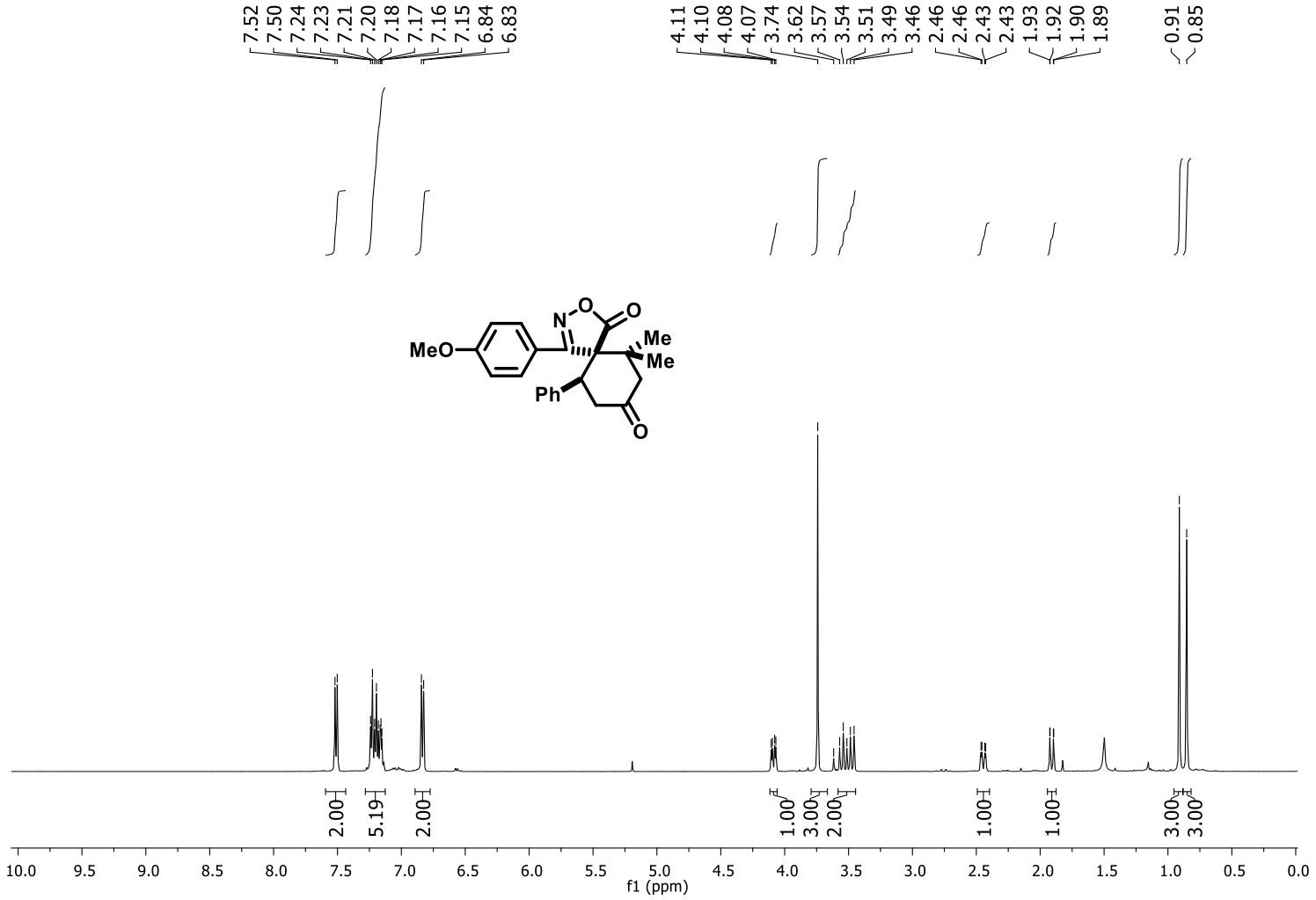


^{13}C (100 MHz, $CDCl_3$)

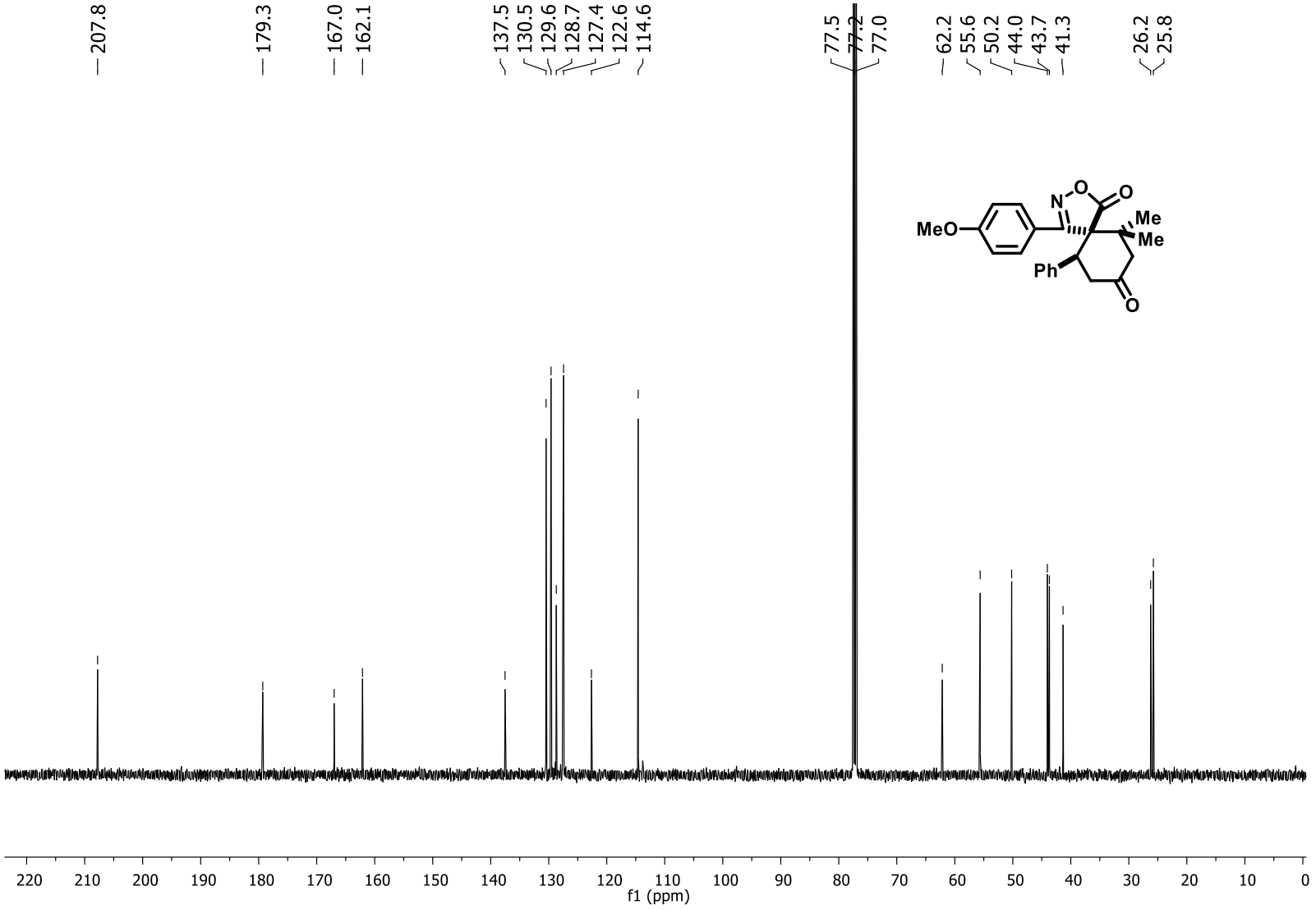


4.13. Molecule 1k

^{1}H (500 MHz, $CDCl_3$)

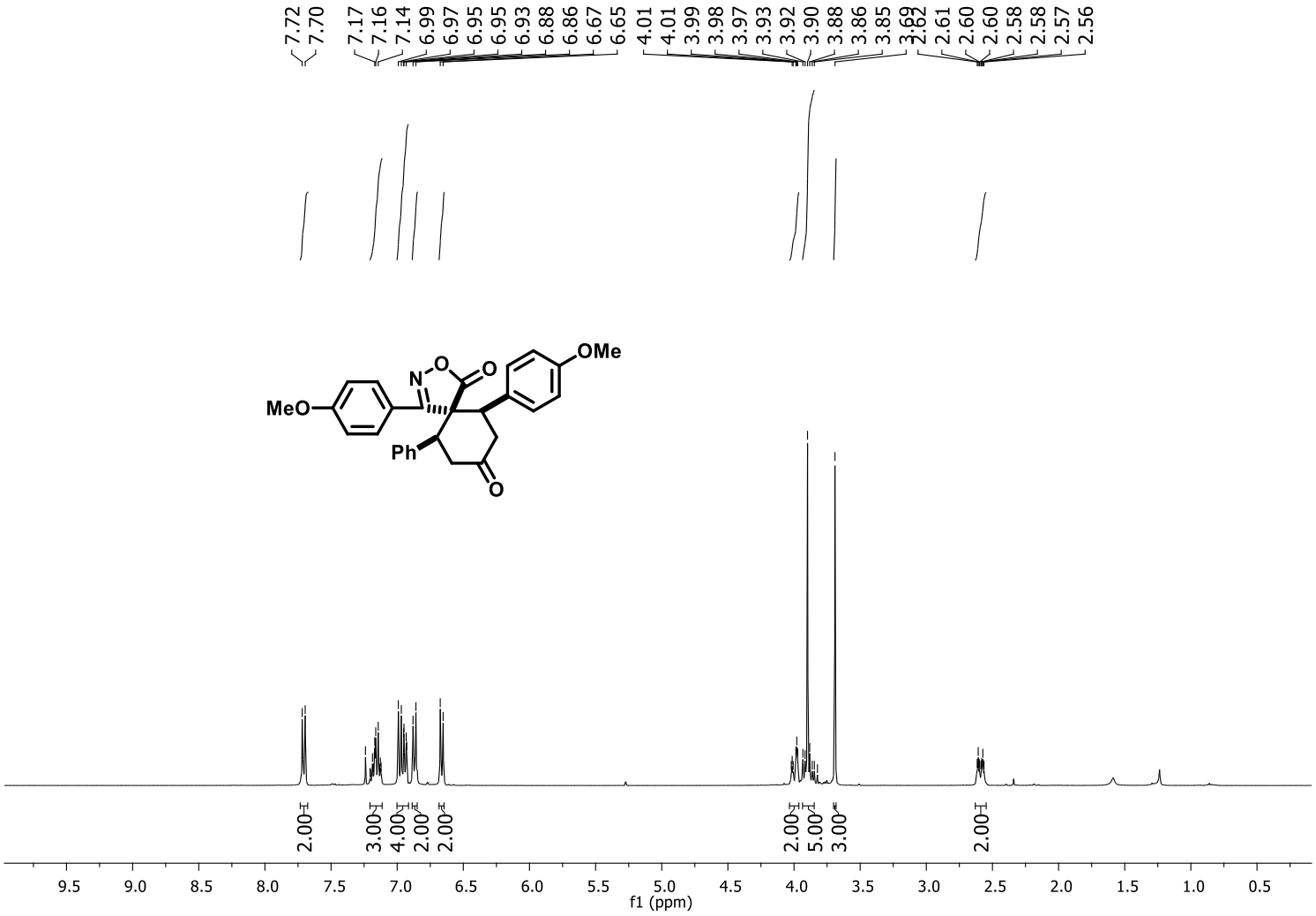


^{13}C (125 MHz, $CDCl_3$)

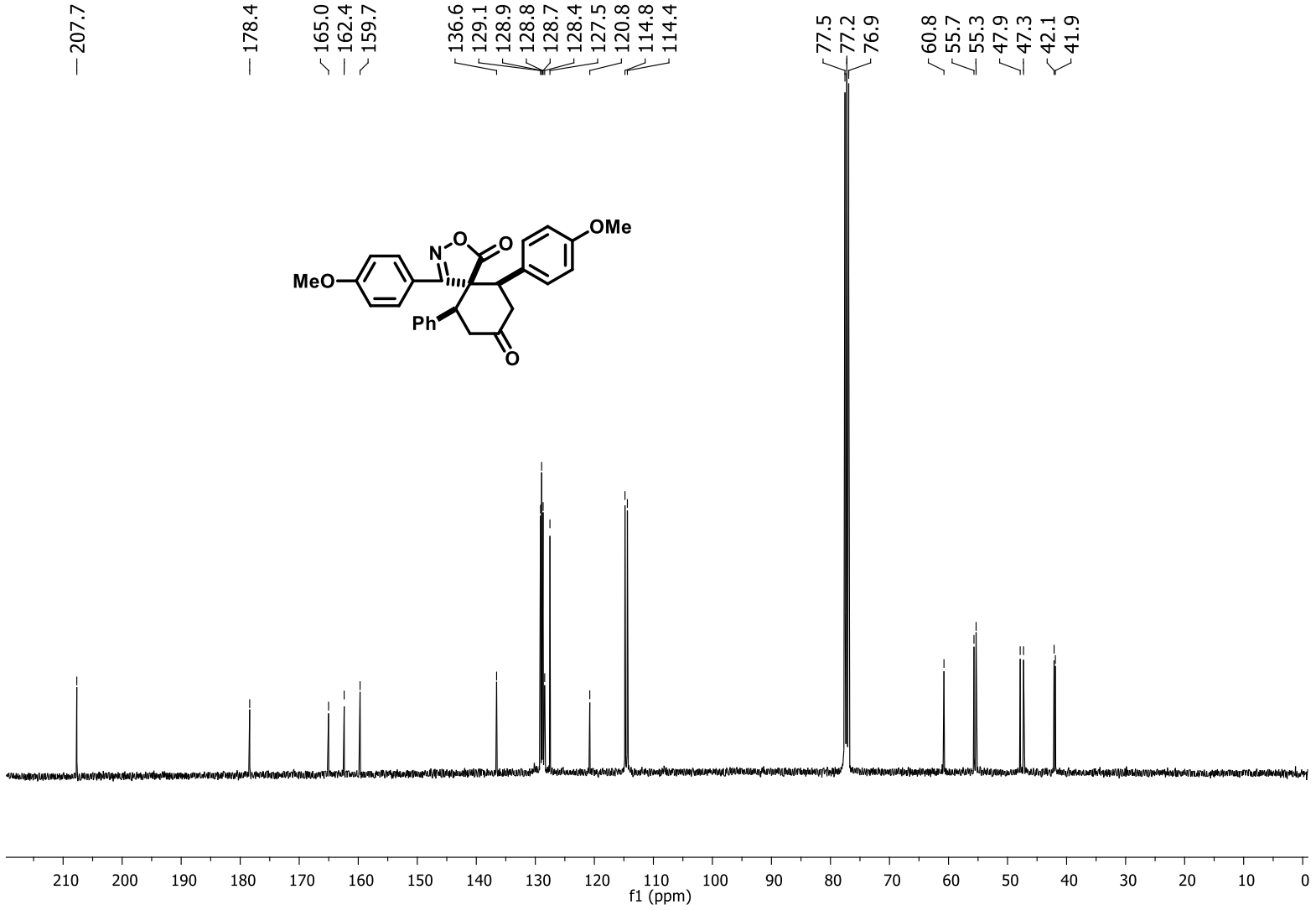


4.14. Molecule 1l

^{1}H (400 MHz, $CDCl_3$)

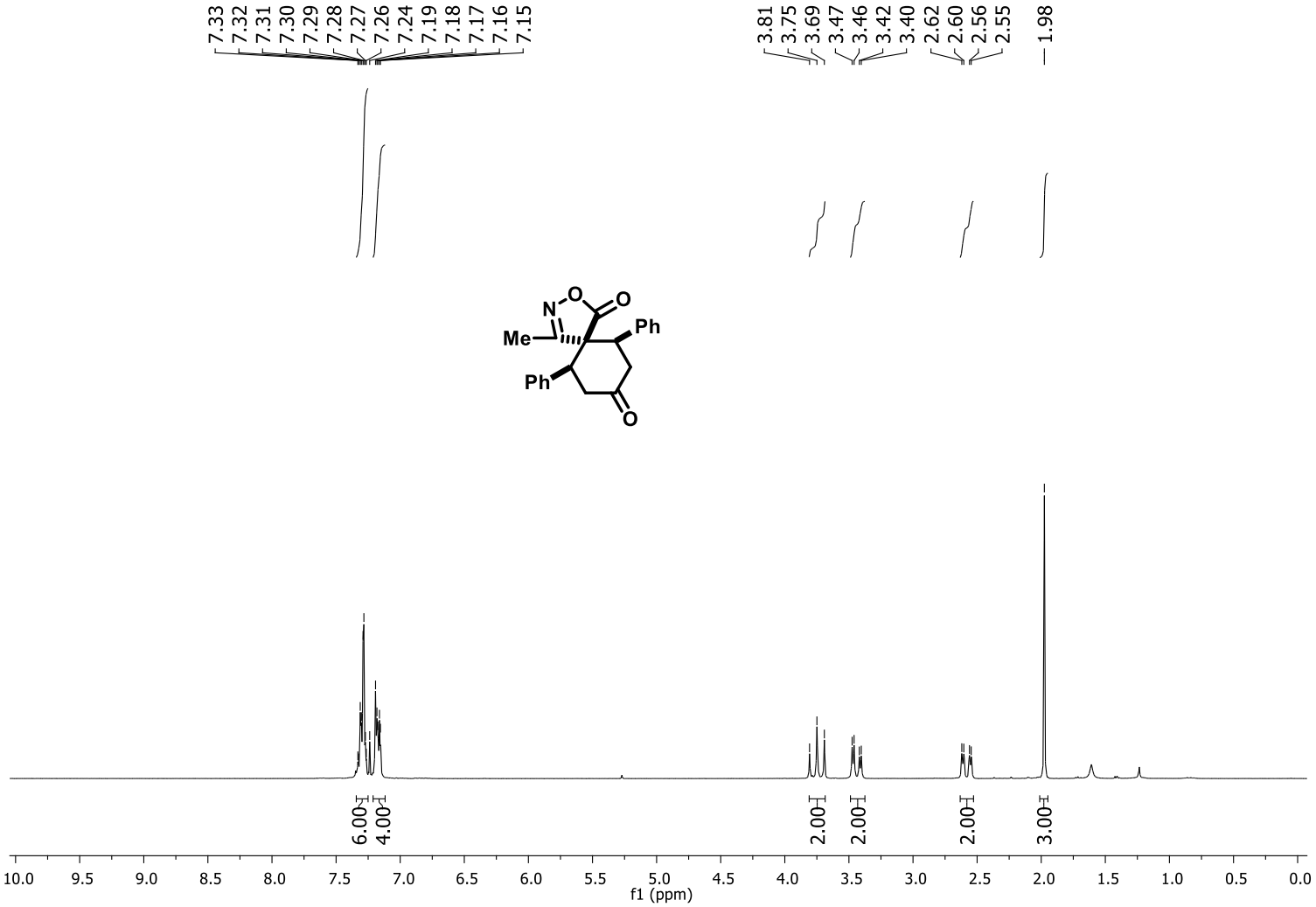


^{13}C (100 MHz, $CDCl_3$)

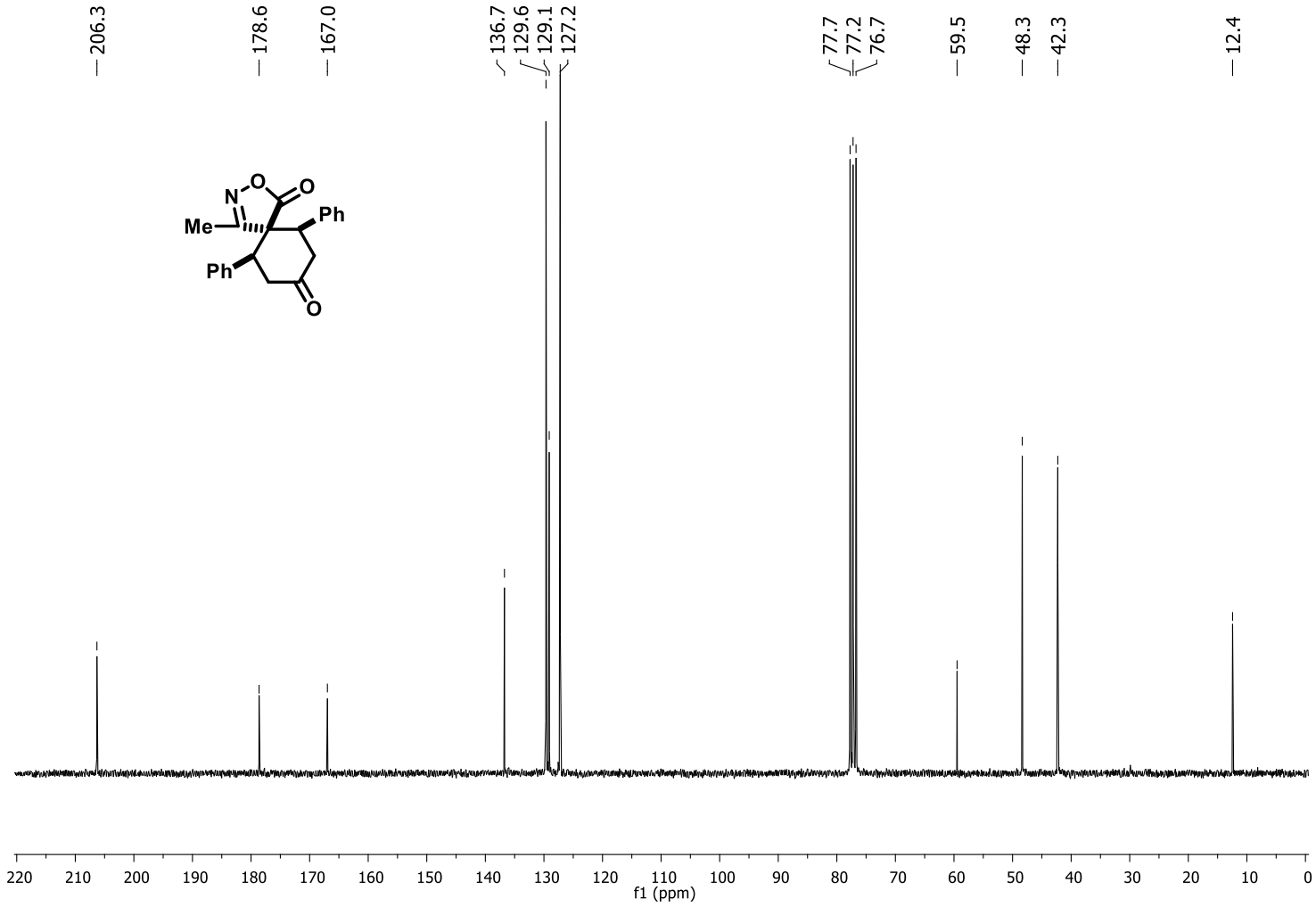


4.15. Molecule 1m

^{1}H (250 MHz, $CDCl_3$)

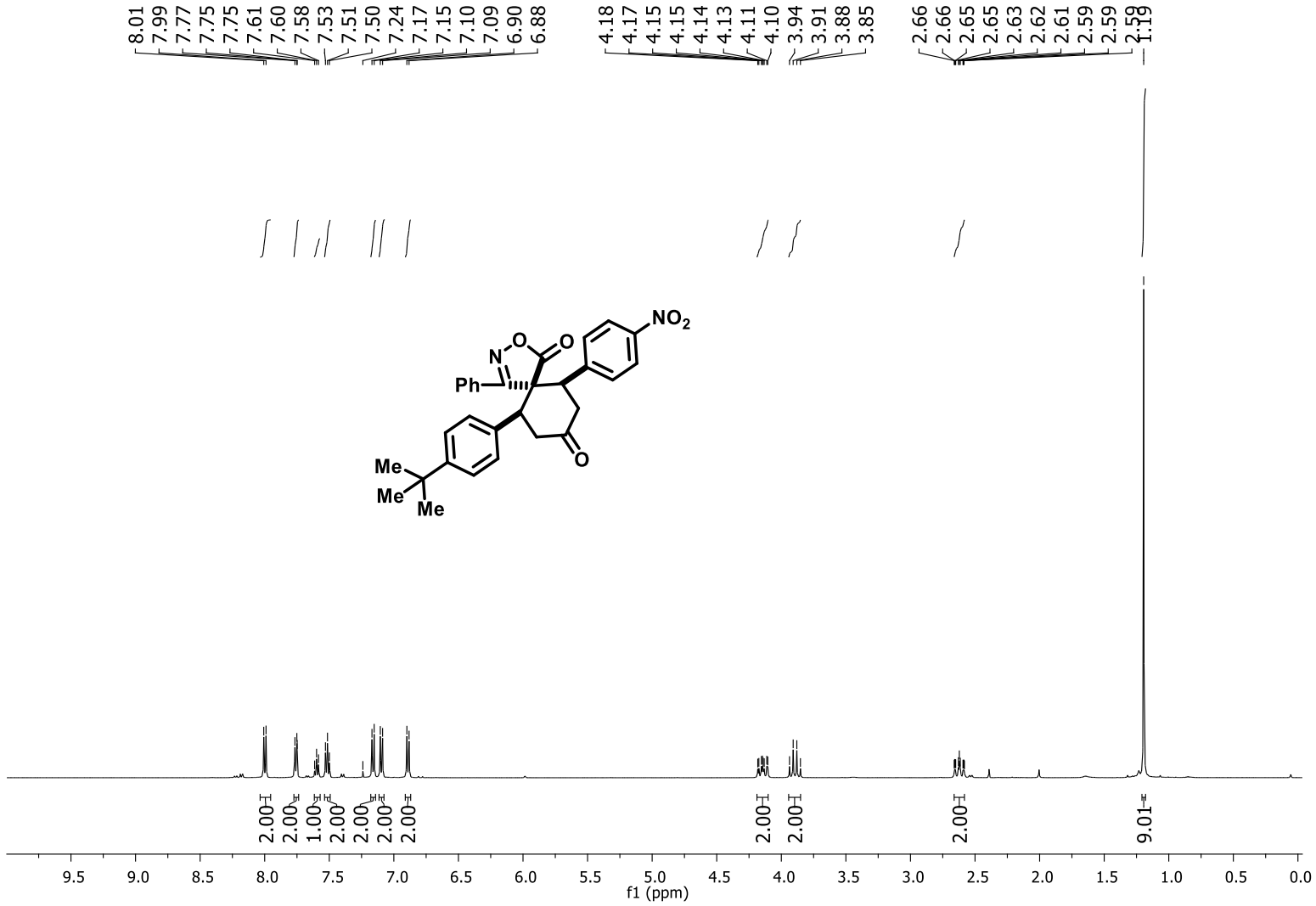


^{13}C (62.5 MHz, $CDCl_3$)

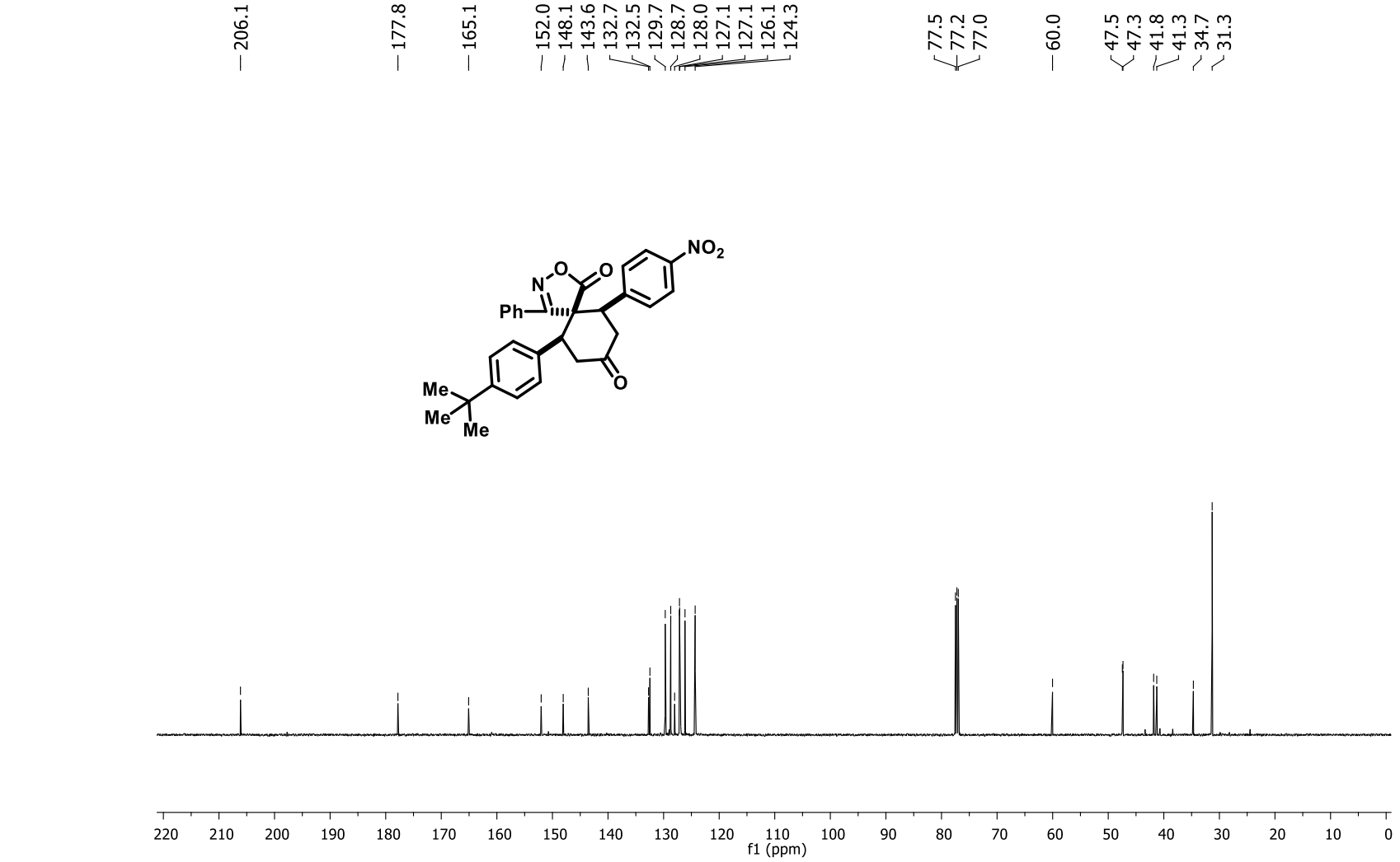


4.16. Molecule 1n

^{1}H (500 MHz, $CDCl_3$)

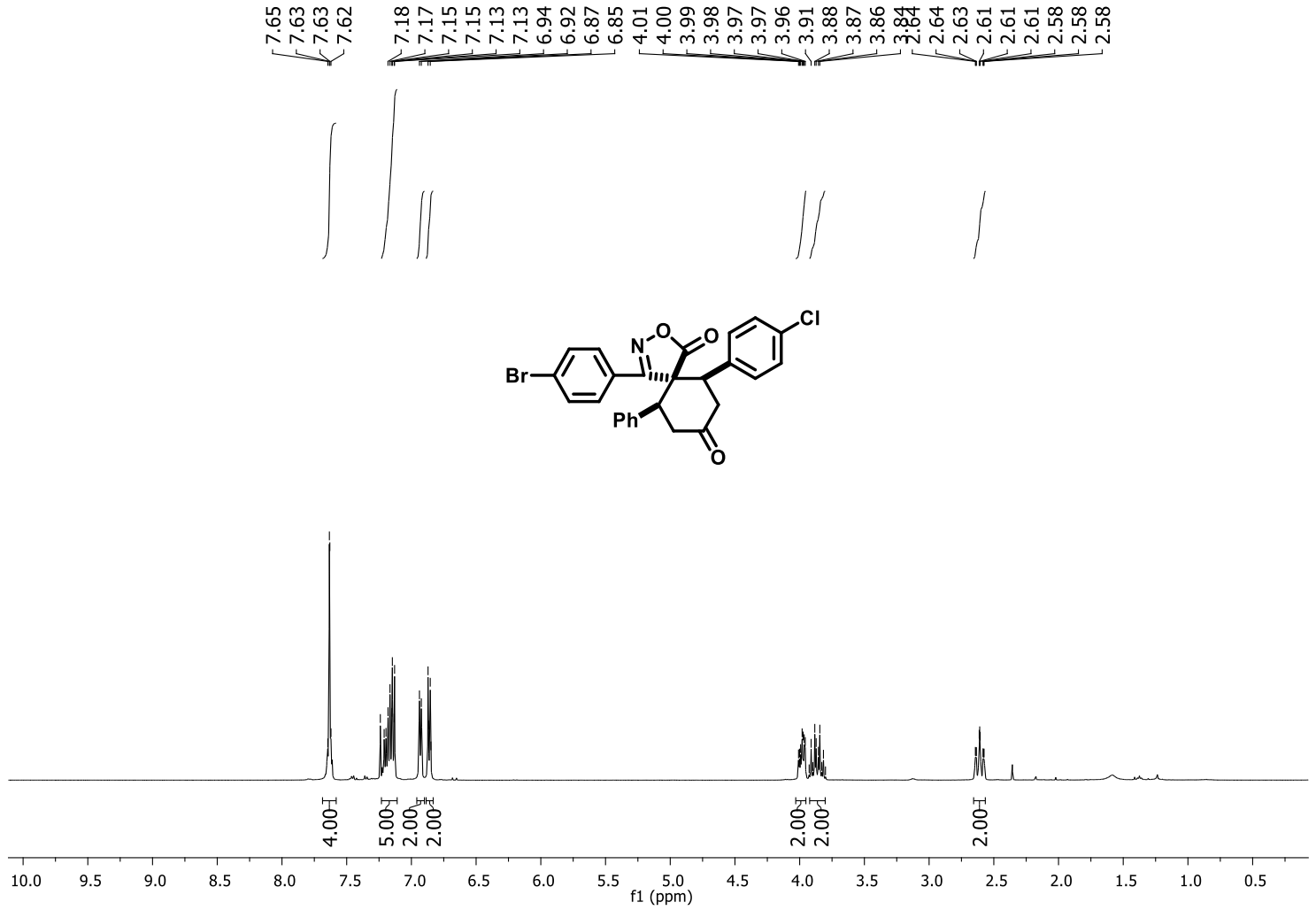


^{13}C (125 MHz, $CDCl_3$)

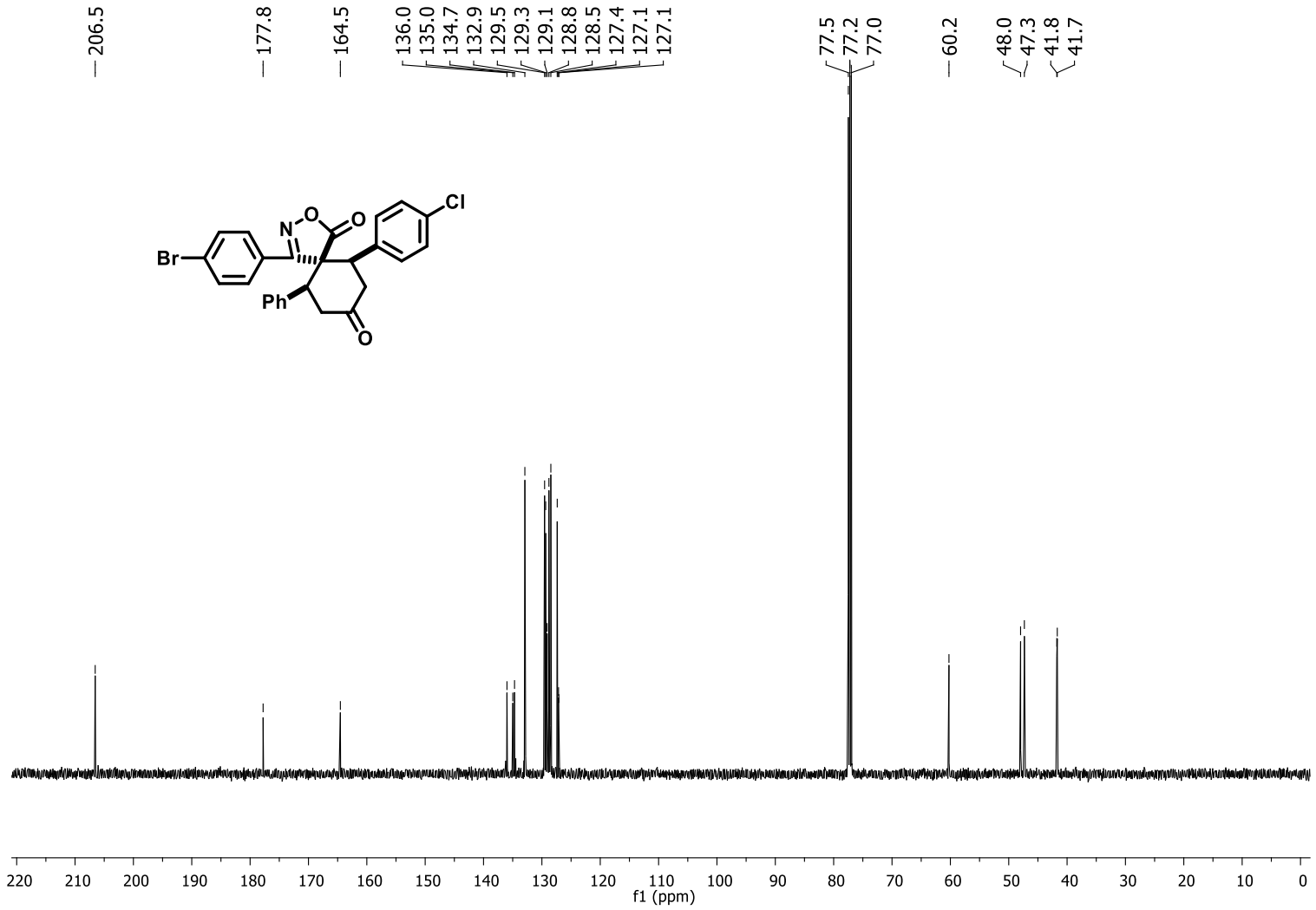


4.17. Molecule 1o

^{1}H (500 MHz, $CDCl_3$)

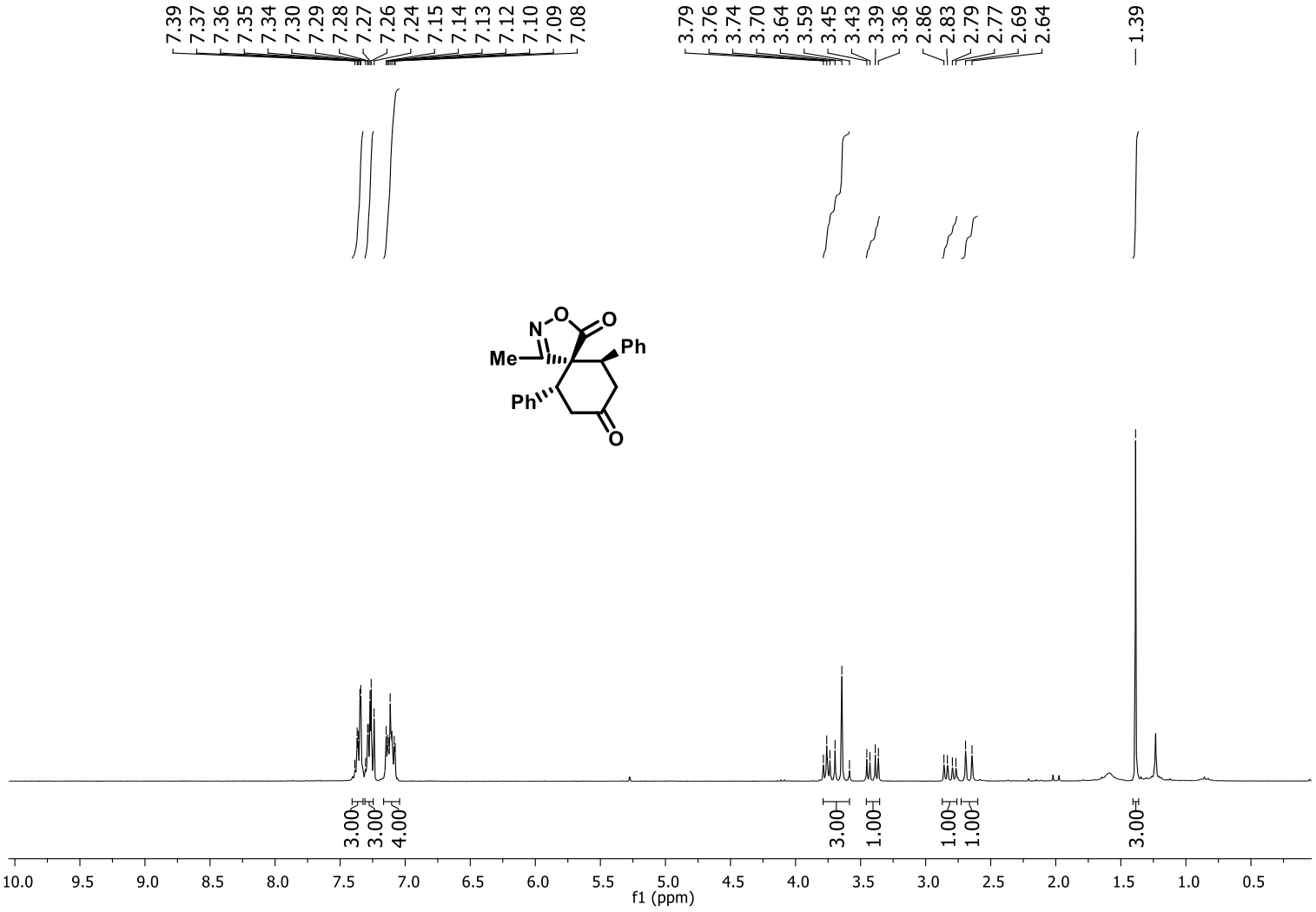


^{13}C (125 MHz, $CDCl_3$)

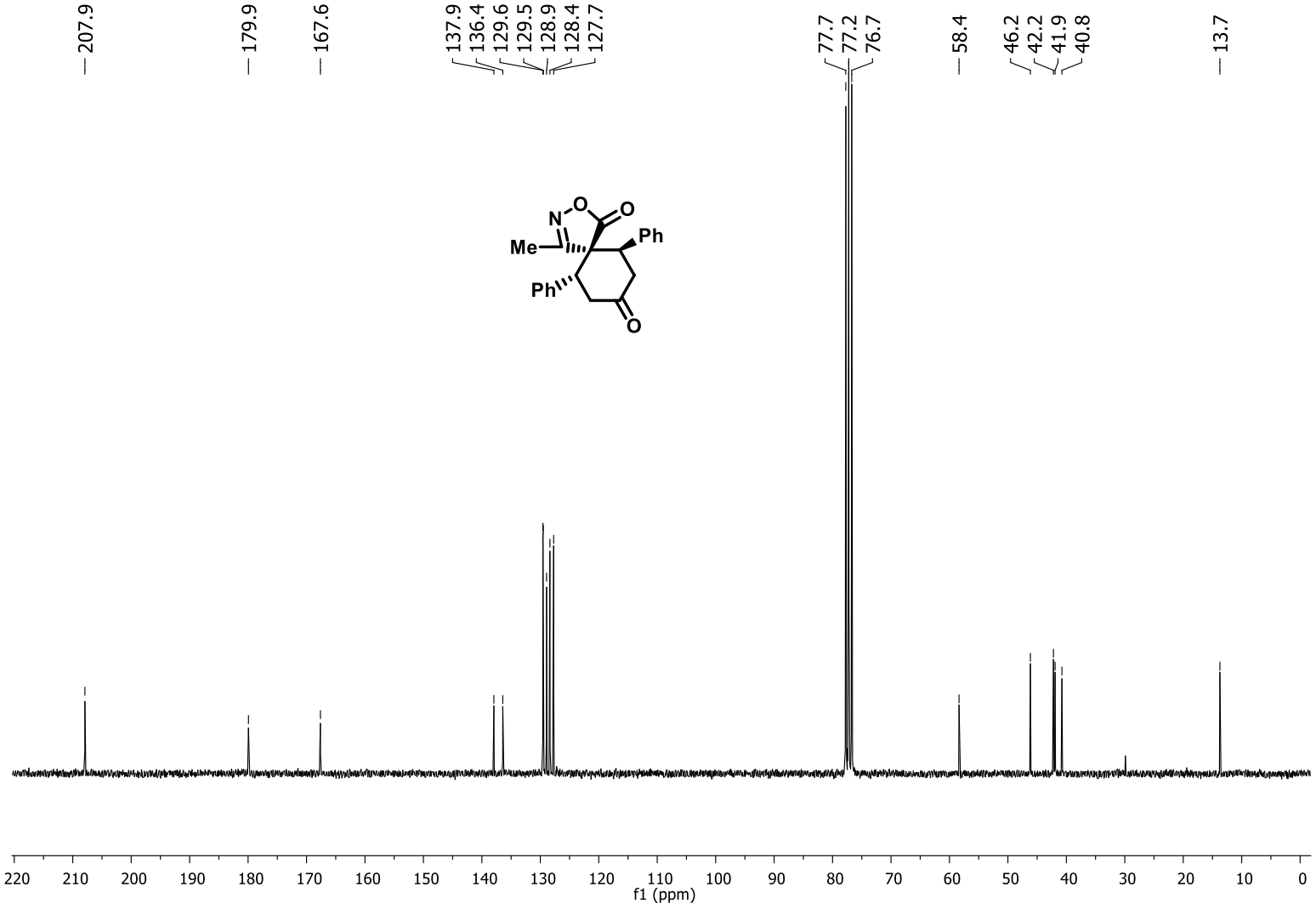


4.18. Molecule 1q

^{1}H (250 MHz, $CDCl_3$)

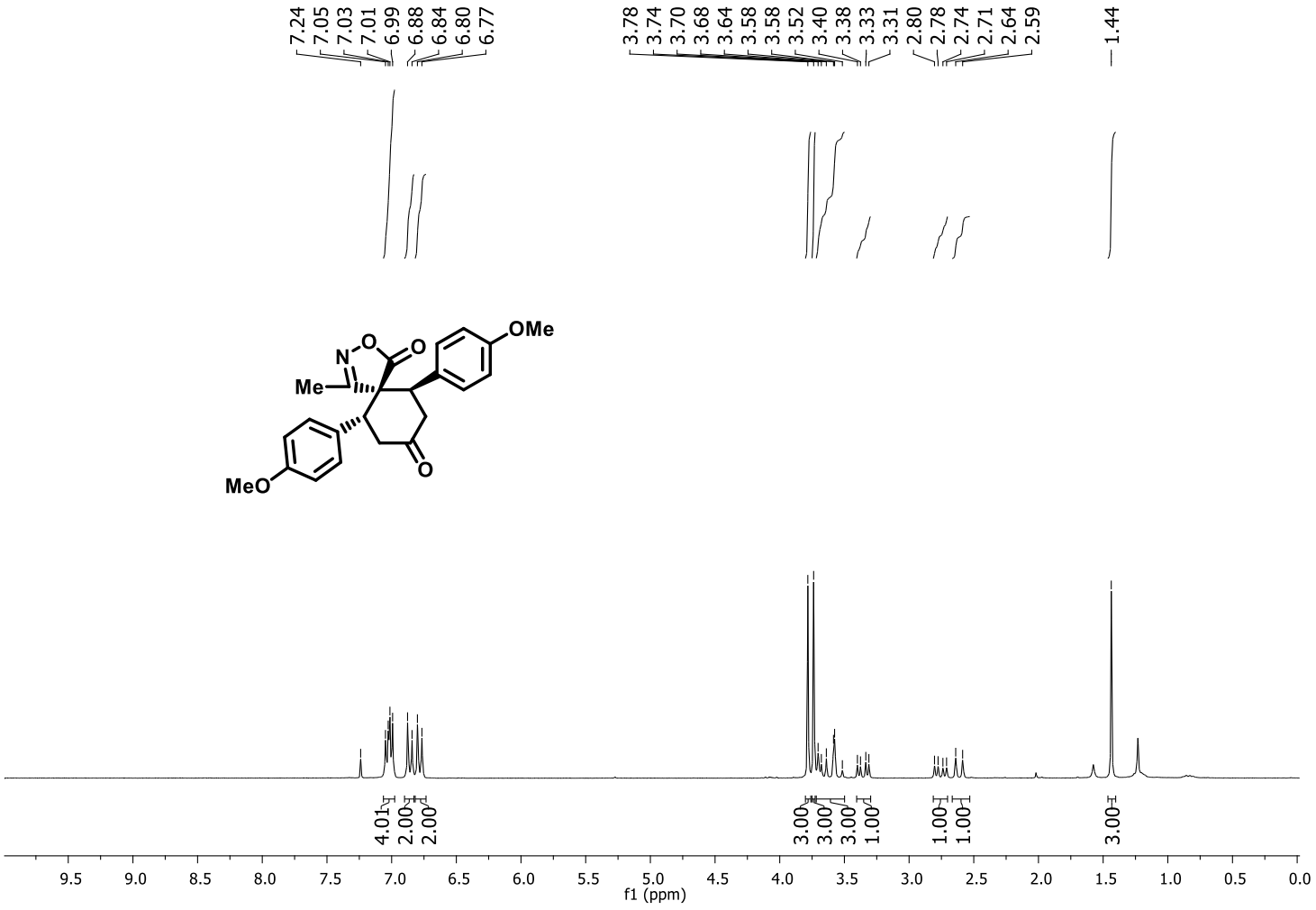


^{13}C (62.5 MHz, $CDCl_3$)

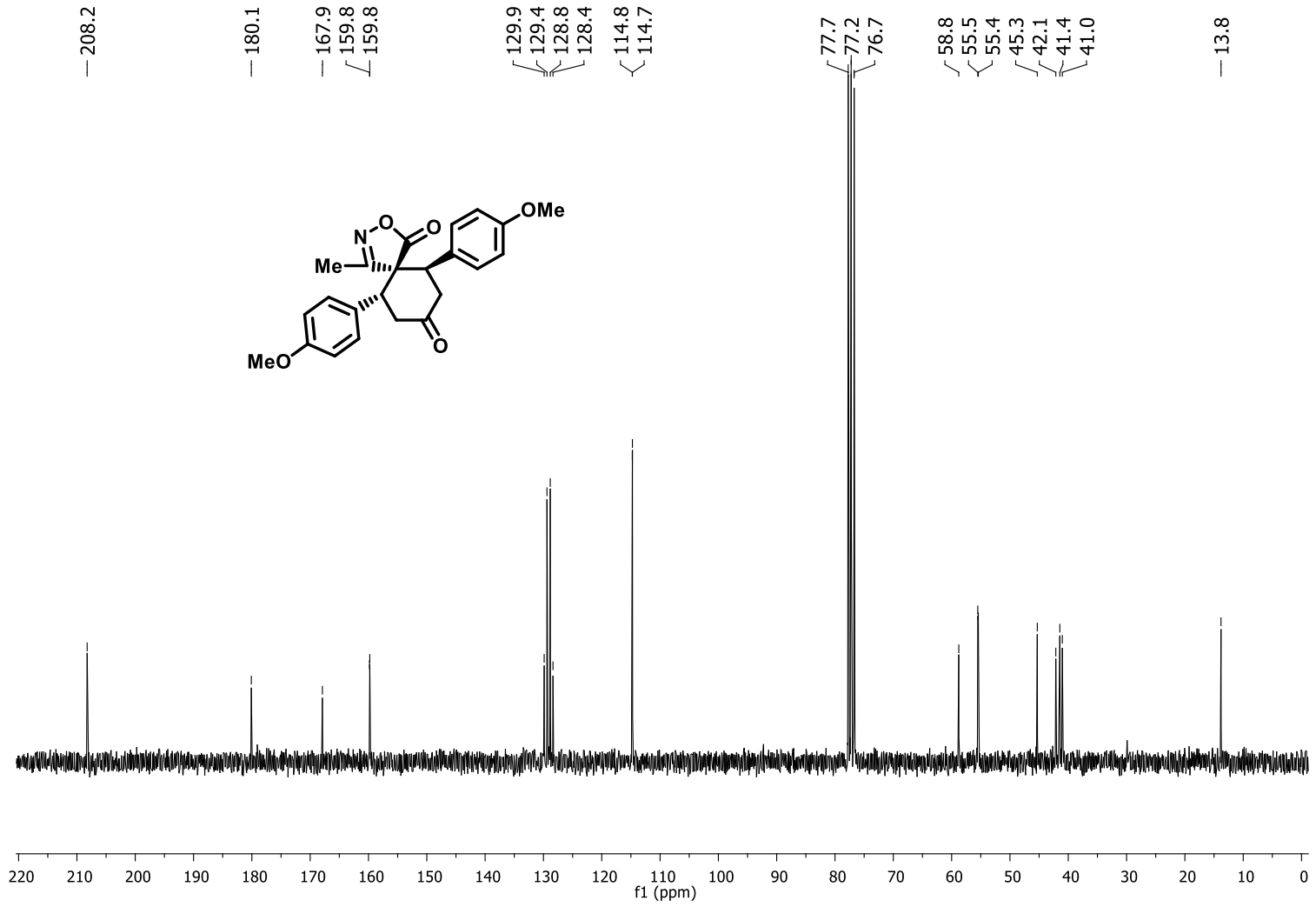


4.19. Molecule 1r

^{1}H (250 MHz, $CDCl_3$)

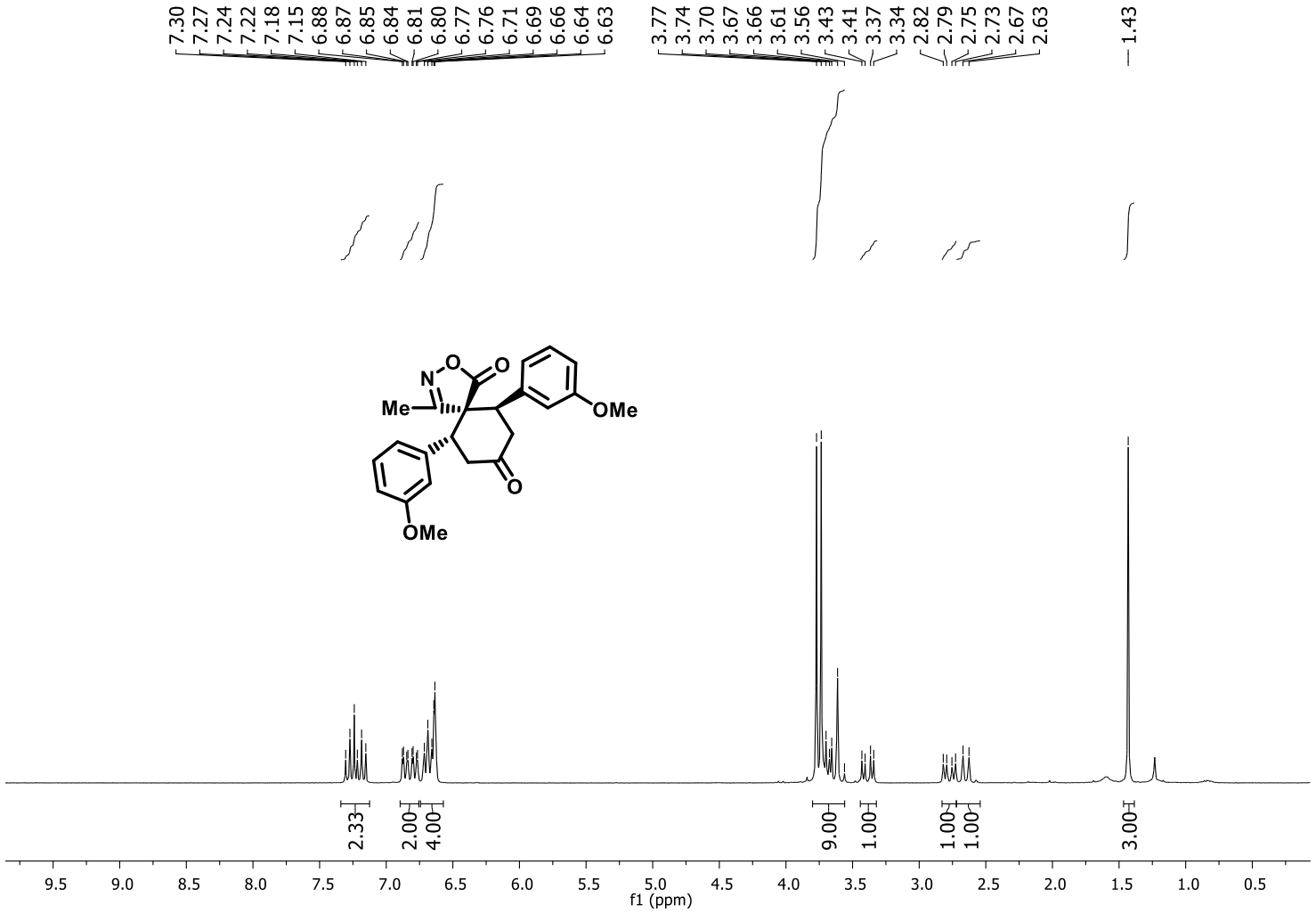


^{13}C (62.5 MHz, $CDCl_3$)

