Supporting Information

Arylation of enelactams using TIPSOTf: reaction scope and mechanistic insight

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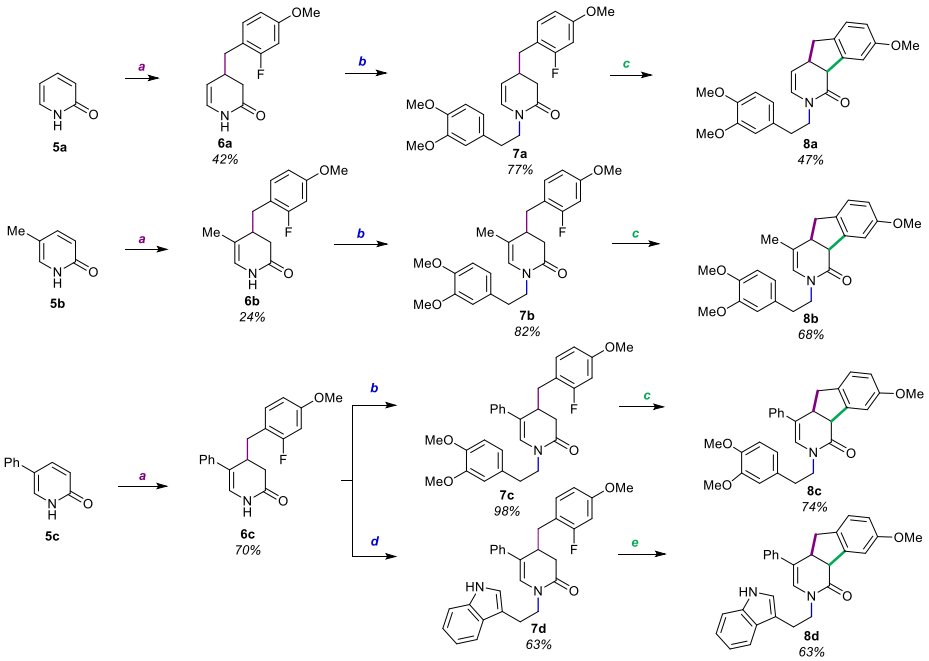
1. General information

Melting points were determined on a Boetius hot stage apparatus. ^{1}H, ^{13}C, ^{19}F and ^{29}Si NMR spectroscopic measurements were performed on a Bruker DPX 400 Avance III HD spectrometer, operating at 400.2, 100.6, 376.6 and 79.5 MHz, respectively. TMS (internal standard, $\delta_{H,C,Si}$ = 0 ppm) and $PhCF_3$ (external standard, 0.05% in $CDCl_3$, δ_F = –62.61 ppm) was used as reference and spectra were acquired in 5 mm probes at 21°C. For NMR analyses MestReNova (version: 12.0.4) program was used. Conformational analyses were performed on the basis of PM3 calculated structures (HyperChem 7.52) and calculated vicinal coupling constants by MSpin program (version: 2.3.4.). For detailed peak assignments, 2D spectra were acquired using Bruker software (^{1}H,^{1}H DFQCOSY; ^{13}C,^{1}H COSY; ^{1}H, ^{13}C HMQC; ^{1}H,^{1}H NOESY; ^{1}H,^{13}C HMBC). In the ^{1}H,^{1}H NOESY spectra the optimized mixing time, varied from 0.7 s to 0.8 s, was used. The ^{1}H,^{13}C HMBC long-range correlations were acquired for $J_{C,H}$=10 Hz. The standard abbreviation for multiplicities were used (s = singlet, d =doublet, t = triplet, q =quartet, quint = quintet, m = multiplet, sxt = sextet, spt = septet, etc. The DOSY spectrum parameters have been optimized in the range of the gradient power between 2 and 95%. After optimization, the DOSY spectrum was taken with a gradient length of 1500 μs, a diffusion time of 50 ms and a relaxation delay of 5 ms. Gas chromatography-mass spectrometry (GC-MS) measurements were carried out on a Hewlett-Packard instrument model HP 6890 equipped with a mass detector HP 5973 and on an Agilent 78206b GC system equipped with a mass (Agilent 5977E MSD) and FID detectors. HRMS analyses (ESI+) were performed on a Waters LCT premier XE (TOF) using acetonitrile as solvent. Crude post-reaction mixtures were analyzed by GC-MS and ^{1}H NMR spectroscopy. *n*-BuLi (2.5 M in hexane), *sec*-BuLi (1.4 M in cyclohexane), MeLi (3.1 M in diethoxymethane), *i*-PrMgCl (2.0M in THF), BnMgCl (2.0M in THF), AllMgCl (2.0M in THF), LDA (2.0M in THF), allyl bromide, metallic magnesium (Mg), methyl acrylate, 3-(2-bromoethyl)-1H-indole, $PhB(OH)_2$, $Pd(PPh_3)_4$, 1,3,5-trimethoxybenzene, piperidine, furfurylamine, tryptamine, 4-methoxybenzylamine, phenylethylamine and Grubbs catalyst second generation were purchased from Aldrich. TIPSOTf, 1-(2-bromoethyl)-3-methylbenzene, 5-(2-bromoethyl)-2,3-dihydrobenzofuran and phenylacetaldehyde were purchased from Fluorochem. Homoveratrylamine, propionaldehyde, isovaleraldehyde, 1-benzyl-4-piperidone was purchased from TCI Chemicals. Pyrrolidine and phenylpropylamine were purchased from Fluka. DIPEA was purchased from Abcr GmbH. Aniline (distilled form zinc powder) was purchased from POCH. 2-(3,4-Dimethoxyphenyl)bromoethane was prepared from corresponding alcohol as described earlier.[1] Reactions in tetrahydrofuran (THF),

dichloromethane (DCM), acetonitrile (MeCN) and chlorobenzene (PhCl) solutions were performed under argon in flame-dried flasks and liquid components were added from a syringe. Anhydrous toluene and THF were purified by distillation over sodium metal under argon prior to use. Anhydrous DCM was purified by distillation over CaH_2 under argon prior to use. Anhydrous MeCN was purified by filtration through a pad of Al_2O_3. Anhydrous PhCl was purified by distillation over P_2O_5, then stored over a layer of dry silica gel and collected in this form for the reaction. Products were purified by flash column chromatography on silica gel (63-200 μm, Merck) using appropriate solvents.

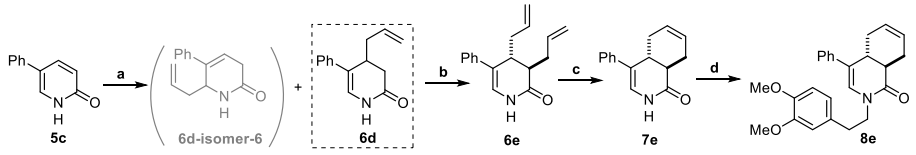
2. Sequences of preparation of enelactams 8

Scheme S1 Synthesis of compounds **8a-8d**



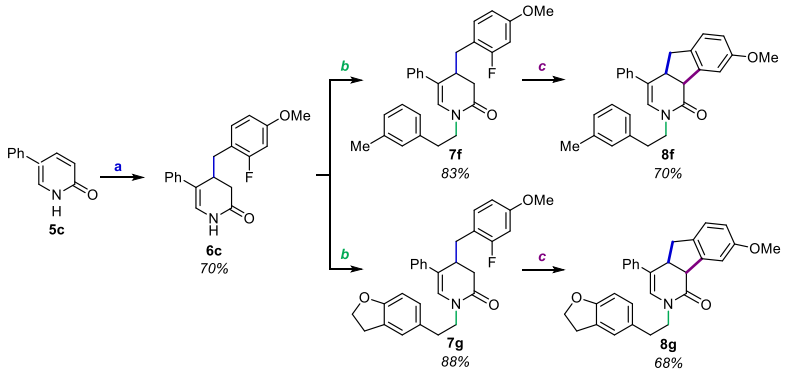
Conditions: ***a*** - **1.** MeLi (1.05 eq.), 0ºC, 15 min, THF **2.** (2-fluoro-4-methoxybenzyl)magnesium chloride (1.1 eq.), MeLi (2.2 eq.), 0ºC to rt, 2.5h, THF; ***b*** - 4-(2-bromoethyl)-1,2-dimethoxybenzene (1.5 eq.), TBAI (0.5 eq.), KOH (1.5 eq.), rt, **7a**, **7b** – 24h, **7c** – 16h, THF; ***c*** - **1.** *i*-PrMgCl (2.02 eq.), *s*-BuLi (4.04 eq.), 0ºC, 1h, THF **2.** *n*-BuLi (5.0 eq.), -80ºC, 3h, THF **3.** 0ºC, 3 min., THF (vigorous stirring) **4.** NH_4Cl_{aq}, 0ºC to rt; ***d*** - 3-(2-bromoethyl)-1*H*-indole (2.5 eq.), TBAI (0.5 eq.), KOH (5.0 eq.), rt, 18h, THF; ***e*** - **1.** *i*-PrMgCl (3.03 eq.), *s*-BuLi (6.06 eq.), 0ºC, 1h, THF **2.** *n*-BuLi (5.0 eq.), -80ºC, 3h, THF **3.** 0ºC, 3 min., THF (vigorous stirring) **4.** NH_4Cl_{aq}, 0ºC to rt.

Scheme S2 Synthesis of compound **8e** from 2-pyridone **5c**



Conditions: ***a*** - 1. MeLi (1.05 eq.), 0ºC, 0.5h, THF 2. AllMgCl (1.25 eq.), MeLi (2.5 eq.), 0ºC, 3h, THF (**6d** – 35%, **6d-isomer-6** – 41%); ***b*** - 1. LDA (2.0 eq.), 0ºC, 0.5h, THF 2. AllBr (1.0 eq.), -80ºC (1h) then 0ºC (1h), THF (**6e** – 65%); ***c*** - Grubbs catalyst 2nd gen. (2% mol.), 70ºC, 2h, PhMe (**7e** – 80%); ***d*** - 4-(2-bromoethyl)-1,2-dimethoxybenzene (1.5 eq.), TBAI (0.5 eq.), KOH (1.5eq.), rt, 24h, THF (**8e** – 80%).

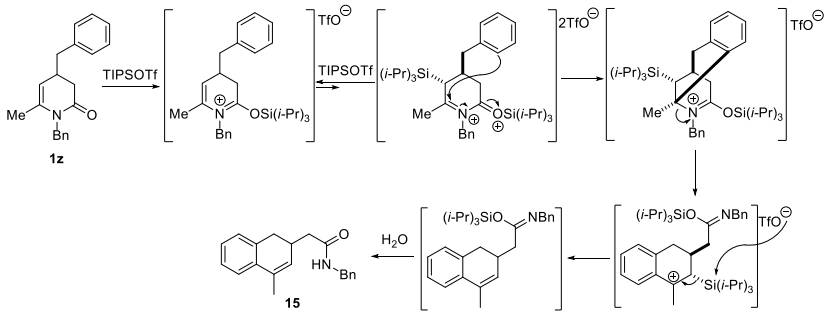
Scheme S3 Synthesis of compounds **8f** and **8g**



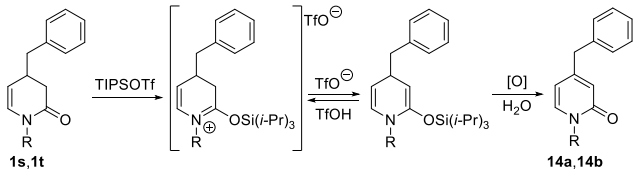
Conditions: ***a*** - **1.** MeLi (1.05 eq.), 0ºC, 15 min, THF **2.** (2-fluoro-4-methoxybenzyl)magnesium chloride (1.1 eq.), MeLi (2.2 eq.), 0ºC to rt, 2.5h, THF; ***b*** - 1-(2-bromoethyl)-3-methylbenzene (1.5 eq.) or 5-(2-bromoethyl)-2,3-dihydrobenzofuran (1.5 eq.), TBAI (0.5 eq.), KOH (1.5 eq.), rt, **7f** – 24h, **7g** – 18h, THF; ***c*** - **1.** *i*-PrMgCl (2.02 eq.), *s*-BuLi (4.04 eq.), 0ºC, 1h, THF **2.** *n*-BuLi (5.0 eq.), -80ºC, 3h, THF **3.** 0ºC, 3 min., THF (vigorous stirring) **4.** NH_4Cl_{aq}, 0ºC to rt.

3. Additional mechanistic aspects

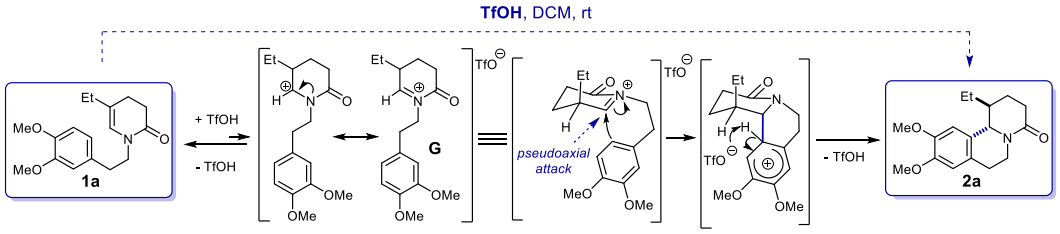
Scheme S4 Possible route of compound **15** formation



Scheme S5 Possible route of compound **14** formation



Scheme S6 Mechanism of the reaction of **1a** upon treatment with TfOH



4. The diagnostic NOEs found in NOESY spectra and vicinal coupling constants for representative compounds

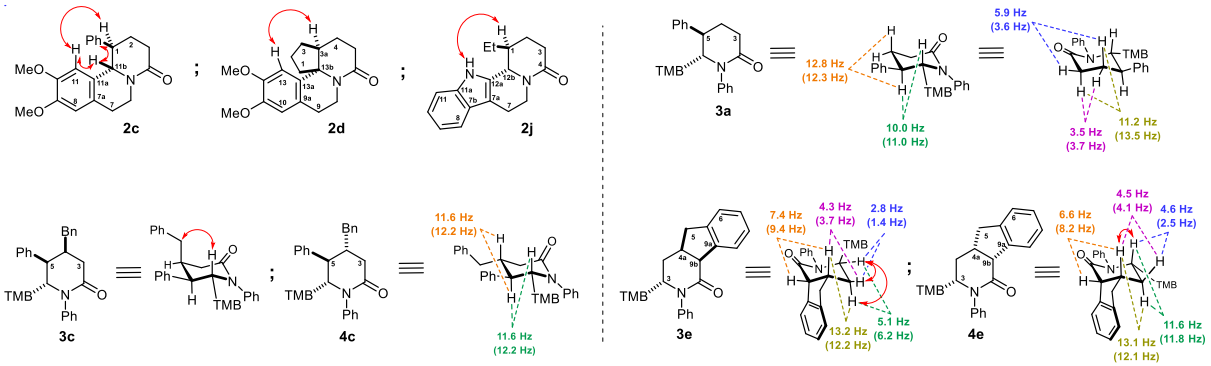


Figure S1 Selected experimental and calculated (given in the parenthesis) $^{3}J_{H,H}$ coupling constants for representative compounds **3a**, **4c**, **3e** and **4e** as well as the diagnostic NOE effects found in ^{1}H, ^{1}H NOESY spectra of compounds **2c**, **2d**, **2j**, **3c**, **3e** and **4e** (for more details see also below)

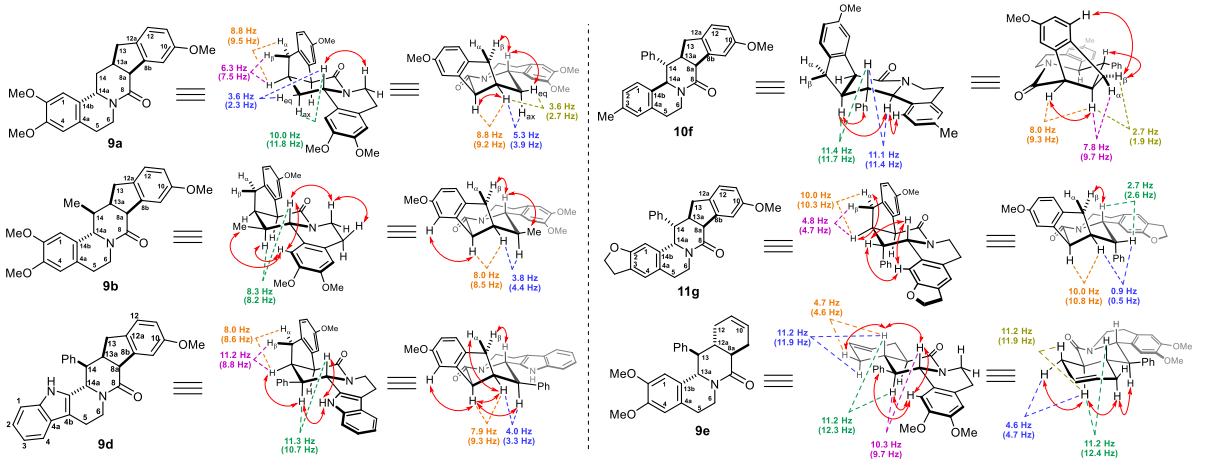


Figure S2 Selected experimental and calculated (given in the parenthesis) $^{3}J_{H,H}$ coupling constants as well as the diagnostic NOE effects found in ^{1}H, ^{1}H NOESY spectra for representative compounds **9a**, **9b**, **9d**, **10f**, **11g** and **9e** (for more details see also below)

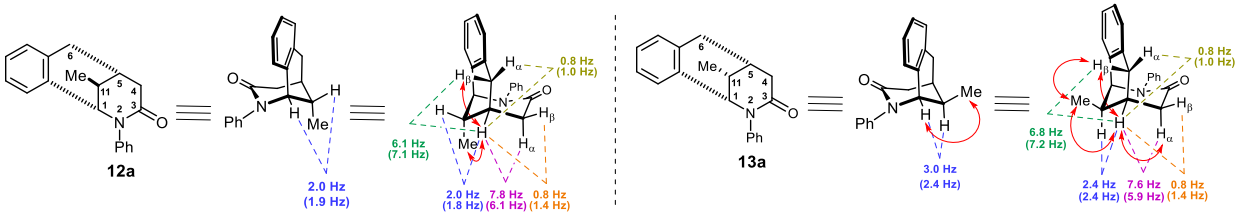
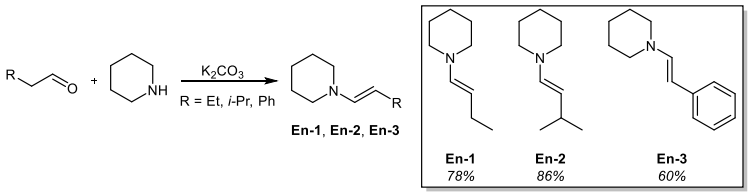


Figure S3 Selected experimental and calculated (given in the parenthesis) $^{3}J_{H,H}$ coupling constants and the diagnostic NOE effects found in ^{1}H, ^{1}H NOESY spectra for representative diasteroisomeric benzomorphanones **12a**, **13a** (for more details see also below)

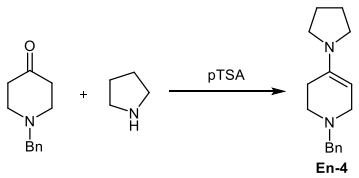
5. Preparation of starting materials

5a. Procedure 1**: Synthesis of enamines **En-1**, **En-2** and **En-3



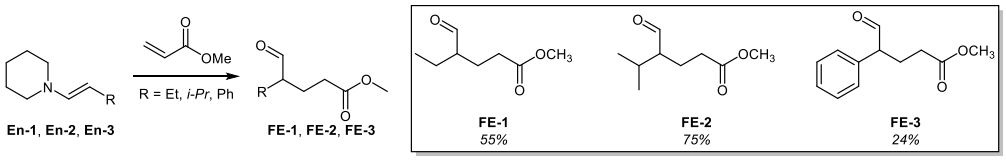
Compounds **En-1**, **En-2** and **En-3** were prepared in 5g scale according to the procedure described earlier[2]. The resulting crude products were purified by distillation under reduced pressure to give respectively 7.615g (78%) of **En-1** as colorless oil (bp 76-77°C/18 mm Hg; reported[3] bp 90-91°C/45 mm Hg), 7.610g (86%) of **En-2** as colorless oil (bp 80-82°C/18 mm Hg; reported[4] bp 83.5-85°C/18 mm Hg) and 4.664g (60%) of **En-3** as yellow oil (bp 85-88°C/0.02 mm Hg). ^{1}H and ^{13}C NMR data for **En-1**[2]**, En-3**[5] matched those reported previously**.**

***5b. Procedure 2:** Synthesis of N-Benzyl-4-pyrrolidinyl-1,2,5,6-tetrahydropyridine (**En-4**)*



N-Benzyl-4-pyrrolidinyl-1,2,5,6-tetrahydropyridine was prepared according to the procedure described earlier[6], however, toluene was used instead of benzene and heating was continued for 4 hours. The resulting crude product was purified by distillation under reduced pressure to give 36% of **En-4** as yellowish oil (bp 145-150°C/0.02 mm Hg, reported[7] 138-140°C/0.05 mm Hg). ^{1}H NMR data for **En-4** matched those reported previously.[5]

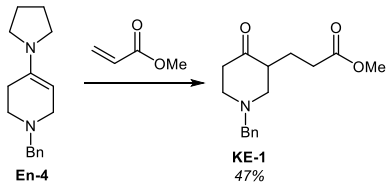
***5c. Procedure 3:** Synthesis of formyl esters*



Compounds **FE-1**, **FE-2** and **FE-3** were prepared according to the procedure described earlier[2]. The resulting crude products were purified by distillation under reduced pressure to give products with 55% yield of **FE-1** as colorless oil (bp 30-32°C/0,01 mm Hg), 75% yield of **FE-2** as colorless oil (bp 56-58°C/0,01 mm Hg) and 24% yield of **FE-3** as yellowish oil bp 102-

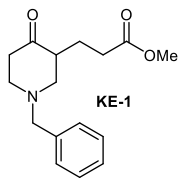
110°C/0.01 mm Hg). ^{1}H and ^{13}C NMR data for **FE-1**[2]**, FE-2**[8]**, FE-3**[9] matched those reported previously**.**

5d. Procedure 4: *Synthesis of methyl 3-(1-benzyl-4-oxopiperidin-3-yl)propanoate*[5]



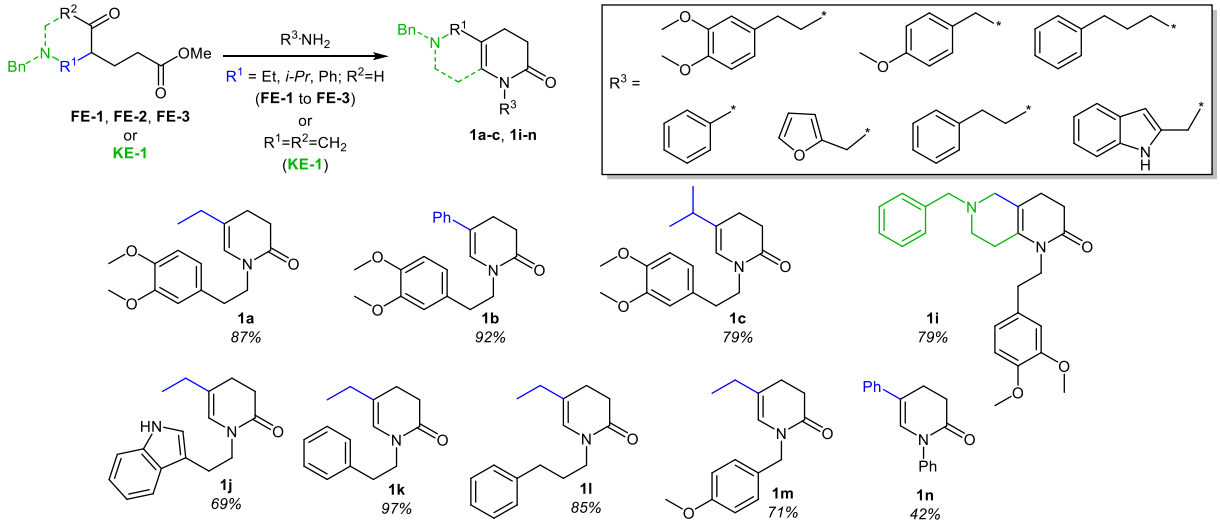
The mixture of enamine **En-4** (1.362g, 5.62 mmol) and methyl acrylate (0.51 mL, 5.62 mmol) in dry MeCN (10 mL) was refluxed for 2 h under Argon. Water (5 mL) was added and the solution was heated for one more hour. After rotary-evaporation, the residue was taken into DCM, washed with water, dried, and the solvent removed in vacuo. The crude product was distilled (130-140°C, 0.01 mmHg) to yield ketoester **KE-1** (0.635g, 47%).

Methyl 3-(1-benzyl-4-oxopiperidin-3-yl)propanoate (**KE-1**):



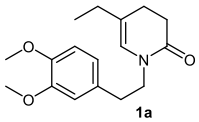
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.54 (dtd, *J* = 14.2, 8.7, 6.7, 5.5 Hz, 1H, C<u>H</u>H), 2.08 (dq, *J* = 14.2, 8.1, 6.5 Hz, 1H, CH<u>H</u>), 2.21 (t, *J* = 10.6 Hz, 1H, NC<u>H</u>H), 2.25 – 2.43 (m, 3H, CH_2, C<u>H</u>H), 2.46 (dd, *J* = 11.0, 3.4 Hz, 1H, NC<u>H</u>H), 2.52 – 2.63 (m, 2H, CH, CH<u>H</u>), 2.97 – 3.09 (m, 2H, two NCH<u>H</u>), 3.57 (d, *J* = 13.2 Hz, 1H, NC<u>H</u>HPh), 3.63 (d, *J* = 13.3 Hz, 1H, NCH<u>H</u>Ph), 3.64 (s, 3H, OCH_3), 7.25 – 7.36 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 22.77 (CH_2), 31.63 (CH_2), 41.05 (CH_2), 48.89 (CH), 51.57 (OCH_3), 53.57, 58.88 (two NCH_2), 61.77 (NCH_2Ph), 127.35, 128.41, 128.85, 138.06 (C_6H_5), 173.71 (O-C=O), 210.29 (C=O). GC-MS (EI, 70eV): m/z = 275 (17), [M+], 244 (15), 202 (75), 189 (24), 188 (20), 152 (19), 91 (100), 65 (10). HRMS (ESI-TOF): *m/z* calcd for $C_{16}H_{22}NO_3[M + H]^+$, 276.1600; found, 276.1599.

5e. Procedure 5: *Procedures for the synthesis of 1,5-disubstited-3,4-dihydropyridin-2(1H)-ones* ***1a-1c***, ***1j-1n*** *and 6-benzyl-1-(3,4-dimethoxyphenethyl)-3,4,5,6,7,8-hexahydro-1,6-naphthyridin-2(1H)-one (**1i**)*



Methyl 4-formylhexanoate (**FE-1**) 0.598g (3.78 mmol), homoveratrylamine 0.685g (3.78 mmol) and dry toluene (10 mL) were placed in a 50 mL round-bottomed flask equipped with a magnetic stirrer and Dean-Stark trap. The reaction mixture was heated at 160°C and the reaction progress was monitored by GC-MS. (Heating time is given separately for each product). The solvent was removed by rotary evaporation and the crude product was purified by column chromatography on silica gel, using a mixture hexane and ethyl acetate (1:1 v/v) as the eluent, yielding the product **1a** as yellow oil 0.951g (87%). (Following this procedure compounds **1b-1c**, **1j-1n** and **1i** were obtained.)

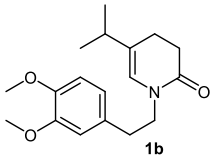
1-(3,4-Dimethoxyphenethyl)-5-ethyl-3,4-dihydropyridin-2(1*H*)-one (**1a**)[10]:



Yield 87% (0.951g, reaction time: 4h). The crude product purified by column chromatography (SiO_2, n-hexane:ethyl acetate, 1:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.97 (t, *J* = 7.5 Hz, 3H, CH_3), 2.00 (qd, *J* = 7.5, 1.4 Hz, 2H, $\underline{CH_2}CH_3$), 2.19 (t, *J* = 8.8, 7.2 Hz, 2H, CH_2-4), 2.47 (dd, *J* = 8.8, 7.2 Hz, 2H, CH_2-3), 2.80 (t, *J* = 8.4, 6.7 Hz, 2H, $NCH_2\underline{CH_2}$), 3.63 (dd, *J* = 8.4, 6.7 Hz, 2H, NCH_2), 3.85 (s, 3H, OCH_3), 3.87 (s, 2H, OCH_3), 5.61 (t, *J* = 1.4 Hz, 1H, =CH-6), 6.73 – 6.76 (m, 2H, CH-5', CH-6'), 6.79 (d, *J* = 8.0 Hz, 1H, CH-2'). ^{13}C NMR (101 MHz, $CDCl_3$) δ 12.37 (CH_3), 24.17 (CH_2-4), 26.72 ($\underline{CH_2}CH_3$), 31.36 (CH_2-3), 34.41 ($NCH_2\underline{CH_2}$), 48.05 (NCH_2), 55.85, 55.89 (two OCH_3), 111.21 (CH-5'), 112.12 (CH-2'), 120.80 (CH-6'), 121.25 (=C-5), 123.70 (=CH-6), 131.38 (C-1'),

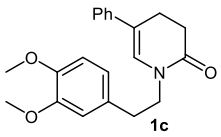
147.55, 148.83 (C-3', C-4'), 168.68 (C=O). GC-MS (EI, 70eV): m/z = 289 (13), [M^+], 164 (100), 151 (10), 138 (11), 110 (18), 84 (7).

1-(3,4-Dimethoxyphenethyl)-5-isopropyl-3,4-dihydropyridin-2(1*H*)-one (**1b**):



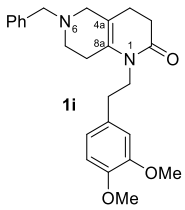
Yield 92% (0.810g, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.96 (d, *J* = 6.8 Hz, 6H, two CH_3), 2.17 (t, *J* = 8.9, 7.4 Hz, 2H, CH-4), 2.23 [hd, *J* = 6.8, 1.2 Hz, 1H, $\underline{CH}(CH_3)_2$], 2.45 (t, *J* = 8.9, 7.4 Hz, 1H, CH-3), 2.80 (dd, *J* = 8.2, 6.6 Hz, 1H, $NCH_2\underline{CH_2}$), 3.64 (dd, *J* = 8.2, 6.6 Hz, 1H, NCH_2), 3.85 (s, 3H, OCH_3), 3.87 (s, 3H, OCH_3), 5.57 (q, *J* = 1.2 Hz, 1H, =CH-6), 6.70 – 6.76 (m, 2H, CH-5', CH-6'), 6.79 (d, *J* = 7.9 Hz, 1H, CH-2'). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.05 (two CH_3), 22.21 (CH_2-4), 31.60 (CH_2-3), 31.88 ($CH(CH_3)_2$), 34.44 ($NCH_2\underline{CH_2}$), 48.12 (NCH_2), 55.87 and 55.93 (two OCH_3), 111.29 (CH-5'), 112.20 (CH-2'), 120.85 (CH-6'), 123.12 (=CH-6), 125.52 (=C-5), 131.46 (C-1'), 147.62 and 148.89 (two OCH_3), 168.91 (C=O). GC-MS (EI, 70eV): m/z = 303 (23), [M^+], 164 (100), 152 (15), 124 (17). HRMS (ESI-TOF): *m/z* calcd for $C_{18}H_{26}NO_3[M + H]^+$, 304.1913; found, 304.1916.

1-(3,4-Dimethoxyphenethyl)-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**1c**):



Yield 79% (0.646g, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.60 – 2.67 (m, 2H, CH_2-4), 2.70 (ddt, *J* = 8.0, 5.9, 1.2 Hz, 2H, CH_2-3), 2.86 (dd, *J* = 8.2, 6.6 Hz, 2H, $NCH_2\underline{CH_2}$), 3.76 (dd, *J* = 8.2, 6.6 Hz, 2H, NCH_2), 3.85 and 3.86 (two s, 6H, two OCH_3), 6.25 (d, *J* = 1.2 Hz, 1H, =CH-6), 6.71 – 6.84 (m, 3H, C_6H_3), 7.16 – 7.24 (m, 3H, C_6H_5), 7.28 – 7.35 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 23.64 (CH_2-4), 31.34 (CH_2-3), 34.70 ($NCH_2\underline{CH_2}$), 48.51 (NCH_2), 55.92 (two OCH_3), 111.38 (CH-5'), 112.20 (CH-2'), 118.11 (=C-5), 120.95 (CH-6'), 124.29 (C_6H_5), 126.61 (C_6H_5), 126.92 (=CH-6), 128.62 (C_6H_5), 131.12 (C_6H_5), 138.40 (C-1'), 147.74, 149.01 (C-3', C-4'), 168.72 (C=O). GC-MS (EI, 70eV): m/z = 337 (17), [M^+], 186 (8), 173 (27), 164 (100), 158 (19), 151 (14), 132 (14), 115 (13), 91 (23). HRMS (ESI-TOF): *m/z* calcd for $C_{21}H_{24}NO_3[M + H]^+$, 338.1756; found, 338.1756.

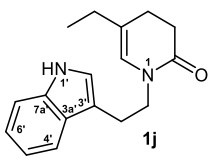
6-Benzyl-1-(3,4-dimethoxyphenethyl)-3,4,5,6,7,8-hexahydro-1,6-naphthyridin-2(1*H*)-one (**1i**):



1i

Yield 79% (0.742g, reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave orange oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.05 (dd, *J* = 8.7, 6.9 Hz, 2H, CH_2-4), 2.23 (tt, *J* = 5.6, 2.0 Hz, 2H, CH_2-8), 2.48 (dd, *J* = 8.7, 6.9 Hz, 2H, CH_2-3), 2.59 (t, *J* = 5.6 Hz, 2H, CH_2-7), 2.75 (dd, *J* = 9.2, 6.3 Hz, 2H, $NCH_2\underline{CH_2}$), 2.96 (d, *J* = 2.0 Hz, 2H, CH_2-5), 3.57 (s, 2H, $N\underline{CH_2}Ph$), 3.72 (dd, *J* = 9.1, 6.2 Hz, 2H, $N\underline{CH_2}CH_2$), 3.82 and 3.84 (two s, 6H, two OCH_3), 6.71 – 6.80 (m, 3H, C_6H_3), 7.23 – 7.35 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 23.03 (CH_2-4), 26.13 (CH_2-8), 31.49 (CH_2-3), 35.08 ($NCH_2\underline{CH_2}$), 42.72 ($N\underline{CH_2}CH_2$), 49.57 (CH_2-7), 55.21 (CH_2-5), 55.80, 55.85 (two OCH_3), 62.14 $N\underline{CH_2}Ph$, 111.28 (CH-5'), 112.14 (CH-2'), 112.23 (=C-4a), 120.70 (CH-6'), 127.17, 128.27, 129.03 (C_6H_5), 129.86 (C-1'), 131.55 (=C-8a), 137.91 (C_6H_5), 147.56, 148.84 (C-3', C-4'), 169.52 (C=O). GC-MS (EI, 70eV): m/z = 406 (91), [M^+], 405 (100), 315 (21), 267 (59), 255 (29), 242 (39), 241 (32), 165 (32), 164 (45), 151 (17), 91 (65). HRMS (ESI-TOF): *m/z* calcd for $C_{25}H_{31}N_2O_3$[M + H]$^+$, 407.2335; found, 407.2329. [(Compound **1i** exists in equilibrium with the second ene-isomer (~92:8).]

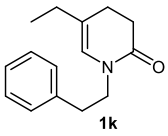
1-(2-(1*H*-Indol-3-yl)ethyl)-5-ethyl-3,4-dihydropyridin-2(1*H*)-one (**1j**)[11]:



1j

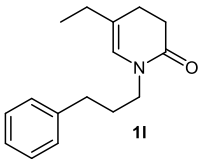
Yield 69% (0.818g, reaction time: 32h). The crude product purified by column chromatography (SiO_2, n-hexane:ethyl acetate, 1:1) gave beige solid, mp 84−86 °C (hexane:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.92 (t, *J* = 7.4 Hz, 3H, CH_3), 1.96 (qd, *J* = 7.5, 1.4 Hz, 2H, $\underline{CH_2}CH_3$), 2.07 – 2.22 (m, 2H, CH_2-4), 2.49 (dd, *J* = 8.9, 7.3 Hz, 2H, CH_2-3), 2.83 – 3.20 (m, 2H, $NCH_2\underline{CH_2}$), 3.59 – 3.82 (m, 2H, NCH_2), 5.65 (t, *J* = 1.4 Hz, 1H, CH-6), 6.97 (d, *J* = 2.4 Hz, 1H, CH-2'), 7.10 (td, *J* = 7.8, 7.0, 1.1 Hz, 1H, CH-5"), 7.16 (td, *J* = 8.1, 7.0, 1.1 Hz, 1H, CH-6'), 7.33 (dd, *J* = 8.1, 1.1 Hz, 1H, CH-7'), 7.64 (dd, *J* = 7.8, 1.1 Hz, 1H, CH-4'), 8.45 (s, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 12.27 (CH_3), 24.13 (CH_2-4), 24.35 (NCH_2CH_2), 26.68 (CH_2CH_3), 31.37 (CH_2-3), 47.08 (NCH_2), 111.22 (CH-7'), 112.69 (C-3'), 118.67 (CH-4'), 119.20 (CH-5'), 121.30 (=C-5), 121.85 (CH-6'), 122.16 (CH-2'), 123.65 (=CH-6), 127.49 (C-3a'), 136.31 (C-7a'), 168.87 (C=O). GC-MS (EI, 70eV): m/z = 268 (15), [M^+], 143 (100), 130 (32), 110 (10).

5-Ethyl-1-phenethyl-3,4-dihydropyridin-2(1*H*)-one (**1k**):



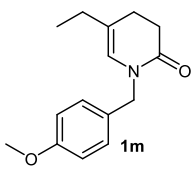
Yield 97% (0.984g, reaction time: 5.5h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.95 (t, *J* = 7.4 Hz, 3H, CH_3), 1.98 (qd, *J* = 7.7, 1.4 Hz, 2H, CH_2), 2.17 (t, *J* = 8.8, 7.2 Hz, 2H, CH_2-4), 2.46 (dd, *J* = 8.8, 7.2 Hz, 2H, CH_2-3), 2.84 (dd, *J* = 8.3, 6.6 Hz, 2H, $C\underline{H_2}$-C_6H_5), 3.65 (dd, *J* = 8.3, 6.6 Hz, 2H, NCH_2), 5.58 (p, *J* = 1.4 Hz, 1H, =CH-6), 7.14 – 7.31 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 12.31 (CH_3), 24.18 (CH_2-4), 26.70 ($\underline{CH_2}CH_3$), 31.34 (CH_2-3), 34.83 ($\underline{CH_2}Ph$), 47.89 (NCH_2), 121.28 (=C-5), 123.68 (=CH-6), 126.37, 128.43, 128.91, 138.81 (C_6H_5), 168.69 (C=O). GC-MS (EI, 70eV): m/z = 229 (54), [M^+], 138 (100), 125 (11), 110 (76), 105 (15), 91 (16), 84 (24). HRMS (ESI-TOF): *m/z* calcd for $C_{15}H_{20}NO[M + H]^+$, 230.1545; found, 230.1551.

5-Ethyl-1-(3-phenylpropyl)-3,4-dihydropyridin-2(1*H*)-one (**1l**):



Yield 85% (0.915g, reaction time: 5.5h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (t, *J* = 7.4 Hz, 3H, CH_3), 1.80 – 1.94 (m, 2H, $\underline{CH_2}CH_2N$), 2.04 (qd, *J* = 7.4, 1.4 Hz, 2H, $\underline{CH_2}CH_3$), 2.20 (t, *J* = 8.8, 7.2 Hz, 2H, CH_2-4), 2.47 (dd, *J* = 8.8, 7.2 Hz, 2H, CH_2-3), 2.62 (t, *J* = 8.7, 7.1 Hz, 1H, $\underline{CH_2}C_6H_5$), 3.48 (t, *J* = 7.8, 7.0 Hz, 2H, NCH_2), 5.71 (p, *J* = 1.4 Hz, 1H, =CH-6), 7.18 (d, *J* = 7.1 Hz, 2H, C_6H_5), 7.23 – 7.31 (m, 3H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 12.40 (CH_3), 24.15 (CH_2-4), 26.78 ($\underline{CH_2}CH_3$), 30.00 ($NCH_2\underline{CH_2}$), 31.35 (CH_2-3), 33.00 ($\underline{CH_2}C_6H_5$), 45.73 (NCH_2), 121.58 (=C-5), 123.33 (=CH-6), 125.88, 128.31, 128.36, 141.51 (C_6H_5), 168.74 (C=O). GC-MS (EI, 70eV): m/z = 243 (100), [M^+], 228 (35), 214 (8), 139 (23), 138 (24), 124 (73), 117 (14), 110 (47), 96 (18), 91 (55), 82 (11), 65 (11). HRMS (ESI-TOF): *m/z* calcd for $C_{16}H_{22}NO[M + H]^+$, 244.1701; found, 244.1701.

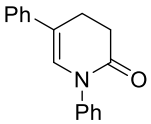
5-Ethyl-1-(4-methoxybenzyl)-3,4-dihydropyridin-2(1*H*)-one (**1m**):



Yield 71% (0.773g, reaction time: 24h). The crude product purified by column chromatography (SiO_2, n-hexane:ethyl acetate, 1:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.98 (t, *J* = 7.4 Hz, 3H, CH_3), 2.01 (qd, *J* = 7.4, 1.3 Hz, 2H, $\underline{CH_2}CH_3$), 2.20 – 2.28 (m, 2H, CH_2-4), 2.50 – 2.59 (m, 2H, CH_2-3), 3.78 (s, 3H, OCH_3), 4.59 (s, 2H, NCH_2), 5.75 (p, *J* = 1.3 Hz, 1H, =CH-6), 6.75 – 6.92 (m,

2H, ArH), 7.07 – 7.23 (m, 2H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 12.34 (CH_3), 24.16 (CH_2-4), 26.77 ($\underline{CH_2}CH_3$), 31.31 (CH_2-3), 48.30 (NCH_2), 55.24 (OCH_3), 113.98 (2C, ArH), 121.94 (C-5), 122.81 (=CH-6), 129.01 (2C, ArH), 129.54 (Ar), 158.93 (Ar), 168.88 (C=O). GC-MS (EI, 70eV): m/z = 245 (14), [M^+], 121 (100). HRMS (ESI-TOF): *m/z* calcd for $C_{15}H_{20}NO_2$[M + H]$^+$, 246.1494; found, 246.1501.

1,5-Diphenyl-3,4-dihydropyridin-2(1*H*)-one (**1n**):

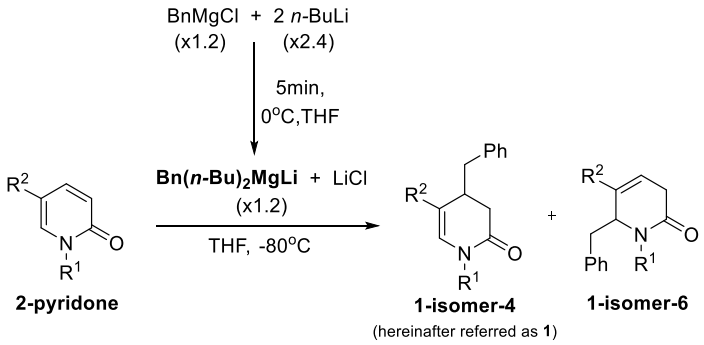


1n

Yield 42% (0.233g, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 86-88ºC (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.61 – 3.07 (m, 4H, CH_2-3, CH_2-4), 6.69 (d, *J* = 1.2 Hz, 1H, =CH-6), 7.19 – 7.27 (m, 1H, C_6H_5), 7.29 – 7.36 (m, 7H, C_6H_5), 7.39 – 7.45 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 23.71 (CH_2-4), 32.04 (CH_2-3), 118.96 (C-5), 124.38 (2C), 126.26 (2C), 126.82, 127.23 (C_6H_5), 127.70 (=CH-6), 128.68 (2C), 129.17 (2C), 138.17, 140.75 (C_6H_5), 168.60 (C=O). GC-MS (EI, 70eV): m/z = 249 (100), 220 (22), 206 (69), 77 (23). HRMS (ESI-TOF): *m/z* calcd for $C_{17}H_{16}NO$[M + H]$^+$, 250.1232; found, 250.1237.

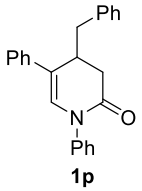
5f. *Synthesis of 4- and 6-benzylsubstituted γ,δ- and β,γ-unsatursted δ-lactams via nucleophilic addition of benzyl magnesiate to 2-pyridone*

Compounds **1o-z** were prepared according to the procedure described earlier.[12]



Spectra of compounds **1o**,[12] **1q**,[13] **1r**,[13] **1t**,[12], **1v-1z**[12] and **1aa**[13] are in agreement with literature data.

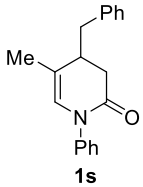
(*4RS*)-4-Benzyl-1,5-diphenyl-3,4-dihydropyridin-2(1*H*)-one (**1p**):



1p

Yield 41% (0.825g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.69 – 2.77 (m, 2H, C<u>H</u>H-3, 4-C<u>H</u>H), 2.87 (ddd, *J* = 16.1, 6.8, 0.6 Hz, 1H, CH<u>H</u>-3), 2.99 (dd, *J* = 13.6, 4.0 Hz, 1H, 4-CH<u>H</u>), 6.70 (d, *J* = 0.6 Hz, 1H, =CH-6), 7.15 – 7.33 (m, 9H, C_6H_5), 7.34 – 7.47 (m, 6H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 36.12 (CH_2-3), 36.42 (CH-4), 38.47 (4-CH_2), 122.45 (=C-5), 124.96 (2C), 126.18 (2C), 126.57, 127.03, 127.22 (C_6H_5), 127.27 (=CH-6), 128.46 (2C), 128.88 (2C), 129.10 (2C), 129.60 (2C), 137.03, 138.37, 140.43 (C_6H_5), 167.90 (C=O). GC-MS (EI, 70eV): m/z = 277 (5), [M^+], 186 (100), 158 (18), 143 (17), 91 (10), 77 (14). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}NONa$ [M + Na]$^+$, 300.1364; found, 300.1367.

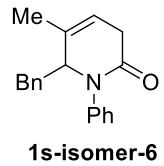
(*4RS*)-4-Benzyl-5-methyl-1-phenyl-3,4-dihydropyridin-2(1*H*)-one (**1s**):



1s

Yield 57% (1.359g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.72 (d, *J* = 1.4 Hz, 3H, CH_3), 2.44 – 2.51 (m, 1H, CH-4), 2.54 (dd, *J* = 16.0, 2.8 Hz, 1H, C<u>H</u>H-3), 2.64 (dd, *J* = 13.3, 8.8 Hz, 1H, 4-C<u>H</u>H), 2.74 (dd, *J* = 16.0, 6.9 Hz, 1H, CH<u>H</u>-3), 2.89 (dd, *J* = 13.3, 5.4 Hz, 1H, 4-CH<u>H</u>), 6.03 (q, *J* = 1.5 Hz, 1H, =CH-6), 7.15 – 7.32 (m, 7H, C_6H_5), 7.34 – 7.40 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 18.46 (CH_3), 36.59 (CH_2-3), 38.11 (4-CH_2), 38.87 (CH-4), 119.50 (=C-5), 125.60, 125.93 (2C), 126.41, 126.77, 128.41 (2C), 128.92 (2C), 129.38 (2C), 138.80, 140.51 (two C_6H_5), 167.73 (C=O). GC-MS (EI, 70eV): m/z = 277 (5), [M^+], 186 (100), 158 (18), 143 (17), 91 (10), 77 (14). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{20}NO$[M + H]$^+$, 278.1545; found, 278.1557. HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}NONa$ [M + Na]$^+$, 300.1364; found, 300.1367.

(*6RS*)-6-Benzyl-5-methyl-1-phenyl-3,6-dihydropyridin-2(1*H*)-one (**1s-isomer-6**) (obtained as regioisomer):

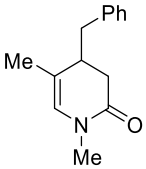


1s-isomer-6

Yield 35% (0.828g). The crude product purified by column chromatography (SiO_2, n-hexane:ethyl acetate, 3:1) gave white solid, mp 104-106°C (petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (dt, *J* = 2.7, 1.3 Hz, 3H, 5-CH_3), 2.02 (ddq, *J* = 20.9, 5.4, 2.7 Hz, 1H, C<u>H</u>H-3), 2.63 (ddt, *J* = 20.9, 5.4, 1.2 Hz, 1H, CH<u>H</u>-3), 2.80 – 2.95 (m, 2H, 6-CH_2), 4.46 (q, *J* = 3.9, 3.5 Hz, 1H, CH-6), 5.47 (dp, *J* = 5.4, 1.7 Hz, 1H, =CH-4), 7.13 – 7.19 (m, 2H, C_6H_5), 7.21 – 7.28 (m, 3H, C_6H_5), 7.29 – 7.34 (m, 1H,

C_6H_5), 7.37 – 7.51 (m, 4H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.49 (CH_3), 32.99 (CH_2-3), 37.04 (6-CH_2), 66.74 (CH-6), 120.50 (=CH-4), 126.90, 127.06, 127.75 (2C), 128.13 (2C), 129.27 (2C), 130.06 (2C), 131.91, 135.79, 141.32 (two C_6H_5), 168.80. GC-MS (EI, 70eV): m/z = 277 (1), [M^+], 186 (100), 158 (17), 143 (17), 91 (12), 77 (14). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{20}NO[M + H]^+$, 278.1545; found, 278.1558. HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}NONa$ $[M + Na]^+$, 300.1364; found, 300.1369.

(4*RS*)-4-Benzyl-1,5-dimethyl-3,4-dihydropyridin-2(1*H*)-one (**1u**):

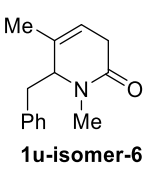


1u

Yield 20% (0.524g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.68 (d, *J* = 1.6 Hz, 3H, 5-CH_3), 2.32 – 2.40 (m, 2H, C<u>H</u>H-3, CH-4), 2.44 – 2.53 (m, 2H, CH<u>H</u>-3, 4-C<u>H</u>H), 2.78 (dd, *J* = 13.2, 5.0 Hz, 1H, 4-CH<u>H</u>), 2.95 (s, 3H, NCH_3), 5.75 (q, *J* = 1.6 Hz, 1H, =CH-6), 7.11 – 7.32 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 18.29 (5-CH_3), 33.28 (NCH_3), 35.42 (CH_2-3), 37.93 (4-CH_2), 38.97 (CH-4), 118.78 (=C-5), 125.46 (=CH-6), 126.31, 128.31, 129.30, 138.98 (C_6H_5), 168.17 (C=O). GC-MS (EI, 70eV): m/z = 215 (25), [M^+], 124 (100), 96 (11), 91 (9), 81 (13). HRMS (ESI-TOF): *m/z* calcd for $C_{14}H_{18}NO[M + H]^+$, 216.1388; found, 216.1386.

(*6RS*)-6-Benzyl-1,5-dimethyl-3,6-dihydropyridin-2(1*H*)-one (**1u-isomer-6**) (obtained as regioisomer):

Yield 70% (1.834 g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave colorless oil.

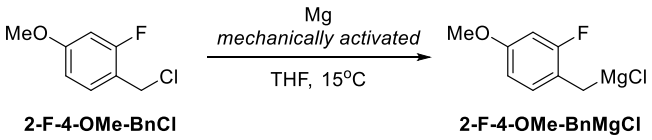


1u-isomer-6

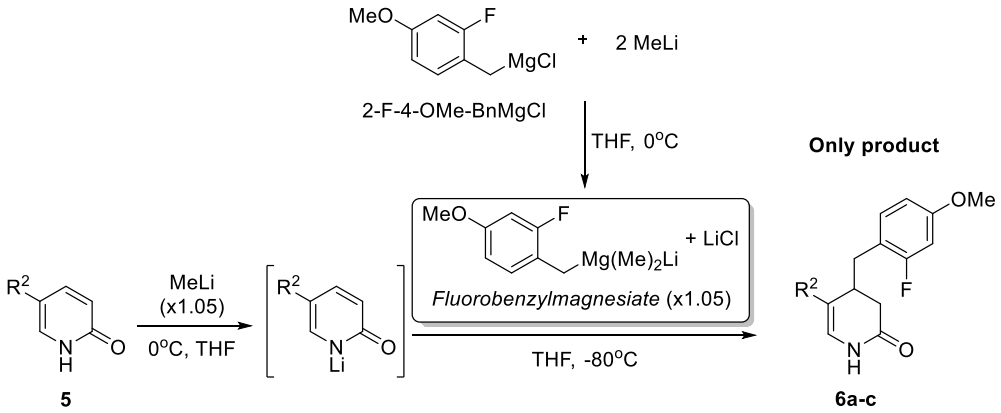
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.60 (dq, *J* = 21.2, 2.7 Hz, 1H, C<u>H</u>H-3), 1.84 (dt, *J* = 2.7, 1.4 Hz, 3H, 5-CH_3), 2.44 (ddt, *J* = 21.2, 5.2, 1.5 Hz, 1H, CH<u>H</u>-3), 2.84 (dd, *J* = 13.8, 3.4 Hz, 1H, 6-C<u>H</u>H), 3.05 (dd, *J* = 13.8, 4.8 Hz, 1H, 6-CH<u>H</u>), 3.07 (s, 3H, NCH_3), 3.91 (qd, *J* = 4.8, 3.4, 1.5 Hz, 1H, CH-6), 5.33 (dt, *J* = 5.2, 1.8 Hz, 1H, =CH-4), 6.97 – 7.04 (m, 2H, C_6H_5), 7.17 – 7.24 (m, 3H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.18 (5-CH_3), 31.91 (CH_2-3), 33.24 (NCH_3), 36.27 (6-CH_2), 65.22 (CH-6), 120.45 (=CH-4), 126.93, 128.08 (2C), 129.97 (2C, C_6H_5), 130.92 (=C-5), 135.41 (C_6H_5), 169.24 (C=O). GC-MS (EI, 70eV): m/z = 215 (<1)), [M^+], 124 (100), 96 (12), 81 (16). HRMS (ESI-TOF): *m/z* calcd for $C_{14}H_{18}NO[M + H]^+$, 216.1388; found, 216.1394.

5g. *Preparation of solution of (2-fluoro-4-methoxybenzyl)magnesium chloride*

Solution of (2-fluoro-4-methoxybenzyl)magnesium chloride (**2-F-4-OMe-BnMgCl**) was prepared[14] and titrated[15] according to the procedures described earlier.

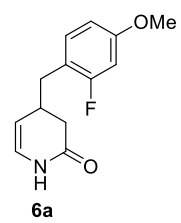


5h. Procedure 6. *Procedure for the synthesis of compounds* ***6a-c*** *via nucleophilic addition of fluorobenzylmagnesiate to NH 2-pyridones*



MeLi (1.7 mL, 5.25 mmol, 3.1M in DEM, 1.05 equiv) was added dropwise to the solution of **5** (5 mmol) in 15 mL of anhydrous THF at 0°C placed in the first Schlenk flask. Resulting suspension was stirred in this temperature for 15 min. Simultaneously, in the second Schlenk flask, MeLi (3.55 mL, 11 mmol, 3.1M in DEM, 2.2 equiv) was added to the solution of (2-fluoro-4-methoxybenzyl)magnesium chloride (55 mL, 5.5 mmol, 0.1 M in THF, 1.1 equiv,) at 0°C and resulting yellow complex was stirred for 10 min. Subsequently, magnesiate complex was transferred to a solution of lithiated **5** with a syringe and stirring was maintained for 2.5h while temperature was slowly raised from 0°C to room temperature. After this time, the mixture was cooled to 0°C, carefully quenched with saturated aqueous ammonium chloride (NH_4Cl, 15 mL) and then diluted with water (ca. 10 mL). The aqueous layer was extracted with ethyl acetate (3 x 70 mL), and the combined organic layers were dried with $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude products were purified by column chromatography on silica gel using the appropriate solvent mixtures to afford the desired products **6**.

