Solvent-triggered stereoselectivity of α,α-cyclopropanation of amino acids in the Ni(II) chiral coordination environment

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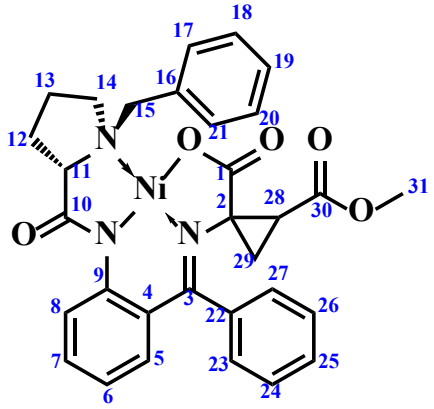
1. Atom numeration and signal assignment in the NMR spectra of complexes **I**



(*R*,*S*)-**I**

NMR ^{1}H ($CDCl_3$ δ, ppm): 8.64 (dd, ^{3}J = 8.7 Hz, ^{4}J = 1.1 Hz, 1H (H-8)), 8.07-8.04 (m, 2H (H-17,21)), 7.61-7.56 (m, 2H (H-18,20)), 7.54-7.49 (m, 2H (H-19,25)), 7.49-7.43 (m, 2H (H-24,26)), 7.33-7.22 (m, 3H (H-7,23,27)), 7.01 (dd, ^{3}J = 8.3 Hz, ^{4}J = 1.7 Hz, 1H (H-5)), 6.75 (ddd, ^{3}J = 8.3 Hz, ^{3}J = 7.0 Hz, ^{4}J = 1.1 Hz, 1H (H-6)), 4.35 (d, ^{2}J = 13.1 Hz, 1H (H-15)), 4.32-4.25 (m, 1H (H-14)), 3.82 (dd, ^{3}J = 8.8 Hz, ^{3}J = 2.6 Hz, 1H (H-11)), 3.68 (s, 3H (H-31)), 3.12 (d, ^{2}J = 13.1 Hz, 1H (H-15)), 2.99-2.91 (m, 1H (H-14)), 2.59 (dd, ^{3}J = 9.0 Hz, ^{3}J = 6.3 Hz, 1H (H-28)), 2.24-2.15 (m, 1H (H-13)), 2.14-1.86 (m, 3H (H-12,12,13)), 1.69 (dd, ^{3}J = 9.0 Hz, ^{2}J = 7.1 Hz, 1H (H-29)), 0.78-0.73 (m, 1H (H-29)).

NMR ^{13}C-{^{1}H} ($CDC1_3$ δ, ppm): 180.65 (C-10), 174.31 (C-1), 172.28 (C-3), 168.62 (C-30), 143.93 (C-9), 135.69 (C-22), 134.70 (C-5), 133.51 (C-16), 133.34 (C-7), 131.35 (C-17,21), 130.76 (C-23), 130.14 (C-19), 129.37 (C-18,20), 129.22 (C-27), 129.15 (C-25), 128.40 (C-24), 128.25 (C-26), 126.51 (C-4), 122.51 (C-8), 120.69 (C-6), 68.15 (C-11), 59.40 (C-2), 59.33 (C-15), 58.28 (C-14), 52.45 (C-31), 34.12 (C-28), 28.97 (C-13), 22.59 (C-12), 22.39 (C-29).

(*S*,*R*)-**I**:

NMR ^{1}H ($CDCl_3$ δ, ppm): 8.14 (d, ^{3}J = 8.6 Hz, 1H (H-8)), 8.05 (d, ^{3}J = 7.3 Hz, 2H (H-17,21)), 7.53-7.47 (m, 1H (H-25)), 7.46-7.40 (m, 2H (H-24,26)), 7.28-7.20 (m, 3H (H-18,20,23)), 7.18-7.13 (m, 1H (H-27)), 7.10-7.04 (m, 2H (H-7,19)), 6.79 (dd, ^{3}J = 8.2 Hz, ^{4}J = 1.4 Hz, 1H (H-5)), 6.70-6.64 (m, 1H (H-6)), 4.24 (d, ^{2}J = 12.7 Hz, 1H (H-15)), 4.09-3.93 (m, 1H (H-13)), 3.73 (s, 3H (H-31)), 3.42-3.32 (m, 3H (H-11,14,15)), 2.77-2.68 (m, 1H (H-12)), 2.67-2.59 (m, 1H (H-12)), 2.56 (dd, 2.05-1.96 ^{3}J = 8.8 Hz, ^{3}J = 6.4 Hz, 1H (H-28)), 2.05-1.96 (m, 1H (H-14)), 1.64 (dd, ^{2}J = 7.3 Hz, ^{3}J = 8.8 Hz, 1H (H-29)), 0.73 (dd, ^{2}J = 7.3 Hz, ^{3}J = 6.4 Hz, 1H (H-29)).

NMR ^{13}C-{^{1}H} ($CDC1_3$ δ, ppm): 179.72 (C-10), 174.14 (C-1), 171.29 (C-3), 168.56 (C-30), 143.30 (C-9), 135.16 (C-22), 134.18 (C-5), 133.40 (C-16), 132.85 (C-7), 131.27 (C-17,21), 130.59 (C-27), 130.26 (C-25), 129.31 (C-23), 128.99 (C-18,20), 128.79 (C-19), 128.30 (C-24,26), 126.93 (C-4), 122.71 (C-8), 120.60 (C-6), 71.20 (C-11), 62.90 (C-15), 59.07 (C-2), 57.09 (C-14), 52.82 (C-31), 34.77 (C-28), 31.05 (C-12), 23.80 (C-13), 22.06 (C-29).

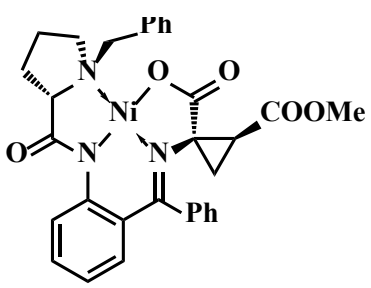
(*S*,*S*)-**I**:

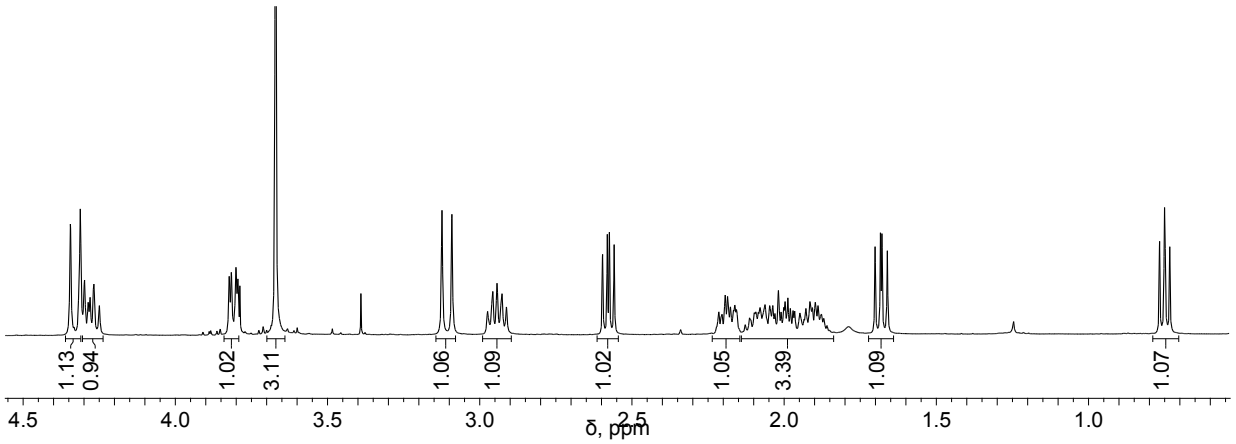
NMR ^{1}H ($CDCl_3$ δ, ppm): 8.13 (m, 2H (H-17,21)), 8.00 (d, ^{3}J = 8.5 Hz, 1H (H-8)), 7.53-7.46 (m, 2H (H-25,26)), 7.41-7.37 (m, 1H (H-24)), 7.31-7.27 (m, 2H (H-18,20)), 7.27-7.24 (m, 1H (H-27)), 7.12-7.08 (m, 1H (H-19)), 7.07-7.04 (m, 1H (H-7)), 6.78 (d, J = 7.6 Hz, 1H (H-23)), 6.61-6.59 (m, 2H (H-5, H-6)), 4.30 (d, ^{2}J = 12.5 Hz, 1H (H-15)), 4.01-3.89 (m, 1H (H-12)), 3.75 (s, 3H (H-31)), 3.48-3.43 (m, 2H (H-11,14)), 3.40 (d, ^{2}J = 12.5 Hz, 1H (H-15)), 2.84-2.77 (m, 1H

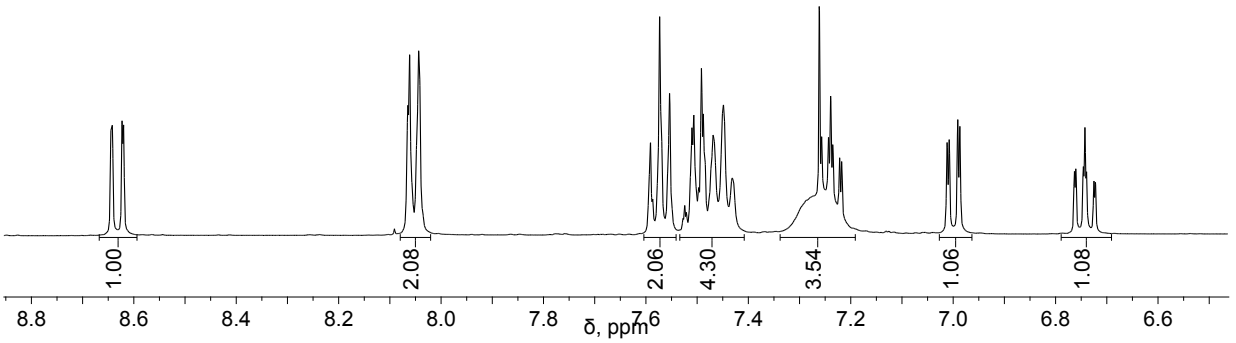
(H-13)), 2.58-2.47 (m, 1H (H-13)), 2.21-2.14 (m, 2H (H-12,29)), 2.06-1.98 (m, 1H (H-14)), 1.82 (dd, ^{2}J = 9.6 Hz, ^{3}J = 7.2 Hz, 1H (H-28)), 0.32 (dd, ^{2}J = 9.6 Hz, ^{3}J = 7.2 Hz, 1H (H-28)).

NMR ^{13}C ($CDC1_3$ δ, ppm): 180.29 (C-10), 172.78 (C-1), 168.09 (C-30), 167.93 (C-3), 142.39 (C-9), 134.63 (C-22), 133.79 (C-16), 133.69 (C-5), 132.55 (C-7), 131.35 (C-17,21), 130.27 (C-25), 129.22 (C-24), 129.16 (C-27), 128.95 (C-18, C-20), 128.83 (C-19), 128.67 (C-26), 127.15 (C-4), 126.71 (C-23), 123.30 (C-8), 120.66 (C-6), 70.82 (C-11), 63.27 (C-15), 59.00 (C-2), 57.58 (C-14), 52.55 (C-31), 35.39 (C-29), 30.74 (C-13), 23.33 (C-12), 22.76 (C-28).

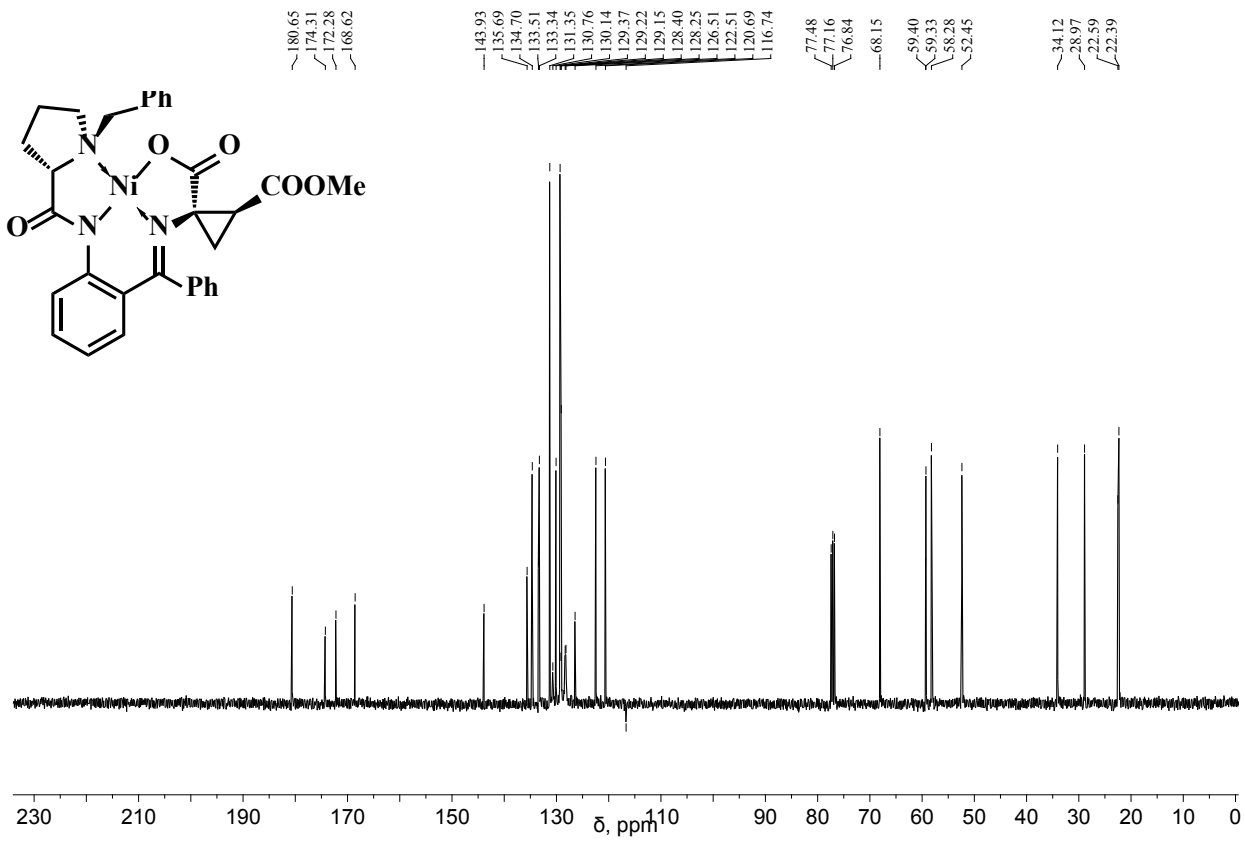
2. ^{1}H NMR spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*R*,2*S*)-**I**))

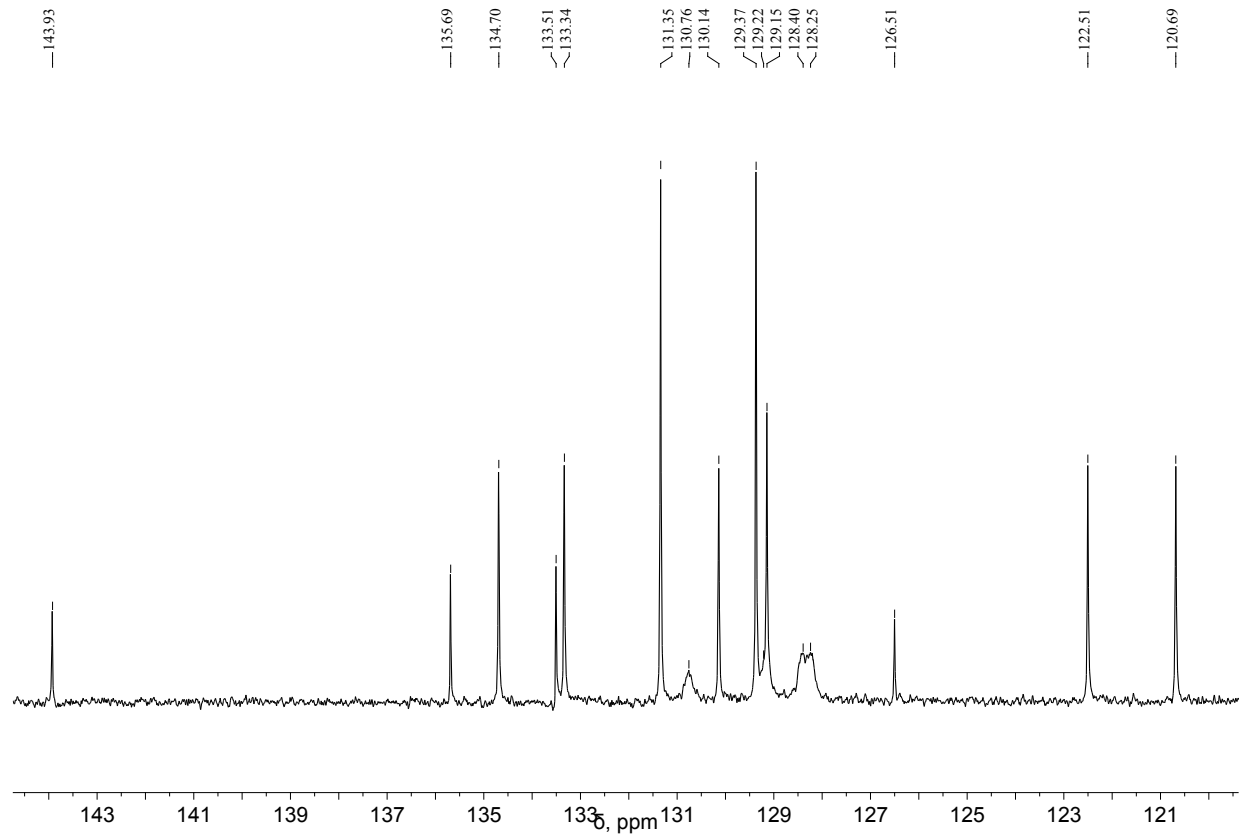




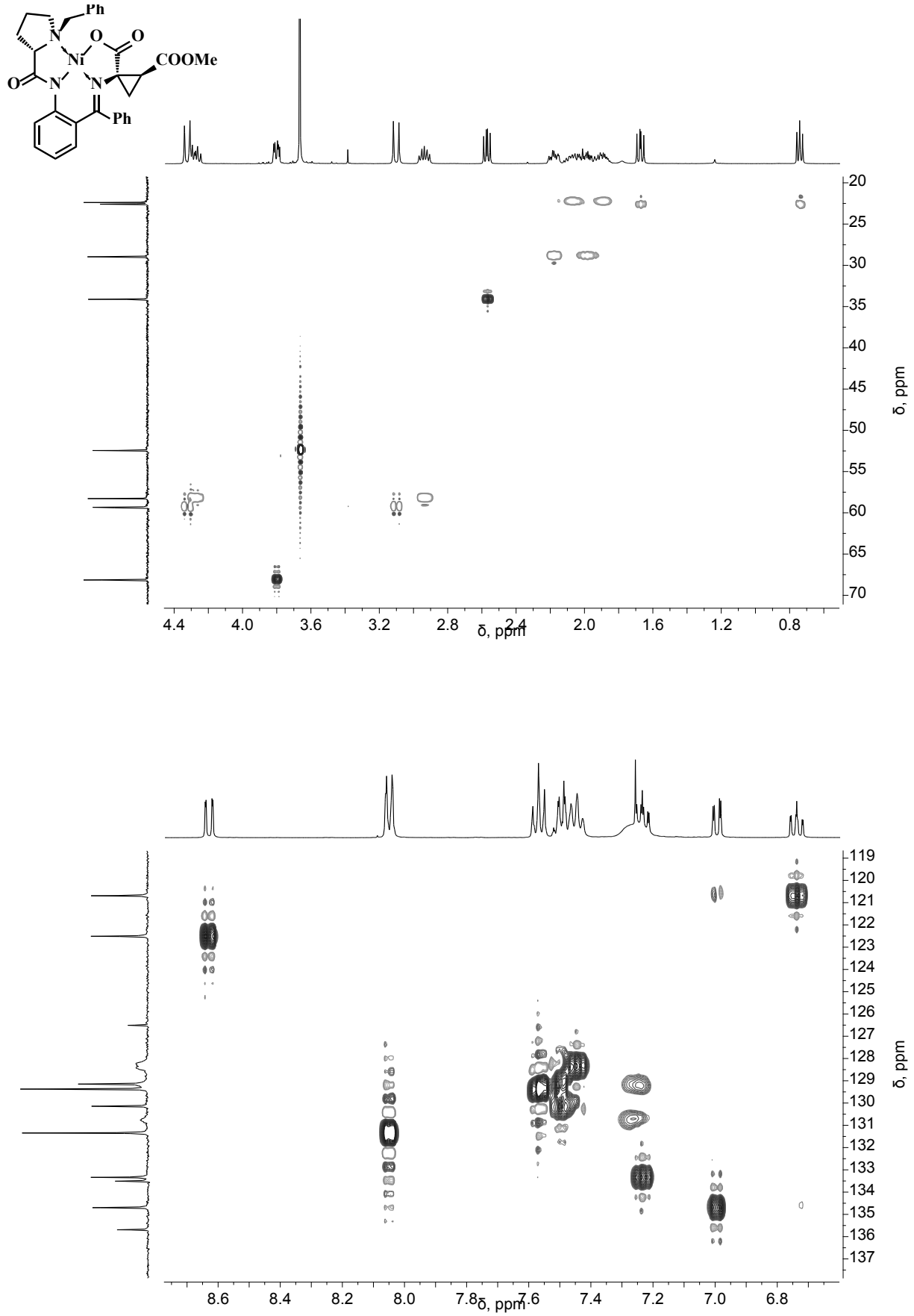


3. ^{13}C NMR spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*R*,2*S*)-**I**))

