Electronic Supplementary Information

Chiral *cis*-iron(II) complexes with metal- and ligand-centered chirality for highly regio- and enantioselective alkylation of N-heteroaromatics

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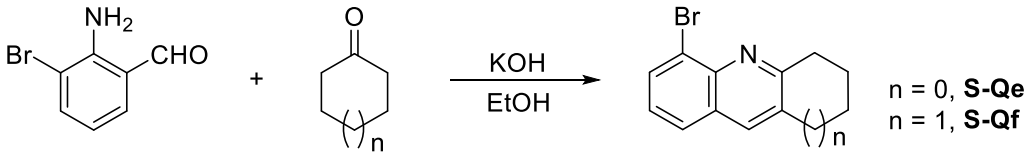
Table of Contents

Experimental section

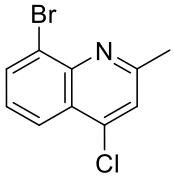
General information

Reagents were obtained commercially and used without further purification unless indicated otherwise. Molecular sieves were dried at 450 ℃ for 5 h prior to use. All solvents used in the reaction were dried and freshly distilled. Flash chromatography was performed using Merck silica gel 60 and a gradient solvent system (EtOAc/*n*-hexane as eluent). Preparative thin layer chromatography was performed on pre-coated silica gel 60 F254 plates. ^{1}H and ^{13}C NMR spectra were recorded on either a Bruker DPX-400 spectrometer. Chemical shifts (δ ppm) were determined with tetramethylsilane (TMS) as internal reference. Mass spectra were determined on a Finnigan MAT 95 mass spectrometer. High performance liquid chromatography was carried out using Agilent 1100 equipped with a variable wavelength detector on chiral stationary columns from DAICEL. Infrared spectra were prepared as KBr pellets and recorded on a Bio-Rad FTS-185 FT-IR spectrometer. $Fe(OTf)_2{\cdot}(CH_3CN)_2$ [1] was prepared by the reported method. Reactions were carried out under nitrogen atmosphere.

Synthesis of iron complexes

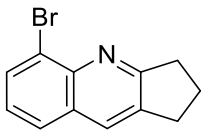


General procedure A:[2,3] A mixture of 2-amino-3-bromobenzaldehyde (5 g, 25 mmol), ketone (1.2 equiv) and KOH (1.3 equiv) in ethanol (150 mL) was refluxed under argon for 20 h. Then the mixture was cooled down to room temperature, quenched with H_2O (80 mL), and extracted with EA (4 × 50 mL); the organic phase was washed with brine (3 × 50 mL), dried with $MgSO_4$, filtered and concentrated under reduced pressure. The crude residue was purified by silica gel flash chromatography (EA/hexane = 1:20 v/v) to afford the product **S-Q**.



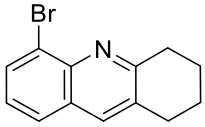
8-Bromo-4-chloro-2-methylquinoline (S-Qd)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.38 Hz, 1H), 8.06 (d, *J* = 7.50 Hz, 1H), 7.44 (s, 1H), 7.40 (t, *J* = 7.89 Hz, 1H), 2.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.17, 145.82, 142.83, 134.13, 126.98, 126.13, 124.71, 124.04, 122.80, 25.65; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{10}H_7BrClN$ 254.9450, found 254.9450.



5-Bromo-2,3-dihydro-1H-cyclopenta[b]quinoline (S-Qe)

Light yellow solid, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.44 Hz, 1H), 7.86 (s,1H), 7.69 (d, *J* = 8.07 Hz, 1H), 7.30 (t, *J* = 7.83 Hz, 1H), 3.25 (t, *J* = 7.64 Hz, 2H), 3.11 (t, *J* = 7.17 Hz, 2H), 2.25-2.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.73, 144.82, 136.88, 132.19, 130.79, 128.98, 127.59, 126.03, 124.18, 35.10, 30.57, 23.84; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{12}H_{10}BrN$ 246.9997, found 246.9989.

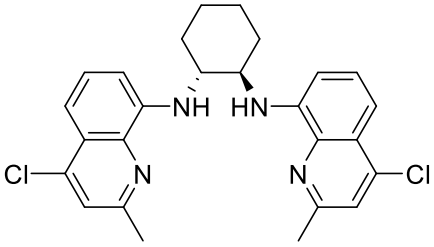


4-Bromo-5,6,7,8-tetrahydroacridine (S-Qf)

Light yellow solid, 89% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (dd, *J* = 1.07, 7.42 Hz, 1H), 7.78 (s, 1H), 7.65 (dd, *J* = 0.94, 8.11 Hz, 1H), 7.28-7.24

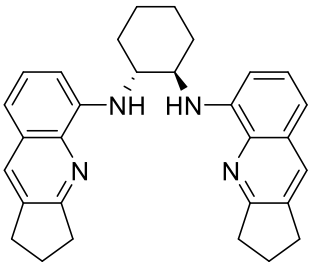
(m, 1H), 3.21 (t, *J* = 6.47 Hz, 2H), 2.99 (t, *J* = 6.09 Hz, 2H), 2.02-1.96 (m, 2H), 1.93-1.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.05, 143.75, 138.23, 135.41, 132.15, 128.56, 127.04, 125.98, 124.03, 33.98, 29.18, 23.23, 22.92; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{13}H_{12}BrN$ 261.0153, found 261.0151.

General procedure B:[4] A mixture of (*R*,*R*)-1,2-diaminocyclohexane (17.5 mmol, 2 g), $Pd_2(dba)_3$ (5 mol%), *rac*-BINAP (10 mol%), 8-bromo-quinoline(**S-Q**, 2.1 equiv) and sodium *t*-butoxide (3 equiv) in dry toluene (200 mL) was stirred at 90 ^{o}C under argon atmosphere for 24-30 h. After cooled to room temperature, the reaction mixture was filtered through a plug of silica and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel (EA/hexane = 1:10 v/v) to afford the corresponding product in high yield.



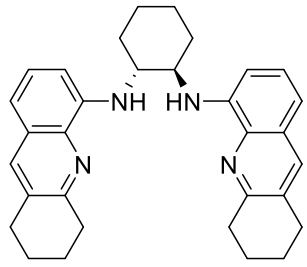
(1*R*,2*R*)-*N*1,*N*2-Bis(4-chloro-2-methylquinolin-8-yl)cyclohexane-1,2-diamine (2d-H_2)

Yellow solid, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (t, *J* = 7.94 Hz, 2H), 7.27 (d, *J* = 8.44 Hz, 2H), 7.19 (s, 2H), 6.87 (d, *J* = 7.64 Hz, 2H), 6.38 (br, 2H), 3.67 (br, 2H), 2.43 (s, 6H), 2.41-2.37 (m, 2H), 1.90 (br, 2H), 1.59-1.55 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.89, 144.57, 142.15, 138.46, 127.64, 125.04, 122.00, 109.76, 106.18, 57.64, 32.30, 24.87, 24.69; HRMS (ESI) *m/z* $[M+H]^+$ Calcd for $C_{26}H_{27}Cl_2N_4$ 465.1535, found 465.1531.



(1*R*,2*R*)-*N*1,*N*2-Bis(2,3-dihydro-1H-cyclopenta[b]quinolin-5-yl)cyclo hexane- 1,2-diamine (2e-H_2)

Yellow solid, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (s, 2H), 7.28 (t, *J* = 7.88 Hz, 2H), 6.91 (dd, *J* = 0.78, 8.10 Hz, 2H), 6.77 (d, *J* = 7.60 Hz, 2H), 6.32 (d, *J* = 5.89 Hz, 2H), 3.71 (b, 2H), 2.97-2.93 (m, 6H), 2.91-2.85 (m, 2H), 2.39 (b, 2H), 2.09-2.04 (m, 4H), 1.84 (b, 2H), 1.55-1.53 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.34, 144.42, 137.64, 135.60, 130.19, 127.66, 126.50, 113.82, 104.81, 56.49, 34.37, 31.68, 30.56, 24.41, 23.85; HRMS (ESI) *m/z* $[M+H]^+$ Calcd for $C_{30}H_{33}N_4$ 449.2705, found 449.2703.

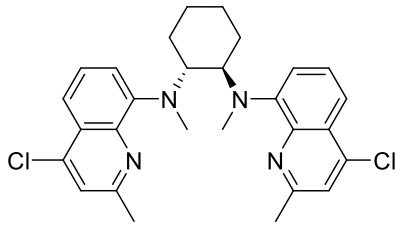


(1*R*,2*R*)-*N*1,*N*2-Bis(5,6,7,8-tetrahydroacridin-4-yl)cyclohex-ane-1,2-diamine (2f-H_2)

Yellow solid, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (s, 2H), 7.29 (t, *J* = 7.96 Hz, 2H), 6.90 (d, *J* = 8.15 Hz, 2H), 6.76 (d, *J* = 7.61 Hz, 2H), 6.37 (d, *J* = 5.31 Hz, 2H), 3.70 (b, 2H), 2.91-2.84 (m, 6H), 2.74-2.68 (m, 2H), 2.40 (b, 2H), 1.89-1.78 (m, 10H), 1.58 (b, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.63, 144.25, 136.92, 134.69, 130.80, 127.47, 126.66, 113.12, 104.28, 56.90, 33.28, 31.94, 29.23, 24.45, 23.44, 23.20; HRMS (ESI) *m/z* $[M+H]^+$ Calcd for $C_{32}H_{37}N_4$ 477.3018, found 477.3018.

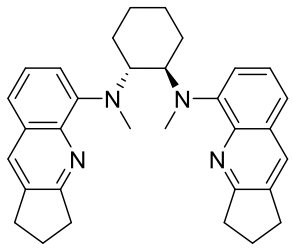
General procedure C:[4] CF_3COOH (1 mL) was slowly added to a solution of the stating material (**L2'**, 4 g) and $(HCHO)_n$ (37 wt.% in H_2O, 20 mL) in CH_3CN (100 mL) at room temperature. After the mixture was stirred for 4 h, $NaB(CN)H_3$ (6 equiv) was added slowly at ice bath temperature. The reaction mixture was stirred overnight at rt Then the reaction was quenched with 0.5 N NaOH aq to pH ≈ 10, and extracted with Et_2O (2 × 150 mL). The organic phase was

washed with 0.5 N NaOH aq (4 × 50 mL) and brine, dried with $MgSO_4$, filtered and concentrated under reduced pressure. The crude residue was purified by silica gel flash chromatography (EA/hexane = 1:10 to 1:5 v/v) to afford the product as a yellow solid.



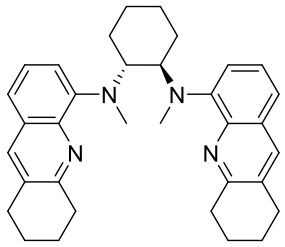
(1*R*,2*R*)-*N*1,*N*2-Bis(4-chloro-2-methylquinolin-8-yl)-*N*1,*N*2-dimethylcyclohexane-1,2-diamine (2d)

Yellow solid, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, *J* = 8.16 Hz, 2H), 7.41 (t, *J* = 7.95 Hz, 2H), 7.35 (s, 2H), 6.71 (d, *J* = 2H), 4.72-4.68 (m, 2H), 2.71 (s, 6H), 2.53-2.51 (m, 2H), 2.48 (s, 6H), 1.90-1.88 (m, 2H), 1.71-1.69 (m, 2H), 1.45-1.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.24, 149.19, 142.53, 142.33, 126.93, 126.21, 121.46, 116.32, 113.65, 63.83, 33.98, 30.78, 26.06, 25.33; HRMS (ESI) *m/z* $[M+H]^+$ Calcd for $C_{28}H_{31}Cl_2N_4$ 493.1926, found 493.1923.



(1*R*,2*R*)-*N*1,*N*2-Bis(2,3-dihydro-1H-cyclopenta[b]quinolin-5-yl)-*N*1,*N*2-dimethylcyclohexane-1,2-diamine (2e)

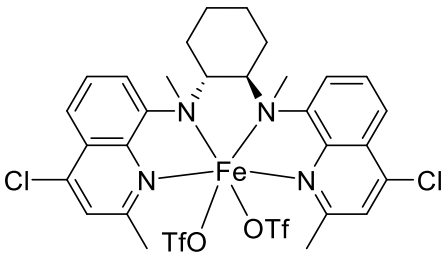
Yellow solid, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (s, 2H), 7.30 (t, *J* = 7.81 Hz, 2H), 7.17 (d, *J* = 7.87 Hz, 2H), 6.74 (d, *J* = 7.14 Hz, 2H), 4.75-4.70 (m, 2H), 3.14 (t, *J* = 7.60 Hz, 4H), 3.08 (t, *J* = 7.37 Hz, 4H), 2.59 (s, 6H), 2.41-2.37 (m, 2H), 2.27-2.16 (m, 4H), 1.83-1.81 (m, 2H), 1.67-1.64 (m, 2H), 1.38-1.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.94, 149.45, 141.61, 134.57, 130.67, 128.78, 125.63, 118.07, 115.34, 63.63, 34.75, 33.90, 30.62, 30.41, 26.18, 23.81; HRMS (ESI) *m/z* $[M+H]^+$ Calcd for $C_{32}H_{37}N_4$ 477.3018, found 477.3018.



(1*R*,2*R*)-*N*1,*N*2-Dimethyl-*N*1,*N*2-bis(5,6,7,8-tetrahydroacri-din-4-yl)cyclohexane-1,2-diamine (2f)

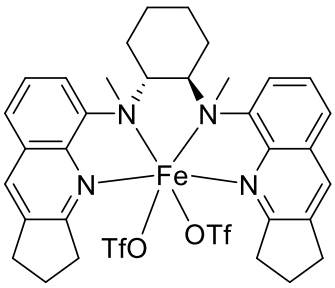
Yellow solid, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (s, 2H), 7.26 (t, *J* = 8.55 Hz, 2H), 7.11 (d, *J* = 7.92 Hz, 2H), 6.60 (d, *J* = 7.64 Hz, 2H), 4.84-4.82 (m, 2H), 3.13-3.09 (m, 4H), 2.95 (t, *J* = 6.36 Hz, 4H), 2.52 (s, 6H), 2.45-2.42 (m, 2H), 2.02-1.98 (m, 4H), 1.95-1.86 (m, 4H), 1.84-1.82 (m, 2H), 1.65-1.60 (m, 2H), 1.41-1.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.02, 148.81, 140.60, 135.18, 130.00, 128.74, 125.83, 117.02, 114.41, 63.45, 33.87, 33.75, 30.73, 29.20, 26.14, 23.67, 23.37; HRMS (ESI) *m/z* $[M+H]^+$ Calcd for $C_{34}H_{41}N_4$ 505.3331, found 505.3328.

General Procedure D:[4] A mixture of ligand (**L2**, 1 g) and $Fe(OTf)_2{\cdot}(CH_3CN)_2$ (0.95 equiv) in dry THF (8 mL) was stirred under argon atmosphere at room temperature for 6 h. The reaction mixture was cooled down with liquid nitrogen for 30 min; then the liquid nitrogen bath was removed and THF was pumped off under reduced pressure carefully. The crude residue was ground into powder and washed with dry Et_2O (3 × 10 mL). The pure product was collected and dried under reduced pressure.



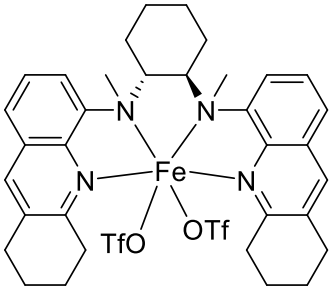
(1*R*,2*R*)-*N*1,*N*2-Bis(4-chloro-2-methylquinolin-8-yl)-*N*1,*N*2-dimethylcyclohexane-1,2-diamine iron(II) bis(tri flate) (1d)

Voluminous orange powder, 95% yield. MS (ESI) *m/z* [M-2OTf]$^{2+}$ 274.1; Elemental analysis for [$C_{30}H_{30}Cl_2F_6FeN_4O_6S_2$•$H_2O$] Calcd for C 41.63, H 3.73, N 6.47, found C 41.69, H 3.78, N 6.43.



(1*R*,2*R*)-*N*1,*N*2-Bis(2,3-dihydro-1H-cyclopenta[b]quinolin-5-yl)-*N*1,*N*2-dimethylcyclohexane-1,2-diamine iron(II) bis(tri flate) (1e)

Voluminous orange powder, 95% yield. IR (KBr): υ_{max} 3412, 2947, 2868, 1496, 1473, 1409, 1249, 1163, 1029, 769, 638, 574, 516 cm^{-1}; MS (ESI) *m/z* [M-2OTf]$^{2+}$ 261.1; Elemental analysis for [$C_{34}H_{36}F_6FeN_4O_6S_2$•$H_2O$] Calcd for C 48.12, H 4.51, N 6.60, found C 48.05, H 4.61, N 6.34.



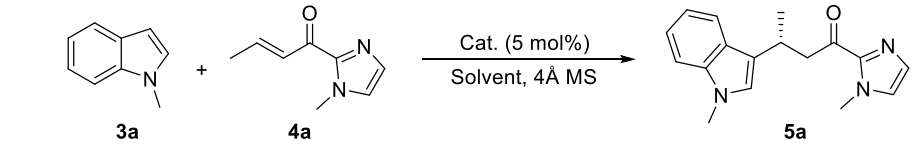
(1*R*,2*R*)-*N*1,*N*2-Dimethyl-*N*1,*N*2-bis(5,6,7,8-tetrahydroacridin-4-yl)cyclohexane-1,2-diamine (1f)

Voluminous orange powder, 92% yield. IR (KBr): υ_{max} 3431, 2943, 2868, 1490, 1465, 1419, 1251, 1161, 1029, 767, 636, 574, 516 cm^{-1}; MS (ESI) *m/z* [M-2OTf]$^{2+}$ 280.2; Elemental analysis for $C_{36}H_{40}F_6FeN_4O_6S_2$•$H_2O$ Calcd for C 49.32, H 4.83, N 6.39, found C 48.97, H 4.93, N 6.03.

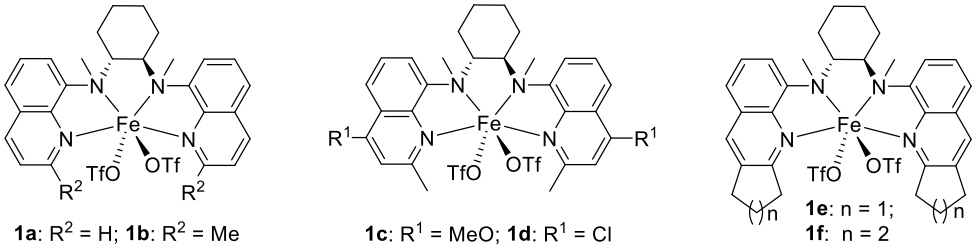
General procedure for iron(II) complexes catalyzed alkylation of N-heteroaromatics with α,β-unsaturated 2-acyl imidazoles

To an oven-dried Schlenk flask equipped with a rubber seal was added N-heteroaromatics (0.45 mmol), α,β-unsaturated 2-acyl imidazoles **4** (0.3 mmol), Fe(II) complexes (5 mol%) and 4 Å MS (100 mg). The flask was evacuated and backfilled with argon three times. Then freshly distilled solvent (3 mL) was added via syringe at reaction temperature. The reaction mixture was stirred at the same temperature until compound **4** was completely consumed (monitored by TLC). The residue was purified by flash chromatography on a silica gel column (eluent: hexane/EA = 8:1–5:1 v/v) to give the corresponding products **5**, **6**, **7**, **9** and **11**.

Table S1 Screening of the iron complexes in the asymmetric alkylation of *N*-methylindole **3a** to α,β-unsaturated 2-acyl imidazole **4a**.[a]



3a **4a** **5a**



1a: R^2 = H; **1b**: R^2 = Me

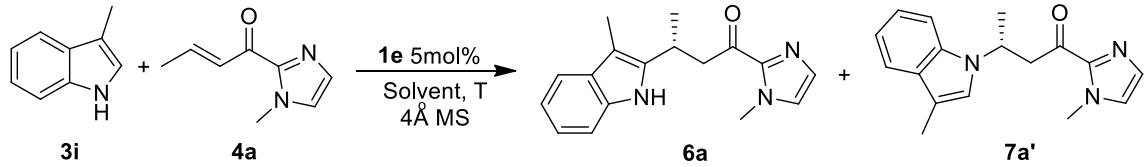
1c: R^1 = MeO; **1d**: R^1 = Cl

1e: n = 1; **1f**: n = 2

Entry	Cat.	Solvent/T (℃)	Time (h)	Yield (%)[b]	ee (%)[c]
1	**1a**	CH_2Cl_2/5	10	91	73
2	**1b**	CH_2Cl_2/5	10	98	79
3	**1c**	CH_2Cl_2/5	15	90	69
4	**1d**	CH_2Cl_2/5	12	87	57
5	**1e**	CH_2Cl_2/5	10	99	85
6	**1f**	CH_2Cl_2/5	10	94	71
7	**1e**	CH_2Cl_2/-15	24	95	90
8	**1e**	$ClCH_2CH_2Cl$/-15	24	97	93
9	**1e**	CH_3Cl/-15	24	96	91
10	**1e**	CH_3CN/-15	20	92	95
11	**1e**	**CH_3CN/-25**	**48**	**91**	**97.5**

[a] Unless otherwise noted, all reactions were carried out with **3a** (0.45 mmol), **4a** (0.3 mmol), Cat. (5 mol%) and 4 Å MS (100 mg) in 3 mL of solvent under argon. [b] Yield of isolated product. [c] Determined by chiral-phase HPLC.

Table S2 Condition optimization of C2 alkylation of 3-methyl-indole **3i** with α,β-unsaturated 2-acyl imidazole **4a** catalyzed by Fe(II) complexes[a]

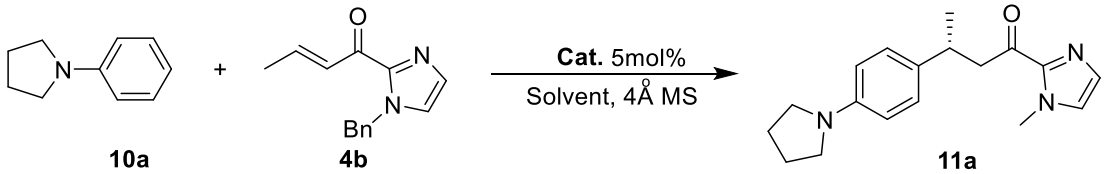


3i 4a 6a 7a'

Entry	Solvent/T (℃)	Time (h)	**6a/7a′** [b]	Yield (%)/**6a** [c]	ee (%)/**6a** [d]
1[e]	CH_2Cl_2/25	3	83:17	80	83
2	CH_2Cl_2/25	3	85:15	83	87
3	$ClCH_2CH_2Cl$/25	3	86:14	85	86
4	CH_3CN/25	12	-	NR[f]	-
5	CH_2Cl_2/0	12	87:13	85	90.5
6	CH_2Cl_2/-20	36	>90:10	84	93
7	**CH_2Cl_2/-40**	**60**	**>90:10**	**85**	**96**

[a] All reactions were carried out with **3i** (0.45 mmol), **4a** (0.3 mmol), Cat. (5 mol%) and 4 Å MS (100 mg) in 3 mL of solvent under argon. [b] Determined by crude ^{1}H NMR. [c] Yield of isolated product. [d] Determined by chiral-phase HPLC. [e] **1b** was used. [f] NR = no reaction.

Table S3 Condition optimization of asymmetric alkylation of 1-phenyl pyrrolidine **10a** with α,β-unsaturated 2-acyl imidazole **4b** catalyzed by Fe(II) complexes[a]



10a 4b 11a

Entry	Cat.	Solvent/T (℃)	Time (h)	Yield (%)[b]	ee (%)[c]
1[d]	**1b**	CH_2Cl_2/25	24	44	59
2	**1b**	CH_2Cl_2/25	20	89	69
3	**1e**	CH_2Cl_2/25	20	85	74
4	**1e**	CH_3Cl/25	20	90	75
5	**1e**	CH_3CN/25	20	88	81
6	**1e**	CH_3CN/0	40	87	88
7	**1e**	**CH_3CN/-25**	**70**	**87**	**94**

[a] All reactions were carried out with **10a** (0.45 mmol), **4b** (0.3 mmol), Cat. (5 mol%) and 4 Å MS (100 mg) in 3 mL of solvent under argon. [b] Yield of isolated product. [c] Determined by chiral-phase HPLC. [d] **4a** instead of **4b**.

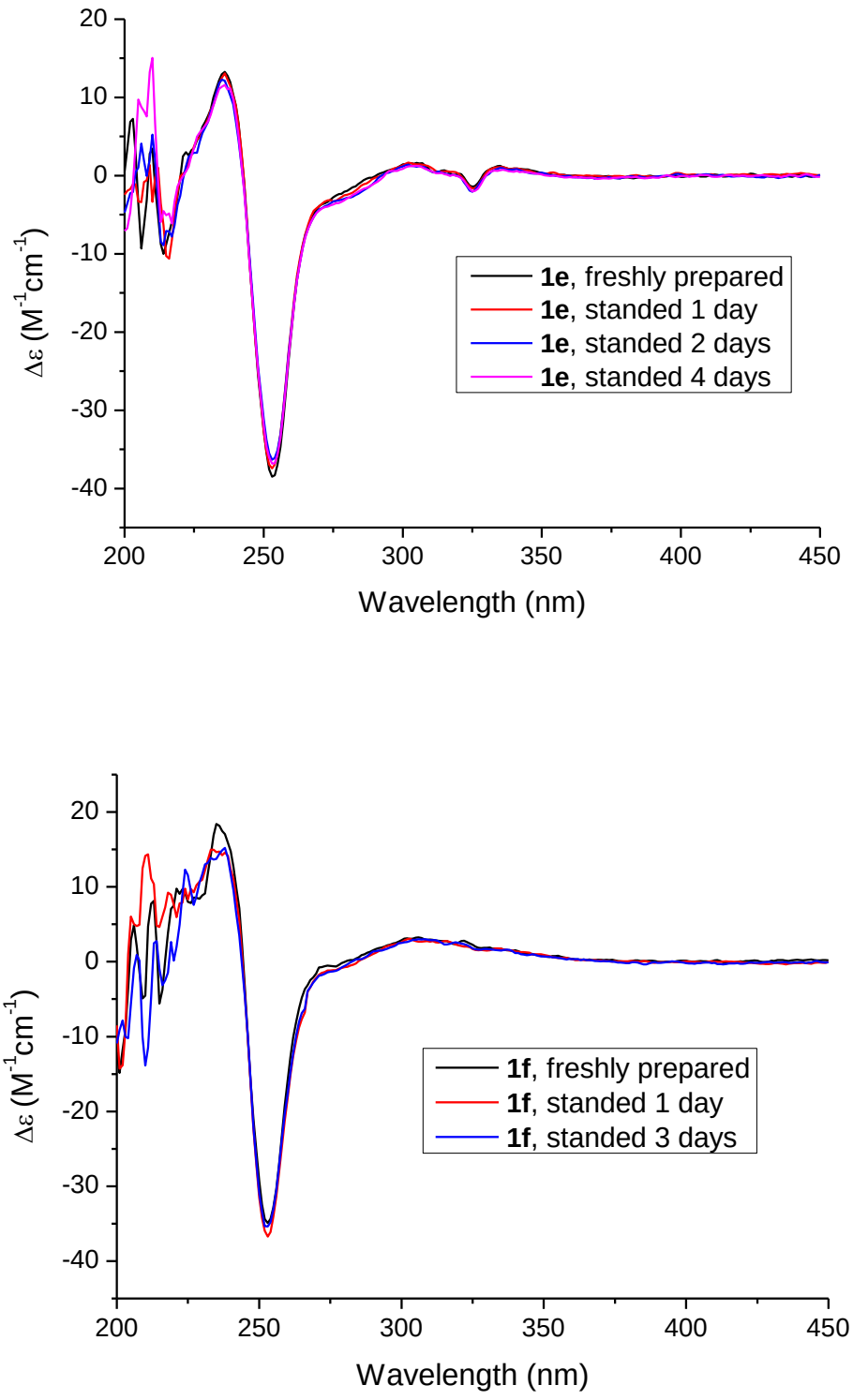


Fig. S1 CD spectra of **1e** (upper) and **1f** (lower) recorded in CH_3CN (0.3 mM) at various time intervals.

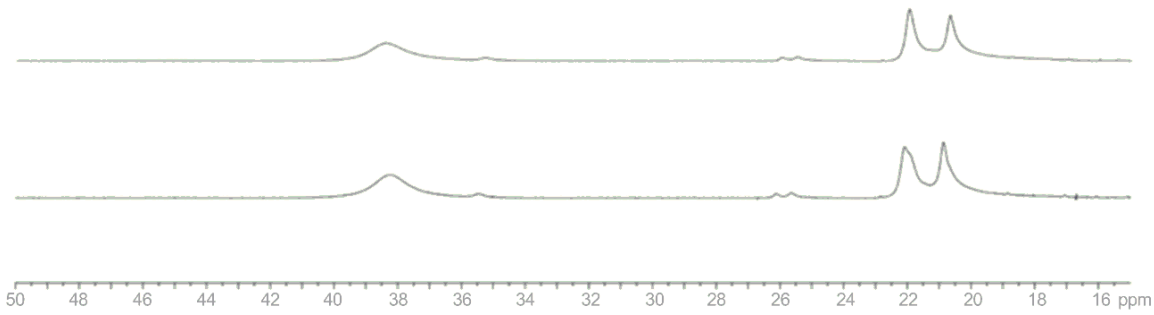


Fig. S2 ^{1}H NMR spectra (in the low-field region of 15–50 ppm) of **1e** in CD_3CN at room temperature measured for freshly prepared solution (bottom) and after the solution was kept standing at room temperature for 8 days (top).

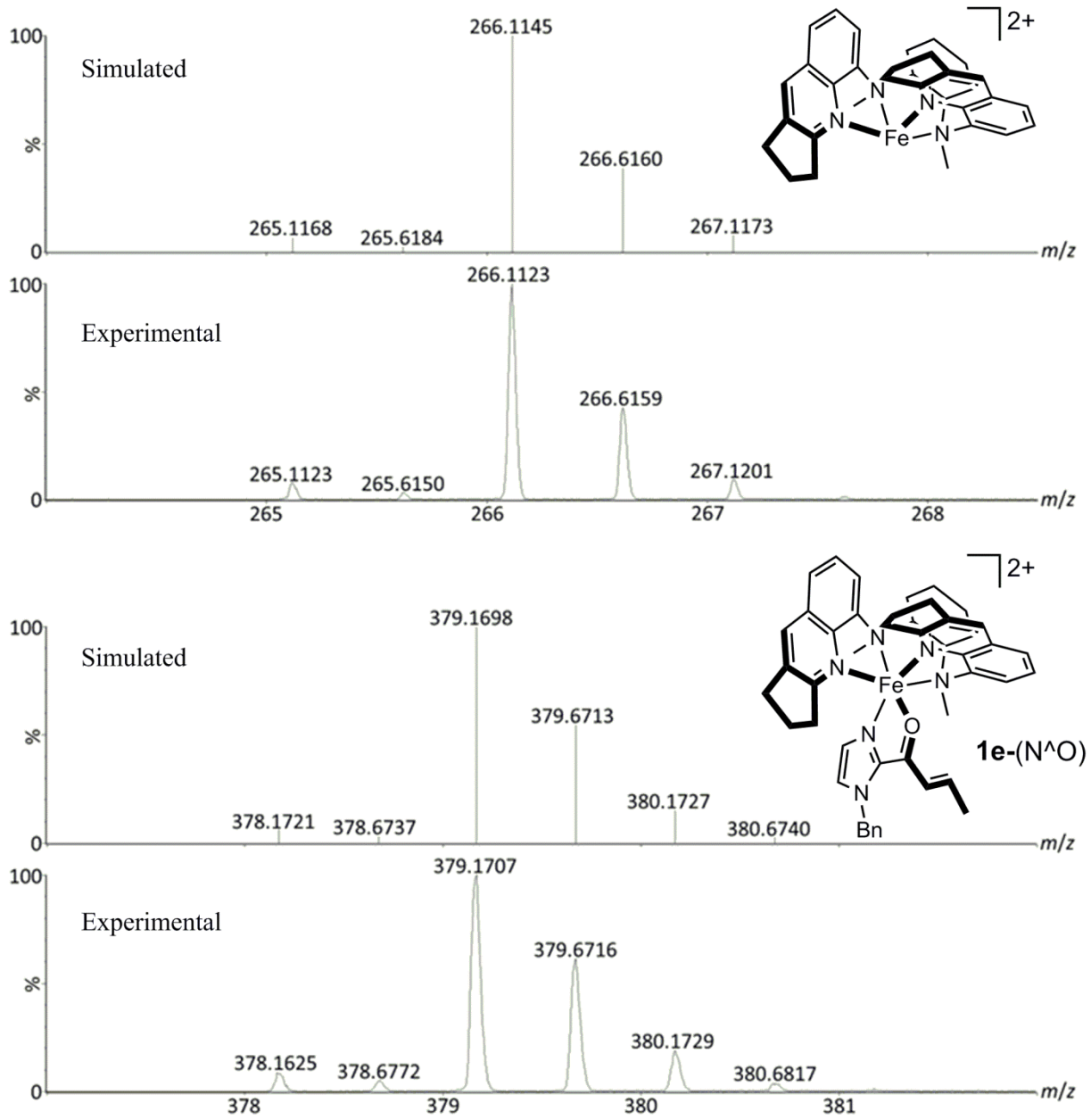


Fig. S3 ESI-MS spectral analysis of the reaction intermediate. Upper: a solution of Fe(II) complex **1e** (1×10^{-5} M) in acetonitrile. Lower: a reaction mixture of Fe complex (1×10^{-5} M) and organic substrate **4b** (2.0 equiv) in acetonitrile.

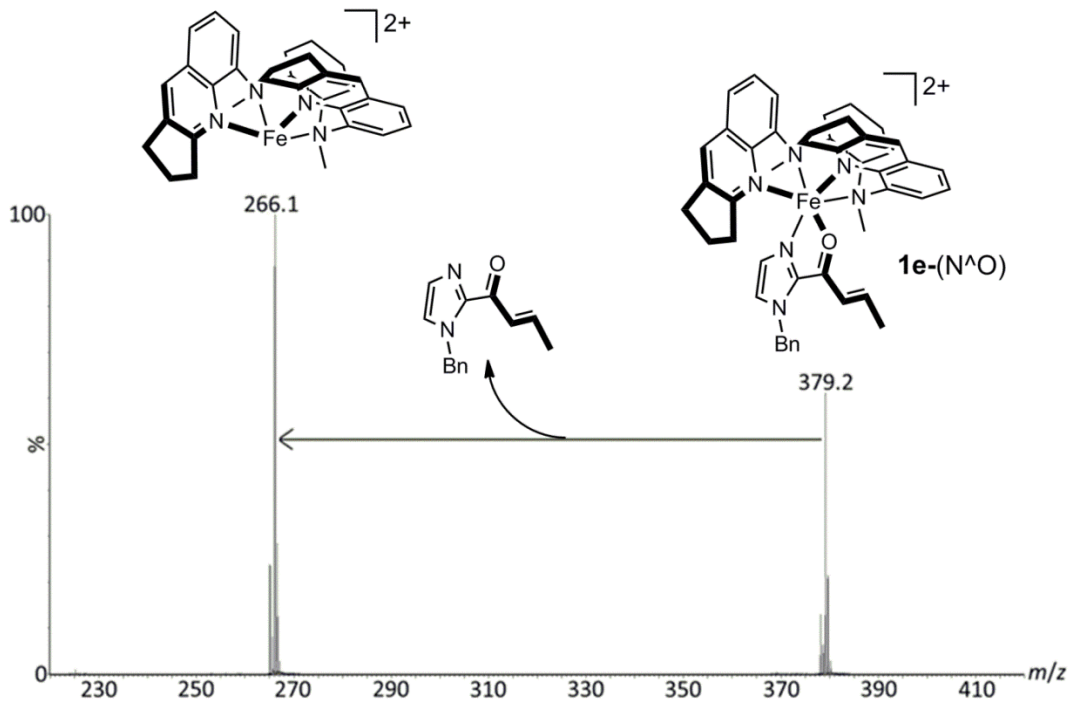


Fig. S4 Collision-induced dissociation of **1e**-(N^O) (*m/z* 379.2) gave $[Fe^{II}(\mathbf{2e})]^{2+}$ (*m/z* 226.1), through the loss of **4b** (collision energy: 8 eV).

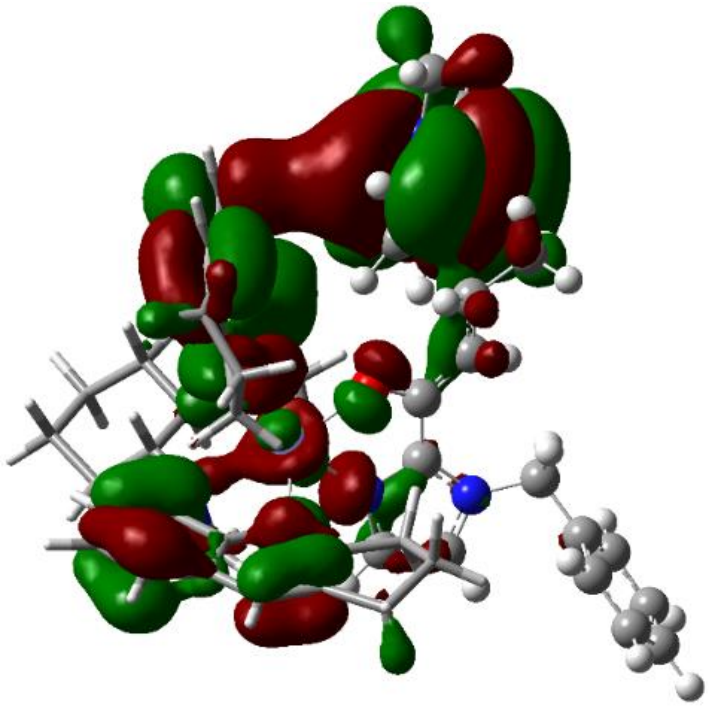


Fig. S5 Molecular orbital of π-π interaction between quinoline and indole moieties in $\mathbf{TSA_{2R}}$.

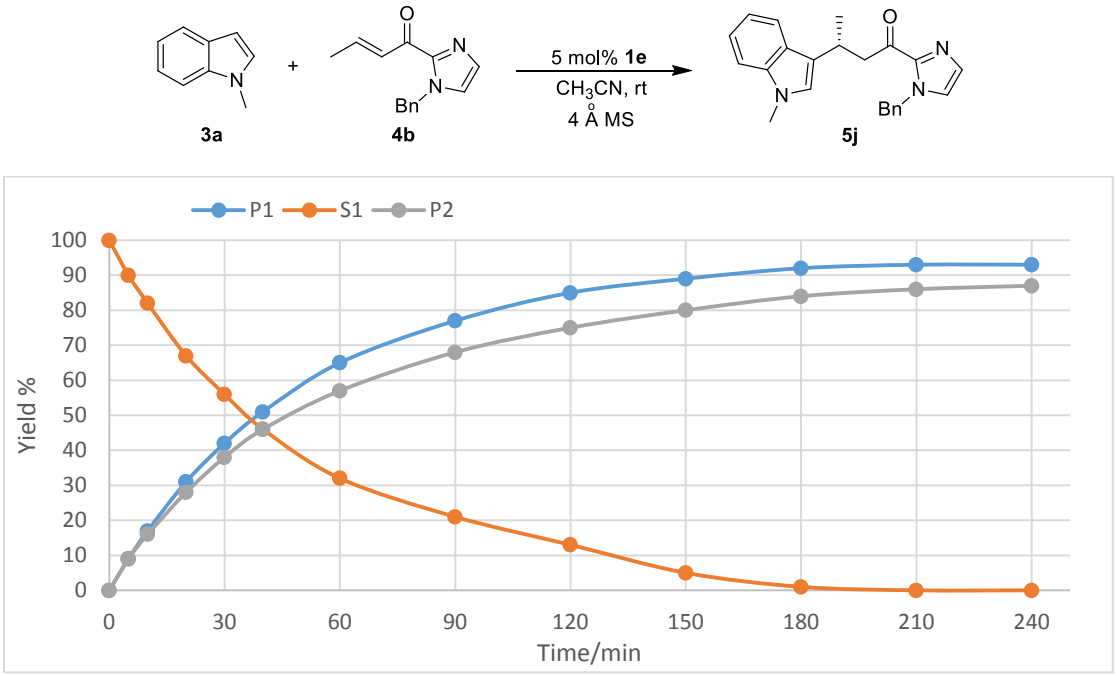
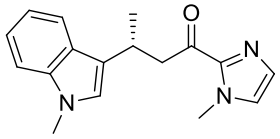
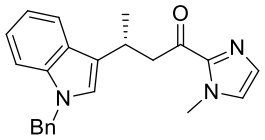
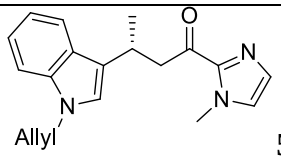
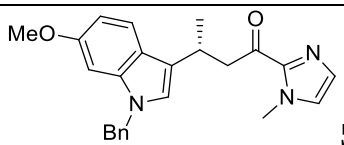
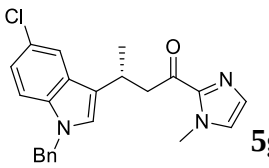
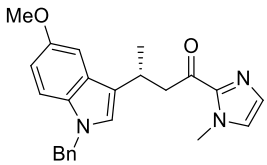
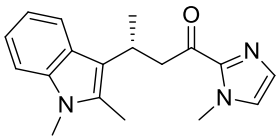
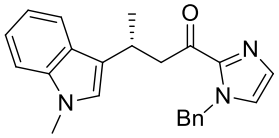
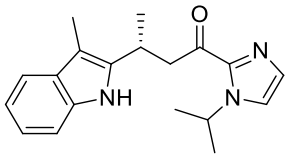
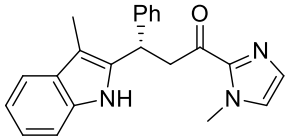


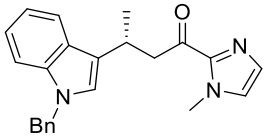
Fig. S6 Time-course plots for alkylation of *N*-methylindole **3a** with **4b** in CH_3CN catalyzed by **1e** at room temperature under conditions A (blue line) and B (grey line). Reaction condition for A: **3a** (0.45 mmol), **4b** (0.3 mmol), **1e** (5 mol%) under argon; reaction condition for B: **3a** (0.45 mmol), **4b** (0.3 mmol), **5j** (0.06 mmol, 20 mol%), **1e** (5 mol%) under argon. P1 and P2: product **5j** generated under conditions A and B, respectively. S1: starting material **4b** (orange line).

Characterization data of products

Table S4 Reported products in literature

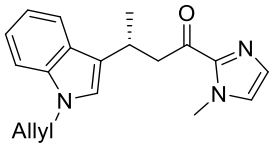
Products	References
 **5a**	(*a*) D. A. Evans, K. R. Fandrick and H.-J. Song, *J. Am. Chem. Soc*., 2005, **127**, 8942; (*b*) D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., 2007, **129**, 10029.
 **5b**	(*a*) D. A. Evans, K. R. Fandrick and H.-J. Song, *J. Am. Chem. Soc*., 2005, **127**, 8942; (*b*) D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., 2007, **129**, 10029.
 **5c**	(*a*) D. A. Evans, K. R. Fandrick and H.-J. Song, *J. Am. Chem. Soc*., 2005, **127**, 8942; (*b*) D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., 2007, **129**, 10029.
 **5e**	(*a*) D. A. Evans, K. R. Fandrick and H.-J. Song, *J. Am. Chem. Soc*., 2005, **127**, 8942; (*b*) D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., 2007, **129**, 10029.
 **5g**	(*a*) D. A. Evans, K. R. Fandrick and H.-J. Song, *J. Am. Chem. Soc*., 2005, **127**, 8942; (*b*) D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., 2007, **129**, 10029.
 **5h**	(*a*) D. A. Evans, K. R. Fandrick and H.-J. Song, *J. Am. Chem. Soc*., 2005, **127**, 8942; (*b*) D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., 2007, **129**, 10029.
 **5i**	D. A. Evans, K. R. Fandrick and H.-J. Song, *J. Am. Chem. Soc*., 2005, **127**, 8942.
 **5j**	D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., 2007, **129**, 10029.

 **6c**	Z. Zhou, Y. Li, L. Gong and E. Meggers, *Org. Lett.*, 2017, **19**, 222.
 **6d**	Z. Zhou, Y. Li, L. Gong and E. Meggers, *Org. Lett.*, 2017, **19**, 222.



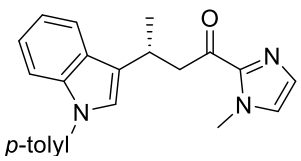
(*R*)-3-(1-Benzyl-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (5b)

^{1}H NMR (400 MHz, $CDCl_3$): 7.68(d, *J*=7.56 Hz, 1H), 7.27-7.21(m, 4H), 7.14-7.06(m, 5H), 7.01(s, 1H), 6.97(s, 1H), 5.24(s, 2H), 3.91(s, 3H), 3.91-3.82(m, 1H), 3.56(dd, *J*=6.28, 15.76 Hz, 1H), 3.46(dd, *J*=8.32, 15.72 Hz, 1H), 1.43(d, *J*=6.96 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.46, 143.08, 137.86, 136.77, 128.99, 128.75, 127.52, 127.35, 126.89, 126.81, 124.60, 121.71, 120.76, 119.57, 118.90, 109.68, 49.98, 46.87, 36.20, 27.33, 21.83; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{23}N_3O$ 357.1841, found 357.1830.



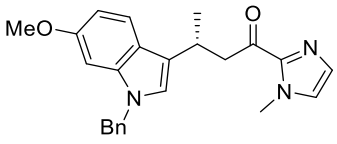
(*R*)-3-(1-Allyl-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (5c)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67(d, *J*=7.88 Hz, 1H), 7.26(d, *J*=8.20 Hz, 1H), 7.17-7.08(m, 3H), 6.97(s, 2H), 5.96-5.92(m, 1H), 5.16(dd, *J*=1.4, 10.24 Hz, 1H), 5.05(dd, *J*=1.44, 17.08 Hz, 1H), 4.66-4.64(m, 2H), 3.91(s, 3H), 3.90-3.83(m, 1H), 3.57-3.43(m, 2H), 1.42(d, *J*=6.88 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.52, 143.53, 136.60, 133.80, 129.05, 127.33, 126.97, 124.19, 121.59, 120.55, 119.60, 118.86, 117.23, 109.61, 48.81, 46.96, 36.28, 27.32, 21.93; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{19}H_{21}N_3O$ 307.1685, found 307.1678.



(*R*)-1-(1-Methyl-1H-imidazol-2-yl)-3-(1-(p-tolyl)-1H-indol-3-yl) butan-1-one (5d)

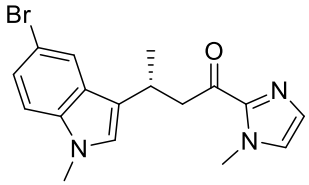
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73(d, *J*=7.28 Hz, 1H), 7.50(d, *J*=7.92 Hz, 1H), 7.34(d, *J*=8.28 Hz, 2H), 7.28(d, *J*=8.12 Hz, 2H), 7.21-7.13(m, 4H), 6.99(s, 1H), 3.94(s, 3H), 3.92-3.86(m, 1H), 3.65(dd, *J*=6.20, 15.84 Hz, 1H), 3.48(dd, *J*=8.16, 15.88 Hz, 1H), 2.42(s, 3H), 1.46(d, *J*=6.92 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.33, 144.01, 143.00, 137.48, 136.28, 135.88, 130.11, 129.04, 128.02, 126.92, 124.34, 124.11, 122.26, 120.26, 119.66, 110.55, 46.68, 36.24, 27.17, 21.74, 21.08; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{23}N_3O$ 357.1841, found 357.1832.



(*R*)-3-(1-Benzyl-6-methoxy-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (5e)

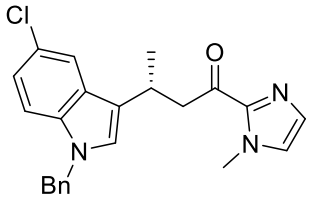
^{1}H NMR (400 MHz, $CDCl_3$):δ 7.54(d, *J*=8.68 Hz, 1H), 7.28-7.25(m, 3H), 7.12(s, 1H), 7.08-7.06(m, 2H), 6.97(s, 1H), 6.88(s, 1H), 6.79-6.6.71(m, 1H), 6.67(s, 1H), 5.18(s, 2H), 3.91(s, 3H), 3.83-3.77(m, 1H), 3.77(s, 3H), 3.53(dd, *J*=6.24, 15.68 Hz, 1H), 3.43(dd, *J*=8.32, 15.68 Hz, 1H), 1.40(d, *J*=6.88 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.54, 156.41, 143.44, 137.86, 137.58, 129.06, 128.81, 127.56, 126.94, 126.86,

123.51, 121.89, 120.89, 120.24, 108.65, 93.57, 55.84, 49.99, 46.98, 36.28, 27.44, 21.87; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O_2$ 387.1947, found 387.1945.



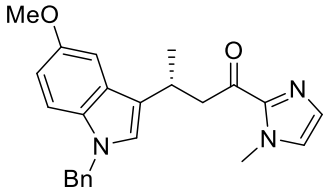
(*R*)-3-(5-Bromo-1-methyl-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (5f)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67(d, *J*=1.63 Hz, 1H), 7.23(dd, *J*=1.84, 8.64 Hz, 1H), 7.13(s, 1H), 7.09(d, *J*=8.64 Hz, 1H), 6.99(s, 1H), 6.91(s, 1H), 3.89(s, 3H), 3.78-3.73(m, 1H), 3.67(s, 3H), 3.49-3.39(m, 2H), 1.39(d, *J*=6.92 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.17, 143.37, 135.79, 129.07, 128.80, 127.07, 126.40, 124.34, 121.98, 119.82, 112.15, 110.73, 47.34, 36.22, 32.92, 27.23, 21.96; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{17}H_{18}N_3OBr$ 359.0633, found 359.0626.



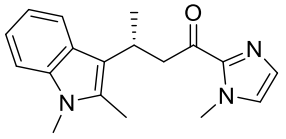
(*R*)-3-(1-Benzyl-5-chloro-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (5g)

^{1}H NMR (400 MHz, CDCl3): δ 7.57(s, 1H), 7.26-7.24(m, 3H), 7.13-6.98(m, 7H), 5.22(s, 2H), 3.90(s, 3H), 3.79-3.77(m, 1H), 3.52-3.39(m, 2H), 1.41(d, *J*=6.92 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.22, 143.41, 137.44, 135.15, 129.09, 128.89, 128.47, 127.76, 127.05, 126.75, 126.05, 124.82, 122.04, 120.53, 119.07, 110.79, 50.28, 47.13, 36.23, 27.32, 21.78; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{22}ClN_3O$ 391.1451, found 391.1449.



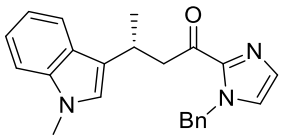
(*R*)-3-(1-Benzyl-5-methoxy-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (5h)

^{1}H NMR (400 MHz, CDCl3): δ 7.27-7.24(m, 3H), 7.18-7.04(m, 5H), 6.99(d, *J*=5.56 Hz, 2H), 6.79(d, *J*=8.84 Hz, 1H), 5.21(s, 2H), 3.92(s, 3H), 3.86(s, 3H), 3.86-3.80(m, 1H), 3.60-3.55(m, 1H), 3.42-3.36(m, 1H), 1.42(dd, *J*=2.40, 6.88 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.60, 153.80, 143.55, 138.02, 132.10, 129.05, 128.79, 127.73, 127.56, 126.95, 126.80, 125.28, 120.32, 112.01, 110.52, 101.47, 56.06, 50.27, 47.01, 36.23, 27.44, 21.66; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O_2$ 387.1947, found 387.1945.



(*R*)-3-(1,2-Dimethyl-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)butan-1-one (5i)

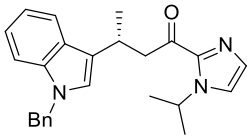
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71(d, *J*=7.88 Hz, 1H), 7.21(d, *J*=8.04 Hz, 1H), 7.11-7.09(m, 2H), 7.05-7.03(m, 1H), 6.92(s, 1H), 3.86(s, 3H), 3.86-3.80(m, 1H), 3.65-3.62(m, 2H), 3.61(s, 3H), 2.42(s, 3H), 1.48(d, *J*=7.16 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.51, 143.46, 136.89, 132.39, 128.95, 126.69, 126.40, 120.26, 119.45, 118.58, 115.00, 108.69, 46.53, 36.11, 29.53, 27.49, 21.49, 10.73; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{18}H_{21}N_3O$ 295.1685, found 295.1676.



(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(1-methyl-1H-indol-3-yl) butan-1-one (5j)

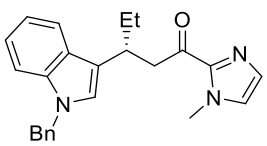
^{1}H NMR (400 MHz, $CDCl_3$): 7.69(d, *J*= 7.92 Hz, 1H), 7.28-7.26(m, 4H), 7.23-7.18(m, 2H), 7.11-7.07(m, 3H), 7.02(s, 1H), 6.90(s, 1H), 5.56(s, 2H), 3.84(q, *J*=7.0, 14.32 Hz, 1H), 3.69(s, 3H), 3.60(dd, *J*=6.52, 15.56 Hz, 1H), 3.46(dd, *J*=8.16, 15.56 Hz, 1H), 1.39(d, *J*=6.88 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.58, 143.03, 137.14,

136.54, 129.44, 128.87, 128.06, 127.64, 127.07, 125.85, 125.18, 121.51, 120.03, 119.54, 118.66, 109.20, 51.79, 47.19, 32.67, 27.45, 21.98; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{23}N_3O$ 357.1841, found 357.1831.



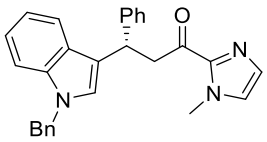
(*R*)-3-(1-Benzyl-1H-indol-3-yl)-1-(1-isopropyl-1H-imidazol-2-yl) butan-1-one (5k)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70(d, *J*=7.52 Hz, 1H), 7.27-7.20(m, 5H), 7.17-7.06(m, 5H), 7.02(s, 1H), 5.51-5.44(m, 1H), 5.25(s, 2H), 3.91-3.85(m, 1H), 3.59(dd, *J*=6.36, 15.68 Hz, 1H), 3.49(dd, *J*=8.32, 15.64 Hz, 1H), 1.44(d, *J*=6.88 Hz, 3H), 1.36(t, *J*=6.80 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.60, 142.79, 137.88, 136.75, 129.47, 128.75, 127.52, 127.39, 126.81, 124.63, 121.69, 121.01, 120.81, 119.62, 118.92, 109.68, 49.99, 49.20, 47.51, 27.44, 23.63, 21.89; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{25}H_{27}N_3O$ 385.2154, found 385.2149.



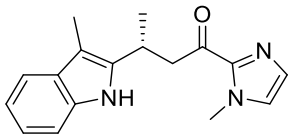
(*R*)-3-(1-Benzyl-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl) pentan-1-one (5l)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66-7.64(m, 1H), 7.26-7.18(m, 4H), 7.12-7.01(m, 6H), 6.93(s, 1H), 5.24(s, 2H), 3.82(s, 3H), 3.70-3.66(m, 1H), 3.54(dd, *J*=0.88, 7.00 Hz, 2H), 1.88-1.80(m, 2H), 0.89(t, *J*=7.32 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.60, 143.57, 138.01, 136.77, 128.96, 128.78, 127.94, 127.53, 126.85, 126.74, 125.71, 121.63, 119.77, 118.89, 118.54, 109.70, 49.99, 45.13, 36.17, 34.24, 29.11, 12.13; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O$ 371.1998, found 371.1996.



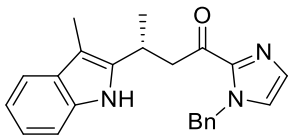
(*S*)-3-(1-Benzyl-1H-indol-3-yl)-1-(1-methyl-1H-imidazol-2-yl)-3-phenyl-propan-1-one (5m)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50(d, *J*=7.92 Hz, 1H), 7.43-7.41(m, 2H), 7.27-7.23(m, 5H), 7.21-7.00(m, 8H), 6.93(s, 1H), 5.24(d, *J*=1.68 Hz, 2H), 5.09(t, *J*=7.68 Hz, 1H), 4.01(dd, *J*=7.40, 16.26 Hz, 1H), 3.89-3.83(m, 1H), 3.85(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.24, 144.62, 143.38, 137.89, 137.00, 129.12, 128.81, 128.48, 128.11, 127.67, 127.59, 127.03, 126.81, 126.29, 125.91, 121.95, 119.89, 119.19, 118.66, 109.70, 50.09, 45.54, 38.42, 36.21; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{28}H_{25}N_3O$ 419.1998, found 419.1995.



(*R*)-1-(1-Methyl-1H-imidazol-2-yl)-3-(3-methyl-1H-indol-2-yl) butan-1-one (6a)

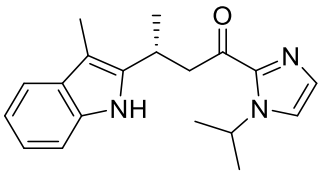
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53(s, 1H), 7.45(d, *J*=8.38 Hz, 1H), 7.25(d, *J*=8.12 Hz, 1H), 7.13-7.04(m, 3H), 6.97(s, 1H), 3.91(s, 3H), 3.86-3.80(m, 1H), 3.72(dd, *J*=8.25, 15.67 Hz, 1H), 3.30(dd, *J*=6.20, 15.67 Hz, 1H), 2.25(s, 3H), 1.39(d, *J*=7.02 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.50, 138.12, 135.41, 129.38, 129.12, 128.70, 127.34, 121.05, 118.95, 118.20, 110.60, 106.40, 44.84, 36.31, 28.04, 21.05, 8.58; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{17}H_{19}N_3O$ 281.1528, found 281.1525.



(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(3-methyl-1H-indol-2-yl) butan-1-one (6b)

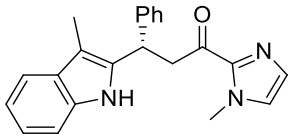
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41(s, 1H), 7.46(d, *J*=6.87 Hz, 1H), 7.26-7.22(m, 4H), 7.16(d, *J*=0.88 Hz, 1H), 7.07-6.99(m, 5H), 5.54(d, *J*=6.92 Hz, 2H), 3.91-3.79(m, 1H), 3.72(dd, *J*=8.38, 15.28 Hz, 1H), 3.30(dd, *J*=6.19, 15.27 Hz,

1H), 2.21(s, 3H), 1.36(d, *J*=6.96 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.65, 142.85, 137.96, 136.23, 135.42, 129.55, 129.37, 128.98, 128.20, 127.60, 126.31, 121.09, 118.96, 118.26, 110.59, 106.49, 51.94, 45.07, 28.29, 21.04, 8.57; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{23}N_3O$ 357.1841, found 357.1830.



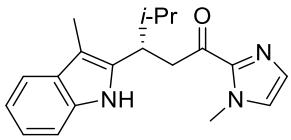
(*R*)-1-(1-Isopropyl-1H-imidazol-2-yl)-3-(3-methyl-1H-indol-2-yl)but-an-1-one (6c)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45(s, 1H), 7.44(d, *J*=7.59 Hz, 1H), 7.26-7.21(m, 2H), 7.15(s, 1H), 7.09-7.01(m, 2H), 5.46-5.39(m, 1H), 3.85-3.80(m, 1H), 3.71(dd, *J*=8.27, 15.51 Hz, 1H), 3.32(dd, *J*=6.31, 15.56 Hz, 1H), 2.23(s, 3H), 1.40-1.33(m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.66, 142.61, 138.12, 135.41, 129.56, 129.37, 127.99, 121.47, 121.04, 118.93, 118.19, 110.55, 49.36, 45.51, 28.18, 23.75, 23.50, 21.06, 8.57; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{19}H_{23}N_3O$ 309.1841, found 309.1837.



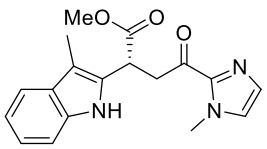
(*S*)-1-(1-Methyl-1H-imidazol-2-yl)-3-(3-methyl-1H-indol-2-yl)-3-phenyl-propan-1-one (6d)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73(s, 1H), 7.45(d, *J*=8.01Hz, 1H), 7.31-7.16(m, 7H), 7.09-7.04(m, 2H), 6.97(s, 1H), 5.07(dd, *J*=6.20, 9.25 Hz, 1H), 4.21(dd, *J*= 9.31, 16.01 Hz, 1H), 3.88(s, 3H), 3.66(dd, *J*=6.20, 15.72 Hz, 1H), 2.24(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.56, 143.23, 142.59, 135.76, 135.65, 129.41, 129.24, 128.78, 127.59, 127.50, 126.69, 121.23, 119.06, 118.38, 110.80, 107.88, 43.27, 38.62, 36.26, 8.71; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{22}H_{21}N_3O$ 343.1685, found 343.1675.



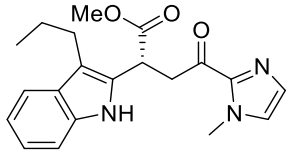
(*S*)-4-Methyl-1-(1-methyl-1H-imidazol-2-yl)-3-(3-methyl-1H-indol-2-yl)pentan-1-one (6e)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.43(s, 1H), 7.44(d, *J*=7.46 Hz, 1H), 7.26-7.21(m, 1H), 7.10-7.02(m, 3H), 6.92(s, 1H), 3.90(dd, *J*=9.96, 15.90 Hz, 1H), 3.82(s, 3H), 3.44-3.39(m, 1H), 3.24(dd, *J*=4.79, 15.90 Hz, 1H), 2.21(s, 3H), 2.07-2.04(m, 1H), 1.02(d, *J*=6.66 Hz, 3H), 0.87(d, *J*=6.71 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.90, 143.31, 136.16, 135.50, 129.21, 128.96, 127.19, 120.90, 118.76, 118.14, 110.52, 108.25, 40.74, 40.01, 36.20, 33.15, 21.02, 20.74, 8.90; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{19}H_{23}N_3O$ 309.1841, found 309.1837.



(*R*)-Methyl-4-(1-methyl-1H-imidazol-2-yl)-2-(3-methyl-1H-indol-2-yl)-4-oxo-butanoate (6f)

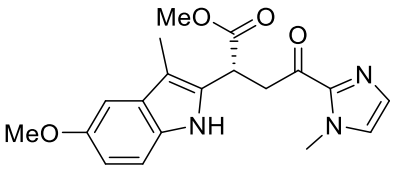
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60(s, 1H), 7.50(d, *J*=7.76 Hz, 1H), 7.27-7.25(m, 1H), 7.16-7.09(m, 2H), 7.07(t, *J*=6.76 Hz, 1H), 7.00(s, 1H), 4.55(dd, *J*=5.48, 9.01 Hz, 1H), 4.03-3.96(m, 4H), 3.77-3.71(m, 4H), 2.29(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.79, 173.42, 142.53, 135.82, 129.80, 129.51, 128.87, 127.36, 122.03, 119.25, 118.71, 110.89, 109.16, 52.69, 41.67, 38.09, 36.23, 8.60; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{18}H_{29}N_3O_3$ 325.1426, found 325.1419.



(*R*)-Methyl-4-(1-methyl-1H-imidazol-2-yl)-4-oxo-2-(3-propyl-1H-indol-2-yl)butanoate (6g)

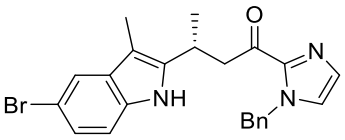
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56(s, 1H), 7.53(d, *J*=7.56 Hz, 1H), 7.26(d, *J*=8.04 Hz, 1H), 7.13-7.11(m, 2H), 7.11-7.08(m, 1H), 7.07-

7.06(m, 1H), 7.01(s, 1H), 4.54(dd, *J*=5.04, 9.41 Hz, 1H), 4.03(dd, *J*=9.42, 18.04 Hz, 1H), 3.97(s, 3H), 3.72-3.66(m, 4H), 2.75-2.70(m, 2H), 1.68-1.63(m, 2H), 0.95(t, *J*=7.37Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.86, 173.55, 142.48, 135.97, 129.79, 129.52, 128.27, 127.36, 121.95, 119.19, 119.04, 114.24, 110.95, 52.68, 42.15, 38.02, 36.25, 26.29, 24.21, 14.36; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{20}H_{23}N_3O_3$ 353.1739, found 353.1738.



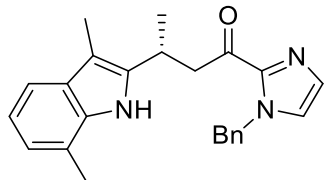
(*R*)-Methyl-2-(5-methoxy-3-methyl-1H-indol-2-yl)-4-(1-methyl-1H-imidaz ol-2-yl)-4-oxo-butanoate (6h)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51(s, 1H), 7.16-7.12(m, 2H), 7.00(s, 1H), 6.93(d, *J*=2.24 Hz, 1H), 6.79(dd, *J*=2.38, 8.72 Hz, 1H), 4.52(dd, *J*=5.44, 9.04 Hz, 1H), 4.02-3.95(m, 4H), 3.84(s, 3H), 3.75-3.69(m, 4H), 2.26(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.79, 173.36, 154.01, 142.53, 130.99, 130.67, 129.48, 129.22, 127.33, 112.06, 111.62, 108.90, 100.81, 56.12, 52.66, 41.64, 38.18, 36.21, 8.67; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{19}H_{21}N_3O_4$ 355.1532, found 355.1519.



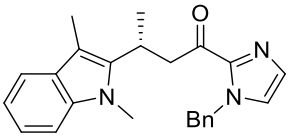
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(5-bromo-3-methyl-1H-indol-2-yl) butan-1-one (6i)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53(s, 1H), 7.55(d, *J*=1.81 Hz, 1H), 7.26-7.22(m, 3H), 7.16-7.14(m, 2H), 7.09(d, *J*=8.49 Hz, 1H), 7.00-7.98(m, 3H), 5.52(s, 2H), 3.77-3.70(m, 2H), 3.28-3.24(m, 1H), 2.14(s, 3H), 1.35(d, *J*=6.82 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.47, 142.74, 139.39, 136.13, 134.01, 131.17, 129.53, 128.98, 128.25, 127.53, 126.43, 123.75, 120.93, 112.20, 111.99, 106.31, 51.96, 44.86, 29.84, 28.37, 20.94; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{22}N_3OBr$ 435.0946, found 435.0940.



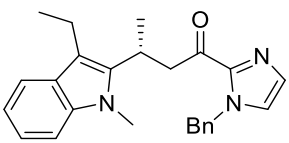
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(3,7-dimethyl-1H-indol-2-yl)butan-1-one (6j)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52(s, 1H), 7.33(d, *J*=7.48 Hz, 1H), 7.26-7.19(m, 4H), 7.03-7.00(m, 4H), 6.90(d, *J*=7.36 Hz, 1H), 5.53(q, *J*=14.89 Hz, 2H), 3.92-3.81(m, 2H), 3.23(dd, *J*=5.45, 14.33 Hz, 1H), 2.44(s, 3H), 2.23(s, 3H), 1.39(d, *J*=6.83 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.83, 143.04, 137.67, 136.19, 134.91, 129.54, 128.99, 128.95, 128.22, 127.61, 126.43, 121.73, 119.91, 119.22, 115.96, 107.04, 51.99, 44.56, 28.70, 21.49, 16.81, 8.73; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O$ 371.1998, found 371.1996.



(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(1,3-dimethyl-1H-indol-2-yl)butan-1-one (6k)

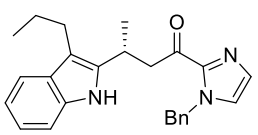
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47(d, *J*=7.76 Hz, 1H), 7.26-7.14(m, 6H), 7.06(t, *J*=7.85 Hz, 1H), 7.00-6.98(m, 3H), 5.50(q, *J*=14.84 Hz, 2H), 4.01-3.95(m, 1H), 3.81-3.75(m, 4H), 3.50(dd, *J*=7.28, 16.04 Hz, 1H), 2.33(s, 3H), 1.42(d, *J*=7.24 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.56, 142.66, 139.22, 136.57, 136.36, 129.58, 128.94, 128.87, 128.14, 127.64, 126.00, 120.85, 118.60, 118.08, 108.85, 106.36, 51.81, 45.28, 30.38, 27.27, 20.04, 9.51; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O$ 371.1998, found 371.1996.



(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(3-ethyl-1-methyl-1H-indol-2-yl) butan-1-one (6l)

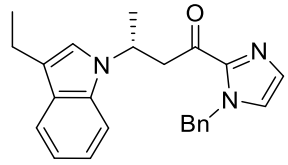
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53(d, *J*=7.80 Hz, 1H), 7.27-7.17(m, 6H), 7.08-7.01(m, 4H), 5.53(q, *J*=14.84 Hz, 2H), 4.05-3.99(m, 1H),

3.82(s, 3H), 3.73(dd, *J*=7.72, 16.04 Hz, 1H), 3.57(dd, *J*=7.56, 16.02 Hz, 1H), 2.82(q, *J*=7.52 Hz, 2H), 1.45(d, *J*=7.28 Hz, 3H), 1.21(t, *J*=7.48 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.50, 142.68, 138.76, 136.99, 136.36, 129.62, 128.95, 128.16, 127.85, 127.67, 126.05, 120.88, 118.60, 118.43, 113.60, 108.94, 51.82, 45.57, 30.69, 27.17, 20.64, 18.02, 16.14; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{25}H_{27}N_3O$ 385.2154, found 385.2149.



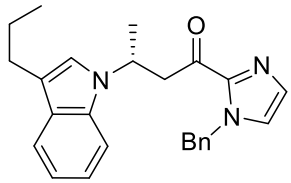
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(3-propyl-1H-indol-2-yl)butan-1-one (6m)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45(s, 1H), 7.49 (d, *J*=7.42 Hz, 1H), 7.26-7.16(m, 5H), 7.08-6.99(m, 5H), 5.55(q, 2H), 3.86-3.80(m, 1H), 3.72-3.66(m, 1H), 3.37-3.31(m, 1H), 2.65(t, *J*=7.16 Hz, 2H), 1.63-1.57(m, 2H), 1.36(d, *J*=7.04 Hz, 3H), 0.93(t, J=7.32 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.65, 142.86, 138.08, 136.22, 135.65, 129.55, 128.98, 128.72, 128.21, 127.61, 126.33, 121.01, 118.87, 118.66, 111.70, 110.67, 51.95, 45.21, 28.11, 26.28, 24.28, 21.57, 14.41; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{25}H_{27}N_3O$ 385.2154, found 385.2149.



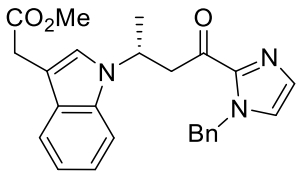
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(3-ethyl-1H-indol-1-yl)butan-1-one (7a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57(d, *J*=7.84 Hz, 1H), 7.38(d, *J*=8.24 Hz, 1H), 7.27-7.26(m, 3H), 7.20-7.11(m, 2H), 7.09-7.02(m, 4H), 6.99(s, 1H), 5.43(s, 2H), 5.29-5.24(m, 1H), 3.71(dd, *J*=7.16, 15.68 Hz, 1H), 3.60(dd, *J*=7.24, 15.64 Hz, 1H), 2.76(q, *J*=7.52 Hz, 2H), 1.55(d, *J*=6.80 Hz, 3H), 1.31(t, *J*=7.48 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.02, 142.57, 136.25, 136.22, 129.77, 128.98, 128.22, 127.93, 127.73, 126.25, 121.45, 120.76, 119.10, 118.71, 118.25, 109.70, 51.78, 47.98, 46.72, 21.42, 18.55, 14.66; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O$ 371.1998, found 371.1996.