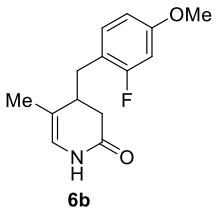
(4*RS*)-4-(2-Fluoro-4-methoxybenzyl)-3,4-dihydropyridin-2(1*H*)-one (**6a**):



6a

Yield 42% (0.568g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 61-63 °C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.32 (dd, *J* = 16.4, 8.6 Hz, 1H, C<u>H</u>H-3), 2.51 (dd, *J* = 16.4, 6.6 Hz, 1H, CH<u>H</u>-3), 2.62 (ddd, *J* = 13.5, 7.8, 1.0 Hz, 1H, 4-C<u>H</u>H), 2.70 (ddd, *J* = 13.5, 7.1, 1.0 Hz, 1H, 4-CH<u>H</u>), 2.73 – 2.83 (m, 1H, CH-4), 3.78 (s, 3H, OCH_3), 5.02 (ddd, *J* = 7.7, 3.8, 1.0 Hz, 1H, =CH-5), 6.06 (ddd, *J* = 7.7, 4.5, 1.5 Hz, 1H, =CH-6), 6.46 – 6.69 (m, 2H, CH-3', CH-5'), 7.04 (t, *J* = 8.6 Hz, 1H, CH-6'), 7.75 (s, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 32.69(CH-4), 33.20 (4-CH_2), 36.21 (CH_2-3), 55.54 (OCH_3), 101.64 (d, $^2J_{C\text{-}F}$ = 25.9 Hz, CH-3'), 109.21 (=CH-5), 109.69 (d, $^4J_{C\text{-}F}$ = 3.2 Hz, CH-5'), 117.58 (d, $^2J_{C\text{-}F}$ = 16.3 Hz, C-1'), 124.38 (=CH-6), 131.75 (d, $^3J_{C\text{-}F}$ = 6.9 Hz, CH-6'), 159.60 (d, *J* = 11.1 Hz, C-4'), 161.67 (d, $^3J_{C\text{-}F}$ = 244.4 Hz, C-2'), 171.23 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –115.66 ppm. GC-MS (EI, 70eV): m/z = 235 (1), [M^+], 139 (100), 96 (52). HRMS (ESI-TOF): *m/z* calcd for $C_{13}H_{15}FNO_2[M + H]^+$, 236.1087; found, 236.1089.

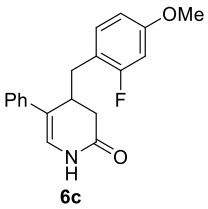
(4*RS*)-4-(2-Fluoro-4-methoxybenzyl)-5-methyl-3,4-dihydropyridin-2(1*H*)-one (**6b**):



6b

Yield 24% (0.169g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 131-133 °C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.68 (d, *J* = 1.6 Hz, 3H, 5-CH_3), 2.29 (dd, *J* = 16.0, 2.4 Hz, 1H, C<u>H</u>H-3), 2.37 – 2.43 (m, 1H, CH-4), 2.46 (d, *J* = 13.3 Hz, 1H, 4-C<u>H</u>H), 2.50 (dd, *J* = 16.3, 6.5 Hz, 1H, CH<u>H</u>-3), 2.84 (ddd, *J* = 13.3, 4.1, 0.9 Hz, 1H, CH<u>H</u>-3), 3.78 (s, 3H, OCH_3), 5.85 (dq, *J* = 4.6, 1.6 Hz, 1H, =CH-6), 6.53 – 6.68 (m, 2H, CH-3', CH-5'), 7.05 (t, *J* = 8.7 Hz, 1H, CH-6'), 7.68 (d, *J* = 4.3 Hz, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 18.20 (5-CH_3), 30.54 (4-CH_2), 34.69 (CH_2-3), 37.40 (CH-4), 55.53 (OCH_3), 101.65 (d, $^2J_{C\text{-}F}$ = 26.0 Hz, CH-3'), 109.59 (d, $^4J_{C\text{-}F}$ = 3.0 Hz, CH-5'), 117.81 (d, $^2J_{C\text{-}F}$ = 16.3 Hz, C-1'), 118.03 (=C-5), 119.38 (=CH-6), 132.04 (d, $^3J_{C\text{-}F}$ = 6.7 Hz, CH-6'), 159.62 (d, $^3J_{C\text{-}F}$ = 10.9 Hz, C-4'), 161.74 (d, $^1J_{C\text{-}F}$ = 244.9 Hz, C-2'), 170.38 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –116.06 ppm. GC-MS (EI, 70eV): m/z = 249 (5), [M^+], 139 (75), 110 (100), 82 (11). HRMS (ESI-TOF): *m/z* calcd for $C_{14}H_{16}FNO_2Na$ [M + Na]$^+$, 272.1063; found, 272.1060.

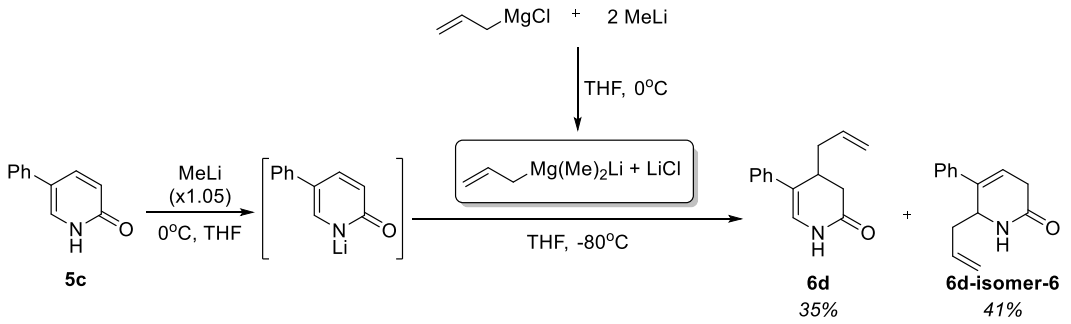
(4*RS*)-4-(2-Fluoro-4-methoxybenzyl)-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**6c**):



6c

Yield 70% (1.100g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 161-162 °C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.46 (dt, *J* = 16.4, 1.6 Hz, 1H, C<u>H</u>H-3), 2.54 (dd, *J* = 13.9, 10.7 Hz, 1H, 4-C<u>H</u>H), 2.62 (dd, *J* = 16.4, 6.5 Hz, 1H, CH<u>H</u>-3), 2.97 (dd, *J* = 13.9, 4.1 Hz, 1H, 4-CH<u>H</u>), 3.16 (dddd, *J* = 10.7, 6.5, 4.1, 1.6 Hz, 1H, CH-4), 3.76 (s, 3H, OCH_3), 6.56 – 6.65 (m, 3H, =CH-6, CH-3', CH-5'), 7.06 (t, *J* = 8.8 Hz, 1H, CH-6'), 7.19 – 7.27 (m, 1H, C_6H_5), 7.36 (dd, *J* = 8.5, 7.0 Hz, 2H, C_6H_5), 7.41 – 7.47 (m, 2H, C_6H_5), 8.32 (d, *J* = 4.8 Hz, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 30.94 (CH_2-3), 34.19 (4-CH_2), 34.84 (CH-4), 55.54 (OCH_3), 101.73 (d, $^2J_{C\text{-}F}$ = 26.0 Hz, CH-3'), 109.64 (d, $^4J_{C\text{-}F}$ = 3.4 Hz, CH-5'), 117.35 (d, $^2J_{C\text{-}F}$ = 16.8 Hz, C-1'), 120.93 (=CH-6), 121.37 (=C-5), 124.60, 126.76, 128.80 (C_6H_5), 132.33 (d, $^3J_{C\text{-}F}$ = 7.1 Hz, CH-6'), 136.93 (C_6H_5), 159.73 (d, $^3J_{C\text{-}F}$ = 11.0 Hz, C-4'), 161.79 (d, $^1J_{C\text{-}F}$ = 244.9 Hz, C-2'), 170.75 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –115.21 ppm. GC-MS (EI, 70eV): m/z = 311 (21), [M^+], 172 (100), 171 (34), 145 (12), 139 (52), 115 (11). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}FNO_2[M + H]^+$, 312.1400; found, 312.1395.

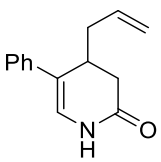
5i. Procedure 7: *Procedure for the synthesis of compounds* ***6d*** *and* ***6d-isomer-6*** *via nucleophilic addition of allylmagnesiate to NH 2-pyridones*



To a cooled and stirred solution of 5-phenylpyridine-2(1*H*)-one **5c** (1.5g, 8.76 mmol) in dry THF (30 mL) at 0°C 2.97 mL (9.2 mmol), MeLi solution (3.1 M in DEM) was added from a syringe over 5 min under argon. The resulting white suspension was stirred at 0°C for 30 min. Simultaneously, in a second Schlenk flask MeLi (3.1 M in DEM, 7.12 mL, 22.08 mmol, 2.5 equiv.) was added from a syringe at 0°C over 5 min to the solution of AllMgCl (5.52 mL, 11.04 mmol, 2.0 M in THF, 1.25 equiv.) in 30 mL of anhydrous THF and resulting solution of yellow complex was stirred for 5 min. Subsequently, the suspension containing the lithium allyldimethylmagnesate was transferred to the solution of lithiated 5-phenylpyridine-2*(1H)*-one

via syringe. The resulting brown-orange solution was stirred for 3h at 0°C. After careful quenching with aqueous saturated NH_4Cl (20 mL) reaction mixture was extracted with ethyl acetate (3x100 mL) and the combined organic layers were dried over $MgSO_4$. Filtration, concentration in vacuo, and purification by column chromatography yielded **6d** and **6d-isomer-6** as white solids.

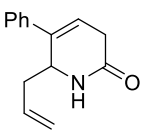
(4*RS*)-4-Allyl-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**6d**):



6d

Yield 35% (0.6473g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 99-101 °C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (dddt, *J* = 14.1, 9.2, 8.1, 1.0 Hz, 1H, 4-C<u>H</u>H), 2.31 (dt, *J* = 14.3, 6.1, 4.5 Hz, 1H, 4-CH<u>H</u>), 2.64 (ddd, *J* = 16.4, 2.5, 0.9 Hz, 1H, C<u>H</u>H-3), 2.72 (dd, *J* = 16.5, 6.8 Hz, 1H, CH<u>H</u>-3), 2.99 (dddd, *J* = 9.2, 6.8, 4.5, 2.5 Hz, 1H, CH-4), 5.05 – 5.15 (m, 2H, $=CH_2$), 5.74 (dddd, *J* = 16.7, 10.1, 8.0, 6.3 Hz, 1H, =CH), 6.50 (d, *J* = 4.8 Hz, 1H, =CH), 7.19 – 7.28 (m, 1H, C_6H_5), 7.31 – 7.40 (m, 4H, C_6H_5), 7.69 (s, 1H. NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 33.87 (CH-4), 34.60 (CH_2-3), 36.51 (4-CH_2), 118.11 ($=CH_2$), 120.92 (=CH-6), 121.28 (=C-5), 124.97, 126.81, 128.76 (C_6H_5), 134.71 (=CH), 137.28 (C_6H_5), 170.69 (C=O). GC-MS (EI, 70eV): m/z = 213 (2), [M^+], 172 (100), 145 (14), 143 (8), 127 (13), 117 (10), 115 (19), 91 (5). HRMS (ESI-TOF): *m/z* calcd for $C_{14}H_{16}NO[M + H]^+$, 214.1232; found, 214.1230.

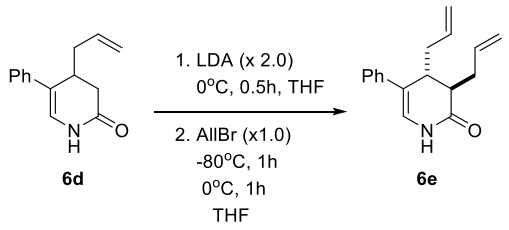
(6*RS*)-6-Allyl-5-phenyl-3,6-dihydropyridin-2(1*H*)-one (**6d-isomer-6**):



6d-isomer-6

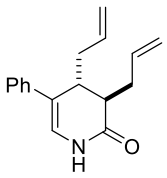
Yield 41% (0.763g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 90-92°C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.17 (dt, *J* = 14.3, 7.3 Hz, 1H, 6-C<u>H</u>H), 2.31 – 2.41 (m, 1H, 6-CH<u>H</u>), 3.08 (t, *J* = 3.8 Hz, 2H, CH_2-3), 4.63 (dp, *J* = 7.0, 3.6 Hz, 1H, CH-6), 5.05 (dq, *J* = 17.0, 1.6 Hz, 1H, =C<u>H</u>H), 5.12 (dd, *J* = 10.2, 1.9 Hz, 1H, =CH<u>H</u>), 5.72 (dddd, *J* = 17.0, 10.2, 7.3, 6.3 Hz, 1H, =CH), 5.93 (t, *J* = 3.8 Hz, 1H, =CH-4), 7.28 – 7.40 (m, 6H, C_6H_5, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 31.94 (CH_2-3), 39.85 (6-CH_2), 54.98 (CH-6), 119.73 ($=CH_2$), 120.42 (=CH-4), 126.35, 127.89, 128.72 (C_6H_5), 132.28 (=CH), 136.18 (=C-5), 138.26 (C_6H_5), 170.32 (C=O). GC-MS (EI, 70eV): m/z = 213 (1), [M^+], 172 (100), 145 (14), 143 (8), 127 (14), 117 (11), 115 (20), 91 (5). HRMS (ESI-TOF): *m/z* calcd for $C_{14}H_{16}NO[M + H]^+$, 214.1232; found, 214.1235.

5j. Procedure 8: *C3-Allylation of compound* ***6d***



Commercially available (Sigma-Aldrich) 2.0 M solution of LDA in THF/heptane/ethylbenzene (2.25 mL, 4.5 mmol, 2.0 equiv.) was added dropwise to a solution of **6d** (0.480g, 2.25 mmol) in dry THF (10 mL) under argon, prepared in a Schlenk flask and cooled to 0°C. The mixture was stirred at 0°C for 0.5h. After this time, reaction flask was transferred to -80°C bath and allyl bromide (0.272g, 2.25 mmol, 1.0 equiv.) was added dropwise for ca. 5 min and the reaction mixture was stirred for 1h at -80°C and 1h at 0°C. Subsequently reaction mixture was carefully quenched with saturated aqueous NH_4Cl (10 mL), then was allowed to warm up to rt and was diluted with water (ca. 10 mL). The aqueous layer was extracted with ethyl acetate (3×60 mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using *n*-hexane/ethyl acetate (1:3) to give product **6e** as a pale yellow oil.

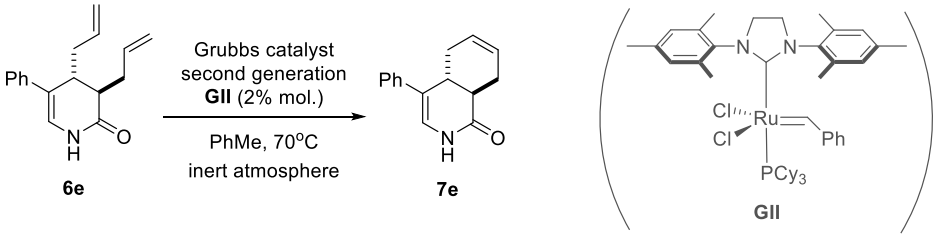
(3*RS*,4*RS*)-3,4-Diallyl-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**6e**):



6e

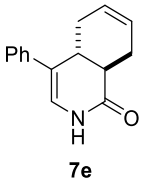
Yield 65% (0.368g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.14 (dt, *J* = 14.3, 8.7 Hz, 1H, 4-C<u>H</u>H), 2.22 – 2.36 (m, 2H, 4-CH<u>H</u>, 3-C<u>H</u>H), 2.47 (dtt, *J* = 14.2, 5.6, 1.6 Hz, 1H, 3-CH<u>H</u>), 2.62 (ddt, *J* = 9.6, 5.5, 1.2 Hz, 1H, CH-3), 2.86 (ddt, *J* = 9.6, 4.4, 1.0 Hz, 1H, CH-4), 5.01 – 5.16 (m, 4H, two =CH2), 5.68 (dddd, *J* = 16.5, 10.1, 8.1, 6.1 Hz, 1H, =CH), 5.81 (dddd, *J* = 17.0, 10.1, 8.5, 5.7 Hz, 1H, =CH), 6.48 (d, *J* = 4.7 Hz, 1H, =CH-6), 7.21 – 7.29 (m, 1H, C_6H_5), 7.34 (d, *J* = 4.3 Hz, 4H, C_6H_5), 8.25 (d, *J* = 4.8 Hz, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.82 (3-CH_2), 36.57 (4-CH_2), 37.98 (CH-4), 44.32 (CH-3), 117.88, 117.93 (two =CH_2), 119.86 (=C-5), 120.06 (=CH-6), 125.18, 126.84, 128.75 (C_6H_5), 134.72, 135.18 (two =CH), 137.78 (C_6H_5), 173.28 (C=O). GC-MS (EI, 70eV): m/z = 253 (9), [M^+], 212 (100), 171 (63), 143 (21), 115 (18). HRMS (ESI-TOF): *m/z* calcd for $C_{17}H_{20}NO[M + H]^+$, 254.1545; found, 254.1550.

5k. Procedure 9: *Procedure for the synthesis of* ***7e*** *via RCM*



To a solution of 3,4-diallyl-5-phenyl-3,4-dihydropyridin-2(1*H*)-one **6e** (0.33g, 1.3mmol) in dry, degassed toluene (10 mL) Grubbs catalyst **GII** was added and the reaction mixture was vigorously stirred under slowly passing stream of argon at 70°C for 2h. After this time toluene was evaporated at reduced pressure, and the residue was left standing for 48 h followed by crystallization from ethyl acetate. The product **7e** was obtained as a white solid in 80% yield.

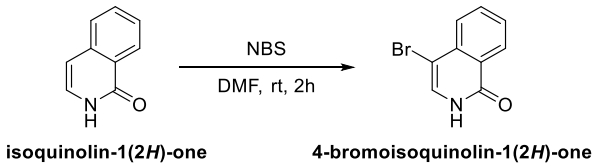
(4a*RS*,8a*RS*)-4-phenyl-4a,5,8,8a-tetrahydroisoquinolin-1(2*H*)-one (**7e**):



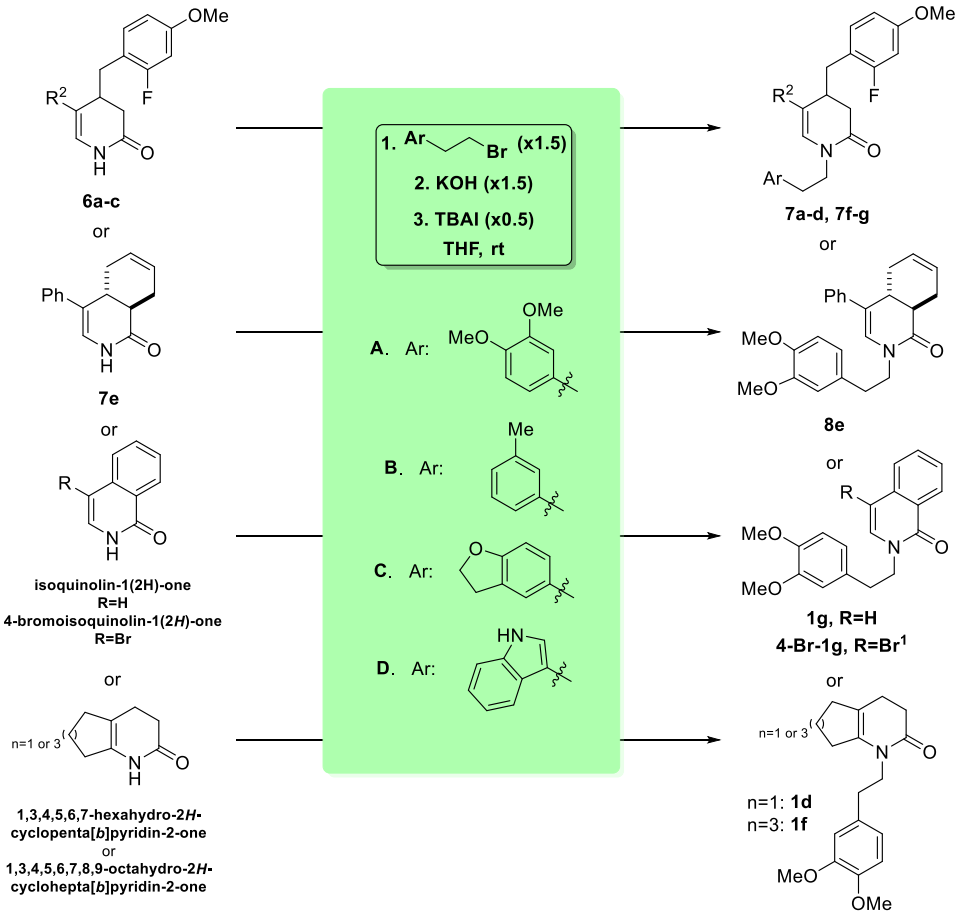
Yield 80% (0.236g). The crude product purified by crystallization from ethyl acetate gave white solid, mp 246-248 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.50 – 1.70 (m, 1H, C<u>H</u>H-5), 2.10 (ddt, *J* = 17.7, 11.3, 4.5, 2.2 Hz, 1H, C<u>H</u>H-8), 2.32 (dt, *J* = 17.4, 5.9, 5.1 Hz, 1H, CH<u>H</u>-5), 2.37 – 2.43 (m, 2H, CH<u>H</u>-8, CH-4a), 2.97 (dddd, *J* = 14.1, 11.3, 5.0, 2.5 Hz, 1H, CH-8a), 5.57 – 5.66 (m, 1H, =CH-6), 5.68 – 5.77 (m, 1H, =CH-7), 6.09 (dd, *J* = 4.9, 2.6 Hz, 1H, =CH-3), 7.05 – 7.27 (m, 3H, C_6H_5), 7.27 – 7.44 (m, 2H, C_6H_5), 9.36 (d, *J* = 4.9 Hz, 1H, NH). ^{13}C NMR (101 MHz, DMSO-d_6) δ 26.37 (CH_2-8), 31.21 (CH_2-5), 34.10 (CH-4a), 40.43 (CH-8a), 120.35 (=C-4), 123.11 (=CH-3), 125.78, 125.92, 125.98 (=CH-6, =CH-7, C_6H_5), 126.90, 127.98, 138.36 (C_6H_5), 170.27 (C=O). GC-MS (EI, 70eV): m/z = 225 (96), [M^+], 208 (11), 196 (17), 184 (14), 171 (100), 170 (21), 143 (37), 128 (11), 115 (28), 91 (12), 77 (16). HRMS (ESI-TOF): *m/z* calcd for $C_{15}H_{16}NO[M + H]^+$, 226.1232; found, 226.1239.

5l. *Synthesis of 4-bromoisoquinolin-1(2H)-one from isoquinolin-1(2H)-one*

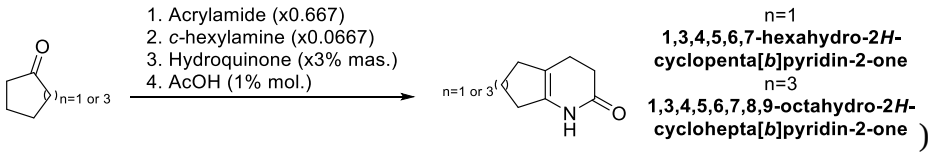
4-Bromoisoquinolin-1(2*H*)-one was prepared according to the procedures described earlier.[16]



5m. Procedure 10: *Procedure for the synthesis of compounds* ***7a-f****,* ***8e****,* ***1d****,* ***1f*** *and* ***1g-h*** *through N-alkylation*



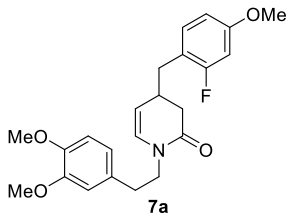
(Note: compounds: 1,3,4,5,6,7-hexahydro-2*H*-cyclopenta[b]pyridin-2-one and 1,3,4,5,6,7,8,9-octahydro-2*H*-cyclohepta[b]pyridin-2-one were prepared according to the procedure described earlier.[17]



(2-Bromoethyl)-aryl derivatives **A-D** (1.5 mmol, 1.5 equiv.), TBAI (0.5 mmol, 0.185g, 0.5 equiv.) and KOH (1.5 mmol, 0.084g, 1.5 equiv.) were added to the solution of enamide: **6a-c**, **6e**, isoquinolin-1(2*H*)-one, 4-bromoisoquinolin-1(2*H*)-one, 1,3,4,5,6,7-hexahydro-2*H*-cyclopenta[b]pyridin-2-one or 1,3,4,5,6,7,8,9-octahydro-2*H*-cyclohepta[b]pyridin-2-one (1

mmol) in dry THF (6 mL) in a Schlenk flask at room temperature under argon and the mixture was stirred for 3-72h was. After full conversion of substrate (checked by GC-MS) aqueous saturated sodium bicarbonate (10 mL) was added and the mixture was stirred for another 5 min and then diluted with water (ca. 10 mL). The aqueous layer was extracted with ethyl acetate (3×60 mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using appropriate mixture of *n*-hexane/ethyl acetate to give desired products.

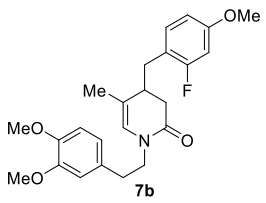
(4*RS*)-1-(3,4-Dimethoxyphenethyl)-4-(2-fluoro-4-methoxybenzyl)-3,4-dihydropyridin-2(1*H*)-one (**7a**):



7a

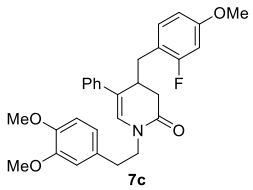
Yield 77% (0.508g, reaction time: 24h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave orange thick oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.31 (dd, *J* = 16.0, 8.8 Hz, 1H, C<u>H</u>H-3), 2.44 – 2.66 (m, 3H, CH<u>H</u>-3, 4-CH_2), 2.66 – 2.72 (m, 1H, CH-4), 2.78 (t, *J* = 7.4 Hz, 2H, CH_2), 3.57 – 3.71 (m, 2H, NCH_2), 3.76 (s, 3H, OCH_3), 3.84 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 4.97 (dd, *J* = 7.8, 3.8 Hz, 1H, =CH-5), 5.86 (dd, *J* = 7.8, 1.5 Hz, 1H, =CH-6), 6.53 – 6.65 (m, 2H, CH-3', CH-5'), 6.69 – 6.75 (m, 2H, ArH), 6.76 – 6.81 (m, 1H, ArH), 6.98 (t, *J* = 8.6 Hz, 1H, CH-6'). ^{13}C NMR (101 MHz, $CDCl_3$) δ 32.81 (CH-4), 33.03 (4-CH_2), 34.41 (CH_2), 37.14 (CH_2-3), 47.84 (NCH_2), 55.49, 55.83, 55.85 (three OCH_3), 101.59 (d, $^2J_{C\text{-}F}$ = 25.9 Hz), 109.62 (d, $^4J_{C\text{-}F}$ = 3.0 Hz, CH-5'), 109.77 (=CH-5), 111.25, 112.10 (ArH), 117.57 (d, $^2J_{C\text{-}F}$ = 16.4 Hz, C-1'), 120.83 (ArH), 129.56 (=CH-6), 131.11 (Ar), 131.72 (d, $^3J_{C\text{-}F}$ = 6.7 Hz, CH-6'*J* = Hz), 147.63, 148.87 (Ar), 159.57 (d, $^3J_{C\text{-}F}$ = 10.9 Hz, C-4'), 161.61 (d, $^1J_{C\text{-}F}$ = 244.9 Hz, C-2'), 168.71 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –115.55 ppm. GC-MS (EI, 70eV): m/z = 399 (3), [M^+], 260 (37), 165 (100), 164 (37), 150 (12), 139 (20). HRMS (ESI-TOF): *m/z* calcd for $C_{23}H_{27}FNO_4$[M + H]$^+$, 400.1924; found, 400.1921.

(4*RS*)-1-(3,4-Dimethoxyphenethyl)-4-(2-fluoro-4-methoxybenzyl)-5-methyl-3,4-dihydropyridin-2(1*H*)-one (**7b**):



Yield 82% (0.164g, reaction time: 24h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.65 (d, *J* = 1.5 Hz, 3H, CH_3), 2.19 – 2.40 (m, 3H, C<u>H</u>H-3, CH-4, 4-C<u>H</u>H), 2.44 – 2.56 (m, 1H, CH<u>H</u>-3), 2.65 – 2.81 (m, 3H, CH_2, 4-CHH), 3.41 (ddd, *J* = 13.4, 8.2, 6.7 Hz, 1H, NC<u>H</u>H), 3.76 (s, 3H, OCH_3), 3.77 – 3.84 (m, 1H, NCH<u>H</u>), 3.85 (s, 3H, OCH_3), 3.88 (s, 3H, OCH_3), 5.72 (q, *J* = 1.5 Hz, 1H, =CH-6), 6.55 – 6.64 (m, 2H, CH-3', CH-5'), 6.73 – 6.84 (m, 3H, ArH), 6.93 – 7.00 (m, 1H, CH-6') ^{13}C NMR (101 MHz, $CDCl_3$) δ 18.36 (CH_3), 30.56 (4-CH_2), 34.34 (CH_2), 35.74 (CH_2-3), 37.43 (CH-4), 47.45 (NCH_2), 55.53, 55.89, 55.92 (three OCH_3), 101.62 (d, $^2J_{C\text{-}F}$ = 26.0 Hz, CH-3'), 109.54 (d, $^4J_{C\text{-}F}$ = 3.3 Hz, CH-5'), 111.25, 112.09 (ArH), 117.79 (d, $^2J_{C\text{-}F}$ = 16.2 Hz, C-1'), 119.00 (=C-5), 120.82 (ArH), 124.36 (=CH-6), 131.19 (Ar), 132.05 (d, $^3J_{C\text{-}F}$ = 6.7 Hz, CH-6'), 147.63, 148.92 (Ar), 159.60 (d, $^3J_{C\text{-}F}$ = 10.9 Hz, C-4'), 161.71 (d, $^1J_{C\text{-}F}$ = 244.9 Hz, C-2'), 167.76 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –116.03 ppm. GC-MS (EI, 70eV): m/z = 413 (2), [M^+], 274 (52), 165 (100), 164 (24), 150 (13), 139 (19), 94 (8). HRMS (ESI-TOF): *m/z* calcd for $C_{24}H_{29}FNO_4$[M + H]$^+$, 414.2081; found, 414.2085.

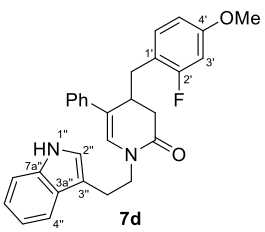
(4*RS*)-1-(3,4-Dimethoxyphenethyl)-4-(2-fluoro-4-methoxybenzyl)-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**7c**):



Yield 98% (0.837g, reaction time: 16h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave red semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.32 (dd, *J* = 13.9, 10.6 Hz, 1H, 4-C<u>H</u>H), 2.46 (dd, *J* = 16.3, 2.1 Hz, 1H, C<u>H</u>H-3), 2.56 (dd, *J* = 16.3, 6.5 Hz, 1H, CH<u>H</u>-3), 2.81 – 2.91 (m, 3H, CH_2, 4-CH<u>H</u>), 3.01 – 3.10 (m, 1H, CH-4), 3.55 (dt, *J* = 13.5, 7.3, 6.3 Hz, 1H, NC<u>H</u>H), 3.76 (s, 3H, OCH_3), 3.83 (s, 3H, OCH_3), 3.87 (s, 3H, OCH_3), 4.08 (dt, *J* = 13.5, 7.7 Hz, 1H, NCH<u>H</u>), 6.36 (s, 1H, =CH-6), 6.55 – 6.63 (m, 2H, CH-3', CH-5'), 6.76 – 6.82 (m, 3H, CH-2", CH-5", CH-6"), 6.94 (t, *J* = 8.8 Hz, 1H, CH-6'), 7.18 – 7.25 (m, 1H, C_6H_5), 7.30 – 7.36 (m, 4H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 30.90 (4-CH_2), 34.71 (CH_2), 34.95 (CH-4), 35.08 (CH-3), 47.90 (NCH_2), 55.54, 55.90, 55.93 (three OCH_3), 101.71 (d, $^2J_{C\text{-}F}$ = 25.9 Hz, CH-3'), 109.55 (d, $^4J_{C\text{-}F}$ = 3.0 Hz, CH-5'), 111.34, 112.17 (CH-2", CH-5"), 117.35 (d, $^2J_{C\text{-}F}$ = 16.4 Hz, C-1'), 121.01 (CH-6"), 121.90 (=C-5), 124.56 (C_6H_5), 126.01 (=CH-6), 126.69, 128.73 (C_6H_5), 130.92 (C-1"), 132.35 (d, $^3J_{C\text{-}F}$ = 6.9 Hz, CH-6'), 137.04 (C_6H_5), 147.77, 149.03 (C-3", C-4"), 159.67 (d, $^3J_{C\text{-}F}$ = 11.1 Hz, C-4'), 161.72 (d, $^1J_{C\text{-}F}$ = 244.5 Hz, C-2'), 168.02 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –115.30 ppm. GC-MS

(EI, 70eV): m/z = 475 (8), [M^+], 336 (62), 165 (100), 156 (9), 150 (15), 139 (19). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{31}FNO_4[M + H]^+$, 476.2237; found, 476.2230.

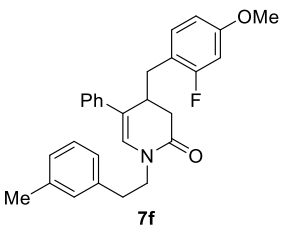
(4*RS*)-1-(2-(1*H*-Indol-3-yl)ethyl)-4-(2-fluoro-4-methoxybenzyl)-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**7d**):



7d

Yield 63% (0.229g, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 10:1) gave pale brown solid, mp 74-76°C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.35 (dd, *J* = 13.9, 10.5 Hz, 1H, 4-C<u>H</u>H), 2.47 (dd, *J* = 16.3, 2.2 Hz, 1H, C<u>H</u>H-3), 2.57 (dd, *J* = 16.3, 6.5 Hz, 1H, CH<u>H</u>-3), 2.81 (dd, *J* = 13.9, 4.2 Hz, 1H, 4-CH<u>H</u>), 2.97 – 3.07 (m, 1H, CH-4), 3.10 (td, *J* = 7.3, 2.7 Hz, 2H, CH_2), 3.64 – 3.73 (m, 1H, NC<u>H</u>H), 3.74 (s, 3H, OCH_3), 4.12 (dt, *J* = 13.6, 7.3 Hz, 1H, NCH<u>H</u>), 6.29 (s, 1H, =CH-6), 6.52 – 6.64 (m, 2H, CH-3', CH-5'), 6.93 (t, *J* = 8.4 Hz, 1H, CH-6'), 7.05 (d, *J* = 2.3 Hz, 1H, CH-2"), 7.11 – 7.30 (m, 7H, C_6H_5, CH-5", CH-6"), 7.37 (dd, *J* = 7.9, 1.1 Hz, 1H, CH-7"), 7.71 (d, *J* = 7.5 Hz, 1H, CH-4"), 8.14 (s, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 24.80 (CH_2), 30.78 (4-CH_2), 34.89 (CH-4), 35.11 (CH_2-3), 47.02 (NCH_2), 55.53 (OCH_3), 101.67 (d, $^2J_{C-F}$ = 25.7 Hz, CH-3'), 109.57 (d, $^4J_{C-F}$ = 2.9 Hz, CH-5'), 111.31 (CH-7"), 112.50 (C-3"), 117.42 (d, $^2J_{C-F}$ = 16.6 Hz, C-1'), 118.83 (CH-4"), 119.55 (CH-5"), 121.38 (=C-5), 122.12 (CH-6"), 122.51 (CH-2"), 124.57 (C_6H_5), 126.36 (=CH-6), 126.52 (C_6H_5), 127.33 (C-3"), 128.64 (C_6H_5), 132.32 (d, $^3J_{C-F}$ = 6.7 Hz, CH-6'), 136.43 (C-7a"), 137.04 (C_6H_5), 159.63 (d, $^3J_{C-F}$ = 10.8 Hz, C-4'), 161.72 (d, $^1J_{C-F}$ = 244.5 Hz, C-2'), 168.12 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –115.39 ppm. GC-MS (EI, 70eV): m/z = 454 (4), [M^+], 315 (14), 207 (7), 172 (8), 144 (100), 143 (33), 139 (15), 130 (10), 115 (6). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{27}FN_2O_2Na$ [M + Na]$^+$, 477.1954; found, 477.1944.

(4*RS*)-4-(2-Fluoro-4-methoxybenzyl)-1-(3-methylphenethyl)-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**7f**):

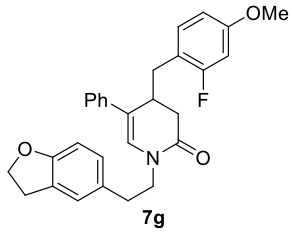


7f

Yield 83% (0.275g, reaction time: 24h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave pale yellow thick oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.31 (s, 3H, CH_3), 2.33 (dd, *J* = 13.9, 10.7 Hz, 1H, 4-C<u>H</u>H), 2.46 (dd, *J* = 16.3, 2.1 Hz, 1H, CHH-3), 2.56 (dd, *J* = 16.3, 6.5 Hz, 1H, CHH-3), 2.81 – 2.92 (m, 3H, 4-CHH, CH_2), 3.05 (dddd, *J* = 10.7, 6.5, 4.1, 2.1 Hz, 1H, CH-4), 3.54 (dt, *J* = 13.5,

7.3 Hz, 1H, NCHH), 3.75 (s, 3H, OCH_3), 4.09 (dt, *J* = 13.5, 7.5 Hz, 1H, NCHH), 6.32 (s, 1H, =CH-6), 6.53 – 6.65 (m, 2H, C-1', C-5'), 6.95 (t, *J* = 8.8 Hz, 1H, CH-6'), 7.01 – 7.11 (m, 3H, ArH), 7.16 – 7.25 (m, 2H, ArH), 7.29 – 7.36 (m, 4H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.34 (CH_3), 30.81 (CH_2), 34.93 (CH-4), 35.06 (CH_2-3, 4-CH_2), 48.02 (NCH_2), 55.53 (OCH_3), 101.69 (d, $^2J_{C\text{-}F}$ = 25.8 Hz, CH-3'), 109.54 (d, $^4J_{C\text{-}F}$ = 2.9 Hz, CH-5'), 117.42 (d, $^2J_{C\text{-}F}$ = 16.2 Hz, C-1'), 121.72 (=C-5), 124.61, 126.00 (ArH), 126.15 (=CH-6), 126.63, 127.31, 128.52, 128.68, 129.92 (ArH), 132.39 (d, $^3J_{C\text{-}F}$ = 6.9 Hz, CH-6'), 137.08, 138.17, 138.37 (Ar), 159.66 (d, $^3J_{C\text{-}F}$ = 11.0 Hz, C-4'), 161.73 (d, $^1J_{C\text{-}F}$ = 245.1 Hz, C-2'), 168.01 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –115.26 ppm. GC-MS (EI, 70eV): m/z = 429 (7), [M^+], 290 (100), 172 (14), 156 (11), 139 (17), 119 (90), 117 (14), 91 (17), 77 (5). HRMS (ESI-TOF): *m/z* calcd for $C_{28}H_{29}FNO_2$ [M + H]$^+$, 430.2182; found, 430.2178.

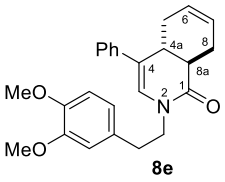
(4*RS*)-1-(2-(2,3-Dihydrobenzofuran-5-yl)ethyl)-4-(2-fluoro-4-methoxybenzyl)-5-phenyl-3,4-dihydropyridin-2(1*H*)-one (**7g**):



7g

Yield 88% (0.260g, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave red semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.35 (dd, *J* = 13.8, 10.6 Hz, 1H, 4-C<u>H</u>H), 2.45 (dd, *J* = 16.3, 2.1 Hz, 1H, C<u>H</u>H-3), 2.56 (dd, *J* = 16.3, 6.5 Hz, 1H, CH<u>H</u>-3), 2.76 – 2.91 (m, 3H, <u>CH_2</u>CH_2N, 4-CH<u>H</u>), 3.05 (dddd, *J* = 10.6, 6.5, 4.0, 2.1 Hz, 1H, CH-4), 3.14 (t, *J* = 8.7 Hz, 2H, <u>CH_2</u>CH_2O), 3.50 (dt, *J* = 13.5, 7.3 Hz, 1H, NC<u>H</u>H), 3.76 (s, 3H, OCH_3), 4.06 (dt, *J* = 13.5, 7.3 Hz, 1H, NCH<u>H</u>), 4.51 (t, *J* = 8.7 Hz, 2H, OCH_2), 6.33 (s, 1H, =CH-6), 6.55 – 6.64 (m, 2H, CH-3', CH-5'), 6.73 (d, *J* = 8.1 Hz, 1H, CH-3"), 6.94 (d, *J* = 8.4 Hz, 1H, CH-6'), 6.99 (dd, *J* = 8.1, 1.7 Hz, 1H, CH-2"), 7.10 (d, *J* = 1.7 Hz, 1H, CH-6'"), 7.18 – 7.25 (m, 1H, C_6H_5), 7.28 – 7.36 (m, 4H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 29.72 (<u>CH_2</u>CH_2O), 30.81 (4-CH_2), 34.58 (<u>CH_2</u>CH_2N), 34.94 (CH-4), 35.06 (CH_2-3), 48.35 (NCH_2), 55.55 (OCH_3), 71.22 (OCH_2), 101.71 (d, $^2J_{C\text{-}F}$ = 26.0 Hz, CH-3'), 109.25 (CH-3"), 109.56 (d, $^4J_{C\text{-}F}$ = 3.0 Hz, CH-5'), 117.42 (d, $^2J_{C\text{-}F}$ = 16.5 Hz, C-1'), 121.65 (=C-5), 124.58 (C_6H_5), 125.70 (CH-6"), 126.19 (=CH-6), 126.65 (C_6H_5), 127.27 (C-5"), 128.47 (CH-2"), 128.72 (C_6H_5), 130.32 (C-1"), 132.36 (d, $^3J_{C\text{-}F}$ = 7.0 Hz, CH-6'), 137.10 (C_6H_5), 158.88 (C-4"), 159.68 (d, $^3J_{C\text{-}F}$ = 11.0 Hz, C-4'), 161.73 (d, $^1J_{C\text{-}F}$ = 244.5 Hz, C-2'), 168.01 (C=O). ^{19}F NMR (376.6 MHz, $CDCl_3$) δ = –115.32 ppm. GC-MS (EI, 70eV): m/z = 457 (7), [M^+], 318 (44), 147 (100), 146 (21), 91 (10). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{29}FNO_3$[M + H]$^+$, 458.2131; found, 458.2132.

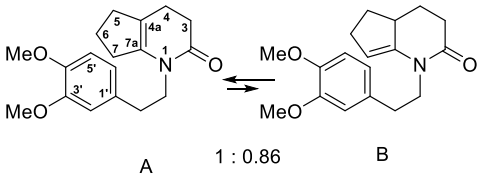
(4a*RS*,8a*RS*)-2-(3,4-dimethoxyphenethyl)-4-phenyl-4a,5,8,8a-tetrahydroisoquinolin-1(2*H*)-one (**8e**):



8e

Yield 80% (0.1384g, reaction time: 24h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.61 – 1.73 (m, 1H, CH<u>H-5$_{ax}$</u>), 2.27 (dddt, *J* = 15.9, 11.2, 4.7, 2.3 Hz, 1H, CH<u>H-8$_{ax}$</u>), 2.33 – 2.40 (m, 1H, CH<u>H-5$_{eq}$</u>), 2.51 (ddd, *J* = 14.4, 11.2, 5.0 Hz, 1H, CH-8a), 2.64 – 2.74 (m, 1H, CH<u>H-8$_{eq}$</u>), 2.77 – 2.90 (m, 2H, CH_2), 2.95 (dddd, *J* = 14.2, 11.4, 5.1, 2.6 Hz, 1H, CH-4a), 3.65 – 3.80 (m, 2H, NCH_2), 3.85 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 5.55 – 5.68 (m, 1H, =CH-6), 5.68 – 5.81 (m, 1H, =CH-7), 5.91 (d, *J* = 2.6 Hz, 1H, =CH-3), 6.71 – 6.84 (m, 3H, C_6H_3), 7.06 – 7.14 (m, 2H, C_6H_5), 7.20 – 7.36 (m, 3H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 27.00 (CH_2-8), 31.47 (CH_2-5), 34.56 (CH_2), 34.73 (CH-4a), 41.62 (CH-8a), 48.67 (NCH_2), 55.88, 55.93 (two OCH_3), 111.34, 112.18, 120.88 (C_6H_3), 123.03 (=C-4), 125.60 (=CH-6), 126.13 (=CH-7), 126.63, 127.29 (C_6H_5), 127.59 (=CH-3), 128.18 (C_6H_5), 131.12 (C_6H_3), 138.25 (C_6H_5), 147.69, 148.96 (C_6H_3), 170.10 (C=O). GC-MS (EI, 70eV): m/z = 389 (22), [M^+], 225 (16), 210 (13), 171 (13), 164 (100), 156 (21), 151 (10), 115 (6), 91 (9), 77 (7). HRMS (ESI-TOF): *m/z* calcd for $C_{25}H_{28}NO_3$[M + H]$^+$, 390.2069; found, 390.2059. HRMS (ESI-TOF): *m/z* calcd for $C_{25}H_{27}NO_3Na$[M + Na]$^+$, 412.1889, found, 412.1887.

1-(3,4-dimethoxyphenethyl)-1,3,4,5,6,7-hexahydro-2*H*-cyclopenta[b]pyridin-2-one (**1d-A**),
1-(3,4-dimethoxyphenethyl)-1,3,4,4a,5,6-hexahydro-2*H*-cyclopenta[b]pyridin-2-one (**1d-B**)[18]:

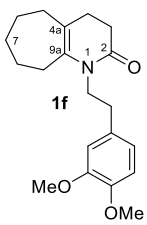


1d

Yield 55% (0.606g, reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.39 – 1.58 (m, 1.92H, two C<u>H</u>H, B), 1.81 – 1.95 (m, 2H, CH_2, A), 1.95 – 2.03 (m, 0.86H, CH<u>H</u>, B), 2.12 – 2.27 [m, 2.86H, CH_2 (A), CH<u>H</u> (B], 2.29 – 2.42 [m, 5.92H, two CH_2 (A), CH_2 (B)], 2.43 – 2.64 [m, 3.92H, CH_2 (A), CH2 (B)], 2.72 – 2.85 [m, 4.58H, CH-4a (B), NCH_2<u>CH_2</u> (A), NCH_2<u>CH_2</u> (B)], 3.63 – 3.69 (m, 2H, NCH_2, A), 3.72 – 3.92 [m, 12.88H, NCH_2 (B), two OCH_3 (A), two OCH_3 (B)], 4.88 (q, *J* = 2.4 Hz, 0.86H, =CH-7, B), 6.69 – 6.83 [m, 5.58H, three CH (A), three CH (B)]. ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.10 (CH_2, A), 21.73 (CH_2, A), 26.99 (CH_2, B), 30.04 (CH_2), 30.56 (CH_2, B), 30.90 (CH_2), 31.79 (CH_2), 32.72 [2C, CH_2, NCH_2<u>CH_2</u> (B)], 33.17 (CH_2), 35.13 (NCH_2<u>CH_2</u>, A), 41.76 (CH-4a, B), 45.01 (NCH_2, B), 45.25 (NCH_2, A), 55.85 (OCH_3), 55.90 (2C, two

OCH_3), 55.93 (OCH_3), 102.35 (=CH-7, B), 111.22, 111.28 (two CH, A, B), 112.14, 112.22 (two CH, A, B), 115.25 (=C-4a, A), 120.71, 120.82 (two CH, A, B), 131.63, 131.71 (two C-1', A, B), 136.65 (=C-7a, A), 143.60 (=C-7a, B), 147.59 (2C), 148.86, 148.90, (C-3', C-4' A, B), 168.88, 169.71 (C=O, A, B). GC-MS (EI, 70eV): m/z = 301 (9), [M^+], 164 (100), 150 (25), 137 (11), 122 (19), 96 (14).

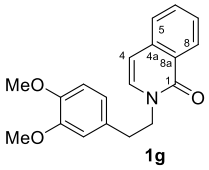
1-(3,4-Dimethoxyphenethyl)-1,3,4,5,6,7,8,9-octahydro-2*H*-cyclohepta[b]pyridin-2-one (**1f**):



1f

Yield 46% (0.462g, reaction time: 72h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.47-1.62 (m, 4H, two CH_2), 1.68 – 1.76 (m, 2H, CH_2), 2.09 – 2.23 (m, 2H, CH_2), 2.30 – 2.43 (m, 2H, CH_2), 2.72 – 2.80 (m, 2H, $\underline{CH_2}CH_2N$), 3.75 – 3.81 (m, 2H, CH_2N), 3.86 and 3.88 (two s, 6H, two OCH_3), 6.68 – 6.83 (m, 3H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 25.89, 26.30, 27.55, 28.70, 31.06, 32.50, 33.35 (seven CH_2), 34.90 ($\underline{CH_2}CH_2N$), 43.50 (NCH_2), 55.88, 55.95 (two OCH_3), 111.24, 112.18, 120.75 (ArH), 122.03 (4a), 131.71 (Ar), 136.86 (C-9a), 147.58, 148.85 (Ar), 170.59 (C=O). GC-MS (EI, 70eV): m/z = 329 (18), [M^+], 178 (21), 165 (58), 164 (100), 150 (53), 124 (22), 91 (12). HRMS (ESI-TOF): *m/z* calcd for $C_{20}H_{28}NO_3[M + H]^+$, 330.2069; found, 330.2070.

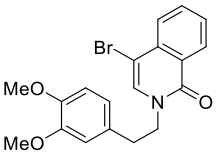
2-(3,4-Dimethoxyphenethyl)isoquinolin-1(2*H*)-one (**1g**)[19]:



1g

Yield 88% (0.938g, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave white solid, mp 111-112 °C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.04 (t, *J* = 7.3 Hz, 2H, CH_2), 3.74 (s, 3H, 3'-OCH_3), 3.85 (s, 3H, 4'-OCH_3), 4.19 (t, *J* = 7.2 Hz, 2H, NCH_2), 6.37 (d, *J* = 7.3 Hz, 1H, =CH-4), 6.66 (d, *J* = 1.9 Hz, 1H, CH-2'), 6.74 (dd, *J* = 8.1, 1.9 Hz, 1H, CH-6'), 6.78 (d, *J* = 7.3 Hz, 1H, =CH-3), 6.79 (d, *J* = 8.1 Hz, 1H, CH-5')7.48 (d, *J* = 8.2 Hz, 1H, CH-5), 7.48 – 7.52 (m, 1H, CH-7), 7.63 (ddd, *J* = 8.2, 7.0, 1.4 Hz, 1H, CH-6), 8.46 (dd, *J* = 8.1, 1.0 Hz, 1H, CH-8). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.74 (CH_2), 51.77 (NCH_2), 55.74 (3'-OCH_3), 55.88 (4'-OCH_3), 105.61 (=CH-4), 111.32 (CH-5'), 112.13 (CH-2'), 120.89 (CH-6'), 125.86 (CH-5 or CH-7), 126.20 (C-8a), 126.75 (CH-5 or CH-7), 127.73 (CH-8), 130.82 (C-1'), 132.09, 132.10 (CH-6, =CH-3), 137.10 (C-4a), 147.74 (C-4'), 148.95 (C-3'), 162.10 (C=O). GC-MS (EI, 70eV): m/z = 309 (2), [M^+], 164 (100), 149 (17), 128 (18), 77 (9).

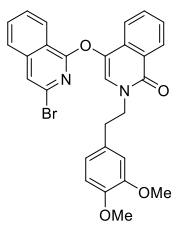
4-Bromo-2-(3,4-dimethoxyphenethyl)isoquinolin-1(2*H*)-one (**4-Br-1g**):



4-Br-1g

Yield 65% (0.653g, reaction time: 3h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave pale yellow solid, mp 80-81 °C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.02 (t, *J* = 7.4 Hz, 2H, CH_2), 3.78 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 4.17 (t, *J* = 7.4 Hz, 2H, NCH_2), 6.69 (d, *J* = 2.0 Hz, 1H, CH-2'), 6.74 (dd, *J* = 8.1, 2.0 Hz, 1H, CH-6'), 6.80 (d, *J* = 8.1 Hz, 1H, CH-5'), 7.12 (s, 1H, =CH-3), 7.56 (ddd, *J* = 8.4, 6.9, 0.9 Hz, 1H, CH-7), 7.74 (ddt, *J* = 8.1, 7.0, 0.9 Hz, 1H, CH-6), 7.79 (dd, *J* = 8.1, 0.9 Hz, 1H, CH-5), 8.46 (dd, *J* = 7.9, 0.9 Hz, 1H, CH-8). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.85 (CH_2), 51.56 (NCH_2), 55.80, 55.93 (two OCH_3), 99.35 (C-4), 111.40 (CH-5'), 112.01 (CH-2'), 120.91 (CH-6'), 125.79 (CH-5), 126.41 (C-8a), 127.78 (CH-7), 128.16 (CH-8), 130.28 (C-1'), 132.52 (=CH-3), 132.95 (CH-6), 135.44 (C-4a), 147.87, 149.04 (C-3', C-4'), 161.15 (C=O). GC-MS (EI, 70eV): m/z = 387 (1), [M^+], 206 (7), 164 (100), 151 (12), 149 (21). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}BrNO_3[M + H]^+$, 388.0548; found, 388.0545.

Next to the product **4-Br-1g** by-product **1g-by-product** was also isolated in 10% yield.

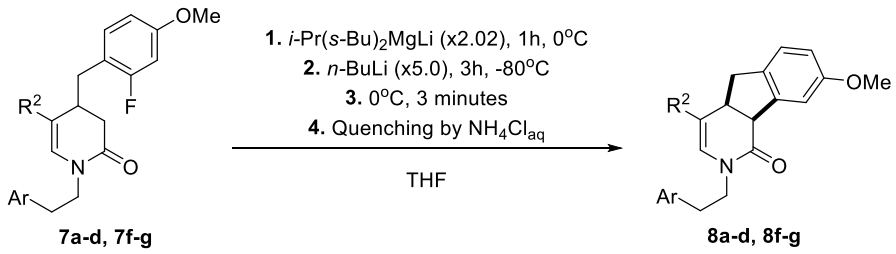


1g-by-product

4-((4-Bromoisoquinolin-1-yl)oxy)-2-(3,4-dimethoxyphenethyl)isoquinolin-1(2*H*)-one (**1g-by-product**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.09 (t, *J* = 7.3 Hz, 2H, CH_2), 3.77 (s, 3H, OCH_3), 3.83 (s, 3H, OCH_3), 4.23 (t, *J* = 7.3 Hz, 2H, NCH_2), 6.67 – 6.79 (m, 3H, CH-2', CH-5', CH-6'), 7.00 (s, 1H, CH-3), 7.38 (dd, *J* = 7.0, 1.4 Hz, 1H, CH-5), 7.48 – 7.64 (m, 2H, CH-6", CH-7"), 7.75 (td, *J* = 8.2, 7.0, 1.2 Hz, 1H, CH-7), 7.90 (td, *J* = 8.4, 7.0, 1.4 Hz, 1H, CH-6), 8.06 (s, 1H, CH-3"), 8.15 (dd, *J* = 8.4, 1.2 Hz, 1H, CH-8), 8.47 – 8.56 (m, 2H, CH-5", CH-8"). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.77 (CH_2), 51.83 (NCH_2), 55.74, 55.84 (two OCH_3), 111.32 (CH-5'), 112.12 (CH-2'), 113.41 (C-4"), 120.09 (C-4a), 120.90, 120.92 (CH-5, CH-6'), 124.34 (CH-8"), 125.02 (=CH-3), 126.08 (C-8a"), 126.19 (CH-8), 127.39 (CH-7"), 128.38 (CH-7), 128.46 (CH-5"), 130.60 (C-1'), 132.11 (C-4a"), 132.16 (CH-6"), 132.28 (CH-6), 133.18 (C-4), 136.80 (C-8a), 140.89 (CH-3"), 147.75, 149.03 (C-3', C-4'), 159.75 (C-1"), 161.02 (C=O).). GC-MS (EI, 70eV): m/z = 530 (<1), [M^+], 366 (4), 207 (7), 164 (100), 149 (9), 127 (8). HRMS (ESI-TOF): *m/z* calcd for $C_{28}H_{24}BrN_2O_4[M + H]^+$, 531.0919; found, 531.0925.