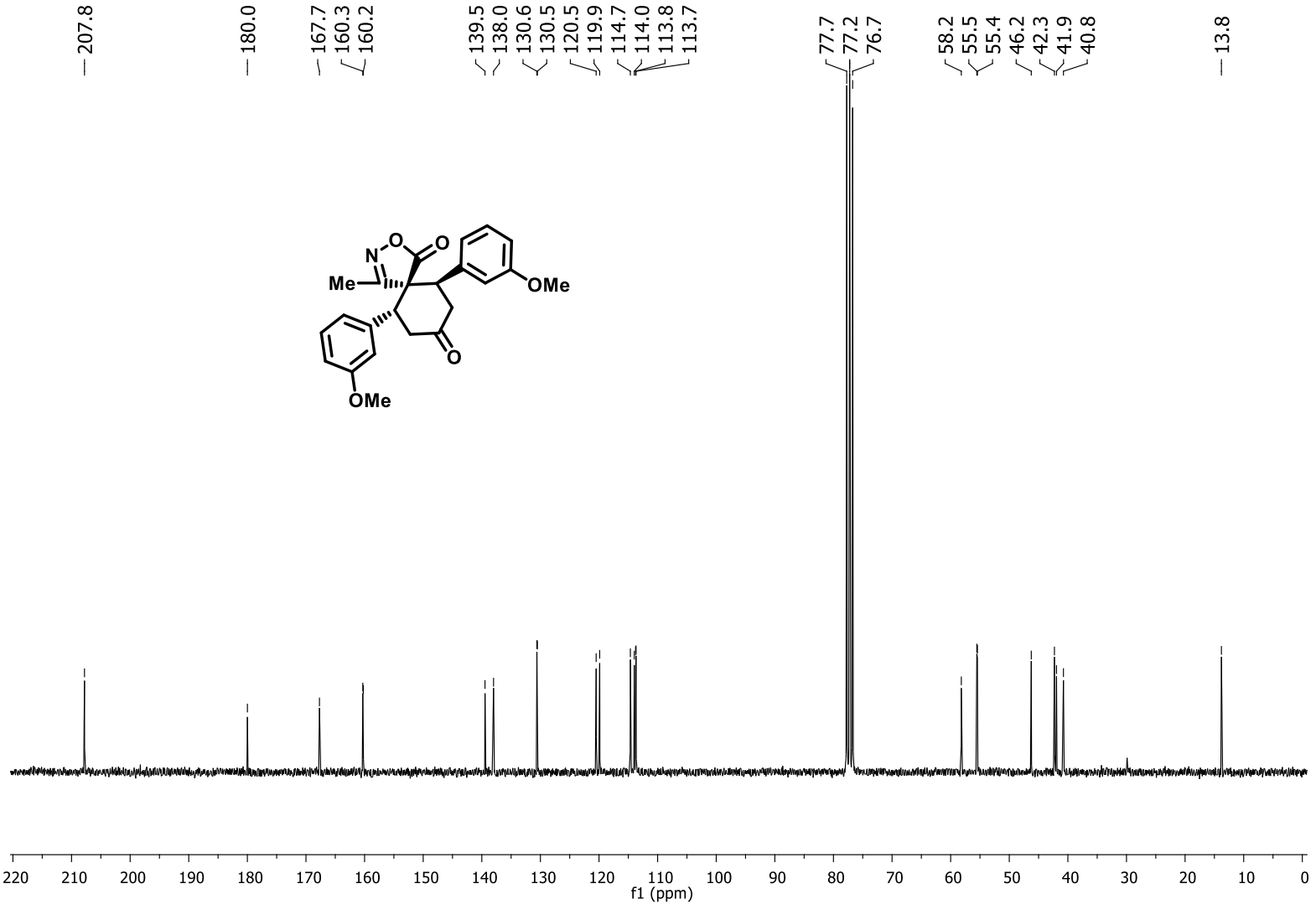


4.20. Molecule 1s

^{1}H (250 MHz, $CDCl_3$)

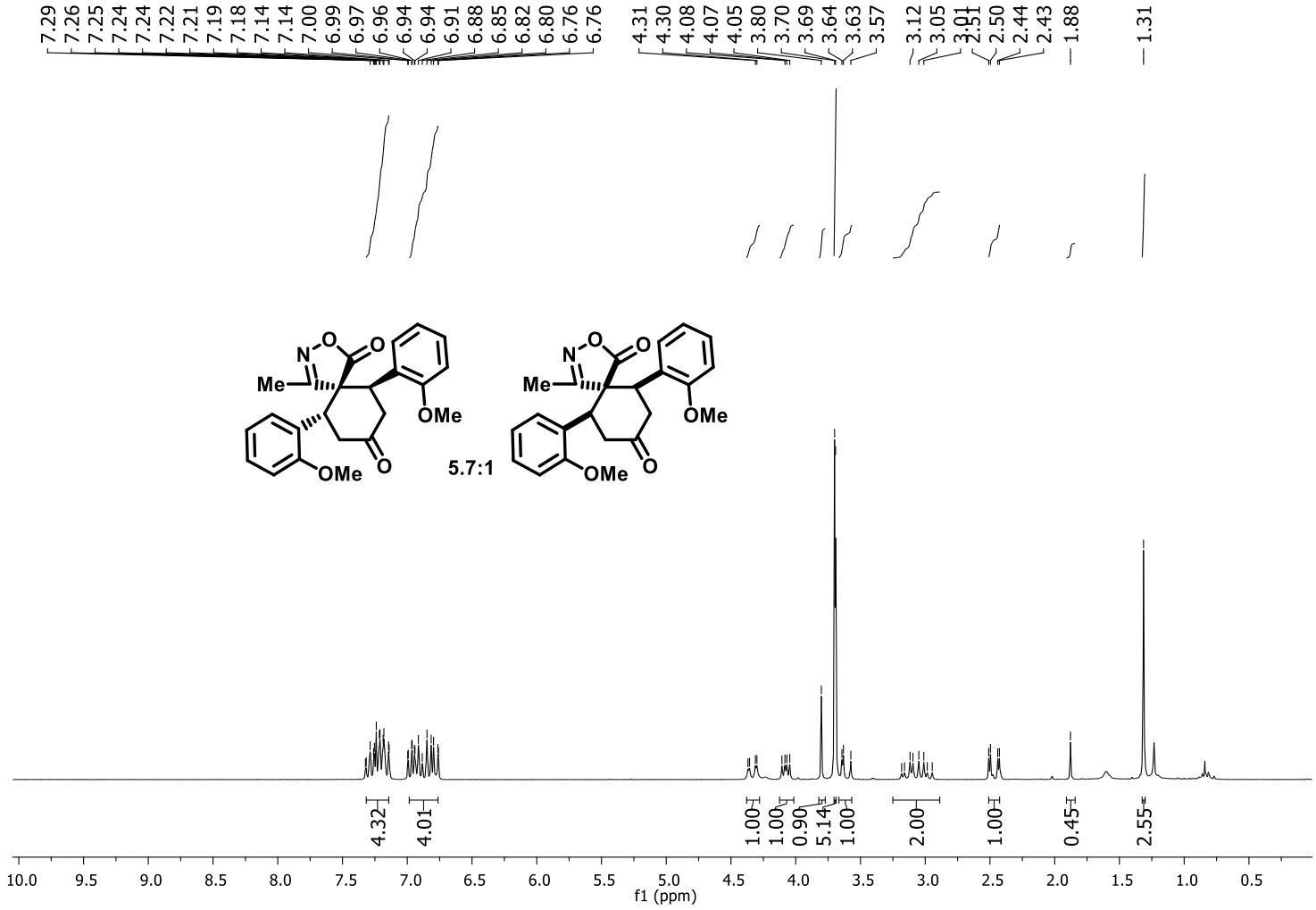


^{13}C (62.5 MHz, $CDCl_3$)

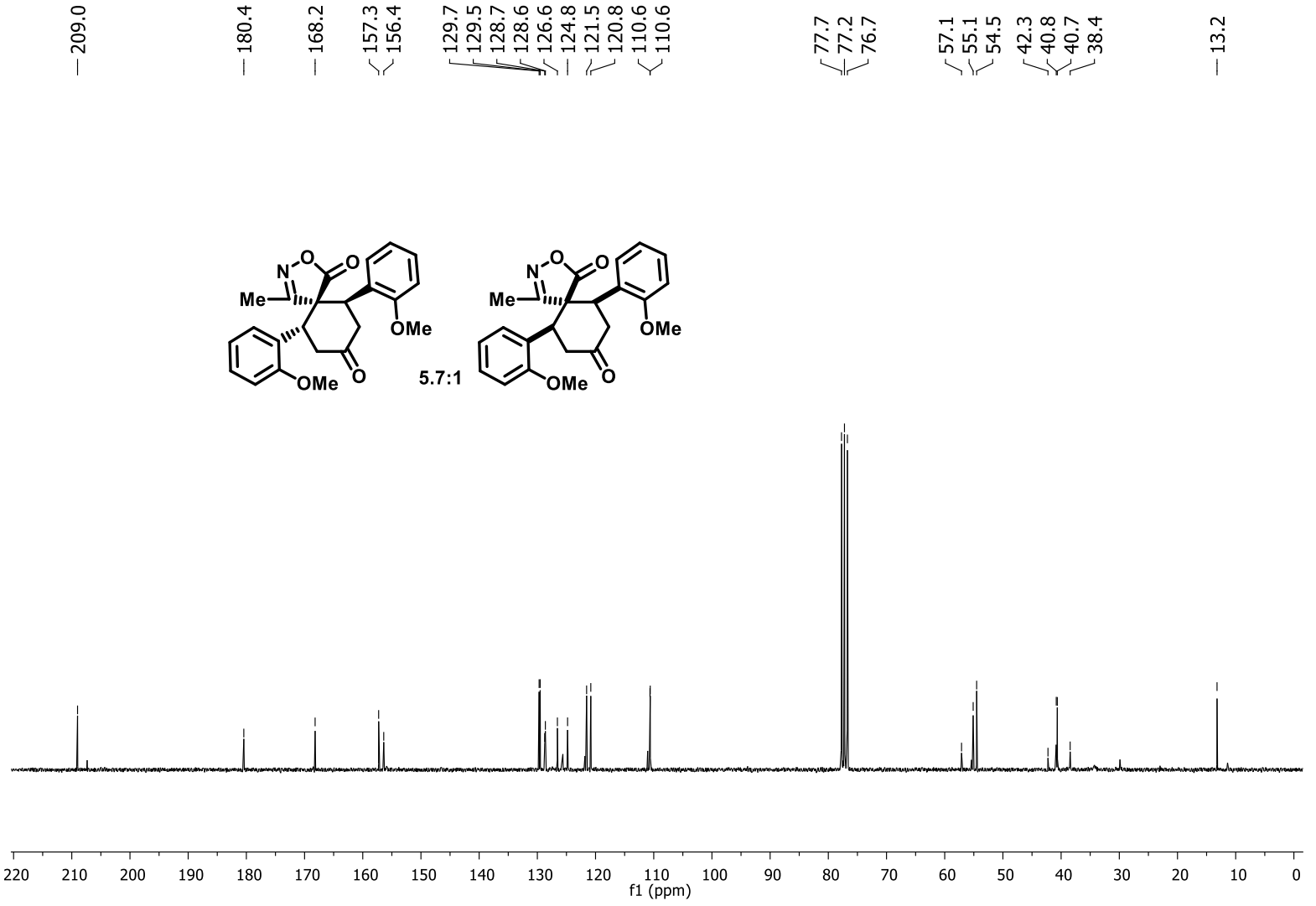


4.21. Molecule 1t

^{1}H (250 MHz, $CDCl_3$)

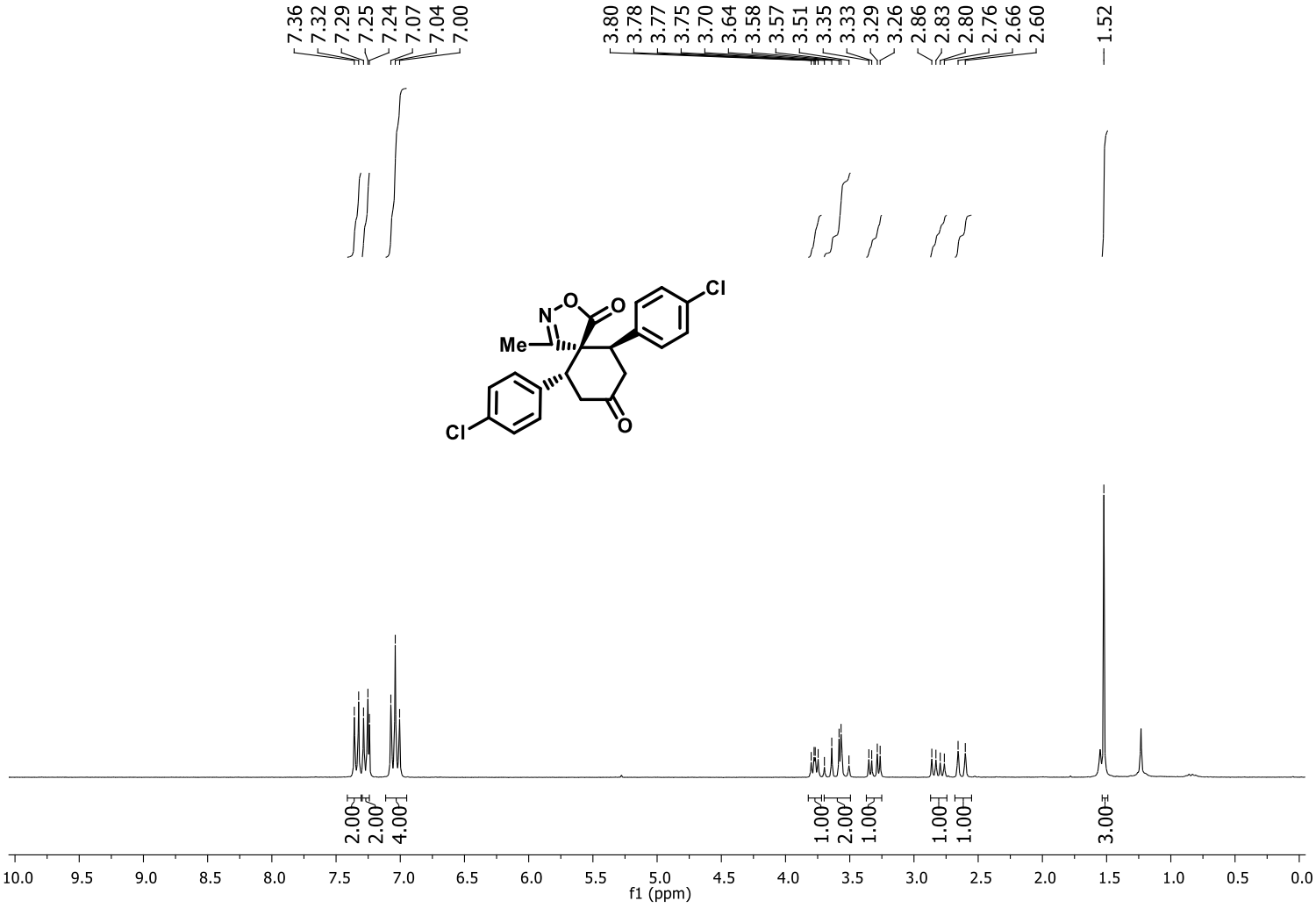


^{13}C (62.5 MHz, $CDCl_3$)

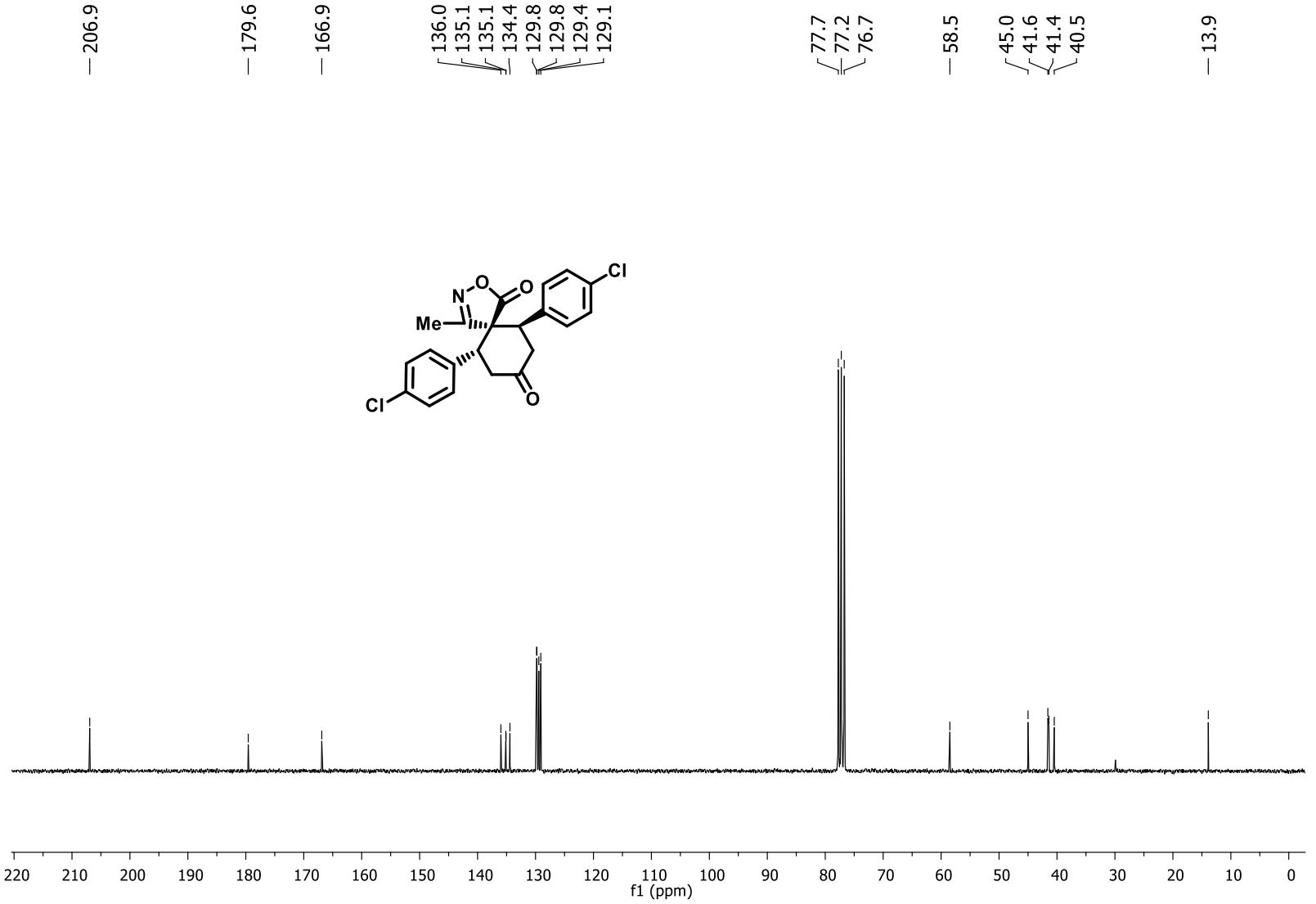


4.22. Molecule 1u

^{1}H (250 MHz, $CDCl_3$)

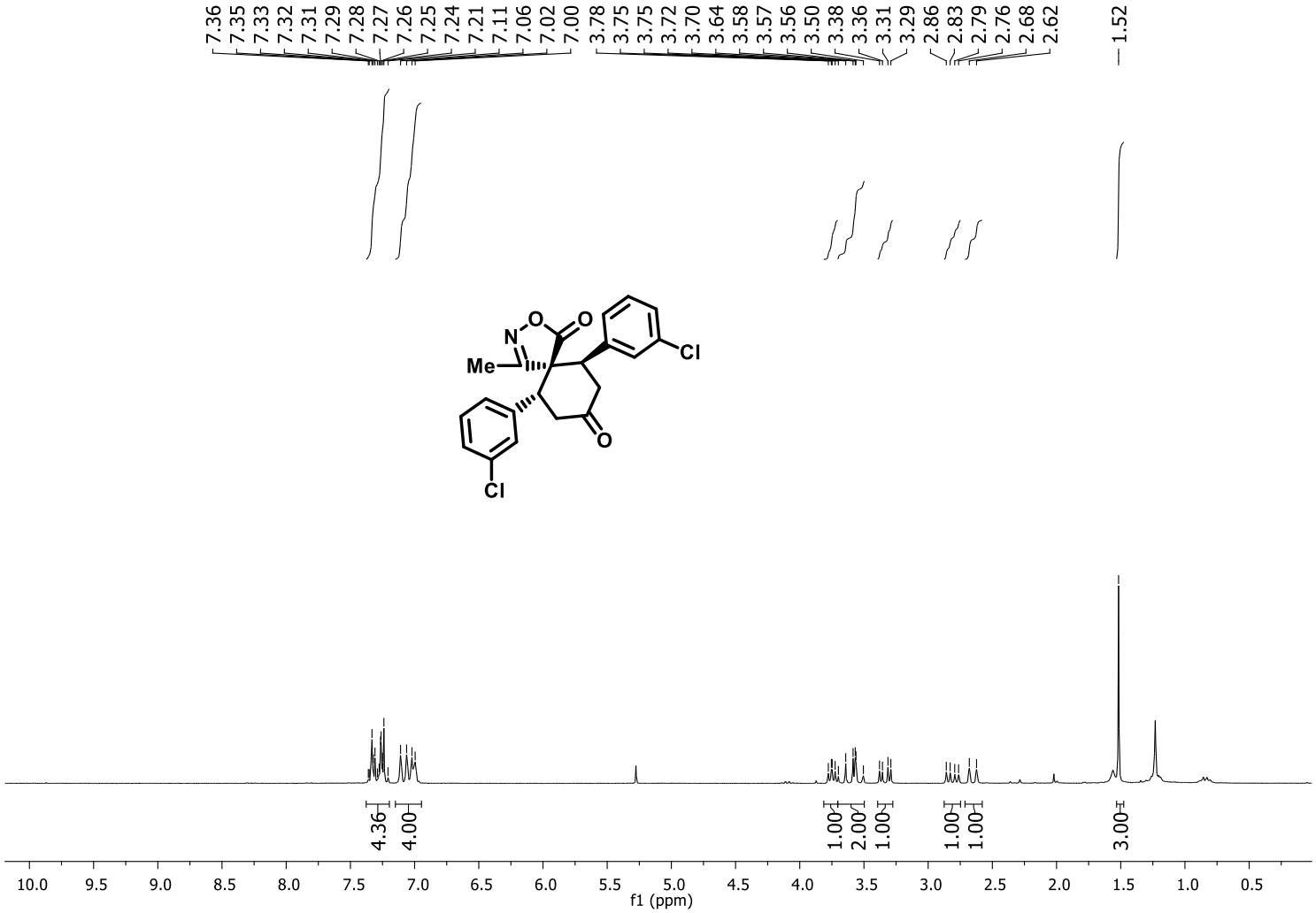


^{13}C (62.5 MHz, $CDCl_3$)

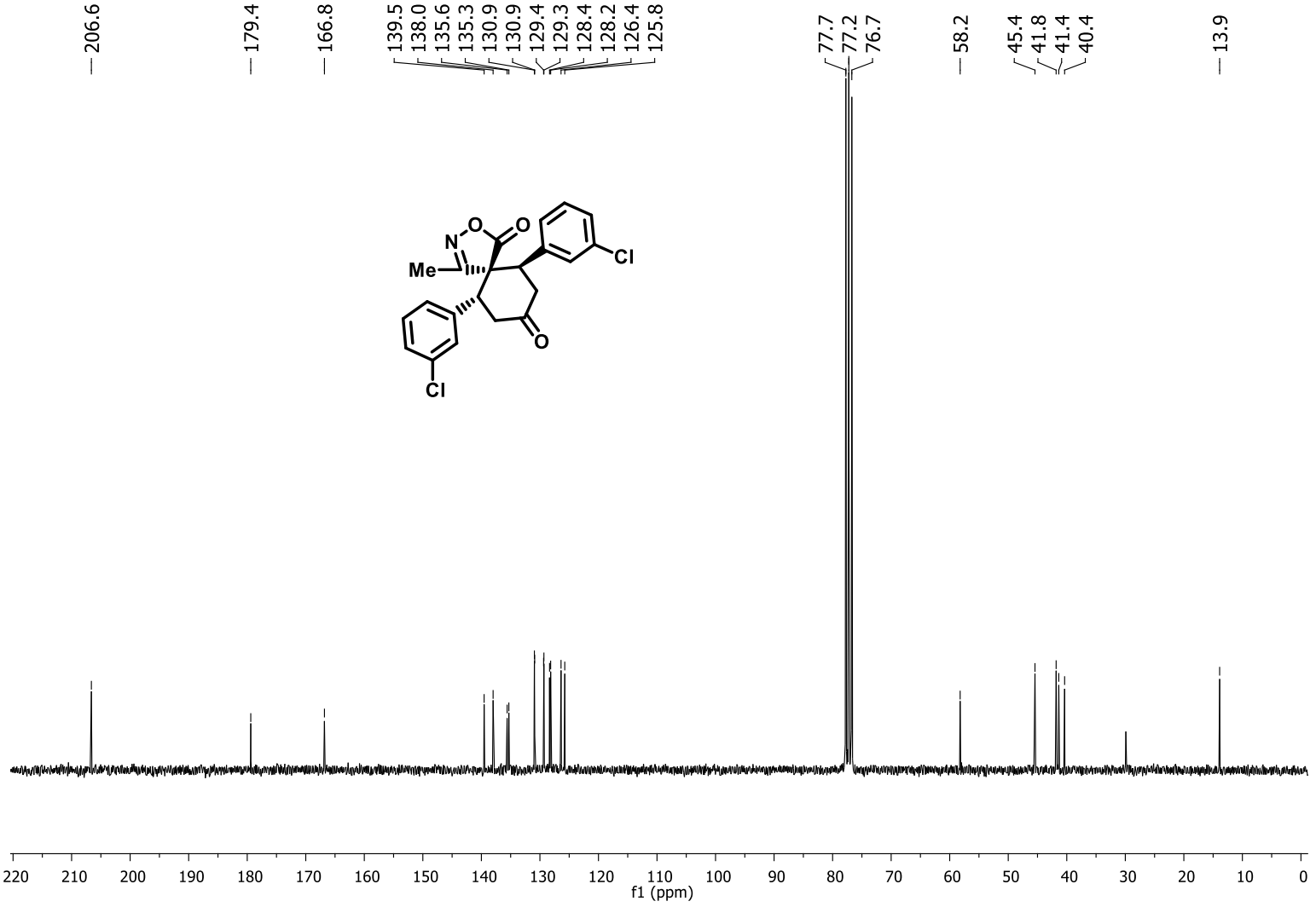


4.23. Molecule 1v

^{1}H (250 MHz, $CDCl_3$)

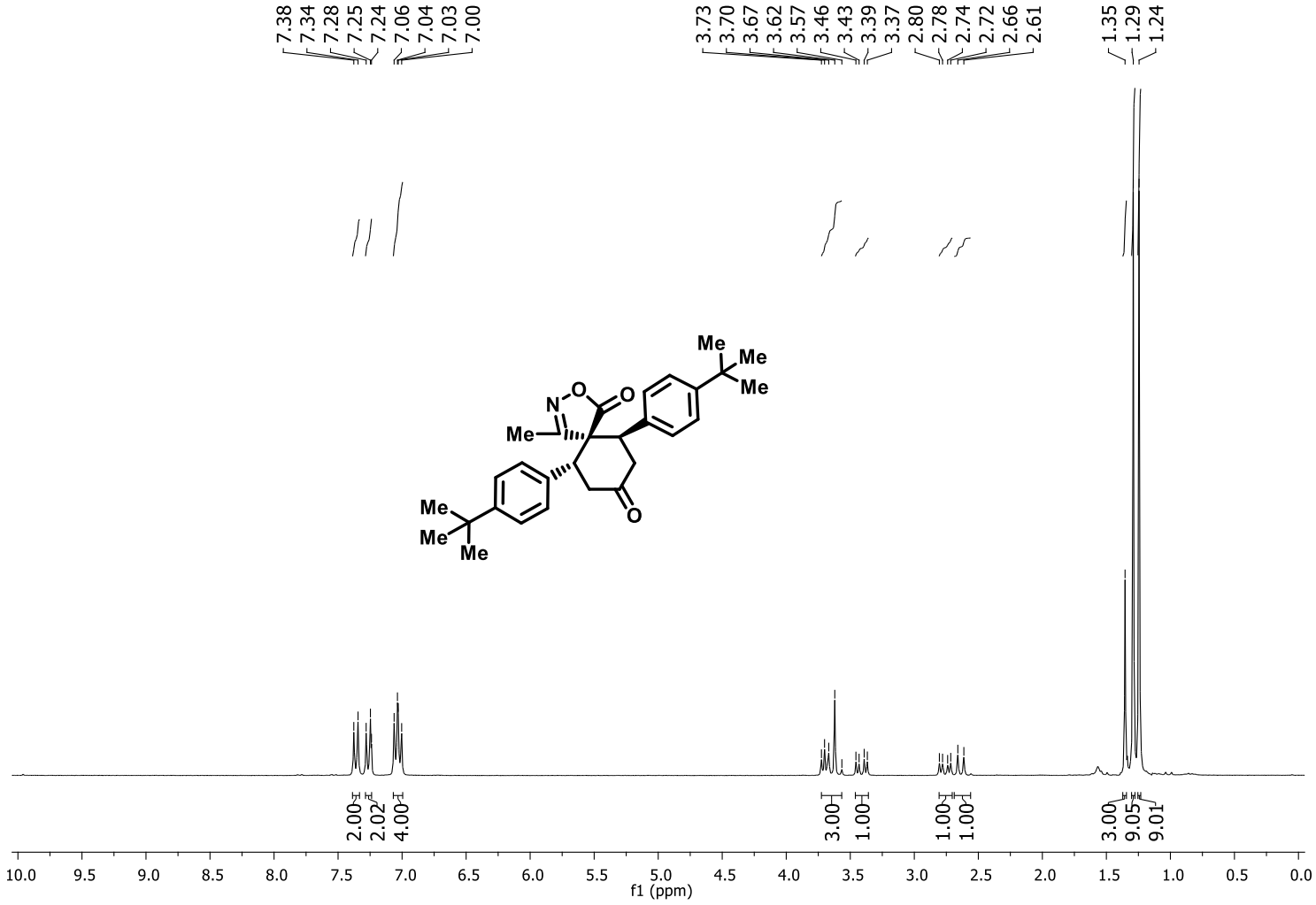


^{13}C (62.5 MHz, $CDCl_3$)

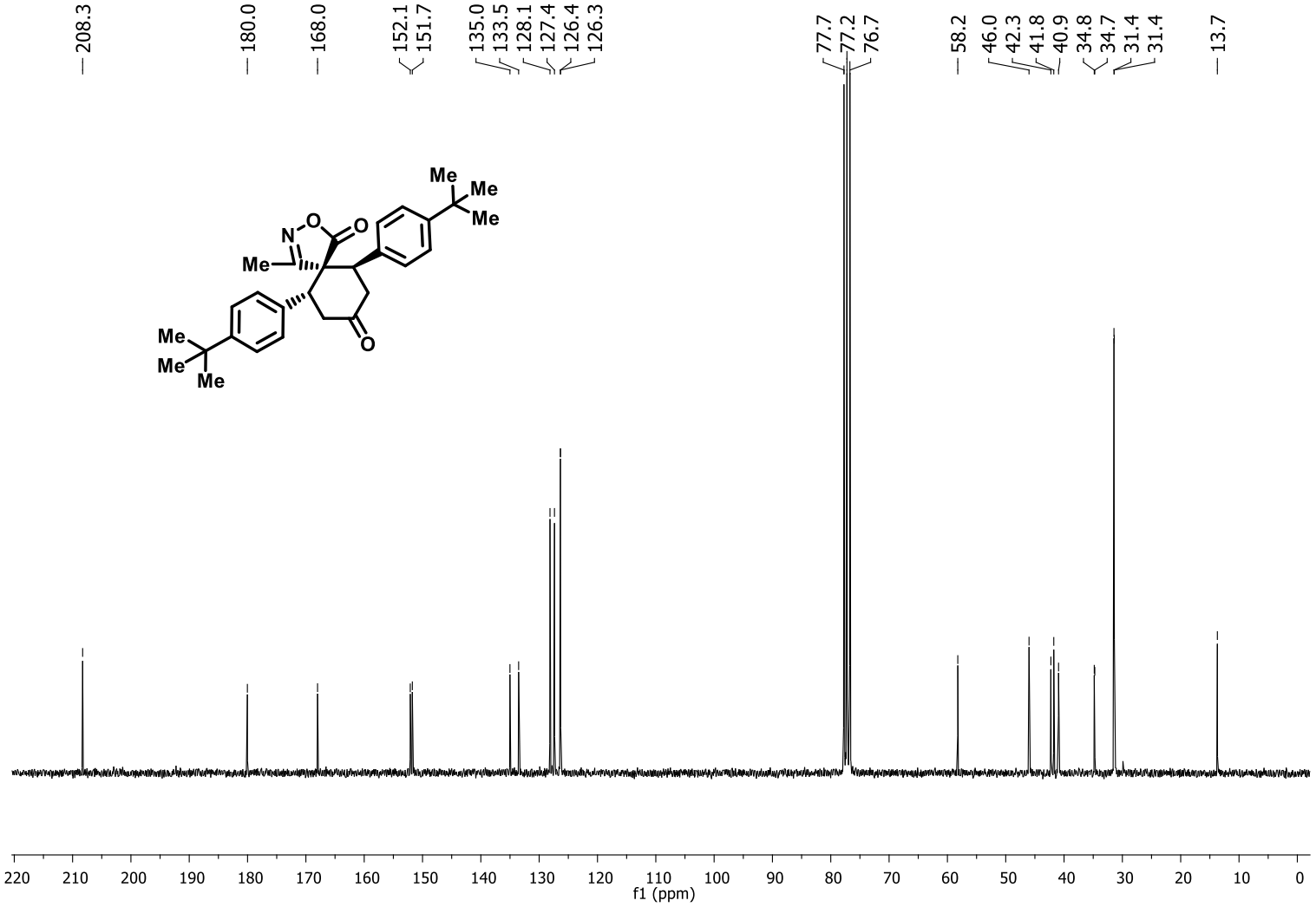


4.24. Molecule 6,10-*trans*-1w

^{1}H (250 MHz, $CDCl_3$)

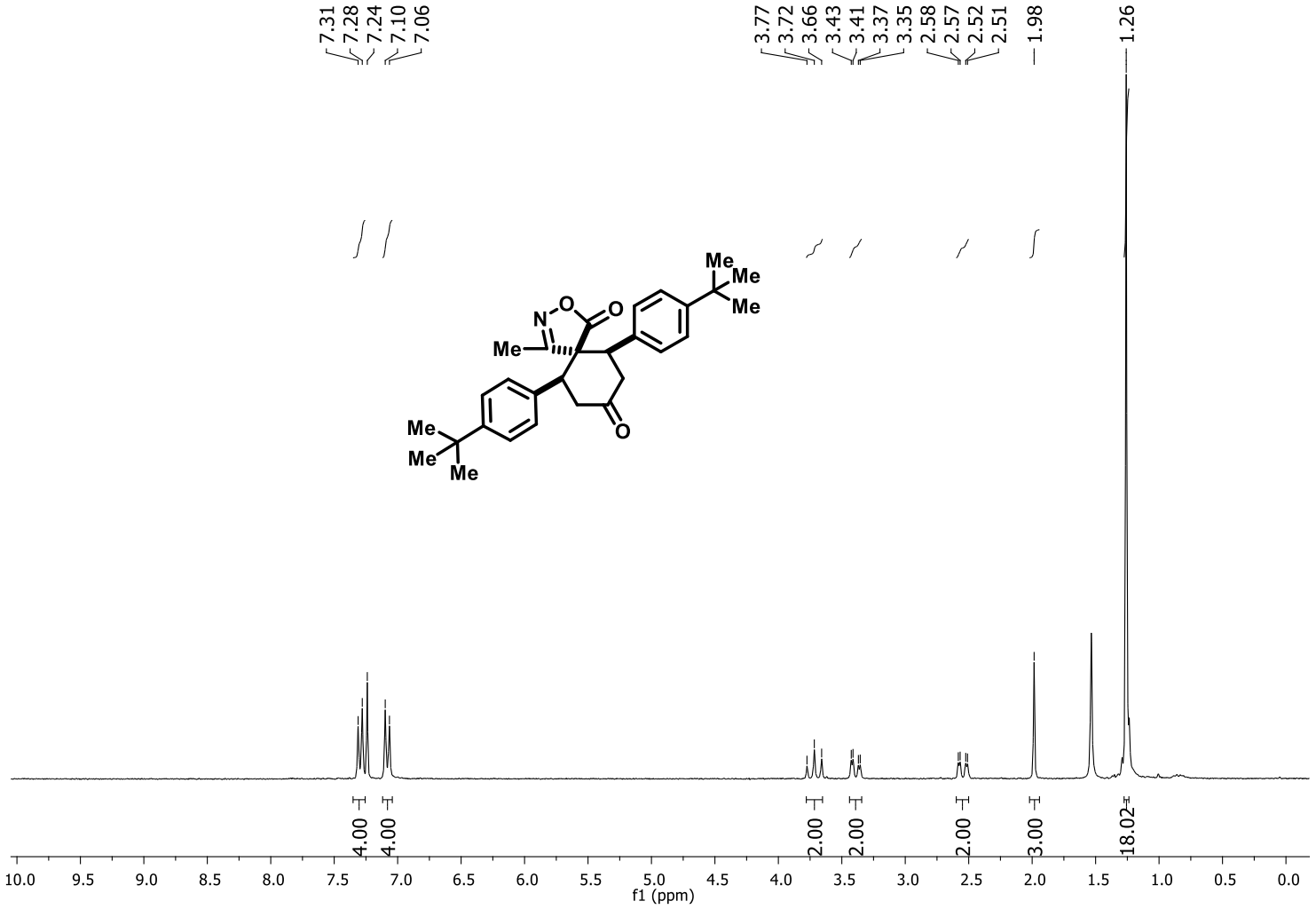


^{13}C (62.5 MHz, $CDCl_3$)

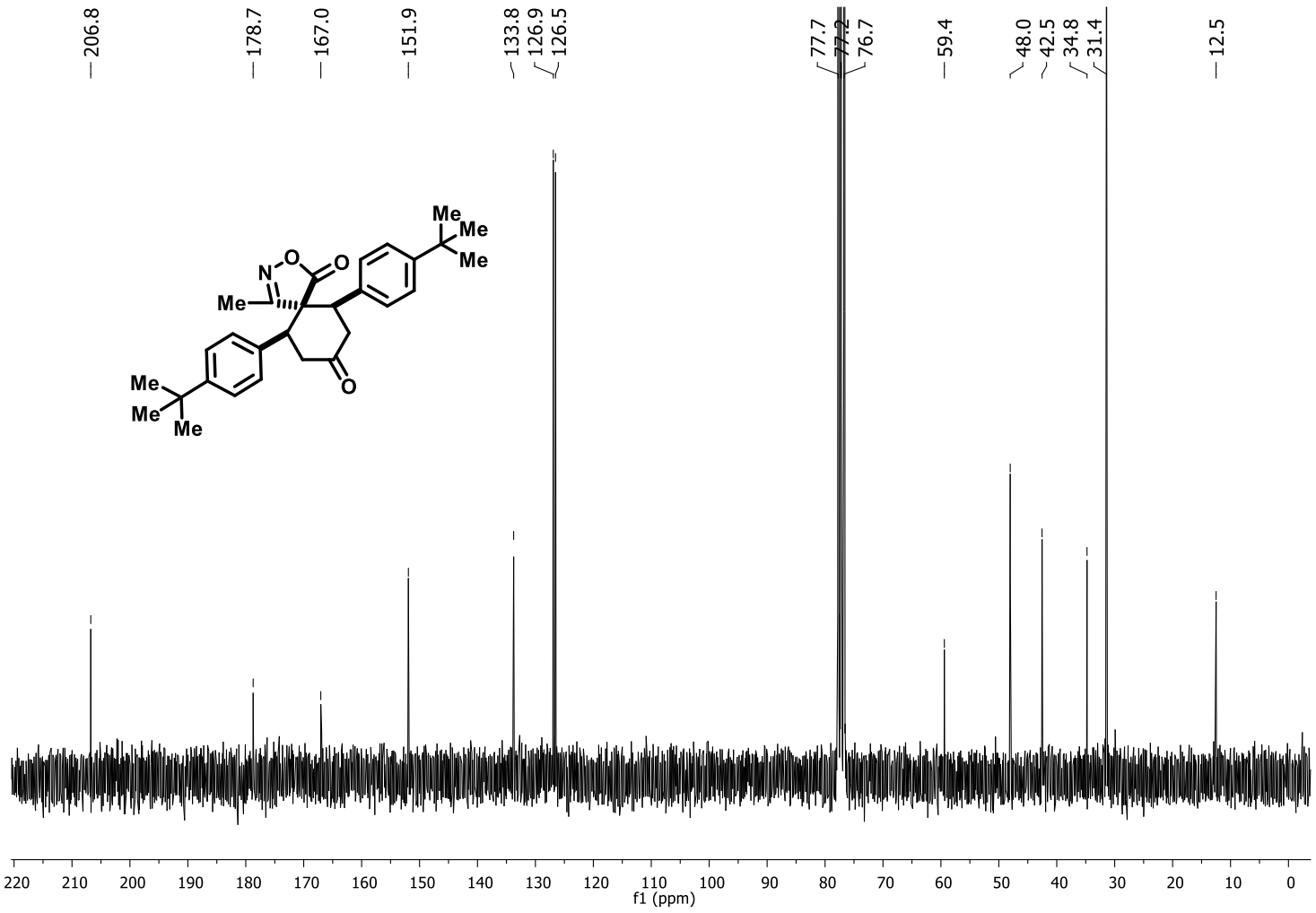


4.25. Molecule 6,10-*cis*-1w

^{1}H (250 MHz, $CDCl_3$)

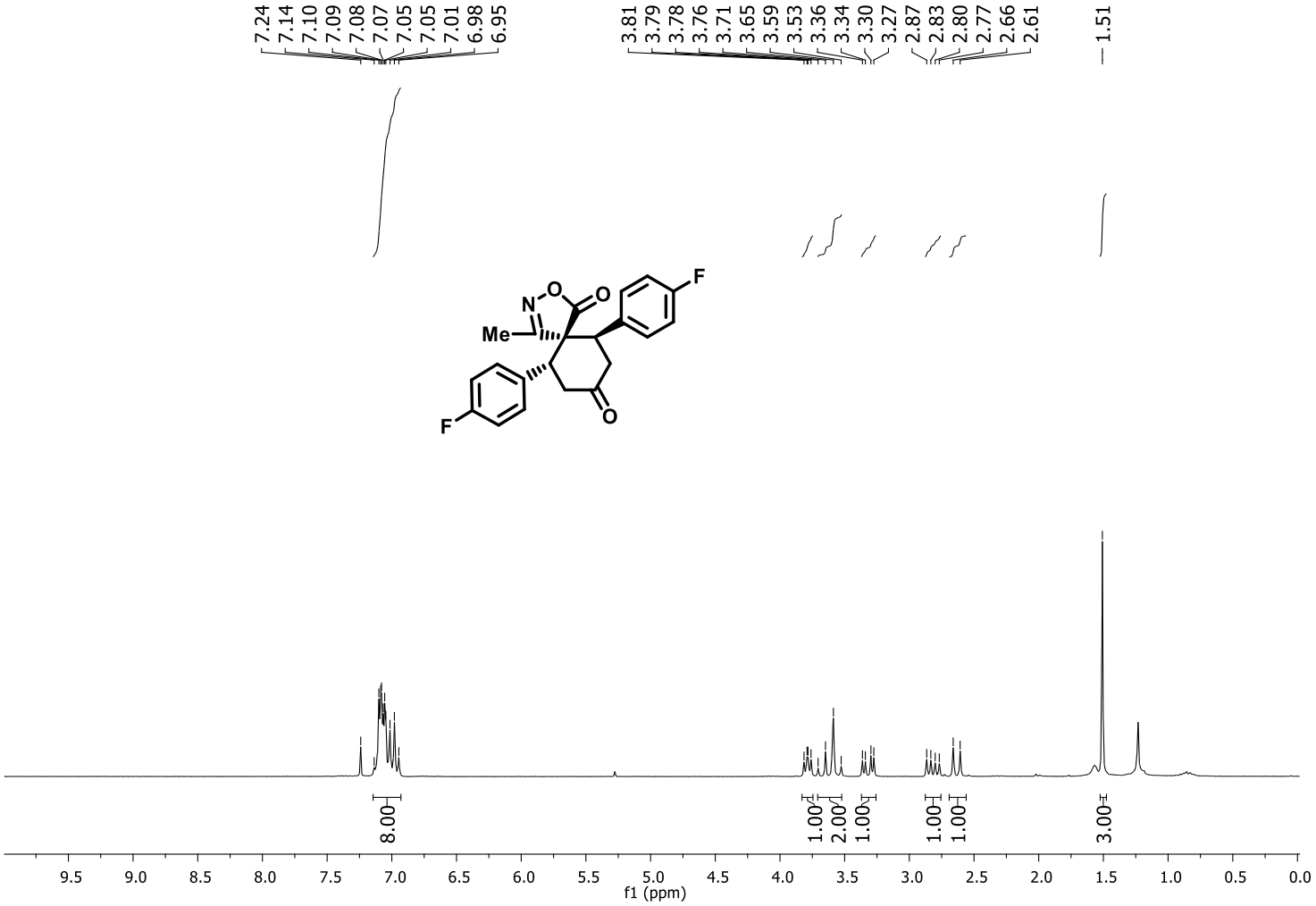


^{13}C (62.5 MHz, $CDCl_3$)

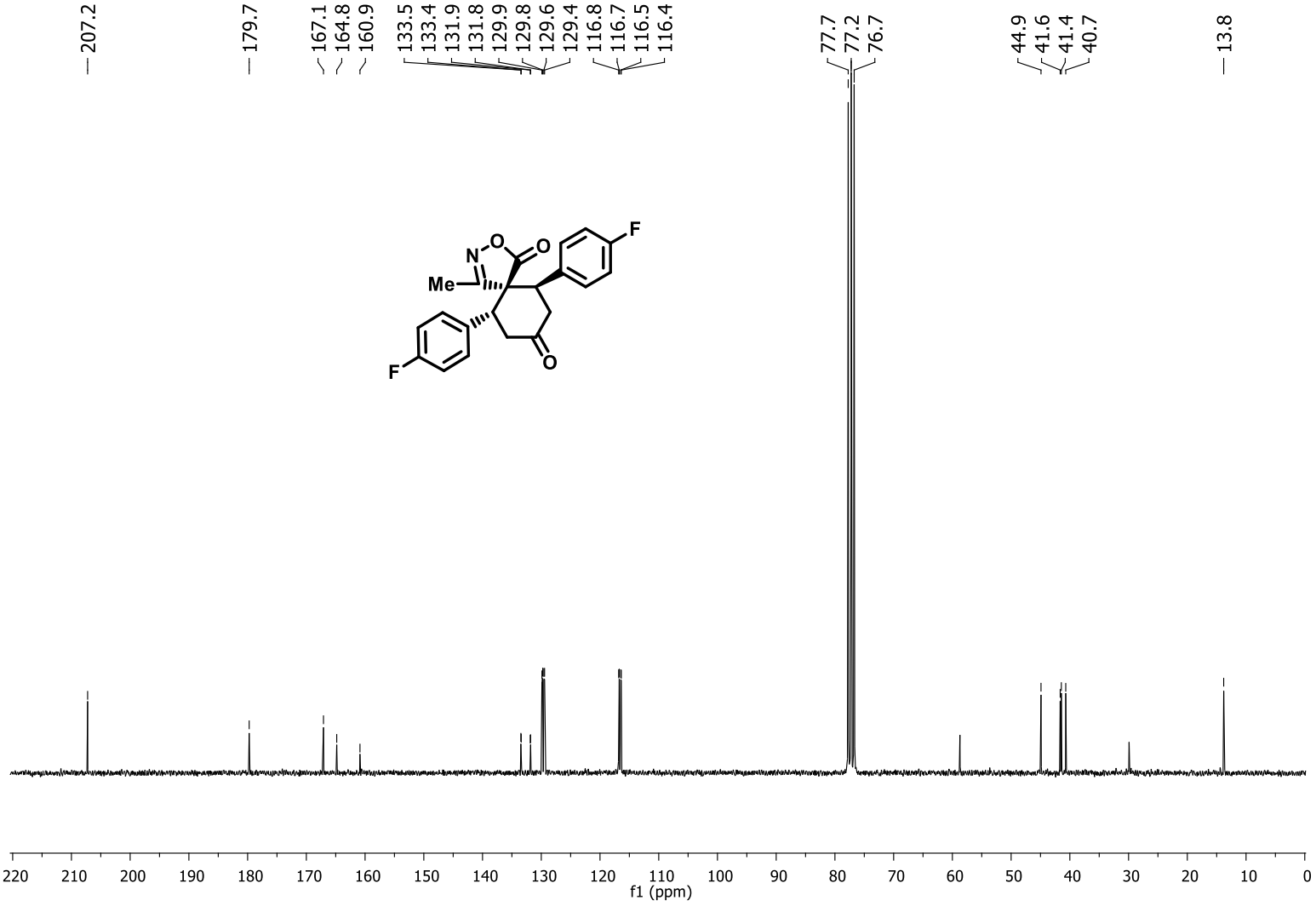


4.26. Molecule 1x

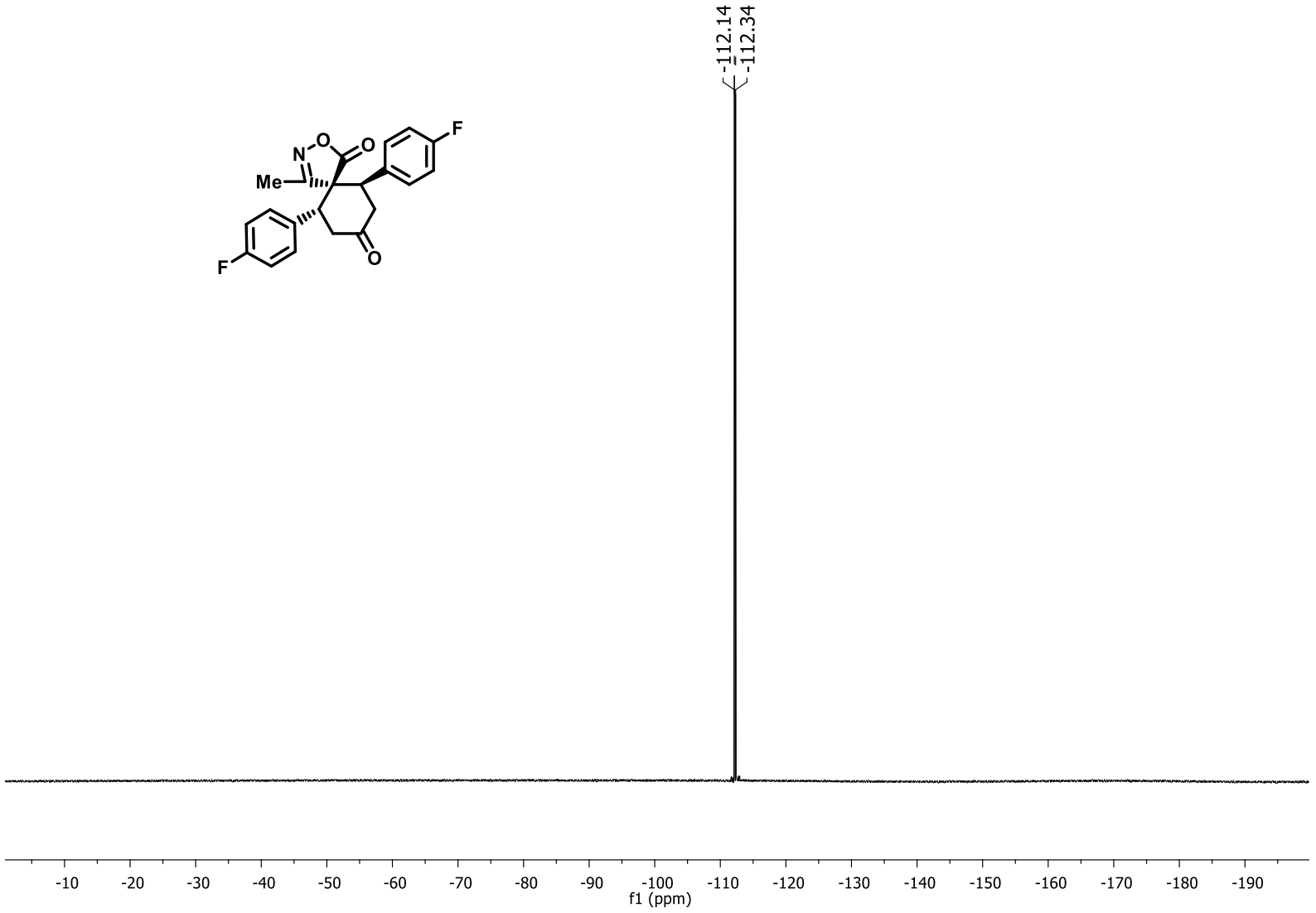
^{1}H (250 MHz, $CDCl_3$)



^{13}C (62.5 MHz, $CDCl_3$)