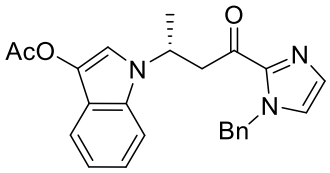
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(3-propyl-1H-indol-1-yl) butan-1-one (7b)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54(d, *J*=7.81 Hz, 1H), 7.36(d, *J*=8.24 Hz, 1H), 7.26-7.24(m, 3H), 7.17-7.15(m, 2H), 7.06-6.99(m, 5H), 5.42(s, 2H), 5.29-5.24(m, 1H), 3.71(dd, *J*=7.18, 15.72 Hz, 1H), 3.59(dd, *J*=7.23, 15.66 Hz, 1H), 2.69(t, *J*=7.40 Hz, 2H), 1.70-1.66(m, 2H), 1.54(d, J=6.80 Hz, 3H), 0.95(t, *J*=7.28 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.01, 142.56, 138.25, 136.19, 129.76, 128.96, 128.20, 128.14, 127.72, 126.23, 121.44, 121.35, 119.16, 118.67, 116.39, 109.66, 51.78, 47.99, 46.71, 27.51, 23.49, 21.43, 14.30; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{25}H_{27}N_3O$ 385.2154, found 385.2149.



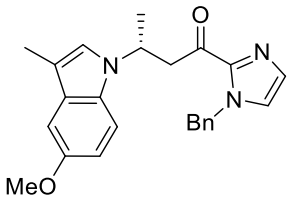
(*R*)-Methyl-2-(1-(4-(1-benzyl-1H-imidazol-2-yl)-4-oxo-butan-2-yl)-1H-indol-3-yl) acetate (7c)

^{1}H NMR (400 MHz, CDCl3): δ 7.57(d, *J*=8.04 Hz, 1H), 7.40(d, *J*=8.12 Hz, 1H), 7.28-7.25(m, 4H), 7.21-7.18(m, 2H), 7.12-7.09(m, 1H), 7.06-7.02(m, 3H), 5.45(s, 2H), 5.29-5.23(m, 1H), 3.75(s, 2H), 3.75-3.59(m, 5H), 1.57(d, *J*=6.80 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.78, 172.60, 142.47, 136.18, 136.02, 129.79, 128.98, 128.22, 127.81, 127.70, 126.28, 123.37, 121.79, 119.42, 119.12, 109.91, 107.82, 52.02, 51.79, 48.17, 46.75, 31.45, 21.34; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{25}H_{25}N_3O_3$ 415.1896, found 415.1885.



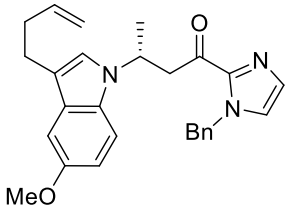
(*R*)-1-(4-(1-Benzyl-1H-imidazol-2-yl)-4-oxo-butan-2-yl)-1H-indol-3-yl acetate (7d)

^{1}H NMR (400 MHz, CDCl3):δ 7.50(d, *J*=7.88 Hz, 1H), 7.44(s, 1H), 7.38(d, *J*=8.36 Hz, 1H), 7.27-7.25(m, 3H), 7.19-7.16(m, 2H), 7.09-7.06(m, 1H), 7.04-7.00(m, 3H), 5.43(s, 2H), 5.30-5.24(m, 1H), 3.68(dd, *J*=7.20, 15.72 Hz, 1H), 3.58(dd, *J*=7.08, 15.72 Hz, 1H), 2.33(s, 3H), 1.55(d, *J*=6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.66, 168.59, 142.43, 136.19, 132.88, 130.24, 129.85, 128.97, 128.22, 127.71, 126.31, 122.36, 120.27, 119.53, 117.68, 113.51, 109.90, 51.78, 48.38, 46.73, 21.27, 21.15; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{23}N_3O_3$ 401.1739, found 407.1731.



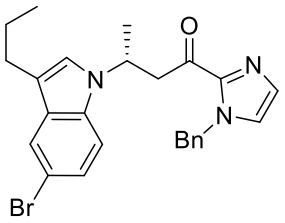
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(5-methoxy-3-methyl-1H -indol-1-yl)bu tan-1-one (7e)

^{1}H NMR (400 MHz, CDCl3):δ 7.28-7.23(m, 4H), 7.16(d, *J*=0.92 Hz, 1H), 7.05-7.01(m, 3H), 6.99(d, *J*=0.88 Hz, 1H), 6.97(d, *J*=2.40 Hz, 1H), 6.82(dd, *J*=2.44, 8.86 Hz, 1H), 5.42(d, *J*=2.8 Hz, 2H), 5.21-5.15(m, 1H), 3.86(s, 3H), 3.66(dd, *J*=7.40, 15.56 Hz, 1H), 3.56(dd, *J*=6.96, 15.60 Hz, 1H), 2.27(s, 3H), 1.52(d, *J*=6.80 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.96, 153.71, 142.52, 136.21, 131.48, 129.75, 128.96, 128.21, 127.74, 126.22, 122.63, 111.59, 110.61, 110.40, 100.89, 56.09, 51.78, 48.18, 46.93, 21.45, 9.94; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O_2$ 387.1947, found 387.1945.



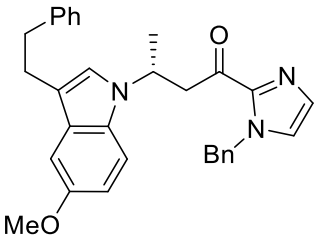
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(3-(but-3-en-1-yl)-5-methoxy-1H-indol-1-yl)butan-1-one (7f)

^{1}H NMR (400 MHz, CDCl3):δ 7.29-7.25(m, 4H), 7.18(d, *J*=0.64 Hz, 1H), 7.05-7.01(m, 5H), 6.84(dd, *J*=2.44, 8.88 Hz, 1H), 5.96-5.87(m, 1H), 5.22-5.16(m, 1H), 5.11-4.97(m, 2H), 3.87(s, 3H), 3.71(dd, *J*=7.32, 15.56 Hz, 1H), 3.56(dd, *J*=7.08, 15.56 Hz, 1H), 2.79(t, *J*=7.12 Hz, 2H), 2.45-2.41(m, 2H), 1.54(d, *J*=6.80 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.96, 153.69, 142.56, 139.02, 136.12, 131.54, 129.75, 128.96, 128.20, 127.71, 126.22, 122.19, 115.18, 114.65, 111.51, 110.45, 101.11, 56.14, 51.79, 48.25, 46.78, 34.40, 29.84, 25.01, 21.40; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{27}H_{29}N_3O_2$ 427.2260, found 427.2247.



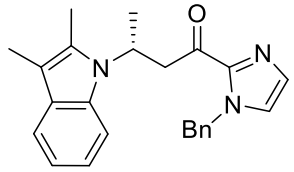
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(5-bromo-3-propyl-1H-indol-1-yl) butan-1-one (7g)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65(s, 1H), 7.26-7.23(m, 3H), 7.19(d, *J*=1.04 Hz, 2H), 7.15(d, *J*=0.80 Hz, 1H), 7.03(s, 1H), 6.99-6.96(m, 3H), 5.40(s, 2H), 5.22-5.16(m, 1H), 3.70(dd, *J*=7.77, 15.48 Hz, 1H), 3.52(dd, *J*=6.72, 15.48 Hz, 1H), 2.62(t, *J*=7.44 Hz, 2H), 1.70-1.61(m, 2H), 1.53(d, *J*=6.80 Hz, 3H), 0.93(t, *J*=7.28 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.67, 142.41, 138.25, 136.06, 134.85, 129.79,129.74, 128.98, 128.25, 127.67, 126.33, 124.07, 122.59, 121.71, 116.11, 111.98, 111.13, 110,13, 51.81, 48.32, 46.72, 27.30, 23.43, 21.46, 14.21; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{25}H_{26}N_3OBr$ 463.1259, found 463.1246.



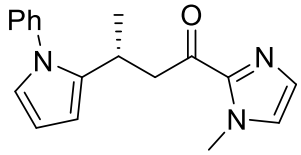
(*R*)-1-(1-Benzyl-1H-imidazol-2-yl)-3-(5-methoxy-3-pheneth yl-1H-indol-1 -yl)butan-1-one (7h)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.19(m, 10H), 7.06-6.98(m, 5H), 6.87-6.85(m, 1H), 5.45(s, 2H), 5.23-5.18(m, 1H), 3.86(s, 3H), 3.70(dd, J=7.32, 15.60 Hz, 1H), 3.57(dd, J=7.04, 15.56 Hz, 1H), 3.04-2.95(m, 4H), 1.53(d, J=6.76 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.95, 153.75, 142.70, 142.55, 136.22, 131.54, 129.77, 128.98, 128.66, 128.42, 128.22, 128.17, 127.74, 126.26, 125.93, 122.29, 115.19, 111.59, 110.50, 101.01, 56.11, 51.79, 48.24, 46.85, 36.73, 27.66, 21.43; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{31}H_{31}N_3O_2$ 477.2416, found 477.2405.



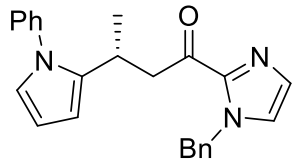
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(2,3-dimethyl-1H-indol-1-yl)butan-1-one (7i)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46(b, d, *J*=7.44 Hz, 2H), 7.29-7.26(m, 3H), 7.14-7.03(m, 5H), 6.97(s, 1H), 5.49-5.27(b, m, 3H), 4.01(b, 1H), 3.76(dd, *J*=6.58, 16.28 Hz, 1H), 2.42(s, 3H), 2.22(s, 3H), 1.61(d, *J*=7.09 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.12, 142.45, 136.28, 132.74, 129.73, 128.98, 128.21, 127.94, 127.75, 126.12, 120.40, 119.41, 118.48, 118.12, 111.05, 110.47, 51.75, 47.36, 45.24, 29.87, 20.38, 9.06; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{25}N_3O$ 371.1998, found 371.1996.



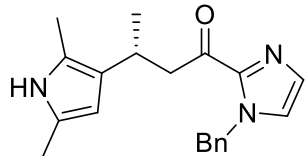
(*R*)-1-(1-Methyl-1*H*-imidazol-2-yl)-3-(1-phenyl-1*H*-pyrrol-2-yl) butanone (9a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.35(m, 5H), 7.11(s, 1H), 6.98(s, 1H), 6.68(d, *J* = 2 Hz, 1H), 6.18-6.13(m, 2H), 3.93(s, 3H), 3.62-3.47(m, 2H), 3.30-3.24(m, 1H), 1.11(d, *J* = 6.71 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.64, 143.35, 140.45, 138.47, 129.22, 129.07, 127.38, 126.95, 126.79, 121.90, 108.00, 105.15, 45.89, 36.26, 26.80, 22.11; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{18}H_{19}N_3O$ 293.1528, found 293.1526.



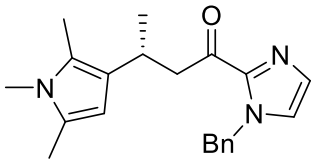
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(1-phenyl-1*H*-pyrrol-2-yl) butanone (9b)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.26(m, 8H), 7.13-7.08(m, 3H), 7.00(s, 1H), 6.68-6.67(m, 1H), 6.18-6.13(m, 2H), 5.57(m, 2H), 3.60-3.50(m, 2H), 3.30-3.21(m, 1H), 1.09(d, *J* = 6.64 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.83, 142.93, 140.42, 138.36, 136.54, 129.51, 129.21, 128.98, 128.14, 127.68, 127.37, 126.81, 125.88, 121.89, 108.02, 105.26, 51.82, 46.11, 27.02, 22.12; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{23}N_3O$ 369.1841, found 369.1838.



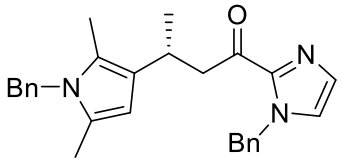
(*R*)-1-(1-Benzyl-1-imidazol-2-yl)-3-(2,5-dimethyl-1*H*-pyrrol-3-yl) butanone (9c)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.26(m, 4H), 7.15-7.12(m, 3H), 7.02(s, 1H), 5.74(s, 1H), 5.64-5.54(m, 2H), 3.39-3.26(m, 3H), 2.18(s, 3H), 2.11(s, 3H), 1.18(d, *J* = 6.59 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.99, 143.16, 136.72, 129.39, 128.91, 128.08, 127.74, 125.69, 125.03, 124.03, 120.98, 104.18, 51.80, 47.95, 27.39, 22.51, 13.15, 11.09; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{20}H_{23}N_3O$ 321.1841, found 321.1837.



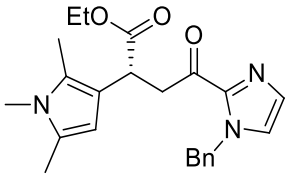
(*R*)-1-(1-Benzyl-imidazol-2-yl)-3-(1,2,5-trimethyl-pyrrol-3-yl) butanone (9d)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.26(m, 3H), 7.17-7.14(m, 3H), 7.03(s, 1H), 5.78(s, 1H), 5.60(m, 2H), 3.44-2.24(m, 6H), 2.17(s, 3H), 2.12(s, 3H), 1.17(d, *J* = 6.57 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.03, 143.18, 136.72, 129.44, 128.93, 128.11, 127.75, 126.81, 125.74, 123.16, 122.95, 103.09, 51.83, 48.03, 30.18, 27.48, 22.65, 12.62, 10.17; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{21}H_{25}N_3O$ 335.1998, found 335.1994.



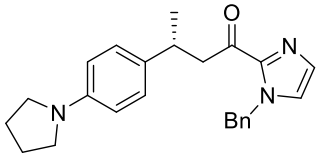
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(1-benzyl-2,5-dimethyl-1*H*-pyrrol-3-yl)butan-1-one (9e)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.23(m, 5H), 7.19-7.13(m, 4H), 7.02(s, 1H), 6.81(d, *J* = 7.17 Hz, 2H), 5.88(s, 1H), 5.55(q, *J*=13.45, 14.86 Hz, 2H), 4.95(s, 2H), 3.45-3.36(m, 2H), 3.30-3.24(m, 1H), 2.10(s, 3H), 1.99(s, 3H), 1.23(d, *J* = 6.59 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.01, 143.14, 139.02, 136.64, 129.43, 128.94, 128.78, 128.12, 127.78, 127.02, 126.98, 125.73, 123.63, 122.87, 103.92, 51.81, 48.35, 46.76, 27.85, 22.59, 12.48, 9.98; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{27}H_{29}N_3O$ 411.2311, found 411.2309.



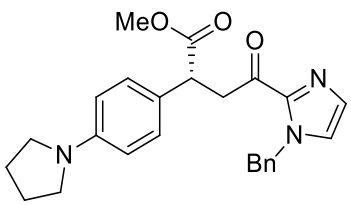
(*R*)-Ethyl 4-(1-benzyl-1*H*-imidazol-2-yl)-4-oxo-2-(1,2,5-trimethyl-1*H*-pyrrol-3-yl) butanoate (9f)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.26(m, 3H), 7.17-7.15(m, 3H), 7.02(s, 1H), 5.83(s, 1H), 5.62-5.58(m, 2H), 4.13-4.03(m, 4H), 3.39-3.33(m, 1H), 3.33(s, 3H), 2.19(s, 3H), 2.15(s, 3H), 1.18(t, *J* = 7.08 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.46, 174.39, 142.53, 136.57, 129.68, 128.95, 128.15, 127.83, 127.24, 125.74, 124.84, 114.68, 104.43, 60.70, 51.75, 42.92, 38.29, 30.33, 14.29, 12.58, 10.37; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{27}N_3O_3$ 393.2052, found 393.2047.



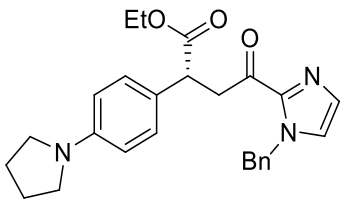
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(4-(pyrrolidin-1-yl) phenyl) butan-1-one (11a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.25(m, 3H), 7.15-7.09(m, 5H), 7.01(s, 1H), 6.49(d, *J* = 8.54 Hz, 2H), 5.62-5.52(m, 2H), 3.43-3.35(m, 3H), 3.24(t, *J* = 6.54 Hz, 4H), 2.01-1.94(m, 4H), 1.22(d, *J* = 6.74 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.59, 146.60, 143.08, 136.61, 133.25, 129.45, 128.94, 128.11, 127.75, 125.83, 111.75, 51.84, 47.80, 47.71, 35.19, 25.60, 22.77; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{24}H_{27}N_3O$ 373.2154, found 373.2153.



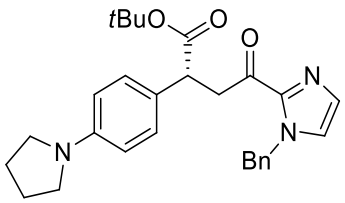
(*R*)-Methyl 4-(1-benzyl-1*H*-imidazol-2-yl)-4-oxo-2-(4-(pyrrolidin-1-yl)phenyl) butanoate (11b)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.26(m, 3H), 7.19-7.13(m, 5H), 7.01(s, 1H), 6.49(d, *J* = 8.61 Hz, 2H), 5.67-5.52(m, 2H), 4.14-4.06(m, 2H), 3.63(s, 3H), 3.51-3.43(m, 1H), 3.25(t, *J* = 6.57 Hz, 4H), 1.99-1.96(m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.95, 174.58, 147.38, 142.42, 136.44, 129.73, 128.98, 128.84, 128.19, 127.82, 125.84, 124.49, 111.87, 52.23, 51.79, 47.72, 45.41, 43.14, 25.61; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{25}H_{27}N_3O_3$ 417.2052, found 417.2048.



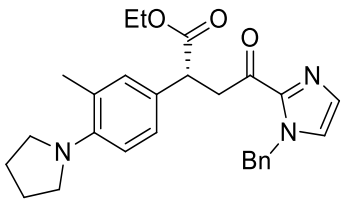
(*R*)-Ethyl 4-(1-benzyl-1H-imidazol-2-yl)-4-oxo-2-(4-(pyrrolidin-1-yl) phenyl) butanoate (11c)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.26(m, 3H), 7.20(d, *J* = 8.59 Hz, 2H), 7.15-7.13(m, 3H), 7.01(s, 1H), 6.50(d, *J* = 8.60 Hz, 2H), 5.59(q, *J* = 14.89 Hz, 2H), 4.15-4.02(m, 4H), 3.51-3.45(m, 1H), 3.25(t, *J* = 6.53 Hz, 4H), 1.99-1.96(m, 4H), 1.16(t, *J* = 7.11 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.99, 174.04, 147.31, 142.44, 136.50, 129.71, 128.97, 128.85, 128.17, 127.82, 125.86, 124.72, 111.86, 60.87, 51.76, 47.75, 45.63, 43.15, 25.61, 14.24; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{26}H_{29}N_3O_3$ 431.2209, found 431.2207.



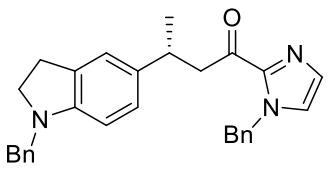
(*R*)-*tert*-Butyl 4-(1-benzyl-1*H*-imidazol-2-yl)-4-oxo-2-(4-(pyrrolidinyl)phenyl) butanoate (11d)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.26(m, 3H), 7.19-7.14(m, 5H), 7.02(s, 1H), 6.49(d, *J* = 8.54 Hz, 2H), 5.59(d, *J* = 4.55 Hz, 2H), 4.10-4.00(m, 2H), 3.37(d, *J* = 13.95 Hz, 1H), 3.25(t, *J* = 6.41 Hz, 4H), 1.97 (t, *J* = 6.41 Hz, 4H), 1.35(s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.16, 173.15, 147.16, 142.48, 136.61, 129.65, 128.95, 128.75, 128.13, 127.78, 125.85, 125.28, 111.81, 80.45, 51.75, 47.74, 46.65, 43.16, 28.05, 25.61; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{28}H_{33}N_3O_3$ 459.2522, found 459.2519.



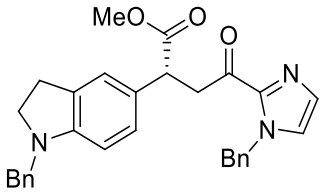
(*R*)-Ethyl 4-(1-benzyl-1*H*-imidazol-2-yl)-2-(3-methyl-4-(pyrrolidin-1-yl)phenyl)-4-oxo-butanoate (11e)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.26(m, 3H), 7.16-7.14(m, 3H), 7.08-7.06(m, 2H), 7.02(s, 1H), 6.79(d, *J* = 8.11 Hz, 1H), 5.59(q, *J* = 14.89 Hz, 2H), 4.14-4.02(m, 4H), 3.49-3.41(m, 1H), 3.16(t, *J* = 6.33 Hz, 4H), 2.29(s, 3H), 1.92-1.89(m, 4H), 1.17(t, *J* = 7.10 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.83, 173.84, 148.79, 142.38, 136.48, 131.25, 129.72, 129.54, 128.97, 128.86, 128.19, 127.80, 125.88, 115.92, 60.93, 51.76, 51.12, 45.65, 43.18, 25.10, 20.77, 14.22; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{27}H_{31}N_3O_3$ 445.2365, found 445.2361.



(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(1-benzylindolin-5-yl)butan-1-one (11f)

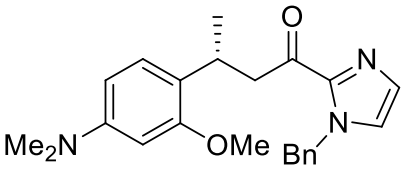
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.24(m, 8H), 7.15-7.02(m, 5H), 6.92(d, *J* = 8.01 Hz, 1H), 6.41(d, *J* = 8.02 Hz, 1H), 5.63-5.54(m, 2H), 4.20(s, 2H), 3.43-3.34(m, 3H), 3.26(t, *J* = 8.26 Hz, 2H), 2.91(t, *J*=8.21 Hz, 2H), 1.25-1.23(m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.49, 151.16, 143.05, 138.85, 136.59, 136.16, 130.40, 129.46, 128.96, 128.57, 128.13, 128.09, 127.71, 127.17, 125.85, 125.81, 123.39, 107.04, 54.30, 54.11, 51.85, 47.77, 35.45, 28.73, 22.78; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{29}H_{29}N_3O$ 435.2311, found 435.2310.



(*R*)-Methyl 4-(1-benzylimidazolyl)-2-(1-benzylindolinyl)-4-oxo-butanoate (11g)

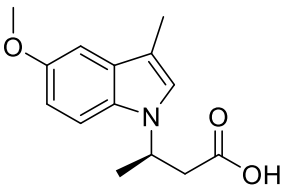
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.26 (m, 8H), 7.16-7.14 (m, 3H), 7.09 (s, 1H), 7.02-7.00 (m, 2H), 6.43 (d, *J* = 8.05 Hz, 1H), 5.60 (q, *J* = 46.88, 14.91 Hz, 2H), 4.23 (s, 2H), 4.16-4.07 (m, 2H), 3.65 (s, 3H), 3.51-3.43 (m, 1H), 3.31 (t, *J* = 8.35 Hz, 2H), 2.94 (t, *J* = 8.26 Hz, 2H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 190.85, 174.56, 152.14, 142.37, 138.54, 136.44, 130.77, 129.76, 129.01, 128.64, 128.22, 128.04, 127.82, 127.28, 127.24, 127.14, 125.91, 124.19, 106.98, 53.81, 53.76, 52.31, 51.79, 45.66, 43.39, 28.57; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{30}H_{29}N_3O_3$ 479.2209, found 479.2209.



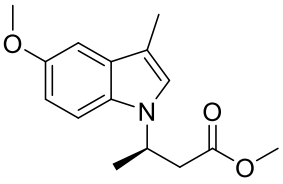
(*R*)-1-(1-Benzylimidazolyl)-3-(4-(dimethylamino)-2-methoxyphenyl)butanone (11h)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.26(m, 3H), 7.15-7.08(m, 4H), 7.01(s, 1H), 6.29-6.25(m, 2H), 5.59(s, 2H), 3.79-3.73(m, 4H), 3.49-3.35(m, 2H), 2.92(s, 6H), 1.22(d, *J* = 6.90 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.91, 157.81, 150.49, 143.22, 136.70, 129.38, 128.93, 128.09, 127.79, 127.63, 125.70, 123.13, 105.02, 96.85, 55.43, 51.81, 46.16, 41.04, 28.90, 21.10; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{23}H_{27}N_3O_2$ 377.2103, found 377.2101.



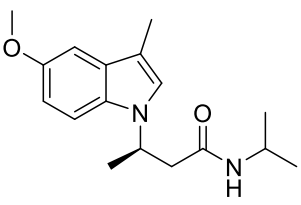
(*R*)-3-(5-Methoxy-3-methyl-1H-indol-1-yl)butanoic acid (12)[5]

To a solution of **7e** (0.3 mmol) in 2ml of dry DMF was added methyl iodide (10 equiv) under argon at rt. After 20h stirring at 60 ^{o}C, the resulting yellow mixture was concentrated in vacuo to remove excess methyl iodide. Then water (5d) and DBU (5 equiv) were added at rt respectively. After 4h of stirring at rt, the reaction was quenched with NH_4Cl aq and purified by silica gel flash chromatography (EA/Hexane = 1:2-2:1) to afford the product as white oil, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28(d, *J*=8.88 Hz, 1H), 7.02(d, *J*=2.39 Hz, 1H), 6.95(s, 1H), 6.90(dd, *J*=2.44, 8.88 Hz, 1H), 4.94-4.88(m, 1H), 3.90(s, 3H), 2.96-2.74(m, 2H), 2.32(s, 3H), 1.57(d, *J*=6.80Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 176.73, 153.88, 131.30, 129.19, 122.24, 111.90, 110.97, 110.25, 101.14, 56.13, 48.10, 41.75, 20.90, 9.90; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{14}H_{17}NO_3$ 247.1208, found 247.1205.



(*R*)-Methyl3-(5-methoxy-3-methyl-1H-indol-1-yl)butanoate (13)[5]

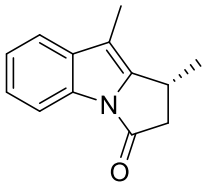
To a solution of **7e** (0.3 mmol) in 2ml of dry DMF was added methyl iodide (10 equiv) under argon at rt. After 20h stirring at 60 ^{o}C, the resulting yellow mixture was concentrated in vacuo to remove excess methyl iodide and DMF. Then anhydrous methanol in 2 ml of dry DCM and DBU (5 equiv) were added at rt respectively. After 6h of stirring at rt, the reaction was quenched with NH_4Cl aq and purified by silica gel flash chromatography (EA/Hexane = 1:10) to afford the product as white oil, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.27(m, 1H), 7.01(d, *J*=2.40 Hz, 1H), 6.95(s, 1H), 6.91-6.88(m, 1H), 4.95-4.90(m, 1H), 3.90(s, 3H), 3.63(s, 3H), 2.91-2.71(m, 2H), 2.31(s, 3H), 1.57(d, *J*=6.82 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.47, 153.84, 131.28, 129.10, 122.26, 111.80, 110.80, 110.24, 101.01, 56.09, 51.98, 48.35, 41.92, 20.93, 9.92; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{15}H_{19}NO_3$ 261.1365, found 261.1365.



(*R*)-*N*-Isopropyl-3-(5-methoxy-3-methyl-1H-indol-1-yl)butanamide (14)[5]

To a solution of **7e** (0.3 mmol) in 2ml of dry DMF was added methyl iodide (10 equiv) under argon at rt. After 20h stirring at 60 ^{o}C, the resulting yellow mixture was concentrated in vacuo to remove excess methyl iodide. Then isopropylamine (10 eq) and DBU (5 equiv) were

added at rt respectively. After 12h of stirring at rt, the reaction was quenched with NH_4Cl aq and purified by silica gel flash chromatography (EA/Hexane = 1:2-1:1) to afford the product as yellow solid, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29(d, *J*=8.90 Hz, 1H), 6.98(d, *J*=2.41 Hz, 1H), 6.92(s, 1H), 6.87(dd, *J*=2.44, 8.88 Hz, 1H), 4.91-4.86(m, 1H), 3.87(s, 3H), 3.87-3.79(m, 1H), 2.62-2.49(m, 2H), 2.29(s, 3H), 1.59(d, *J*=6.88 Hz, 3H), 0.96(d, *J*=6.56 Hz, 3H), 0.68(d, *J*=6.55 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.24, 153.86, 131.37, 129.06, 122.39, 111.90, 110.77, 110.56, 101.11, 56.13, 49.38, 44.98, 41.40, 22.63, 22.09, 21.03, 9.88; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{17}H_{24}N_2O_2$ 288.1838, found 288.1831.



(*R*)-1,9-Dimethyl-1,2-dihydropyrrolo[1,2-a]indol-3-one (15)[5]

To a solution of **6b** (0.3 mmol) in 2ml of dry DMF was added methyl iodide (10 equiv) under argon at rt. After 20h stirring at 60 ^{o}C, the resulting yellow mixture was concentrated in vacuo to remove excess methyl iodide. Then DBU (5 equiv) was added at rt. After 12h of stirring at rt, the reaction was quenched with NH_4Cl aq and purified by silica gel flash chromatography (EA/Hexane = 1:20) to afford the product as yellow solid, 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05-8.03(m, 1H), 7.47-7.44(m, 1H), 7.31-7.27(m, 2H), 3.55-3.51(m, 1H), 3.31(dd, *J*=8.68, 18.14 Hz, 1H), 2.65(dd, *J*=3.82, 18.12 Hz, 1H), 2.26(s, 3H), 1.47(d, *J*=7.06 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.89, 143.73, 136.45, 130.02, 123.85, 123.51, 118.68, 113.78, 108.66, 44.08, 27.08, 20.27, 8.37; HRMS (EI) *m/z* $[M]^+$ Calcd for $C_{13}H_{13}NO$ 199.0997, found 199.0996.

Computational details

All the calculations were performed by Gaussian 09 packages.[6] Molecular structures of all intermediates and transition states were optimized by the M06L functional.[7] The vibrational frequency calculations at the same level were carried out to verify that every optimized structure is an energy minima (no imaginary frequency) or a transition state, and to evaluate its zero-point vibration energy (ZPVE). The 6-31G* Pople basis set[8] was employed for all the atoms except for Fe atom with effective core potential (ECP) type basis set LANL2DZ.[9] The solvent effect was included by the single point calculations for all the optimized gas-phase structures with self-consistent reactions field (SCRF) based on the polarizable continuum model (PCM)[10] in which acetonitrile was the solvent as the experimental condition. The functional of M06[11] was applied in the single point calculations to compute energy; 6-311+G* basis set[12] was applied on all the atoms except for Fe atom with the Hay-Wadt relativistic effective core potentials (RECPs) LANL2TZ(f).[13] Simulation results showed that quintet is the ground state for all the complexes.

References

1 K. S. Hagen, *Inorg. Chem*., 2000, **39**, 5867.

2 J.-L. Lim, S. Chirayil and R. P. Thummel, *J. Org. Chem.*, 1991, **56**, 1492.

3 A.-H. Li, D. J. Beard, H. Coate, A. Honda, M. Kadalbajoo, A. Kleinberg, R. Laufer, K. M. Mulvihill, A. Nigro, P. Rastogi, D. Sherman, K. W. Siu, A. G. Steinig, T. Wang, D. Werner, A. P. Crew and M. J. Mulvihill, *Synthesis,* 2010, **10**, 1678.

4 (*a*) A. Maisonial, M. Traikia, A. Gautier and D. J. Aitken, *Tetrahedron Lett*., 2006, **47**, 8091; (*b*) M. E. Fox, A. Gerlach, I. C. Lennon, G. Meek and C. Praquin, *Synthesis,* 2005, **19**, 3196; (*c*) C. Zang, Y. Liu, Z.-J. Xu, C.-W. Tse, X. Guan, J. Wei, J.-S. Huang and C.-M. Che, *Angew. Chem., Int. Ed.*, 2016, **55**, 10253.

5 D. A. Evans, K. R. Fandrick, H.-J. Song, K. A. Scheidt and R. Xu, *J. Am. Chem. Soc*., **2007**, *129*, 10029.

6 R. D. Gaussian 09, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

7 Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101.

8 (*a*) P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213; (*b*) M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654.

9 P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299.

10 (*a*) S. Miertuš, E. Scrocco and J. Tomasi, *Chem. Phys.*, 1981, **55**, 117; (*b*) J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999.

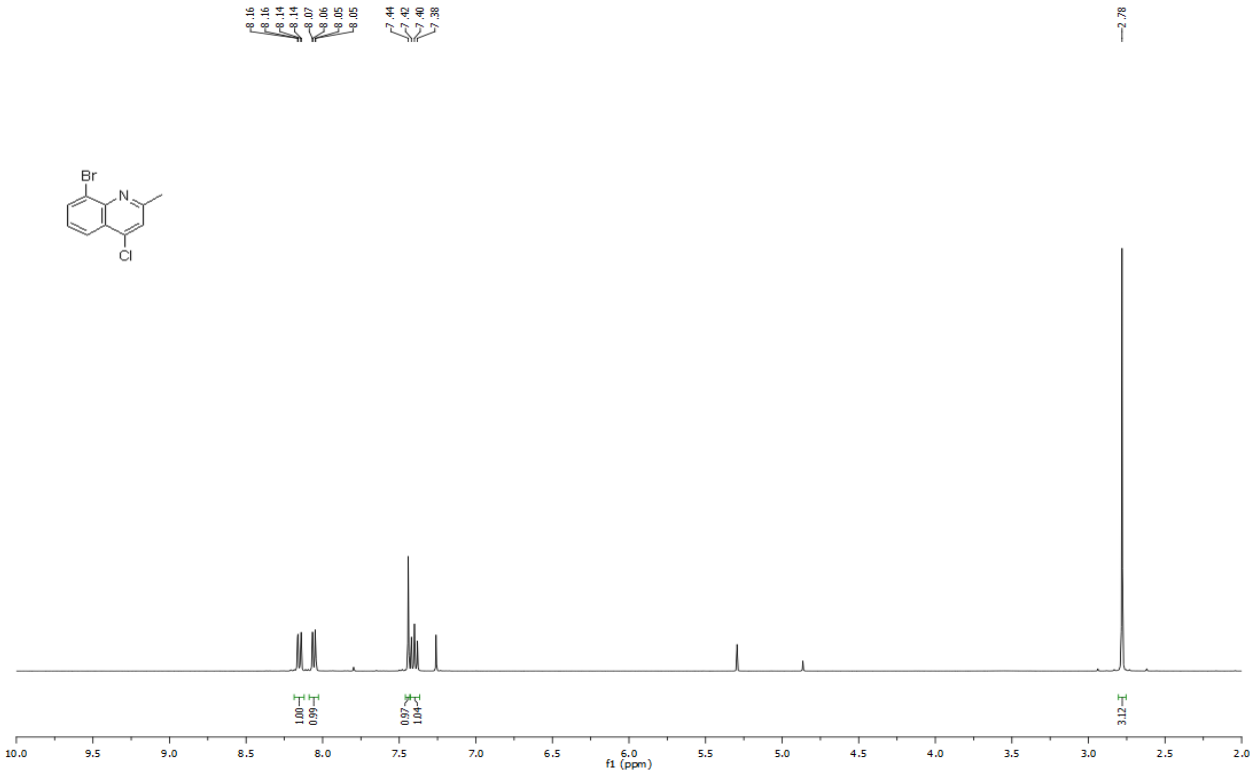
11 Y. Zhao and D. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.

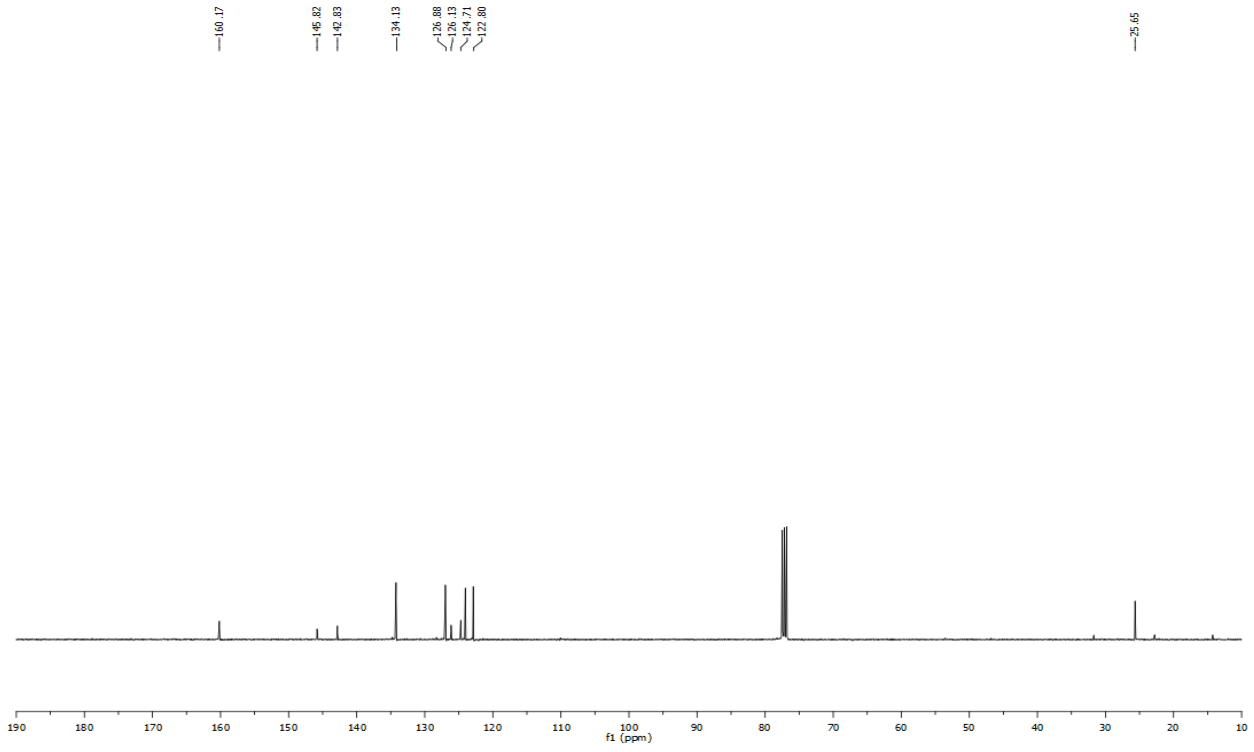
12 (*a*) R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650; (*b*) T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294.

13 L. E. Roy, P. J. Hay and R. L. Martin, *J. Chem. Theory Comput.*, 2008, **4**, 1029.

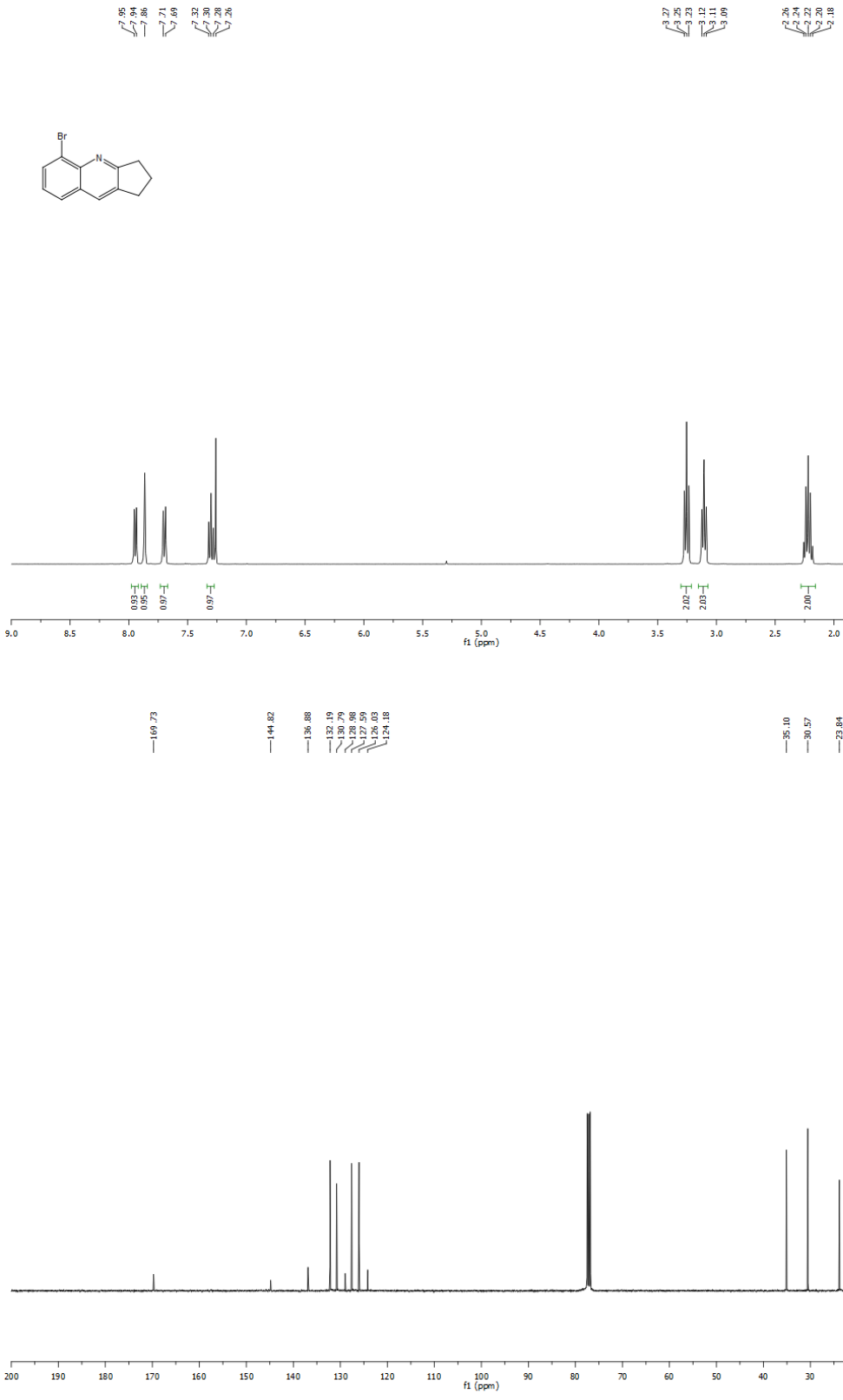
NMR spectra of compounds

8-Bromo-4-chloro-2-methylquinoline (**S-Qd**)

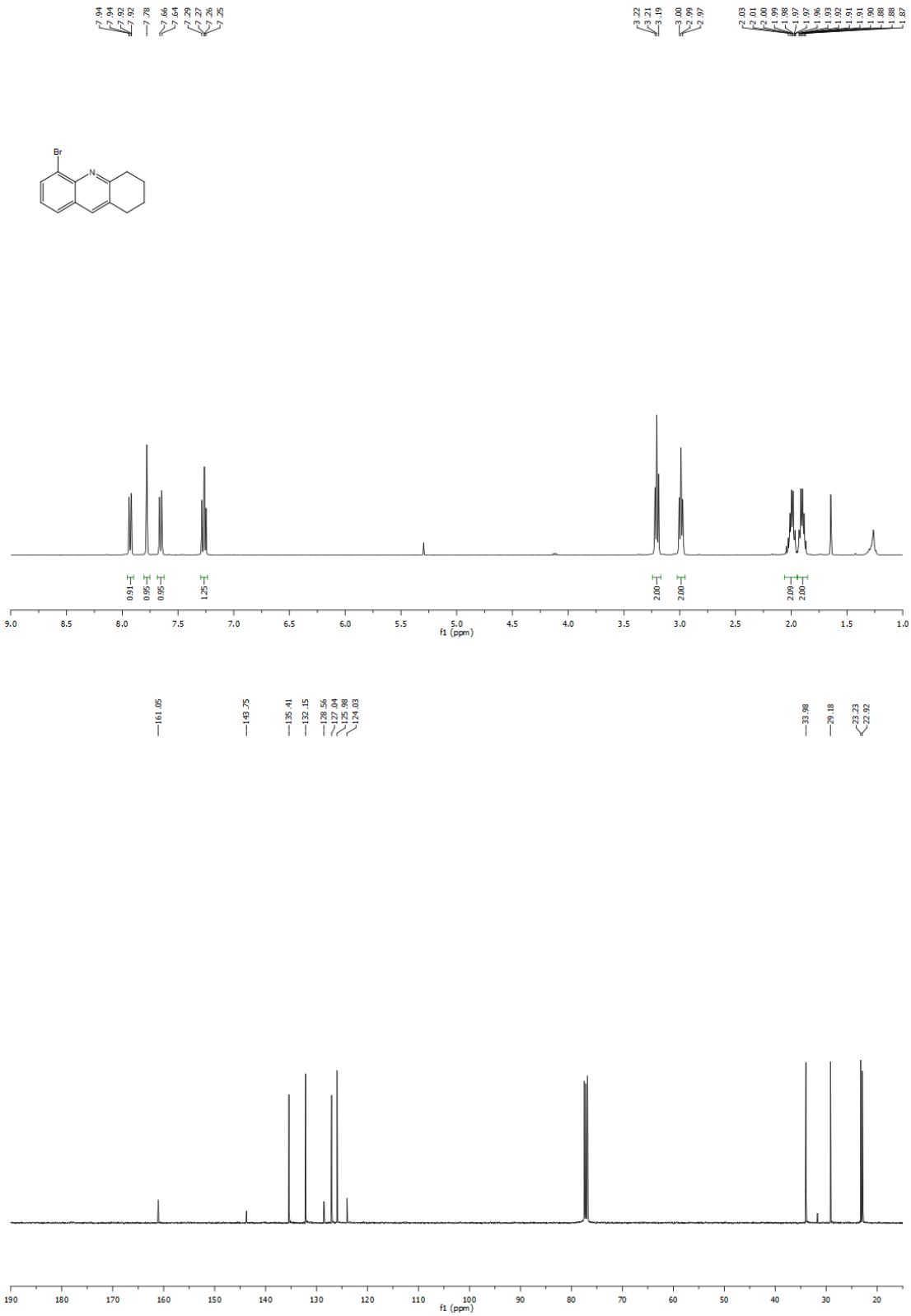




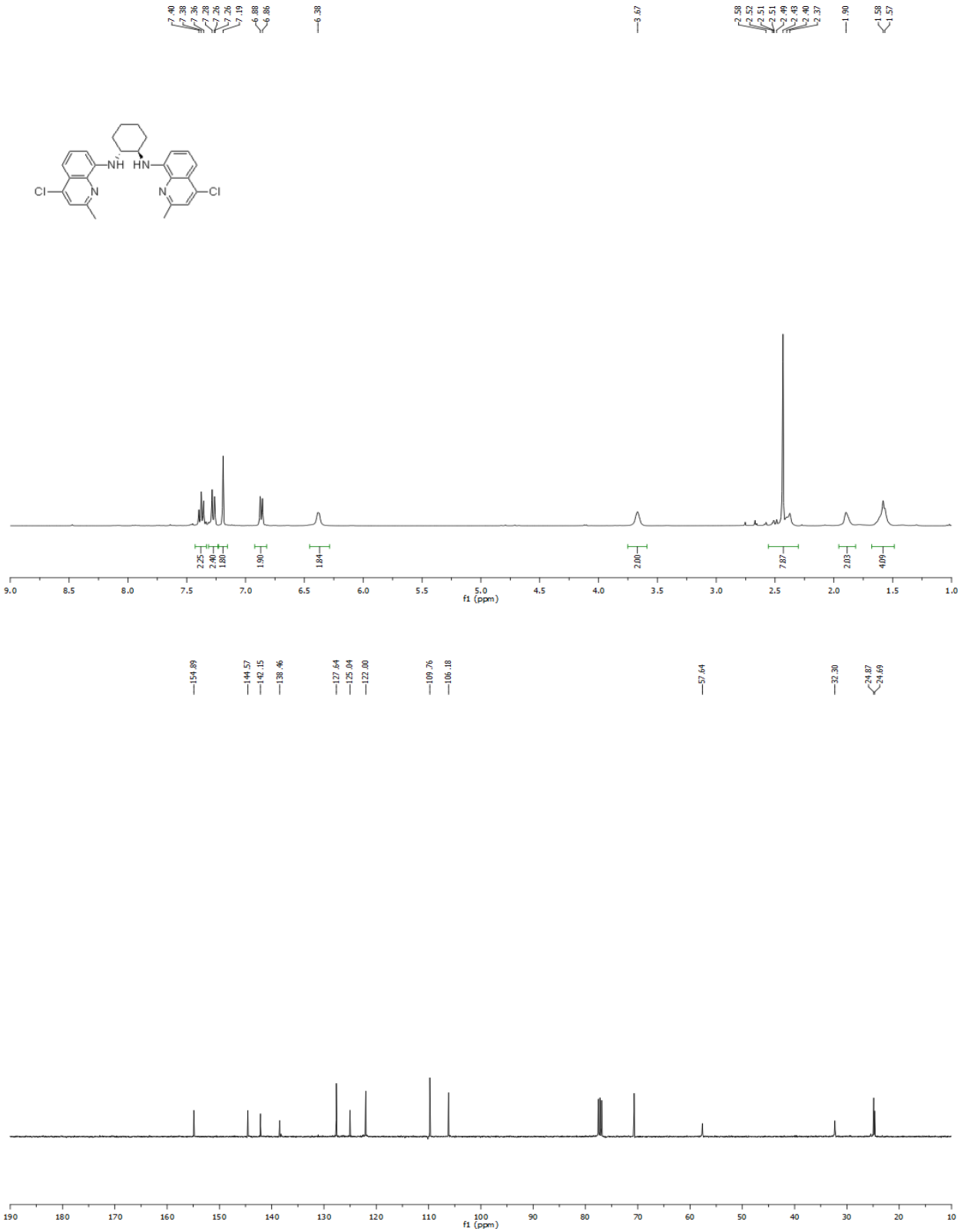
5-Bromo-2,3-dihydro-1*H*-cyclopenta[*b*]quinoline (**S-Qe**)



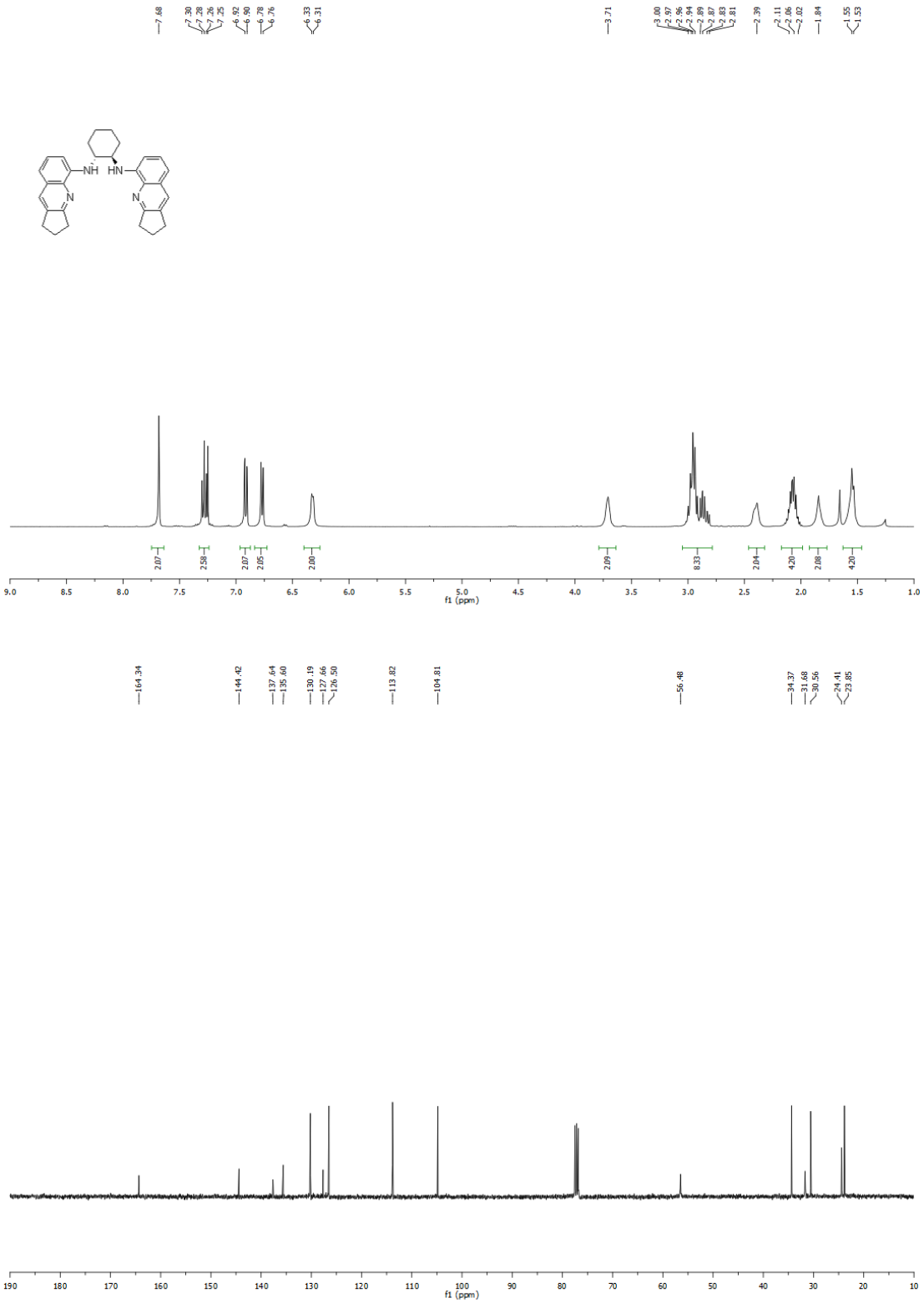
5-Bromo-1,2,3,4-tetrahydroacridine (**S-Qf**)



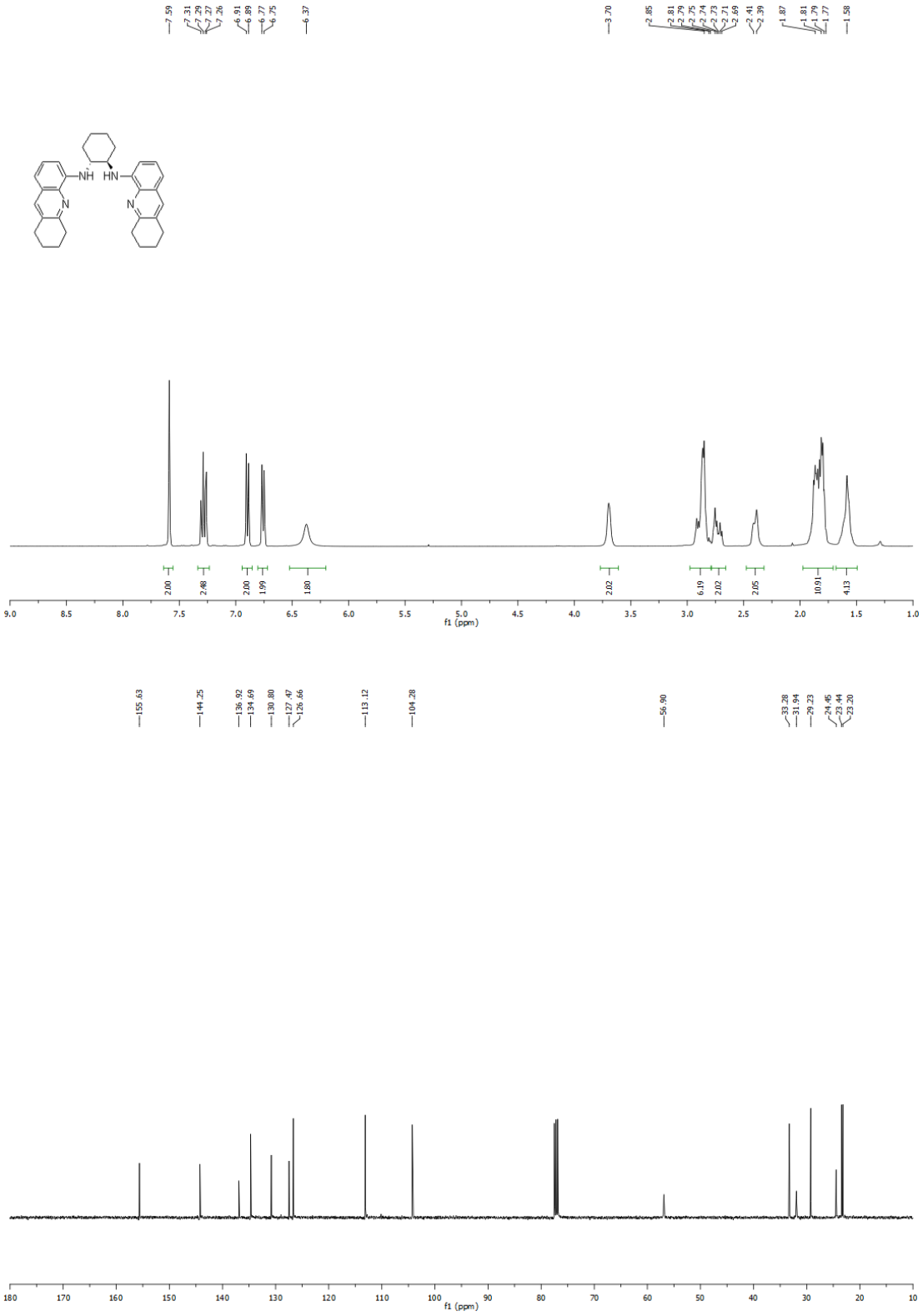
(*R*,*R*)-*N*,*N*-Bis(4-chloro-2-methylquinolin-8-yl)cyclohexane-1,2-diamine (**2d-H$_2$**)



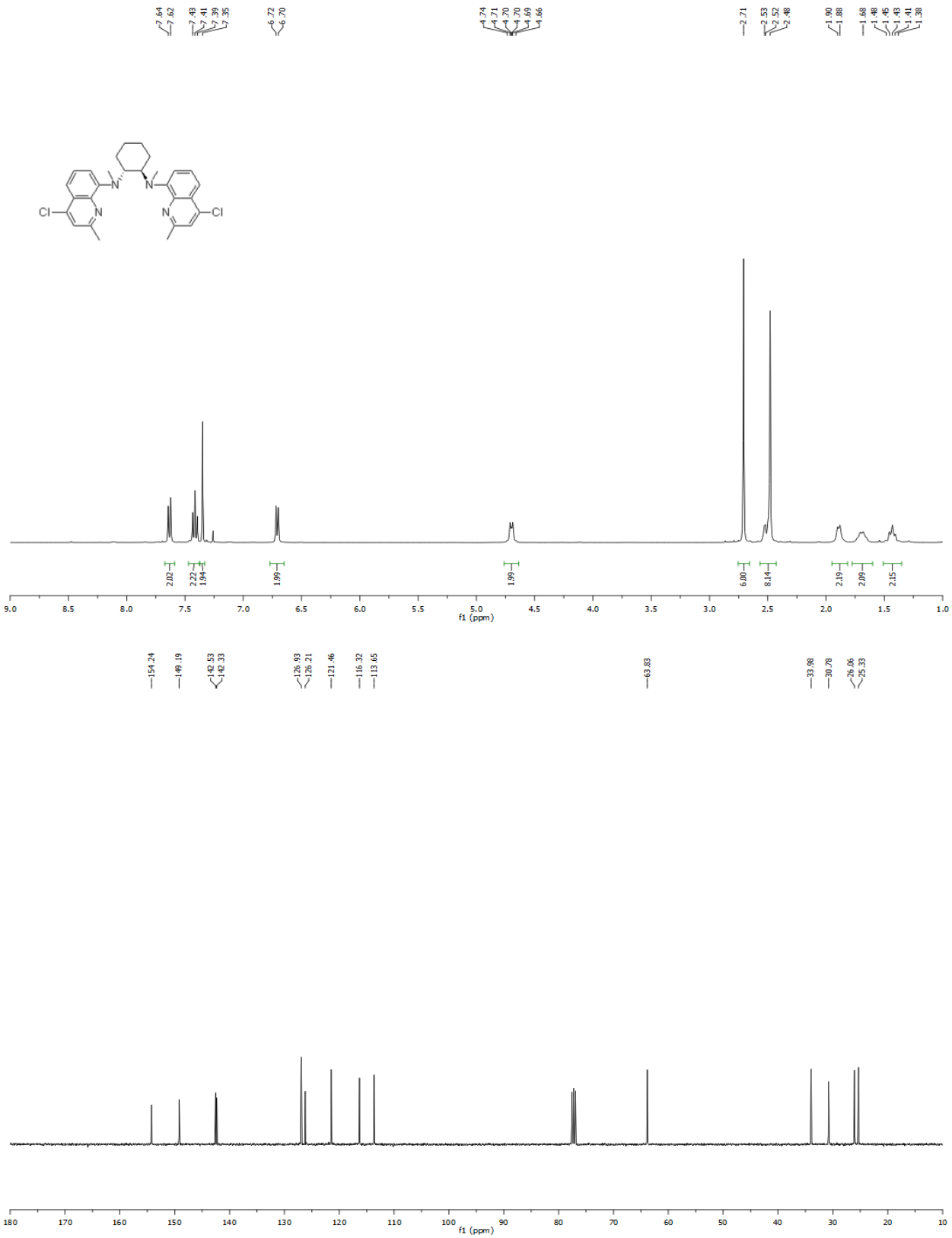
(*R*,*R*)-*N*,*N'*-Bis(2,3-dihydro-1*H*-cyclopenta[*b*]quinolin-5-yl)cyclohexane-1,2-diamine (**2e-H$_2$**)



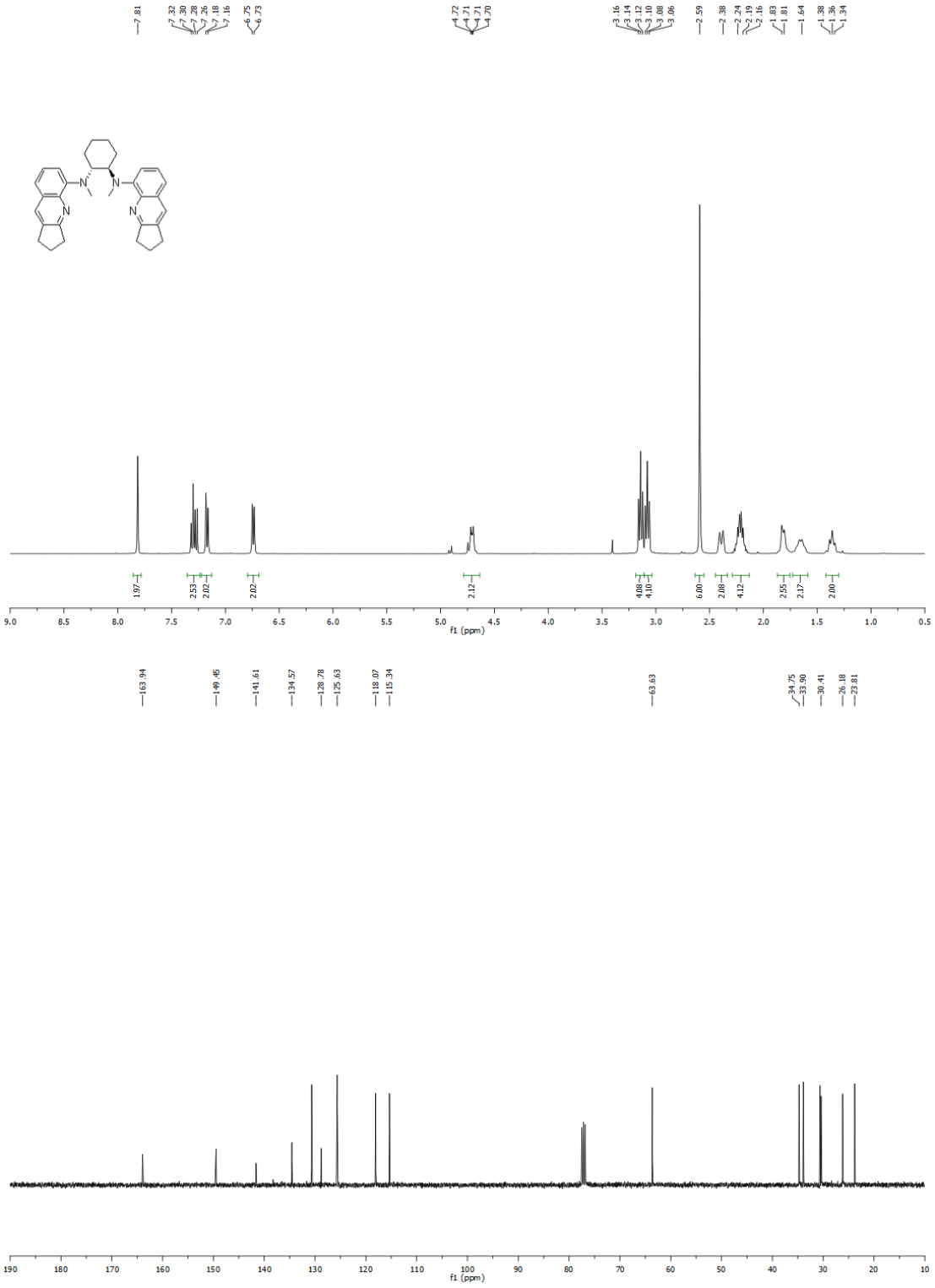
(*R*,*R*)-*N*,*N'*-Bis(5,6,7,8-tetrahydroacridin-4-yl)cyclohexane-1,2-diamine (**2f-H$_2$**)



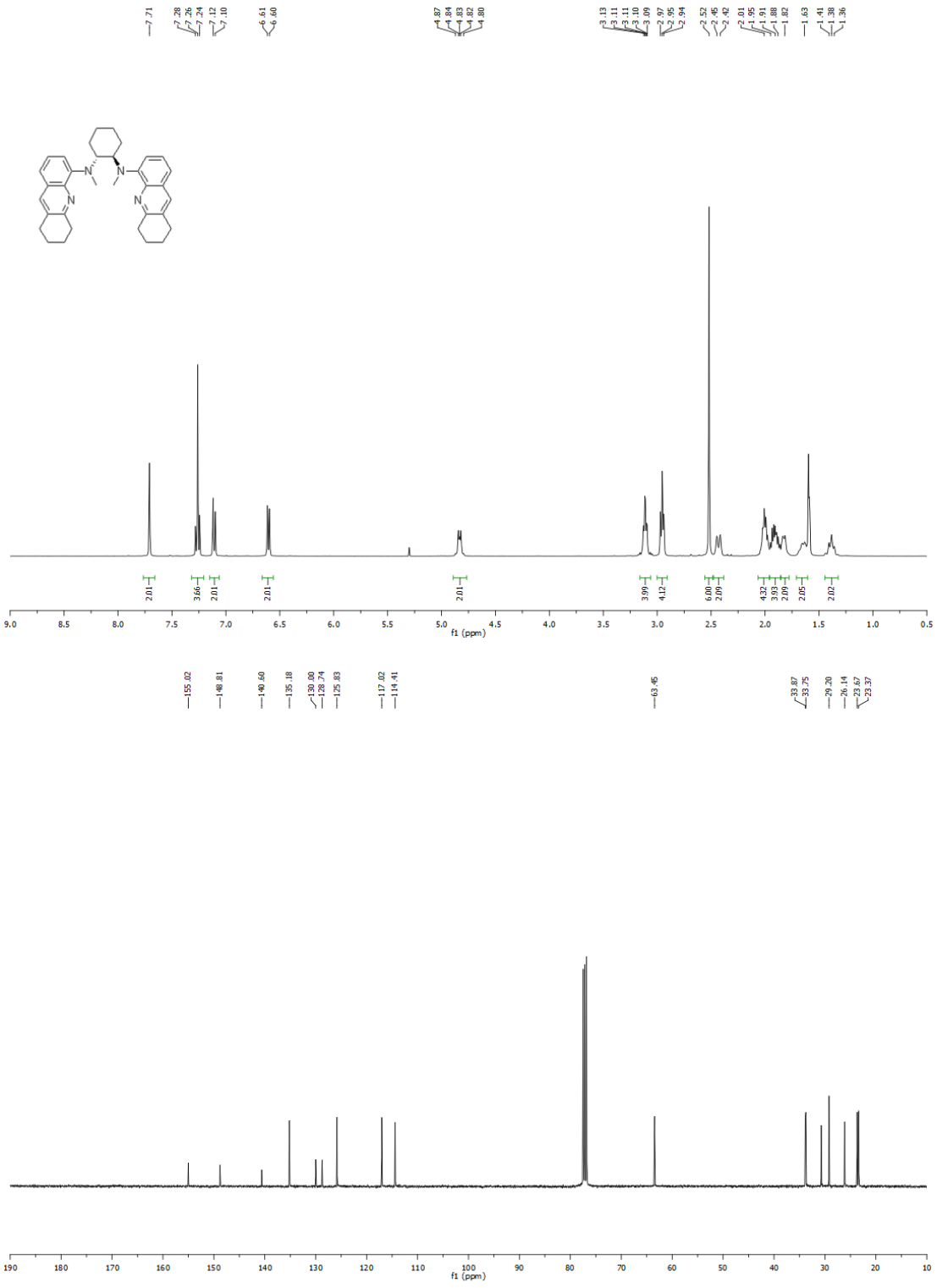
(*R*,*R*)-*N*,*N*-Bis(4-chloro-2-methylquinolin-8-yl)-*N*,*N*-dimethylcyclohexane-1,2-diamine (**2d**)



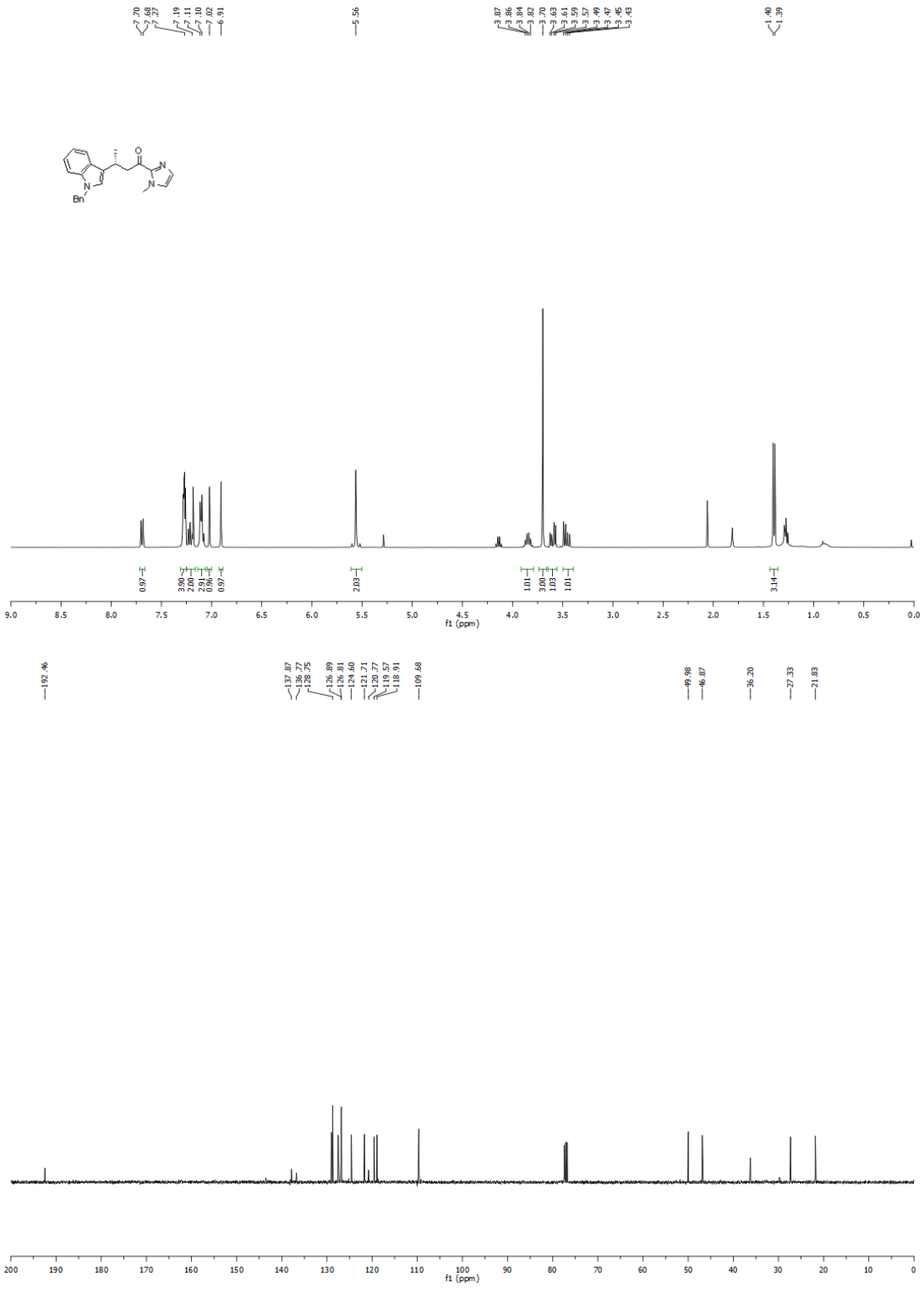
(*R*,*R*)-*N*,*N'*-Bis(2,3-dihydro-1*H*-cyclopenta[*b*]quinolin-5-yl)-*N*,*N'*-dimethylcyclo-hexane-1,2-diamine (**2e**)