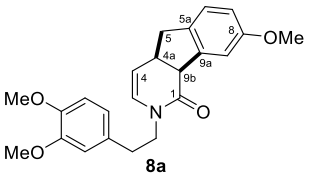
5n. *Synthesis of compounds* ***8a-d*** *and* ***8f-g*** *via "benzyne" cyclization*

Compounds **8a-d** and **8f-g** were prepared according to the procedure described earlier.[14]



7a-d, 7f-g **8a-d, 8f-g**

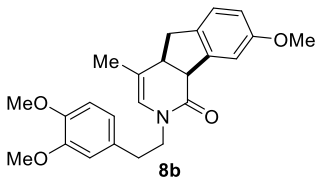
(4a*RS*,9b*SR*)-2-(3,4-Dimethoxyphenethyl)-8-methoxy-2,4a,5,9b-tetrahydro-1*H*-indeno[1,2-c]pyridin-1-one (**8a**):



8a

Yield 47% (0.180g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.73 – 2.81 (m, 3H, CH_2, C<u>H</u>H-5), 3.19 (dd, *J* = 15.2, 7.6 Hz, 1H, CH<u>H</u>-5), 3.46 (ddtd, *J* = 8.4, 7.6, 2.8, 2.3 Hz, 1H, CH-4a), 3.52 (dt, *J* = 13.4, 7.5 Hz, 1H, NC<u>H</u>H), 3.67 (s, 3H, OCH_3), 3.78 (s, 3H, OCH_3), 3.75 – 3.83 (m, 1H, NCH<u>H</u>), 3.84 (s, 3H, OCH_3), 4.03 (d, *J* = 8.4 Hz, 1H, CH-9b), 4.72 (ddd, *J* = 8.1, 2.8, 0.8 Hz, 1H, =CH-4), 5.65 (dd, *J* = 8.1, 2.3 Hz, 1H, CH-3), 6.58 (d, *J* = 1.9 Hz, 1H, CH-2'), 6.68 (dd, *J* = 8.2, 1.9 Hz, 1H, CH-6'), 6.75 (d, *J* = 8.0 Hz, 1H, CH-5'), 6.77 (dd, *J* = 8.0, 2.5 Hz, 1H, CH-7), 6.96 (d, *J* = 2.5 Hz, 1H, CH-9), 7.13 (d, *J* = 8.2 Hz, 1H, CH-6). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.42 (CH_2), 38.61 (CH-4a), 39.07 (CH_2-5), 48.98 (NCH_2), 51.36 (CH-9b), 55.51, 55.66, 55.86 (three OCH_3), 108.79 (=CH-4), 109.55 (CH-9), 111.24 (CH-5'), 112.21 (CH-2'), 114.19 (CH-7), 120.72 (CH-6'), 125.06 (CH-6), 128.91 (=CH-3), 131.25 (C-1'), 133.74 (C-5a), 141.64 (C-9a), 147.55 (C-4'), 148.81 C-3'), 159.28 (C-8), 167.73 (C=O). GC-MS (EI, 70eV): m/z = 379 (6), [M^+], 200 (11), 164 (100). HRMS (ESI-TOF): *m/z* calcd for $C_{23}H_{26}NO_4[M + H]^+$, 380.1862; found, 380.1855.

(4a*SR*,9b*SR*)-2-(3,4-Dimethoxyphenethyl)-8-methoxy-4-methyl-2,4a,5,9b-tetrahydro-1*H*-indeno[1,2-c]pyridin-1-one (**8b**):

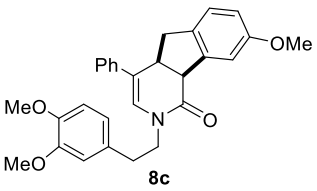


8b

Yield 68% (0.071g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave brown semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.68 (t, *J* = 1.3 Hz, 3H, 4-CH_3), 2.78 (ddd, *J* = 9.0, 6.7, 2.6 Hz, 2H, CH_2), 2.86 (dd, *J* = 15.2, 5.5 Hz, 1H, C<u>H</u>H-5), 3.15 (dd, *J* = 15.2, 8.0 Hz, 1H, CH<u>H</u>-5), 3.26 (dddq, *J* = 9.3, 8.0, 5.5, 1.3 Hz, 1H, CH-4a), 3.54 (ddd, *J* = 13.4, 8.5, 6.9 Hz, 1H, NC<u>H</u>H), 3.68-3.78 (m, 1H, NCH<u>H</u>), 3.75

(s, 3H, OCH_3), 3.80 (s, 3H, OCH_3), 3.84 (s, 3H, OCH_3), 4.01 (d, *J* = 9.2 Hz, 1H, CH-9b), 5.60 (p, *J* = 1.3 Hz, 1H, =CH-3), 6.65 (d, *J* = 1.9 Hz, 1H, CH-2'), 6.71 (dd, *J* = 8.1, 1.9 Hz, 1H, CH-6'), 6.74 – 6.80 (m, 2H, CH-7, CH-5'), 7.07 (d, *J* = 2.2 Hz, 1H, CH-9), 7.11 (d, *J* = 8.2 Hz, 1H, CH-6). ^{13}C NMR (101 MHz, $CDCl_3$) δ 18.27 (4-CH_3), 34.32 (CH_2), 36.85 (CH_2-5), 43.21 (CH-4a), 48.97 (NCH_2), 50.39 (CH-9b), 55.48, 55.72, 55.89 (three OCH_3), 110.38 (CH-9), 111.21 (CH-5'), 112.13 (CH-2'), 114.29 (CH-7), 114.79 (C-4), 120.71 (CH-6'), 123.92 (=CH-3), 124.52 (CH-6), 131.26 (C-1'), 133.22 (C-5a), 142.26 (C-9a), 147.54 (C-4'), 148.83 (C-3'), 159.10 (C-8), 167.24 (C=O). GC-MS (EI, 70eV): m/z = 393 (5), [M^+], 214 (15), 164 (100). HRMS (ESI-TOF): *m/z* calcd for $C_{24}H_{28}NO_4[M + H]^+$, 394.2018; found, 394.2025.

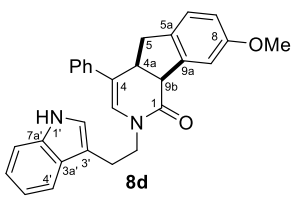
(4a*SR*,9b*SR*)-2-(3,4-Dimethoxyphenethyl)-8-methoxy-4-phenyl-2,4a,5,9b-tetrahydro-1*H*-indeno[1,2-c]pyridin-1-one (**8c**):



8c

Yield 74% (0.480g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 10:1) gave brown solid, mp 53-55 °C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.77 (dd, *J* = 15.4, 6.1 Hz, 1H, C<u>H</u>H-5), 2.82 – 2.90 (m, 2H, CH_2), 3.23 (dd, *J* = 15.4, 7.9 Hz, 1H, CH<u>H</u>-5), 3.56 (dt, *J* = 13.4, 7.6 Hz, 1H, NC<u>H</u>H), 3.68 (s, 3H, OCH_3), 3.82 (s, 3H, OCH_3), 3.84 (s, 3H, OCH_3), 3.86 – 3.94 (m, 1H, CH-4a), 3.98 (dt, *J* = 13.4, 7.6, 6.0 Hz, 1H, NC<u>H</u>H), 4.16 (d, *J* = 9.3 Hz, 1H, CH-9b), 6.05 (d, *J* = 0.9 Hz, 1H, =CH-3), 6.62 (d, *J* = 2.0 Hz, 1H, CH-2'), 6.70 (dd, *J* = 8.2, 2.0 Hz, 1H, CH-6'), 6.74 – 6.81 (m, 2H, CH-5', CH-7), 7.03 (d, *J* = 8.2 Hz, 1H, CH-6), 7.12 (d, *J* = 2.4 Hz, 1H, CH-9), 7.14 – 7.18 (m, 2H, C_6H_5), 7.19 – 7.25 (m, 1H, C_6H_5), 7.28 – 7.34 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.57 (CH_2), 38.32 (CH_2-5), 40.85 (CH-4a), 49.50 (NCH_2), 50.36 (CH-9b), 55.51, 55.70, 55.93 (three OCH_3), 110.51 (CH-9), 111.39 (CH-5'), 112.25 (CH-2'), 114.38 (CH-7), 118.84 (=C-4), 120.86 (CH-6'), 124.64 (CH-6), 125.29 (C_6H_5), 126.39) (=CH-3), 126.68, 128.63 (C_6H_5), 131.11 (C-1'), 133.43 (C-5a), 138.12 (C_6H_5), 141.91 (C-9a), 147.69 (C-4'), 148.97 (C-3'), 159.16 (C-8), 167.37 (C=O). GC-MS (EI, 70eV): m/z = 455 (22), [M^+], 291 (80), 276 (32), 274 (14), 248 (17), 164 (100), 151 (16), 103 (8), 91 (13), 77 (8). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{30}NO_4[M + H]^+$, 456.2175; found 456.2170.

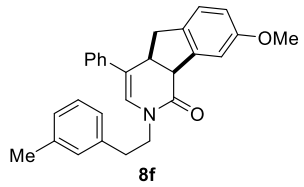
(4a*SR*,9b*SR*)-2-(2-(1*H*-Indol-3-yl)ethyl)-8-methoxy-4-phenyl-2,4a,5,9b-tetrahydro-1*H*-indeno[1,2-c]pyridin-1-one (**8d**):



8d

Yield 63% (0.090g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.73 (dd, *J* = 15.4, 6.6 Hz, 1H, CHH-5), 3.07 (t, *J* = 7.2 Hz, 2H, CH_2), 3.20 (dd, *J* = 15.4, 8.0 Hz, 1H, CHH-5), 3.75 (dt, *J* = 13.5, 7.6 Hz, 1H, NCHH), 3.81 (s, 3H, OCH_3), 3.82 – 3.89 (m, 1H, CH-4a), 3.99 (dt, *J* = 13.5, 6.8 Hz, 1H, NCHH), 4.15 (d, *J* = 9.5 Hz, 1H, CH-9b), 6.04 (d, *J* = 0.8 Hz, 1H, =CH-3), 6.78 (dd, *J* = 8.3, 2.5 Hz, 1H, CH-7), 6.85 (d, *J* = 2.3 Hz, 1H, CH-2'), 6.97 – 7.01 (m, 2H, C_6H_5), 7.03 (d, *J* = 8.3 Hz, 1H, CH-6), 7.09 (ddd, *J* = 7.9, 7.0, 1.1 Hz, 1H, CH-5'), 7.15 (d, *J* = 2.5 Hz, 1H, CH-9), 7.16 – 7.22 (m, 2H, C_6H_5, CH-6'), 7.22 – 7.28 (m, 2H, C_6H_5), 7.34 (dt, *J* = 8.2, 0.9 Hz, 1H, CH-7'), 7.61 (dd, *J* = 7.8, 1.1 Hz, 1H, CH-4'), 8.02 (s, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 24.50 (CH_2-5), 38.43 (CH_2), 40.79 (CH-5a), 48.29 (NCH_2), 50.28 (CH-9b), 55.53 (OCH_3), 110.71 (CH-9), 111.19 (CH-7'), 112.53(C-3'), 114.41 (CH-7), 118.41 (=C-4), 118.77 (CH-4'), 119.57 (CH-5'), 122.08 (CH-6'), 122.49 (CH-2'), 124.58 (CH-6), 125.15 (C_6H_5), 126.37 (=CH-3), 126.49 (C_6H_5), 127.30 (C-3a'), 128.53 (C_6H_5), 133.51 (C-5a), 136.33 (C-5a), 138.09 (C_6H_5), 142.04 (C-9a), 159.07 (C-8), 167.43 (C=O). GC-MS (EI, 70eV): m/z = 434 (9), [M^+], 291 (15), 276 (9), 144 (23), 143 (100), 130 (22), 115 (5). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{27}N_2O_2$[M + H]$^+$, 435.2073; found, 435.2063.

(4a*SR*,9b*SR*)-8-Methoxy-2-(3-methylphenethyl)-4-phenyl-2,4a,5,9b-tetrahydro-1*H*-indeno[1,2-c]pyridin-1-one (**8f**):

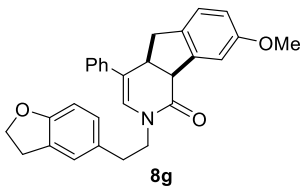


8f

Yield 70% (0.141g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave brown semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.23 (s, 3H, 3'-CH_3), 2.78 (dd, *J* = 15.4, 6.4 Hz, 1H, CHH-5), 2.83 – 2.92 (m, 2H, CH_2), 3.23 (dd, *J* = 15.4, 7.9 Hz, 1H, CHH-5), 3.59 (dt, *J* = 13.4, 7.9 Hz, 1H, NCHH), 3.82 (s, 3H, OCH_3), 3.86 – 3.98 (m, 2H, CH-4a, NCHH), 4.16 (d, *J* = 9.4 Hz, 1H, CH-9b), 6.04 (d, *J* = 0.8 Hz, 1H, =CH-3), 6.78 (ddd, *J* = 8.2, 2.5, 0.7 Hz, 1H, CH-7), 6.93 (d, *J* = 1.8 Hz, 1H, CH-2'), 6.94 – 7.06 (m, 3H, ArH, CH-6), 7.10 – 7.18 (m, 4H, ArH, CH-9), 7.19 – 7.26 (m, 1H, ArH), 7.31 (dd, *J* = 8.2, 6.7 Hz, 2H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.25 (CH_3), 34.86 (CH_2), 38.38 (CH_2-5), 40.85 (CH-4a), 49.49 (NCH_2), 50.31 (CH-9b), 55.51 (OCH_3), 110.60 (CH-9), 114.46 (CH-7), 118.73 (=C-4), 124.60 (CH-6), 125.27 (ArH), 125.93 (=CH-3), 126.37, 126.62, 127.22, 128.50, 128.58 (ArH), 130.01 (CH-2'), 133.43 (C-5a), 138.17 (two Ar), 138.39 (Ar), 141.91 (C-9a), 159.11 (C-8), 167.36 (C=O). GC-MS (EI, 70eV): m/z = 409 (73), [M^+], 304 (48), 291

(33), 276 (100), 274 (18), 248 (16), 232 (11), 202 (12), 119 (17), 115 (12), 103 (15), 91 (27), 77 (16). HRMS (ESI-TOF): *m/z* calcd for $C_{28}H_{28}NO_2[M + H]^+$, 410.2120; found, 410.2131.

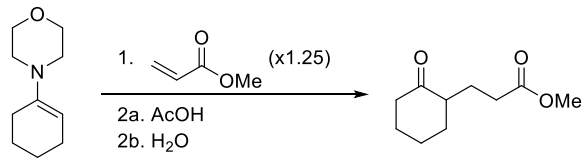
(4a*SR*,9b*SR*)-2-(2-(2,3-Dihydrobenzofuran-5-yl)ethyl)-8-methoxy-4-phenyl-2,4a,5,9b-tetrahydro-1*H*-indeno[1,2-c]pyridin-1-one (**8g**):



8g

Yield 68% (0.144g). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave white solid, mp 53-55°C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.69 – 2.90 (m, 3H, CH_2-2", C<u>H</u>H-5), 2.94 – 3.14 (m, 2H, CH_2-3'), 3.23 (dd, *J* = 15.4, 7.9 Hz, 1H, CH<u>H</u>-5), 3.54 (dt, *J* = 13.4, 7.6 Hz, 1H, NC<u>H</u>H), 3.82 (s, 3H, OCH_3), 3.85 – 3.97 (m, 2H, NCH<u>H</u>, CH-4a), 4.15 (d, *J* = 9.4 Hz, 1H, CH-9b), 4.50 (ddd, *J* = 9.3, 8.2, 1.2 Hz, 2H, CH_2-2'), 6.03 (d, *J* = 0.9 Hz, 1H, =CH-3), 6.68 (d, *J* = 7.9 Hz, 1H, CH-7'), 6.78 (dd, *J* = 8.2, 2.4 Hz, 1H, CH-7), 6.84 – 6.94 (m, 2H, CH-4', CH-6'), 7.04 (d, *J* = 8.2 Hz, 1H, CH-6), 7.12 (d, *J* = 2.4 Hz, 1H, CH-9), 7.14 – 7.19 (m, 2H, C_6H_5), 7.19 – 7.27 (m, 1H, C_6H_5), 7.31 (dd, *J* = 8.2, 6.7 Hz, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 29.65 (CH_2-3), 34.30 (CH_2-2"), 38.38 (CH_2-5), 40.83 (CH-4a), 49.72 (NCH_2), 50.32 (CH-9a), 55.52 (OCH_3), 71.20 (CH_2-2'), 109.19 (CH-7'), 110.62 (CH-9), 114.43 (CH-7), 118.64 (=C-4), 124.56 (CH-6), 125.24 (C_6H_5), 125.81 (CH-4'), 126.40 (=CH-3), 126.64 (C_6H_5), 127.24 (C-3a'), 128.38 (CH-6'), 128.61 (C_6H_5), 130.32 (C-5'), 133.45 (C-5a), 138.17 (C_6H_5), 141.94 (C-9a), 158.80, 159.11 (C-7a', C-8), 167.36 (C=O). GC-MS (EI, 70eV): m/z = 437 (24), [M^+], 291 (100), 290 (20), 276 (33), 274 (17), 248 (23), 146 (63), 133 (29), 115 (9), 103 (11), 91 (16), 77 (12). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{28}NO_3[M + H]^+$, 438.2069; found, 438.2077.

5o. Procedure 11: *Procedure for the synthesis of 3-(2-oxocyclohexyl)propanoate using 4-(cyclohex-1-en-1-yl)morpholine*



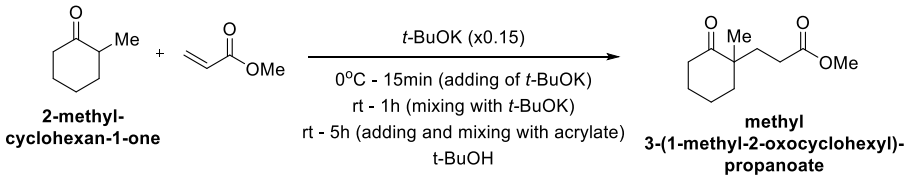
4-(cyclohex-1-en-1-yl)morpholine **3-(2-oxocyclohexyl)propanoate**

A solution of methyl acrylate (1.29g, 14.95 mmol) in 3.5 mL of dry MeCN was slowly added to the flask containing a solution of 4-(cyclohex-1-en-1-yl)morpholine (2.0g, 11.96 mmol) in 8 mL of dry MeCN. A reflux condenser was installed and the oil bath temperature was raised to 110°C. The reaction mixture was refluxed for 48h, then AcOH (0.72 mL) and H_2O (4.8 mL)

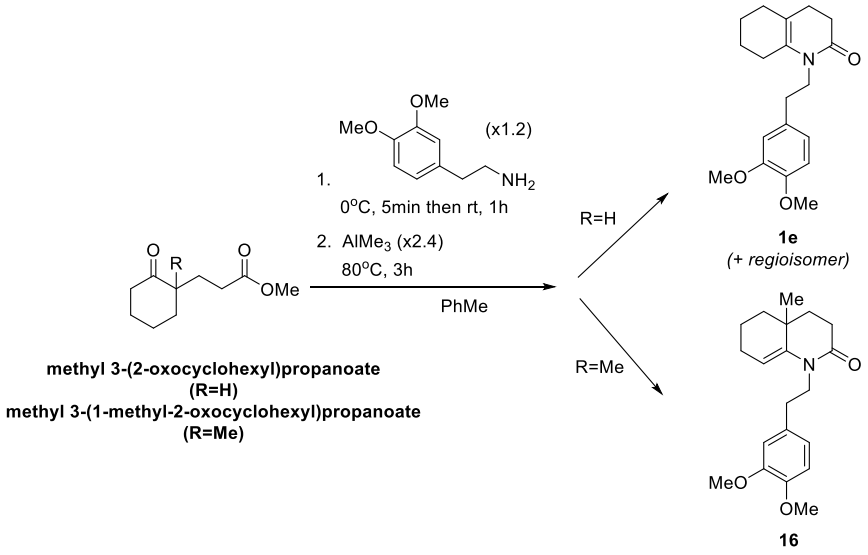
were added and reflux was continued for further 30h. After this time, the reaction mixture was cooled to room temperature and saturated with NaCl, extracted with AcOEt (3x100 mL), washed with 5% HCl (1x30 mL), then with 5% sodium bicarbonate (1x30 mL) and saturated NaCl aqueuos solution (1x30 mL). Combined organic layers were dried over $MgSO_4$. Filtration, concentration *in vacuo*, and purification by distillation (b.p. 60-61^{o}C, 0.01mmHg) yielded methyl 3-(2-oxocyclohexyl)propanoate in 46% (1.009 g, 5.48 mmol) as a colorless oil. ^{1}H and ^{13}C NMR spectra are in agreement with literature data.[20]

***5p**. Synthesis of methyl 3-(1-methyl-2-oxocyclohexyl)-propanoate using 2-methylcyclohexan-1-one and methyl acrylate*

Methyl 3-(1-methyl-2-oxocyclohexyl)propanoate was prepared according to the procedure described earlier.[21]



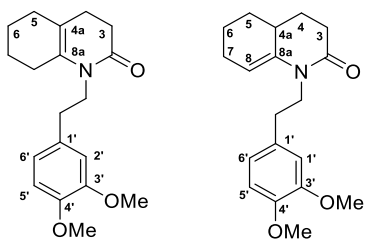
***5q. Procedure 12:** Synthesis of compounds **1e** and **16** via condensation reaction*



Solution of *homoveratrylamine* (0.492g, 2.71 mmol for the synthesis of **1e** or 0.768g, 4.24 mmol for the synthesis of **16**) in toluene (6.5 mL for the synthesis of **1e** or 20 mL for the synthesis of **16**) was treated with two equivalents of a 2.0M $AlMe_3$ solution in toluene (2.18 mL, 5.43 mmol - for the synthesis of **1e** or 4.25 mL, 8.5 mmol - for the synthesis of **16**) at 0^{o}C

and stirred for 1h at room temperature. After this time methyl 3-(2-oxocyclohexyl)propanoate (0.5g, 2.71mmol) or methyl 3-(1-methyl-2-oxocyclohexyl)propanoate (0.7g, 3.53 mmol) was added dropwise and the mixture was heated at 80°C for 3h in a pre-heated oil bath. After this time the reaction mixture was allowed to cool to room temperature and saturated solution of sodium bicarbonate (20 mL) was added dropwise, and the reaction mixture was stirred for another 15 minutes. The aqueous phase was extracted with ethyl acetate (3x80mL), the combined extracts were dried over $MgSO_4$, and the solvent was removed in vacuum. The crude product was purified by column chromatography on silica gel (*n*-hexane/ethyl acetate = 3:1) giving product **1e** with 45% yield (0.383g, 1.21 mmol, as a mixture of regioisomers) as a yellow oil or product **16** in 8.5% yield (0.098g, 0.296mmol). ^{1}H and ^{13}C NMR spectra of **16** are in agreement with literature data.[22]

1-(3,4-Dimethoxyphenethyl)-3,4,5,6,7,8-hexahydroquinolin-2(1H)-one (**1e-A**)[23]:
1-(3,4-Dimethoxyphenethyl)-3,4,4a,5,6,7-hexahydroquinolin-2(1H)-one (**1e-B**):



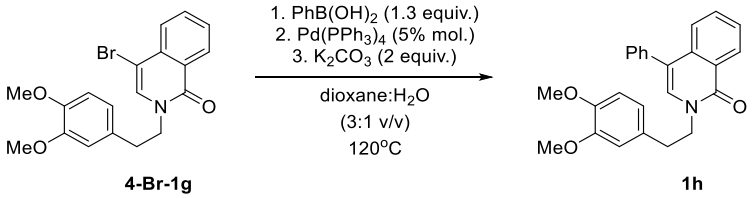
1e

From 1:0.65 mixture of A : B

Yield 45% (0.383g, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (tdd, *J* = 12.9, 10.6, 2.7 Hz, 0.65H, C<u>H</u>H-5, B), 1.45 [qd, *J* = 12.9, 5.4 Hz, 0.65H, C<u>H</u>H-6(7), B], 1.51 – 1.57 [m, 2H, CH_2-6(7), A], 1.62 – 1.70 (m, 2.65H, CH_2-7(6), A; C<u>H</u>H-4, B), 1.75 – 1.87 [m, 1.3H, CH<u>H</u>-6(7), CH<u>H</u>-4, B], 1.88 – 2.00 (m, 0.65H, CH<u>H</u>-5, B), 2.00 – 2.10 (m, 6.65H, CH_2-4, CH_2-5, CH_2-8, A; CH<u>H</u>-6(7), B), 2.13 – 2.32 (m, 1.3H, CHH-6(7), CH-4a, B), 2.41 – 2.47 (m, 2.0H, CH_2-3, A), 2.50 (dd, *J* = 13.2, 6.0 Hz, 0.65H, NCH_2C<u>H</u>H, B), 2.60 (ddd, *J* = 17.7, 5.3, 1.8 Hz, 0.65H, C<u>H</u>H-3, B), 2.71 – 2.76 (m, 2.65H, NCH_2<u>CH_2</u>, A; CH<u>H</u>-3, B), 2.83 (ddd, *J* = 13.2, 10.7, 5.5 Hz, 0.65H, NCH_2C<u>H</u>H, B), 3.73 – 3.82 (m, 2.65H, NCH_2, A; NC<u>H</u>H, B), 3.85 (s, 3H, OCH_3, A), 3.86 (s, 1.95H, OCH_3, B), 3.87 (s, 3H, OCH_3, A), 3.89 (s, 1.95H, OCH_3, B), 3.98 (ddd, *J* = 13.6, 10.8, 5.5 Hz, 0.65H, NCH<u>H</u>, B), 5.16 (dt, *J* = 5.1, 2.3 Hz, 0.65H, =CH-8, B), 6.55 – 6.87 (m, 4.95H, ArH, A, B). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.46 [CH_2-6(7), B], 22.10 [CH_2-6(7), A], 22.94 [CH_2-7(6), A], 24.61 [CH_2-7(6), B], 25.49, 25.53 (CH_2-4, CH_2-5, A), 27.48 [CH_2-4, B], 29.04 [CH_2-8, A], 30.55, [CH_2-5, B], 31.77 [CH_2-3, A], 32.87 [NCH_2<u>CH_2</u>, B], 32.92 [CH_2-3, B], 34.99 [CH-4a, B], 35.17 [NCH_2<u>CH_2</u>, A], 42.32 (NCH_2, A), 44.13 (NCH_2, B), 55.87, 55,90, 55.92, 55.95 (four OCH_3, A, B), 103.87 (=CH-8, B), 111.23 (ArH, A), 111.26 (ArH, B),

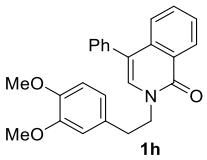
112.15 (ArH, B), 112.25 (ArH, A), 115.32 (=C-4a, A), 120.65 (ArH, B), 120.80 (ArH, A), 131.11, 131.81 (C-1', C-8a, A), 131.87 (C-1', B), 138.48 (=C-8a, B), 147.56 (Ar, B), 147.59 (Ar, A), 148.83 (Ar, A), 148.91 (Ar, B), 168.84 (C=O, B), 170.06 (C=O, A). GC-MS (EI, 70eV): m/z = 315 (10), [M^+], 164 (100), 151 (28), 136 (40), 110 (12).

5r. Procedure 13: *Arylation of* ***4-Br-1g*** *under Suzuki reaction conditions*



To a solution of **4-Br-1g** (0.5g, 1.3mmol) in dry, degassed mixture of 1,4-dioxane and H_2O in 3:1 volume ratio (9.75 mL/3.25 mL), $PhB(OH)_2$ (0.204g, 1.67 mmol, 1.3 equiv.), $Pd(PPh_3)_4$ (0.0744g, 0.064 mmol, 5% mol.) and K_2CO_3 (0.3560g, 2.6 mmol, 2.0 equiv.) was added and the reaction mixture was heated to 120°C under an argon atmosphere and stirred at this temperature for 2h. After this time reaction mixture was allowed to cool to room temperature, 5 mL of AcOEt was added and stirring was maintained for 5 min. Aqueous layer was extracted with ethyl acetate (3x80mL), the combined extracts were dried over $MgSO_4$, and the solvent was removed *in vacuo*. The crude product was purified by column chromatography on silica gel (*n*-hexane/ethyl acetate = 1:1) giving product **1h** with 93% yield (0.460g, 1.2 mmol) as a white solid.

2-(3,4-Dimethoxyphenethyl)-4-phenylisoquinolin-1(2*H*)-one (**1h**):

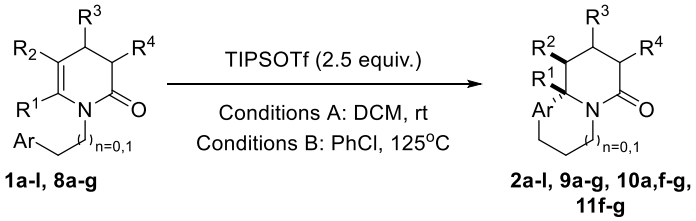


Yield 93% (0.460g). Mp 138-140°C (petroleum ether:ethyl acetate). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.07 (dd, *J* = 7.9, 6.6 Hz, 2H, CH_2), 3.71 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 4.24 (dd, *J* = 7.9, 6.6 Hz, 2H, NCH_2), 6.67 (d, *J* = 2.0 Hz, 1H, CH-2'), 6.72 (s, 1H, =CH-3), 6.74 (dd, *J* = 8.2, 2.0 Hz, 1H, CH-6'), 6.79 (d, *J* = 8.2 Hz, 1H, CH-5'), 7.23 – 7.28 (m, 2H, C_6H_5), 7.36 – 7.46 (m, 3H, C_6H_5), 7.49 – 7.57 (m, 2H, CH-5, CH-7), 7.57 – 7.65 (m, 1H, CH-6), 8.56 (dd, *J* = 8.2, 1.5 Hz, 1H, CH-8). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.77 (CH_2), 51.81 (NCH_2), 55.74, 55.94 (two OCH_3), 111.46 (CH-5'), 112.24 (CH-2'), 119.23 (C-4), 120.98 (CH-6'), 124.63 (CH-5), 125.87 (C-8a), 126.89 (CH-7), 127.66 (C_6H_5), 128.14 (CH-8), 128.61, 129.90 (C_6H_5), 130.75 (C-1'), 131.16 (=CH-3), 132.14 (CH-6), 136.22, 136.36 (C-4a, C_6H_5), 147.86, 149.07 (C-3', C-4'), 161.69 (C=O).

GC-MS (EI, 70eV): m/z = 385 (1), [M^+], 221 (9), 164 (100), 149 (9). HRMS (ESI-TOF): *m/z* calcd for $C_{25}H_{24}NO_3[M + H]^+$, 386.1756; found, 386.1755.

6. Synthesis of compounds 2a-l, 9a-g, 10a, f-g, 11f-g

6a. Procedure 14. *General procedure for intramolecular arylation of enelactams using TIPSOTf*



Conditions A:

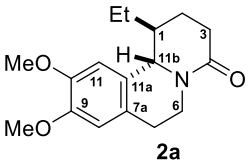
Enelactam **1a-f** or **1i** or **8a-e** (1 mmol) was dissolved in 10 mL of anhydrous DCM, placed in a dry Schlenk flask. TIPSOTf (0.766g, 2.5 mmol, 2.5 equiv.) was added to the resulting solution with a syringe and was stirred at room temperature. Reaction time (2-66h) was monitored by GC-MS. After completation of the reaction 10 mL of saturated sodium bicarbonate solution was added to the reaction flask and the mixture was stirred for 5 minutes. The aqueous layer was extracted with ethyl acetate (3×80 mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using the appropriate mixture of n-hexane/AcOEt to give desired products **2a-f**, **2i**, **9a-9e**.

Conditions B:

Enelactam **1g** or **1j** or **8f-g** (1 mmol) was dissolved in 5 ml of anhydrous PhCl, which was placed in a dry Schlenk flask. TIPSOTf (0.766g, 2.5 mmol, 2.5 equiv.) was added to this solution with a syringe and the mixture was stirred at room temperature for 5 minutes. Subsequently, a reflux condenser was attached to the flask and the bath temperature was raised to 125°C. Reaction time (4-96h) was monitored by GC-MS. After completation of the reaction a heater was removed and the reaction mixture was allowed to cool to room temperature. Subsequently, 10 mL of saturated sodium bicarbonate solution was added to the reaction flask and the mixture was stirred for 5 minutes. The aqueous layer was extracted with ethyl acetate

(3×80 mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using the appropriate mixture of *n*-hexane/AcOEt to give desired products **2g**, **2j**, **9f-g**, **10f-g**, **11f-g**.

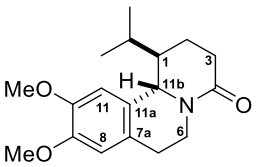
(1*SR*,11b*SR*)-1-Ethyl-9,10-dimethoxy-1,2,3,6,7,11b-hexahydro-4*H*-pyrido[2,1-a]isoquinolin-4-one (**2a**):



2a

Yield 92% (0.220g, reaction conditions **A**; reaction time: 18h). The crude product purified by cristalization from ethyl acetate:petroleum ether gave white solid, mp 212-213°C. ^{1}H NMR (400 MHz, DMSO) δ 1.03 (t, *J* = 7.4 Hz, 3H, CH_3), 1.39 – 1.82 (m, 4H, CH_2-2, $\underline{CH_2}CH_3$), 2.09 (dt, *J* = 17.2, 5.5 Hz, 1H, C$\underline{H}$H-3), 2.21 – 2.28 (m, 1H, CH-1), 2.30 (ddd, *J* = 17.2, 9.8, 5.8 Hz, 1H, CH$\underline{H}$-3), 2.66 (dt, *J* = 15.5, 4.9 Hz, 1H, C$\underline{H}$H-7), 2.84 (ddd, *J* = 15.5, 9.3, 5.9 Hz, 1H, CH$\underline{H}$-7), 3.00 (ddd, *J* = 12.4, 9.3, 5.0 Hz, 1H, NC$\underline{H}$H), 3.73 (s, 3H, OCH_3), 3.75 (s, 3H, OCH_3), 4.15 (dt, *J* = 12.6, 5.4 Hz, 1H, NCH$\underline{H}$), 4.34 (d, *J* = 4.7 Hz, 1H, CH-11b), 6.78 (s, 1H, ArH), 6.79 (s, 1H, ArH). ^{13}C NMR (101 MHz, DMSO) δ 11.41 (CH_3), 21.87, 24.71 (CH_2-2, $\underline{CH_2}CH_3$), 27.22 (CH_2-7), 28.91 (CH_2-3), 36.20 (CH-1), 41.80 (NCH_2), 55.42, 55.73 (two OCH_3), 59.62 (CH-11b), 108.34, 112.23 (CH-8, CH-11), 128.72, 129.45 (CH-7a, C-11a), 146.89, 147.64 (C-9, C-10), 168.54. GC-MS (EI, 70eV): m/z = 289 (39), [M^+], 233 (24), 232 (26), 191 (100), 190 (31), 176 (22). HRMS (ESI-TOF): *m/z* calcd for $C_{17}H_{24}NO_3$ [M + H]$^+$, 290.1756; found, 290.1752.

(1*RS*,11b*SR*)-1-Isopropyl-9,10-dimethoxy-1,2,3,6,7,11b-hexahydro-4*H*-pyrido[2,1-a]isoquinolin-4-one (**2b**):

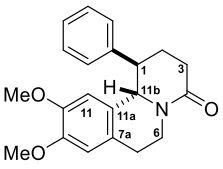


2b

Yield 81% (0.171g, conditions **A**; reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave white solid, mp 129-131°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (d, *J* = 6.1 Hz, 3H, CH_3), 1.13 (d, *J* = 6.1 Hz, 3H, CH_3), 1.66 – 1.81 (m, 2H, CH_2-2), 1.94 – 2.05 [m, 2H, CH-1, $\underline{CH}(CH_3)_2$], 2.24 (dt, *J* = 17.3, 5.6 Hz, 1H, C$\underline{H}$H-3), 2.44 (ddd, *J* = 17.3, 9.5, 5.8 Hz, 1H, CH$\underline{H}$-3), 2.64 – 2.76 (m, 1H, C$\underline{H}$H-7), 2.97 – 3.12 (m, 2H, CH$\underline{H}$-7, NC$\underline{H}$H), 3.87 (s, 3H, OCH_3), 3.88 (s, 3H, OCH_3), 4.39 – 4.47 (m, 1H, NCH$\underline{H}$), 4.50 (d, *J* = 4.2 Hz, 1H, CH-11b), 6.67 and 6.70 (two s, 2H, CH-8, CH-11). ^{13}C NMR (101 MHz, $CDCl_3$) δ 18.73 (CH_3), 19.41 (CH_2-2), 21.75 (CH_3), 27.55 [$\underline{CH}(CH_3)_2$], 28.08 (CH_2-7), 29.86 (CH_2-3), 42.20 (CH-1), 42.67 (NCH_2), 55.95 and 56.23 (two OCH_3), 58.38 (CH-11b), 107.74 and 111.93 (CH-8, CH-11), 129.33 and 129.75 (C-7a, C-11a),

147.30 and 148.12 (C-9, C-10), 170.25 (C=O). GC-MS (EI, 70eV): m/z = 303 (29), [M^+], 233 (24), 232 (25), 192 (23), 191 (100), 190 (29), 176 (19). HRMS (ESI-TOF): *m/z* calcd for $C_{18}H_{26}NO_3[M + H]^+$, 304.1913; found, 304.1920.

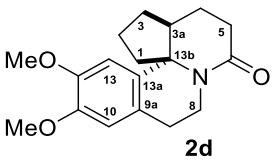
(1*RS*,11b*SR*)-9,10-Dimethoxy-1-phenyl-1,2,3,6,7,11b-hexahydro-4*H*-pyrido[2,1-a]isoquinolin-4-one (**2c**):



2c

Yield 99% (0.212g, conditions **A**; reaction time: 42h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave white solid, mp 221-223°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.86 (dtd, *J* = 13.3, 5.1, 4.5 Hz, 1H, C<u>H</u>H-2), 1.97 – 2.12 (m, 1H, CH<u>H</u>-2), 2.30 – 2.47 (m, 2H, CH_2-3), 2.69 (dt, *J* = 15.3, 4.6 Hz, 1H, C<u>H</u>H-7), 2.79 (ddd, *J* = 15.3, 9.9, 5.0 Hz, 1H, CH<u>H</u>-7), 2.96 (td, *J* = 12.3, 9.9, 4.6 Hz, 1H, NC<u>H</u>H), 3.16 (td, *J* = 9.9, 9.5, 4.5 Hz, 1H, CH-1), 3.23 (s, 3H, 10-OCH_3), 3.68 (s, 3H, 9-OCH_3), 4.36 (dt, *J* = 12.3, 4.6 Hz, 1H, NCH<u>H</u>), 5.05 (dd, *J* = 81.9, 9.5 Hz, 1H, CH-11b), 6.20 (s, 1H, CH-11), 6.73 (s, 1H, CH-8), 7.27 (dd, *J* = 7.5, 7.1 Hz, 1H, C_6H_5), 7.38 (t, *J* = 7.5 Hz, 2H, C_6H_5), 7.43 (d, *J* = 7.5 Hz, 2H, C_6H_5). ^{13}C NMR (101 MHz, DMSO-d_6) δ 27.83 (CH_2-7), 29.11 (CH_2-2), 31.43 (CH_2-3), 40.63 (NCH_2), 45.99 (CH-1), 54.67 (10-OCH_3), 55.29 (9-OCH_3), 59.36 (CH-11b), 109.87 (CH-11), 111.63 (CH-8), 126.59, 127.83 (C_6H_5), 128.30 (C-7a), 128.62 (C-11a), 128.71 (C_6H_5), 144.37 (C_6H_5), 146.07 (CH-10), 147.07 (CH-9), 168.43 (C=O). GC-MS (EI, 70eV): m/z = 337 (16), [M^+], 233 (32), 232 (21), 192 (20), 191 (100), 190 (29), 176 (26). HRMS (ESI-TOF): *m/z* calcd for $C_{21}H_{24}NO_3[M + H]^+$, 338.1756; found, 338.1748.

(3a*SR*,13b*SR*)-11,12-Dimethoxy-1,2,3,3a,4,5,8,9-octahydro-6*H*-cyclopenta[2,3]pyrido[2,1-a]isoquinolin-6-one (**2d**):

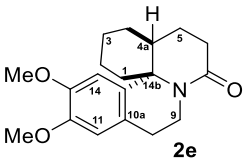


2d

Yield 81% (0.162g, conditions **A**; reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave white solid, mp 110-112°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.68 – 1.74 (m, 2H, CH_2-4), 1.74 – 1.89 (m, 3H, CH_2-2, C<u>H</u>H-3), 2.00 (dt, *J* = 13.1, 7.4 Hz, 1H, C<u>H</u>H-1), 2.10 – 2.26 (m, 2H, CH<u>H</u>-1, CH<u>H</u>-3), 2.31 (dtd, *J* = 17.4, 4.7, 1.0 Hz, 1H, C<u>H</u>H-5), 2.49 (ddd, *J* = 17.4, 9.8, 6.9 Hz, 1H, CH<u>H</u>-5), 2.53 – 2.65 (m, 1H, C<u>H</u>H-9), 2.80 (dq, *J* = 10.8, 5.2 Hz, 1H, CH-3a), 2.94 – 3.10 (m, 2H, CH<u>H</u>-9, NC<u>H</u>H), 3.86 and 3.88 (two s, 6H, two OCH_3), 4.85 (dt, *J* = 9.0, 1.9 Hz, 1H,

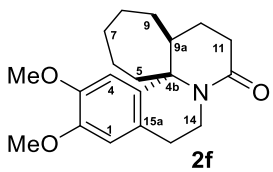
NCHH), 6.57 (s, 1H, CH-10), 6.70 (s, 1H, CH-13). ^{13}C NMR (101 MHz, $CDCl_3$) δ 22.61 (CH_2-4), 24.14 (CH_2-2), 28.45 (CH_2-9), 28.59 (CH_2-5), 30.08 (CH_2-3), 37.48 (NCH_2), 43.79 (CH-3a), 44.20 (CH_2-1), 55.84 and 56.23 (two OCH_3), 70.05 (C-13b), 108.25 (CH-13), 111.67 (CH-10), 127.95 (C-9a), 133.82 (C-13a), 147.38 (C-12), 147.78 (C-11), 170.29 (C=O). GC-MS (EI, 70eV): m/z = 301 (23), [M^+], 272 (61), 259 (100), 258 (46), 244 (34), 230 (20), 216 (11), 115 (10). HRMS (ESI-TOF): *m/z* calcd for $C_{18}H_{24}NO_3[M + H]^+$, 302.1756; found, 302.1753.

(4a*SR*,14b*SR*)-12,13-Dimethoxy-2,3,4,4a,5,6,9,10-octahydroisoquinolino[1,2-j]quinolin-7(1*H*)-one (**2e**)[24]:



Yield 91% (0.245g, conditions **A**; reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.35 – 1.70 (m, 6H, CH_2-3, CH_2-5, CHH-1, CHH-2), 1.77 – 1.90 (m, 3H, CHH-2, CH_2-4), 2.26 (dd, *J* = 18.4, 6.7 Hz, 1H, CHH-1), 2.30 – 2.37 (m, 1H, CHH-6), 2.46 – 2.60 (m, 3H, CHH-6, CH-4a, CHH-10), 3.17 (ddd, *J* = 16.5, 12.2, 8.0 Hz, 1H, CHH-10), 3.26 (td, *J* = 12.2, 4.8 Hz, 1H, NCHH), 3.84 and 3.87 (two s, 6H, two OCH_3), 4.71 – 4.81 (m, 1H, NCHH), 6.57 (s, 1H, CH-11), 6.68 (s, 1H, CH-14). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.65 (CH_2-5), 22.53 (CH_2-2), 25.90, 26.09 (CH_2-3, CH_2-4), 26.92 (CH_2-9), 28.72 (CH_2-6), 35.20 (NCH_2), 36.11 (CH-4a), 40.82 (CH_2-1), 55.80 and 56.28 (two OCH_3), 61.56 (C-14b), 106.18 (CH-14), 112.47 (CH-11), 127.23 (C-10a), 135.77 (C-14a), 147.18, 147.74 (C-12, C13), 172.42 (C=O). GC-MS (EI, 70eV): m/z = 315 (24), [M^+], 273 (18), 272 (100), 259 (20), 244 (15), 230 (7).

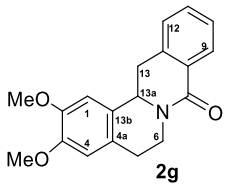
(4b*SR*,9a*SR*)-2,3-dimethoxy-5,6,7,8,9,9a,10,11,14,15-decahydro-12H-cyclohepta[2,3]pyrido-[2,1-a]isoquinolin-12-one (**2f**):



Yield 68% (0.135g, conditions **A**, reaction time: 66h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave white solid, mp 141-143°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.30 – 1.60 (m, 6H, CH_2-6, CH_2-8, CH_2-10), 1.65 – 1.94 (m, 5H, CHH-5, CH_2-7, CH_2-9), 1.97 – 2.16 (m, 2H, CHH-5, CHH-11), 2.33 (ddd, *J* = 17.5, 13.7, 6.4 Hz, 1H, CHH-11), 2.55 (dd, *J* = 16.5, 5.4 Hz, 1H, CHH-15), 2.65 – 2.78 (m, 1H, CH-9a), 2.87 (ddd, *J* = 16.5, 11.9, 7.5 Hz, 1H, CHH-15), 3.16 (ddd, *J* = 13.3, 11.9, 5.4 Hz, 1H, NCHH), 3.70 and 3.76 (two s, 6H, two OCH_3), 4.58 (dd, *J* = 13.3, 7.5 Hz, 1H, NCHH), 6.66 (s, 1H, CH-1), 6.90 (s, 1H, CH-4). ^{13}C NMR (101 MHz, DMSO-d_6) δ

20.46 (CH_2-10), 25.13 (CH_2-6), 26.76 (CH_2-15), 27.81, 27.89, 28.02, 28.70 (CH_2-7, CH_2-8, CH_2-9, CH_2-11), 34.37 (NCH_2), 38.79 (CH-9a), 41.99 (CH_2-5), 55.28 and 56.03 (two OCH_3), 64.06 (C-4b), 107.64 (CH-4), 113.18 (CH-1), 126.17 (C-15a), 135.92 (C-4a), 146.65, 147.35 (C-2, C-3), 169.34 (C=O). GC-MS (EI, 70eV): m/z = 329 (29), [M^+], 286 (16), 273 (19), 272 (100), 259 (46), 258 (42), 245 (37), 244 (36), 230 (14), 216 (10). HRMS (ESI-TOF): *m/z* calcd for $C_{20}H_{28}NO_3$[M + H]+, 330.2069; found, 330.2078.

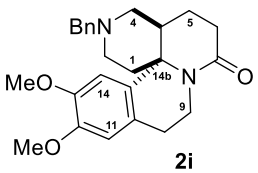
(13a*RS*)-2,3-Dimethoxy-5,6,13,13a-tetrahydro-8*H*-isoquinolino[3,2-a]isoquinolin-8-one (**2g**)[25]:



2g

Yield 79% (0.197g, conditions **B**, reaction time: 72h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave white solid, mp 141-142°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.73 – 2.82 (m, 1H, C<u>H</u>H-5), 2.89 – 3.07 (m, 3H, CH<u>H</u>-5, C<u>H</u>H-13, NC<u>H</u>H), 3.22 (dd, *J* = 15.7, 3.7 Hz, 1H, CH<u>H</u>-13), 3.90 (s, 3H, OCH_3), 3.92 (s, 3H, OCH_3), 4.87 (dd, *J* = 13.4, 3.7 Hz, 1H, CH-13a), 4.96 – 5.08 (m, 1H, NCH<u>H</u>), 6.70 and 6.72 (two s, 2H, CH-1, CH-4), 7.27 (dd, *J* = 7.6, 1.0 Hz, 1H, CH-12), 7.39 (td, *J* = 7.6, 1.0 Hz, 1H, CH-10), 7.46 (td, *J* = 7.6, 1.0 Hz, 1H, CH-11), 8.14 (dd, *J* = 7.6, 1.0 Hz, 1H, CH-9). ^{13}C NMR (101 MHz, $CDCl_3$) δ 29.21 (CH_2-5), 38.13 (CH_2-13), 38.72 (NCH_2), 55.00 (CH-3a), 55.94, 56.16 (two OCH_3), 108.83, 111.46 (CH-1, CH-4), 126.87 (CH-12), 127.30 (C-4a), 127.34 (CH-10), 127.65 (C-13b), 128.60 (CH-9), 129.10 (C-8a), 131.81 (CH-11), 137.30 (C-12a), 147.96, 148.03 (C-2, C-3), 164.64 (C=O). GC-MS (EI, 70eV): m/z = 309 (100), [M^+], 308 (93), 294 (46), 280 (28), 278 (38), 190 (19), 176 (11), 119 (31), 118 (73), 90 (68), 89 (25), 77 (8).

(4a*RS*,14b*SR*)-3-Benzyl-12,13-dimethoxy-2,3,4,4a,5,6,9,10-octahydroisoquinolino[1,2-j][1,6]naphthyridin-7(1*H*)-one (**2i**):

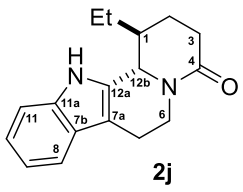


2i

Yield 87% (0.113g, conditions **B**, reaction time: 4h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave white solid, mp 141-143°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.46 (ddd, *J* = 13.5, 6.8, 2.6 Hz, 1H, C<u>H</u>H-5), 1.76 (dddd, *J* = 13.5, 10.1, 6.8, 3.4 Hz, 1H, CH<u>H</u>-5), 1.85 (td, *J* = 14.8, 12.7, 3.5 Hz, 1H, C<u>H</u>H-1), 2.12 (ddd, *J* = 13.2, 11.3, 1.8 Hz, 1H, C<u>H</u>H-2), 2.28 (dd, *J* = 18.8, 6.8 Hz, 1H, CHH-6), 2.32 (dt, *J* = 14.8, 2.3, 1.8 Hz, 1H, CH<u>H</u>-1), 2.40 – 2.52 (m, 2H, CH<u>H</u>-6, C<u>H</u>H-4), 2.56 (d,

J = 14.8 Hz, 1H, CHH-10), 2.73 (dt, *J* = 11.3, 2.6 Hz, 1H, CHH-2), 2.78 – 2.88 (m, 2H, CH-4a, CHH-4), 3.03 – 3.33 (m, 2H, CHH-9, CHH-10), 3.52 (d, *J* = 13.0 Hz, 1H, NCHHPh), 3.56 (d, *J* = 13.0 Hz, 1H, NCHHPh), 3.84 and 3.85 (two s, 6H, two OCH_3), 4.74 – 4.84 (m, 1H, CHH-9), 6.57 (s, 1H, CH-11) 6.71 (s, 1H, C-14), 7.21 – 7.42 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.61 (CH_2-5), 27.06 (CH_2-10), 28.98 (CH_2-6), 35.36 (CH_2-9), 35.94 (CH-4a), 39.50 (CH_2-1), 49.36 (CH_2-2), 53.39 (CH_2-4), 55.81, 56.22 (two OCH_3), 60.23 (C-14b), 63.40 (NCH_2Ph), 106.17 (CH-14), 112.41 (CH-11), 127.21 (C_6H_5), 127.46 (C-10a), 128.36, 129.18 (C_6H_5), 134.36 (C-14), 138.04 (C_6H_5), 147.38, 147.93 (C-12, C-13), 172.16 (C=O). GC-MS (EI, 70eV): m/z = 406 (35), [M^+], 315 (45), 287 (19), 260 (55), 218 (25), 146 (100), 91 (91). HRMS (ESI-TOF): *m/z* calcd for $C_{25}H_{31}N_2O_3[M + H]^+$, 407.2335; found, 407.2329.

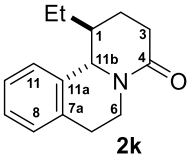
(1*SR*,12b*SR*)-1-Ethyl-2,3,6,7,12,12b-hexahydroindolo[2,3-a]quinolizin-4(1*H*)-one (**2j**)[26]:



2j

Yield 86% (0.198g, conditions **A**, reaction time: 18h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave pale yellow solid, mp 213-215°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.5 Hz, 3H, CH_2CH_3), 1.61 – 1.75 (m, 2H, $CHHCH_3$, CHH-2), 1.81 – 1.96 (m, 2H, $CHHCH_3$, CHH-2), 2.03 – 2.13 (m, 1H, CH-1), 2.27 (ddd, *J* = 17.5, 7.2, 5.2 Hz, 1H, CHH-3), 2.50 (ddd, *J* = 17.5, 8.6, 5.2 Hz, 1H, CHH-3), 2.69 (ddt, *J* = 15.0, 4.2, 1.3 Hz, 1H, CHH-7), 2.87 (ddd, *J* = 12.4, 4.2 Hz, 1H, NCHH), 3.02 (dddd, *J* = 15.0, 12.1, 5.4, 2.5 Hz, 1H, CHH-7), 4.62 (dt, *J* = 4.6, 2.0 Hz, 1H, CH-12b), 5.04 (ddd, *J* = 12.4, 5.5, 1.1 Hz, 1H, NCHH), 7.11 (td, *J* = 8.1, 7.2, 1.0 Hz, 1H, CH-9), 7.18 (td, *J* = 8.1, 7.2, 1.0 Hz, 1H, CH-10), 7.34 (dt, *J* = 8.2, 1.0 Hz, 1H, CH-11), 7.48 (dd, *J* = 7.2, 1.0 Hz, 1H, CH-8), 8.16 (s, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 11.73 (CH_3), 20.99 (CH_2-7), 22.97 (CH_2CH_3), 26.07 (CH_2-2), 29.87 (CH_2-3), 38.29 (CH-1), 42.56 (NCH_2), 59.47 (CH-12b), 110.84 (C-7a), 111.01 (CH-11), 118.29 (CH-8), 119.88 (CH-9), 122.19 (CH-10), 127.10 (C-7b), 133.82 (C-12a), 135.84 (C-11a), 170.00 (C=O). GC-MS (EI, 70eV): m/z = 268 (78), [M^+], 239 (31), 211 (27), 170 (100), 154 (9), 143 (12), 115 (16).

(1*SR*,11b*SR*)-1-Ethyl-1,2,3,6,7,11b-hexahydro-4*H*-pyrido[2,1-a]isoquinolin-4-one (**2k**):

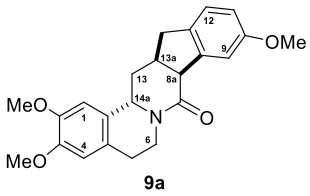


2k

Yield 76% (0.151g, conditions **B**, reaction time: 96h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.08 (t, *J* = 7.4 Hz, 3H, CH_3), 1.46 – 1.59 (m, 1H, $CHHCH_3$), 1.60 – 1.70 (m, 1H, CHH-2), 1.71 – 1.82 (m, 1H,

CHHCH$_3$), 1.91 (dddd, *J* = 13.2, 9.3, 5.5, 4.0 Hz, 1H, CHH-2), 2.17 – 2.32 (m, 2H, CH-1, CHH-3), 2.48 (ddd, *J* = 17.4, 9.0, 5.6 Hz, 1H, CHH-3), 2.80 (dt, *J* = 16.0, 5.5 Hz, 1H, CHH-7), 3.06 (ddd, *J* = 16.0, 8.3, 5.5 Hz, 1H, CHH-7), 3.19 (ddd, *J* = 12.9, 8.3, 5.5 Hz, 1H, NCHH), 4.29 (dt, *J* = 12.9, 6.2 Hz, 1H, NCHH), 4.33 (dd, *J* = 5.6, 4.3 Hz, 1H, CH-11b), 6.87 – 7.62 (m, 4H, C$_6$H$_4$). ^{13}C NMR (101 MHz, CDCl$_3$) δ 11.74 (CH$_3$), 22.74 (CH$_2$-2), 25.71 (CH$_2$CH$_3$), 28.38 (CH$_2$-7), 29.75 (CH$_2$-3), 37.13 (CH-1), 42.38 (NCH$_2$), 60.40 (CH-11b), 123.69, 126.35, 127.25, 128.73, 137.06, 137.47 (C$_6$H$_4$), 169.90 (C=O). GC-MS (EI, 70eV): m/z = 229 (49), [M$^+$], 173 (21), 145 (100), 132 (30), 131 (60), 130 (45), 117 (14), 103 (11), 77 (13). HRMS (ESI-TOF): *m/z* calcd for C$_{15}$H$_{20}$NO[M + H]$^+$, 230.1545; found, 230.1537.