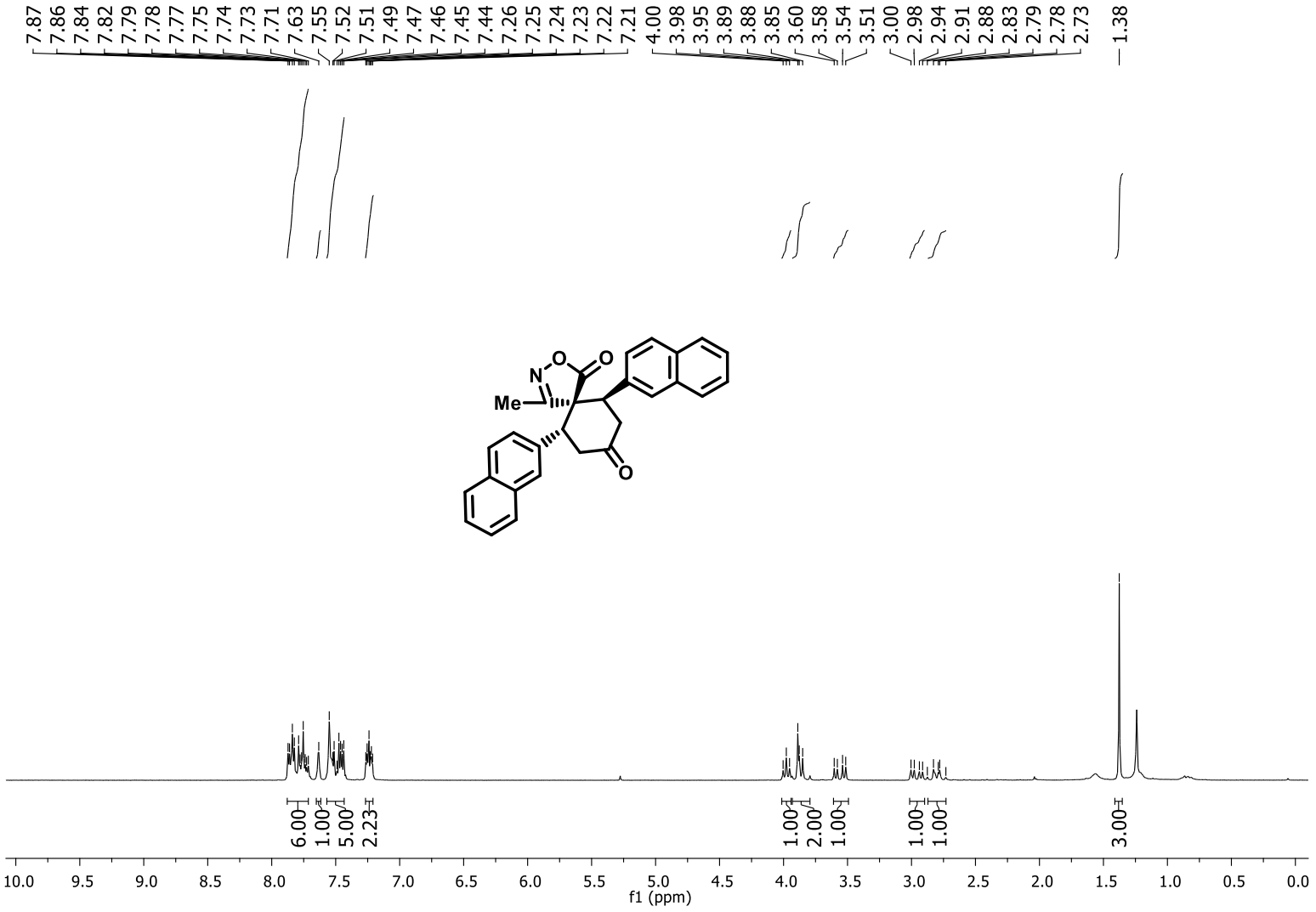


^{19}F (235 MHz, $CDCl_3$)

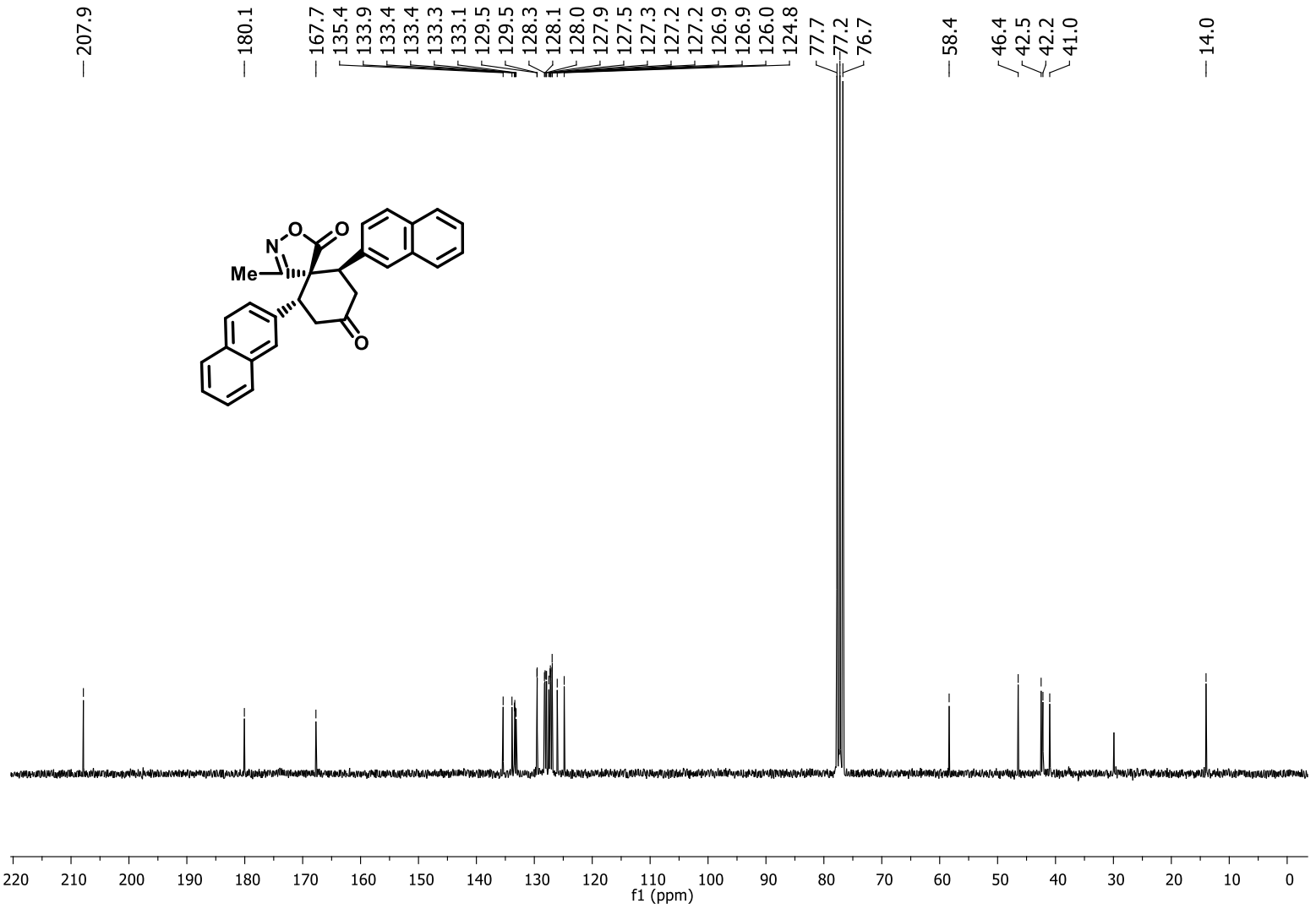


4.27. Molecule 1y

^{1}H (250 MHz, $CDCl_3$)

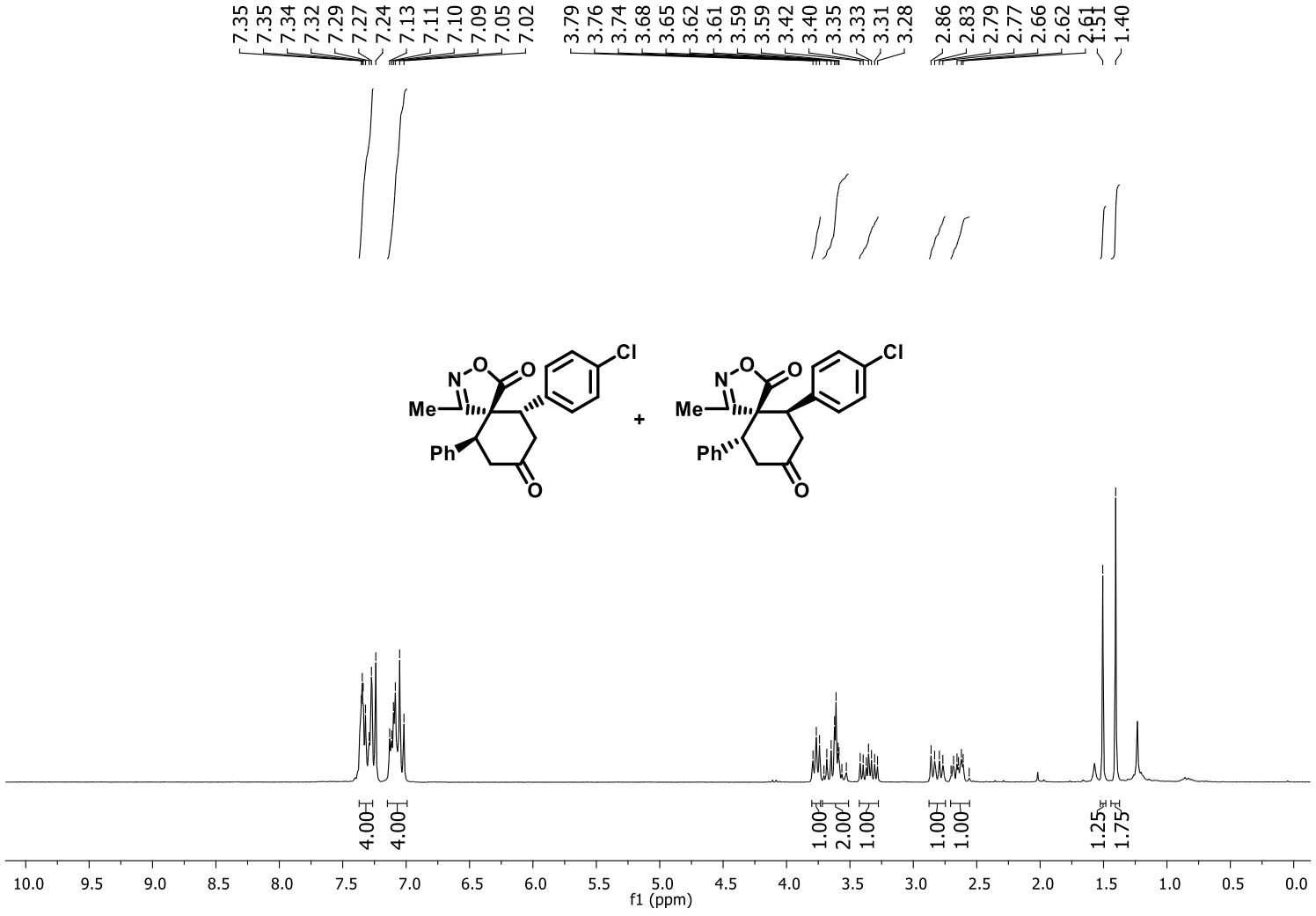


^{13}C (62.5 MHz, $CDCl_3$)

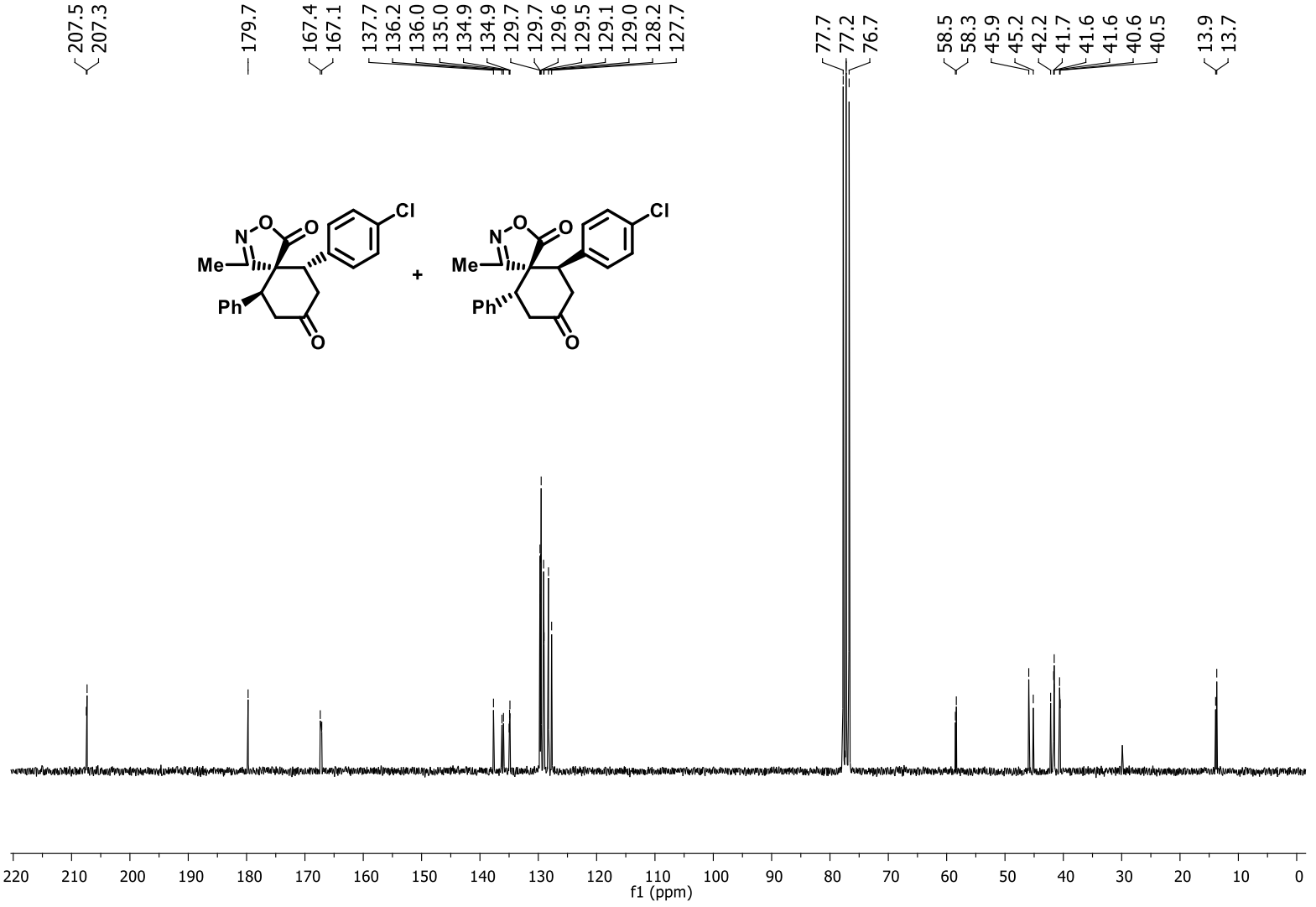


4.28. Molecule 1z

^{1}H (250 MHz, $CDCl_3$)

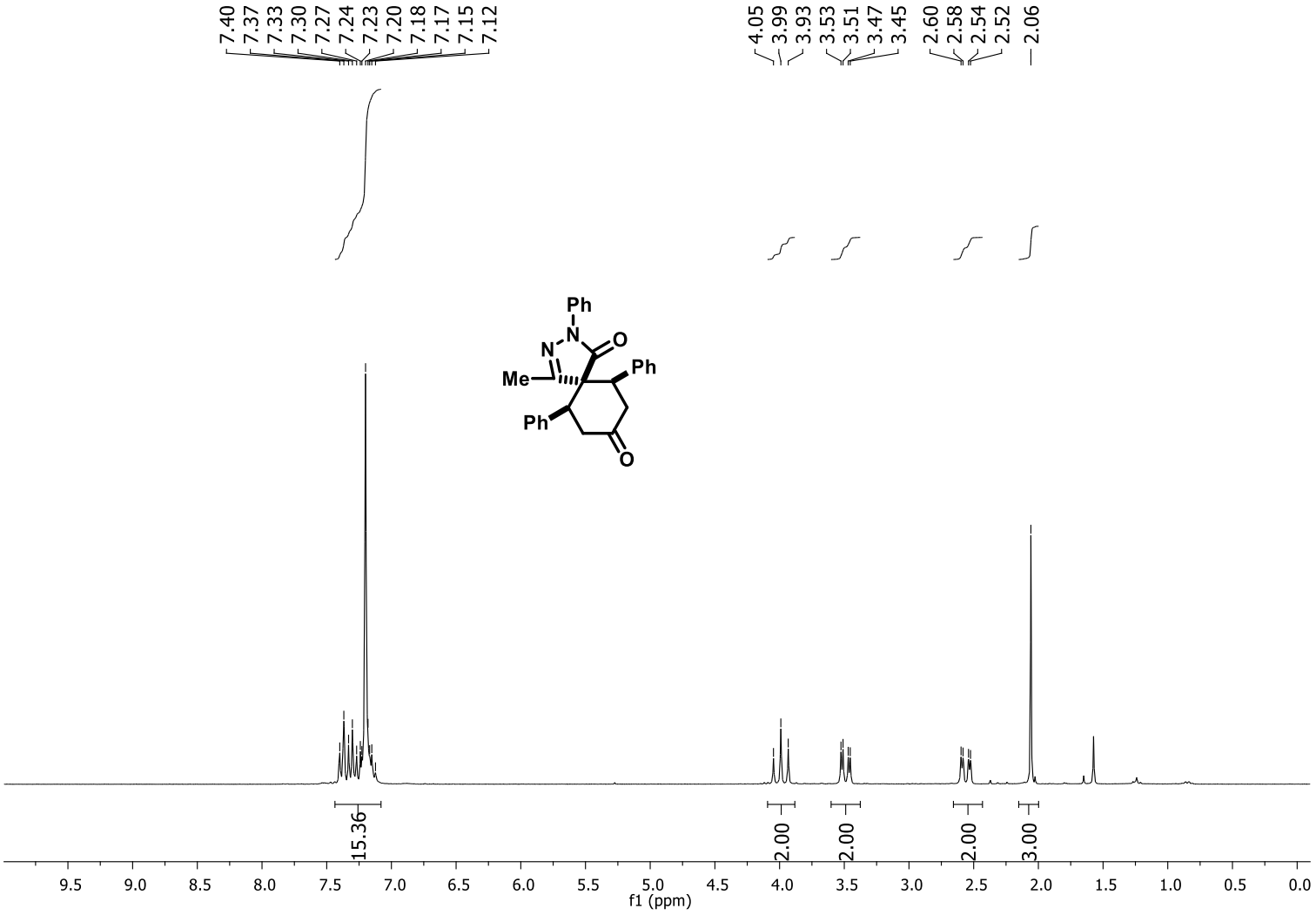


^{13}C (62.5 MHz, $CDCl_3$)

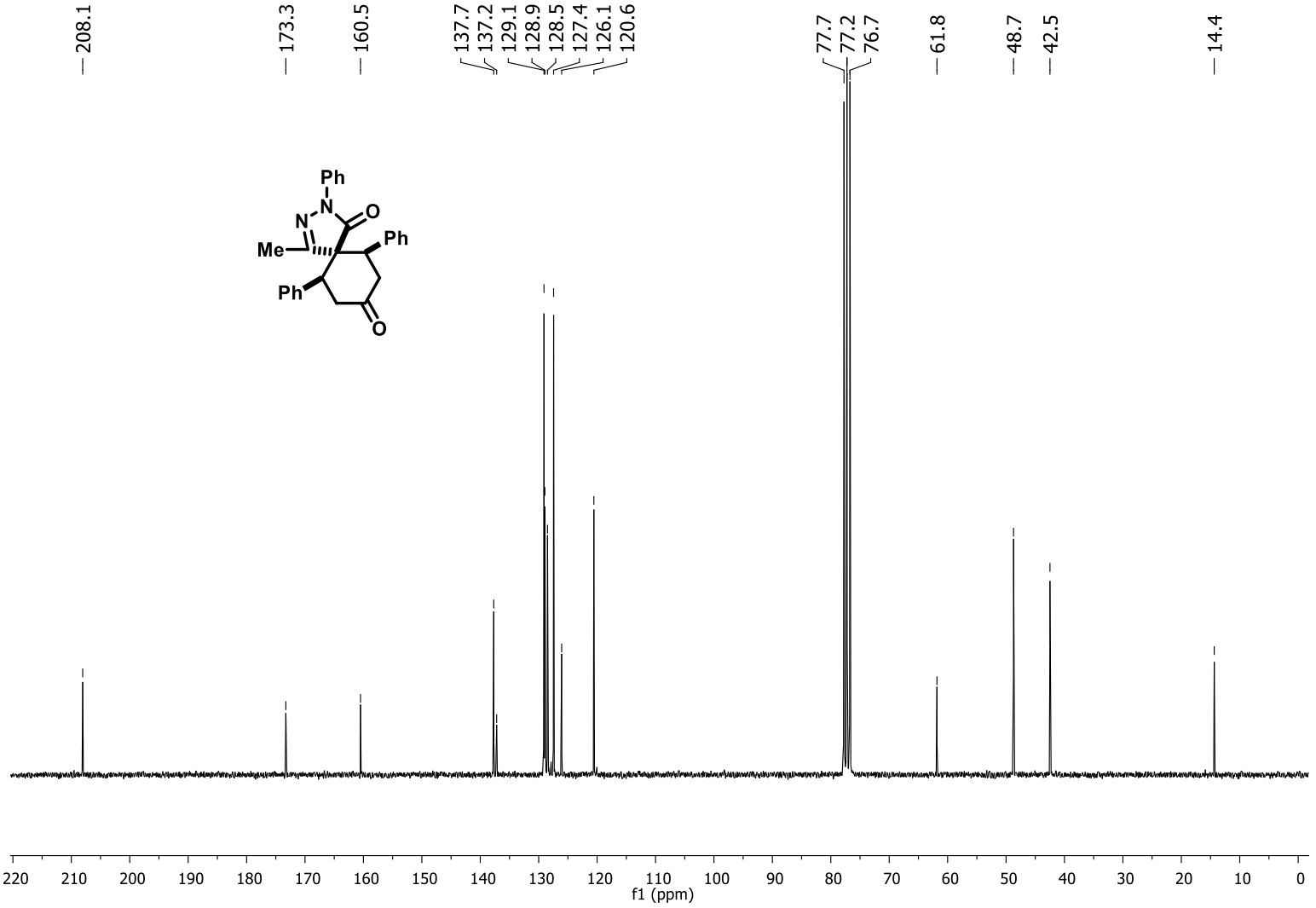


4.29. Molecule 7m

^{1}H (250 MHz, $CDCl_3$)

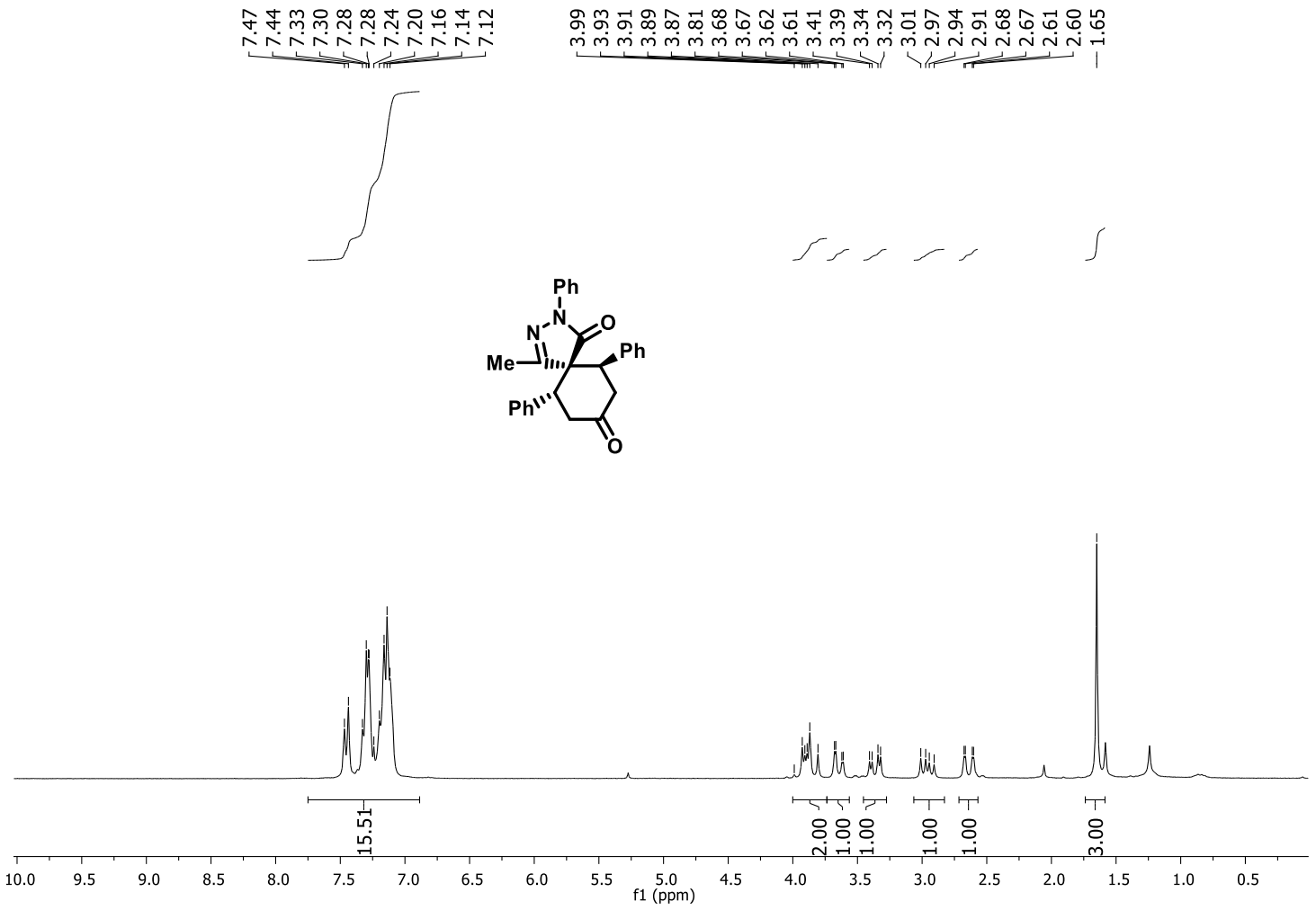


^{13}C (62.5 MHz, $CDCl_3$)

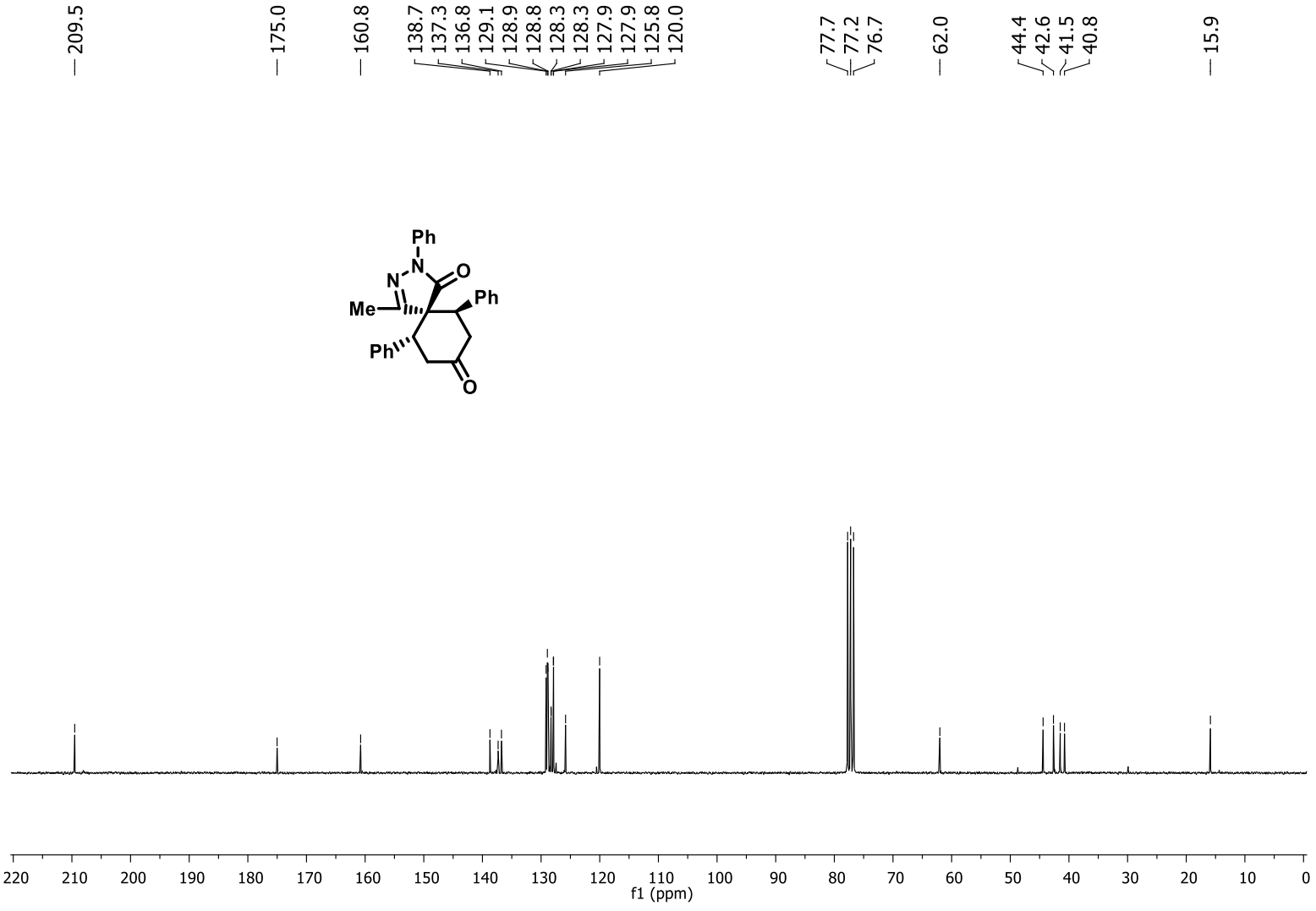


4.30. Molecule 7q

^{1}H (250 MHz, $CDCl_3$)

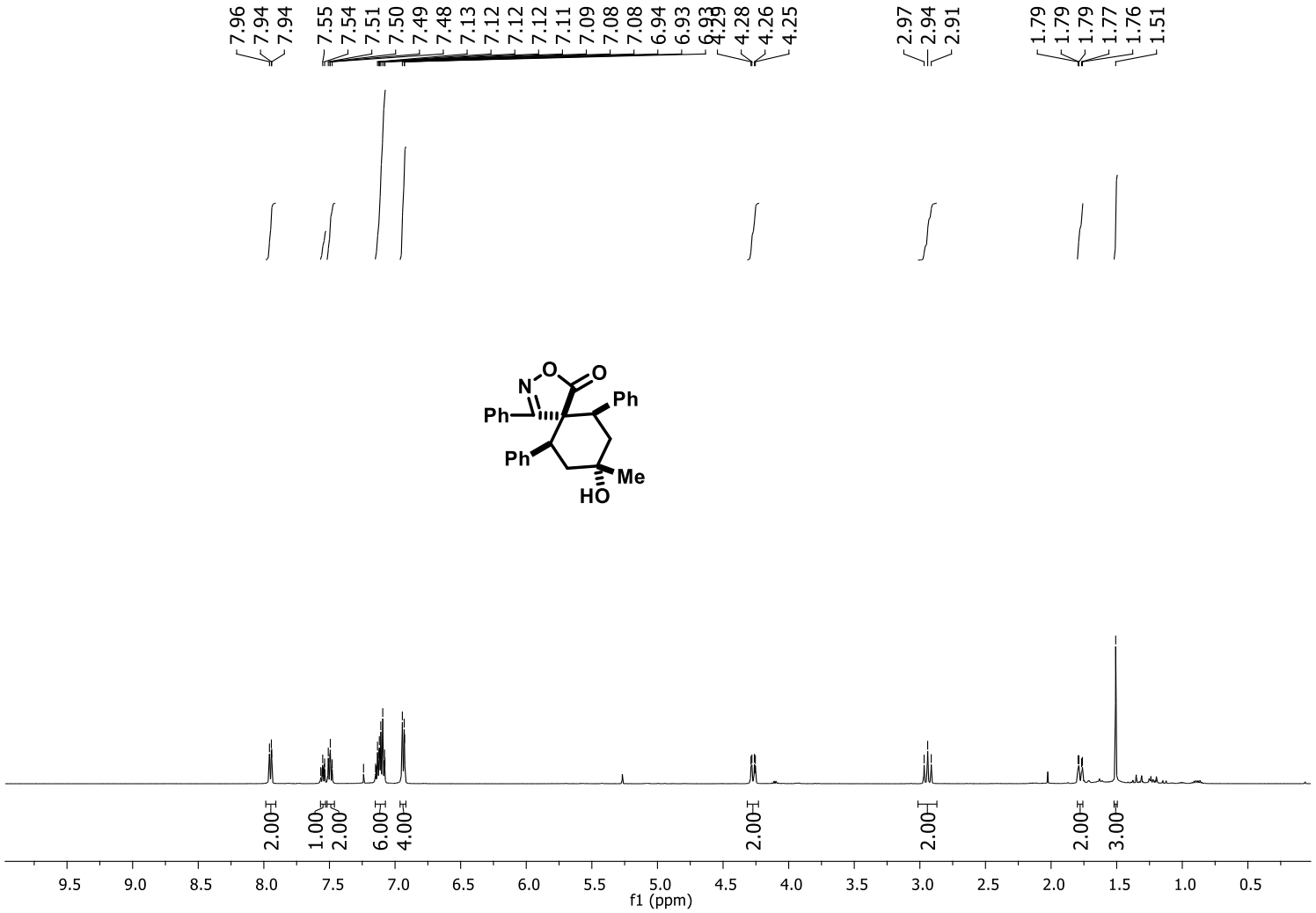


^{13}C (62.5 MHz, $CDCl_3$)

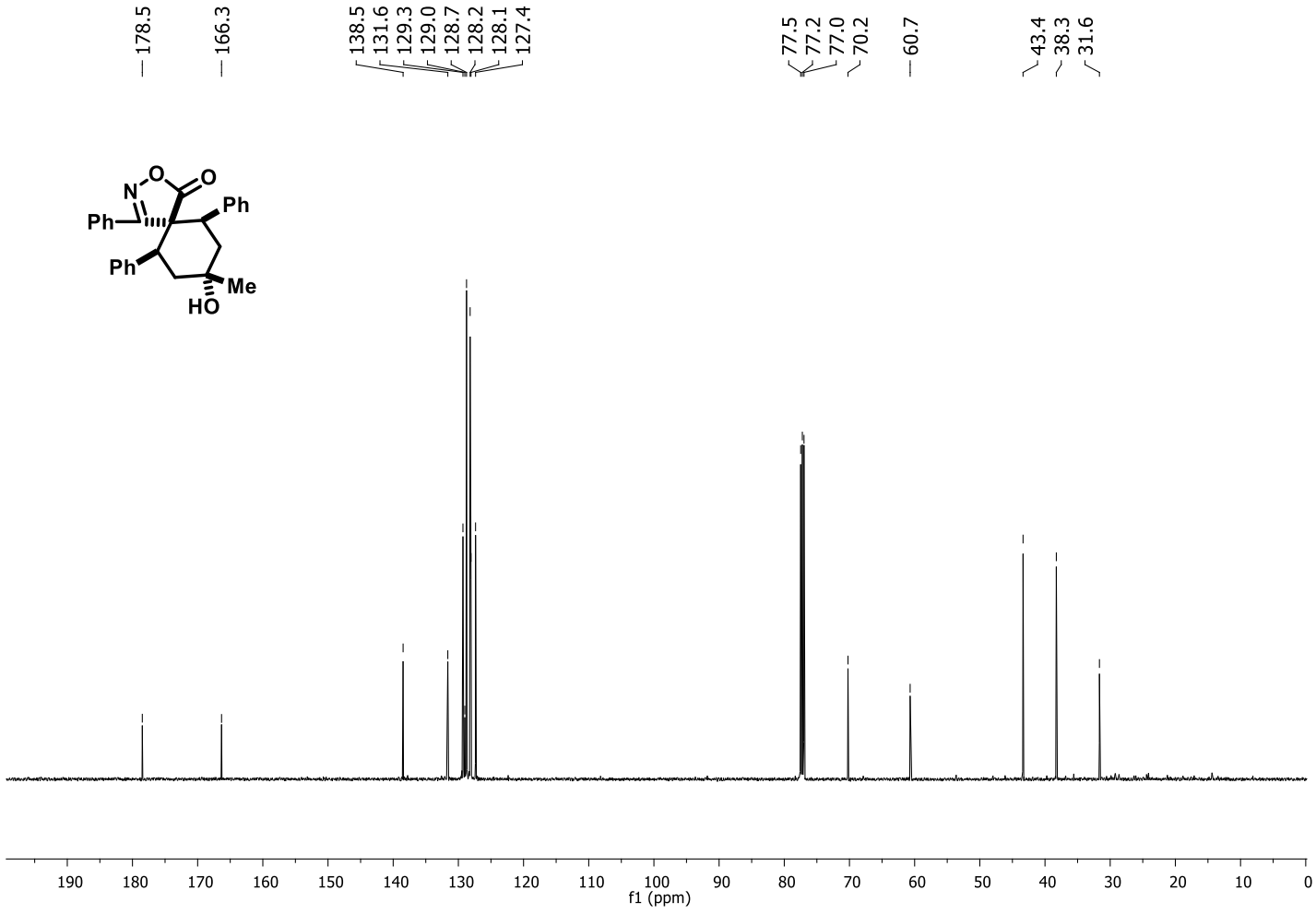


4.31. Molecule 12

^{1}H (500 MHz, $CDCl_3$)

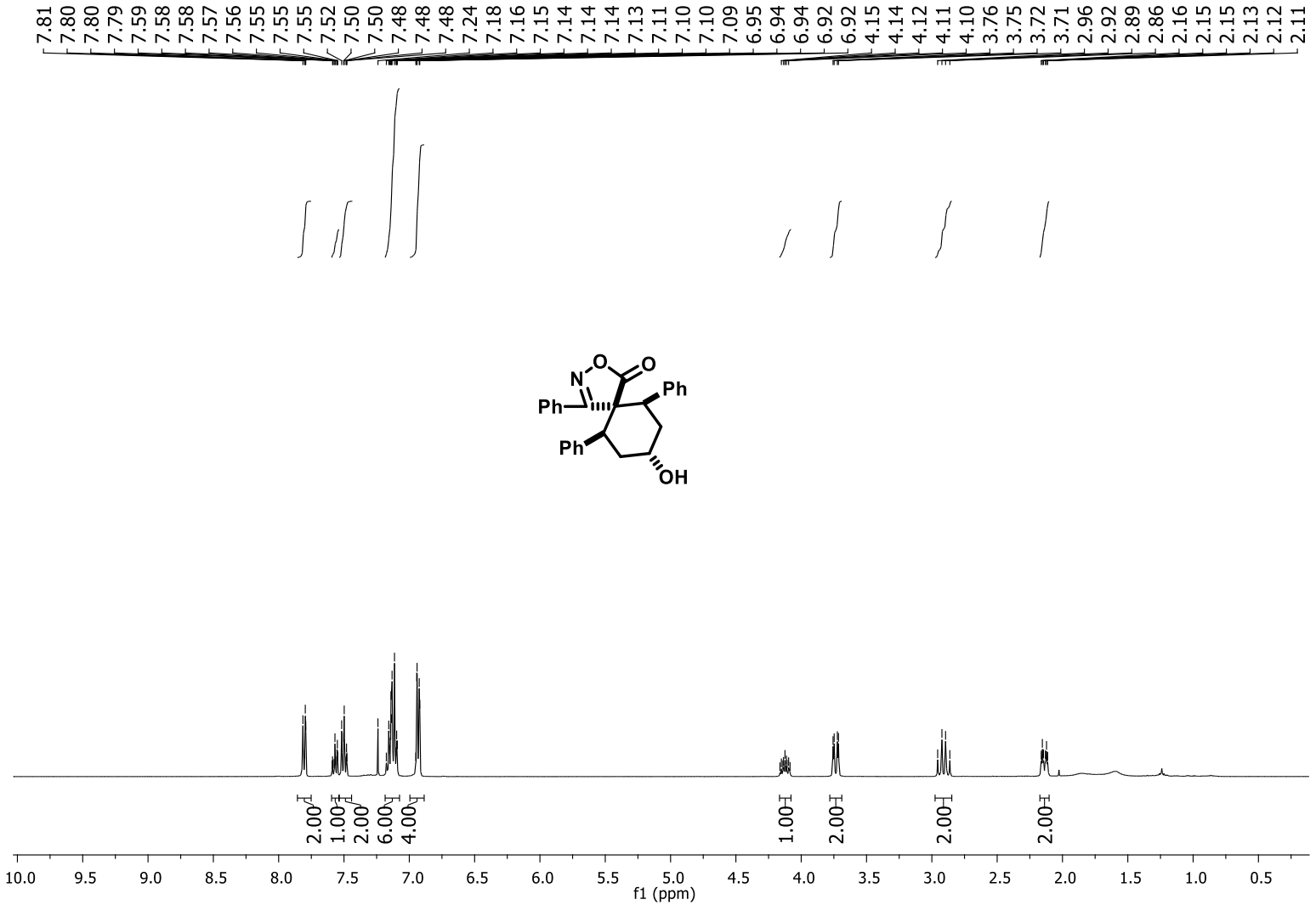


^{13}C (125 MHz, $CDCl_3$)

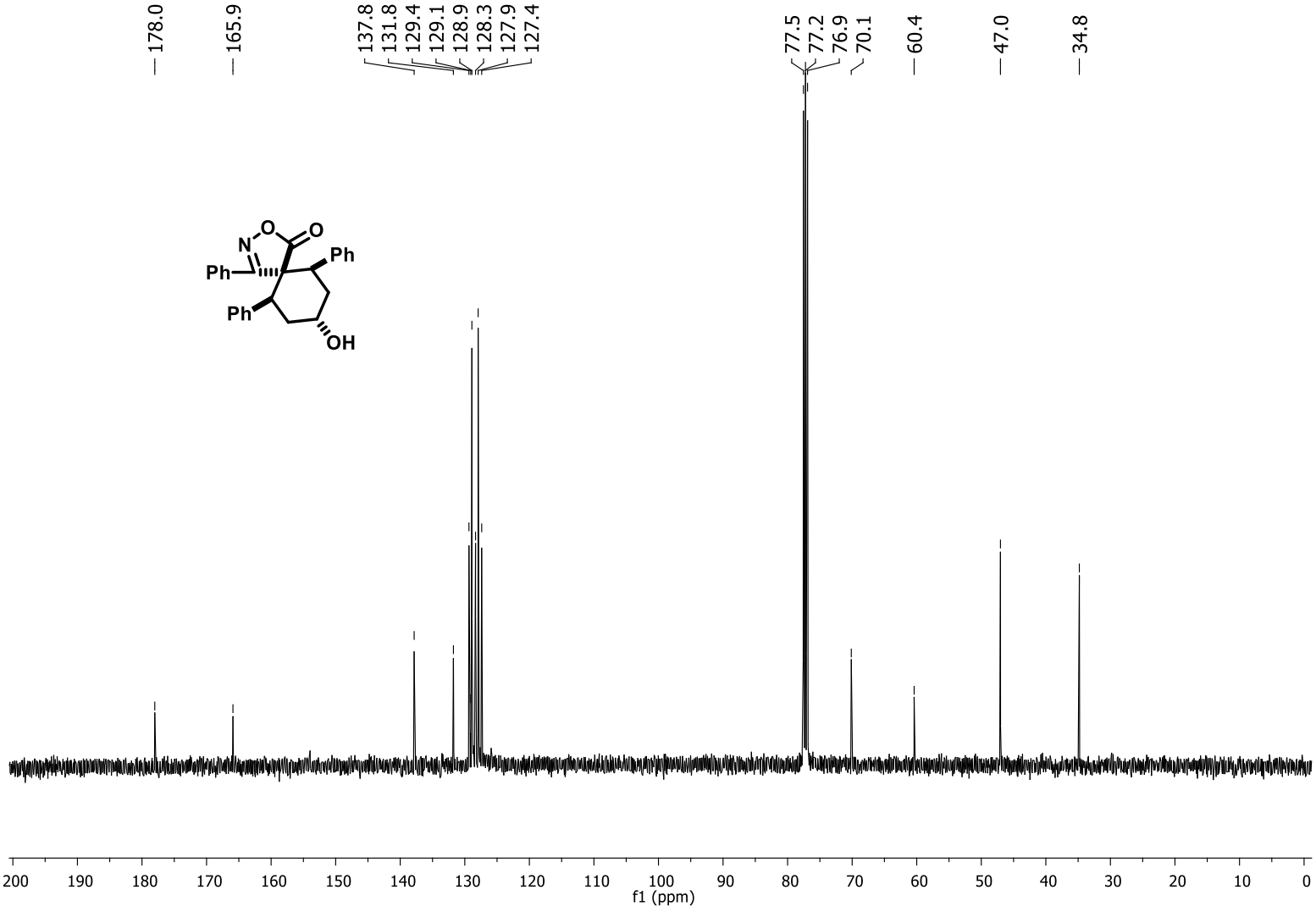


4.32. Molecule 13

^{1}H (400 MHz, $CDCl_3$)

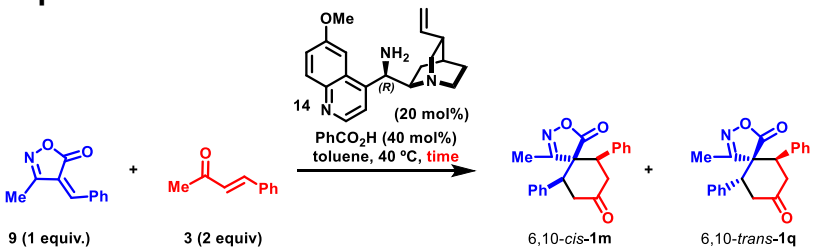


^{13}C (100 MHz, $CDCl_3$)



5. HPLC traces

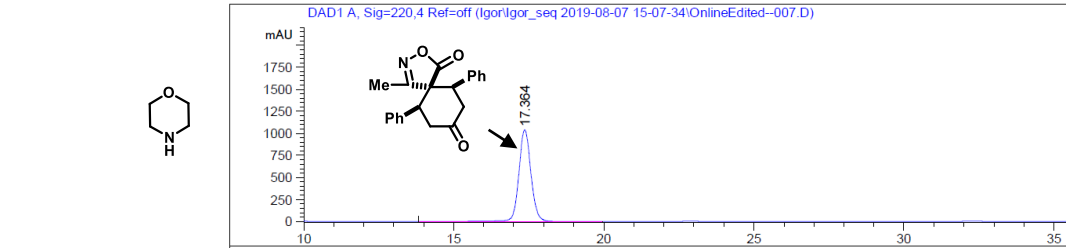
5.1. Reaction monitoring for the formation of spiroisoxazol-5-ones 6,10-*cis*-1m vs 6,10-*trans*-1q:

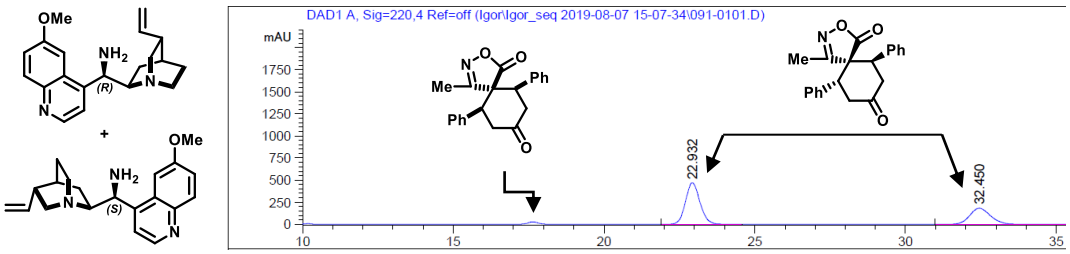


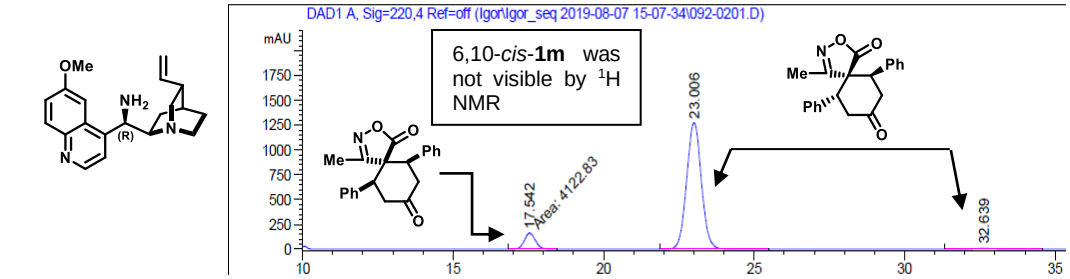
time	6,10-*cis*-**1m** (%)[a]	6,10-*trans*-**1q** (%)[a]/ *er* [b]
3h	0	70/ 99:1
20h	45	55/ 99:1
5 days	63	37/ >99:1

[a]Estimated by ^{1}H NMR of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard. [b]Measured by HPLC analysis.