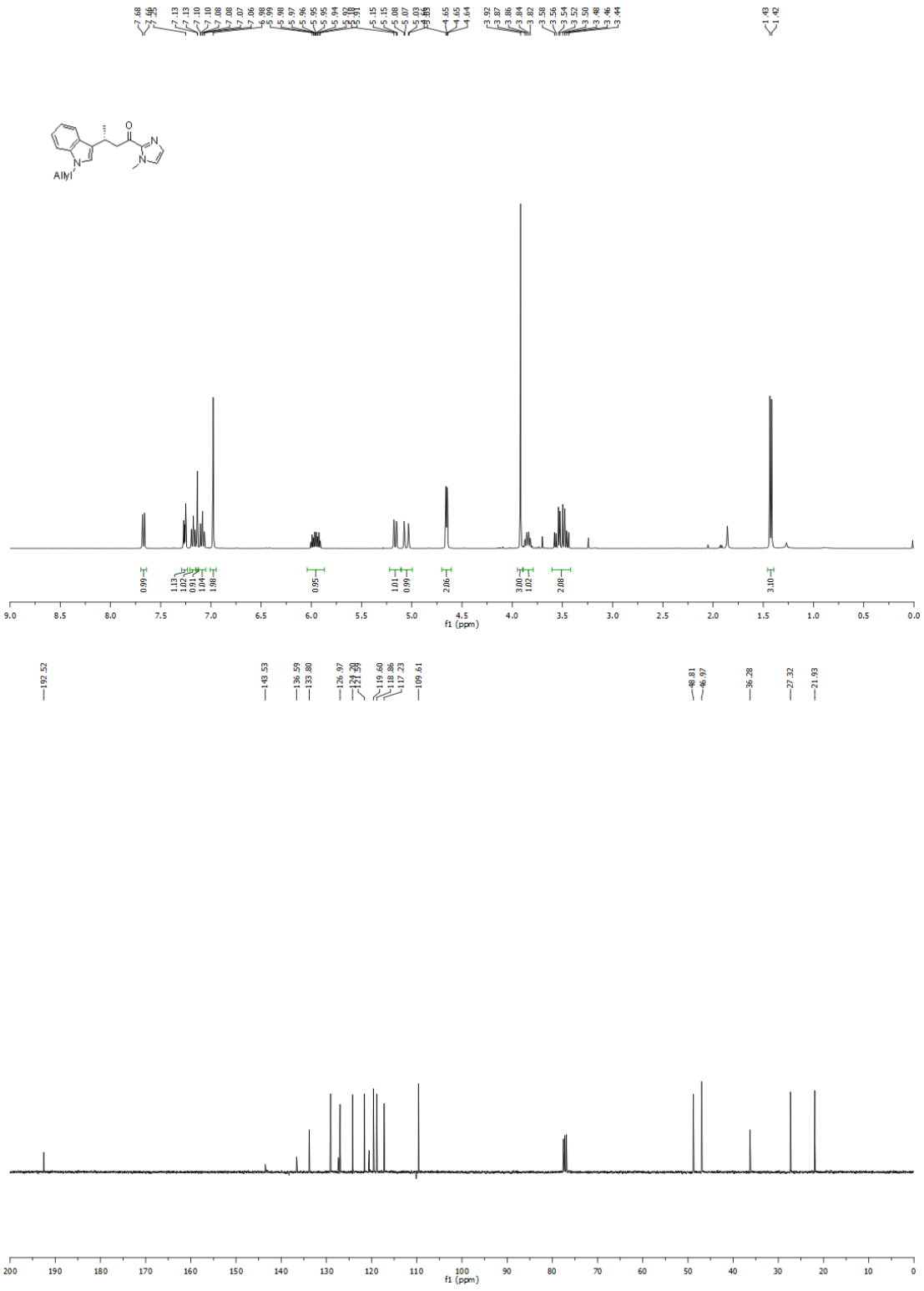
(*R*,*R*)-*N*,*N'*-Dimethyl-*N*,*N'*-bis(5,6,7,8-tetrahydroacridin-4-yl)cyclohexane-1,2-diamine (**2f**)



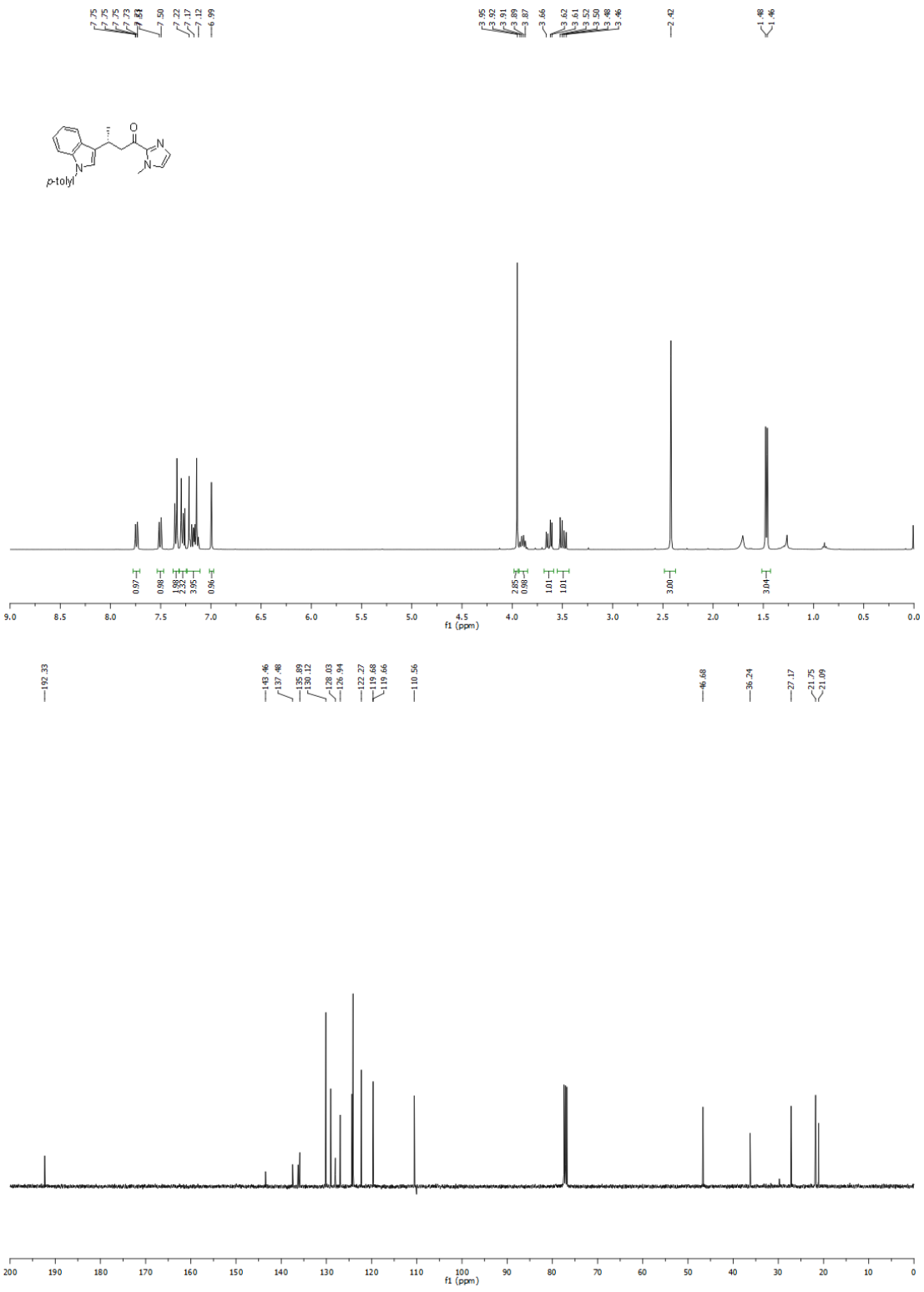
(*R*)-3-(1-Benzyl-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one (**5b**)



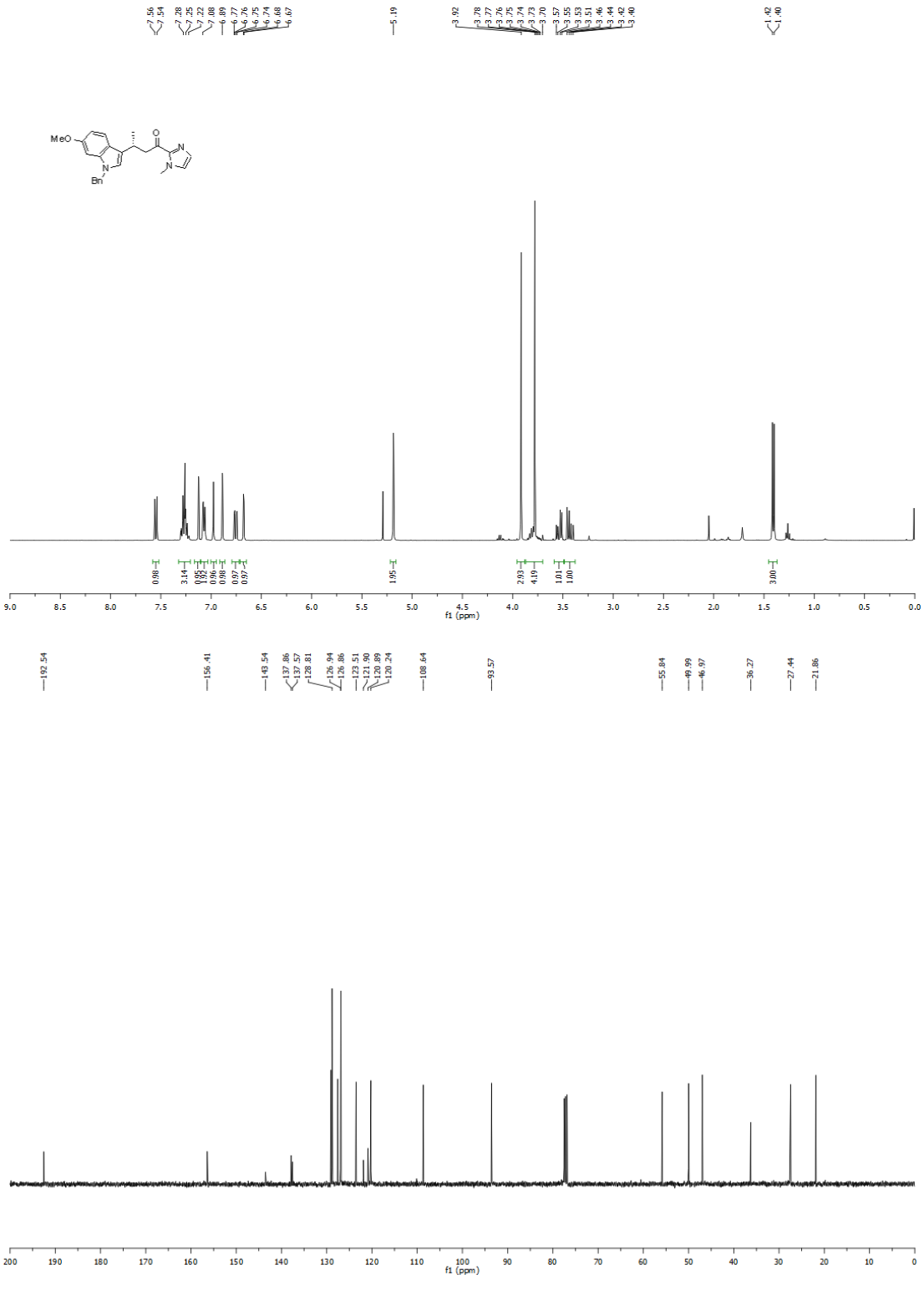
(*R*)-3-(1-Allyl-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one (**5c**)



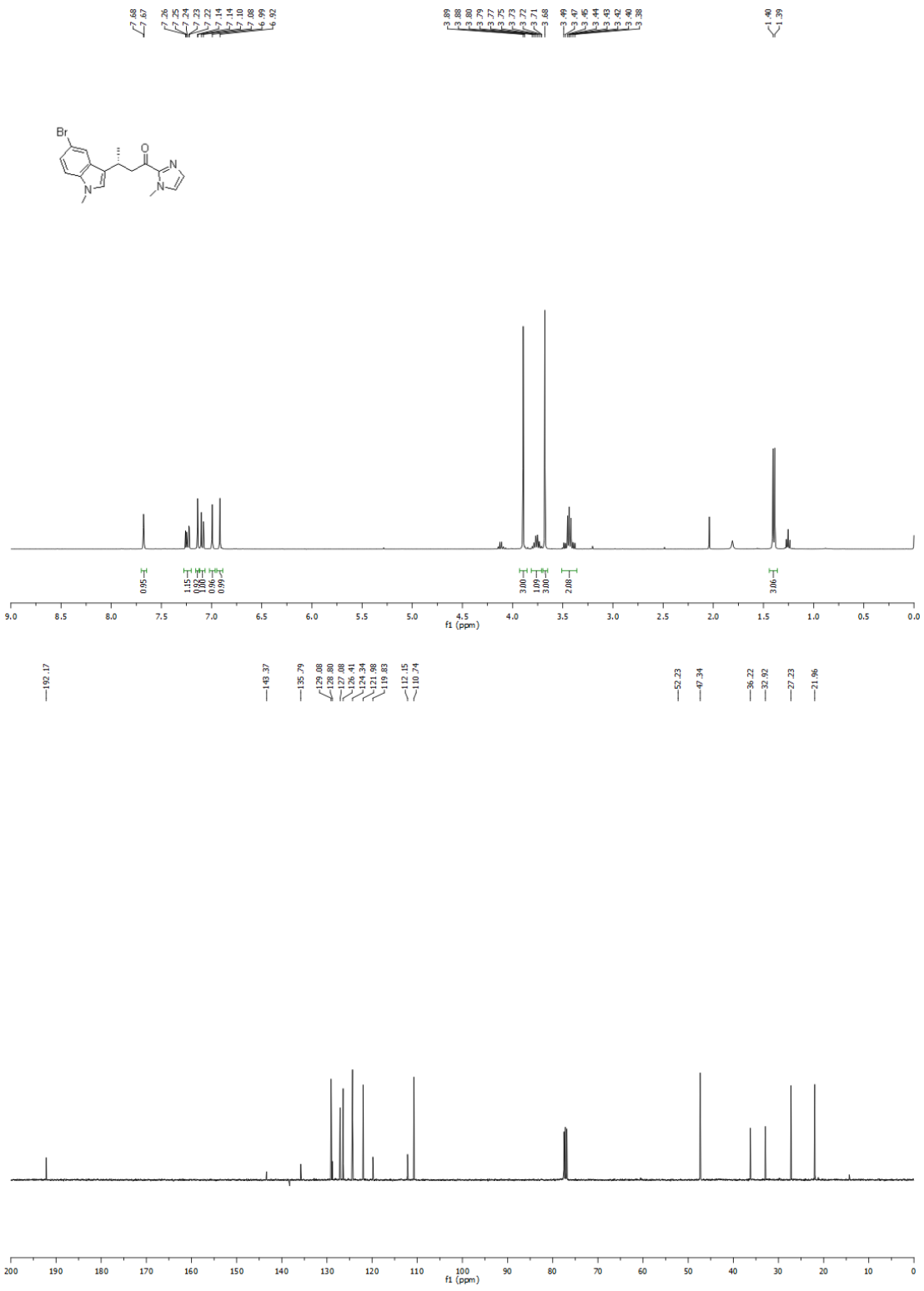
(*R*)-1-(1-Methyl-1*H*-imidazol-2-yl)-3-(1-(p-tolyl)-1*H*-indol-3-yl)butan-1-one (**5d**)



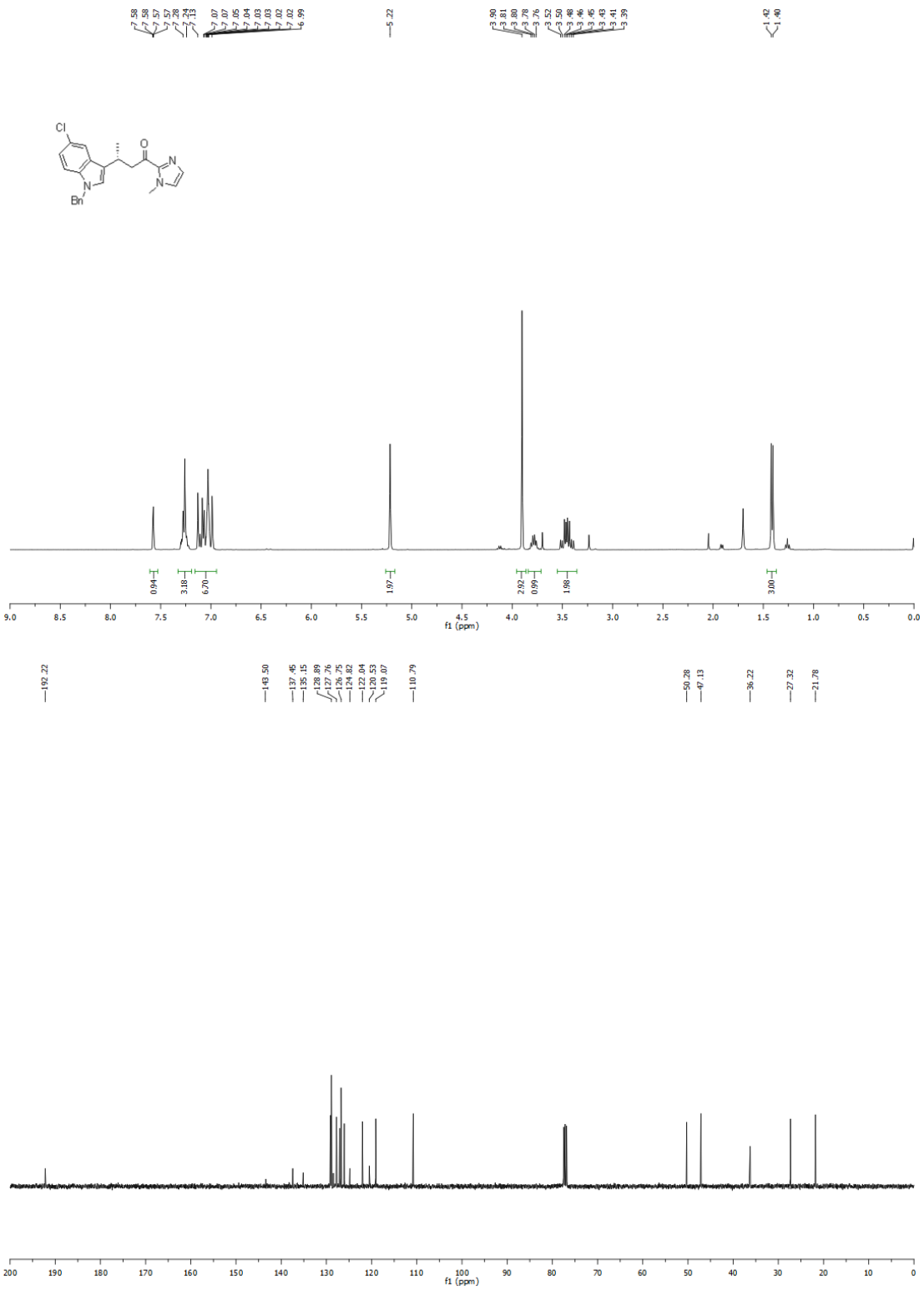
(*R*)-3-(1-Benzyl-6-methoxy-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one (**5e**)



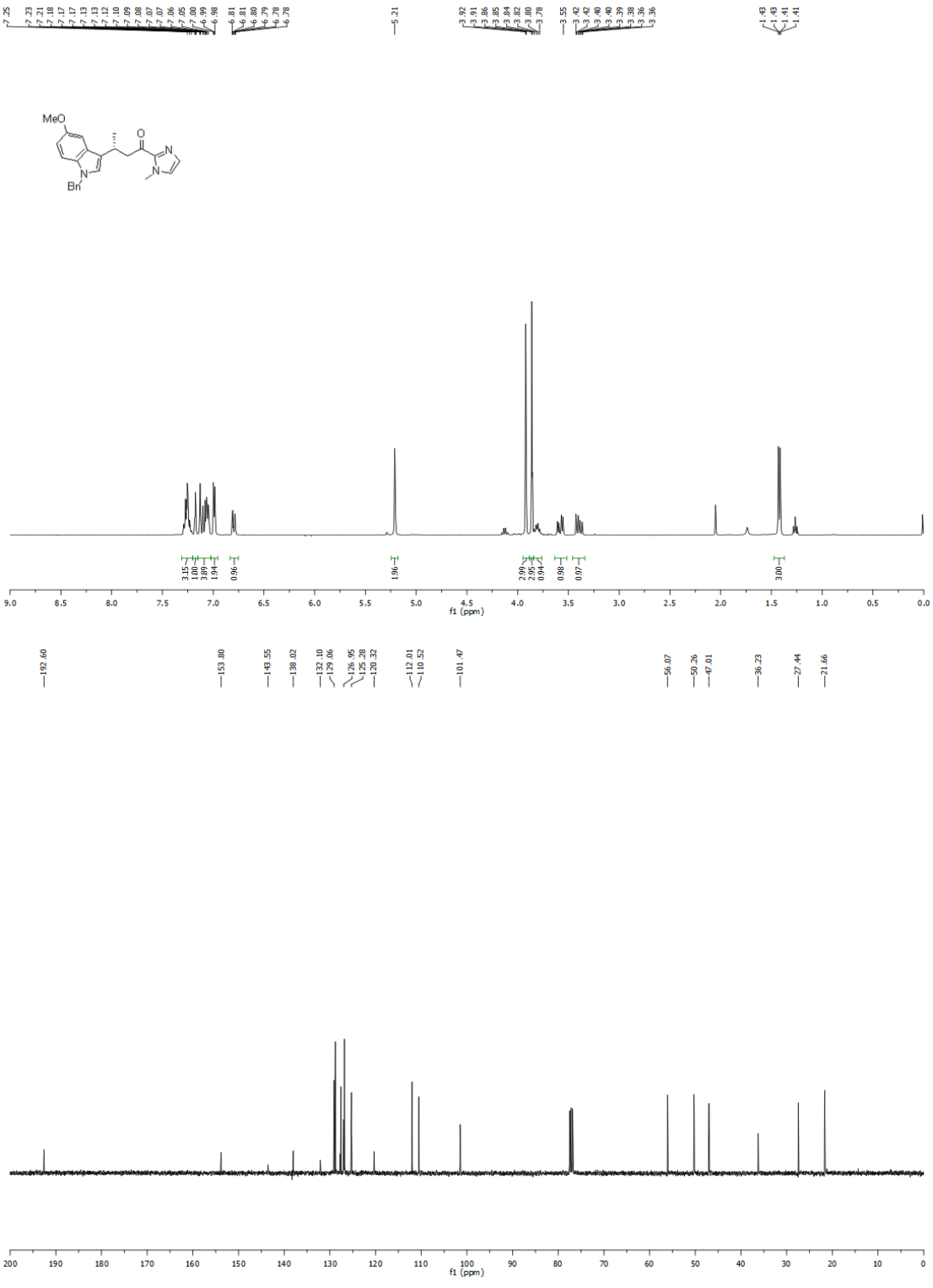
(*R*)-3-(5-Bromo-1-methyl-1*H*-indolyl)-1-(1-methyl-1*H*-imidazolyl)butan-1-one (**5f**)



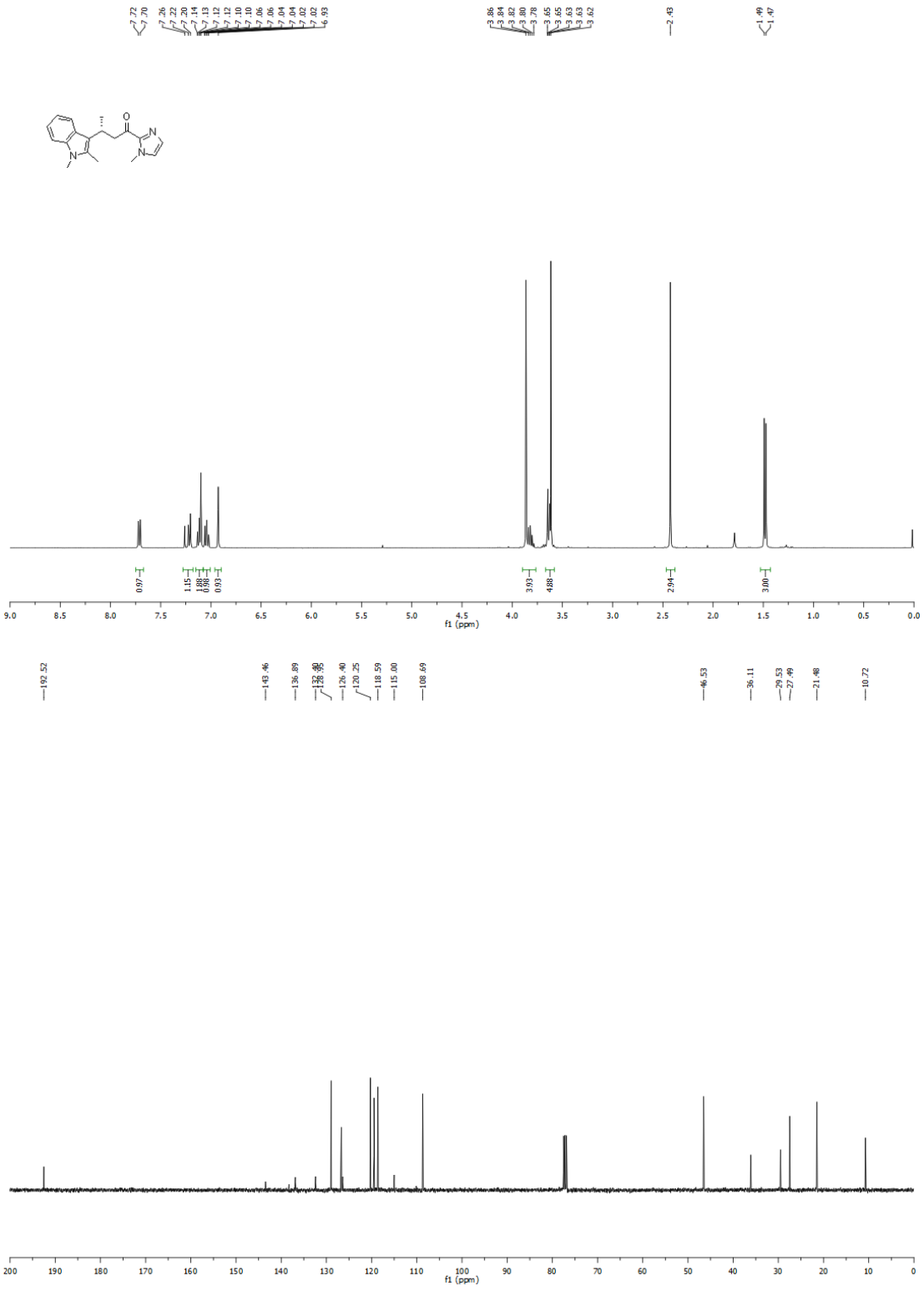
(*R*)-3-(1-Benzyl-5-chloro-1*H*-indolyl)-1-(1-methyl-1*H*-imidazolyl)butan-1-one (**5g**)



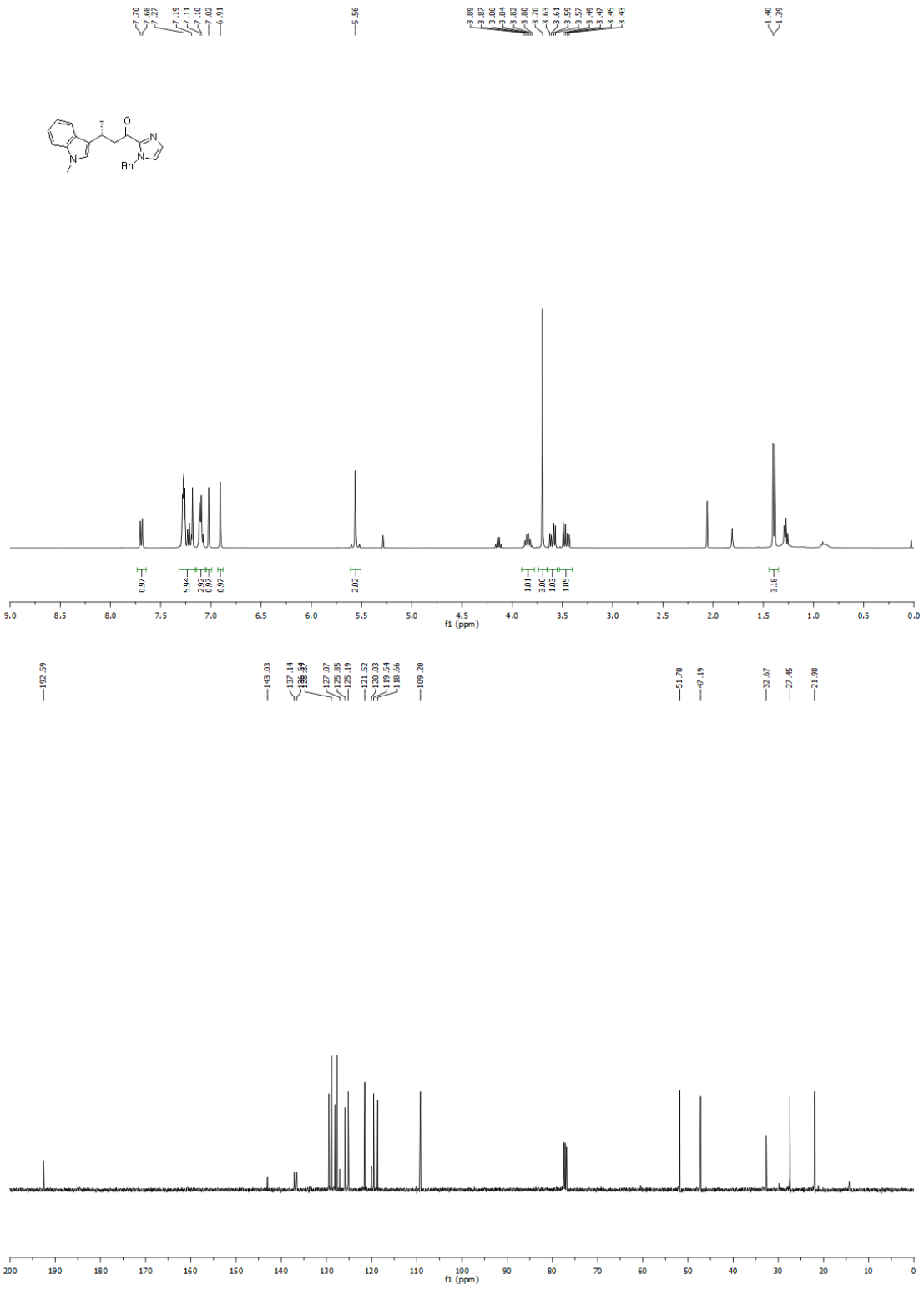
(*R*)-3-(1-Benzyl-5-methoxy-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one (**5h**)



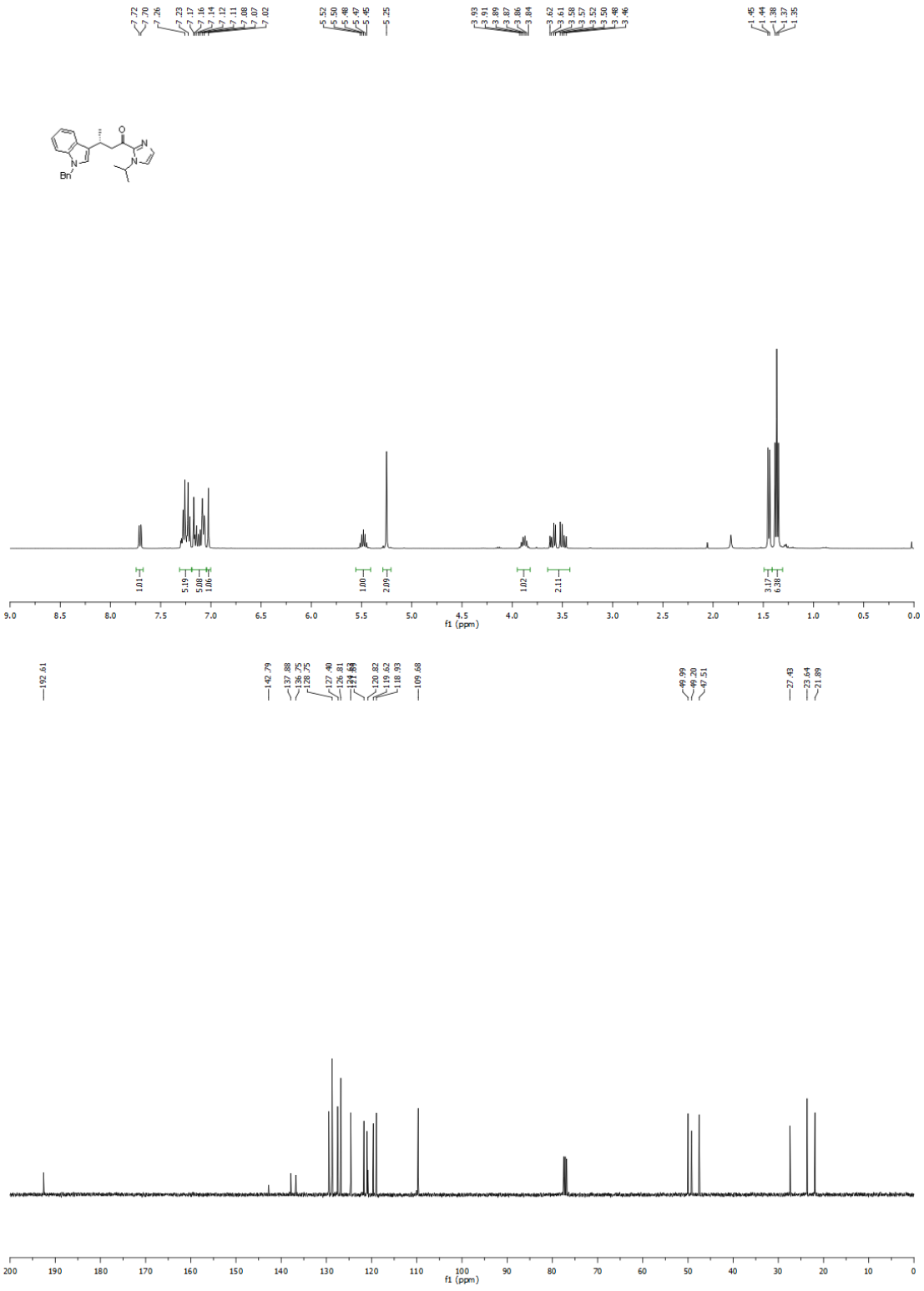
(*R*)-3-(1,2-Dimethyl-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)butan-1-one (**5i**)



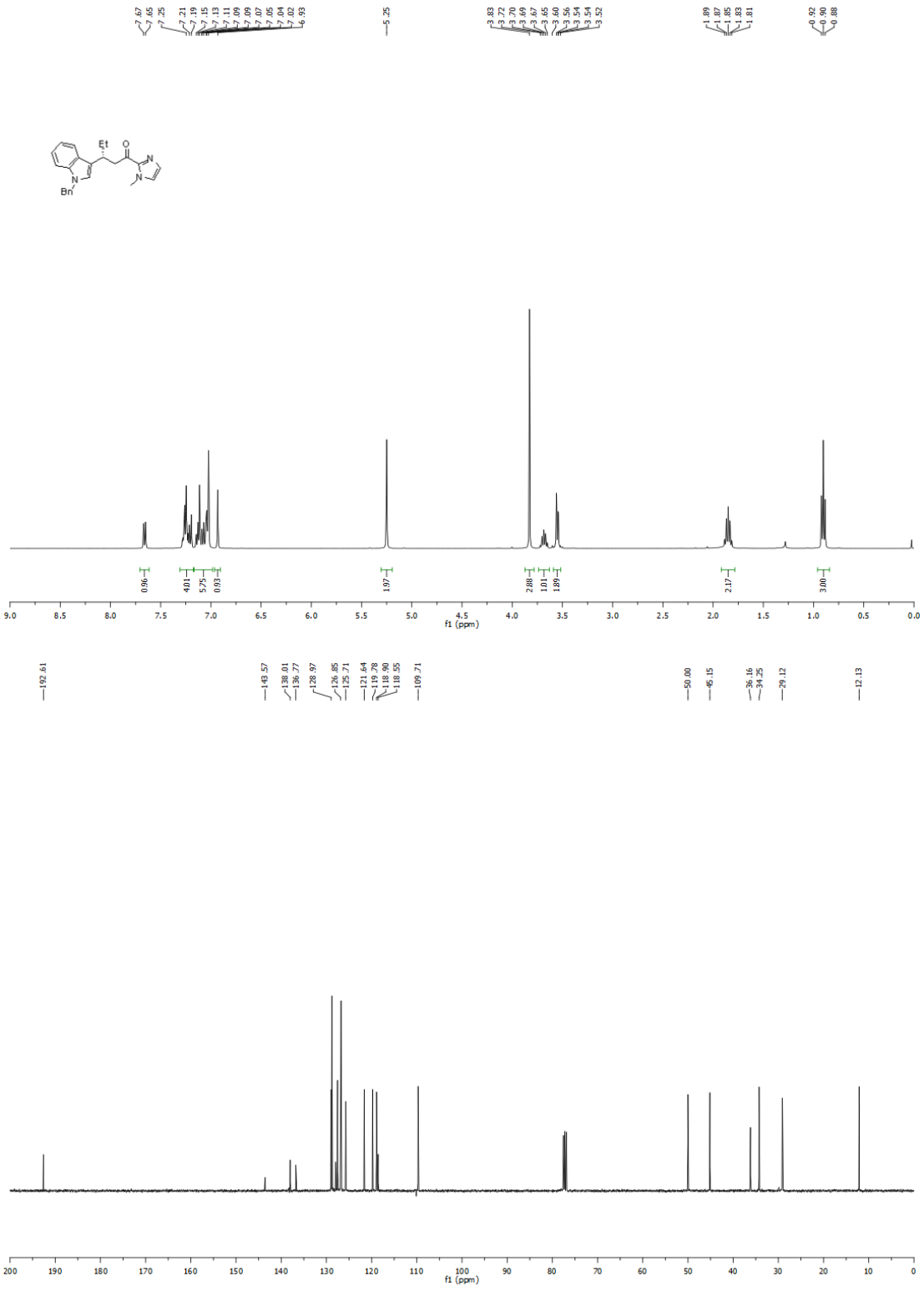
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(1-methyl-1*H*-indol-3-yl) butan-1-one (**5j**)



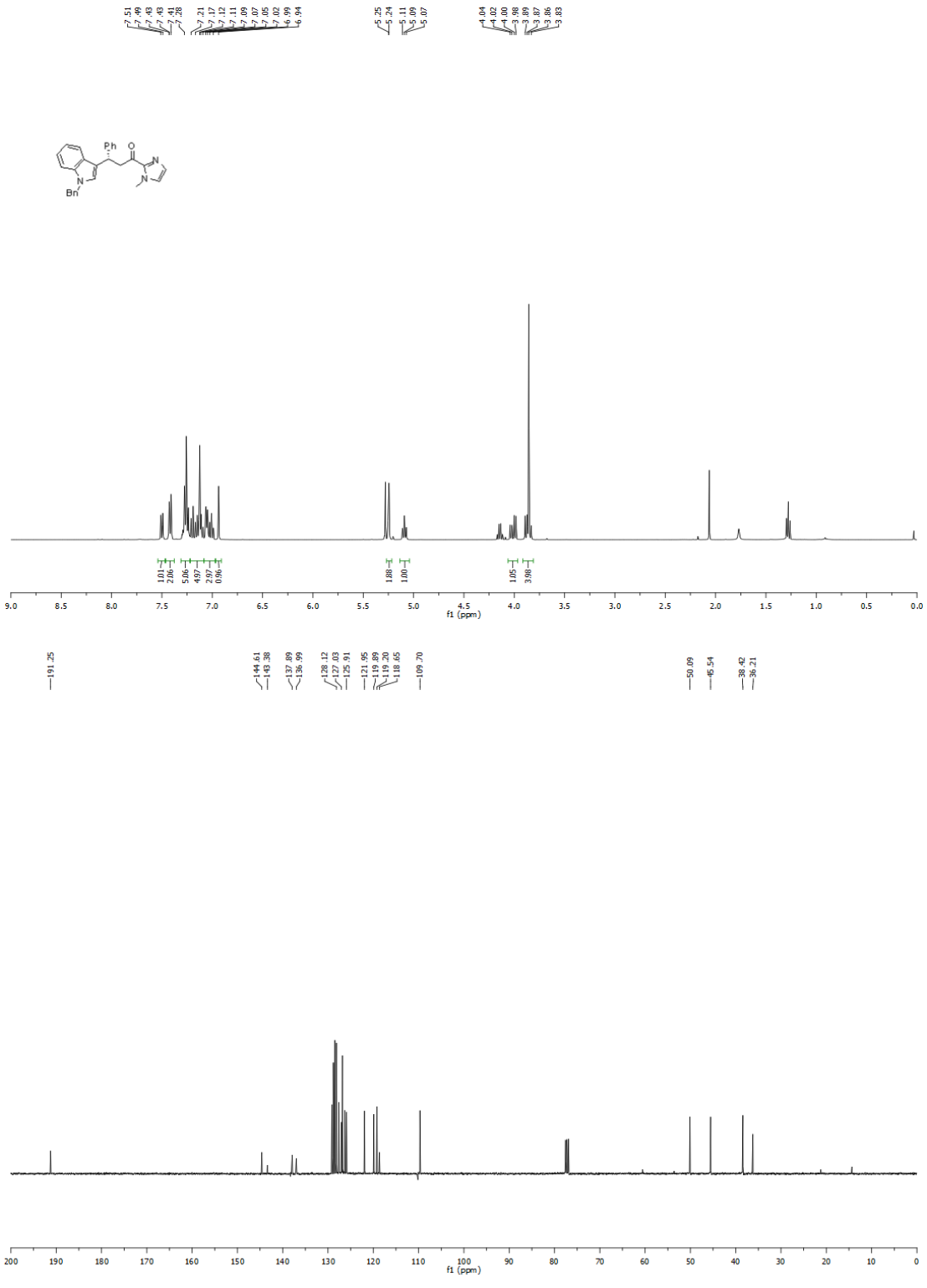
(*R*)-3-(1-Benzyl-1*H*-indol-3-yl)-1-(1-isopropyl-1*H*-imidazol-2-yl) butan-1-one (**5k**)



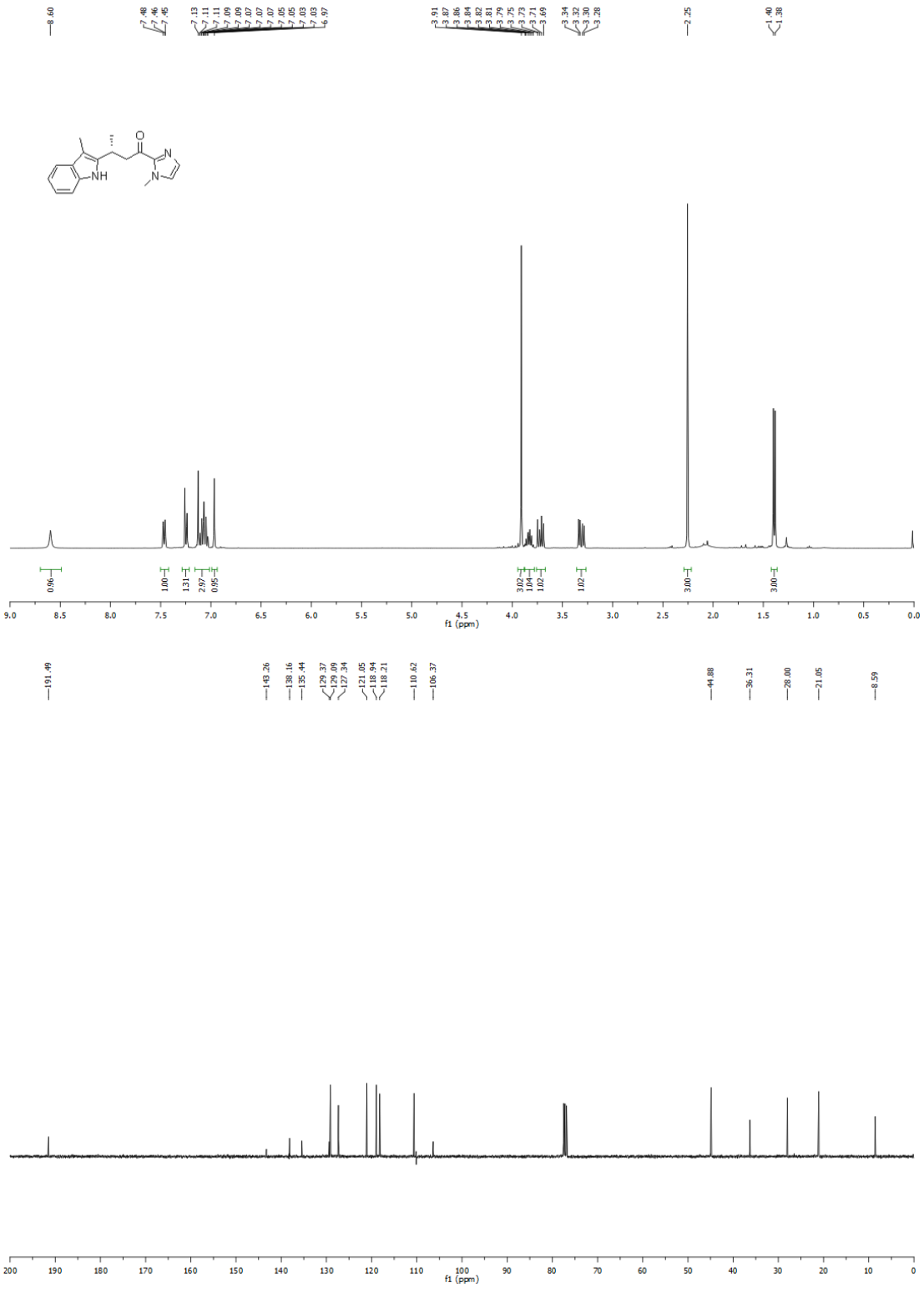
(*R*)-3-(1-Benzyl-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)pentan-1-one (**5l**)



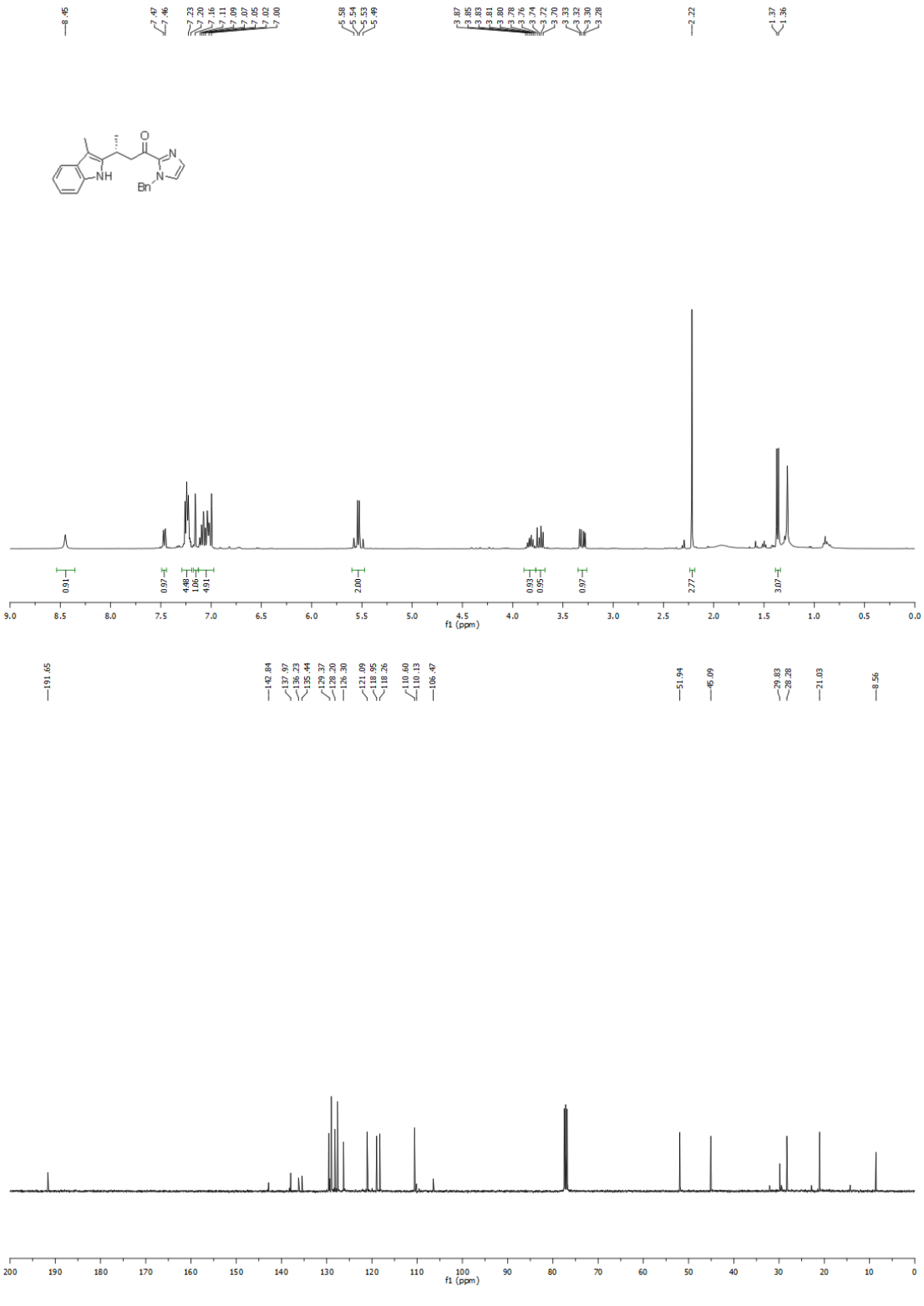
(*S*)-3-(1-Benzyl-1*H*-indol-3-yl)-1-(1-methyl-1*H*-imidazol-2-yl)-3-phenyl-propan-1-one (**5m**)



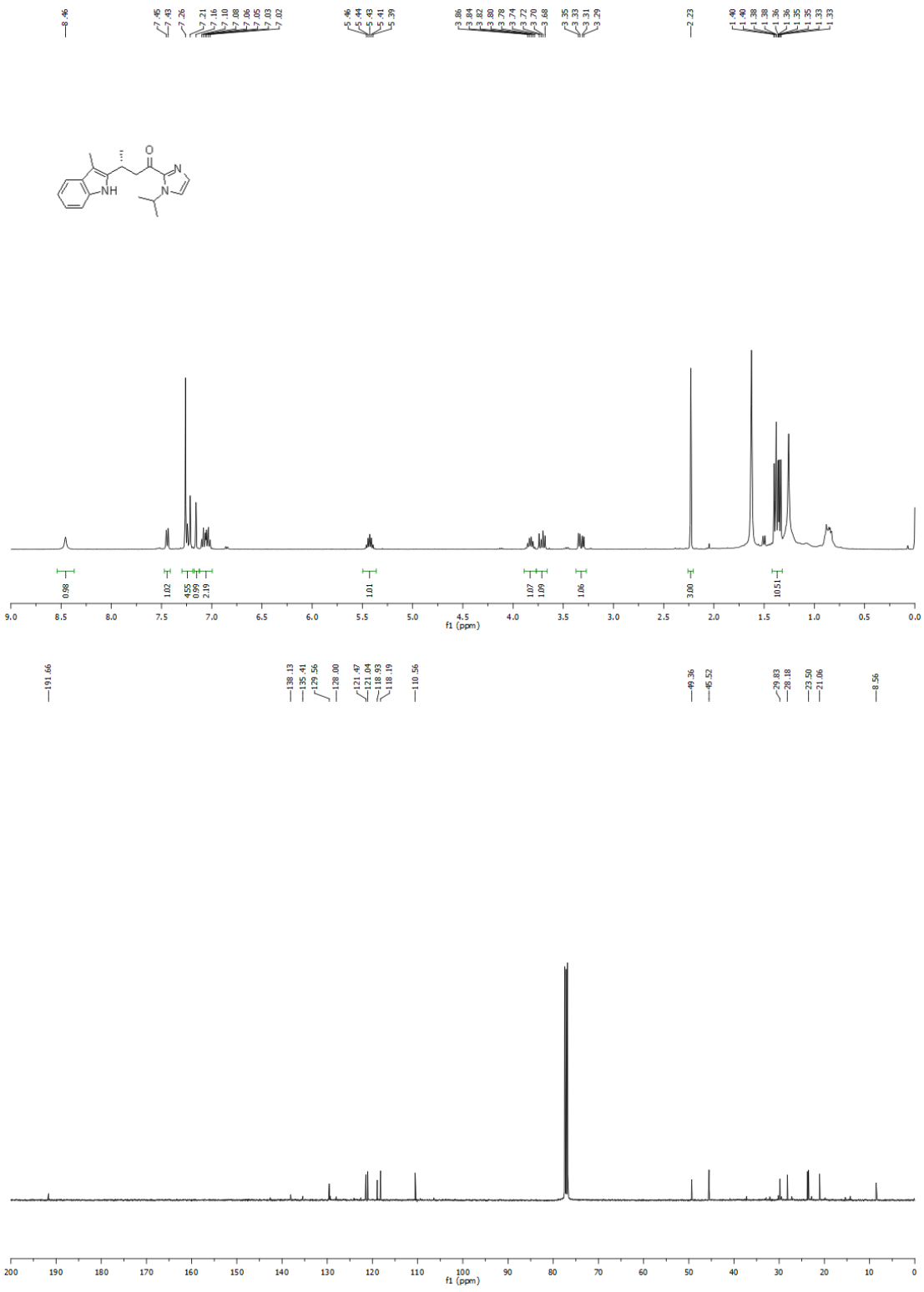
(*R*)-1-(1-Methyl-1*H*-imidazol-2-yl)-3-(3-methyl-1*H*-indol-2-yl)butan-1-one (**6a**)



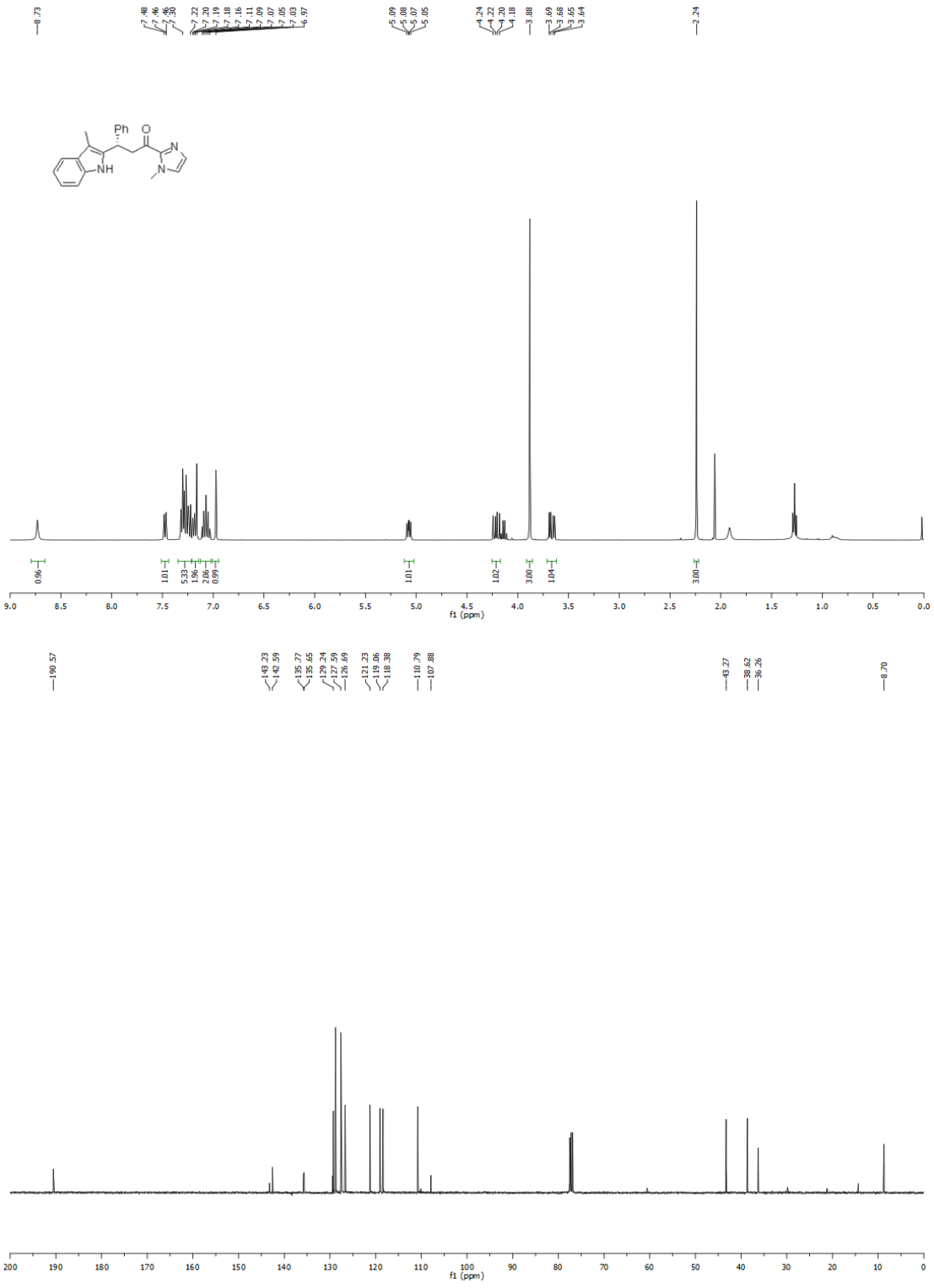
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(3-methyl-1*H*-indol-2-yl) butan-1-one (**6b**)



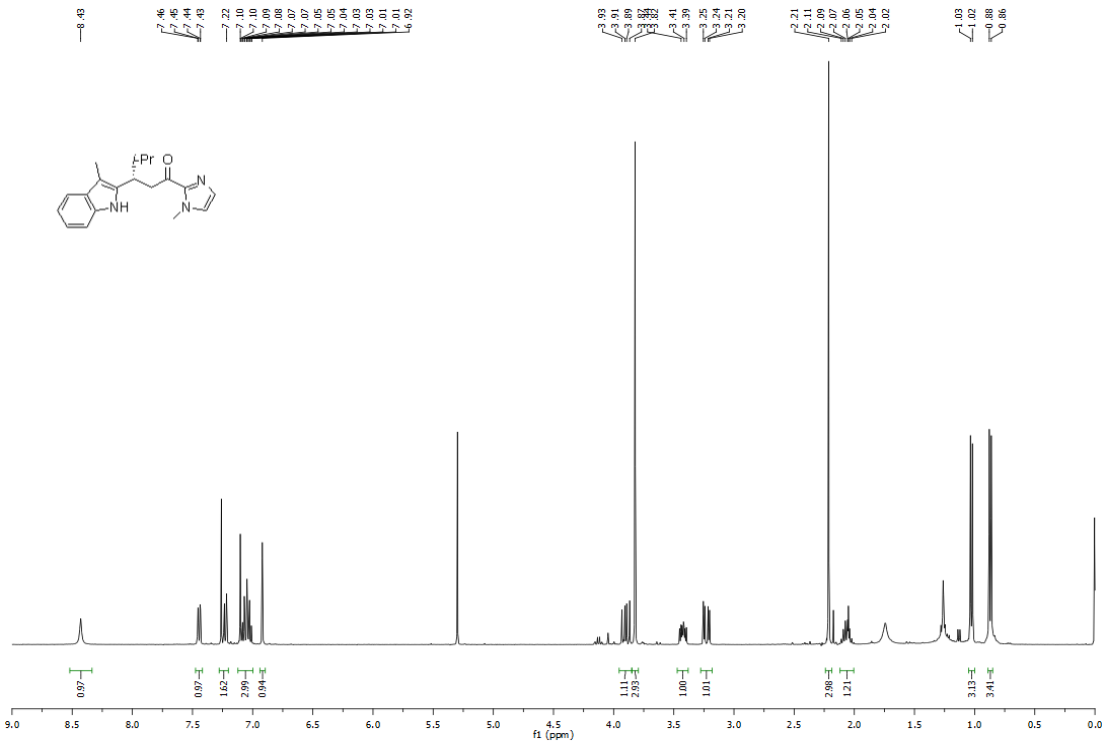
(*R*)-1-(1-Isopropyl-1*H*-imidazol-2-yl)-3-(3-methyl-1*H*-indol-2-yl) butan-1-one (**6c**)

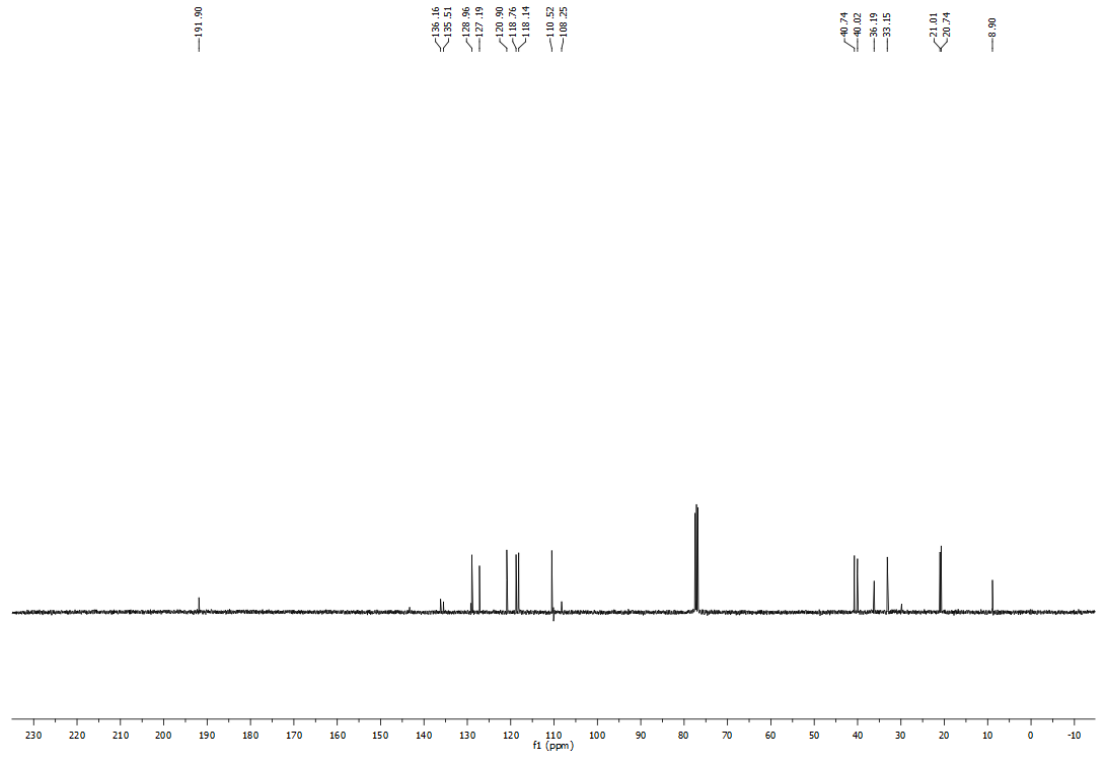


(*S*)-1-(1-Methyl-1*H*-imidazol-2-yl)-3-(3-methyl-1*H*-indol-2-yl)-3-phenyl-propan-1-one (**6d**)

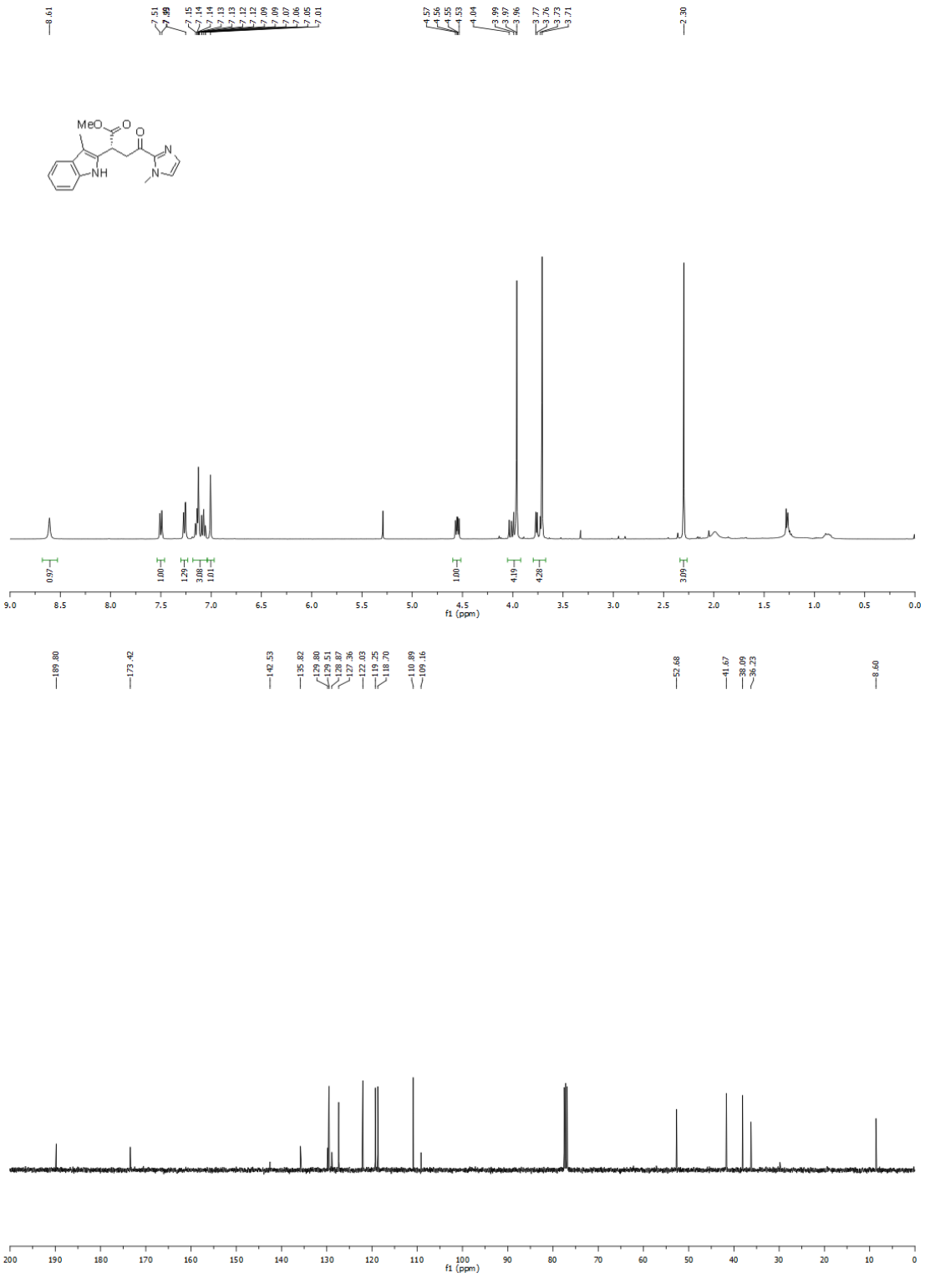


(*S*)-4-Methyl-1-(1-methyl-1*H*-imidazol-2-yl)-3-(3-methyl-1*H*-indol-2-yl)pentan-1-one (**6e**)

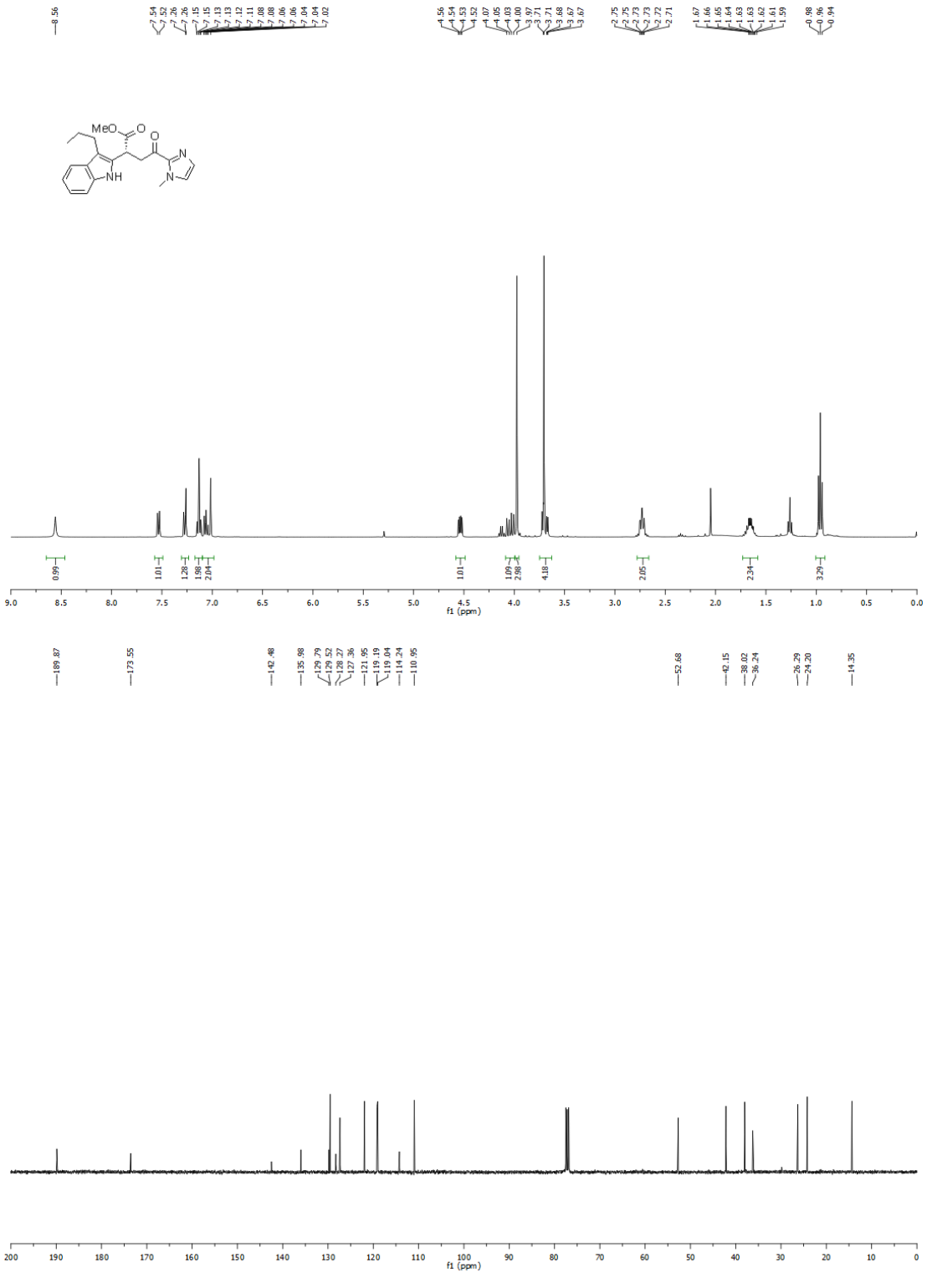




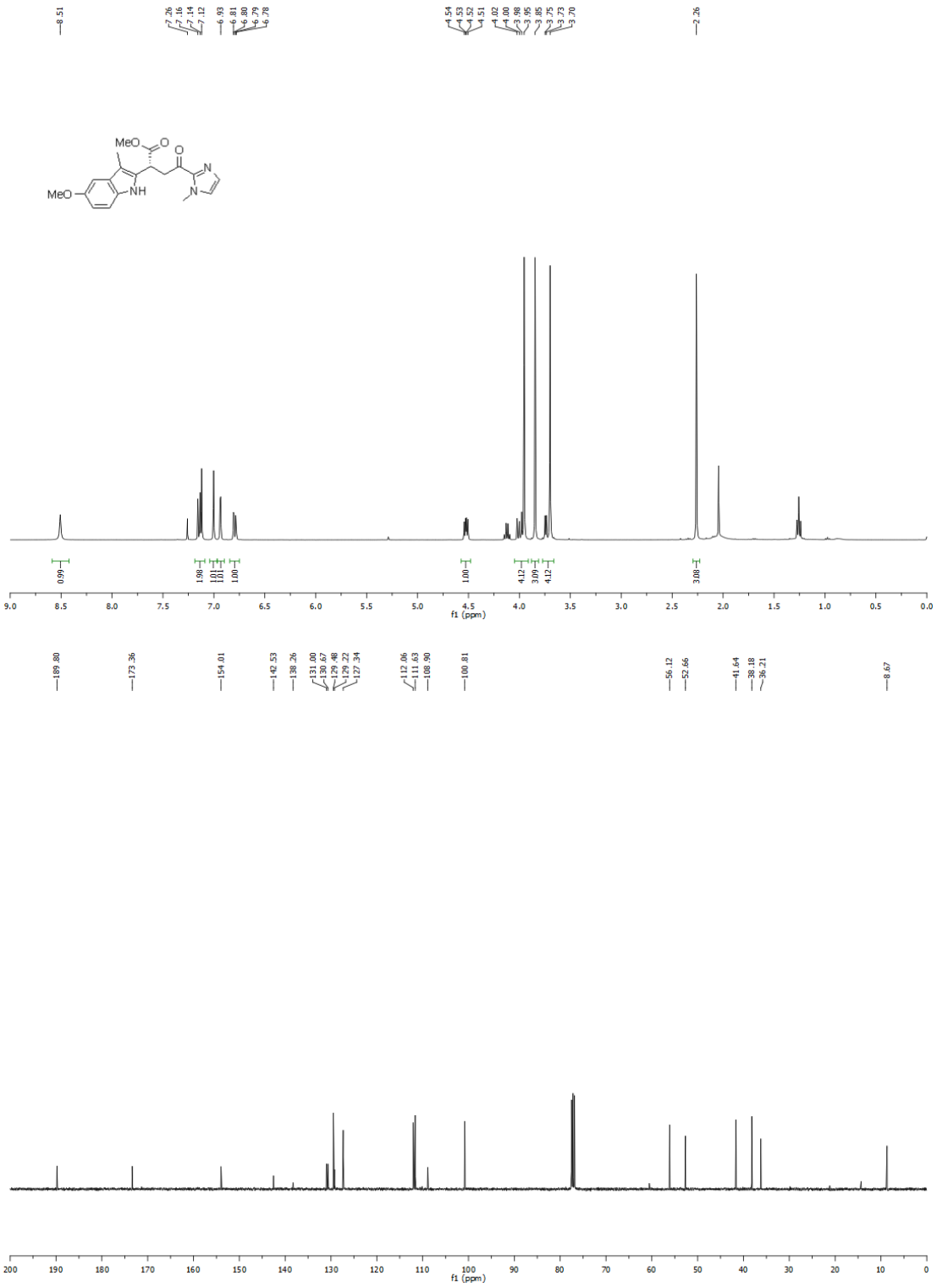
(*R*)-Methyl-4-(1-methyl-1*H*-imidazol-2-yl)-2-(3-methyl-1*H*-indol-2-yl)-4-oxobutanoate (**6f**)