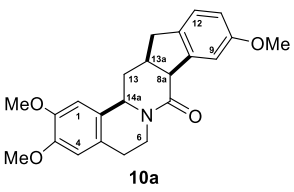
(8a*SR*,13a*RS*,14a*SR*)-2,3,10-Trimethoxy-5,8a,13,13a,14,14a-hexahydroindeno[2',1':4,5]pyrido-[2,1-a]isoquinolin-8(6*H*)-one (**9a**):



9a

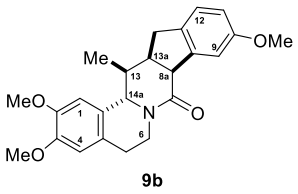
Yield 69% (0.066g, conditions **A**, reaction time: 5h). The crude product purified by column chromatography (SiO$_2$, *n*-hexane:ethyl acetate, 1:1) gave pale purple solid, mp 148-150°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, CDCl$_3$) δ 2.03 (ddd, *J* = 14.0, 10.0, 5.3 Hz, 1H, CHH-14$_{ax}$), 2.25 (dt, *J* = 14.0, 3.6 Hz, 1H, CHH-14$_{eq}$), 2.63 (ddd, *J* = 15.4, 3.3, 2.5 Hz, 1H, CHH-5$_{eq}$), 2.74 (ddd, *J* = 12.5, 11.9, 3.3 Hz, 1H, CHH-6$_{ax}$), 2.91 (ddd, *J* = 15.4, 11.9, 4.8 Hz, 1H, CHH-5$_{ax}$), 2.95 (dd, *J* = 15.5, 6.3 Hz, 1H, CHH-13$_β$), 3.07 (tddd, *J* = 8.8, 6.3, 5.3, 3.6 Hz, 1H, CH-13a), 3.23 (dd, *J* = 15.5, 8.8 Hz, 1H, CHH-13$_α$), 3.81 (s, 3H, 10-OCH$_3$), 3.87 (s, 3H, OCH$_3$), 3.88 (s, 3H, OCH$_3$), 4.04 (d, *J* = 8.8 Hz, 1H, CH-8a), 4.63 (dd, *J* = 10.0, 3.6 Hz, 1H, CH-14a), 4.83 (ddd, *J* = 12.5, 4.8, 2.5 Hz, 1H, CHH-6$_{eq}$), 6.61 (s, 1H, CH-1), 6.63 (s, 1H, CH-4), 6.79 (dd, *J* = 8.3, 2.5 Hz, 1H, CH-11), 7.13 (d, *J* = 8.3 Hz, 1H, CH-12), 7.19 (d, *J* = 2.5 Hz, 1H, CH-9). ^{13}C NMR (101 MHz, CDCl$_3$) δ 28.53 (CH$_2$-5), 34.63 (CH-13a), 36.31 (CH$_2$-14), 37.14 (CH$_2$-13), 39.82 (CH$_2$-6), 51.18 (CH-8a), 52.68 (CH-14a), 55.49 (10-OCH$_3$), 55.89, 56.20 (two OCH$_3$), 108.61 (CH-4), 110.04 (CH-9), 111.58 (CH-1), 114.87 (CH-11), 124.91 (CH-12), 127.71 (C-4a), 128.38 (C-14b), 134.24 (C-12a), 142.74 (C-8b), 147.74, 147.78 (C-2, C-3), 159.12 (C-10), 169.86 (C=O). GC-MS (EI, 70eV): m/z = 379 (14), [M$^+$], 258 (100), 192 (17), 191 (18), 190 (12), 176 (8), 159 (8), 146 (14), 115 (7), 103 (6). HRMS (ESI-TOF): *m/z* calcd for C$_{23}$H$_{26}$NO$_4$[M + H]$^+$, 380.1862; found, 380.1860.

(8a*SR*,13a*RS*,14a*RS*)-2,3,10-Trimethoxy-5,8a,13,13a,14,14a-hexahydroindeno[2',1':4,5]-pyrido[2,1-a]isoquinolin-8(6*H*)-one (**10a**):



Yield 15% (0.0145g, conditions **A**, reaction time: 5h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.50 (ddd, *J* = 13.3, 13.0, 11.6 Hz, 1H, CH<u>H</u>-14$_{ax}$), 2.30 (dt, *J* = 13.3, 3.9, 3.0 Hz, 1H, CH<u>H</u>-14$_{eq}$), 2.57 – 3.01 (m, 5H, C<u>H</u>H-13$_β$, CH-13a, CH_2-5, NC<u>H</u>H), 3.20 (dd, *J* = 15.6, 7.3 Hz, 1H, C<u>H</u>H-13$_α$), 3.79 (s, 3H, OCH_3), 3.83 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 4.05 (d, *J* = 7.0 Hz, 1H, CH-8a), 4.71 (dd, *J* = 11.6, 3.0 Hz, 1H, CH-14a), 4.88 – 4.98 (m, 1H, NCH<u>H</u>), 6.57 (s, 1H, CH-1), 6.63 (s, 1H, CH-4), 6.73 (ddd, *J* = 8.2, 2.6, 1.0 Hz, 1H, CH-11), 7.08 (d, *J* = 8.2 Hz, 1H, CH-12), 7.32 (dd, *J* = 2.6, 1.2 Hz, 1H, CH-9). ^{13}C NMR (101 MHz, $CDCl_3$) δ 28.64 (CH_2-5), 35.66 (CH_2-14), 36.42 (CH-13a), 37.82 (CH_2-13), 39.31 (CH_2-6), 50.40 (CH-8a), 55.49 (10-OCH_3), 55.80 (CH-14a), 55.90, 56.10 (two OCH_3), 108.45 (CH-4), 109.99 (CH-9), 111.38 (CH-1), 114.35 (CH-11), 125.37 (CH-12), 127.29 (C-4a), 128.50 (C-14b), 132.61 (C-12a), 142.01 (C-8b), 147.71 (2C, C-2, C-3), 159.07 (C-10), 168.94 (C=O). GC-MS (EI, 70eV): m/z = 379 (29), [M^+], 281 (19), 258 (100), 244 (20), 207 (44), 192 (23), 191 (36), 190 (23), 176 (11), 159 (13), 146 (25), 115 (13), 103 (10). HRMS (ESI-TOF): *m/z* calcd for $C_{23}H_{26}NO_4[M + H]^+$, 380.1862; found, 380.1869.

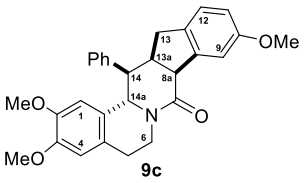
(8a*SR*,13a*RS*,14*SR*,14a*SR*)-2,3,10-Trimethoxy-14-methyl-5,8a,13,13a,14,14a-hexahydroindeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(6*H*)-one (**9b**):



Yield 70% (0.028g, conditions **A**, reaction time: 5h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave grayish-pink solid, mp 173-175°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.01 (d, *J* = 7.0 Hz, 3H, 14-CH_3), 2.27 (dqd, *J* = 8.3, 7.0, 3.8 Hz, 1H, CH-14), 2.64 (dt, *J* = 15.0, 3.4 Hz, 1H, CH$_{eq}$-5), 2.77 (ddd, *J* = 12.7, 10.8, 3.2 Hz, 1H, CH$_{ax}$-6), 2.90 (ddd, *J* = 15.0, 10.8, 4.3 Hz, 1H, CH$_{ax}$-5), 2.97 – 3.12 (m, 3H, CH_2-13, CH13a), 3.81 (s, 3H, 10-OCH_3), 3.88 (s, 6H, 2-OCH_3, 3-OCH_3), 4.11 (d, *J* = 8.0 Hz, 1H, CH-8a), 4.34 (d, *J* = 8.3 Hz, 1H, CH-14a), 4.73 (dt, *J* = 12.7, 4.3 Hz, 1H, CH$_{eq}$-6), 6.62 (s, 1H, CH-1), 6.67 (s, 1H, CH-4), 6.79 (ddd, *J* = 8.3, 2.4, 0.8 Hz, 1H, CH-11), 7.13 (d, *J* = 8.3 Hz, 1H, CH-12), 7.21 (d, *J* = 2.4 Hz, 1H, CH-9). ^{13}C NMR (101 MHz, $CDCl_3$) δ 16.96 (14-CH_3), 29.05 (CH_2-5), 32.86 (CH_2-13), 37.63 (CH-14), 40.48 (CH-13a), 41.35 (CH_2-6), 51.36 (CH-8a), 55.51 (10-OCH_3), 55.91, 56.25 (2-OCH_3, 3-OCH_3), 58.14 (CH-14a), 109.42 (CH-9), 110.73 (CH-1), 111.60 (CH-4), 115.01 (CH-11), 124.73 (CH-12), 126.68 (C-14b), 129.80 (C-4a), 133.95 (C-12a), 142.72 (C-8b), 146.88 (C-2), 147.95 (C-

3), 159.15 (C-10), 169.99 (C=O). GC-MS (EI, 70eV): m/z = 393 (10), [M^+], 272 (100), 219 (17), 207 (18), 192 (68), 191 (61), 159 (29), 176 (21), 146 (43), 115 (11). HRMS (ESI-TOF): *m/z* calcd for $C_{24}H_{28}NO_4[M + H]^+$, 394.2018; found, 394.2013.

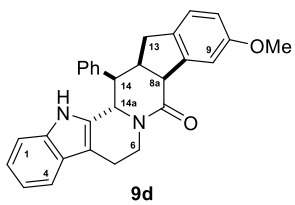
(8a*SR*,13a*RS*,14*RS*,14a*SR*)-2,3,10-Trimethoxy-14-phenyl-5,8a,13,13a,14,14a-hexahydroindeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(6*H*)-one (**9c**):



9c

Yield 85% (0.124g, conditions **A**, reaction time: 5h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:2) gave white solid, mp 209-211°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 – 2.75 (m, 2H, CH<u>H</u>-5, CH<u>H</u>$_\alpha$-13), 2.93 – 3.11 (m, 3H, NC<u>H</u>H, CH<u>H</u>-5, CH-13a), 3.21 (s, 3H, 3-OMe), 3.23 (dd, *J* = 14.8, 10.9 Hz, 1H, CH<u>H</u>$_\beta$-13), 3.55 (dd, *J* = 10.8, 4.1 Hz, 1H, CH-14), 3.81 (s, 3H, OMe), 3.82 (s, 3H, OMe), 3.91 (d, *J* = 7.7 Hz, 1H, CH-8a), 4.35 (dt, *J* = 12.1, 4.6 Hz, 1H, NCH<u>H</u>), 5.39 (d, *J* = 10.8 Hz, 1H, CH-14a), 6.27 (s, 1H, CH-1), 6.61 (s, 1H, CH-4), 6.75 (dd, *J* = 8.2, 2.5 Hz, 1H, CH-11), 7.03 (d, *J* = 8.2 Hz, 1H, CH-12), 7.22 (d, *J* = 2.5 Hz, 1H, CH-9), 7.27 – 7.35 (m, 1H, 14-Ph), 7.37 – 7.48 (m, 4H, 14-Ph). ^{13}C NMR (101 MHz, $CDCl_3$) δ 28.55 (CH_2-5), 32.25 (CH_2-13), 42.71 (NCH_2), 46.01 (CH-13a), 47.27 (CH-14), 51.20 (CH-8a), 55.02 (2-OMe), , 55.43 (10-OMe), 55.79 (3-OMe), 56.24 (CH-14a), 109.97 (CH-1), 111.01 (CH-4), 111.24 (CH-9), 114.68 (C-11), 124.81 (CH-12), 127.15 (5-Ph), 128.27 (5-Ph), 128.75 (C-14b), 129.22 (5-Ph C-4a), 133.60 (C-12a), 142.60 (5-Ph), 143.31 (C-8b), 146.57 (C-2), 147.46 (C-3), 158.91 (C-10), 168.79 (C=O). GC-MS (EI, 70eV): m/z = 455 (18), [M^+], 364 (5), 334 (35), 281 (91), 236 (12), 220 (8), 207 (34), 192 (100), 191 (85), 190 (22), 178 (9), 176 (28), 146 (67), 145 (57), 131 (9), 115 (12), 91 (27), 77 (7), 73 (7). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{30}NO_4[M + H]^+$, 456.2175; found, 456.2168.

(8a*SR*,13a*RS*,14*RS*,14a*SR*)-10-Methoxy-14-phenyl-5,6,8a,13,13a,14,14a,15-octahydro-8*H*-indeno[1,2-g]indolo[2,3-a]quinolizin-8-one (**9d**):

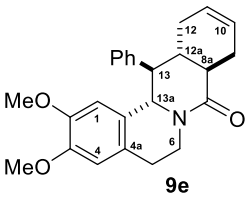


9d

Yield 72% (0.036g, conditions **A**, reaction time: 2h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave yellow solid, mp 155-157°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.70 (dd, *J* = 14.8, 8.0 Hz, 1H, CH<u>H</u>$_\alpha$-13), 2.72–2.79 (m, 1H, CH<u>H</u>$_{eq}$-5), 2.82 (td, *J* = 12.0, 3.0 Hz, 1H,

CH$\underline{H}_{ax}$-6), 2.95 (dddd, *J* = 14.3, 12.0, 4.6, 2.3 Hz, 1H, CH$\underline{H}_{ax}$-5), 2.99–3.08 (m, 1H, CH-13a), 3.28 (dd, *J* = 14.8, 11.2 Hz, 1H, CH$\underline{H}_{\beta}$-13), 3.53 (dd, *J* = 11.3, 4.0 Hz, 1H, CH-14), 3.82 (s, 3H, OCH_3), 3.97 (d, *J* = 7.9 Hz, 1H, CH-8a), 5.09 (ddd, *J* = 12.0, 4.6, 1.2 Hz, 1H, CH$\underline{H}_{eq}$-6), 5.54 (d, *J* = 11.3 Hz, 1H, CH-14a), 6.66 (s, 1H, NH), 6.77 (dd, *J* = 8.3, 2.5 Hz, 1H, CH-11), 6.91 – 6.96 (m, 1H, CH-1), 7.02 – 7.09 (m, 3H, CH-2, CH-3, CH-12), 7.25 (d, *J* = 2.5 Hz, 1H, CH-9), 7.42 – 7.61 (m, 6H, CH-4, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.03 (CH_2-5), 31.76 (CH_2-13), 41.55 (NCH_2), 45.25 (CH-13a), 47.16 (CH-14, 51.53 (CH-8a), 54.50 (CH-14a), 55.45 (OCH_3), 110.82 (CH-1), 110.96 (C-4b), 111.42 (CH-9), 114.80 (CH-11), 118.18 (CH-4), 119.63 (CH-3), 122.13 (CH-2), 124.85 (CH-12), 126.02 (C-4a), 128.42, 129.78 br, 129.82 br (C_6H_5) 132.68 (C-14b), 133.40 (C-12a), 135.32 (C-15a), 140.60 (C_6H_5), 143.02 (C-8b), 158.99 (C-10), 168.73 (C=O). GC-MS (EI, 70eV): m/z = 434 (63), [M^+], 343 (9), 313 (24), 291 (7), 281 (7), 260 (33), 245 (12), 235 (7), 230 (7), 217 (11), 207 (17), 191 (8), 171 (43), 170 (79), 169 (100), 157 (16), 146 (36), 145 (42), 143 (20), 115 (19), 103 (8), 91 (22), 77 (6). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{27}N_2O_2[M + H]^+$, 435.2073; found, 435.2072.

(8a*RS*,12a*SR*,13*RS*,13a*SR*)-2,3-Dimethoxy-13-phenyl-5,6,8a,9,12,12a,13,13a-octahydro-8*H*-isoquinolino[3,2-a]isoquinolin-8-one (**9e**):

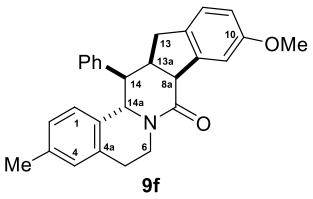


9e

Yield 80% (0.080g, conditions: **A**, reaction time: 7h). The crude product purified by cristalization from ethyl acetate gave white solid, mp 186-188°C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.30 (dt, *J* = 17.8, 0.7 Hz, 1H, CH$\underline{H}_{eq}$-12), 1.63 (dd, *J* = 17.8, 11.2 Hz, 1H, CH$\underline{H}_{ax}$ -12), 1.95 (dd, *J* = 15.8, 11.2 Hz, 1H, CH$\underline{H}_{ax}$-9), 2.08 (qd, *J* = 11.2, 4.7 Hz, 1H, CH-12a), 2.24 (td, *J* = 11.2, 4.6 Hz, 1H, CH-8a), 2.57 (br d, *J* = 15.8 Hz, 1H, CH$\underline{H}_{eq}$-9), 2.70 (dt, *J* = 15.2, 5.1 Hz, 1H, CH$\underline{H}_{eq}$-5), 2.79 (ddd, *J* = 15.2, 8.7, 5.1 Hz, 1H, CH$\underline{H}_{ax}$-5), 2.96 (dd, *J* = 11.1, 10.3 Hz, 1H, CH-13), 3.05 (ddd, *J* = 12.7, 8.7, 5.1 Hz, 1H, NCH$\underline{H}_{ax}$), 3.25 (s, 3H, OCH_3), 3.67 (s, 3H, OCH_3), 4.23 (dt, *J* = 12.7, 5.1 Hz, 1H, NCH$\underline{H}_{eq}$), 5.12 (d, *J* = 10.3 Hz, 1H, CH-13a), 5.47 – 5.54 (m, 1H, =CH-11), 5.64 – 5.72 (m, 1H, =CH-10), 6.34 (s, 1H, CH-1), 6.72 (s, 1H, CH-4), 7.29 (t, *J* = 7.5 Hz, 1H, C_6H_5), 7.41 (t, *J* = 7.5 Hz, 2H, C_6H_5), 7.50 (d, *J* = 7.5 Hz, 2H, C_6H_5). ^{13}C NMR (101 MHz, DMSO-d_6) δ 28.36 (CH_2-5), 28.66 (CH_2-9), 30.89 (CH_2-12), 38.38 (CH-12a), 41.76 (CH-8a), 41.82 (NCH_2), 51.72 (CH-13), 55.23, 55.88 (2 OCH_3), 59.86 (CH-13a), 110.44 (CH-1), 112.13 (CH-4), 126.18 (=CH-11), 126.57 (=CH-10), 127.37 (C_6H_5), 129.21 (C-13b), 129.32 br (C_6H_5), 129.97 (C-4a), 142.69 (C_6H_5), 146.62, 147.56 (C-1, C-2), 170.18 (C=O). GC-MS (EI, 70eV): m/z = 389 (39), [M^+], 361 (35), 298 (26), 281 (33), 259 (10), 233 (17), 232 (17), 192

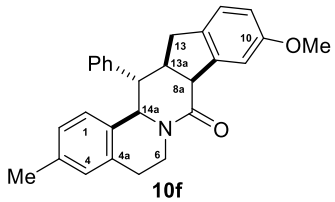
(100), 191 (94), 176 (41), 165 (8), 128 (9), 115 (14), 91 (25), 79 (15), 77 (16). HRMS (ESI-TOF): *m/z* calcd for $C_{25}H_{27}NO_3Na$ $[M + Na]^+$, 412.1889; found, 412.1883.

(8a*SR*,13a*RS*,14*RS*,14a*SR*)-10-Methoxy-3-methyl-14-phenyl-5,8a,13,13a,14,14a-hexahydroindeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(6*H*)-one (**9f**):



Yield 27% (0.026g, conditions: neat/100°C; reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave pale beige solid, mp 232-234°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.25 (s, 3H, 3-CH_3), 2.46 – 2.61 (m, 1H, C<u>H</u>H-13), 2.86 (ddd, *J* = 15.2, 10.0, 4.8 Hz, 1H, CH<u>H$_{ax}$</u>-5), 2.98 (ddd, *J* = 15.2, 6.3, 4.8 Hz, 1H, CH<u>H$_{eq}$</u>-5), 3.05 – 3.17 (m, 2H, CHH-13, CH-13a), 3.42 (ddd, *J* = 12.6, 6.3, 4.8 Hz, 1H, 6-C<u>H</u>H), 3.70 (dd, *J* = 10.7, 3.5 Hz, 1H, CH-14), 3.81 (s, 3H, 10-OCH_3), 3.85 – 3.97 (m, 2H, CH-8a, 6-CH<u>H</u>), 5.34 (d, *J* = 10.7 Hz, 1H, CH-14a), 6.65 – 6.79 (m, 3H, CH-1, CH-2, CH-11), 6.90 – 7.05 (m, 2H, CH-4, CH-12), 7.21 (d, *J* = 2.5 Hz, 1H, CH-9), 7.26 – 7.43 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.85 (3-CH_3), 28.65 (CH_2-5), 32.23 (CH_2-13), 43.32 (NCH_2), 45.23 (CH-14), 46.12 (CH-13a), 50.95 (CH-8a), 54.99 (CH-14a), 55.44 (OCH_3), 111.20 (CH-9), 114.68 (CH-11), 124.76 (CH-12), 125.90 (CH-2), 126.79 (CH-1), 126.99, 127.68 (C_6H_5), 128.48 (CH-4), 129.06 (C_6H_5), 133.58 (C-14b), 134.00 (C-12a), 136.86 (C-4a), 137.62 (C-3), 142.07 (C_6H_5), 143.38 (C-8b), 158.88 (C-10), 168.91 (C=O).GC-MS (EI, 70eV): m/z = 409 (10), [M^+], 288 (11), 235 (42), 207 (17), 146 (100), 145 (39), 91 (17). HRMS (ESI-TOF): *m/z* calcd for $C_{28}H_{28}NO_2$ $[M + H]^+$, 410.2120; found, 410.2127.

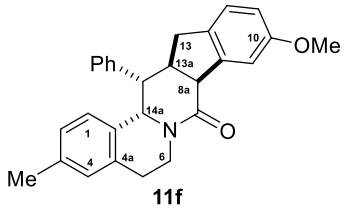
(8a*SR*,13a*RS*,14*SR*,14a*RS*)-10-Methoxy-3-methyl-14-phenyl-5,8a,13,13a,14,14a-hexahydroindeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(6*H*)-one (**10f**):



Yield 24.2% (0.023g, conditions: neat/100°C; reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave reddish solid, mp 95-97°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 3H, 3-CH_3), 2.51 (dd, *J* = 16.0, 2.7 Hz, 1H, CH<u>H$_{\beta}$</u>-13), 2.63 – 2.76 (m, 2H, C<u>H</u>H-5, CH-14), 2.80 – 2.92 (m, 2H, CH<u>H</u>-5, CH<u>H$_{\alpha}$</u>-13), 2.98 (ddd, *J* = 12.2, 11.1, 3.4 Hz, 1H, NC<u>H</u>H), 3.24 (dddd, *J* = 11.4, 8.0, 2.7 Hz, 1H, CH-13a), 3.81 (10-OCH_3), 4.18 (d, *J* = 8.0 Hz, 1H, CH-8a), 4.75 (ddd, *J* = 12.2, 4.8, 3.7 Hz, 1H, NCHH), 5.00 (d, *J* = 10.1 Hz, 1H, CH-14a), 6.10 (d, *J* =

8.1 Hz, 1H, CH-1), 6.50 (dd, *J* = 8.1, 1.6 Hz, 1H, CH-2), 6.75 (dd, *J* = 8.1, 2.8 Hz, 1H, CH-11), 6.87 (d, *J* = 1.6 Hz, 1H, CH-4), 7.02 (d, *J* = 8.1 Hz, 1H, CH-12), 7.04 – 7.13 (m, 2H, C_6H_5), 7.26 – 7.37 (m, 4H, C_6H_5, CH-9). ^{13}C NMR (101 MHz, $CDCl_3$) δ 20.76 (3-CH_3), 29.88 (CH_2-5), 35.92 (CH_2-13), 41.14 (NCH_2) 43.90 (CH-13a), 50.12 (CH-8a), 50.60 (CH-14), 55.51 (10-OCH_3), 61.46 (CH-14a), 110.45 (CH-9), 114.38 (CH-11), 125.10 (CH-12), 125.91 (CH-2), 127.21 (C_6H_5), 127.57 (CH-1), 128.71 (C_6H_5), 128.80 (CH-4), 129.44 (C_6H_5), 131.94 (C-14b), 132.89 (C-12a) 136.19 (C-4a), 136.88 (C-3), 141.50 (C_6H_5), 142.02 (C-8b), 158.98 (C-10), 169.10 (C=O). GC-MS (EI, 70eV): m/z = 409 (8), [M^+], 281 (39), 253 (17), 235 (25), 207 (100), 191 (14), 146 (63), 145 (24), 133 (12), 91 (13), 73 (25). HRMS (ESI-TOF): *m/z* calcd for $C_{28}H_{28}NO_2$[M + H]$^+$, 410.2120; found, 410.2129.

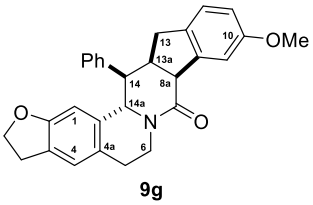
(8a*SR*,13a*RS*,14*SR*,14a*SR*)-10-Methoxy-3-methyl-14-phenyl-5,8a,13,13a,14,14a-hexahydroindeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(6*H*)-one (**11f**):



11f

Yield 14% (0.0135g, conditions: neat/100ºC; reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave brownish solid, mp 199-201°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.15 – 1.38 (m, 1H, CH$\underline{H}_{ax}$-5), 2.14 (ddd, *J* = 15.2, 2.9, 2.1 Hz, 1H, CH$\underline{H}_{eq}$-5), 2.28 (s, 3H, 3-CH_3), 2.55 (td, *J* = 12.7, 2.9 Hz, 1H, CH$\underline{H}_{ax}$-6), 3.11 (dd, *J* = 16.6, 4.8 Hz, 1H, CH$\underline{H}_{\beta}$-13), 3.23 (dd, *J* = 2.5, 0.8 Hz, 1H, CH-14), 3.35 (tdd, *J* = 9.9, 4.8, 0.8 Hz, 1H, CH-13a), 3.67 (dd, *J* = 16.6, 9.9 Hz, 1H, CH$\underline{H}_{\alpha}$-13), 3.81 (s, 3H, 10-OCH_3), 4.54 (d, *J* = 9.9 Hz, 1H, CH-8a), 4.55 (ddd, *J* = 12.7, 4.6, 2.1 Hz, 1H, CH$\underline{H}_{eq}$-6), 4.80 (d, *J* = 2.5 Hz, 1H, CH-14a), 6.56 – 6.63 (m, 2H, C_6H_5), 6.66 (s, 1H, CH-4), 6.84 (ddd, *J* = 8.2, 2.5, 0.9 Hz, 1H, CH-11), 7.01 – 7.11 (m, 4H, CH-1, CH-2, C_6H_5), 7.13-7.14 (m, 2H, CH-9, C_6H_5), 7.19 (d, *J* = 8.2 Hz, 1H, CH-12). ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.02 (3-CH_3), 27.57 (CH_2-5), 38.47 (CH_2-6), 40.31 (CH-13a), 41.11 (CH_2-13), 52.18 (CH-8a), 55.58 (10-OCH_3), 55.96 (CH-14a), 56.64 (CH-14), 109.11 (CH-9), 115.39 (CH-11), 124.79 (CH-12), 126.63, 127.26, 127.67, 128.48, 128.88, (C_6H_5, CH-1, CH-2, CH-4), 130.97 (C-14b), 134.40 (C-12a) 136.23 (C-4a), 136.98 (C-3), 139.80 (Ph), 142.02 (C-8b), 159.48 (C-10), 170.56 (C=O). GC-MS (EI, 70eV): m/z = 409 (12), [M^+], 281 (13), 235 (44), 207 (35), 146 (100), 145 (41), 115 (10), 91 (18). HRMS (ESI-TOF): *m/z* calcd for $C_{28}H_{28}NO_2$ [M + H]$^+$, 410.2120; found, 410.2119.

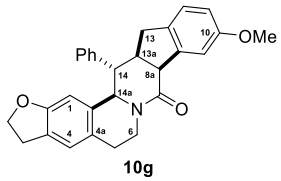
(8a*SR*,13a*RS*,14*RS*,14a*SR*)-10-Methoxy-14-phenyl-3,5,6,8a,13,13a,14,14a-octahydrofuro[3,2-g]indeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(2*H*)-one (**9g**):



9g

Yield 30.3% (0.029g, conditions: **B**, reaction time: 48h,). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave pale beige solid, mp 239-241°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.49 – 2.56 (m, 1H, CH<u>H</u>-13$_\alpha$), 2.82 – 2.87 (m, 1H, C<u>H</u>H-5), 2.93 (dt, *J* = 15.3, 5.2 Hz, 1H, CH<u>H</u>-5), 3.03 – 3.10 (m, 3H, CH_2CH_2O, CH<u>H</u>-13$_\beta$), 3.10 (qd, *J* = 9.2, 8.1, 7.1, 3.8 Hz, 1H, CH-13a), 3.47 (dt, *J* = 12.7, 5.2 Hz, 1H, NC<u>H</u>H), 3.72 (dd, *J* = 10.7, 3.8 Hz, 1H, CH-14), 3.77 – 3.86 (m, 1H, NCHH), 3.80 (s, 3H, OCH_3), 3.90 (d, *J* = 7.1 Hz, 1H, CH-8a), 4.41 – 4.49 (m, 2H, OCH_2), 5.28 (d, *J* = 10.7 Hz, 1H, CH-14a), 6.36 (s, 1H, CH-1), 6.72 (dd, *J* = 8.3, 2.5 Hz, 1H, CH-11), 6.98 (d, *J* = 8.3 Hz, 1H, CH-12), 7.00 (s, 1H, CH-4), 7.20 (d, *J* = 2.5 Hz, 1H, CH-9), 7.27 – 7.38 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 28.21 (CH_2-5), 29.37 (<u>CH_2</u>CH_2O), 32.21 (CH_2-13), 43.91 (NCH_2), 44.77 (CH-14), 46.14 (CH-13a), 50.87 (CH-8a), 55.02 (CH-14a), 55.44 (OCH_3), 71.09 (OCH_2), 107.39 (CH-1), 111.21 (CH-9), 114.65 (CH-11), 124.00 (CH-4), 124.73 (CH-12), 125.86 (C-3), 127.10, 127.53, 129.15 (C_6H_5), 129.88 (C-4a), 133.56 (C-12a), 136.71 (C-14b), 141.76 (C_6H_5), 143.38 (C-8b), 158.50 (C-2), 158.86 (C-10), 168.95 (C=O). GC-MS (EI, 70eV): m/z = 437 (26), [M^+], 316 (23), 281 (36), 263 (72), 253 (14), 236 (15), 207 (97), 191 (21), 174 (100), 173 (35), 146 (98), 145 (69), 133 (14), 115 (20), 103 (13), 96 (12), 91 (35), 73 (26). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{28}NO_3$ [M + H]$^+$, 438.2069; found, 438.2061.

(8a*SR*,13a*RS*,14*SR*,14a*RS*)-10-Methoxy-14-phenyl-3,5,6,8a,13,13a,14,14a-octahydrofuro[3,2-g]indeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(2*H*)-one (**10g**):

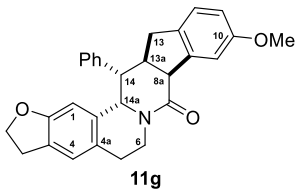


10g

Yield 22.3% (0.0212g, conditions: **B**, reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave pale orange solid, mp 121-123°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.53 (dd, *J* = 16.0, 2.7 Hz, 1H, CH<u>H</u>-13$_\beta$), 2.63 – 2.75 (m, 2H, CH-14, C<u>H</u>H-5), 2.79 – 2.84 (m, 1H, CH<u>H</u>-5), 2.85 (dd, *J* = 16.0, 7.3 Hz, 1H, CH<u>H</u>-13$_\alpha$), 2.98 – 3.10 (m, 3H, <u>CH_2</u>CH_2O, NC<u>H</u>H) 3.20 (dddd, *J* = 11.5, 7.7, 7.3, 2.7 Hz, 1H, CH-13a), 3.81 (s, 3H, OCH_3), 4.16 (d, *J* = 7.7 Hz, 1H, CH-8a), 4.30 – 4.43 (m, 2H, OCH_2), 4.61 (ddd, *J* = 12.3, 4.6, 4.0 Hz, 1H, NCH<u>H</u>), 4.95 (d, *J* = 10.0 Hz, 1H, CH-14a), 5.75 (s, 1H, CH-1), 6.75 (ddd, *J* = 8.2, 2.5, 0.8 Hz, 1H, CH-11), 6.88 (s, 1H, CH-4), 7.03 (d, *J* = 8.2 Hz, 1H, CH-12), 7.13 (dd, *J* = 8.0, 1.0 Hz, 2H, C_6H_5), 7.25 – 7.37 (m, 4H, C_6H_5, CH-9). ^{13}C

NMR (101 MHz, $CDCl_3$) δ 29.38 (CH_2-5), 29.42 (CH_2CH_2O), 35.84 (CH_2-13), 41.74 (NCH_2), 44.04 (CH-13a), 49.93 (CH-14), 50.10 (CH-8a), 55.51 (OCH_3), 61.51 (CH-14a), 71.04 (OCH_2), 108.63 (CH-1), 110.40 (CH-9), 114.34 (CH-11), 124.32 (CH-4), 125.15 (CH-12), 125.55 (C-3), 127.38, 128.84 (C_6H_5), 129.09 (C-4a), 129.25 (C_6H_5), 132.88 (C-12a), 134.81 (C-14b), 141.43 (C_6H_5), 142.02 (C-8b), 157.86 (C-2), 158.98 (C-10), 169.03 (C=O). GC-MS (EI, 70eV): m/z = 437 (19), [M^+], 316 (13), 281 (35), 263 (38), 253 (16), 207 (100), 191 (18), 174 (49), 173 (12), 146 (45), 145 (31), 133 (13), 115 (10), 96 (11), 91 (20), 73 (28). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{28}NO_3[M + H]^+$, 438.2069; found, 438.2068.

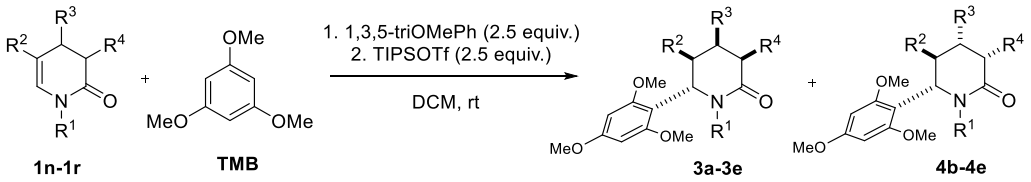
(8a*SR*,13a*RS*,14*SR*,14a*SR*)-10-Methoxy-14-phenyl-3,5,6,8a,13,13a,14,14a-octahydrofuro[3,2-g]indeno[2',1':4,5]pyrido[2,1-a]isoquinolin-8(2*H*)-one (**11g**):



11g

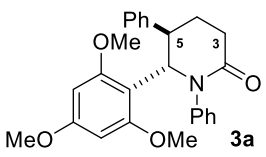
Yield 15% (0.014g, conditions: **B**, reaction time: 48h). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave pale orange solid, mp 117-119°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20 (ddd, *J* = 15.2, 12.6, 4.6 Hz, 1H, CH$\underline{H}_{ax}$-5), 2.11 (dt, *J* = 15.2, 2.7 Hz, 1H, CH$\underline{H}_{eq}$-5), 2.53 (td, *J* = 12.6, 3.0 Hz, 1H, CH$\underline{H}_{ax}$-6), 3.08 (dd, *J* = 16.6, 4.8 Hz, 1H, CH$\underline{H}$-13$_\beta$), 3.12 – 3.22 (m, 2H, $\underline{CH_2}CH_2O$), 3.23 (dd, *J* = 2.7, 0.9 Hz, 1H, CH-14), 3.34 (tdd, *J* = 10.0, 4.8, 0.9 Hz, 1H, CH-13a), 3.67 (dd, *J* = 16.6, 10.0 Hz, 1H, CH$\underline{H}$-13$_\alpha$), 3.81 (s, 3H, OCH_3), 4.48 – 4.65 (m, 4H, NCH$\underline{H}$, CH_2O, CH-8a), 4.73 (d, *J* = 2.7 Hz, 1H, CH-14a), 6.58 (s, 1H, CH-1), 6.63 – 6.69 (m, 3H, CH-4, C_6H_5), 6.84 (ddd, *J* = 8.3, 2.5, 0.9 Hz, 1H, CH-11), 7.06 – 7.16 (m, 4H, C_6H_5, CH-9), 7.19 (d, *J* = 8.3 Hz, 1H, CH-12). ^{13}C NMR (101 MHz, $CDCl_3$) δ 27.25 ($\underline{CH_2}CH_2N$), 29.46 ($\underline{CH_2}CH_2O$), 38.77 (NCH_2), 40.26 (CH-13a), 41.07 (CH_2-13), 52.16 (CH-8a), 55.58 (OCH_3), 56.39 (CH-14a), 56.55 (CH-14), 71.34 (OCH_2), 107.01 (CH-1), 109.13 (CH-9), 115.37 (CH-11), 124.25 (CH-4), 124.83 (CH-12), 125.91 (C-3), 126.66, 127.65, 128.89 (C_6H_5), 129.25 (C-4a), 133.48 (C-12a), 134.40 (C-14b), 139.78 (C_6H_5), 141.96 (C-8b), 158.91 (C-2), 159.48 (C-10), 170.53 (C=O). GC-MS (EI, 70eV): m/z = 437 (22), [M^+], 316 (25), 281 (34), 263 (73), 253 (12), 236 (15), 207 (100), 191 (17), 174 (97), 173 (30), 146 (86), 145 (65), 133 (13), 115 (21), 96 (11), 91 (33), 73 (23). HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{28}NO_3[M + H]^+$, 438.2069; found, 438.2078.

6b. Procedure 15. *General procedure for intermolecular arylation of enelactams with 1,3,5-trimethoxybenzene using TIPSOTf*



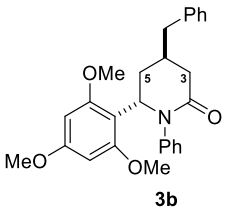
A representative procedure is presented for the synthesis of **3a**. Enelactam **1n** (0.21g, 0.85mmol) and TMB (0.359g, 2.14mmol) were dissolved in 3 mL of anhydrous DCM placed in a dry Schlenk flask. TIPSOTf (0.654g, 2.14mmol) was added to the resulting solution with a syringe and the mixture was stirred at room temperature. Reaction time was monitored by GC-MS. After completation of the reaction 10 mL of saturated sodium bicarbonate solution was added to the reaction flask and the resulting mixture was stirred for 5 minutes. The aqueous layer was extracted with ethyl acetate (3x80mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica (*n*-hexane/ethyl acetate = 1:3) giving product **3a** with 77% yield (0.2761g) as a white solid.

(5*RS*,6*SR*)-1,5-Diphenyl-6-(2,4,6-trimethoxyphenyl)piperidin-2-one (**3a**):



Yield 77% (0.276g, reaction time: 18h, substrate: **1n** (0.21g, 0.85 mmol), TIPSOTf (0.655g, 2.14 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:3) gave white solid, mp 200-202°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.06 – 2.19 (m, 1H, CH$\underline{H}_{eq}$-4), 2.37 (tdd, *J* = 12.8, 11.2, 5.9 Hz, 1H, CH$\underline{H}_{ax}$-4), 2.69 – 2.85 (m, 2H, CH_2-3), 3.08 [br s, 3H, 2'(6')-OCH_3], 3.60 (ddd, *J* = 12.8, 10.0, 3.5 Hz, 1H, CH_{ax}-5), 3.65 (s, 3H, 4'-OCH_3), 3.92 (br s, 3H, OCH_3), 5.47 (d, *J* = 10.0 Hz, 1H, CH_{ax}-6), 5.59 [br s, 1H, CH-3'(5')], 6.00 [br s, 1H, CH-5'(3')], 6.97 – 7.21 (m, 10H, two C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 28.08 (CH_2-4), 33.53 (CH_2-3), 45.05 (CH-5), 54.99 (4'-OCH_3), 55.59 br (2'-OCH_3, 6'-OCH_3), 61.23 (CH-6), 90.39 br (CH-3', CH-5'), 108.36 (C-1'), 126.28, 126.50, 127.20, 127.79, 127.92, 128.09, 141.35, 142.79 (two C_6H_5), 158.89 br (C-2', C-6'), 160.44 (C-4'), 170.75 (C=O). GC-MS (EI, 70eV): m/z = 417 (90), [M^+], 325 (13), 282 (81), 272 (100), 194 (12), 181 (32), 179 (70), 121 (13), 91 (12). HRMS (ESI-TOF): *m/z* calcd for $C_{26}H_{28}NO_4[M + H]^+$, 418.2018; found, 418.2023.

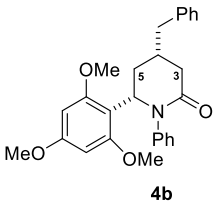
(4*RS*,6*SR*)-4-Benzyl-1-phenyl-6-(2,4,6-trimethoxyphenyl)piperidin-2-one (**3b**):



3b

Yield 21% (0.035g, reaction time: 2h, substrate: **1o** (0.1g, 0.38 mmol), TIPSOTf (0.292g, 0.95 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave white semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94 (ddd, *J* = 13.3, 8.5, 6.0 Hz, 1H, CH$\underline{H}_{ax}$-5), 2.16 (dddd, *J* = 13.3, 6.0, 3.6, 1.2 Hz, 1H, CH$\underline{H}_{eq}$-5), 2.32 (ddd, *J* = 16.9, 7.5, 0.9 Hz, 1H, CH$\underline{H}_{ax}$-3), 2.39 – 2.49 (m, 1H, CH-4), 2.60 – 2.72 (m, 2H, CH$\underline{H}_{eq}$-6, 4-C$\underline{H}$H), 2.80 (dd, *J* = 13.5, 6.6 Hz, 1H, 4-CH$\underline{H}$), 3.72 (br s, 6H, 2'-OCH_3, 6'-OCH_3), 3.75 (s, 3H, 4'-OCH_3), 5.53 (t, *J* = 6.0 Hz, 1H, CH-6), 6.01 (br s, 2H, CH-3', CH-5'), 7.06 – 7.13 (m, 2H, C_6H_5), 7.20 (m, 6H, C_6H_5), 7.24 – 7.32 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 32.60 (CH-4), 34.36 (CH_2-5), 38.56 (CH_2-3), 41.15 (4-CH_2), 54.31 (CH-6), 55.18 (4'-OCH_3), 55.62 br (2'-OCH_3, 6'-OCH_3), 90.68 (CH-3', CH-5'), 109.44 (C-1'), 126.09, 126.26, 126.80, 128.37, 128.46, 129.12, 139.75, 142.39 (two C_6H_5), 158.88 br (C-2', C-6'), 160.38 (C-4'), 170.75 (C=O). GC-MS (EI, 70eV): m/z = 431 (14), [M^+], 340 (100), 272 (13), 221 (48), 181 (37), 179 (24), 168 (17), 151 (12), 146 (23), 121 (20), 117 (12), 115 (11), 91 (31), 77 (15). HRMS (ESI-TOF): *m/z* calcd for $C_{27}H_{30}NO_4$[M + H]$^+$, 432.2175; found, 432.2179.

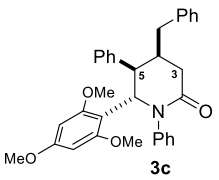
(4*SR*,6*SR*)-4-Benzyl-1-phenyl-6-(2,4,6-trimethoxyphenyl)piperidin-2-one (**4b**):



4b

Yield 48% (0.079g, reaction time: 2h, substrate: **1o** (0.1g, 0.38 mmol), TIPSOTf (0.292g, 0.95 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave white semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 – 2.19 (m, 2H, CH_2-5), 2.27 – 2.42 (m, 2H, CH-4, C$\underline{H}$H-3), 2.55 – 2.73 (m, 3H, CH$\underline{H}$-3, 4-CH_2), 3.52 (br s, 3H, OCH_3), 3.68 (s, 3H, OCH_3), 3.83 (br s, 3H, OCH_3), 5.46 (dd, *J* = 10.8, 6.5 Hz, 1H, CH-6), 5.80 and 5.98 (two br s, 2H, CH-3' or CH-5'), 6.96 – 7.04 (m, 3H, ArH), 7.08 – 7.14 (m, 2H, ArH), 7.16 – 7.23 (m, 3H, ArH), 7.25 – 7.33 (m, 2H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.03 (CH_2-5), 34.98 (CH-4), 39.76 (CH_2-3), 42.54 (4-CH_2), 54.40 (CH-6), 55.11 (OCH_3), 55.33 br and 55.89 br (two OCH_3), 90.10 br and 90.91 br (CH-3', CH-5') , 109.28 (C-1'), 126.17, 126.23, 127.14, 128.00, 128.38, 129.20, 139.46, 141.15 (two C_6H_5), 158.10 br and 159.29 br (C-2', C-6'), 160.52 (C-4'), 170.42 (C=O). GC-MS (EI, 70eV): m/z = 431 (16), [M^+], 340 (100), 272 (13), 221 (48), 181 (36), 179 (24), 168 (17), 151 (11), 146 (23), 121 (20), 91 (31), 77 (15). HRMS (ESI-TOF): *m/z* calcd for $C_{27}H_{30}NO_4$[M + H]$^+$, 432.2175; found, 432.2179.

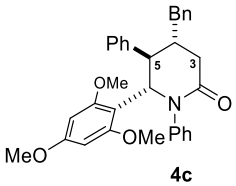
(4*SR*,5*RS*,6*SR*)-4-Benzyl-1,5-diphenyl-6-(2,4,6-trimethoxyphenyl)piperidin-2-one (**3c**):



3c

Yield 34% (0.050g, reaction time: 48h, substrate: **1p** (0.098g, 0.29 mmol), TIPSOTf (0.221g, 0.72 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave white solid, mp 89-91°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (dd, *J* = 13.2, 10.1 Hz, 1H, 4-C<u>H</u>H), 2.46 – 2.50 (m, 1H, C<u>H</u>H-3), 2.62 – 2.71 (m, 2H, CH<u>H</u>-3, CH-4), 2.78 (dd, *J* = 13.2, 3.8 Hz, 1H, 4-CH<u>H</u>), 3.53 (s, 3H, OCH_3), 3.67 – 3.73 (m, 4H, OCH_3, CH-5), 3.85 (s, 3H, OCH_3), 5.75 (d, *J* = 6.3 Hz, 1H, CH-6), 5.85 and 6.08 (two s, 2H, CH-3' and CH-5'), 7.00 (d, *J* = 7.5 Hz, 2H, C_6H_5), 7.07 – 7.30 (m, 7H, C_6H_5), 7.34 (t, *J* = 7.5 Hz, 2H, C_6H_5), 7.42 (d, *J* = 7.5 Hz, 2H,). ^{13}C NMR (101 MHz, $CDCl_3$) δ 36.23 (4-CH_2), 36.83 (CH_2-3), 38.55 (CH-4), 48.82 (CH-5), 55.12 br (OCH_3), 55.43 (OCH_3), 55.75 br (OCH_3), 59.03 (CH-6), 90.44, 91.04 (CH-3', CH-5'), 108.96 (C-1'), 125.97, 126.50, 126.79, 127.09, 128.31, 128.35, 128.48, 128.76, 129.00, 139.95, 141.11, 142.15 (three C_6H_5), 158.36 br, 159.60 br (C-2', C-6'), 160.53 (C-4'), 170.66 (C=O). HRMS (ESI-TOF): *m/z* calcd for $C_{33}H_{34}NO_4[M + H]^+$, 508.2488; found, 508.2485.

(4*RS*,5*RS*,6*SR*)-4-Benzyl-1,5-diphenyl-6-(2,4,6-trimethoxyphenyl)piperidin-2-one (**4c**):

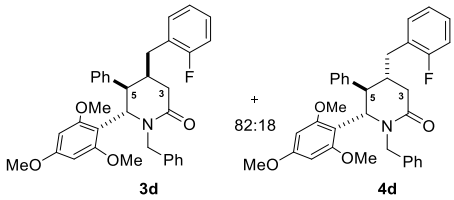


4c

Yield 22% (0.0325g, reaction time: 48h, substrate: **1p** (0.098g, 0.29 mmol), TIPSOTf (0.221g, 0.72 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave 25 : 75 mixture of **3c** : **4c** isomers as white solid. Analyses for **4c** were performed from 25 : 75 mixture of **3c** : **4c** isomers. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.11 (dd, *J* = 13.9, 10.2 Hz, 1H, 4-C<u>H</u>H), 2.42 (dd, *J* = 16.7, 12.2 Hz, 1H, CH<u>H$_{ax}$</u>-3), 2.60 – 2.72 (m, 3H, CH-4, CH<u>H$_{eq}$</u>-3, 4-CH<u>H</u>), 3.00 (s, 3H, OCH_3), 3.35 (dd, *J* = 11.6, 10.2 Hz, 1H, CH_{ax}-5), 3.64 (s, 3H, OCH_3), 3.90 (s, 3H, OCH_3), 5.50 (d, *J* = 10.2 Hz, 1H, CH_{ax}-6), 5.54 and 5.99 (two d, *J* = 2.2 Hz, 2H, CH-3', CH-5'), 6.94 – 7.27 (m, 15H, three C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 38.55 (CH_2-3), 39.04 (CH-4), 39.96 (4-CH_2), 51.30 (CH-5), 54.97 (OCH_3), 55.41 br, 55.71 br (two OCH_3), 61.30 (CH-6), 90.11, 90.87 (CH-3', CH-5'), 108.40 (C-1'), 126.09, 126.36, 126.63, 127.21 (2C), 128.09 (2C), 128.13 (2C), 128.31 (2C), 128.70 (2C), 129.11 (2C), 139.38, 141.03, 141.10 (three C_6H_5), 158.59, 159.00 (C-2', C-6'), 160.41 (C-4'), 170.35 (C=O). GC-MS (EI, 70eV): m/z = 507 (16), [M^+], 282 (46), 272 (100), 257 (19), 207 (14), 194 (11), 181 (19), 179 (86), 151 (12), 121 (15), 117 (19), 115 (15), 91 (33), 77 (8). HRMS (ESI-TOF): *m/z* calcd for $C_{33}H_{34}NO_4[M + H]^+$, 508.2488; found, 508.2493.

(4*SR*,5*RS*,6*SR*)-1-Benzyl-4-(2-fluorobenzyl)-5-phenyl-6-(2,4,6-trimethoxyphenyl)piperidin-2-one (**3d**):

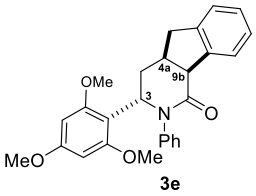
(4*RS*,5*RS*,6*SR*)-1-Benzyl-4-(2-fluorobenzyl)-5-phenyl-6-(2,4,6-trimethoxyphenyl)piperidin-2-one (**4d**):



Yield 75% (0.076g, reaction time: 18h, substrate: **1q** (0.07g, 0.27 mmol), TIPSOTf (0.206g, 0.67 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave 82 : 18 mixture of **3d** : **4d** isomers as pale yellow solid. Analyses for **3d** and **4d** were performed from 82 : 18 mixture of **3d** : **4d** isomers. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.09 [dd, *J* = 13.4, 10.4 Hz, 0.22H, 4-C<u>H</u>H (**4d**)], 2.25 [dd, *J* = 13.2, 10.9 Hz, 1H, 4-C<u>H</u>H (**3d**)], 2.31 [dd, *J* = 17.3, 7.0 Hz, 1H, CH<u>H$_{ax}$</u>-3 (**3d**)], 2.33-2.37 [m, 0.22, C<u>H</u>H-3 (**4d**)], 2.51 [dd, *J* = 17.2, 5.2 Hz, 1H, CH<u>H$_{eq}$</u>-3 (**3d**)], 2.52-2.56 [m, 0.44, CH-4, CH<u>H</u>-3 (**4d**)], 2.55 – 2.62 [m, 1H, CH-4 (**3d**)], 2.65 [dd, *J* = 13.5, 3.9 Hz, 1H, 4-CH<u>H</u> (**3d**)]), 3.02 [s, 0.66H, OCH_3 (**4d**)], 3.15 [dd, *J* = 11.6, 10.1 Hz, 0.22H, CH-5 (**4d**)], 3.55 [dd, *J* = 6.4, 4.0 Hz, 1H, CH-5 (**3d**)], 3.59 [d, *J* = 14.6 Hz, 1H, NC<u>H</u>H (**3d**)], 3.60 [s, 3H, OCH_3 (**3d**)], 3.70 [s, 3H, OCH_3 (**3d**)], 3.73 [s, .0.66H, OCH_3 (**4d**)], 3.74 [s, 0.66H, OCH_3 (**4d**)]), 3.75 [d, *J* = 14.6 Hz, 0.22, NC<u>H</u>H (**4d**)], 3.78 [s, 3H, OCH_3 (**3d**)]), 4.88 [d, *J* = 14.6 Hz, 0.22H, NCH<u>H</u> (**4d**)]), 5.00 [d, *J* = 10.1 Hz, 0.22H, CH-6 (**4d**)], 5.29 [d, *J* = 6.4 Hz, 1H, CH-6 (**3d**)], 5.32 [d, *J* = 14.3 Hz, 1H, NCH<u>H</u> (**3d**)], 5.78 [d, *J* = 2.2 Hz, 0.22H, CH-3'(5') (**4d**)], 5.98 [d, *J* = 2.2 Hz, 0.22H, CH-5'(3') (**4d**)], 6.03 (d, *J* = 2.3 Hz, 1H, CH-3'(5') (**3d**)], 6.05 (d, *J* = 2.3 Hz, 1H, CH-5'(3') (**3d**)], 6.87 – 7.29 [m, 17.08H, ArH(**3d**), ArH(**4d**)]. ^{13}C NMR (101 MHz, $CDCl_3$) δ 29.86 (**3d**, CH_2-3), 33.25 (**4d**, CH_2-3), 35.50 (**3d**, 4-CH_2), 36.71 (**3d**, CH-4), 37.57 (**4d**, CH-4), 38.10 (**4d**, 4-CH_2), 47.23 (**4d**, NCH_2), 47.69 (**3d**, NCH_2), 48.84 (**3d**, CH-5A), 52.24 (**4d**, CH-5), 54.39 (**3d**, CH-6), 55.18, 55.19 (**4d**, two OCH_3), 55.22, 55.41 (**3d**, two OCH_3), 55.56 (**4d**, OCH_3), 55.65 (**3d**, OCH_3), 58.38 (**4d**, CH-6), 90.12 (**4d**, CH-3'(5') 90.40 (**3d**, CH-5'(3') 90.94 (**4d**, CH-5'(3'), 91.11 (**3d**, CH-5'(3'), 107.89 (**4d**, CH-1'), 108.34 (**3d**, CH-1'), 115.22 (**3d**, d, *J*=22.0 Hz, CH-3") 115.27 (**4d**, d, *J*=22.0 Hz, CH-3"), 123.89 (**3d**, **4d**, d, *J* = 3.6 Hz), 126.41 (**3d**, **4d**, d, *J* = 12.8 Hz, C-1"), 126.50 (**4d**, ArH), 126.55 (**3d**, ArH), 126.81 (**4d**, ArH), 126.98 (**3d**, ArH), 127.65, 127.73, 127.80 (**4d**, three ArH), 127.87 (**3d**, ArH), 127.88 (**3d**, B C-4' overlapped), 127.95 (**3d**, ArH), 128.44 (**4d**, ArH), 128.76, 129.21 (**3d**, two ArH), 131.29 (**3d**, d, *J* = 4.9 Hz, CH-6"), 131.35 (**4d**, d, *J* = 5.0 Hz, CH-6"), 137.71 (**3d**, Ar), 138.14 (**4d**, Ar), 140.51 (**3d**, Ar), 140.96 (**4d**, Ar), 158.74 (**3d**, Ar), 158.93, 159.49, (**4d**, two Ar), 159.80, 160.74

(**3d**, two Ar), 160.80 (**4d**, Ar), 162.39 (**4d**, d, *J* = 243.9 Hz, CF-2"), 162.43 (**3d**, d, *J* = 245.0 Hz, CF-2"), 170.66 (**3d**, C=O), 170.88 (**4d**, C=O). **3d**: GC-MS (EI, 70eV): m/z = 539 (8), [M^+], 448 (66), 371 (25), 296 (23), 286 (47), 284 (16), 281 (18), 257 (16), 207 (45), 181 (98), 179 (24), 117 (16), 109 (29), 91 (100), 73 (13). **4d**: GC-MS (EI, 70eV): m/z = 539 (7), [M^+], 448 (61), 371 (23), 296 (21), 286 (46), 284 (17), 281 (17), 257 (16), 207 (41), 181 (100), 179 (23), 117 (19), 109 (27), 91 (99), 73 (12). HRMS (ESI-TOF): *m/z* calcd for $C_{34}H_{34}FNO_4[M + H]^+$, 540.2550; found, 540.2552.