5.1.1. Reaction time: 3h

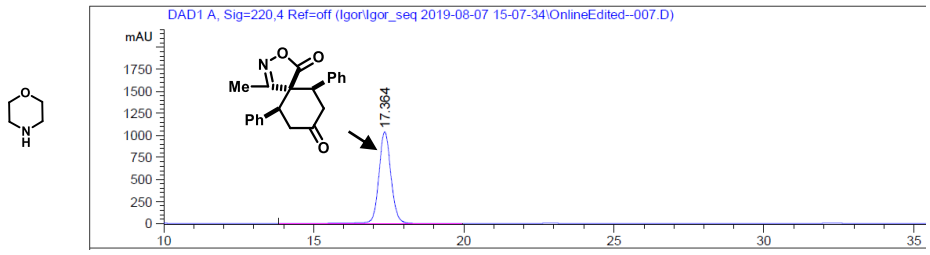


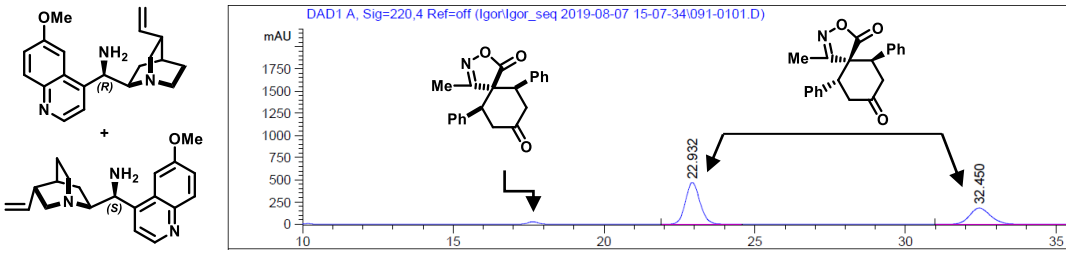


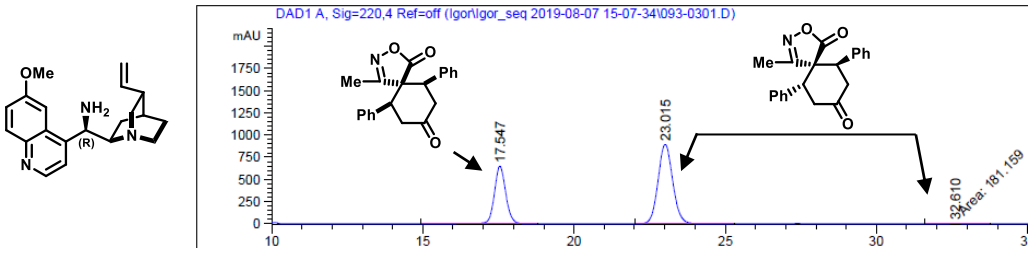


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.542	MM	0.4245	4122.83154	161.86179	8.5876
2	23.006	BB	0.5340	4.34253e4	1273.08057	90.4518
3	32.639	BB	0.7223	461.18393	9.50102	0.9606

5.1.2. Reaction time: 20h

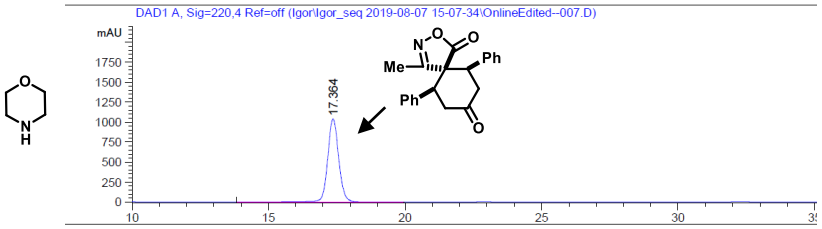


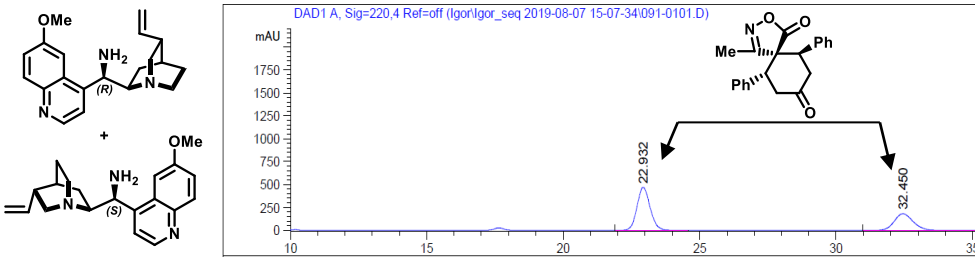


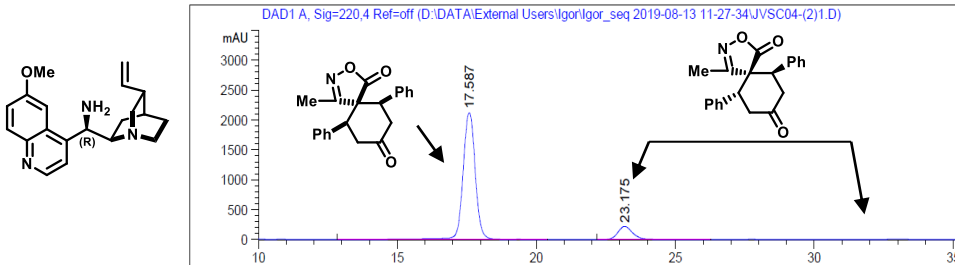


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.547	BB	0.4055	1.70787e4	647.89661	36.0513
2	23.015	BB	0.5233	3.01135e4	893.23975	63.5663
3	32.610	MM	0.7811	181.15910	3.86525	0.3824

5.1.3. Reaction time: 5 days

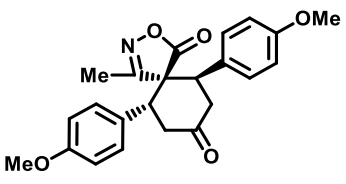


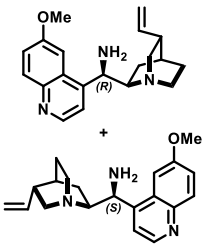


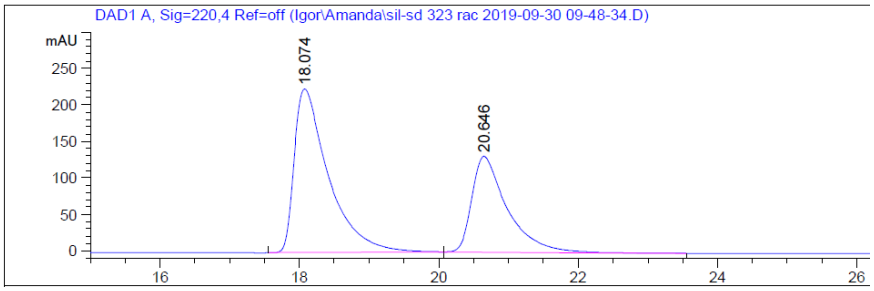


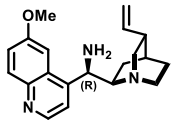
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.587	VV R	0.4777	6.50494e4	2116.88672	89.0150
2	23.175	BV	0.5603	8027.52881	216.64095	10.9850

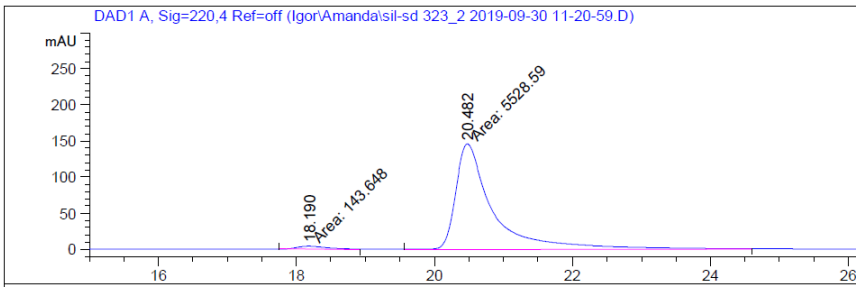
5.2. Molecule 6,10-*trans*-1r:





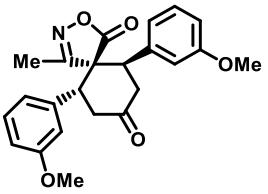


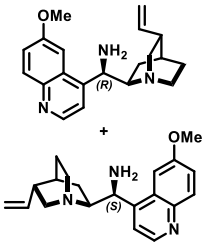


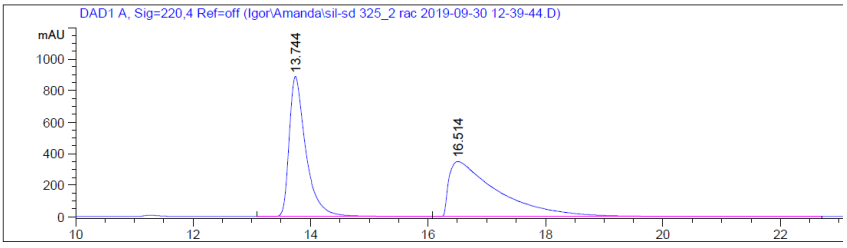


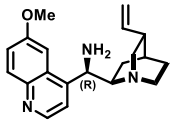
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.190	MM	0.5432	143.64821	4.40785	2.5325
2	20.482	MM	0.6309	5528.59131	146.05893	97.4675

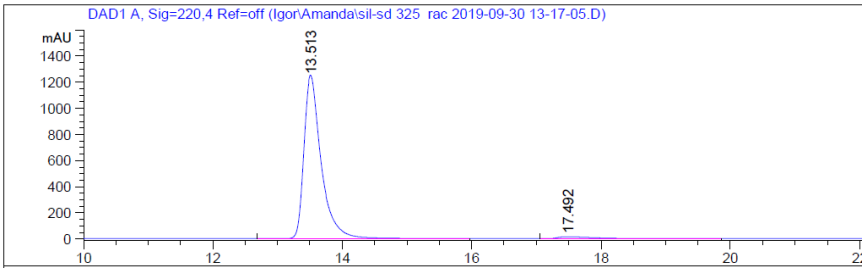
5.3. Molecule 6,10-*trans*-1s:





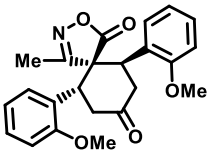


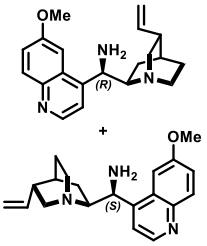


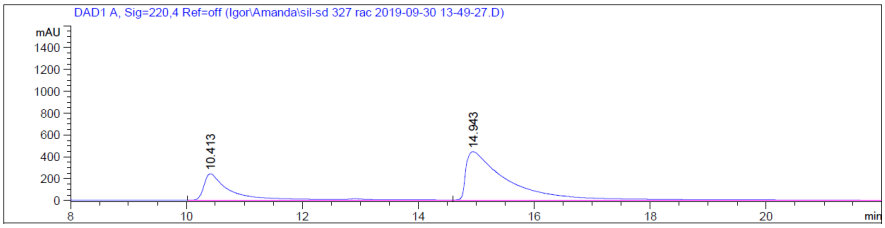


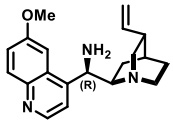
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.513	BB	0.2762	2.31749e4	1250.71106	97.5165
2	17.492	BB	0.5598	590.21643	15.24022	2.4835

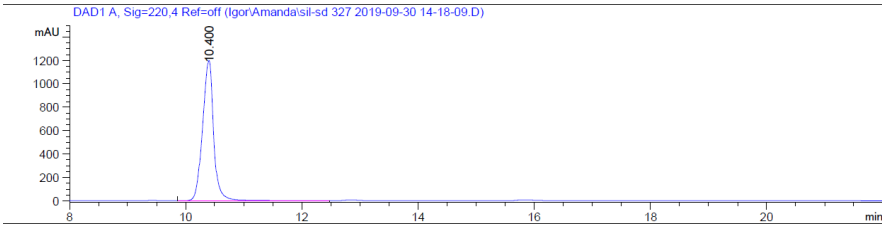
5.4. Molecule 6,10-*trans*-1t:





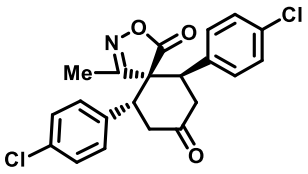


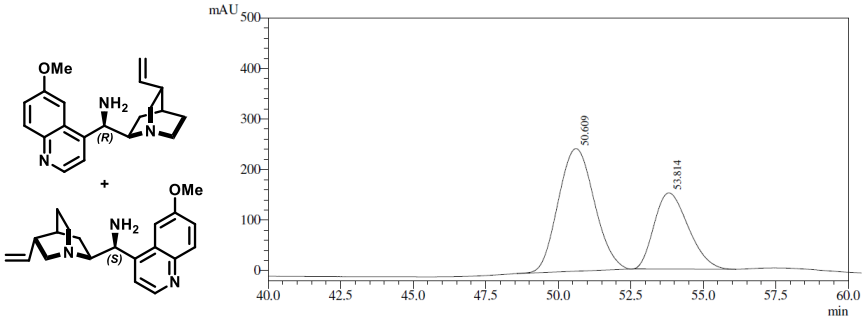


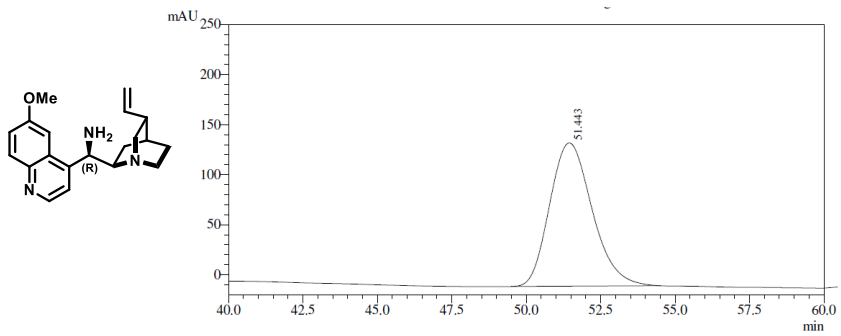


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.400	BB	0.2008	1.59139e4	1199.40991	100.0000

5.5. Molecule 6,10-*trans*-1u:

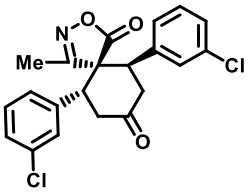


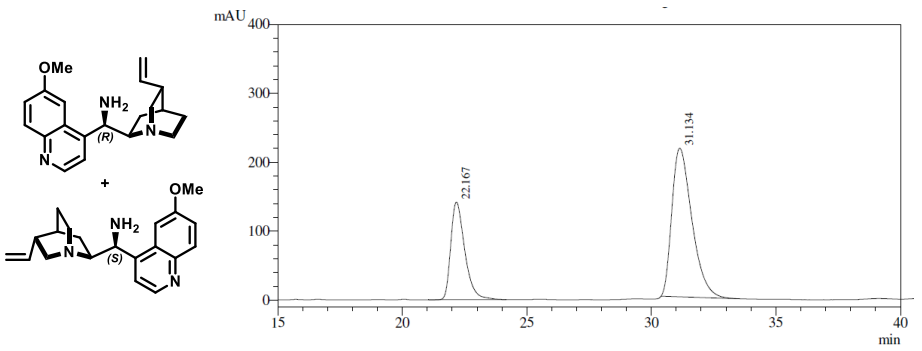


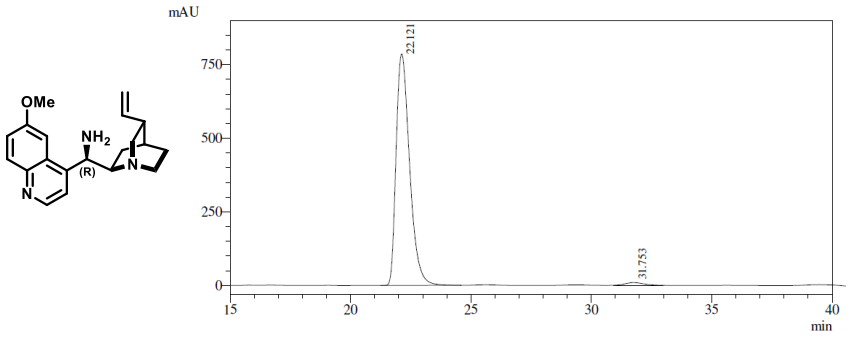


Peak#	Ret. Time	Area	Height	Area %	Height %
1	51.443	14225302	143152	100.000	100.000
Total		14225302	143152	100.000	100.000

5.6. Molecule 6,10-*trans*-1v:

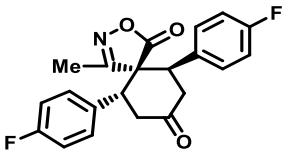


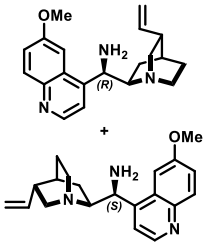


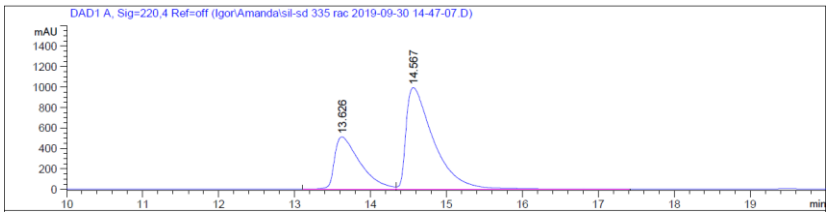


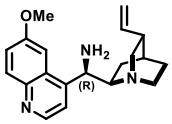
Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.121	30659638	786362	98.417	98.857
2	31.753	493177	9091	1.583	1.143
Total		31152815	795453	100.000	100.000

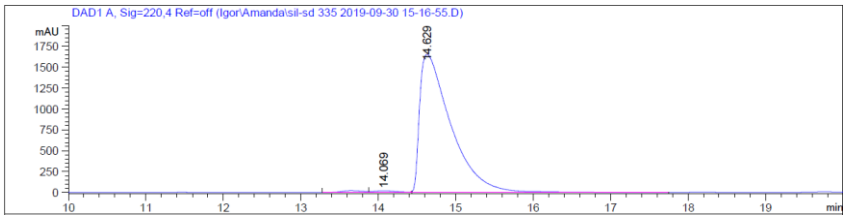
5.7. Molecule 6,10-*trans*-1x:





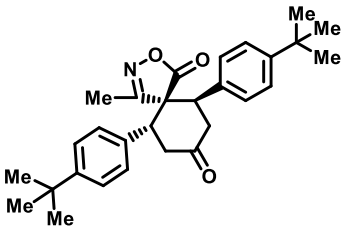


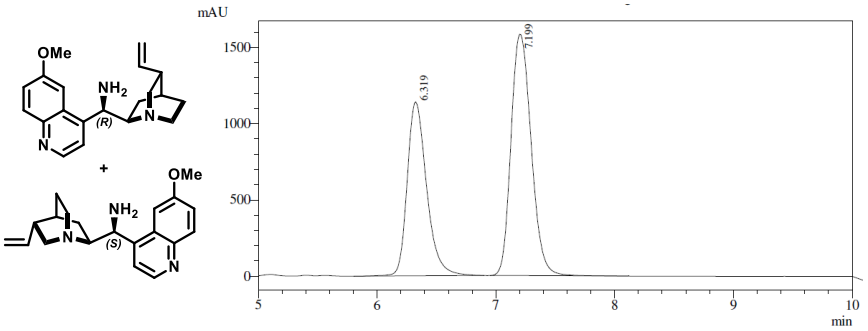


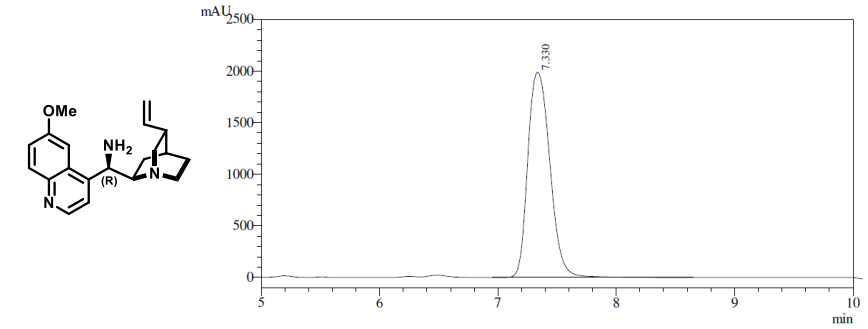


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.069	VV E	0.2949	438.91629	21.98682	0.9318
2	14.629	VB R	0.4127	4.66643e4	1650.74304	99.0682

5.8. Molecule 6,10-*trans*-1w:

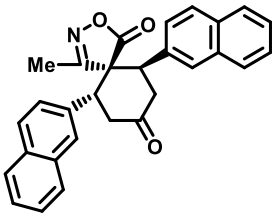


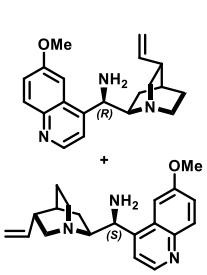


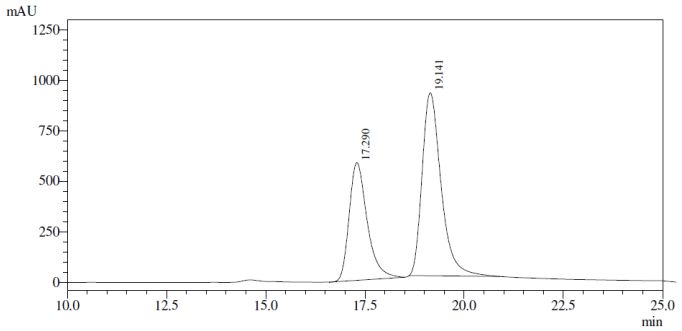


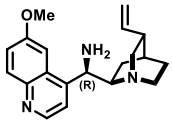
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.330	25838917	1989119	100.000	100.000
Total		25838917	1989119	100.000	100.000

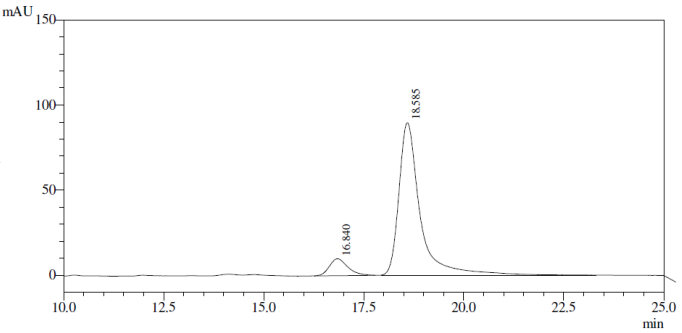
5.9. Molecule 6,10-*trans*-1y:





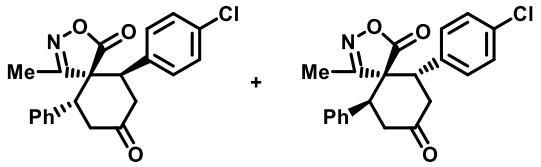


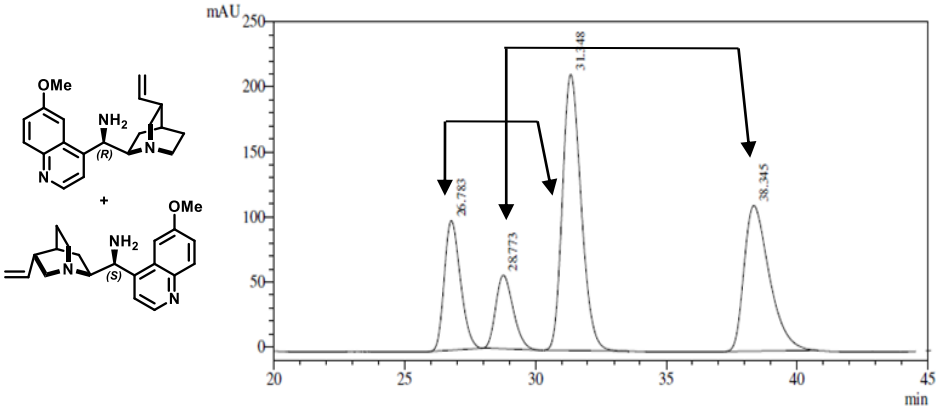


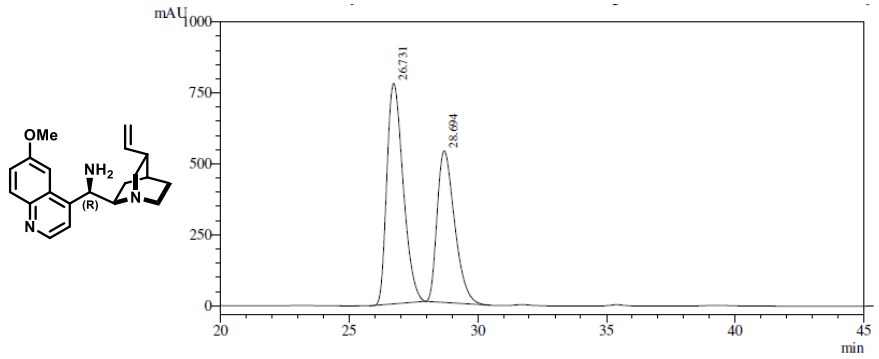


Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.840	317632	9964	8.757	10.008
2	18.585	3309731	89594	91.243	89.992
Total		3627363	99558	100.000	100.000

5.10. Molecules 6,10-*trans*-1z + 1z':

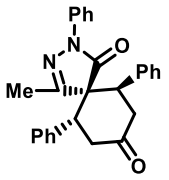


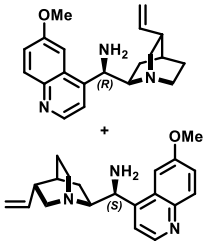


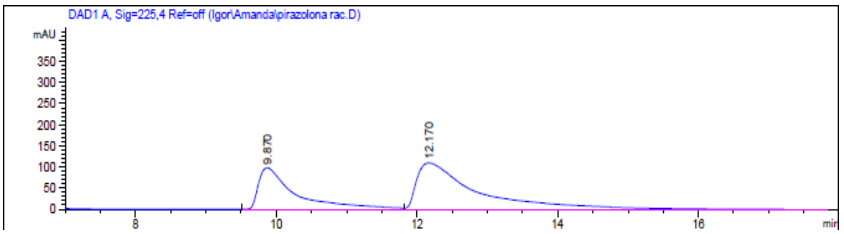


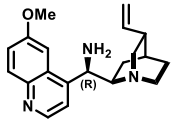
Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.731	34288776	776974	57.556	59.276
2	28.694	25286101	533804	42.444	40.724
Total		59574877	1310778	100.000	100.000

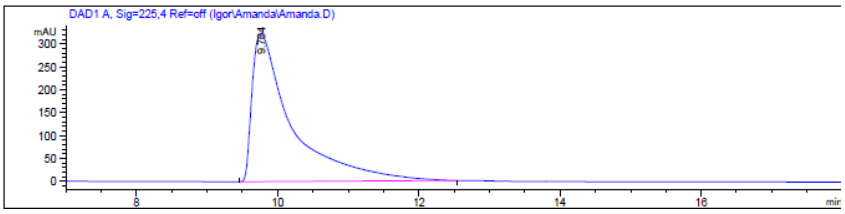
5.11. Molecule 6,10-*trans*-7q







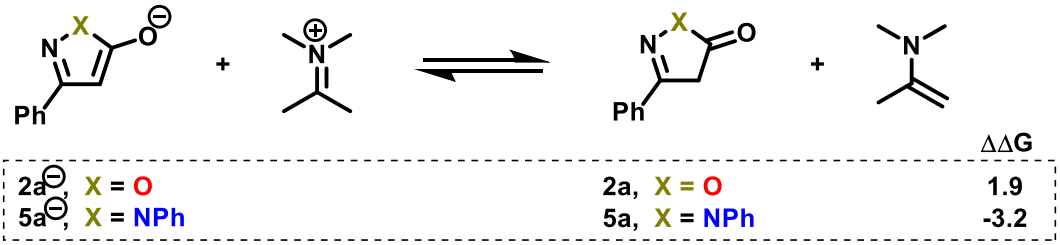




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.764	BB	0.5533	1.25956e4	322.76804	100.0000
Totals :				1.25956e4	322.76804	

6. Tables of Energy

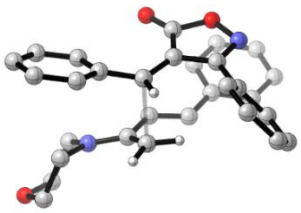
Table S1: Comparison of stability between pyrazol-5-one and isoxazol-5-one, in acetonitrile. Summary of energies (in Hartree).



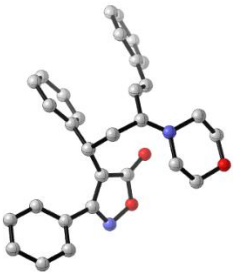
	M06-2X/6-31+G(d,p)/IEF-PCM			M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM	
	ΔE_{ele}	Thermal correction to Gibbs Free Energy	Imaginary Frequency (cm^{-1})	ΔE_{ele}	ΔG*
enamine	-251.7687169	0.124518	-	-251.8237112	-251.6991932
iminium	-252.2317921	0.136256	-	-252.2853411	-252.1490851
2a⁻	-551.6823707	0.096820	-	-551.8085230	-551.7117030
2a	-552.1425115	0.108918	-	-552.2675265	-552.1586085
5a⁻	-762.8071458	0.184790	-	-762.9702185	-762.7854285
5a	-763.2735753	0.195422	-	-763.4358507	-763.2404287

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **M06-2X/6-311+G(d,p)/IEF-PCM**.

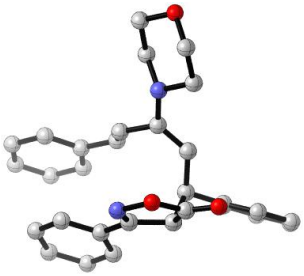
Table S2: Summary of lowest energies (in Hartree) intermediates and transition states of Scheme 3 of the main text, in acetonitrile.



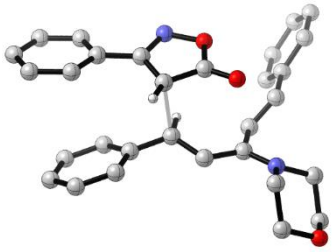
TS(15b→16b)



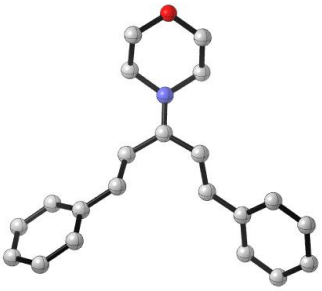
16b



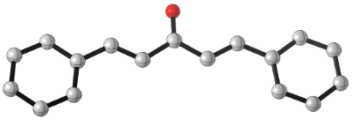
17b



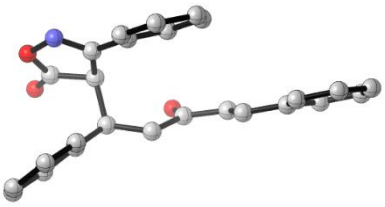
TS(17b→18b)



18b



6b

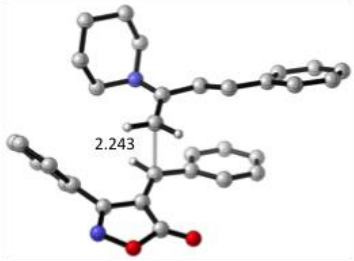


19b

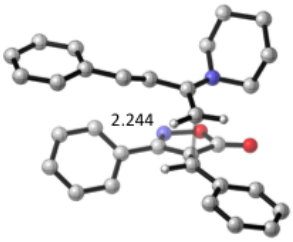
	M06-2X/6-31+G(d,p)/IEF-PCM			M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM	
	ΔE_{ele}	Thermal correction to Gibbs Free Energy	Imaginary Frequency (cm^{-1})	ΔE_{ele}	ΔG^*
9b	-821.18764520	0.188130	-	-821.36461889	-821.17648889
3a	-462.12356972	0.135526	-	-462.22358341	-462.08805741
morpholine	-287.68956949	0.108258	-	-287.75781722	-287.64955922
15b-s-cis-conf1	-673.40031258	0.242466	-	-673.54476485	-673.30229885
H_2O	-76.40321234	0.003849	-	-76.42868486	-76.42483586
TS(15b→16b)	-1494.59231371	0.455149	-299.90	-1494.91473584	-1494.45958684
16b-conf1	-1494.6241290	0.459936	-	-1494.9462851	-1494.4863491
17b	-1494.6234141	0.457812	-	-1494.9462427	-1494.4884307
TS(17b→18b)	-1494.58981487	0.453296	-334.64	-1494.91263758	-1494.45934158
$2a^-$	-551.68237142	0.096870	-	-551.80852682	-551.71165682
18b	-942.9027042	0.335393	-	-943.0980564	-942.7626634
2a	-552.14251170	0.108913	-	-552.26752312	-552.15861012
6b	-731.1665065	0.213763	-	-731.3187928	-731.1050298
19b	-1283.344766	0.351158	-	-1283.623246	-1283.2720884

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **M06-2X/6-311+G(d,p)/IEF-PCM**.

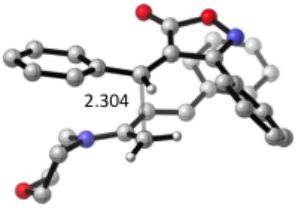
Table S3: Transition state geometries obtained for **TS(15b→16b)**. Energies in Hartree, in acetonitrile.



TS(15b→16b)-conf2



TS(15b→16b)-conf3

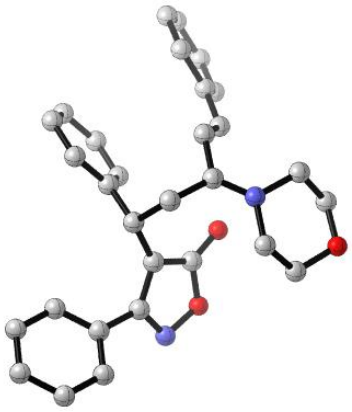


TS(15b→16b)

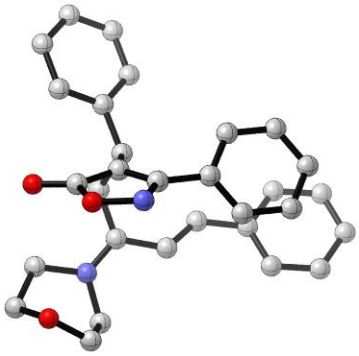
	M06-2X/6-31+G(d,p)/IEF-PCM			**M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM**	
	ΔE_{ele}	**Thermal correction to Gibbs Free Energy**	**Imaginary Frequency (cm^{-1})**	**ΔE_{ele}**	**ΔG***
TS(15b→16b)-conf2	-1494.58936455	0.455282	-375.80	-1494.91182856	-1494.45654656
TS(15b→16b)-conf3	-1494.58993995	0.457730	-339.57	-1494.91234543	-1494.45461543
TS(15b→16b)	-1494.59231371	0.455149	-299.90	-1494.91473584	-1494.45958684

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and Thermal correction to Gibbs Free Energy at **M06-2X/6-311+G(d,p)/IEF-PCM**.

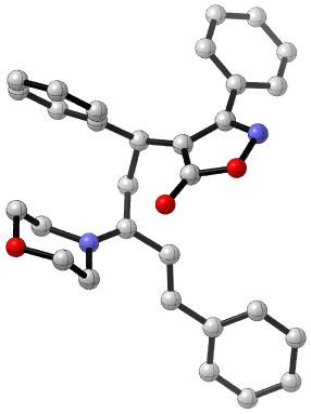
Table S4: Geometries obtained for **16b**. Energies in Hartree, in acetonitrile.



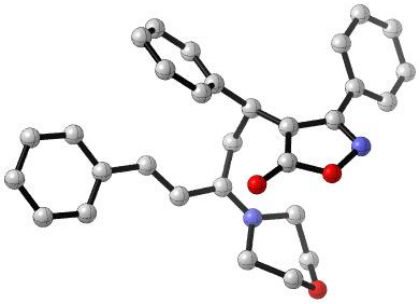
16b



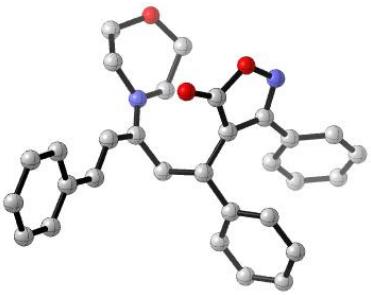
16b-conf2



16b-conf3



16b-conf4

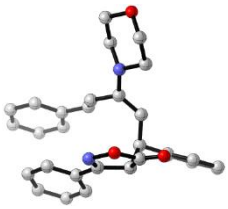


16b-conf5

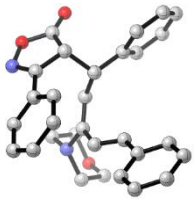
	M06-2X/6-31+G(d,p)/IEF-PCM			M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM	
	ΔE_{ele}	Thermal correction to Gibbs Free Energy	Imaginary Frequency (cm^{-1})	ΔE_{ele}	ΔG*
16b	-1494.6241290	0.459936	-	-1494.9462851	-1494.4863491
16b-conf2	-1494.6221679	0.460769	-	-1494.9443789	-1494.4836099
16b-conf3	-1494.6221365	0.460429	-	-1494.9441296	-1494.4837006
16b-conf4	-1494.6220769	0.461054	-	-1494.9441916	-1494.4831376
16b-conf4	-1494.6211648	0.459458	-	-1494.9432995	-1494.4838415

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and Thermal correction to Gibbs Free Energy at **M06-2X/6-311+G(d,p)/IEF-PCM**.

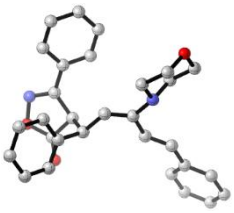
Table S5: Geometries obtained for **17b**. Energies in Hartree, in acetonitrile.



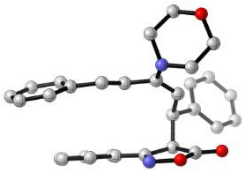
17b



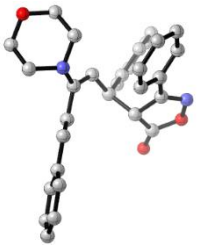
17b-conf2



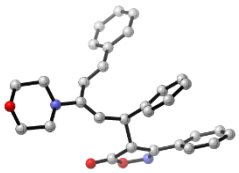
17b-conf3



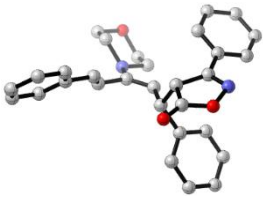
17b-conf4



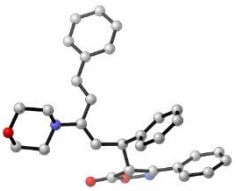
17b-conf5



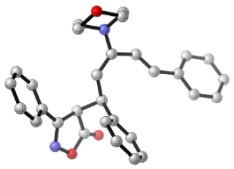
17b-conf6



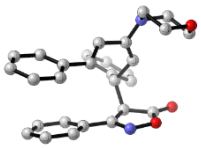
17b-conf7



17b-conf8



17b-conf9

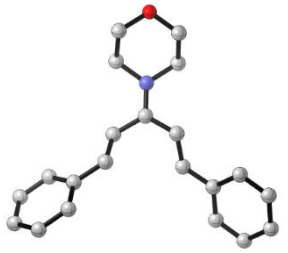


17b-conf10

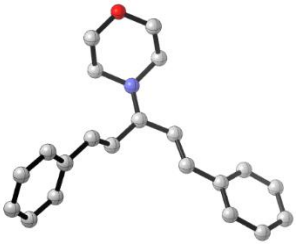
	M06-2X/6-31+G(d,p)/IEF-PCM			M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM	
	ΔE_{ele}	Thermal correction to Gibbs Free Energy	Imaginary Frequency (cm^{-1})	ΔE_{ele}	ΔG^*
17b	-1494.6234141	0.457812	-	-1494.9462427	-1494.4884307
17b-conf2	-1494.6221530	0.457465	-	-1494.9447918	-1494.4873268
17b-conf3	-1494.6216214	0.456762	-	-1494.9438534	-1494.4870914
17b-conf4	-1494.6212477	0.458128	-	-1494.9442689	-1494.4861409
17b-conf5	-1494.6209391	0.458058	-	-1494.9435619	-1494.4855039
17b-conf6	-1494.6203578	0.456411	-	-1494.9429393	-1494.4865283
17b-conf7	-1494.6202004	0.455467	-	-1494.9424425	-1494.4869755
17b-conf8	-1494.6197542	0.456695	-	-1494.9423099	-1494.4856149
17b-conf9	-1494.6192775	0.457861	-	-1494.9405398	-1494.4826788
17b-conf10	-1494.6190881	0.458334	-	-1494.9417792	-1494.4834452

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and Thermal correction to Gibbs Free Energy at **M06-2X/6-311+G(d,p)/IEF-PCM**.

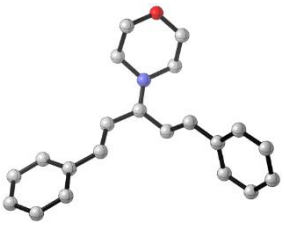
Table S6: Geometries obtained for **18b**. Energies in Hartree, in acetonitrile.



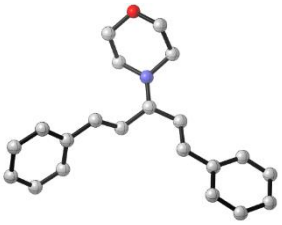
18b



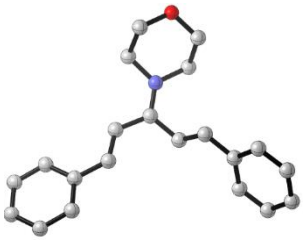
18b-conf2



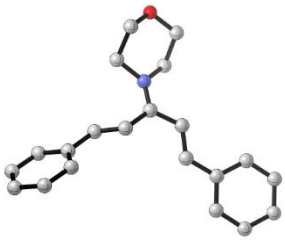
18b-conf3



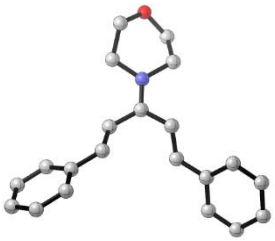
18b-conf4



18b-conf5



18b-conf6

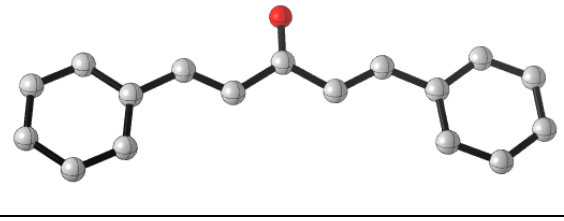
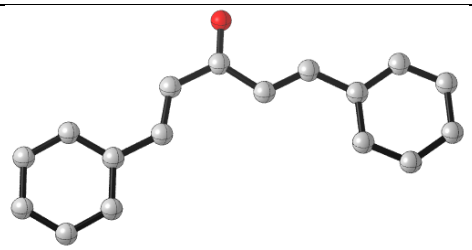


18b-conf7

	M06-2X/6-31+G(d,p)/IEF-PCM			M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM	
	ΔE_{ele}	Thermal correction to Gibbs Free Energy	Imaginary Frequency (cm^{-1})	ΔE_{ele}	ΔG*
18b	-942.9027042	0.335393	-	-943.0980564	-942.7626634
18b-conf2	-942.8995289	0.334349	-	-943.0949676	-942.7606186
18b-conf3	-942.8995288	0.334267	-	-943.0949675	-942.7607005
18b-conf4	-942.8995288	0.334246	-	-943.0949676	-942.7607216
18b-conf5	-942.8995271	0.333691	-	-943.0949679	-942.7612769
18b-conf6	-942.8994233	0.334765	-	-943.0948142	-942.7600492
18b-conf7	-942.8981905	0.334024	-	-943.0937629	-942.7597389

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **M06-2X/6-311+G(d,p)/IEF-PCM**.

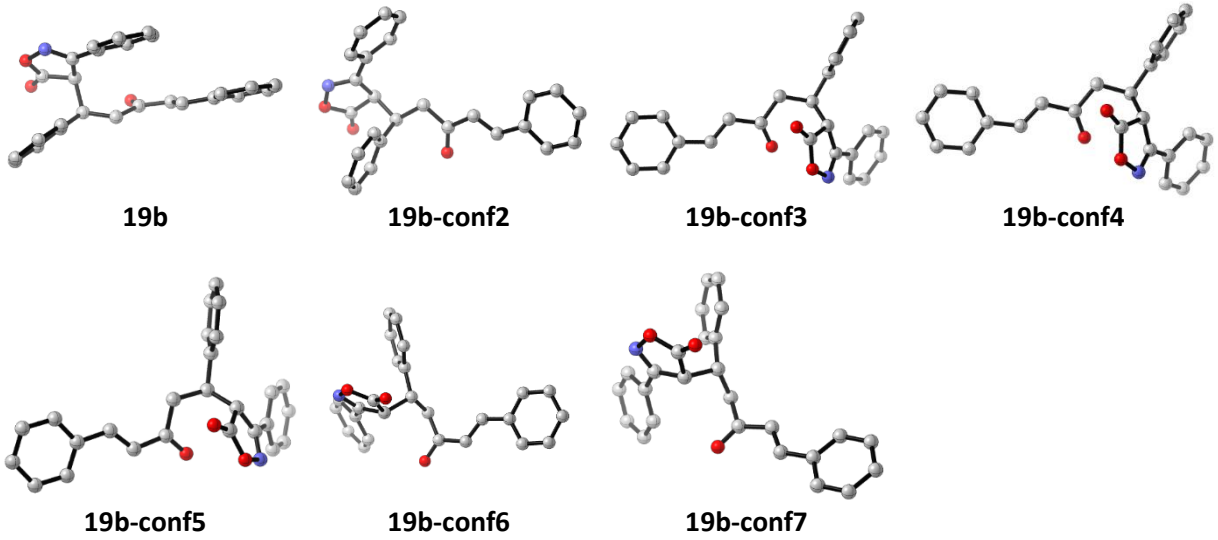
Table S7: Geometries obtained for **6b**. Energies in Hartree, in acetonitrile.

	
6b	**6b-conf2**

	M06-2X/6-31+G(d,p)/IEF-PCM			**M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM**	
	ΔE_{ele}	**Thermal correction to Gibbs Free Energy**	**Imaginary Frequency (cm^{-1})**	**ΔE_{ele}**	**ΔG***
6b	-731.1678933	0.214267	-	-731.3199917	-731.1057247
6b-conf2	-731.1665065	0.213763	-	-731.3187928	-731.1050298

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **M06-2X/6-311+G(d,p)/IEF-PCM**.

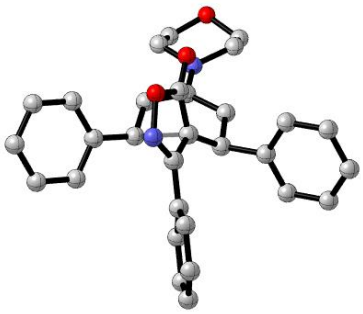
Table S8: Geometries obtained for **19b**. Energies in Hartree, in acetonitrile.



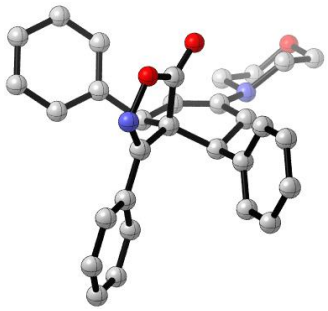
	M06-2X/6-31+G(d,p)/IEF-PCM			M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM	
	ΔE_{ele}	Thermal correction to Gibbs Free Energy	Imaginary Frequency (cm^{-1})	ΔE_{ele}	ΔG^*
19b	-1283.344766	0.351158	-	-1283.623246	-1283.2720884
19b-conf2	-1283.341823	0.348965	-	-1283.619936	-1283.2709708
19b-conf3	-1283.341577	0.349268	-	-1283.619397	-1283.2701291
19b-conf4	-1283.341577	0.349276	-	-1283.619397	-1283.2701212
19b-conf5	-1283.341351	0.349876	-	-1283.619427	-1283.2695509
19b-conf6	-1283.341104	0.350132	-	-1283.619381	-1283.2692492
19b-conf7	-1283.340903	0.349366	-	-1283.619052	-1283.2696856

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **M06-2X/6-311+G(d,p)/IEF-PCM**.

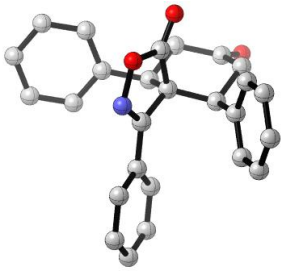
Table S9: Lowest energy geometries of transition states and intermediates potentially involved in the conversion of **16b** to spirocycles **6,10-*cis*-1b**, **6,10-*cis*-1b'**, and **6,10-*trans*-1b**. Energies in Hartree, in acetonitrile.



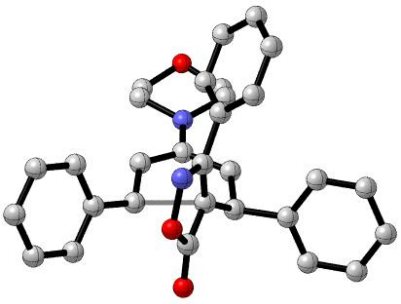
TS(16b→6,10-*cis*-1b)



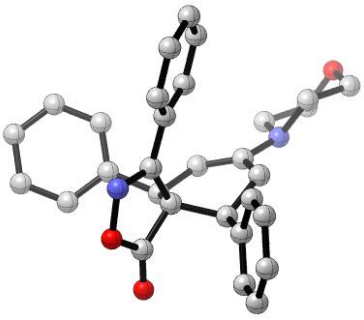
pre-6,10-*cis*-1b



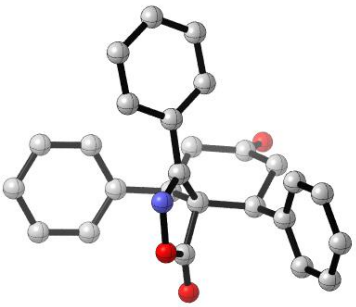
6,10-*cis*-1b



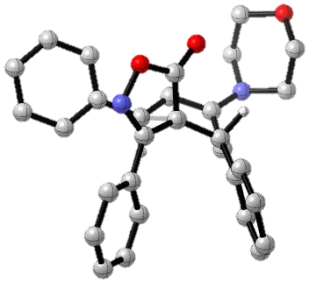
TS(16b→6,10-*cis*-1b')



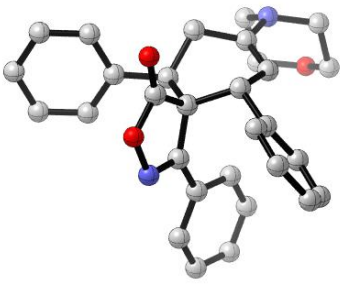
pre-6,10-*cis*-1b'



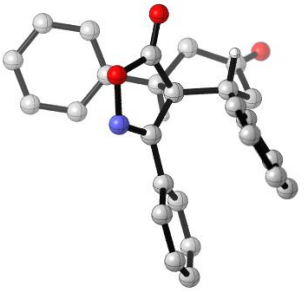
6,10-*cis*-1b'



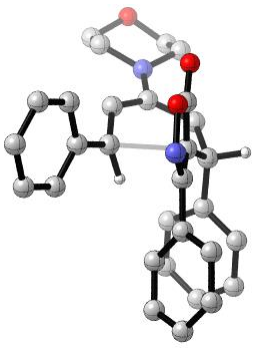
TS(16b→6,10-*trans*-1b)



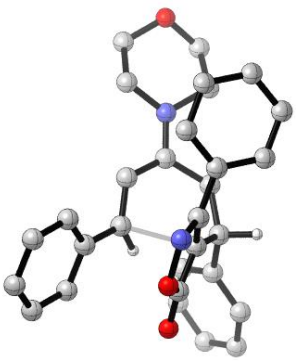
pre-6,10-*trans*-1b



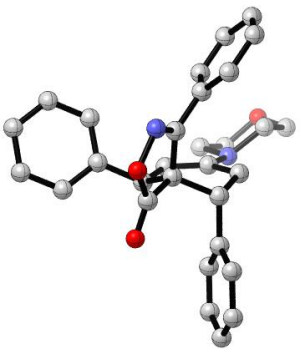
6,10-*trans*-1b



TS(16b→6,10-*trans*-1b')



TS(16b→6,10-*trans*-1b'')



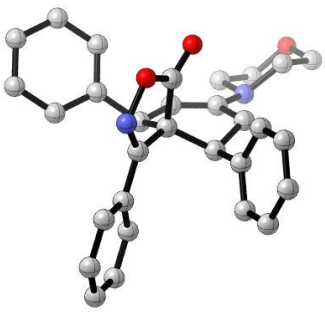
pre-6,10-*trans*-1b''

Table S9: Lowest energy geometries of transition states and intermediates potentially involved in the conversion of **16b** to spirocycles **6,10-*cis*-1b**, **6,10-*cis*-1b'**, and **6,10-*trans*-1b**. Energies in Hartree, in acetonitrile (continued).

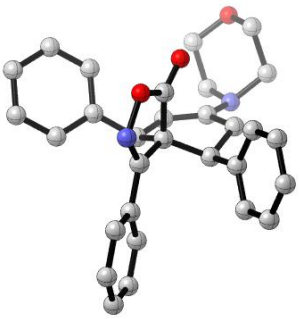
	ΔE_{ele}	**Thermal correction to Gibbs Free Energy**	**Imaginary Frequency (cm^{-1})**	ΔE_{ele}	**ΔG***
TS(16b→6,10-*cis*-1b)	-1494.60976249	0.460116	-258.12	-1494.93155767	-1494.47144167
pre-6,10-*cis*-1b	-1494.65113306	0.463548	-	-1494.97307949	-1494.50953149
6,10-*cis*-1b	-1283.36780814	0.356991	-	-1283.64586342	-1283.28887242
TS(16b→6,10-*cis*-1b')	-1494.60428422	0.460990	-251.10	-1494.92623872	-1494.46524872
pre-6,10-*cis*-1b'	-1494.648861	0.464071	-	-1494.97076381	-1494.50669281
6,10-*cis*-1b'	-1283.35904971	0.357374	-	-1283.63714557	-1283.27977157
TS(16b→6,10-*trans*-1b')	-1494.616392	0.462340	-269.10	-1494.93889	-1494.47654951
pre-6,10-*trans*-1b	-1494.645398	0.463761	-	-1494.96757	-1494.50380937
6,10-*trans*-1b	-1283.362572	0.357483	-	-1283.640862	-1283.28337925
TS(16b→6,10-*trans*-1b')	-1494.600907	0.462269	-263.04	-1494.923179	-1494.46090985
TS(16b→6,10-*trans*-1b'')	-1494.599868	0.461676	-266.76	-1494.922481	-1494.46080536
pre-6,10-*trans*-1b''	-1494.642209	0.464249	-	-1494.964131	-1494.49988231

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **M06-2X/6-311+G(d,p)/IEF-PCM**.

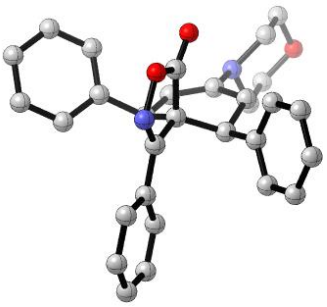
Table S10: Geometries obtained for **pre-1b**. Energies in Hartree, in acetonitrile.



pre-1b



pre-1b-conf2

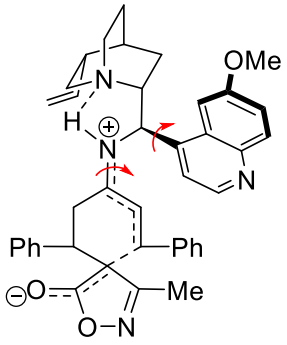


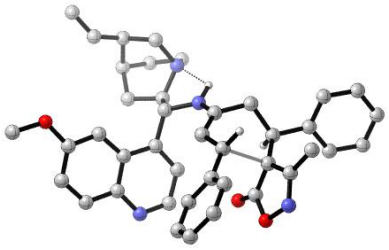
pre-1b-conf3

	M06-2X/6-31+G(d,p)/IEF-PCM			**M06-2X/6-311+G(d,p)/IEF-PCM // M06-2X/6-31+G(d,p)/IEF-PCM**	
	ΔE_{ele}	**Thermal correction to Gibbs Free Energy**	**Imaginary Frequency (cm^{-1})**	**ΔE_{ele}**	**ΔG***
pre-1b	-1494.65113306	0.463548	-	-1494.97307949	-1494.50953149
pre-1b-conf2	-1494.64875750	0.464263	-	-1494.9708236	-1494.50656060
pre-1b-conf3	-1494.64436070	0.461759	-	-1494.9660594	-1494.50430040

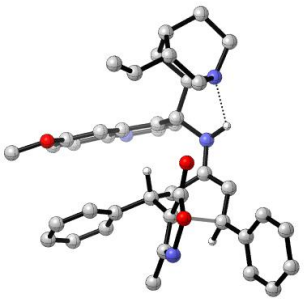
* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **M06-2X/6-31+G(d,p)/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **M06-2X/6-311+G(d,p)/IEF-PCM**.

Table S11: Geometries obtained for transition states involved in enantioselective studies. Energies in Hartree, in toluene.

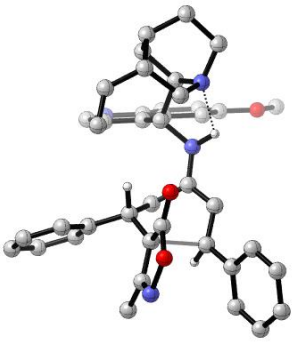




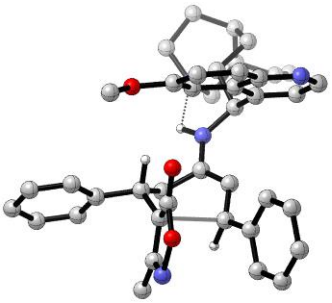
TS(6,10-*trans*-ent-1q)



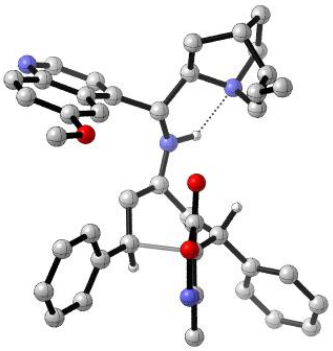
TS(6,10-*trans*-ent-1q)-conf3



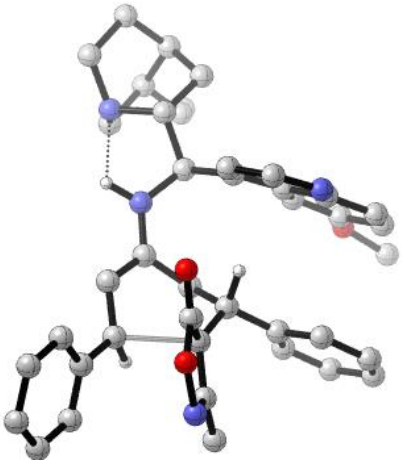
TS(6,10-*trans*-ent-1q)-conf4



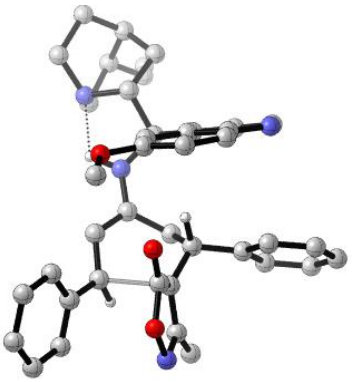
TS(6,10-*trans*-ent-1q)-conf2



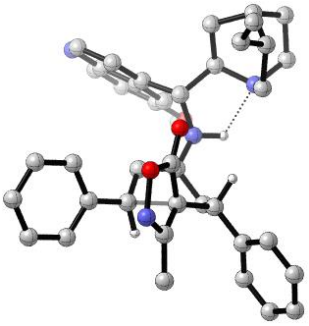
TS(6,10-*trans*-1q)



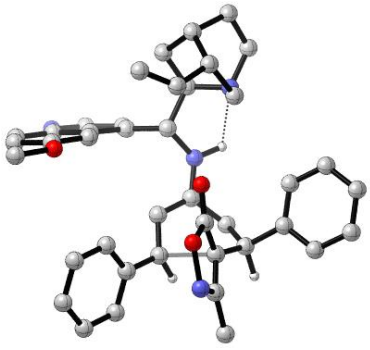
TS(6,10-*trans*-1q)-conf3



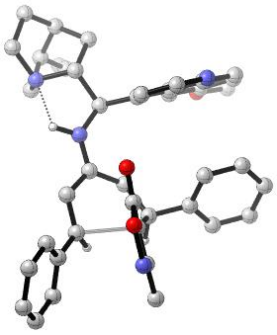
TS(6,10-*trans*-1q)-conf4



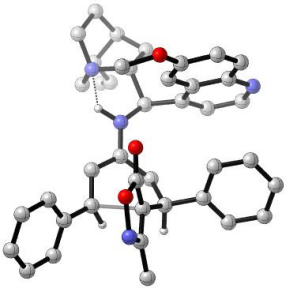
TS(6,10-*trans*-1q)-conf2



TS(6,10-*cis*-1m)-conf2

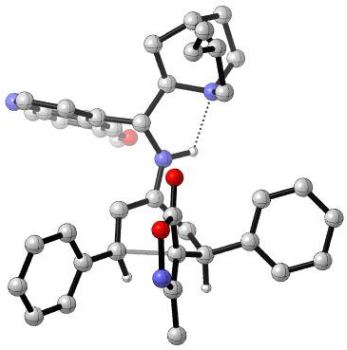


TS(6,10-*cis*-1m)-conf3



TS(6,10-*cis*-1m)-conf4

Table S11: Geometries obtained for transition states involved in enantioselective studies. Energies in Hartree, in toluene (continued).