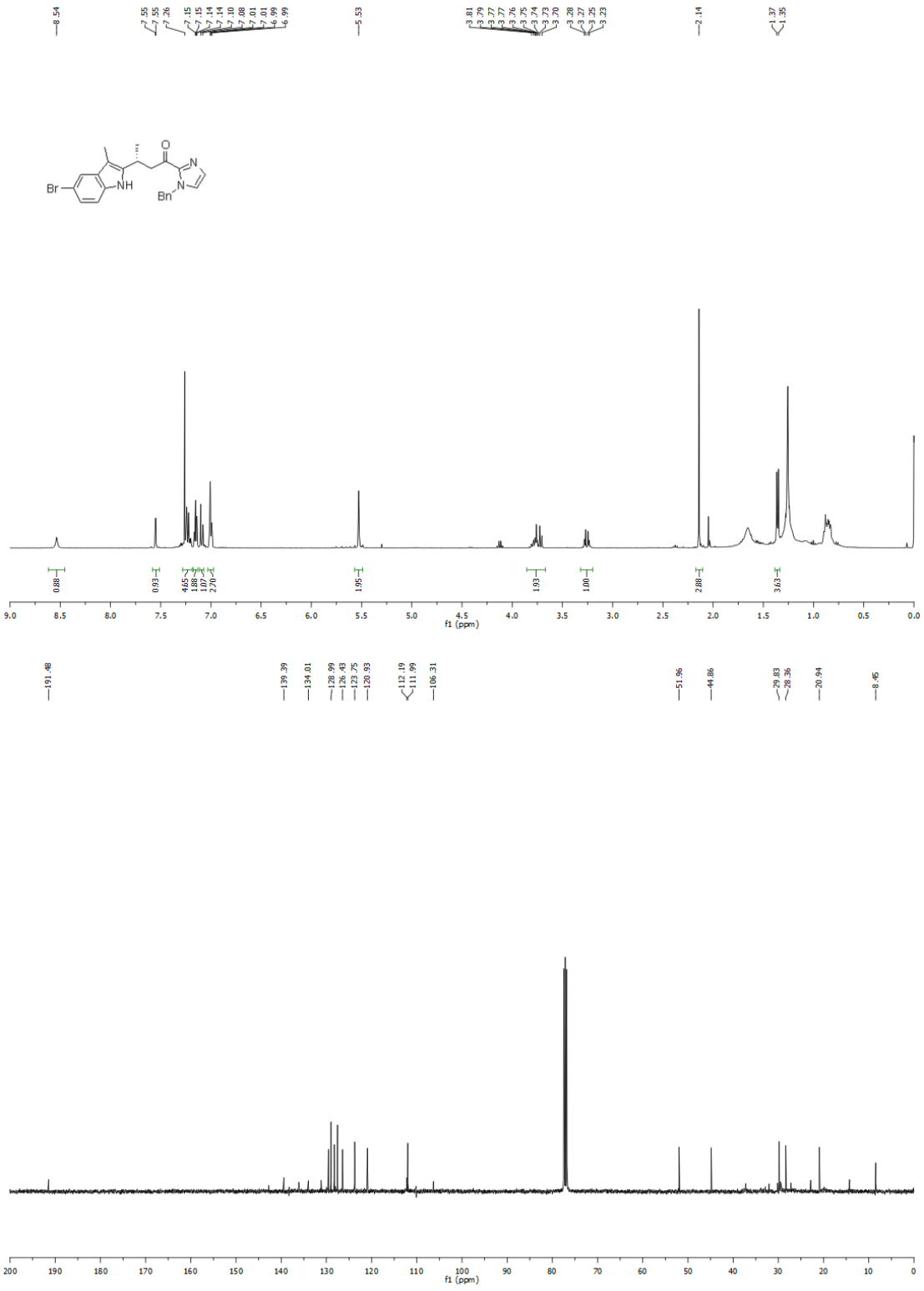
(*R*)-Methyl-4-(1-methyl-1*H*-imidazol-2-yl)-4-oxo-2-(3-propyl-1*H*-indol-2-yl) butanoate (**6g**)



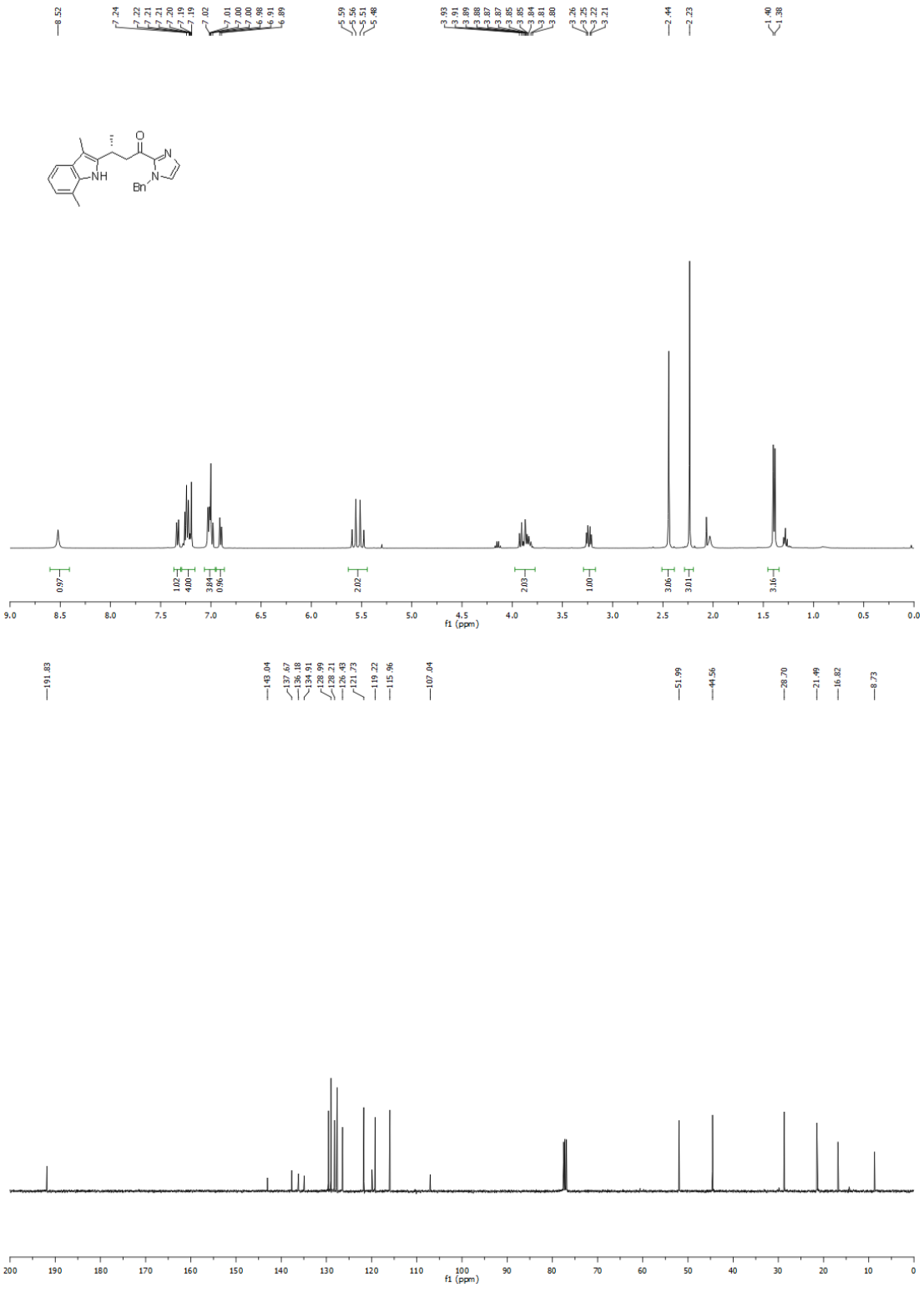
(*R*)-Methyl-2-(5-methoxy-3-methyl-1*H*-indol-2-yl)-4-(1-methyl-1*H*-imidazol-2-yl)-4-oxobutanoate (**6h**)



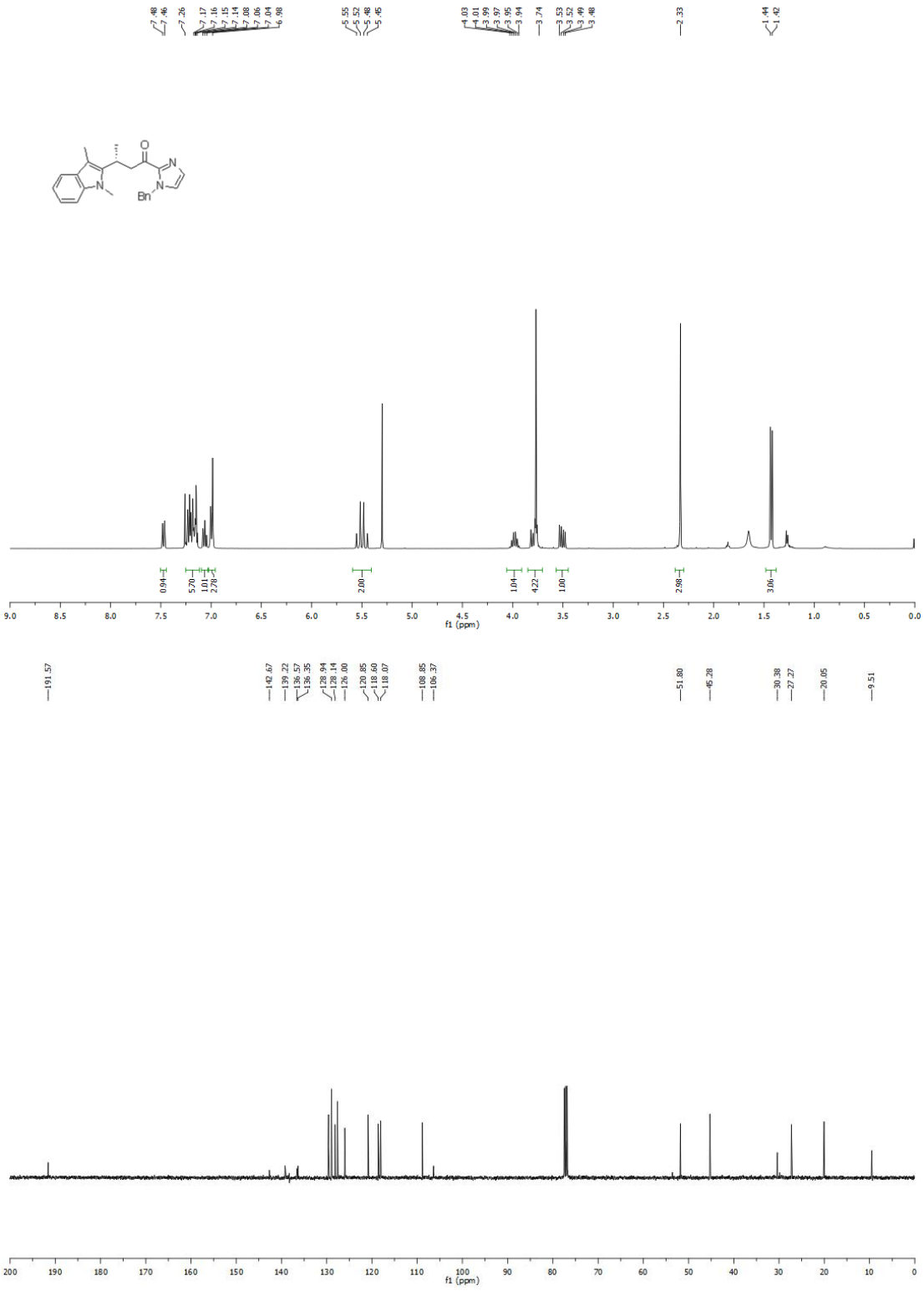
(*R*)-1-(1-Benzyl-1*H*-imidazolyl)-3-(5-bromo-3-methyl-1*H*-indolyl)butan-1-one (**6i**)



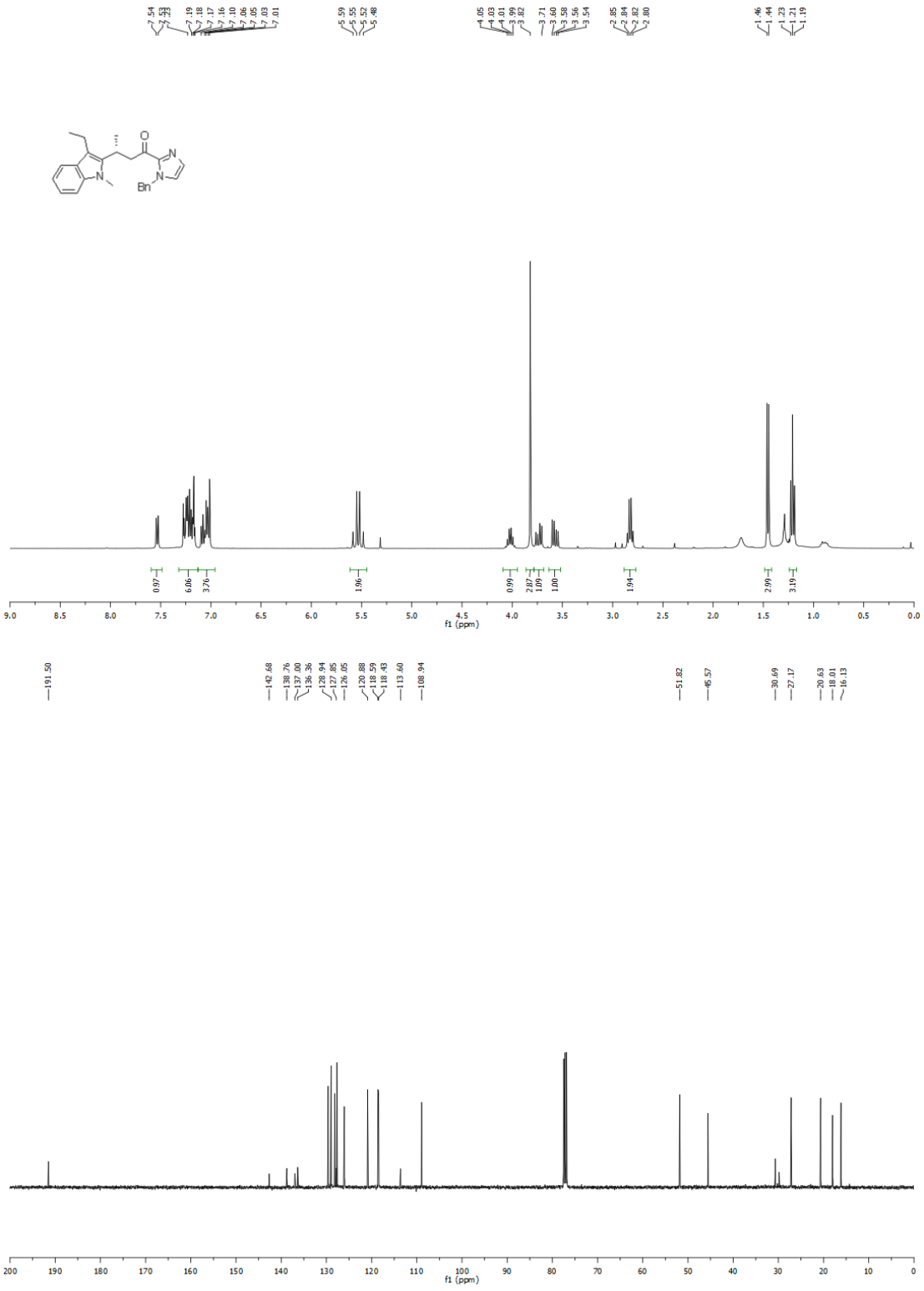
(*R*)-1-(1-Benzyl-1*H*-imidazolyl)-3-(3,7-dimethyl-1*H*-indol-2-yl)butan-1-one (**6j**)



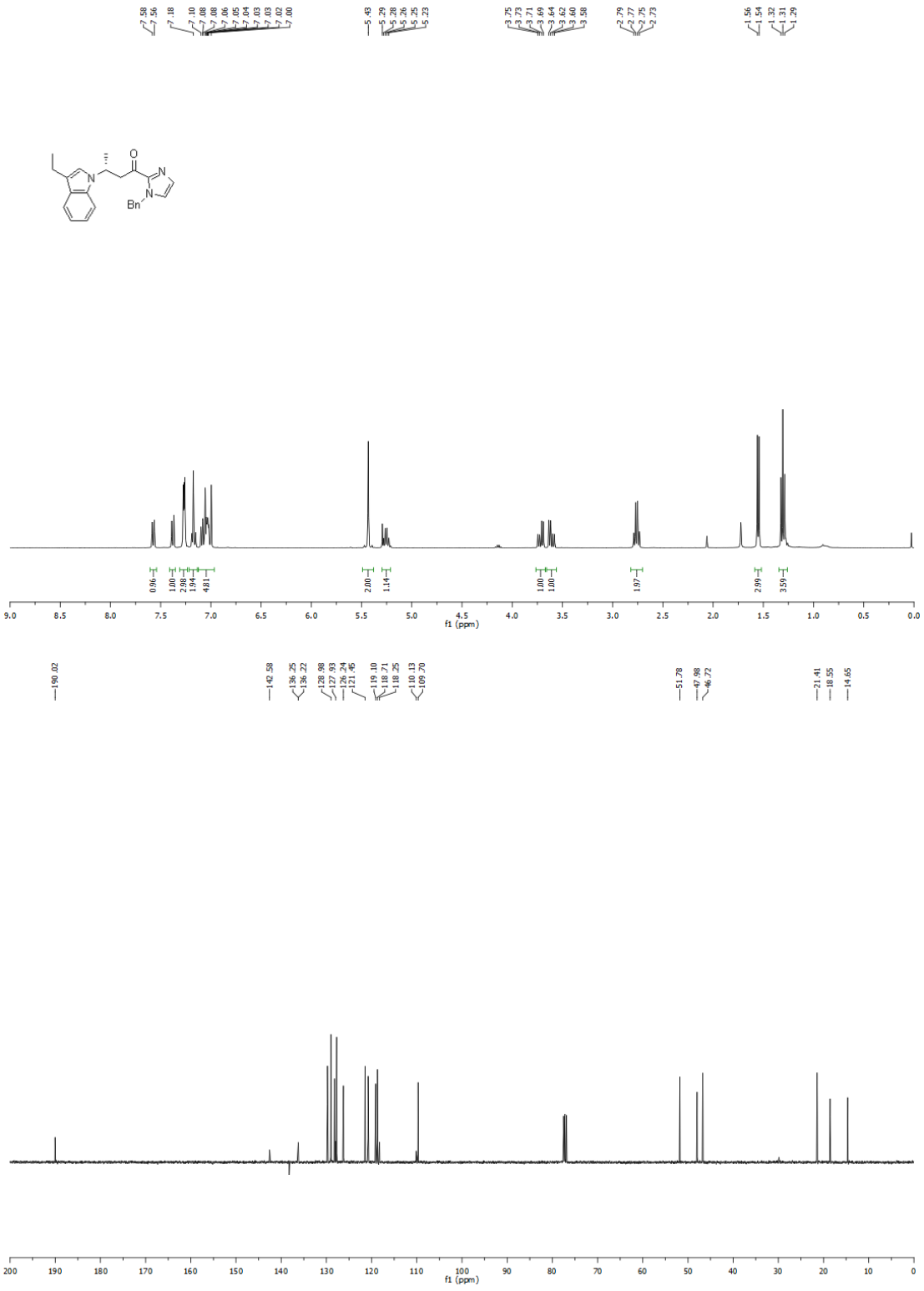
(*R*)-1-(1-Benzyl-1*H*-imidazolyl)-3-(1,3-dimethyl-1*H*-indol-2-yl) butan-1-one (**6k**)



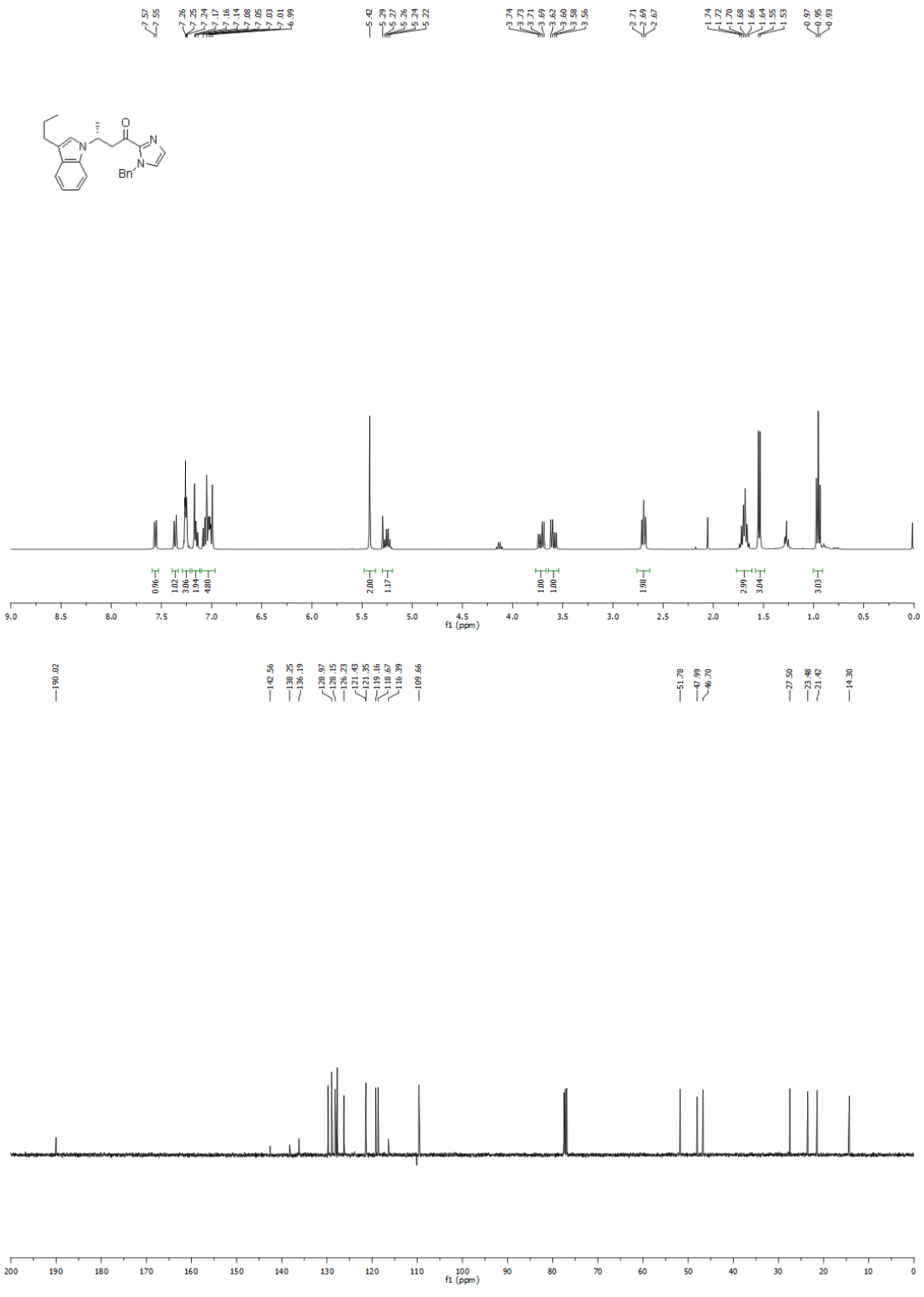
(*R*)-1-(1-Benzyl-1*H*-imidazolyl)-3-(3-ethyl-1-methyl-1*H*-indolyl) butan-1-one (**6l**)



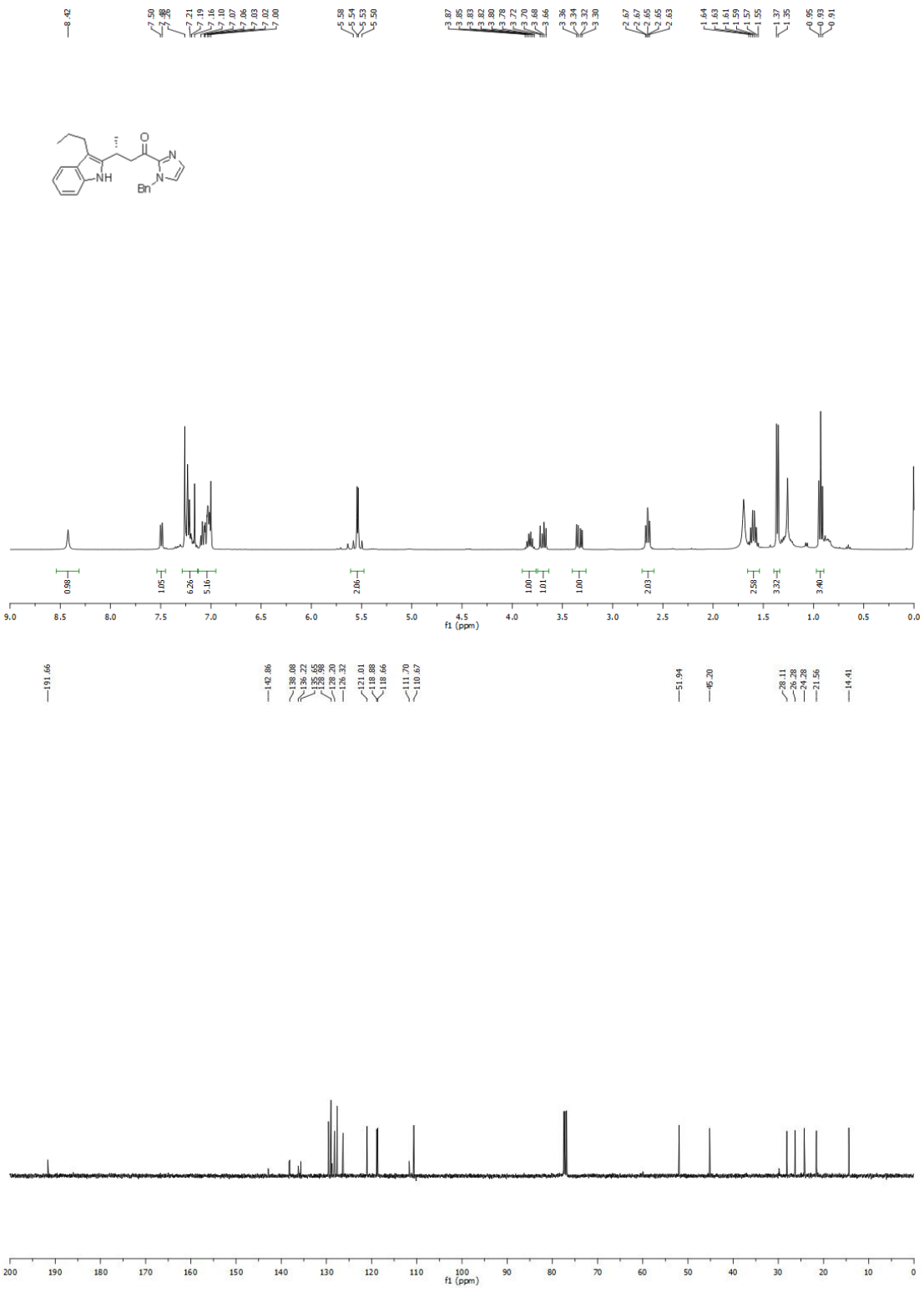
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(3-ethyl-1*H*-indol-1-yl)butan-1-one (**7a**)



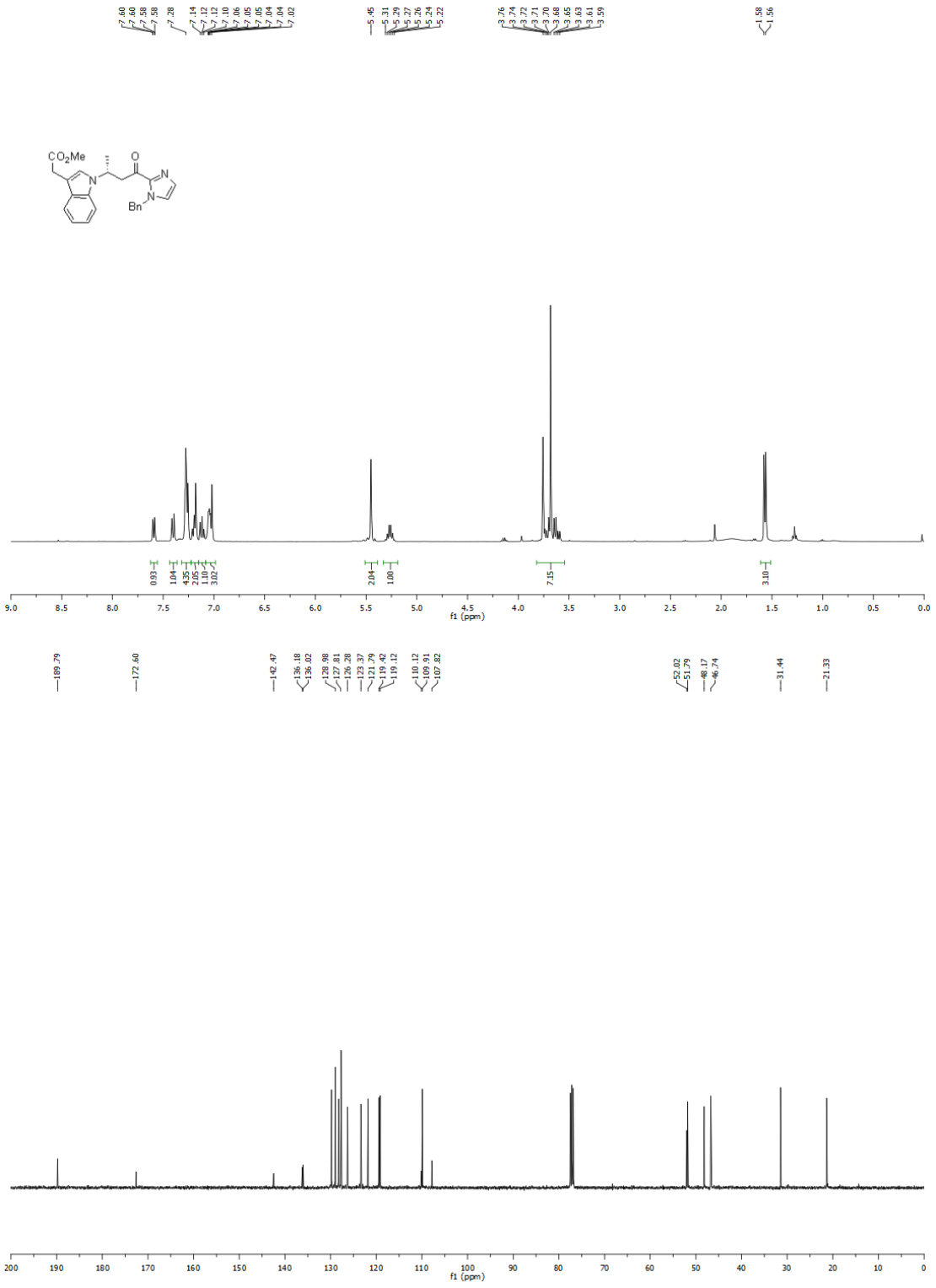
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(3-propyl-1*H*-indol-1-yl)butan-1-one (**7b**)



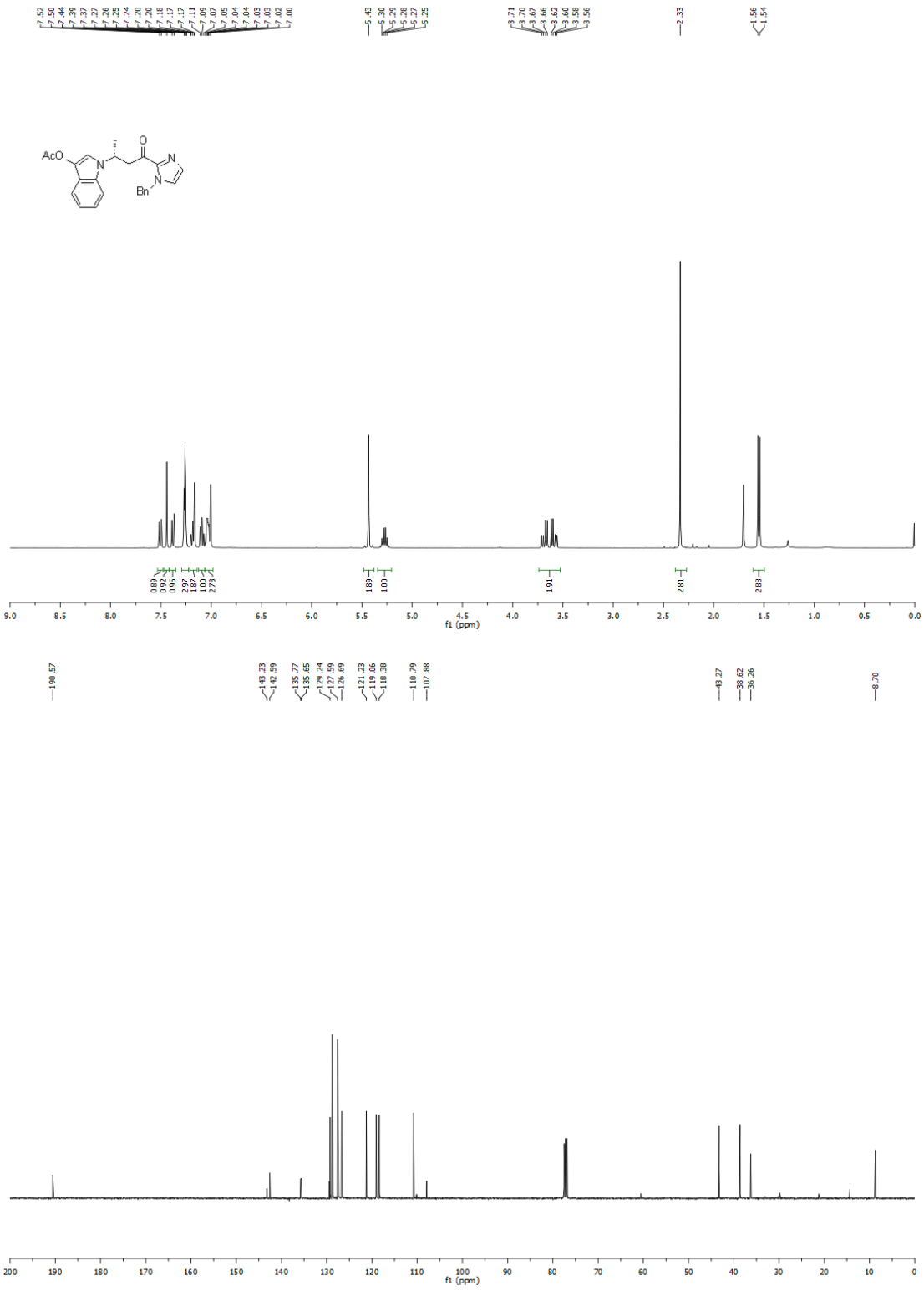
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(3-propyl-1*H*-indolyl)butan-1-one (**7b'**)



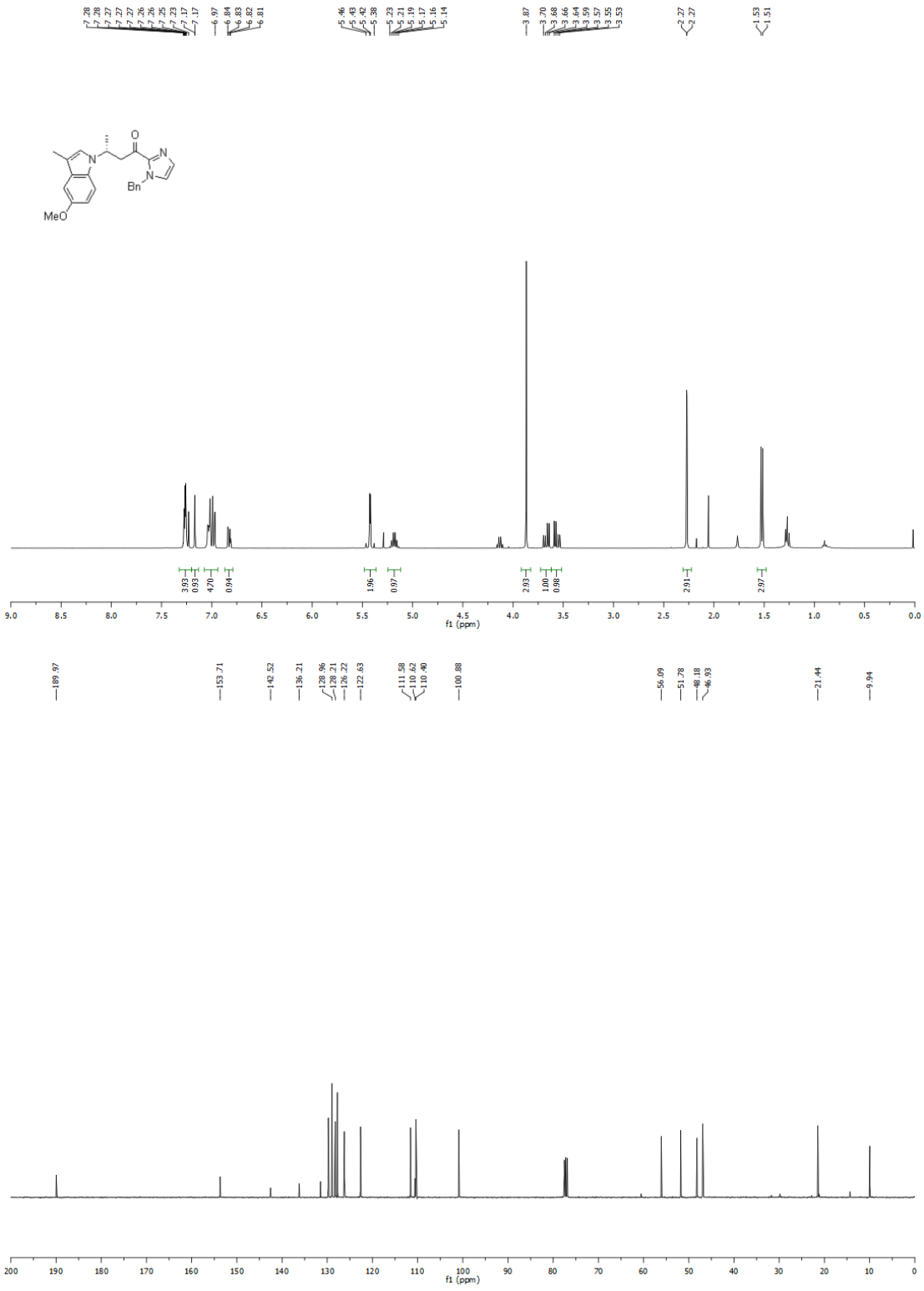
(*R*)-Methyl-2-(1-(4-(1-benzyl-1*H*-imidazol-2-yl)-4-oxobutan-2-yl)-1*H*-indol-3-yl) acetate (**7c**)



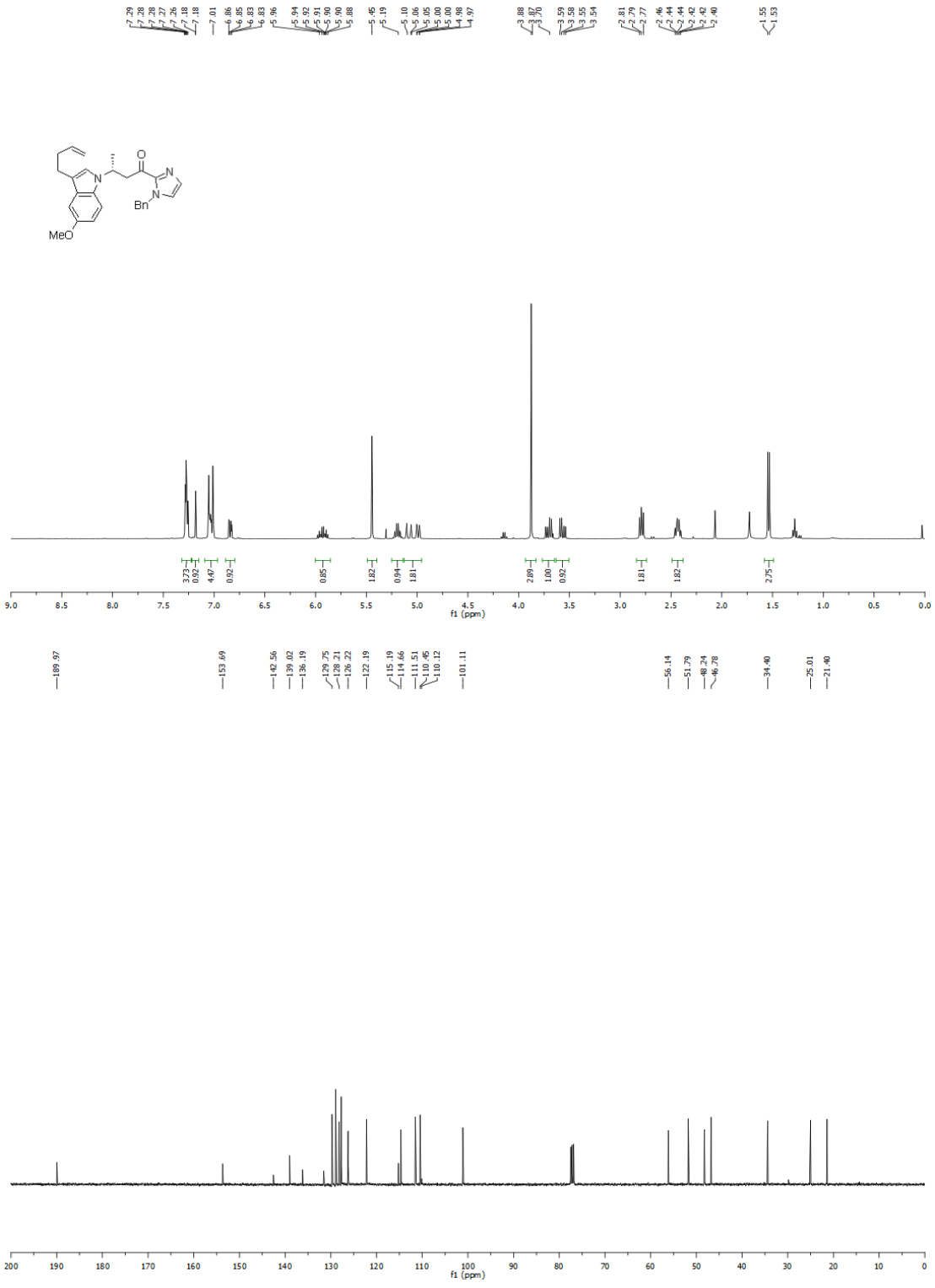
(*R*)-1-(4-(1-Benzyl-1*H*-imidazolyl)-4-oxobutan-2-yl)-1*H*-indol-3-yl acetate (**7d**)



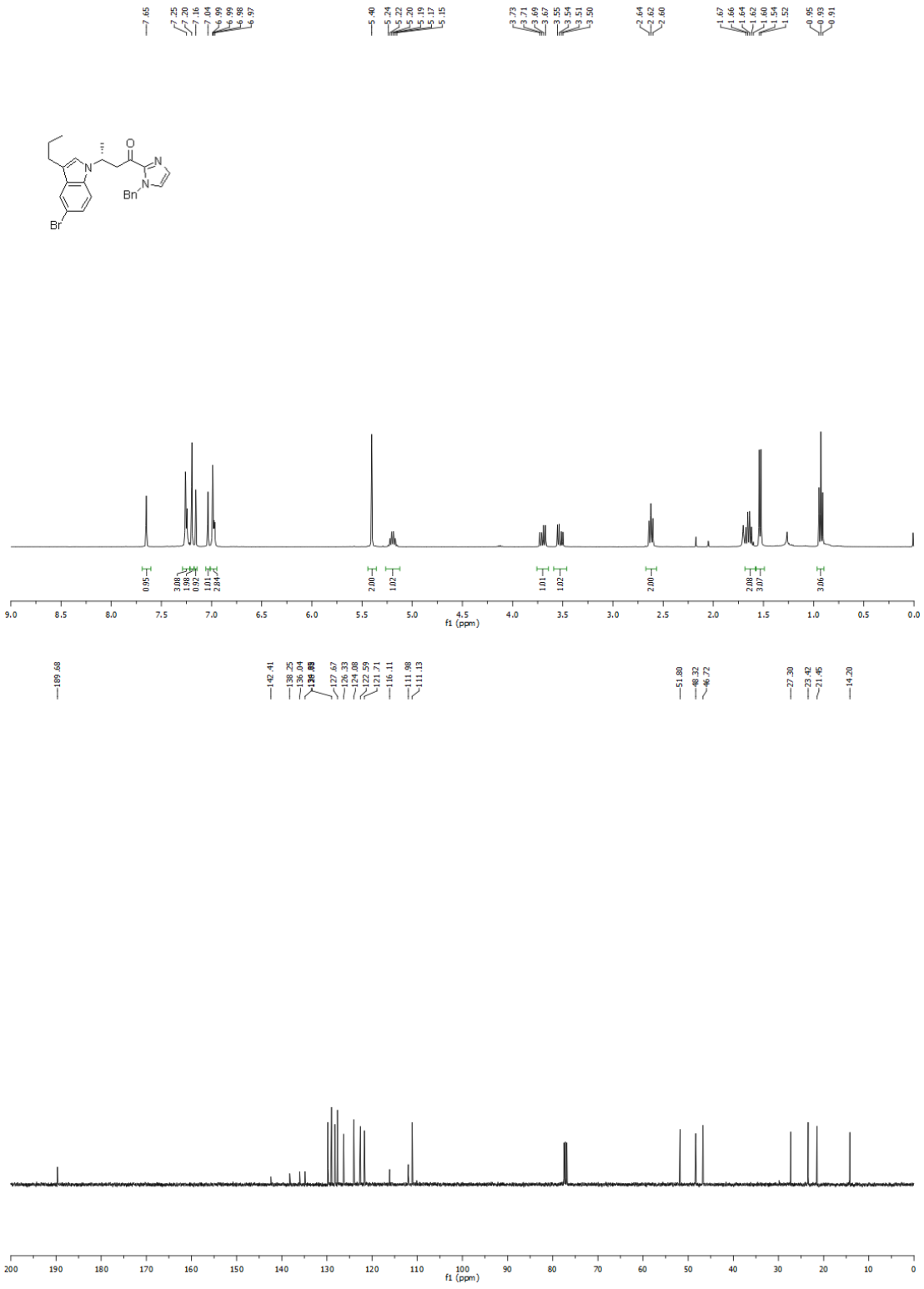
(*R*)-(Benzyl-1*H*-imidazolyl)-3-(5-methoxy-3-methyl-1*H*-indolyl) butan-1-one (**7e**)



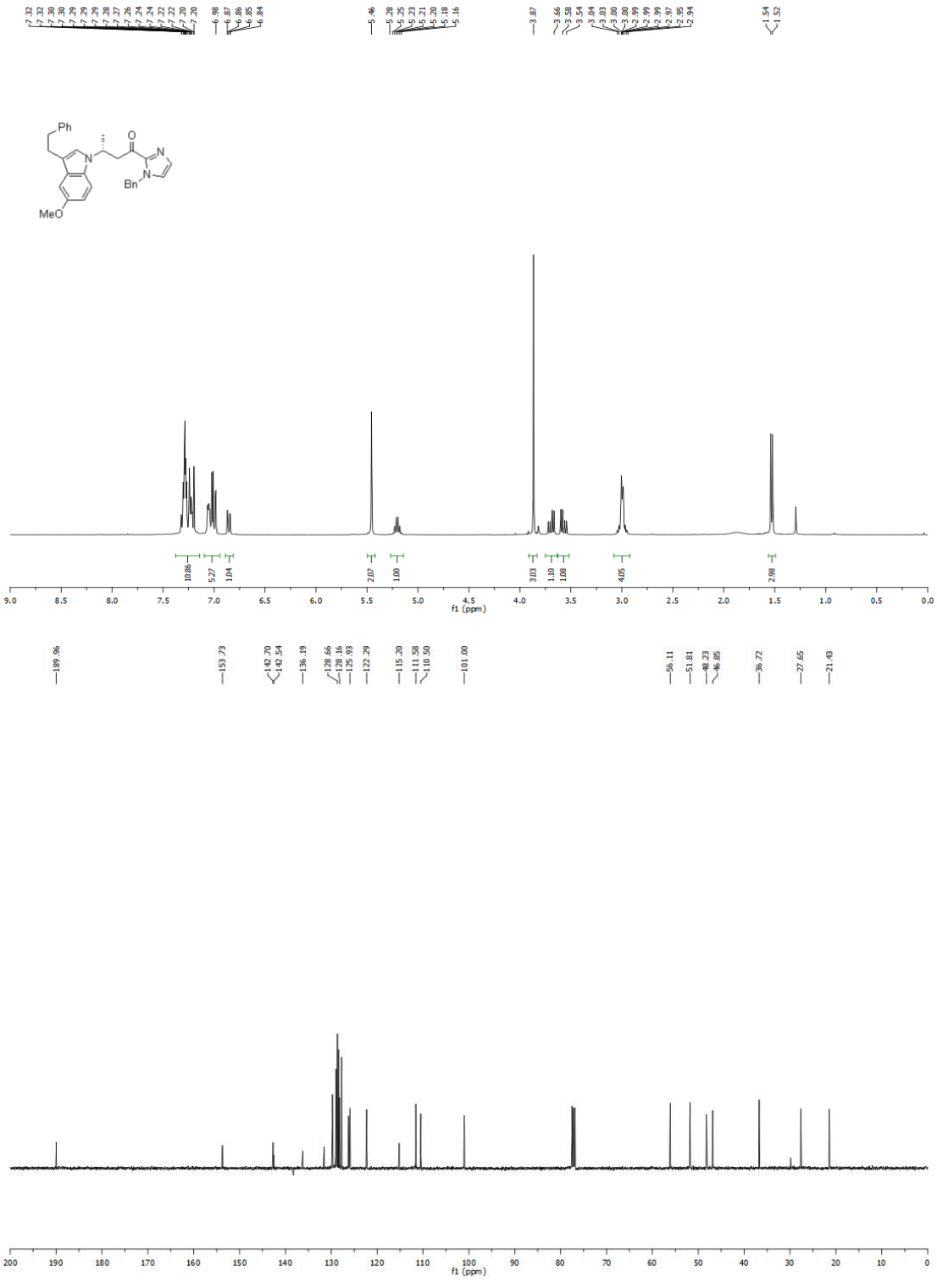
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(3-(but-3-en-1-yl)-5-methoxy-1*H*-indol-1-yl) butan-1-one (**7f**)



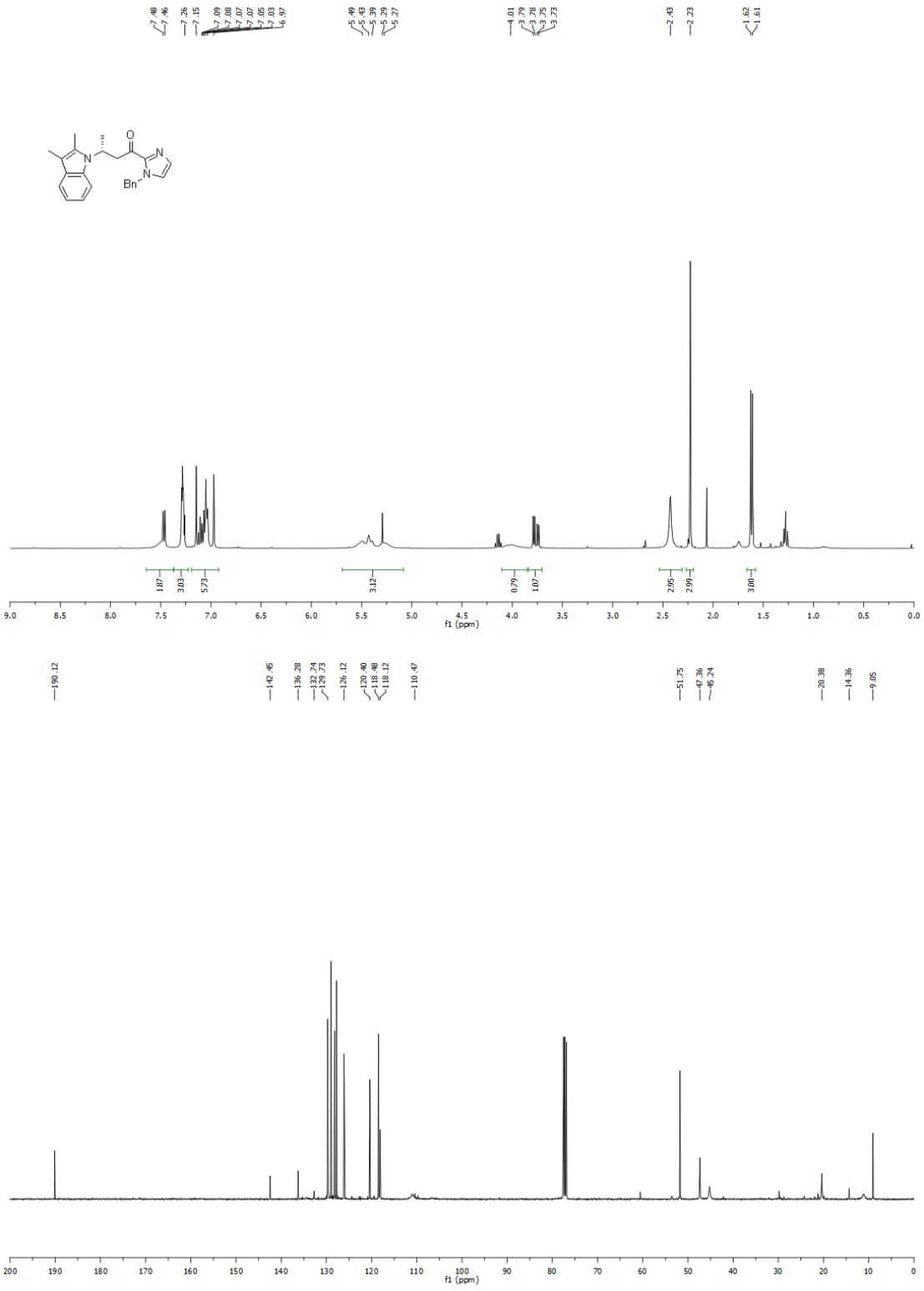
(*R*)-(1-Benzyl-1*H*-imidazolyl)-3-(5-bromo-3-propyl-1*H*-indolyl)butan-1-one (**7g**)



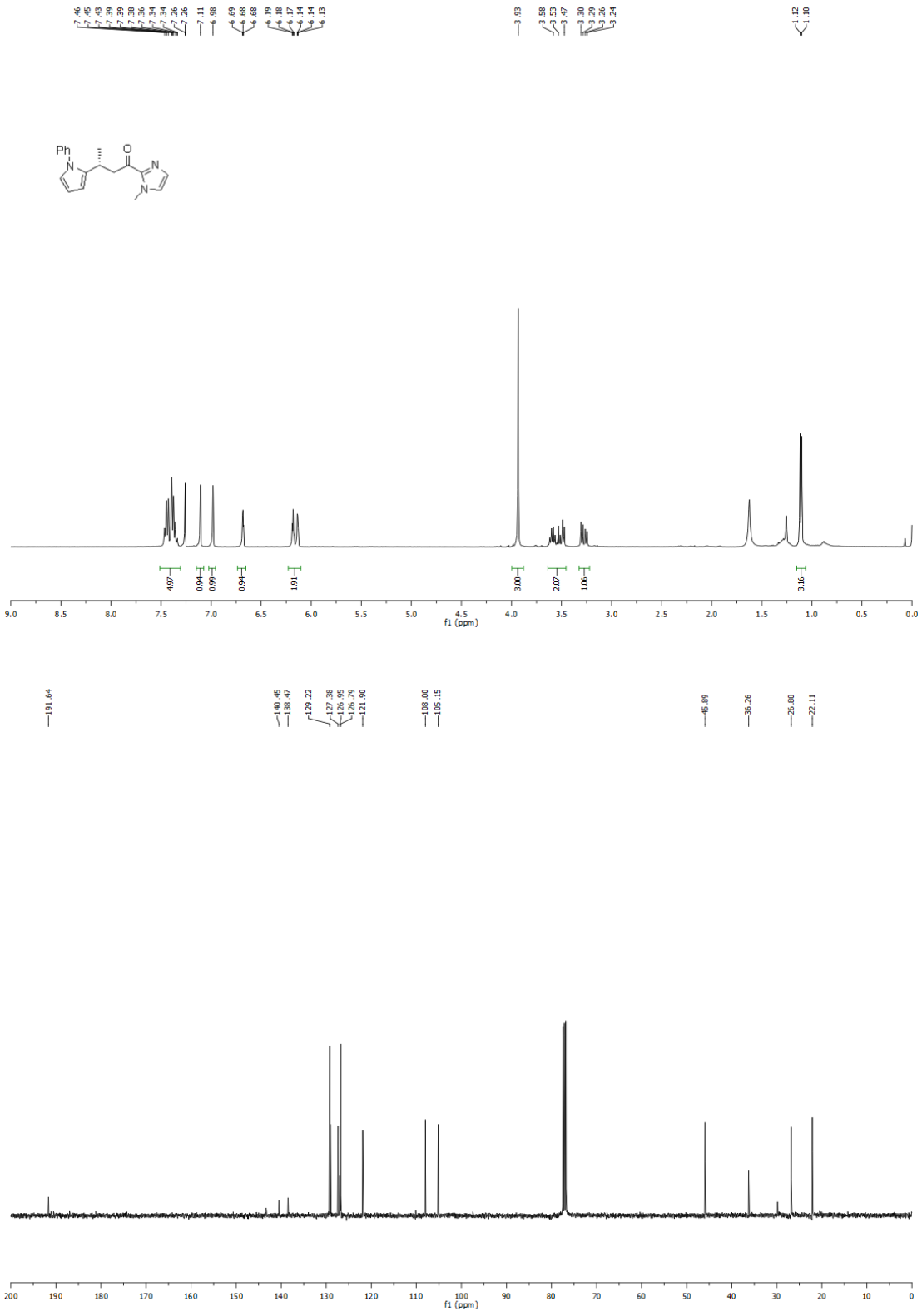
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(5-methoxy-3-phenethyl-1*H*-indol-1-yl)butan-1-one (**7h**)



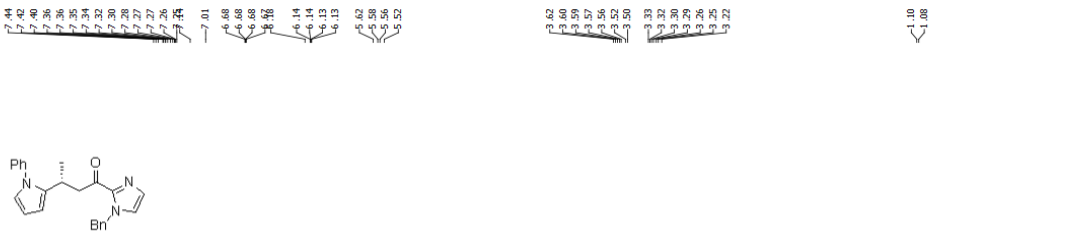
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(2,3-dimethyl-1*H*-indolyl)butan-1-one (**7i**)

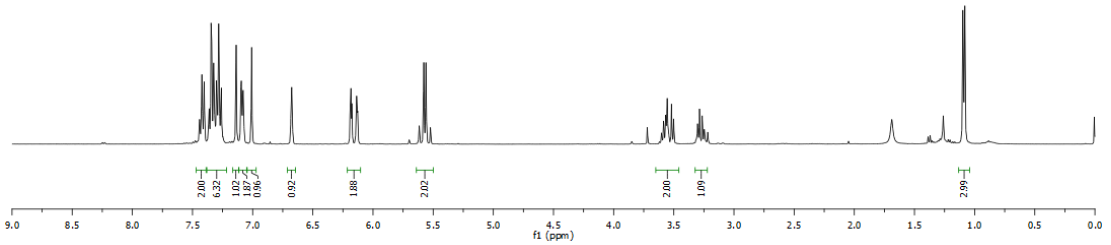


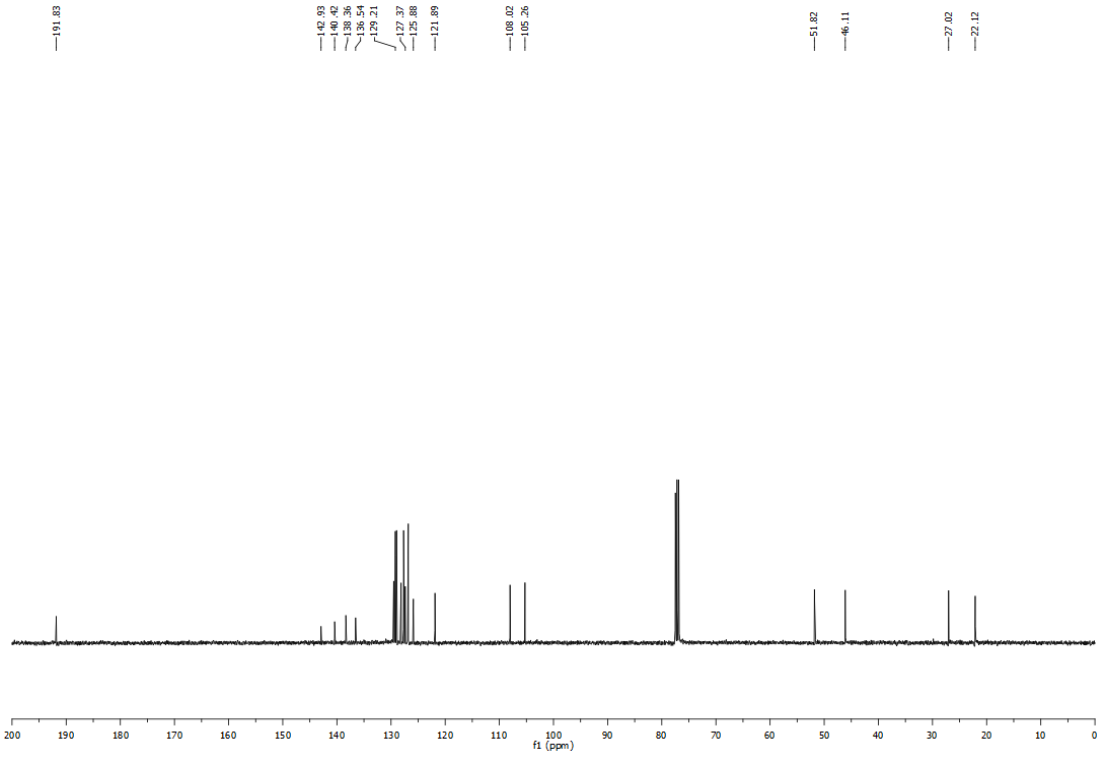
(*R*)-1-(1-Methyl-1*H*-imidazol-2-yl)-3-(1-phenyl-1*H*-pyrrol-2-yl) butan-1-one (**9a**)



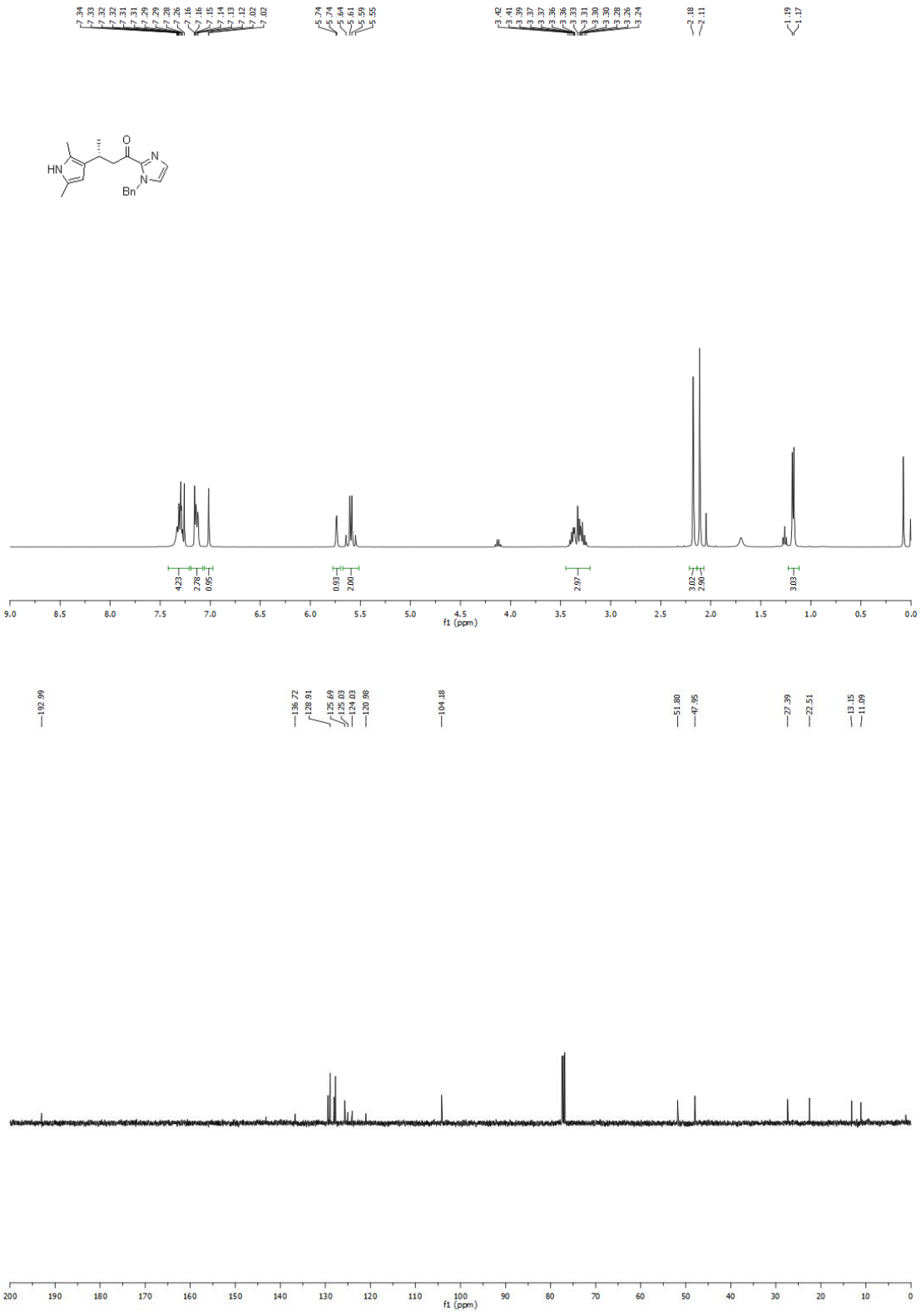
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(1-phenyl-1*H*-pyrrol-2-yl) butanone (**9b**)