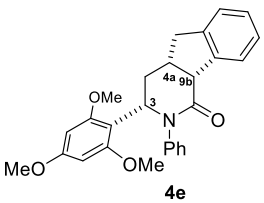
(3*SR*,4a*RS*,9b*SR*)-2-Phenyl-3-(2,4,6-trimethoxyphenyl)-2,3,4,4a,5,9b-hexahydro-1*H*-indeno[1,2-c]pyridin-1-one (**3e**):



3e

Yield 41% (0.030g, reaction time: 5h, substrate: **1r** (0.045g, 0.17 mmol), TIPSOTf (0.132g, 0.43 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave 71 : 29 mixture of **3e** : **4e** isomers as white solid. Analyses for **3e** were performed from 71 : 29 mixture of **3e** : **4e** isomers. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.89 (ddd, *J* = 13.2, 4.3, 2.8 Hz, 1H, CH$\underline{H}_{eq}$-4), 2.06 (td, *J* = 13.2, 5.1 Hz, 1H, CH$\underline{H}_{ax}$-4), 2.61 (dd, *J* = 15.9, ~1.0 Hz, 1H, CH$\underline{H}_{\beta}$-5), 2.90 – 3.06 (m, 1H, CH-4a), 3.17 (ddd, *J* = 15.9, 6.3, 1.2 Hz, 1H, CH$\underline{H}_{\alpha}$-5), 3.80 (br. s, 9H, three OCH_3), 4.17 (d, *J* = 7.4 Hz, 1H, CH-9b), 5.32 (dd, *J* = 5.1, 2.8 Hz, 1H, CH-3), 6.11 [br. s, 2H, $C_6H_2(OMe)_3$], 7.07 – 7.31 (m, 8H, ArH), 7.78 – 7.85 (m, 1H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 33.63 (CH_2-4), 35.23 (CH-4a), 38.20 (CH_2-5), 52.01 (CH-9b), 55.25 (OCH_3), 55.65 (two OCH_3), 56.14 (CH-3), 90.72, 109.15 [$C_6H_2(OMe)_3$], 124.88, 126.08, 126.19, 126.54, 126.59, 127.07, 128.65, 141.24, 141.76, 143.14 (C_6H_5, C_6H_4), 158.98 br., 160.40 [$C_6H_2(OMe)_3$], 171.24 (C=O). GC-MS (EI, 70eV): m/z = 429 (9), [M^+], 398 (5), 308 (5), 281 (10), 261 (87), 248 (9), 214 (7), 207 (24), 194 (90), 181 (100), 179 (82), 168 (17), 165 (10), 151 (17), 142 (12), 128 (9), 121 (29), 115 (24), 91 (12), 77 (16). HRMS (ESI-TOF): *m/z* calcd for $C_{27}H_{28}NO_4[M + H]^+$, 430.2018; found, 430.2058.

(3*SR*,4a*SR*,9b*RS*)-2-Phenyl-3-(2,4,6-trimethoxyphenyl)-2,3,4,4a,5,9b-hexahydro-1*H*-indeno[1,2-c]pyridin-1-one (**4e**):

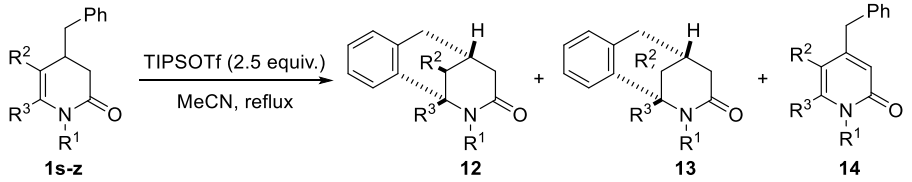


4e

Yield 29% (0.0223g, reaction time: 5h, substrate: **1r** (0.045g, 0.17 mmol), TIPSOTf (0.132g, 0.43 mmol)). The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 94-97°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz,

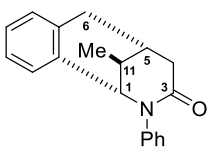
$CDCl_3$) δ 1.76 (dtd, *J* = 13.4, 4.6, 1.4 Hz, 1H, CH$\underline{H_{eq}}$-4), 2.33 (ddd, *J* = 13.4, 13.1, 11.6 Hz, 1H, CH$\underline{H_{ax}}$-4), 2.63 (dd, *J* = 15.6, ~1.0 Hz, 1H, CH$\underline{H_{\alpha}}$-5), 3.01 (dtd, *J* = 13.1, 6.5, 4.5 Hz, 1H, H-4a), 3.22 (dd, *J* = 15.5, 6.5 Hz, 1H, CH$\underline{H_{\beta}}$-5), 3.31 (s, 3H, OCH_3), 3.63 (s, 3H, OCH_3), 3.67 (s, 3H, OCH_3), 4.15 (d, *J* = 6.5 Hz, 1H, CH-9b), 5.64 (dd, *J* = 11.6, 4.6 Hz, 1H, CH-3), 5.73 [d, *J* = 2.3 Hz, 1H, $C_6H_2(OMe)_3$], 5.80 [d, *J* = 2.3 Hz, 1H, $C_6H_2(OMe)_3$], 6.96 – 7.04 (m, 1H, ArH), 7.09 – 7.15 (m, 4H, ArH), 7.18 – 7.30 (m, 3H, ArH), 7.78 – 7.85 (m, 1H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 30.34 (CH_2-4), 36.83 (CH-4a), 38.61 (CH_2-5), 51.20 (CH-9b), 53.62 (CH-3), 54.46, 55.05, 55.90 (three OCH_3) , 89.86, 90.60, 108.85 [$C_6H_2(OMe)_3$], 125.06, 125.07, 125.98, 126.32, 126.82, 126.89, 127.66, 140.89, 141.30, 141.59 (C_6H_5, C_6H_4), 157.90, 159.19, 160.41 [$C_6H_2(OMe)_3$], 169.54 (C=O). GC-MS (EI, 70eV): m/z = 429 (6), [M^+], 398 (5), 308 (5), 281 (5), 261 (100), 248 (8), 214 (5), 207 (12), 194 (67), 181 (79), 179 (65), 168 (15), 165 (7), 151 (13), 142 (7), 128 (8), 121 (24), 115 (21), 91 (9), 77 (11). HRMS (ESI-TOF): *m/z* calcd for $C_{27}H_{28}NO_4[M + H]^+$, 430.2018; found, 430.2058.

6c. Procedure 16. *General procedure for the cyclisation of 4-benzyl enelactams using TIPSOTf*



Enelactam (**1t-z)** (0.36-0.97 mmol) was dissolved in anhydrous MeCN or PhCl (**1s**) (to obtain 0.07M solution) in a dry Schlenk flask. TIPSOTf (2.5 equiv.) was added with a syringe and the mixture was stirred at room temperature for 5 minutes. Subsequently, the reaction was refluxed for 9-96h. Reaction time was monitored by ^{1}H NMR by sampling the reactions at the time intervals. After full conversion the reaction mixture was allowed to cool to room temperature and 10 mL of saturated sodium bicarbonate solution was added to the reaction flask and the mixture was stirred for 5 minutes. The aqueous layer was extracted with ethyl acetate (3×80 mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using a mixture of appropriate mixture of *n*-hexane/AcOEt to give desired products **12a-h**, **13a-e**, **14a-b** and by-product **15**.

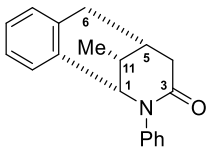
(1*SR*,5*RS*,11*SR*)-11-Methyl-2-phenyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12a**):



12a

Yield 61% [0.061g; reaction conditions: substrate **1s** (0.36 mmol, 0.1g), neat/100°C/24h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 176-178°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.46 (d, *J* = 6.9 Hz, 3H, 11-CH_3), 2.32 – 2.40 (m, 1H, CH-11), 2.38 (dd, *J* = 18.8, 0.8 Hz, 1H, CH$\underline{H}_\beta$-4), 2.45 (dddt, *J* = 7.8, 6.1, 2.0, 0.8, 0.8 Hz, 1H, CH-5), 2.93 (dd, *J* = 17.4, 0.8 Hz, 1H, CH$\underline{H}_\alpha$-6), 2.90 – 2.98 (m, 1H, CH$\underline{H}_\alpha$-4), 3.25 (ddd, *J* = 17.4, 6.1, 0.8 Hz, 1H, CH$\underline{H}_\beta$-6), 4.38 (t, *J* = 2.0 Hz, 1H, CH-1), 6.50 (dd, *J* = 7.7, 1.2 Hz, 1H, CH-10), 6.91 – 7.07 (m, 3H, C_6H_5, CH-9), 7.12 – 7.25 (m, 2H, CH-7, CH-8), 7.25 – 7.33 (m, 1H, C_6H_5), 7.35 – 7.43 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 17.16 (11-CH_3), 31.62 (CH-5), 32.67 (CH-11), 35.87 (CH_2-4), 38.38 (CH_2-6), 64.96 (CH-1), 125.46 (CH-9), 127.08, 128.08 (C_6H_5), 128.20 (CH-8), 128.55 (CH-10), 129.18 (C_6H_5), 129.98 (CH-7), 132.89 (C-6a), 136.90 (C-10a), 142.38 (C_6H_5), 169.47 (C=O). GC-MS (EI, 70eV): m/z = 277 (100), [M^+], 172 (22), 157 (10), 143 (41), 141 (29), 135 (39), 134 (42), 129 (35), 128 (56), 115 (29), 92 (48), 91 (19), 77 (23). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{20}NO$ [M + H]$^+$, 278.1545; found, 278.1539. HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}NONa$[M + Na]$^+$, 300.1364; found, 300.1373.

(1*SR*,5*RS*,11*RS*)-11-Methyl-2-phenyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**13a**):

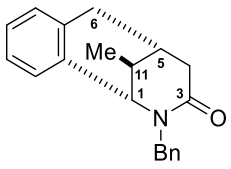


13a

Yield 4% [0.0044g; reaction conditions: substrate **1s** (0.36 mmol, 0.1g), neat/100°C/18h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 195-197°C (ethyl acetate:petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.04 (d, *J* = 7.1 Hz, 3H, 11-CH_3), 2.46 (ddddt, *J* = 7.6, 6.8, 2.4, 1.7, 0.8 Hz, 1H, CH-5), 2.55 (dd, *J* = 18.6, 0.8 Hz, 1H, CH$\underline{H}_\beta$-4), 2.77 (m, 1H, CH-11), 2.83 (dd, *J* = 18.2, 0.8 Hz, 1H, CH$\underline{H}_\alpha$-6), 3.01 (ddd, *J* = 18.6, 7.6, 1.4 Hz, 1H, CH$\underline{H}_\alpha$-4), 3.25 (dddd, *J* = 18.1, 6.8, 1.4, 0.8 Hz, 1H, CH$\underline{H}_\beta$-6), 4.33 (dd, *J* = 3.0, 1.7 Hz, 1H, CH-1), 6.42 (d, *J* = 7.6 Hz, 1H CH-10), 6.92 – 7.00 (m, 3H, C_6H_5, CH-9), 7.17 (d, *J* = 7.4 Hz, 1H, CH-7), 7.22 (td, *J* = 7.4, 1.3 Hz, 1H, CH-8), 7.26 – 7.31 (m, 1H, C_6H_5), 7.33 – 7.40 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 16.11 (11-CH_3), 30.99 (CH-5), 32.17 (CH_2-6), 33.61 (CH-11), 41.20 (CH_2-4), 64.64 (CH-1), 125.47 (CH-9), 127.22 (C_6H_5), 128.15 (CH-8), 128.23 (C_6H_5), 129.15 (C_6H_5), 129.70 (CH-7), 129.74 (CH-10), 132.77 (C-6a), 133.91 (C-10a), 142.07 (C_6H_5), 169.78 (C=O). GC-MS (EI, 70eV): m/z = 277 (72), [M^+], 207 (16),

172 (22), 143 (32), 141 (36), 135 (94), 134 (82), 129 (31), 128 (71), 115 (34), 92 (100), 91 (26), 77 (29). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{20}NO$ $[M + H]^+$, 278.1545 found, 278.1537

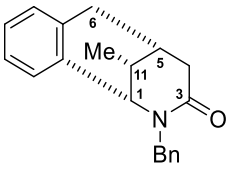
(1*SR*,5*RS*,11*SR*)-2-Benzyl-11-methyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12b**):



12b

Yield 73% [0.079g; reaction conditions: substrate **1t** (0.37 mmol, 0.109g), MeCN/reflux/24h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 2:1) gave white solid, mp 147-149°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.00 (d, *J* = 6.9 Hz, 3H, 11-CH_3), 2.09 – 2.17 (m, 1H, CH-11), 2.26 – 2.37 (m, 2H, CH-5, CH$\underline{H}_\beta$-4), 2.88 (d, *J* = 17.9 Hz, 1H, CH$\underline{H}_\alpha$-6), 2.98 (ddd, *J* = 18.7, 8.1, 1.3 Hz, 1H, CH$\underline{H}_\alpha$-4), 3.21 (dd, *J* = 17.9, 6.1 Hz, 1H, CH$\underline{H}_\beta$-6), 3.68 (d, *J* = 14.9 Hz, 1H, NC$\underline{H}$H), 3.87 (t, *J* = 2.1 Hz, 1H, CH-1), 5.56 (d, *J* = 14.9 Hz, 1H, NCH$\underline{H}$), 7.07 – 7.11 (m, 1H, CH-10), 7.12 – 7.19 (m, 2H, CH-7, CH-9), 7.21 – 7.27 (m, 1H, CH-8), 7.28 – 7.41 (m, 5H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 16.56 (11-CH_3), 31.24 (CH-5), 32.35 (CH-11), 35.82 (CH_2-4), 38.11 (CH_2-6), 46.85 (NCH_2), 57.73 (CH-1), 125.57 (CH-9), 127.53 (C_6H_5), 127.97 (CH-8), 128.18 (CH-10), 128.61, 129.03 (C6H5), 130.14 (CH-7), 133.69 (C-6a), 137.00 (C-10a), 137.24 (C_6H_5), 169.63 (C=O). GC-MS (EI, 70eV): m/z = 291 (62), [M^+], 207 (11), 149 (45), 148 (100), 143 (35), 129 (55), 128 (56), 118 (18), 115 (30), 107 (45), 104 (28), 91 (78), 77 (16), 65 (17). HRMS (ESI-TOF): *m/z* calcd for $C_{20}H_{22}NO$ $[M + H]^+$, 292.1701; found, 292.1700.

(1*SR*,5*RS*,11*RS*)-2-benzyl-11-methyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**13b**):

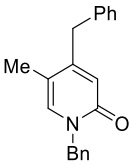


13b

Yield 9% [0.0097g; reaction conditions: substrate **1t** (0.37 mmol, 0.109g), MeCN/reflux/24h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 2:1) gave colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.86 (d, *J* = 6.8 Hz, 3H, 11-CH_3), 2.26 – 2.44 (m, 2H, CH-5, CH-11), 2.49 (d, *J* = 18.4 Hz, 1H, CH$\underline{H}_\beta$-4), 2.78 (d, *J* = 18.2 Hz, 1H, CH$\underline{H}_\alpha$-6), 2.97 (ddd, *J* = 18.4, 7.2, 1.5 Hz, 1H, CH$\underline{H}_\alpha$-4), 3.19 (dd, *J* = 18.2, 7.1 Hz, 1H, CH$\underline{H}_\beta$-6), 3.71 (d, *J* = 15.4 Hz, 1H, NC$\underline{H}$H), 3.84 (dd, *J* = 3.0, 1.8 Hz, 1H, CH-1), 5.49 (d, *J* = 15.4 Hz, 1H, NCH$\underline{H}$), 7.07 (dd, *J* = 7.8, 1.4 Hz, 1H, CH-10), 7.12 – 7.20 (m, 2H, CH-7, CH-9), 7.20 – 7.28 (m, 1H, CH-8), 7.32 (d, *J* = 8.1 Hz, 3H, C_6H_5), 7.35 – 7.41 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 16.14 (11-CH_3), 30.85 (CH-5), 32.19 (CH_2-6), 33.34 (CH-11), 41.17 (CH_2-4), 46.76 (NCH_2), 58.07

(CH-1), 125.73 (CH-9), 127.34, 127.98 (C_6H_5), 128.14 (CH-8), 128.76 (C_6H_5), 129.19 (CH-10), 129.86 (CH-7), 133.58 (C-6a), 134.17 (C-10a), 137.35 (C_6H_5), 169.80 (C=O). GC-MS (EI, 70eV): m/z = 291 (96), [M^+], 186 (19), 147 (32), 146 (67), 144 (70), 143 (59), 141 (21), 129 (100), 128 (67), 119 (28), 115 (35), 106 (57), 104 (55), 91 (91), 77 (19), 65 (23). HRMS (ESI-TOF): *m/z* calcd for $C_{20}H_{22}NO$ [M + H]$^+$, 292.1701; found, 292.1700.

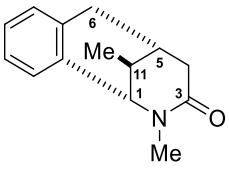
1,4-Dibenzyl-5-methylpyridin-2(1*H*)-one (**14b**):



14b

Yield 28% [0.035g; reaction conditions: substrate **1t** (0.43 mmol, 0.126g), PhCl/110ºC/24h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 2:1) gave yellow solid, mp 123-125°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.91 (d, *J* = 1.0 Hz, 3H, CH_3), 3.76 (s, 2H, 4-CH_2), 5.10 (s, 2H, NCH_2), 6.36 (s, 1H, CH-3), 6.98 (q, *J* = 1.0 Hz, 1H, CH-6), 7.15 (dd, *J* = 7.0, 1.7 Hz, 2H, C_6H_5), 7.18 – 7.40 (m, 8H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 15.56 (CH_3), 39.33 (4-CH_2), 51.24 (NCH_2), 115.53 (C-5), 120.35 (CH-3), 126.70, 127.89, 128.09, 128.71, 128.84, 129.04 (two C_6H_5), 134.65 (CH-6), 136.75, 137.30 (two C_6H_5), 153.42 (C-4), 162.34 (C=O). GC-MS (EI, 70eV): m/z = 289 (57), [M^+], 281 (23), 253 (11), 212 (14), 207 (60), 183 (30), 91 (100), 65 (18). HRMS (ESI-TOF): *m/z* calcd for $C_{20}H_{20}NO$ [M + H]$^+$, 290.1545; found, 290.1544.

(1*SR*,5*RS*,11*SR*)-2,11-Dimethyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12c**):

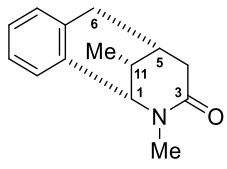


12c

Yield 40% [0.080g; reaction conditions: substrate **1u** (0.94 mmol, 0.203g), MeCN/reflux/96h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.24 (d, *J* = 7.0 Hz, 3H, 11-CH_3), 2.20 (d, *J* = 18.7 Hz, 1H, CH$\underline{H}_\alpha$-4), 2.21 – 2.29 (m, 1H, CH-11), 2.35 (dddd, *J* = 7.4, 6.6, 2.1, 1.5 Hz, 1H, CH-5), 2.79 (dd, *J* = 18.7, 7.4 Hz, 1H, CH$\underline{H}_\beta$-4), 2.84 (d, *J* = 17.6 Hz, 1H, CH$\underline{H}_\alpha$-6), 2.97 (s, 1H, NCH_3), 3.21 (dd, *J* = 17.6, 6.6 Hz, 1H, CH$\underline{H}_\beta$-6), 3.91 (t, *J* = 2.1 Hz, 1H, CH-1), 7.08 – 7.16 (m, 3H, CH-7, CH-9, CH-10), 7.22 (ddd, *J* = 8.0, 6.0, 2.5 Hz, 1H, CH-8). ^{13}C NMR (101 MHz, $CDCl_3$) δ 16.75 (11-CH_3), 31.61 (CH-5), 32.72 (CH-11), 34.06 (NCH_3), 35.55 (CH_2-4), 38.08 (CH_2-6), 62.98 (CH-1), 125.61 (CH-9), 127.81 (CH-10), 128.14 (CH-8), 130.08 (CH-7), 133.27 (C-6a), 137.16 (C-10a), 169.69 (C=O). GC-MS (EI, 70eV): m/z = 215 (96), [M^+], 200 (32), 160 (16),

144 (72), 143 (54), 141 (38), 129 (100), 128 (74), 124 (31), 115 (51), 91 (18), 77 (13), 73 (93), 65 (9). HRMS (ESI-TOF): *m/z* calcd for $C_{14}H_{18}NO$ $[M + H]^+$, 216.1388; found, 216.1382.

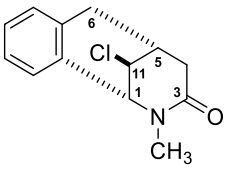
(1*SR*,5*RS*,11*RS*)-2,11-Dimethyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**13c**):



13c

Yield 13% [0.027g; reaction conditions: substrate **1u** (0.94 mmol, 0.203g), MeCN/reflux/96h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 1:1) gave white semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.97 (d, *J* = 7.0 Hz, 3H, 11-CH_3), 2.31 – 2.37 (m, 1H, CH-5), 2.37 (d, *J* = 18.1 Hz, 1H, CH$\underline{H}_\alpha$-4), 2.45 – 2.55 (m, 1H, CH-11), 2.73 (d, *J* = 18.3 Hz, 1H, CH$\underline{H}_\alpha$-6), 2.83 (dd, *J* = 18.1, 7.3 Hz, 1H, CH$\underline{H}_\beta$-4), 2.92 (s, 3H, NCH_3), 3.18 (dd, *J* = 18.3, 7.4 Hz, 1H, CH$\underline{H}_\beta$-6), 3.87 (dd, *J* = 3.1, 1.7 Hz, 1H, CH-1), 7.04 – 7.18 (m, 3H, C_6H_4), 7.23 (td, *J* = 7.3, 1.8 Hz, 1H, C_6H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 16.06 (11-CH_3), 31.05 (CH-5), 32.09 (CH_2-6), 33.04 (CH-11), 33.45 (NCH_3), 40.94 (CH_2-4), 62.67 (CH-1), 125.72, 128.10, 129.04, 129.84, 133.24, 134.05 (C_6H_4), 169.93 (C=O). GC-MS (EI, 70eV): m/z = 215 (72), $[M^+]$, 200 (9), 160 (11), 144 (44), 143 (42), 142 (36), 141 (32), 129 (61), 128 (53), 127 (13), 124 (31), 115 (28), 91 (11), 73 (100). HRMS (ESI-TOF): *m/z* calcd for $C_{14}H_{18}NO$ $[M + H]^+$, 216.1388; found, 216.1381.

(1*RS*,5*RS*,11*SR*)-11-Chloro-2-methyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12d**):

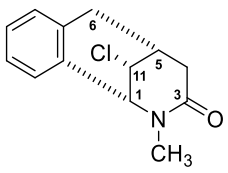


12d

Yield 49% [0.0854g; reaction conditions: substrate **1v** (0.73 mmol, 0.173g), MeCN/reflux/17h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 2:1) gave white solid, mp 126-128°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.31 (dd, *J* = 18.4, 0.6 Hz, 1H, CH$\underline{H}_\beta$-4), 2.82 (dddd, *J* = 7.6, 6.7, 3.1, 1.9 Hz, 1H, CH-5), 3.00 (s, 3H, NCH_3), 3.01 (dd, *J* = 17.8, 0.6 Hz, 1H, CH$\underline{H}_\alpha$-6), 3.08 (dd, *J* = 18.6, 7.6 Hz, 1H, CH$\underline{H}_\alpha$-4), 3.34 (ddd, *J* = 17.8, 6.7, 1.3 Hz, 1H, CH$\underline{H}_\beta$-6), 4.28 (dd, *J* = 3.1, 1.9 Hz, 1H, CH-1), 4.57 (t, *J* = 3.1 Hz, 1H, CH-11), 7.13 (dd, *J* = 7.7, 1.5 Hz, 1H, CH-10), 7.15 – 7.22 (m, 2H, CH-7, CH-9), 7.28 (td, *J* = 7.3, 1.5 Hz, 1H, CH-8). ^{13}C NMR (101 MHz, $CDCl_3$) δ 33.87 (NCH_3), 34.07 (CH-5), 35.28 (CH_2-4), 37.55 (CH_2-6), 57.59 (CH-11), 63.48 (CH-1), 126.38 (CH-9), 128.02 (CH-10), 129.04 (CH-8), 129.86 (CH-7), 131.63, 135.20 (C-6a, CH-10a), 168.38 (C=O). GC-MS (EI, 70eV): m/z = 235 (39), $[M^+]$, 200 (19), 155 (13), 143 (22), 142 (41), 141 (52), 132 (12), 129 (44), 128 (100),

118 (17), 115 (30). HRMS (ESI-TOF): *m/z* calcd for $C_{13}H_{15}ClNO$ $[M + H]^+$, 236.0842; found, 236.0845.

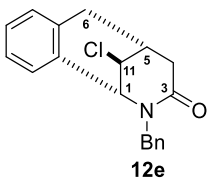
(1*RS*,5*RS*,11*RS*)-11-Chloro-2-methyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**13d**):



13d

Yield 47% [0.081g; reaction conditions: substrate **1v** (0.73 mmol, 0.173g), MeCN/reflux/17h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 2:1) gave white solid, mp 192-194°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.51 (dd, *J* = 18.2, 0.8 Hz, 1H, CH$\underline{H}_\beta$-4), 2.74 – 2.80 (m, 1H, CH-5), 2.79 (dd, *J* = 17.8, 0.8 Hz, 1H, CH$\underline{H}_\alpha$-6), 2.90 (dd, *J* = 18.2, 6.9 Hz, 1H, CH$\underline{H}_\alpha$-4), 2.94 (s, 3H, NCH_3), 3.45 (dd, *J* = 18.0, 6.5 Hz, 1H, CH$\underline{H}_\beta$-6), 4.25 (dd, *J* = 3.5, 1.8 Hz, 1H, CH-1), 4.72 (t, *J* = 3.5 Hz, 1H, CH-11), 7.12 – 7.21 (m, 3H, CH-7, CH-9, CH-10), 7.24 – 7.31 (m, 1H, CH-8). ^{13}C NMR (101 MHz, $CDCl_3$) δ 32.05 (CH_2-6), 32.99 (CH-5), 33.69 (NCH_3), 39.41 (CH_2-4), 55.35 (CH-11), 61.72 (CH-1), 126.16 (CH-9), 128.65 (CH-8), 128.92 (CH-7), 129.82 (CH-10), 132.06, 132.32 (C-6a, C-10a), 168.41 (C=O). GC-MS (EI, 70eV): m/z = 235 (41), $[M^+]$, 200 (31), 160 (12), 155 (13), 143 (30), 142 (49), 141 (63), 132 (15), 129 (53), 128 (100), 118 (21), 115 (41), 89 (10), 73 (27). HRMS (ESI-TOF): *m/z* calcd for $C_{13}H_{15}ClNO$ $[M + H]^+$, 236.0842; found, 236.0846.

(1*RS*,5*RS*,11*SR*)-2-Benzyl-11-chloro-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12e**):

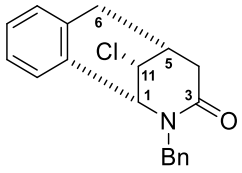


12e

Yield 51% [0.0653g; reaction conditions: substrate **1w** (0.41 mmol, 0.128g), MeCN/reflux/19h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 2:1) gave white solid, mp 172-174°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.44 (dd, *J* = 18.6, 0.8 Hz, 1H, CH$\underline{H}_\beta$-4), 2.74 – 2.86 (m, 1H, CH-5), 3.06 (dd, *J* = 17.8, 0.8 Hz, 1H, CH$\underline{H}_\alpha$-6), 3.23 (ddd, *J* = 18.6, 7.6, 1.4 Hz, 1H, CH$\underline{H}_\alpha$-4), 3.35 (ddd, *J* = 17.8, 7.0, 0.8 Hz, 1H, CH$\underline{H}_\beta$-6), 3.75 (d, *J* = 15.2 Hz, 1H, NC$\underline{H}$H), 4.24 (t, *J* = 3.2, 2.1 Hz, 1H, CH-1), 4.47 (t, *J* = 3.2 Hz, 1H, CH-11), 5.55 (d, *J* = 15.2 Hz, 1H, NCH$\underline{H}$), 7.02 (dd, *J* = 8.0, 1.4 Hz, 1H, CH-10), 7.14 – 7.20 (m, 2H, CH-7, CH-9), 7.24 – 7.42 (m, 6H, CH-8, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 33.72 (CH_2-5), 35.67 (CH_2-4), 37.44 (CH_2-6), 46.77 (NCH_2), 57.26 (CH-11), 58.50 (CH-1), 126.18 (CH-9), 127.59 (C_6H_5), 128.20 (CH-10), 128.57 (2C), 128.90 (2C), (C_6H_5), 129.00 (CH-8), 129.81 (CH-7), 132.05 (C-6a), 135.13 (C_6H_5), 135.94 (CH-10a), 168.47 (C=O). GC-MS (EI, 70eV): m/z = 311

(25), [M^+], 275 (13), 147 (79), 146 (68), 142 (100), 141 (90), 129 (73), 128 (93), 127 (25), 119 (31), 118 (40), 115 (35), 106 (30), 104 (55), 91 (85), 77 (18), 65 (22). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}ClNO$ [M + H]$^+$, 312.1155; found, 312.1147.

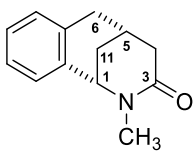
(1*RS*,5*RS*,11*RS*)-2-Benzyl-11-chloro-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**13e**):



13e

Yield 37% [0.047g; reaction conditions: substrate **1w** (0.41 mmol, 0.128g), MeCN/reflux/19h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 2:1) gave white solid, mp 134-140°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (dd, *J* = 18.4, 0.8 Hz, 1H, CH$\underline{H}_b$-4), 2.71 – 2.82 (m, 1H, CH-5), 2.84 (d, *J* = 18.0 Hz, 1H, CH$\underline{H}_\alpha$-6), 3.05 (ddd, *J* = 18.4, 7.6, 1.4 Hz, 1H, CH$\underline{H}_\alpha$-4), 3.46 (ddd, *J* = 18.0, 6.5, 0.8 Hz, 1H, CH$\underline{H}_\beta$-6), 3.73 (d, *J* = 15.3 Hz, 1H, NC$\underline{H}$H), 4.21 (dd, *J* = 3.5, 1.8 Hz, 1H, CH-1), 4.58 (t, *J* = 3.5 Hz, 1H, CH-11), 5.47 (d, *J* = 15.3 Hz, 1H, NCH$\underline{H}$), 7.12 (dd, *J* = 7.8, 1.4 Hz, 1H, CH-10), 7.17 – 7.24 (m, 2H, CH-9, CH-7), 7.27 – 7.44 (m, 6H, CH-8, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 32.18 (CH_2-6), 32.84 (CH-5), 39.64 (CH_2-4), 47.19 (NCH_2), 55.73 (CH-11), 57.26 (CH-1), 126.20 (CH-9), 127.81, 128.14 (2C) (C_6H_5), 128.73 (CH-8), 129.00 (2C) (C_6H_5), 129.12 (CH-7), 129.87 (CH-10), 132.40, 132.42 (C-6a, C-10a), 136.46 (C_6H_5), 168.25 (C=O). GC-MS (EI, 70eV): m/z = 311 (11), [M^+], 275 (14), 147 (82), 146 (54), 142 (94), 141 (82), 129 (94), 128 (92), 127 (27), 119 (25), 118 (28), 115 (35), 106 (53), 104 (45), 91 (100), 77 (18), 65 (23). HRMS (ESI-TOF): *m/z* calcd for $C_{19}H_{19}ClNO$ [M + H]$^+$, 312.1155; found, 312.1151.

(1*SR*,5*SR*)-2-Methyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12f**):

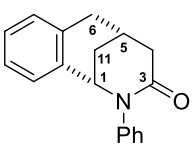


12f

Yield 32% [0.038g; reaction conditions: substrate **1x** (0.59 mmol, 0.118g), MeCN/reflux/24h]. The crude product purified by column chromatography (SiO_2, ethyl acetate) gave colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.08 (dq, *J* = 12.8, 2.9 Hz, 1H, C$\underline{H}$H-11), 2.29 (dtd, *J* = 12.8, 3.4, 1.3 Hz, 1H, CH$\underline{H}$-11), 2.36 (dt, *J* = 18.4, 1.3 Hz, 1H, C$\underline{H}$H-6), 2.61 – 2.70 (m, 1H, CH-5), 2.81 (d, *J* = 18.4, 1H, CH$\underline{H}$-6), 2.82 (d, *J* = 17.9 Hz, 1H, C$\underline{H}$H-4), 2.96 (s, 3H, NCH_3), 3.21 (ddt, *J* = 17.9, 7.0, 1.0 Hz, 1H, CH$\underline{H}$-4), 4.18 (ddd, *J* = 3.4, 2.9, 1.3 Hz, 1H, CH-1), 7.08 – 7.17 (m, 3H, C_6H_4), 7.20 – 7.26 (m, 1H, C_6H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 25.61 (CH-5), 29.43 (CH-11), 33.57 (NCH_3), 35.94 (CH_2-4), 39.57 (CH_2-6), 57.30 (CH-1), 125.60, 127.90, 128.25, 130.14, 133.81, 136.12 (C_6H_4), 170.29 (C=O). GC-MS (EI, 70eV): m/z = 201 (96), [M^+], 141 (19), 130 (44),

129 (75), 128 (77), 115 (37), 110 (21), 73 (100). HRMS (ESI-TOF): *m/z* calcd for $C_{13}H_{16}NO$ $[M + H]^+$, 202.1232; found, 202.1234.

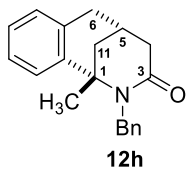
(1*SR*,5*SR*)-2-Phenyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12g**):



12g

Yield 50% [0.127g; reaction conditions: substrate **1y** (0.97 mmol, 0.254g), MeCN/reflux/23h]. The crude product purified by column chromatography (Al_2O_3, *n*-hexane:ethyl acetate, 1:1) gave white solid, mp 171-173°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.23 (dq, *J* = 12.9, 3.2, 1.7 Hz, 1H, C<u>H</u>H-11), 2.52 (dt, *J* = 18.7, 1.4 Hz, 1H, C<u>H</u>H-6), 2.54 (dq, *J* = 12.9, 3.2, 1.3 Hz, 1H, CH<u>H</u>-11), 2.70 – 2.82 (m, 1H, CH-5), 2.92 (d, *J* = 17.8 Hz, 1H, C<u>H</u>H-4), 2.98 (ddd, *J* = 18.6, 7.8, 1.4 Hz, 1H, CH<u>H</u>-6), 3.26 (dd, *J* = 17.8, 6.5 Hz, 1H, CH<u>H</u>-4), 4.66 (td, *J* = 3.2, 1.3 Hz, 1H, CH-1), 6.47 (dd, *J* = 7.5, 1.3 Hz, 1H, C_6H_4), 6.89 – 7.03 (m, 3H, C_6H_5, C_6H_4), 7.14 – 7.32 (m, 3H, C_6H_5, C_6H_4), 7.34 – 7.40 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 25.68 (CH-5), 30.01 (CH-11), 36.32 (CH_2-4), 39.84 (CH_2-6), 59.29 (CH-1), 125.38, 127.20, 128.11 (2C), 128.24, 128.62, 129.19 (2C), 129.98, 133.37, 135.98, 142.2 (C_6H_5, C_6H_4), 169.79 (C=O). GC-MS (EI, 70eV): m/z = 263 (65), [M^+], 141 (23), 135 (78), 134 (79), 129 (53), 128 (80), 115 (28), 93 (28), 92 (100), 77 (29). HRMS (ESI-TOF): *m/z* calcd for $C_{18}H_{18}NO$ $[M + H]^+$, 264.1388; found, 264.1390.

(1*SR*,5*SR*)-2-Benzyl-1-methyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12h**):

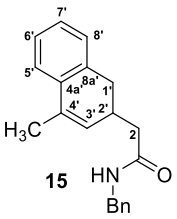


12h

Yield 35% [0.060g; reaction conditions: substrate **1z** (0.58 mmol, 0.169g), MeCN/reflux/51h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave white semi-solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.54 (s, 3H, 1-CH_3), 2.12 (dt, *J* = 13.2, 3.6, 2.3 Hz, 1H, C<u>H</u>H-11), 2.25 (ddd, *J* = 13.2, 3.3, 1.3 Hz, 1H, CH<u>H</u>-11), 2.51 (dt, *J* = 18.1, 1.9 Hz, 1H, C<u>H</u>H-6), 2.57 – 2.70 (m, 1H, CH-5), 2.88 (d, *J* = 17.9 Hz, 1H, C<u>H</u>H-4), 2.96 (ddd, *J* = 18.1, 7.1, 1.2 Hz, 1H, CH<u>H</u>-6), 3.28 (ddd, *J* = 17.9, 7.5, 1.2 Hz, 1H, CH<u>H</u>-4), 4.06 (d, *J* = 16.2 Hz, 1H, NC<u>H</u>H), 5.03 (d, *J* = 16.2 Hz, 1H, NCH<u>H</u>), 7.10 – 7.31 (m, 8H, C_6H_5, C_6H_4), 7.40 (dd, *J* = 7.0, 2.2 Hz, 1H, CH-10). ^{13}C NMR (101 MHz, $CDCl_3$) δ 24.25 (CH_2-5), 25.82 (1-CH_3), 36.27 (CH_2-4), 39.36 (CH_2-11), 40.00 (CH_2-6), 45.32 (NCH_2), 56.26 (C-1), 124.13, 125.63, 126.48, 126.60 (2C), 127.71, 128.38 (2C), 130.20, 133.88, 139.77, 139.81 (C_6H_5, C_6H_4), 171.74 (C=O). GC-MS (EI, 70eV): m/z = 291 (30), [M^+], 186 (15), 158 (12), 149 (64), 148 (100), 143 (76), 142

(67), 130 (34), 129 (34), 128 (76), 115 (34), 107 (50), 106 (72), 91 (89), 77 (19), 65 (18). HRMS (ESI-TOF): *m/z* calcd for $C_{20}H_{22}NO$ $[M + H]^+$, 292.1701; found, 292.1703.

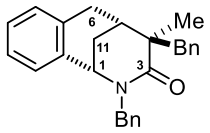
(2'*RS*)-N-benzyl-2-(4-methyl-1,2-dihydronaphthalen-2-yl)acetamide (**15**):



15

Yield 40% [0.068g; reaction conditions: substrate **1z** (0.58 mmol, 0.169g), MeCN/reflux/51h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 3:1) gave white solid, mp 140-142°C (ethyl acetate:hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.04 (t, *J* = 1.4 Hz, 3H, 4'-CH_3), 2.17 (dd, *J* = 14.1, 7.6 Hz, 1H, C<u>H</u>H-2), 2.24 (dd, *J* = 14.1, 6.8 Hz, 1H, CH<u>H</u>-2), 2.59 (dd, *J* = 17.5, 10.3 Hz, 1H, C<u>H</u>H-1'), 2.88 – 3.05 (m, 2H, CH<u>H</u>-1', CH-2'), 4.44 (d, *J* = 5.7 Hz, 2H, NCH_2), 5.72 (t, *J* = 5.7 Hz, 1H, NH), 5.77 (dd, *J* = 4.2, 1.4 Hz, 1H, =CH-3'), 7.07 (dt, *J* = 7.1, 0.9 Hz, 1H, CH-8'), 7.11 – 7.16 (m, 1H, C_6H_4), 7.17 – 7.24 (m, 2H, C_6H_4), 7.25 – 7.30 (m, 3H, C_6H_5), 7.31 – 7.38 (m, 2H, C_6H_5). ^{13}C NMR (101 MHz, $CDCl_3$) δ 19.27 (CH_3), 31.03 (CH-2'), 34.04 (CH_2-1'), 40.76 (CH_2-2), 43.58 (NCH_2), 122.91, 126.57, 127.07, 127.56, 127.83 (2C), 127.94 (C_6H_5, C_6H_4), 128.50 (=CH-3), 128.73 (2C), 132.55 (=C-4'), 134.61, 135.12, 138.34 (C_6H_5, C_6H_4), 171.46 (C=O). GC-MS (EI, 70eV): m/z = 291 (1<), [M^+], 155 (12), 149 (100), 148 (22), 141 (22), 128 (29), 115 (13), 106 (23), 91 (52). HRMS (ESI-TOF): *m/z* calcd for $C_{20}H_{22}NO$ $[M + H]^+$, 292.1701; found, 292.1704.

(1*SR*,4*RS*,5*SR*)-2,4-Dibenzyl-4-methyl-1,4,5,6-tetrahydro-1,5-methanobenzo[c]azocin-3(2*H*)-one (**12i**):

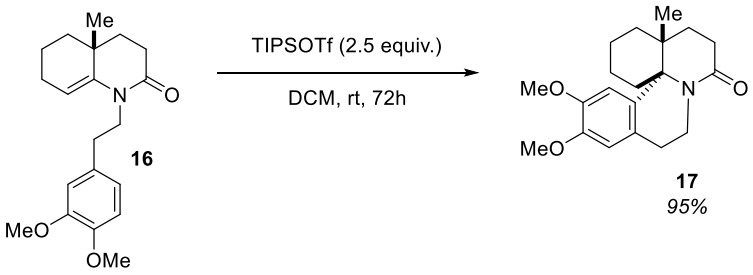


12i

Yield 72% [0.108 g; reaction conditions: substrate **1aa** (0.39 mmol, 0.150g), MeCN/reflux/2h]. The crude product purified by column chromatography (SiO_2, *n*-hexane:ethyl acetate, 6:1) gave colorless thick oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (s, 3H, 4-CH_3), 1.69 – 1.83 (m, 2H, CH_2-11), 2.44 (dtd, *J* = 6.2, 2.8, 1.4 Hz, 1H, CH-5), 2.79 (d, *J* = 13.0 Hz, 1H, 4-C<u>H</u>HPh), 2.86 (dd, *J* = 18.0, 6.2 Hz, 1H, CH<u>H$_b$</u>-6), 3.06 (d, *J* = 18.0 Hz, 1H, CH<u>H$_a$</u>-6), 3.45 (d, *J* = 13.0 Hz, 1H, 4-CH<u>H</u>Ph), 3.75 (d, *J* = 15.4 Hz, 1H, NC<u>H</u>H), 3.98 (ddd, *J* = 3.0, 1.4 Hz, 1H, CH-1), 5.57 (d, *J* = 15.4 Hz, 1H, NCH<u>H</u>), 7.03 (dd, *J* = 7.4, 1.6 Hz, 1H, ArH), 7.11 (t, *J* = 7.6 Hz, 2H, ArH), 7.17 – 7.39 (m, 11H, ArH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 24.53 (CH_3), 27.91 (CH_2-11), 32.49 (CH_2-6), 33.17 (CH-5), 46.00 (C-4), 47.23 (NCH_2), 48.46 (4-CH_2Ph), 52.69 (CH-1), 125.64, 126.64, 127.28, 127.88, 128.09 (2C), 128.14, 128.17 (2C), 128.66 (2C), 129.59, 130.61 (2C) (ArH), 134.43, 136.68, 137.39, 138.39 (Ar), 175.69 (C=O). GC-MS (EI, 70eV): m/z = 381 (24), [$M^{+\cdot}$], 290

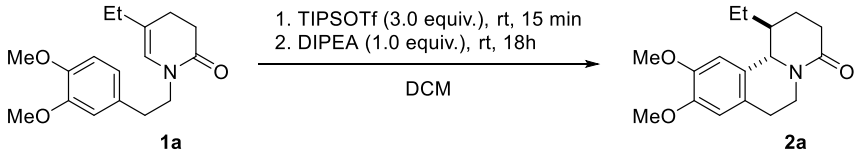
(44), 252 (20), 199 (15), 129 (41), 128 (23), 115 (17), 91 (100), 65 (12). HRMS (ESI-TOF): *m/z* calcd for $C_{27}H_{27}NO$ $[M + H]^+$, 382.2171; found, 382.2169.

6d. Procedure 17. *Procedure for the cyclisation of compound* ***16*** *using TIPSOTf*



Bicyclic enelactam **16** (0.05g, 0.152 mmol) was dissolved in 2 mL of anhydrous DCM, in a dry Schlenk flask. TIPSOTf (0.1163 g, 0.38 mmol, 2.5 equiv.) was added with a syringe and the mixture was stirred at room temperature. After 72h, 5 mL of saturated sodium bicarbonate solution was added to the reaction flask and the mixture was stirred for 5 minutes. The aqueous layer was extracted with ethyl acetate (3×50 mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using mixture of n-hexane/AcOEt (1:1) to give product **17** with 95% as a light beige solid. ^1H and ^{13}C NMR spectra of **17** are in agreement with literature data.[22]

7. Procedure 18. Procedure for the cyclisation of compound 1a using TIPSOTf in presence of DIPEA



Enelactam **1a** (0.05g, 0.17 mmol) was dissolved in 2 mL of anhydrous DCM, which was placed in a dry Schlenk flask. TIPSOTf (0.1588 g, 0.52 mmol, 3.0 equiv.) was added to the resulting solution using syringe and stirred at room temperature for 15 min. Subsequently, *N*,*N*-diisopropylethylamine (DIPEA), 0.0223g, 0.17 mmol, 1.0 equiv.) was added and resulting yellow solution was stirred for 18h at room temperature. After this time, 10 mL of saturated

sodium bicarbonate solution was added to the reaction flask and stirred for 5 minutes. The aqueous layer was extracted with ethyl acetate (3×50 mL), and the combined organic layers were dried over $MgSO_4$. The mixture was filtered, and the solvents were evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel using mixture of *n*-hexane/AcOEt (1:3) to give desired product **2a** with 80% yield (0.04g, 0.14mmol) as a white solid.

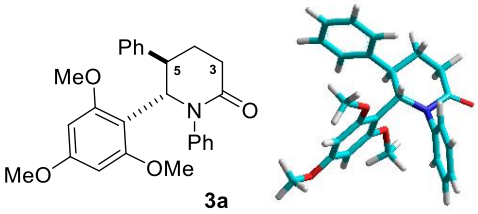
8. Antiproliferative activity

The antiproliferative activity of compounds was evaluated using the Cell Proliferation Reagent WST-1 assay (Sigma-Aldrich, Germany). The WST-1 test is based on the reduction of the tetrazolium salt WST-1 to a soluble red formazan by mitochondrial dehydrogenase. The amount of formazan dye is directly correlated to the number of metabolically active cells. In the present study, A375 cells were seeded in 96-well plate at an initial density of 1.5×103 cells/well and then cultured in 100 μL medium in standard conditions. After 24 h the culture medium was removed and the cells were treated with compounds at a single dose 10 μM for 48 h. All the tested compounds were dissolved in DMSO. In the final concentrations the amount of DMSO did not exceed 0.2%. The cells without the tested compounds were used as controls. After 48 h, WST-1 reagent was added, incubated with the cells for 30 min and absorbance was measured at 450 nm (with 620 nm background correction), using a spectrophotometric microplate reader (Infinite 200 Pro, Tecan, Switzerland). The interaction between compounds (without cells) and WST-1 reagents was also determined (Ablank). Results were normalized to the control cells, and the cell viability was calculated using the following formula: number of viable cells (% of control) = [(Atest – Ablank)/(Acontrol − Ablank)] × 100%. The readings were acquired from three independent experiments (each conducted in triplicate). Results are expressed as mean ± standard deviation. Only compounds which satisfy pre-determined cytotoxicity (viability at 10 μM less than 80%) will progress to the further study in order to estimate the inhibitory concentration causing 50% growth inhibition (IC50) using an online calculator (AAT Bioquest, Inc., 2020, September 10, Quest Graph™ IC50 Calculator (v.1). Retrieved from https://www.aatbio.com/tools/ic50-calculator-v1). Statistical analysis was carried out using Statistica 13.3 (StatSoft Inc., Tulsa, Oklahoma, USA). Experimental data were assessed using the Student's t-test. A p-value level of < 0.05 was considered statistically significant.

9. Conformational analysis data for representative compounds

(Calculated $J^3_{H,H}$ coupling constants were obtained using Haasnoot's correlation [27] on the basis of dihedral angles read from PM3 optimized structure.)

Table S1. Experimental and calculated $^3J_{H,H}$ coupling constants for **3a**

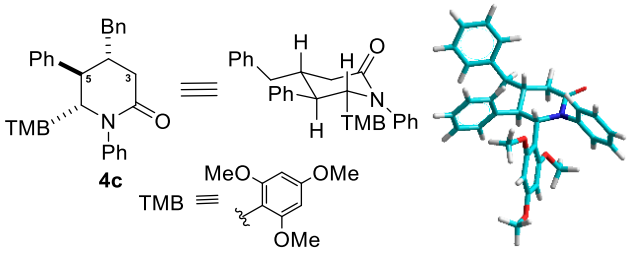


3a

Vicinal hydrogen atoms 3a	Experimental J^3_{HH} [Hz]	Calculated J^3_{HH} [Hz]
CH-6_{ax} vs CH-5_{ax}	10.0	11.0
CH-5_{ax} vs CH-4_{ax}	12.8	12.3
CH-4_{ax} vs CH-3_{ax}	11.2	13.5
CH-4_{ax} vs CH-3_{eq}	5.9	3.6
CH-5_{ax} vs CH-4_{eq}	3.5	3.7
CH-5_{eq} vs CH-4_{eq}	-[a]	3.0

[a] – Could not be assigned.

Table S2. Experimental and calculated $^3J_{H,H}$ coupling constants for **4c**

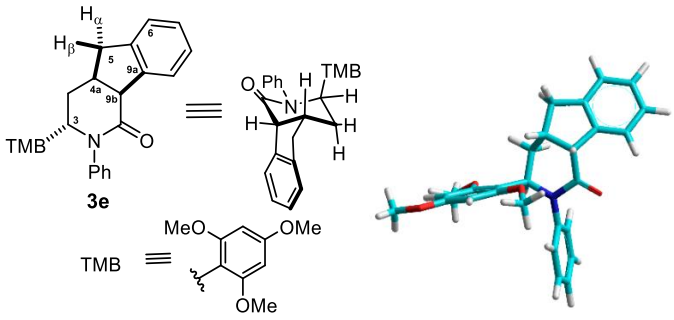


4c

Vicinal hydrogen atoms 4c	Experimental J^3_{HH} [Hz]	Calculated J^3_{HH} [Hz]
CH-6_{ax} vs CH-5_{ax}	10.2	11.0
CH-5_{ax} vs CH-4_{ax}	11.6	12.2
CHH-3_{ax} vs CH-4_{ax}	12.2	12.3
CHH-3_{eq} vs CH-4_{ax}	-[a]	3.2

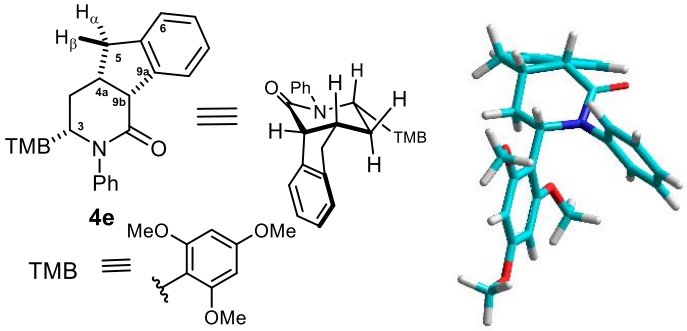
[a] – Could not be assigned.

Table S3. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **3e**



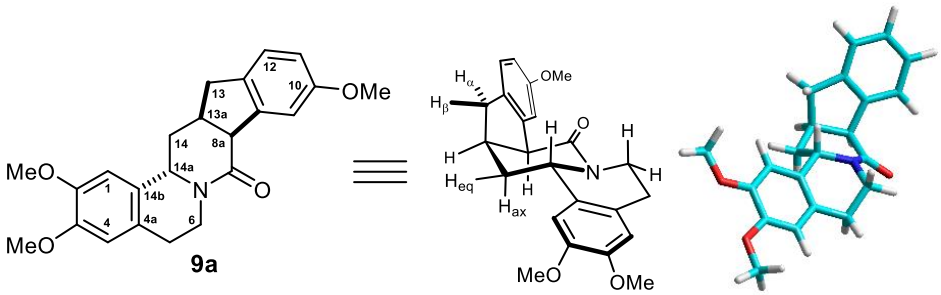
Vicinal hydrogen atoms 3e	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-3_{eq} vs CH-4_{ax}	5.1	6.2
CH-3_{eq} vs CH-4_{eq}	2.8	1.4
CH-4a vs CH-9b	7.4	9.4
CH-4a vs CHH-5_{β}	~1	1.9
CH-4a vs CHH-5_{α}	6.3	9.7
CH-4a vs CH<u>H</u>-4_{ax}	13.2	12.2
CH-4a vs C<u>H</u>H-4_{eq}	4.3	3.7

Table S4. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **4e**



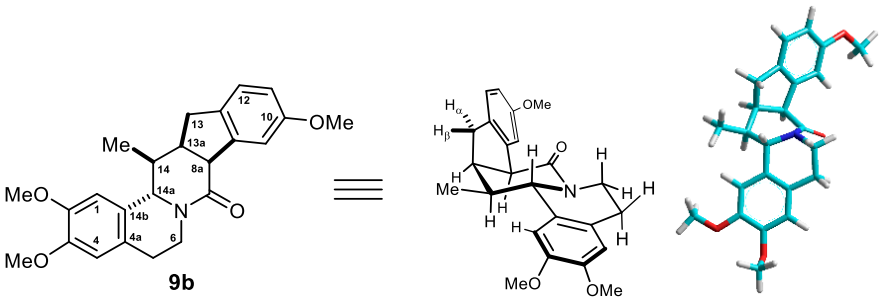
Vicinal hydrogen atoms 4e	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-3_{ax} vs CH-4_{ax}	11.6	11.8
CH-3_{ax} vs CH-4_{eq}	4.6	2.5
CH-4a vs CH-9b	6.6	8.2
CH-4a vs CH-5_{α}	~1	1.3
CH-4a vs CH-5_{β}	6.5	8.9
CH-4a vs CH-4_{ax}	13.1	12.1
CH-4a vs CH-4_{eq}	4.5	4.1

Table S5. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **9a**



Vicinal hydrogen atoms 9a	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a	8.8	10.2
CH-14a vs CH-14_{ax}	10.0	11.8
CH-14a vs CH-14_{eq}	3.6	2.3
CH-13a vs CH-13_{β}	6.3	7.5
CH-13a vs CH-13_{α}	8.8	9.5
CH-13a vs CH-14_{eq}	3.6	2.7
CH-13a vs CH-14_{ax}	5.3	3.9
CH-5_{ax} vs CH-6_{ax}	11.9	12.6
CH-5_{ax} vs CH-6_{eq}	4.8	3.3
CH-6_{ax} vs CH-5_{eq}	3.3	3.0
CH-6_{eq} vs CH-5_{eq}	2.5	2.6

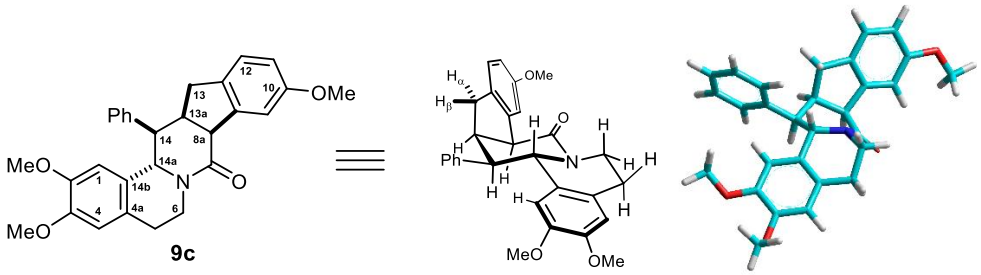
Table S6. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **9b**



Vicinal hydrogen atoms 9b	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a	8.0	8.5
CH-14_{ax} vs CH-13a	3.8	4.4
CH-$14a_{ax}$ vs CH-14_{ax}	8.3	8.2
CH-13a vs CH-13_{β}	-[a]	9.5
CH-13a vs CH-13_{α}	-[a]	8.2
CH-5_{ax} vs CH-6_{ax}	10.8	11.7
CH-5_{ax} vs CH-6_{eq}	3.4	5.1
CH-6_{ax} vs CH-5_{eq}	4.3	6.1
CH-6_{eq} vs CH-5_{eq}	3.2	1.1

[a] – Could not be assigned.