TS(6,10-*cis*-1m)

	B3LYP-GD3/6-31G/IEF-PCM			M06-2X/6-311+G(d,p)/IEF-PCM // B3LYP-GD3/6-31G/IEF-PCM	
	ΔE_{ele}	Thermal correction to Gibbs Free Energy	Imaginary Frequency (cm^{-1})	ΔE_{ele}	ΔG*
TS(6,10-*trans*-ent-1q)	-2031.78646655	0.68344700	-162.5750	-2031.92234464	-2031.23889764
TS(6,10-*trans*-ent-1q)-conf3	-2031.78616063	0.68423200	-210.6885	-2031.92095946	-2031.23672746
TS(6,10-*trans*-ent-1q)-conf4	-2031.78618223	0.68529800	-227.3546	-2031.92109288	-2031.23579488
TS(6,10-*trans*-ent-1q)-conf2	-2031.79160326	0.68655700	-123.0051	-2031.92241008	-2031.23585308
TS(6,10-*trans*-1q)	-2031.79459166	0.68663300	-286.4699	-2031.92868780	-2031.24205480
TS(6,10-*trans*-1q)-conf3	-2031.78561882	0.68408900	-178.0495	-2031.92324019	-2031.23915119
TS(6,10-*trans*-1q)-conf4	-2031.79156116	0.68644200	-146.5338	-2031.92147559	-2031.23503359
TS(6,10-*trans*-1q)-conf2	-2031.78987572	0.68495200	-288.4435	-2031.92593192	-2031.24097992
TS(6,10-*cis*-1m)-conf2	-2031.79601165	0.68844700	-190.9851	-2031.92603402	-2031.23758702
TS(6,10-*cis*-1m)-conf3	-2031.78159877	0.68374900	-144.1760	-2031.91404432	-2031.23029532
TS(6,10-*cis*-1m)-conf4	-2031.78785728	0.68475400	-167.5726	-2031.91737420	-2031.23262020
TS(6,10-*cis*-1m)	-2031.78879733	0.68429400	-207.6649	-2031.92306652	-2031.23877252

* Obtained from the sum of ΔE_{ele} at **M06-2X/6-311+G(d,p)/IEF-PCM** // **B3LYP-GD3/6-31G/IEF-PCM** and **Thermal correction to Gibbs Free Energy** at **B3LYP-GD3/6-31G/IEF-PCM**.

7. Intrinsic Reaction Coordinates

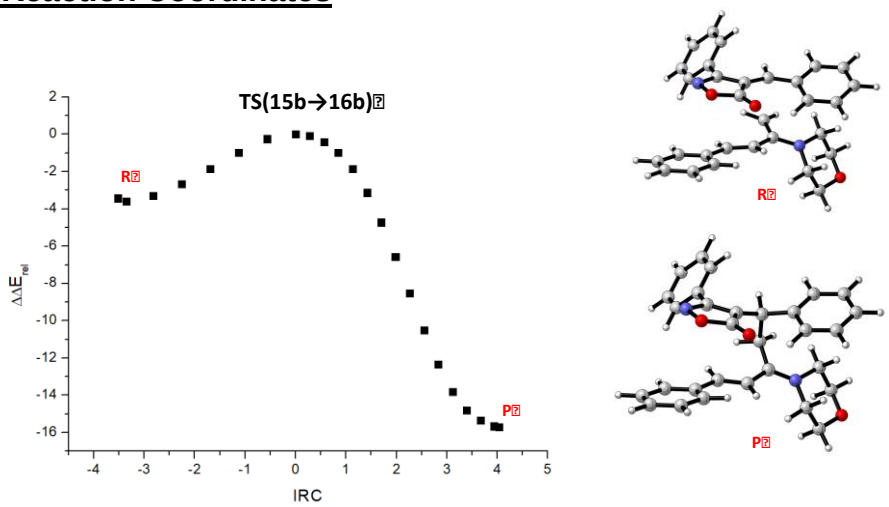


Figure S1. Intrinsic Reaction Coordinate (IRC) of **TS(15b→16b)**.

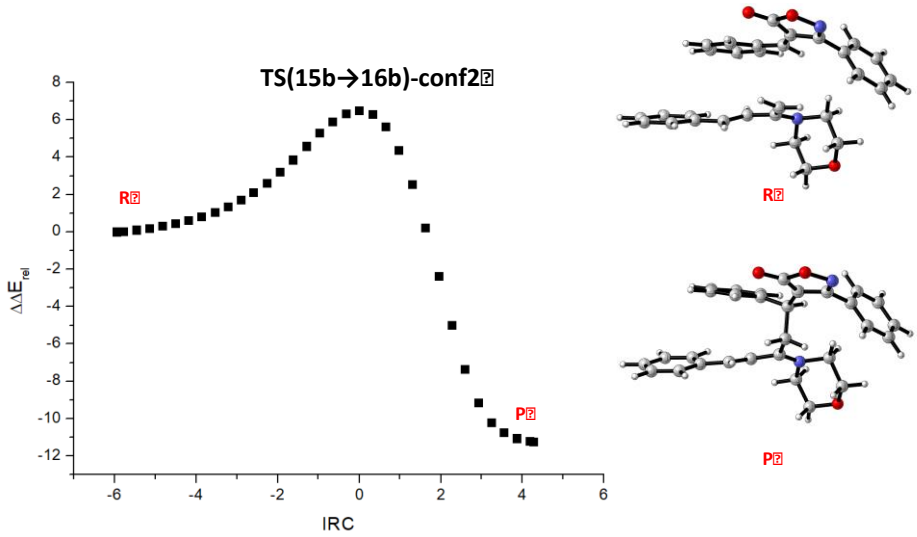


Figure S2. Intrinsic Reaction Coordinate (IRC) of **TS(15b→16b)-conf2**.

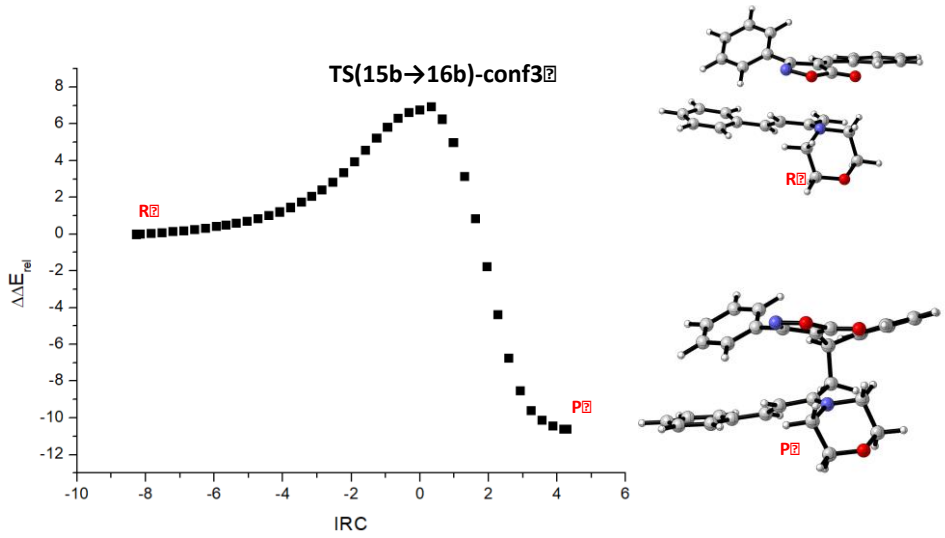


Figure S3. Intrinsic Reaction Coordinate (IRC) of **TS(15b→16b)-conf3**.

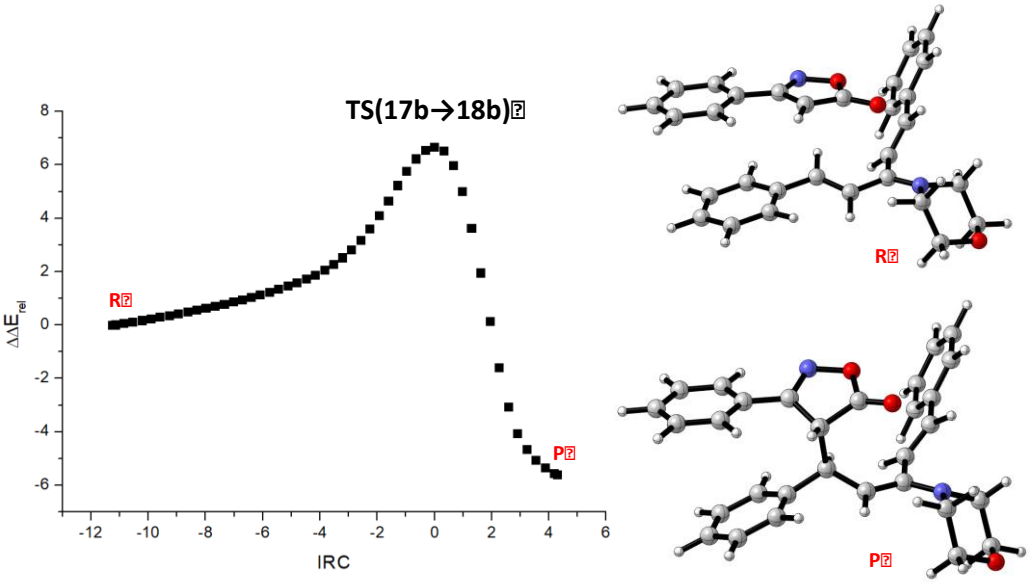


Figure S4. Intrinsic Reaction Coordinate (IRC) of **TS(17b→18b)**.

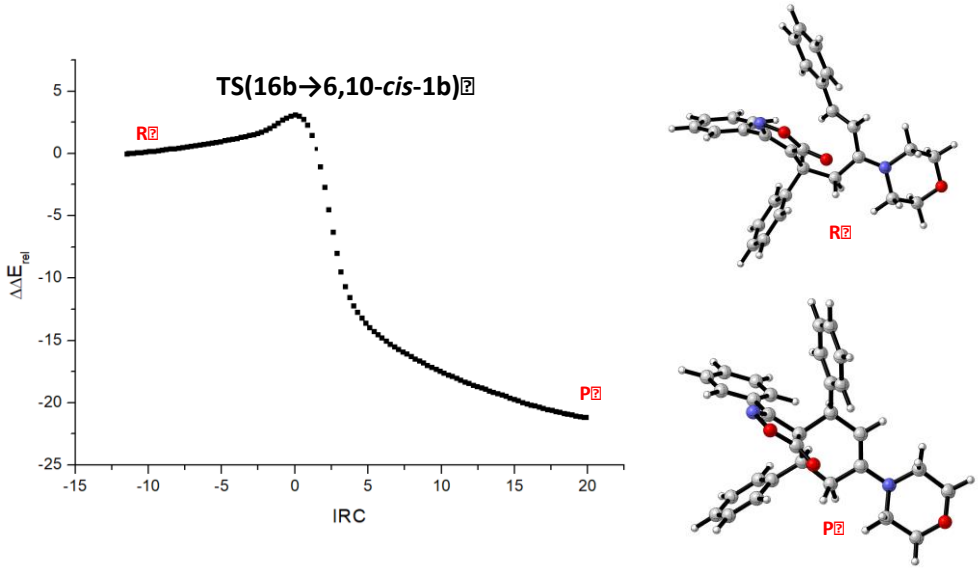


Figure S5. Intrinsic Reaction Coordinate (IRC) of **TS(16b→6,10-*cis*-1b)**.

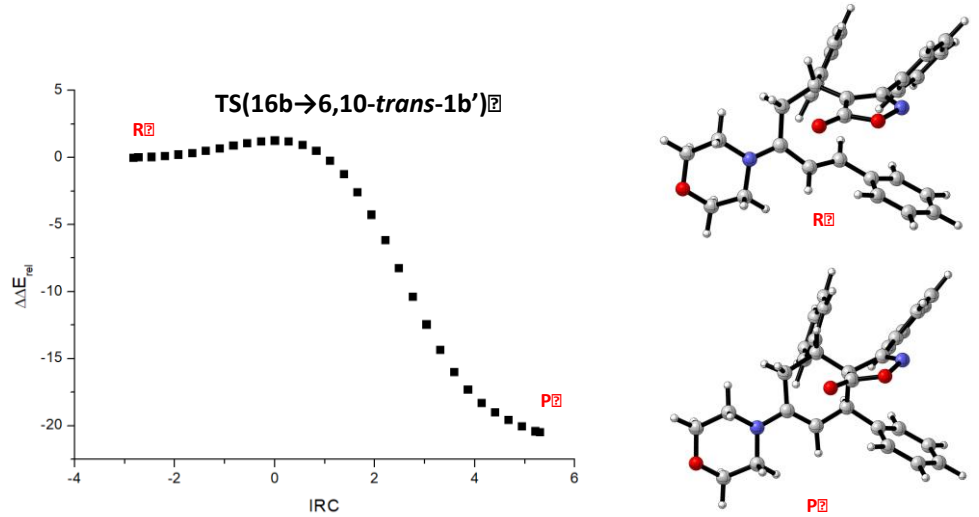


Figure S6. Intrinsic Reaction Coordinate (IRC) of **TS(16b→6,10-*trans*-1b')**.

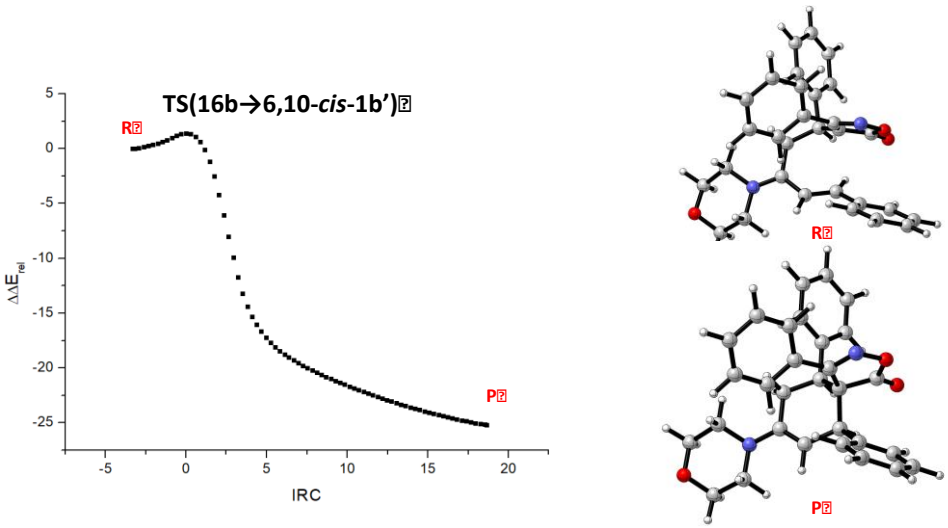


Figure S7. Intrinsic Reaction Coordinate (IRC) of **TS(16b→6,10-*cis*-1b')**.

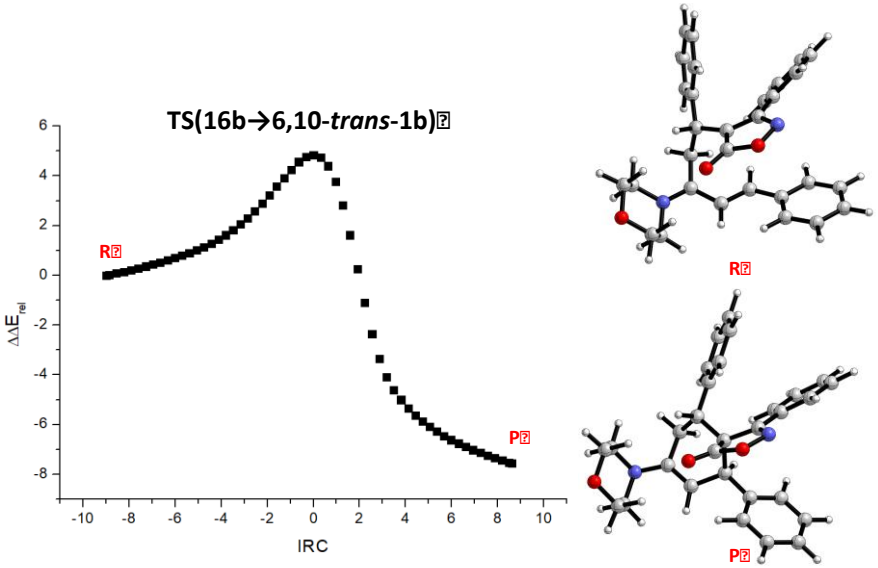


Figure S8. Intrinsic Reaction Coordinate (IRC) of **TS(16b→6,10-*trans*-1b)**.

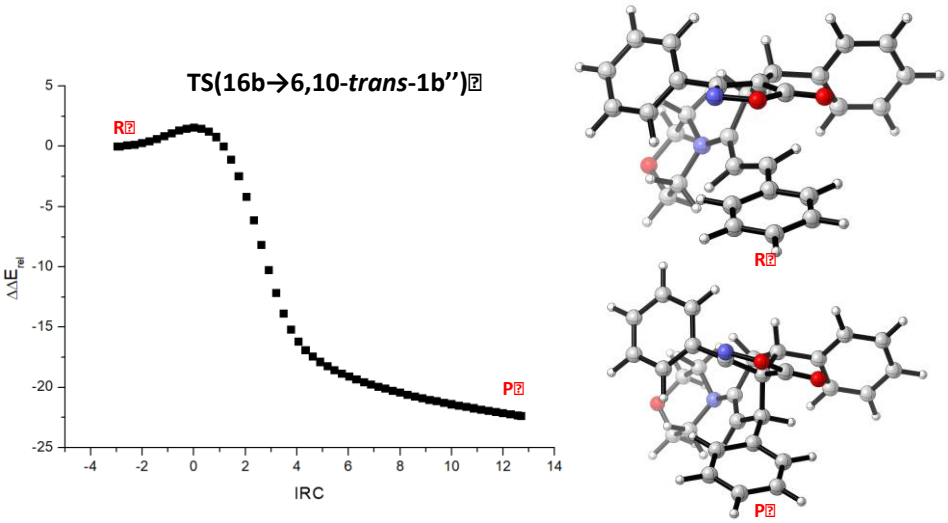


Figure S9 Intrinsic Reaction Coordinate (IRC) of **TS(16b→6,10-*trans*-1b'')**

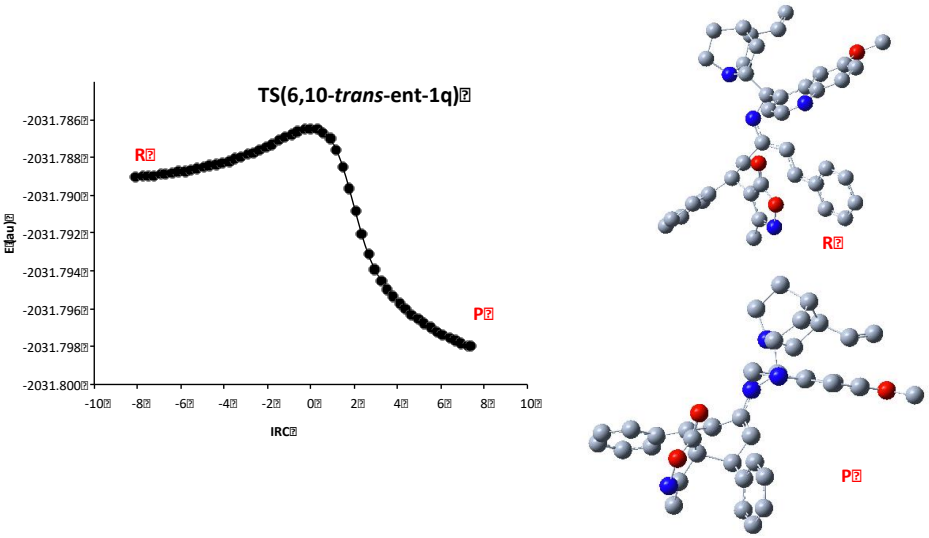


Figure S10 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-ent-1q)**.

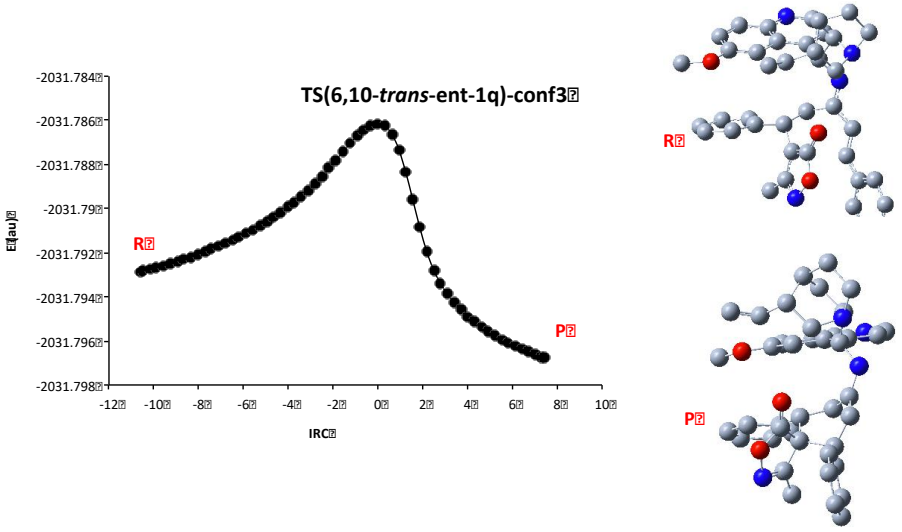


Figure S11 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-ent-1q)-conf3**.

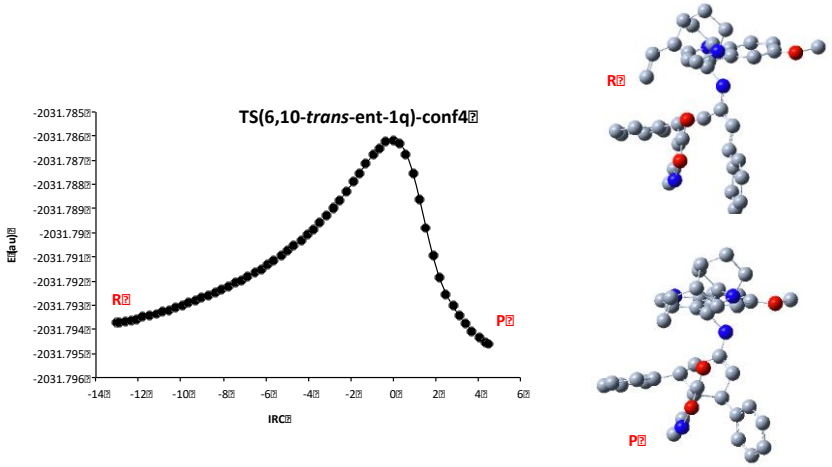


Figure S12 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-ent-1q)-conf4**.

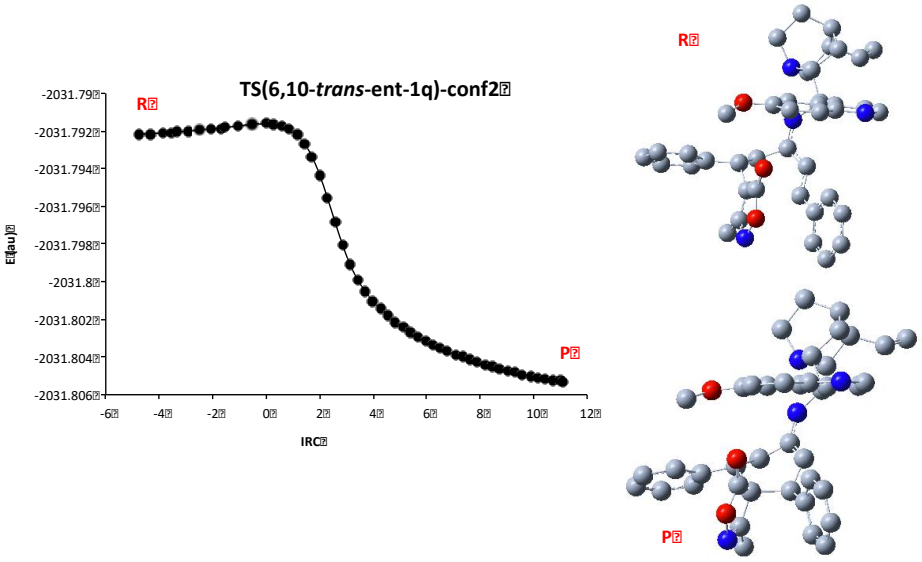


Figure S13 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-ent-1q)-conf2**.

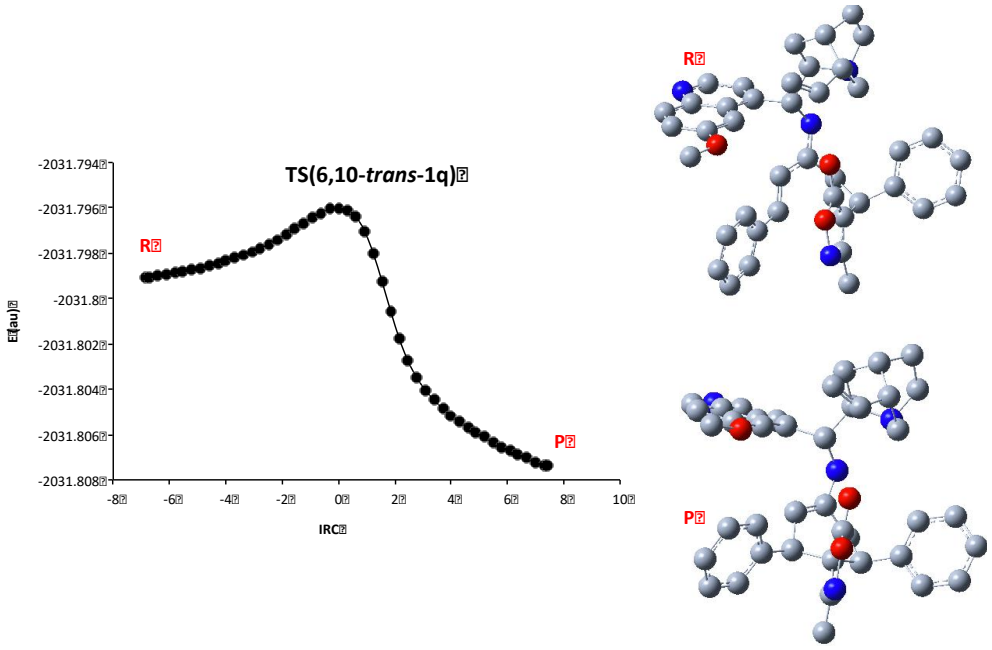


Figure S14 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-1q)**.

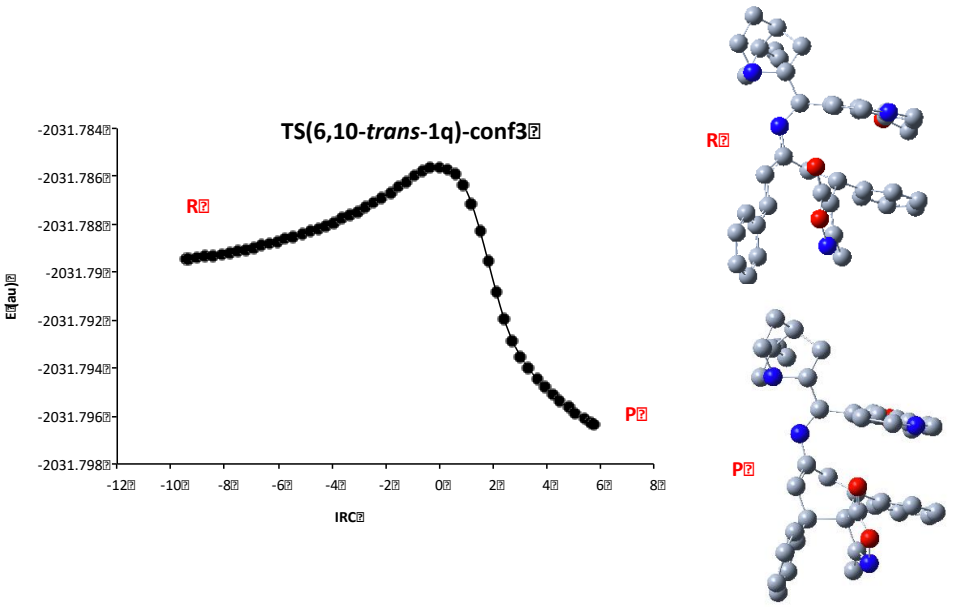


Figure S15 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-1q)-conf3**.

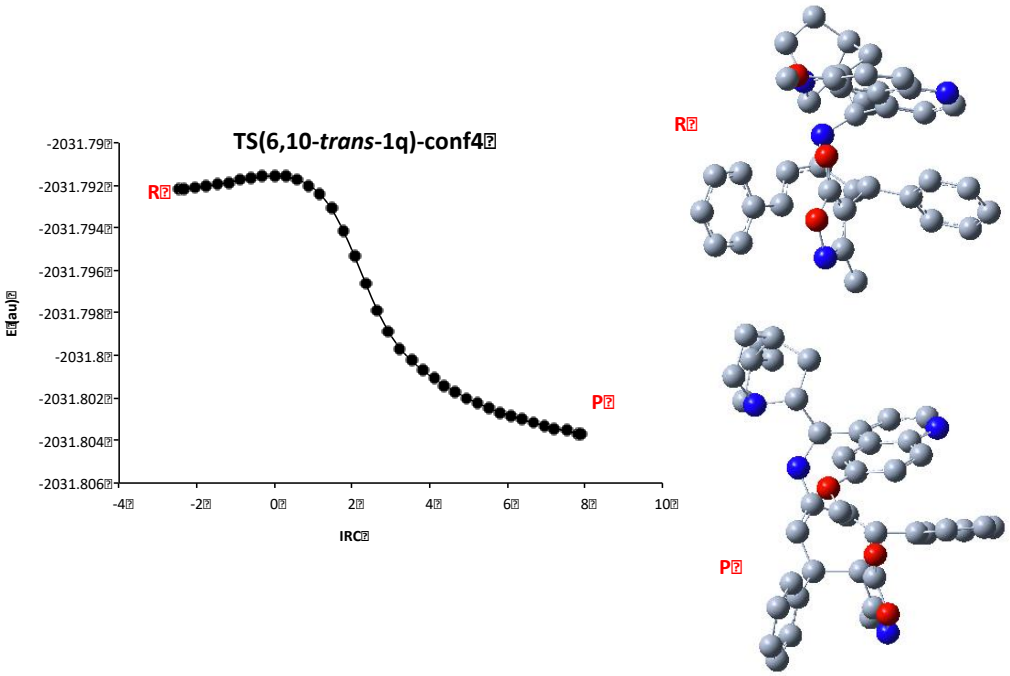


Figure S16 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-1q)-conf4**.

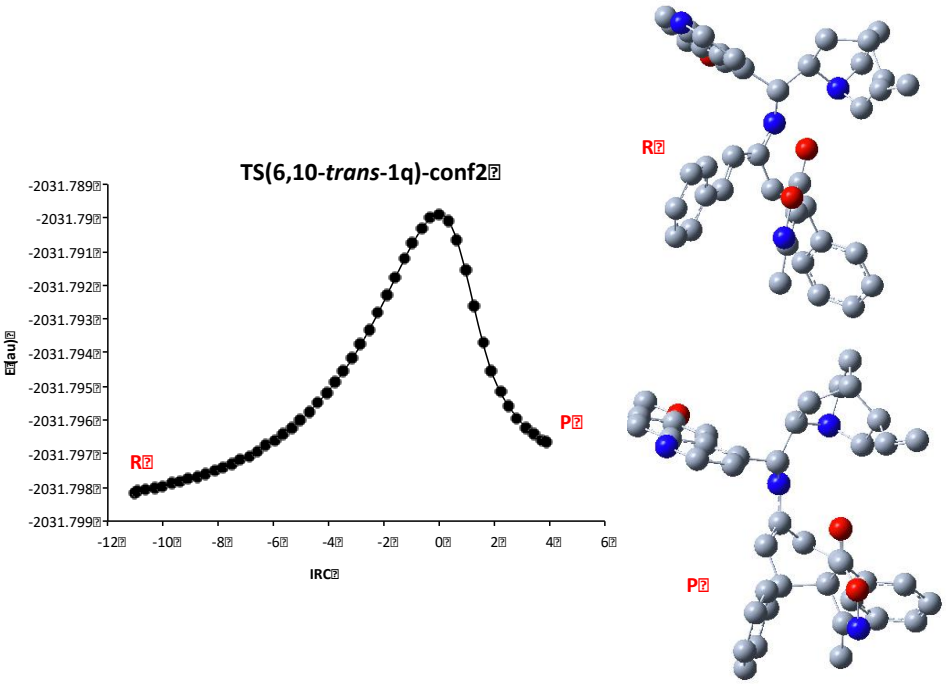


Figure S17 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*trans*-1q)-conf2**.

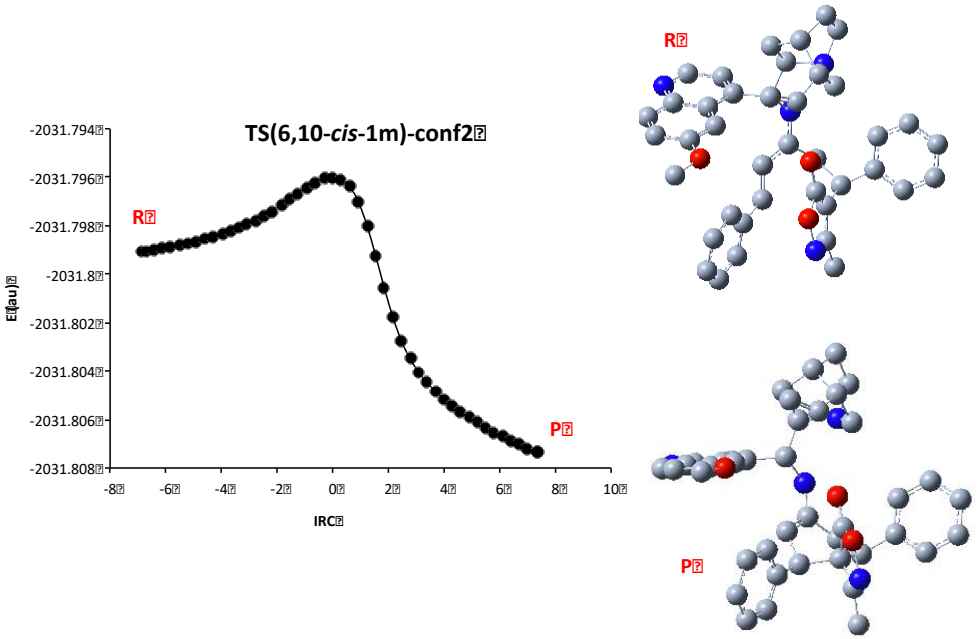


Figure S18 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*cis*-1m)-conf2**.

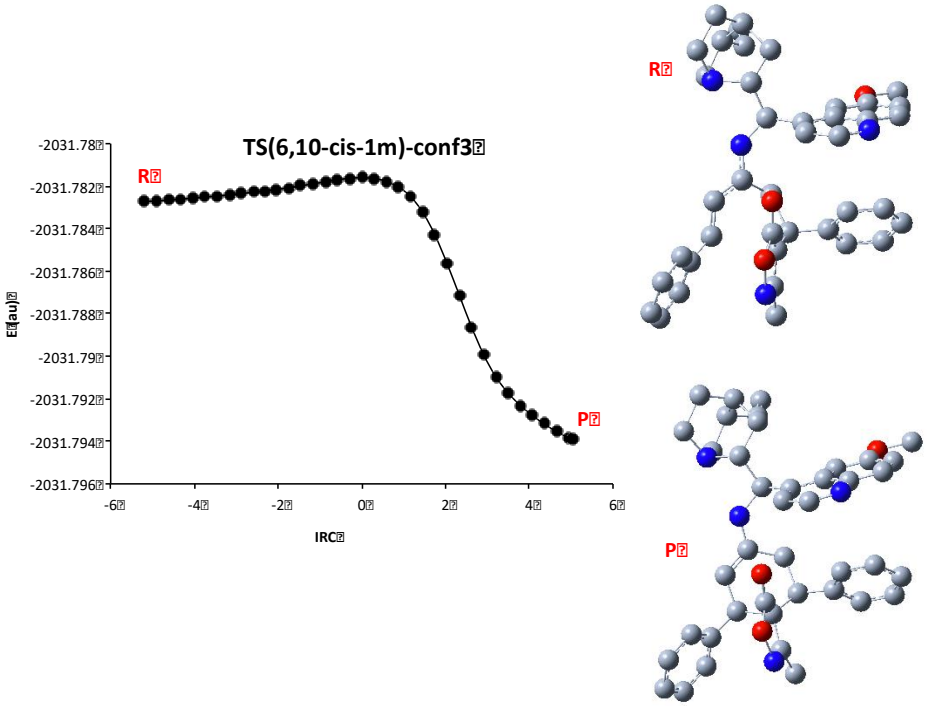


Figure S19 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*cis*-1m)-conf3**.

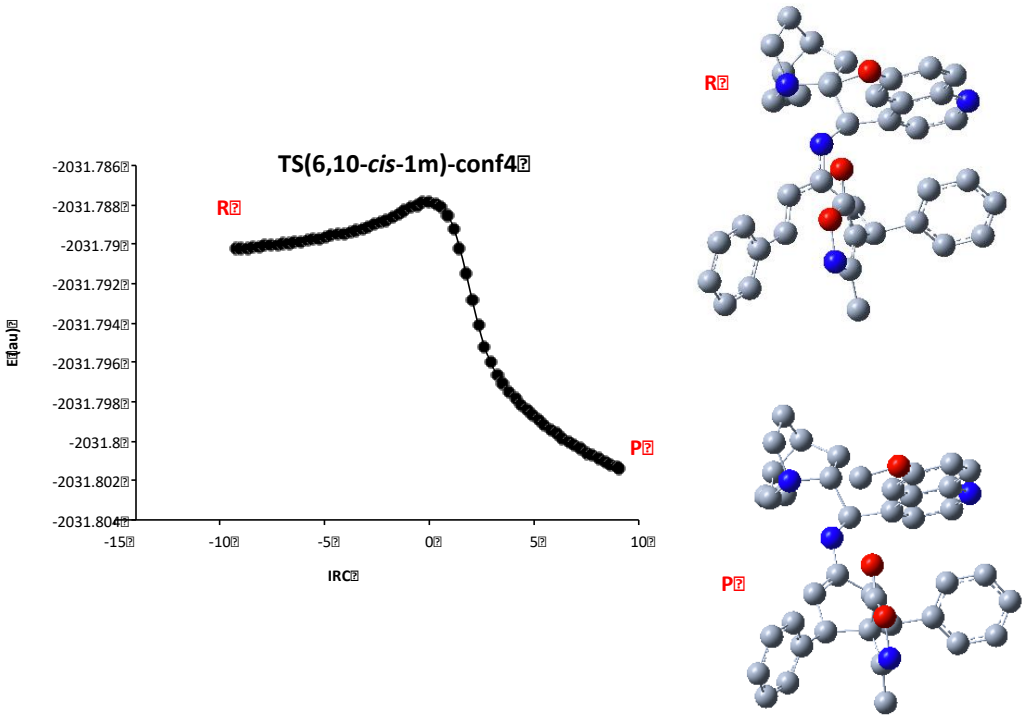


Figure S20 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*cis*-1m)-conf4**.

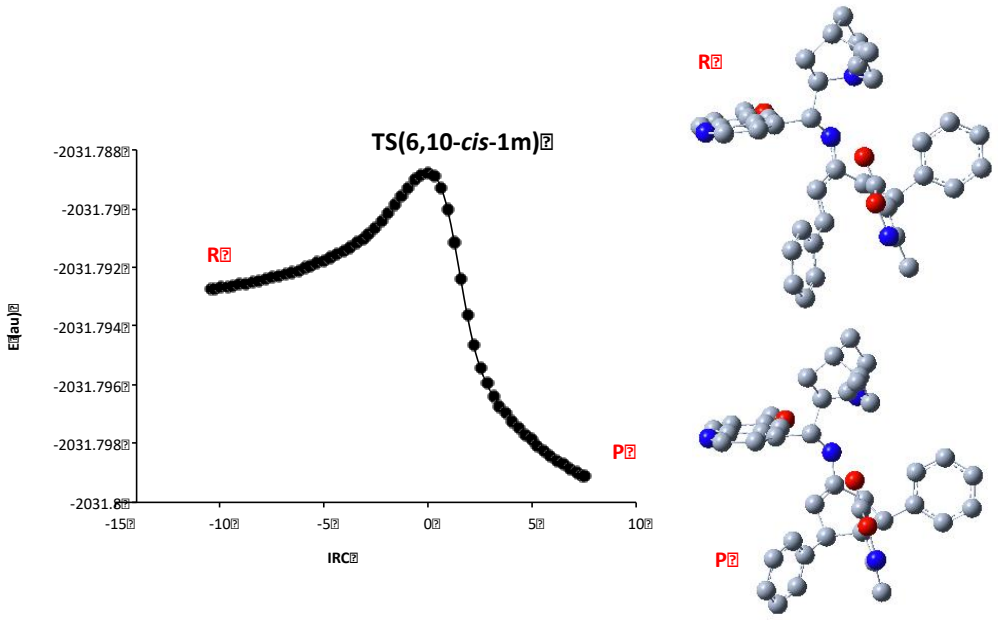


Figure S21 Intrinsic Reaction Coordinate (IRC) of **TS(6,10-*cis*-1m)**.

8. Cartesian Coordinates

enamine

C	0.71591	0.20147	-0.03891
C	1.17261	1.44800	0.20737
H	2.23985	1.61492	0.29067
H	0.52524	2.30905	0.31198
C	1.67593	-0.95964	-0.13168
H	1.51093	-1.53405	-1.04874
H	2.70242	-0.59144	-0.13069
H	1.56159	-1.64400	0.71474
C	-1.13213	-1.37268	0.23419
H	-1.19178	-1.38819	1.33407
H	-2.13387	-1.53716	-0.16745
H	-0.50096	-2.19869	-0.09280
C	-1.57253	0.99022	-0.11501
H	-1.61202	1.36388	0.92146
H	-1.29725	1.82023	-0.77016
H	-2.56697	0.64171	-0.39892
N	-0.62799	-0.10006	-0.27142

iminium

C	0.66992	-0.00002	0.00001
C	1.43801	-1.27951	-0.05397
H	0.93846	-2.04403	-0.64792
H	2.42681	-1.08540	-0.46934
H	1.57429	-1.65640	0.96688
C	1.43821	1.27944	0.05393
H	0.94000	2.04260	0.65082
H	2.42815	1.08483	0.46625
H	1.57145	1.65855	-0.96648
C	-1.41992	1.23724	-0.05140
H	-0.88135	2.01646	-0.58367
H	-2.34237	1.01328	-0.58500
H	-1.65485	1.55820	0.96578
C	-1.41984	-1.23723	0.05141
H	-1.65177	-1.56031	-0.96579
H	-0.88249	-2.01520	0.58679
H	-2.34386	-1.01247	0.58191
N	-0.62296	0.00005	-0.00001

2a$^-$

C	0.65594	-0.11754	0.02283
C	2.84696	0.31366	-0.06038
O	2.60745	-1.03160	0.18086
N	1.23249	-1.28832	0.23109
O	4.02883	0.70388	-0.13920
C	1.58668	0.92362	-0.16268
H	1.40424	1.96576	-0.37022
C	-0.82088	-0.02620	0.00558
C	-1.45149	1.21615	0.13823
C	-1.60957	-1.17493	-0.14315
C	-2.84246	1.31055	0.12359
H	-0.85088	2.11232	0.26241
C	-2.99893	-1.08067	-0.15422
H	-1.12332	-2.13881	-0.25496
C	-3.62092	0.16248	-0.02175
H	-3.31741	2.28103	0.22897
H	-3.59838	-1.97819	-0.27193
H	-4.70392	0.23517	-0.03347

2a

C	0.61075	0.15693	-0.00001
C	2.88290	-0.25432	0.00000
O	2.60100	1.08157	0.00017
N	1.20560	1.29523	0.00007
O	4.01338	-0.65831	-0.00002
C	1.56911	-0.99183	-0.00020
H	1.48499	-1.62715	0.88623
H	1.48510	-1.62684	-0.88686
C	-0.85581	0.05316	-0.00004
C	-1.45810	-1.20921	0.00009
C	-1.65571	1.20521	-0.00008
C	-2.84763	-1.32137	0.00012
H	-0.84848	-2.10769	0.00019
C	-3.04024	1.08801	-0.00008
H	-1.18660	2.18362	-0.00011
C	-3.63937	-0.17496	-0.00000
H	-3.30786	-2.30376	0.00020
H	-3.65579	1.98151	-0.00013
H	-4.72109	-0.26206	0.00003

5a$^-$

C	-1.11764	0.54153	0.00000
C	0.70029	1.87871	0.00000
N	-0.08842	-0.30017	0.00000
O	1.55294	2.81105	0.00000
C	-0.71139	1.88947	0.00000
H	-1.31837	2.78197	0.00000
C	-2.49686	0.01101	0.00000
C	-3.59610	0.87944	0.00000
C	-2.73487	-1.37129	-0.00001
C	-4.89866	0.38182	0.00000
H	-3.43302	1.95298	0.00001
C	-4.03531	-1.86848	-0.00001
H	-1.88707	-2.04888	-0.00001
C	-5.12487	-0.99444	-0.00000
H	-5.73733	1.07149	0.00001
H	-4.20055	-2.94178	-0.00001
H	-6.13852	-1.38280	-0.00000
N	1.02624	0.50166	0.00000
C	2.29435	-0.10157	0.00000
C	2.38658	-1.50460	0.00001
C	3.47677	0.65856	-0.00001
C	3.63117	-2.12659	0.00001
H	1.47686	-2.09060	0.00001
C	4.71392	0.01527	-0.00001
H	3.40920	1.73713	-0.00001
C	4.80763	-1.37563	0.00000
H	3.67786	-3.21178	0.00001
H	5.61669	0.61940	-0.00001

H	5.77608	-1.86521	0.00000

5a

C	-1.12530	0.49424	0.01354
C	0.76355	1.86040	0.10949
N	-0.09397	-0.27360	-0.05996
O	1.56895	2.76989	0.20262
C	-0.74863	1.94122	0.12211
H	-1.10603	2.54277	-0.71960
H	-1.09736	2.41147	1.04645
C	-2.49546	-0.03433	-0.01929
C	-3.58301	0.84339	0.05092
C	-2.72784	-1.41414	-0.11986
C	-4.88687	0.35036	0.02065
H	-3.41615	1.91365	0.12898
C	-4.02884	-1.90164	-0.14964
H	-1.88329	-2.09343	-0.17412
C	-5.11236	-1.02106	-0.07957
H	-5.72372	1.03888	0.07527
H	-4.20162	-2.97018	-0.22769
H	-6.12707	-1.40528	-0.10329
N	1.04904	0.51452	-0.02072
C	2.31630	-0.11524	-0.01981
C	2.40683	-1.46468	0.33920
C	3.46461	0.59753	-0.38315
C	3.64825	-2.09455	0.33748
H	1.51046	-2.00720	0.61350
C	4.69963	-0.04855	-0.37162
H	3.39054	1.63829	-0.66831
C	4.80112	-1.39200	-0.01373
H	3.71110	-3.14139	0.61712
H	5.58755	0.50814	-0.65406
H	5.76661	-1.88689	-0.01071

Geometries involving spiroisoxal-5-one

9b

C	-1.39528	1.05877	0.03422
O	-0.60162	3.09185	-0.03142
N	-1.76383	2.29487	-0.01407
C	-2.40532	-0.01647	0.05154
C	-2.30717	-1.06649	0.97272
C	-3.48056	0.02779	-0.84307
C	-3.27865	-2.06448	0.99497
H	-1.48843	-1.09065	1.68610
C	-4.44799	-0.97366	-0.81752
H	-3.54569	0.84160	-1.55834
C	-4.34723	-2.02087	0.09912
H	-3.20288	-2.87270	1.71484
H	-5.27768	-0.93869	-1.51594
H	-5.10085	-2.80158	0.11583
C	0.05922	0.91974	0.06184
C	0.72372	-0.25928	-0.04648
H	0.07230	-1.12540	-0.16518
C	2.13775	-0.59767	-0.05972
C	2.46361	-1.90411	-0.47544
C	3.17258	0.26713	0.34338
C	3.78587	-2.32697	-0.52100
H	1.66769	-2.58306	-0.76838
C	4.49277	-0.16769	0.31126
H	2.93901	1.26737	0.68264
C	4.80370	-1.45685	-0.12676
H	4.02278	-3.33202	-0.85319
H	5.28461	0.50177	0.63044
H	5.83781	-1.78543	-0.15277
C	0.52443	2.32062	0.04283
O	1.61780	2.83535	0.05032

3b

C	-3.00099	-0.21608	-0.00000
C	-1.55792	-0.53704	0.00006
H	-1.33675	-1.60116	0.00028
C	-0.59048	0.39568	-0.00011
H	-0.87822	1.44614	-0.00031
O	-3.81960	-1.12779	0.00006
C	-3.45071	1.22654	-0.00014
H	-3.07110	1.74790	0.88324
H	-3.07096	1.74779	-0.88352
H	-4.53974	1.25773	-0.00022
C	0.85936	0.15889	-0.00003
C	1.71692	1.26871	-0.00023
C	1.42203	-1.12814	0.00022
C	3.10034	1.10316	-0.00017
H	1.29179	2.26885	-0.00042
C	2.80229	-1.29352	0.00028
H	0.78247	-2.00495	0.00037
C	3.64638	-0.17926	0.00008
H	3.74877	1.97331	-0.00032
H	3.22383	-2.29356	0.00047
H	4.72337	-0.31337	0.00013

morpholine

C	1.17332	-0.75265	0.19787
C	1.19885	0.71460	-0.20134
C	-1.19864	0.71493	-0.20134
C	-1.17353	-0.75233	0.19787
H	2.08929	1.19427	0.21492
H	1.20625	-0.83791	1.29477
H	2.02282	-1.29049	-0.22851
H	-2.08895	1.19485	0.21492
H	-1.25052	0.77949	-1.30190
H	-1.20649	-0.83758	1.29477
H	-2.02318	-1.28993	-0.22851
H	1.25073	0.77914	-1.30190
N	0.00019	1.36187	0.33177
H	0.00033	2.34797	0.08924
O	-0.00019	-1.39002	-0.29108

15b-s-cis-conf1

C	-1.33273	0.86764	0.19530
H	-1.26717	1.72750	0.86130

C	-0.21030	0.43650	-0.39883
H	-0.21892	-0.46512	-1.01017
C	1.09783	1.11705	-0.27681
C	1.19077	2.46257	-0.27090
H	0.30105	3.06053	-0.42617
H	2.13110	2.98513	-0.14846
C	-2.67155	0.26909	0.06278
C	-3.67591	0.65655	0.96191
C	-2.99061	-0.67355	-0.92824
C	-4.95503	0.10800	0.88989
H	-3.44599	1.39294	1.72762
C	-4.26682	-1.22305	-1.00019
H	-2.24246	-0.96998	-1.65720
C	-5.25453	-0.83695	-0.09041
H	-5.71640	0.41981	1.59801
H	-4.49582	-1.94873	-1.77443
H	-6.25012	-1.26472	-0.15195
C	3.52262	0.86951	-0.25063
C	2.13235	-0.83869	0.72491
C	4.59342	-0.18949	-0.46548
H	3.70813	1.39508	0.70279
H	3.57701	1.60181	-1.06123
C	3.24534	-1.84129	0.47208
H	2.22886	-0.43401	1.74713
H	1.16557	-1.34168	0.64989
H	5.58693	0.25560	-0.38365
H	4.47963	-0.63155	-1.46672
H	3.24524	-2.61215	1.24525
H	3.10161	-2.31575	-0.51043
N	2.20466	0.24852	-0.25844
O	4.51626	-1.21220	0.51439

water

O	0.00000	0.00000	0.11701
H	0.00000	0.76588	-0.46803
H	0.00000	-0.76588	-0.46803

TS(15b→16b)-conf2

C	-2.56046	0.67252	-1.03219
H	-2.19772	0.27041	-1.97686
C	-1.67993	1.22370	-0.17933
H	-2.02925	1.65485	0.75445
C	-0.22460	1.22058	-0.38968
C	-4.00911	0.55914	-0.82430
C	-4.78626	-0.01199	-1.84255
C	-4.64879	0.97576	0.35506
C	-6.16340	-0.16401	-1.69341
H	-4.30154	-0.34231	-2.75751
C	-6.02291	0.82688	0.50355
H	-4.07231	1.40598	1.16827
C	-6.78604	0.25587	-0.51901
H	-6.74741	-0.60986	-2.49215
H	-6.50219	1.15133	1.42184
H	-7.85822	0.13915	-0.39738
C	1.94610	2.24350	0.20856
C	-0.06853	3.50192	0.56582
C	2.36944	3.24633	-0.86007
H	2.30472	2.58711	1.18555
H	2.37477	1.25945	0.02123
C	0.40423	4.48300	-0.50670
H	0.29382	3.81882	1.54927
H	-1.15672	3.47886	0.58342
H	3.45526	3.36153	-0.87073
H	2.03273	2.90416	-1.85105
H	0.06822	5.49488	-0.27177
H	-0.00917	4.18225	-1.48192
N	0.48640	2.17527	0.27661
C	0.37650	0.16637	-1.06438
H	-0.26356	-0.53957	-1.57666
H	1.40125	0.22864	-1.40947
C	0.78400	-1.33145	0.55486
H	1.36834	-0.57663	1.07849
C	-0.57327	-1.46750	1.10566
C	-0.87615	-0.71039	2.24891
C	-1.59138	-2.22615	0.50730
C	-2.15493	-0.73078	2.80017
H	-0.10146	-0.09775	2.70406
C	-2.87109	-2.23606	1.05520
H	-1.37760	-2.80037	-0.38595
C	-3.15710	-1.49463	2.20235
H	-2.36987	-0.14391	3.68771
H	-3.65393	-2.81647	0.57627
H	-4.15920	-1.50202	2.61995
C	1.56637	-2.29872	-0.09224
C	1.23389	-3.54993	-0.73486
C	2.96709	-2.13319	-0.38498
O	2.40258	-4.01424	-1.29697
O	0.21322	-4.21138	-0.85921
N	3.45909	-3.11495	-1.07957
C	3.81753	-0.98053	-0.01783
C	3.96692	-0.60749	1.32371
C	4.44996	-0.23531	-1.01938
C	4.73652	0.50507	1.65768
H	3.48758	-1.19406	2.10276
C	5.21540	0.88013	-0.68163
H	4.32548	-0.52534	-2.05839
C	5.35525	1.25404	0.65550
H	4.84999	0.78900	2.69889
H	5.69659	1.46010	-1.46281
H	5.94571	2.12669	0.91620
O	1.81991	4.52474	-0.57704

TS(15b→16b)-conf3

C	1.86071	0.81070	-1.54772
H	1.49457	0.51583	-2.52996
C	0.98829	1.19836	-0.60374
H	1.35916	1.46559	0.38203
C	-0.47160	1.23378	-0.79365
C	3.31485	0.72643	-1.35102
C	4.05481	-0.17088	-2.13331