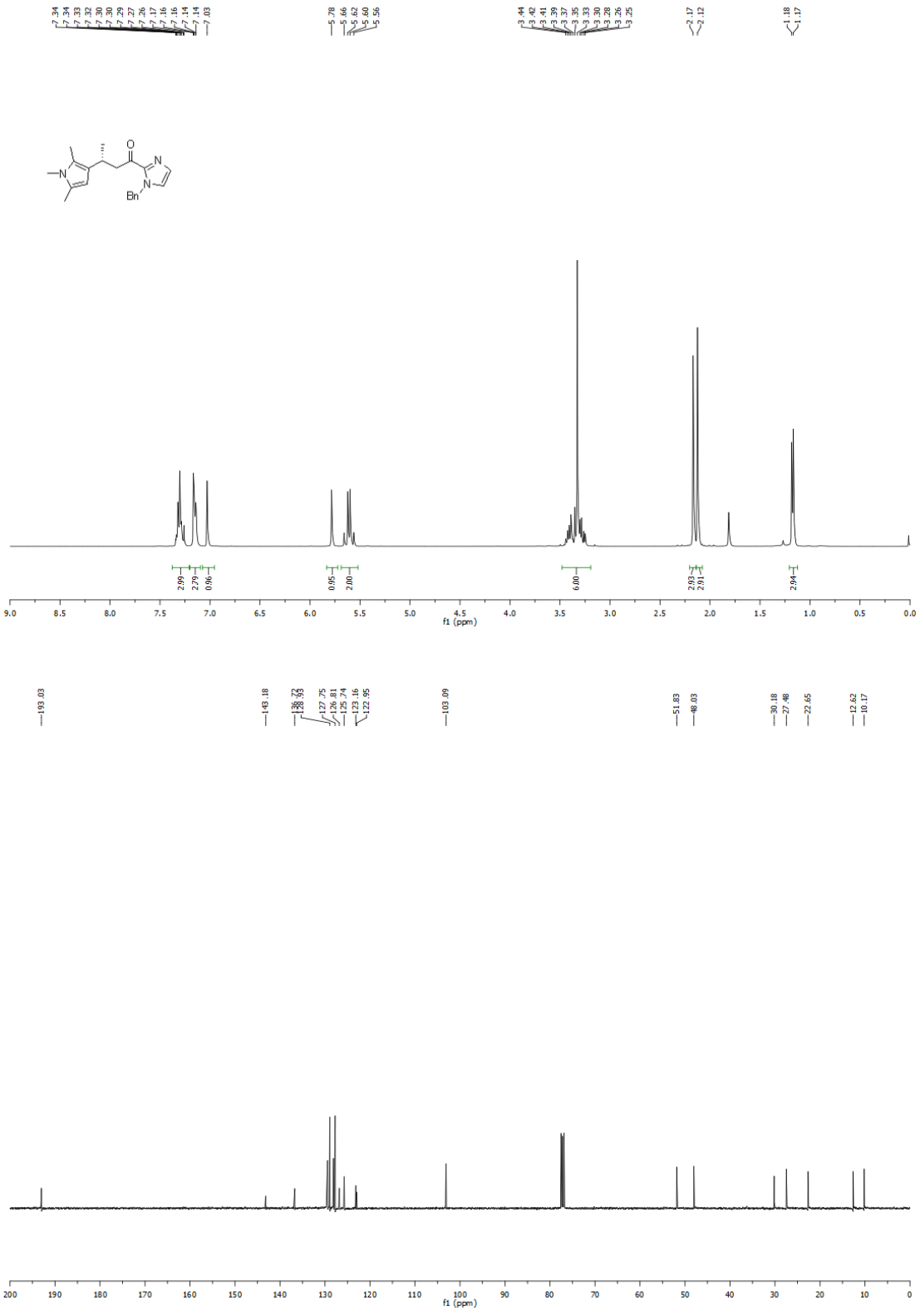




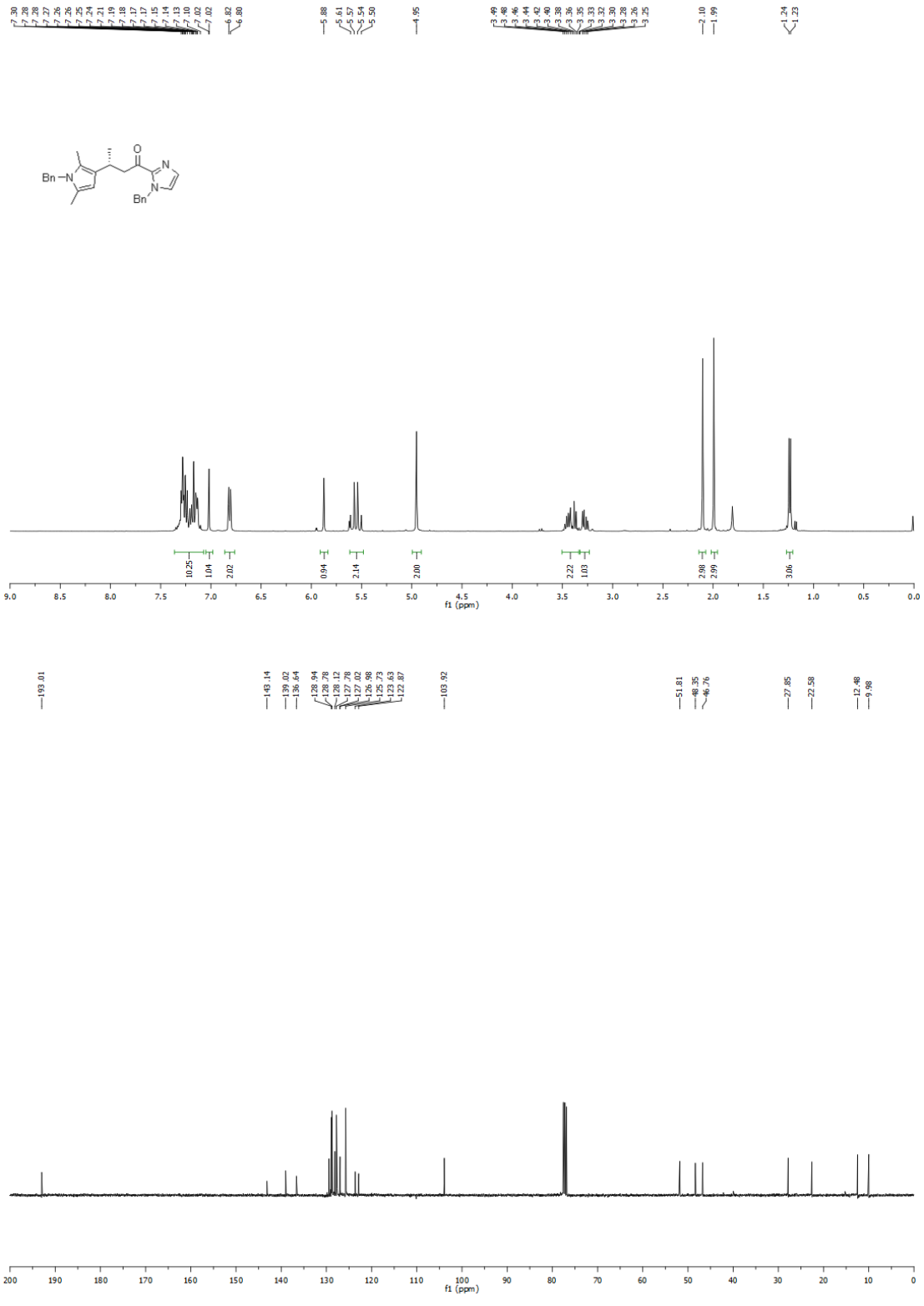
(*R*)-1-(1-Benzyl-1-imidazol-2-yl)-3-(2,5-dimethyl-1*H*-pyrrol-3-yl) butan-1-one (**9c**)



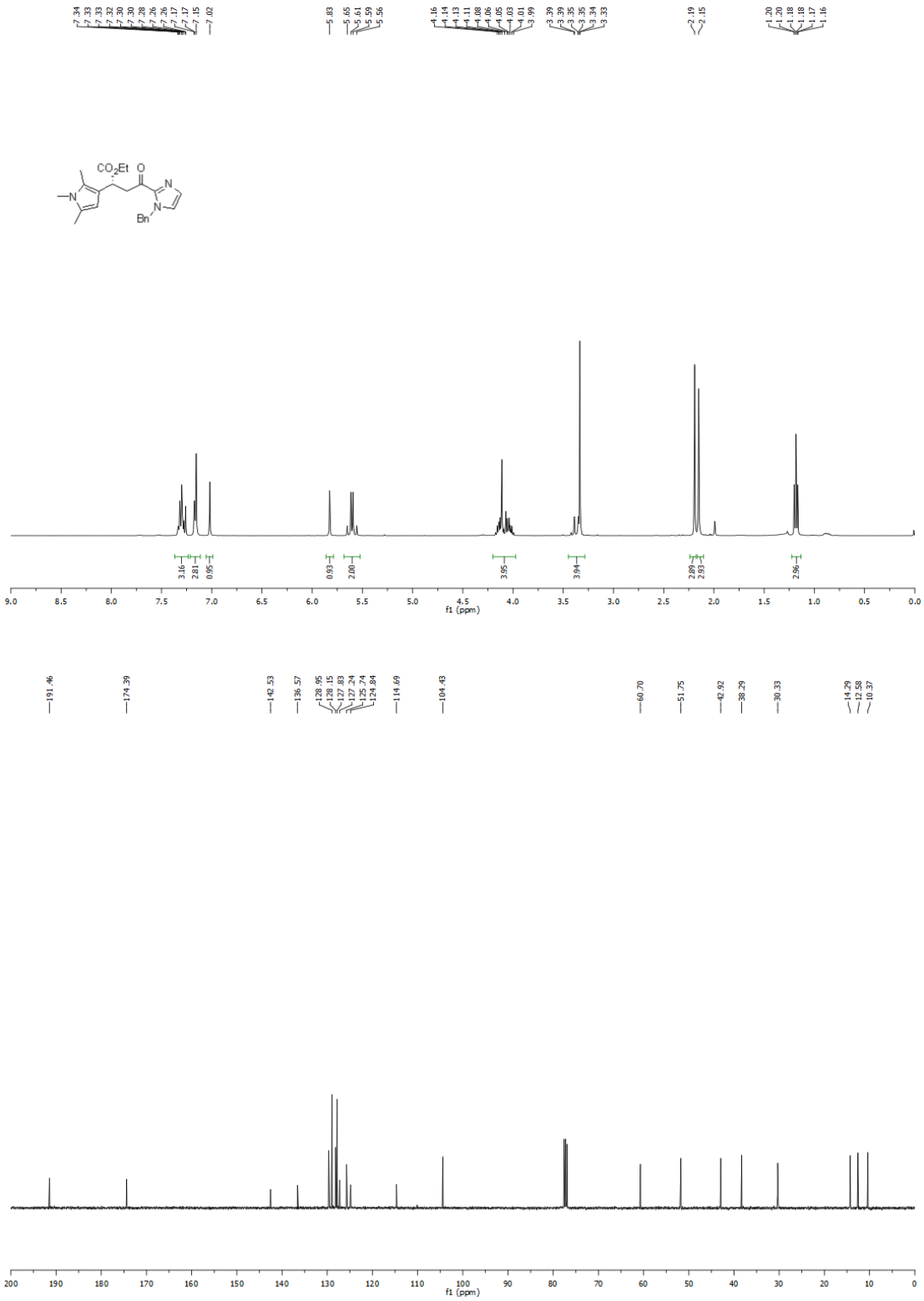
(*R*)-1-(1-Benzyl-imidazol-2-yl)-3-(1,2,5-trimethyl-pyrrol-3-yl) butan-1-one (**9d**)



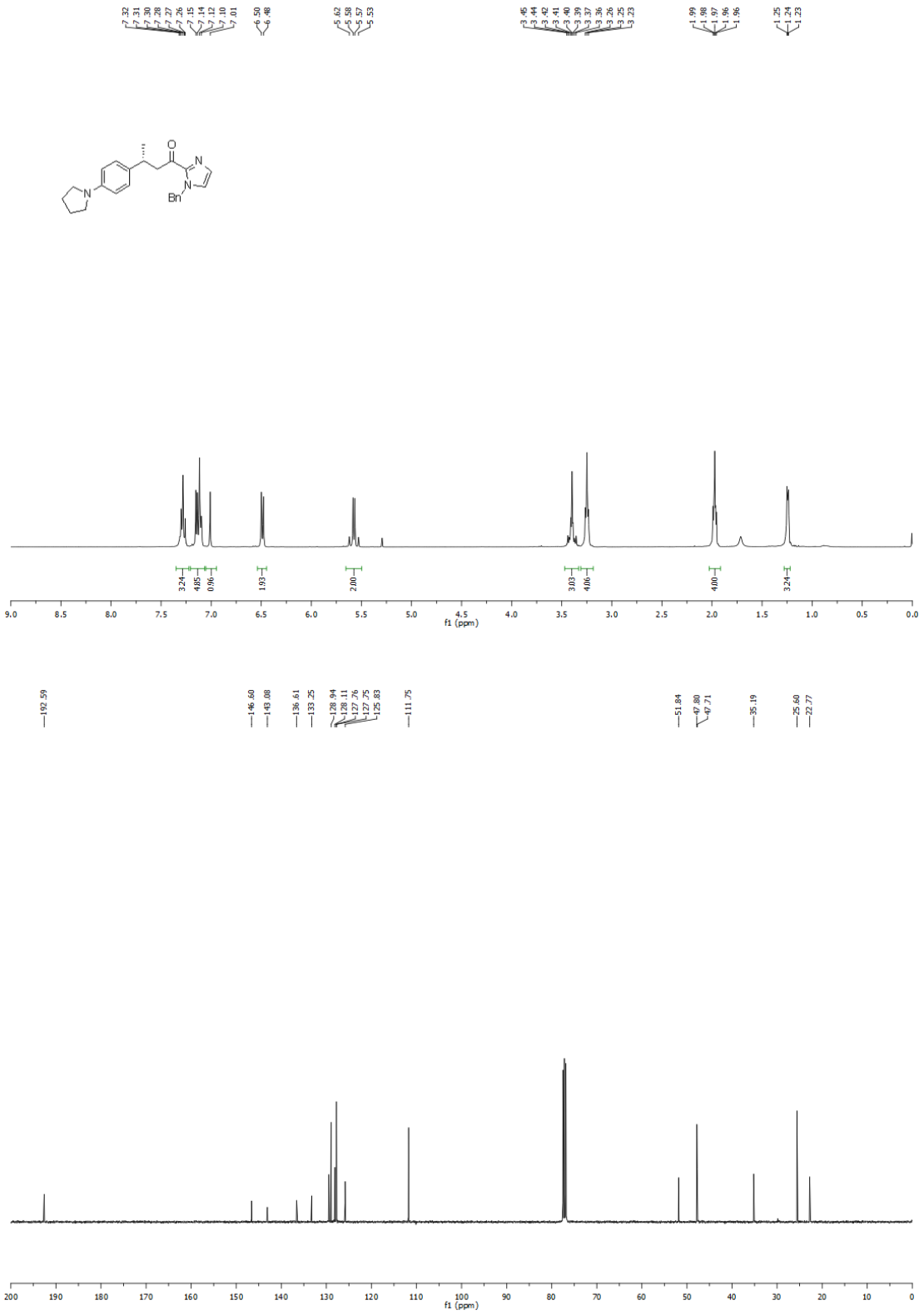
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(1-benzyl-2,5-dimethyl-1*H*-pyrrol-3-yl)butan-1-one (**9e**)



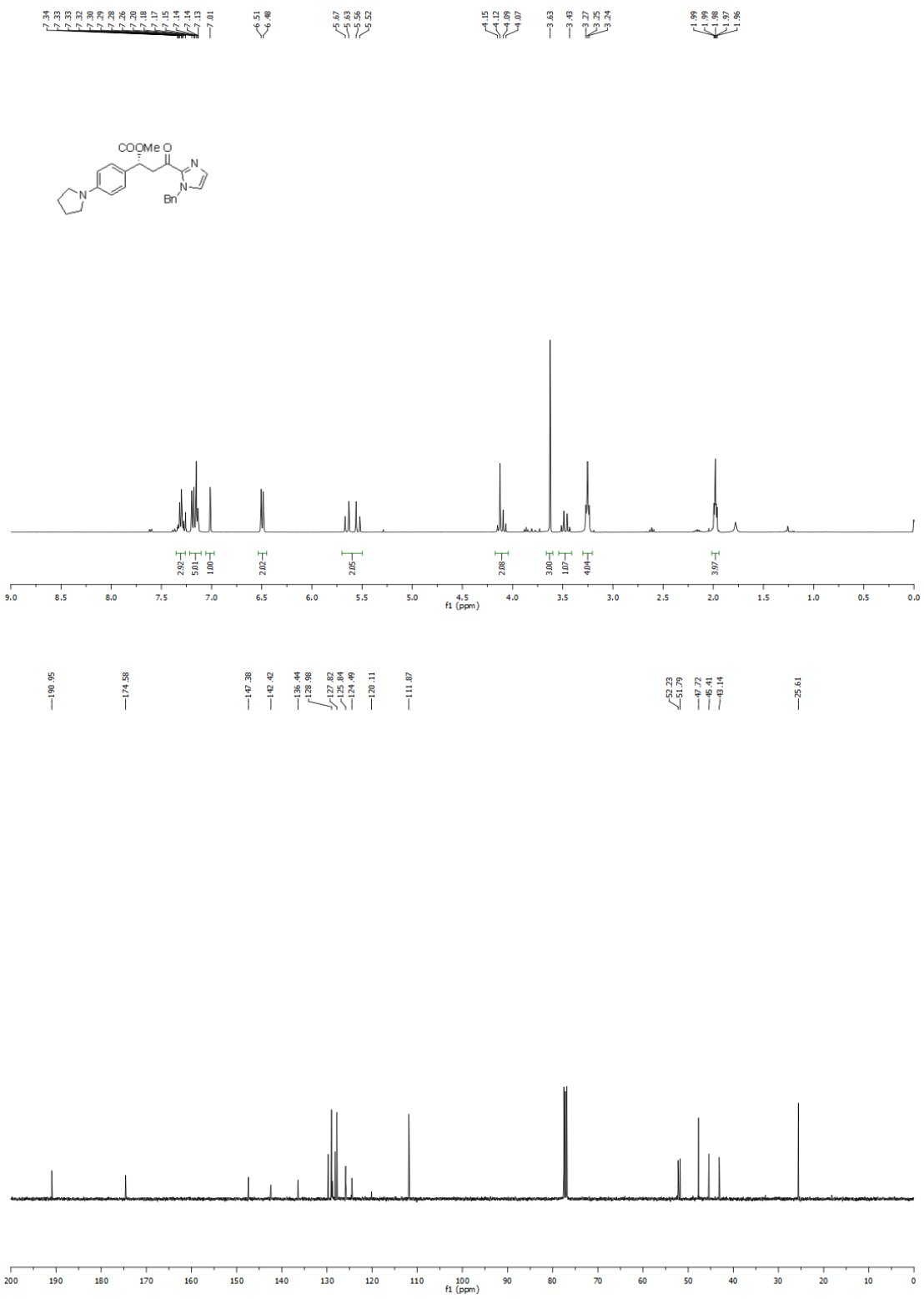
(*R*)-Ethyl 4-(1-benzyl-1*H*-imidazol-2-yl)-4-oxo-2-(1,2,5-trimethyl-1*H*-pyrrol-3-yl)butanoate (**9f**)



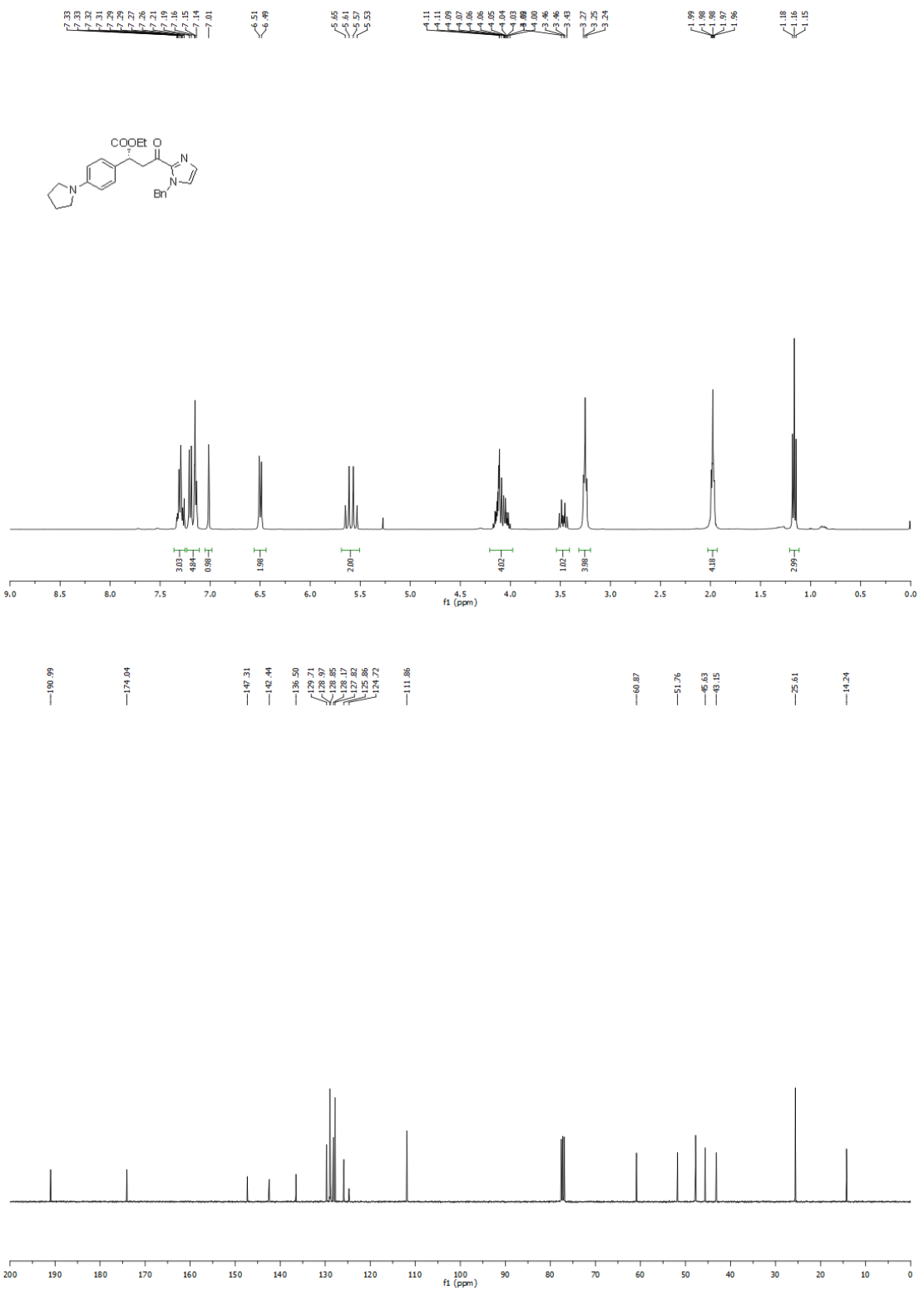
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(4-(pyrrolidin-1-yl) phenyl)butan-1-one (**11a**)



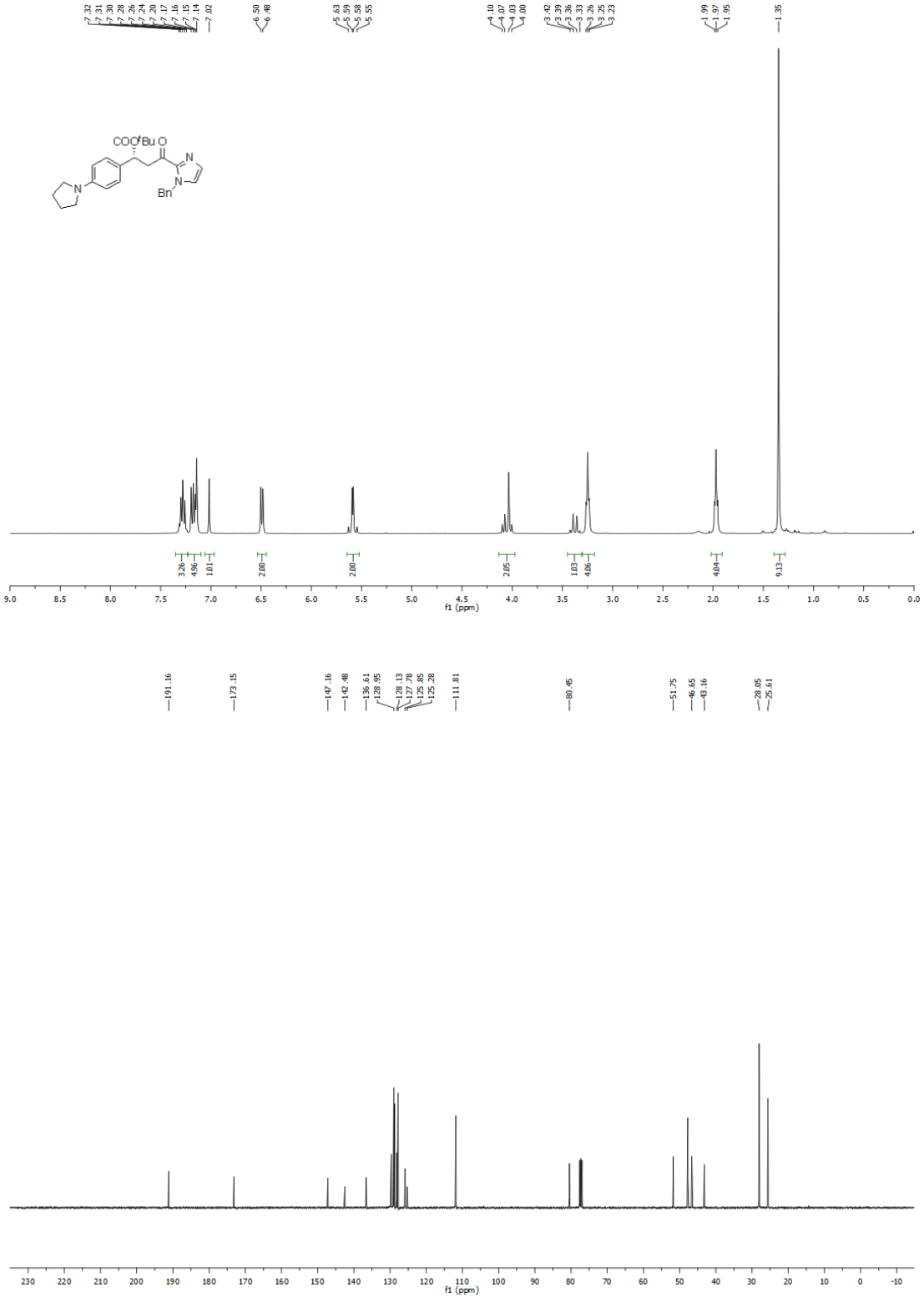
(*R*)-Methyl 4-(1-benzyl-1*H*-imidazol-2-yl)-4-oxo-2-(4-(pyrrolidin-1-yl)phenyl) butanoate (**11b**)



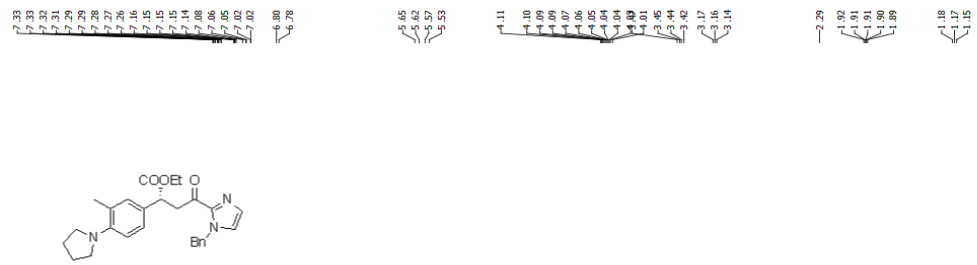
(*R*)-Ethyl 4-(1-benzyl-1H-imidazol-2-yl)-4-oxo-2-(4-(pyrrolidin-1-yl)phenyl) butanoate (**11c**)

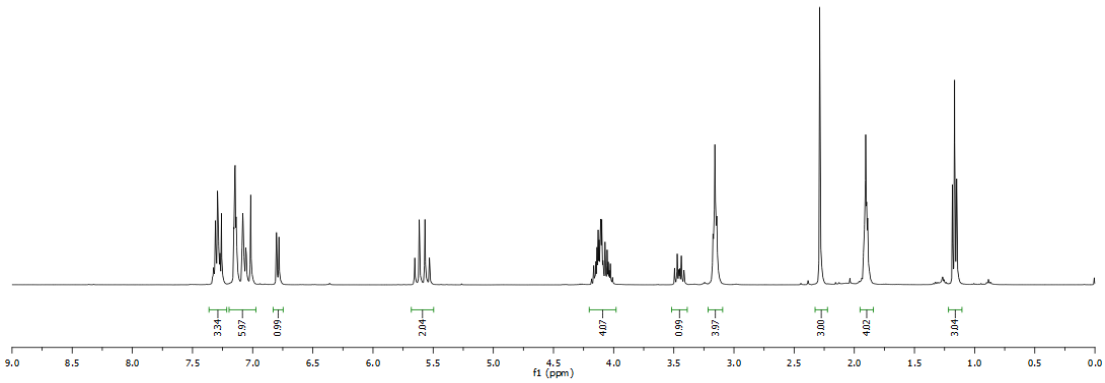


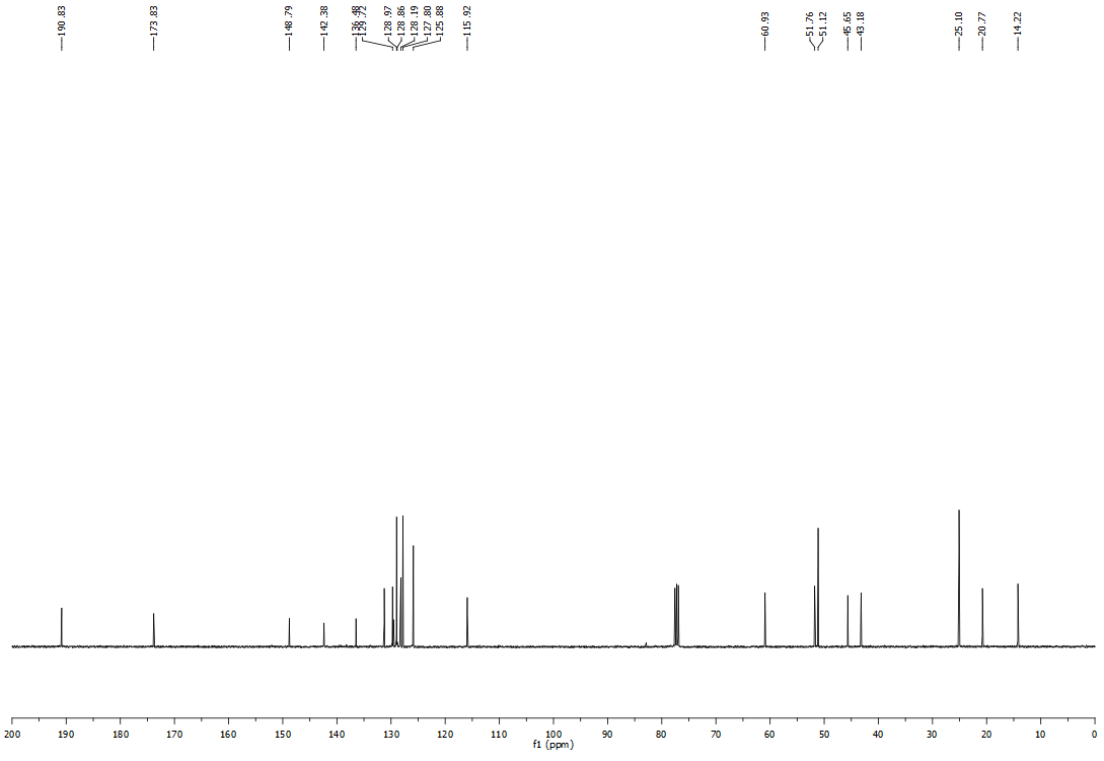
(*R*)-*tert*-Butyl 4-(1-benzyl-1*H*-imidazol-2-yl)-4-oxo-2-(4-(pyrrolidin-1-yl) phenyl) butanoate (**11d**)



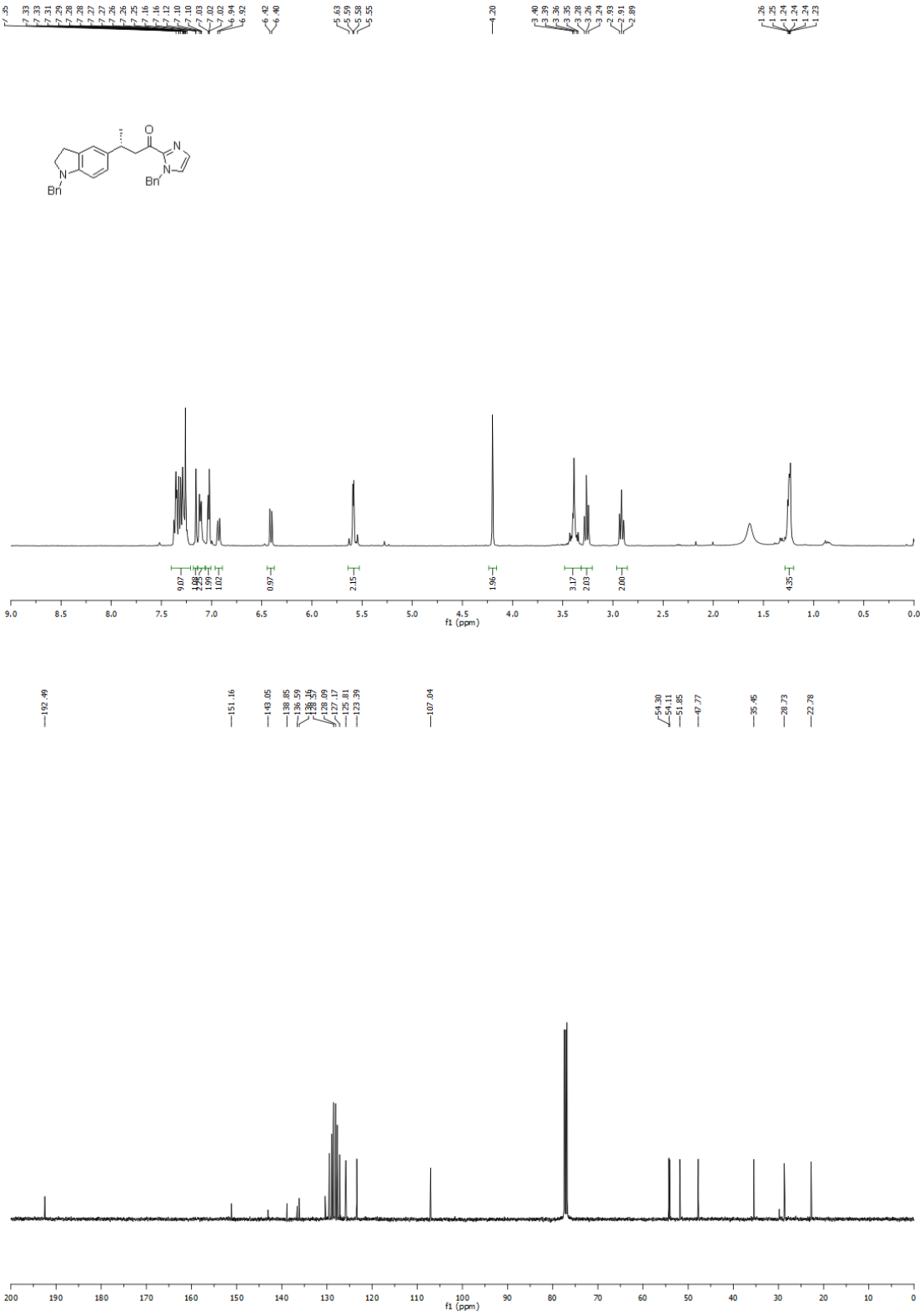
(*R*)-Ethyl 4-(1-benzyl-1*H*-imidazol-2-yl)-2-(3-methyl-4-(pyrrolidin-1-yl) phenyl)-4-oxo-butanoate (**11e**)



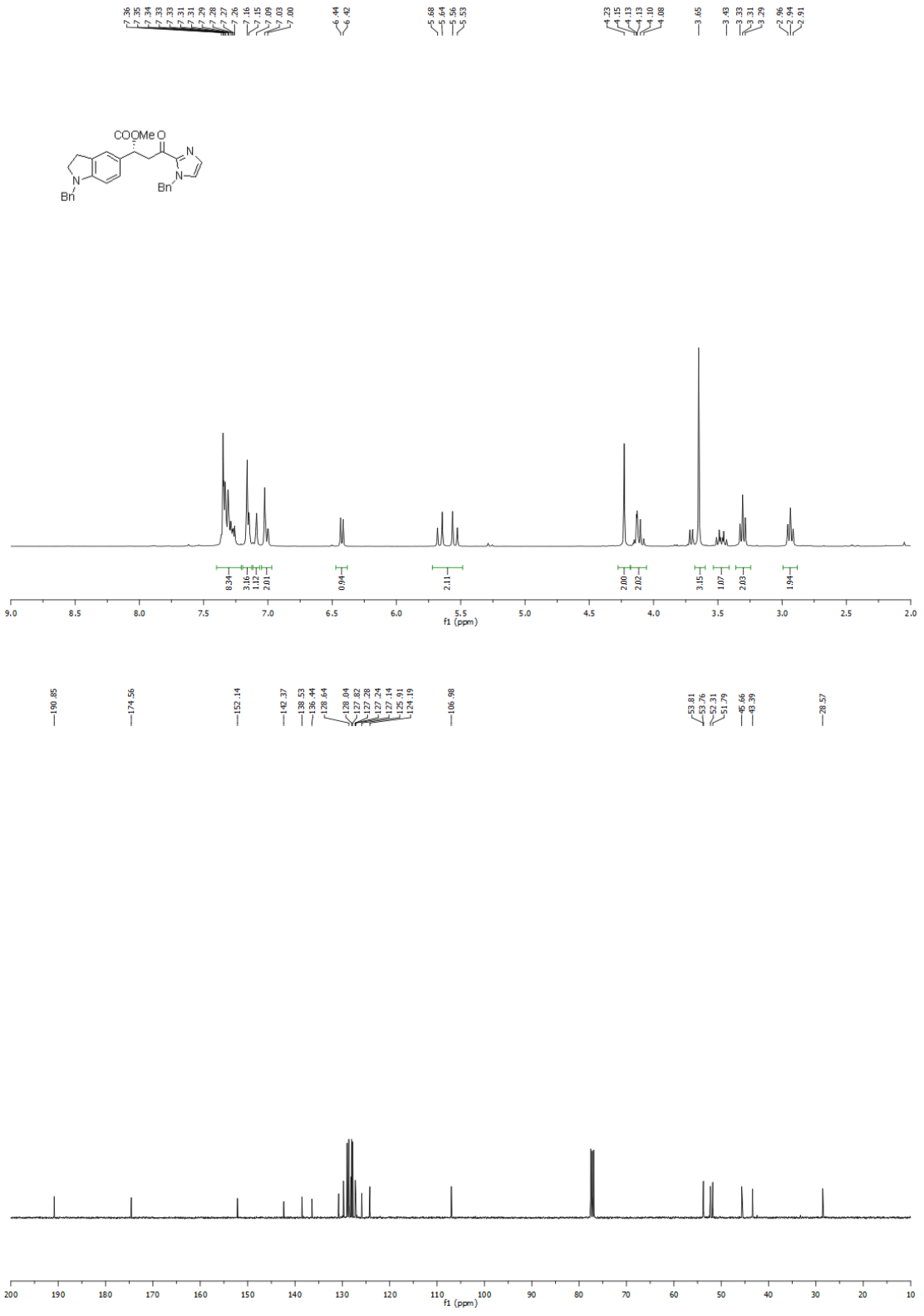




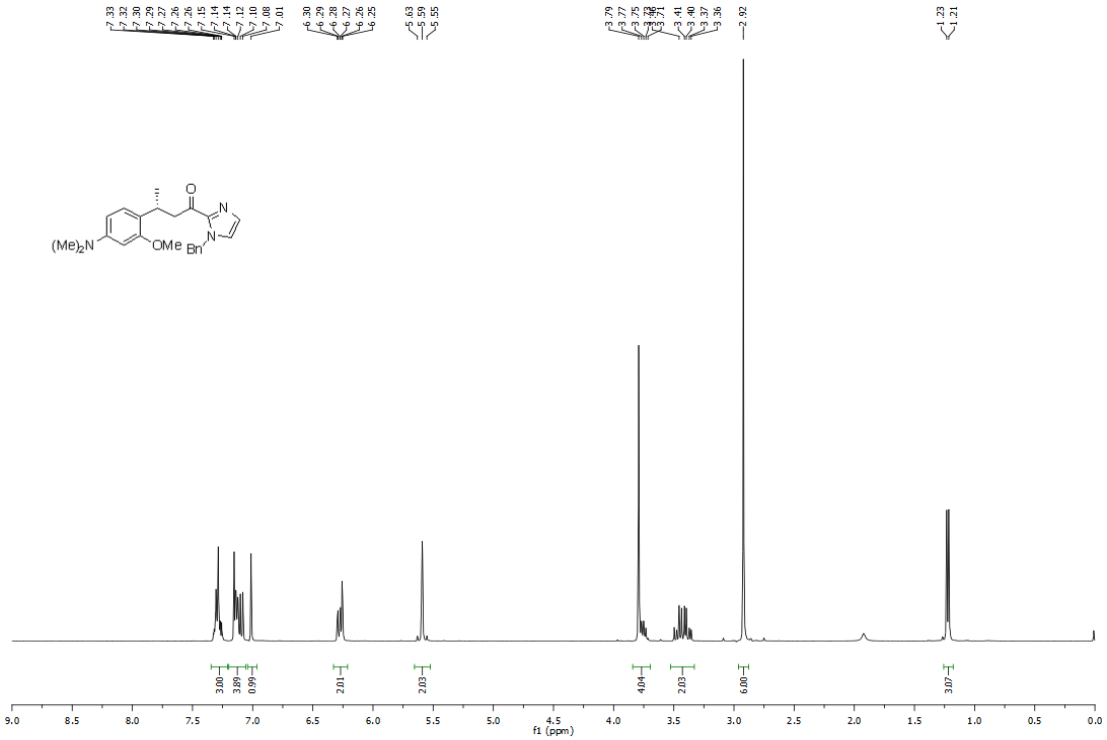
(*R*)-1-(1-Benzyl-1*H*-imidazol-2-yl)-3-(1-benzylindolin-5-yl)butan-1-one (**11f**)

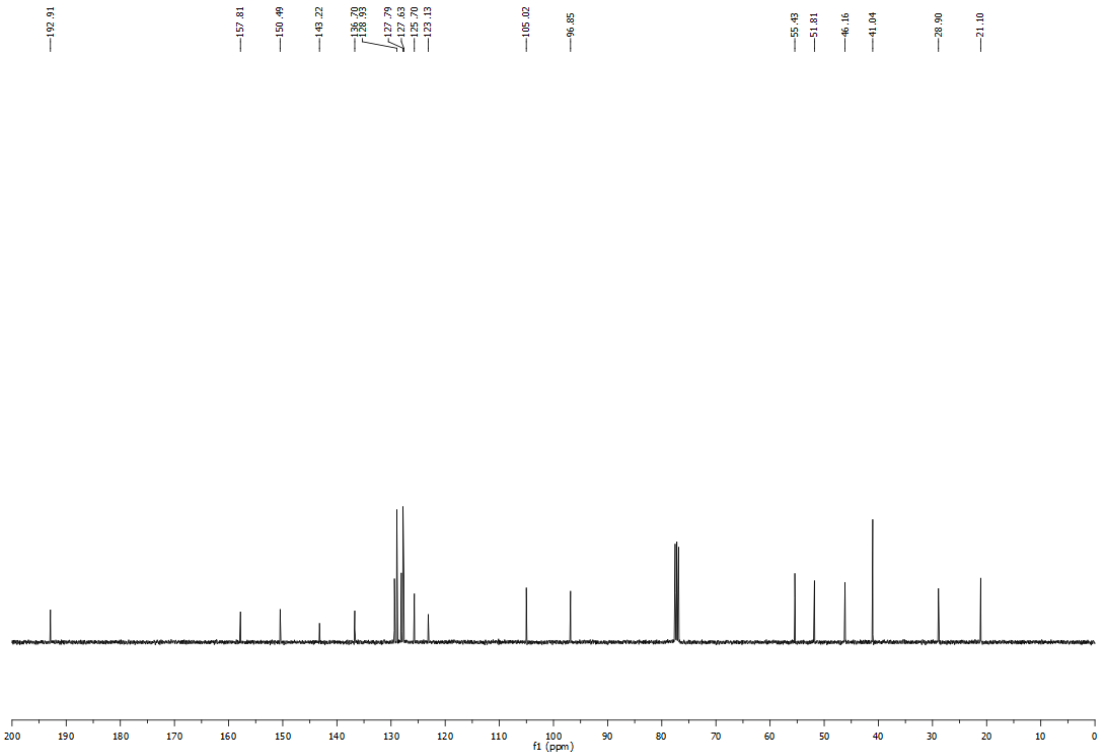


(*R*)-Methyl 4-(1-benzylimidazolyl)-2-(1-benzylindolinyl)-4-oxo-butanoate (**11g**)

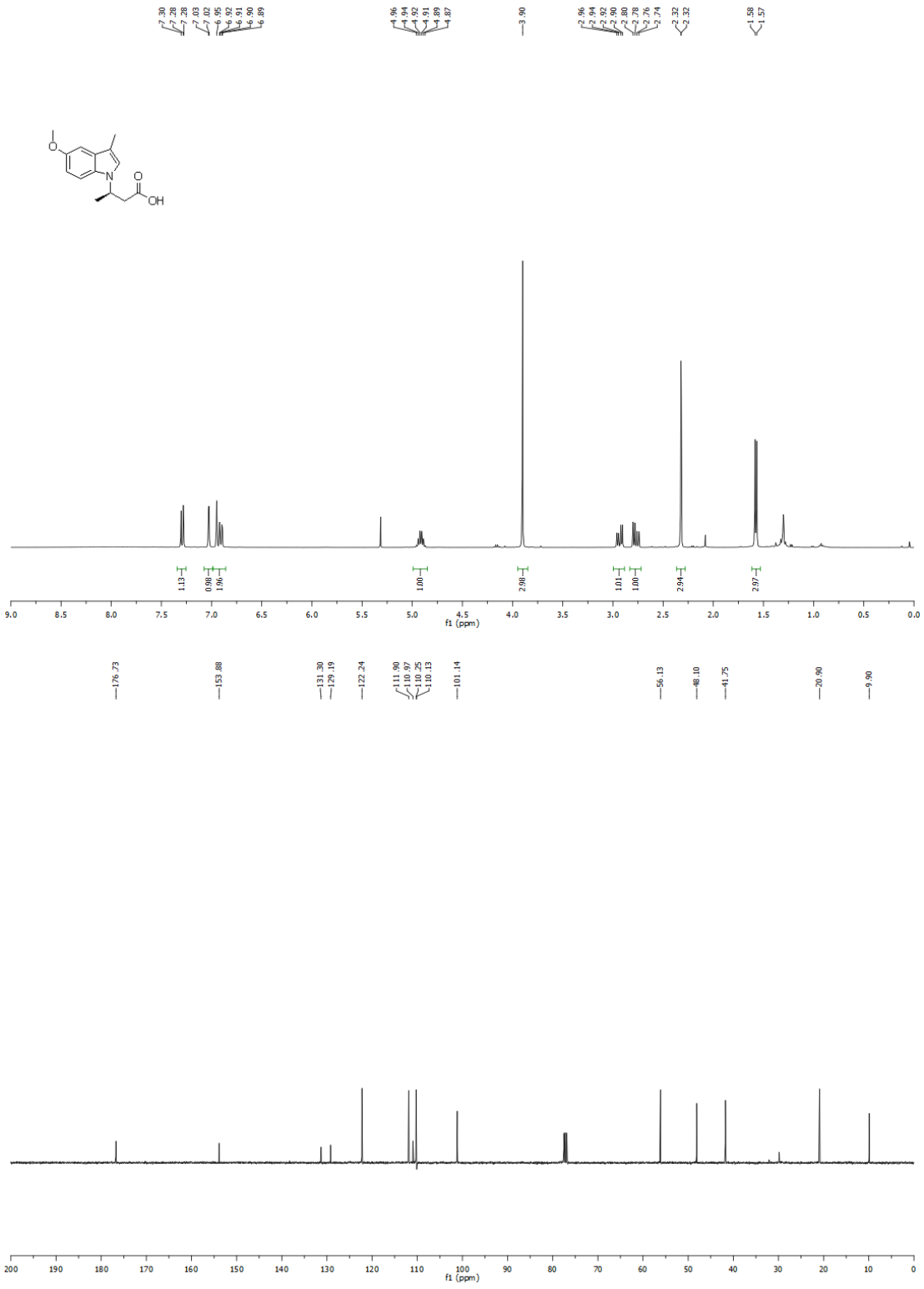


(*R*)-1-(1-Benzylimidazol-2-yl)-3-(4-(dimethylamino)-2-methoxyphenyl)butan-1-one (**11h**)

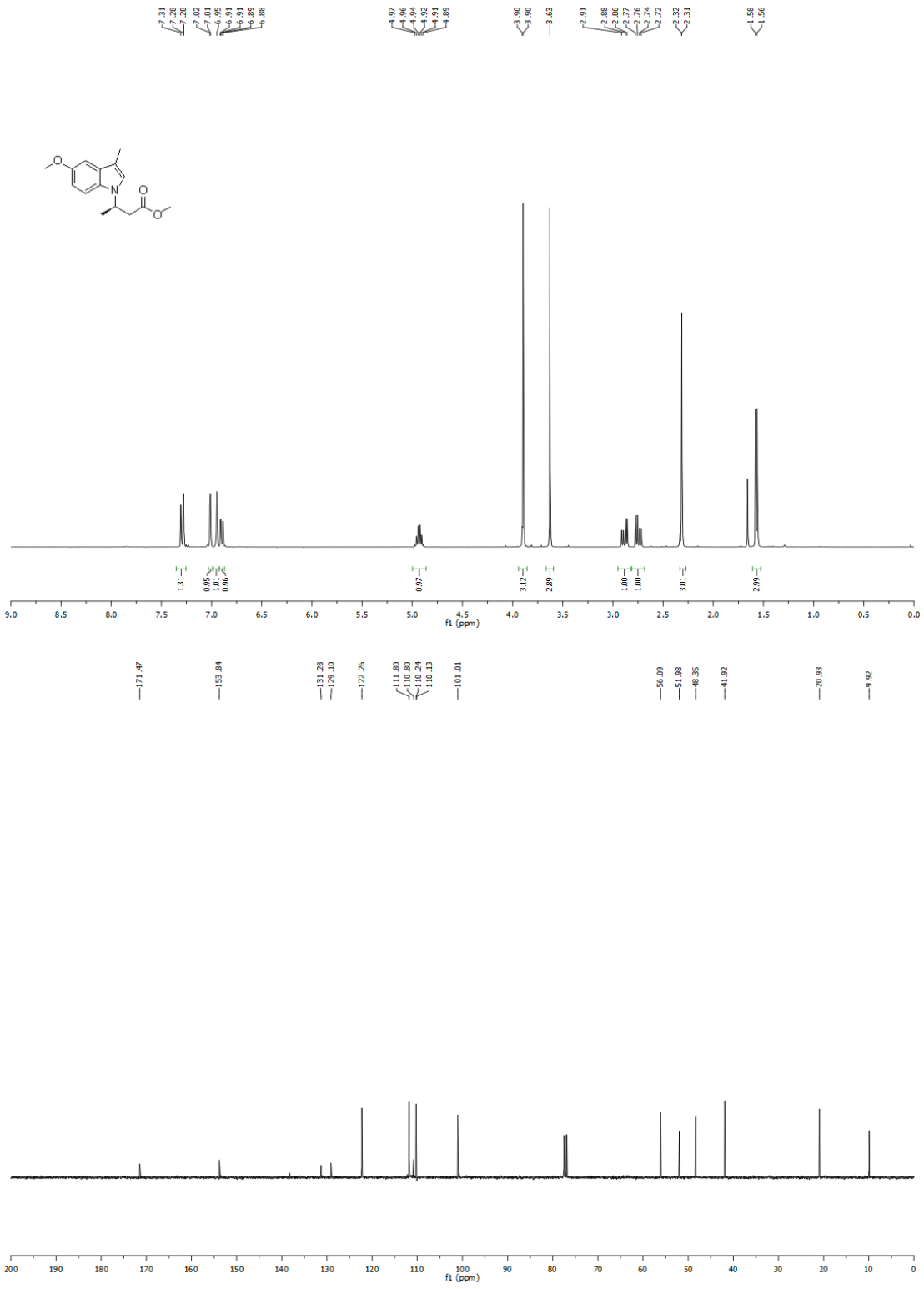




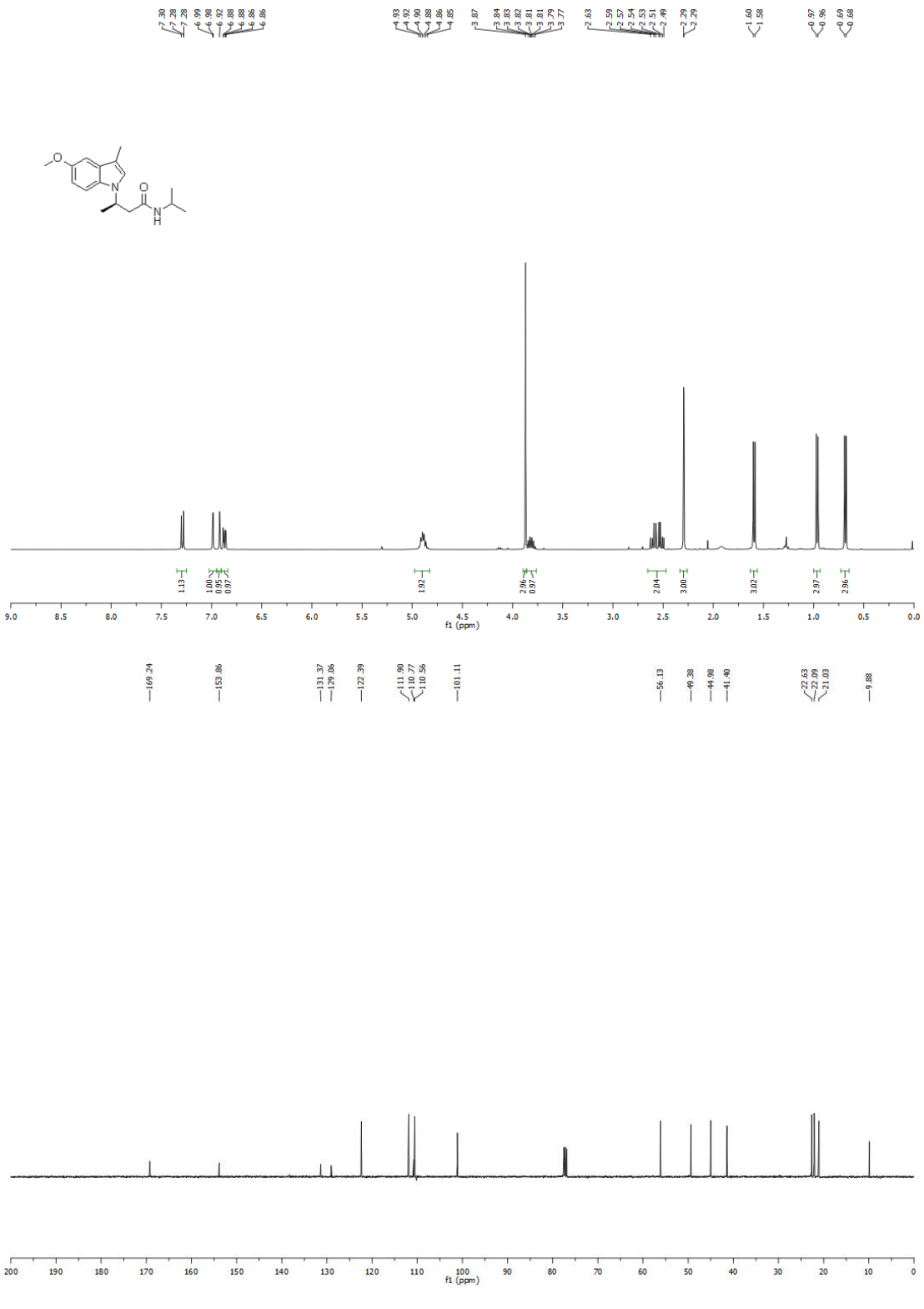
(*R*)-3-(5-Methoxy-3-methyl-1*H*-indol-1-yl) butanoic acid (**12**)



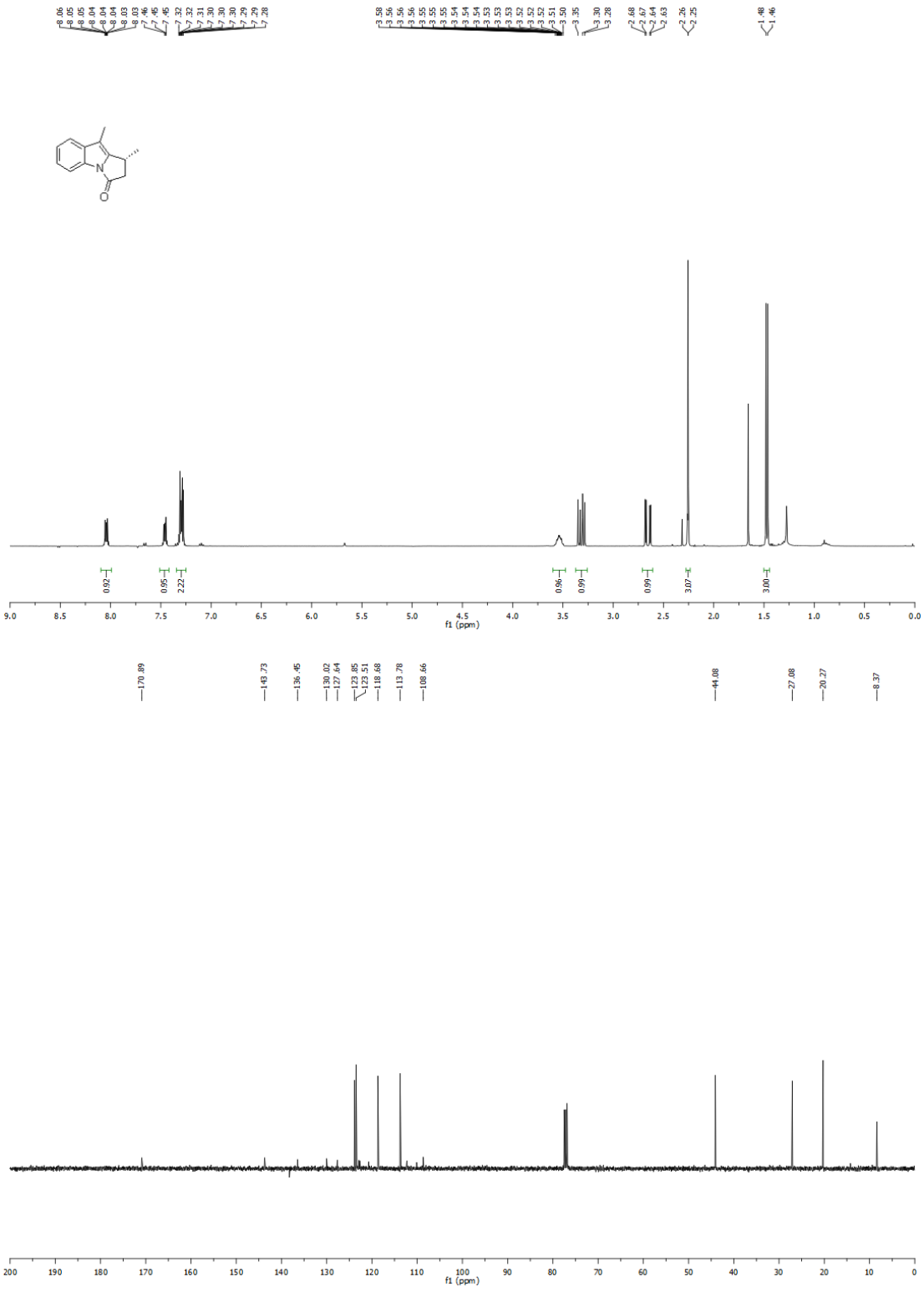
(*R*)-Methyl 3-(5-methoxy-3-methyl-1*H*-indol-1-yl) butanoate (**13**)



(*R*)-*N*-Isopropyl-3-(5-methoxy-3-methyl-1*H*-indol-1-yl) butanamide **(14)**



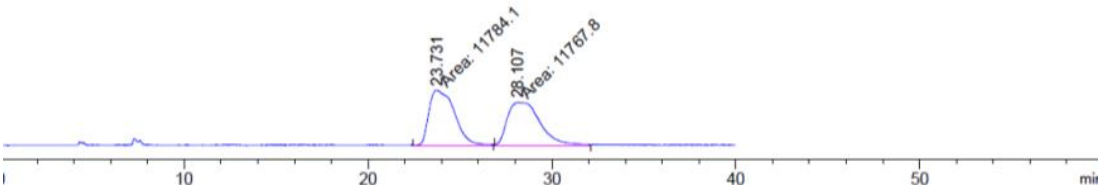
(*R*)-1,9-Dimethyl-1,2-dihydropyrrolo[1,2-*a*]indol-3-one (**15**)



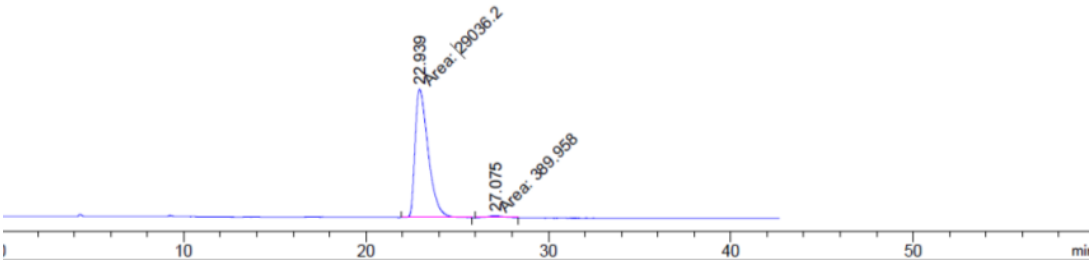
Chiral HPLC chromatographic analysis

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5a**

Condition: chiral OD-H column, *n*-hexane/2-propanol = 90: 10, flow rate: 0.7 ml/min, λ = 280 nm, retention time: t (major) = 22.94 min, t (minor) = 27.07 min.



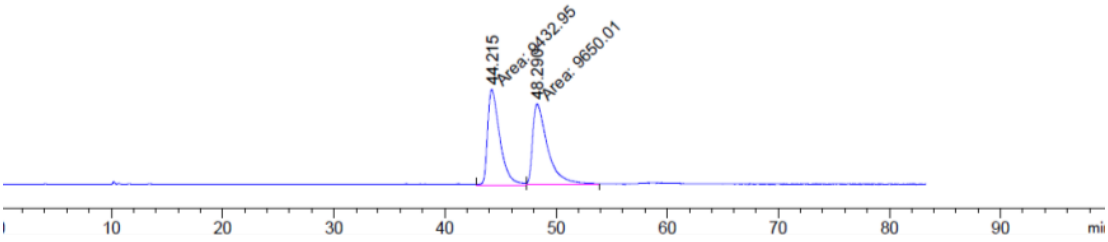
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.731	MM	1.5980	1.17841e4	122.90300	50.0346
2	28.107	MM	2.0579	1.17678e4	95.30473	49.9654



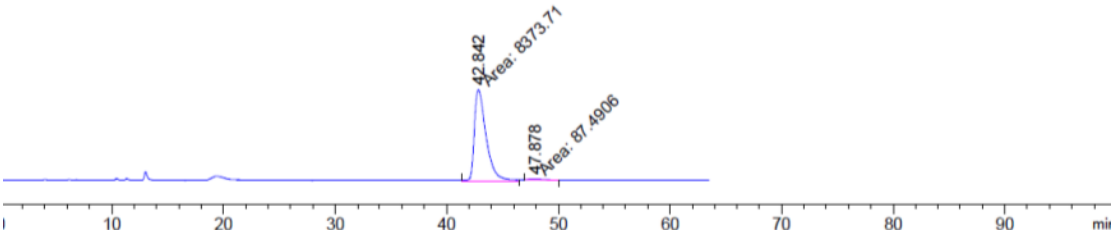
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.939	MM	0.8307	2.90362e4	582.54944	98.6748
2	27.075	MM	0.8108	389.95764	8.01572	1.3252

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5b**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 92: 8, flow rate: 0.7 ml/min, λ = 280 nm, retention time: t (major) = 42.84 min, t (minor) = 47.87 min.



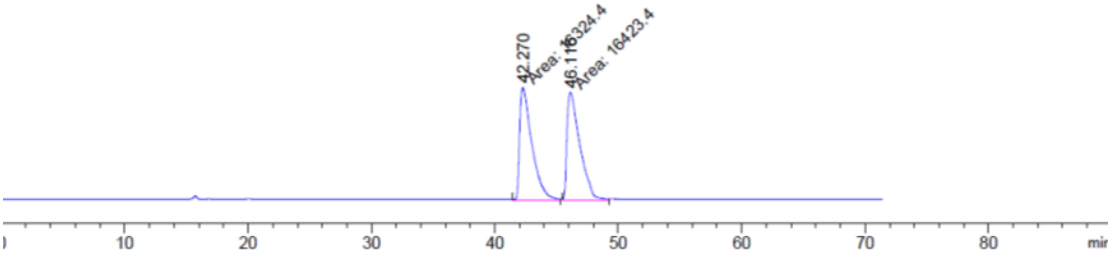
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	44.215	MM	1.2884	9432.94531	122.02751	49.4313
2	48.290	MM	1.5671	9650.01367	102.63039	50.5687



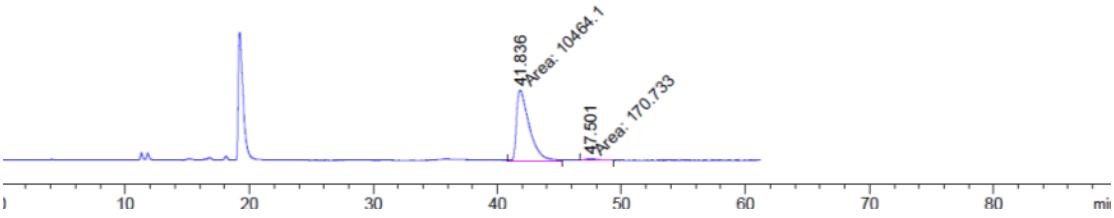
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	42.842	MM	1.2156	8373.70898	114.81345	98.9660
2	47.878	MM	1.2506	87.49060	1.16596	1.0340

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5c**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 97: 3, flow rate: 0.7 ml/min, λ = 280 nm, retention time: t (major) = 41.84 min, t (minor) = 47.50 min.



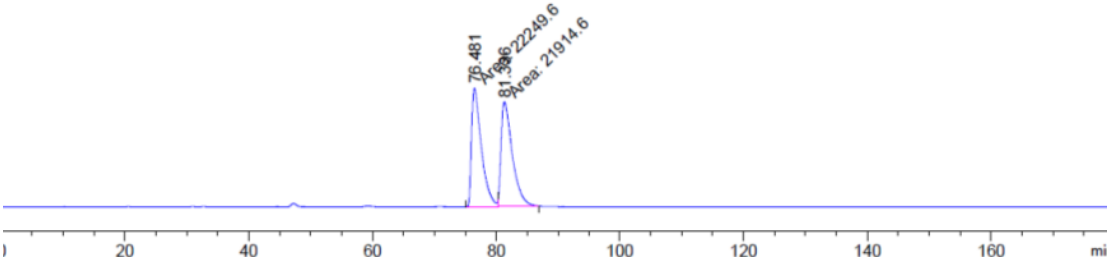
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	42.270	MM	1.1471	1.63244e4	237.18617	49.8489
2	46.116	MM	1.2045	1.64234e4	227.24606	50.1511



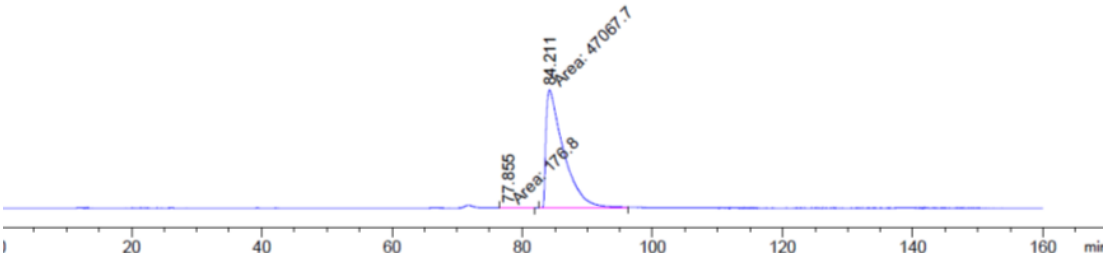
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	41.836	MM	1.1741	1.04641e4	148.53560	98.3946
2	47.501	MM	1.0980	170.73346	2.59152	1.6054

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5d**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 99: 1, flow rate: 0.3 ml/min, λ = 280 nm, retention time: t (major) = 84.21 min, t (minor) = 77.85 min.



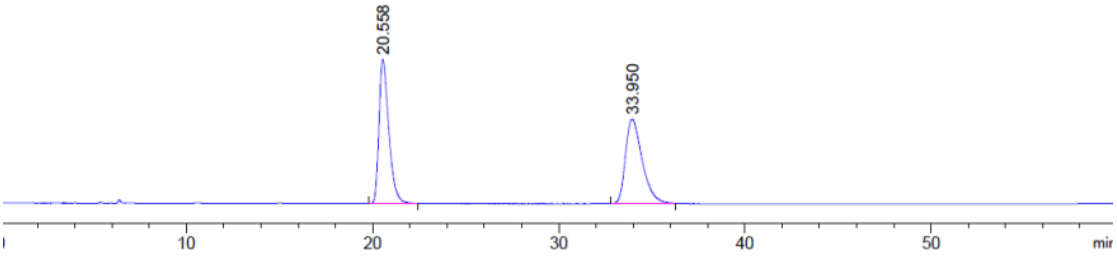
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	76.481	MM	1.8498	2.22496e4	200.46718	50.3793
2	81.336	MM	2.0843	2.19146e4	175.23637	49.6207



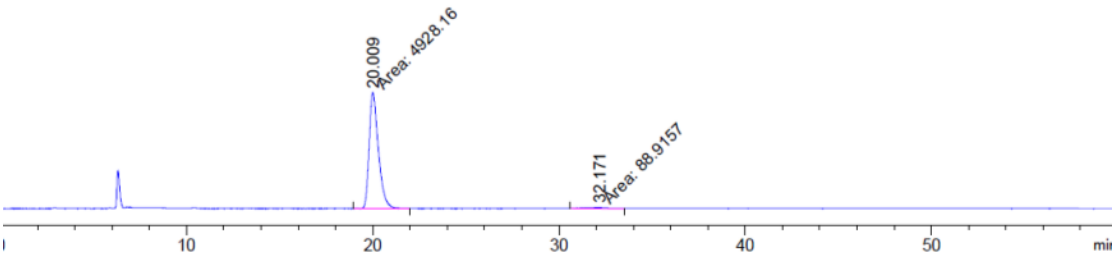
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	77.855	MM	4.2443	176.79971	6.94257e-1	0.3742
2	84.211	MM	3.1752	4.70677e4	247.06026	99.6258

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5e**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 20.01 min, t (minor) = 32.17 min.



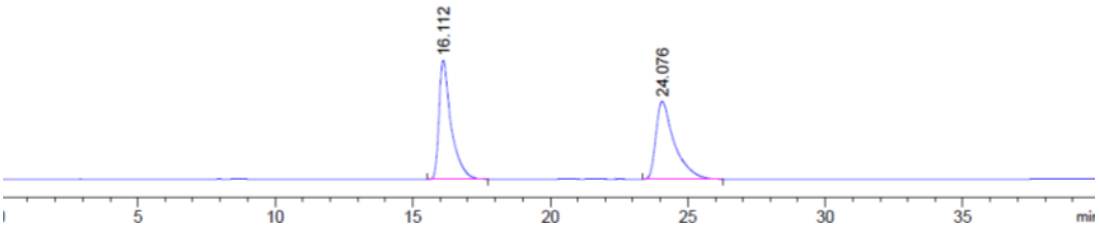
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.558	BB	0.5525	1.30966e4	358.23447	50.1971
2	33.950	BB	0.8692	1.29938e4	210.20258	49.8029



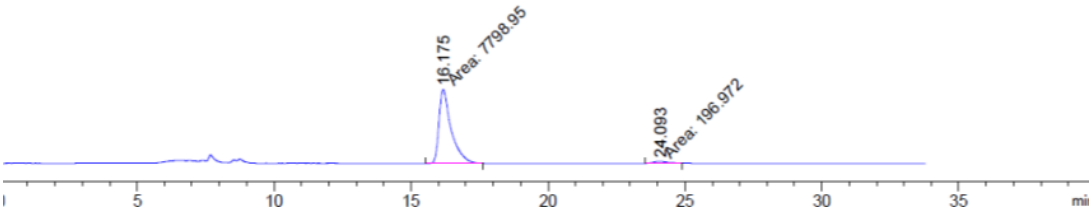
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.009	MM	0.5775	4928.16455	142.22926	98.2277
2	32.171	MM	1.1514	88.91572	1.28706	1.7723

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5f**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 93: 7, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 16.17 min, t (minor) = 24.09 min.