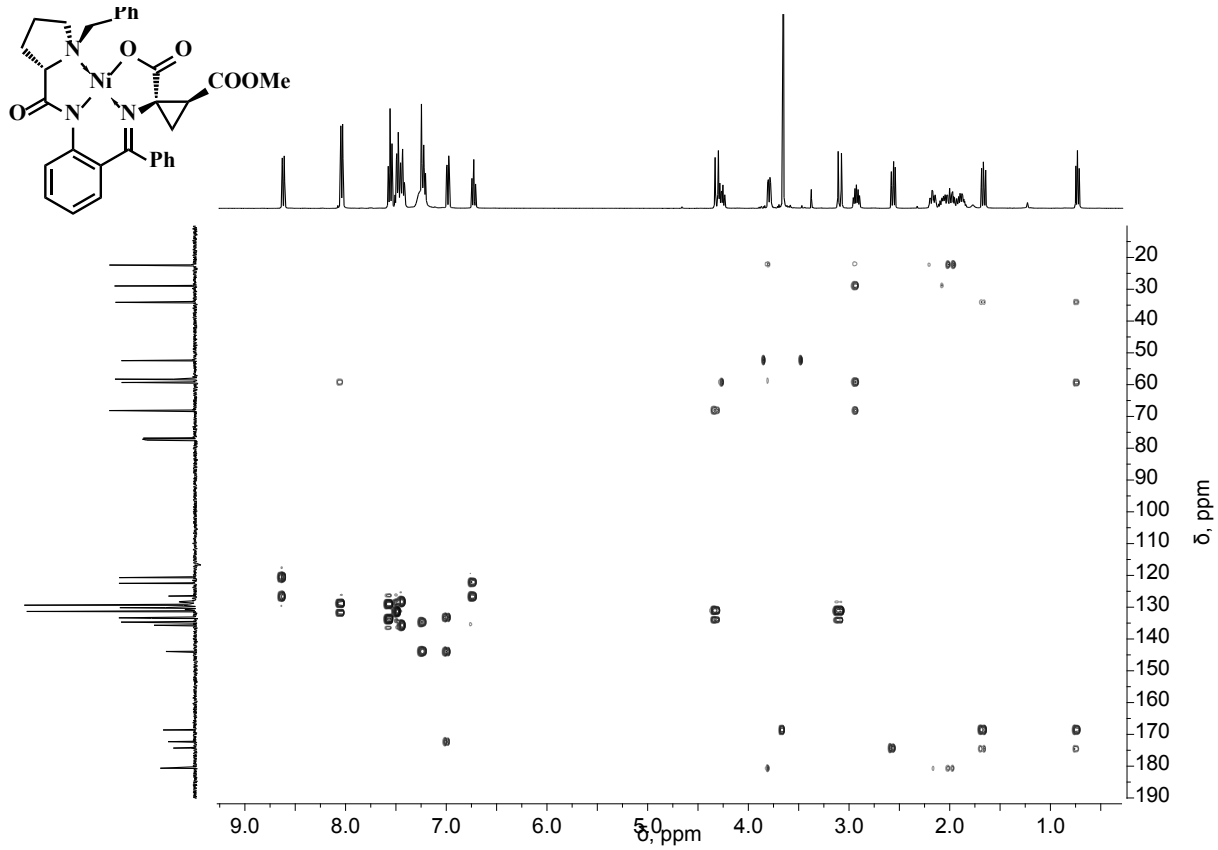




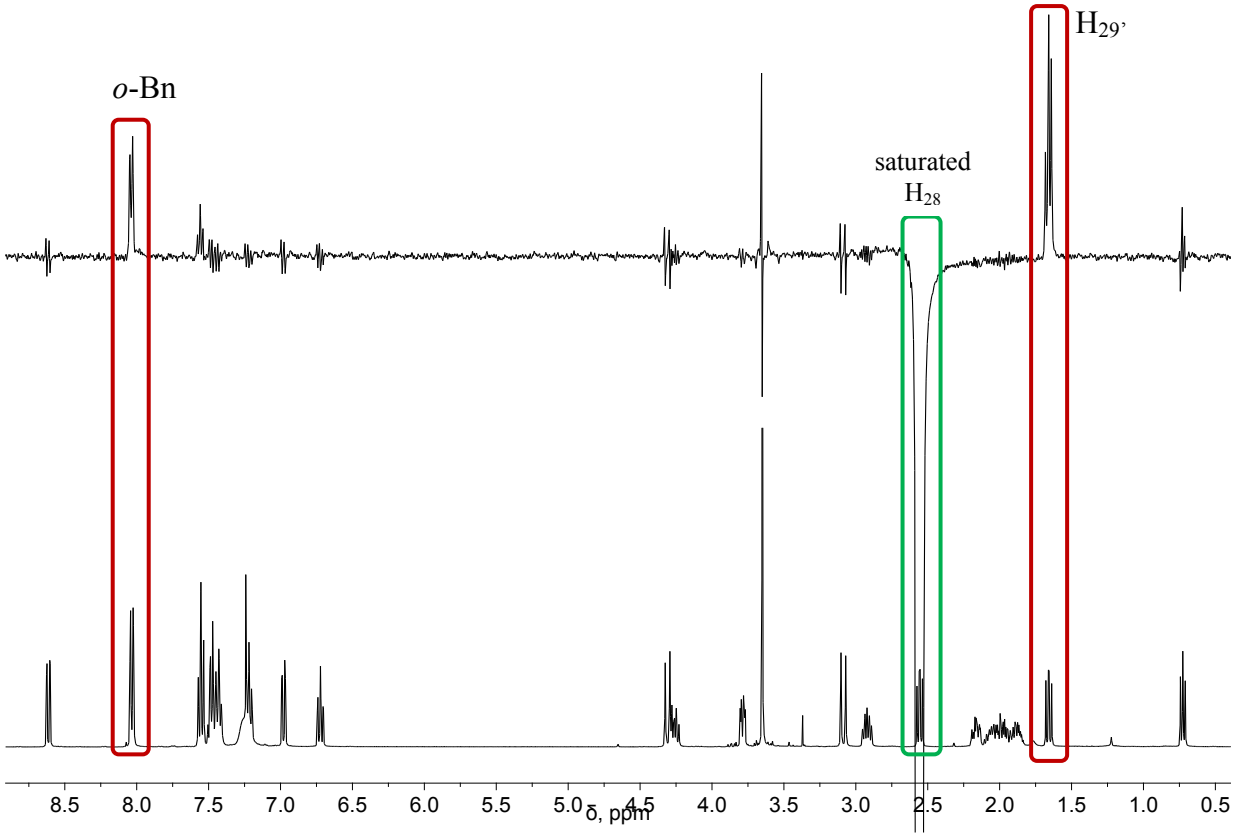
4. HSQC spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*R*,2*S*)-**I**))

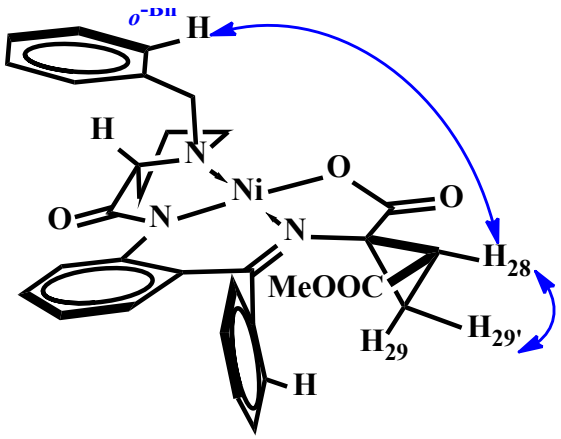


5. HMBC spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*R*,2*S*)-**I**))

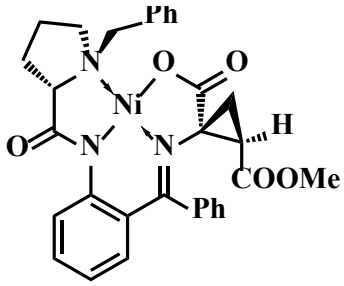


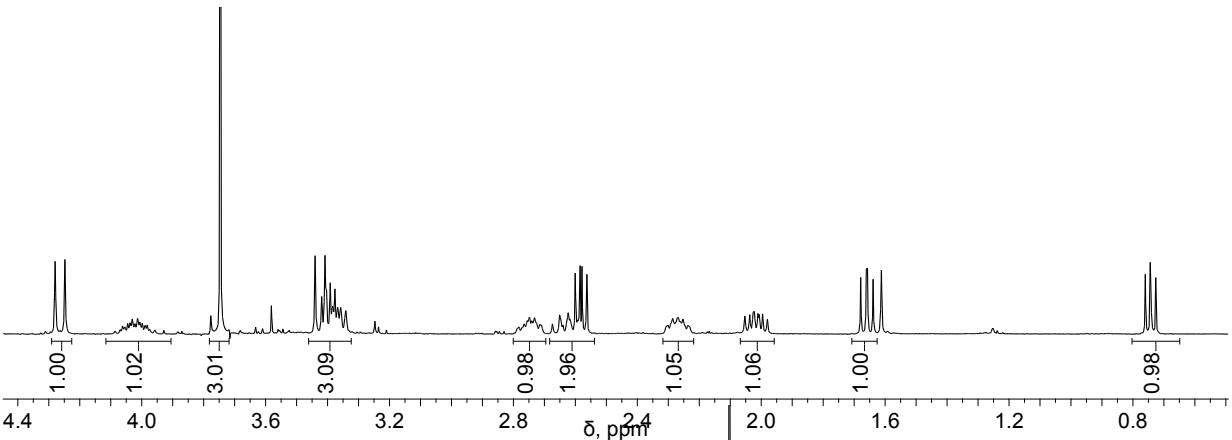
6. NOESY-1D spectrum (saturation of proton H_{28}) (upper) and ^1H NMR spectrum (bottom) of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*R*,2*S*)-**I**))

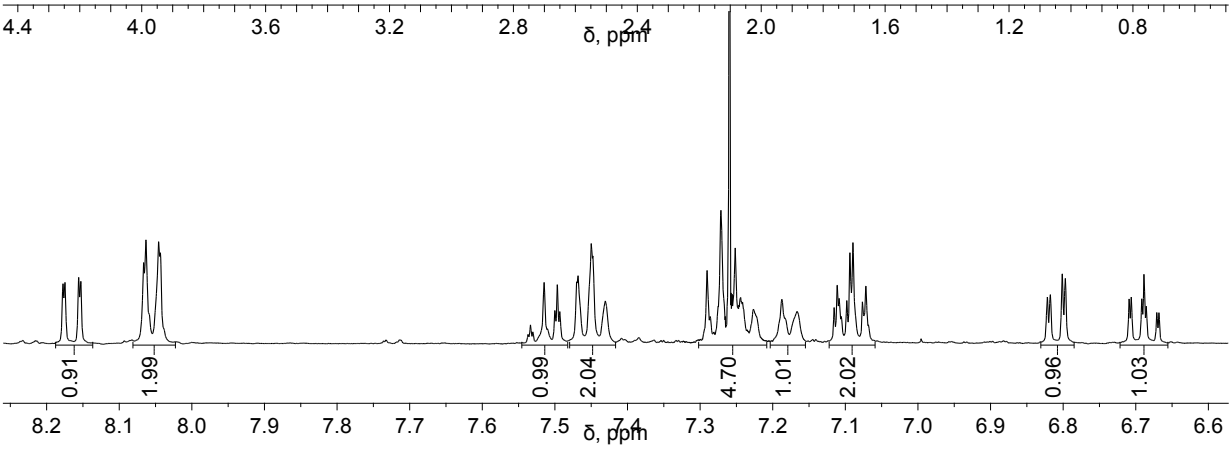




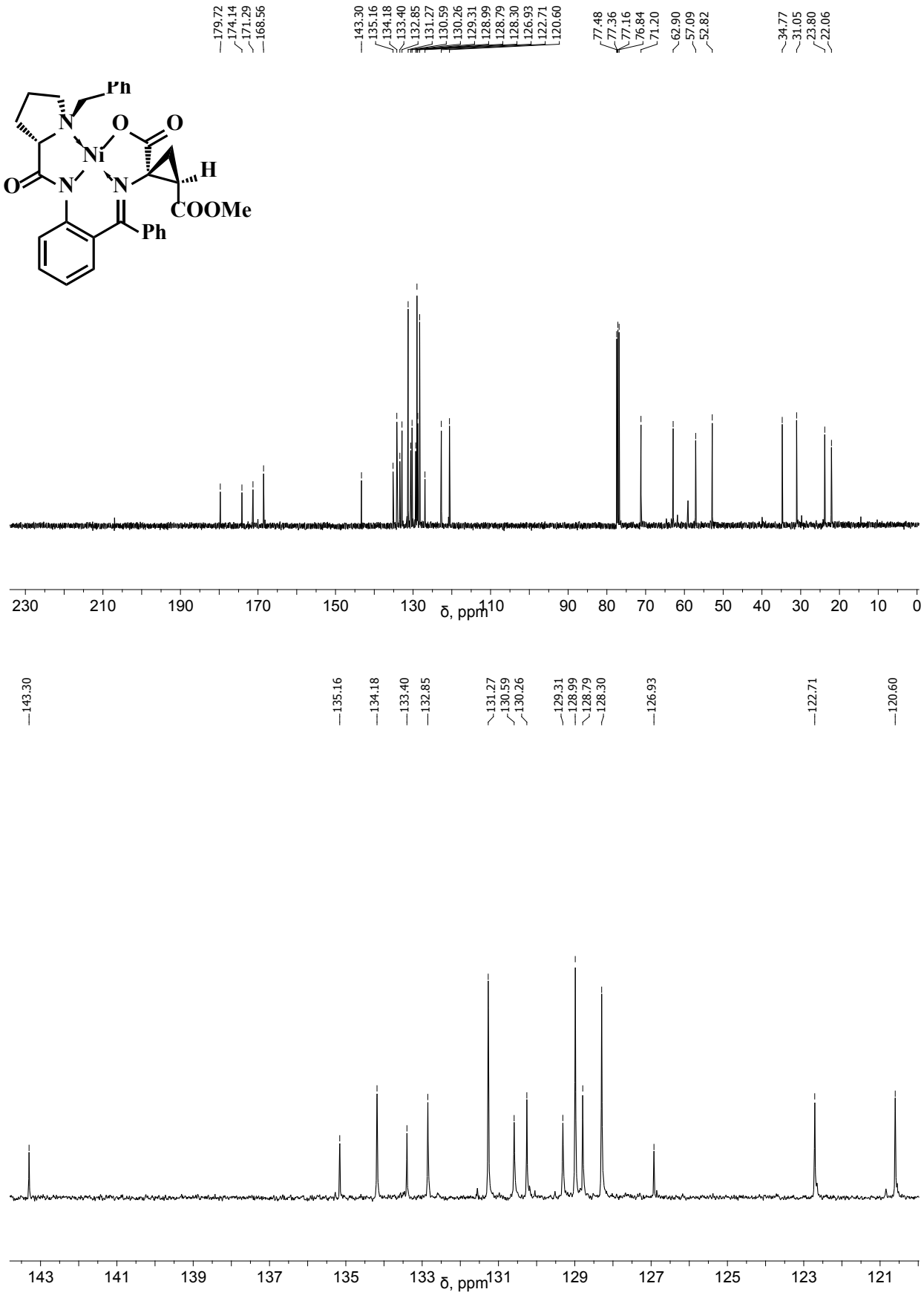
7. ^{1}H NMR spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*R*)-**I**))



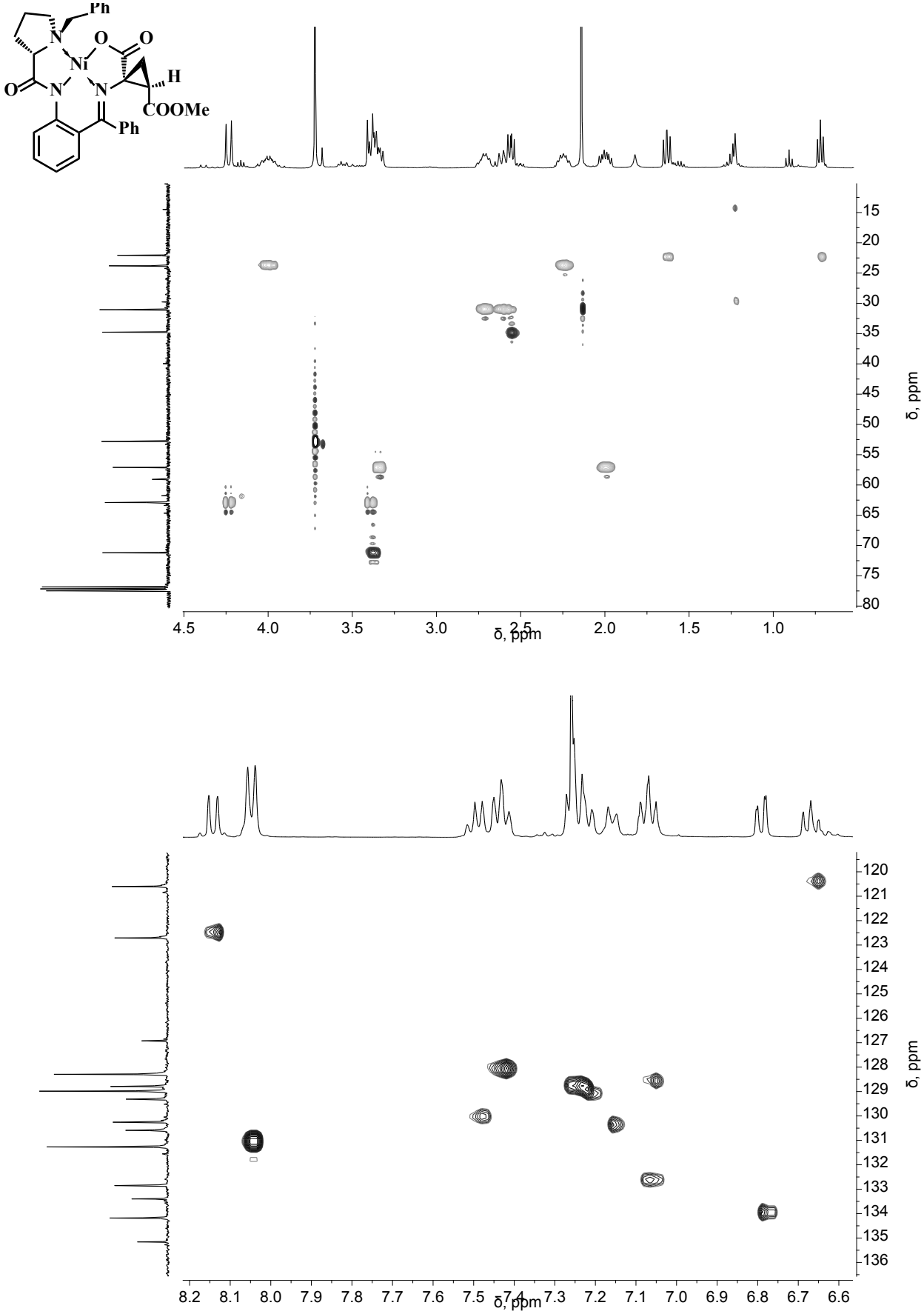




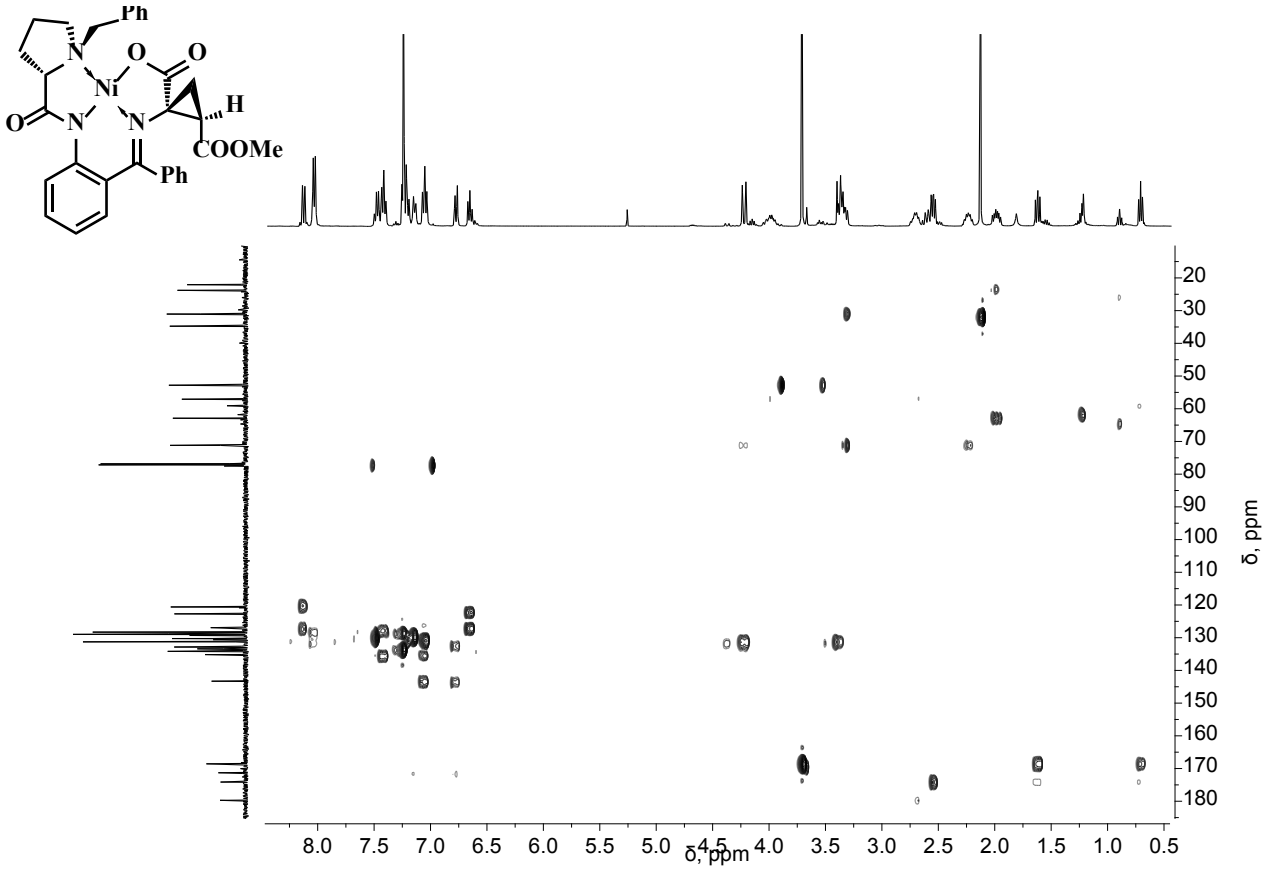
8. ^{13}C NMR spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*R*)-**I**))