C	3.98671	1.50244	-0.39373
C	5.42539	-0.32337	-1.93514
H	3.54564	-0.76574	-2.88707
C	5.35783	1.36065	-0.20568
H	3.43793	2.23389	0.19298
C	6.08031	0.44049	-0.96910
H	5.98218	-1.03402	-2.53767
H	5.86568	1.97129	0.53420
H	7.14942	0.32905	-0.81858
C	-2.62853	2.19227	-0.08676
C	-0.60403	3.28066	0.60104
C	-2.95856	3.39085	-0.97098
H	-3.01528	2.36121	0.92252
H	-3.07810	1.26984	-0.45136
C	-0.99380	4.47268	-0.27444
H	-1.01708	3.39670	1.60803
H	0.47997	3.22033	0.67184
H	-4.03763	3.54481	-1.02458
H	-2.56434	3.23100	-1.98628
H	-0.65248	5.40422	0.18082
H	-0.52537	4.36159	-1.26468
N	-1.17430	2.06035	0.01756
C	-1.08969	0.27704	-1.58836
H	-0.46008	-0.34291	-2.21347
H	-2.11331	0.39049	-1.91600
C	-1.43136	-1.30304	-0.03139
H	-0.55296	-1.80310	-0.43088
C	-2.68102	-1.81768	-0.63124
C	-2.54910	-2.69243	-1.72371
C	-3.96828	-1.50392	-0.17056
C	-3.66791	-3.24289	-2.33922
H	-1.55585	-2.94206	-2.08937
C	-5.08758	-2.05566	-0.79231
H	-4.08674	-0.83182	0.67178
C	-4.94528	-2.92319	-1.87516
H	-3.54419	-3.92040	-3.17800
H	-6.07815	-1.80594	-0.42493
H	-5.82181	-3.34905	-2.35306
C	-1.21714	-0.80607	1.26520
C	-2.04343	-0.02585	2.15838
C	0.07213	-0.80607	1.91893
O	-1.22527	0.37581	3.19131
O	-3.21955	0.31673	2.17490
N	0.06801	-0.13766	3.03602
C	1.30293	-1.52207	1.51370
C	1.23727	-2.84781	1.06529
C	2.54959	-0.89504	1.61394
C	2.40058	-3.52594	0.70572
H	0.27878	-3.35706	1.01893
C	3.71058	-1.57290	1.25042
H	2.60421	0.13172	1.96464
C	3.63844	-2.88819	0.79212
H	2.33877	-4.55371	0.36261
H	4.66900	-1.06559	1.30765
H	4.54313	-3.41335	0.50196
O	-2.40015	4.57224	-0.41548

TS(15b→16b)

C	0.22907	-1.49886	-0.68343
C	1.19846	-0.47033	-1.08655
H	0.57916	-2.24543	0.02337
C	-0.82843	0.85787	1.22389
C	0.37408	1.46225	0.84654
H	0.24679	2.43639	0.38160
C	-1.06697	-1.49602	-1.04461
H	-1.41053	-0.76896	-1.77949
C	0.73855	0.81355	-1.33368
H	1.38640	1.59817	-1.70225
H	-0.31990	0.96350	-1.49384
C	-2.10340	-2.40960	-0.55038
C	-3.39632	-2.30225	-1.08291
C	-1.86558	-3.36457	0.45207
C	-4.42655	-3.12526	-0.63295
H	-3.59273	-1.56333	-1.85563
C	-2.89240	-4.18737	0.89944
H	-0.88136	-3.45474	0.90062
C	-4.17668	-4.07125	0.35975
H	-5.42128	-3.02605	-1.05546
H	-2.69502	-4.91804	1.67742
H	-4.97613	-4.71368	0.71503
C	3.03819	-2.14804	-0.91280
C	3.59749	0.18443	-1.14960
C	3.92732	-2.43229	-2.12231
H	3.62242	-2.24620	0.01234
H	2.22930	-2.87601	-0.89787
C	4.44929	-0.16693	-2.36281
H	3.20776	1.19626	-1.23004
H	4.21905	0.13728	-0.24448
H	4.39838	-3.41178	-2.01912
H	3.31390	-2.42081	-3.03589
H	5.30343	0.50872	-2.43766
H	3.84670	-0.09220	-3.28058
N	2.51748	-0.78563	-0.99837
O	4.97077	-1.48056	-2.23565
C	1.72021	1.27880	1.41122
C	2.58152	2.39058	1.38643
C	2.20002	0.06585	1.93100
C	3.87349	2.30621	1.89248
H	2.22654	3.32833	0.96597
C	3.49933	-0.01885	2.42822
H	1.55119	-0.80138	1.95547
C	4.33745	1.09666	2.41511
H	4.51955	3.17796	1.87483
H	3.85880	-0.96304	2.82580
H	5.34761	1.02398	2.80573
C	-2.12732	1.27751	0.75238
C	-2.43952	2.39618	-0.16301
C	-1.99363	3.69513	0.11033
C	-3.19819	2.15436	-1.31389
C	-2.30061	4.73724	-0.76213

H	-1.42849	3.89383	1.01682
C	-3.50262	3.19861	-2.18507
H	-3.54394	1.14545	-1.51966
C	-3.05128	4.49001	-1.91229
H	-1.95814	5.74291	-0.54084
H	-4.08938	3.00305	-3.07683
H	-3.28660	5.30280	-2.59189
O	-2.49389	-0.46047	1.99330
C	-1.12641	-0.31775	2.01690
O	-0.45910	-1.12010	2.65423
N	-3.08991	0.52231	1.19085

16b

C	2.70275	0.61199	-0.25233
H	2.42386	1.34681	0.50033
C	1.90115	0.46372	-1.32243
C	0.63125	1.17430	-1.46073
C	3.84891	-0.23881	0.07570
C	4.36658	-0.17685	1.37724
C	4.41815	-1.13722	-0.84084
C	5.41588	-1.00740	1.76508
H	3.93029	0.51831	2.08970
C	5.46868	-1.96095	-0.45572
H	4.04288	-1.19232	-1.85828
C	5.96699	-1.90271	0.84961
H	5.80143	-0.95512	2.77805
H	5.90258	-2.65139	-1.17185
H	6.78548	-2.55053	1.14698
C	-0.76298	3.19674	-1.25792
C	1.65736	3.40318	-1.24320
C	-0.77556	4.09480	-0.01700
H	-0.85176	3.79945	-2.16736
H	-1.59349	2.49836	-1.18827
C	1.54584	4.23051	0.03058
H	1.56756	4.06926	-2.10805
H	2.59631	2.86110	-1.30316
H	-1.67384	4.71355	-0.05036
H	-0.78681	3.47531	0.88675
H	2.36633	4.94833	0.07099
H	1.57506	3.57750	0.91333
N	0.51974	2.46665	-1.33309
C	-0.53855	0.30787	-1.83330
H	-1.37121	0.89813	-2.21252
H	-0.18194	-0.31102	-2.66507
C	-1.06949	-0.65014	-0.71598
H	-1.93368	-1.11617	-1.20319
C	-0.08767	-1.78297	-0.42890
C	0.68566	-1.83738	0.73397
C	0.06620	-2.79599	-1.38326
C	1.60397	-2.87035	0.92744
H	0.59416	-1.04769	1.47348
C	0.97940	-3.83218	-1.19174
H	-0.53900	-2.77521	-2.28804
C	1.75592	-3.87000	-0.03291
H	2.21086	-2.88580	1.82847
H	1.08005	-4.60976	-1.94293
H	2.47293	-4.67096	0.11939
C	-1.60139	0.08030	0.48323
C	-0.91820	0.96228	1.34016
C	-2.93384	0.09207	0.96107
O	-1.84826	1.45582	2.23269
O	0.26526	1.35349	1.42666
N	-3.10789	0.89608	1.99209
C	-4.08543	-0.69275	0.46282
C	-5.33693	-0.09015	0.29039
C	-3.93964	-2.05787	0.18337
C	-6.42380	-0.83958	-0.15683
H	-5.44883	0.96835	0.50412
C	-5.02677	-2.80578	-0.26532
H	-2.97573	-2.53755	0.33741
C	-6.27085	-2.19785	-0.43789
H	-7.38961	-0.36210	-0.28978
H	-4.90372	-3.86394	-0.47383
H	-7.11723	-2.78020	-0.78822
O	0.33703	4.96960	0.01057
H	2.04012	-0.36015	-2.01666

16b-conf2

C	1.48869	-0.40993	-1.58963
H	1.13642	0.45118	-2.15583
C	0.59312	-1.31049	-1.13759
C	-0.84382	-1.15328	-1.33431
C	2.93766	-0.46347	-1.39740
C	3.60208	-1.59618	-0.89934
C	3.68859	0.67653	-1.72223
C	4.98000	-1.57913	-0.72236
H	3.04664	-2.49734	-0.65817
C	5.06753	0.69618	-1.53529
H	3.17981	1.55526	-2.11029
C	5.71518	-0.43258	-1.03468
H	5.48422	-2.46036	-0.33920
H	5.63461	1.58816	-1.78077
H	6.79124	-0.42356	-0.89230
C	-3.10549	-2.14377	-1.35315
C	-1.13435	-3.59027	-1.29927
C	-3.65919	-3.41725	-0.69903
H	-3.42266	-1.28735	-0.75882
H	-3.44117	-2.04802	-2.39087
C	-1.57475	-4.23397	0.01992
H	-0.05849	-3.64048	-1.43532
H	-1.59404	-4.08749	-2.15720
H	-4.66149	-3.20792	-0.32378
H	-3.72516	-4.25619	-1.40296
H	-0.88496	-3.97295	0.82628
H	-1.58912	-5.32370	-0.10464
N	-1.62060	-2.20217	-1.32973
C	-1.41173	0.23170	-1.50162
H	-1.02266	0.64159	-2.44219
H	-2.49625	0.20816	-1.59579
C	-1.00672	1.15634	-0.31767

H	0.07602	1.28859	-0.37714
C	-1.61221	2.53564	-0.51911
C	-0.83646	3.55017	-1.08941
C	-2.93981	2.81322	-0.17185
C	-1.36970	4.82129	-1.30854
H	0.19850	3.34493	-1.35810
C	-3.47489	4.08188	-0.39330
H	-3.54557	2.02638	0.27109
C	-2.69294	5.08975	-0.96099
H	-0.75116	5.59926	-1.74562
H	-4.50560	4.28601	-0.11876
H	-3.11163	6.07733	-1.12799
C	-1.27669	0.49788	1.00547
C	-2.47967	-0.07104	1.46168
C	-0.32246	0.13452	1.98509
O	-2.19883	-0.69134	2.66059
O	-3.64564	-0.12211	1.01111
N	-0.84081	-0.56172	2.97850
C	1.12766	0.42613	1.97506
C	2.05111	-0.58225	2.27170
C	1.59477	1.70646	1.64991
C	3.41898	-0.31590	2.24150
H	1.68822	-1.57784	2.51017
C	2.96291	1.96934	1.61503
H	0.88198	2.50002	1.43750
C	3.87833	0.95776	1.90789
H	4.12763	-1.10903	2.45999
H	3.31419	2.96409	1.35795
H	4.94437	1.15918	1.86743
O	-2.85418	-3.75632	0.41400
H	0.93087	-2.16420	-0.56067

16b-conf3

C	3.24338	-0.36758	-0.71563
H	3.51132	-1.32314	-1.16508
C	1.94888	-0.10155	-0.47267
C	0.86628	-1.00083	-0.87402
C	4.36331	0.54795	-0.46866
C	4.23030	1.70765	0.31226
C	5.61473	0.24377	-1.02326
C	5.32039	2.54576	0.51602
H	3.27836	1.94871	0.77592
C	6.70584	1.08587	-0.82061
H	5.72801	-0.65709	-1.62035
C	6.56023	2.23991	-0.05223
H	5.20689	3.43680	1.12493
H	7.66720	0.83960	-1.25953
H	7.40881	2.89654	0.11086
C	0.08982	-3.29423	-1.37201
C	1.86132	-2.92456	0.27073
C	-0.59944	-4.21001	-0.36911
H	-0.64549	-2.81129	-2.00785
H	0.77424	-3.88013	-1.99497
C	1.05466	-3.82132	1.20566
H	2.35247	-2.14794	0.85131
H	2.59658	-3.51182	-0.28791
H	-1.33229	-3.64289	0.21858
H	-1.11202	-5.00669	-0.91133
H	0.35887	-3.19737	1.78302
H	1.74059	-4.33094	1.88438
N	0.93250	-2.29047	-0.68966
C	-0.28717	-0.32644	-1.56269
H	0.09411	0.60492	-1.98536
H	-0.66238	-0.92368	-2.39440
C	-1.47681	0.05917	-0.60704
H	-2.06856	0.73014	-1.24151
C	-2.38820	-1.12748	-0.29087
C	-2.68411	-1.51852	1.01819
C	-3.01369	-1.81211	-1.34315
C	-3.56451	-2.57441	1.26874
H	-2.22431	-0.99661	1.84952
C	-3.88414	-2.87163	-1.09909
H	-2.83149	-1.50513	-2.37158
C	-4.16187	-3.25964	0.21361
H	-3.77673	-2.86136	2.29412
H	-4.35411	-3.38567	-1.93185
H	-4.84188	-4.08292	0.40825
C	-1.04534	0.85699	0.58548
C	-0.19689	0.43002	1.62173
C	-1.35271	2.19745	0.91400
O	-0.02684	1.50082	2.47156
O	0.38854	-0.64727	1.86074
N	-0.76438	2.60438	2.02262
C	-2.24295	3.13013	0.18823
C	-3.50543	2.70458	-0.24461
C	-1.84542	4.44977	-0.05509
C	-4.35419	3.58418	-0.91426
H	-3.82957	1.68752	-0.03633
C	-2.69585	5.32894	-0.72347
H	-0.86537	4.77727	0.27801
C	-3.95031	4.89766	-1.15671
H	-5.33252	3.24584	-1.24088
H	-2.37746	6.34985	-0.90999
H	-4.61096	5.58235	-1.67914
O	0.34902	-4.81695	0.48831
H	1.62451	0.87807	-0.13314

16b-conf4

C	2.67845	0.18915	-0.88469
H	2.27022	-0.75247	-1.24158
C	1.86159	1.24985	-0.69947
C	0.43463	1.20404	-0.95369
C	4.11592	0.15326	-0.62165
C	4.77498	-1.07724	-0.77187
C	4.85796	1.27760	-0.21997
C	6.13993	-1.18877	-0.52102
H	4.20252	-1.94992	-1.07620
C	6.22064	1.16588	0.02524
H	4.37638	2.24288	-0.10181
C	6.86482	-0.06658	-0.12266

H	6.63542	-2.14710	-0.63654
H	6.78546	2.03973	0.33283
H	7.92939	-0.14767	0.07227
C	-1.73036	2.41053	-1.06385
C	0.23819	3.43917	0.02214
C	-2.01978	3.87440	-1.35844
H	-1.95509	1.82904	-1.95512
H	-2.35162	2.04512	-0.23813
C	-0.90135	4.17471	0.70704
H	0.77133	4.09122	-0.67777
H	0.90921	3.07351	0.79813
H	-1.37091	4.22024	-2.17382
H	-3.05881	3.96919	-1.68046
H	-0.48911	5.01741	1.26484
H	-1.39418	3.49501	1.41424
N	-0.29907	2.26586	-0.70949
C	-0.21159	-0.05294	-1.44755
H	-1.10530	0.17857	-2.02296
H	0.46556	-0.58095	-2.11984
C	-0.66124	-1.02926	-0.28340
H	-1.37203	-1.68142	-0.80156
C	0.47550	-1.93878	0.15660
C	0.84219	-2.99287	-0.69141
C	1.18995	-1.75551	1.34409
C	1.90350	-3.83777	-0.37229
H	0.28798	-3.15347	-1.61442
C	2.25572	-2.59967	1.66478
H	0.92845	-0.93310	2.00176
C	2.61805	-3.63993	0.81050
H	2.16875	-4.64988	-1.04235
H	2.80772	-2.43774	2.58591
H	3.44924	-4.29131	1.06255
C	-1.43813	-0.32755	0.79130
C	-1.00239	0.66453	1.69609
C	-2.84643	-0.32930	0.93021
O	-2.13314	1.16914	2.30808
O	0.10547	1.15009	2.00088
N	-3.28455	0.54127	1.81877
C	-3.82863	-1.16041	0.19903
C	-3.64550	-2.54481	0.08924
C	-4.95749	-0.57103	-0.38178
C	-4.57703	-3.32647	-0.59132
H	-2.77936	-3.00927	0.55449
C	-5.88906	-1.35429	-1.06176
H	-5.09493	0.50317	-0.30065
C	-5.69994	-2.73238	-1.16948
H	-4.42916	-4.39922	-0.66579
H	-6.76035	-0.88796	-1.51094
H	-6.42468	-3.34135	-1.70060
O	-1.84454	4.70076	-0.21671
H	2.28229	2.18261	-0.34925

16b-conf5

C	-3.24030	-0.71405	-0.69265
H	-2.75539	-1.45140	-1.32761
C	-2.63827	0.46901	-0.45614
C	-1.30986	0.80178	-0.95369
C	-4.55347	-1.12131	-0.18810
C	-5.10394	-2.31956	-0.66806
C	-5.27542	-0.37331	0.75743
C	-6.35056	-2.75680	-0.22801
H	-4.54795	-2.90805	-1.39287
C	-6.51796	-0.81227	1.19807
H	-4.86497	0.54719	1.16003
C	-7.06034	-2.00279	0.70530
H	-6.76452	-3.68392	-0.61043
H	-7.06525	-0.22884	1.93116
H	-8.03104	-2.34108	1.05338
C	0.39712	2.52375	-1.43033
C	-1.86606	3.15453	-0.65188
C	0.78430	3.71580	-0.56830
H	1.12814	1.73827	-1.26700
H	0.37115	2.78655	-2.49266
C	-1.37272	4.47081	-1.22809
H	-1.90402	3.18284	0.44422
H	-2.86059	2.94564	-1.04707
H	0.79327	3.41327	0.48661
H	1.79113	4.03579	-0.84604
H	-2.06181	5.26169	-0.92764
H	-1.36914	4.41986	-2.32472
N	-0.94898	2.05424	-1.03174
C	-0.34077	-0.29776	-1.25495
H	-0.88231	-1.11551	-1.73325
H	0.43026	0.02318	-1.95616
C	0.27616	-0.81492	0.08443
H	-0.58678	-1.15438	0.67744
C	1.16620	-2.03529	-0.12402
C	1.80188	-2.59185	0.99428
C	1.37011	-2.63509	-1.36801
C	2.63081	-3.70180	0.86991
H	1.65704	-2.13050	1.96810
C	2.20178	-3.75101	-1.49779
H	0.90384	-2.23437	-2.26249
C	2.83913	-4.28588	-0.38252
H	3.11852	-4.11062	1.74970
H	2.35293	-4.19368	-2.47761
H	3.49022	-5.14847	-0.48349
C	0.91466	0.27781	0.89913
C	0.15179	1.09884	1.75153
C	2.24965	0.70714	1.09939
O	1.02946	1.94028	2.40005
O	-1.07170	1.18555	1.97938
N	2.33952	1.69048	1.97881
C	3.50680	0.21757	0.48853
C	3.57557	-0.10166	-0.87144
C	4.65545	0.07730	1.27707
C	4.76500	-0.56020	-1.43371
H	2.69467	0.00143	-1.49853
C	5.84647	-0.37924	0.71591
H	4.60125	0.31657	2.33443

C	5.90388	-0.70231	-0.64046
H	4.80062	-0.80775	-2.49012
H	6.72798	-0.49081	1.33957
H	6.82960	-1.06437	-1.07659
O	-0.08811	4.82712	-0.74636
H	-3.13042	1.21134	0.15842

17b

C	-1.12329	0.92304	-1.21913
H	-0.73914	0.24311	-1.98063
C	-0.26060	1.45441	-0.34337
H	-0.60691	2.14969	0.42201
C	1.19674	1.17602	-0.33233
C	-2.57835	1.14691	-1.24273
C	-3.39114	0.22962	-1.92193
C	-3.18591	2.24374	-0.61178
C	-4.77594	0.38276	-1.94713
H	-2.93030	-0.62017	-2.42022
C	-4.56743	2.40203	-0.64308
H	-2.57460	2.98323	-0.10230
C	-5.36900	1.46866	-1.30506
H	-5.39040	-0.34593	-2.46697
H	-5.02187	3.25696	-0.15176
H	-6.44711	1.59385	-1.32619
C	1.69046	3.37577	-1.25140
C	3.42454	2.16422	-0.08560
C	2.39206	4.66918	-0.87404
H	2.02655	3.05409	-2.25190
H	0.61217	3.54484	-1.29320
C	4.06740	3.50364	0.24397
H	3.88985	1.74474	-0.99472
H	3.60525	1.47361	0.74368
H	2.24069	5.42255	-1.64957
H	1.98988	5.04605	0.07849
H	5.15268	3.39685	0.29465
H	3.69603	3.86138	1.21599
N	1.98802	2.33517	-0.25983
C	1.71808	-0.07250	-0.29612
H	2.79699	-0.19767	-0.31414
C	0.94245	-1.34905	-0.05970
H	-0.09269	-1.21232	-0.37422
C	1.49683	-2.51106	-0.86183
C	2.71929	-3.11443	-0.54516
C	0.77614	-2.98036	-1.96402
C	3.20783	-4.16610	-1.31953
H	3.28715	-2.76294	0.31242
C	1.26489	-4.03094	-2.74124
H	-0.17777	-2.52125	-2.21490
C	2.48379	-4.62656	-2.42033
H	4.15627	-4.62737	-1.06178
H	0.69151	-4.38436	-3.59260
H	2.86619	-5.44566	-3.02115
C	2.04342	-1.13100	2.26067
C	-0.23897	-0.85655	2.12286
O	1.59523	-0.15055	3.09290
O	3.20762	-1.43053	2.22494
N	0.19153	-0.01659	2.99347
C	-1.66966	-0.96164	1.79652
C	-2.55808	0.06366	2.14373
C	-2.14642	-2.09434	1.12487
C	-3.90880	-0.05237	1.83413
H	-2.18104	0.95304	2.63949
C	-3.50024	-2.20538	0.81678
H	-1.46656	-2.89567	0.84730
C	-4.38243	-1.18570	1.17127
H	-4.59098	0.75089	2.09276
H	-3.86272	-3.08558	0.29585
H	-5.43524	-1.26640	0.91993
O	3.79188	4.47299	-0.75353
C	0.85688	-1.65618	1.47909
H	0.74422	-2.73170	1.65346

17b-conf2

C	1.62569	-0.33328	1.17051
H	0.93038	-1.01353	1.66518
C	1.14496	0.81980	0.68534
H	1.80213	1.54766	0.20787
C	-0.28658	1.20003	0.74049
C	3.01703	-0.80670	1.08455
C	3.31697	-2.09633	1.54598
C	4.05720	-0.02901	0.54955
C	4.61435	-2.60146	1.47268
H	2.52097	-2.70815	1.96302
C	5.35216	-0.53109	0.47788
H	3.85590	0.97359	0.18450
C	5.63689	-1.82019	0.93729
H	4.82448	-3.60338	1.83357
H	6.14413	0.08418	0.06198
H	6.64867	-2.20863	0.87886
C	-1.85125	3.07436	1.13224
C	0.23078	3.01457	2.31313
C	-2.58420	2.73611	2.42868
H	-2.39760	2.72545	0.25282
H	-1.76147	4.16465	1.06001
C	-0.53711	2.67221	3.58528
H	0.32910	4.10250	2.22603
H	1.23094	2.57830	2.34596
H	-3.56305	3.21921	2.46266
H	-2.71952	1.64857	2.52791
H	-0.04616	3.09310	4.46562
H	-0.59812	1.57742	3.69812
N	-0.49682	2.52810	1.13400
C	-1.27367	0.36576	0.32969
H	-2.30868	0.68737	0.42425
C	-1.06450	-0.91359	-0.43476
H	0.00820	-1.07994	-0.55868
C	-1.64275	-2.16580	0.20826
C	-1.31300	-3.41835	-0.32547
C	-2.47698	-2.11352	1.32659
C	-1.81521	-4.58955	0.23538

H	-0.64675	-3.48044	-1.18394
C	-2.98489	-3.28597	1.89057
H	-2.73013	-1.15398	1.76711
C	-2.65950	-4.52615	1.34610
H	-1.54484	-5.55087	-0.19040
H	-3.63397	-3.22584	2.75876
H	-3.05339	-5.43715	1.78543
C	-3.08638	-0.45754	-1.96966
C	-1.07584	0.52090	-2.52450
O	-3.25431	0.76634	-2.55093
O	-4.02703	-1.11507	-1.61380
N	-2.00086	1.33841	-2.87441
C	0.34646	0.88219	-2.62838
C	0.73251	2.22772	-2.58109
C	1.32170	-0.11936	-2.70036
C	2.08233	2.56486	-2.61333
H	-0.02759	2.99756	-2.49151
C	2.67175	0.22238	-2.72924
H	1.03105	-1.16612	-2.73376
C	3.05304	1.56322	-2.68444
H	2.37835	3.60785	-2.56742
H	3.42439	-0.55788	-2.77760
H	4.10602	1.82749	-2.69466
O	-1.84816	3.22122	3.54588
C	-1.60258	-0.73429	-1.89356
H	-1.38006	-1.62588	-2.49054

17b-conf3

C	3.33451	-0.04170	0.31242
H	3.60356	0.81659	0.92739
C	2.03495	-0.23378	0.03117
H	1.73591	-1.09723	-0.55670
C	0.95460	0.65761	0.49329
C	4.45517	-0.89339	-0.11337
C	5.72939	-0.63623	0.41427
C	4.31249	-1.95134	-1.02688
C	6.82708	-1.41589	0.05454
H	5.85536	0.18326	1.11705
C	5.40747	-2.72953	-1.38697
H	3.34399	-2.16504	-1.46857
C	6.66961	-2.46728	-0.84702
H	7.80348	-1.20076	0.47716
H	5.27856	-3.54160	-2.09570
H	7.52178	-3.07587	-1.13215
C	0.39904	2.74663	1.64523
C	1.89040	2.78342	-0.22468
C	1.08751	3.99639	2.17403
H	-0.46916	3.04689	1.03078
H	0.03675	2.14645	2.48510
C	2.53946	4.03245	0.34705
H	1.07463	3.07653	-0.90809
H	2.62606	2.21348	-0.79417
H	0.37393	4.62414	2.71150
H	1.90016	3.70802	2.85744
H	2.88659	4.68502	-0.45659
H	3.39683	3.74767	0.97623
N	1.35490	1.96204	0.87126
C	-0.32512	0.23731	0.60089
H	-1.08412	0.94786	0.90945
C	-0.80468	-1.16449	0.33098
H	0.02830	-1.86786	0.42286
C	-1.88135	-1.62241	1.30363
C	-1.77628	-2.88029	1.90662
C	-3.00195	-0.83249	1.58973
C	-2.76532	-3.34126	2.77557
H	-0.91182	-3.50370	1.69311
C	-3.99299	-1.29169	2.45549
H	-3.11077	0.15135	1.14002
C	-3.87773	-2.54785	3.05140
H	-2.66391	-4.31884	3.23624
H	-4.85470	-0.66560	2.66481
H	-4.64877	-2.90382	3.72721
C	-1.71157	-2.76826	-1.37503
C	-2.56282	-0.63333	-1.52165
O	-3.03700	-2.77227	-1.68547
O	-1.07812	-3.78397	-1.26961
N	-3.51689	-1.44701	-1.80208
C	-2.79101	0.82135	-1.57343
C	-4.06250	1.33953	-1.29276
C	-1.74519	1.68942	-1.90873
C	-4.28287	2.71219	-1.34899
H	-4.86453	0.66233	-1.01500
C	-1.97310	3.06239	-1.97062
H	-0.75621	1.29580	-2.12362
C	-3.23908	3.57518	-1.68863
H	-5.26642	3.10964	-1.12124
H	-1.16168	3.73200	-2.23701
H	-3.41155	4.64583	-1.72932
O	1.61247	4.78287	1.11608
C	-1.28893	-1.33469	-1.15497
H	-0.46226	-1.07848	-1.82591

17b-conf4

C	1.85461	1.61934	0.08918
H	1.79792	2.40046	-0.66869
C	0.71562	1.03592	0.49372
H	0.76131	0.21850	1.20855
C	-0.62356	1.39916	-0.01544
C	3.20357	1.25164	0.54291
C	3.43459	0.52580	1.72167
C	4.30521	1.61625	-0.24536
C	4.72486	0.14981	2.08058
H	2.60253	0.25722	2.36620
C	5.59782	1.23925	0.11288
H	4.13981	2.18730	-1.15554
C	5.81174	0.49905	1.27554
H	4.88520	-0.41584	2.99343
H	6.43651	1.52258	-0.51557
H	6.81733	0.20400	1.55850
C	-1.90198	3.06368	-1.32964

C	-0.42021	3.82422	0.39824
C	-3.09328	3.53418	-0.49726
H	-2.17047	2.22013	-1.97070
H	-1.59089	3.89431	-1.97566
C	-1.64509	4.25436	1.19689
H	-0.07204	4.66523	-0.21392
H	0.38423	3.53423	1.07486
H	-3.89618	3.89511	-1.14399
H	-3.48325	2.72159	0.13304
H	-1.41936	5.12845	1.81222
H	-1.97208	3.43094	1.85219
N	-0.75057	2.71040	-0.50221
C	-1.61610	0.47838	-0.09763
H	-2.60085	0.77746	-0.44441
C	-1.46836	-1.00435	0.15225
H	-0.59607	-1.18621	0.78756
C	-2.67419	-1.54521	0.90744
C	-2.81092	-1.16791	2.25049
C	-3.64641	-2.37099	0.34096
C	-3.88643	-1.61275	3.01279
H	-2.06044	-0.51933	2.69763
C	-4.72917	-2.81756	1.10425
H	-3.58388	-2.66110	-0.70287
C	-4.85257	-2.44312	2.43934
H	-3.97025	-1.31503	4.05340
H	-5.47643	-3.45870	0.64702
H	-5.69304	-2.79288	3.03037
C	-1.93092	-1.17299	-2.34825
C	0.23790	-1.53326	-1.65900
O	-1.02432	-0.64116	-3.21439
O	-3.11219	-1.10086	-2.55915
N	0.29294	-0.90144	-2.77563
C	1.46153	-1.97587	-0.97123
C	1.37921	-2.91434	0.06404
C	2.71441	-1.47782	-1.35616
C	2.53811	-3.35790	0.70030
H	0.41631	-3.31318	0.37143
C	3.86625	-1.92547	-0.72209
H	2.77435	-0.72689	-2.13794
C	3.78120	-2.86725	0.30605
H	2.46570	-4.08672	1.50078
H	4.83113	-1.52102	-1.01142
H	4.68295	-3.20578	0.80669
O	-2.71103	4.62412	0.33251
C	-1.16706	-1.76164	-1.18048
H	-1.38860	-2.83008	-1.08190

17b-conf5

C	-2.91140	0.06138	-0.16780
H	-3.05548	0.96725	0.42213
C	-1.76532	-0.06694	-0.85695
H	-1.57315	-0.97248	-1.42761
C	-0.68261	0.93720	-0.84267
C	-4.00378	-0.92147	-0.10374
C	-4.06176	-2.05333	-0.93389
C	-5.03460	-0.72238	0.82652
C	-5.11099	-2.95944	-0.82412
H	-3.29095	-2.22408	-1.67909
C	-6.08591	-1.63056	0.93771
H	-5.00557	0.15317	1.46994
C	-6.12685	-2.75394	0.11335
H	-5.14100	-3.82732	-1.47541
H	-6.87213	-1.45907	1.66612
H	-6.94500	-3.46238	0.19465
C	-2.09112	2.86280	-1.47077
C	-0.05471	3.25758	-0.26528
C	-1.44440	3.50764	-2.69138
H	-2.80986	2.10567	-1.78593
H	-2.62424	3.62845	-0.89427
C	0.54045	3.90704	-1.51234
H	0.71854	2.80525	0.36163
H	-0.54831	4.03862	0.32725
H	-0.95164	2.73578	-3.30407
H	-2.19260	4.01946	-3.30111
H	1.08898	3.17016	-2.11735
H	1.22138	4.71601	-1.23829
N	-1.07290	2.26234	-0.59677
C	0.61057	0.54024	-0.90786
H	1.39701	1.28517	-0.89113
C	1.07276	-0.89629	-0.88624
H	0.50156	-1.49877	-1.60330
C	2.54111	-1.03321	-1.25183
C	3.52291	-0.24393	-0.63951
C	2.93993	-1.99297	-2.18773
C	4.87003	-0.41283	-0.95469
H	3.23998	0.51384	0.08776
C	4.28696	-2.16244	-2.50751
H	2.18832	-2.61395	-2.66808
C	5.25613	-1.37324	-1.89016
H	5.61712	0.20750	-0.46964
H	4.57671	-2.91014	-3.23908
H	6.30500	-1.50316	-2.13707
C	1.37722	-2.97644	0.49919
C	1.49930	-1.00364	1.67576
O	2.36938	-3.00414	1.43411
O	1.13004	-3.92747	-0.19333
N	2.38415	-1.79393	2.16852
C	1.26363	0.32230	2.27452
C	-0.03946	0.83074	2.34265
C	2.32916	1.06339	2.79894
C	-0.27500	2.06343	2.94390
H	-0.86978	0.26603	1.92687
C	2.08977	2.30399	3.38591
H	3.33910	0.66959	2.73240
C	0.78868	2.80324	3.46265
H	-1.28746	2.45169	2.99299
H	2.91919	2.88143	3.78088
H	0.60505	3.77049	3.91949
O	-0.48984	4.48642	-2.30382
C	0.78206	-1.59105	0.50075

H	-0.30257	-1.63283	0.64693

17b-conf6

C	-1.50847	1.78934	0.16118
H	-0.84930	1.51913	0.98583
C	-2.26655	0.82404	-0.38056
H	-2.99524	1.05065	-1.15819
C	-2.20574	-0.59056	0.04400
C	-1.46887	3.20921	-0.22359
C	-2.19929	3.73380	-1.30215
C	-0.65774	4.07831	0.52070
C	-2.12473	5.08690	-1.61547
H	-2.82562	3.08305	-1.90461
C	-0.58081	5.43401	0.20602
H	-0.08297	3.68158	1.35444
C	-1.31617	5.94339	-0.86299
H	-2.69613	5.47647	-2.45222
H	0.05257	6.08983	0.79507
H	-1.25952	6.99813	-1.11256
C	-4.43552	-0.50514	1.01129
C	-3.50049	-2.63997	0.39536
C	-5.82221	-1.09454	0.81605
H	-4.45158	0.55733	0.75762
H	-4.14189	-0.60023	2.07109
C	-4.92039	-3.15850	0.22242
H	-3.14491	-2.88266	1.41269
H	-2.84606	-3.13513	-0.32798
H	-6.53141	-0.63498	1.50737
H	-6.15888	-0.91734	-0.21657
H	-4.96788	-4.21972	0.47459
H	-5.23842	-3.02308	-0.82222
N	-3.47003	-1.20316	0.15466
C	-1.04811	-1.26386	0.22954
H	-1.09341	-2.28986	0.58279
C	0.32957	-0.76226	-0.12033
H	0.24204	0.09745	-0.79410
C	1.14007	-0.32031	1.08919
C	1.22846	-1.12177	2.23076
C	1.82970	0.89461	1.06102
C	2.00862	-0.72517	3.31586
H	0.69148	-2.06646	2.27435
C	2.60845	1.29687	2.14516
H	1.76478	1.52669	0.17699
C	2.70386	0.48394	3.27452
H	2.07310	-1.36058	4.19376
H	3.14292	2.24120	2.10433
H	3.31279	0.79190	4.11871
C	0.34859	-2.25589	-2.16239
C	2.39140	-1.40387	-1.52351
O	1.07562	-1.81757	-3.23149
O	-0.70949	-2.80465	-2.30860
N	2.33787	-1.34854	-2.80621
C	3.62442	-1.00303	-0.82258
C	4.00011	-1.64694	0.36121
C	4.42358	0.02244	-1.34197
C	5.16424	-1.26497	1.02174
H	3.38376	-2.44098	0.77135
C	5.58592	0.40246	-0.67684
H	4.11680	0.52983	-2.25114
C	5.95681	-0.23881	0.50633
H	5.44780	-1.76436	1.94256
H	6.19741	1.20501	-1.07634
H	6.85914	0.06406	1.02800
O	-5.82608	-2.48782	1.08393
C	1.10647	-1.88292	-0.90701
H	1.23231	-2.75957	-0.26311

17b-conf7

C	2.67126	0.05559	-0.35755
H	2.01227	-0.27110	-1.16104
C	2.16963	0.85758	0.59239
H	2.81171	1.25844	1.37579
C	0.75943	1.29940	0.66131
C	4.05508	-0.43737	-0.45905
C	4.38373	-1.29146	-1.52147
C	5.06101	-0.09268	0.45828
C	5.67720	-1.78968	-1.66828
H	3.61370	-1.56775	-2.23740
C	6.35236	-0.58771	0.31129
H	4.83820	0.56492	1.29275
C	6.66689	-1.43843	-0.75206
H	5.90973	-2.45084	-2.49709
H	7.11806	-0.31044	1.02905
H	7.67573	-1.82316	-0.86218
C	-0.72187	3.16692	1.23379
C	1.34226	3.57617	0.06400
C	-0.64852	4.59088	1.76464
H	-1.19727	2.53192	1.98719
H	-1.34303	3.14686	0.32030
C	1.34750	4.98452	0.63329
H	0.85815	3.58238	-0.92849
H	2.37082	3.23038	-0.06192
H	-1.65382	4.99523	1.89802
H	-0.12734	4.59696	2.73371
H	1.81306	5.67689	-0.07090
H	1.90964	5.00007	1.57922
N	0.62329	2.67030	0.96957
C	-0.30478	0.47462	0.53906
H	-1.29632	0.91139	0.58430
C	-0.26591	-1.02550	0.43253
H	0.75829	-1.37536	0.59457
C	-1.15393	-1.70613	1.46642
C	-2.48422	-1.31767	1.67015
C	-0.64396	-2.76969	2.21877
C	-3.28360	-1.97898	2.60074
H	-2.90832	-0.49119	1.10509
C	-1.44097	-3.43163	3.15301
H	0.38671	-3.08158	2.07034
C	-2.76428	-3.03848	3.34557
H	-4.31250	-1.66411	2.74434

H	-1.02586	-4.25256	3.72925
H	-3.38666	-3.55145	4.07185
C	-0.51500	-3.04007	-1.04102
C	-2.04881	-1.37115	-1.44704
O	-1.74678	-3.54394	-1.32871
O	0.42884	-3.75007	-0.81971
N	-2.65190	-2.49392	-1.60981
C	-2.75717	-0.10388	-1.69614
C	-2.04928	1.02371	-2.12865
C	-4.14379	-0.02565	-1.50941
C	-2.72422	2.21622	-2.37952
H	-0.97332	0.97434	-2.26731
C	-4.81253	1.16901	-1.75706
H	-4.68428	-0.89826	-1.15543
C	-4.10425	2.29096	-2.19299
H	-2.17007	3.08694	-2.71487
H	-5.88486	1.22792	-1.60266
H	-4.62728	3.22297	-2.38152
O	0.02597	5.44828	0.85860
C	-0.62335	-1.53344	-1.00947
H	0.07540	-1.09455	-1.72816

17b-conf8

C	-3.06625	1.02327	-0.36514
H	-3.89578	0.35323	-0.59001
C	-1.89609	0.47855	0.00633
H	-1.04284	1.11816	0.21698
C	-1.66544	-0.97095	0.14485
C	-3.34578	2.45901	-0.52050
C	-2.44008	3.46269	-0.13674
C	-4.57374	2.84762	-1.07631
C	-2.75246	4.80594	-0.31651
H	-1.48842	3.19687	0.31406
C	-4.88753	4.19353	-1.25697
H	-5.28647	2.08209	-1.37200
C	-3.97653	5.17845	-0.87893
H	-2.04098	5.56745	-0.01256
H	-5.84274	4.47119	-1.69141
H	-4.21697	6.22795	-1.01563
C	-3.57079	-1.54209	1.54591
C	-2.66389	-3.20377	0.07950
C	-4.92034	-2.23434	1.45719
H	-3.00722	-1.94468	2.40560
H	-3.71492	-0.47156	1.70172
C	-4.03884	-3.85309	0.02232
H	-2.07789	-3.67799	0.88718
H	-2.13844	-3.36368	-0.86677
H	-5.46626	-2.13230	2.39736
H	-5.51269	-1.78477	0.64535
H	-3.94451	-4.93517	-0.08936
H	-4.60180	-3.45021	-0.83291
N	-2.82054	-1.77135	0.30383
C	-0.42275	-1.49189	0.06145
H	-0.27969	-2.55926	0.19586
C	0.81441	-0.67858	-0.25041
H	0.56787	0.10136	-0.98128
C	1.39015	0.00601	0.98122
C	1.74154	1.35683	0.93672
C	1.59608	-0.71048	2.16421
C	2.30992	1.97989	2.04811
H	1.58656	1.92212	0.01980
C	2.16728	-0.09293	3.27459
H	1.31347	-1.75958	2.21699
C	2.52941	1.25421	3.21793
H	2.58512	3.02886	1.99578
H	2.32958	-0.66260	4.18440
H	2.97659	1.73505	4.08229
C	1.33959	-2.19459	-2.20439
C	3.06318	-0.83986	-1.49061
O	2.03477	-1.66003	-3.24861
O	0.44584	-2.97677	-2.38260
N	3.10584	-0.87139	-2.77412
C	4.09448	-0.09987	-0.74142
C	4.53247	-0.56670	0.50253
C	4.63852	1.07368	-1.27666
C	5.50463	0.13789	1.20656
H	4.11282	-1.47428	0.92532
C	5.60929	1.77603	-0.56794
H	4.28106	1.43976	-2.23392
C	6.04202	1.31067	0.67482
H	5.83673	-0.22575	2.17361
H	6.02119	2.69113	-0.98082
H	6.79310	1.86367	1.22992
O	-4.76607	-3.62528	1.21978
C	1.89032	-1.59392	-0.92673
H	2.18343	-2.38851	-0.23176

17b-conf9

C	2.66193	0.62071	-0.02330
H	2.13437	0.12846	0.79709
C	1.96252	1.43185	-0.83199
H	2.43782	1.97094	-1.65279
C	0.50875	1.67796	-0.66433
C	4.09698	0.29612	-0.12036
C	4.61857	-0.68645	0.73556
C	4.96436	0.92632	-1.02846
C	5.96813	-1.03935	0.68397
H	3.95579	-1.17989	1.44475
C	6.31174	0.57619	-1.07932
H	4.58953	1.69822	-1.69643
C	6.81961	-0.40869	-0.22462
H	6.35248	-1.80470	1.35335
H	6.97014	1.07438	-1.78642
H	7.87157	-0.67856	-0.26714
C	-1.25449	3.40545	-0.82151
C	0.91908	4.02594	-0.01461
C	-1.82888	3.63367	0.57393
H	-1.81868	2.64319	-1.36610
H	-1.31325	4.34682	-1.38309
C	0.30228	4.24277	1.36467

H	0.89455	4.96568	-0.58049
H	1.95698	3.69882	0.08402
H	-2.85177	4.01632	0.52694
H	-1.81448	2.70100	1.15924
H	0.80188	5.05459	1.89946
H	0.37186	3.31644	1.95625
N	0.14775	3.02470	-0.74837
C	-0.39498	0.67988	-0.51213
H	-1.42853	0.93991	-0.30156
C	-0.09023	-0.79068	-0.62585
H	0.87635	-0.91851	-1.12529
C	-0.00924	-1.50683	0.71756
C	0.92475	-2.53551	0.89991
C	-0.85157	-1.16374	1.78290
C	1.00926	-3.21493	2.11767
H	1.59681	-2.80117	0.08470
C	-0.77332	-1.84552	2.99875
H	-1.56990	-0.35341	1.66973
C	0.15708	-2.87379	3.16997
H	1.74441	-4.00591	2.24324
H	-1.43592	-1.56748	3.81465
H	0.22200	-3.39954	4.11900
C	-0.64596	-2.93010	-1.82528
C	-2.45675	-1.80888	-0.96531
O	-1.56547	-3.79303	-1.31458
O	0.37291	-3.31987	-2.32970
N	-2.69068	-3.06101	-0.81464
C	-3.47536	-0.81832	-0.55932
C	-3.70632	0.31719	-1.34764
C	-4.23065	-1.02679	0.60310
C	-4.68196	1.23985	-0.97064
H	-3.13114	0.47962	-2.25716
C	-5.20115	-0.09895	0.97846
H	-4.03659	-1.90344	1.21662
C	-5.42703	1.03520	0.19359
H	-4.85915	2.11764	-1.58658
H	-5.77568	-0.25772	1.88687
H	-6.18111	1.75978	0.48919
O	-1.06520	4.62693	1.25366
C	-1.11563	-1.51673	-1.56653
H	-1.18684	-0.96262	-2.50887

17b-conf10

C	-1.27310	1.25278	-0.45015
H	-1.06501	1.32210	0.61872
C	-0.24690	1.28863	-1.30961
H	-0.43257	1.33096	-2.38370
C	1.17792	1.33939	-0.89004
C	-2.69356	1.17423	-0.83907
C	-3.10385	0.47983	-1.98554
C	-3.66535	1.79550	-0.04235
C	-4.45163	0.42572	-2.33590
H	-2.36560	-0.04163	-2.58917
C	-5.01136	1.74766	-0.39494
H	-3.35797	2.31894	0.85976
C	-5.40890	1.06183	-1.54393
H	-4.75604	-0.12325	-3.22168
H	-5.75118	2.23806	0.23018
H	-6.45882	1.01550	-1.81559
C	1.18584	3.78009	-1.17832
C	3.27662	2.63327	-1.01435
C	1.40410	4.32198	0.23020
H	1.62053	4.47205	-1.90817
H	0.11985	3.68169	-1.38827
C	3.46363	3.19586	0.39330
H	3.69783	3.34527	-1.73333
H	3.79741	1.68254	-1.14337
H	0.97119	5.31894	0.33940
H	0.93561	3.64587	0.96452
H	4.51874	3.38481	0.60260
H	3.07037	2.49616	1.14639
N	1.85768	2.48261	-1.33372
C	1.77274	0.30976	-0.24226
H	2.81269	0.39174	0.05949
C	1.16823	-1.05833	-0.03321
H	0.16553	-1.06092	-0.46704
C	1.98002	-2.11530	-0.76422
C	1.52708	-2.58884	-1.99916
C	3.19006	-2.59848	-0.25399
C	2.26647	-3.53121	-2.71415
H	0.58748	-2.21642	-2.40220
C	3.93013	-3.54044	-0.96764
H	3.55603	-2.23298	0.70311
C	3.47096	-4.00968	-2.19937
H	1.89911	-3.89337	-3.66940
H	4.86681	-3.90889	-0.56062
H	4.04719	-4.74483	-2.75217
C	1.91819	-0.63716	2.39413
C	-0.33167	-0.96634	2.03771
O	1.15373	0.14287	3.20829
O	3.11871	-0.62173	2.46052
N	-0.21953	-0.09705	2.97662
C	-1.64702	-1.43984	1.57869
C	-2.82165	-0.80702	2.00563
C	-1.72719	-2.53020	0.70275
C	-4.05818	-1.26165	1.56223
H	-2.75776	0.04825	2.67147
C	-2.96849	-2.98066	0.25901
H	-0.82547	-3.03658	0.36823
C	-4.13470	-2.34693	0.68693
H	-4.96351	-0.75881	1.88649
H	-3.02244	-3.82518	-0.41993
H	-5.10136	-2.69420	0.33604
O	2.79207	4.44507	0.51377
C	0.98912	-1.41117	1.48454
H	1.14302	-2.48418	1.64590

TS(17b→18b)

C	2.83701	0.98439	0.01896
H	3.22880	0.67449	0.98758

C	2.08207	0.10992	-0.66173
H	1.60088	0.38728	-1.59505
C	1.77371	-1.23729	-0.13631
C	3.14510	2.36310	-0.38290
C	3.71031	3.22658	0.56642
C	2.89367	2.85305	-1.67467
C	4.00324	4.55003	0.24318
H	3.91293	2.85461	1.56733
C	3.18825	4.17310	-1.99822
H	2.47807	2.19880	-2.43498
C	3.74143	5.02722	-1.04024
H	4.43608	5.20583	0.99180
H	2.99170	4.53757	-3.00150
H	3.97068	6.05656	-1.29689
C	2.58453	-3.19361	1.13102
C	4.18262	-1.88427	-0.11646
C	2.98160	-4.42497	0.32615
H	3.24219	-3.11418	2.00530
H	1.55649	-3.24588	1.48463
C	4.54775	-3.15943	-0.87527
H	4.82708	-1.77050	0.76277
H	4.30983	-1.01995	-0.76484
H	2.90515	-5.32579	0.93752
H	2.32968	-4.52893	-0.55440
H	5.60631	-3.14606	-1.14208
H	3.94540	-3.22066	-1.79433
N	2.78953	-1.98803	0.32953
C	0.44860	-1.69963	-0.15885
H	0.24748	-2.74548	0.04113
C	-0.63657	-0.84105	-0.38355
H	-0.41469	0.16810	-0.72890
C	-1.94955	-1.35417	-0.83672
C	-2.68344	-0.60352	-1.76359
C	-2.48094	-2.56492	-0.37202
C	-3.91694	-1.05626	-2.22764
H	-2.28529	0.34430	-2.11743
C	-3.71718	-3.01281	-0.82805
H	-1.93800	-3.15036	0.36559
C	-4.43793	-2.26113	-1.75926
H	-4.47400	-0.46179	-2.94512
H	-4.12210	-3.94771	-0.45347
H	-5.40343	-2.61134	-2.11061
C	-0.01126	0.41013	1.96625
C	-2.01917	1.10906	1.20960
O	0.01598	1.75178	1.63458
O	0.98644	-0.14311	2.41038
N	-1.24922	2.16771	1.19697
C	-3.43758	1.20448	0.81505
C	-4.32326	0.17112	1.13804
C	-3.90694	2.31218	0.09689
C	-5.65844	0.24091	0.74683
H	-3.96886	-0.69565	1.68787
C	-5.24108	2.37970	-0.29320
H	-3.21636	3.10752	-0.16527
C	-6.12058	1.34333	0.02906
H	-6.33500	-0.57044	0.99657
H	-5.59514	3.23808	-0.85549
H	-7.15949	1.39501	-0.28132
O	4.33578	-4.31812	-0.08602
C	-1.29586	-0.07489	1.56768
H	-1.71023	-1.00712	1.91989

2a^{-}

C	-0.65597	0.11755	-0.02254
C	-1.58671	-0.92282	0.16693
H	-1.40443	-1.96408	0.37900
N	-1.23276	1.28706	-0.23714
O	-2.60752	1.03073	-0.18558
C	-2.84701	-0.31351	0.06168
O	-4.02873	-0.70330	0.14236
C	0.82089	0.02624	-0.00512
C	1.45161	-1.21566	-0.14123
C	1.60953	1.17456	0.14701
C	2.84262	-1.31000	-0.12684
H	0.85123	-2.11161	-0.26812
C	2.99890	1.08035	0.15782
H	1.12333	2.13813	0.26171
C	3.62103	-0.16234	0.02176
H	3.31755	-2.28019	-0.23509
H	3.59825	1.97761	0.27821
H	4.70405	-0.23494	0.03325

18b

C	1.42323	-0.82259	-0.46577
H	0.64275	-1.24511	-1.09558
C	1.27312	0.44141	-0.01608
H	2.05263	0.91860	0.56787
C	0.08209	1.23214	-0.30560
C	2.56920	-1.69855	-0.22377
C	2.58429	-2.95250	-0.85380
C	3.64267	-1.34334	0.61101
C	3.64747	-3.83111	-0.66334
H	1.75540	-3.23445	-1.49705
C	4.70178	-2.22160	0.80150
H	3.65320	-0.38368	1.11754
C	4.70804	-3.46626	0.16432
H	3.64688	-4.79664	-1.15798
H	5.52558	-1.93916	1.44855
H	5.53852	-4.14811	0.31645
C	-0.95745	3.46358	-0.46333
C	1.46000	3.25555	-0.62453
C	-0.72382	4.51463	0.62369
H	-1.01913	3.93455	-1.44880
H	-1.88053	2.92900	-0.25158
C	1.59517	4.30511	0.47263
H	1.41576	3.75076	-1.60037
H	2.29643	2.56147	-0.62933
H	-1.52218	5.25678	0.58274
H	-0.73311	4.02851	1.60967
H	2.49922	4.89304	0.30999

H	1.65164	3.81881	1.45704
N	0.18591	2.53576	-0.46418
C	-1.22297	0.59595	-0.43146
H	-1.93377	1.06446	-1.10335
C	-1.55541	-0.51351	0.26260
H	-0.83461	-0.91765	0.97071
C	-2.82817	-1.23015	0.19184
C	-3.84883	-0.89115	-0.71318
C	-3.02755	-2.30829	1.06806
C	-5.03630	-1.61134	-0.73152
H	-3.71827	-0.06850	-1.40868
C	-4.21909	-3.02818	1.04973
H	-2.24096	-2.57823	1.76717
C	-5.22538	-2.68008	0.15009
H	-5.81783	-1.34289	-1.43453
H	-4.36050	-3.85799	1.73407
H	-6.15534	-3.23914	0.13160
O	0.49802	5.19836	0.43058

18b-conf2

C	1.99416	-0.49152	-0.04764
H	1.28219	-1.26677	0.23153
C	1.51674	0.71605	-0.42119
H	2.19137	1.52504	-0.67407
C	0.08759	0.95937	-0.52995
C	3.39956	-0.87679	0.05243
C	3.69936	-2.15061	0.56068
C	4.45453	-0.03515	-0.34183
C	5.01975	-2.57441	0.68232
H	2.88824	-2.80732	0.86272
C	5.77112	-0.46068	-0.22235
H	4.25164	0.94987	-0.74943
C	6.05731	-1.72946	0.29128
H	5.23740	-3.56043	1.07889
H	6.57869	0.19455	-0.53139
H	7.08812	-2.05637	0.38253
C	-1.72942	2.59311	-0.96864
C	0.40530	3.36018	-0.09499
C	-2.43278	3.38399	0.12782
H	-1.57310	3.24532	-1.83473
H	-2.30328	1.72337	-1.27535
C	-0.38871	4.11636	0.97189
H	0.57759	3.99364	-0.97033
H	1.35542	3.04550	0.32916
H	-3.38767	3.75372	-0.24771
H	-2.61456	2.75000	1.00756
H	0.15348	5.02299	1.24323
H	-0.49969	3.48255	1.86333
N	-0.38264	2.18787	-0.51896
C	-0.80308	-0.19582	-0.69015
H	-0.46308	-0.95884	-1.38248
C	-1.89987	-0.36538	0.07038
H	-2.14378	0.40154	0.80548
C	-2.80569	-1.51685	0.05067
C	-2.67936	-2.56651	-0.87429
C	-3.84514	-1.56079	0.99135
C	-3.57094	-3.63162	-0.85145
H	-1.88855	-2.55300	-1.61745
C	-4.73797	-2.62971	1.01345
H	-3.95076	-0.75087	1.70808
C	-4.60186	-3.66689	0.09233
H	-3.46583	-4.43664	-1.57126
H	-5.53732	-2.65129	1.74670
H	-5.29606	-4.50096	0.10568
O	-1.65819	4.50978	0.49367