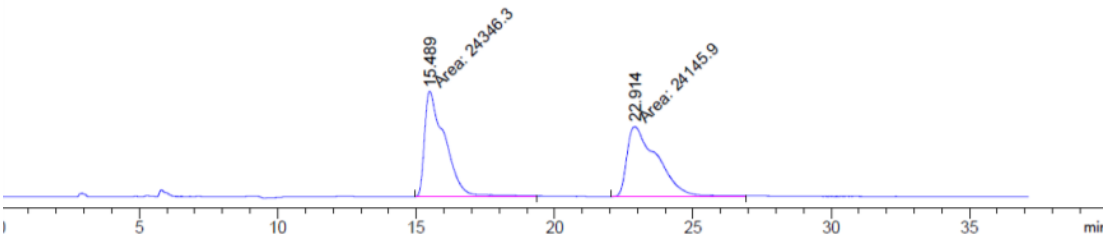
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.112	BB	0.4441	1.21497e4	398.00253	50.0679
2	24.076	BB	0.6634	1.21167e4	260.13638	49.9321



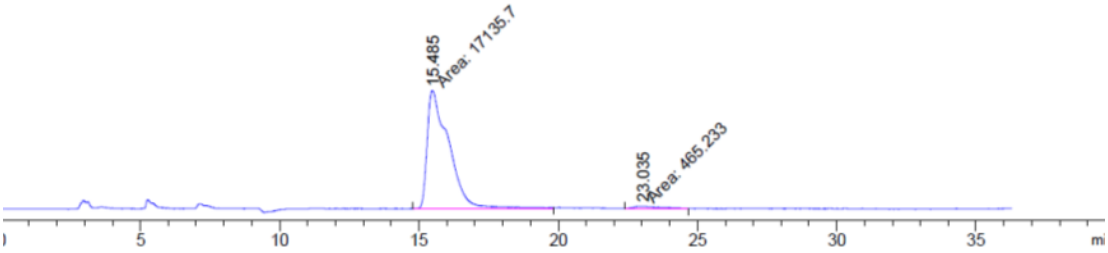
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.175	MM	0.5215	7798.94580	249.25296	97.5366
2	24.093	MM	0.5860	196.97183	5.60257	2.4634

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5g**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 0.7 ml/min, λ = 230 nm, retention time: t (major) = 15.48 min, t (minor) = 23.03 min.



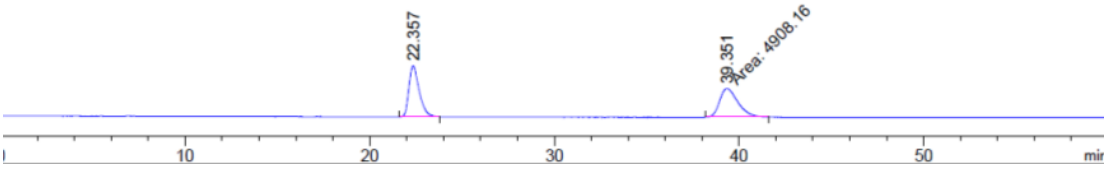
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.489	MM	0.8704	2.43463e4	466.17526	50.2067
2	22.914	MM	1.2952	2.41459e4	310.72086	49.7933



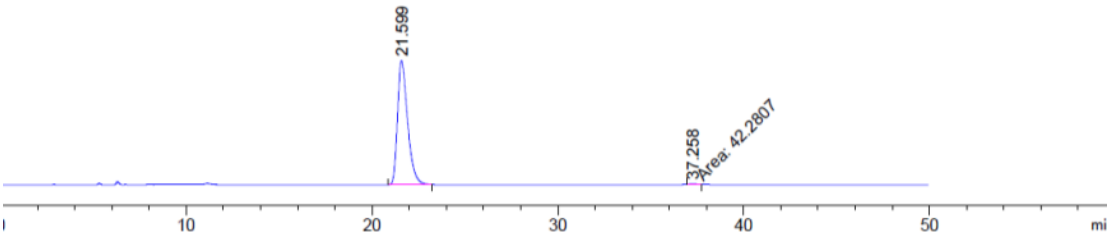
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.485	MM	0.9180	1.71357e4	311.10327	97.3568
2	23.035	MM	1.2058	465.23312	6.43044	2.6432

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5h**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 21.60 min, t (minor) = 37.26 min.



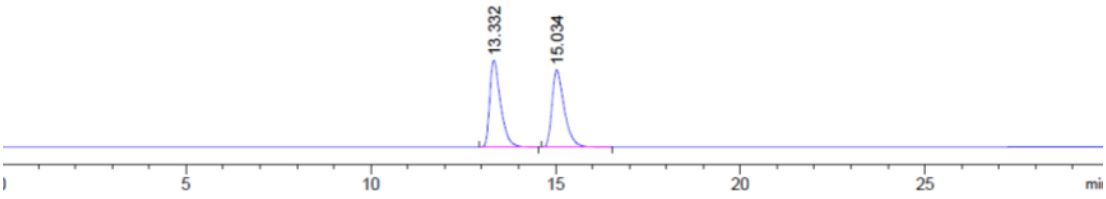
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.357	BB	0.5823	4960.85938	127.95944	50.2670
2	39.351	MM	1.1398	4908.15576	71.76692	49.7330



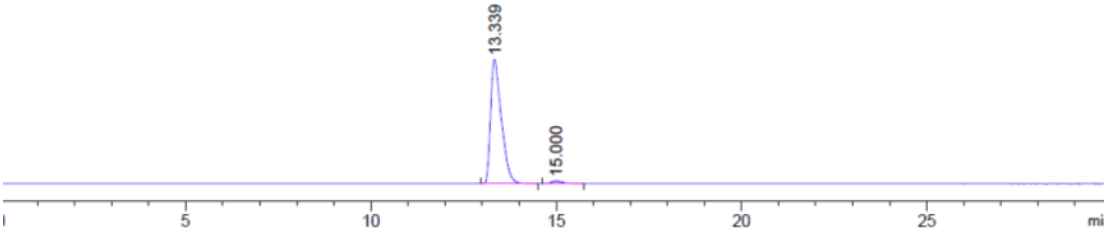
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.599	BV	0.5651	1.17104e4	309.73575	99.6402
2	37.258	MM	0.5733	42.28070	1.22927	0.3598

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5i**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 93: 7, flow rate: 0.8 ml/min, λ = 280 nm, retention time: t (major) = 13.34 min, t (minor) = 15.00 min.



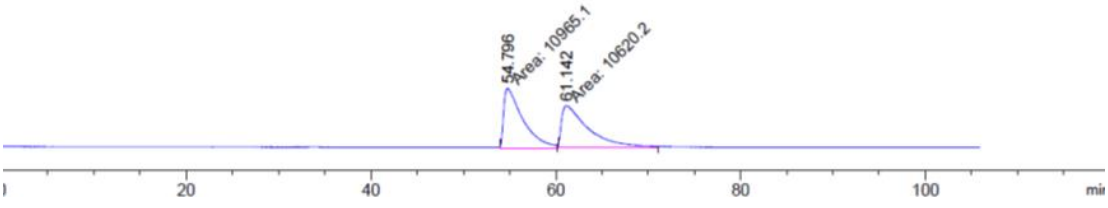
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.332	BB	0.3041	7309.16846	358.07965	49.9810
2	15.034	BB	0.3418	7314.72119	318.62088	50.0190



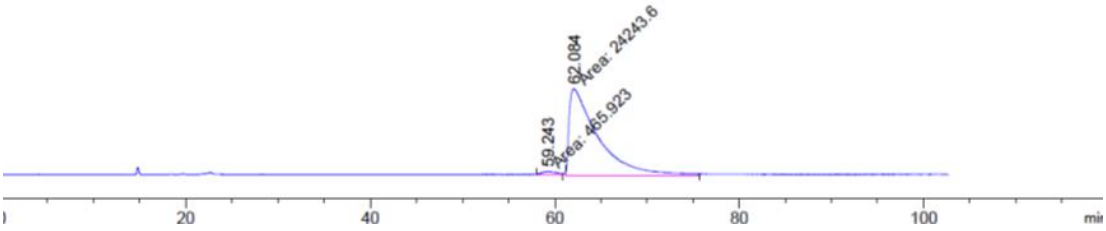
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.339	BB	0.2979	1.03341e4	511.04984	97.4477
2	15.000	BB	0.3031	270.66534	12.18657	2.5523

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5j**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 94: 6, flow rate: 0.7 ml/min, λ = 280 nm, retention time: t (major) = 62.08 min, t (minor) = 59.24 min.



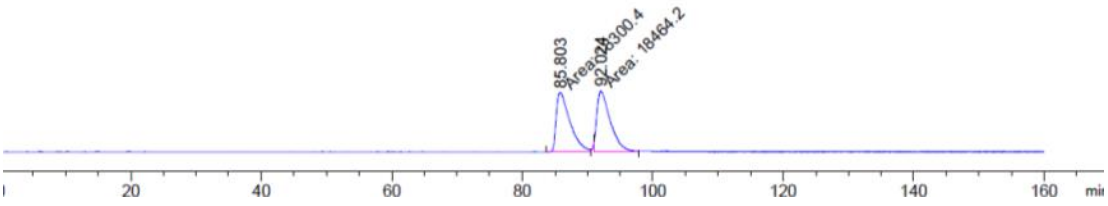
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	54.796	MM	2.4060	1.09651e4	75.95802	50.7989
2	61.142	MM	3.3363	1.06202e4	53.05419	49.2011



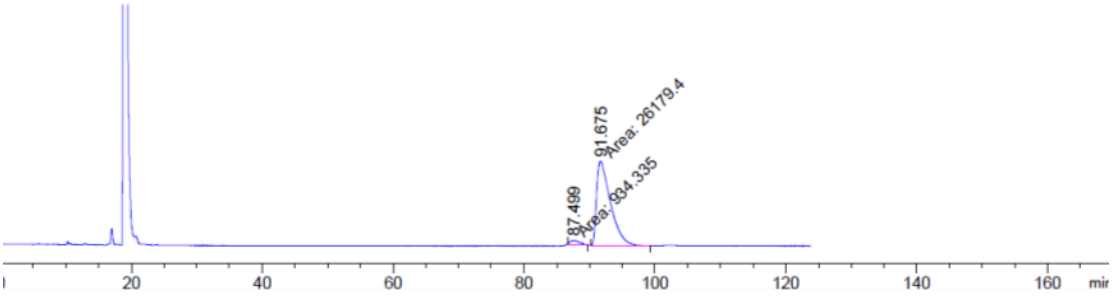
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	59.243	MM	1.9087	465.92279	4.06850	1.8856
2	62.084	MM	3.6415	2.42436e4	110.96034	98.1144

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5k**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 98: 2, flow rate: 0.5 ml/min, λ = 280 nm, retention time: t (major) = 91.67 min, t (minor) = 87.50 min.



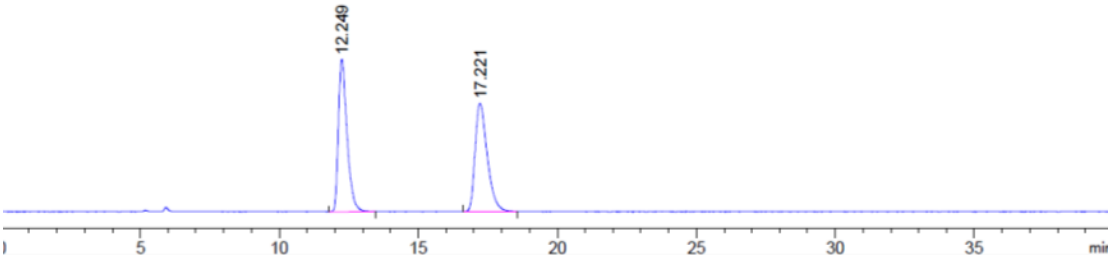
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	85.803	MM	2.4568	1.83004e4	124.14713	49.7772
2	92.024	MM	2.4210	1.84642e4	127.11095	50.2228



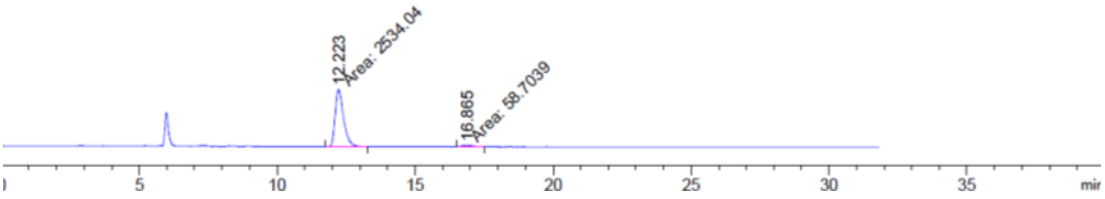
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	87.499	MM	1.6665	934.33521	9.34401	3.4460
2	91.675	MM	2.4704	2.61794e4	176.62206	96.5540

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5l**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 12.22 min, t (minor) = 16.86 min.



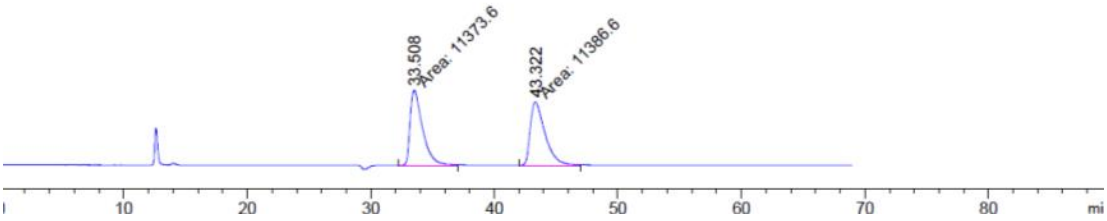
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.249	BB	0.3290	8137.52148	375.21893	49.9994
2	17.221	BV	0.4656	8137.70996	266.95889	50.0006



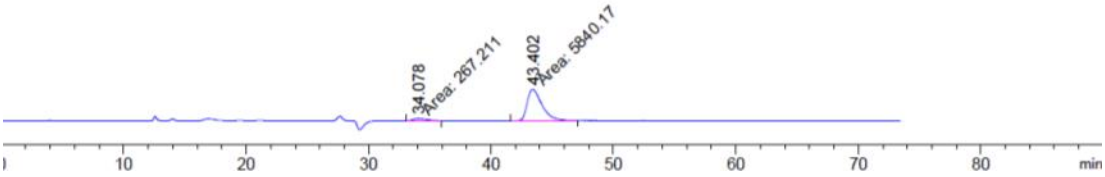
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.223	MM	0.3547	2534.04199	119.06854	97.7358
2	16.865	MM	0.3694	58.70388	2.64865	2.2642

Chiral HPLC chromatographic analysis of C3-alkylated indole of **5m**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 0.7 ml/min, λ = 280 nm, retention time: t (major) = 43.40 min, t (minor) = 34.07 min.



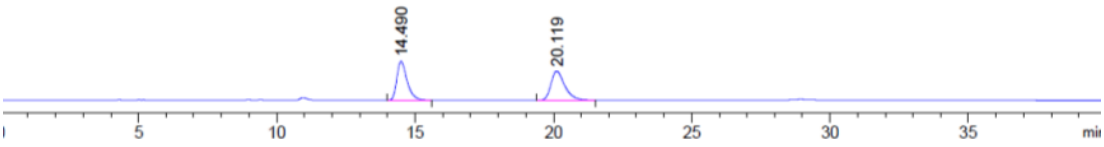
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	33.508	MM	1.1866	1.13736e4	159.74542	49.9714
2	43.322	MM	1.4062	1.13866e4	134.95337	50.0286



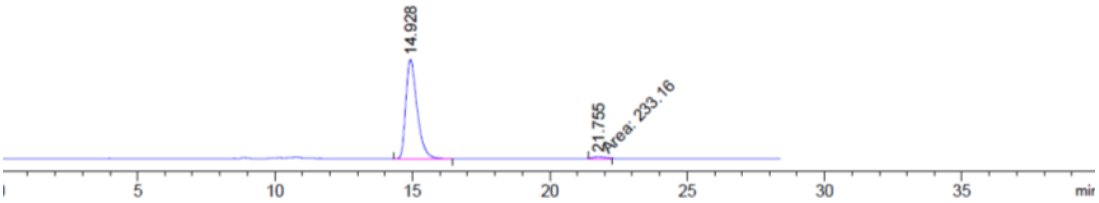
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	34.078	MM	1.0563	267.21069	4.21596	4.3752
2	43.402	MM	1.4253	5840.17236	68.29041	95.6248

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6a**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 95: 5, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 14.93 min, t (minor) = 21.75 min.



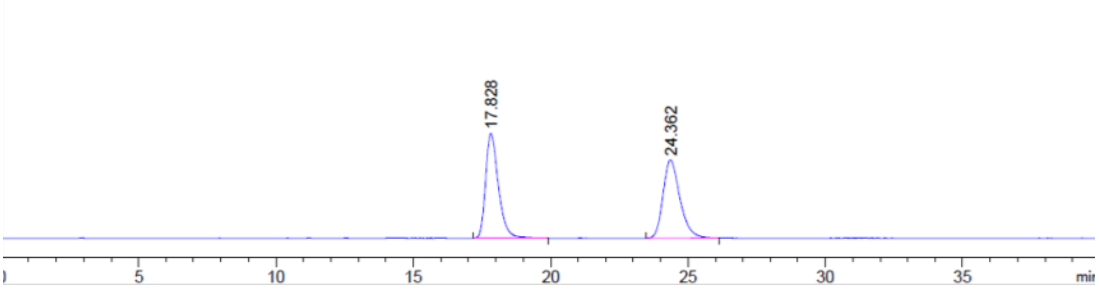
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.490	BB	0.3879	4046.45313	157.40800	49.9850
2	20.119	BB	0.5226	4048.88477	117.91042	50.0150



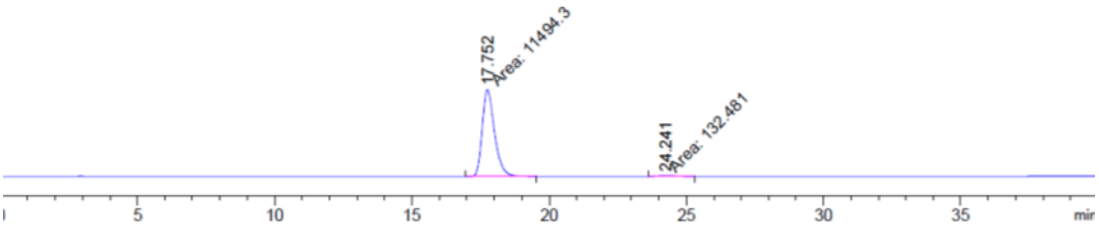
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.928	BB	0.4385	1.15284e4	404.48044	98.0176
2	21.755	MM	0.5377	233.15968	7.22748	1.9824

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6b**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 92: 8, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 17.75 min, t (minor) = 24.24 min.



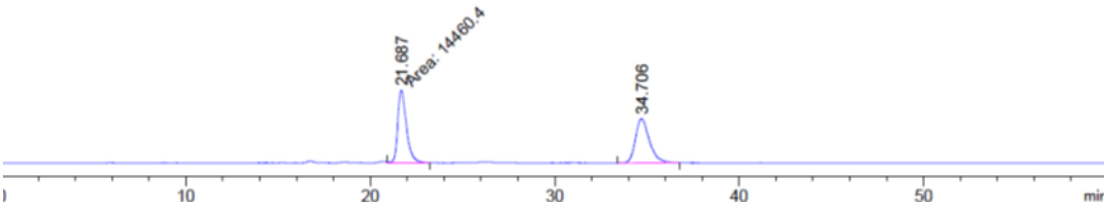
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.828	VB	0.4912	1.42089e4	439.49539	50.3947
2	24.362	BB	0.6334	1.39864e4	328.04382	49.6053



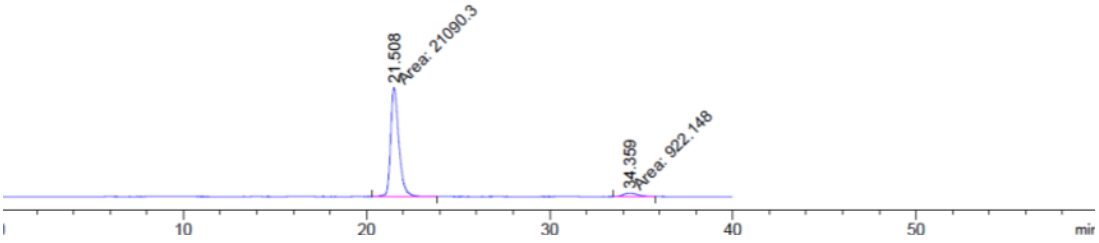
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.752	MM	0.5249	1.14943e4	364.93936	98.8606
2	24.241	MM	0.5566	132.48140	3.96684	1.1394

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6c**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 95: 5, flow rate: 0.5 ml/min, λ = 280 nm, retention time: t (major) = 21.51 min, t (minor) = 34.36 min.



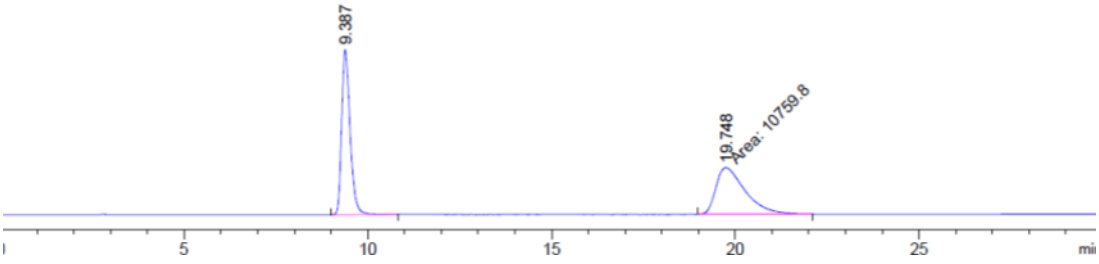
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.687	MM	0.5453	1.44604e4	441.99899	50.5978
2	34.706	BB	0.7637	1.41187e4	269.27759	49.4022



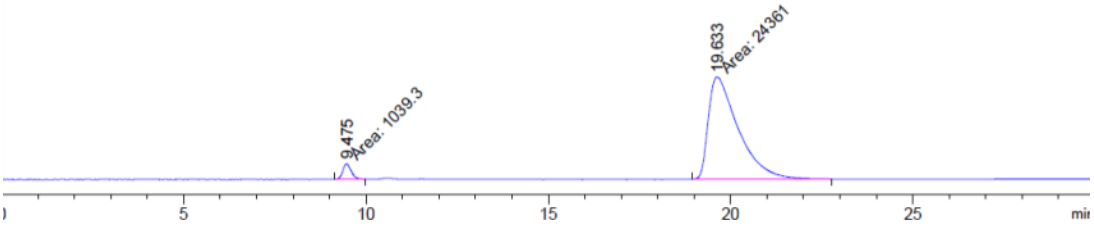
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.508	MM	0.5252	2.10903e4	669.27502	95.8108
2	34.359	MM	0.8221	922.14758	18.69481	4.1892

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6d**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 19.63 min, t (minor) = 9.47 min.



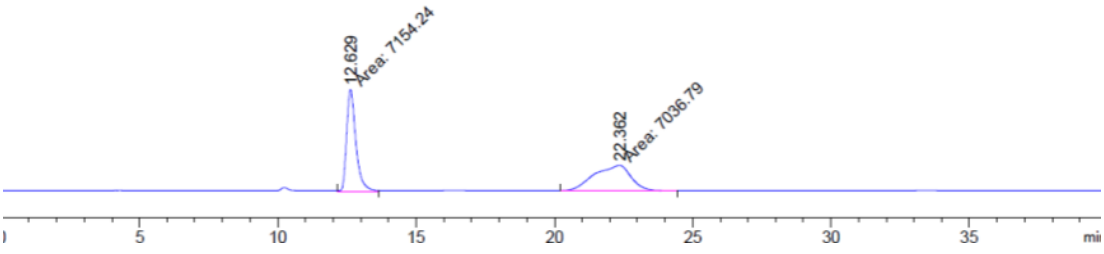
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.387	BB	0.2472	1.08740e4	677.67993	50.2638
2	19.748	MM	0.9347	1.07598e4	191.86763	49.7362



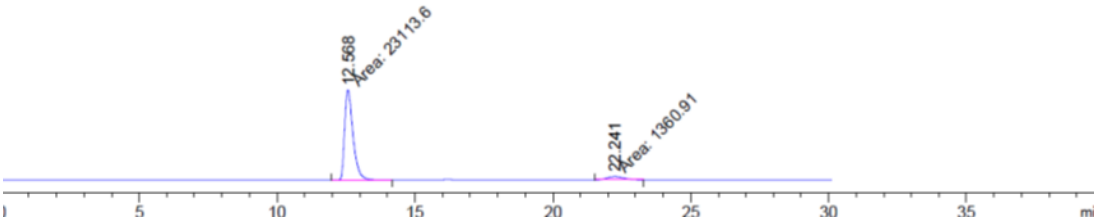
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.475	MM	0.2709	1039.29956	63.93324	4.0917
2	19.633	MM	0.9615	2.43610e4	422.26038	95.9083

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6e**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 95: 5, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 12.56 min, t (minor) = 22.24 min.



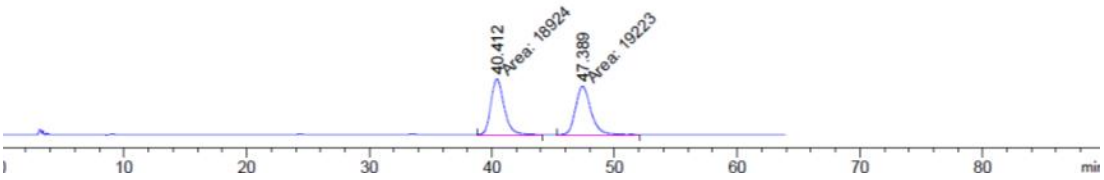
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.629	MM	0.3887	7154.24072	306.73462	50.4138
2	22.362	MM	1.5369	7036.78955	76.30802	49.5862



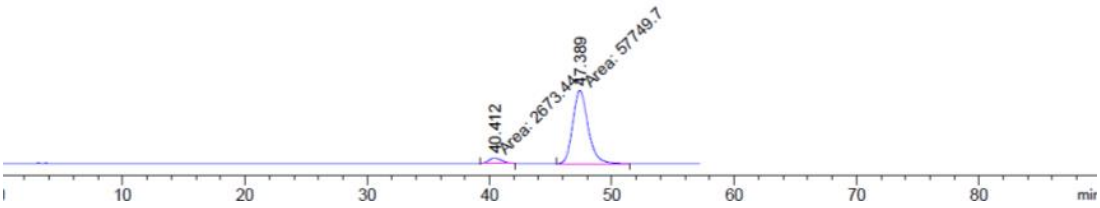
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.568	MM	0.3518	2.31136e4	1094.94543	94.4395
2	22.241	MM	0.6341	1360.91113	35.77253	5.5605

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6f**

Condition: chiral AD-H column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 220 nm, retention time: t (major) = 47.39 min, t (minor) = 40.41 min.



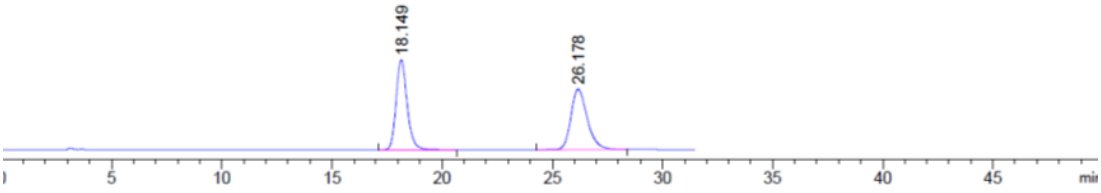
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	40.412	MM	1.2744	1.89240e4	247.49606	49.6081
2	47.389	MM	1.4887	1.92230e4	215.20364	50.3919



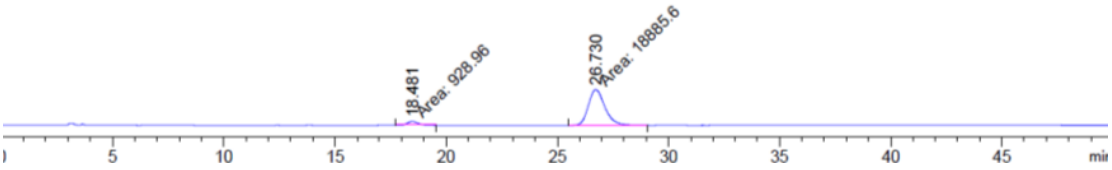
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	40.412	MM	1.0106	2673.43677	44.08809	4.4245
2	47.389	MM	1.4729	5.77497e4	653.45898	95.5755

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6g**

Condition: chiral AD-H column, *n*-hexane/2-propanol = 85: 15, flow rate: 1 ml/min, λ = 220 nm, retention time: t (major) = 26.73 min, t (minor) = 18.48 min.



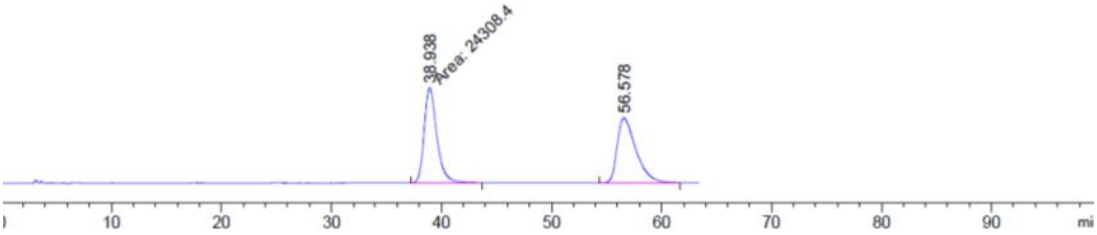
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.149	BB	0.5301	2.44503e4	705.98035	49.9123
2	26.178	BB	0.7884	2.45363e4	475.20380	50.0877



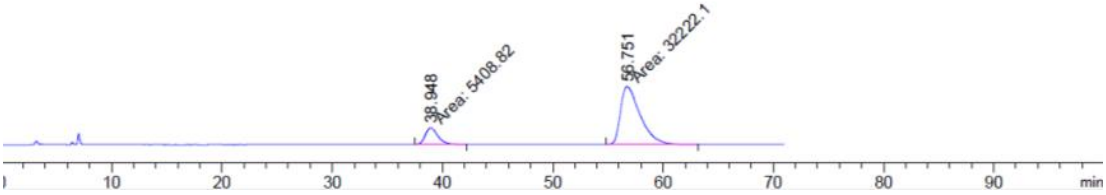
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.481	MM	0.4695	928.96021	32.97385	4.6883
2	26.730	MM	0.8772	1.88856e4	358.82593	95.3117

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6h**

Condition: chiral AD-H column, *n*-hexane/2-propanol = 85: 15, flow rate: 1 ml/min, λ = 220 nm, retention time: t (major) = 56.75 min, t (minor) = 38.95 min.



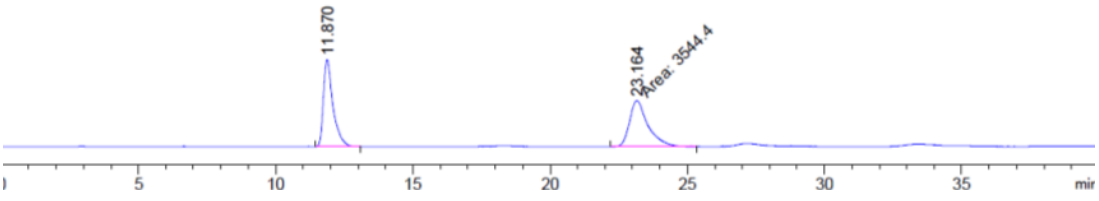
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.938	MM	1.3428	2.43084e4	301.72333	49.9656
2	56.578	BB	1.7089	2.43419e4	205.65544	50.0344



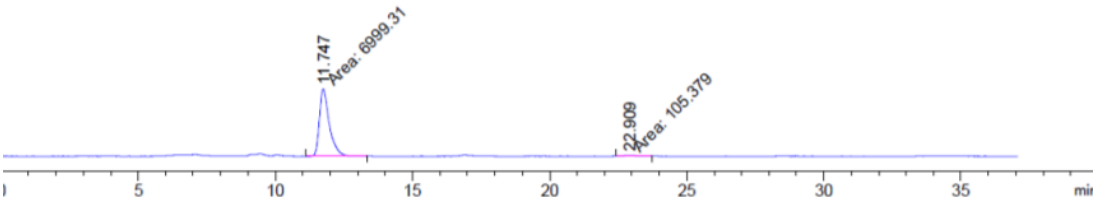
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.948	MM	1.2392	5408.81982	72.74702	14.3733
2	56.751	MM	2.0516	3.22221e4	261.77008	85.6267

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6i**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 82: 8, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 11.75 min, t (minor) = 22.91 min.



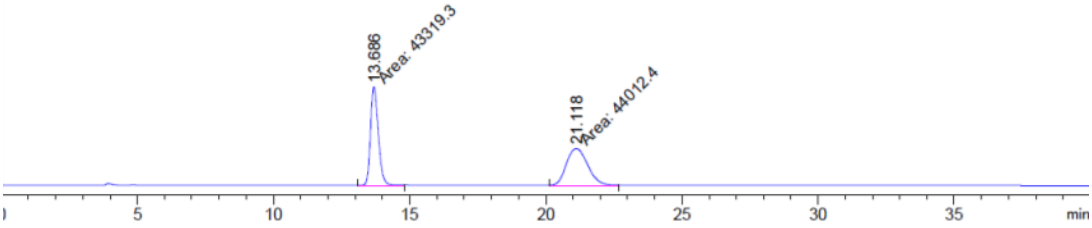
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.870	BB	0.3475	3527.33057	146.20004	49.8793
2	23.164	MM	0.7709	3544.39990	76.62571	50.1207



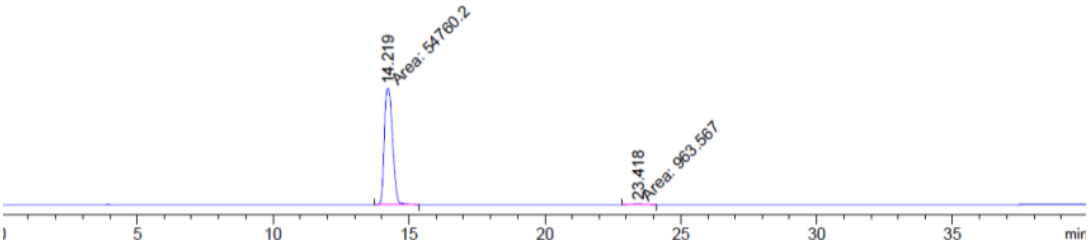
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.747	MM	0.4183	6999.30664	278.90451	98.5168
2	22.909	MM	0.6649	105.37888	2.64141	1.4832

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6j**

Condition: chiral AD-H column, *n*-hexane/2-propanol = 95: 5, flow rate: 0.8 ml/min, λ = 220 nm, retention time: t (major) = 14.22 min, t (minor) = 23.42 min.



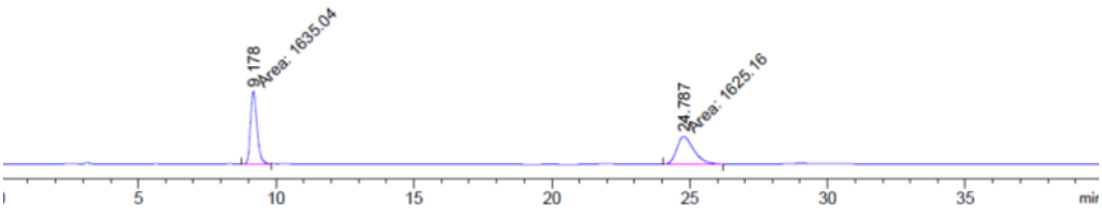
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.686	MM	0.3344	4.33193e4	2159.02124	49.6032
2	21.118	MM	0.9138	4.40124e4	802.73938	50.3968



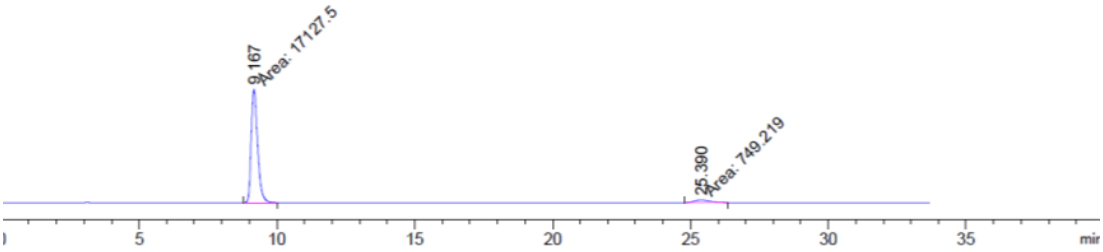
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.219	MM	0.3533	5.47602e4	2583.51611	98.2708
2	23.418	MM	0.7551	963.56677	21.26761	1.7292

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6k**

Condition: chiral AD-H column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 254 nm, retention time: t (major) = 9.17 min, t (minor) = 25.39 min.



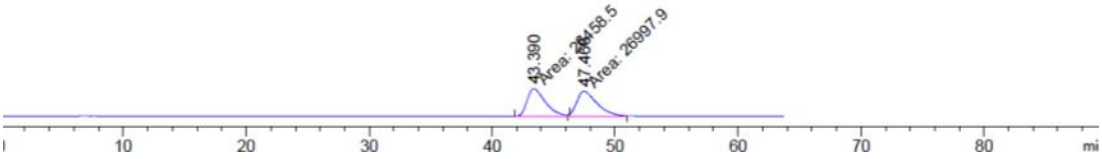
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.178	MM	0.2751	1635.03674	99.04852	50.1515
2	24.787	MM	0.7231	1625.16113	37.45817	49.8485



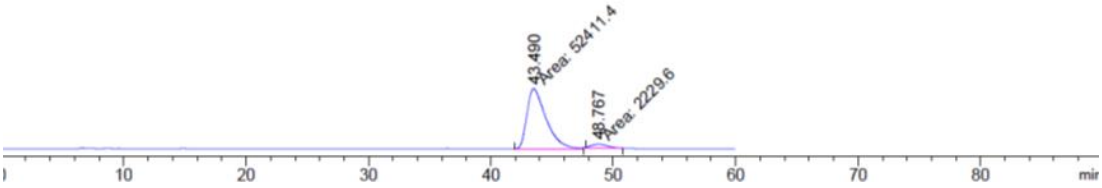
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.167	MM	0.2758	1.71275e4	1035.15576	95.8090
2	25.390	MM	0.6118	749.21936	20.41064	4.1910

Chiral HPLC chromatographic analysis of C2-alkylated indole of **6l**

Condition: chiral OD-H column, *n*-hexane/2-propanol = 98: 2, flow rate: 0.5 ml/min, λ = 230 nm, retention time: t (major) = 43.49 min, t (minor) = 48.77 min.



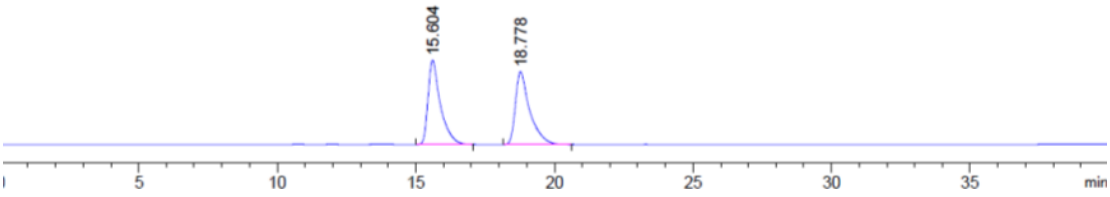
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	43.388	BV	1.3783	5453.89258	53.36655	49.5881
2	47.466	VB	1.5324	5544.49609	48.47564	50.4119



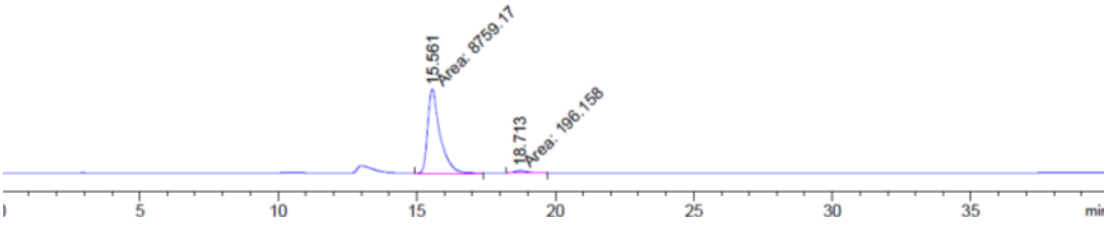
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	43.490	MM	1.8439	5.24114e4	473.74878	95.9195
2	48.767	MM	1.4584	2229.60229	25.47966	4.0805

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7a**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 95: 5, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 15.56 min, t (minor) = 18.71 min.



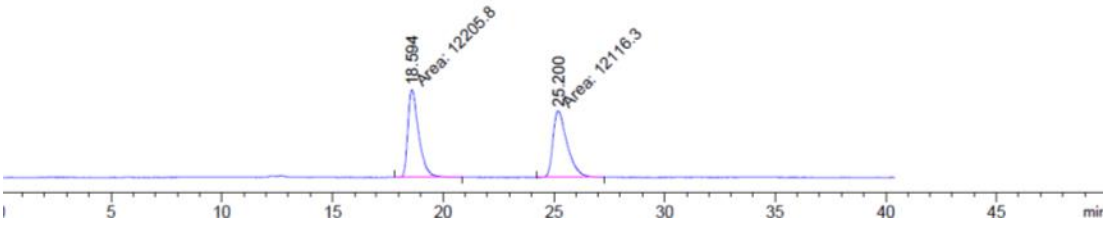
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.604	BV	0.4575	8652.42188	279.21481	50.0006
2	18.778	BV	0.5228	8652.20605	241.04968	49.9994



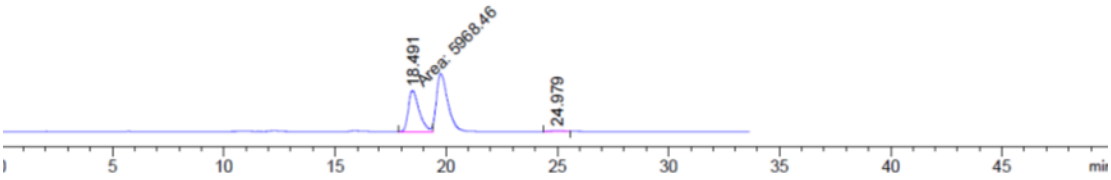
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.561	MM	0.5200	8759.16895	280.74469	97.8096
2	18.713	MM	0.4712	196.15848	6.93867	2.1904

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7b**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 92: 8, flow rate: 0.5 ml/min, λ = 280 nm, retention time: t (major) = 18.49 min, t (minor) = 24.98 min.



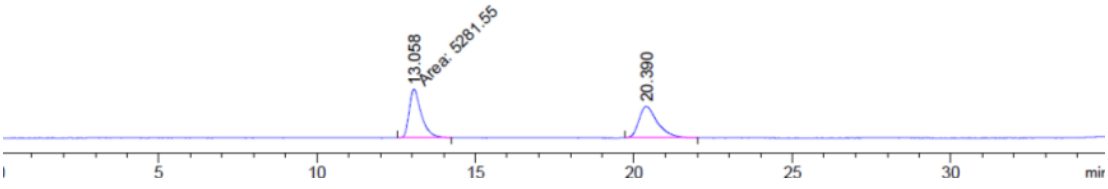
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.594	MM	0.5657	1.22058e4	359.58835	50.1841
2	25.200	MM	0.7415	1.21163e4	272.35587	49.8159



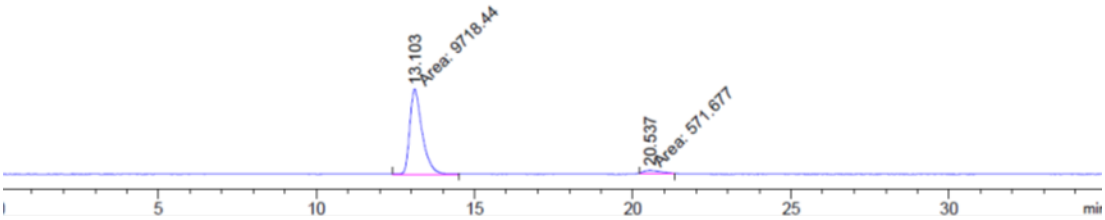
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.491	MM	0.5875	5968.46045	169.30614	97.5176
2	24.979	BV	0.4590	151.93427	3.93009	2.4824

Chiral HPLC chromatographic analysis of C2-alkylated indole of **7b'**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 94: 6, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 13.10 min, t (minor) = 20.54 min.



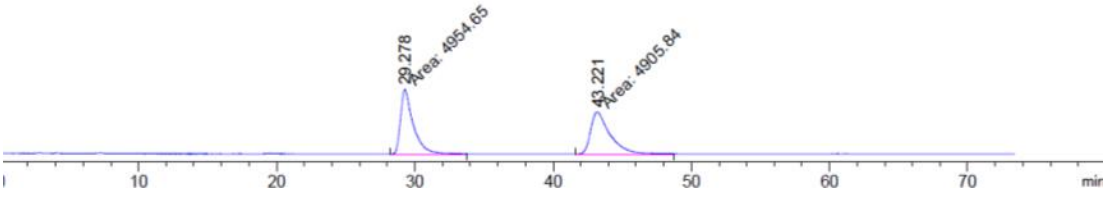
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.058	MM	0.4440	5281.54688	198.23958	50.0966
2	20.390	BB	0.5904	5261.18506	128.82924	49.9034



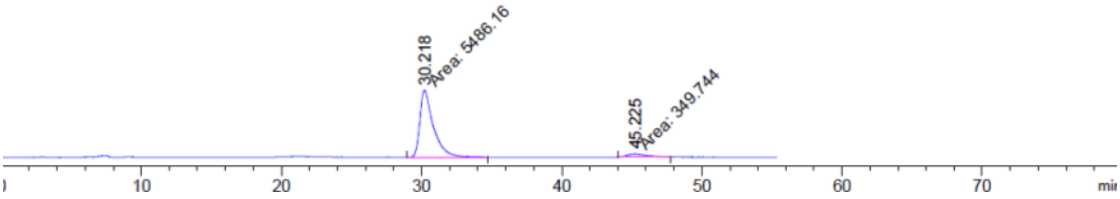
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.103	MM	0.4624	9718.44141	350.30307	94.4444
2	20.537	MM	0.6724	571.67664	14.16922	5.5556

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7c**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 30.22 min, t (minor) = 45.22 min.



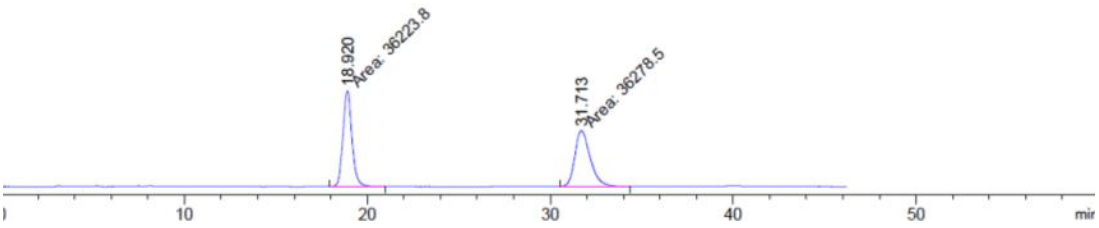
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.278	MM	1.0678	4954.64990	77.33517	50.2475
2	43.221	MM	1.6273	4905.83887	50.24450	49.7525



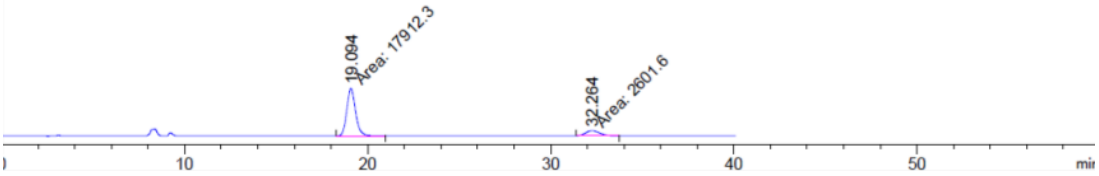
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.218	MM	1.1478	5486.16064	79.66487	94.0070
2	45.225	MM	1.5511	349.74353	3.75808	5.9930

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7d**

Condition: chiral AD-H column, *n*-hexane/2-propanol = 85: 15, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 19.09 min, t (minor) = 32.26 min.



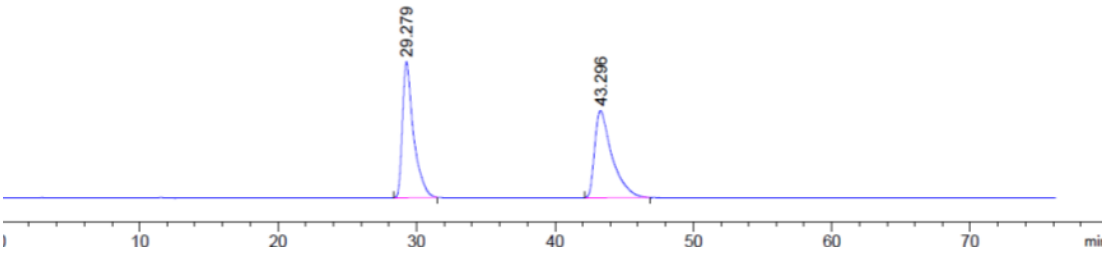
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.920	MM	0.5767	3.62238e4	1046.81250	49.9623
2	31.713	MM	0.9881	3.62785e4	611.92621	50.0377



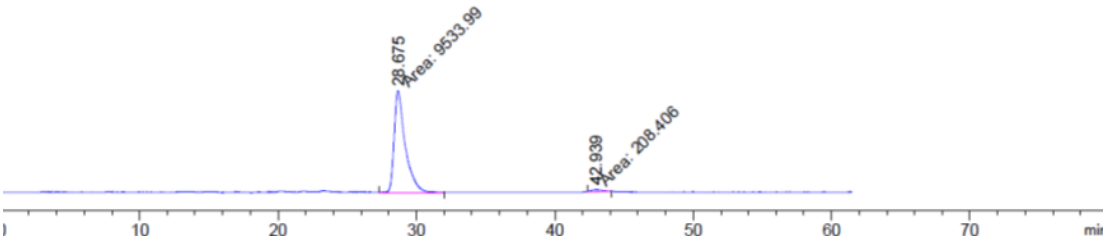
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.094	MM	0.5705	1.79123e4	523.30646	87.3179
2	32.264	MM	0.8347	2601.59985	51.94750	12.6821

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7e**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 95: 5, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 28.67 min, t (minor) = 42.94 min.



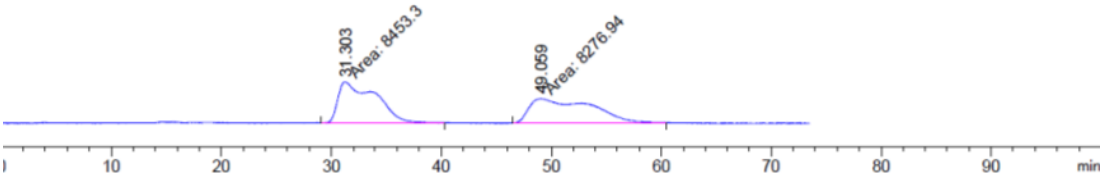
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.279	BB	0.7960	9675.87012	173.66272	49.9676
2	43.296	BV	1.0436	9688.43164	111.07635	50.0324



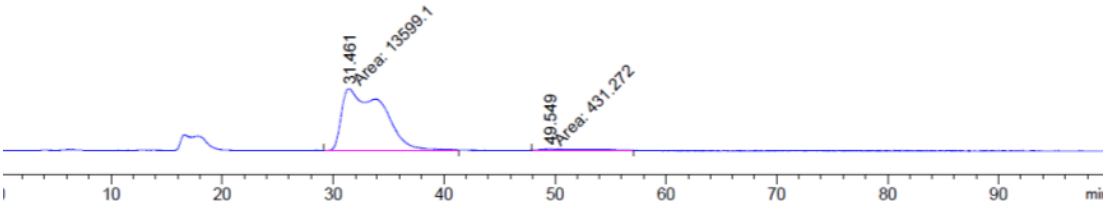
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.675	MM	0.9393	9533.99023	169.16603	97.8608
2	42.939	MM	1.0112	208.40565	3.43485	2.1392

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7f**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 96: 4, flow rate: 0.8 ml/min, λ = 280 nm, retention time: t (major) = 31.46 min, t (minor) = 49.55 min.



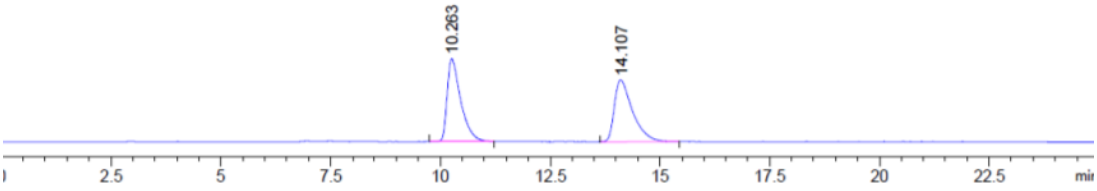
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.303	MM	3.9922	8453.29688	35.29079	50.5270
2	49.059	MM	6.5575	8276.94434	21.03675	49.4730



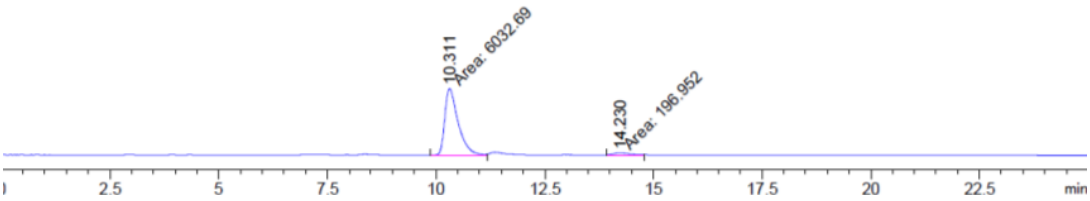
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.461	MM	4.3056	1.35991e4	52.64136	96.9261
2	49.549	MM	5.5520	431.27240	1.29464	3.0739

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7g**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 94: 6, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 10.31 min, t (minor) = 14.23 min.



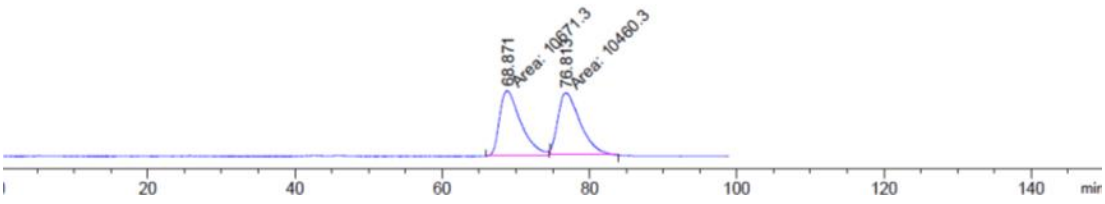
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.263	BB	0.3217	7368.64893	341.56470	50.0355
2	14.107	BB	0.4305	7358.18164	255.14725	49.9645



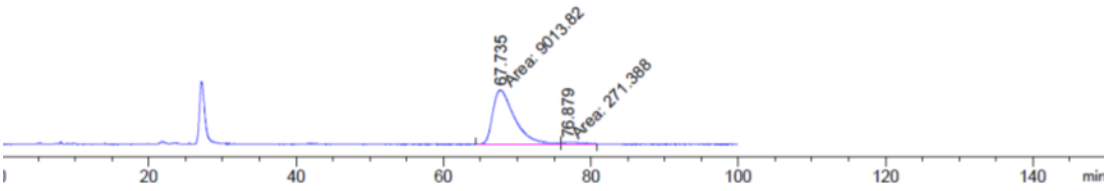
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.311	MM	0.3612	6032.68750	278.35477	96.8385
2	14.230	MM	0.4272	196.95183	7.68345	3.1615

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7h**

Condition: chiral OD-H column, *n*-hexane/2-propanol = 95: 5, flow rate: 0.6 ml/min, λ = 280 nm, retention time: t (major) = 67.74 min, t (minor) = 76.88 min.



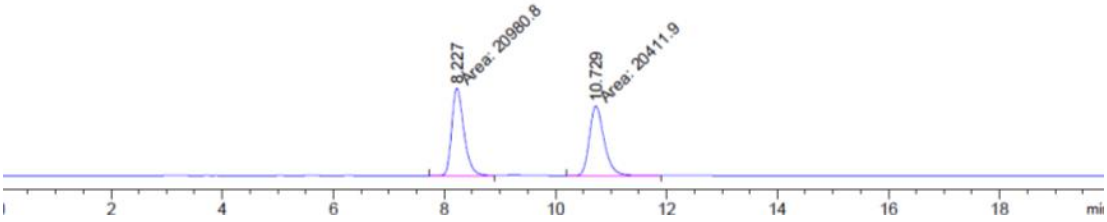
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	68.871	MM	3.3700	1.06713e4	52.77581	50.4993
2	76.813	MM	3.4715	1.04603e4	50.22012	49.5007



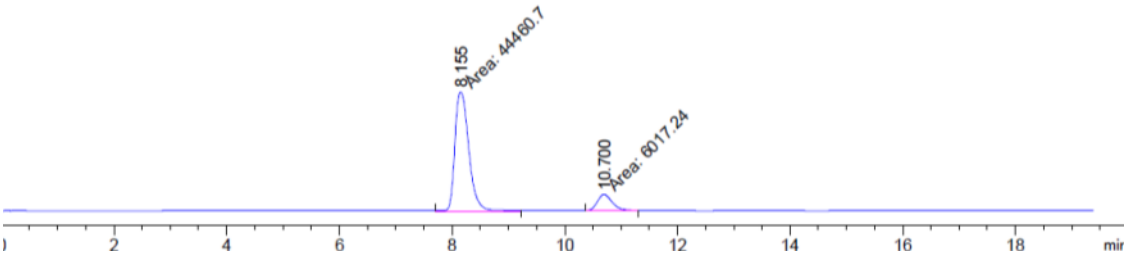
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	67.735	MM	3.4211	9013.81543	43.91257	97.0772
2	76.879	MM	3.0459	271.38773	1.48499	2.9228

Chiral HPLC chromatographic analysis of N1-alkylated indole of **7i**

Condition: chiral AD-H column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 8.15 min, t (minor) = 10.70 min.



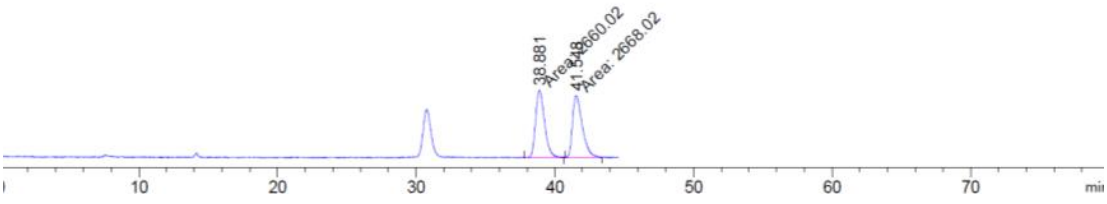
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.227	MM	0.2564	2.09808e4	1363.54358	50.6872
2	10.729	MM	0.3130	2.04119e4	1086.91394	49.3128



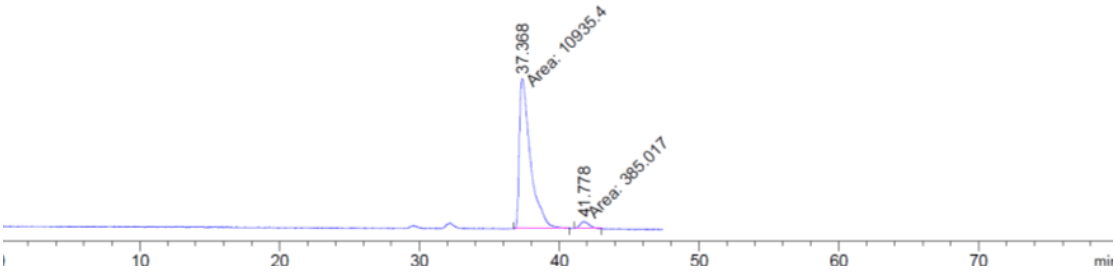
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.155	MM	0.2850	4.44607e4	2599.58765	88.0795
2	10.700	MM	0.2913	6017.23828	344.24915	11.9205

Chiral HPLC chromatographic analysis of C2-alkylated pyrrole of **9a**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 98: 2, flow rate: 0.4 ml/min, λ = 254 nm, retention time: t (major) = 37.37 min, t (minor) = 41.77 min.



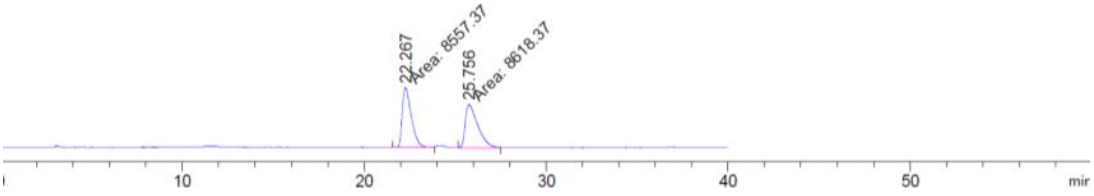
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.881	MM	0.7483	2660.01538	59.24261	49.9249
2	41.548	MM	0.8158	2668.01904	54.51048	50.0751



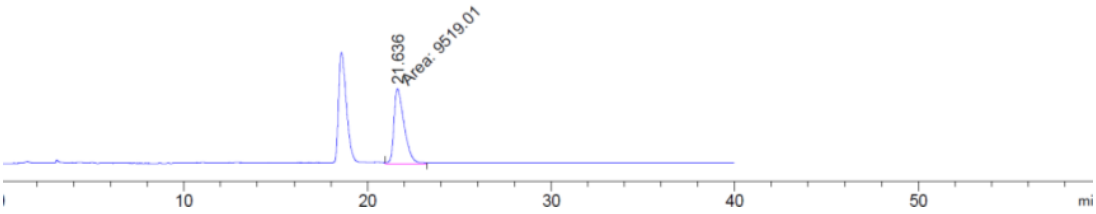
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.368	MM	0.9153	1.09354e4	199.12209	96.5989
2	41.778	MM	0.7202	385.01730	8.91000	3.4011

Chiral HPLC chromatographic analysis of C2-alkylated pyrrole of **9b**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 98: 2, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 21.64 min.



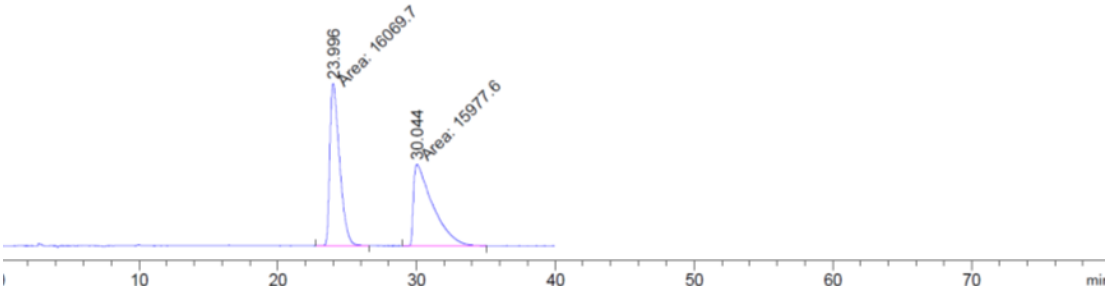
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.267	MM	0.5738	8557.36621	248.53770	49.8224
2	25.756	MM	0.8007	8618.36816	179.40320	50.1776



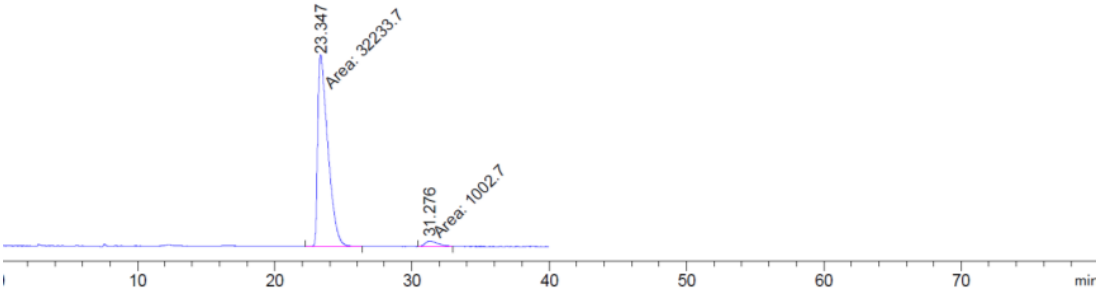
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.636	MM	0.6367	9519.01270	249.16541	100.0000

Chiral HPLC chromatographic analysis of C3-alkylated pyrrole of **9c**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 85: 15, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 23.35 min, t (minor) = 31.27 min.



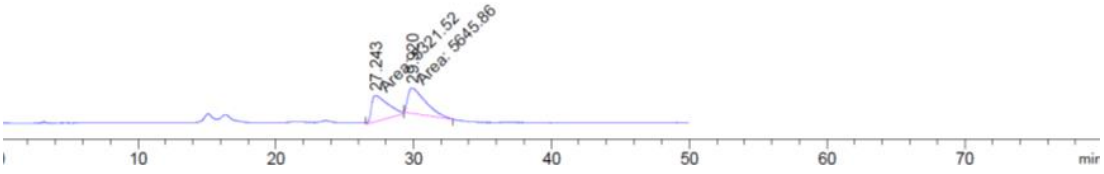
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.996	MM	0.8108	1.60697e4	330.30765	50.1438
2	30.044	MM	1.6078	1.59776e4	165.62183	49.8562



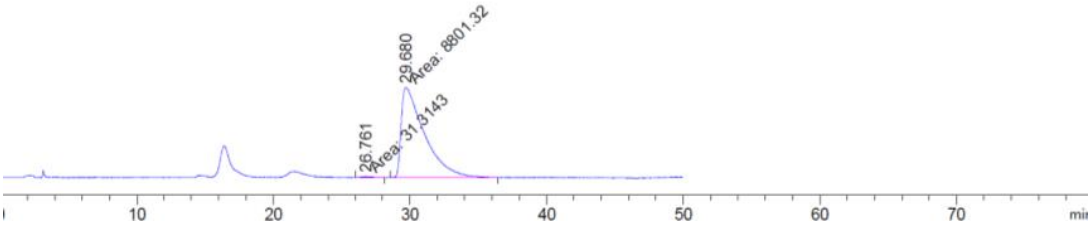
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.347	MM	0.8500	3.22337e4	632.02692	96.9831
2	31.276	MM	0.9837	1002.70020	16.98913	3.0169

Chiral HPLC chromatographic analysis of C3-alkylated pyrrole of **9d**

Condition: chiral OD-H column, *n*-hexane/2-propanol = 95: 5, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 29.68 min, t (minor) = 26.76 min.



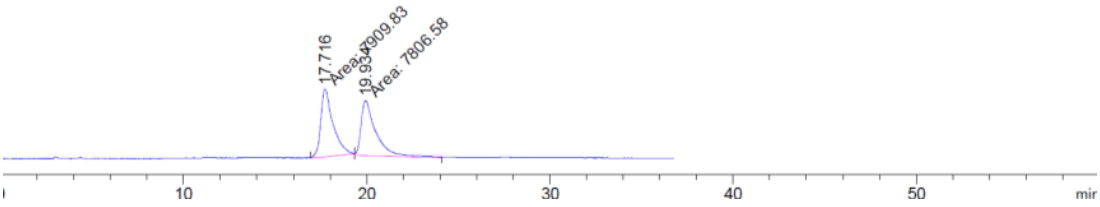
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.243	MM	0.9644	5321.52100	65.34373	48.5213
2	29.920	MM	1.4900	5645.86279	63.15380	51.4787



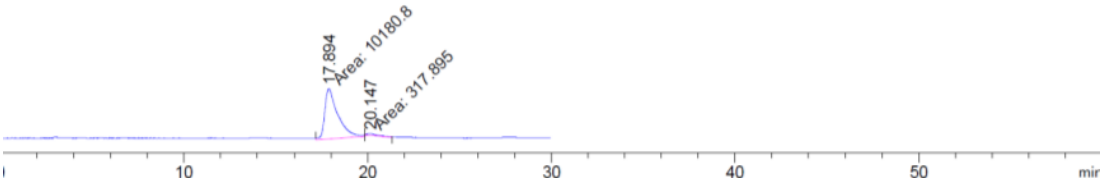
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.761	MM	0.6423	31.31428	8.12562e-1	0.3545
2	29.680	MM	1.9445	8801.31543	75.43927	99.6455

Chiral HPLC chromatographic analysis of C3-alkylated pyrrole of **9e**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 95: 5, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 17.89 min, t (minor) = 20.15 min.



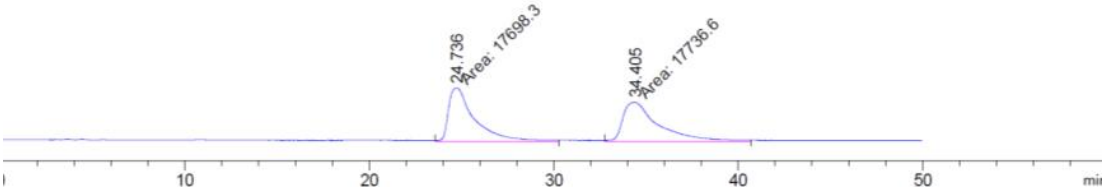
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.716	MM	0.7764	7909.83301	169.78731	50.3285
2	19.934	MM	0.9481	7806.57764	137.23320	49.6715



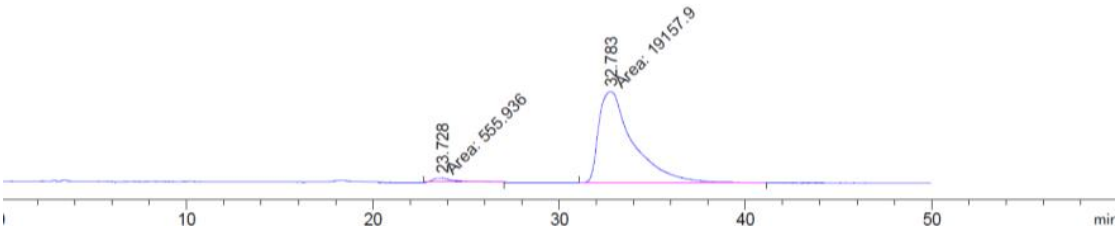
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.894	MM	0.8260	1.01808e4	205.42078	96.9721
2	20.147	MM	0.7391	317.89493	7.16841	3.0279

Chiral HPLC chromatographic analysis of C3-alkylated pyrrole of **9f**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 85: 15, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 32.78 min, t (minor) = 23.73 min.



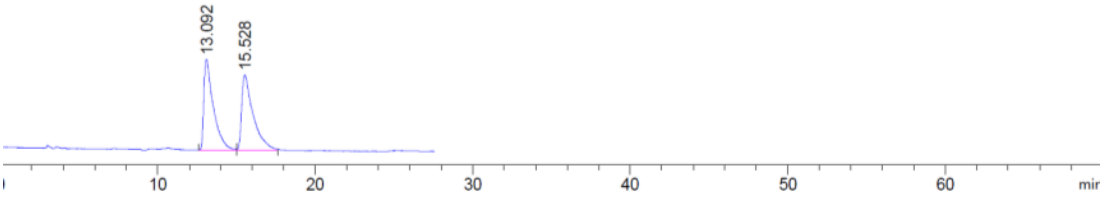
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.736	MM	1.6434	1.76983e4	179.48587	49.9460
2	34.405	MM	2.2601	1.77366e4	130.79332	50.0540



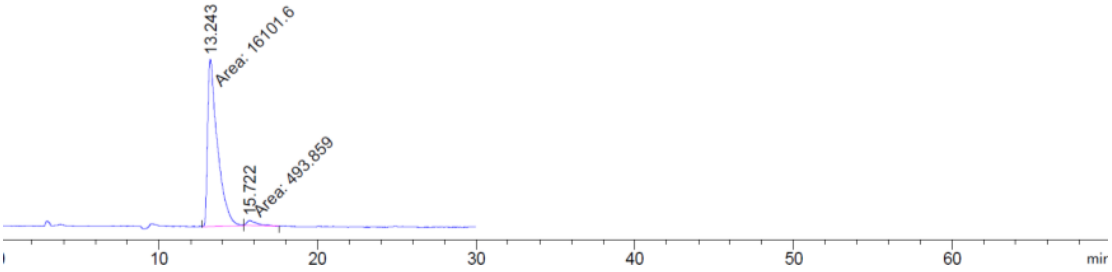
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.728	MM	1.4107	555.93640	6.56791	2.8200
2	32.783	MM	2.1332	1.91579e4	149.68059	97.1800

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11a**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 254 nm, retention time: t (major) = 13.24 min, t (minor) = 15.72 min.