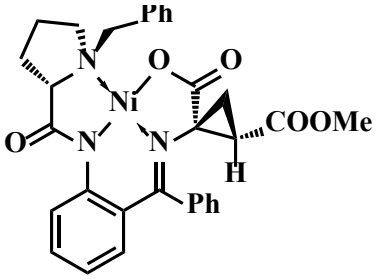
9. HSQC spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*R*)-**I**))

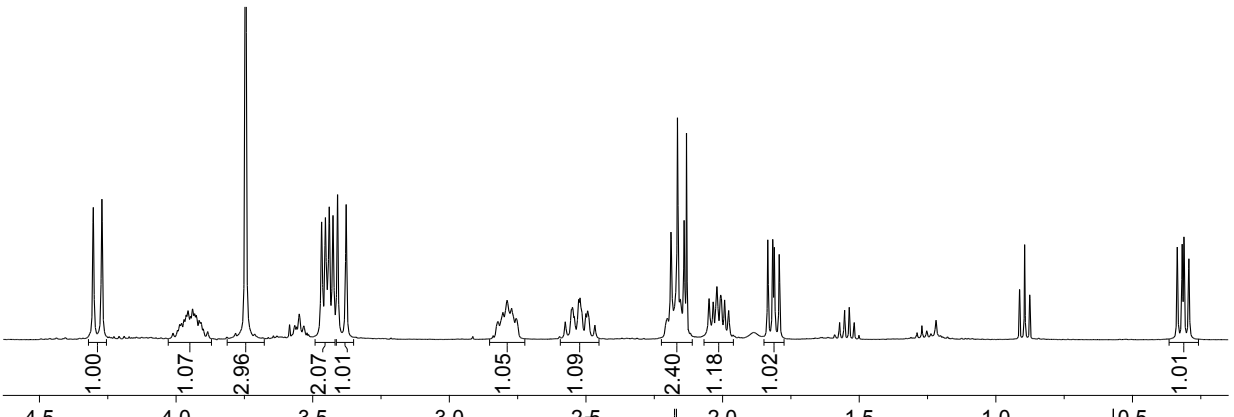


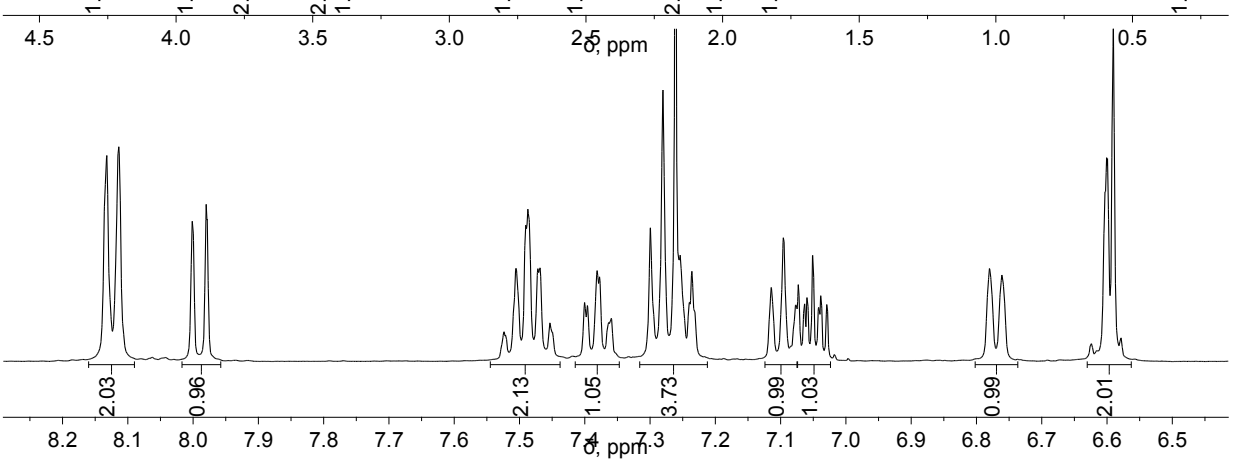
10. HMBC spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*R*)-**I**))



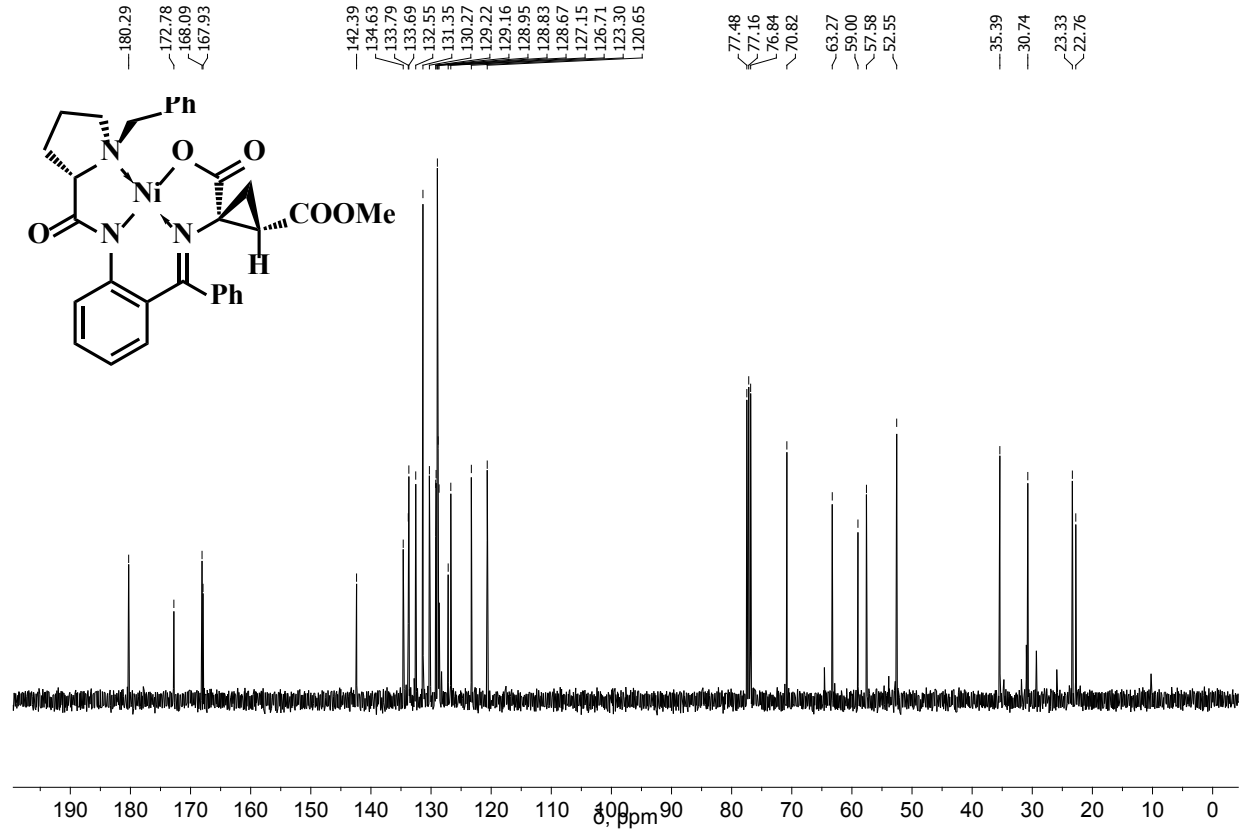
11. ^{1}H NMR spectrum of the Ni complex of Shiff base of (1*S*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*S*)-**I**))

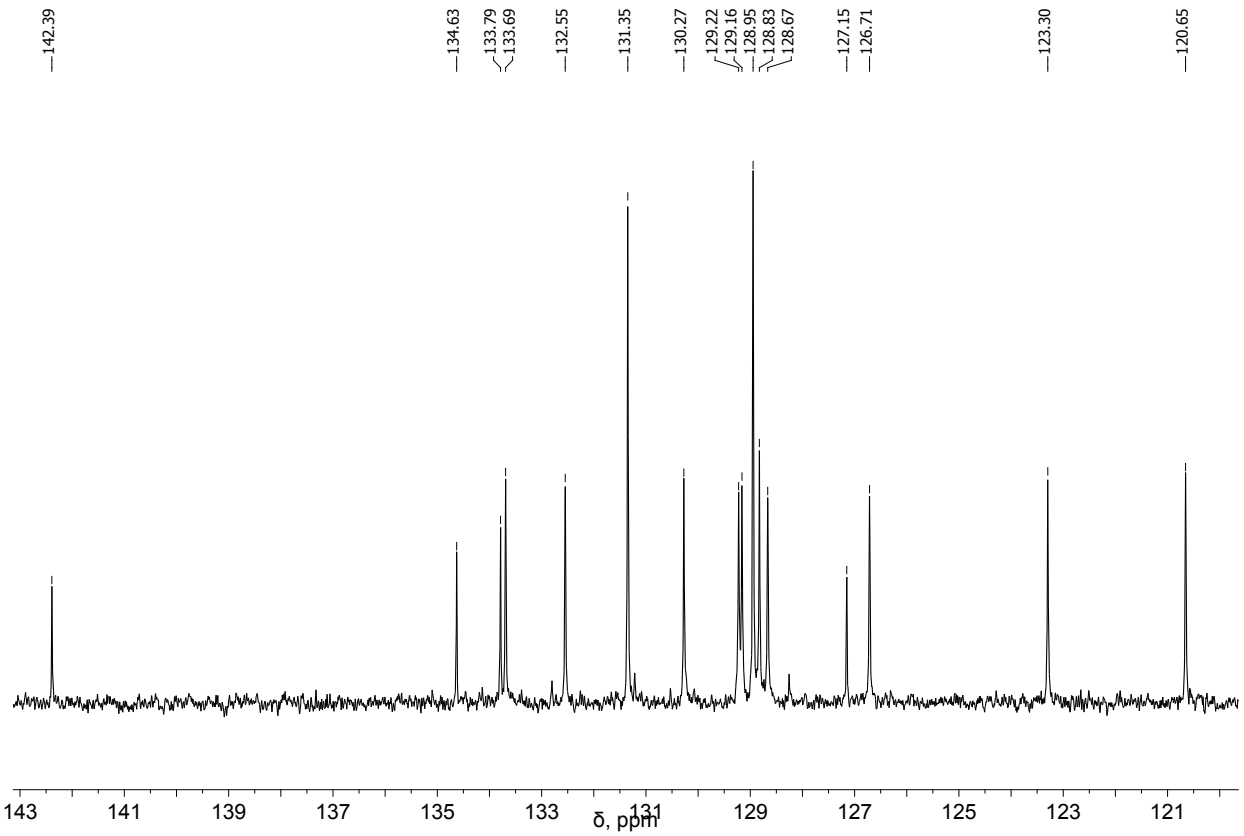




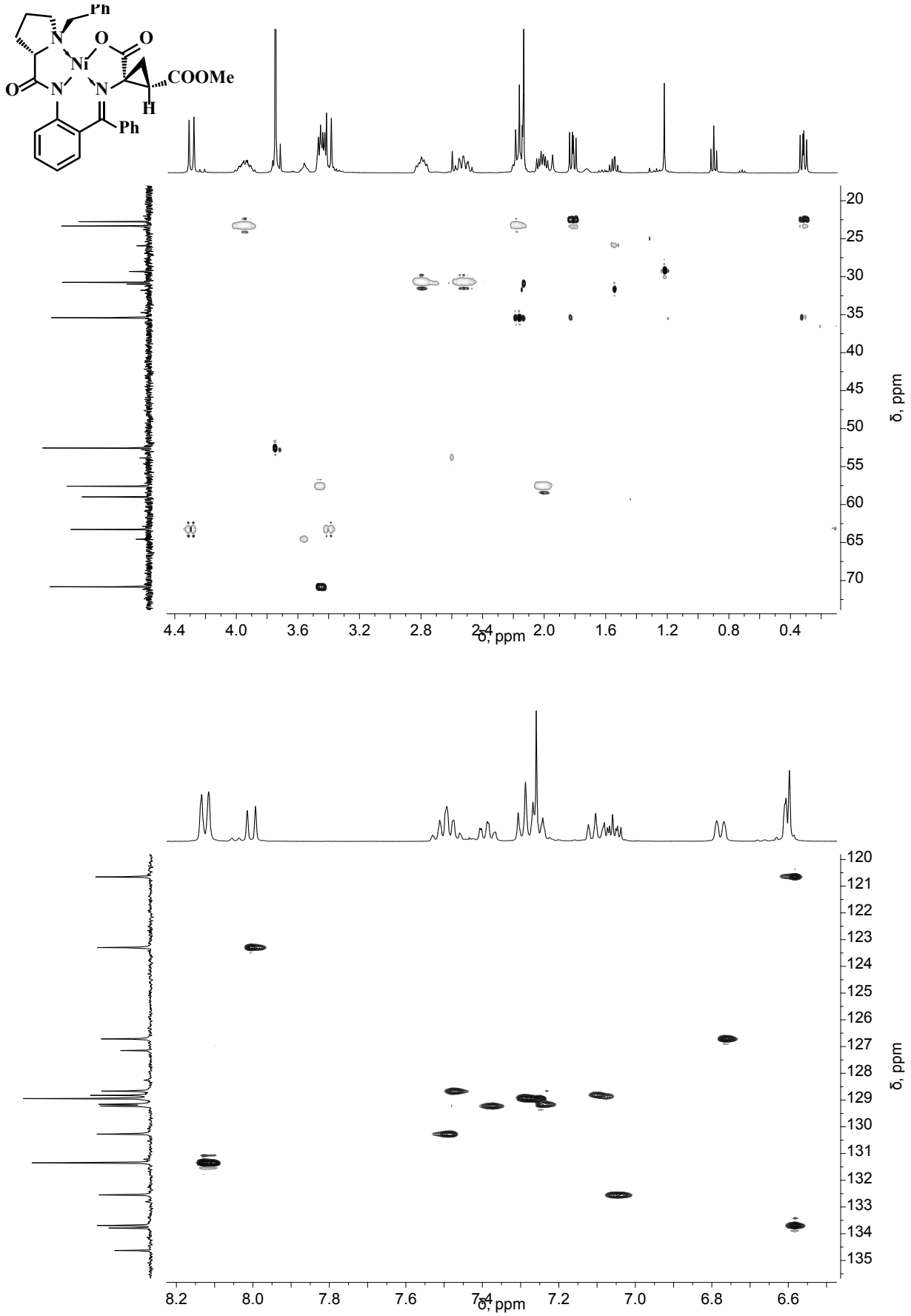


12. ^{13}C NMR spectrum of the Ni complex of Shiff base of (1*S*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*S*)-**I**))

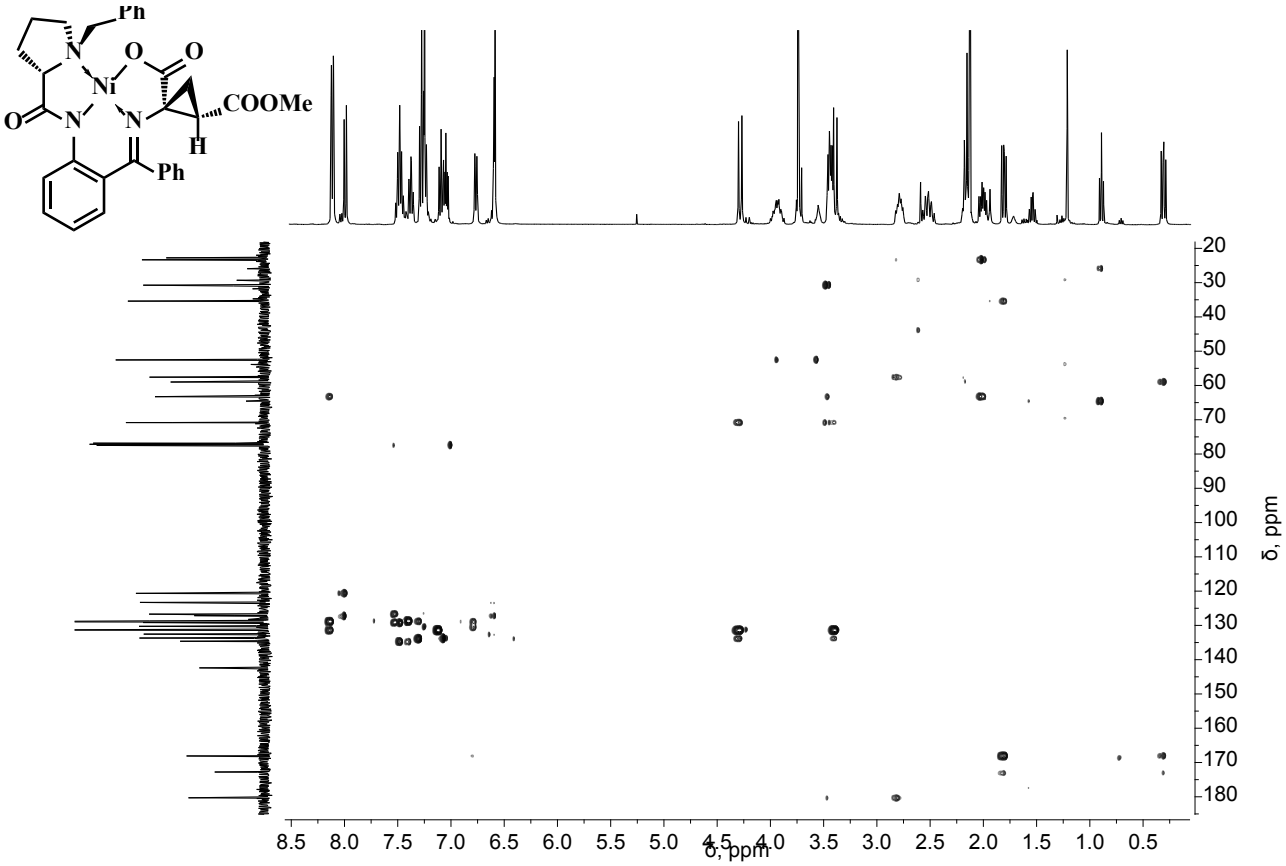




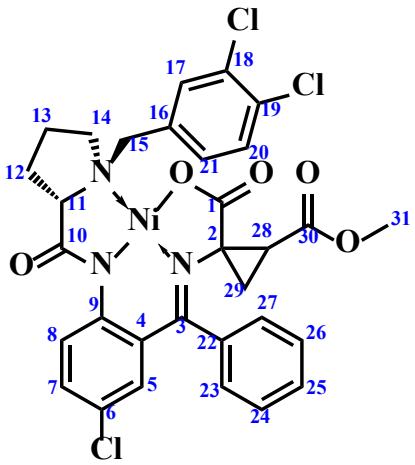
13. HSQC spectrum of the Ni complex of Shiff base of (1*S*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*S*)-**I**))



14. HMBC spectrum of the Ni complex of Shiff base of (1*S*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*S*)-**I**))



15. Atom numeration and signal assignment in the NMR spectra of complexes **II**



(1*R*,2*S*)-**II**:

NMR ^{1}H ($CDCl_3$ δ, ppm): 8.66 (d, ^{3}J = 9.3 Hz, 1H (H-8)), 8.22 (dd, ^{3}J = 8.3 Hz, ^{4}J = 2.1 Hz, 1H (H-21)), 7.74 (d, ^{3}J = 8.3 Hz, 1H (H-20)), 7.60 (d, ^{4}J = 2.1 Hz, 1H (H-17)), 7.57-7.52 (m, 1H (H-25)), 7.51-7.44 (m, 1H (H-24,26)), 7.33-7.27 (m, 1H (H-23)), 7.24-7.21 (m, 1H (H-27)), 7.19 (dd, ^{3}J = 9.3 Hz, ^{4}J = 2.6 Hz, 1H (H-7)), 6.96 (d, ^{4}J = 2.6 Hz, 1H (H-5)), 4.36-4.29 (m, 1H (H-14)), 4.08 (d, ^{2}J = 13.0 Hz, 1H (H-15)), 3.81 (dd, ^{3}J = 8.4 Hz, ^{3}J = 2.6 Hz, 1H (H-11)), 3.62 (s, 3H (H-31)), 3.00 (d, ^{3}J = 13.0 Hz, 1H (H-15)), 2.98-2.90 (m, 1H (H-14)), 2.54 (dd, ^{3}J = 9.1 Hz, ^{3}J = 6.3 Hz, 1H (H-28)), 2.30-2.22 (m, 1H (H-13)), 2.15-2.04 (m, 2H (H-12,13)), 2.00-1.91 (m, 1H (H-12)), 1.67 (dd, ^{2}J = 7.2 Hz, ^{3}J = 9.1 Hz, 1H (H-29)), 0.71 (dd, ^{2}J = 7.2 Hz, ^{3}J = 6.3 Hz (H-29)).