18b-conf3

C	1.89997	-0.36526	0.07042
H	2.14372	0.40166	0.80558
C	0.80321	-0.19580	-0.69019
H	0.46326	-0.95889	-1.38248
C	-0.08756	0.95931	-0.53014
C	2.80588	-1.51663	0.05071
C	3.84494	-1.56083	0.99182
C	2.67997	-2.56600	-0.87463
C	4.73777	-2.62975	1.01399
H	3.95024	-0.75112	1.70884
C	3.57156	-3.63110	-0.85175
H	1.88950	-2.55220	-1.61815
C	4.60205	-3.66667	0.09250
H	5.53680	-2.65156	1.74758
H	3.46677	-4.43590	-1.57185
H	5.29625	-4.50073	0.10590
C	-0.40562	3.36008	-0.09531
C	1.72935	2.59325	-0.96856
C	0.38810	4.11638	0.97172
H	-0.57781	3.99350	-0.97070
H	-1.35579	3.04529	0.32866
C	2.43243	3.38424	0.12802
H	1.57309	3.24544	-1.83467
H	2.30337	1.72358	-1.27516
H	-0.15424	5.02296	1.24291
H	0.49897	3.48260	1.86319
H	3.38732	3.75409	-0.24737
H	2.61417	2.75028	1.00779
N	0.38254	2.18785	-0.51909
C	-1.51674	0.71590	-0.42162
H	-2.19133	1.52474	-0.67507
C	-1.99410	-0.49155	-0.04763
H	-1.28207	-1.26664	0.23181
C	-3.39947	-0.87693	0.05252
C	-4.45458	-0.03503	-0.34081
C	-3.69910	-2.15114	0.55989
C	-5.77112	-0.46074	-0.22141
H	-4.25187	0.95040	-0.74751
C	-5.01944	-2.57514	0.68142
H	-2.88788	-2.80802	0.86129
C	-6.05713	-1.72996	0.29123
H	-6.57880	0.19471	-0.52971
H	-5.23694	-3.56148	1.07728

H	-7.08790	-2.05701	0.38243
O	1.65763	4.50993	0.49373

18b-conf4

C	1.99406	-0.49155	-0.04770
H	1.28202	-1.26664	0.23171
C	1.51672	0.71591	-0.42168
H	2.19132	1.52473	-0.67514
C	0.08754	0.95933	-0.53019
C	3.39943	-0.87695	0.05250
C	4.45457	-0.03495	-0.34052
C	3.69901	-2.15127	0.55962
C	5.77110	-0.46069	-0.22110
H	4.25191	0.95060	-0.74698
C	5.01934	-2.57530	0.68117
H	2.88777	-2.80821	0.86081
C	6.05706	-1.73003	0.29127
H	6.57880	0.19485	-0.52916
H	5.23681	-3.56172	1.07682
H	7.08782	-2.05710	0.38248
C	-1.72936	2.59329	-0.96855
C	0.40564	3.36010	-0.09536
C	-2.43239	3.38429	0.12805
H	-1.57311	3.24548	-1.83467
H	-2.30339	1.72363	-1.27514
C	-0.38804	4.11640	0.97169
H	0.57783	3.99351	-0.97075
H	1.35582	3.04529	0.32860
H	-3.38730	3.75415	-0.24731
H	-2.61411	2.75032	1.00781
H	0.15432	5.02297	1.24288
H	-0.49889	3.48262	1.86317
N	-0.38254	2.18788	-0.51912
C	-0.80324	-0.19576	-0.69026
H	-0.46334	-0.95882	-1.38261
C	-1.89996	-0.36524	0.07041
H	-2.14366	0.40166	0.80561
C	-2.80588	-1.51662	0.05072
C	-2.68001	-2.56594	-0.87468
C	-3.84486	-1.56087	0.99190
C	-3.57157	-3.63107	-0.85176
H	-1.88961	-2.55210	-1.61826
C	-4.73765	-2.62982	1.01411
H	-3.95013	-0.75118	1.70895
C	-4.60198	-3.66670	0.09258
H	-3.46682	-4.43584	-1.57190
H	-5.53662	-2.65167	1.74776
H	-5.29615	-4.50080	0.10602
O	-1.65758	4.50997	0.49374

18b-conf5

C	-1.99415	-0.49404	-0.05134
H	-1.28155	-1.26973	0.22491
C	-1.51720	0.71272	-0.42785
H	-2.19173	1.52017	-0.68556
C	-0.08811	0.95736	-0.53473
C	-3.39927	-0.87924	0.05304
C	-3.69584	-2.16816	0.52377
C	-4.45721	-0.02303	-0.29994
C	-5.01548	-2.59475	0.64387
H	-2.88270	-2.83502	0.79682
C	-5.77306	-0.45092	-0.18115
H	-4.25793	0.97697	-0.67119
C	-6.05576	-1.73637	0.29131
H	-5.23046	-3.59305	1.00999
H	-6.58289	0.21608	-0.45739
H	-7.08604	-2.06506	0.38215
C	1.72761	2.59348	-0.97045
C	-0.41010	3.35797	-0.10187
C	2.42742	3.38588	0.12722
H	2.30340	1.72444	-1.27551
H	1.57230	3.24511	-1.83715
C	0.38047	4.11579	0.96639
H	-1.36068	3.04214	0.32040
H	-0.58145	3.99073	-0.97790
H	2.60819	2.75259	1.00767
H	3.38261	3.75677	-0.24637
H	0.49029	3.48261	1.85842
H	-0.16363	5.02178	1.23606
N	0.38039	2.18653	-0.52360
C	0.80452	-0.19667	-0.69213
H	0.46709	-0.96077	-1.38455
C	1.90004	-0.36371	0.07078
H	2.14071	0.40404	0.80610
C	2.80832	-1.51326	0.05359
C	2.68769	-2.56234	-0.87276
C	3.84435	-1.55580	0.99812
C	3.58137	-3.62564	-0.84744
H	1.89985	-2.54965	-1.61907
C	4.73923	-2.62294	1.02276
H	3.94559	-0.74623	1.71589
C	4.60872	-3.65964	0.10027
H	3.48075	-4.43019	-1.56842
H	5.53585	-2.64350	1.75900
H	5.30461	-4.49226	0.11554
O	1.65046	4.51077	0.49083

18b-conf6

C	1.82197	-0.76170	-0.06993
H	1.04147	-1.51147	-0.19071
C	1.46025	0.53666	0.02390
H	2.21110	1.31047	0.12501
C	0.06086	0.93266	0.02765
C	3.18560	-1.28545	-0.04581
C	4.31901	-0.46530	0.09468
C	3.36131	-2.67332	-0.16237
C	5.58957	-1.02529	0.11922
H	4.21355	0.61085	0.18540
C	4.63573	-3.23304	-0.13798
H	2.48985	-3.31273	-0.27140

C	5.75147	-2.40944	0.00316
H	6.45823	-0.38466	0.22869
H	4.75694	-4.30729	-0.22821
H	6.74688	-2.84131	0.02274
C	-1.59763	2.77641	0.04176
C	0.61125	3.14857	-0.90313
C	-1.36001	4.02397	0.89318
H	-2.08860	3.04001	-0.89973
H	-2.21513	2.07141	0.59186
C	0.75894	4.37233	-0.00691
H	0.13061	3.43977	-1.84292
H	1.57180	2.69852	-1.13721
H	-2.31472	4.52392	1.06271
H	-0.93145	3.72948	1.86193
H	1.36363	5.12507	-0.51416
H	1.24646	4.09472	0.93873
N	-0.28912	2.16595	-0.26988
C	-0.94433	-0.07459	0.38462
H	-0.68508	-0.73141	1.20810
C	-2.05536	-0.26119	-0.35168
H	-2.22343	0.39043	-1.20933
C	-3.07561	-1.29157	-0.14585
C	-4.11573	-1.39008	-1.08177
C	-3.05808	-2.17283	0.94818
C	-5.11561	-2.34842	-0.93446
H	-4.13678	-0.70987	-1.92876
C	-4.05685	-3.12734	1.09459
H	-2.26880	-2.11243	1.69077
C	-5.08718	-3.21886	0.15379
H	-5.91388	-2.41400	-1.66625
H	-4.03582	-3.80197	1.94412
H	-5.86475	-3.96646	0.27303
O	-0.50821	4.94804	0.24697

18b-conf7

C	1.50738	-0.72328	-0.34151
H	0.76127	-1.15541	-1.00562
C	1.25304	0.48006	0.21729
H	2.00122	0.98053	0.82275
C	-0.00021	1.18786	-0.00001
C	2.72983	-1.50888	-0.18009
C	3.74323	-1.16463	0.73100
C	2.88604	-2.65925	-0.96885
C	4.88451	-1.94886	0.83788
H	3.63951	-0.29024	1.36531
C	4.03213	-3.44256	-0.86276
H	2.10320	-2.93442	-1.67020
C	5.03327	-3.08753	0.04008
H	5.66051	-1.67684	1.54563
H	4.14193	-4.32741	-1.48071
H	5.92726	-3.69657	0.12731
C	-1.24309	3.30215	-0.00696
C	1.24164	3.30280	0.00691
C	-0.97874	4.63376	0.67925
H	-1.57415	3.45269	-1.04039
H	-2.01536	2.76170	0.54133
C	0.97656	4.63430	-0.67922
H	2.01417	2.76279	-0.54145
H	1.57267	3.45347	1.04033
H	-1.90271	5.21402	0.69577
H	-0.66282	4.45491	1.71498
H	0.66072	4.45533	-1.71495
H	1.90023	5.21505	-0.69573
N	-0.00052	2.50370	-0.00001
C	-1.25318	0.47954	-0.21729
H	-2.00159	0.97973	-0.82271
C	-1.50701	-0.72390	0.34151
H	-0.76071	-1.15574	1.00559
C	-2.72914	-1.51000	0.18010
C	-2.88485	-2.66047	0.96882
C	-3.74271	-1.16615	-0.73095
C	-4.03060	-3.44427	0.86272
H	-2.10187	-2.93533	1.67015
C	-4.88366	-1.95087	-0.83784
H	-3.63938	-0.29168	-1.36523
C	-5.03191	-3.08963	-0.04008
H	-4.14001	-4.32919	1.48064
H	-5.65979	-1.67915	-1.54557
H	-5.92563	-3.69906	-0.12732
O	-0.00129	5.40922	0.00004

2a

C	-0.61083	0.15704	-0.00003
C	-1.56906	-0.99159	-0.00000
H	-1.48497	-1.62655	0.88656
H	-1.48496	-1.62653	-0.88659
N	-1.20519	1.29583	-0.00003
O	-2.60148	1.08151	-0.00003
C	-2.88279	-0.25376	-0.00007
O	-4.01304	-0.65914	0.00011
C	0.85589	0.05312	-0.00001
C	1.45795	-1.20922	-0.00002
C	1.65575	1.20512	0.00002
C	2.84747	-1.32144	-0.00001
H	0.84831	-2.10763	-0.00005
C	3.04023	1.08789	0.00003
H	1.18673	2.18351	0.00003
C	3.63922	-0.17512	0.00002
H	3.30764	-2.30381	-0.00002
H	3.65589	1.98125	0.00006
H	4.72088	-0.26225	0.00003

6b

C	-2.45040	-0.76953	-0.00006
H	-2.44152	-1.85939	-0.00012
C	-1.25611	-0.15338	0.00001
H	-1.16325	0.92880	0.00014
C	0.00000	-0.94079	-0.00006
C	-3.77461	-0.13967	-0.00003
C	-3.95662	1.25372	-0.00055

C	-4.90788	-0.96661	0.00054
C	-5.23579	1.79739	-0.00044
H	-3.09719	1.91675	-0.00108
C	-6.19025	-0.42188	0.00065
H	-4.77722	-2.04540	0.00091
C	-6.35693	0.96200	0.00017
H	-5.36233	2.87526	-0.00086
H	-7.05593	-1.07626	0.00111
H	-7.35385	1.39106	0.00024
C	1.25611	-0.15338	0.00001
H	1.16325	0.92880	0.00009
C	2.45040	-0.76953	-0.00005
H	2.44152	-1.85939	-0.00015
C	3.77461	-0.13967	-0.00001
C	4.90788	-0.96661	-0.00034
C	3.95662	1.25372	0.00034
C	6.19025	-0.42188	-0.00034
H	4.77722	-2.04540	-0.00060
C	5.23579	1.79739	0.00034
H	3.09719	1.91675	0.00063
C	6.35693	0.96200	-0.00001
H	7.05593	-1.07626	-0.00061
H	5.36233	2.87526	0.00061
H	7.35385	1.39106	-0.00001
O	0.00000	-2.17015	-0.00015

6b-conf2

C	-1.92040	0.15308	-0.00456
H	-1.23760	-0.69339	-0.00628
C	-1.42741	1.40400	-0.01492
H	-2.08501	2.26931	-0.02219
C	0.00607	1.76629	-0.02249
C	-3.34118	-0.22116	0.00321
C	-4.38065	0.72151	0.06922
C	-3.67109	-1.58327	-0.05629
C	-5.70767	0.30805	0.07088
H	-4.15649	1.78187	0.12390
C	-5.00114	-1.99771	-0.05548
H	-2.87462	-2.32104	-0.10520
C	-6.02323	-1.05221	0.00780
H	-6.50054	1.04719	0.12353
H	-5.23759	-3.05572	-0.10329
H	-7.06093	-1.37004	0.00990
C	1.04277	0.70433	-0.00895
H	0.72902	-0.33262	0.00754
C	2.34397	1.03771	-0.01481
H	2.58209	2.10079	-0.03032
C	3.49191	0.12389	-0.00163
C	3.35499	-1.27439	0.01431
C	4.78276	0.67299	-0.00498
C	4.47819	-2.09309	0.02702
H	2.36853	-1.72727	0.01663
C	5.90900	-0.14736	0.00786
H	4.89946	1.75331	-0.01762
C	5.75909	-1.53298	0.02393
H	4.35761	-3.17157	0.03928
H	6.90001	0.29485	0.00523
H	6.63337	-2.17599	0.03386
O	0.31333	2.95778	-0.03946

19b

C	2.65852	-1.00759	0.34572
H	2.04464	-0.41314	1.02037
C	2.06041	-1.83584	-0.52826
H	2.62943	-2.41611	-1.25006
C	0.59867	-1.98061	-0.66380
C	4.10080	-0.76486	0.46706
C	4.52820	0.33235	1.22940
C	5.06449	-1.57394	-0.15634
C	5.88382	0.62748	1.35511
H	3.78795	0.95971	1.71959
C	6.41749	-1.28225	-0.02582
H	4.75890	-2.44057	-0.73409
C	6.83127	-0.17932	0.72662
H	6.19886	1.48279	1.94393
H	7.15358	-1.91746	-0.50787
H	7.88866	0.04441	0.82541
C	-0.32805	-1.33249	0.35191
H	-0.27235	-1.93723	1.26669
H	0.04190	-0.34092	0.62313
C	-1.78716	-1.27669	-0.10666
H	-2.08008	-2.28401	-0.42058
C	-2.72242	-0.83610	1.00528
C	-2.45777	0.29655	1.78547
C	-3.89813	-1.55582	1.24501
C	-3.34956	0.70043	2.77800
H	-1.54889	0.87205	1.62757
C	-4.79159	-1.15463	2.23781
H	-4.11436	-2.43721	0.64692
C	-4.51974	-0.02373	3.00642
H	-3.12769	1.58053	3.37339
H	-5.69739	-1.72720	2.41051
H	-5.21291	0.29048	3.78021
C	-3.44549	-0.42721	-1.77195
C	-1.78877	1.07453	-1.22883
O	-3.92409	0.84540	-1.67835
O	-4.15232	-1.35078	-2.07233
N	-2.87376	1.74376	-1.38066
C	-0.52269	1.76754	-0.92994
C	0.67739	1.29092	-1.46966
C	-0.51345	2.89693	-0.10129
C	1.87788	1.93466	-1.17907
H	0.67762	0.42182	-2.12292
C	0.68905	3.53561	0.18815
H	-1.44614	3.25289	0.32605
C	1.88560	3.05422	-0.34727
H	2.80612	1.55564	-1.59552
H	0.69422	4.40345	0.83934
H	2.82309	3.54836	-0.11273
O	0.13906	-2.63578	-1.59190

C	-1.98393	-0.40460	-1.38911
H	-1.37918	-0.82849	-2.19774

19b-conf2

C	3.62831	-0.96784	-0.42742
H	3.56244	-2.05445	-0.48105
C	2.48467	-0.28175	-0.58854
H	2.44552	0.80344	-0.55028
C	1.20762	-0.99390	-0.82920
C	4.96611	-0.41861	-0.18377
C	5.21702	0.96054	-0.08920
C	6.03897	-1.31059	-0.03966
C	6.50522	1.42770	0.14318
H	4.40461	1.67233	-0.19677
C	7.33046	-0.84236	0.19294
H	5.85434	-2.37907	-0.11111
C	7.56615	0.52832	0.28492
H	6.68577	2.49545	0.21438
H	8.14928	-1.54603	0.30210
H	8.57047	0.89772	0.46616
C	-0.01417	-0.11060	-1.01427
H	0.00754	0.68014	-0.25683
H	0.11371	0.40059	-1.97907
C	-1.31732	-0.90554	-0.99829
H	-1.21707	-1.71576	-1.72907
C	-1.62425	-1.53892	0.34925
C	-2.09479	-2.85549	0.40306
C	-1.48903	-0.82606	1.54605
C	-2.42728	-3.44664	1.62109
H	-2.19383	-3.42285	-0.51892
C	-1.82078	-1.41436	2.76640
H	-1.12193	0.19708	1.53892
C	-2.29218	-2.72600	2.80755
H	-2.78693	-4.47058	1.64240
H	-1.70889	-0.84560	3.68425
H	-2.54847	-3.18433	3.75742
C	-3.73416	-0.96739	-1.62434
C	-3.07599	0.96548	-0.55903
O	-4.68935	-0.50983	-0.76994
O	-3.89405	-1.95557	-2.28815
N	-4.26495	0.69242	-0.15872
C	-2.40114	2.18495	-0.08095
C	-2.63776	2.65230	1.21843
C	-1.53467	2.88754	-0.92609
C	-2.01161	3.81203	1.66464
H	-3.29646	2.09135	1.87444
C	-0.91338	4.05022	-0.47609
H	-1.35270	2.53728	-1.93796
C	-1.14915	4.51204	0.81875
H	-2.19000	4.16583	2.67469
H	-0.24636	4.59387	-1.13676
H	-0.65899	5.41426	1.17001
O	1.13213	-2.21104	-0.89985
C	-2.52661	-0.06274	-1.50661
H	-2.28877	0.35995	-2.48914

19b-conf3

C	3.59528	0.41712	-0.30204
H	3.27680	1.45164	-0.17406
C	2.63022	-0.51779	-0.31966
H	2.84323	-1.57596	-0.44247
C	1.21062	-0.13264	-0.16741
C	5.03926	0.20303	-0.43880
C	5.88647	1.32070	-0.41401
C	5.60746	-1.07248	-0.59439
C	7.26593	1.17349	-0.54253
H	5.45559	2.31087	-0.29303
C	6.98350	-1.21941	-0.72222
H	4.97435	-1.95391	-0.61436
C	7.81724	-0.09734	-0.69715
H	7.90742	2.04846	-0.52179
H	7.41026	-2.21002	-0.84144
H	8.89130	-0.21681	-0.79730
C	0.20260	-1.25938	-0.18712
H	0.32809	-1.80834	-1.12900
H	0.45620	-1.96712	0.61159
C	-1.25276	-0.78575	-0.08236
H	-1.42547	-0.10122	-0.91998
C	-2.17776	-1.97720	-0.24703
C	-2.31008	-2.92182	0.77728
C	-2.87959	-2.16857	-1.43926
C	-3.13308	-4.03400	0.61351
H	-1.76322	-2.78837	1.70965
C	-3.70536	-3.28146	-1.60635
H	-2.78453	-1.43828	-2.23962
C	-3.83428	-4.21598	-0.58013
H	-3.22708	-4.75838	1.41644
H	-4.24946	-3.41383	-2.53628
H	-4.47782	-5.08061	-0.70726
C	-0.50006	0.11431	2.26851
C	-1.88612	1.47853	1.04751
O	-0.39084	1.41621	2.64460
O	0.17040	-0.74839	2.77368
N	-1.24459	2.22905	1.86661
C	-2.83812	2.04421	0.08027
C	-3.85954	1.24124	-0.44109
C	-2.72806	3.38084	-0.32534
C	-4.77051	1.77354	-1.35089
H	-3.95178	0.20281	-0.13308
C	-3.64060	3.90789	-1.23319
H	-1.92178	3.99260	0.06640
C	-4.66261	3.10614	-1.74706
H	-5.56204	1.14697	-1.74866
H	-3.55093	4.94245	-1.54775
H	-5.36986	3.51932	-2.45897
O	0.84669	1.02894	-0.02792
C	-1.58003	0.01820	1.21631
H	-2.43712	-0.45222	1.71967

19b-conf4

C	3.59527	0.41724	-0.30200

H	3.27676	1.45177	-0.17418
C	2.63024	-0.51768	-0.31967
H	2.84327	-1.57584	-0.44259
C	1.21063	-0.13259	-0.16743
C	5.03927	0.20319	-0.43867
C	5.60771	-1.07251	-0.59184
C	5.88625	1.32108	-0.41625
C	6.98374	-1.21938	-0.71981
H	4.97480	-1.95413	-0.60965
C	7.26570	1.17392	-0.54497
H	5.45519	2.31138	-0.29703
C	7.81724	-0.09709	-0.69727
H	7.41069	-2.21015	-0.83711
H	7.90701	2.04907	-0.52613
H	8.89130	-0.21651	-0.79752
C	0.20265	-1.25935	-0.18727
H	0.32816	-1.80819	-1.12922
H	0.45628	-1.96717	0.61135
C	-1.25271	-0.78575	-0.08250
H	-1.42536	-0.10108	-0.92002
C	-2.17767	-1.97719	-0.24740
C	-2.87954	-2.16836	-1.43962
C	-2.30987	-2.92201	0.77675
C	-3.70528	-3.28126	-1.60686
H	-2.78455	-1.43792	-2.23985
C	-3.13283	-4.03420	0.61283
H	-1.76295	-2.78870	1.70910
C	-3.83410	-4.21597	-0.58080
H	-4.24943	-3.41349	-2.53678
H	-3.22674	-4.75874	1.41562
H	-4.47762	-5.08060	-0.70807
C	-0.50006	0.11399	2.26849
C	-1.88616	1.47833	1.04769
O	-0.39086	1.41581	2.64472
O	0.17040	-0.74881	2.77352
N	-1.24468	2.22876	1.86690
C	-2.83819	2.04415	0.08057
C	-2.72844	3.38095	-0.32455
C	-3.85938	1.24112	-0.44112
C	-3.64106	3.90810	-1.23226
H	-1.92235	3.99279	0.06747
C	-4.77044	1.77352	-1.35079
H	-3.95140	0.20256	-0.13348
C	-4.66284	3.10628	-1.74648
H	-3.55164	4.94280	-1.54643
H	-5.56180	1.14689	-1.74881
H	-5.37016	3.51954	-2.45827
O	0.84667	1.02898	-0.02784
C	-1.58003	0.01796	1.21629
H	-2.43707	-0.45256	1.71962

19b-conf5

C	-3.45935	-0.03779	-0.35375
H	-3.10006	0.98459	-0.24511
C	-2.56399	-1.04080	-0.36979
H	-2.85935	-2.08122	-0.47519
C	-1.11063	-0.83634	-0.23895
C	-4.91735	-0.16115	-0.47110
C	-5.68809	1.01057	-0.45572
C	-5.57056	-1.39823	-0.59810
C	-7.07558	0.95391	-0.56635
H	-5.19174	1.97224	-0.35661
C	-6.95497	-1.45461	-0.70834
H	-4.99873	-2.32051	-0.60981
C	-7.71209	-0.27960	-0.69321
H	-7.65700	1.87001	-0.55305
H	-7.44778	-2.41657	-0.80560
H	-8.79285	-0.32887	-0.77930
C	-0.55105	0.56632	-0.09723
H	-0.85304	1.15271	-0.97276
H	-1.00252	1.05047	0.77551
C	0.98221	0.59577	-0.00925
H	1.36486	0.10830	-0.91226
C	1.44722	2.04032	-0.01651
C	2.03084	2.59111	-1.15962
C	1.26056	2.85219	1.10817
C	2.42784	3.92927	-1.17953
H	2.18217	1.96703	-2.03740
C	1.65540	4.18819	1.09148
H	0.80051	2.43764	2.00410
C	2.24151	4.73017	-0.05405
H	2.88551	4.34215	-2.07306
H	1.50544	4.80599	1.97127
H	2.55195	5.77003	-0.06695
C	0.60567	-0.77474	2.19991
C	2.36897	-1.42491	0.88025
O	0.95226	-2.07089	2.41861
O	-0.31633	-0.26019	2.77801
N	2.03014	-2.44228	1.58438
C	3.45399	-1.50796	-0.10837
C	3.81219	-2.74117	-0.66858
C	4.13291	-0.34575	-0.49323
C	4.84815	-2.80786	-1.59437
H	3.26902	-3.63574	-0.38139
C	5.16922	-0.41768	-1.42160
H	3.86106	0.61524	-0.06397
C	5.52797	-1.64749	-1.97220
H	5.12112	-3.76383	-2.02904
H	5.69377	0.48622	-1.71345
H	6.33242	-1.70274	-2.69855
O	-0.35241	-1.80050	-0.24206
C	1.57790	-0.18999	1.20214
H	2.22281	0.48507	1.78288

19b-conf6

C	3.16222	-0.65020	-0.46005
H	2.61434	0.11820	-1.00384
C	2.48430	-1.68174	0.07537
H	2.98275	-2.46518	0.63985
C	1.02245	-1.84586	-0.01059

C	4.61008	-0.42263	-0.38542
C	5.49612	-1.33601	0.20963
C	5.12693	0.75964	-0.93542
C	6.85868	-1.06582	0.25457
H	5.12408	-2.26229	0.63548
C	6.49241	1.03093	-0.88868
H	4.44895	1.47027	-1.40050
C	7.36123	0.11830	-0.29270
H	7.53347	-1.77961	0.71586
H	6.87589	1.95125	-1.31688
H	8.42605	0.32463	-0.25472
C	0.16791	-0.82203	-0.73512
H	0.69027	-0.40735	-1.60051
H	-0.72164	-1.33925	-1.10008
C	-0.20716	0.33867	0.20852
H	0.71763	0.70307	0.67459
C	-0.85101	1.51028	-0.51313
C	-1.72925	1.32413	-1.58657
C	-0.60075	2.81220	-0.06468
C	-2.35088	2.41611	-2.19087
H	-1.93840	0.32446	-1.95764
C	-1.22246	3.90545	-0.66724
H	0.09041	2.97143	0.75988
C	-2.10177	3.70929	-1.73134
H	-3.03048	2.25396	-3.02169
H	-1.01476	4.90825	-0.30768
H	-2.58568	4.55844	-2.20319
C	-1.04962	0.94163	2.48563
C	-2.57792	-0.16741	1.16599
O	-2.31398	1.39627	2.68771
O	-0.10688	1.39437	3.07780
N	-3.22757	0.68063	1.87887
C	-3.30338	-1.05627	0.24252
C	-2.82896	-2.34949	-0.00409
C	-4.48010	-0.61199	-0.37527
C	-3.53372	-3.19410	-0.86055
H	-1.91109	-2.69541	0.46472
C	-5.17600	-1.45864	-1.23149
H	-4.82783	0.40034	-0.19458
C	-4.70445	-2.75098	-1.47464
H	-3.16534	-4.19736	-1.04802
H	-6.08167	-1.10921	-1.71630
H	-5.24724	-3.40842	-2.14622
O	0.48447	-2.79321	0.55480
C	-1.09493	-0.11984	1.40786
H	-0.71535	-1.06552	1.81360

19b-conf7

C	-3.69292	0.94932	-0.05147
H	-3.54876	1.84677	0.55012
C	-2.59530	0.41386	-0.61454
H	-2.63380	-0.48011	-1.23029
C	-1.26979	1.03760	-0.41093
C	-5.07104	0.46289	-0.15511
C	-5.42465	-0.66766	-0.91096
C	-6.07762	1.15825	0.53145
C	-6.74813	-1.08677	-0.97267
H	-4.66522	-1.22123	-1.45404
C	-7.40428	0.73781	0.46978
H	-5.81269	2.03411	1.11746
C	-7.74193	-0.38607	-0.28246
H	-7.00905	-1.96126	-1.55990
H	-8.17115	1.28610	1.00716
H	-8.77423	-0.71724	-0.33363
C	-0.07671	0.33482	-1.02729
H	-0.37384	-0.18169	-1.94482
H	0.67846	1.08276	-1.27735
C	0.47665	-0.72078	-0.04746
H	-0.36608	-1.34346	0.28177
C	1.50706	-1.64017	-0.68089
C	2.44210	-1.16971	-1.60962
C	1.55982	-2.98379	-0.29294
C	3.41370	-2.02262	-2.13141
H	2.42171	-0.13201	-1.93112
C	2.53172	-3.83811	-0.81307
H	0.83108	-3.36502	0.41866
C	3.46306	-3.35842	-1.73301
H	4.13198	-1.64095	-2.85032
H	2.55608	-4.87787	-0.50271
H	4.21920	-4.02165	-2.14071
C	1.15989	-1.17986	2.31369
C	2.46355	0.38043	1.23118
O	2.46511	-1.27180	2.68024
O	0.31818	-1.90908	2.76566
N	3.23175	-0.28676	2.01493
C	3.01640	1.48618	0.43058
C	4.34229	1.42889	-0.01939
C	2.22501	2.60203	0.13581
C	4.87028	2.48312	-0.75710
H	4.94129	0.54959	0.19624
C	2.76226	3.65702	-0.60038
H	1.19250	2.64610	0.47344
C	4.08164	3.59906	-1.04756
H	5.89410	2.43230	-1.11288
H	2.14761	4.52249	-0.82525
H	4.49483	4.41883	-1.62646
O	-1.11278	2.04878	0.26437
C	1.03752	-0.09372	1.26726
H	0.35603	0.68590	1.62904

TS(16b→6,10-*cis*-1b)

C	1.76321	1.31448	-0.40218
C	0.41265	1.52723	-0.67663
C	-0.57324	-0.11654	0.56900
C	0.00855	-1.19387	-0.31500
C	1.55528	-1.23911	-0.31238
H	2.33039	2.13810	0.01313
H	-0.31220	-1.01985	-1.34711
H	1.86764	-1.69979	0.63126

H	1.85780	-1.92238	-1.11409
H	-0.06177	0.95794	-1.46805
C	-0.51939	-2.57341	0.05799
C	-1.14141	-3.37500	-0.90078
C	-0.39324	-3.05629	1.36635
C	-1.63074	-4.63921	-0.56363
H	-1.25124	-3.00535	-1.91787
C	-0.87648	-4.31746	1.70534
H	0.08277	-2.43654	2.12393
C	-1.49835	-5.11327	0.73974
H	-2.11665	-5.24871	-1.31928
H	-0.77211	-4.67948	2.72353
H	-1.87871	-6.09460	1.00523
C	-0.26209	2.78697	-0.34060
C	-1.38167	3.19311	-1.08145
C	0.15662	3.57268	0.74446
C	-2.04917	4.37407	-0.76792
H	-1.72452	2.58169	-1.91222
C	-0.51406	4.74970	1.06095
H	0.99223	3.24618	1.35726
C	-1.61424	5.15608	0.30269
H	-2.90874	4.68137	-1.35466
H	-0.18495	5.34736	1.90486
H	-2.13622	6.07447	0.55203
C	0.00565	0.32186	1.79545
O	1.14064	0.21525	2.26163
O	-0.95968	1.03945	2.46421
C	-1.94927	0.26293	0.69427
N	-2.17296	0.97416	1.77170
C	-3.08410	-0.04663	-0.20139
C	-2.92672	-0.11706	-1.59068
C	-4.35226	-0.27591	0.34991
C	-4.01412	-0.40534	-2.41345
H	-1.95910	0.06790	-2.04595
C	-5.43835	-0.56409	-0.47253
H	-4.47380	-0.23555	1.42748
C	-5.27245	-0.63135	-1.85669
H	-3.87604	-0.45147	-3.48890
H	-6.41387	-0.74390	-0.03196
H	-6.11815	-0.86087	-2.49701
C	2.36075	0.04192	-0.41175
C	4.57784	1.08347	-0.40575
C	4.38389	-1.32120	0.03192
C	5.86918	0.76773	-1.14989
H	4.79504	1.39612	0.62414
H	4.07745	1.89803	-0.92778
C	5.68003	-1.50131	-0.74507
H	4.60104	-1.25336	1.10640
H	3.75387	-2.18947	-0.14170
H	6.55504	1.61101	-1.05519
H	5.65097	0.60214	-2.21510
H	6.22422	-2.35851	-0.34559
H	5.45816	-1.68011	-1.80740
N	3.69510	-0.08791	-0.37508
O	6.51813	-0.36932	-0.61552

pre-6,10-*cis*-1b

C	-1.74847	0.86742	0.72044
C	-0.29731	1.24156	0.54642
C	0.47898	0.16115	-0.27867
C	0.07695	-1.26236	0.20231
C	-1.42190	-1.49721	-0.00600
H	-2.37391	1.67840	1.07755
H	0.26203	-1.27865	1.28158
H	-1.63257	-1.65821	-1.06854
H	-1.69417	-2.41885	0.52004
H	0.17445	1.26707	1.53562
C	0.93965	-2.34218	-0.42518
C	1.89095	-3.00912	0.35417
C	0.83196	-2.67459	-1.78183
C	2.72137	-3.97990	-0.20495
H	1.98482	-2.76278	1.40912
C	1.66337	-3.64256	-2.34417
H	0.09309	-2.18506	-2.41107
C	2.61193	-4.29688	-1.55826
H	3.45263	-4.48636	0.41722
H	1.56651	-3.88646	-3.39742
H	3.25793	-5.05059	-1.99701
C	-0.10600	2.63209	-0.04516
C	1.00914	3.39071	0.32812
C	-0.99979	3.16195	-0.98175
C	1.23387	4.64946	-0.22685
H	1.70564	2.99397	1.06463
C	-0.77769	4.42159	-1.53811
H	-1.87123	2.58310	-1.27530
C	0.33985	5.16756	-1.16401
H	2.10256	5.22555	0.07597
H	-1.48034	4.82028	-2.26324
H	0.51029	6.14866	-1.59592
C	0.18859	0.37025	-1.75786
O	-0.83904	0.27601	-2.37480
O	1.34559	0.73660	-2.37165
C	1.97370	0.38708	-0.29599
N	2.41456	0.71473	-1.45748
C	2.93872	0.24065	0.81577
C	2.52965	0.07832	2.14500
C	4.31284	0.24364	0.52458
C	3.47256	-0.06978	3.16187
H	1.47997	0.06022	2.41192
C	5.24929	0.09697	1.54020
H	4.63832	0.35124	-0.50424
C	4.83257	-0.06026	2.86430
H	3.13664	-0.19461	4.18585
H	6.30705	0.09792	1.29832
H	5.56503	-0.17857	3.65618
C	-2.26651	-0.35761	0.51563
C	-4.44442	0.37353	1.32950
C	-4.30107	-1.45561	-0.23382
C	-5.78129	-0.18677	1.78968
H	-4.61076	1.15259	0.56446
H	-3.94897	0.83632	2.18750

C	-5.63938	-1.95233	0.28663
H	-4.46397	-0.82184	-1.12261
H	-3.70447	-2.31878	-0.53346
H	-6.43987	0.62522	2.10394
H	-5.62376	-0.86931	2.63838
H	-6.19294	-2.44938	-0.51239
H	-5.47587	-2.66567	1.10862
N	-3.60062	-0.69650	0.81063
O	-6.44333	-0.87804	0.74397

6,10-*cis*-1b

C	-1.63601	-2.16631	1.42520
C	-1.44982	-0.73497	0.88873
C	-0.13741	-0.62068	0.04040
C	1.10050	-1.08410	0.86874
C	0.90501	-2.51187	1.41128
H	-1.81945	-2.86414	0.60004
H	-2.49185	-2.19806	2.10282
H	1.15025	-0.41030	1.73145
H	0.88725	-3.23184	0.58442
H	1.72887	-2.77149	2.07941
H	-1.30811	-0.08636	1.75800
C	2.39611	-0.91567	0.09352
C	3.23101	0.17216	0.37296
C	2.76757	-1.80546	-0.92188
C	4.40607	0.37419	-0.34951
H	2.95771	0.86861	1.16224
C	3.94140	-1.60338	-1.64704
H	2.14763	-2.66723	-1.15321
C	4.76283	-0.51238	-1.36485
H	5.04143	1.22298	-0.11702
H	4.21418	-2.30295	-2.43073
H	5.67695	-0.35740	-1.92894
C	-2.66106	-0.21343	0.13522
C	-3.10704	1.09111	0.37567
C	-3.32829	-0.98669	-0.82202
C	-4.19003	1.61686	-0.32664
H	-2.60305	1.70122	1.12158
C	-4.41118	-0.46170	-1.52696
H	-3.01171	-2.00589	-1.02531
C	-4.84421	0.84096	-1.28298
H	-4.52251	2.63002	-0.12428
H	-4.91752	-1.07504	-2.26545
H	-5.68846	1.24678	-1.83101
C	-0.29511	-1.43472	-1.23571
O	-0.45451	-2.61937	-1.38131
O	-0.25333	-0.59122	-2.29390
C	0.05876	0.74763	-0.57812
N	-0.02341	0.72900	-1.86012
C	0.37415	2.02496	0.09649
C	0.27842	2.18093	1.48445
C	0.81176	3.11026	-0.68000
C	0.60268	3.39733	2.08365
H	-0.04602	1.36702	2.12102
C	1.13228	4.32164	-0.08004
H	0.90858	2.99172	-1.75355
C	1.02882	4.47016	1.30509
H	0.52188	3.49951	3.16057
H	1.47174	5.15016	-0.69286
H	1.28425	5.41540	1.77278
C	-0.40510	-2.66107	2.15230
O	-0.46853	-3.16946	3.25535

TS(16b→6,10-*cis*-1b')

C	-0.14812	-1.89731	-0.65329
C	1.10312	-1.45785	-1.07817
C	1.14179	0.78491	-0.38901
C	-0.03256	1.09499	-1.28784
C	-1.34999	0.32547	-1.05119
H	-0.17516	-2.77799	-0.02148
H	0.31696	0.85304	-2.29851
H	-1.84101	0.74351	-0.16275
H	-2.00506	0.56279	-1.89686
H	1.21028	-0.92116	-2.01716
C	-0.33604	2.58987	-1.31069
C	-0.04838	3.34005	-2.45394
C	-0.88137	3.24388	-0.19825
C	-0.29217	4.71455	-2.48843
H	0.37522	2.84466	-3.32397
C	-1.12651	4.61484	-0.22922
H	-1.11006	2.68404	0.70584
C	-0.83185	5.35608	-1.37556
H	-0.05986	5.28051	-3.38532
H	-1.54771	5.10545	0.64306
H	-1.02278	6.42430	-1.39885
C	2.33662	-2.07028	-0.58092
C	3.45558	-2.15931	-1.42394
C	2.43566	-2.52781	0.74269
C	4.63874	-2.72737	-0.96263
H	3.38615	-1.77976	-2.43879
C	3.62390	-3.08543	1.20458
H	1.58879	-2.42147	1.41566
C	4.72420	-3.19151	0.35151
H	5.49627	-2.80268	-1.62331
H	3.69605	-3.42898	2.23139
H	5.65004	-3.62736	0.71354
C	2.46729	0.90276	-0.90313
O	2.90147	0.94443	-2.05670
O	3.32514	0.88572	0.16876
C	1.32810	0.83493	1.02799
N	2.59617	0.86236	1.36332
C	0.32897	0.90881	2.12271
C	-0.68285	-0.04566	2.26649
C	0.40310	1.96666	3.03769
C	-1.61716	0.06355	3.29555
H	-0.72686	-0.89050	1.58721
C	-0.53074	2.07588	4.06623
H	1.18590	2.71030	2.92391
C	-1.54702	1.12802	4.19399
H	-2.39522	-0.68685	3.39674

H	-0.46856	2.90484	4.76408
H	-2.27784	1.21687	4.99144
C	-1.34225	-1.17307	-0.83136
C	-2.64257	-3.18497	-0.30745
C	-3.77516	-1.00854	-0.37708
C	-3.90450	-3.77493	-0.92555
H	-2.65339	-3.31150	0.78313
H	-1.78497	-3.71367	-0.72073
C	-4.96504	-1.72217	-1.00304
H	-3.91848	-0.92896	0.70892
H	-3.71153	-0.00709	-0.79363
H	-4.02696	-4.80208	-0.57878
H	-3.81314	-3.77569	-2.02140
H	-5.88409	-1.20960	-0.71491
H	-4.87513	-1.70988	-2.09898
N	-2.52955	-1.75383	-0.61802
O	-5.06047	-3.05627	-0.54445

pre-6,10-*cis*-1b'

C	1.42830	0.84655	-1.21502
C	-0.01115	1.26157	-1.38350
C	-1.03544	0.21309	-0.83257
C	-0.52911	-1.22404	-1.16489
C	0.85708	-1.49205	-0.57912
H	2.14512	1.63007	-1.43598
H	-0.42772	-1.21772	-2.25810
H	0.79751	-1.63800	0.50571
H	1.22080	-2.43503	-1.00202
H	-0.22097	1.28045	-2.46378
C	-1.55062	-2.28967	-0.80836
C	-1.69355	-2.77502	0.49773
C	-2.39937	-2.78918	-1.80339
C	-2.66547	-3.72742	0.80076
H	-1.04778	-2.41306	1.29294
C	-3.37154	-3.74303	-1.50330
H	-2.29624	-2.42602	-2.82270
C	-3.50867	-4.21376	-0.19834
H	-2.76120	-4.08996	1.81954
H	-4.01801	-4.11854	-2.29023
H	-4.26391	-4.95641	0.03843
C	-0.31506	2.66317	-0.86523
C	0.43267	3.26439	0.15158
C	-1.39319	3.37376	-1.40994
C	0.09561	4.53053	0.63172
H	1.29440	2.75154	0.56710
C	-1.73507	4.63628	-0.92992
H	-1.96327	2.94442	-2.23076
C	-0.99361	5.21745	0.09901
H	0.69009	4.97955	1.42131
H	-2.57363	5.16892	-1.36733
H	-1.25538	6.20219	0.47275
C	-2.33317	0.42171	-1.60088
O	-2.52021	0.37269	-2.78798
O	-3.32541	0.70325	-0.72734
C	-1.56934	0.41093	0.57683
N	-2.82527	0.68904	0.58953
C	-0.91260	0.25568	1.89672
C	-1.70706	-0.09863	3.00021
C	0.46006	0.44372	2.08279
C	-1.13823	-0.24326	4.26018
H	-2.76726	-0.27741	2.85660
C	1.02797	0.29660	3.34763
H	1.09273	0.70119	1.24204
C	0.23249	-0.04347	4.43927
H	-1.76305	-0.52358	5.10186
H	2.09524	0.44788	3.47435
H	0.67673	-0.16225	5.42227
C	1.84459	-0.39382	-0.89994
C	4.17525	0.25367	-1.18280
C	3.60485	-1.55166	0.30953
C	5.56171	-0.35756	-1.31524
H	4.18471	1.03412	-0.40101
H	3.91133	0.72415	-2.13392
C	5.00772	-2.10215	0.11581
H	3.58391	-0.91162	1.20880
H	2.92200	-2.38806	0.46806
H	6.30453	0.42787	-1.46700
H	5.58281	-1.04215	-2.17637
H	5.34100	-2.61089	1.02242
H	5.01265	-2.81684	-0.72099
N	3.19586	-0.78150	-0.87315
O	5.93468	-1.06142	-0.14253

6,10-*cis*-1b'

C	0.98211	-0.28145	2.36585
C	0.87682	-1.17921	1.12361
C	-0.29363	-0.74399	0.19030
C	-1.63588	-0.67712	1.00452
C	-1.56669	0.09633	2.32971
H	1.24688	0.74435	2.08172
H	1.76336	-0.65388	3.03260
H	-1.78896	-1.72748	1.28289
H	-1.61489	1.17896	2.17496
H	-2.43739	-0.16467	2.93665
H	0.59196	-2.18425	1.46395
C	-2.81667	-0.27474	0.14093
C	-3.72690	-1.24933	-0.28144
C	-3.01158	1.04965	-0.26816
C	-4.80868	-0.91060	-1.09445
H	-3.58660	-2.28157	0.02921
C	-4.09047	1.39110	-1.08079
H	-2.32072	1.82932	0.04186
C	-4.99267	0.41103	-1.49630
H	-5.50582	-1.67989	-1.41080
H	-4.22532	2.42293	-1.38902
H	-5.83367	0.67758	-2.12832
C	2.18882	-1.31541	0.36609
C	2.46441	-2.51032	-0.31178
C	3.12497	-0.27783	0.29965
C	3.63482	-2.65803	-1.05410

H	1.75975	-3.33579	-0.25031
C	4.29763	-0.42427	-0.44109
H	2.95004	0.65879	0.82085
C	4.55464	-1.61203	-1.12379
H	3.82989	-3.59272	-1.57015
H	5.00972	0.39413	-0.48208
H	5.46815	-1.72473	-1.69885
C	-0.55989	-1.85570	-0.82260
O	-0.83433	-3.00684	-0.61483
O	-0.49414	-1.34122	-2.07037
C	0.04737	0.37083	-0.78783
N	-0.08441	0.00445	-2.01329
C	0.64346	1.71271	-0.57336
C	0.30834	2.54753	0.49623
C	1.60571	2.15175	-1.49754
C	0.91415	3.79412	0.64240
H	-0.43116	2.24377	1.22439
C	2.20824	3.39623	-1.35301
H	1.89499	1.49602	-2.31159
C	1.86571	4.22173	-0.28082
H	0.63803	4.42660	1.47930
H	2.95658	3.71610	-2.07062
H	2.34229	5.18941	-0.16291
C	-0.31739	-0.20160	3.13366
O	-0.35863	-0.33849	4.34069

TS(16b→6,10-*trans*-1b)

C	-1.95747	0.81888	1.15103
C	-0.63254	1.28726	1.04153
C	0.13400	-0.01215	-0.59023
C	-0.24401	-1.40335	-0.11594
C	-0.97555	-1.43556	1.26329
H	-2.76672	1.49103	0.90040
H	-0.99734	-1.74603	-0.84030
H	-0.29885	-1.08760	2.04983
H	-1.22915	-2.46475	1.51211
H	0.13638	0.82007	1.64842
C	0.90810	-2.39934	-0.19737
C	1.53953	-2.58485	-1.43490
C	1.36139	-3.13867	0.89617
C	2.60798	-3.46524	-1.57048
H	1.19494	-2.01970	-2.29847
C	2.43315	-4.02557	0.76452
H	0.90229	-3.02245	1.87289
C	3.06402	-4.18837	-0.46534
H	3.08587	-3.58778	-2.53754
H	2.77519	-4.58274	1.63126
H	3.89978	-4.87343	-0.56635
C	-0.31874	2.67739	0.68072
C	0.90585	3.22498	1.09003
C	-1.19538	3.46777	-0.07909
C	1.23602	4.54161	0.77862
H	1.59927	2.61112	1.66058
C	-0.86344	4.78100	-0.39472
H	-2.12875	3.04736	-0.44304
C	0.34946	5.32284	0.03802
H	2.18340	4.95466	1.10945
H	-1.54765	5.38258	-0.98436
H	0.60419	6.34865	-0.20901
C	-0.70159	0.59300	-1.59475
O	-1.87941	0.40648	-1.87425
O	0.04619	1.53850	-2.24299
C	1.42576	0.57980	-0.85078
N	1.36331	1.51142	-1.76494
C	2.71733	0.35110	-0.17258
C	2.76760	-0.15876	1.12853
C	3.91572	0.67648	-0.82321
C	3.99011	-0.33572	1.77401
H	1.85231	-0.42914	1.64580
C	5.13632	0.49850	-0.17926
H	3.88020	1.05978	-1.83776
C	5.17755	-0.00732	1.12194
H	4.01165	-0.73385	2.78344
H	6.05798	0.74849	-0.69507
H	6.13050	-0.14937	1.62157
C	-2.18300	-0.54960	1.25593
C	-4.61499	-0.25506	1.22691
C	-3.71457	-2.41502	0.68495
C	-5.06804	-0.09252	-0.22133
H	-5.39561	-0.77280	1.79407
H	-4.42363	0.70046	1.71374
C	-4.21691	-2.21555	-0.74663
H	-4.49033	-2.88913	1.29448
H	-2.83693	-3.05891	0.68068
H	-5.98734	0.49306	-0.27874
H	-4.27752	0.39636	-0.80960
H	-4.51922	-3.17211	-1.17797
H	-3.41304	-1.77204	-1.35423
N	-3.41881	-1.09920	1.26453
O	-5.35622	-1.37063	-0.77537

TS(16b→6,10-*trans*-1b')

C	1.74366	0.92281	-0.45321
C	0.38160	0.95598	-0.71345
C	-0.47944	0.08095	1.28558
C	0.18766	-1.28016	1.15165
C	1.72693	-1.23454	0.94280
H	2.29066	1.85495	-0.53077
H	0.09350	-1.75451	2.13873
H	2.16750	-1.09668	1.93571
H	2.02894	-2.22992	0.60103
H	-0.12362	0.06509	-1.06634
C	-0.49478	-2.24667	0.19531
C	-1.56226	-3.02012	0.66501
C	-0.07827	-2.41920	-1.12812
C	-2.22691	-3.91032	-0.17361
H	-1.88280	-2.90939	1.69866
C	-0.74790	-3.30193	-1.97748
H	0.78132	-1.87148	-1.51042
C	-1.82890	-4.04422	-1.50450

H	-3.05811	-4.49470	0.20901
H	-0.41579	-3.41510	-3.00481
H	-2.34816	-4.73238	-2.16412
C	-0.31223	2.22341	-0.98048
C	-1.39261	2.26554	-1.87379
C	0.07684	3.40428	-0.32906
C	-2.05685	3.46308	-2.12614
H	-1.70108	1.36021	-2.38801
C	-0.59181	4.59892	-0.57558
H	0.88620	3.37527	0.39552
C	-1.65816	4.63180	-1.47663
H	-2.88516	3.48365	-2.82695
H	-0.28793	5.50362	-0.05885
H	-2.18005	5.56429	-1.66686
C	0.13058	1.08814	2.08937
O	1.28836	1.22776	2.49246
O	-0.81954	2.04110	2.35354
C	-1.85385	0.48796	1.23309
N	-2.04914	1.64771	1.81946
C	-3.05032	-0.13905	0.61662
C	-3.05699	-0.59559	-0.70570
C	-4.22653	-0.23201	1.37054
C	-4.21456	-1.12840	-1.26571
H	-2.15111	-0.56020	-1.30063
C	-5.38375	-0.77554	0.81422
H	-4.22384	0.11640	2.39852
C	-5.38164	-1.22287	-0.50686
H	-4.19912	-1.48134	-2.29226
H	-6.28560	-0.84983	1.41380
H	-6.28177	-1.64668	-0.94100
C	2.41904	-0.18388	0.10358
C	4.54886	0.74634	-0.68056
C	4.57338	-1.10962	0.91821
C	5.75897	0.09544	-1.33972
H	4.86790	1.52964	0.01914
H	3.93749	1.19344	-1.46309
C	5.77464	-1.66170	0.16393
H	4.91475	-0.50243	1.76704
H	3.98970	-1.94269	1.29962
H	6.39238	0.87079	-1.77344
H	5.42419	-0.58164	-2.13917
H	6.41981	-2.20182	0.85860
H	5.43753	-2.35145	-0.62369
N	3.75599	-0.25202	0.04717
O	6.54342	-0.62110	-0.40689

pre-6,10-*trans*-1b

C	-0.87692	1.52697	0.48736
C	0.51853	1.31507	1.01970
C	1.15296	-0.02718	0.50504
C	0.76023	-0.26323	-0.98874
C	-0.75773	-0.34459	-1.14445
H	-1.39978	2.35027	0.96285
H	1.11055	0.64152	-1.50191
H	-1.13228	-1.29003	-0.73256
H	-0.99100	-0.35131	-2.21495
H	0.45130	1.21780	2.11188
C	1.48190	-1.44370	-1.61526
C	2.61078	-1.21921	-2.41245
C	1.06034	-2.76313	-1.41301
C	3.30733	-2.28312	-2.98365
H	2.94790	-0.20005	-2.58117
C	1.75600	-3.83018	-1.98050
H	0.17723	-2.97082	-0.81632
C	2.88340	-3.59375	-2.76620
H	4.17947	-2.08664	-3.59929
H	1.41234	-4.84571	-1.80992
H	3.42414	-4.42394	-3.20932
C	1.38917	2.54255	0.76921
C	2.27950	2.97018	1.75859
C	1.31359	3.26224	-0.42643
C	3.09522	4.08113	1.55264
H	2.33881	2.42467	2.69818
C	2.13342	4.37010	-0.63991
H	0.60235	2.96135	-1.19106
C	3.02848	4.78126	0.34770
H	3.77999	4.40046	2.33211
H	2.06706	4.91632	-1.57583
H	3.66229	5.64708	0.18369
C	2.67568	-0.02927	0.56211
O	3.47135	0.66446	-0.00903
O	3.07820	-1.05504	1.36009
C	0.88545	-1.21033	1.41618
N	1.96107	-1.74424	1.87058
C	-0.39576	-1.84588	1.81408
C	-1.48848	-1.10710	2.28386
C	-0.48521	-3.24462	1.76297
C	-2.65869	-1.75861	2.66775
H	-1.43372	-0.02860	2.35961
C	-1.65795	-3.89100	2.14420
H	0.36707	-3.81871	1.41236
C	-2.75050	-3.14798	2.59123
H	-3.49912	-1.17541	3.03030
H	-1.71761	-4.97299	2.08914
H	-3.66708	-3.64969	2.88447
C	-1.46638	0.81269	-0.48632
C	-3.45397	2.21800	-0.39292
C	-3.63488	-0.07026	-1.12672
C	-4.72382	2.51924	-1.17371
H	-3.70698	2.00566	0.66132
H	-2.81078	3.10223	-0.42033
C	-4.89445	0.31333	-1.88471
H	-3.90750	-0.45593	-0.12898
H	-3.12938	-0.86713	-1.67506
H	-5.29072	3.30950	-0.67786
H	-4.46286	2.84907	-2.19052
H	-5.58737	-0.52980	-1.91519
H	-4.63382	0.60275	-2.91405
N	-2.74791	1.09432	0.99724
O	-5.57028	1.38429	1.24742

6,10-*trans*-1b

C	-0.54487	2.15622	1.51230
C	-0.57470	1.71943	0.04441
C	0.45110	0.56643	-0.24807
C	1.61740	0.53253	0.81673
C	1.99294	1.96753	1.20235
H	-0.80542	1.32794	2.18517
H	-1.26489	2.95779	1.69423
H	1.20995	0.05248	1.71025
H	2.86483	1.98309	1.86099
H	2.23822	2.56104	0.31132
H	-0.20702	-2.57188	-0.54249
C	2.78722	0.32009	0.36134
C	2.75461	1.70070	0.58942
C	3.88872	-0.22738	-0.30521
C	3.79343	2.52063	0.15381
H	1.90952	2.13883	1.11706
C	4.93071	0.59122	-0.74039
H	3.94057	-1.29622	-0.49014
C	4.88469	1.96632	-0.51520
H	3.75176	3.58881	0.34098
H	5.77931	0.15114	-1.25430
H	5.69684	2.60168	-0.85370
C	-1.96159	1.38403	-0.47962
C	-3.03807	1.10922	0.36734
C	-2.15636	1.29692	-1.86367
C	-4.27728	0.73990	-0.15656
H	-2.91830	1.16337	1.44504
C	-3.38999	0.92090	-2.38985
H	-1.33720	1.52998	-2.54201
C	-4.45585	0.63755	-1.53464
H	-5.10046	0.52436	0.51758
H	-3.51966	0.85579	-3.46550
H	-5.41868	0.34465	-1.94099
C	1.10153	0.78316	-1.60512
O	1.63756	1.76759	-2.04032
O	1.01874	-0.36914	-2.31359
C	-0.14115	-0.80188	-0.49503
N	0.21219	-1.30357	-1.62303
C	-1.12299	-1.53837	0.32793
C	-2.13556	-2.24558	0.33606
C	-1.11365	-1.50726	1.72707
C	-3.11783	-2.91194	0.38854
H	-2.16239	-2.23732	-1.42088
C	-2.10062	-2.17470	2.44958
H	-0.34090	-0.97812	2.27243
C	-3.10511	-2.87531	1.78363
H	-3.90342	-3.44590	-0.13614
H	-2.08141	-2.14501	3.53389
H	-3.87692	-3.38733	2.34913
C	0.83455	2.64793	1.90116
O	1.00028	3.52901	2.72045