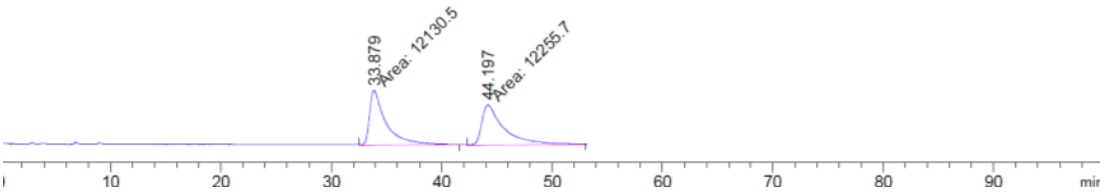
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.092	VV	0.5902	6313.91992	151.50896	50.1634
2	15.528	VV	0.6630	6272.77881	124.67211	49.8366



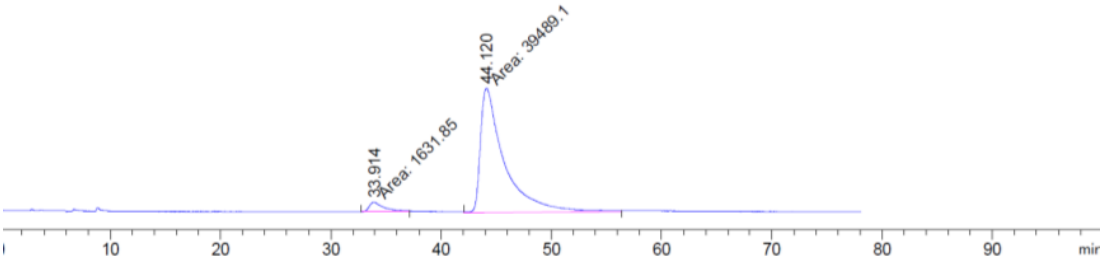
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.243	MM	0.7228	1.61016e4	371.26733	97.0241
2	15.722	MM	0.7274	493.85925	11.31632	2.9759

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11b**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 85: 15, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 44.12 min, t (minor) = 33.91 min.



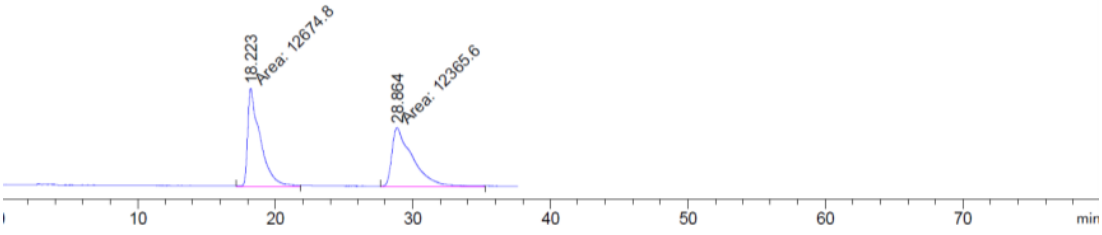
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	33.879	MM	1.7588	1.21305e4	114.94885	49.7432
2	44.197	MM	2.4127	1.22557e4	84.65962	50.2568



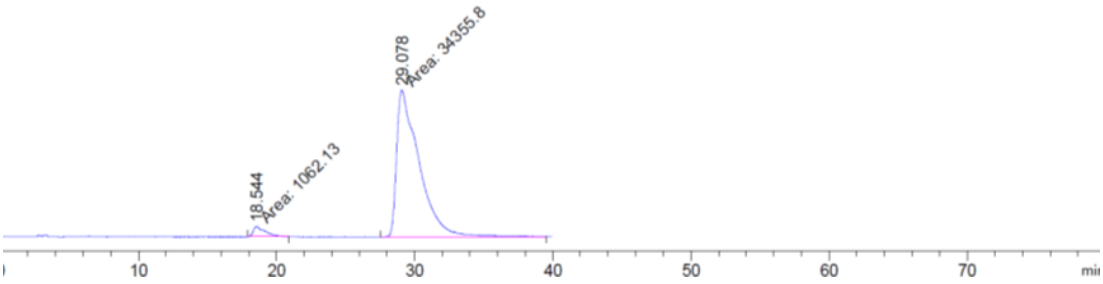
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	33.914	MM	1.4349	1631.84570	18.95401	3.9684
2	44.120	MM	2.5354	3.94891e4	259.58527	96.0316

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11c**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 75: 25, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 29.08 min, t (minor) = 18.54 min.



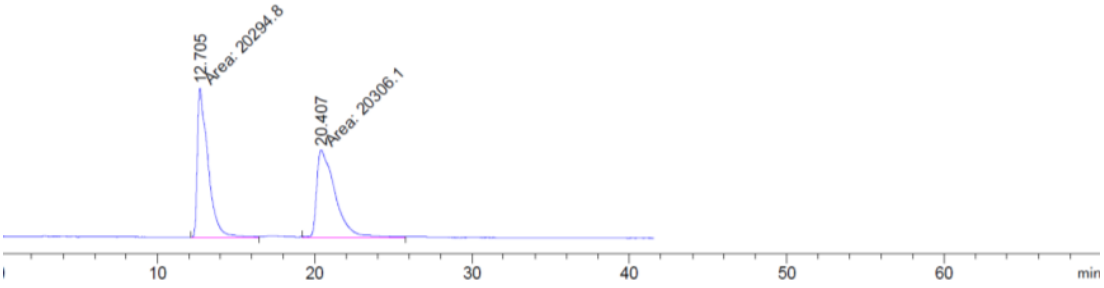
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.223	MM	1.0497	1.26748e4	201.23907	50.6173
2	28.864	MM	1.7105	1.23656e4	120.48938	49.3827



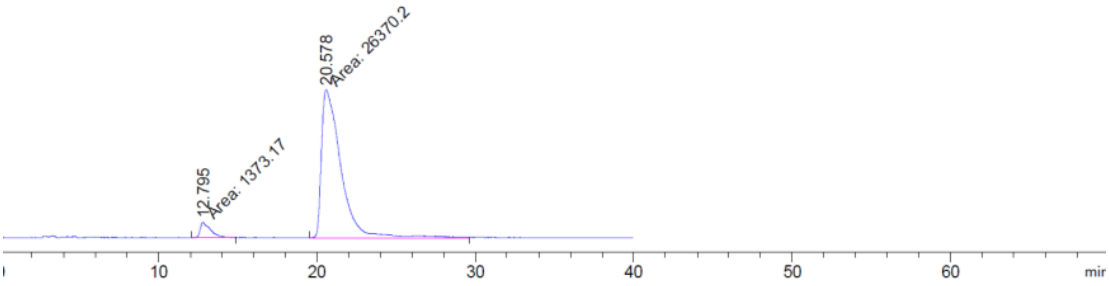
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.544	MM	0.9064	1062.13232	19.53116	2.9989
2	29.078	MM	1.9010	3.43558e4	301.21399	97.0011

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11d**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 80: 20, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 20.58 min, t (minor) = 12.79 min.



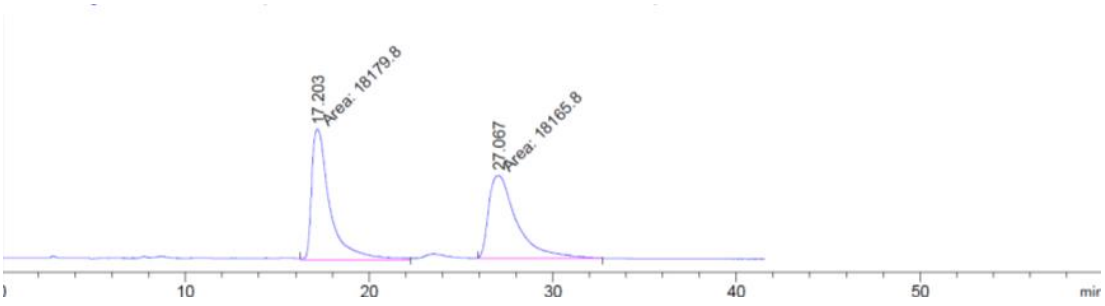
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.705	MM	0.7807	2.02948e4	433.23657	49.9861
2	20.407	MM	1.3350	2.03061e4	253.50861	50.0139



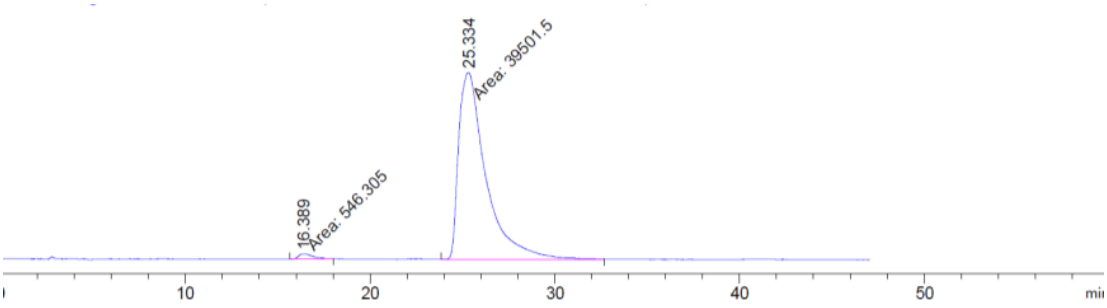
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.795	MM	0.7460	1373.16541	30.67795	4.9495
2	20.578	MM	1.4466	2.63702e4	303.81403	95.0505

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11e**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 80: 20, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 25.33 min, t (minor) = 16.39 min.



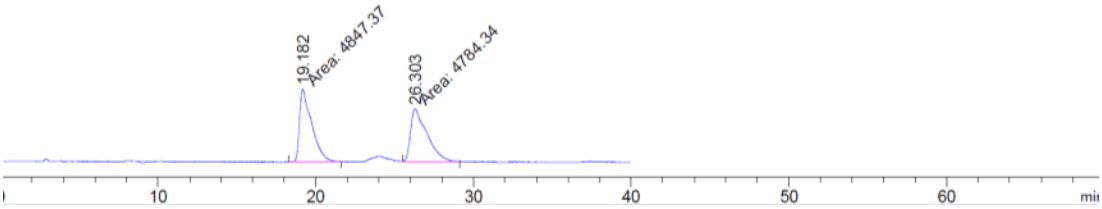
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.203	MM	1.1364	1.81798e4	266.63797	50.0192
2	27.067	MM	1.7765	1.81658e4	170.42595	49.9808



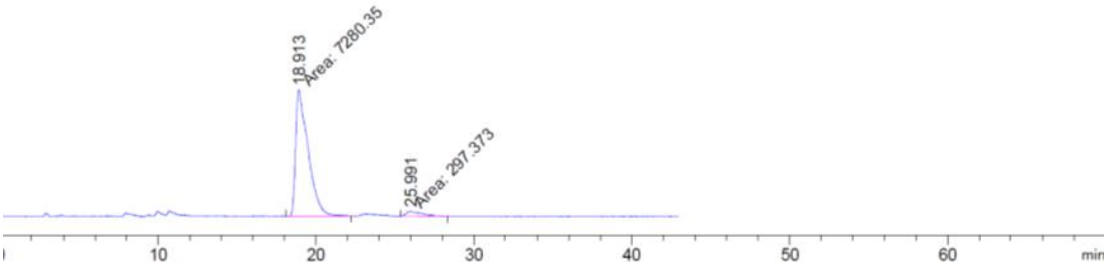
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.389	MM	0.8801	546.30536	10.34603	1.3641
2	25.334	MM	1.7210	3.95015e4	382.55389	98.6359

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11f**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 18.91 min, t (minor) = 25.99 min.



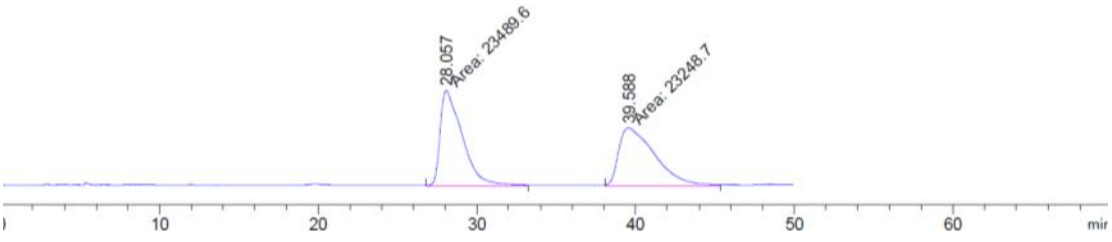
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.182	MM	0.8994	4847.36719	89.82850	50.3272
2	26.303	MM	1.2114	4784.33594	65.82258	49.6728



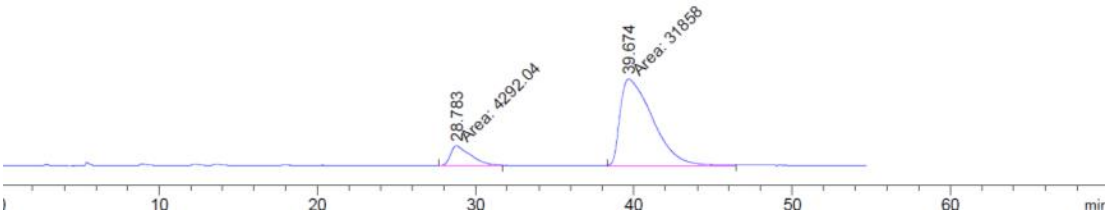
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.913	MM	0.9189	7280.35352	132.04611	96.0757
2	25.991	MM	1.0553	297.37329	4.69628	3.9243

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11g**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 75: 25, flow rate: 1 ml/min, λ = 280 nm, retention time: t (major) = 39.67 min, t (minor) = 28.78 min.



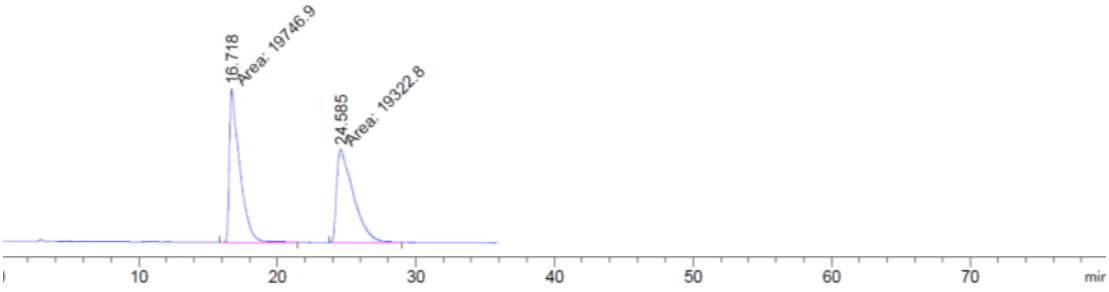
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.057	MM	1.6351	2.34896e4	239.42758	50.2577
2	39.588	MM	2.6762	2.32487e4	144.78821	49.7423



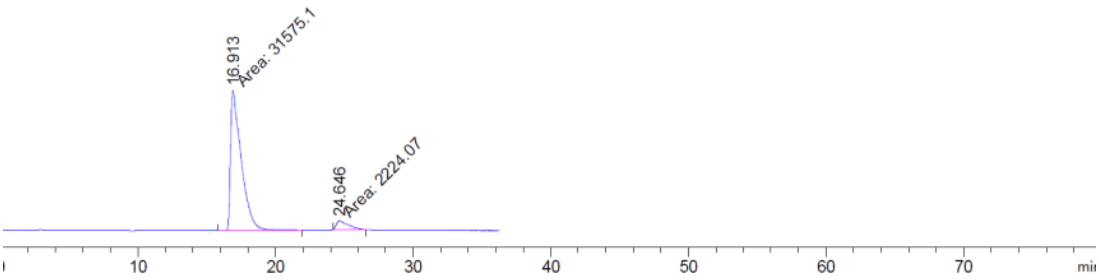
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.783	MM	1.4378	4292.03516	49.75124	11.8728
2	39.674	MM	2.4268	3.18580e4	218.78955	88.1272

Chiral HPLC chromatographic analysis of *para*-alkylated pyrrole of **11h**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 1 ml/min, λ = 254 nm, retention time: t (major) = 16.91 min, t (minor) = 24.65 min.



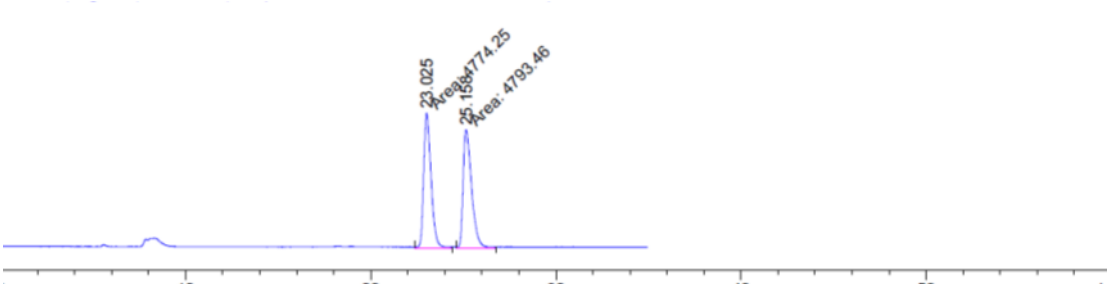
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.718	MM	0.8705	1.97469e4	378.09497	50.5428
2	24.585	MM	1.4035	1.93228e4	229.46420	49.4572



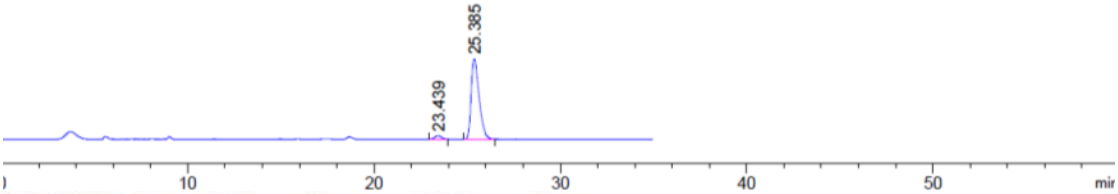
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.913	MM	0.9017	3.15751e4	583.62183	93.4197
2	24.646	MM	0.9989	2224.07495	37.10903	6.5803

Chiral HPLC chromatographic analysis of indole derivative of **13**

Condition: chiral OD-3 column, *n*-hexane/2-propanol = 90: 10, flow rate: 0.5 ml/min, λ = 280 nm, retention time: t (major) = 25.38 min, t (minor) = 23.44 min.



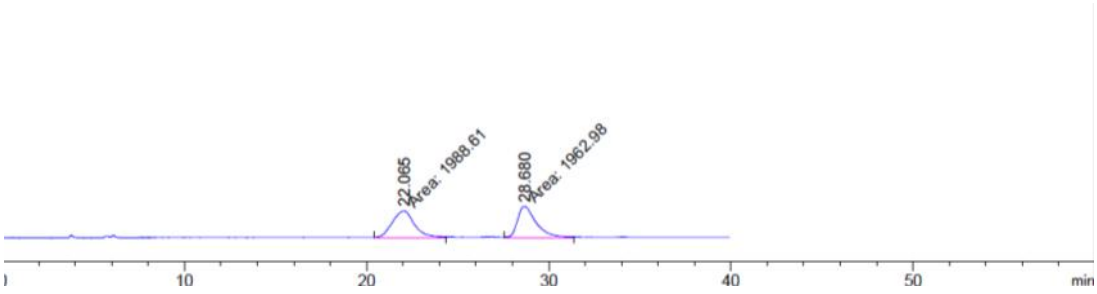
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.025	MM	0.4633	4774.25391	171.75862	49.8996
2	25.158	MM	0.5309	4793.46240	150.49553	50.1004



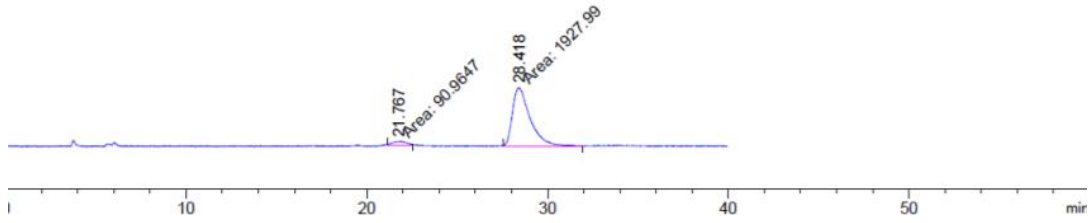
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.439	BB	0.3090	110.49870	4.39946	3.5222
2	25.385	BB	0.4399	3026.73877	102.07632	96.4778

Chiral HPLC chromatographic analysis of indole derivative of **14**

Condition: chiral AD-3 column, *n*-hexane/2-propanol = 95: 5, flow rate: 0.8 ml/min, λ = 280 nm, retention time: t (major) = 28.42 min, t (minor) = 21.76 min.



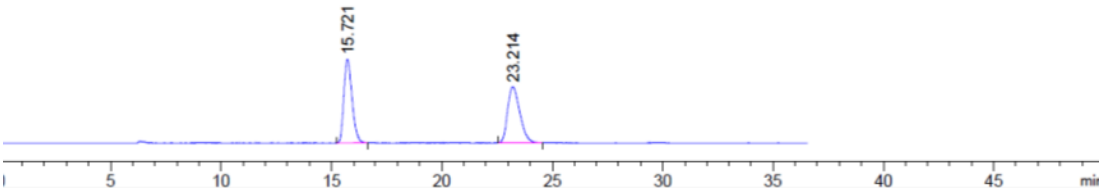
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.065	MM	1.4245	1988.61304	23.26722	50.3244
2	28.680	MM	1.2041	1962.97656	27.17184	49.6756



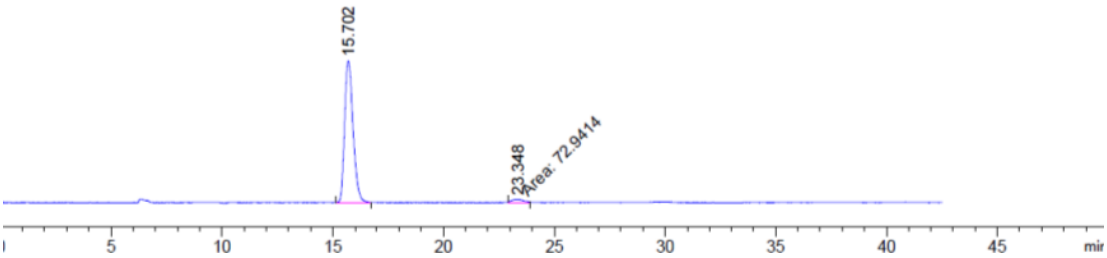
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.767	MM	0.8709	90.96465	1.74083	4.5055
2	28.418	MM	1.1501	1927.98657	27.93885	95.4945

Chiral HPLC chromatographic analysis of indole derivative of **15**

Condition: chiral OD-H column, *n*-hexane/2-propanol = 95: 5, flow rate: 0.5 ml/min, λ = 280 nm, retention time: t (major) = 15.70 min, t (minor) = 23.35 min.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.721	VB	0.3944	3590.00610	139.42899	49.9421
2	23.214	BB	0.5621	3598.33032	93.68615	50.0579



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.702	BB	0.3955	3159.11206	119.86357	97.7432
2	23.348	MM	0.5601	72.94143	2.17032	2.2568

Coordinates

1e			
Fe	3.94414	1.2861	2.32742
N	4.16879	-0.69098	2.85118
N	2.45441	0.48184	1.0325
N	4.9858	1.81648	0.5248
N	5.31251	2.57899	3.09187
C	5.06269	-1.25521	3.65726
C	5.00017	-2.60687	4.06896
C	3.93141	-3.3733	3.67329
H	3.81999	-4.40638	4.00178
C	2.94048	-2.80414	2.83572
C	1.78049	-3.5035	2.43505
H	1.64124	-4.52945	2.76948
C	0.83164	-2.88497	1.6546
H	-0.07378	-3.41447	1.37048
C	1.02794	-1.56872	1.19759
H	0.26688	-1.11496	0.56725
C	2.17142	-0.86781	1.5289
C	3.11594	-1.45688	2.40193
C	1.2354	1.33244	1.06047
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H	0.7426	1.23661	2.03152
H	0.52266	1.05231	0.27428
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H	2.61602	1.43079	-0.82274
C	2.64995	-0.65361	-1.26383
H	3.0728	-1.58243	-0.85288
H	1.55997	-0.76979	-1.23761
C	3.11708	-0.46542	-2.70245
H	2.83662	-1.34434	-3.29233
H	2.58901	0.3884	-3.15218
C	4.61589	-0.22578	-2.76049
H	4.93804	-0.03459	-3.78954
H	5.15507	-1.12631	-2.43036
C	4.99751	0.95553	-1.87844
H	4.48192	1.85655	-2.24345
H	6.06753	1.1698	-1.96037
C	4.59327	0.71781	-0.41733
H	5.08647	-0.18933	-0.03065
C	4.62231	3.17436	0.04421
H	5.25947	3.48625	-0.79141
H	4.74585	3.88838	0.86275
H	3.57773	3.19447	-0.28029
C	6.4677	2.36747	2.36157
C	6.34258	1.84031	1.04623
C	7.48286	1.45538	0.37098
H	7.42026	1.02433	-0.62297
C	8.75486	1.63663	0.95288
H	9.63523	1.32999	0.39435
C	8.89379	2.23397	2.18447
H	9.88076	2.41221	2.60606
C	7.75019	2.61077	2.9259

C	7.81386	3.18158	4.22377
H	8.78911	3.38247	4.66694
C	6.65058	3.44197	4.90904
C	5.41568	3.08992	4.31465
C	6.26197	-0.57827	4.24446
H	6.04707	0.43678	4.60668
H	7.03873	-0.47561	3.46812
C	6.69902	-1.54261	5.36056
H	7.77815	-1.5271	5.53216
H	6.21786	-1.25015	6.30131
C	6.18335	-2.92697	4.93028
H	6.93759	-3.46504	4.33783
H	5.93807	-3.57522	5.77775
C	4.28149	3.32784	5.25643
H	3.52546	2.52966	5.23245
H	3.76125	4.25632	4.97374
C	4.98785	3.47147	6.61503
H	5.06377	2.48666	7.09264
H	4.44587	4.12336	7.30397
C	6.39812	3.99082	6.28167
H	6.41707	5.08992	6.24963
H	7.15366	3.69017	7.01451

4b

C	-5.86911	18.91224	4.64995
C	-5.93356	17.3093	6.06297
H	-5.62967	16.3953	6.56034
C	-6.99699	18.12348	6.37369
H	-7.79394	18.0501	7.10271
N	-5.24676	17.7929	4.9942
N	-6.95184	19.15692	5.47496
C	-7.99633	20.17479	5.34718
H	-7.87042	20.64164	4.36341
C	-5.38992	19.80549	3.57004
C	-5.53455	21.26614	3.77011
H	-5.86345	21.63277	4.74503
O	-4.84127	19.33772	2.5797
C	-5.21036	22.13224	2.79885
H	-4.87075	21.70048	1.85426
C	-5.26471	23.60928	2.90493
H	-5.60845	23.94355	3.89003
H	-4.27692	24.05232	2.71908
H	-5.93164	24.03746	2.14429
H	-7.83386	20.96147	6.0979
C	-9.38047	19.60165	5.48484
C	-10.27786	20.13092	6.41175
C	-9.7866	18.53572	4.67529
C	-11.56552	19.61103	6.52728
H	-9.96409	20.95744	7.05037
C	-11.06895	18.01406	4.79195
H	-9.08386	18.10891	3.95922
C	-11.96249	18.55132	5.71829
H	-12.25569	20.03175	7.25621
H	-11.37353	17.18278	4.15877
H	-12.96583	18.13972	5.81077

3e

C	-3.27051	0.39994	-11.18164
C	-2.9799	0.61645	-9.80745
C	-1.74514	1.18683	-9.4662
C	-0.85303	1.51865	-10.47419
C	-1.16393	1.29321	-11.82661
C	-2.37676	0.73118	-12.19985
C	-5.02271	-0.30518	-9.98242
H	-1.4921	1.36669	-8.42196
H	0.10778	1.96162	-10.21739
H	-0.44122	1.56345	-12.59452
H	-2.61819	0.55484	-13.24748
H	-6.00753	-0.7352	-9.83979
N	-4.52508	-0.16354	-11.26221
C	-5.1889	-0.53859	-12.48178
H	-5.32115	0.32788	-13.14247
H	-4.61916	-1.30398	-13.0248
H	-6.17481	-0.94561	-12.24354
C	-4.11388	0.15781	-9.06952
H	-4.24327	0.1687	-7.99432

IntA$_1$

N	4.09796	-0.32223	2.89455
N	2.36988	0.50749	0.83706
N	5.05227	1.52775	0.44648
N	5.48935	2.87781	2.72923
C	4.95613	-0.76588	3.8036
C	4.90206	-2.05534	4.39419
C	3.85651	-2.88094	4.07873
H	3.74157	-3.86159	4.54064
C	2.88508	-2.43823	3.14828
C	1.74583	-3.21244	2.83903
H	1.62442	-4.18266	3.31701
C	0.80195	-2.73498	1.96186
H	-0.08667	-3.31849	1.73519
C	0.99766	-1.49935	1.32278
H	0.25348	-1.16149	0.60633
C	2.12249	-0.73051	1.56109
C	3.06525	-1.16043	2.53148
C	1.10988	1.22275	0.5488
H	1.34577	2.24158	0.22726
H	0.49715	1.26334	1.45409
H	0.52431	0.74068	-0.24634
C	3.09623	0.29712	-0.48102
H	2.78783	1.16347	-1.08645
C	2.66789	-0.96662	-1.22653
H	2.96643	-1.84826	-0.64018
H	1.57259	-1.0018	-1.29617
C	3.28862	-1.04865	-2.61482
H	2.98781	-1.98549	-3.09656
H	2.89614	-0.237	-3.24585
C	4.8029	-0.93778	-2.53283
H	5.24835	-0.93947	-3.5337
H	5.21588	-1.81298	-2.00792

C		5.19074	0.33692	-1.79665
H		4.77675	1.19512	-2.34718
H		6.27631	0.48118	-1.79677
C		4.62452	0.35329	-0.36828
H		4.97506	-0.52985	0.18893
C		4.93472	2.8108	-0.28852
H		5.64208	2.87108	-1.12426
H		5.14133	3.62982	0.40454
H		3.91404	2.92425	-0.67099
C		6.58875	2.28498	2.16177
C		6.36692	1.4341	1.04427
C		7.39411	0.61464	0.62047
H		7.24413	-0.10085	-0.18191
C		8.67303	0.70371	1.21138
H		9.46428	0.05439	0.84503
C		8.93799	1.62478	2.19735
H		9.93864	1.72344	2.61331
C		7.89467	2.43148	2.70798
C		8.06337	3.33021	3.79161
H		9.05678	3.47184	4.21724
C		6.96483	3.97591	4.30189
C		5.68725	3.68404	3.76037
C		6.11607	-0.00046	4.36228
H		5.87607	1.0501	4.56682
H		6.93727	-0.0019	3.62765
C		6.49909	-0.79292	5.62099
H		7.56273	-0.71559	5.8622
H		5.94244	-0.40253	6.48179
C		6.05273	-2.23529	5.33614
H		6.85363	-2.80435	4.84101
H		5.79103	-2.79456	6.24048
C		4.61482	4.38852	4.53519
H		3.74215	3.74794	4.71718
H		4.25516	5.25418	3.955
C		5.33741	4.82625	5.81926
H		5.22547	4.04648	6.58265
H		4.93233	5.74979	6.24247
C		6.82168	4.95051	5.43094
H		7.05299	5.96594	5.07645
H		7.50258	4.75397	6.26564
Fe	3.68335		1.72744	2.21994
C		1.62917	3.78024	2.93387
C		2.69371	4.88257	1.41388
H		3.3968	5.08565	0.61611
C		1.77703	5.74965	1.97582
H		1.56202	6.79273	1.78601
N		2.60732	3.67264	2.01559
N		1.11111	5.05066	2.93453
C		0.09755	5.63398	3.85403
H		0.28979	5.19502	4.83953
C		1.31653	2.612	3.73929
C		0.10293	2.48191	4.51109
H		-0.63597	3.2785	4.4696
O		2.15797	1.66989	3.67373
C		-0.15495	1.36821	5.23554
H		0.60582	0.5838	5.23506
C		-1.3783	1.1293	6.02087

H	-2.09082	1.95732	5.96767
H	-1.87898	0.2115	5.68374
H	-1.12864	0.94725	7.0751
H	-0.89039	5.29748	3.51664
C	0.16983	7.12814	3.90695
C	-0.78177	7.90701	3.24608
C	1.2039	7.7529	4.61315
C	-0.70571	9.29678	3.29563
H	-1.59279	7.42434	2.70065
C	1.28194	9.13956	4.65817
H	1.94485	7.14498	5.13643
C	0.32584	9.91221	3.99939
H	-1.4562	9.89793	2.78783
H	2.08153	9.62198	5.21563
H	0.38252	10.99734	4.0417

TSA_{2S}

N	4.25931	-0.32763	2.69716
N	2.43197	0.52553	0.74742
N	5.08372	1.62451	0.33523
N	5.52293	2.92556	2.64134
C	5.15883	-0.78473	3.55488
C	5.18444	-2.11035	4.06705
C	4.1737	-2.96734	3.72659
H	4.12415	-3.98345	4.12033
C	3.13812	-2.50495	2.87837
C	1.99813	-3.2901	2.60207
H	1.92928	-4.28724	3.03383
C	0.98789	-2.78842	1.81798
H	0.0977	-3.37995	1.61878
C	1.11934	-1.51991	1.22769
H	0.32966	-1.16849	0.56872
C	2.24047	-0.73689	1.43395
C	3.24573	-1.18614	2.33201
C	1.14891	1.21323	0.50299
H	1.35472	2.24241	0.19521
H	0.56137	1.2286	1.42638
H	0.55385	0.73101	-0.2859
C	3.14044	0.37223	-0.58583
H	2.79968	1.24652	-1.16146
C	2.7286	-0.88065	-1.35829
H	3.06512	-1.77095	-0.80642
H	1.63305	-0.94467	-1.40273
C	3.31914	-0.90585	-2.76169
H	3.03146	-1.83469	-3.26694
H	2.89336	-0.08491	-3.35833
C	4.83197	-0.75918	-2.70791
H	5.25582	-0.72106	-3.7176
H	5.27626	-1.63944	-2.21783
C	5.20599	0.50141	-1.94124
H	4.76355	1.36654	-2.45812
H	6.28829	0.66939	-1.95731
C	4.6696	0.46485	-0.50153
H	5.05365	-0.42548	0.02107
C	4.91244	2.92424	-0.35774
H	5.60419	3.03457	-1.20196

H	5.09686	3.73038	0.35621
H	3.88202	3.01308	-0.71843
C	6.62693	2.37696	2.04333
C	6.40697	1.54916	0.90711
C	7.44825	0.76581	0.44986
H	7.30399	0.06761	-0.369
C	8.7328	0.87194	1.02583
H	9.53463	0.25185	0.63226
C	8.99095	1.77527	2.03022
H	9.99539	1.88807	2.4336
C	7.93646	2.54417	2.57509
C	8.09711	3.42132	3.67794
H	9.09236	3.57756	4.09428
C	6.98929	4.02771	4.21623
C	5.71274	3.71442	3.68517
C	6.28159	0.00674	4.15186
H	5.98793	1.03366	4.40104
H	7.10721	0.07867	3.42591
C	6.69464	-0.82828	5.37233
H	7.74578	-0.69563	5.64342
H	6.09372	-0.52721	6.2407
C	6.3483	-2.27722	4.99525
H	7.18633	-2.75824	4.46914
H	6.12376	-2.90839	5.86272
C	4.62943	4.37064	4.4855
H	3.77725	3.69891	4.65617
H	4.23698	5.23665	3.92774
C	5.35621	4.79976	5.77019
H	5.2768	3.99976	6.51731
H	4.93259	5.70274	6.21974
C	6.83267	4.97346	5.36818
H	7.03035	6.00263	5.0334
H	7.52883	4.77894	6.19097
Fe	3.70963	1.79534	2.13634
C	1.58777	3.73152	2.87277
C	2.5816	4.95016	1.38879
H	3.27117	5.21347	0.59647
C	1.62855	5.74367	1.97957
H	1.35476	6.77963	1.83328
N	2.56002	3.7095	1.95122
N	1.00564	4.96619	2.92072
C	-0.03496	5.43812	3.85718
H	0.13946	4.90273	4.79842
C	1.34272	2.51648	3.65214
C	0.17205	2.22858	4.34761
H	-0.64251	2.94571	4.40557
O	2.31945	1.66425	3.61295
C	0.05211	0.96911	4.99203
H	0.71208	0.20446	4.5739
C	-1.28464	0.46615	5.43211
H	-1.89881	1.24802	5.89324
H	-1.83431	0.09387	4.55781
H	-1.19782	-0.37575	6.1294
H	-1.01325	5.12453	3.47091
C	0.01331	6.92168	4.06279
C	-0.96017	7.74849	3.50032
C	1.04987	7.4912	4.81046

C	-0.90314	9.12782	3.68627
H	-1.77151	7.30976	2.91919
C	1.10906	8.8672	4.99335
H	1.812	6.84635	5.25298
C	0.13095	9.68714	4.43111
H	-1.66895	9.76512	3.25027
H	1.91349	9.30424	5.58106
H	0.17451	10.76382	4.57866
C	1.54539	-0.3638	6.93531
C	0.75576	-0.75053	8.03172
C	0.74486	-2.04488	8.53858
C	1.57902	-2.96551	7.9113
C	2.37687	-2.59957	6.81751
C	2.362	-1.30354	6.31221
C	0.37813	1.43096	7.69416
H	0.12526	-2.33196	9.38534
H	1.61112	-3.98803	8.27896
H	3.02119	-3.34846	6.35959
H	2.97207	-1.019	5.45414
H	-0.06796	2.40269	7.87839
N	0.05086	0.38516	8.46411
C	-0.91112	0.37956	9.54922
H	-1.75069	-0.27984	9.30475
H	-0.43352	0.02333	10.46687
H	-1.284	1.39236	9.70927
C	1.23819	1.02683	6.64323
H	1.96312	1.69508	6.19029

TSA_{2R}

N	3.66066	-0.15461	3.12942
N	1.89285	0.72228	1.13331
N	4.62892	1.45626	0.55698
N	5.32746	2.89029	2.71801
C	4.51768	-0.62287	4.0244
C	4.37722	-1.86318	4.70504
C	3.25029	-2.60747	4.48891
H	3.07404	-3.54771	5.01268
C	2.27795	-2.13285	3.57491
C	1.05982	-2.81674	3.36672
H	0.88096	-3.74513	3.90742
C	0.11616	-2.30651	2.50761
H	-0.83342	-2.81616	2.3608
C	0.38662	-1.132	1.78628
H	-0.36659	-0.76368	1.09437
C	1.58553	-0.45493	1.92349
C	2.54052	-0.91317	2.87247
C	0.69467	1.55265	0.91168
H	1.00368	2.51121	0.48564
H	0.20867	1.73739	1.87565
H	-0.03399	1.09021	0.23015
C	2.51391	0.40291	-0.21133
H	2.26438	1.27998	-0.82806
C	1.91172	-0.82715	-0.89047
H	2.14005	-1.71762	-0.28622
H	0.81709	-0.74018	-0.90626
C	2.44966	-1.02321	-2.30169
H	2.02157	-1.93342	-2.7365

H	2.12285	-0.19069	-2.94305
C	3.96878	-1.08532	-2.29145
H	4.36139	-1.17519	-3.31042
H	4.30456	-1.98329	-1.74983
C	4.53333	0.16172	-1.62659
H	4.19365	1.04119	-2.19416
H	5.62708	0.18118	-1.67829
C	4.04307	0.29909	-0.17657
H	4.32639	-0.59218	0.40598
C	4.6044	2.71107	-0.23481
H	5.29911	2.67698	-1.08303
H	4.88632	3.54145	0.41717
H	3.58935	2.89371	-0.60385
C	6.32544	2.14747	2.14217
C	5.95312	1.25693	1.09813
C	6.86383	0.30553	0.68301
H	6.59629	-0.43593	-0.06353
C	8.17532	0.29274	1.2046
H	8.8739	-0.45855	0.8446
C	8.59004	1.24066	2.11066
H	9.618	1.25743	2.46753
C	7.66784	2.18787	2.61297
C	7.9888	3.13719	3.61676
H	9.01367	3.20048	3.98275
C	6.99353	3.93424	4.12547
C	5.66359	3.74343	3.67111
C	5.77018	0.06104	4.47982
H	5.63975	1.14167	4.61044
H	6.55572	-0.07558	3.71944
C	6.13357	-0.67507	5.7767
H	7.20877	-0.67805	5.97587
H	5.6485	-0.17945	6.62703
C	5.55208	-2.08683	5.60729
H	6.27688	-2.75315	5.11589
H	5.28883	-2.56593	6.55652
C	4.71285	4.61424	4.43435
H	3.79235	4.08287	4.70946
H	4.40679	5.4645	3.80243
C	5.54844	5.07222	5.64108
H	5.39755	4.37342	6.4733
H	5.26709	6.06566	6.00214
C	7.01456	5.00174	5.17675
H	7.3325	5.95564	4.73039
H	7.71519	4.79644	5.99313
Fe	3.36806	1.95686	2.36517
C	1.55525	4.20633	3.01137
C	2.60834	5.12293	1.36053
H	3.27205	5.20771	0.50936
C	1.82361	6.10058	1.92276
H	1.68869	7.14766	1.68782
N	2.44646	3.95563	2.04291
N	1.16414	5.51504	2.97069
C	0.2731	6.22221	3.91687
H	0.45883	5.77558	4.90099
C	1.22638	3.14078	3.9582
C	0.12241	3.16456	4.81044
H	-0.67043	3.89245	4.65229

O	2.03283	2.12891	3.92476
C	-0.05175	2.1811	5.81137
H	0.87391	1.73197	6.17314
C	-1.14465	2.35531	6.81451
H	-2.09716	2.61243	6.33597
H	-1.29551	1.46516	7.43345
H	-0.88778	3.17957	7.49286
H	-0.76479	5.99789	3.63949
C	0.51704	7.69964	3.9328
C	-0.34904	8.5678	3.26539
C	1.62853	8.21958	4.60395
C	-0.11048	9.93968	3.27059
H	-1.22035	8.16773	2.74605
C	1.86734	9.58871	4.60893
H	2.30342	7.54355	5.13278
C	0.99721	10.45006	3.94136
H	-0.7941	10.61037	2.75517
H	2.72739	9.98885	5.14147
H	1.18081	11.52207	3.95099
C	-2.70202	-0.21055	5.14591
C	-1.88589	0.58861	4.31997
C	-2.49313	1.38112	3.34466
C	-3.87865	1.34475	3.22067
C	-4.66523	0.53974	4.05675
C	-4.08755	-0.25244	5.04225
C	-0.59024	-0.55663	5.79185
H	-1.89664	2.02072	2.69503
H	-4.36576	1.95077	2.46018
H	-5.74533	0.53558	3.93453
H	-4.6974	-0.87256	5.69574
H	0.21047	-0.98953	6.38316
N	-1.86664	-0.89477	6.03763
C	-2.34158	-1.78293	7.07922
H	-2.97194	-1.23424	7.78725
H	-2.92843	-2.59521	6.63929
H	-1.48875	-2.20582	7.61278
C	-0.51845	0.42909	4.78548
H	0.37483	0.55118	4.17563

$IntA_{3S}$

N	0.80097	-1.94708	-0.42002
N	-0.66744	-1.21911	-2.71553
N	1.92582	0.02952	-2.76046
N	2.09104	1.19122	-0.33931
C	1.44191	-2.30111	0.68287
C	1.47359	-3.61611	1.2143
C	0.75072	-4.59424	0.58957
H	0.71885	-5.61674	0.96821
C	-0.02859	-4.25244	-0.54068
C	-0.91661	-5.18054	-1.12528
H	-0.94961	-6.19585	-0.73201
C	-1.74553	-4.79155	-2.14934
H	-2.45455	-5.49152	-2.58417
C	-1.66809	-3.48267	-2.65413
H	-2.32753	-3.20284	-3.47174
C	-0.76742	-2.55623	-2.15659
C	0.03942	-2.90992	-1.04015

C	-2.00749	-0.63475	-2.93869
H	-1.89363	0.43549	-3.14012
H	-2.60183	-0.75913	-2.03012
H	-2.53997	-1.09562	-3.78289
C	0.1262	-1.14338	-3.9991
H	-0.19576	-0.18889	-4.44409
C	-0.18357	-2.25188	-5.00696
H	0.09439	-3.22218	-4.57127
H	-1.26558	-2.29039	-5.18947
C	0.56394	-2.07123	-6.32209
H	0.327	-2.90349	-6.99427
H	0.21744	-1.15738	-6.82813
C	2.05972	-1.97619	-6.07248
H	2.60353	-1.81136	-7.00938
H	2.43242	-2.92602	-5.65891
C	2.34154	-0.83791	-5.10383
H	1.96611	0.09289	-5.55379
H	3.41785	-0.6873	-4.96407
C	1.63647	-1.04385	-3.75462
H	1.98101	-1.98035	-3.28684
C	1.82726	1.39161	-3.34724
H	2.64688	1.59695	-4.0464
H	1.85734	2.1278	-2.53994
H	0.87022	1.49358	-3.87033
C	3.25393	0.66254	-0.83708
C	3.16855	-0.09325	-2.03903
C	4.25659	-0.85049	-2.42652
H	4.20765	-1.48782	-3.30416
C	5.46805	-0.78868	-1.70574
H	6.31048	-1.38595	-2.04565
C	5.60912	0.04881	-0.62495
H	6.56284	0.13522	-0.1078
C	4.49978	0.79004	-0.15708
C	4.5432	1.60858	1.00021
H	5.48824	1.73567	1.52876
C	3.38403	2.19269	1.44485
C	2.17316	1.91975	0.7606
C	2.20819	-1.37694	1.5825
H	1.70263	-0.412	1.7075
H	3.19736	-1.16174	1.15026
C	2.34219	-2.17401	2.88809
H	3.24174	-1.91585	3.45482
H	1.47878	-1.96149	3.5359
C	2.30009	-3.65058	2.46313
H	3.3113	-4.02328	2.24266
H	1.88761	-4.31157	3.23436
C	1.00773	2.51095	1.49739
H	0.14629	1.82865	1.52725
H	0.663	3.42319	0.98453
C	1.59988	2.82792	2.88048
H	1.47795	1.95293	3.53692
H	1.11289	3.67432	3.3747
C	3.1011	3.05978	2.63453
H	3.29608	4.11352	2.38633
H	3.72332	2.82698	3.50515
Fe	0.32077	0.13575	-1.16964
C	-1.71708	2.16463	-0.4332

C	-0.63998	3.33665	-1.90023
H	0.05799	3.56097	-2.69667
C	-1.51826	4.18895	-1.28475
H	-1.72573	5.24114	-1.42047
N	-0.76146	2.08256	-1.36915
N	-2.19344	3.4398	-0.35153
C	-3.1982	3.95162	0.59998
H	-2.9208	3.55311	1.58499
C	-2.04724	0.96845	0.34363
C	-3.04791	0.81603	1.261
H	-3.75368	1.60866	1.48542
O	-1.23067	-0.04158	0.09144
C	-3.22745	-0.50384	1.93275
H	-3.35681	-1.27678	1.15584
C	-4.40732	-0.54627	2.88933
H	-4.3216	0.22143	3.66932
H	-5.34392	-0.35953	2.35381
H	-4.49777	-1.5218	3.38106
H	-4.16973	3.51943	0.32769
C	-3.25908	5.44735	0.62713
C	-4.18635	6.13533	-0.15879
C	-2.3647	6.1699	1.42224
C	-4.221	7.52681	-0.14739
H	-4.88832	5.57669	-0.7784
C	-2.39964	7.55972	1.436
H	-1.63977	5.63435	2.03844
C	-3.3285	8.23916	0.64989
H	-4.95122	8.05538	-0.75598
H	-1.70769	8.1158	2.06483
H	-3.36055	9.32621	0.66392
C	-1.7787	-2.40404	3.0327
C	-1.31445	-2.4559	4.35156
C	-1.05826	-3.63654	5.03509
C	-1.30803	-4.81616	4.33662
C	-1.78769	-4.7916	3.02166
C	-2.02406	-3.58969	2.35397
C	-1.51052	-0.27805	3.85059
H	-0.69629	-3.65271	6.06081
H	-1.13813	-5.77085	4.82804
H	-1.98368	-5.73298	2.51152
H	-2.3892	-3.58364	1.32725
H	-1.49516	0.79436	4.02692
N	-1.17362	-1.1204	4.80549
C	-0.7241	-0.77903	6.14549
H	-1.40944	-1.20948	6.88119
H	0.27791	-1.18797	6.30756
H	-0.70122	0.30556	6.25759
C	-1.88872	-0.97582	2.62818
H	-1.14813	-0.74668	1.81889

$IntA_{3R}$

N	1.17039	-2.05131	0.16471
N	-0.65273	-1.20593	-1.78876
N	2.06181	-0.52981	-2.46977
N	2.83022	0.97767	-0.37595
C	2.04907	-2.50636	1.04317
C	1.88603	-3.69581	1.80807

C	0.71362	-4.39117	1.69953
H	0.52033	-5.28719	2.29057
C	-0.28159	-3.92254	0.80598
C	-1.54235	-4.55238	0.70109
H	-1.73739	-5.44	1.30328
C	-2.49906	-4.04956	-0.14999
H	-3.47388	-4.52735	-0.23581
C	-2.21199	-2.93362	-0.95317
H	-2.98048	-2.57208	-1.63222
C	-0.97565	-2.3117	-0.91514
C	0.00444	-2.76482	0.01379
C	-1.82238	-0.34452	-2.03459
H	-1.48596	0.57407	-2.52337
H	-2.2714	-0.07911	-1.07203
H	-2.58582	-0.81863	-2.67009
C	-0.06968	-1.6322	-3.11756
H	-0.34409	-0.8113	-3.79725
C	-0.68262	-2.91616	-3.67396
H	-0.42267	-3.7553	-3.01102
H	-1.77846	-2.83969	-3.65596
C	-0.19461	-3.21553	-5.08549
H	-0.61552	-4.16719	-5.42915
H	-0.56889	-2.44518	-5.77667
C	1.32523	-3.24138	-5.13659
H	1.67529	-3.39572	-6.1634
H	1.70634	-4.09125	-4.54908
C	1.89053	-1.93971	-4.58583
H	1.50421	-1.10681	-5.19289
H	2.97947	-1.90279	-4.69329
C	1.46132	-1.7222	-3.12544
H	1.77251	-2.58223	-2.51123
C	1.98787	0.68768	-3.31346
H	2.61103	0.60418	-4.2126
H	2.33199	1.54297	-2.72701
H	0.94803	0.87005	-3.60766
C	3.81146	0.22979	-0.97313
C	3.40775	-0.69552	-1.97515
C	4.31314	-1.64974	-2.39698
H	4.02472	-2.41767	-3.10787
C	5.64478	-1.63325	-1.92994
H	6.33712	-2.38731	-2.2963
C	6.08417	-0.65435	-1.06985
H	7.12526	-0.61563	-0.75539
C	5.17131	0.29644	-0.55779
C	5.52275	1.27618	0.40601
H	6.56131	1.35991	0.72645
C	4.54002	2.07488	0.93546
C	3.19474	1.85709	0.54256
C	3.35053	-1.85434	1.39923
H	3.26552	-0.76472	1.48018
H	4.08973	-2.05836	0.60777
C	3.74979	-2.53479	2.71497
H	4.83289	-2.57988	2.85762
H	3.33554	-1.96992	3.55934
C	3.09584	-3.9243	2.66072
H	3.76123	-4.65157	2.17164
H	2.86342	-4.33616	3.64873

C	2.26461	2.73179	1.32599
H	1.36594	2.19324	1.65517
H	1.91453	3.55915	0.68658
C	3.14553	3.23462	2.48176
H	3.04051	2.55899	3.33978
H	2.86641	4.23456	2.82632
C	4.59119	3.17075	1.95603
H	4.87437	4.1161	1.46951
H	5.33024	2.99844	2.7457
Fe	0.84927	0.07416	-0.63305
C	-0.88945	2.3414	0.06939
C	0.12242	3.24444	-1.61933
H	0.7503	3.31253	-2.4987
C	-0.59909	4.24006	-1.01488
H	-0.71326	5.29241	-1.23538
N	-0.05457	2.07109	-0.94089
N	-1.23271	3.66182	0.05987
C	-2.06489	4.37528	1.04818
H	-1.81858	3.9412	2.02548
C	-1.22487	1.27194	1.01523
C	-2.26313	1.30118	1.90408
H	-2.97591	2.12097	1.90799
O	-0.44238	0.21563	0.91173
C	-2.51276	0.15639	2.82066
H	-1.56928	-0.1145	3.31967
C	-3.58446	0.45039	3.85666
H	-4.54745	0.67964	3.3832
H	-3.74011	-0.39371	4.54047
H	-3.30304	1.31641	4.46436
H	-3.11784	4.14431	0.83898
C	-1.83245	5.85479	1.03412
C	-2.73665	6.70834	0.39916
C	-0.69416	6.39219	1.64297
C	-2.50912	8.08181	0.37479
H	-3.62892	6.29469	-0.07187
C	-0.46556	7.76292	1.61854
H	0.01075	5.72727	2.14552
C	-1.37386	8.60917	0.98348
H	-3.22279	8.74088	-0.1144
H	0.41703	8.17609	2.10219
H	-1.1985	9.68256	0.97009
C	-4.91138	-2.24455	1.61488
C	-4.16088	-1.12948	1.22552
C	-4.70446	-0.25331	0.29404
C	-5.96576	-0.53723	-0.23135
C	-6.68148	-1.67364	0.16007
C	-6.16391	-2.5557	1.10603
C	-3.0022	-2.36094	2.77947
H	-4.16012	0.63913	-0.00885
H	-6.40646	0.14062	-0.95845
H	-7.66068	-1.86733	-0.26988
H	-6.72241	-3.43272	1.42579
H	-2.28768	-2.76492	3.49167
N	-4.15807	-2.9525	2.58475
C	-4.62046	-4.17851	3.21178
H	-5.56331	-3.99063	3.73335
H	-4.78351	-4.93974	2.44196

H	-3.87242	-4.53012	3.92356
C	-2.86724	-1.14535	1.97304
H	-1.98351	-1.23928	1.30811

TSA_{4S}

N	3.87657	-0.3312	2.91102
N	2.39667	0.46505	0.65107
N	5.05402	1.59922	0.58717
N	5.26754	2.76861	2.99029
C	4.57367	-0.73862	3.96221
C	4.61873	-2.0758	4.43312
C	3.8282	-3.01321	3.8285
H	3.79731	-4.04739	4.1728
C	2.98717	-2.61352	2.76367
C	2.04572	-3.49999	2.1999
H	2.00296	-4.52404	2.56813
C	1.17903	-3.06095	1.22842
H	0.42956	-3.72913	0.81159
C	1.27918	-1.74603	0.74338
H	0.60254	-1.43323	-0.04786
C	2.2337	-0.86279	1.21832
C	3.06709	-1.26149	2.29817
C	1.08825	1.10545	0.40102
H	1.25156	2.16286	0.16964
H	0.47647	1.03078	1.30439
H	0.5413	0.64957	-0.43625
C	3.20264	0.48121	-0.63122
H	2.92237	1.43806	-1.09868
C	2.84841	-0.6359	-1.61491
H	3.09148	-1.60667	-1.1595
H	1.76499	-0.63908	-1.79249
C	3.59625	-0.50865	-2.93591
H	3.32814	-1.34634	-3.58926
H	3.27923	0.40552	-3.46037
C	5.09541	-0.45981	-2.69448
H	5.63916	-0.32855	-3.63663
H	5.43924	-1.41424	-2.26692
C	5.41992	0.68451	-1.74667
H	5.0712	1.61966	-2.20931
H	6.50104	0.80304	-1.61604
C	4.7165	0.5229	-0.38999
H	5.02735	-0.41955	0.0894
C	4.99101	2.95642	-0.01565
H	5.80811	3.12819	-0.72647
H	5.05726	3.69961	0.78301
H	4.03114	3.08369	-0.52764
C	6.41642	2.21502	2.48857
C	6.30385	1.45066	1.29512
C	7.37229	0.6684	0.90457
H	7.30255	0.02214	0.03492
C	8.59142	0.71515	1.61466
H	9.41939	0.09912	1.27281
C	8.75841	1.55811	2.68786
H	9.71785	1.62776	3.19677
C	7.66722	2.32248	3.1617
C	7.72775	3.13338	4.32421
H	8.67565	3.23785	4.85248

C	6.58026	3.73483	4.77724
C	5.36477	3.49522	4.08928
C	5.41951	0.13308	4.8419
H	4.9344	1.09406	5.05932
H	6.36799	0.36669	4.33608
C	5.66926	-0.73281	6.0851
H	6.62634	-0.51659	6.56902
H	4.87969	-0.54691	6.82549
C	5.55552	-2.18422	5.59588
H	6.53201	-2.56384	5.26053
H	5.20263	-2.87523	6.3701
C	4.21424	4.1224	4.81587
H	3.32214	3.48086	4.81155
H	3.92545	5.05846	4.31153
C	4.80028	4.39166	6.21067
H	4.64942	3.50451	6.84402
H	4.33156	5.2386	6.72046
C	6.30941	4.59054	5.97868
H	6.53111	5.64312	5.74869
H	6.91971	4.3293	6.84953
Fe	3.47982	1.76174	2.18543
C	1.35706	3.77614	2.81734
C	2.55233	4.92413	1.42568
H	3.32732	5.14181	0.70269
C	1.59079	5.76959	1.91099
H	1.37416	6.81134	1.72005
N	2.40723	3.68573	1.99013
N	0.83869	5.03608	2.79688
C	-0.29224	5.54785	3.59735
H	-0.16694	5.13406	4.60637
C	0.95379	2.61287	3.5883
C	-0.17328	2.40582	4.31044
H	-0.95797	3.1527	4.36228
O	1.88336	1.62628	3.51846
C	-0.38508	1.09058	5.0041
H	-0.60183	0.33358	4.22778
C	-1.54577	1.11296	5.98977
H	-1.38203	1.85748	6.77844
H	-2.48418	1.36444	5.48316
H	-1.67577	0.13705	6.4691
H	-1.21759	5.12981	3.18009
C	-0.34355	7.04398	3.62846
C	-1.2259	7.74058	2.80021
C	0.50923	7.75759	4.4767
C	-1.25958	9.13232	2.82262
H	-1.89649	7.18947	2.14054
C	0.47687	9.14688	4.49883
H	1.19782	7.2161	5.12793
C	-0.40862	9.83557	3.671
H	-1.95579	9.66747	2.18097
H	1.13565	9.69594	5.16806
H	-0.43915	10.92249	3.693
C	1.19381	-0.80507	5.96011
C	2.03223	-0.84437	7.09034
C	2.51591	-2.02702	7.64196
C	2.10231	-3.20963	7.03907
C	1.24921	-3.19671	5.92502

C	0.79876	-2.00469	5.36853
C	1.54189	1.30638	6.72573
H	3.16751	-2.03399	8.51407
H	2.43471	-4.16075	7.44873
H	0.92917	-4.14282	5.49243
H	0.1407	-2.01093	4.50006
H	1.53839	2.3754	6.92113
N	2.22302	0.47569	7.5232
C	3.01715	0.85139	8.67768
H	2.67697	0.29496	9.55595
H	4.07681	0.63062	8.50603
H	2.89805	1.91978	8.86619
C	0.92379	0.60282	5.65746
H	1.66034	0.9569	4.62672

TSA_{4R}

N	3.07983	0.02057	3.32819
N	1.50803	0.79453	1.13349
N	4.26973	1.39575	0.6095
N	5.06488	2.67988	2.829
C	3.76437	-0.32424	4.40733
C	3.69903	-1.60083	5.02577
C	2.83212	-2.53211	4.52016
H	2.73725	-3.52668	4.95908
C	1.99364	-2.17232	3.4365
C	0.96727	-3.02642	2.97772
H	0.87129	-4.0193	3.41683
C	0.08645	-2.5916	2.01671
H	-0.73333	-3.22696	1.68932
C	0.24581	-1.32068	1.43897
H	-0.46873	-1.00082	0.6854
C	1.29441	-0.48685	1.78702
C	2.1599	-0.87852	2.84518
C	0.26817	1.59577	1.11394
H	0.49003	2.57434	0.6782
H	-0.07591	1.73948	2.14324
H	-0.54299	1.12778	0.53779
C	2.07317	0.67943	-0.26458
H	1.94154	1.69331	-0.67613
C	1.33112	-0.29599	-1.17976
H	1.40044	-1.3084	-0.75854
H	0.26459	-0.03541	-1.20615
C	1.90638	-0.33063	-2.58854
H	1.34251	-1.0472	-3.1961
H	1.78504	0.6497	-3.07408
C	3.38049	-0.69516	-2.53565
H	3.81737	-0.71548	-3.54019
H	3.50203	-1.7087	-2.12326
C	4.12017	0.31846	-1.67667
H	3.99472	1.30452	-2.14603
H	5.19933	0.12701	-1.67026
C	3.57704	0.38162	-0.24198
H	3.73079	-0.58744	0.26068
C	4.46896	2.68588	-0.10333
H	5.2689	2.61948	-0.85016
H	4.72599	3.46165	0.62172
H	3.53705	2.97119	-0.6012

C	5.95911	1.78556	2.29711
C	5.51732	0.984	1.20931
C	6.30201	-0.07388	0.79575
H	5.97302	-0.73199	-0.00359
C	7.56387	-0.30178	1.38433
H	8.16278	-1.13834	1.03298
C	8.06146	0.54551	2.34644
H	9.05913	0.39857	2.7555
C	7.26926	1.61351	2.82685
C	7.69219	2.50241	3.84883
H	8.69623	2.40244	4.26162
C	6.81789	3.45661	4.30609
C	5.49694	3.48153	3.78833
C	4.67553	0.57499	5.18666
H	4.26487	1.58917	5.27147
H	5.64686	0.66574	4.67831
C	4.83307	-0.15385	6.53001
H	5.79532	0.04411	7.01032
H	4.05498	0.18416	7.22747
C	4.62303	-1.642	6.20436
H	5.57347	-2.11823	5.92152
H	4.23083	-2.22158	7.04814
C	4.67232	4.50816	4.50296
H	3.658	4.15299	4.72507
H	4.55968	5.39737	3.86163
C	5.5086	4.81965	5.75456
H	5.20717	4.14876	6.56999
H	5.37235	5.843	6.11593
C	6.96413	4.51515	5.35709
H	7.44705	5.4041	4.92464
H	7.58776	4.20743	6.20314
Fe	2.99461	2.02599	2.36763
C	1.48016	4.47682	3.09696
C	2.41296	5.11825	1.24973
H	2.96463	5.0495	0.32158
C	1.83955	6.22783	1.80851
H	1.80006	7.26136	1.49454
N	2.19905	4.03227	2.05595
N	1.25883	5.81663	2.98433
C	0.59598	6.69918	3.96713
H	0.9343	6.36328	4.95585
C	1.12445	3.5663	4.17309
C	0.25081	3.75477	5.19019
H	-0.34381	4.65961	5.25597
O	1.79229	2.38998	4.06885
C	0.05823	2.69871	6.24121
H	0.93791	2.72241	6.91059
C	-1.1902	2.93434	7.08237
H	-2.0968	2.89882	6.46723
H	-1.28938	2.17649	7.86674
H	-1.15191	3.9162	7.56706
H	-0.48612	6.52482	3.90715
C	0.92289	8.14346	3.74519
C	0.03208	8.97563	3.06421
C	2.14058	8.66233	4.19599
C	0.35271	10.31174	2.83862
H	-0.9202	8.57655	2.71423

C	2.46167	9.99596	3.97047
H	2.83546	8.01409	4.73345
C	1.56702	10.82143	3.29061
H	-0.34907	10.95642	2.31442
H	3.40586	10.39669	4.3324
H	1.8153	11.86638	3.11889
C	-1.12408	-0.61935	5.03322
C	-1.04764	0.76709	4.8066
C	-1.96318	1.35427	3.93045
C	-2.90925	0.54298	3.31281
C	-2.95389	-0.83912	3.54864
C	-2.05745	-1.44735	4.41852
C	0.50472	0.15523	6.35069
H	-1.94755	2.42854	3.74847
H	-3.64204	0.98941	2.64434
H	-3.71345	-1.44191	3.05653
H	-2.0969	-2.51713	4.61545
H	1.27228	0.10503	7.11806
N	-0.15068	-0.95052	5.98508
C	0.04641	-2.28475	6.5156
H	-0.84153	-2.59958	7.07303
H	0.22198	-2.98891	5.69559
H	0.91014	-2.28469	7.18369
C	0.06584	1.28779	5.61275
H	1.04557	1.5653	4.7784

$IntA_{5S}$

N	0.74189	-1.85769	-0.30565
N	-0.68319	-0.86126	-2.51352
N	2.05878	0.07044	-2.54102
N	2.31297	1.13987	-0.08564
C	1.45104	-2.38182	0.68835
C	1.38565	-3.73915	1.09359
C	0.448	-4.55503	0.52253
H	0.31699	-5.58876	0.8419
C	-0.40114	-4.02501	-0.47668
C	-1.46799	-4.77709	-1.01281
H	-1.62041	-5.79538	-0.65898
C	-2.31309	-4.21604	-1.93934
H	-3.15519	-4.77897	-2.3337
C	-2.06903	-2.91584	-2.41248
H	-2.72685	-2.51019	-3.17667
C	-0.99946	-2.16555	-1.95624
C	-0.18424	-2.68012	-0.91405
C	-1.90748	-0.08554	-2.80303
H	-1.62945	0.95107	-3.01802
H	-2.56198	-0.10402	-1.92669
H	-2.46449	-0.47668	-3.66582
C	0.14907	-0.93499	-3.78083
H	-0.0625	0.02118	-4.2843
C	-0.26247	-2.0593	-4.73232
H	-0.0727	-3.02793	-4.24761
H	-1.3442	-2.01161	-4.91288
C	0.49315	-2.00219	-6.05365
H	0.19168	-2.84515	-6.68512
H	0.21557	-1.08993	-6.60303
C	1.99362	-2.0092	-5.81146

H	2.54163	-1.91689	-6.75554
H	2.29923	-2.96922	-5.36768
C	2.37002	-0.86391	-4.88253
H	2.06052	0.07953	-5.35698
H	3.45559	-0.79118	-4.75993
C	1.66176	-0.98176	-3.52397
H	1.91523	-1.9409	-3.04419
C	2.06339	1.43221	-3.13497
H	2.87035	1.55598	-3.86686
H	2.2044	2.16566	-2.33681
H	1.10172	1.62389	-3.62381
C	3.44328	0.57511	-0.61817
C	3.30435	-0.14402	-1.83652
C	4.34365	-0.95006	-2.25583
H	4.24889	-1.56845	-3.14272
C	5.56485	-0.96932	-1.54904
H	6.3696	-1.60332	-1.91233
C	5.7621	-0.16768	-0.44929
H	6.7231	-0.14954	0.06079
C	4.69801	0.61551	0.05459
C	4.78809	1.37661	1.24792
H	5.74063	1.43116	1.77491
C	3.65993	1.98863	1.73533
C	2.43359	1.80808	1.0492
C	2.41963	-1.64213	1.56371
H	2.02419	-0.66874	1.88664
H	3.34736	-1.43963	1.0094
C	2.67604	-2.60821	2.73022
H	3.68242	-2.51091	3.14749
H	1.96334	-2.39888	3.53721
C	2.38497	-4.00821	2.1739
H	3.29067	-4.46126	1.74412
H	2.01501	-4.70544	2.93402
C	1.30065	2.40994	1.82402
H	0.40921	1.76642	1.82093
H	0.99635	3.36403	1.36516
C	1.91142	2.61672	3.21876
H	1.74815	1.71104	3.81948
H	1.46537	3.45303	3.76434
C	3.42122	2.7944	2.97707
H	3.66583	3.85082	2.79224
H	4.03548	2.47943	3.82704
Fe	0.50845	0.28126	-0.95804
C	-1.67752	2.22462	-0.12493
C	-0.43111	3.37827	-1.47199
H	0.38287	3.60277	-2.14825
C	-1.43423	4.20804	-1.05016
H	-1.66349	5.24081	-1.27067
N	-0.58395	2.14436	-0.89895
N	-2.22109	3.47011	-0.19845
C	-3.43177	3.95736	0.50259
H	-3.26635	3.79289	1.5752
C	-2.11554	1.07428	0.63428
C	-3.17732	0.8797	1.43809
H	-3.87267	1.69242	1.62169
O	-1.23077	0.02995	0.40051
C	-3.46493	-0.45942	2.06791

H	-3.65486	-1.1637	1.23525
C	-4.72335	-0.41536	2.93426
H	-4.59243	0.27498	3.77574
H	-5.5945	-0.08928	2.3544
H	-4.94343	-1.40382	3.34877
H	-4.26398	3.31472	0.18782
C	-3.72396	5.39714	0.21655
C	-4.54284	5.74959	-0.86005
C	-3.15946	6.40075	1.00919
C	-4.79556	7.08915	-1.13892
H	-4.9914	4.96993	-1.47631
C	-3.41218	7.74	0.73024
H	-2.52679	6.1294	1.85502
C	-4.22985	8.08428	-0.34442
H	-5.44186	7.35689	-1.97151
H	-2.97898	8.516	1.35703
H	-4.43361	9.13097	-0.55809
C	-1.96175	-2.40617	2.9969
C	-0.90683	-2.48034	3.9426
C	-0.36364	-3.69641	4.3622
C	-0.9004	-4.85445	3.81696
C	-1.94751	-4.80354	2.87799
C	-2.48252	-3.59406	2.46239
C	-1.4347	-0.32384	3.67662
H	0.43354	-3.7402	5.10341
H	-0.51703	-5.82108	4.13764
H	-2.35623	-5.73423	2.4886
H	-3.30552	-3.56994	1.74766
H	-1.38016	0.74037	3.88696
N	-0.60311	-1.19216	4.33933
C	0.34881	-0.83594	5.36665
H	0.20193	-1.46399	6.25136
H	1.38467	-0.95445	5.02186
H	0.19262	0.20531	5.65758
C	-2.28552	-1.01498	2.83461
H	-1.26458	-0.58987	1.17311

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N	0.60871	-1.94062	0.28693
N	-0.94455	-1.22426	-1.92586
N	1.79653	-0.60168	-2.47592
N	2.61232	0.62976	-0.2286
C	1.29426	-2.27186	1.37338
C	1.30779	-3.56909	1.94761
C	0.5297	-4.54692	1.38877
H	0.49527	-5.55743	1.79843
C	-0.3026	-4.21716	0.29257
C	-1.2456	-5.13208	-0.22394
H	-1.28336	-6.13901	0.19034
C	-2.12809	-4.73703	-1.19962
H	-2.89056	-5.42044	-1.56603
C	-2.05203	-3.43919	-1.73271
H	-2.77923	-3.14073	-2.48264
C	-1.07908	-2.54272	-1.32717
C	-0.22101	-2.89657	-0.25347
C	-2.2215	-0.48513	-1.84695
H	-2.07109	0.52785	-2.23479

H	-2.53439	-0.429	-0.7982
H	-3.03222	-0.96578	-2.41165
C	-0.42045	-1.24678	-3.34431
H	-0.5456	-0.20313	-3.6786
C	-1.19153	-2.14428	-4.31346
H	-1.12954	-3.18441	-3.96758
H	-2.25421	-1.86757	-4.30819
C	-0.62907	-2.09433	-5.72703
H	-1.22397	-2.7432	-6.37911
H	-0.71548	-1.07743	-6.13953
C	0.82916	-2.52044	-5.71018
H	1.25978	-2.4967	-6.71728
H	0.91058	-3.56126	-5.36154
C	1.61563	-1.59	-4.79988
H	1.53821	-0.57823	-5.22099
H	2.68448	-1.83435	-4.80314
C	1.07865	-1.57215	-3.36193
H	1.22027	-2.56222	-2.89855
C	2.03828	0.69926	-3.15641
H	2.84485	0.62651	-3.89495
H	2.31032	1.45152	-2.41242
H	1.12106	1.01881	-3.66072
C	3.48103	-0.28709	-0.76721
C	3.02775	-1.05886	-1.87242
C	3.79062	-2.12268	-2.30854
H	3.45298	-2.74866	-3.13004
C	5.04227	-2.39371	-1.71634
H	5.6246	-3.23539	-2.08276
C	5.55333	-1.57767	-0.7348
H	6.5464	-1.75396	-0.32629
C	4.78656	-0.49752	-0.23991
C	5.2385	0.38099	0.77869
H	6.24084	0.25365	1.18793
C	4.39716	1.36664	1.23061
C	3.07381	1.42592	0.72199
C	2.13236	-1.34371	2.20128
H	1.67923	-0.34924	2.29878
H	3.11445	-1.20053	1.72611
C	2.28493	-2.09722	3.53066
H	3.20749	-1.84269	4.05999
H	1.45096	-1.84085	4.19735
C	2.19928	-3.58415	3.15183
H	3.19085	-3.97806	2.8833
H	1.82586	-4.2196	3.96281
C	2.28773	2.48732	1.4311
H	1.26538	2.16905	1.67085
H	2.19307	3.36922	0.77684
C	3.14445	2.79165	2.67055
H	2.8269	2.14592	3.4998
H	3.04609	3.82512	3.01456
C	4.5856	2.43144	2.26816
H	5.09771	3.2971	1.8224
H	5.20285	2.11199	3.11446
Fe	0.53462	0.02449	-0.7376
C	-0.98718	2.50014	0.09533
C	-0.02512	3.08586	-1.75683
H	0.5389	2.99077	-2.67439