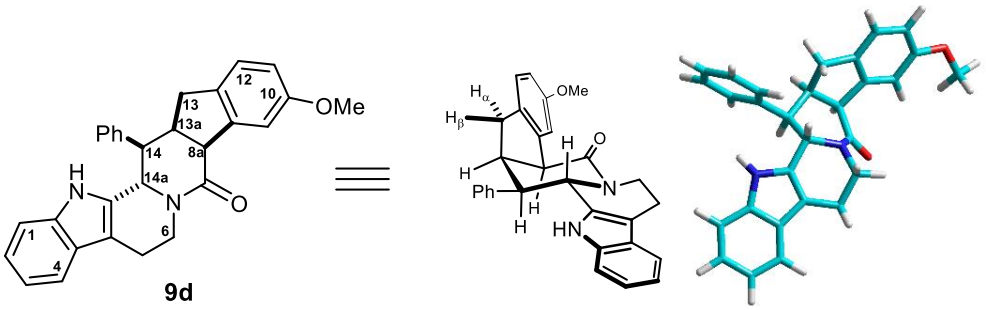
Table S7. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **9c**



Vicinal hydrogen atoms 9c	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a	7.7	9.2
CH-14_{ax} vs CH-13a	4.1	3.8
CH-$14a_{ax}$ vs CH-14_{ax}	10.8	9.8
CH-13a vs CH-13_{β}	10.9	8.7
CH-13a vs CH-13_{α}	-[a]	8.8
CH-5_{ax} vs CH-6_{ax}	12.1	12.3
CH-5_{ax} vs CH-6_{eq}	-[a]	5.0
CH-6_{ax} vs CH-5_{eq}	4.6	4.0
CH-6_{eq} vs CH-5_{eq}	-[a]	1.7

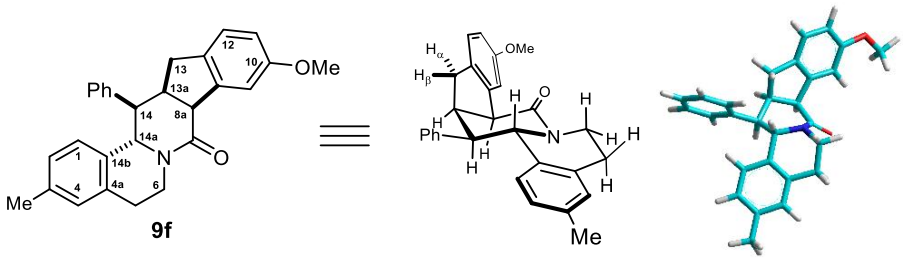
[a] – Could not be assigned.

Table S8. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **9d**



Vicinal hydrogen atoms 9d	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a	7.9	9.3
CH-14_{ax} vsCH-13a	4.0	3.3
CH-$14a_{ax}$ vs CH-14_{ax}	11.3	10.7
CH-13a vs CH-13_{β}	11.2	8.6
CH-13a vs CH-13_{α}	8.0	8.8
CH-5_{ax} vs CH-6_{ax}	12.0	12.1
CH-5_{ax} vs CH-6_{eq}	4.6	5.4
CH-6_{ax} vs CH-5_{eq}	3.0	4.6
CH-6_{eq} vs CH-5_{eq}	1.2	1.3

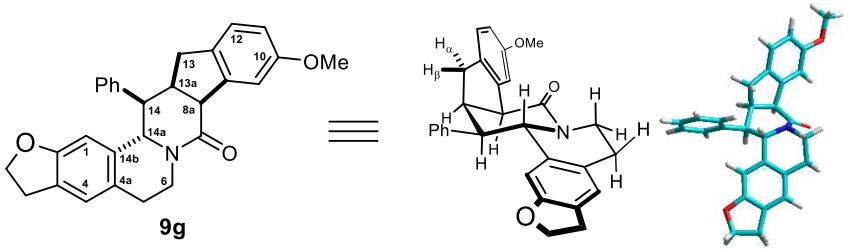
Table S9. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **9f**



Vicinal hydrogen atoms 9f	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a	-[a]	9.2
CH-14_{ax} vs CH-13a	3.5	3.8
CH-$14a_{ax}$ vs CH-14_{ax}	10.7	9.7
CH-13a vs CH-13_{β}	-[a]	8.7
CH-13a vs CH-13_{α}	-[a]	8.7
CH-5_{ax} vs CH-6_{ax}	10.0	12.2
CH-5_{ax} vs CH-6_{eq}	4.8	5.2
CH-6_{ax} vs CH-5_{eq}	6.3	4.2
CH-6_{eq} vs CH-5_{eq}	-[a]	1.6

[a] – Could not be assigned.

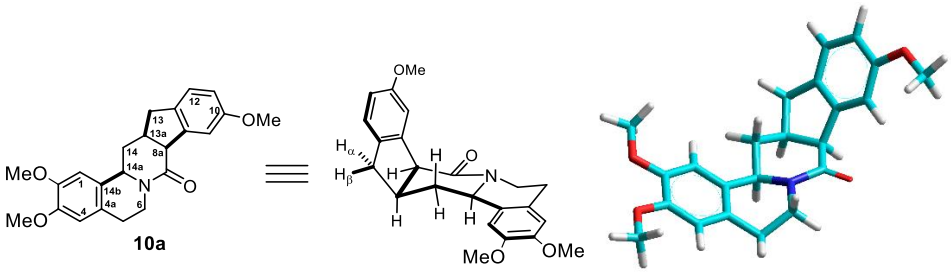
Table S10. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **9g**



Vicinal hydrogen atoms 9g	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a	7.1	9.1
CH-14_{ax} vsCH-13a	3.8	3.9
CH-$14a_{ax}$ vs CH-14_{ax}	10.7	9.5
CH-13a vs CHH-13_{β}	~9.2	8.7
CH-13a vs CHH-13_{α}	~8.2	8.7
CH-5_{ax} vs CH-6_{ax}	12.7	12.1
CH-5_{ax} vs CH-6_{eq}	5.2	5.4
CH-6_{ax} vs CH-5_{eq}	5.2	4.4
CH-6_{eq} vs CH-5_{eq}	-[a]	1.5

[a] – Could not be assigned.

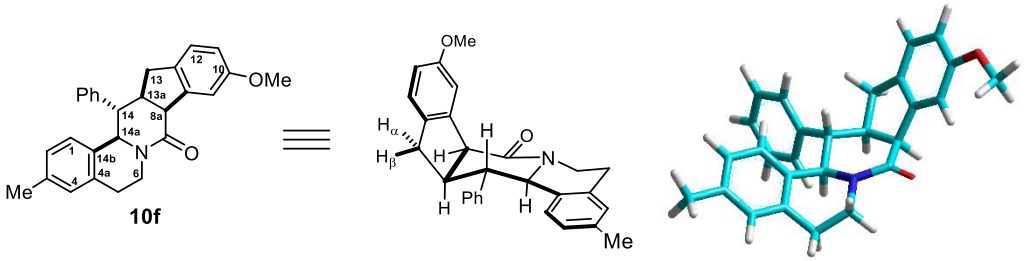
Table S11. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **10a**



Vicinal hydrogen atoms 10a	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a$_{ax}$	7.0	8.8
CH-14$_{ax}$ vs CH-13a$_{ax}$	13.0	12.2
CH-14$_{eq}$ vs CH-13a$_{ax}$	3.9	3.8
CH-13a$_{ax}$ vs CH-13$_{\beta}$	7.3	9.3
CH-13a$_{ax}$ vs CH-13$_{\alpha}$	-[a]	1.6
CH-14a$_{ax}$ vs CH-14$_{ax}$	11.6	11.7
CH-14a$_{ax}$ vs CH-14$_{eq}$	3.0	1.9
CH-5$_{ax}$ vs CH-6$_{ax}$	-[a]	12.1
CH-5$_{ax}$ vs CH-6$_{eq}$	-[a]	5.1
CH-6$_{ax}$ vs CH-5$_{eq}$	-[a]	4.3
CH-6$_{eq}$ vs CH-5$_{eq}$	-[a]	1.7

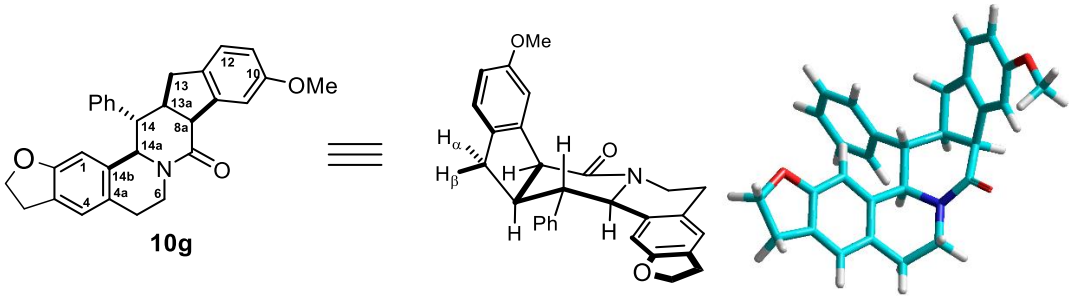
[a] – Could not be assigned.

Table S12. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **10f**



Vicinal hydrogen atoms 10f	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a$_{ax}$	8.0	9.3
CH-14$_{ax}$ vs CH-13a$_{ax}$	11.4	11.7
CH-13a$_{ax}$ vs CH-13$_{\beta}$	2.7	1.9
CH-13a$_{ax}$ vs CH-13$_{\alpha}$	7.8	9.7
CH-14a$_{ax}$ vs CH-14$_{ax}$	10.1	11.4
CH-5$_{ax}$ vs CH-6$_{ax}$	11.1	12.1
CH-5$_{ax}$ vs CH-6$_{eq}$	4.2	5.0
CH-6$_{ax}$ vs CH-5$_{eq}$	3.4	4.3
CH-6$_{eq}$ vs CH-5$_{eq}$	3.7	1.7

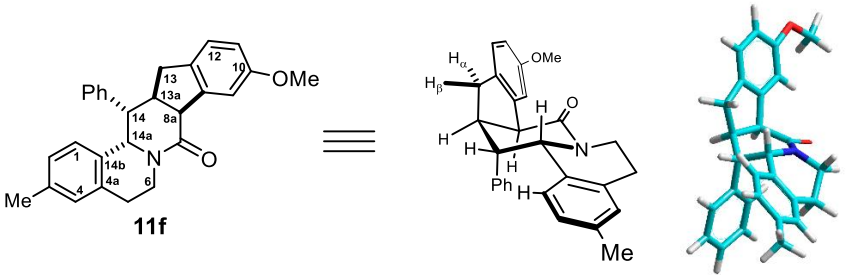
Table S13. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **10g**



Vicinal hydrogen atoms 10g	Experimental J^3_{HH} [Hz]	Calculated J^3_{HH} [Hz]
CH-8a vs CH-13a$_{ax}$	7.7	8.4
CH-14a$_{ax}$ vs CH-14$_{ax}$	10.0	10.8
CH-13a$_{ax}$ vs CH-13$_{\beta}$	2.7	1.3
CH-13a$_{ax}$ vs CH-13$_{\alpha}$	7.3	8.9
CH-13a$_{ax}$ vs CH-14$_{ax}$	11.5	12.3
CH-5$_{ax}$ vs CH-6$_{ax}$	-[a]	12.4
CH-5$_{ax}$ vs CH-6$_{eq}$	4.6	4.3
CH-6$_{ax}$ vs CH-5$_{eq}$	-[a]	3.7
CH-6$_{eq}$ vs CH-5$_{eq}$	4.0	2.1

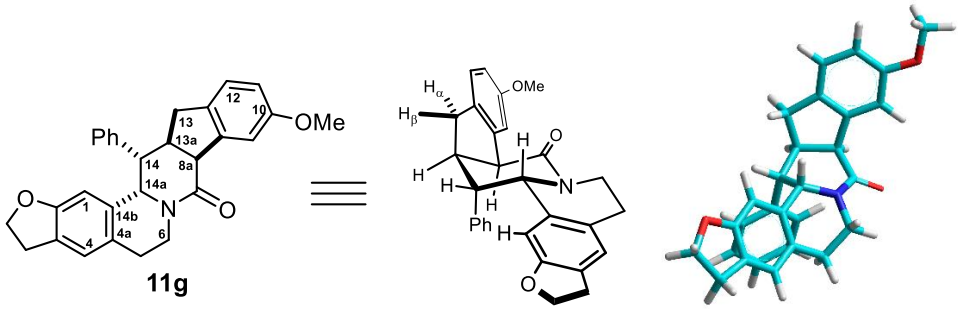
[a] – Could not be assigned.

Table S14. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **11f**



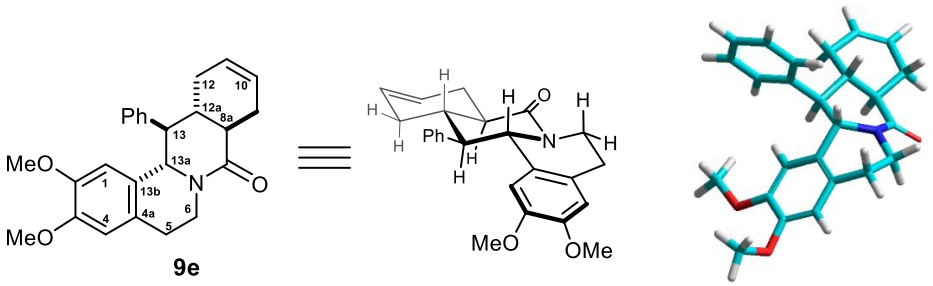
Vicinal hydrogen atoms 11f	Experimental J^3_{HH} [Hz]	Calculated J^3_{HH} [Hz]
CH-8a vs CH-13a	9.9	10.1
CH-14a vs CH-14	2.5	3.0
CH-13a vs CH-13$_{\beta}$	4.8	8.2
CH-13a vs CH-13$_{\alpha}$	9.9	9.1
CH-13a vs CH-14	0.8	0.9
CH-5$_{ax}$ vs CH-6$_{ax}$	12.7	12.6
CH-5$_{ax}$ vs CH-6$_{eq}$	4.6	3.0
CH-6$_{ax}$ vs CH-5$_{eq}$	2.9	2.4
CH-6$_{eq}$ vs CH-5$_{eq}$	2.1	3.2

Table S15. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **11g**



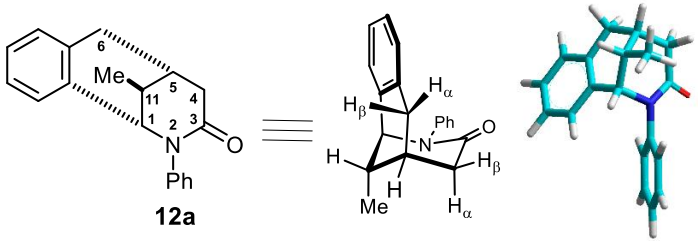
Vicinal hydrogen atoms 11g	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-8a vs CH-13a	10.0	10.8
CH-14a vs CH-14	2.7	2.6
CH-13a vs CH-13$_{\beta}$	4.8	4.7
CH-13a vs CH-13$_{\alpha}$	10.0	10.3
CH-13a vs CH-14	0.9	0.5
CH-5$_{ax}$ vs CH-6$_{ax}$	12.6	12.6
CH-5$_{ax}$ vs CH-6$_{eq}$	4.6	3.3
CH-6$_{ax}$ vs CH-5$_{eq}$	3.0	2.6
CH-6$_{eq}$ vs CH-5$_{eq}$	2.7	3.0

Table S16. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **9e**



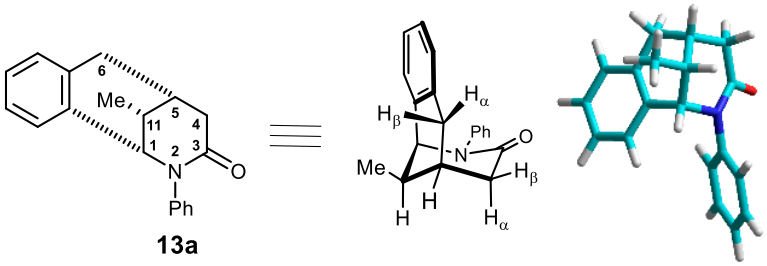
Vicinal hydrogen atoms 9e	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-13a$_{ax}$ vs CH-13$_{ax}$	10.3	9.7
CH-13$_{ax}$ vs CH-12a$_{ax}$	11.2	12.3
CH-12a$_{ax}$ vsCH-8a$_{ax}$	11.2	12.4
CH-8a$_{ax}$ vs CH-9$_{ax}$	11.2	11.9
CH-8a$_{ax}$ vs CH-9$_{eq}$	4.6	4.7
CH-12a$_{ax}$ vs CH-12$_{ax}$	11.2	11.9
CH-12a vs CH-12$_{eq}$	4.7	4.6
CH-6$_{eq}$ vs CH-5$_{eq}$	5.1	1.6
CH-6$_{eq}$ vs CH-5$_{ax}$	5.1	5.1
CH-6$_{ax}$ vs CH-5$_{eq}$	5.1	4.1
CH-6$_{ax}$ vs CH-5$_{ax}$	8.7	12.1

Table S17. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **12a**



Vicinal hydrogen atoms 12a	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-1 vs CH-11	2.0	1.8
CH-11 vs CH-5	2.0	1.9
CH-5 vs CH-4$_\alpha$	7.8	6.1
CH-5 vs CH-4$_\beta$	0.8	1.4
CH-5 vs CH-6$_\alpha$	0.8	1.0
CH-5 vs CH-6$_\beta$	6.1	7.1

Table S18. Experimental and calculated $^{3}J_{H,H}$ coupling constants for **13a**



Vicinal hydrogen atoms 13a	Experimental J^{3}_{HH} [Hz]	Calculated J^{3}_{HH} [Hz]
CH-1 vs CH-11	3.0	2.4
CH-11 vs CH-5	2.4	2.4
CH-5 vs CH-4$_\alpha$	7.6	5.9
CH-5 vs CH-4$_\beta$	0.8	1.4
CH-5 vs CH-6$_\alpha$	0.8	1.0
CH-5 vs CH-6$_\beta$	6.8	7.2

10. ^{1}H NMR, ^{13}C NMR, ^{13}C DEPT-135 spectra of monitoring the cyclization of enelactam 1a in presence of 0.5, 1.5 and 2.5 fold excess of TIPSOTf

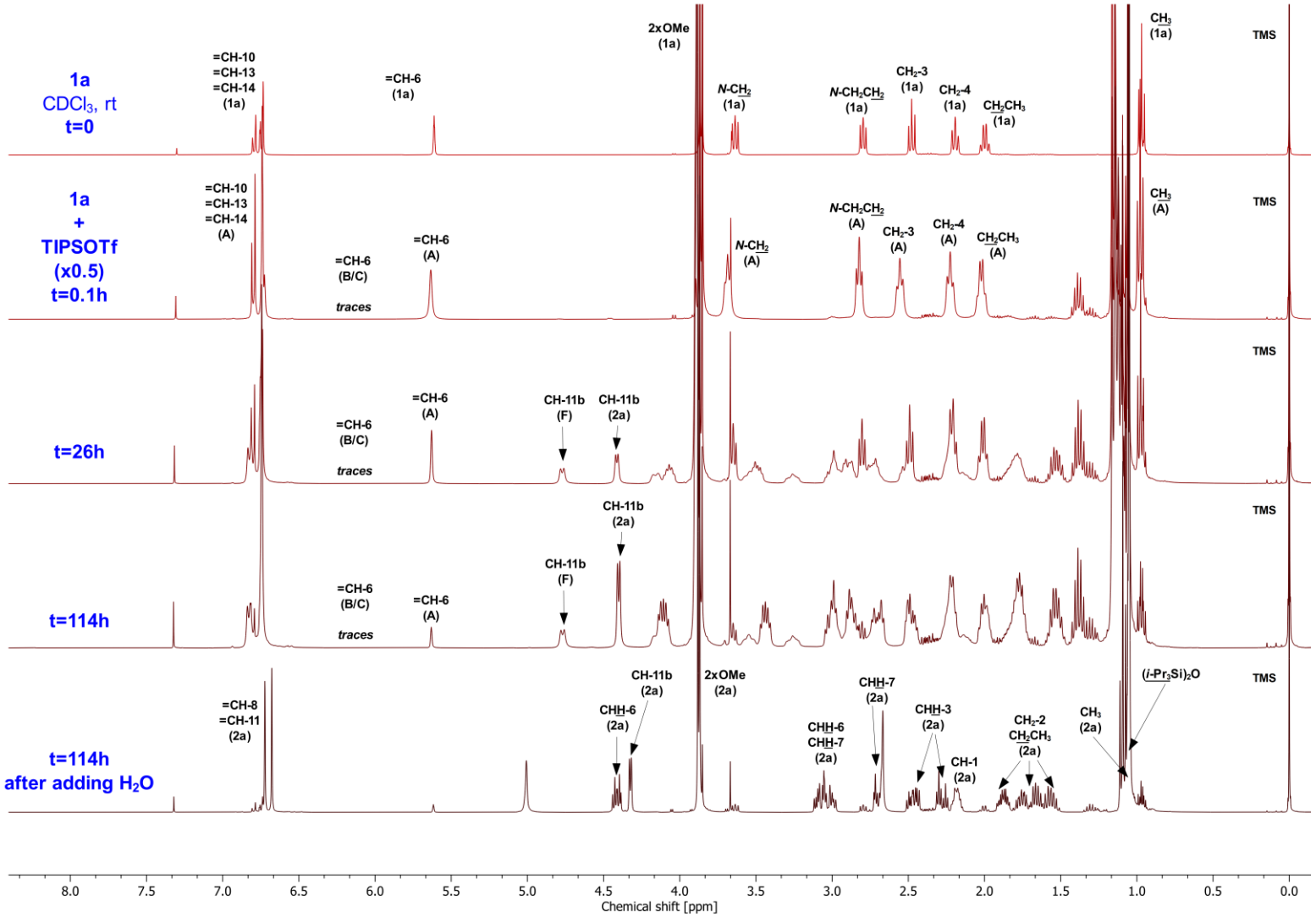


Figure S4. ^{1}H NMR spectra recorded at different time intervals of the cyclization reaction of **1a** in the presence of 0.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^{o}C)

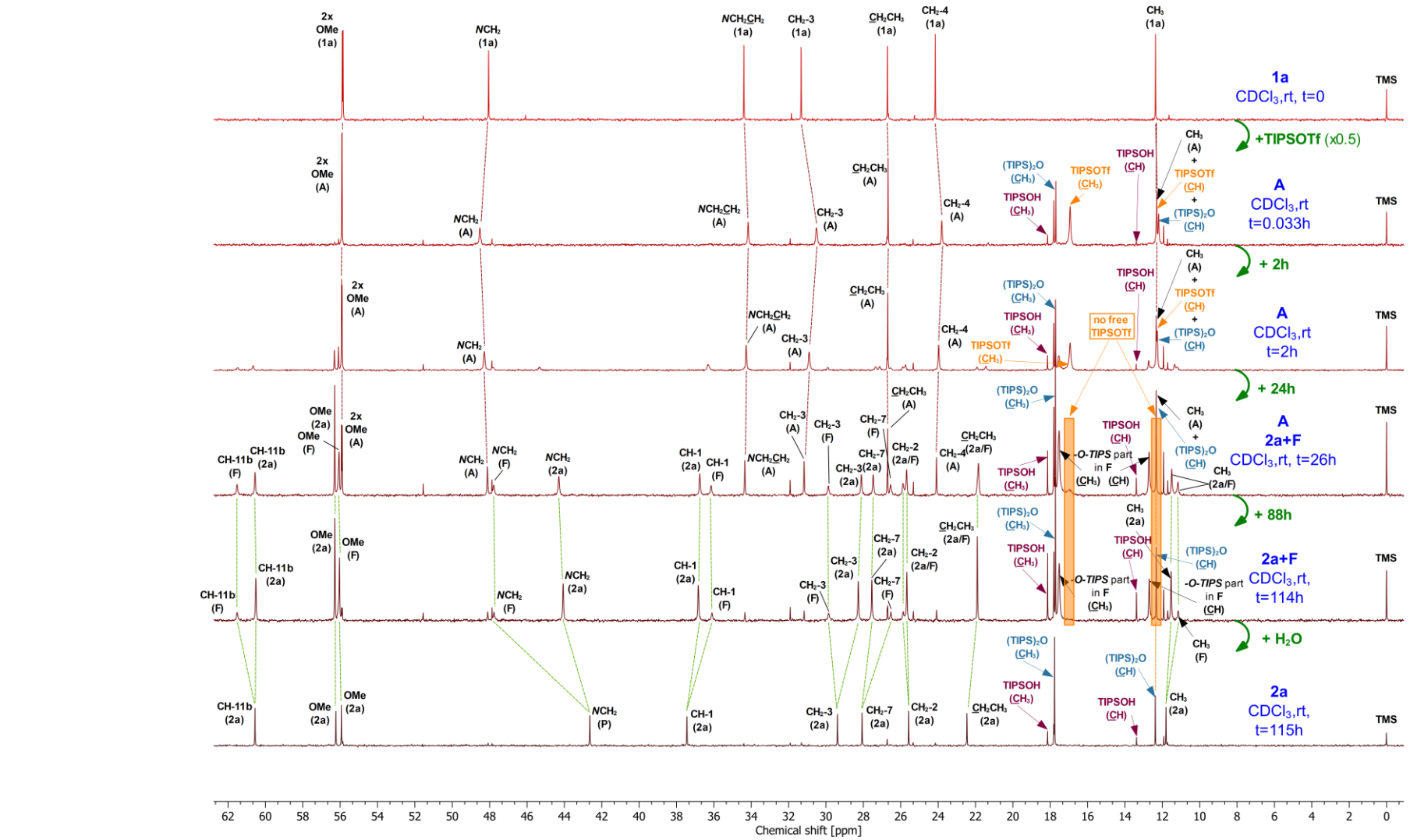


Figure S5. Partial ^{13}C NMR spectra (0-62.5ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 0.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^{o}C)

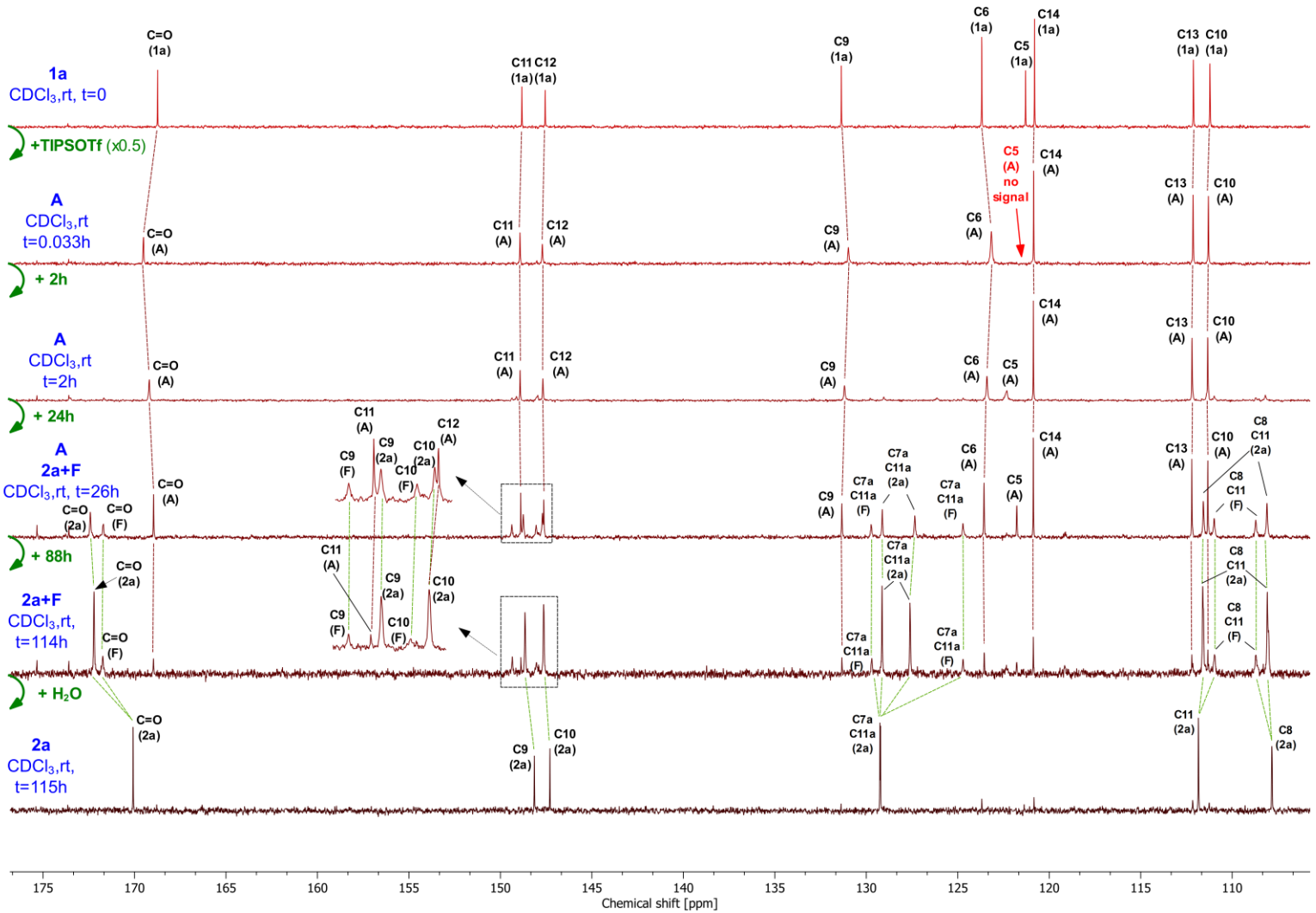


Figure S6. Partial ^{13}C NMR spectra (100-175ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 0.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^oC)

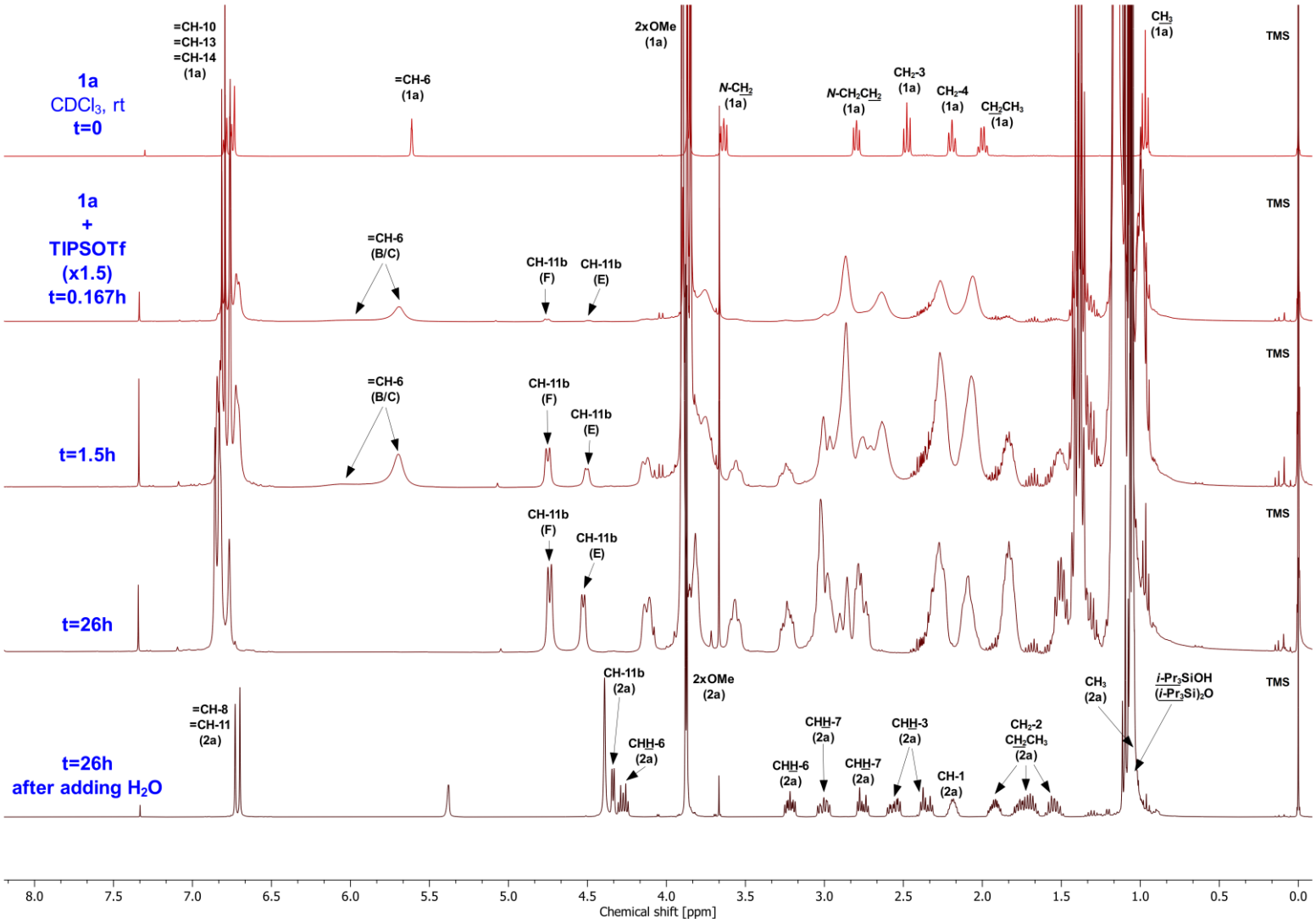


Figure S7. ^{1}H NMR spectra recorded at different time intervals of the cyclization reaction of **1a** in the presence of 1.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^{o}C)

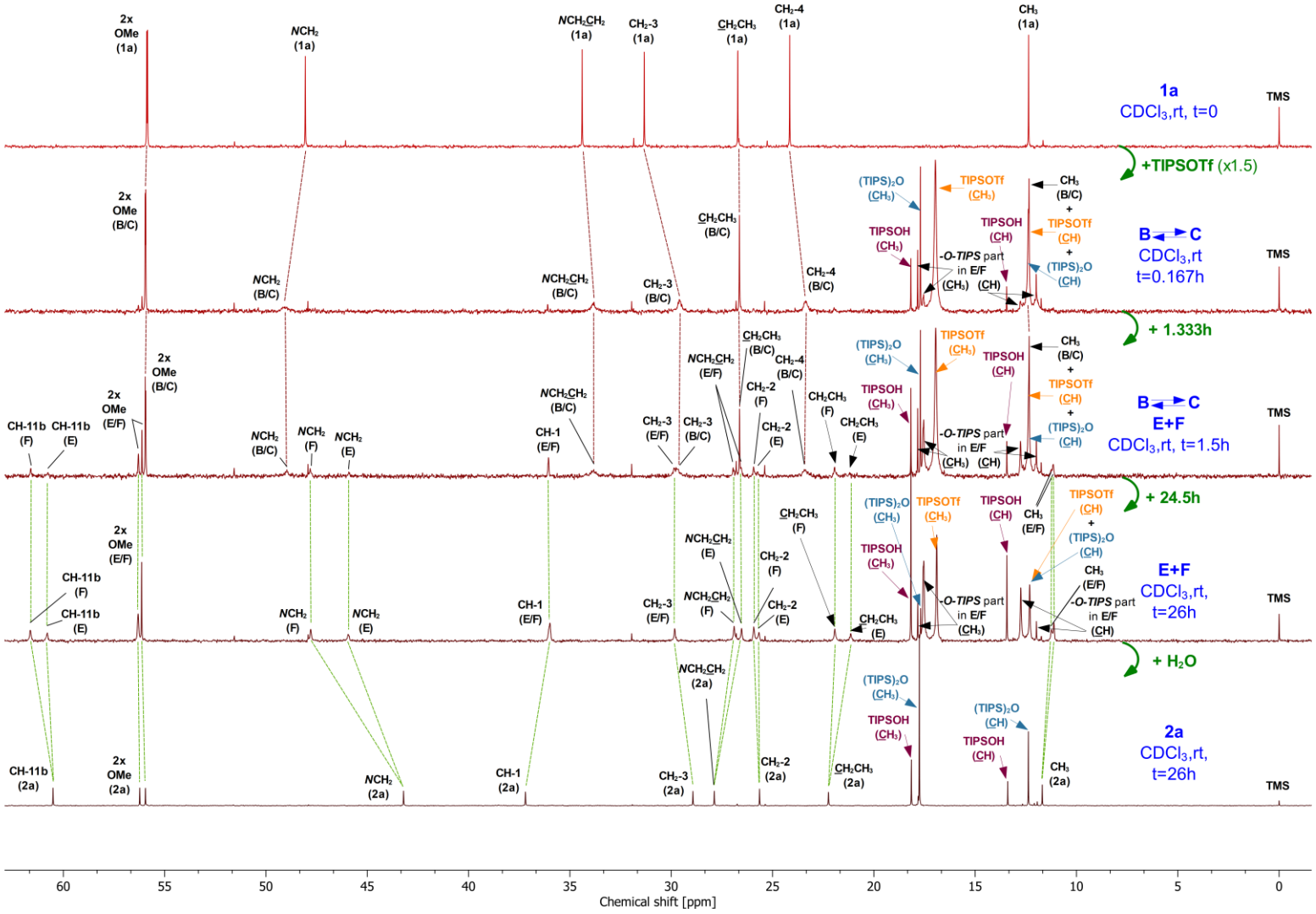


Figure S8. Partial ^{13}C NMR spectra (0-62.5ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 1.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^{o}C)

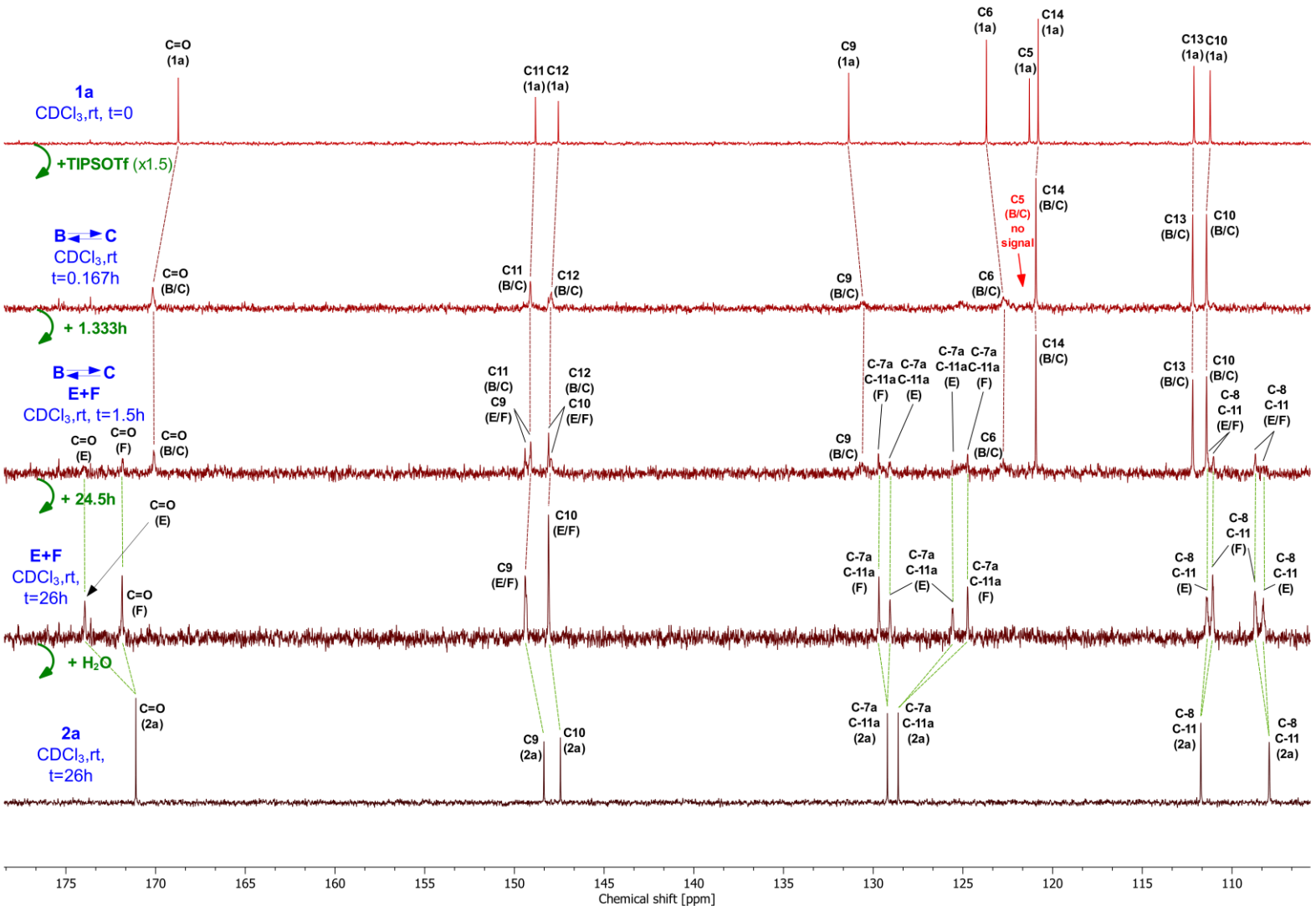


Figure S9. Partial ^{13}C NMR spectra (100-175ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 1.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^{o}C)

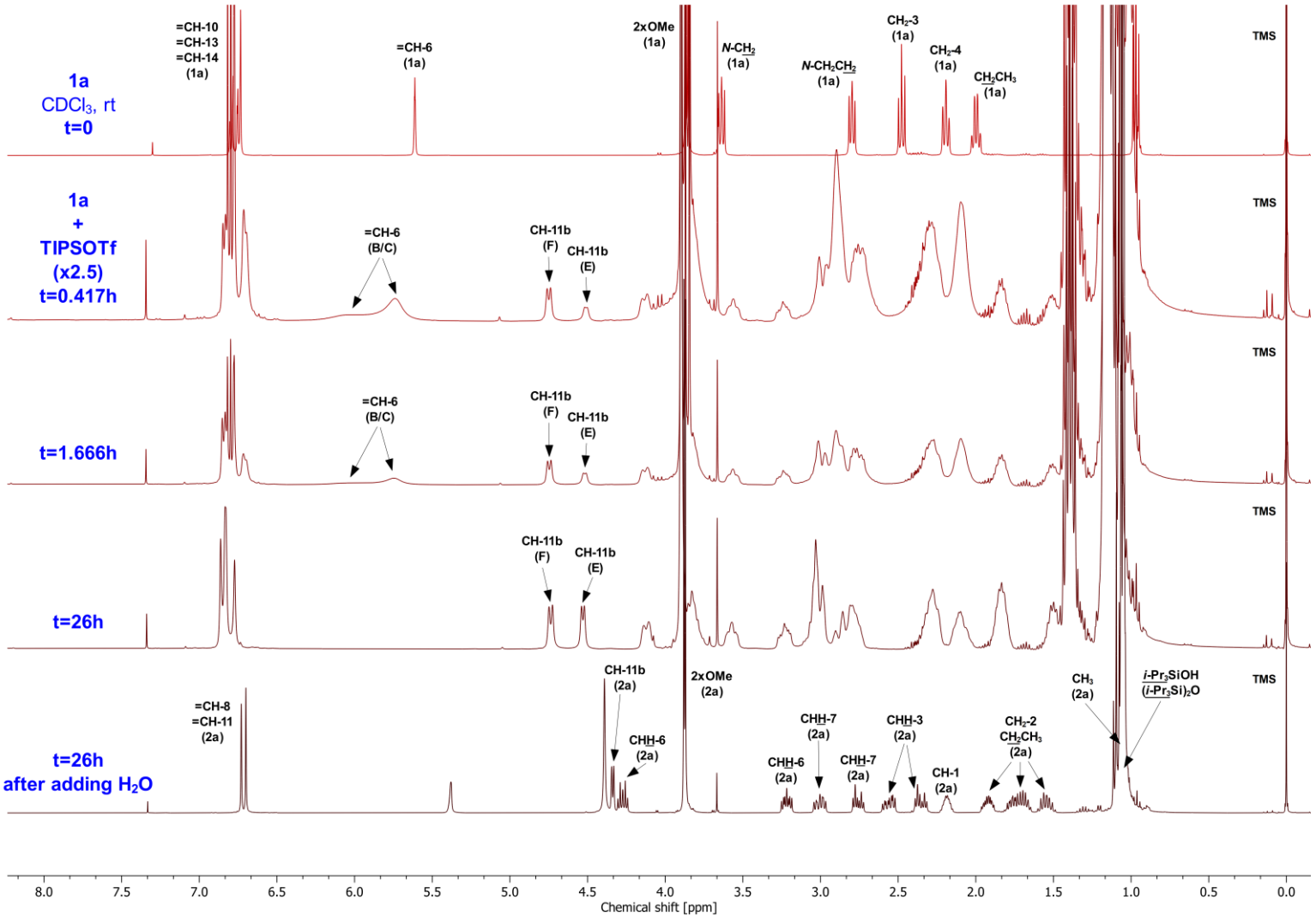


Figure S10. ^{1}H NMR spectra recorded at different time intervals of the cyclization reaction of **1a** in the presence of 2.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^{o}C)

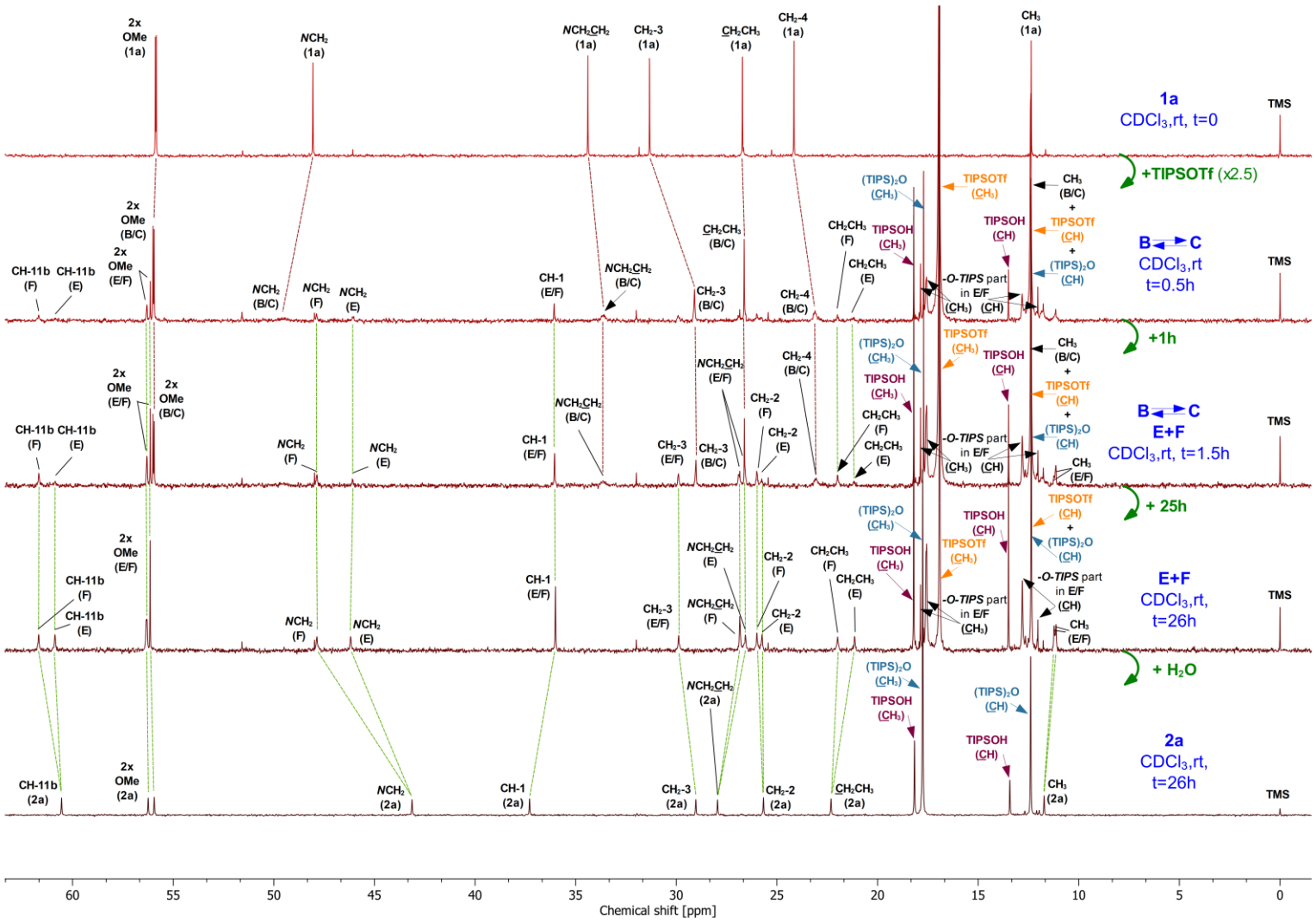


Figure S11. Partial ^{13}C NMR spectra (0-62.5ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 2.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^oC)

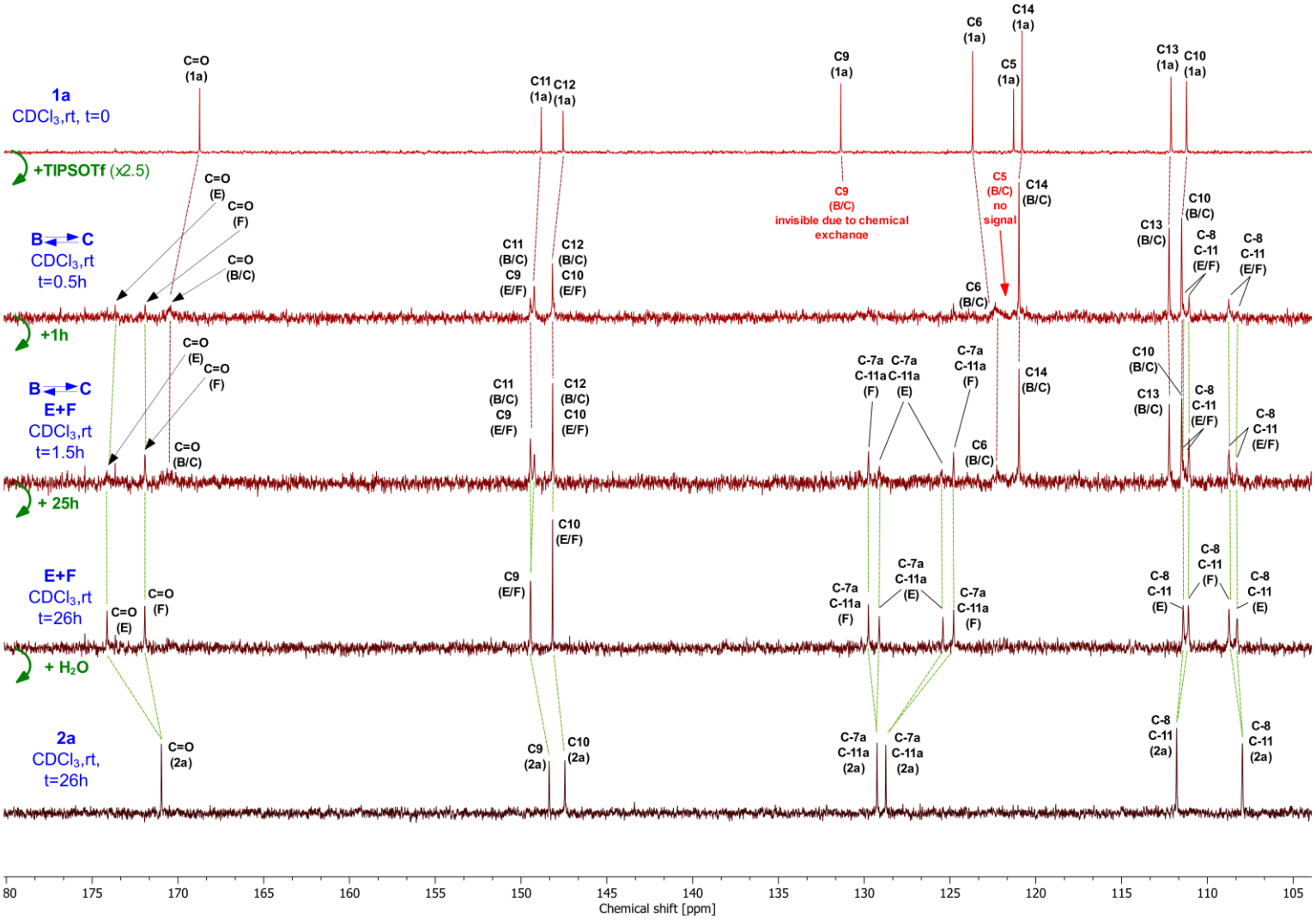


Figure S12. Partial ^{13}C NMR spectra (100-180ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 2.5 equiv. of TIPSOTf in $CDCl_3$ (23 ^oC)

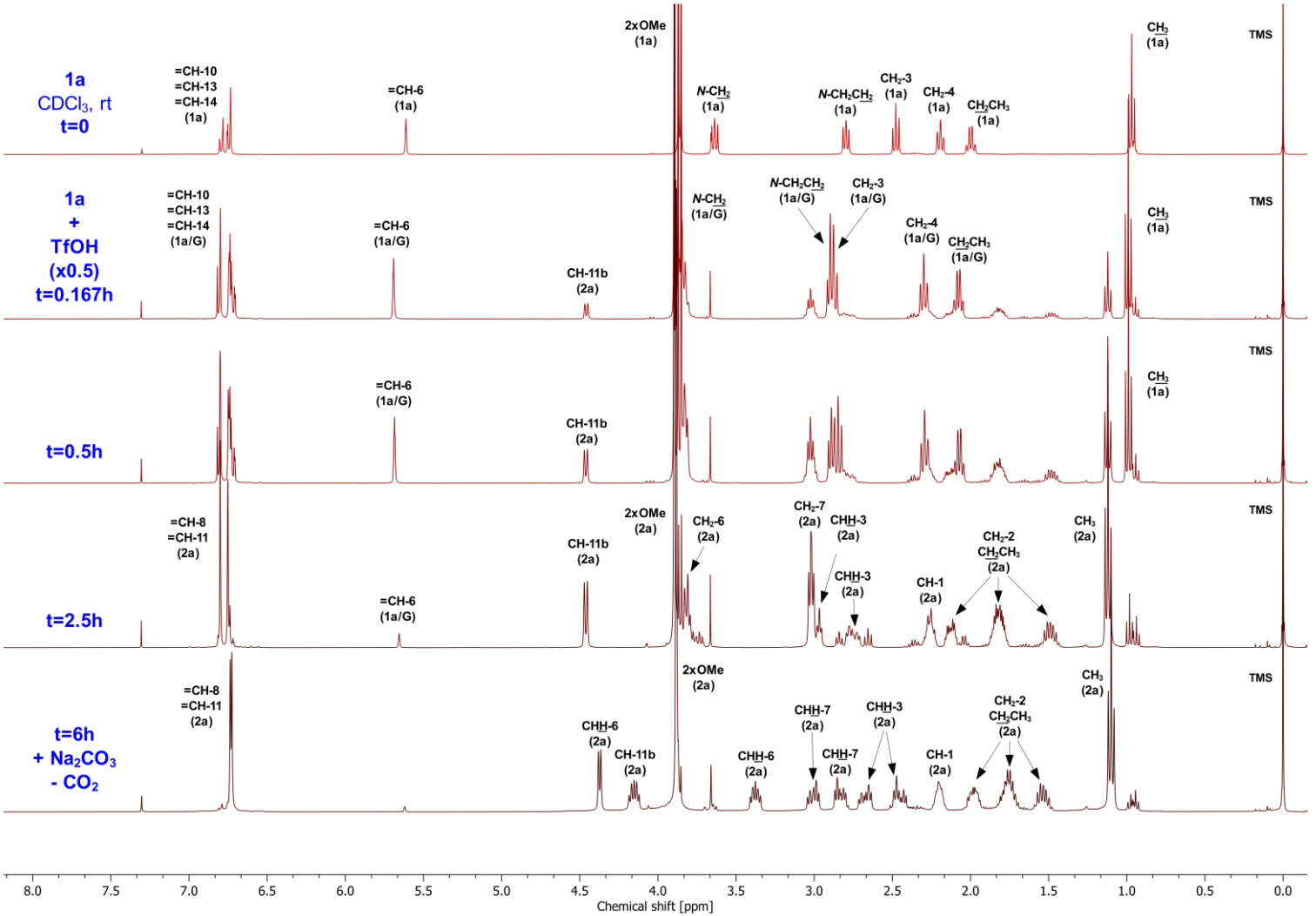


Figure S13. ^{1}H NMR spectra recorded at different time intervals of the cyclization reaction of **1a** in the presence of 0.5 equiv. of TfOH in $CDCl_3$ (23 ^{o}C)