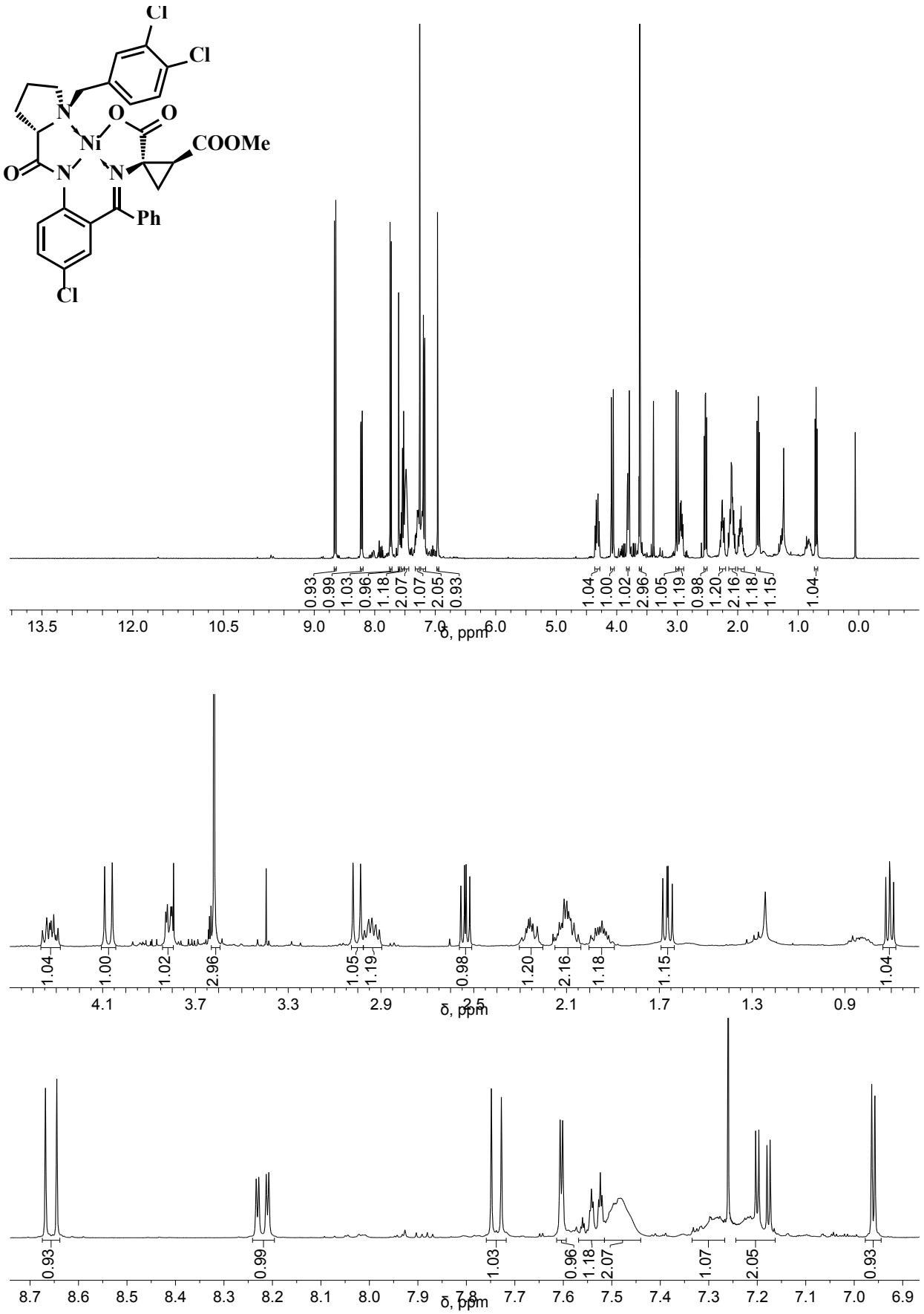
NMR ^{13}C-{^{1}H} ($CDC1_3$ δ, ppm): 180.20 (C-10), 174.04 (C-1), 171.82 (C-3), 168.41 (C-30), 142.36 (C-9), 135.02 (C-22), 133.97 (C-19), 133.77 (C-16), 133.66 (C-17), 133.50 (C-18), 133.43 (C-5), 133.22 (C-7), 131.56 (C-20), 130.71 (C-25), 130.66 (C-23) 130.59 (C-21), 129.19 (C-27), 128.71 (C-24,26), 127.68 (C-4), 125.67 (C-6), 123.89 (C-8), 68.27 (C-11), 59.53 (C-2), 59.14 (C-14), 58.04 (C-15), 52.62 (C-31), 34.31 (C-28), 28.89 (C-13), 22.69 (C-29), 22.31 (C-12).

(1*S*,2*R*)-**II**:

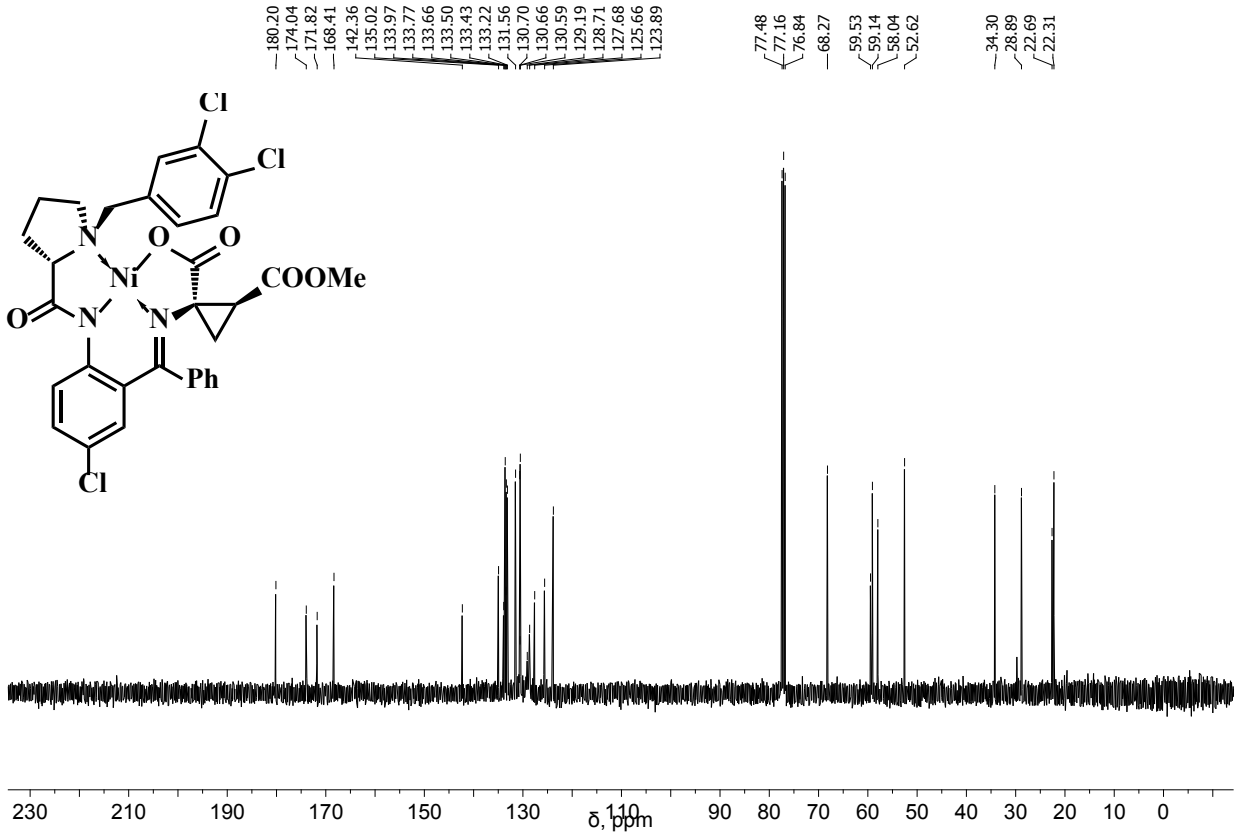
NMR ^{1}H ($CDCl_3$ δ, ppm): 8.92 (d, ^{4}J = 2.1 Hz, 1H (H-17)), 8.14 (d, ^{3}J = 9.3 Hz, 1H (H-8)), 7.73 (dd, ^{3}J = 8.2 Hz, ^{4}J = 2.1 Hz 1H (H-21)), 7.57-7.52 (m, 1H (H-25)), 7.51-7.45 (m, 2H (H-24,26)), 7.29 (d, ^{3}J = 8.2 Hz, 1H (H-20)), 7.26-7.23 (m, 1H (H-23)), 7.16-7.12 (m, 1H (H-27)), 7.08 (dd, ^{3}J = 9.3 Hz, ^{4}J = 2.6 Hz, 1H (H-7)), 6.77 (d, ^{4}J = 2.6 Hz, 1H (H-5)), 4.16 (d, ^{2}J = 12.5 Hz, 1H (H-15)), 4.07-3.93 (m, 1H (H-12)), 3.72 (s, 3H (H-31)), 3.45-3.39 (m, 1H (H-14)), 3.34-3.28 (m, 1H (H-11)), 3.08 (d, ^{2}J = 12.5 Hz, 1H (H-15)), 2.71-2.63 (m, 2H (H-13)), 2.58 (dd, ^{3}J = 8.8 Hz, ^{3}J = 6.4 Hz, 1H (H-28)), 2.36-2.27 (m, 1H (H-12)), 2.09-2.00 (m, 1H (H-14)), 1.64 (dd, ^{2}J = 7.3 Hz, ^{3}J = 8.8 Hz, 1H (H-29)), 0.72 (dd, ^{2}J = 7.3 Hz ^{3}J = 6.4 Hz, 1H (H-29)).

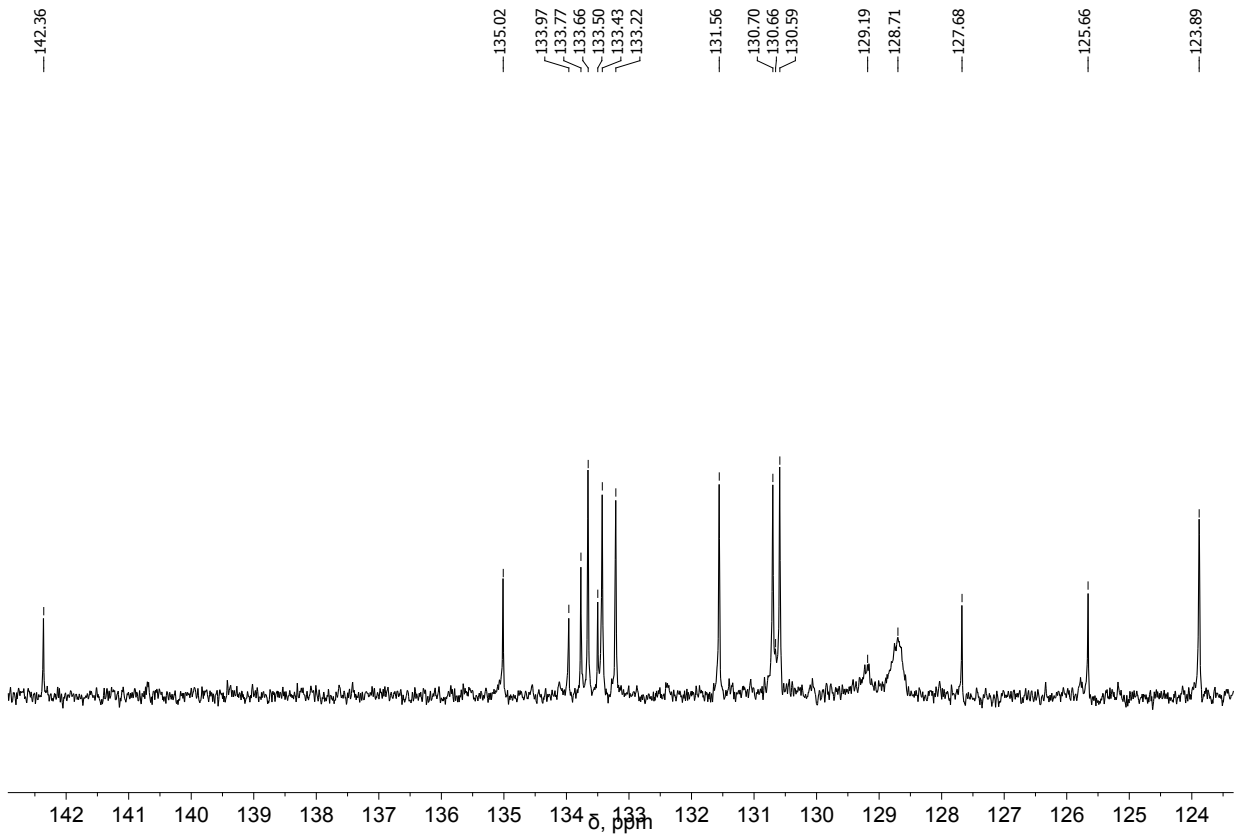
NMR ^{13}C-{^{1}H} ($CDC1_3$ δ, ppm): 179.52 (C-10), 173.85 (C-1), 170.86 (C-3), 168.44 (C-30), 141.52 (C-9), 135.23 (C-18), 134.40 (C-22), 133.72 (C-16), 133.44 (C-17), 133.40 (C-19), 133.15 (C-5), 132.97 (C-7), 131.26 (C-20), 130.80 (C-25), 130.30 (C-23), 129.57 (C-21), 129.41 (C-27), 128.72 (C-24), 128.69 (C-26), 127.95 (C-6), 125.95 (C-4), 123.13 (C-8), 72.38 (C-11), 62.81 (C-15), 59.10 (C-2), 58.48 (C-14), 52.93 (C-31), 35.05 (C-28), 31.36 (C-13), 23.80 (C-12), 22.03 (C-29).

16. ^{1}H NMR spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*R*,2*S*)-**II**))

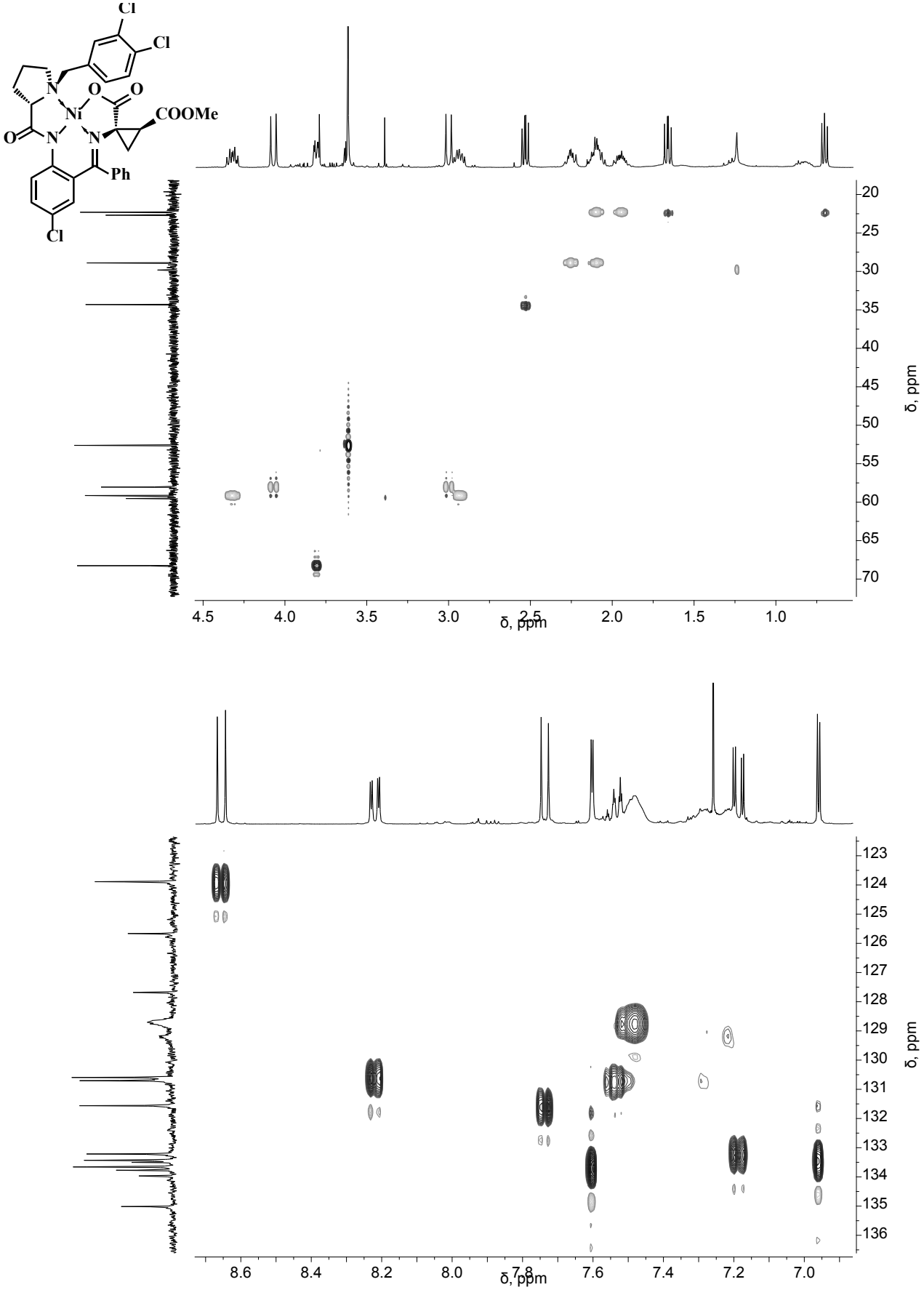


17. ^{13}C NMR spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*R*,2*S*)-**II**))