C	-0.60186	4.21051	-1.23624
H	-0.63384	5.23496	-1.57932
N	-0.25665	2.02115	-0.92489
N	-1.19992	3.8353	-0.05695
C	-1.87844	4.75249	0.88686
H	-1.56633	4.44112	1.89188
C	-1.38471	1.63716	1.18704
C	-2.2985	1.83265	2.15471
H	-2.88797	2.74451	2.12522
O	-0.63809	0.4696	1.11169
C	-2.57168	0.87154	3.28512
H	-1.71896	0.94399	3.98429
C	-3.83079	1.2848	4.05129
H	-4.72144	1.21003	3.41698
H	-3.98646	0.63439	4.91663
H	-3.75403	2.31717	4.41157
H	-2.95971	4.58458	0.80316
C	-1.5344	6.18677	0.6307
C	-2.40595	7.00543	-0.09091
C	-0.32266	6.7097	1.09299
C	-2.07136	8.33281	-0.34601
H	-3.35477	6.60405	-0.4476
C	0.01185	8.03469	0.83782
H	0.3559	6.07388	1.66461
C	-0.86282	8.84665	0.11686
H	-2.75796	8.96742	-0.90146
H	0.9506	8.43945	1.20909
H	-0.60417	9.88498	-0.07752
C	-3.41807	-2.53769	1.94099
C	-3.55655	-1.12759	1.86999
C	-4.48504	-0.58151	0.96892
C	-5.23702	-1.43881	0.17977
C	-5.08556	-2.83384	0.27254
C	-4.17876	-3.40329	1.15492
C	-2.03359	-1.64384	3.44932
H	-4.62498	0.49772	0.90192
H	-5.97382	-1.02914	-0.50783
H	-5.70718	-3.48014	-0.3437
H	-4.08155	-4.48413	1.24178
H	-1.33068	-1.65743	4.27687
N	-2.47115	-2.82647	2.90535
C	-2.19201	-4.14613	3.4219
H	-3.01198	-4.50674	4.05426
H	-2.05127	-4.85062	2.59472
H	-1.27409	-4.11831	4.01611
C	-2.65767	-0.56936	2.84585
H	-1.08991	-0.23551	1.64272

IntA$_{6S}$

N	0.6099	-2.08595	0.09325
N	-0.92325	-1.17124	-2.09485
N	1.87082	-0.55081	-2.55592
N	2.5983	0.64126	-0.2564
C	1.31128	-2.52469	1.13133
C	1.13504	-3.79085	1.73749
C	0.10568	-4.58508	1.31202

H	-0.10568	-5.54771	1.77862
C	-0.73198	-4.1252	0.26987
C	-1.87633	-4.84881	-0.12562
H	-2.09362	-5.7958	0.36554
C	-2.71396	-4.34463	-1.09045
H	-3.61384	-4.88201	-1.37847
C	-2.40083	-3.13133	-1.72478
H	-3.07545	-2.7583	-2.49124
C	-1.25822	-2.41542	-1.40958
C	-0.42372	-2.8757	-0.35647
C	-2.11846	-0.31505	-2.24648
H	-1.79798	0.69008	-2.54071
H	-2.6453	-0.26193	-1.29038
H	-2.81924	-0.68909	-3.00561
C	-0.29642	-1.36368	-3.46217
H	-0.45852	-0.39337	-3.95802
C	-0.96909	-2.44103	-4.31562
H	-0.85228	-3.41511	-3.81977
H	-2.04789	-2.24759	-4.37118
C	-0.38594	-2.52682	-5.71973
H	-0.88325	-3.33173	-6.27191
H	-0.59692	-1.59791	-6.27109
C	1.11555	-2.74892	-5.65869
H	1.54997	-2.76927	-6.66423
H	1.33475	-3.72779	-5.20516
C	1.75713	-1.63706	-4.84309
H	1.52147	-0.67987	-5.33191
H	2.84974	-1.7129	-4.85146
C	1.21826	-1.5943	-3.40538
H	1.41153	-2.55196	-2.89514
C	2.00924	0.75186	-3.25501
H	2.74402	0.70484	-4.06725
H	2.33818	1.50073	-2.53068
H	1.03824	1.05741	-3.66004
C	3.5509	-0.14266	-0.85707
C	3.15083	-0.9116	-1.9826
C	3.99672	-1.89775	-2.4495
H	3.69832	-2.54696	-3.26709
C	5.28019	-2.06707	-1.88854
H	5.92768	-2.84388	-2.28745
C	5.73209	-1.23947	-0.88794
H	6.74012	-1.34397	-0.49158
C	4.87129	-0.26284	-0.33756
C	5.22785	0.55716	0.76337
H	6.23643	0.49226	1.17192
C	4.27996	1.38042	1.31717
C	2.96203	1.35772	0.79436
C	2.3841	-1.75824	1.84296
H	2.05763	-0.7332	2.06857
H	3.2794	-1.68044	1.20926
C	2.65882	-2.58108	3.11202
H	3.71228	-2.56117	3.40609
H	2.07678	-2.1614	3.93944
C	2.14939	-4.00116	2.81659
H	2.95876	-4.64918	2.44983
H	1.73239	-4.49671	3.70128
C	2.04582	2.19034	1.64183

H	1.07367	1.705	1.81791
H	1.84204	3.15081	1.14078
C	2.85961	2.38468	2.93142
H	2.63697	1.55359	3.61602
H	2.61883	3.31408	3.45727
C	4.33328	2.30068	2.4989
H	4.71023	3.28731	2.19116
H	4.99824	1.9498	3.29501
Fe	0.59264	-0.09552	-0.76472
C	-0.99472	2.37129	-0.07565
C	0.24697	3.1909	-1.63824
H	0.96265	3.23105	-2.44913
C	-0.46321	4.24248	-1.09233
H	-0.46499	5.30207	-1.31192
N	-0.07732	2.0394	-1.00635
N	-1.2423	3.72189	-0.10789
C	-2.15095	4.52931	0.74875
H	-2.14894	4.05975	1.73671
C	-1.52679	1.31633	0.76296
C	-2.6318	1.48113	1.73725
H	-3.32444	2.27503	1.43689
O	-0.97653	0.19673	0.65155
C	-2.11973	1.76764	3.17955
H	-1.53022	2.70292	3.14526
C	-3.34007	2.01178	4.07022
H	-3.95571	1.1075	4.14218
H	-3.02772	2.27921	5.08399
H	-3.9699	2.82159	3.68067
H	-3.16256	4.44453	0.33315
C	-1.71261	5.95785	0.84313
C	-2.3821	6.95616	0.13299
C	-0.61373	6.29588	1.6405
C	-1.96033	8.28057	0.22221
H	-3.24367	6.69794	-0.48284
C	-0.1918	7.61693	1.72723
H	-0.09505	5.51565	2.20242
C	-0.866	8.61024	1.01692
H	-2.49153	9.05598	-0.32444
H	0.65659	7.87777	2.35585
H	-0.54024	9.64522	1.09005
C	-0.39852	-1.22184	4.67248
C	-1.42613	-0.71405	3.83204
C	-2.36346	-1.62304	3.31279
C	-2.26855	-2.96537	3.64543
C	-1.25568	-3.43554	4.49858
C	-0.30753	-2.57002	5.0247
C	-0.10924	0.98261	4.5019
H	-3.1826	-1.28862	2.67752
H	-3.00467	-3.66591	3.25574
H	-1.22474	-4.49012	4.76622
H	0.46705	-2.92677	5.70317
H	0.34354	1.9419	4.73559
N	0.40349	-0.16598	5.05652
C	1.45582	-0.23403	6.04352
H	1.07037	-0.60357	7.00075
H	2.26757	-0.89593	5.71602
H	1.86711	0.76611	6.19956

C	-1.22433	0.70828	3.7432
H	-3.19876	0.54404	1.75123

$IntA_{6R}$

N	0.60614	-2.0866	0.09796
N	-0.92744	-1.17441	-2.09102
N	1.86687	-0.55788	-2.55642
N	2.59968	0.63468	-0.25893
C	1.30689	-2.5234	1.1373
C	1.13052	-3.78852	1.74551
C	0.10179	-4.58382	1.32044
H	-0.10952	-5.54584	1.78831
C	-0.73539	-4.12578	0.27709
C	-1.87932	-4.85034	-0.11788
H	-2.09654	-5.7967	0.37452
C	-2.71673	-4.34774	-1.08371
H	-3.61636	-4.88577	-1.37129
C	-2.40388	-3.13509	-1.71941
H	-3.07867	-2.7631	-2.48622
C	-1.26157	-2.41839	-1.40489
C	-0.42721	-2.87712	-0.35097
C	-2.1228	-0.31791	-2.23994
H	-1.80287	0.68691	-2.5358
H	-2.64672	-0.26394	-1.2823
H	-2.8259	-0.69229	-2.99673
C	-0.30315	-1.3669	-3.45949
H	-0.4642	-0.39585	-3.95428
C	-0.97903	-2.44239	-4.31281
H	-0.86372	-3.41696	-3.81757
H	-2.05745	-2.24664	-4.36727
C	-0.39752	-2.52894	-5.71754
H	-0.89738	-3.33236	-6.26959
H	-0.60671	-1.59926	-6.26828
C	1.10345	-2.75483	-5.658
H	1.53684	-2.77618	-6.66397
H	1.32063	-3.7343	-5.20479
C	1.7485	-1.6446	-4.843
H	1.5148	-0.68689	-5.33173
H	2.84092	-1.72313	-4.85233
C	1.21117	-1.60038	-3.40477
H	1.40319	-2.55828	-2.8945
C	2.00796	0.74399	-3.25651
H	2.74244	0.69475	-4.0689
H	2.33867	1.49263	-2.53277
H	1.03752	1.05133	-3.66152
C	3.54961	-0.15262	-0.85954
C	3.14656	-0.92143	-1.98412
C	3.98952	-1.91001	-2.45113
H	3.68871	-2.55894	-3.26807
C	5.27301	-2.08235	-1.89113
H	5.91813	-2.86111	-2.29009
C	5.72781	-1.25545	-0.89128
H	6.7358	-1.36244	-0.49551
C	4.87002	-0.27621	-0.34086
C	5.22955	0.54307	0.75965
H	6.23807	0.47518	1.16784
C	4.28433	1.36918	1.31371

C	2.96618	1.35054	0.79126
C	2.37871	-1.7552	1.84847
H	2.05108	-0.73015	2.07234
H	3.27437	-1.6774	1.21529
C	2.65331	-2.57603	3.1189
H	3.70672	-2.55545	3.41313
H	2.07103	-2.15505	3.94546
C	2.14422	-3.99671	2.82565
H	2.95389	-4.64532	2.46061
H	1.7267	-4.49068	3.71099
C	2.05313	2.18656	1.63881
H	1.07865	1.70567	1.81408
H	1.85437	3.14836	1.13835
C	2.86737	2.37678	2.9287
H	2.64217	1.54555	3.61232
H	2.62947	3.30632	3.4556
C	4.34068	2.28876	2.49583
H	4.72039	3.27448	2.18855
H	5.00485	1.93549	3.29156
Fe	0.59166	-0.09844	-0.76418
C	-0.98989	2.37355	-0.07931
C	0.25123	3.18776	-1.64509
H	0.96587	3.22498	-2.45705
C	-0.45652	4.2417	-1.10051
H	-0.45679	5.3008	-1.32238
N	-0.07415	2.03812	-1.01038
N	-1.23528	3.72449	-0.11406
C	-2.14135	4.53522	0.7422
H	-2.13943	4.06719	1.73089
C	-1.5232	1.32131	0.76179
C	-2.62779	1.48994	1.7359
H	-3.31885	2.28468	1.4341
O	-0.97493	0.20049	0.65247
C	-2.1155	1.7778	3.17783
H	-1.52412	2.71184	3.14211
C	-3.33561	2.02597	4.0677
H	-3.95313	1.12308	4.14095
H	-3.02304	2.29448	5.08112
H	-3.96361	2.83643	3.67654
H	-3.15356	4.45194	0.32771
C	-1.69993	5.96299	0.8339
C	-2.36843	6.96164	0.12333
C	-0.59928	6.29995	1.62929
C	-1.94394	8.28535	0.21015
H	-3.23133	6.70426	-0.49098
C	-0.1746	7.62027	1.71358
H	-0.08139	5.51946	2.19158
C	-0.84785	8.61394	1.00287
H	-2.47439	9.06106	-0.33681
H	0.67516	7.88032	2.34067
H	-0.51995	9.64838	1.07415
C	-0.40104	-1.21233	4.67722
C	-1.42703	-0.70413	3.83505
C	-2.36525	-1.61243	3.31618
C	-2.27273	-2.95443	3.65083
C	-1.26152	-3.42494	4.50576
C	-0.31255	-2.56013	5.03154

C	-0.10727	0.99123	4.50256
H	-3.18297	-1.27773	2.67923
H	-3.00942	-3.65442	3.26122
H	-1.23244	-4.47918	4.77491
H	0.46082	-2.91711	5.71126
H	0.34734	1.95004	4.73463
N	0.40273	-0.15729	5.05984
C	1.4547	-0.22543	6.04721
H	1.06797	-0.59003	7.00582
H	2.26399	-0.89151	5.72215
H	1.86961	0.77379	6.19947
C	-1.22243	0.71765	3.74369
H	-3.19667	0.55404	1.75129

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N	4.17921	-0.47736	3.13334
N	2.32887	0.5458	1.26631
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N	5.76435	2.49191	3.17822
C	5.00002	-0.95682	4.05857
C	5.16863	-2.33457	4.34135
C	4.40299	-3.24188	3.65855
H	4.47148	-4.31198	3.85468
C	3.45424	-2.77507	2.7162
C	2.54561	-3.65383	2.08885
H	2.61892	-4.72022	2.29374
C	1.55838	-3.15836	1.2723
H	0.82978	-3.8257	0.81949
C	1.48294	-1.77864	1.0174
H	0.67971	-1.41293	0.3839
C	2.39969	-0.8849	1.54629
C	3.37929	-1.36897	2.45454
C	0.97024	1.0596	1.53901
H	0.98766	2.15245	1.47111
H	0.67107	0.76445	2.54896
H	0.2184	0.68201	0.83288
C	2.74192	0.93682	-0.14012
H	2.41542	1.98691	-0.21644
C	2.05564	0.13887	-1.25162
H	2.32218	-0.92146	-1.14606
H	0.96585	0.20569	-1.13811
C	2.46759	0.58927	-2.64646
H	1.94613	-0.01957	-3.39325
H	2.15363	1.62963	-2.82041
C	3.97427	0.47751	-2.79895
H	4.29632	0.80605	-3.79323
H	4.28459	-0.57421	-2.70281
C	4.64656	1.33122	-1.73656
H	4.32538	2.37023	-1.89366
H	5.7363	1.33593	-1.8544
C	4.26489	0.9111	-0.30968
H	4.61438	-0.11568	-0.11317
C	4.88694	3.21356	0.38417
H	5.60745	3.43477	-0.41096
H	5.12762	3.80439	1.26909
H	3.88201	3.49533	0.05993

C	6.70194	1.91256	2.35894
C	6.25044	1.38871	1.11826
C	7.11315	0.61765	0.36472
H	6.78869	0.16714	-0.56873
C	8.44843	0.42721	0.77792
H	9.10623	-0.17803	0.15945
C	8.93524	1.03648	1.91048
H	9.98145	0.93331	2.19168
C	8.07159	1.79864	2.73058
C	8.48478	2.43429	3.93065
H	9.53118	2.37886	4.23091
C	7.55292	3.09443	4.69208
C	6.19211	3.06157	4.29181
C	5.83736	-0.13628	4.99254
H	5.31167	0.76343	5.33797
H	6.74884	0.20773	4.47843
C	6.17854	-1.12653	6.11541
H	7.12552	-0.89655	6.61157
H	5.39412	-1.09317	6.8823
C	6.17269	-2.50752	5.44043
H	7.16013	-2.74143	5.01563
H	5.92883	-3.32475	6.12696
C	5.32685	3.73138	5.315
H	4.39574	3.18148	5.50742
H	5.03129	4.72551	4.94324
C	6.24696	3.8318	6.54302
H	6.11564	2.93932	7.16864
H	6.02608	4.6987	7.17118
C	7.67884	3.85105	5.97899
H	8.00609	4.88094	5.77327
H	8.41808	3.42548	6.66573
Fe	3.80603	1.59282	2.67502
C	1.72194	2.80976	4.41059
C	1.93899	0.84786	5.30898
H	2.34012	-0.14395	5.47972
C	0.89639	1.47724	5.95463
H	0.24026	1.15445	6.75161
N	2.4392	1.67227	4.35677
N	0.76369	2.71051	5.38458
C	-0.27799	3.70674	5.76203
H	-0.71256	4.07064	4.82431
C	2.0612	3.86016	3.45774
C	1.51971	5.19843	3.51904
H	0.87512	5.46656	4.35248
O	2.90229	3.52035	2.57974
C	1.81961	6.13163	2.58751
H	2.47474	5.82917	1.76675
C	1.33193	7.52294	2.58814
H	0.69025	7.74998	3.44426
H	2.17468	8.22751	2.58483
H	0.77501	7.73806	1.66607
H	0.23597	4.54373	6.24991
C	-1.32835	3.12774	6.65637
C	-1.24976	3.29958	8.04075
C	-2.38717	2.39394	6.1113
C	-2.21995	2.74611	8.87138
H	-0.43122	3.87861	8.46924

C	-3.35462	1.83967	6.9417
H	-2.45783	2.26649	5.03042
C	-3.27076	2.01532	8.32219
H	-2.15959	2.8924	9.94722
H	-4.18212	1.27986	6.51195
H	-4.03218	1.58862	8.97103

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N	3.94681	-0.60615	2.86925
N	2.6891	0.61779	0.68773
N	5.40632	1.54579	0.87804
N	5.69203	2.14588	3.49644
C	4.44971	-1.18118	3.9527
C	4.39402	-2.57269	4.22592
C	3.73291	-3.38997	3.35012
H	3.64166	-4.46265	3.52179
C	3.09363	-2.81373	2.22624
C	2.27184	-3.58093	1.37322
H	2.18303	-4.65084	1.55305
C	1.56135	-2.97373	0.36659
H	0.89577	-3.55374	-0.26754
C	1.68924	-1.59093	0.15461
H	1.0976	-1.12816	-0.63079
C	2.54403	-0.81159	0.91547
C	3.23589	-1.40559	2.00436
C	1.37064	1.27997	0.6673
H	1.52335	2.3653	0.65411
H	0.82552	1.01408	1.57726
H	0.76088	1.00149	-0.2038
C	3.47046	0.97848	-0.55215
H	3.28193	2.05909	-0.66853
C	3.00783	0.27898	-1.8321
H	3.13307	-0.80558	-1.71286
H	1.93553	0.45916	-1.98628
C	3.79815	0.71058	-3.05917
H	3.42698	0.17479	-3.94005
H	3.64004	1.78199	-3.25796
C	5.27782	0.44583	-2.8384
H	5.86821	0.75535	-3.70801
H	5.44925	-0.63449	-2.71472
C	5.7449	1.201	-1.60447
H	5.5759	2.27197	-1.78645
H	6.82467	1.09141	-1.45085
C	4.97885	0.79282	-0.3383
H	5.16426	-0.27026	-0.11327
C	5.56434	3.00156	0.61353
H	6.46952	3.20992	0.02997
H	5.61125	3.54049	1.56191
H	4.68778	3.36448	0.06857
C	6.747	1.50444	2.89617
C	6.5742	1.04588	1.56024
C	7.52297	0.20387	1.01407
H	7.397	-0.20033	0.0137
C	8.69136	-0.12486	1.73258
H	9.42177	-0.78604	1.27294
C	8.93783	0.42184	2.96938
H	9.86796	0.21405	3.49498

C	7.97145	1.25318	3.5809
C	8.14048	1.82364	4.86857
H	9.07391	1.65765	5.40698
C	7.11485	2.55435	5.41336
C	5.89241	2.65186	4.70132
C	5.09947	-0.46802	5.10073
H	4.59064	0.47593	5.33194
H	6.14276	-0.21817	4.85387
C	5.03829	-1.49848	6.23685
H	5.84272	-1.37481	6.96765
H	4.08898	-1.38947	6.77821
C	5.0678	-2.86348	5.53219
H	6.10337	-3.19202	5.35818
H	4.581	-3.65992	6.10461
C	4.85991	3.36015	5.52611
H	3.87505	2.87827	5.46471
H	4.72765	4.387	5.1487
C	5.46498	3.34219	6.93883
H	5.12062	2.44377	7.46836
H	5.16947	4.20477	7.54283
C	6.98757	3.25651	6.73091
H	7.43185	4.26063	6.6634
H	7.50587	2.74521	7.54909
Fe	3.79799	1.57894	2.44975
C	1.65501	2.83192	4.06207
C	1.59975	0.81913	4.8636
H	1.81329	-0.24102	4.93517
C	0.80481	1.59206	5.67357
H	0.227	1.36051	6.5575
N	2.12855	1.59364	3.87693
N	0.8513	2.86646	5.166
C	0.22485	4.05227	5.79201
H	-0.65798	4.32369	5.19913
C	2.12543	3.89253	3.16377
C	1.59198	5.17823	3.1211
O	3.09156	3.53082	2.38492
C	2.19938	6.19269	2.33903
H	3.2698	6.0474	2.17266
C	1.77134	7.61371	2.51842
H	0.68235	7.71061	2.59689
H	2.19828	8.00434	3.45127
H	2.12837	8.2633	1.71202
H	0.95485	4.86572	5.69922
C	-0.13994	3.81347	7.22468
C	0.84505	3.87739	8.2154
C	-1.45223	3.49618	7.58089
C	0.52086	3.62999	9.5442
H	1.87067	4.12777	7.93782
C	-1.77766	3.24791	8.91184
H	-2.22411	3.4475	6.81234
C	-0.79181	3.31457	9.89301
H	1.28885	3.69295	10.31198
H	-2.80309	3.00818	9.1831
H	-1.04682	3.12615	10.93338
C	1.83064	7.66658	-0.92871
C	2.71941	6.71703	-0.38909
C	4.09045	6.89448	-0.57566

C	4.52547	7.99629	-1.30493
C	3.61806	8.92425	-1.83508
C	2.24708	8.77856	-1.65093
C	0.58113	6.13632	0.12191
H	4.80731	6.18806	-0.15909
H	5.59017	8.14597	-1.46759
H	3.99129	9.77598	-2.39792
H	1.54338	9.50314	-2.05474
H	-0.33263	5.68246	0.49142
H	0.65514	5.39901	3.62722
N	0.52899	7.27301	-0.58456
C	-0.66125	8.03349	-0.91172
H	-0.61879	9.01986	-0.438
H	-0.7342	8.16216	-1.99577
H	-1.54318	7.49942	-0.5547
C	1.92289	5.7589	0.36262
H	2.2263	4.72774	0.53023

TSB_{2R}

N	4.06114	-0.61738	3.07205
N	2.51198	0.22077	0.8885
N	5.27818	0.95631	0.5324
N	5.89504	2.26604	2.80996
C	4.76658	-1.02428	4.11967
C	4.59921	-2.27764	4.7665
C	3.60451	-3.11325	4.33932
H	3.41178	-4.07104	4.82318
C	2.77351	-2.69829	3.27211
C	1.65866	-3.46413	2.86999
H	1.46707	-4.41286	3.36821
C	0.81686	-2.99863	1.88939
H	-0.05918	-3.5708	1.59501
C	1.09416	-1.7791	1.25052
H	0.41911	-1.4354	0.4705
C	2.20661	-1.02173	1.57529
C	3.05183	-1.447	2.63406
C	1.29783	1.03926	0.69531
H	1.59817	2.04292	0.37688
H	0.76195	1.11249	1.64613
H	0.61554	0.62338	-0.05964
C	3.19286	0.03447	-0.44901
H	3.00343	0.98589	-0.97029
C	2.60624	-1.08937	-1.305
H	2.7527	-2.04889	-0.78876
H	1.52122	-0.95086	-1.40049
C	3.2475	-1.16864	-2.68409
H	2.81351	-2.00624	-3.24147
H	3.01307	-0.25997	-3.25947
C	4.75563	-1.3141	-2.56156
H	5.22873	-1.33159	-3.54975
H	5.00301	-2.27367	-2.0815
C	5.31345	-0.16128	-1.74075
H	5.05943	0.77827	-2.25415
H	6.4079	-0.19107	-1.69918
C	4.71357	-0.12171	-0.32811
H	4.92769	-1.06473	0.20037
C	5.35034	2.26492	-0.16904

H		6.1263	2.26686	-0.94389
H		5.56553	3.05056	0.55852
H		4.3788	2.48764	-0.62206
C		6.88339	1.48164	2.27311
C		6.54274	0.66292	1.16106
C		7.42711	-0.322	0.76622
H		7.17705	-1.00704	-0.03839
C		8.69074	-0.44231	1.38123
H		9.36778	-1.22098	1.03853
C		9.09091	0.43777	2.35865
H		10.08782	0.37474	2.79072
C		8.19242	1.42069	2.83428
C		8.50346	2.31174	3.89326
H		9.50048	2.28857	4.33367
C		7.52988	3.16121	4.35648
C		6.22802	3.07276	3.80175
C		5.81893	-0.23186	4.83601
H		5.55292	0.8277	4.92383
H		6.76536	-0.27949	4.27577
C		5.94626	-0.94722	6.18845
H		6.93819	-0.83822	6.63589
H		5.22247	-0.52136	6.89595
C		5.57327	-2.40721	5.89662
H		6.45482	-2.97894	5.5702
H		5.16467	-2.93552	6.76461
C		5.28651	3.98585	4.5221
H		4.3029	3.52699	4.68938
H		5.1129	4.88462	3.90831
C		6.04772	4.32952	5.8112
H		5.79109	3.59952	6.58992
H		5.79828	5.32061	6.20272
C		7.53825	4.18541	5.45135
H		7.94314	5.1353	5.07139
H		8.16234	3.90503	6.30656
Fe	3.89512		1.46536	2.22611
C		1.78828	2.95114	3.70657
C		1.94201	1.17589	4.94124
H		2.29621	0.2058	5.26962
C		0.97508	1.97152	5.50639
H		0.35341	1.84553	6.38185
N		2.4403	1.7883	3.83502
N		0.88189	3.093	4.72205
C		-0.04435	4.22535	4.95645
H		-0.68511	4.30629	4.06999
C		2.15302	3.81345	2.57658
C		1.54127	5.02931	2.28716
H		0.80794	5.45362	2.9643
O		3.12735	3.35831	1.85898
C		1.97886	5.82874	1.20202
H		2.43705	5.27756	0.37881
C		1.16021	7.0216	0.82133
H		0.17793	6.6904	0.46109
H		0.98028	7.67873	1.68136
H		1.61811	7.61105	0.02117
H		0.56863	5.13476	5.01012
C		-0.86245	4.06706	6.1993
C		-0.37365	4.528	7.42502

C	-2.11466	3.44866	6.14842
C	-1.12665	4.3754	8.58441
H	0.60118	5.01671	7.4665
C	-2.86905	3.29687	7.30769
H	-2.50391	3.09359	5.1939
C	-2.37544	3.75975	8.52546
H	-0.74449	4.74502	9.53312
H	-3.84776	2.82493	7.25907
H	-2.96929	3.64838	9.42989
C	3.57648	8.6684	2.68543
C	3.49621	7.30676	3.03475
C	3.1006	6.96708	4.32911
C	2.80533	7.98928	5.22739
C	2.89301	9.33656	4.8522
C	3.27913	9.70131	3.5665
C	4.15394	7.50157	0.86753
H	3.03081	5.92263	4.63273
H	2.50501	7.74173	6.24358
H	2.65742	10.11144	5.57721
H	3.34157	10.747	3.27338
H	4.46926	7.35469	-0.16037
N	3.98243	8.74206	1.34518
C	4.12991	9.97992	0.6051
H	3.15928	10.47706	0.50203
H	4.81833	10.6476	1.13144
H	4.53115	9.7642	-0.38637
C	3.77689	6.53538	1.83042
H	4.2017	5.5316	1.82564

IntB$_{3S}$

N	0.49711	-2.82524	0.1897
N	-0.74964	-1.60353	-1.99624
N	1.97555	-0.68902	-1.79715
N	2.2601	-0.08769	0.82305
C	0.98628	-3.39777	1.28022
C	0.92016	-4.78796	1.56016
C	0.26226	-5.60609	0.68322
H	0.16362	-6.67744	0.85924
C	-0.36552	-5.03117	-0.44783
C	-1.18631	-5.79743	-1.30259
H	-1.28203	-6.86608	-1.11854
C	-1.88839	-5.19076	-2.31548
H	-2.55357	-5.77006	-2.95076
C	-1.75324	-3.80922	-2.5309
H	-2.33976	-3.34517	-3.31955
C	-0.89872	-3.03139	-1.76825
C	-0.21372	-3.62481	-0.6745
C	-2.06445	-0.93608	-2.01516
H	-1.90479	0.14859	-2.01766
H	-2.60947	-1.20281	-1.10547
H	-2.67511	-1.20848	-2.88827
C	0.0376	-1.24416	-3.23009
H	-0.14343	-0.16178	-3.34348
C	-0.42501	-1.93753	-4.51376
H	-0.30771	-3.02306	-4.39576
H	-1.49605	-1.751	-4.67027
C	0.37211	-1.51047	-5.73774

H	-0.00098	-2.04047	-6.62147
H	0.22496	-0.43674	-5.93421
C	1.84875	-1.7887	-5.51296
H	2.44473	-1.48438	-6.38074
H	2.00922	-2.87073	-5.3899
C	2.31878	-1.0397	-4.27657
H	2.16289	0.03344	-4.45833
H	3.39669	-1.16129	-4.11853
C	1.54491	-1.43916	-3.0123
H	1.72093	-2.50347	-2.78578
C	2.14533	0.76502	-2.05832
H	3.06038	0.97066	-2.62796
H	2.17773	1.30265	-1.10838
H	1.27892	1.13274	-2.61685
C	3.30872	-0.74202	0.22664
C	3.13437	-1.19998	-1.10978
C	4.07386	-2.05664	-1.65021
H	3.94659	-2.46129	-2.65028
C	5.23453	-2.40084	-0.92665
H	5.95684	-3.07381	-1.38203
C	5.48431	-1.85531	0.30995
H	6.40897	-2.07597	0.84003
C	4.5276	-1.00903	0.9159
C	4.69959	-0.44026	2.20404
H	5.62811	-0.62008	2.74657
C	3.68168	0.30385	2.74479
C	2.46327	0.4166	2.02782
C	1.6282	-2.6827	2.43128
H	1.11961	-1.73643	2.65285
H	2.67476	-2.43863	2.19331
C	1.55202	-3.70732	3.5716
H	2.3511	-3.58416	4.30846
H	0.5989	-3.59069	4.1045
C	1.58054	-5.07596	2.87379
H	2.61594	-5.41088	2.71084
H	1.08425	-5.86711	3.44551
C	1.43481	1.13258	2.84994
H	0.44557	0.66179	2.77772
H	1.31492	2.16275	2.47726
C	2.0324	1.10034	4.26539
H	1.67856	0.20062	4.78666
H	1.74098	1.9609	4.87437
C	3.55536	1.00318	4.06407
H	4.00758	2.0042	4.00172
H	4.06635	0.48517	4.8827
Fe	0.35038	-0.62749	-0.22761
C	-1.76071	0.58658	1.4303
C	-1.84481	-1.44537	2.18443
H	-1.65084	-2.51103	2.22458
C	-2.61004	-0.68132	3.02528
H	-3.18251	-0.92358	3.90954
N	-1.31521	-0.65419	1.20613
N	-2.54501	0.60805	2.54793
C	-3.13377	1.79109	3.20616
H	-3.98991	2.12665	2.60631
C	-1.27908	1.66582	0.55865
C	-1.71631	2.96252	0.58274

O	-0.34313	1.27946	-0.2807
C	-1.06755	3.981	-0.27881
H	0.02425	3.84393	-0.22399
C	-1.43209	5.40892	0.08954
H	-2.51714	5.57388	0.04917
H	-1.11365	5.6288	1.11366
H	-0.95255	6.14172	-0.56931
H	-2.36814	2.5762	3.16289
C	-3.54138	1.51516	4.62083
C	-2.57833	1.51048	5.63474
C	-4.87051	1.22776	4.93734
C	-2.93966	1.22358	6.94598
H	-1.5395	1.73748	5.38876
C	-5.23391	0.94123	6.25073
H	-5.62574	1.23263	4.15086
C	-4.26891	0.9378	7.25454
H	-2.18701	1.23036	7.73148
H	-6.2723	0.72471	6.49079
H	-4.55295	0.71813	8.28118
C	-1.55702	5.22587	-3.58561
C	-0.61328	4.56415	-2.79297
C	0.73367	4.84307	-2.97987
C	1.08836	5.7713	-3.95983
C	0.12167	6.41543	-4.73991
C	-1.23479	6.15386	-4.56493
C	-2.73548	3.90756	-2.2065
H	1.49736	4.35858	-2.37321
H	2.13813	6.00491	-4.1202
H	0.43261	7.13554	-5.49214
H	-1.99027	6.65719	-5.1641
H	-3.62115	3.48202	-1.74302
H	-2.55985	3.26582	1.19537
N	-2.84223	4.78427	-3.1788
C	-4.07667	5.28734	-3.76141
H	-4.13273	6.36937	-3.61172
H	-4.08568	5.0728	-4.83368
H	-4.92927	4.80494	-3.28248
C	-1.33843	3.68294	-1.83088
H	-1.05387	2.61746	-1.90544

$IntB_{3R}$

N	0.61891	-2.90485	0.20085
N	-1.01723	-2.08113	-1.91846
N	1.7203	-1.27939	-2.34889
N	2.35328	0.05269	-0.09505
C	1.36563	-3.30568	1.2205
C	1.23935	-4.56412	1.86847
C	0.24255	-5.41315	1.47305
H	0.08122	-6.37575	1.95887
C	-0.63208	-5.00558	0.43787
C	-1.75033	-5.78423	0.07027
H	-1.91137	-6.73851	0.5688
C	-2.63283	-5.32484	-0.87719
H	-3.51048	-5.90791	-1.14427
C	-2.39503	-4.09789	-1.51752
H	-3.10059	-3.7576	-2.27156
C	-1.28184	-3.32864	-1.22754

C	-0.39336	-3.74753	-0.20295
C	-2.24964	-1.28381	-2.08096
H	-1.97191	-0.26819	-2.38151
H	-2.77304	-1.23753	-1.12137
H	-2.93398	-1.70065	-2.83395
C	-0.36599	-2.257	-3.27072
H	-0.59337	-1.31497	-3.79414
C	-0.94541	-3.40023	-4.10604
H	-0.7625	-4.35278	-3.5885
H	-2.03573	-3.28952	-4.17316
C	-0.33952	-3.46991	-5.50138
H	-0.7659	-4.3213	-6.0437
H	-0.61326	-2.5704	-6.07405
C	1.17477	-3.57439	-5.42003
H	1.6211	-3.58449	-6.42081
H	1.46067	-4.52442	-4.94249
C	1.72318	-2.40314	-4.61906
H	1.42856	-1.4732	-5.12871
H	2.81884	-2.40228	-4.60852
C	1.16155	-2.37369	-3.19013
H	1.41497	-3.30865	-2.66481
C	1.72855	0.02978	-3.04944
H	2.47492	0.0573	-3.85311
H	1.94639	0.81982	-2.32726
H	0.73453	0.22536	-3.46508
C	3.35318	-0.69815	-0.65404
C	3.0096	-1.53102	-1.75527
C	3.91624	-2.48723	-2.16979
H	3.66838	-3.18444	-2.96464
C	5.19947	-2.56037	-1.58756
H	5.89393	-3.31624	-1.94611
C	5.59646	-1.6624	-0.62486
H	6.60715	-1.6887	-0.22177
C	4.67786	-0.70881	-0.12797
C	4.98452	0.20402	0.91409
H	5.99365	0.22243	1.32639
C	3.99375	1.02437	1.3948
C	2.68182	0.88183	0.87841
C	2.43198	-2.49968	1.89957
H	2.15249	-1.44461	2.00099
H	3.35784	-2.532	1.30525
C	2.61996	-3.21757	3.2436
H	3.62617	-3.09581	3.65467
H	1.9165	-2.80474	3.97866
C	2.25761	-4.6822	2.96047
H	3.13473	-5.23951	2.5986
H	1.89094	-5.21915	3.84178
C	1.72355	1.76975	1.60686
H	0.76887	1.26903	1.81578
H	1.4815	2.64016	0.97464
C	2.50907	2.18227	2.8608
H	2.29271	1.47701	3.67328
H	2.24104	3.18027	3.22234
C	3.99596	2.0681	2.47154
H	4.37133	3.02047	2.06793
H	4.64315	1.81865	3.31934
Fe	0.36111	-0.79331	-0.61491

C	-1.76237	0.53383	0.94761
C	-1.53456	-1.282	2.11352
H	-1.12125	-2.23654	2.41713
C	-2.58169	-0.58944	2.66173
H	-3.23489	-0.80204	3.49585
N	-1.03273	-0.58275	1.05526
N	-2.72325	0.5593	1.91869
C	-3.74951	1.59955	2.13915
H	-4.28093	1.73199	1.18833
C	-1.44215	1.46261	-0.14377
C	-2.07119	2.65605	-0.37793
H	-2.82002	3.04776	0.30217
O	-0.45706	1.05056	-0.91042
C	-1.66126	3.5089	-1.516
H	-1.55581	2.88803	-2.41878
C	-2.61898	4.65882	-1.77299
H	-3.62687	4.2766	-1.96426
H	-2.68196	5.32938	-0.90673
H	-2.32636	5.25937	-2.64334
H	-3.22318	2.53877	2.35772
C	-4.69944	1.25141	3.24322
C	-4.41967	1.62568	4.56023
C	-5.85523	0.5147	2.97079
C	-5.28285	1.26827	5.59117
H	-3.51994	2.20254	4.77743
C	-6.71933	0.1575	4.00087
H	-6.08013	0.2241	1.94422
C	-6.43245	0.53248	5.31172
H	-5.06169	1.56838	6.61297
H	-7.62096	-0.40928	3.77984
H	-7.10982	0.25667	6.11694
C	0.47627	6.19571	-0.60166
C	0.01259	4.96819	-0.11425
C	-0.23034	4.84186	1.24881
C	0.00486	5.9448	2.07174
C	0.47314	7.15697	1.55445
C	0.71791	7.30748	0.19193
C	0.3167	4.85426	-2.38784
H	-0.59872	3.9042	1.66182
H	-0.18144	5.86329	3.14021
H	0.64618	7.99608	2.22313
H	1.07795	8.2488	-0.21689
H	0.35772	4.58156	-3.43852
N	0.63542	6.07071	-2.00448
C	1.06332	7.16706	-2.85877
H	0.35168	7.99329	-2.77132
H	2.05236	7.51035	-2.54258
H	1.10613	6.8281	-3.89424
C	-0.15593	4.03616	-1.26938
H	0.40042	3.08384	-1.18683

TSB_{4S}

N	3.75711	-0.38346	2.74056
N	2.48362	1.20983	0.82424
N	5.20367	2.16852	1.10989
N	5.53329	2.19812	3.77322
C	4.27265	-1.14356	3.69637

C	4.29754	-2.56087	3.67282
C	3.71427	-3.21114	2.61873
H	3.68425	-4.29907	2.55976
C	3.07695	-2.44768	1.61067
C	2.33733	-3.06156	0.57708
H	2.31095	-4.14834	0.52399
C	1.62128	-2.29524	-0.30963
H	1.01179	-2.76415	-1.07789
C	1.66181	-0.89366	-0.21924
H	1.05064	-0.31293	-0.90451
C	2.44397	-0.24527	0.7218
C	3.13273	-1.01902	1.6935
C	1.1133	1.73529	0.97594
H	1.17076	2.81221	1.16581
H	0.64277	1.25458	1.83785
H	0.48509	1.5572	0.0912
C	3.19753	1.91097	-0.30844
H	2.99375	2.98171	-0.11917
C	2.67543	1.5588	-1.70338
H	2.82027	0.48427	-1.87566
H	1.5923	1.74036	-1.75334
C	3.40354	2.30218	-2.8132
H	2.97412	2.02856	-3.78435
H	3.26946	3.39081	-2.69937
C	4.88595	1.97459	-2.75273
H	5.43794	2.49217	-3.54534
H	5.03605	0.8974	-2.92101
C	5.4307	2.38945	-1.39595
H	5.29286	3.47672	-1.30753
H	6.51198	2.21802	-1.32837
C	4.71616	1.70239	-0.22263
H	4.90757	0.61739	-0.25592
C	5.44282	3.63592	1.13929
H	6.36805	3.90647	0.61477
H	5.4979	3.97545	2.17505
H	4.60271	4.14871	0.66576
C	6.55789	1.6484	3.04001
C	6.3584	1.49167	1.64114
C	7.28065	0.77129	0.90945
H	7.13855	0.60895	-0.15577
C	8.44345	0.26156	1.52451
H	9.15373	-0.29917	0.92198
C	8.71255	0.51395	2.84914
H	9.64005	0.17114	3.30338
C	7.77771	1.22243	3.63944
C	7.97766	1.51961	5.01208
H	8.91057	1.22318	5.49214
C	6.98472	2.16298	5.70848
C	5.75803	2.44401	5.0539
C	4.8686	-0.64654	4.97838
H	4.3181	0.21273	5.3846
H	5.9021	-0.30955	4.80665
C	4.84361	-1.88783	5.88163
H	5.63064	-1.87661	6.64107
H	3.88304	-1.93814	6.41106
C	4.95581	-3.07838	4.91512
H	6.01002	-3.31856	4.71097

H	4.4979	-3.99541	5.30051
C	4.76371	3.01214	6.02104
H	3.76361	2.57791	5.89492
H	4.65807	4.09561	5.84872
C	5.39049	2.70811	7.39237
H	5.01207	1.74366	7.75647
H	5.1422	3.45614	8.15052
C	6.90452	2.6013	7.13882
H	7.39307	3.57993	7.25613
H	7.41013	1.92056	7.83193
Fe	3.63568	1.81153	2.70818
C	1.60014	3.09438	4.39116
C	1.54826	1.04269	5.10526
H	1.72957	-0.02521	5.1041
C	0.85799	1.79638	6.01425
H	0.35173	1.54492	6.93588
N	2.01811	1.8519	4.10483
N	0.90421	3.09669	5.56036
C	0.35908	4.27085	6.27252
H	-0.59091	4.54972	5.79862
C	1.96227	4.20005	3.51593
C	1.42587	5.44585	3.46816
O	2.91447	3.85072	2.62288
C	1.94472	6.43611	2.46432
H	2.97331	6.7082	2.76033
C	1.11178	7.70757	2.38525
H	0.07453	7.48627	2.10529
H	1.09264	8.22249	3.35219
H	1.51994	8.40281	1.64412
H	1.07187	5.08651	6.09693
C	0.1794	4.0161	7.73793
C	1.2967	3.97057	8.57823
C	-1.09182	3.81042	8.2762
C	1.14459	3.7232	9.93689
H	2.28968	4.1425	8.15922
C	-1.2457	3.56711	9.63909
H	-1.96674	3.84937	7.62719
C	-0.12891	3.52214	10.46864
H	2.01659	3.69977	10.58682
H	-2.23991	3.41809	10.05373
H	-0.25005	3.33768	11.53369
C	2.51752	5.88286	-1.19543
C	3.05919	6.21606	0.06003
C	4.31753	6.81935	0.11268
C	4.98791	7.06297	-1.08065
C	4.42995	6.70978	-2.31959
C	3.17846	6.1113	-2.39952
C	0.99326	5.30518	0.33494
H	4.76291	7.10271	1.06577
H	5.96048	7.54916	-1.05814
H	4.97881	6.92298	-3.23343
H	2.73552	5.85298	-3.35969
H	0.03612	4.94442	0.70077
H	0.5971	5.73261	4.10731
N	1.24938	5.32692	-0.97798
C	0.36788	4.87796	-2.03914
H	0.09216	5.72279	-2.67793

H	0.87114	4.12167	-2.65139
H	-0.53596	4.44833	-1.60326
C	2.11306	5.75898	1.08594
H	2.61393	4.66936	1.60835

TSB_{4R}

N	4.15418	-0.37635	3.0992
N	2.37674	0.47369	1.10678
N	5.03577	1.51389	0.667
N	5.56249	2.76898	2.98955
C	5.019	-0.8246	4.00043
C	4.97602	-2.11895	4.58344
C	3.93655	-2.95135	4.26656
H	3.83253	-3.93724	4.72001
C	2.95574	-2.50655	3.34787
C	1.81477	-3.28238	3.04844
H	1.70434	-4.257	3.52016
C	0.85361	-2.79895	2.19424
H	-0.03768	-3.38248	1.97822
C	1.03198	-1.55276	1.57094
H	0.27125	-1.20247	0.87787
C	2.15747	-0.78218	1.7989
C	3.12322	-1.22032	2.74245
C	1.1106	1.20593	0.89616
H	1.34511	2.23889	0.61923
H	0.53455	1.20888	1.82565
H	0.49386	0.76198	0.10146
C	3.05249	0.31399	-0.2393
H	2.72043	1.19985	-0.80276
C	2.60516	-0.92252	-1.01886
H	2.92633	-1.82484	-0.47807
H	1.50848	-0.96085	-1.05335
C	3.17732	-0.94738	-2.43052
H	2.86702	-1.86776	-2.93759
H	2.75554	-0.11581	-3.01541
C	4.6926	-0.82441	-2.40083
H	5.09994	-0.78336	-3.41718
H	5.13246	-1.71508	-1.92616
C	5.0966	0.42344	-1.62853
H	4.65308	1.29884	-2.12788
H	6.18005	0.57927	-1.66408
C	4.58424	0.37554	-0.18062
H	4.96034	-0.529	0.32298
C	4.86338	2.82787	0.00172
H	5.53276	2.9389	-0.86118
H	5.07695	3.61959	0.72546
H	3.82259	2.93905	-0.32305
C	6.63906	2.22383	2.33895
C	6.37394	1.412	1.20171
C	7.38785	0.61795	0.7028
H	7.20691	-0.07269	-0.11479
C	8.69175	0.70123	1.2356
H	9.47035	0.07048	0.8136
C	8.99543	1.59662	2.23413
H	10.01452	1.69436	2.60358
C	7.9707	2.37489	2.82048
C	8.18541	3.25489	3.91287

H	9.19837	3.40313	4.28764
C	7.10499	3.86663	4.49703
C	5.80353	3.54515	4.0327
C	6.1741	-0.05539	4.56563
H	5.91755	0.98719	4.78534
H	6.99277	-0.03294	3.82914
C	6.57123	-0.85853	5.81288
H	7.63585	-0.77612	6.04858
H	6.01784	-0.48107	6.68183
C	6.13306	-2.30077	5.51699
H	6.93475	-2.85908	5.01086
H	5.88088	-2.87135	6.4171
C	4.76023	4.14839	4.91636
H	3.9491	3.44177	5.1358
H	4.29331	5.00448	4.40645
C	5.55695	4.5892	6.15463
H	5.54808	3.78497	6.90099
H	5.13715	5.47755	6.63605
C	6.99763	4.80696	5.65907
H	7.13694	5.84158	5.30913
H	7.75335	4.63674	6.43314
Fe	3.69086	1.73561	2.47028
C	1.35014	2.92262	3.87271
C	1.68127	1.08563	4.98716
H	2.16125	0.15896	5.27657
C	0.56643	1.67599	5.51567
H	-0.09159	1.3909	6.32412
N	2.16552	1.86191	3.96937
N	0.3614	2.83747	4.80494
C	-0.72751	3.81091	5.04054
H	-1.31462	3.87109	4.11523
C	1.59484	3.91732	2.83804
C	0.84971	5.00234	2.50986
H	-0.06171	5.25107	3.04178
O	2.7301	3.65405	2.15442
C	1.29086	5.90575	1.39162
H	1.12901	5.37551	0.43442
C	0.51744	7.2173	1.35426
H	-0.55789	7.03118	1.25773
H	0.67599	7.799	2.26975
H	0.82722	7.83788	0.50686
H	-0.25199	4.78828	5.19743
C	-1.59569	3.43331	6.20012
C	-1.25507	3.82448	7.49803
C	-2.7373	2.65418	5.99522
C	-2.04651	3.44186	8.57647
H	-0.36728	4.43609	7.6625
C	-3.52926	2.27165	7.07348
H	-3.00985	2.3521	4.98355
C	-3.18315	2.66431	8.36441
H	-1.78059	3.7565	9.58312
H	-4.42167	1.67315	6.90515
H	-3.80482	2.37069	9.20715
C	4.646	7.42942	2.05419
C	3.44406	6.9029	2.56094
C	3.09901	7.17088	3.88778
C	3.96746	7.93556	4.65978

C	5.17965	8.41367	4.13991
C	5.54302	8.16675	2.82123
C	3.63226	6.39867	0.35035
H	2.16563	6.79513	4.30528
H	3.70118	8.17501	5.68688
H	5.83687	9.00608	4.77184
H	6.47215	8.55523	2.40951
H	3.49878	6.06535	-0.67508
N	4.7183	7.0973	0.69443
C	5.82127	7.46285	-0.17477
H	5.95415	8.54873	-0.16514
H	6.74665	6.98709	0.16573
H	5.6015	7.1408	-1.19387
C	2.81209	6.13191	1.48147
H	3.07335	4.8848	1.72762

$IntB_{5S}$

N	0.35349	-2.62628	-0.1123
N	-0.95034	-0.87966	-1.90269
N	1.84788	-0.17441	-1.71141
N	2.21234	0.08606	0.93314
C	0.95451	-3.4572	0.72877
C	0.72571	-4.85573	0.77742
C	-0.21891	-5.39635	-0.05282
H	-0.46055	-6.45898	-0.03211
C	-0.93242	-4.54463	-0.93114
C	-1.98804	-5.02957	-1.73253
H	-2.23015	-6.09002	-1.69716
C	-2.71351	-4.16604	-2.51648
H	-3.54601	-4.52827	-3.11413
C	-2.37486	-2.80405	-2.55848
H	-2.96072	-2.14484	-3.19295
C	-1.31434	-2.29118	-1.83179
C	-0.59599	-3.15254	-0.96065
C	-2.15338	-0.02497	-1.83236
H	-1.84311	1.01923	-1.72546
H	-2.74751	-0.31281	-0.96068
H	-2.78364	-0.09529	-2.73116
C	-0.15167	-0.50545	-3.13674
H	-0.27034	0.58946	-3.20373
C	-0.68553	-1.10888	-4.43664
H	-0.61631	-2.20448	-4.38651
H	-1.75279	-0.87023	-4.54394
C	0.08626	-0.62749	-5.65781
H	-0.32468	-1.0928	-6.56097
H	-0.04368	0.46041	-5.77844
C	1.5655	-0.93577	-5.50053
H	2.13511	-0.57265	-6.36316
H	1.71901	-2.0252	-5.46369
C	2.08315	-0.28327	-4.22842
H	1.91773	0.80235	-4.31195
H	3.16579	-0.41519	-4.12307
C	1.34791	-0.78861	-2.97783
H	1.49229	-1.87521	-2.86092
C	2.04353	1.29497	-1.83939
H	2.93247	1.53741	-2.43405
H	2.15107	1.73347	-0.84408

H	1.17048	1.74096	-2.32679
C	3.25502	-0.46693	0.23107
C	3.03644	-0.76368	-1.14184
C	3.96204	-1.53828	-1.81127
H	3.80026	-1.83094	-2.84449
C	5.15429	-1.94125	-1.17277
H	5.86892	-2.54215	-1.72965
C	5.44505	-1.53766	0.10931
H	6.39313	-1.8005	0.57445
C	4.4979	-0.79037	0.84674
C	4.69419	-0.38318	2.18991
H	5.64409	-0.59783	2.67982
C	3.67492	0.25679	2.8508
C	2.43029	0.42937	2.1938
C	1.94014	-3.06679	1.78708
H	1.67006	-2.12661	2.28543
H	2.93058	-2.91248	1.33109
C	1.95098	-4.28099	2.72751
H	2.9057	-4.4088	3.24492
H	1.17962	-4.15313	3.49807
C	1.58679	-5.47715	1.83408
H	2.48726	-5.91267	1.37583
H	1.09187	-6.28948	2.37634
C	1.41815	1.01913	3.12919
H	0.44534	0.51701	3.05878
H	1.24459	2.07489	2.86619
C	2.07736	0.86764	4.51103
H	1.74386	-0.07223	4.96936
H	1.80868	1.67328	5.20001
C	3.5911	0.79922	4.24436
H	4.04354	1.80122	4.27929
H	4.13061	0.19353	4.98019
Fe	0.34222	-0.43555	-0.0913
C	-1.78548	0.83674	1.6137
C	-1.70733	-1.25183	2.21489
H	-1.43398	-2.2989	2.17
C	-2.50583	-0.60701	3.11752
H	-3.03542	-0.94532	3.99724
N	-1.25366	-0.35181	1.28575
N	-2.542	0.71642	2.73618
C	-3.21803	1.79731	3.48471
H	-4.19982	1.97136	3.02631
C	-1.51814	2.02583	0.82877
C	-2.28415	3.12595	0.70903
O	-0.33765	1.85129	0.11884
C	-1.95435	4.31764	-0.16038
H	-1.00933	4.74797	0.21509
C	-3.03277	5.39225	-0.04276
H	-4.00006	5.01917	-0.40057
H	-3.16052	5.71405	0.99707
H	-2.77464	6.27042	-0.64088
H	-2.61218	2.69777	3.32294
C	-3.35858	1.48189	4.94281
C	-2.22758	1.43679	5.76555
C	-4.61765	1.23934	5.49342
C	-2.3573	1.15607	7.12
H	-1.2424	1.63238	5.33789

C	-4.74864	0.96417	6.85268
H	-5.50223	1.27679	4.85769
C	-3.61977	0.9222	7.66535
H	-1.47607	1.13227	7.75722
H	-5.73424	0.78761	7.27679
H	-3.72181	0.71242	8.72769
C	-0.68781	3.43502	-3.59953
C	-0.45714	3.97257	-2.30234
C	0.82486	4.45924	-1.98674
C	1.82171	4.39257	-2.94778
C	1.57388	3.84217	-4.21975
C	0.31932	3.35717	-4.56542
C	-2.61681	3.36688	-2.47143
H	1.02656	4.90745	-1.0134
H	2.81064	4.7871	-2.72461
H	2.37476	3.81868	-4.9558
H	0.12196	2.97202	-5.56526
H	-3.67478	3.16331	-2.33915
H	-3.23074	3.14347	1.24477
N	-2.01494	3.07536	-3.67369
C	-2.6707	2.56124	-4.85406
H	-2.65947	3.29895	-5.66408
H	-2.17193	1.64909	-5.20705
H	-3.70916	2.3221	-4.61499
C	-1.70484	3.90738	-1.59194
H	-0.32697	2.47363	-0.64142

IntB$_{5R}$

N	0.70527	-2.7144	0.1419
N	-1.10512	-1.93389	-1.85353
N	1.50908	-0.78099	-2.33695
N	1.95481	0.558	-0.05053
C	1.59672	-3.12442	1.03364
C	1.61237	-4.41762	1.61705
C	0.60387	-5.29136	1.30974
H	0.54147	-6.27901	1.76669
C	-0.40249	-4.88833	0.39735
C	-1.5162	-5.7061	0.10697
H	-1.58678	-6.68456	0.57824
C	-2.50303	-5.25733	-0.73711
H	-3.37411	-5.87345	-0.94445
C	-2.37849	-4.00655	-1.3645
H	-3.15816	-3.68838	-2.05174
C	-1.28015	-3.19447	-1.14924
C	-0.29283	-3.5976	-0.21195
C	-2.40214	-1.26044	-2.08296
H	-2.21157	-0.22381	-2.37537
H	-2.98647	-1.26899	-1.15885
H	-2.98972	-1.74341	-2.87607
C	-0.42131	-2.09051	-3.20188
H	-0.79158	-1.23019	-3.78064
C	-0.82091	-3.35999	-3.95348
H	-0.46266	-4.23719	-3.39498
H	-1.91517	-3.44273	-3.98557
C	-0.24993	-3.39394	-5.36536
H	-0.52692	-4.33637	-5.85062
H	-0.70245	-2.59197	-5.96801

C	1.2596	-3.21589	-5.33905
H	1.66595	-3.18343	-6.35598
H	1.73148	-4.07843	-4.84377
C	1.61698	-1.93618	-4.59715
H	1.14334	-1.08948	-5.11732
H	2.69411	-1.74207	-4.63645
C	1.10653	-1.96461	-3.14801
H	1.52032	-2.83677	-2.61728
C	1.30231	0.5007	-3.0503
H	1.99473	0.61896	-3.89427
H	1.46118	1.32445	-2.34821
H	0.27212	0.5533	-3.41896
C	3.06291	0.02997	-0.6686
C	2.84678	-0.81479	-1.7915
C	3.89996	-1.57334	-2.26412
H	3.75747	-2.28435	-3.07188
C	5.19163	-1.42783	-1.71581
H	6.00224	-2.03041	-2.11809
C	5.44229	-0.50906	-0.72354
H	6.44992	-0.36637	-0.33796
C	4.37784	0.23476	-0.16432
C	4.53914	1.12701	0.9265
H	5.53883	1.31096	1.3206
C	3.42907	1.70447	1.48949
C	2.14685	1.3508	0.99399
C	2.72217	-2.30266	1.58283
H	2.42456	-1.26717	1.793
H	3.53494	-2.25532	0.84043
C	3.1585	-3.08159	2.83254
H	4.21951	-2.9524	3.06304
H	2.59296	-2.72446	3.70201
C	2.78189	-4.54375	2.5444
H	3.60432	-5.06866	2.03598
H	2.56031	-5.12034	3.44859
C	1.07118	1.95868	1.83428
H	0.25264	1.25622	2.03758
H	0.62861	2.81583	1.30141
C	1.82044	2.41976	3.09476
H	1.78557	1.62891	3.85448
H	1.37812	3.3174	3.53705
C	3.27579	2.64073	2.6475
H	3.41587	3.67568	2.30037
H	4.00706	2.47234	3.44505
Fe	0.201	-0.6705	-0.49895
C	-2.14815	0.60459	0.90889
C	-1.87	-1.30938	1.90375
H	-1.42767	-2.27465	2.11703
C	-2.93756	-0.70069	2.50278
H	-3.58557	-1.00257	3.31318
N	-1.37954	-0.49794	0.91647
N	-3.10919	0.50886	1.86813
C	-4.1524	1.50916	2.19644
H	-4.70333	1.71122	1.26892
C	-1.91237	1.66525	-0.04987
C	-2.49071	2.87517	-0.18256
H	-3.2463	3.18621	0.532
O	-0.92186	1.26388	-0.93939

C	-2.13315	3.84097	-1.29054
H	-2.36444	3.33536	-2.24565
C	-2.97958	5.11027	-1.21916
H	-4.04868	4.87171	-1.24446
H	-2.78011	5.6745	-0.30099
H	-2.75893	5.76973	-2.06313
H	-3.63179	2.43062	2.48653
C	-5.06841	1.0525	3.28788
C	-4.77031	1.34724	4.62133
C	-6.21522	0.31206	2.98654
C	-5.60915	0.90966	5.64104
H	-3.88089	1.93133	4.85991
C	-7.05394	-0.12552	4.00638
H	-6.45646	0.08677	1.94732
C	-6.75092	0.17267	5.33356
H	-5.37725	1.15152	6.67559
H	-7.95035	-0.69209	3.76506
H	-7.41124	-0.16328	6.12988
C	1.46171	4.82421	-0.74366
C	0.12565	4.75423	-0.27046
C	-0.16562	5.25447	1.00964
C	0.85885	5.80426	1.76408
C	2.17659	5.86063	1.27184
C	2.49995	5.36528	0.01686
C	0.2231	3.87688	-2.34242
H	-1.18088	5.21818	1.40382
H	0.6423	6.21565	2.74757
H	2.95367	6.31666	1.88202
H	3.51823	5.42006	-0.3648
H	0.02198	3.48003	-3.33378
N	1.49625	4.2814	-2.01075
C	2.67711	4.16015	-2.83252
H	3.17347	5.1304	-2.93969
H	3.39087	3.44667	-2.39662
H	2.39067	3.81053	-3.8273
C	-0.65423	4.13962	-1.30802
H	-0.46329	2.0769	-1.27187

IntB$_{6S}$

N	0.8037	-2.5825	0.34085
N	-0.85863	-1.022	-1.32743
N	1.89751	-0.24857	-1.8053
N	2.90732	0.05326	0.65372
C	1.55145	-3.31525	1.15615
C	1.44484	-4.72186	1.29012
C	0.46784	-5.37544	0.58699
H	0.32055	-6.45174	0.6771
C	-0.41043	-4.6272	-0.2342
C	-1.51738	-5.22931	-0.86969
H	-1.66187	-6.30314	-0.76758
C	-2.416	-4.45862	-1.56615
H	-3.29164	-4.91047	-2.02535
C	-2.20302	-3.07635	-1.6967
H	-2.9301	-2.48788	-2.24988
C	-1.09062	-2.45133	-1.15835
C	-0.19583	-3.21668	-0.36269
C	-2.07912	-0.25227	-0.99745

H	-1.82264	0.81104	-0.91822
H	-2.47865	-0.60842	-0.04237
H	-2.86436	-0.35116	-1.76183
C	-0.38724	-0.62211	-2.7186
H	-0.55603	0.46761	-2.74649
C	-1.18251	-1.25903	-3.8636
H	-1.09271	-2.35191	-3.7956
H	-2.24832	-1.01798	-3.75048
C	-0.70239	-0.831	-5.24476
H	-1.29141	-1.35216	-6.00824
H	-0.88535	0.24365	-5.38423
C	0.78107	-1.11048	-5.40536
H	1.13947	-0.77334	-6.38442
H	0.97458	-2.19365	-5.35863
C	1.53617	-0.39019	-4.3013
H	1.30679	0.68308	-4.37945
H	2.62123	-0.47833	-4.42796
C	1.11104	-0.87779	-2.91021
H	1.29148	-1.96204	-2.82111
C	2.08925	1.21566	-2.01146
H	2.78636	1.41245	-2.83372
H	2.47652	1.65902	-1.09278
H	1.12082	1.678	-2.2249
C	3.72994	-0.5614	-0.25616
C	3.17728	-0.86641	-1.52829
C	3.89689	-1.67034	-2.39031
H	3.4892	-1.96657	-3.35234
C	5.1972	-2.10018	-2.049
H	5.74366	-2.72194	-2.75378
C	5.79417	-1.70297	-0.87565
H	6.81783	-1.99222	-0.64662
C	5.07177	-0.92148	0.05489
C	5.59551	-0.50226	1.30517
H	6.62507	-0.75106	1.56265
C	4.78761	0.19616	2.1676
C	3.43404	0.4192	1.80906
C	2.58767	-2.78812	2.10353
H	2.27104	-1.85506	2.58774
H	3.51731	-2.5596	1.55867
C	2.79253	-3.95169	3.08506
H	3.79899	-3.97346	3.51192
H	2.08864	-3.85241	3.92104
C	2.45392	-5.21681	2.28092
H	3.34166	-5.597	1.75406
H	2.08628	-6.04015	2.90215
C	2.69732	1.09508	2.92422
H	1.69077	0.68309	3.07774
H	2.56422	2.15962	2.67321
C	3.63461	0.90831	4.12882
H	3.37	-0.01807	4.6553
H	3.56205	1.72115	4.85621
C	5.04565	0.76814	3.52863
H	5.53083	1.75064	3.43213
H	5.71438	0.15411	4.14092
Fe	0.82126	-0.43226	0.13257
C	-1.10835	0.93436	1.95249
C	-1.27606	-1.13727	2.58488

H	-1.04039	-2.19254	2.65205
C	-2.27916	-0.43712	3.2163
H	-3.07144	-0.74993	3.88423
N	-0.56513	-0.28946	1.80321
N	-2.1689	0.86384	2.81665
C	-3.15127	1.89767	3.21129
H	-3.01004	2.73805	2.5293
C	-0.48896	2.02196	1.19989
C	-0.69336	3.48881	1.41713
O	0.34132	1.65329	0.34226
C	-0.85438	4.22566	0.07712
H	0.09443	4.09393	-0.46346
C	-1.08448	5.71618	0.30152
H	-2.01185	5.89335	0.86069
H	-0.25987	6.17401	0.86045
H	-1.17557	6.24109	-0.65478
H	-2.89988	2.2414	4.22147
C	-4.55746	1.37995	3.13296
C	-5.3759	1.36896	4.26214
C	-5.05763	0.91214	1.91196
C	-6.68548	0.9009	4.17276
H	-4.99183	1.7349	5.21405
C	-6.36141	0.43991	1.82566
H	-4.41359	0.92012	1.02821
C	-7.17754	0.43483	2.95755
H	-7.31976	0.89964	5.0558
H	-6.7477	0.07627	0.87524
H	-8.19889	0.06768	2.88919
C	-3.07164	2.68911	-2.53438
C	-1.82223	3.23521	-2.13756
C	-0.79795	3.35055	-3.09221
C	-1.03919	2.92313	-4.38955
C	-2.2867	2.38145	-4.75674
C	-3.31666	2.24883	-3.83652
C	-3.21199	3.2476	-0.37495
H	0.15693	3.80716	-2.82952
H	-0.26631	3.03633	-5.14803
H	-2.4539	2.08001	-5.78885
H	-4.28532	1.84842	-4.13192
H	-3.73905	3.41152	0.56155
H	-1.53723	3.70313	2.0801
N	-3.90385	2.70353	-1.43863
C	-5.28838	2.29483	-1.4428
H	-5.84461	2.82395	-2.22424
H	-5.38131	1.21392	-1.61895
H	-5.73901	2.53177	-0.47583
C	-1.93044	3.58543	-0.75413
H	0.19603	3.86858	1.94514

IntB_{6R}

N	0.81714	-2.57722	0.27302
N	-0.67599	-1.53236	-1.88035
N	1.93125	-0.27479	-1.93482
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C	1.48189	-3.07262	1.30878
C	1.61393	-4.45535	1.58695
C	0.97138	-5.35169	0.77519

H	1.01469	-6.42518	0.95986
C	0.1911	-4.87044	-0.3038
C	-0.58213	-5.74271	-1.09898
H	-0.5381	-6.81204	-0.90105
C	-1.40485	-5.23866	-2.07651
H	-2.03202	-5.9013	-2.66714
C	-1.44121	-3.85548	-2.31948
H	-2.11773	-3.48013	-3.08218
C	-0.6444	-2.96623	-1.61765
C	0.15421	-3.46006	-0.55075
C	-2.06344	-1.0288	-1.82345
H	-2.04457	0.06704	-1.83563
H	-2.53247	-1.37887	-0.89942
H	-2.67665	-1.37097	-2.67031
C	-0.03521	-1.10484	-3.18822
H	-0.35955	-0.05672	-3.3053
C	-0.50584	-1.88991	-4.41502
H	-0.24381	-2.94927	-4.28779
H	-1.60105	-1.84143	-4.49023
C	0.13501	-1.40412	-5.70797
H	-0.24562	-1.99304	-6.55049
H	-0.14707	-0.35626	-5.89804
C	1.64687	-1.49287	-5.60268
H	2.12662	-1.13965	-6.52226
H	1.95517	-2.54179	-5.47302
C	2.10374	-0.64608	-4.42686
H	1.77909	0.38766	-4.6162
H	3.19702	-0.61156	-4.35471
C	1.49438	-1.11088	-3.09611
H	1.82302	-2.1391	-2.87041
C	1.94882	1.18116	-2.26984
H	2.79014	1.42342	-2.92884
H	2.02608	1.76147	-1.34934
H	1.00969	1.4584	-2.7563
C	3.42345	-0.13978	-0.0332
C	3.198	-0.64287	-1.34201
C	4.19163	-1.37983	-1.95573
H	4.03697	-1.81069	-2.9407
C	5.44207	-1.55939	-1.32805
H	6.20817	-2.13573	-1.84059
C	5.71646	-0.9743	-0.11432
H	6.70058	-1.07067	0.33991
C	4.71159	-0.24723	0.56388
C	4.90568	0.35774	1.83276
H	5.88581	0.30104	2.30667
C	3.84893	0.9892	2.43945
C	2.57819	0.9582	1.80828
C	2.1694	-2.26941	2.37088
H	1.59382	-1.38102	2.66155
H	3.13841	-1.90628	1.99424
C	2.36342	-3.28111	3.50995
H	3.23809	-3.06006	4.12763
H	1.48776	-3.26133	4.17119
C	2.44768	-4.65039	2.8158
H	3.48464	-4.88349	2.53196
H	2.10664	-5.47759	3.44698
C	1.54593	1.60639	2.68044

H	0.58964	1.06655	2.68163
H	1.33583	2.61783	2.29646
C	2.23309	1.66124	4.05437
H	2.00391	0.74386	4.61258
H	1.89765	2.5025	4.66682
C	3.74025	1.70817	3.74938
H	4.08543	2.74629	3.63361
H	4.35439	1.26711	4.54165
Fe	0.51665	-0.50106	-0.22669
C	-1.78704	0.82558	1.1384
C	-1.76208	-1.09968	2.13232
H	-1.44325	-2.10616	2.37536
C	-2.80987	-0.37848	2.66771
H	-3.54257	-0.62276	3.4252
N	-1.13606	-0.35332	1.19205
N	-2.81984	0.8311	2.03807
C	-3.78536	1.92973	2.31668
H	-4.13356	2.29559	1.34342
C	-1.28174	1.82953	0.21766
C	-1.82332	3.2065	0.06546
H	-2.25788	3.5773	1.00043
O	-0.32269	1.45955	-0.49382
C	-2.88335	3.33957	-1.0681
H	-3.7604	2.73564	-0.77545
C	-3.31936	4.80299	-1.1435
H	-3.69898	5.16215	-0.17906
H	-2.48102	5.44552	-1.43775
H	-4.10925	4.93082	-1.88953
H	-3.22396	2.73764	2.80125
C	-4.93026	1.48747	3.1725
C	-4.90707	1.71654	4.55068
C	-6.02194	0.82487	2.60213
C	-5.96458	1.2915	5.34958
H	-4.06284	2.24136	4.99876
C	-7.07675	0.3983	3.40113
H	-6.04847	0.65203	1.52548
C	-7.04819	0.63153	4.77517
H	-5.94637	1.48392	6.41974
H	-7.92816	-0.10675	2.95077
H	-7.87838	0.30656	5.39803
C	-1.24552	2.42172	-4.33089
C	-1.19757	3.13505	-3.10149
C	-0.09103	3.96433	-2.85495
C	0.91646	4.05514	-3.80345
C	0.85172	3.3286	-5.00584
C	-0.23108	2.50621	-5.28817
C	-3.12135	1.97742	-3.20637
H	-0.02634	4.55763	-1.94365
H	1.76473	4.71247	-3.62469
H	1.64712	3.43537	-5.74031
H	-0.30428	1.98322	-6.24134
H	-4.10262	1.53786	-3.05526
N	-2.42944	1.71138	-4.36626
C	-2.96627	1.04095	-5.52764
H	-3.28149	1.7577	-6.29543
H	-2.21664	0.37183	-5.96512
H	-3.83193	0.44263	-5.2315

C	-2.40631	2.8191	-2.38876
H	-0.97522	3.85693	-0.17713