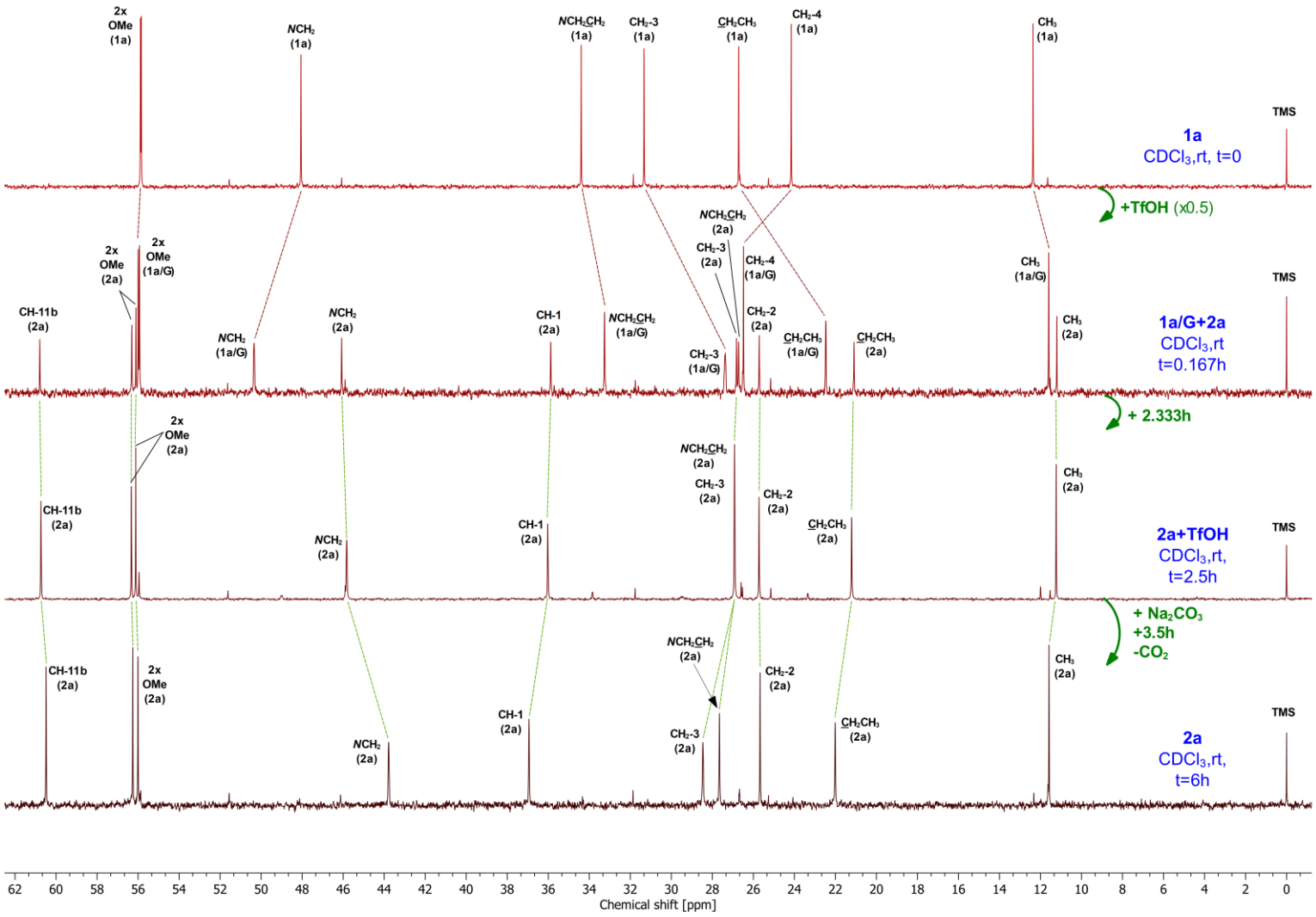


Figure S14. Partial ^{13}C NMR spectra (0-62.5ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 0.5 equiv. of TfOH in $CDCl_3$ (23 ^{o}C)

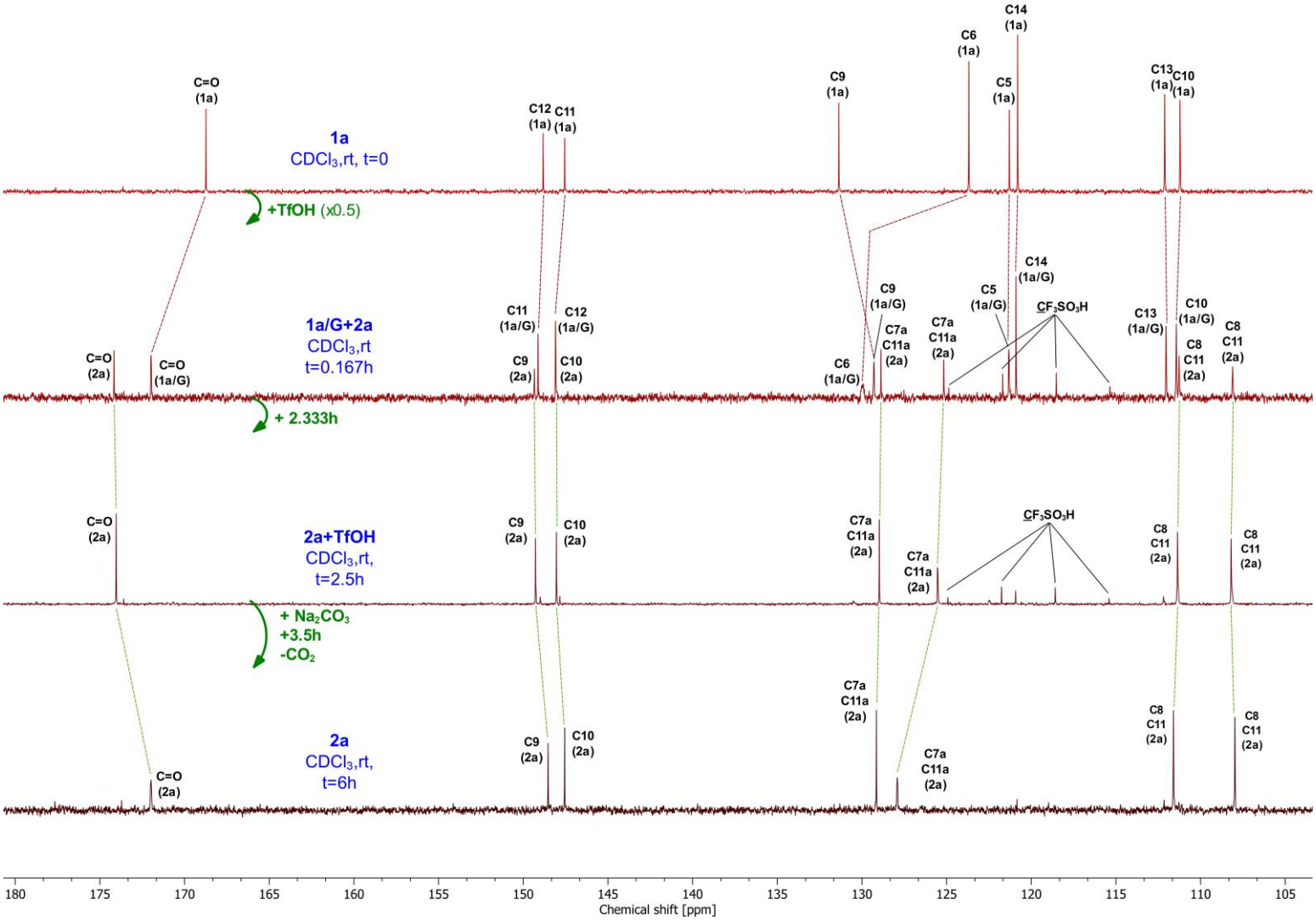


Figure S15. Partial ^{13}C NMR spectra (100-180ppm) recorded at different time intervals of the cyclization reaction of **1a** in the presence of 0.5 equiv. of TfOH in $CDCl_3$ (23 ^oC)

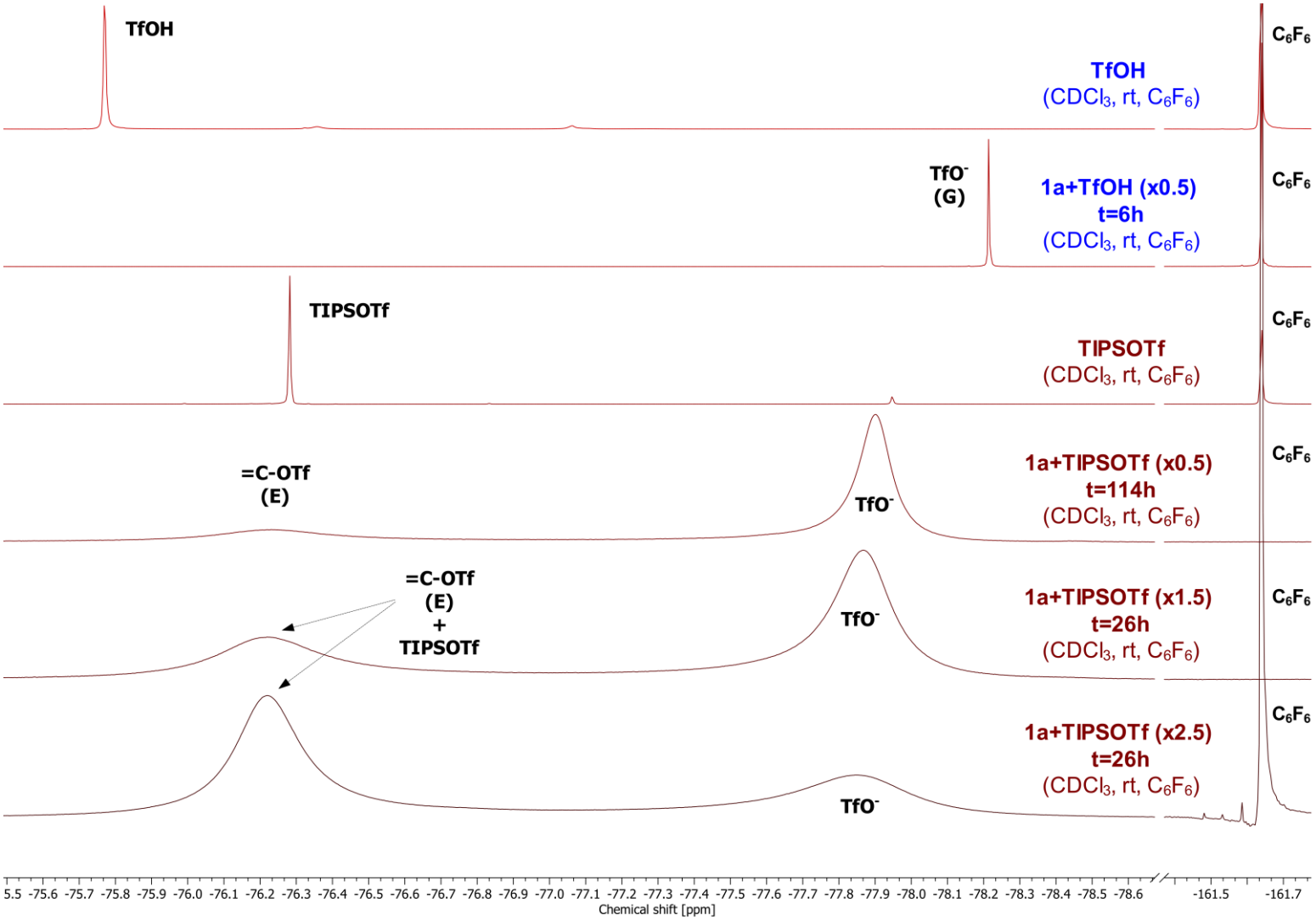
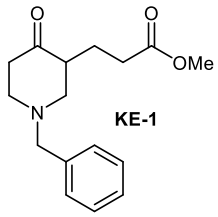


Figure S16. ^{19}F NMR spectra (with C_6F_6 as the internal standard) of TfOH, the mixture of **1a** and TfOH, TIPSOTf, and the mixtures of **1a** and TIPSOTf (0.5 eq.; 1.5 eq.; and 2.5 eq.) recorded at the end of the reaction conducted in $CDCl_3$ (23ºC)

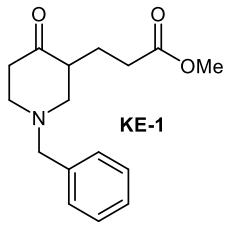
11. ^{1}H, ^{13}C, ^{13}C DEPT-135 and ^{19}F NMR spectra

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



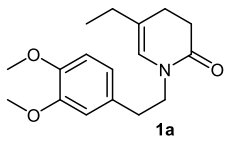
KE-1

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



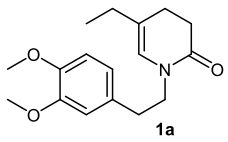
KE-1

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



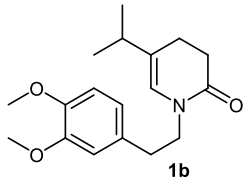
1a

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



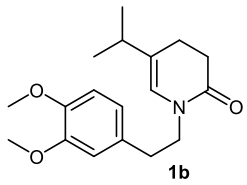
1a

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



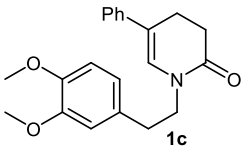
1b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



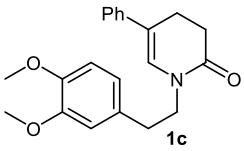
1b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



1c

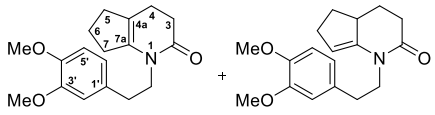
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.63
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



1c

^{13}C DEPT-135

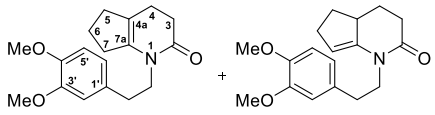
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



A 1 : 0.86 B

1d

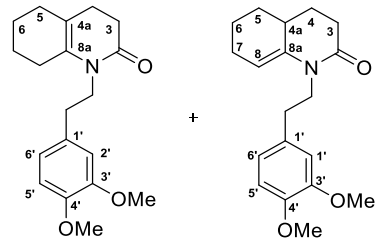
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



A 1 : 0.86 B

1d

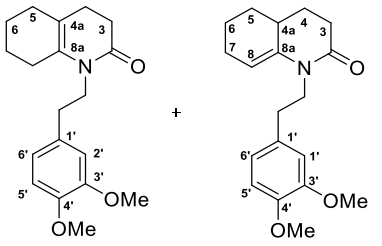
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



A ~1:0.65 B

1e

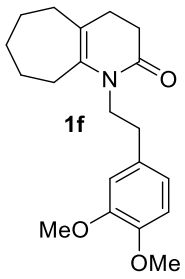
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



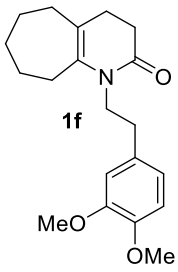
A ~1:0.65 B

1e

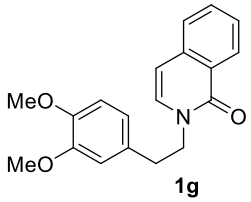
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

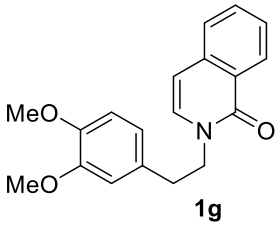


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



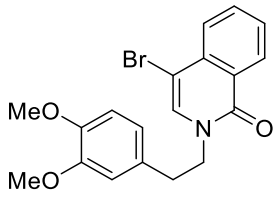
1g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



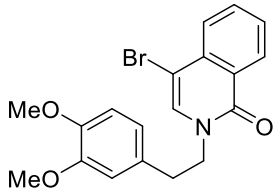
1g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



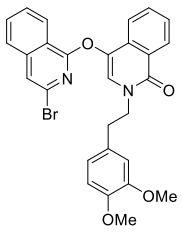
4-Br-1g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



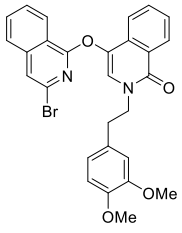
4-Br-1g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



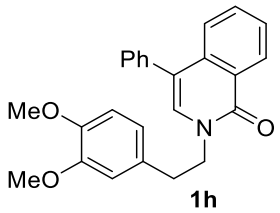
1g-by-product

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



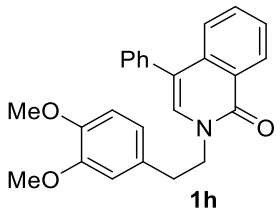
1g-by-product

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

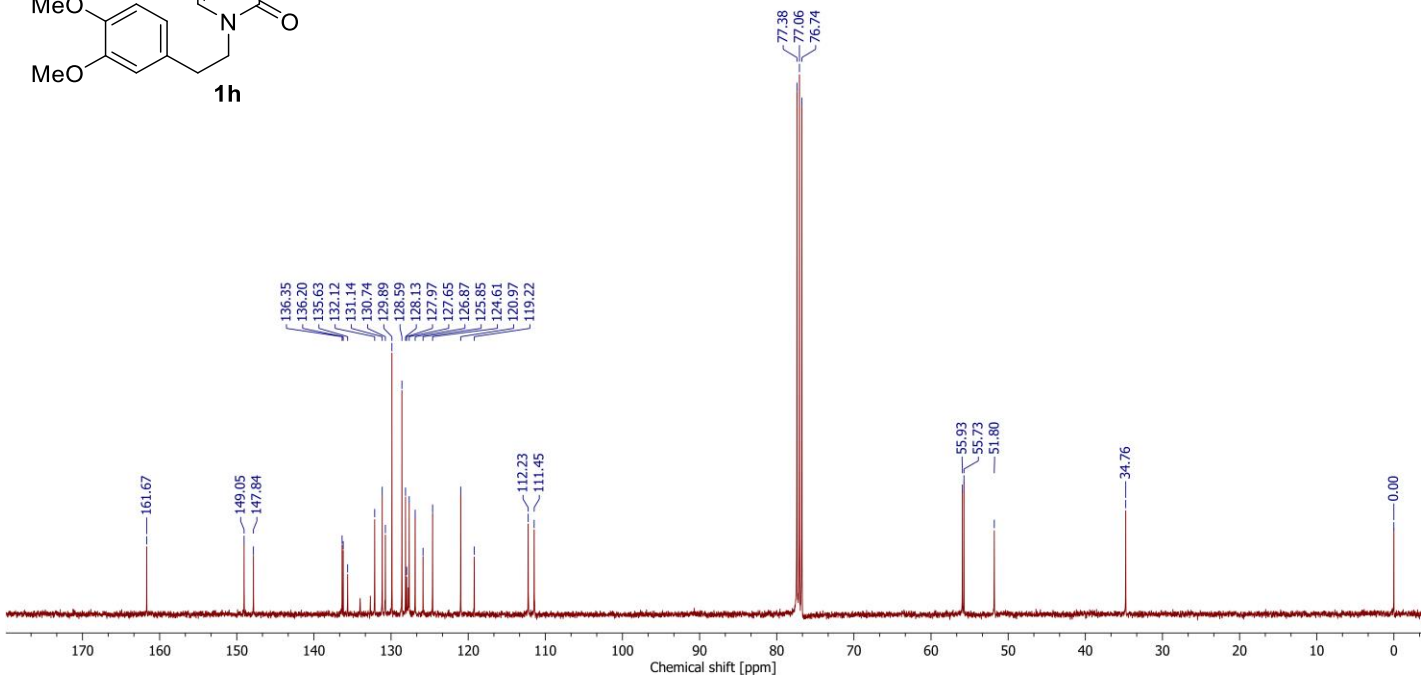


1h

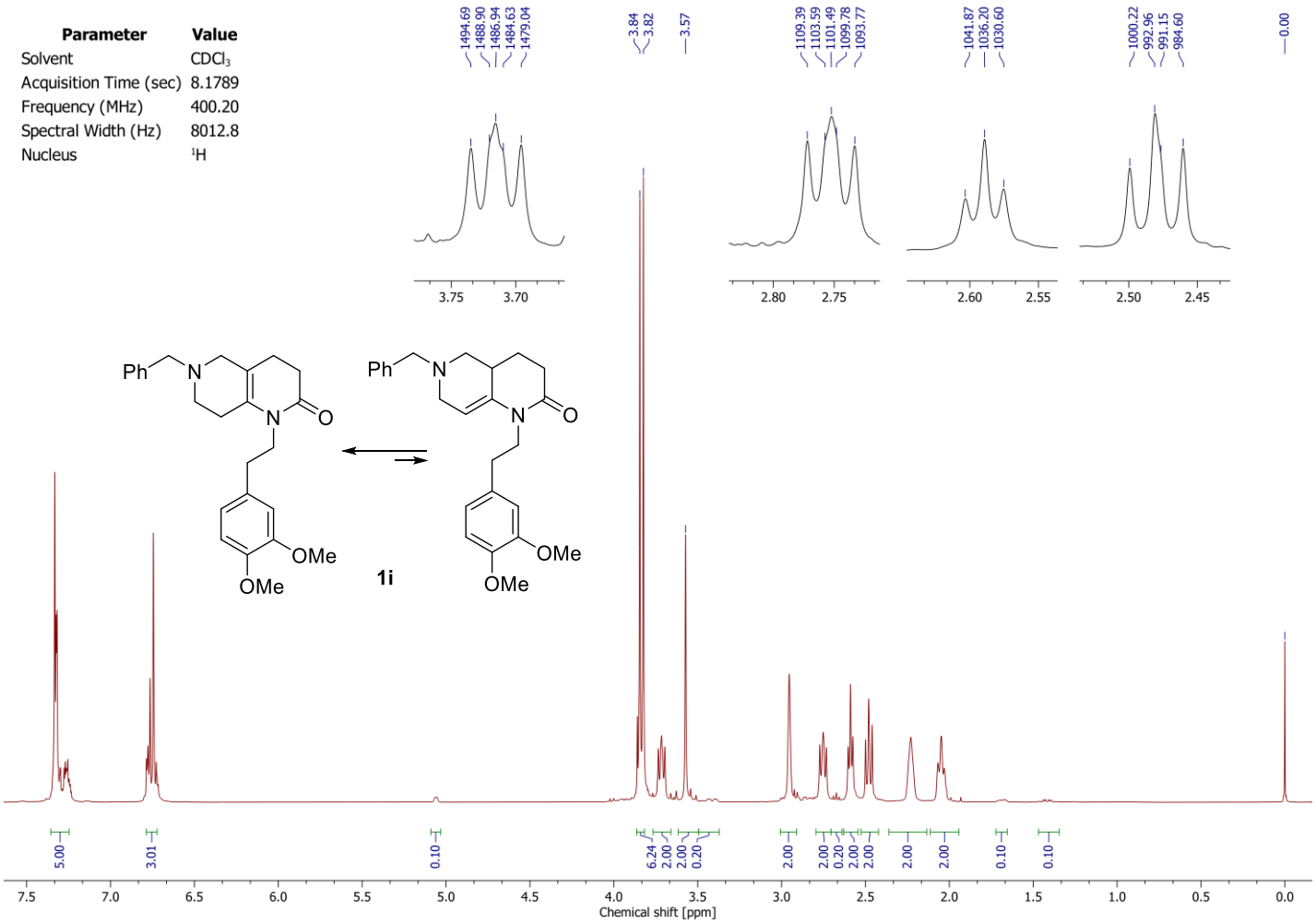
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



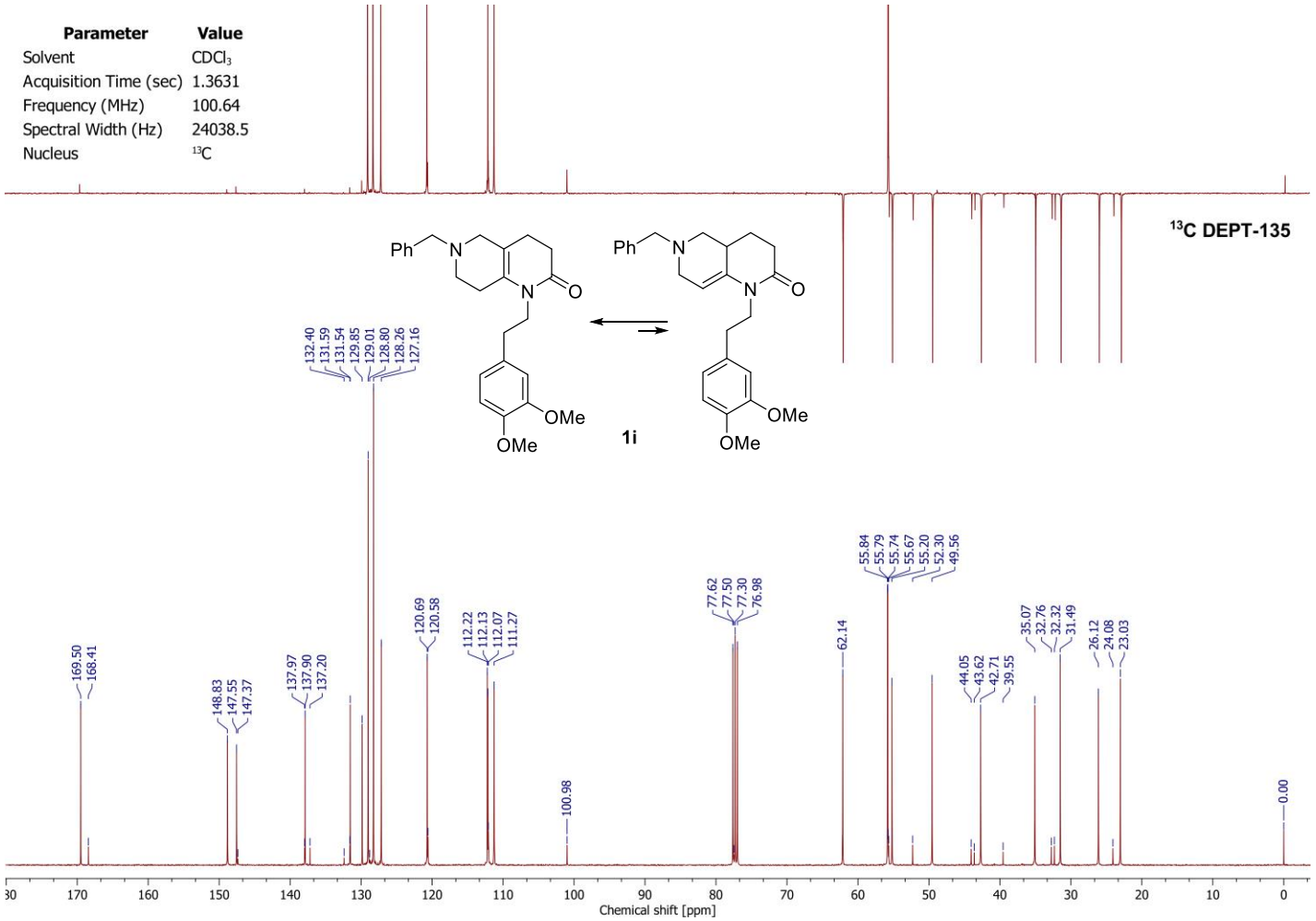
1h



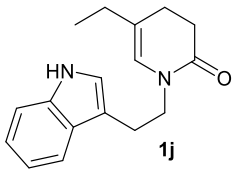
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

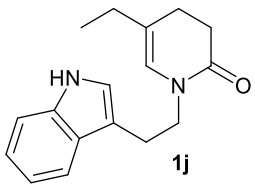


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



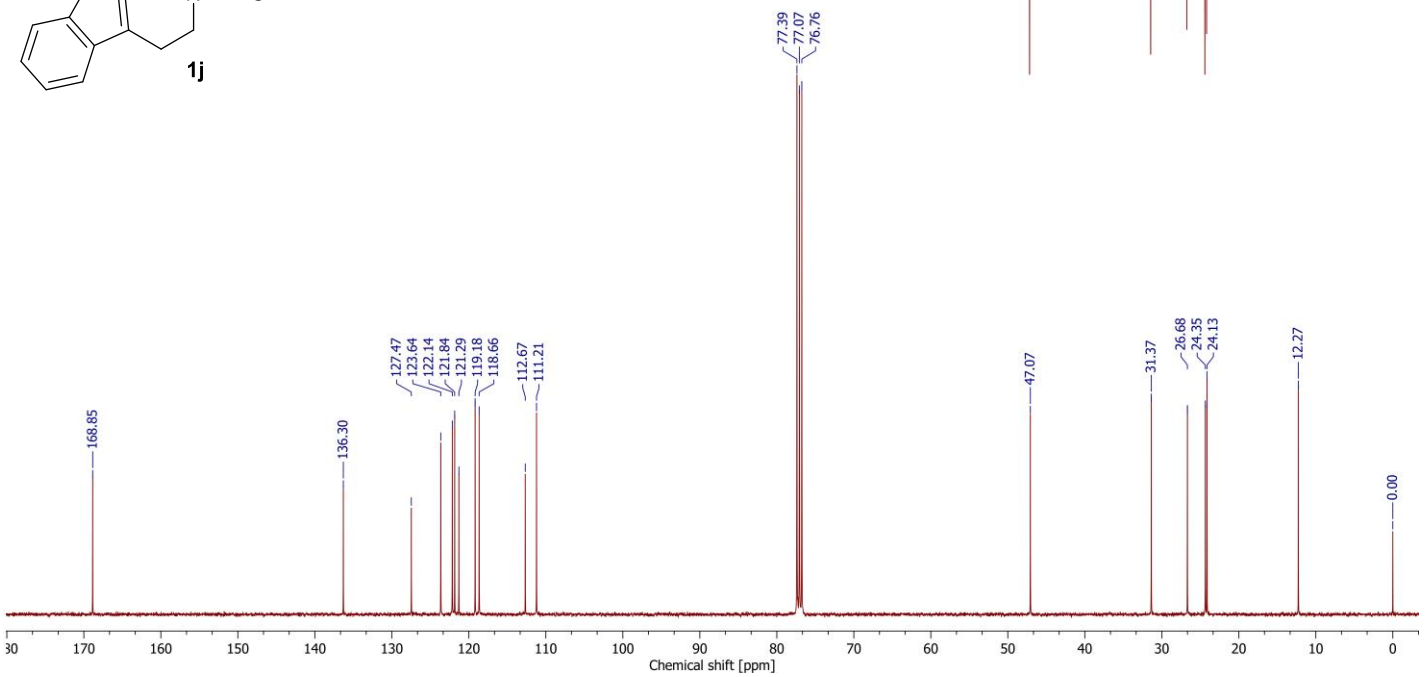
1j

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

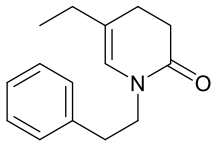


1j

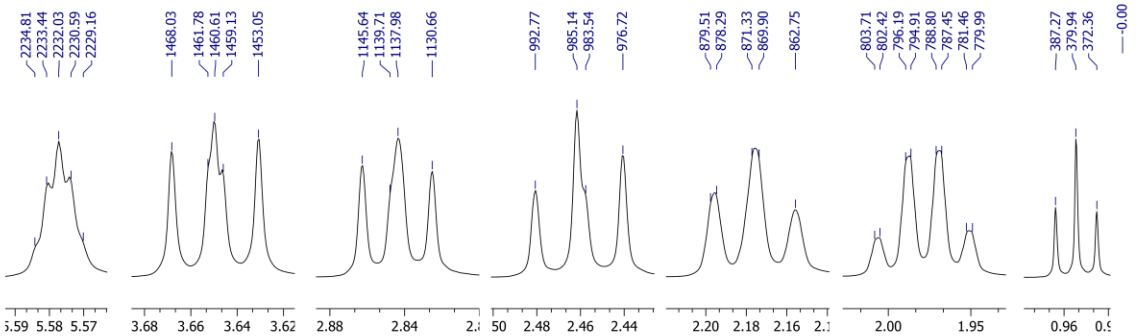
^{13}C DEPT-135

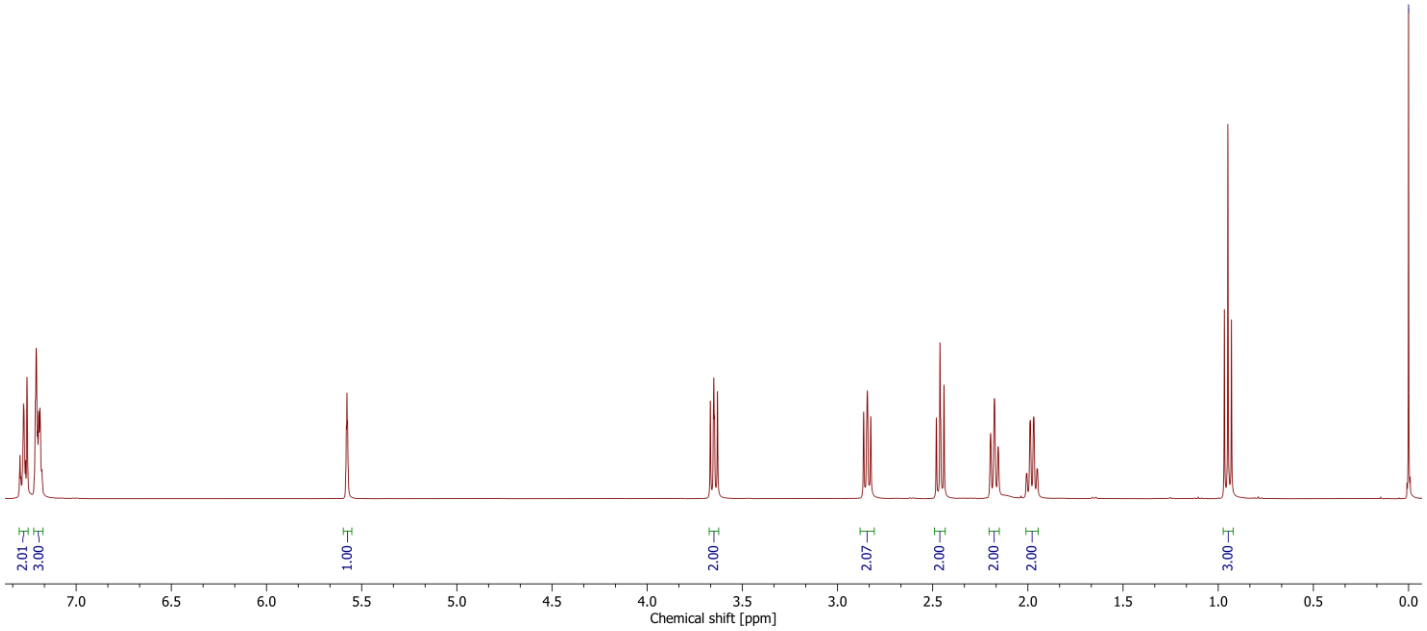


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

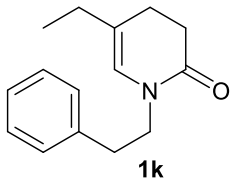


1k



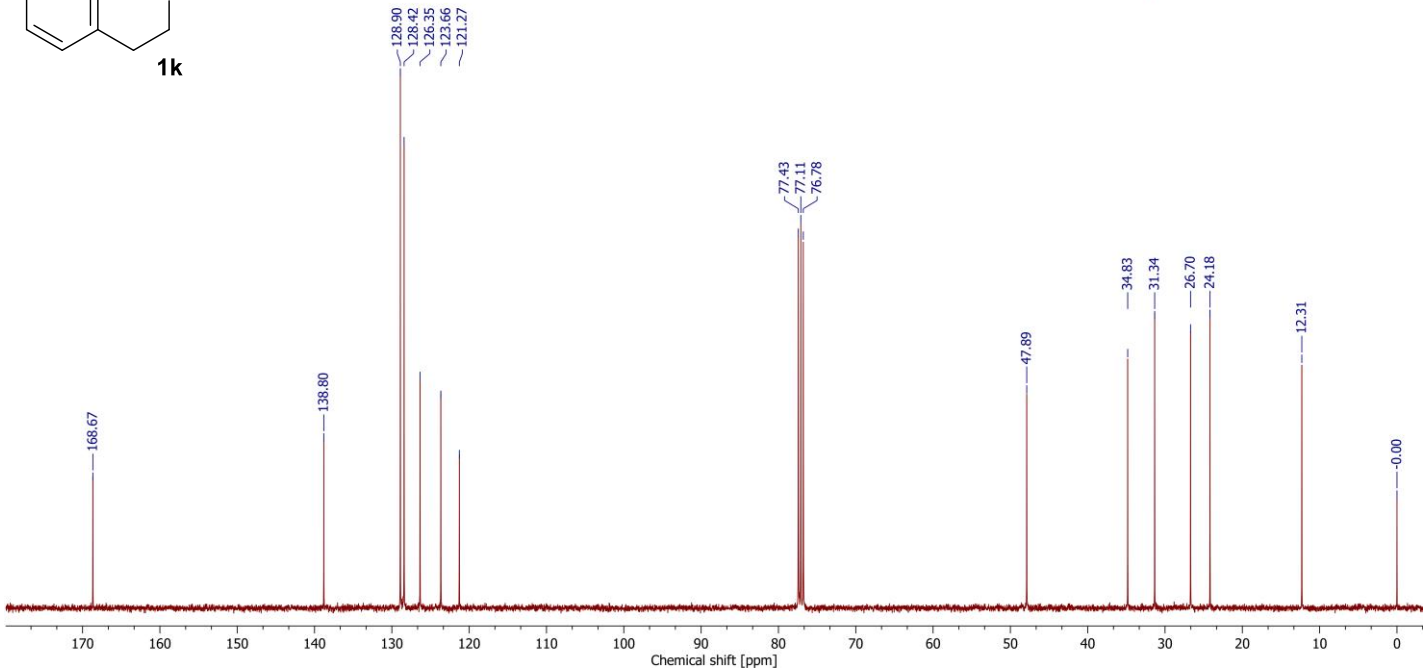


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

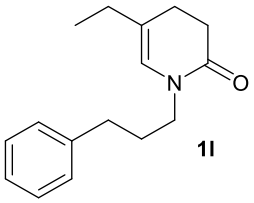


1k

^{13}C DEPT-135

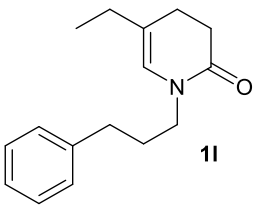


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



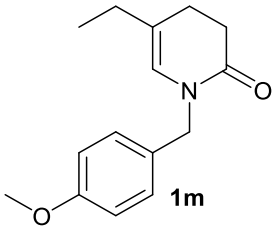
1l

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



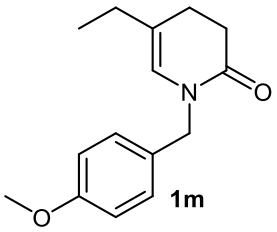
1l

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



1m

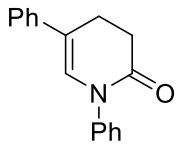
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



1m

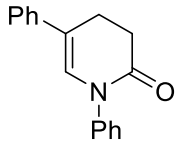
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



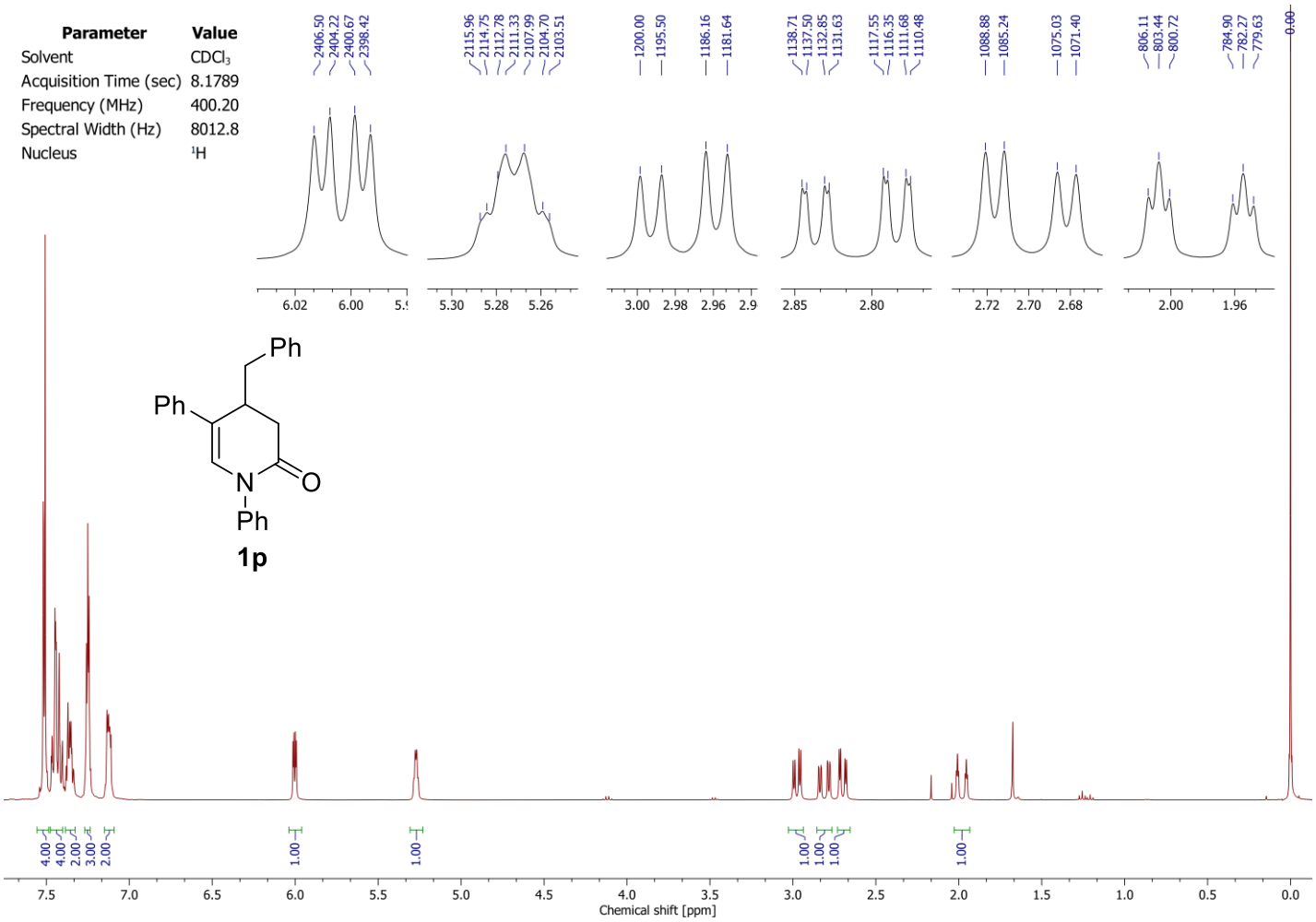
1n

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

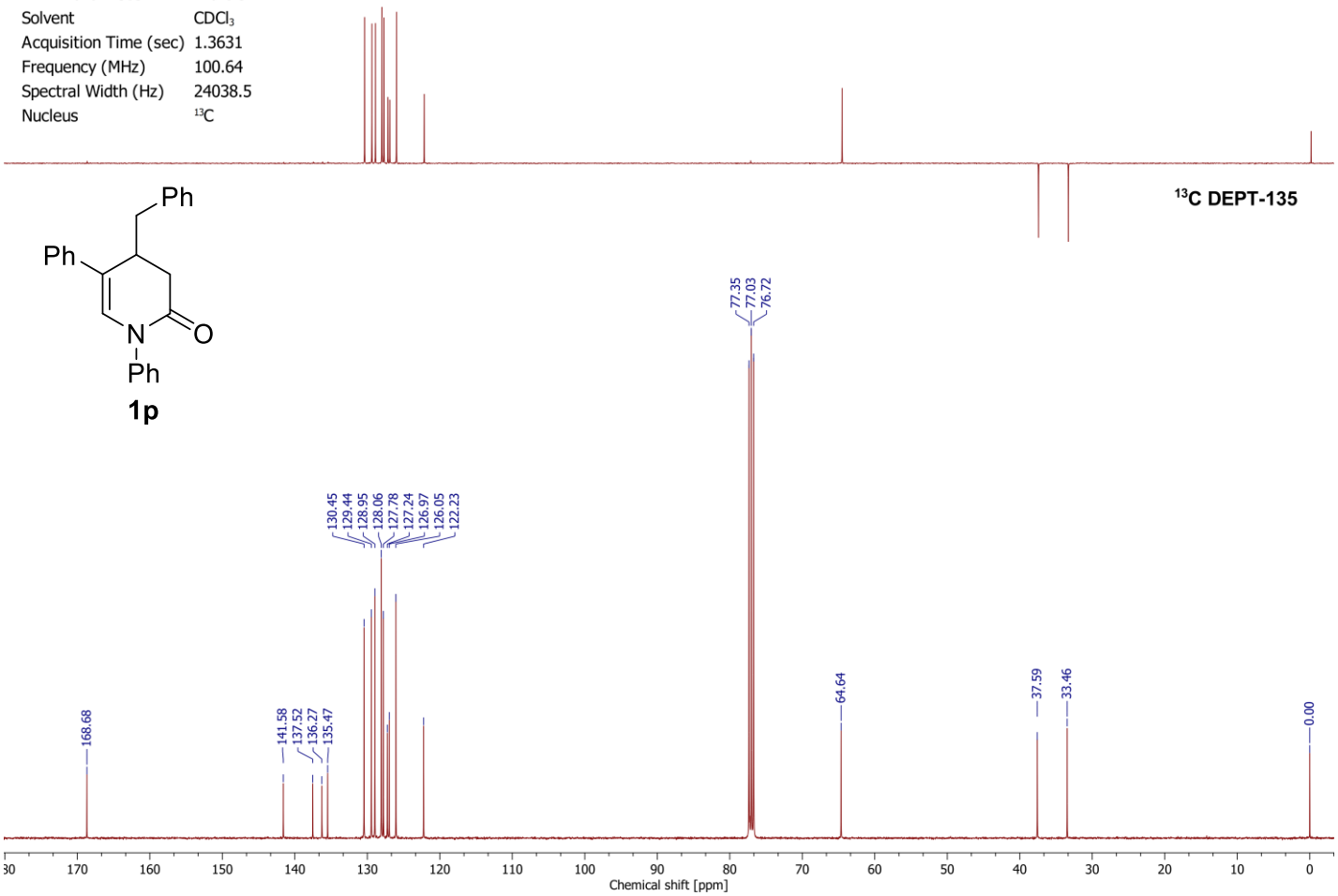


1n

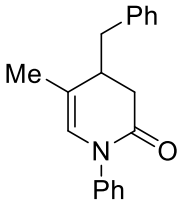
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



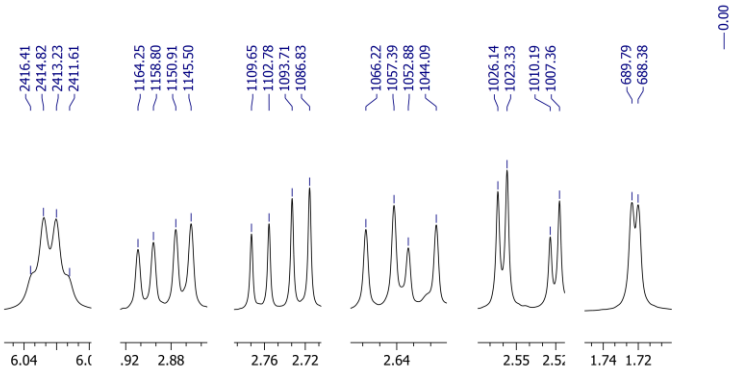
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

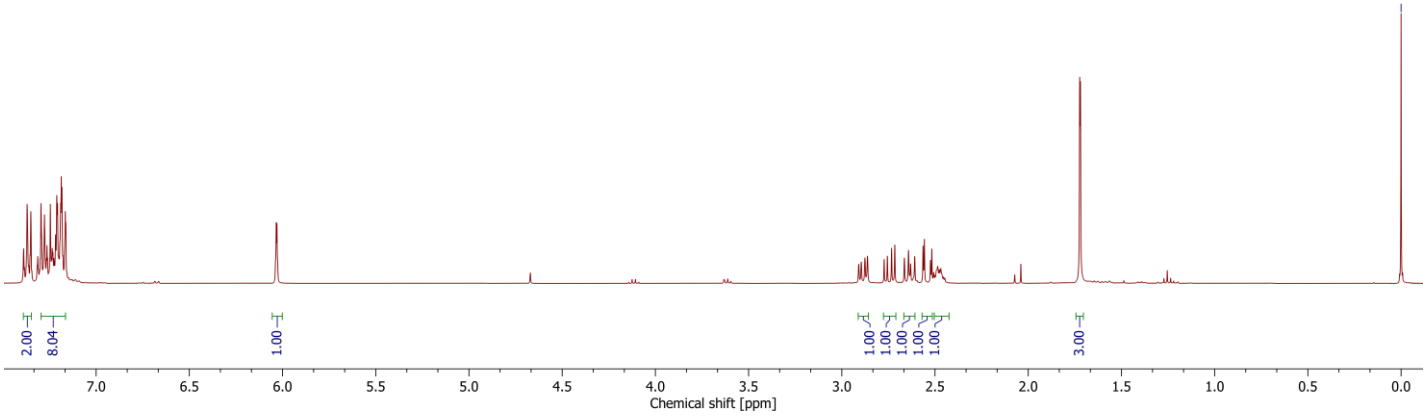


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

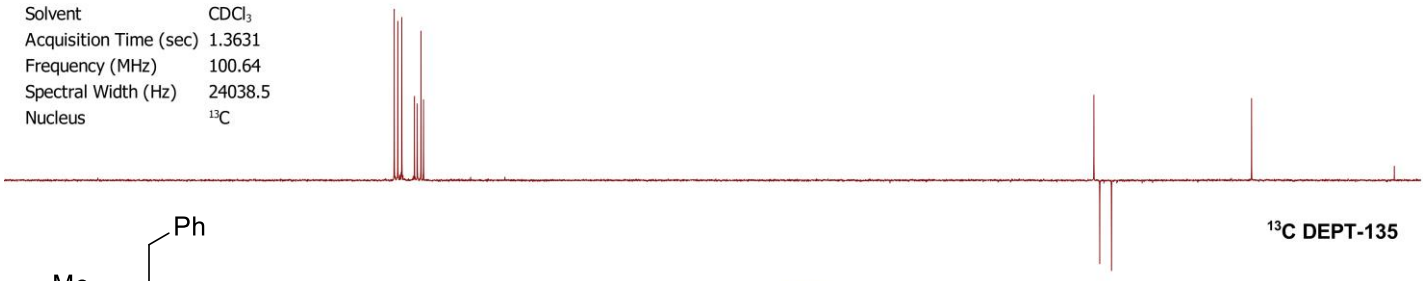


1s

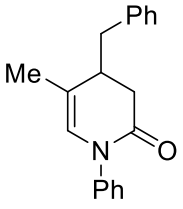




Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

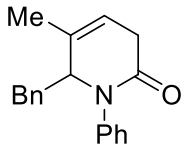


^{13}C DEPT-135



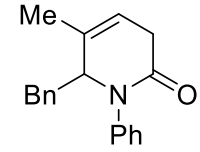
1s

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



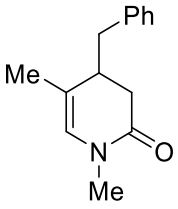
1s-isomer-6

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



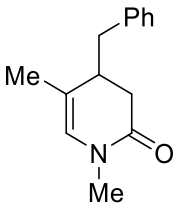
1s-isomer-6

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



1u

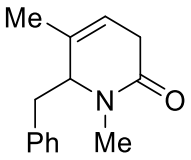
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



1u

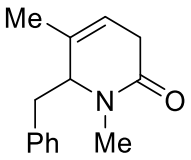
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



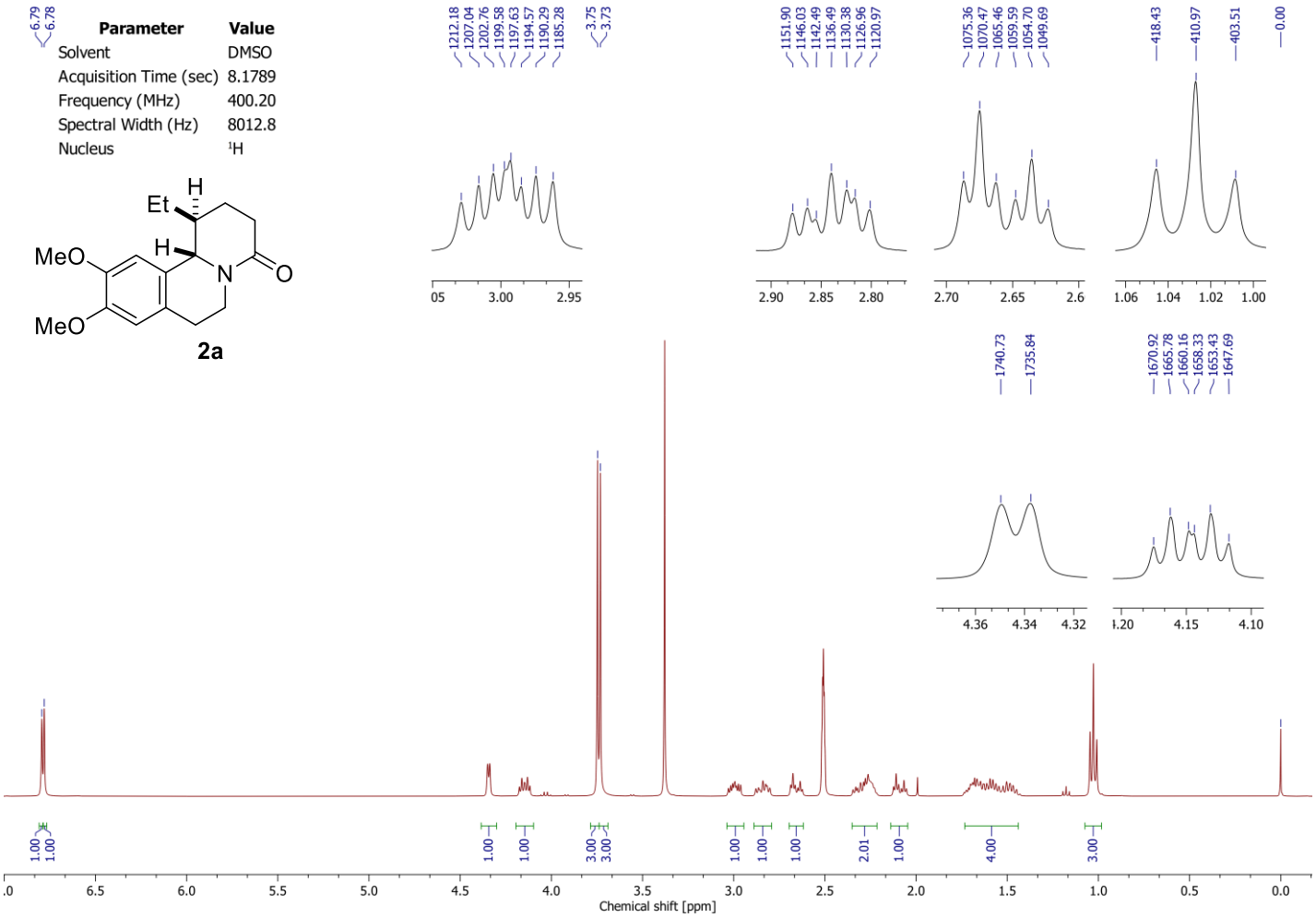
1u-isomer-6

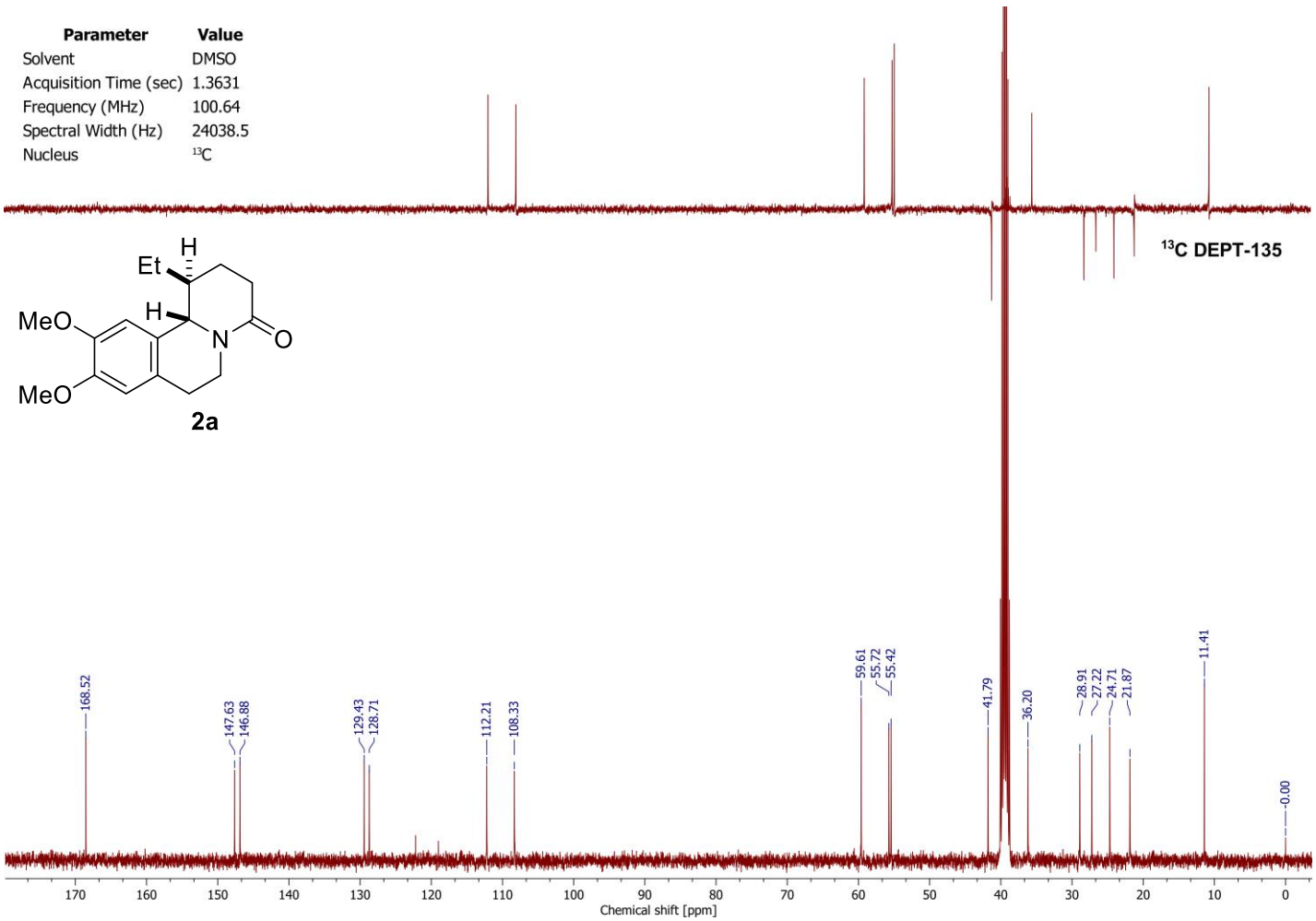
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