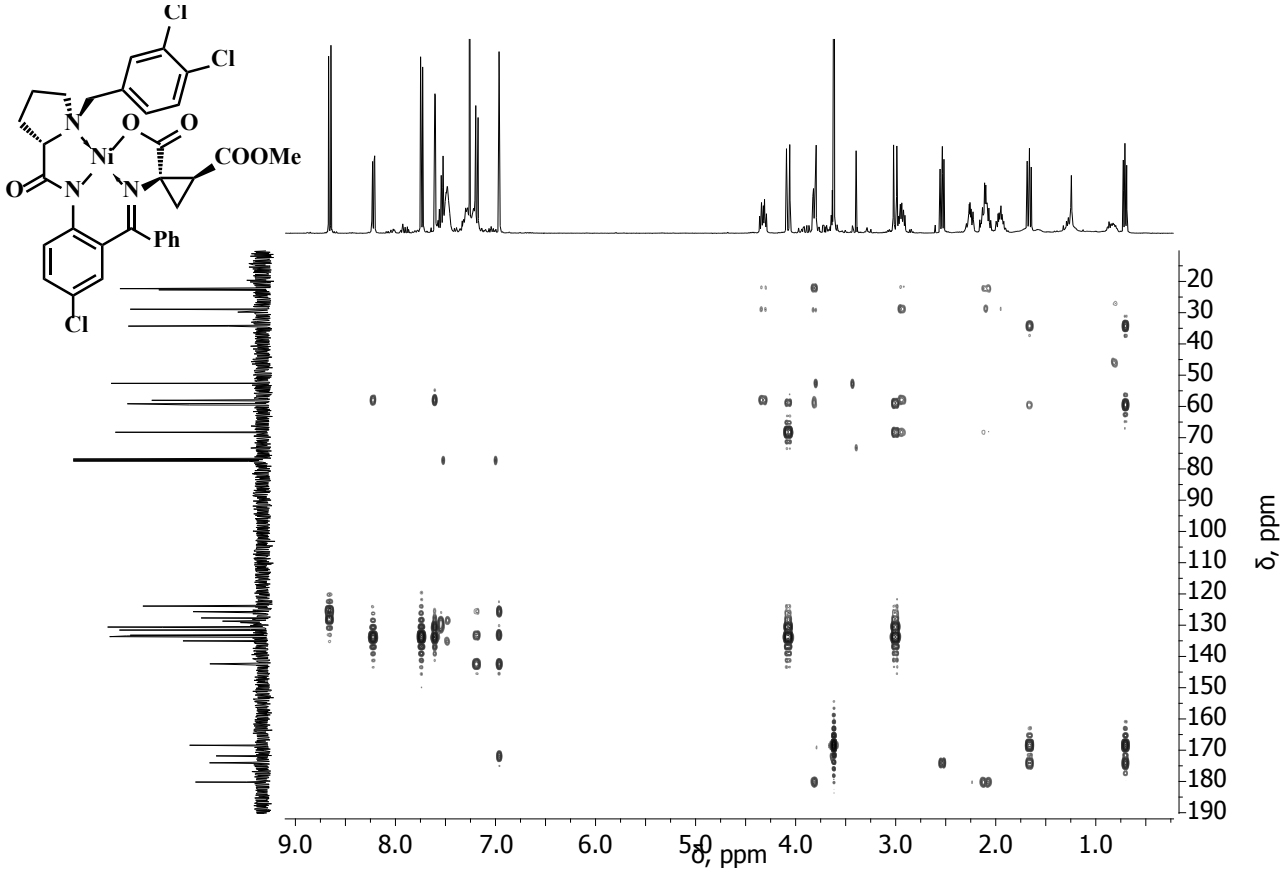




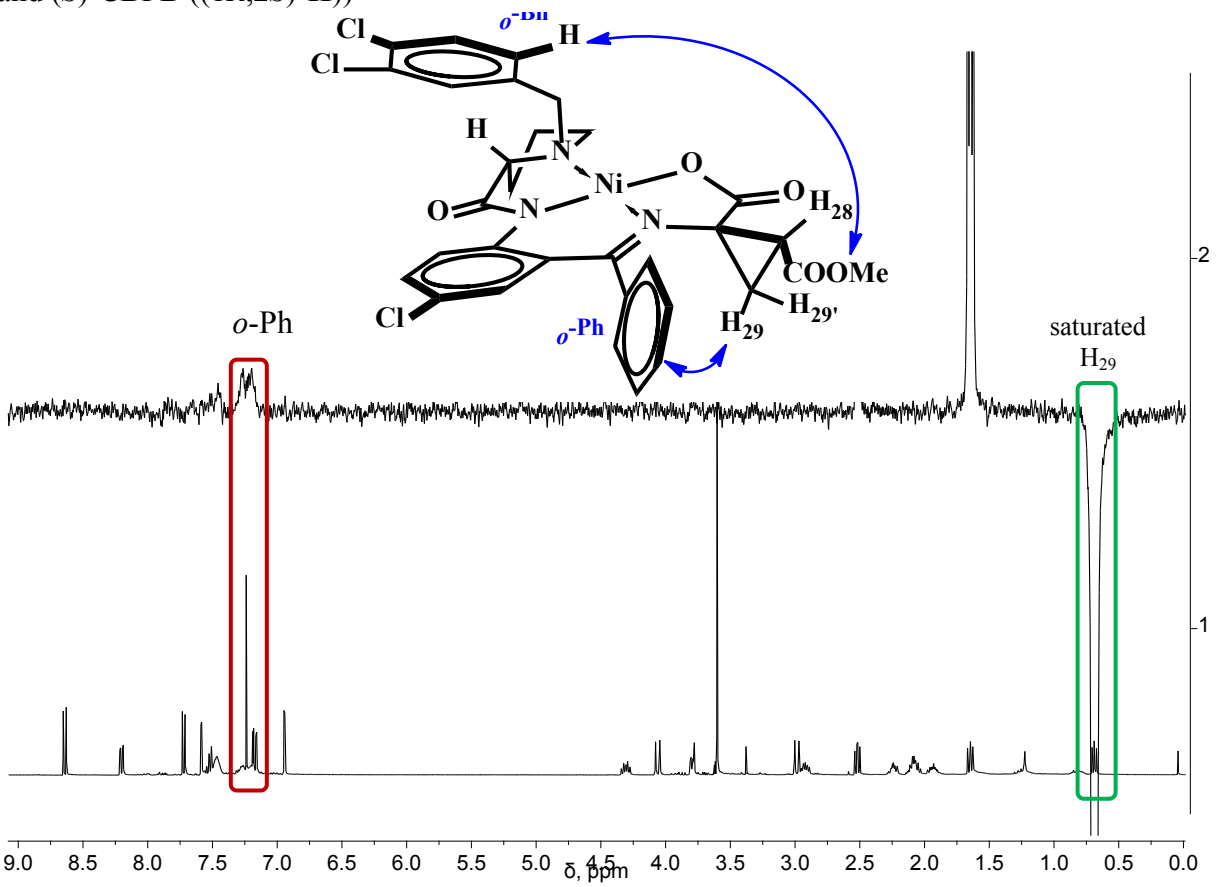
18. HSQC spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*R*,2*S*)-**II**))



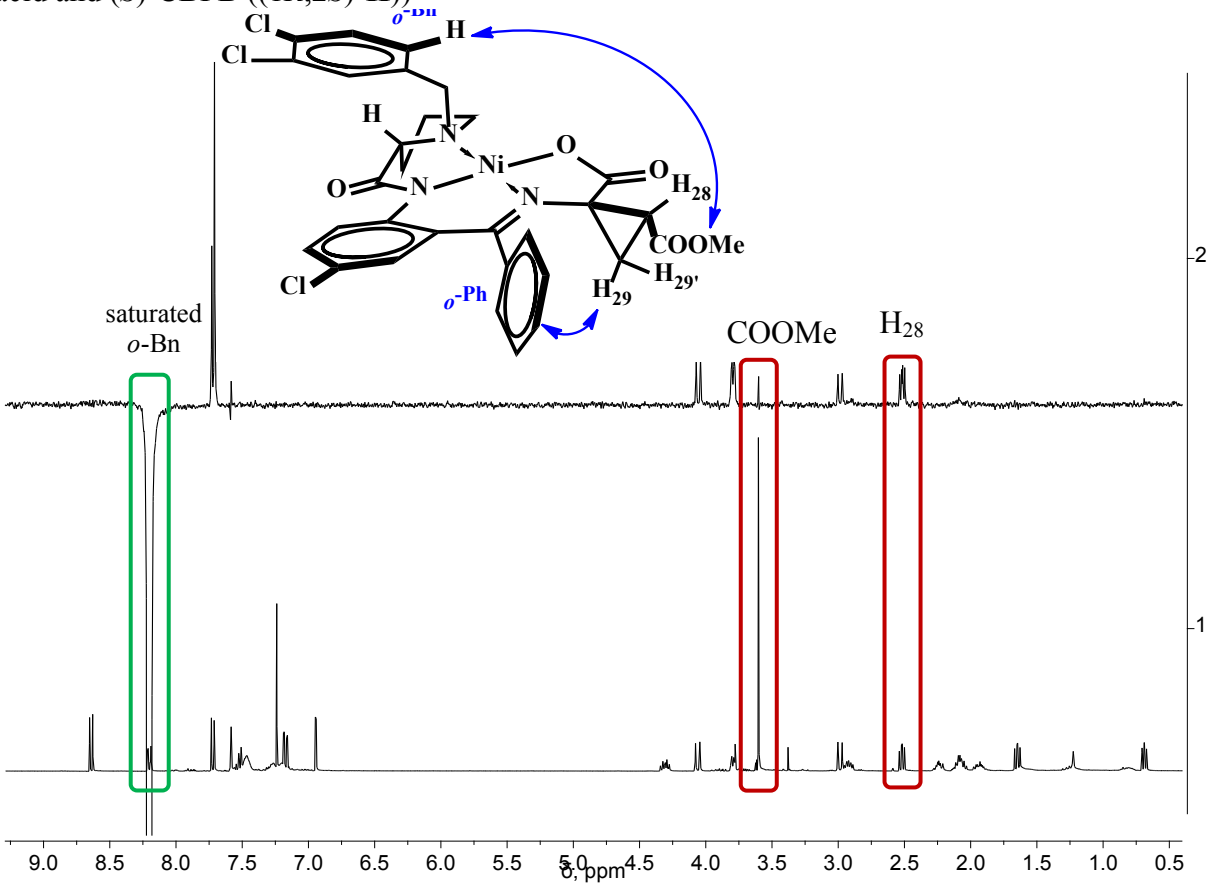
19. HMBC spectrum of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*R*,2*S*)-**II**))



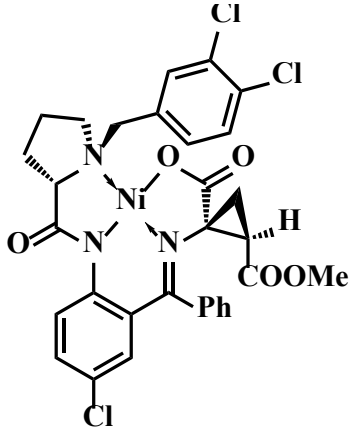
20. NOESY-1D spectra (saturation of proton H_{29}) (upper) and ^{1}H NMR spectrum (bottom) of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*R*,2*S*)-**II**))

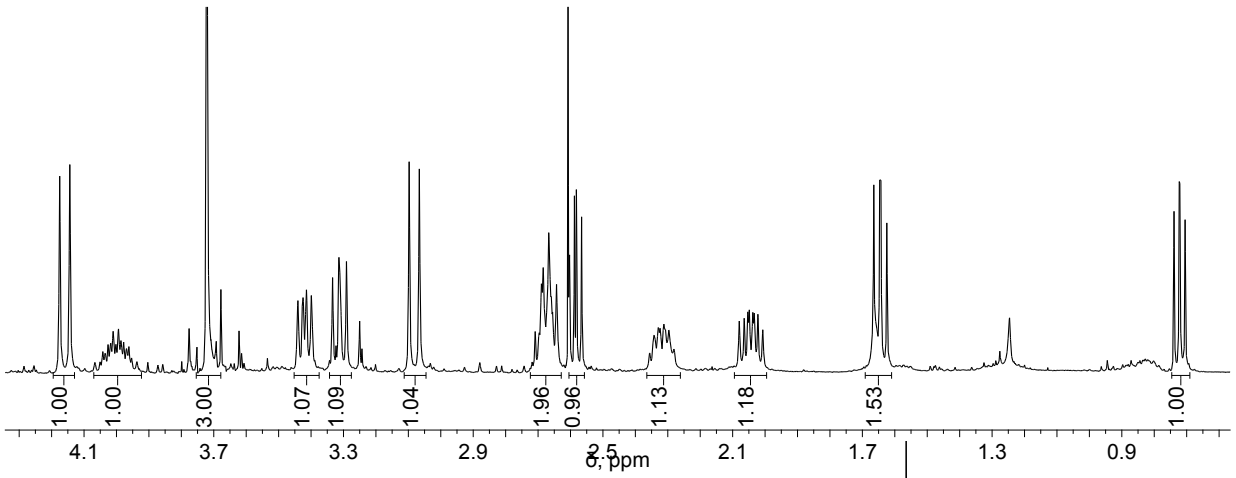


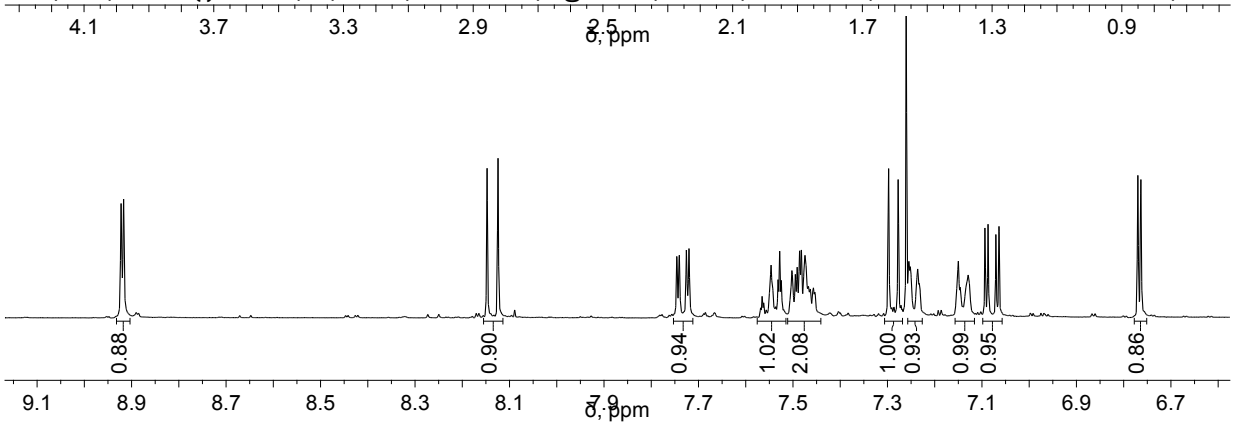
21. NOESY-1D spectra (saturation of proton *o*-Bn) (upper) and ^{1}H NMR spectrum (bottom) of the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*R*,2*S*)-**II**))



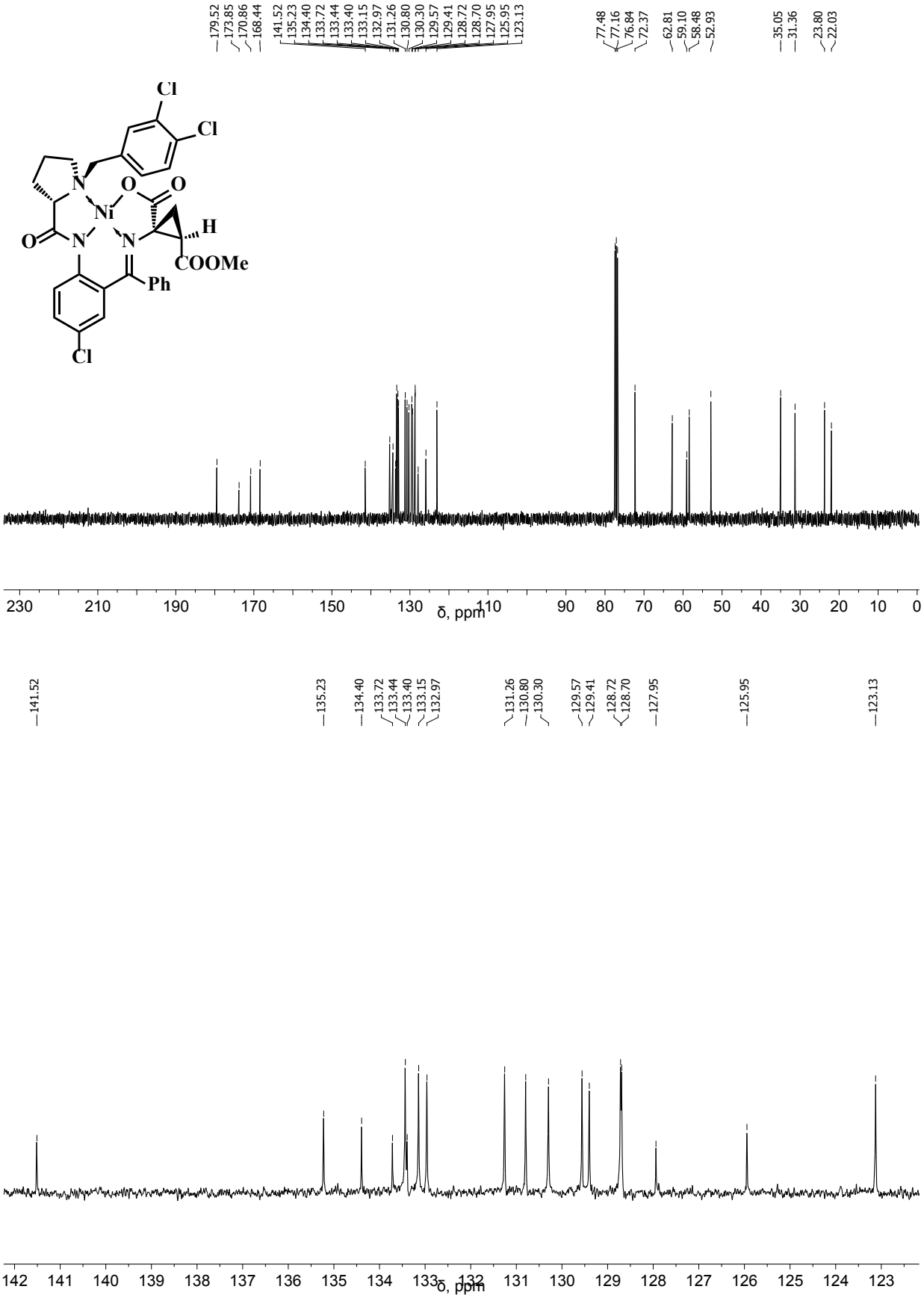
22. ^{1}H NMR spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*S*,2*R*)-**II**))