TS(16b→6,10-*trans*-1b'')

C	-0.40916	-0.47821	-1.25613
C	0.97402	-0.49653	-1.07801
C	1.11436	0.12076	1.18589
C	0.58862	1.51994	0.92637
C	-0.78100	1.60350	0.18281
H	-0.87177	-1.38661	-1.61918
H	0.35257	1.94715	1.91061
H	-1.54692	1.58852	0.96205
H	-0.84679	2.59905	-0.27057
H	1.55058	0.42103	-1.12011
C	1.63408	2.47009	0.34879
C	2.58447	3.02468	1.21328
C	1.66168	2.84554	-0.99668
C	3.55034	3.90987	0.74572
H	2.56840	2.74811	2.26492
C	2.63276	3.72909	-1.47432
H	0.92061	2.45822	-1.69310
C	3.58167	4.26181	-0.60563
H	4.27813	4.32758	1.43453
H	2.63781	4.00350	-2.52462
H	4.33348	4.95271	-0.97381
C	1.76465	-1.70773	-1.29014
C	3.11765	-1.58464	-1.64854
C	1.21948	-2.99046	-1.11326
C	3.90052	-2.71709	-1.84624
H	3.54597	-0.59392	-1.76436
C	2.00638	-4.12123	-1.30275
H	0.18357	-3.10388	-0.81037
C	3.34650	-3.98665	-1.67203
H	4.94258	-2.61198	-2.13003
H	1.57828	-5.10759	-1.15684
H	3.95885	-4.87066	-1.81981
C	2.47125	-0.32523	1.23242
O	3.54678	0.14261	0.86122
O	2.44179	-1.60825	1.75192
C	0.38477	-0.94667	1.79815
N	1.13801	-1.97255	2.09831
C	-1.07139	-0.99938	2.07213
C	-1.87925	-1.96537	1.46392
C	-1.65326	-0.06858	2.94186
C	-3.25227	-1.99222	1.71029
H	-1.42978	-2.69075	0.79278
C	-3.02347	-0.09951	3.19303
H	-1.02843	0.67617	3.42865
C	-3.82631	-1.05894	2.57328
H	-3.87147	-2.74289	1.22903
H	-3.46382	0.62390	3.87172
H	-4.89485	-1.07882	2.76291
C	-1.23544	0.56753	-0.82176
C	-3.11761	-0.45940	-1.99901
C	-3.52727	1.43004	-0.46409
C	-4.31591	0.03723	-2.79551
H	-3.40944	-1.29504	-1.34688
H	-2.37211	-0.80944	-2.71223
C	-4.69062	1.80616	-1.36942
H	-3.89343	0.86381	0.40438

H	-3.07064	2.35348	-0.11465
H	-4.80216	-0.81337	-3.27563
H	-3.98156	0.74112	-3.57153
H	-5.46170	2.29636	-0.77303
H	-4.34870	2.49995	-2.15145
N	-2.53538	0.60564	-1.17323
O	-5.27322	0.66593	-1.96758

pre-6,10-*trans*-1b''

C	0.48915	0.19535	1.32565
C	-0.97222	0.00261	1.01955
C	-1.24586	-0.07355	-0.51394
C	-0.52873	1.10912	-1.24803
C	0.98327	1.08281	-0.95831
H	0.78641	-0.07635	2.33238
H	-0.65438	0.93129	-2.32239
H	1.46137	0.36581	-1.63478
H	1.39164	2.06754	-1.21184
H	-1.51898	0.90688	1.32899
C	-1.15878	2.46206	-0.95867
C	-2.07471	2.99345	-1.87230
C	-0.83638	3.21228	0.17815
C	-2.67058	4.23383	-1.65275
H	-2.32724	2.42684	-2.76566
C	-1.43249	4.45311	0.40272
H	-0.11144	2.83329	0.89385
C	-2.35376	4.96688	-0.50933
H	-3.37880	4.62746	-2.37517
H	-1.17161	5.01999	1.29109
H	-2.81501	5.93372	-0.33430
C	-1.61038	-1.15257	1.77657
C	-2.85680	-0.97391	2.38780
C	-0.99524	-2.40576	1.86975
C	-3.47836	-2.02241	3.06594
H	-3.34319	-0.00348	2.33210
C	-1.61252	-3.45631	2.54653
H	-0.02061	-2.56642	1.42013
C	-2.85830	-3.26838	3.14538
H	-4.44406	-1.86226	3.53509
H	-1.11754	-4.42045	2.60776
H	-3.33855	-4.08546	3.67432
C	-2.76249	-0.03728	-0.65429
O	-3.55138	0.78248	-0.26954
O	-3.17268	-1.18839	-1.24803
C	-0.98051	-1.39597	-1.21611
N	-2.06005	-1.97034	-1.61073
C	0.28672	-2.01005	-1.69751
C	1.41275	-2.22805	-0.89344
C	0.32794	-2.40112	-3.04434
C	2.54764	-2.83425	-1.42599
H	1.42044	-1.90868	0.14136
C	1.46751	-3.00140	-3.57476
H	-0.53585	-2.21827	-3.67480
C	2.58045	-3.22234	-2.76553
H	3.41069	-3.00107	-0.78909
H	1.48462	-3.29038	-4.62048
H	3.47026	-3.68884	-3.17585
C	1.36847	0.74519	0.46545
C	3.11181	0.73272	2.16633
C	3.73040	0.74270	-0.16895
C	4.46270	1.36022	2.47407
H	3.16774	-0.36262	2.29680
H	2.38241	1.12574	2.87961
C	5.04967	1.38302	0.22910
H	3.86169	-0.35041	-0.23636
H	3.45112	1.11581	-1.15528
H	4.81360	1.02979	3.45360
H	4.36737	2.45645	2.47896
H	5.83893	1.07384	-0.45889
H	4.95446	2.47902	0.19902
N	2.68881	1.07388	0.81290
O	5.44544	0.97647	1.52785

TS(6,10-*cis*-1m)-conf2

C	0.20588	1.01769	1.46998
C	0.97509	2.21215	1.33172
C	2.67302	1.44084	0.26010
C	3.26044	0.48058	1.28622
C	2.22884	-0.07857	2.36337
H	-0.77278	0.99993	1.01998
H	3.98168	1.06619	1.87093
H	2.58486	-1.05011	2.71657
H	2.27436	0.60245	3.22133
H	1.66015	2.48537	2.13423
C	4.06463	-0.62758	0.59706
C	5.38144	-0.35181	0.18813
C	3.53376	-1.89810	0.32999
C	6.14876	-1.31764	-0.46881
H	5.80688	0.62902	0.38265
C	4.30098	-2.86855	-0.32478
H	2.51920	-2.13779	0.61511
C	5.60955	-2.58398	-0.72746
H	7.16347	-1.08377	-0.77554
H	3.87039	-3.84585	-0.51968
H	6.20272	-3.33727	-1.23602
C	0.42552	3.36619	0.59590
C	0.78708	4.67667	0.96538
C	-0.44597	3.18914	-0.49967
C	0.27052	5.78053	0.28367
H	1.46610	4.82659	1.80055
C	-0.96008	4.29243	-1.18040
H	-0.69949	2.19245	-0.83820
C	-0.60849	5.59082	-0.79000
H	0.55399	6.78383	0.58526
H	-1.61987	4.13046	-2.02587
H	-1.00545	6.44794	-1.32488
C	1.94960	0.97775	-0.91536
O	1.21945	-0.01783	-1.08556
O	2.08430	1.96224	-1.90748
C	3.35094	2.64226	-0.19156

N	3.01443	3.02120	-1.40752
C	0.80125	-0.14982	1.89986
H	0.76841	-2.20896	1.90826
N	0.19906	-1.37300	1.81395
C	-2.26137	-1.01013	1.60526
C	-1.15436	-3.11290	0.75461
C	-3.11935	-0.11348	0.88199
C	-2.60634	-1.33868	2.90251
H	-1.38599	-3.56933	1.72492
C	-2.28076	-3.44809	-0.27536
N	0.15093	-3.71248	0.33123
C	-2.85493	0.35081	-0.43173
C	-4.28587	0.38140	1.56414
C	-3.78932	-0.81842	3.48384
H	-1.95895	-1.98192	3.48879
C	-1.64798	-4.23194	-1.45037
H	-3.06227	-4.05407	0.19762
H	-2.75919	-2.53804	-0.64525
C	0.59250	-3.18791	-0.99746
C	-0.01916	-5.19049	0.23203
C	-3.68968	1.27606	-1.03337
H	-2.00317	0.00635	-1.00069
C	-5.13341	1.30648	0.90409
N	-4.61180	0.01074	2.84925
H	-4.06135	-1.08919	4.49954
C	-0.50983	-3.39032	-2.09917
C	-1.03937	-5.54919	-0.90135
H	-2.41543	-4.46525	-2.19623
H	0.85799	-2.13625	-0.89954
H	1.51014	-3.72391	-1.25764
H	-0.35813	-5.55868	1.20646
H	0.96561	-5.62760	0.03836
C	-4.84735	1.75796	-0.36882
O	-3.30004	1.69270	-2.30415
H	-6.00495	1.65511	1.44570
H	-0.07508	-3.99699	-2.90992
C	-0.93956	-2.06416	-2.70272
H	-1.83819	-6.19481	-0.51616
H	-0.54433	-6.09568	-1.71377
H	-5.50149	2.47736	-0.84484
C	-4.11313	2.66935	-3.01018
H	-0.15799	-1.30417	-2.73035
C	-2.15491	-1.75416	-3.17368
H	-3.60646	2.82232	-3.96230
H	-5.12712	2.29168	-3.18715
H	-4.16154	3.61664	-2.45988
H	-2.98695	-2.45398	-3.16019
H	-2.36873	-0.76666	-3.57159
C	-0.99508	-1.59171	0.98357
H	-0.80425	-1.11068	0.01856
C	4.27395	3.50146	0.61047
H	3.79241	3.82101	1.54332
H	5.19171	2.96493	0.87860
H	4.54627	4.39146	0.03839

TS(6,10-*cis*-1m)-conf3

C	2.06094	-1.85658	-0.43281
C	3.22651	-1.30756	-1.01697
C	3.13617	0.77928	-0.16450
C	1.96195	1.20286	-1.01334
C	0.72866	0.19968	-1.05876
H	2.15273	-2.73769	0.19388
H	2.34555	1.26537	-2.04060
H	-0.12541	0.71236	-0.61910
H	0.47936	0.05823	-2.12117
H	3.12944	-0.78984	-1.96863
C	1.45475	2.60419	-0.66117
C	1.46355	3.62372	-1.62449
C	0.95127	2.88487	0.62130
C	0.97548	4.90095	-1.31714
H	1.84859	3.41767	-2.62035
C	0.45765	4.15484	0.92743
H	0.94765	2.10527	1.37377
C	0.46778	5.16782	-0.04159
H	0.98998	5.68027	-2.07331
H	0.05299	4.33968	1.91688
H	0.08348	6.15464	0.19732
C	4.56415	-1.85293	-0.76344
C	5.55207	-1.78716	-1.76750
C	4.90903	-2.39899	0.49051
C	6.83657	-2.28294	-1.54009
H	5.30148	-1.35380	-2.73209
C	6.19549	-2.88909	0.71788
H	4.18148	-2.39311	1.29408
C	7.16076	-2.83894	-0.29601
H	7.58407	-2.23119	-2.32528
H	6.45209	-3.29109	1.69233
H	8.16204	-3.21551	-0.11294
C	3.06271	0.38763	1.22035
O	2.10923	-0.04819	1.89992
O	4.37172	0.45586	1.74070
C	4.48590	1.24718	-0.34870
N	5.26639	1.04991	0.69933
C	0.85524	-1.17035	-0.43587
H	-0.23202	-2.73062	0.33868
N	-0.25080	-1.73729	0.11843
C	-1.60619	0.09662	1.16773
C	-2.45839	-2.25405	0.96449
C	-2.39658	1.24747	0.83105
C	-0.86196	0.12554	2.33142
H	-2.10521	-2.34222	1.99847
C	-3.98493	-1.92821	0.95066
N	-2.19776	-3.59012	0.34439
C	-3.15010	1.38570	-0.36244
C	-2.38297	2.34750	1.75890
C	-0.90740	1.26039	3.17871
H	-0.18710	-0.68500	2.57108
C	-4.73962	-3.17453	0.42635
H	-4.32977	-1.67940	1.96024
H	-4.20488	-1.05687	0.32681

C	-2.74752	-3.65735	-1.03680
C	-2.83196	-4.64490	1.18571
C	-3.86349	2.54334	-0.62342
H	-3.18183	0.60802	-1.11406
C	-3.13143	3.51369	1.46359
N	-1.64539	2.33603	2.92065
H	-0.30717	1.28320	4.08163
C	-4.31360	-3.48742	-1.04539
C	-4.37245	-4.39362	1.31061
H	-5.81950	-2.99612	0.45647
H	-2.26511	-2.88145	-1.63867
H	-2.45731	-4.62009	-1.46807
H	-2.34238	-4.63715	2.16466
H	-2.61857	-5.61111	0.71772
C	-3.86297	3.62189	0.29904
O	-4.55784	2.56111	-1.82844
H	-3.09546	4.32085	2.18581
H	-4.77651	-4.44514	-1.32060
C	-4.76713	-2.44575	-2.03470
H	-4.65177	-4.18942	2.35147
H	-4.94085	-5.27487	0.98955
H	-4.41985	4.52719	0.09419
C	-5.29909	3.75461	-2.19999
H	-4.34108	-1.44883	-1.91085
C	-5.63115	-2.66158	-3.03356
H	-5.73013	3.52857	-3.17470
H	-6.10111	3.96627	-1.48267
H	-4.63776	4.62546	-2.28131
H	-6.07899	-3.63894	-3.20011
H	-5.92400	-1.87334	-3.72036
C	-1.58451	-1.15624	0.29413
H	-2.00619	-0.92222	-0.69018
C	5.05187	1.85132	-1.59206
H	4.52609	2.77973	-1.84546
H	6.11323	2.07122	-1.45497
H	4.94748	1.16361	-2.44140

TS(6,10-*cis*-1m)-conf4

C	1.24376	-1.97198	-0.22798
C	2.55621	-1.95294	-0.77175
C	3.01594	0.18281	-0.60517
C	2.04935	0.66465	-1.66497
C	0.63591	-0.08220	-1.74264
H	1.04539	-2.57229	0.65356
H	2.53858	0.44193	-2.62198
H	-0.13523	0.68172	-1.82569
H	0.63319	-0.63565	-2.69276
H	2.65649	-1.80493	-1.84640
C	1.84582	2.18107	-1.63971
C	2.23160	2.94864	-2.74998
C	1.26116	2.82759	-0.53609
C	2.03772	4.33556	-2.76513
H	2.68267	2.45845	-3.60960
C	1.06546	4.21133	-0.55291
H	0.96531	2.24924	0.33065
C	1.45071	4.96999	-1.66598
H	2.34134	4.91395	-3.63251
H	0.60333	4.69260	0.30166
H	1.29181	6.04356	-1.67483
C	3.65789	-2.72314	-0.17550
C	4.67729	-3.24206	-0.99906
C	3.74938	-2.91891	1.21784
C	5.74108	-3.96219	-0.45315
H	4.62477	-3.08467	-2.07309
C	4.81573	-3.63510	1.76291
H	3.00760	-2.47221	1.87019
C	5.81116	-4.16337	0.93100
H	6.51507	-4.36010	-1.10158
H	4.88145	-3.76514	2.83802
H	6.64203	-4.71479	1.35925
C	2.80411	0.27857	0.82314
O	1.74973	0.30520	1.49139
O	4.06227	0.19199	1.44161
C	4.45377	0.23165	-0.76065
N	5.11719	0.19161	0.37854
C	0.28871	-1.06434	-0.65524
H	-1.19640	-1.82285	0.53438
N	-0.95288	-1.05718	-0.09607
C	-2.14289	1.18278	-0.46972
C	-3.32387	-0.86018	0.36766
C	-1.80192	1.92419	0.71045
C	-2.61589	1.88306	-1.56937
H	-3.20573	-0.38640	1.34707
C	-4.73330	-0.53104	-0.20846
N	-3.19128	-2.32809	0.62549
C	-1.23130	1.34581	1.87906
C	-2.05748	3.33984	0.68751
C	-2.79144	3.28488	-1.51020
H	-2.87039	1.35504	-2.48373
C	-5.61123	-1.80074	-0.08369
H	-5.18687	0.29913	0.34343
H	-4.66984	-0.20911	-1.25415
C	-3.53000	-3.11940	-0.58929
C	-4.11173	-2.70152	1.73816
C	-0.95714	2.13860	2.98157
H	-0.92665	0.31200	1.85753
C	-1.77944	4.11458	1.84808
N	-2.54555	3.99704	-0.41492
H	-3.15567	3.82862	-2.37607
C	-5.04130	-2.94121	-0.98933
C	-5.58101	-2.29016	1.38768
H	-6.63895	-1.57797	-0.38828
H	-2.87012	-2.79849	-1.40147
H	-3.29979	-4.16967	-0.38708
H	-3.76167	-2.20806	2.65020
H	-4.02157	-3.78173	1.89058
C	-1.24909	3.53185	2.97248
O	-0.39889	1.68384	4.15705
H	-1.99161	5.17614	1.79864
H	-5.59002	-3.85957	-0.73891

C	-5.20842	-2.68143	-2.46332
H	-5.92946	-1.48704	2.04844
H	-6.26594	-3.13666	1.51683
H	-1.01691	4.10317	3.86312
C	0.08301	0.30352	4.22119
H	-4.66024	-1.82548	-2.86104
C	-5.95630	-3.41903	-3.29254
H	-0.75167	-0.40077	4.10570
H	0.83985	0.13117	3.45141
H	0.51059	0.20555	5.21835
H	-6.51339	-4.28467	-2.94105
H	-6.04174	-3.18879	-4.35018
C	-2.15663	-0.34274	-0.52990
H	-2.37754	-0.61664	-1.57401
C	5.20583	0.25769	-2.05095
H	4.93484	-0.60203	-2.67713
H	4.97760	1.16972	-2.61544
H	6.28086	0.22176	-1.86008

TS(6,10-*cis*-1m)

C	-0.64016	-1.54956	0.32665
C	-1.94028	-2.09922	0.55353
C	-3.08903	-0.31055	0.66927
C	-2.55808	0.24522	1.98402
C	-1.03851	-0.12111	2.30663
H	-0.13296	-1.79136	-0.59508
H	-3.14384	-0.24192	2.77396
H	-0.58735	0.71482	2.84751
H	-1.05716	-0.97048	3.00004
H	-2.23053	-2.31455	1.58233
C	-2.82154	1.74614	2.10738
C	-3.95541	2.19886	2.80110
C	-1.96376	2.69348	1.52416
C	-4.23224	3.56624	2.90811
H	-4.62464	1.47755	3.26295
C	-2.23868	4.05976	1.63062
H	-1.09801	2.35702	0.97114
C	-3.37304	4.50240	2.32197
H	-5.11303	3.89802	3.44911
H	-1.56874	4.77961	1.17050
H	-3.58478	5.56384	2.40283
C	-2.56232	-3.00715	-0.42907
C	-3.39783	-4.05237	0.01149
C	-2.37111	-2.83347	-1.81478
C	-4.00468	-4.91700	-0.90152
H	-3.55841	-4.19196	1.07722
C	-2.98162	-3.69539	-2.72693
H	-1.77422	-2.00241	-2.17303
C	-3.79610	-4.74131	-2.27490
H	-4.63951	-5.72192	-0.54513
H	-2.83582	-3.54172	-3.79099
H	-4.27289	-5.40675	-2.98738
C	-2.73633	0.26126	-0.62589
O	-1.69328	0.81699	-1.01984
O	-3.78376	-0.03616	-1.51431
C	-4.45875	-0.76143	0.49377
N	-4.89427	-0.68140	-0.74607
C	-0.20218	-0.50691	1.11747
H	0.97624	1.17307	1.28716
N	0.87924	0.26925	0.82540
C	2.31336	-0.97750	-0.84216
C	2.43429	1.52495	-0.57145
C	3.29790	-1.55844	0.02917
C	2.13333	-1.54806	-2.09012
H	3.30449	1.33673	0.06652
C	2.91126	1.84069	-2.02117
N	1.75342	2.71408	0.03076
C	3.58345	-1.09090	1.33635
C	4.03933	-2.68615	-0.47324
C	2.90900	-2.66288	-2.49575
H	1.38728	-1.14557	-2.76844
C	2.76538	3.36387	-2.25096
H	3.95320	1.53052	-2.15757
H	2.31957	1.29045	-2.76143
C	0.67374	3.23213	-0.86300
C	2.77321	3.78174	0.24139
C	4.55948	-1.70014	2.10746
H	3.02459	-0.27455	1.76906
C	5.02955	-3.28505	0.34459
N	3.83632	-3.22054	-1.72650
H	2.75959	-3.10234	-3.47712
C	1.25396	3.76268	-2.22144
C	3.49153	4.12041	-1.10837
H	3.19103	3.64014	-3.22124
H	-0.05489	2.43618	-1.03187
H	0.15469	4.03127	-0.32551
H	3.48355	3.43516	0.99901
H	2.25336	4.65457	0.64916
C	5.29586	-2.80788	1.61188
O	4.75133	-1.15610	3.37386
H	5.56711	-4.13140	-0.06674
H	1.21417	4.86111	-2.23563
C	0.46986	3.24719	-3.40275
H	4.54497	3.81481	-1.07690
H	3.47248	5.19981	-1.30147
H	6.05772	-3.28328	2.21657
C	5.74512	-1.74562	4.25425
H	0.20788	2.18873	-3.37779
C	0.07016	3.99619	-4.43711
H	5.69939	-1.15545	5.16892
H	5.50967	-2.79295	4.47916
H	6.75155	-1.67953	3.82329
H	0.28697	5.06128	-4.48942
H	-0.49549	3.57874	-5.26441
C	1.51713	0.27456	-0.49406
H	0.71330	0.37297	-1.24028
C	-5.33699	-1.36660	1.53982
H	-5.58106	-0.63794	2.32184
H	-6.26776	-1.71813	1.08865
H	-4.83875	-2.21839	2.01902

TS(6,10-*trans*-1q)

C	-0.32336	0.85530	-1.51295
C	-1.41029	1.73588	-1.17290
C	-2.46606	0.58260	0.18218
C	-2.71390	-0.74458	-0.54958
C	-2.04255	-0.83535	-1.97726
H	0.68278	1.16793	-1.27845
H	-2.17934	-1.49944	0.04370
H	-2.56491	-0.17339	-2.67428
H	-2.16453	-1.85955	-2.34446
H	-2.27082	1.74511	-1.84216
C	-4.18409	-1.15529	-0.56009
C	-4.75865	-1.60169	0.64507
C	-4.99777	-1.08190	-1.70052
C	-6.11019	-1.94652	0.71344
H	-4.13942	-1.66011	1.53588
C	-6.35345	-1.43150	-1.63666
H	-4.58905	-0.74428	-2.64614
C	-6.91563	-1.86027	-0.43065
H	-6.53437	-2.28167	1.65456
H	-6.96711	-1.36493	-2.52967
H	-7.96630	-2.12718	-0.38088
C	-1.13068	3.06609	-0.58560
C	-1.96254	4.15819	-0.89924
C	-0.05852	3.26844	0.30666
C	-1.71535	5.42379	-0.36285
H	-2.80149	4.01237	-1.57438
C	0.18485	4.53172	0.84585
H	0.56713	2.43770	0.60533
C	-0.63730	5.61444	0.51016
H	-2.36285	6.25603	-0.61981
H	1.00713	4.65948	1.54137
H	-0.44817	6.59571	0.93404
C	-1.47552	0.54798	1.26154
O	-0.44804	-0.15042	1.37083
O	-1.81385	1.52589	2.19434
C	-3.47488	1.52164	0.67373
N	-3.12463	2.13883	1.78118
C	-0.59895	-0.44507	-1.86461
N	0.33278	-1.45099	-1.85974
H	0.00245	-2.41424	-1.91088
C	1.53708	-1.35051	-1.01858
H	1.21766	-0.89096	-0.07862
C	2.65379	-0.51956	-1.63680
C	3.27838	0.56161	-0.92679
C	3.09739	-0.80555	-2.91479
C	2.87122	1.01501	0.35544
C	4.34862	1.25682	-1.59433
C	4.16551	-0.07129	-3.48508
H	2.61443	-1.58777	-3.49072
C	3.48034	2.11450	0.93694
H	2.05445	0.55459	0.89762
C	4.97464	2.35158	-0.94698
H	4.51737	-0.30766	-4.48472
C	4.55345	2.78467	0.29350
H	5.78253	2.84433	-1.47519
H	5.03381	3.63584	0.75917
N	4.78616	0.92156	-2.85548
O	2.94581	2.51686	2.15641
C	3.54244	3.63867	2.86131
H	2.96164	3.73522	3.77773
H	4.59311	3.44303	3.10656
H	3.46642	4.56353	2.27632
C	2.04267	-2.78526	-0.72152
H	2.55086	-3.15631	-1.61918
C	3.01818	-2.82655	0.49639
C	0.22011	-3.46097	0.79883
C	1.41210	-5.11910	-0.52963
C	2.59952	-4.00906	1.40260
H	4.05189	-2.95476	0.15599
H	2.98414	-1.88895	1.06248
C	1.17959	-3.74991	2.00747
H	-0.11173	-2.42030	0.81663
H	-0.67294	-4.09281	0.84532
C	2.53460	-5.30051	0.54705
H	1.78339	-5.33318	-1.53731
H	0.56442	-5.78564	-0.34059
H	3.31833	-4.12839	2.21986
H	0.87516	-4.68302	2.50309
H	3.50760	-5.47602	0.07091
H	2.32570	-6.16605	1.18738
N	0.89300	-3.72133	-0.50900
C	1.15170	-2.63946	3.03109
H	1.11693	-1.62211	2.64317
C	1.13839	-2.83758	4.35489
H	1.13805	-3.83705	4.78658
H	1.12094	-2.00944	5.05688
C	-4.74515	1.93655	0.00246
H	-4.56775	2.15698	-1.05672
H	-5.49613	1.14257	0.04985
H	-5.14227	2.83167	0.48738

TS(6,10-*trans*-1q)-conf3

C	1.60426	-2.16498	-0.66990
C	2.82943	-1.56071	-1.09157
C	2.83399	0.30180	0.05756
C	1.41683	0.83466	-0.09709
C	0.51749	0.00454	-1.08545
H	1.62752	-3.13954	-0.19547
H	0.96111	0.69017	0.88675
H	0.95356	0.06350	-2.08994
H	-0.46330	0.47595	-1.13889
H	2.79740	-0.93727	-1.98341
C	1.35249	2.33651	-0.37635
C	1.76263	3.21793	0.64225
C	0.88830	2.88160	-1.58259
C	1.72113	4.60069	0.45583
H	2.10439	2.80809	1.58779
C	0.84003	4.27017	-1.77103
H	0.55812	2.23477	-2.38731

C	1.25866	5.13462	-0.75509
H	2.04207	5.26055	1.25560
H	0.48127	4.67013	-2.71491
H	1.22778	6.20973	-0.90268
C	4.12282	-2.23043	-0.88994
C	5.18652	-1.97467	-1.77752
C	4.34443	-3.10214	0.19775
C	6.42393	-2.60003	-1.61122
H	5.03584	-1.28395	-2.60237
C	5.58159	-3.72227	0.36504
H	3.56308	-3.24555	0.93583
C	6.62256	-3.48061	-0.54226
H	7.23204	-2.39343	-2.30537
H	5.74294	-4.37936	1.21329
H	7.58569	-3.96197	-0.40550
C	3.18677	-0.31505	1.33171
O	2.47408	-0.90841	2.15925
O	4.58257	-0.20483	1.47801
C	4.06980	0.90158	-0.41081
N	5.11682	0.59796	0.33095
C	0.43471	-1.43595	-0.67328
N	-0.74986	-1.95564	-0.22380
H	-0.86536	-2.96031	-0.14179
C	-1.91291	-1.18255	0.22268
H	-2.36116	-0.67222	-0.63637
C	-1.53094	-0.15110	1.28658
C	-1.81941	1.24753	1.14435
C	-0.78731	-0.56011	2.37898
C	-2.49211	1.82014	0.03427
C	-1.29392	2.13051	2.15252
C	-0.33408	0.38112	3.33501
H	-0.47052	-1.59168	2.47208
C	-2.60232	3.19375	-0.09597
H	-2.90110	1.21412	-0.76373
C	-1.46229	3.53001	2.00559
H	0.27309	0.05374	4.17063
C	-2.09300	4.06372	0.90275
H	-1.04405	4.16186	2.77977
H	-2.17747	5.13716	0.79741
N	-0.57247	1.68545	3.23619
O	-3.22611	3.64225	-1.25458
C	-3.17760	5.06143	-1.57041
H	-3.63176	5.14812	-2.55703
H	-3.75393	5.65261	-0.84897
H	-2.14185	5.41968	-1.60159
C	-2.95661	-2.17356	0.79205
H	-2.57052	-2.53795	1.75061
C	-4.35492	-1.50728	0.99919
C	-3.67583	-3.05433	-1.39057
C	-3.91367	-4.39853	0.62224
C	-5.41846	-2.39385	0.30636
H	-4.58239	-1.41939	2.06723
H	-4.37500	-0.48981	0.59323
C	-5.13734	-2.48698	-1.22939
H	-3.02702	-2.33544	-1.89895
H	-3.67703	-3.96487	-1.99732
C	-5.34288	-3.82248	0.90362
H	-3.40594	-4.68289	1.54953
H	-3.95693	-5.28699	-0.01564
H	-6.41624	-1.97052	0.46210
H	-5.85126	-3.21124	-1.64536
H	-5.54266	-3.78144	1.98137
H	-6.11688	-4.45682	0.45481
N	-3.06856	-3.38676	-0.07354
C	-5.32348	-1.17838	-1.95232
H	-4.63253	-0.37836	-1.68148
C	-6.25249	-0.94307	-2.88635
H	-6.96033	-1.71004	-3.19326
H	-6.34216	0.02073	-3.37816
C	4.27802	1.70041	-1.65743
H	3.87146	1.17268	-2.53006
H	3.76877	2.66701	-1.59557
H	5.34615	1.86941	-1.81587

TS(6,10-*trans*-1q)-conf4

C	0.73167	-1.73636	-1.09774
C	2.05872	-1.59187	-1.59589
C	2.68715	0.46012	-0.88745
C	1.35275	1.14194	-0.70158
C	0.22531	0.62074	-1.66803
H	0.49492	-2.61076	-0.49972
H	1.04015	0.85363	0.30611
H	0.61313	0.57436	-2.69315
H	-0.60506	1.32712	-1.66867
H	2.17804	-1.16928	-2.58974
C	1.47307	2.66612	-0.69672
C	1.98701	3.28582	0.45628
C	1.08822	3.47153	-1.77975
C	2.10608	4.67492	0.52718
H	2.27627	2.66759	1.30054
C	1.21127	4.86593	-1.71188
H	0.68583	3.01990	-2.68111
C	1.71839	5.47170	-0.55826
H	2.49017	5.13588	1.43131
H	0.90823	5.47448	-2.55870
H	1.80787	6.55194	-0.50258
C	3.12561	-2.50400	-1.18075
C	4.23459	-2.72160	-2.02391
C	3.09949	-3.12555	0.08965
C	5.27581	-3.56197	-1.62604
H	4.27832	-2.22212	-2.98609
C	4.14290	-3.96197	0.48110
H	2.29131	-2.90746	0.77929
C	5.23048	-4.18746	-0.37520
H	6.12507	-3.71752	-2.28301
H	4.12073	-4.42600	1.46214
H	6.04389	-4.83404	-0.06139
C	3.43606	0.03251	0.28198
O	3.05627	-0.24766	1.43409
O	4.78209	-0.09323	-0.10300

C	3.69958	0.73778	-1.88417
N	4.91586	0.37864	-1.51712
C	-0.21842	-0.74046	-1.21895
N	-1.49975	-0.95339	-0.79168
H	-1.82330	-1.91031	-0.65377
C	-2.49124	0.02342	-0.32699
H	-2.95030	0.52816	-1.19086
C	-1.94924	1.10993	0.59790
C	-1.05929	0.83201	1.69287
C	-2.33017	2.42296	0.38144
C	-0.54106	-0.45095	2.00456
C	-0.59195	1.96043	2.45693
C	-1.86529	3.45885	1.22896
H	-2.97709	2.67294	-0.45417
C	0.45799	-0.60469	2.94975
H	-0.84055	-1.32858	1.45451
C	0.39631	1.75805	3.45485
H	-2.17869	4.48415	1.06108
C	0.93356	0.51115	3.68836
H	0.73523	2.63214	3.99841
H	1.72991	0.39056	4.41032
N	-1.02093	3.24766	2.23146
O	0.94209	-1.89082	3.10942
C	2.22197	-2.08338	3.79476
H	2.43975	-3.14501	3.67729
H	2.99449	-1.48015	3.31283
H	2.13436	-1.84684	4.86180
C	-3.60012	-0.78122	0.41689
H	-3.19300	-1.05820	1.39474
C	-4.91891	0.02827	0.60777
C	-4.59915	-1.85773	-1.55772
C	-4.69501	-2.93842	0.62233
C	-6.10499	-0.88372	0.20732
H	-5.02400	0.34792	1.65008
H	-4.91558	0.94154	0.00179
C	-6.02505	-1.23799	-1.31392
H	-3.98880	-1.20362	-2.18773
H	-4.67391	-2.81930	-2.07421
C	-6.01957	-2.20297	1.01799
H	-4.09239	-3.18468	1.50205
H	-4.89741	-3.87208	0.08810
H	-7.05349	-0.37536	0.40903
H	-6.78857	-2.00375	-1.50852
H	-6.03428	-1.97574	2.09098
H	-6.89394	-2.83036	0.80749
N	-3.87393	-2.07741	-0.27649
C	-6.29434	-0.06553	-2.22013
H	-5.56152	0.74260	-2.18382
C	-7.33915	0.03916	-3.04985
H	-8.08921	-0.74512	-3.12460
H	-7.48611	0.90769	-3.68466
C	3.49390	1.29457	-3.25615
H	2.78495	0.68572	-3.83298
H	3.08806	2.31011	-3.19987
H	4.44459	1.32272	-3.79461

TS(6,10-*trans*-1q)-conf2

C	0.45078	1.43992	0.38338
C	1.81154	1.90305	0.45279
C	2.86452	0.16350	0.08212
C	2.32533	-0.83956	1.11269
C	1.13153	-0.29064	1.98921
H	-0.20182	1.84756	-0.37462
H	1.86998	-1.64157	0.51517
H	1.50450	0.45576	2.69667
H	0.72984	-1.12360	2.57525
H	2.26347	1.96925	1.44257
C	3.42514	-1.48616	1.95065
C	4.25446	-2.44291	1.33537
C	3.67139	-1.15275	3.29092
C	5.31023	-3.03470	2.03217
H	4.07560	-2.70763	0.29694
C	4.72700	-1.74799	3.99470
H	3.05186	-0.42178	3.79799
C	5.55240	-2.68645	3.36825
H	5.94169	-3.76498	1.53627
H	4.90291	-1.47422	5.03036
H	6.37204	-3.14422	3.91254
C	2.27736	2.97412	-0.45654
C	3.24045	3.89978	-0.01199
C	1.79631	3.08188	-1.77672
C	3.69248	4.92146	-0.84985
H	3.62874	3.81922	0.99959
C	2.25039	4.10071	-2.61506
H	1.09262	2.34721	-2.15233
C	3.19558	5.02603	-2.15421
H	4.43155	5.62970	-0.48937
H	1.87849	4.16519	-3.63230
H	3.54947	5.81496	-2.81009
C	2.44915	-0.05923	-1.30553
O	1.38816	-0.54055	-1.74756
O	3.44508	0.44388	-2.14298
C	4.23954	0.64760	-0.04554
N	4.59907	0.89046	-1.28736
C	0.09474	0.31611	1.09106
N	-1.03403	-0.41585	0.84702
H	-1.11370	-1.34463	1.26266
C	-1.72080	-0.36220	-0.45080
H	-0.93516	-0.32882	-1.22015
C	-2.61978	0.84502	-0.67812
C	-3.63304	1.26442	0.25049
C	-2.50156	1.53983	-1.86930
C	-3.86261	0.65334	1.50829
C	-4.46549	2.37292	-0.13787
C	-3.36620	2.62447	-2.16246
H	-1.73805	1.25742	-2.58775
C	-4.87201	1.10883	2.34027
H	-3.23697	-0.15487	1.85706
C	-5.48676	2.81332	0.74015
H	-3.26584	3.16300	-3.09979
C	-5.69766	2.19839	1.95768

H	-6.09370	3.65044	0.41554
H	-6.48523	2.55354	2.61017
N	-4.32155	3.03579	-1.33715
O	-5.00572	0.43309	3.54975
C	-6.02860	0.85939	4.48868
H	-5.92639	0.19043	5.34258
H	-5.86930	1.89555	4.81111
H	-7.03316	0.75839	4.06004
C	-2.53095	-1.67921	-0.62335
H	-3.46102	-1.58389	-0.05337
C	-2.85881	-1.98437	-2.11764
C	-0.60672	-3.21333	-0.80707
C	-2.73796	-3.98910	0.08704
C	-2.55025	-3.47813	-2.37916
H	-3.91172	-1.76937	-2.33176
H	-2.26214	-1.35646	-2.78917
C	-1.01603	-3.74547	-2.22543
H	0.04121	-2.33826	-0.90115
H	-0.05504	-3.97368	-0.24457
C	-3.30198	-4.33905	-1.33117
H	-3.53953	-3.73238	0.78722
H	-2.17995	-4.82834	0.51468
H	-2.86018	-3.75379	-3.39249
H	-0.88287	-4.83625	-2.26168
H	-4.37767	-4.12915	-1.38585
H	-3.16731	-5.40453	-1.55343
N	-1.80378	-2.83039	0.00061
C	-0.18003	-3.12928	-3.32290
H	0.06179	-2.07243	-3.21320
C	0.29074	-3.80528	-4.37810
H	0.10249	-4.86950	-4.50946
H	0.88734	-3.32353	-5.14684
C	5.18975	1.01048	1.05088
H	4.68524	1.61164	1.81617
H	5.58413	0.11766	1.54491
H	6.02232	1.58706	0.64040

TS(6,10-*trans*-ent-1q)

N	-0.45951	-1.50788	-0.35678
H	-0.51253	-2.52339	-0.40201
C	-1.74577	-0.92743	0.04386
H	-2.29518	-0.63585	-0.85971
C	-1.63297	0.28377	0.96254
C	-2.47411	1.43761	0.78967
C	-0.69022	0.30411	1.97066
C	-3.45454	1.57781	-0.22569
C	-2.28113	2.53239	1.70364
C	-0.55325	1.44371	2.80472
H	0.01227	-0.51021	2.08702
C	-4.22718	2.72338	-0.31764
H	-3.62805	0.80805	-0.96583
C	-3.08921	3.68991	1.58039
H	0.23608	1.46974	3.54494
C	-4.05135	3.79438	0.59602
H	-2.91526	4.49092	2.28942
H	-4.65445	4.69048	0.52411
N	-1.32135	2.52282	2.69225
O	-5.16029	2.73513	-1.35033
C	-5.99320	3.91105	-1.53594
H	-6.61861	3.68257	-2.39831
H	-6.62649	4.09457	-0.65956
H	-5.38711	4.80072	-1.74493
C	-2.51614	-2.06691	0.76541
H	-1.96429	-2.26588	1.69175
C	-4.00176	-1.73205	1.09737
C	-3.30432	-3.27199	-1.23331
C	-2.85751	-4.47243	0.83607
C	-4.87056	-2.95340	0.70769
H	-4.11080	-1.51595	2.16562
H	-4.34145	-0.83842	0.56666
C	-4.82528	-3.17188	-0.83922
H	-3.00139	-2.41041	-1.83581
H	-3.11590	-4.16500	-1.83685
C	-4.29829	-4.22033	1.39403
H	-2.12614	-4.58062	1.64308
H	-2.81555	-5.38170	0.22780
H	-5.90743	-2.78919	1.01862
H	-5.31281	-4.13442	-1.04745
H	-4.27525	-4.06994	2.48036
H	-4.94936	-5.08107	1.19955
N	-2.42944	-3.33495	-0.02918
C	-5.54473	-2.10288	-1.61960
H	-5.15158	-1.08957	-1.52300
C	-6.60420	-2.31448	-2.40939
H	-7.03009	-3.30696	-2.54059
H	-7.08555	-1.50726	-2.95295
C	0.63442	-0.85950	-0.85264
C	0.75928	0.50753	-0.95889
C	1.85361	-1.70363	-1.08856
C	2.01430	1.10838	-1.28691
H	-0.04192	1.15322	-0.63434
C	2.93670	-1.39850	0.01043
H	2.27385	-1.50496	-2.08070
H	1.60741	-2.76991	-1.04373
H	2.58594	0.68010	-2.10749
C	2.21995	2.54919	-1.09167
C	3.42609	0.03982	0.03499
H	2.41187	-1.53496	0.96734
C	4.09555	-2.39772	-0.00839
C	3.17652	3.23434	-1.86691
C	1.50758	3.26648	-0.10365
C	3.17766	0.81924	1.23955
C	4.67554	0.56556	-0.48315
C	4.93463	-2.46083	1.12032
C	4.37858	-3.23424	-1.09873
C	3.39197	4.60287	-1.68973
H	3.74860	2.68806	-2.61089
C	1.72733	4.63054	0.07350
H	0.81921	2.74803	0.55351
O	2.29370	0.69539	2.10573

O	4.13508	1.84693	1.28233
N	5.09595	1.64304	0.15076
C	5.43714	0.09460	-1.68039
C	6.02699	-3.32955	1.15578
H	4.72889	-1.81218	1.96706
C	5.47453	-4.10824	-1.06547
H	3.75822	-3.20779	-1.98774
C	2.66478	5.30483	-0.72246
H	4.13233	5.11599	-2.29467
H	1.18092	5.16350	0.84451
H	4.78341	0.02704	-2.55998
H	5.85812	-0.90116	-1.51059
H	6.24979	0.79143	-1.90104
C	6.30269	-4.15844	0.05923
H	6.66307	-3.35941	2.03473
H	5.67879	-4.74493	-1.92091
H	2.83772	6.36647	-0.57687
H	7.15240	-4.83313	0.08371

TS(6,10-*trans*-ent-1q)-conf3

N	-0.20750	1.71970	-1.70575
H	0.07265	2.69886	-1.61907
C	-1.48374	1.50312	-0.99518
H	-1.26627	1.02250	-0.03778
C	-2.47482	0.64176	-1.76654
C	-3.10908	-0.50203	-1.17090
C	-2.76035	0.93630	-3.08658
C	-2.87168	-0.94905	0.15319
C	-3.99443	-1.27326	-2.00422
C	-3.67124	0.13487	-3.81801
H	-2.26115	1.76721	-3.57294
C	-3.46572	-2.10385	0.63226
H	-2.20677	-0.42714	0.82661
C	-4.59386	-2.44603	-1.47841
H	-3.90180	0.37646	-4.85098
C	-4.33725	-2.86636	-0.18957
H	-5.25336	-3.00199	-2.13458
H	-4.79786	-3.77149	0.18498
N	-4.27291	-0.93624	-3.30912
O	-3.14960	-2.43982	1.93937
C	-3.60710	-3.71086	2.47648
H	-3.18006	-3.76292	3.47712
H	-4.70120	-3.74630	2.53893
H	-3.23332	-4.54604	1.87479
C	-2.08320	2.89780	-0.68265
H	-2.45809	3.31402	-1.62513
C	-3.23244	2.83343	0.37335
C	-0.44313	3.43733	1.09194
C	-1.57081	5.20762	-0.14494
C	-2.89927	3.83339	1.50718
H	-4.19131	3.09702	-0.08720
H	-3.34806	1.82258	0.77865
C	-1.55457	3.44089	2.20493
H	0.04427	2.46269	1.00965
H	0.35246	4.14748	1.33424
C	-2.74071	5.24909	0.89598
H	-1.91143	5.50167	-1.14341
H	-0.75680	5.88182	0.13858
H	-3.70132	3.82979	2.25280
H	-1.33267	4.23057	2.93595
H	-3.68016	5.55180	0.41681
H	-2.53291	5.97652	1.69002
N	-1.00363	3.83290	-0.23572
C	-1.62925	2.12955	2.94531
H	-1.65439	1.23007	2.32964
C	-1.65670	2.00067	4.27637
H	-1.61453	2.86567	4.93474
H	-1.71013	1.02934	4.75816
C	0.80897	0.79073	-1.67584
C	2.13399	1.15283	-1.61539
C	0.48086	-0.66172	-1.50452
C	3.13511	0.14929	-1.39256
H	2.40575	2.20000	-1.54183
C	0.86586	-1.12183	-0.05194
H	1.04173	-1.26172	-2.22953
H	-0.57403	-0.86505	-1.67305
H	3.05176	-0.76881	-1.97256
C	4.52970	0.52271	-1.09456
C	2.33783	-0.90834	0.28870
H	0.32725	-0.43663	0.61780
C	0.36111	-2.52614	0.27864
C	5.57937	-0.32809	-1.49197
C	4.84591	1.70269	-0.38888
C	2.63701	0.10333	1.29917
C	3.35577	-1.92855	0.49170
C	0.35461	-2.93065	1.62686
C	-0.10395	-3.42642	-0.69137
C	6.90964	0.00408	-1.22710
H	5.34657	-1.25116	-2.01549
C	6.17436	2.03109	-0.12097
H	4.04705	2.33115	-0.01088
O	2.02104	1.14390	1.58706
O	3.85113	-0.25012	1.90711
N	4.28255	-1.58173	1.36063
C	3.50404	-3.22035	-0.24561
C	-0.08706	-4.20279	1.99294
H	0.70729	-2.24036	2.38750
C	-0.55639	-4.70160	-0.32631
H	-0.12285	-3.14659	-1.73815
C	7.21064	1.18812	-0.54494
H	7.70651	-0.66124	-1.54316
H	6.40276	2.93517	0.43376
H	3.49137	-3.05148	-1.33013
H	2.68105	-3.90259	-0.01192
H	4.45022	-3.69626	0.02365
C	-0.54445	-5.09713	1.01471
H	-0.07678	-4.49583	3.03804
H	-0.91366	-5.38249	-1.09253
H	8.24306	1.44550	-0.33093
H	-0.88246	-6.08987	1.29577

TS(6,10-*trans*-ent-1q)-conf4

N	1.02581	-0.99733	0.10007
H	1.09782	-1.80421	0.72235
C	1.81813	0.12709	0.62633
H	1.13655	0.87895	1.04760
C	2.69748	0.84687	-0.38766
C	3.60961	0.17159	-1.26971
C	2.65992	2.23086	-0.42526
C	3.74400	-1.23649	-1.35421
C	4.43859	0.99326	-2.11377
C	3.50975	2.95450	-1.29909
H	1.96838	2.77275	0.21288
C	4.66407	-1.80721	-2.21870
H	3.11041	-1.89216	-0.77589
C	5.36662	0.37431	-2.98771
H	3.47137	4.03917	-1.32165
C	5.48877	-0.99906	-3.04492
H	5.97439	1.02359	-3.60701
H	6.20587	-1.44760	-3.72070
N	4.37737	2.36962	-2.11646
O	4.70984	-3.19659	-2.21529
C	5.62736	-3.87879	-3.11196
H	5.46531	-4.94033	-2.92857
H	5.40677	-3.64791	-4.16114
H	6.66998	-3.62125	-2.88949
C	2.67017	-0.42290	1.80703
H	3.48672	-1.01719	1.38420
C	3.24647	0.71286	2.70876
C	0.69667	-0.70809	3.28331
C	2.73271	-1.99056	3.65814
C	2.73724	0.48452	4.15202
H	4.34219	0.70182	2.68946
H	2.93464	1.69913	2.34896
C	1.17752	0.49992	4.16315
H	-0.02702	-0.40669	2.52475
H	0.19671	-1.46569	3.89287
C	3.23674	-0.89272	4.65493
H	3.56733	-2.48321	3.14838
H	2.15475	-2.76506	4.17141
H	3.11287	1.28030	4.80666
H	0.86287	0.32060	5.20376
H	4.33185	-0.89225	4.71611
H	2.85565	-1.07805	5.66676
N	1.85562	-1.38194	2.61950
C	0.62435	1.85362	3.75433
H	1.27091	2.70196	3.98948
C	-0.57188	2.08794	3.19719
H	-1.28106	1.29498	2.97378
H	-0.89389	3.10031	2.96833
C	-0.15598	-0.85362	-0.58302
C	-1.14451	-1.80935	-0.53548
C	-0.49123	0.45639	-1.23026
C	-2.42956	-1.53287	-1.11199
H	-1.01870	-2.68843	0.08685
C	-1.61553	1.15881	-0.38656
H	-0.84729	0.29754	-2.25408
H	0.37329	1.11501	-1.29230
H	-2.43367	-1.07754	-2.10191
C	-3.56711	-2.44802	-0.89336
C	-2.90858	0.35225	-0.28492
H	-1.22119	1.18466	0.63790
C	-1.84884	2.61359	-0.78937
C	-4.55866	-2.57694	-1.88468
C	-3.70824	-3.18012	0.30404
C	-3.29747	-0.10316	1.04794
C	-4.17636	0.64710	-0.94090
C	-2.57712	3.43859	0.08936
C	-1.37308	3.16770	-1.98723
C	-5.64350	-3.43792	-1.70451
H	-4.47241	-2.00041	-2.80141
C	-4.79427	-4.03612	0.48475
H	-2.99305	-3.03748	1.10658
O	-2.58632	-0.40897	2.02296
O	-4.69234	-0.22387	1.06856
N	-5.22981	0.28052	-0.24227
C	-4.37694	1.19348	-2.31738
C	-2.82817	4.77596	-0.22321
H	-2.95624	3.01814	1.01648
C	-1.62250	4.51099	-2.30263
H	-0.80999	2.56139	-2.68772
C	-5.76117	-4.17388	-0.52038
H	-6.39752	-3.52729	-2.47976
H	-4.89726	-4.58396	1.41569
H	-3.81357	0.60627	-3.05418
H	-4.02344	2.22697	-2.38392
H	-5.43703	1.16097	-2.58067
C	-2.35071	5.31865	-1.42456
H	-3.39528	5.39330	0.46624
H	-1.24725	4.92080	-3.23526
H	-6.60686	-4.83825	-0.37421
H	-2.54504	6.35767	-1.67031

TS(6,10-*trans*-ent-1q)-conf2

N	1.51974	0.55590	-0.78424
H	1.90503	1.49717	-0.71074
C	2.53174	-0.44546	-0.43164
H	2.97940	-0.83809	-1.35871
C	2.04655	-1.65256	0.36238
C	1.15730	-1.55231	1.48523
C	2.48056	-2.91078	-0.02013
C	0.62108	-0.33719	1.97352
C	0.72821	-2.78660	2.09248
C	2.05101	-4.06504	0.67964
H	3.13293	-3.02574	-0.88032
C	-0.34620	-0.33891	2.96232
H	0.89714	0.61164	1.53924
C	-0.24076	-2.74702	3.12758
H	2.40438	-5.04733	0.38211
C	-0.78334	-1.55438	3.55056
H	-0.55238	-3.69394	3.55220

H	-1.55773	-1.55092	4.30548
N	1.19285	-4.01877	1.69286
O	-0.84445	0.90286	3.31641
C	-2.08739	0.96590	4.08099
H	-2.34308	2.02496	4.10752
H	-2.86745	0.39381	3.57117
H	-1.94010	0.60142	5.10450
C	3.63367	0.30938	0.36874
H	3.21834	0.52313	1.35883
C	4.95714	-0.49674	0.51865
C	4.69302	1.51354	-1.50176
C	4.66995	2.47328	0.73594
C	6.13961	0.47263	0.26854
H	5.02717	-0.93220	1.52101
H	4.99299	-1.33476	-0.18710
C	6.13435	0.95113	-1.21978
H	4.14394	0.85405	-2.18116
H	4.74342	2.49606	-1.98045
C	5.96923	1.71907	1.17614
H	4.01722	2.68486	1.58829
H	4.90292	3.42727	0.25230
H	7.08888	-0.02800	0.48471
H	6.86209	1.77039	-1.30067
H	5.90026	1.40294	2.22424
H	6.84727	2.37022	1.09088
N	3.90480	1.64896	-0.24471
C	6.52387	-0.12172	-2.20209
H	5.84855	-0.97669	-2.26650
C	7.60864	-0.08724	-2.98509
H	8.30467	0.74833	-2.95955
H	7.84356	-0.88827	-3.67933
C	0.25843	0.37553	-1.26794
C	-0.36545	-0.84640	-1.42141
C	-0.55885	1.62939	-1.42390
C	-1.70689	-0.95457	-1.88632
H	0.12130	-1.74555	-1.07370
C	-1.72731	1.62187	-0.36965
H	-0.97371	1.71178	-2.43463
H	0.06583	2.51243	-1.25503
H	-2.00197	-0.34297	-2.73329
C	-2.46818	-2.18999	-1.71779
C	-2.83620	0.64883	-0.69409
H	-1.29271	1.26199	0.57242
C	-2.28498	3.02041	-0.08643
C	-3.53314	-2.48780	-2.59360
C	-2.19808	-3.07232	-0.64526
C	-3.36790	-0.21321	0.34401
C	-3.93532	0.83181	-1.61553
C	-3.00315	3.21224	1.10852
C	-2.13891	4.10700	-0.96204
C	-4.28654	-3.65081	-2.42522
H	-3.76933	-1.79984	-3.39855
C	-2.95342	-4.23080	-0.48190
H	-1.43426	-2.82181	0.08176
O	-2.87894	-0.59580	1.42428
O	-4.64269	-0.63819	-0.07781
N	-4.97899	0.06545	-1.35226
C	-3.97107	1.70217	-2.83097
C	-3.55718	4.45497	1.42011
H	-3.12723	2.37168	1.78323
C	-2.69478	5.35643	-0.65100
H	-1.59633	3.99093	-1.89452
C	-3.99546	-4.52665	-1.37334
H	-5.10559	-3.86622	-3.10334
H	-2.74216	-4.89466	0.34983
H	-3.15845	1.45353	-3.52680
H	-3.85720	2.75544	-2.55409
H	-4.92315	1.57392	-3.35231
C	-3.40416	5.53534	0.53972
H	-4.10898	4.58239	2.34639
H	-2.57256	6.18515	-1.34187
H	-4.58639	-5.42695	-1.23736
H	-3.83474	6.50216	0.78007