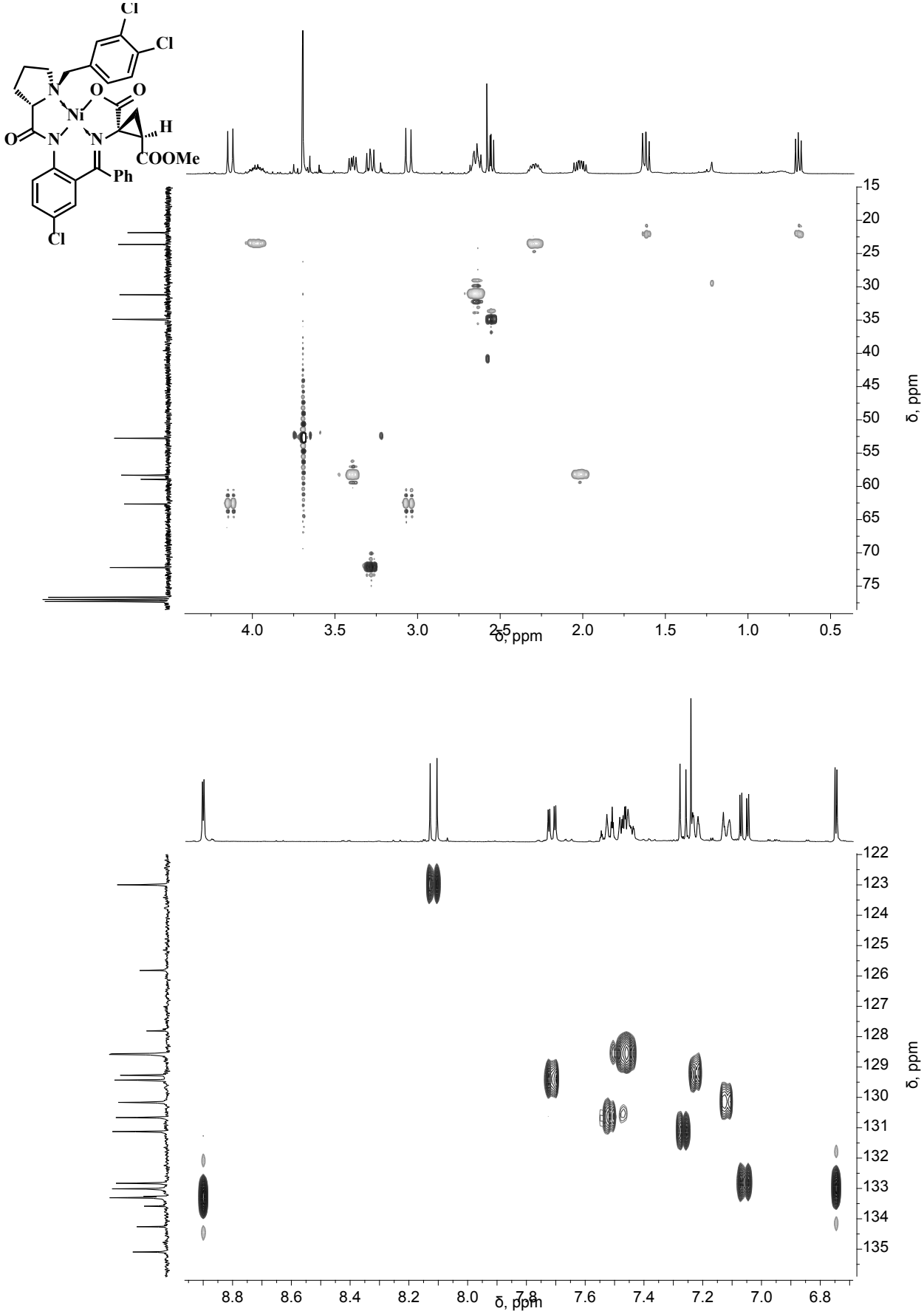




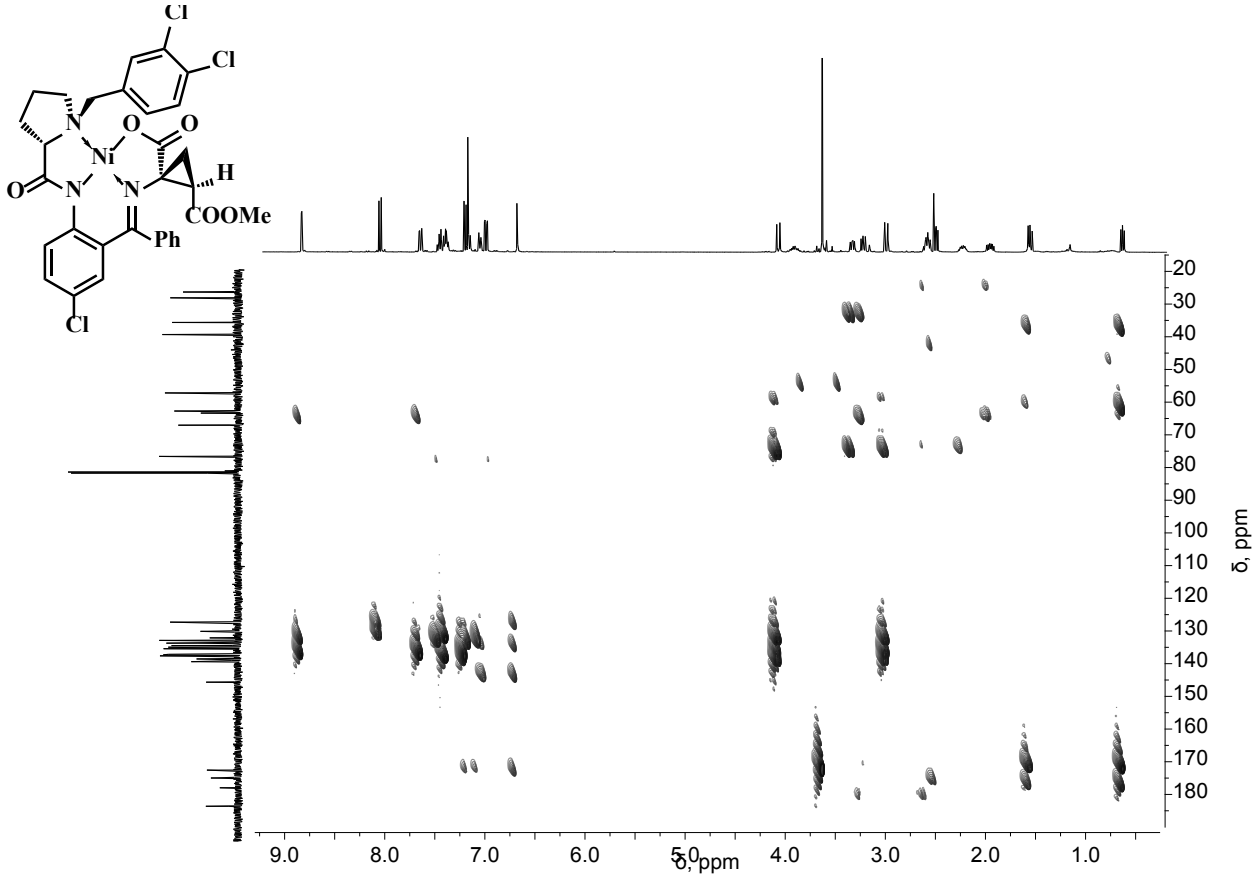
23. ^{13}C NMR spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*S*,2*R*)-**II**))



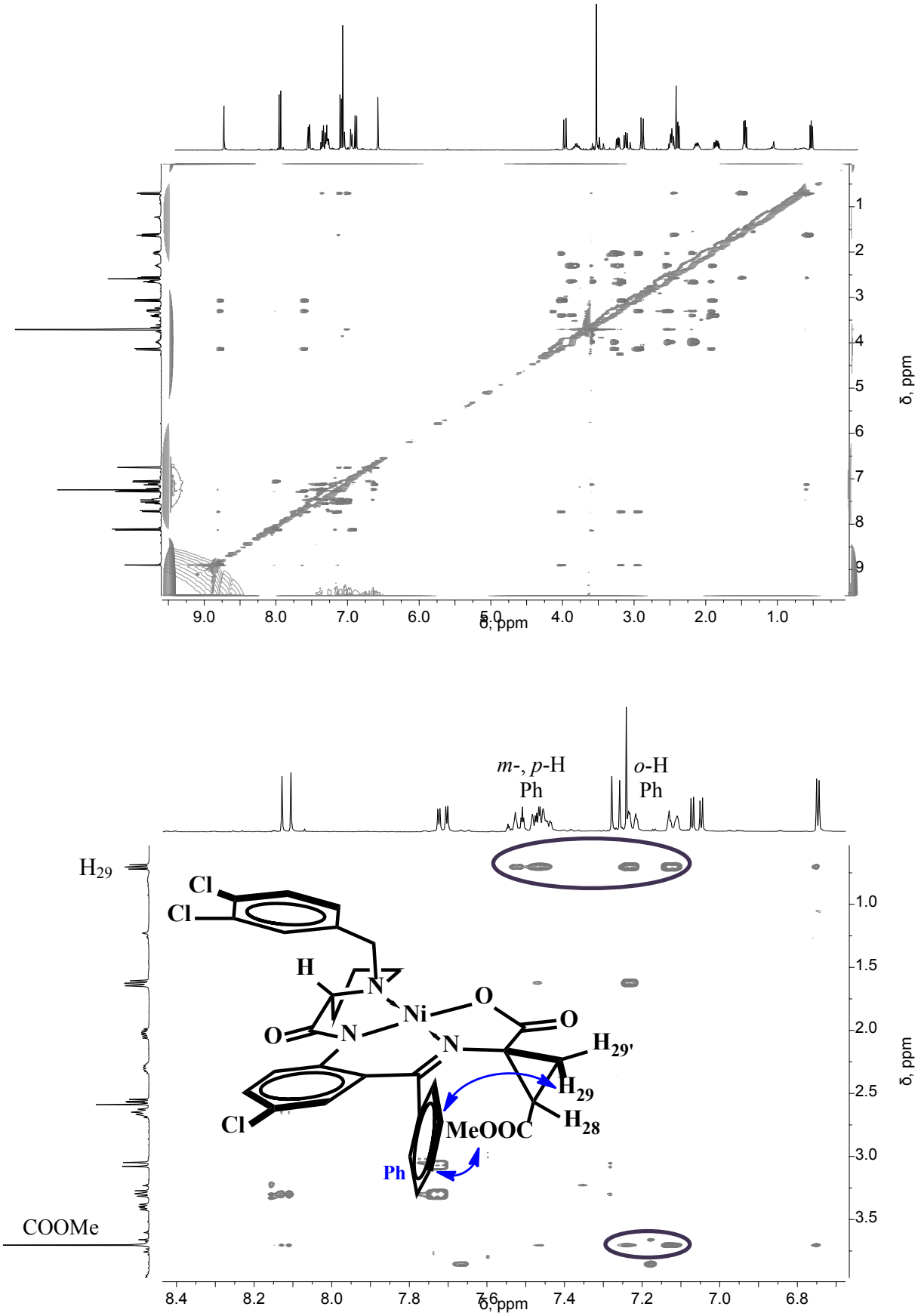
24. HSQC spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*S*,2*R*)-**II**))



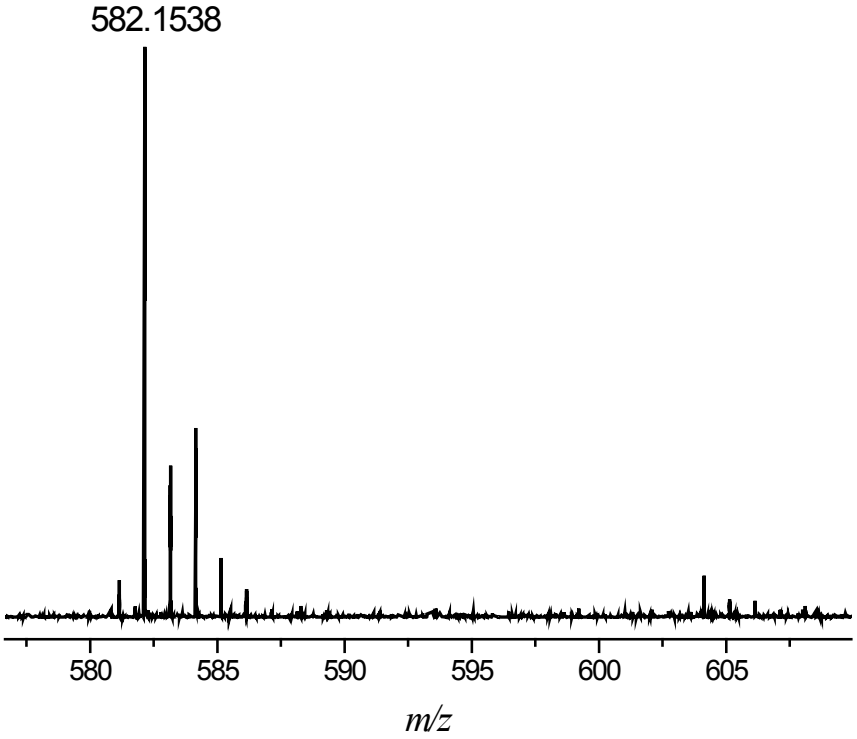
25. HMBC spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*S*,2*R*)-**II**))



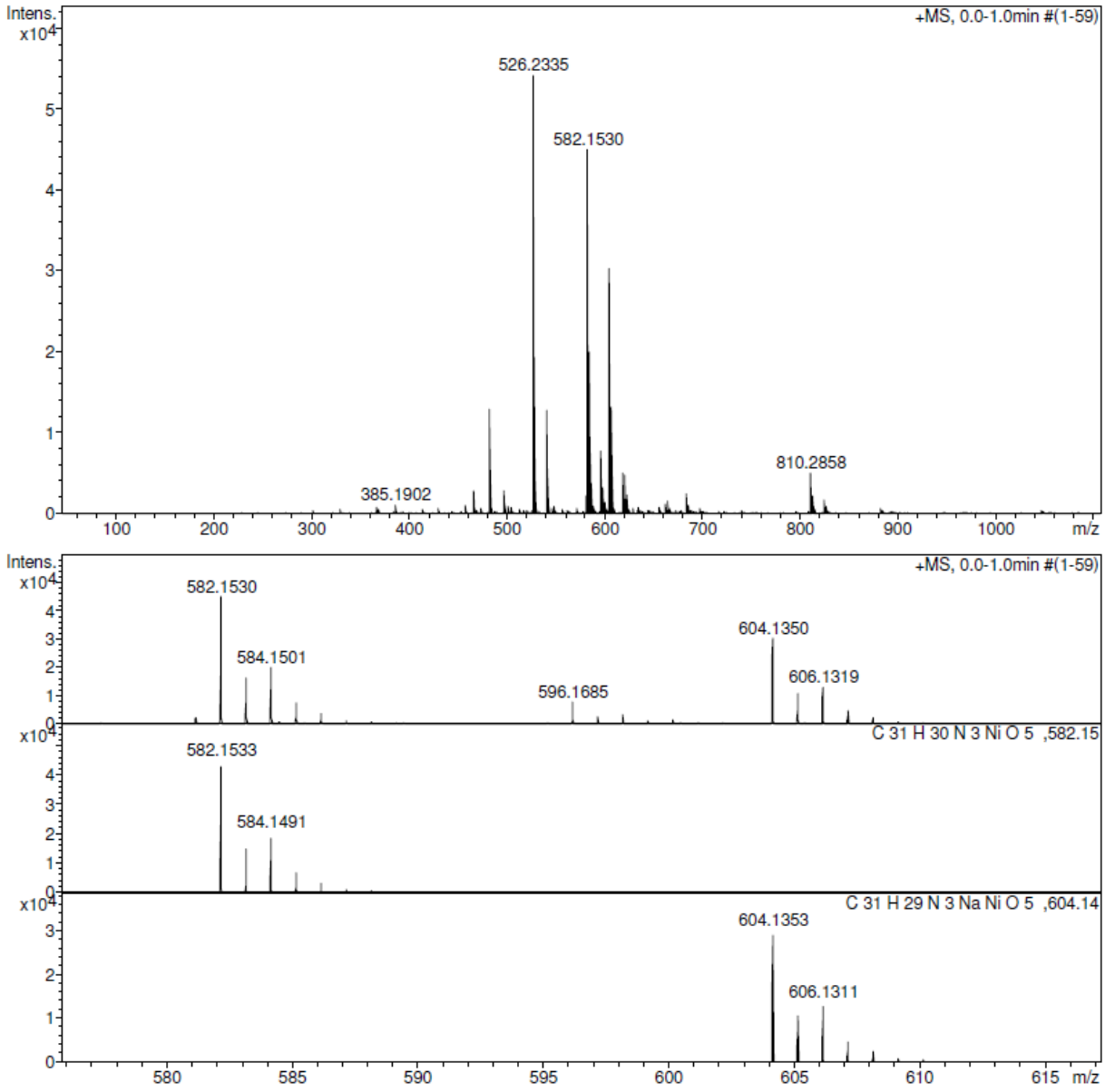
26. NOESY-2D spectrum of the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*S*,2*R*)-**II**))



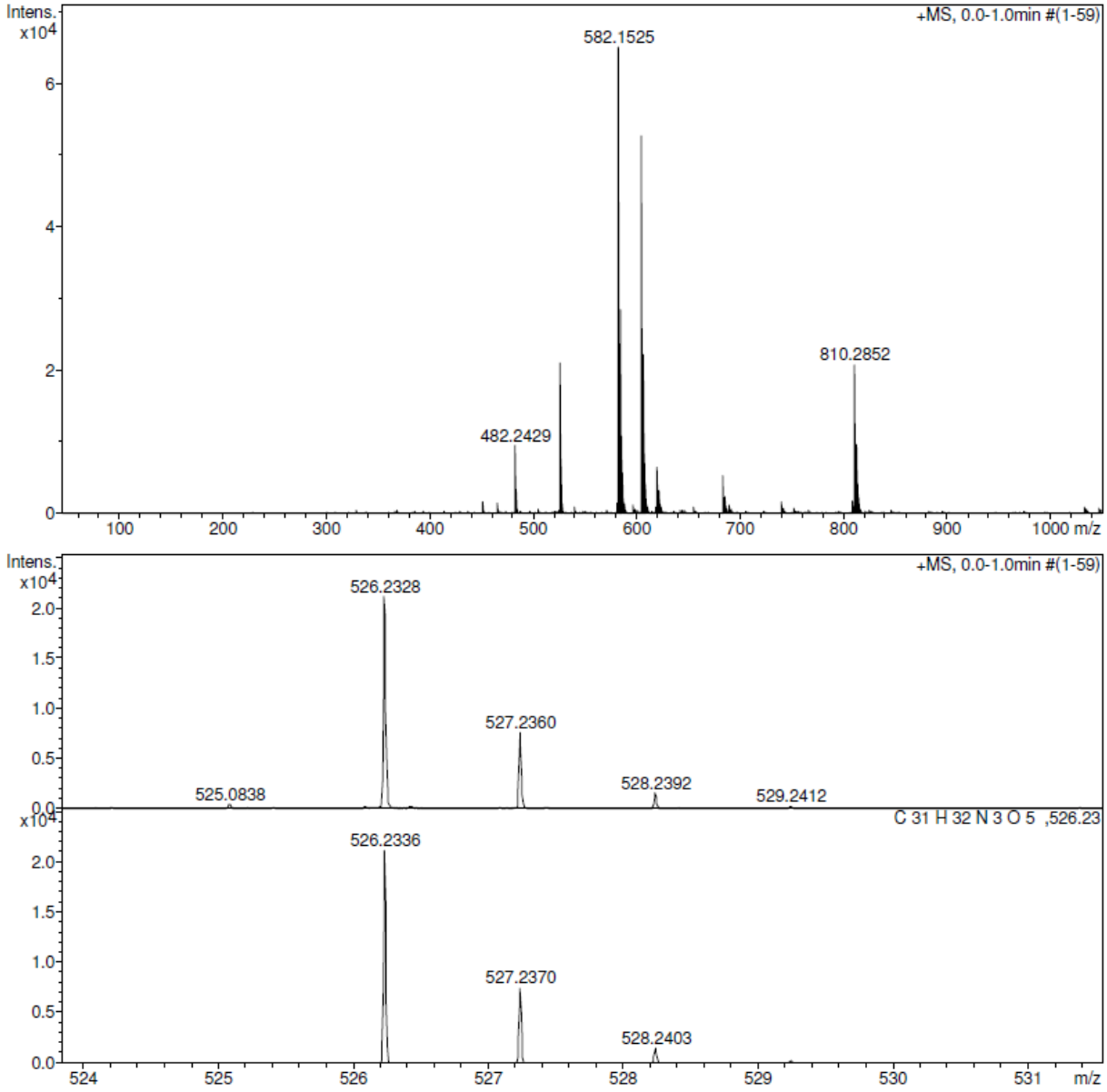
27. ESI-HRMS data for the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*R*,2*S*)-**I**))



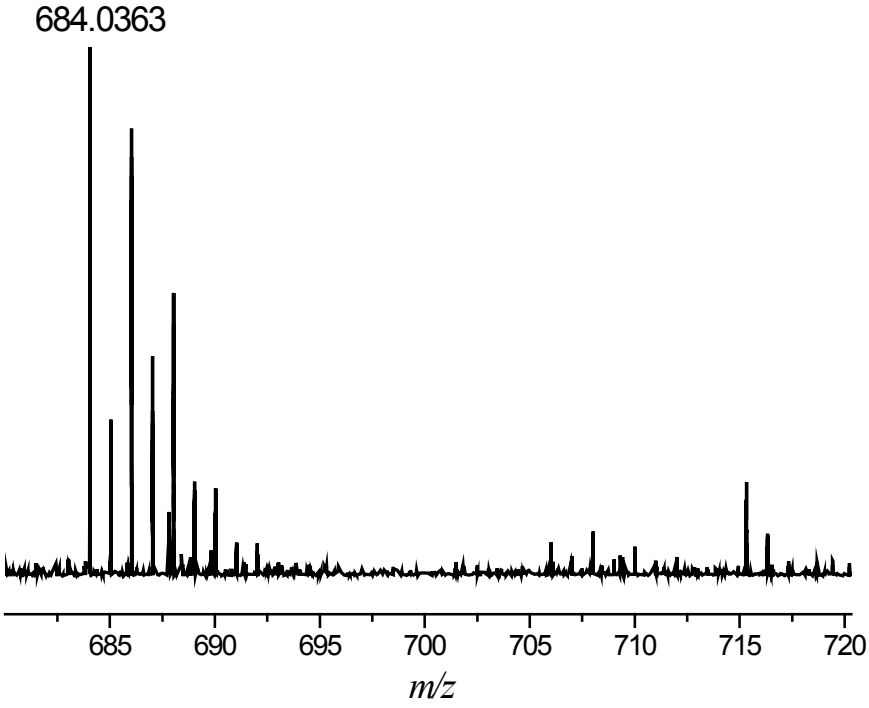
28. ESI-HRMS data for the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*R*)-**I**))



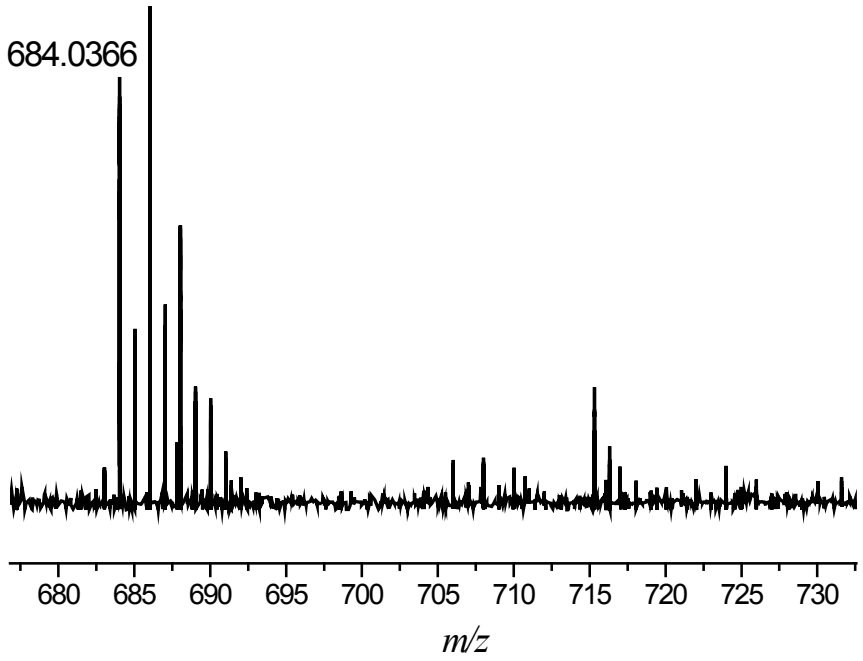
29. ESI-HRMS data for the Ni complex of Shiff base of (1*S*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-BPB ((1*S*,2*S*)-**I**))



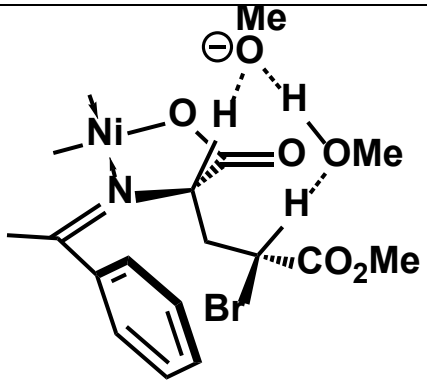
30. ESI-HRMS data for the Ni complex of Shiff base of (1*R*,2*S*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*R*,2*S*)-**II**))



31. ESI-HRMS data for the Ni complex of Shiff base of (1*S*,2*R*)-1-amino-2-(methoxycarbonyl)cyclopropanecarboxylic acid and (*S*)-CBPB ((1*S*,2*R*)-**II**))



32. Optimized structures and energies of intermediates and transition states.



(S,R)

Electronic energy: E_{el} = -6048.61213772 Hartree
Zero-point energy E_0 = 0.63464287 Hartree
Thermal contribution to Gibbs free energy:
$G - E_{el}$ = 0.56459760 Hartree

Cartesian coordinates:

Element	x	y	z
C	-1.020760000000	-1.961254000000	1.533748000000
C	-0.803217000000	-3.018557000000	2.459126000000
C	-1.784661000000	-3.429755000000	3.358717000000
C	-3.037893000000	-2.789085000000	3.334716000000
C	-3.287692000000	-1.753247000000	2.435733000000
C	-2.293615000000	-1.296900000000	1.525842000000
N	-2.519293000000	-0.219108000000	0.674185000000

C	0.087265000000	-1.602758000000	0.638068000000
H	0.180279000000	-3.507902000000	2.474599000000
H	-1.577799000000	-4.241963000000	4.071714000000
H	-3.832153000000	-3.094841000000	4.034018000000
H	-4.266647000000	-1.265081000000	2.427021000000
C	3.292336000000	-3.690404000000	0.402536000000
C	2.803905000000	-4.849199000000	-0.220554000000
C	1.443988000000	-4.930889000000	-0.566184000000
C	0.582187000000	-3.866808000000	-0.271433000000
C	1.074813000000	-2.692796000000	0.347472000000
C	2.442087000000	-2.606297000000	0.680994000000
H	2.867635000000	-1.675332000000	1.106000000000
H	4.357387000000	-3.619204000000	0.671949000000
H	3.481361000000	-5.688705000000	-0.442070000000
H	1.049971000000	-5.831139000000	-1.062780000000
H	-0.484992000000	-3.935901000000	-0.532591000000
N	0.178973000000	-0.401612000000	0.106626000000
C	1.315858000000	0.010160000000	-0.735495000000
C	1.258713000000	1.526670000000	-0.889579000000
O	2.173341000000	2.160343000000	-1.434497000000
O	0.195589000000	2.102865000000	-0.394540000000
C	-3.779298000000	0.207752000000	0.336463000000
C	-3.776646000000	1.538716000000	-0.396625000000
O	-4.851487000000	-0.392109000000	0.520193000000
C	-3.880319000000	1.371201000000	-1.943188000000
N	-2.504877000000	2.292074000000	-0.157083000000
H	-4.637348000000	2.130509000000	-0.020263000000
H	-4.810225000000	1.852785000000	-2.299798000000
H	-3.925497000000	0.304158000000	-2.234423000000
C	-2.512973000000	3.176272000000	1.046513000000
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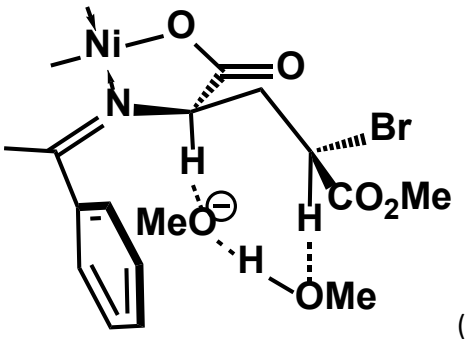
H	-3.425658000000	3.810899000000	1.013101000000
H	-1.236848000000	3.434217000000	-1.435932000000
H	-2.971557000000	3.944151000000	-1.408554000000
C	-2.638622000000	2.085429000000	-2.507651000000
C	-1.168062000000	2.029115000000	2.850383000000
C	-3.589993000000	1.992083000000	3.022378000000
C	-1.071851000000	1.231993000000	4.000117000000
H	-0.254274000000	2.373289000000	2.341351000000
C	-3.494245000000	1.196533000000	4.176534000000
H	-4.580222000000	2.285097000000	2.640218000000
H	-4.409809000000	0.871408000000	4.693574000000
H	-0.081686000000	0.938874000000	4.381052000000
C	-2.236281000000	0.810218000000	4.663089000000

H	-2.161761000000	0.178357000000	5.561271000000
H	-2.839450000000	2.591738000000	-3.471234000000
H	-1.793995000000	1.385346000000	-2.672045000000
Ni	-1.140835000000	0.897434000000	0.108402000000
C	1.324707000000	-0.738400000000	-2.091910000000
H	0.301350000000	-0.737677000000	-2.521784000000
C	2.294066000000	-0.135368000000	-3.094023000000
H	1.612741000000	-1.787808000000	-1.904167000000
C	1.730807000000	1.082508000000	-3.804451000000
O	2.704646000000	1.847861000000	-4.325367000000
O	0.537427000000	1.330343000000	-3.917651000000
C	2.269232000000	3.056215000000	-4.968369000000
H	3.183259000000	3.549313000000	-5.344021000000
H	1.581487000000	2.835320000000	-5.809290000000
H	1.753336000000	3.714087000000	-4.239542000000
Br	2.659939000000	-1.465074000000	-4.547731000000
H	2.290649000000	-0.169727000000	-0.193800000000
O	4.894906000000	-0.004295000000	-1.367029000000
H	3.289452000000	0.079182000000	-2.643792000000
C	5.263916000000	-1.344981000000	-1.556897000000
H	5.895857000000	-1.744084000000	-0.720892000000
H	4.395663000000	-2.044388000000	-1.661364000000
H	5.863788000000	-1.450089000000	-2.490965000000
O	3.848567000000	0.033862000000	0.898511000000
H	4.429254000000	0.051169000000	-0.398866000000
C	3.594946000000	1.282249000000	1.434521000000
H	2.494291000000	1.509047000000	1.555232000000
H	4.026162000000	1.423896000000	2.467559000000
H	3.997326000000	2.137930000000	0.824432000000



(R,R)

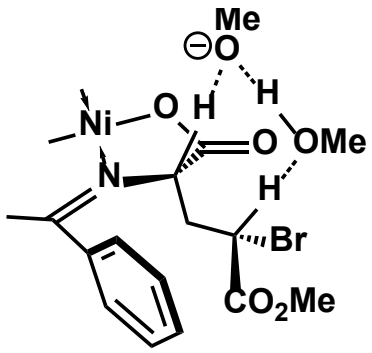
Electronic energy: E_{el} = -6048.60200959 Hartree
Zero-point energy E_0 = 0.63493632 Hartree
Thermal contribution to Gibbs free energy:
$G - E_{el}$ = 0.56318252 Hartree

Cartesian coordinates:

Element	x	y	z
C	-1.845602000000	-2.009302000000	0.594624000000
C	-1.998299000000	-3.425026000000	0.668646000000
C	-3.180590000000	-4.029866000000	1.082888000000
C	-4.270238000000	-3.212579000000	1.441516000000

C	-4.161126000000	-1.825812000000	1.381032000000
C	-2.961816000000	-1.179198000000	0.958698000000
N	-2.899988000000	0.203482000000	0.834267000000
C	-0.561421000000	-1.493545000000	0.112320000000
H	-1.156113000000	-4.058787000000	0.361778000000
H	-3.260023000000	-5.126876000000	1.116906000000
H	-5.222112000000	-3.662576000000	1.764691000000
H	-5.020103000000	-1.209353000000	1.666550000000
C	2.120374000000	-3.799232000000	1.489367000000
C	2.737362000000	-4.272955000000	0.319832000000
C	2.271461000000	-3.846816000000	-0.932776000000
C	1.203386000000	-2.939158000000	-1.034629000000
C	0.583989000000	-2.464233000000	0.138193000000
C	1.041471000000	-2.911035000000	1.400400000000
H	0.555625000000	-2.542231000000	2.316829000000
H	2.480258000000	-4.123639000000	2.477640000000
H	3.584624000000	-4.973356000000	0.387630000000
H	2.750596000000	-4.219989000000	-1.850744000000
H	0.891494000000	-2.554683000000	-2.025811000000
N	-0.401021000000	-0.250978000000	-0.305305000000
C	0.882436000000	0.199493000000	-0.888787000000
C	0.670803000000	1.578584000000	-1.505416000000
O	1.502739000000	2.106317000000	-2.249340000000
O	-0.455875000000	2.163558000000	-1.175569000000
C	-3.793860000000	1.027395000000	1.493593000000
C	-3.977997000000	2.356354000000	0.784361000000
O	-4.476427000000	0.739834000000	2.485598000000
C	-5.059653000000	2.220767000000	-0.328952000000
N	-2.720111000000	2.760291000000	0.084189000000
H	-4.272788000000	3.130308000000	1.518873000000
H	-5.802079000000	3.034036000000	-0.209970000000
H	-5.606523000000	1.260443000000	-0.259585000000
C	-1.906622000000	3.753965000000	0.850165000000
C	-3.141696000000	3.295157000000	-1.247538000000
H	-1.170080000000	4.168704000000	0.139126000000
C	-1.183100000000	3.167904000000	2.042449000000
H	-2.583686000000	4.578621000000	1.165147000000
H	-2.273202000000	3.300564000000	-1.930126000000
H	-3.499211000000	4.340833000000	-1.112713000000
C	-4.286585000000	2.379835000000	-1.646549000000
C	0.208258000000	2.944488000000	1.973769000000
C	-1.855961000000	2.855840000000	3.242584000000
C	0.905379000000	2.401968000000	3.063524000000
H	0.752784000000	3.204973000000	1.053351000000
C	-1.163937000000	2.293057000000	4.326413000000
H	-2.933190000000	3.054944000000	3.344527000000

H	-1.708854000000	2.045186000000	5.250584000000
H	1.993863000000	2.247588000000	2.992764000000
C	0.217941000000	2.059825000000	4.239701000000
H	0.761120000000	1.626331000000	5.093698000000
H	-4.905630000000	2.812550000000	-2.455806000000
H	-3.892589000000	1.405360000000	-2.000481000000
Ni	-1.623092000000	1.135565000000	-0.146566000000
C	2.025404000000	0.219585000000	0.145402000000
H	2.168626000000	-0.798233000000	0.549042000000
C	3.366824000000	0.655881000000	-0.434451000000
H	1.731248000000	0.847540000000	1.007933000000
H	1.144105000000	-0.468411000000	-1.756867000000
O	3.339621000000	-0.386217000000	-3.396889000000
H	3.347419000000	0.693876000000	-1.548494000000
C	4.074656000000	-1.543021000000	-3.105361000000
H	3.944589000000	-1.908343000000	-2.053819000000
H	3.801564000000	-2.407541000000	-3.764221000000
H	5.166172000000	-1.362997000000	-3.250624000000
O	1.011393000000	-1.255541000000	-3.559882000000
H	2.313525000000	-0.703165000000	-3.468799000000
C	4.516868000000	-0.242931000000	-0.001994000000
C	0.048257000000	-0.397103000000	-4.049390000000
H	-0.612839000000	-0.864416000000	-4.836304000000
H	-0.677103000000	-0.025875000000	-3.263842000000
H	0.457633000000	0.539164000000	-4.523445000000
Br	3.852492000000	2.505149000000	0.133427000000
O	5.639109000000	0.034234000000	-0.687499000000
O	4.439260000000	-1.129243000000	0.837266000000
C	6.781317000000	-0.781578000000	-0.381747000000
H	7.592069000000	-0.430477000000	-1.043854000000
H	7.077717000000	-0.661738000000	0.679992000000
H	6.565312000000	-1.851491000000	-0.577140000000



(S,S)

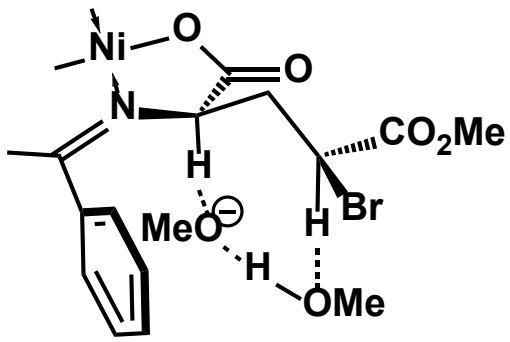
Electronic energy: E_{el} = -6048.60399736 Hartree
Zero-point energy E_0 = 0.63390833 Hartree
Thermal contribution to Gibbs free energy:
$G - E_{el}$ = 0.67797083 Hartree

Cartesian coordinates:

Element	x	y	z
C	-1.051736000000	-1.611398000000	1.414600000000
C	-0.788419000000	-2.725082000000	2.259155000000

C	-1.705863000000	-3.166967000000	3.209939000000
C	-2.937910000000	-2.496008000000	3.327557000000
C	-3.234136000000	-1.408822000000	2.507203000000
C	-2.309314000000	-0.929035000000	1.538382000000
N	-2.588506000000	0.185306000000	0.751417000000
C	-0.000048000000	-1.210783000000	0.473542000000
H	0.181257000000	-3.234268000000	2.170344000000
H	-1.465481000000	-4.023920000000	3.856795000000
H	-3.678775000000	-2.820167000000	4.075398000000
H	-4.198086000000	-0.900682000000	2.605761000000
C	3.191811000000	-3.255181000000	-0.101676000000
C	2.675183000000	-4.350740000000	-0.810098000000
C	1.297190000000	-4.415543000000	-1.079102000000
C	0.448450000000	-3.393754000000	-0.634228000000
C	0.971345000000	-2.278150000000	0.063139000000
C	2.353718000000	-2.213551000000	0.333276000000
H	2.792304000000	-1.325826000000	0.837981000000
H	4.269922000000	-3.202391000000	0.116165000000
H	3.343907000000	-5.154462000000	-1.155569000000
H	0.879058000000	-5.269085000000	-1.635259000000
H	-0.631604000000	-3.447256000000	-0.841990000000
N	0.062201000000	0.012584000000	-0.011027000000
C	1.169121000000	0.450262000000	-0.881594000000
C	1.143438000000	1.977205000000	-0.937709000000
O	2.086490000000	2.640561000000	-1.375259000000
O	0.033403000000	2.521332000000	-0.496015000000
C	-3.870089000000	0.622027000000	0.523919000000
C	-3.931175000000	1.982500000000	-0.150079000000
O	-4.925645000000	0.011608000000	0.761966000000
C	-4.228741000000	1.882169000000	-1.676280000000
N	-2.627423000000	2.712525000000	-0.036877000000
H	-4.729830000000	2.565464000000	0.353860000000
H	-5.153912000000	2.443626000000	-1.906825000000
H	-4.390211000000	0.833883000000	-1.992615000000
C	-2.501879000000	3.586105000000	1.169406000000
C	-2.511437000000	3.500293000000	-1.300242000000
H	-1.623836000000	4.234708000000	0.987181000000
C	-2.305278000000	2.799259000000	2.442571000000
H	-3.404239000000	4.233104000000	1.231446000000
H	-1.467204000000	3.833033000000	-1.429981000000
H	-3.174511000000	4.390459000000	-1.222060000000
C	-3.015790000000	2.535203000000	-2.359223000000
C	-1.003501000000	2.423709000000	2.838779000000
C	-3.403130000000	2.358778000000	3.204888000000
C	-0.808145000000	1.604464000000	3.960150000000
H	-0.136696000000	2.784587000000	2.263278000000

C	-3.208196000000	1.539168000000	4.329284000000
H	-4.423429000000	2.650924000000	2.911643000000
H	-4.076260000000	1.193940000000	4.911364000000
H	0.212526000000	1.314398000000	4.253948000000
C	-1.911639000000	1.154616000000	4.703763000000
H	-1.759018000000	0.504181000000	5.578648000000
H	-3.279951000000	3.047380000000	-3.304069000000
H	-2.228335000000	1.787028000000	-2.588668000000
Ni	-1.255818000000	1.306641000000	0.090489000000
C	1.059581000000	-0.184183000000	-2.282774000000
H	0.076210000000	0.066381000000	-2.730994000000
C	2.208620000000	0.210421000000	-3.211925000000
H	1.075686000000	-1.281755000000	-2.157397000000
H	2.149639000000	0.185161000000	-0.414524000000
O	4.621122000000	0.701941000000	-1.315049000000
H	3.023166000000	0.724070000000	-2.640970000000
C	5.221519000000	-0.541922000000	-1.550082000000
H	5.848359000000	-0.891856000000	-0.688995000000
H	4.490671000000	-1.366935000000	-1.755307000000
H	5.893802000000	-0.492100000000	-2.438844000000
O	3.676332000000	0.422300000000	0.963349000000
H	4.172150000000	0.639163000000	-0.329612000000
C	3.132444000000	1.515920000000	1.604988000000
H	2.000681000000	1.533166000000	1.606644000000
H	3.413298000000	1.581269000000	2.696649000000
H	3.429283000000	2.508613000000	1.164406000000
Br	1.619076000000	1.540534000000	-4.563523000000
C	2.897297000000	-0.913471000000	-3.976742000000
O	3.855534000000	-0.747391000000	-4.715649000000
O	2.366871000000	-2.123998000000	-3.716188000000
C	3.031125000000	-3.249985000000	-4.312052000000
H	2.437013000000	-4.137229000000	-4.032774000000
H	3.071522000000	-3.142595000000	-5.414455000000
H	4.062870000000	-3.345477000000	-3.918968000000



Electronic energy: E_{el} = -6048.60829937 Hartree
Zero-point energy E_0 = 0.63527983 Hartree
Thermal contribution to Gibbs free energy:
$G - E_{el}$ = 0.56603040 Hartree

(R,S)

Cartesian coordinates:

Element	x	y	z

C	-1.598679000000	-2.294334000000	0.647237000000
C	-1.756272000000	-3.709374000000	0.734811000000
C	-2.932928000000	-4.307480000000	1.173697000000
C	-4.014631000000	-3.484655000000	1.542891000000
C	-3.901705000000	-2.099083000000	1.469769000000
C	-2.706768000000	-1.459106000000	1.025036000000
N	-2.644902000000	-0.077680000000	0.890899000000
C	-0.323165000000	-1.787914000000	0.130841000000
H	-0.923549000000	-4.350038000000	0.417527000000
H	-3.014503000000	-5.403985000000	1.217050000000
H	-4.963173000000	-3.929027000000	1.883200000000
H	-4.754588000000	-1.477445000000	1.761914000000
C	2.354956000000	-4.163502000000	1.395121000000
C	2.898637000000	-4.661573000000	0.199295000000
C	2.394291000000	-4.217417000000	-1.032401000000
C	1.356351000000	-3.272042000000	-1.086811000000
C	0.806179000000	-2.777287000000	0.112911000000
C	1.305718000000	-3.236605000000	1.353972000000
H	0.873882000000	-2.851945000000	2.290713000000
H	2.747498000000	-4.501246000000	2.366315000000
H	3.719378000000	-5.395364000000	0.230050000000
H	2.820183000000	-4.604315000000	-1.970332000000
H	1.012744000000	-2.873403000000	-2.060448000000
N	-0.162262000000	-0.547332000000	-0.293132000000
C	1.094211000000	-0.110720000000	-0.940350000000
C	0.890117000000	1.287030000000	-1.496210000000
O	1.747285000000	1.836703000000	-2.204456000000
O	-0.235985000000	1.865542000000	-1.177898000000
C	-3.531481000000	0.751958000000	1.554958000000
C	-3.720181000000	2.074810000000	0.837175000000
O	-4.202968000000	0.471253000000	2.555920000000
C	-4.795359000000	1.932466000000	-0.282295000000
N	-2.461165000000	2.477076000000	0.141561000000
H	-4.020449000000	2.852247000000	1.565590000000
H	-5.563198000000	2.718291000000	-0.144561000000
H	-5.311792000000	0.953854000000	-0.237797000000
C	-1.630110000000	3.434996000000	0.933713000000
C	-2.883975000000	3.051792000000	-1.171575000000
H	-0.858765000000	3.824051000000	0.244777000000
C	-0.966263000000	2.803237000000	2.136754000000
H	-2.281724000000	4.282836000000	1.239642000000
H	-2.017109000000	3.080494000000	-1.855394000000
H	-3.244399000000	4.091402000000	-1.002718000000
C	-4.026108000000	2.143864000000	-1.596190000000
C	0.381457000000	2.395505000000	2.054076000000
C	-1.657952000000	2.604988000000	3.348688000000

C	1.018689000000	1.788305000000	3.145529000000
H	0.939587000000	2.556368000000	1.121490000000
C	-1.027647000000	1.980545000000	4.437250000000
H	-2.700527000000	2.940330000000	3.452123000000
H	-1.586216000000	1.824287000000	5.373275000000
H	2.076110000000	1.492462000000	3.064610000000
C	0.310423000000	1.567248000000	4.338656000000
H	0.805035000000	1.085538000000	5.196314000000
H	-4.650419000000	2.599828000000	-2.388515000000
H	-3.627069000000	1.184928000000	-1.985365000000
Ni	-1.384537000000	0.842433000000	-0.119622000000
C	2.335324000000	-0.167437000000	-0.016710000000
H	2.507644000000	-1.219697000000	0.260298000000
C	3.608194000000	0.331977000000	-0.690590000000
H	2.141947000000	0.390780000000	0.919399000000
H	1.268699000000	-0.761219000000	-1.853486000000
O	3.518155000000	-0.881453000000	-3.575170000000
H	3.716686000000	-0.046014000000	-1.734053000000
C	4.175225000000	-2.112965000000	-3.420732000000
H	4.306753000000	-2.418307000000	-2.351286000000
H	3.636179000000	-2.950376000000	-3.930591000000
H	5.198757000000	-2.074345000000	-3.865070000000
O	1.114074000000	-1.520258000000	-3.552879000000
H	2.465628000000	-1.103504000000	-3.567155000000
Br	5.185859000000	-0.423434000000	0.299056000000
C	3.869112000000	1.827091000000	-0.710959000000
O	4.609774000000	2.383204000000	-1.507519000000
O	3.242814000000	2.473541000000	0.295048000000
C	3.403699000000	3.899686000000	0.316597000000
H	2.891968000000	4.254923000000	1.228679000000
H	4.475888000000	4.177287000000	0.349850000000
H	2.937220000000	4.351893000000	-0.581917000000
C	0.209189000000	-0.622778000000	-4.084781000000
H	-0.461040000000	-1.073261000000	-4.872542000000
H	-0.507501000000	-0.196124000000	-3.320954000000
H	0.679546000000	0.276996000000	-4.571816000000

Transition state of cyclization reaction leading to (R,R)-isomer

Electronic energy: E_{el} = -5933.08921590 Hartree
Zero-point energy E_0 = 0.58359905 Hartree
Thermal contribution to Gibbs free energy: $G - E_{el}$ = 0.51755728 Hartree

Cartesian coordinates:

Element	x	y	z
C	-1.013290000000	-2.150839000000	1.220580000000
C	-0.745369000000	-3.321560000000	1.992451000000
C	-1.191774000000	-3.475842000000	3.302805000000

C	-1.930334000000	-2.437828000000	3.901631000000
C	-2.296860000000	-1.323140000000	3.146540000000
C	-1.923616000000	-1.183575000000	1.781553000000
N	-2.446096000000	-0.160869000000	0.991362000000
C	-0.302620000000	-1.962569000000	-0.038718000000
H	-0.136949000000	-4.120302000000	1.550096000000
H	-0.941641000000	-4.389311000000	3.863511000000
H	-2.240759000000	-2.504805000000	4.955791000000
H	-2.907538000000	-0.537769000000	3.602608000000
C	2.231778000000	-4.777341000000	-0.657810000000
C	1.758777000000	-5.284515000000	-1.878888000000
C	0.627725000000	-4.707553000000	-2.481744000000
C	-0.027507000000	-3.631850000000	-1.864888000000
C	0.435873000000	-3.119151000000	-0.632924000000
C	1.575714000000	-3.703936000000	-0.036405000000
H	1.980331000000	-3.291751000000	0.898924000000
H	3.129645000000	-5.207896000000	-0.189829000000
H	2.274421000000	-6.127078000000	-2.364429000000
H	0.252096000000	-5.097657000000	-3.439718000000
H	-0.911394000000	-3.178758000000	-2.339422000000
N	-0.285201000000	-0.780262000000	-0.676694000000
C	0.701100000000	-0.384607000000	-1.579199000000
C	0.346699000000	0.827783000000	-2.347193000000
O	1.021854000000	1.285052000000	-3.287330000000
O	-0.784439000000	1.392424000000	-1.958453000000
C	-3.675850000000	0.380992000000	1.282499000000
C	-4.100077000000	1.474762000000	0.324592000000
O	-4.471994000000	0.020189000000	2.166288000000
C	-5.146742000000	0.975636000000	-0.715794000000
N	-2.941236000000	1.983838000000	-0.474718000000
H	-4.533987000000	2.300865000000	0.925627000000
H	-6.048654000000	1.614471000000	-0.662108000000
H	-5.463991000000	-0.063779000000	-0.507325000000
C	-2.257938000000	3.168229000000	0.130643000000
C	-3.494291000000	2.288729000000	-1.827185000000
H	-1.547387000000	3.539346000000	-0.632400000000
C	-1.526427000000	2.824014000000	1.406584000000
H	-3.022433000000	3.956377000000	0.308391000000
H	-2.664380000000	2.383003000000	-2.549248000000
H	-4.045347000000	3.254640000000	-1.774112000000
C	-4.451900000000	1.134854000000	-2.077034000000
C	-0.186290000000	2.384745000000	1.355368000000
C	-2.185049000000	2.848409000000	2.650696000000
C	0.469148000000	1.949864000000	2.516381000000
H	0.356505000000	2.383570000000	0.398840000000
C	-1.534056000000	2.405007000000	3.814130000000

H	-3.223550000000	3.208873000000	2.712034000000
H	-2.067235000000	2.418611000000	4.777581000000
H	1.515658000000	1.618196000000	2.441612000000
C	-0.209174000000	1.945824000000	3.746864000000
H	0.298770000000	1.592203000000	4.657541000000
H	-5.161104000000	1.349196000000	-2.899162000000
H	-3.882278000000	0.221215000000	-2.349137000000
Ni	-1.614760000000	0.530839000000	-0.528485000000
C	2.064264000000	-0.977721000000	-1.774550000000
H	2.509282000000	-0.537197000000	-2.683891000000
C	2.521199000000	-0.283429000000	-0.545139000000
H	2.185812000000	-2.071133000000	-1.765399000000
C	2.992712000000	1.119214000000	-0.546615000000
H	2.097290000000	-0.602469000000	0.415601000000
Br	4.712584000000	-1.365610000000	0.150140000000
O	3.435227000000	1.518241000000	-1.755378000000
O	2.982936000000	1.856308000000	0.439592000000
C	3.818240000000	2.894167000000	-1.858965000000
H	4.118063000000	3.050049000000	-2.910467000000
H	2.966255000000	3.558899000000	-1.609024000000
H	4.668644000000	3.102278000000	-1.180171000000
H	5.791322000000	0.587047000000	-0.087292000000
O	6.298480000000	1.383744000000	-0.400835000000
C	6.747298000000	1.064778000000	-1.703581000000
H	7.259424000000	1.955257000000	-2.126734000000
H	7.478845000000	0.219505000000	-1.714466000000
H	5.917545000000	0.790862000000	-2.395998000000

Transition state of cyclization reaction leading to (S,R)-isomer

Electronic energy: E_{el} = -5933.10019812 Hartree
Zero-point energy E_0 = 0.58368216 Hartree
Thermal contribution to Gibbs free energy:
$G - E_{el}$ = 0.51489890 Hartree

Cartesian coordinates:

Element	x	y	z
C	-0.314102000000	-1.552839000000	1.701188000000
C	-0.187300000000	-2.541903000000	2.719321000000
C	-1.262329000000	-2.951685000000	3.505026000000
C	-2.527737000000	-2.374548000000	3.287490000000
C	-2.687015000000	-1.386027000000	2.316575000000
C	-1.602029000000	-0.933180000000	1.518883000000
N	-1.754772000000	0.129355000000	0.628303000000
C	0.852992000000	-1.228292000000	0.893048000000
H	0.800553000000	-2.989178000000	2.895538000000
H	-1.116539000000	-3.716569000000	4.283123000000
H	-3.394964000000	-2.683954000000	3.891959000000
H	-3.670290000000	-0.930380000000	2.162022000000

C	4.438586000000	-2.352358000000	1.466696000000
C	4.375575000000	-3.716252000000	1.131096000000
C	3.154413000000	-4.274711000000	0.718869000000
C	2.003348000000	-3.476248000000	0.641035000000
C	2.057348000000	-2.104088000000	0.971686000000
C	3.290568000000	-1.552254000000	1.385196000000
H	3.343163000000	-0.484327000000	1.647830000000
H	5.390187000000	-1.908925000000	1.798889000000
H	5.278442000000	-4.343320000000	1.192790000000
H	3.097167000000	-5.341195000000	0.450825000000
H	1.051715000000	-3.914797000000	0.306650000000
N	0.908079000000	-0.125774000000	0.137384000000
C	1.849922000000	0.150072000000	-0.834192000000
C	1.984723000000	1.587380000000	-1.109476000000
O	2.887100000000	2.077172000000	-1.824276000000
O	1.070731000000	2.338207000000	-0.511866000000
C	-2.969406000000	0.539338000000	0.155413000000
C	-2.929244000000	1.914455000000	-0.495129000000
O	-4.040885000000	-0.098158000000	0.165572000000
C	-2.940215000000	1.841664000000	-2.051545000000
N	-1.682746000000	2.665501000000	-0.132832000000
H	-3.818650000000	2.476438000000	-0.136484000000
H	-3.868115000000	2.305263000000	-2.437450000000
H	-2.910202000000	0.793970000000	-2.407121000000
C	-1.773888000000	3.476435000000	1.117250000000
C	-1.398567000000	3.530836000000	-1.313807000000
H	-0.914848000000	4.175330000000	1.092900000000
C	-1.717216000000	2.646446000000	2.376941000000
H	-2.705228000000	4.083745000000	1.081284000000
H	-0.355455000000	3.889779000000	-1.261069000000
H	-2.093919000000	4.400238000000	-1.290551000000
C	-1.690679000000	2.623486000000	-2.496849000000
C	-0.468295000000	2.207624000000	2.868585000000
C	-2.889660000000	2.243955000000	3.040640000000
C	-0.399233000000	1.366595000000	3.988652000000
H	0.458396000000	2.540830000000	2.374833000000
C	-2.820917000000	1.408355000000	4.169209000000
H	-3.869865000000	2.580204000000	2.666332000000
H	-3.747399000000	1.093883000000	4.673990000000
H	0.580494000000	1.023255000000	4.355114000000
C	-1.576978000000	0.963312000000	4.640322000000
H	-1.523953000000	0.293915000000	5.512564000000
H	-1.852381000000	3.195940000000	-3.430622000000
H	-0.841754000000	1.930228000000	-2.663610000000
Ni	-0.347332000000	1.235889000000	0.108833000000
C	2.559219000000	-0.838308000000	-1.712878000000

H	2.592399000000	-1.870193000000	-1.328661000000
C	1.612351000000	-0.689292000000	-2.866611000000
H	3.579252000000	-0.500860000000	-1.977804000000
C	0.189873000000	-1.108767000000	-2.689208000000
H	1.679152000000	0.258307000000	-3.422579000000
Br	2.288495000000	-2.014747000000	-4.598653000000
O	0.059628000000	-2.164968000000	-1.859444000000
O	-0.762176000000	-0.581285000000	-3.260614000000
C	-1.278925000000	-2.635523000000	-1.646435000000
H	-1.198919000000	-3.489200000000	-0.950305000000
H	-1.916315000000	-1.846514000000	-1.201116000000
H	-1.731494000000	-2.970441000000	-2.601861000000
H	2.281959000000	0.115060000000	-5.470979000000
O	2.322169000000	1.091634000000	-5.620850000000
C	3.609195000000	1.517363000000	-5.192077000000
H	3.768324000000	2.554802000000	-5.555381000000
H	3.704766000000	1.535846000000	-4.080921000000
H	4.431651000000	0.888952000000	-5.606599000000

Transition state of cyclization reaction leading to (S,S)-isomer

Electronic energy: E_{el} = -5933.09251652 Hartree
Zero-point energy E_0 = 0.58271931 Hartree
Thermal contribution to Gibbs free energy:
$G - E_{el}$ = 0.51540236 Hartree

Cartesian coordinates:

Element	x	y	z
C	-0.646418000000	-1.887841000000	1.136980000000
C	-0.474927000000	-3.120209000000	1.833819000000
C	-1.520407000000	-3.765769000000	2.487431000000
C	-2.801471000000	-3.182679000000	2.463219000000
C	-3.006528000000	-1.968675000000	1.810244000000
C	-1.952754000000	-1.277583000000	1.148981000000
N	-2.151843000000	-0.007894000000	0.608997000000
C	0.511119000000	-1.315157000000	0.462784000000
H	0.526254000000	-3.570531000000	1.860411000000
H	-1.340768000000	-4.716419000000	3.011113000000
H	-3.648088000000	-3.671084000000	2.970615000000
H	-4.003836000000	-1.517803000000	1.808817000000
C	4.119376000000	-2.379765000000	0.972123000000
C	4.180437000000	-3.571711000000	0.229275000000
C	3.036110000000	-4.040584000000	-0.435234000000
C	1.833727000000	-3.322265000000	-0.357545000000
C	1.766378000000	-2.118853000000	0.376381000000
C	2.921361000000	-1.654628000000	1.043800000000
H	2.873932000000	-0.716501000000	1.617952000000
H	5.013476000000	-2.011274000000	1.498340000000
H	5.125373000000	-4.133008000000	0.164805000000

H	3.082930000000	-4.962789000000	-1.031546000000
H	0.940501000000	-3.683011000000	-0.890215000000
N	0.523077000000	-0.063210000000	0.001065000000
C	1.491381000000	0.486691000000	-0.836464000000
C	1.591322000000	1.955154000000	-0.687312000000
O	2.541137000000	2.634413000000	-1.120471000000
O	0.582615000000	2.484929000000	-0.017611000000
C	-3.398840000000	0.509013000000	0.370413000000
C	-3.436372000000	2.027832000000	0.265429000000
O	-4.463356000000	-0.122357000000	0.238592000000
C	-3.823319000000	2.535914000000	-1.149492000000
N	-2.105045000000	2.648383000000	0.582675000000
H	-4.191941000000	2.365765000000	1.006917000000
H	-4.655533000000	3.262080000000	-1.066948000000
H	-4.170154000000	1.704010000000	-1.792571000000
C	-1.950474000000	3.114924000000	1.994304000000
C	-1.943903000000	3.775004000000	-0.385920000000
H	-1.048951000000	3.758424000000	2.009125000000
C	-1.785302000000	1.972117000000	2.968202000000
H	-2.828195000000	3.745168000000	2.258048000000
H	-0.875348000000	4.043038000000	-0.456414000000
H	-2.520141000000	4.649801000000	-0.009564000000
C	-2.557180000000	3.232939000000	-1.666469000000
C	-0.506089000000	1.411663000000	3.180553000000
C	-2.897452000000	1.387631000000	3.600604000000
C	-0.351382000000	0.274692000000	3.987065000000
H	0.374785000000	1.875889000000	2.710768000000
C	-2.742789000000	0.249507000000	4.411250000000
H	-3.899364000000	1.818779000000	3.448323000000
H	-3.624144000000	-0.205791000000	4.887943000000
H	0.649198000000	-0.160969000000	4.131227000000
C	-1.471482000000	-0.313817000000	4.598024000000
H	-1.352652000000	-1.218215000000	5.214070000000
H	-2.776103000000	4.036457000000	-2.396195000000
H	-1.863539000000	2.514225000000	-2.151301000000
Ni	-0.781318000000	1.218889000000	0.311424000000
C	2.308362000000	-0.226928000000	-1.870125000000
H	2.688773000000	-1.235115000000	-1.644460000000
C	1.116393000000	-0.229184000000	-2.760117000000
H	3.116239000000	0.435504000000	-2.228496000000
C	0.629305000000	0.994240000000	-3.435792000000
Br	1.646384000000	-1.544050000000	-4.780124000000
H	0.300343000000	-0.910088000000	-2.481741000000
O	1.624359000000	1.843875000000	-3.760415000000
O	-0.556664000000	1.217701000000	-3.684342000000
C	1.223310000000	3.116485000000	-4.278795000000

H	2.153685000000	3.692287000000	-4.430430000000
H	0.687137000000	3.003576000000	-5.243261000000
H	0.565981000000	3.648624000000	-3.561153000000
H	3.225668000000	-2.761032000000	-3.670451000000
O	3.993972000000	-3.283371000000	-3.321014000000
C	5.048992000000	-2.378744000000	-3.075798000000
H	5.982497000000	-2.960069000000	-2.916400000000
H	5.231892000000	-1.680046000000	-3.927321000000
H	4.896287000000	-1.756601000000	-2.160604000000

Transition state of cyclization reaction leading to (R,S)-isomer

Electronic energy: E_{el} = -5933.09410568 Hartree
Zero-point energy E_0 = 0.58415786 Hartree
Thermal contribution to Gibbs free energy:
$G - E_{el}$ = 0.62563468 Hartree

Cartesian coordinates:

Element	x	y	z
C	-0.338440000000	-2.620903000000	-1.156476000000
C	-0.197625000000	-3.993497000000	-1.513445000000
C	-1.159232000000	-4.953175000000	-1.203637000000
C	-2.324261000000	-4.558880000000	-0.519446000000
C	-2.506264000000	-3.221246000000	-0.164447000000
C	-1.539129000000	-2.224164000000	-0.466251000000
N	-1.779747000000	-0.881254000000	-0.165991000000
C	0.731710000000	-1.694376000000	-1.508533000000
H	0.699174000000	-4.301597000000	-2.067579000000
H	-1.007704000000	-6.001320000000	-1.502899000000
H	-3.103691000000	-5.295673000000	-0.269754000000
H	-3.416732000000	-2.922374000000	0.367328000000
C	4.029355000000	-3.608552000000	-1.733950000000
C	4.455017000000	-3.265103000000	-3.028194000000
C	3.663148000000	-2.414151000000	-3.818325000000
C	2.456781000000	-1.905764000000	-3.315756000000
C	2.022578000000	-2.244181000000	-2.015150000000
C	2.821858000000	-3.103719000000	-1.229763000000
H	2.496380000000	-3.355020000000	-0.210820000000
H	4.646147000000	-4.271896000000	-1.107707000000
H	5.403389000000	-3.661838000000	-3.422457000000
H	3.985632000000	-2.146924000000	-4.836665000000
H	1.838985000000	-1.239231000000	-3.937197000000
N	0.551997000000	-0.369183000000	-1.491469000000
C	1.546243000000	0.588130000000	-1.572619000000
C	1.039880000000	1.902258000000	-2.015234000000
O	1.782047000000	2.863360000000	-2.300517000000
O	-0.279938000000	1.969596000000	-2.093797000000
C	-2.658809000000	-0.482375000000	0.805598000000
C	-3.052943000000	0.994310000000	0.694074000000

O	-3.124852000000	-1.179211000000	1.724507000000
C	-4.575036000000	1.212535000000	0.792775000000
N	-2.654205000000	1.505192000000	-0.651843000000
H	-2.495189000000	1.544079000000	1.478121000000
H	-4.792209000000	2.173783000000	1.297181000000
H	-5.024258000000	0.408339000000	1.406255000000
C	-2.555900000000	3.001274000000	-0.702577000000
C	-3.790888000000	1.059858000000	-1.528148000000
H	-2.057588000000	3.235482000000	-1.663783000000
C	-1.800566000000	3.652285000000	0.430119000000
H	-3.579370000000	3.427461000000	-0.740313000000
H	-3.619088000000	-0.001569000000	-1.786621000000
H	-3.781343000000	1.643139000000	-2.467645000000
C	-5.068736000000	1.222566000000	-0.677548000000
C	-0.556400000000	3.168046000000	0.884779000000
C	-2.336063000000	4.806600000000	1.038231000000
C	0.131511000000	3.817914000000	1.920015000000
H	-0.137933000000	2.252387000000	0.442521000000
C	-1.639487000000	5.471592000000	2.060077000000
H	-3.313669000000	5.189773000000	0.703850000000
H	-2.073087000000	6.374065000000	2.518296000000
H	1.085967000000	3.400352000000	2.274514000000
C	-0.402250000000	4.978373000000	2.504960000000
H	0.140688000000	5.491062000000	3.314184000000
H	-5.594005000000	2.168228000000	-0.914574000000
H	-5.774962000000	0.397348000000	-0.890223000000
Ni	-1.045164000000	0.515941000000	-1.145935000000
C	2.974101000000	0.473744000000	-1.124119000000
H	3.631962000000	1.149453000000	-1.700435000000
C	2.663172000000	1.013516000000	0.235018000000
H	3.390706000000	-0.545048000000	-1.085131000000
Br	4.673583000000	1.228456000000	1.469418000000
H	2.432148000000	2.085872000000	0.295531000000
C	1.875028000000	0.120184000000	1.125449000000
O	1.182693000000	0.819572000000	2.053683000000
O	1.838126000000	-1.103084000000	1.035442000000
C	0.416350000000	0.046306000000	2.987623000000
H	-0.200124000000	0.769995000000	3.551336000000
H	-0.233402000000	-0.684862000000	2.466661000000
H	1.105692000000	-0.488599000000	3.672681000000
H	3.827618000000	0.011141000000	3.215702000000
O	3.539229000000	-0.679377000000	3.865748000000
C	4.028296000000	-1.914040000000	3.371428000000
H	3.706706000000	-2.717593000000	4.067219000000
H	3.632926000000	-2.158598000000	2.358855000000
H	5.143470000000	-1.945192000000	3.317795000000