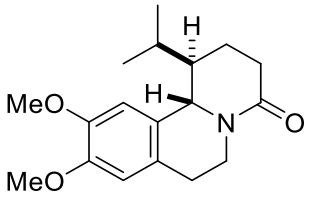
1u-isomer-6

^{13}C DEPT-135


Parameter Value
Solvent DMSO
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
Et
H
MeO
MeO
N
O
2a
Chemical shift [ppm]

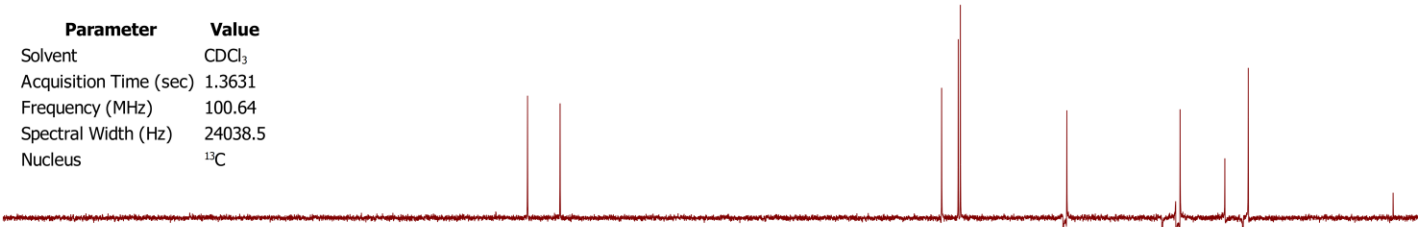

Parameter Value
Solvent DMSO
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
Et
H
MeO
MeO
N
O
2a
Chemical shift [ppm]

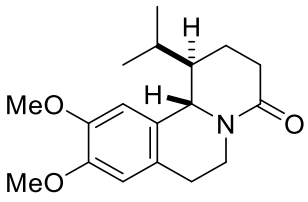
Parameter	Value
Solvent	CDCl3
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



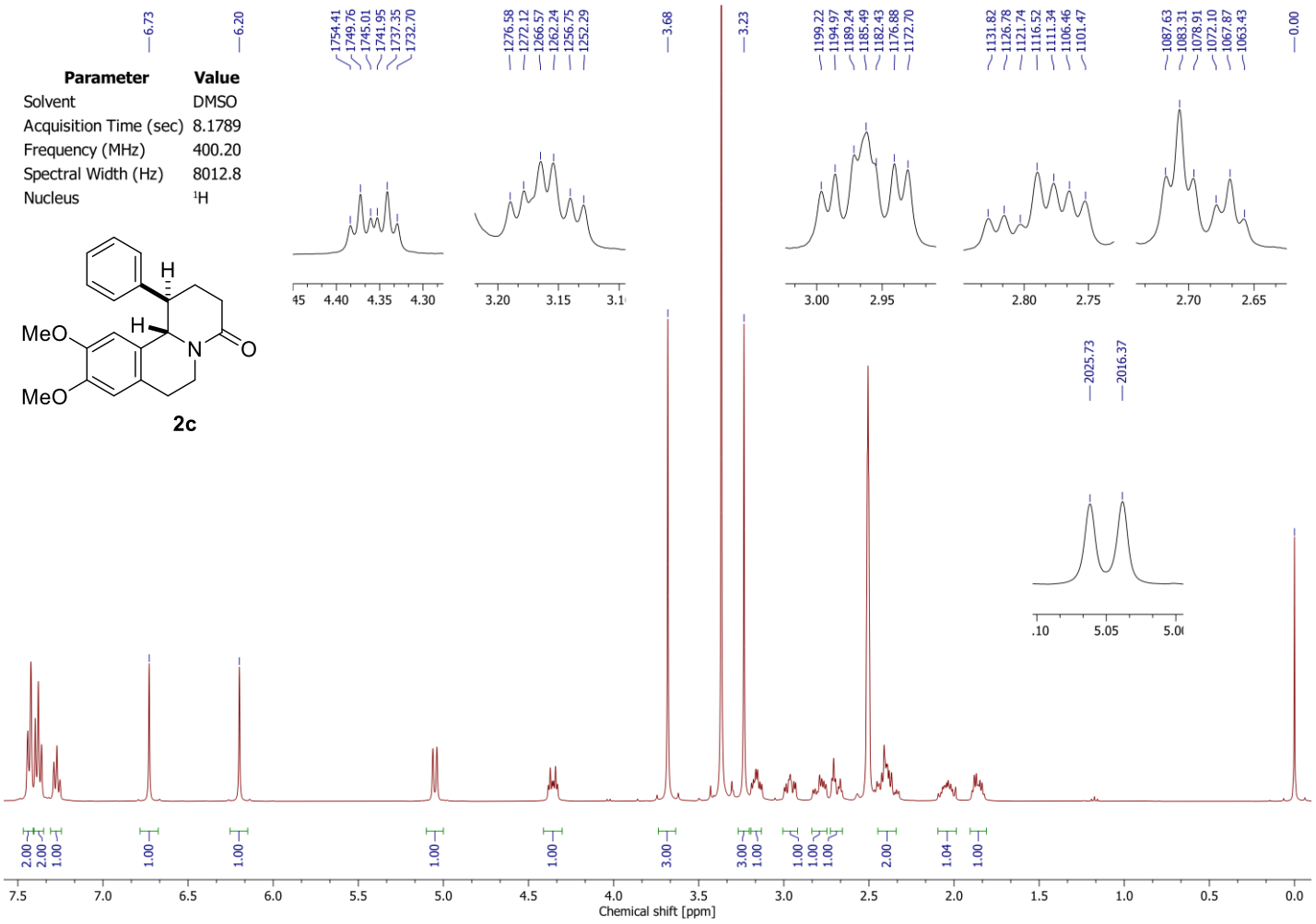
2b

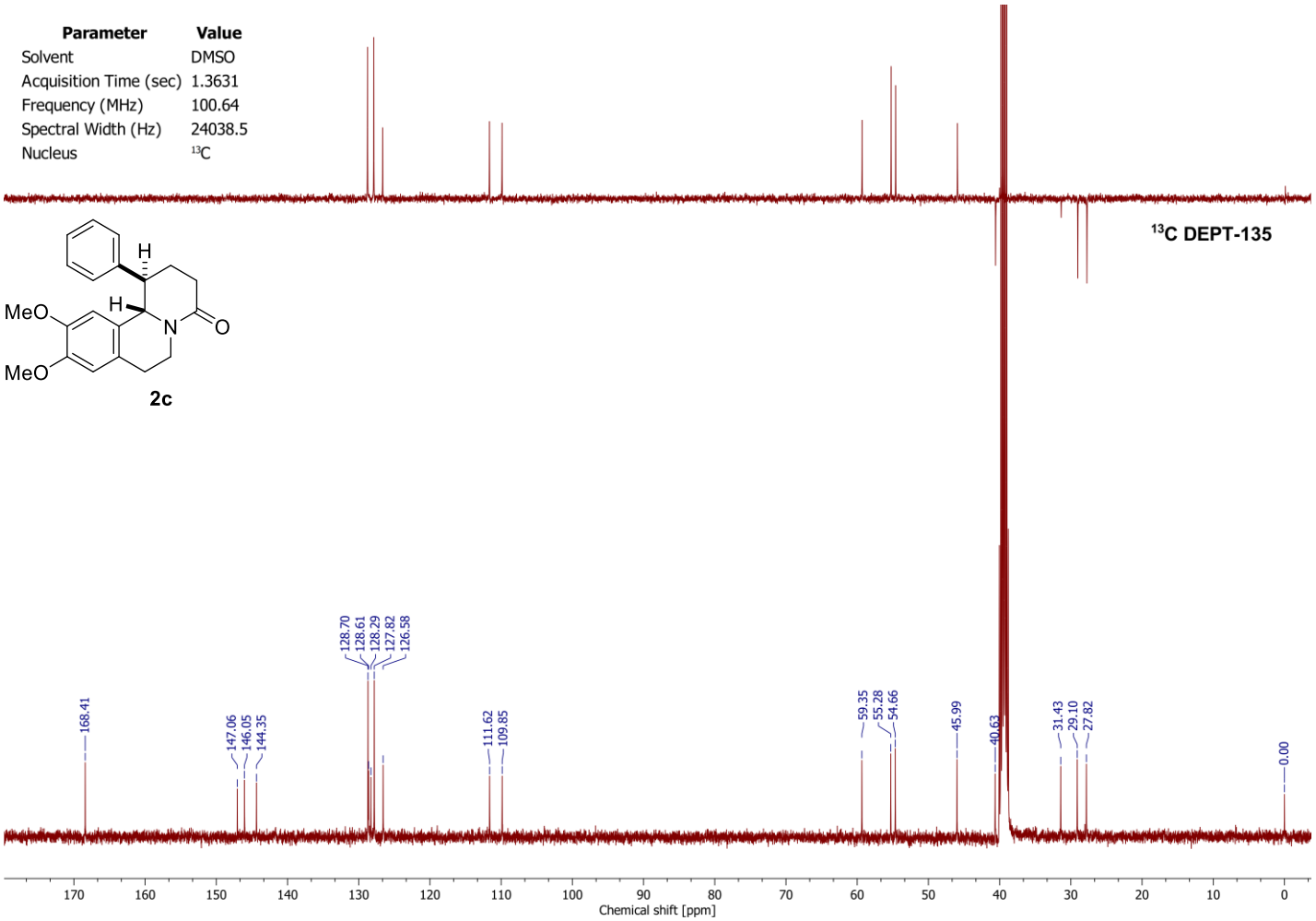
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

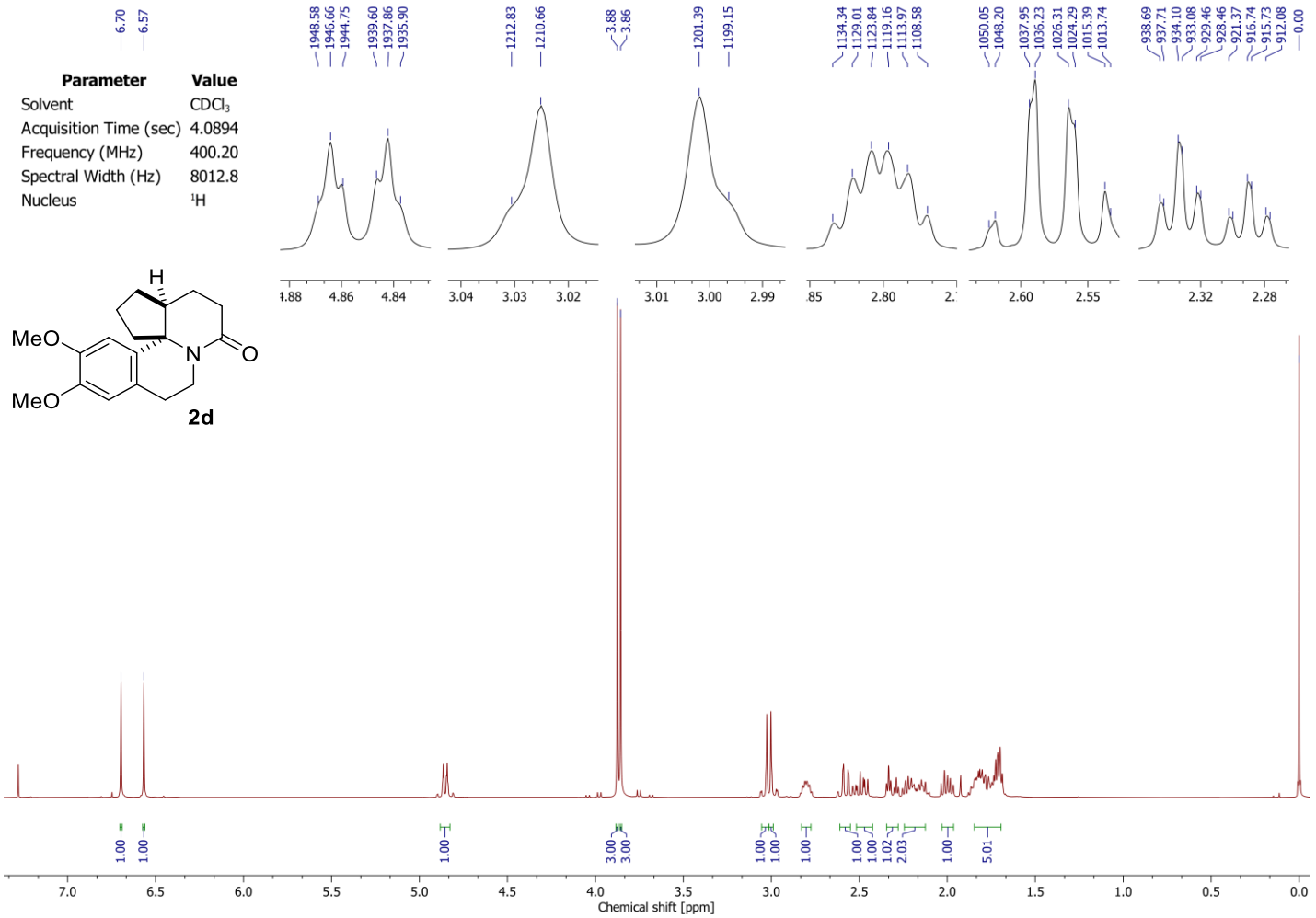


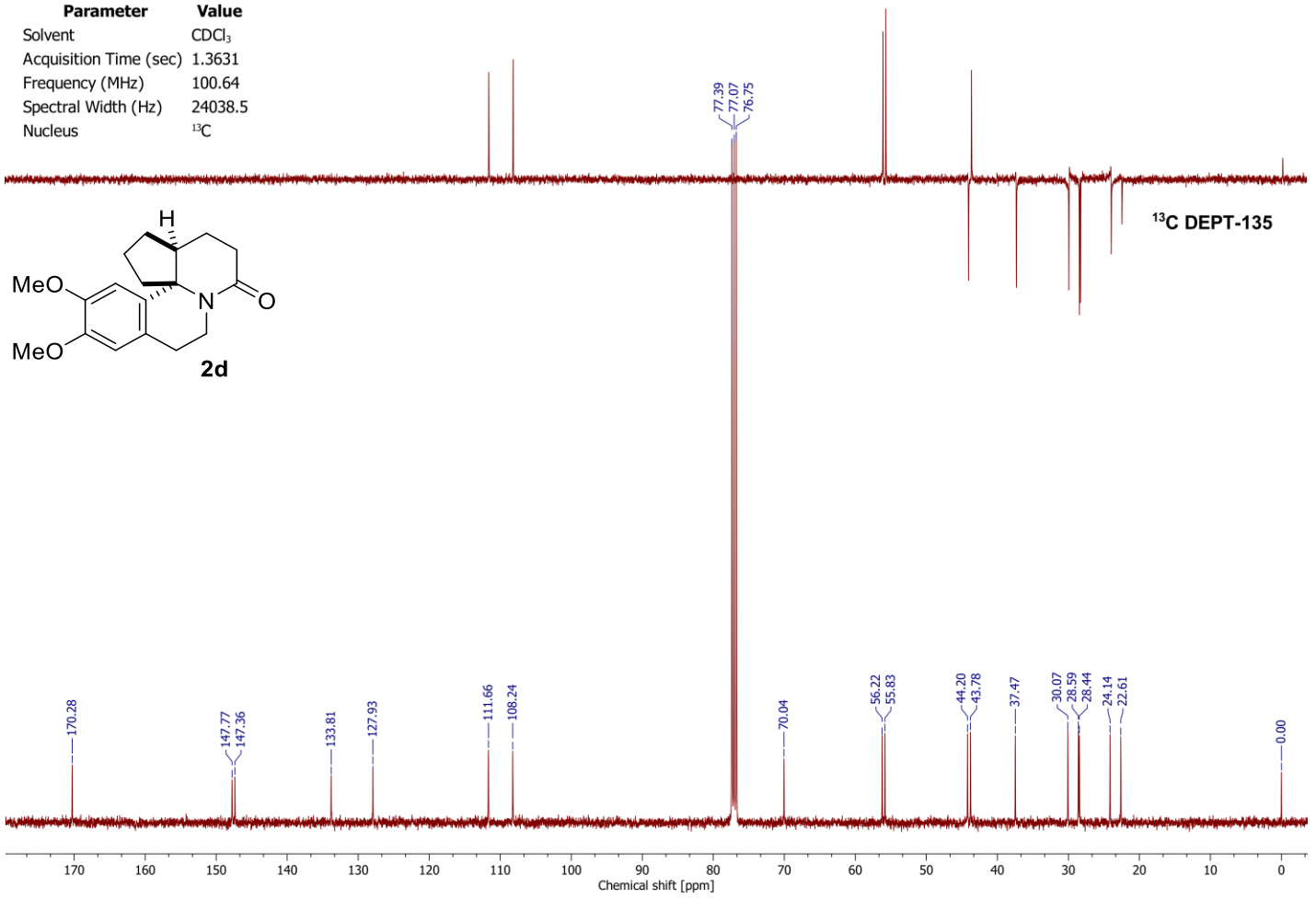


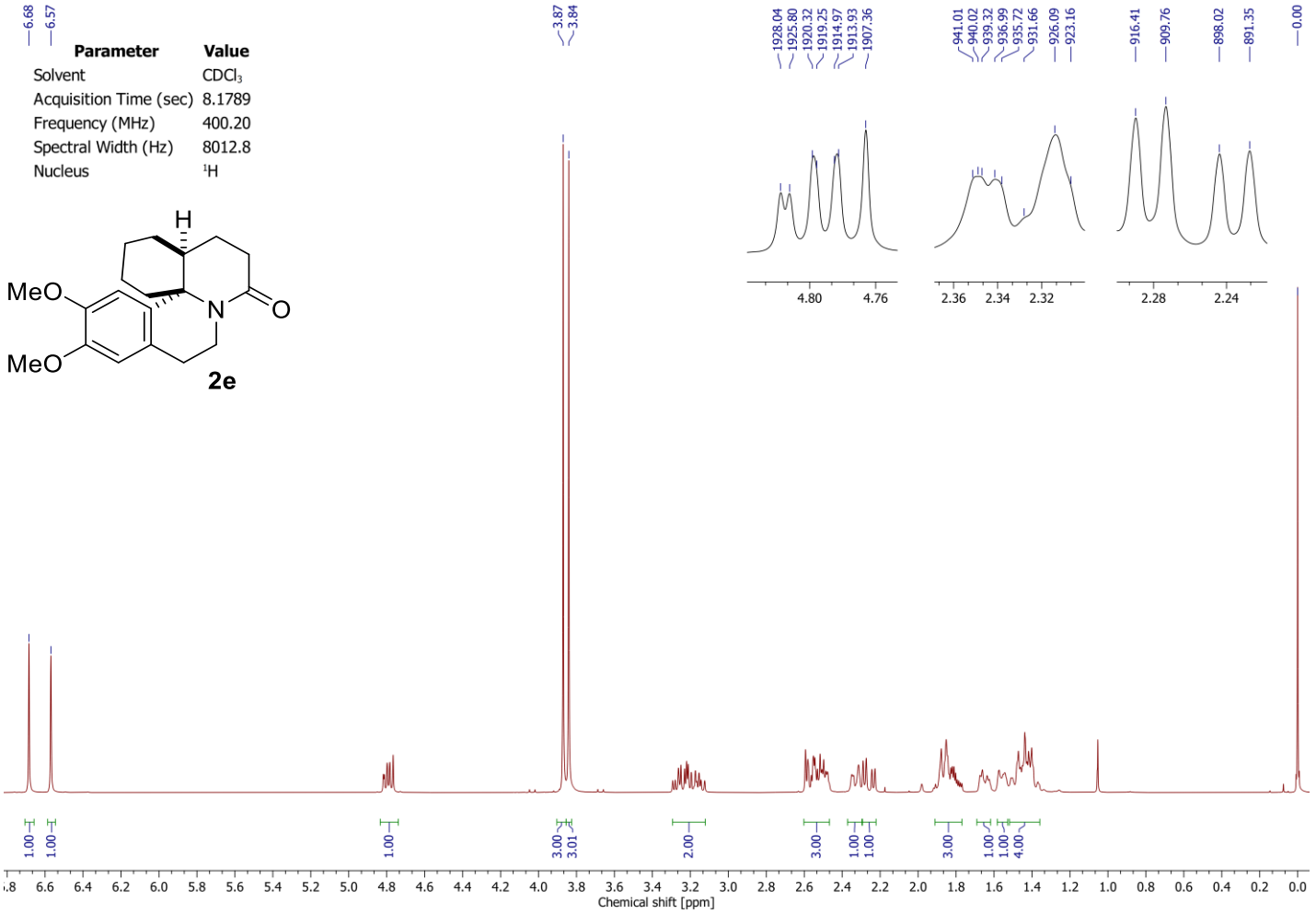
2b

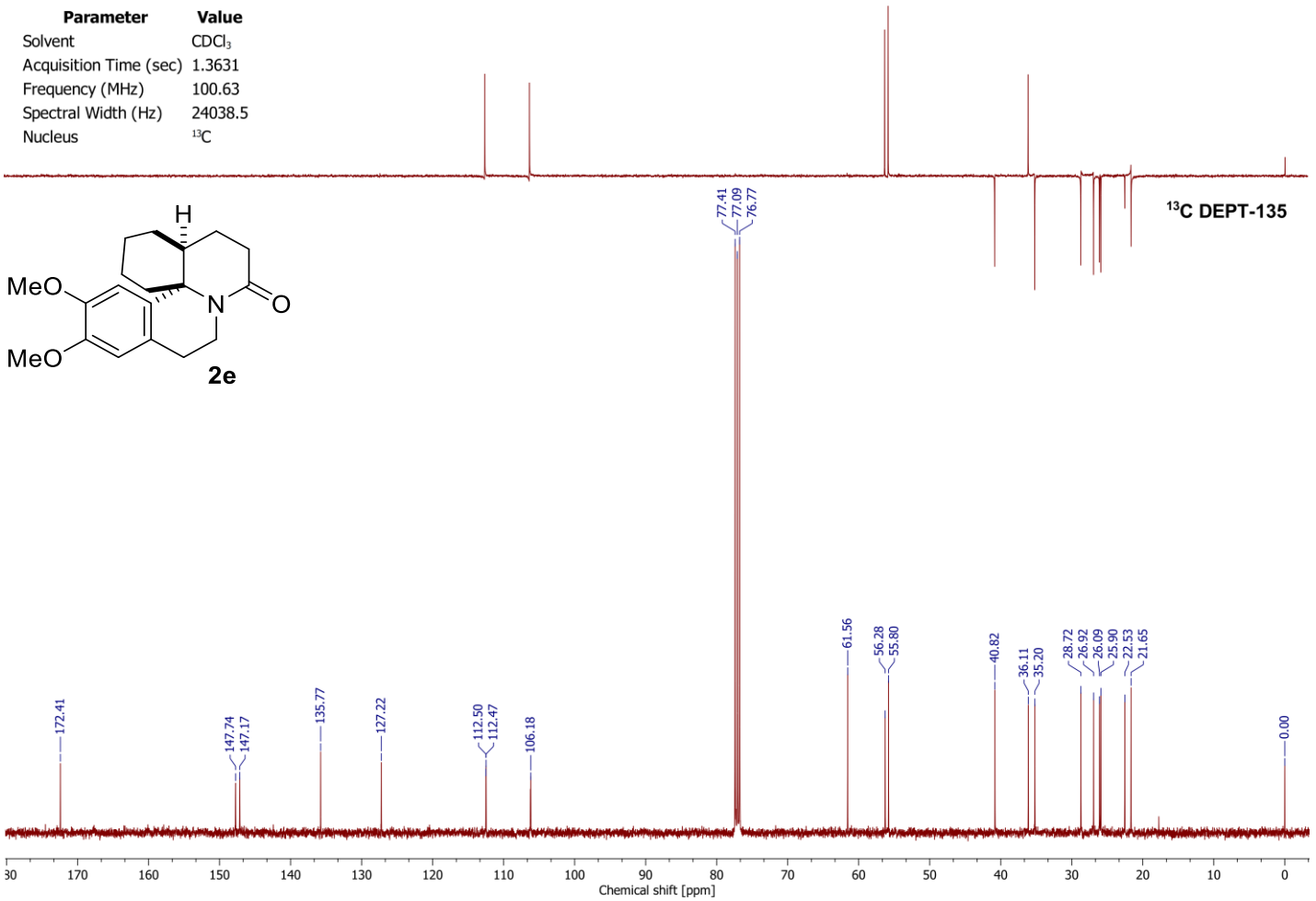

Parameter Value
Solvent DMSO
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
MeO
MeO
H
H
N
O
2c
Chemical shift [ppm]


Parameter Value
Solvent DMSO
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
MeO
MeO
H
H
N
O
2c
Chemical shift [ppm]

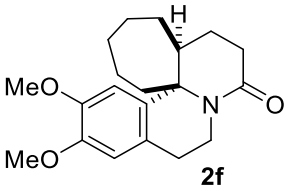

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 4.0894
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
MeO
MeO
N
O
H
2d
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
MeO
MeO
N
O
H
2d
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
MeO
MeO
N
O
H
2e
Chemical shift [ppm]

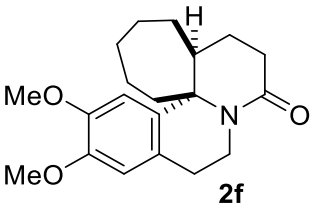

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.63
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
MeO
MeO
N
O
H
2e
Chemical shift [ppm]

Parameter	Value
Solvent	DMSO
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

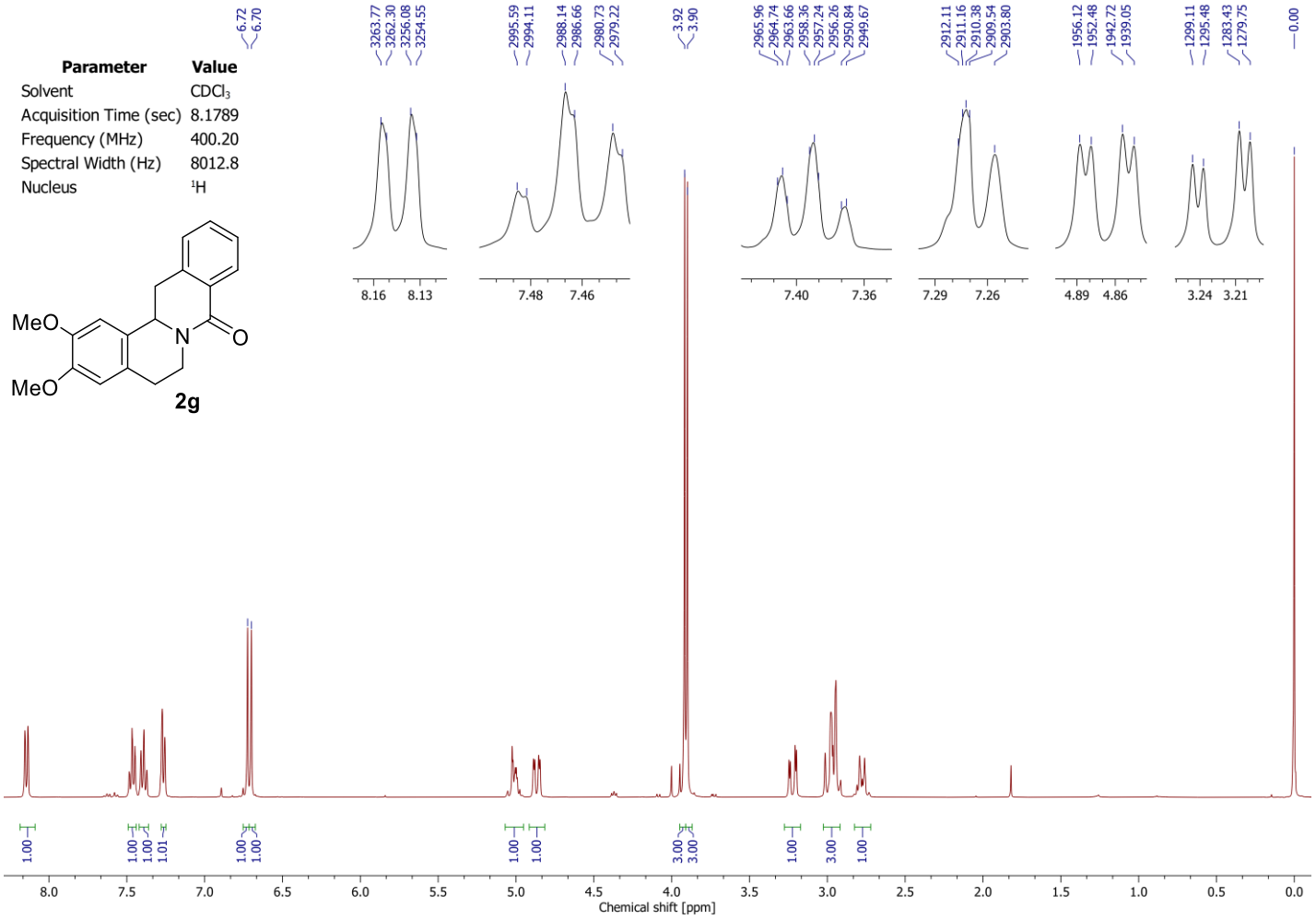


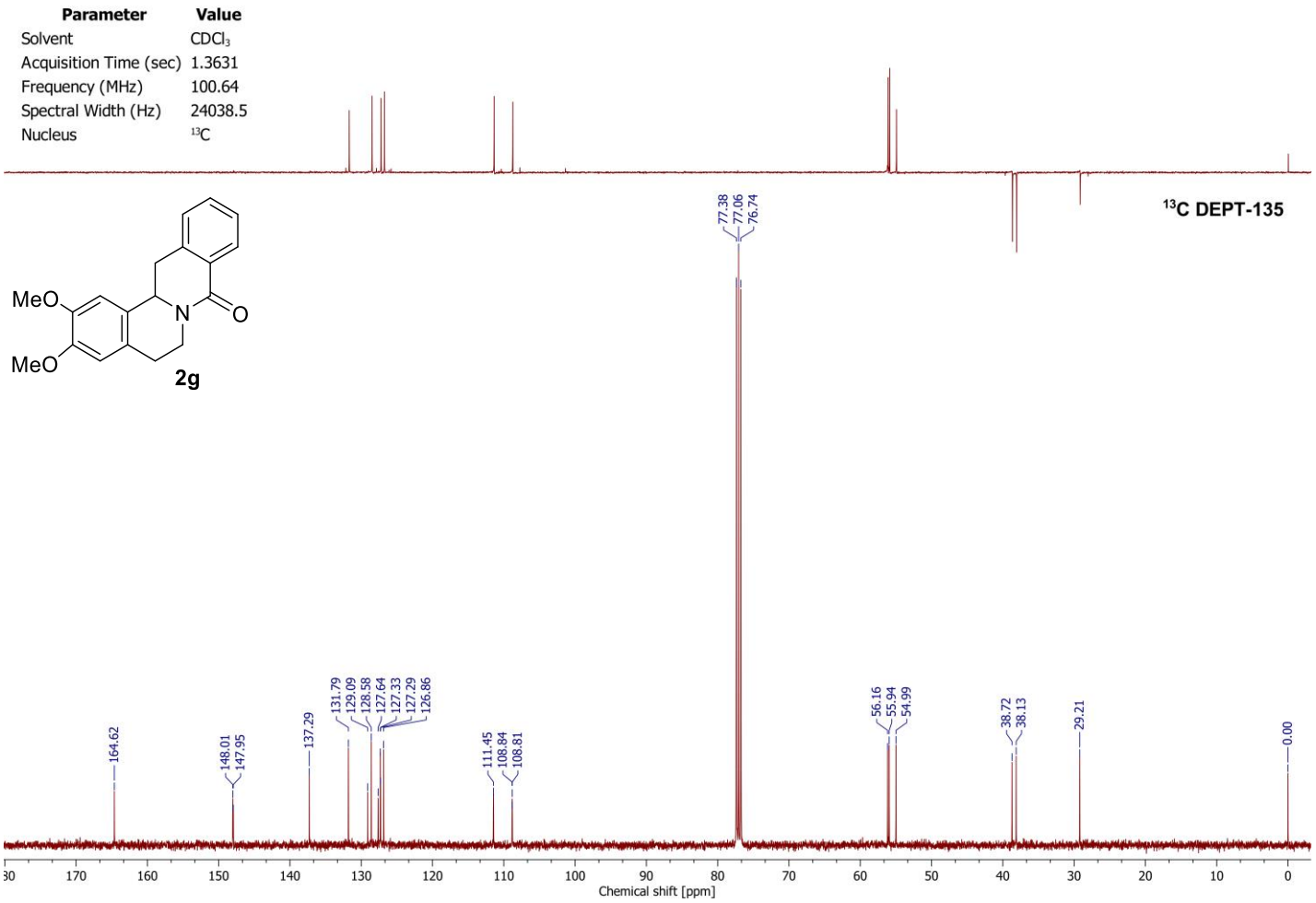
2f

Parameter	Value
Solvent	DMSO
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

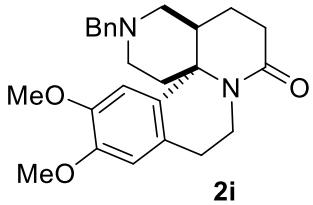


2f


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
MeO
MeO
N
O
2g
Chemical shift [ppm]

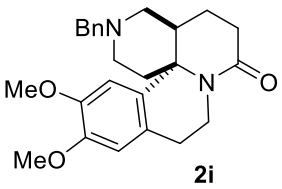

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
MeO
MeO
N
O
2g
Chemical shift [ppm]

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



2i

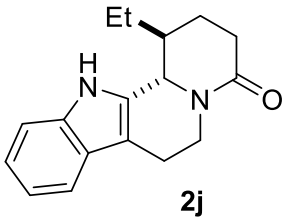
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



2i

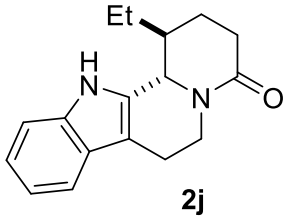
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



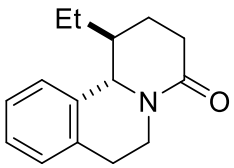
2j

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



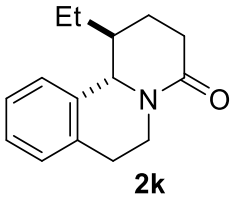
2j

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H

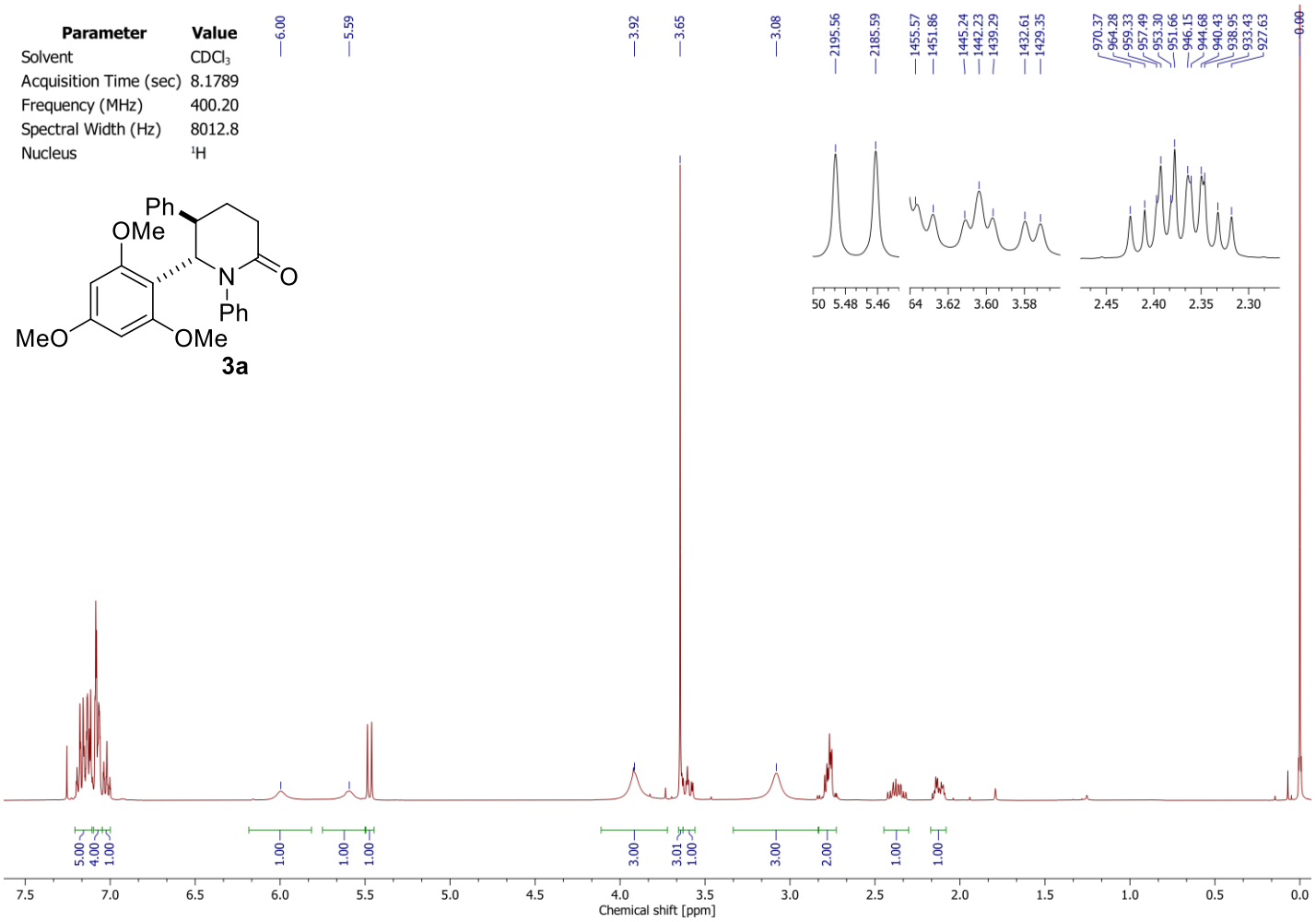


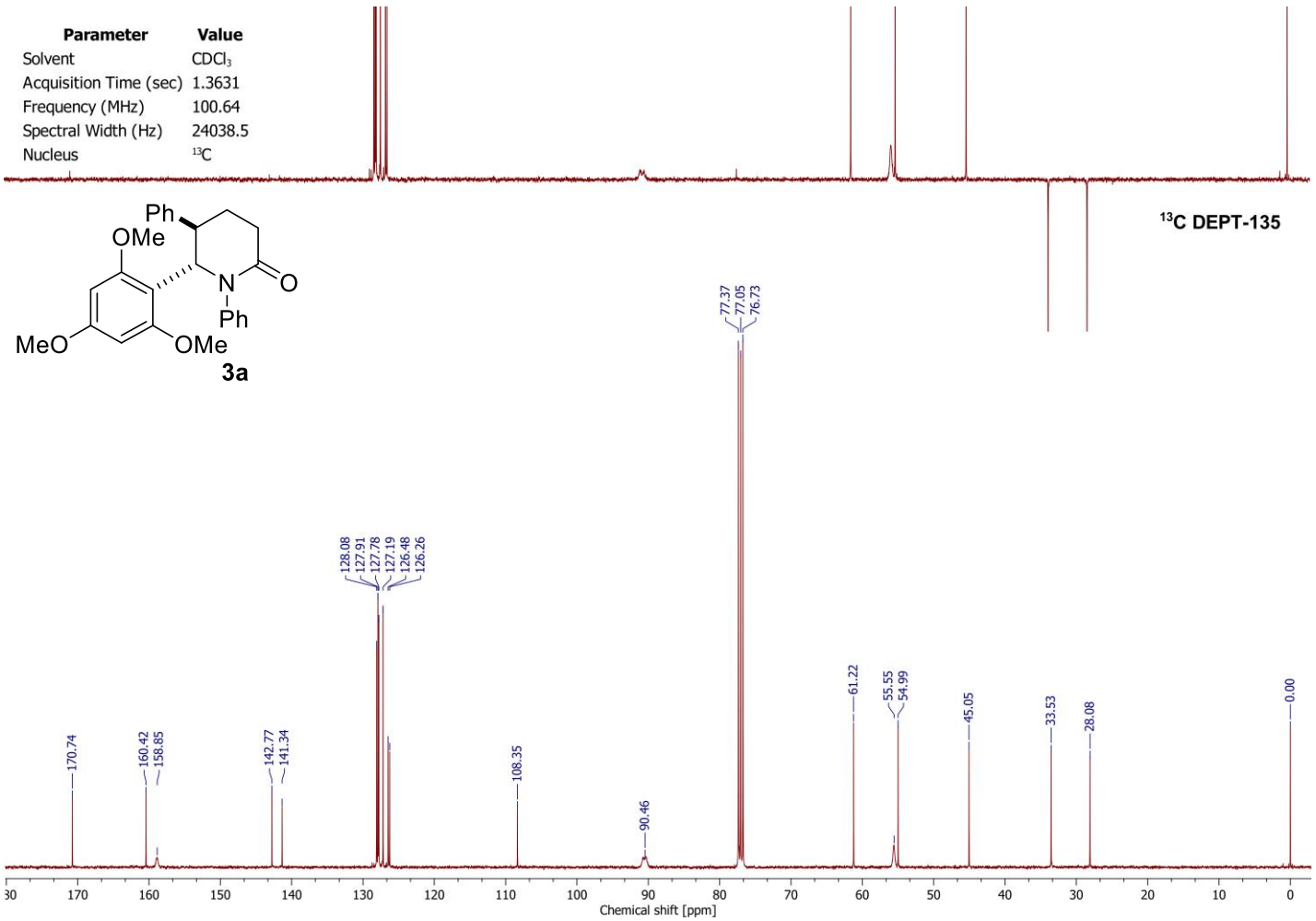
2k

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

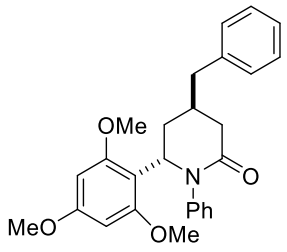


2k


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
Ph
OMe
N
O
Ph
MeO
OMe
3a
6.00
5.59
3.92
3.65
3.08
2195.56
2185.59
1455.57
1451.86
1445.24
1442.23
1439.29
1432.61
1429.35
970.37
964.28
959.33
957.49
953.30
951.66
946.15
944.68
940.43
938.95
933.43
927.63
0.00
5.00
4.00
1.00
1.00
1.00
1.00
3.00
3.01
1.00
3.00
2.00
1.00
1.00
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
Ph
OMe
N
O
Ph
MeO
OMe
3a
77.37
77.05
76.73
128.08
127.91
127.78
127.19
126.48
126.26
170.74
160.42
158.85
142.77
141.34
108.35
90.46
61.22
55.55
54.99
45.05
33.53
28.08
0.00
Chemical shift [ppm]

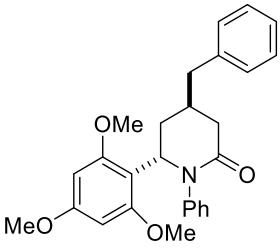
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



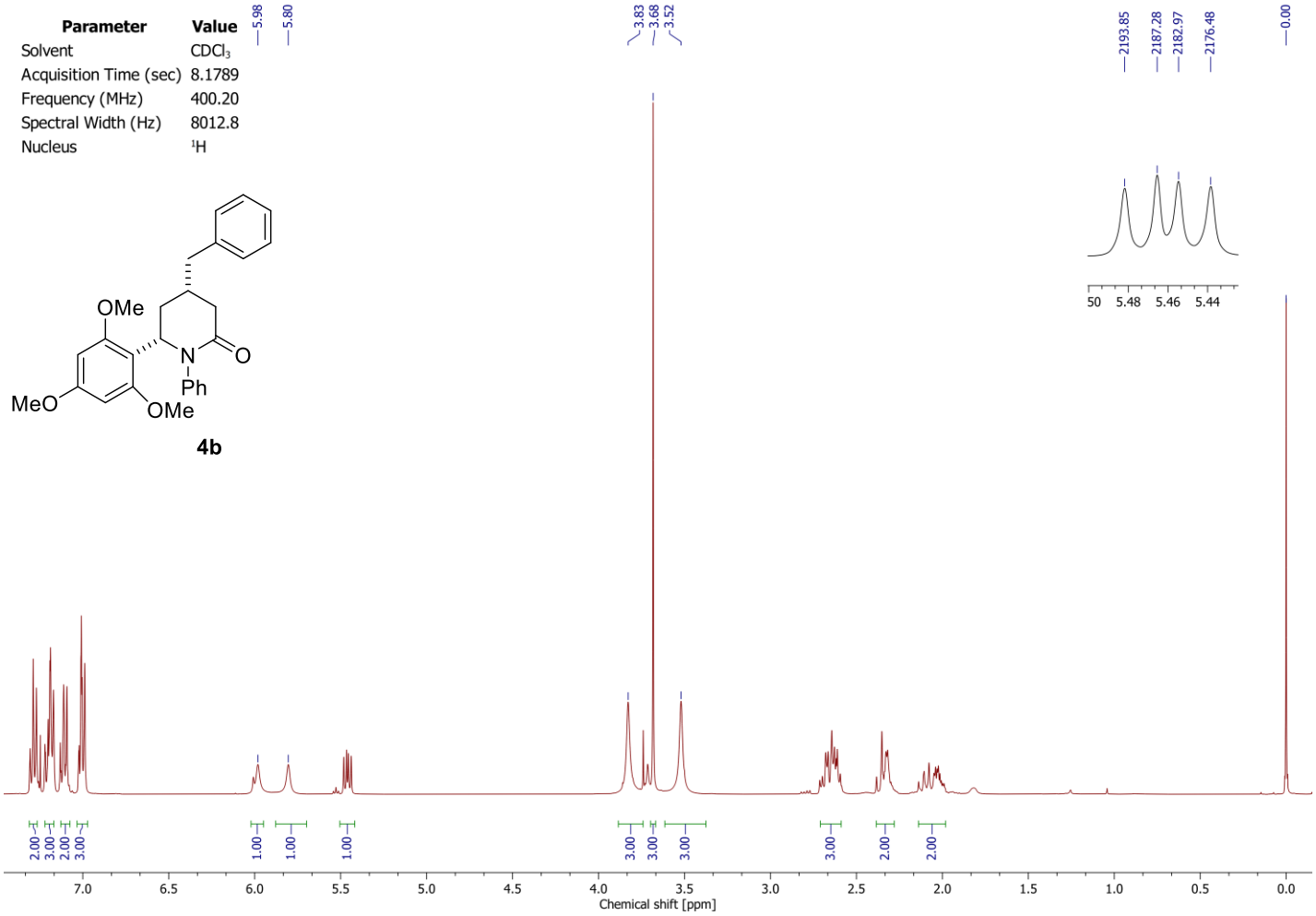
3b

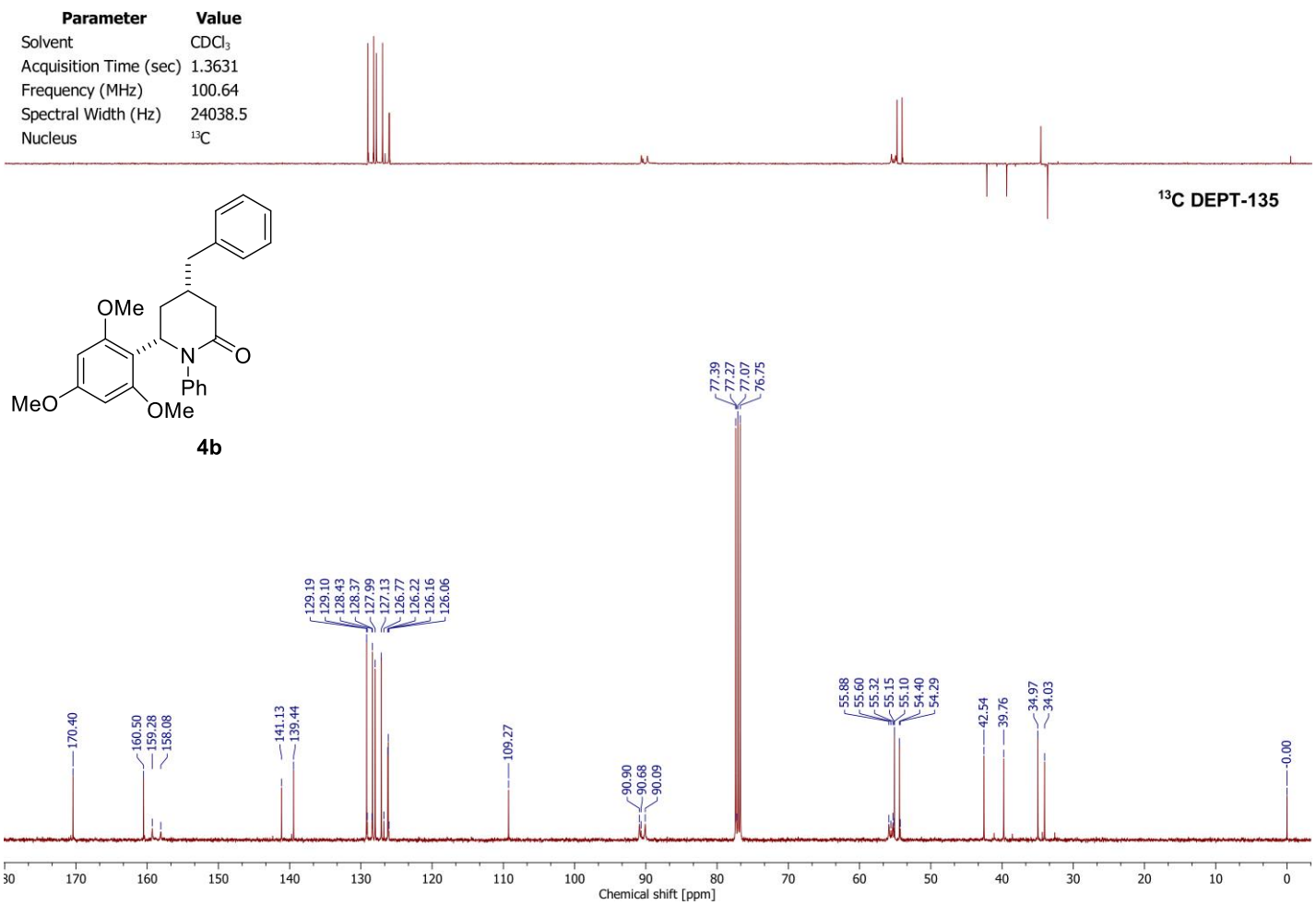
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

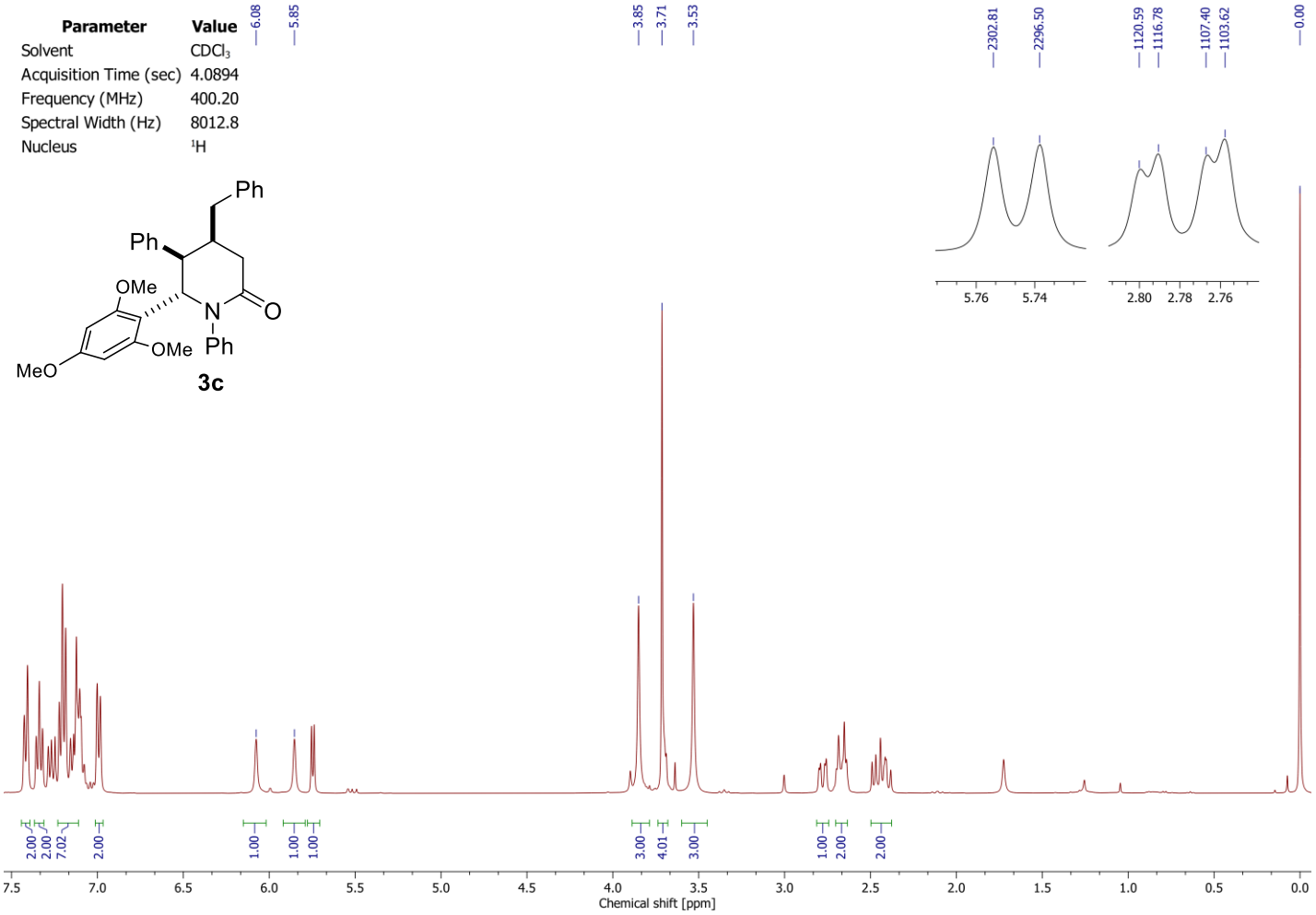
^{13}C DEPT-135

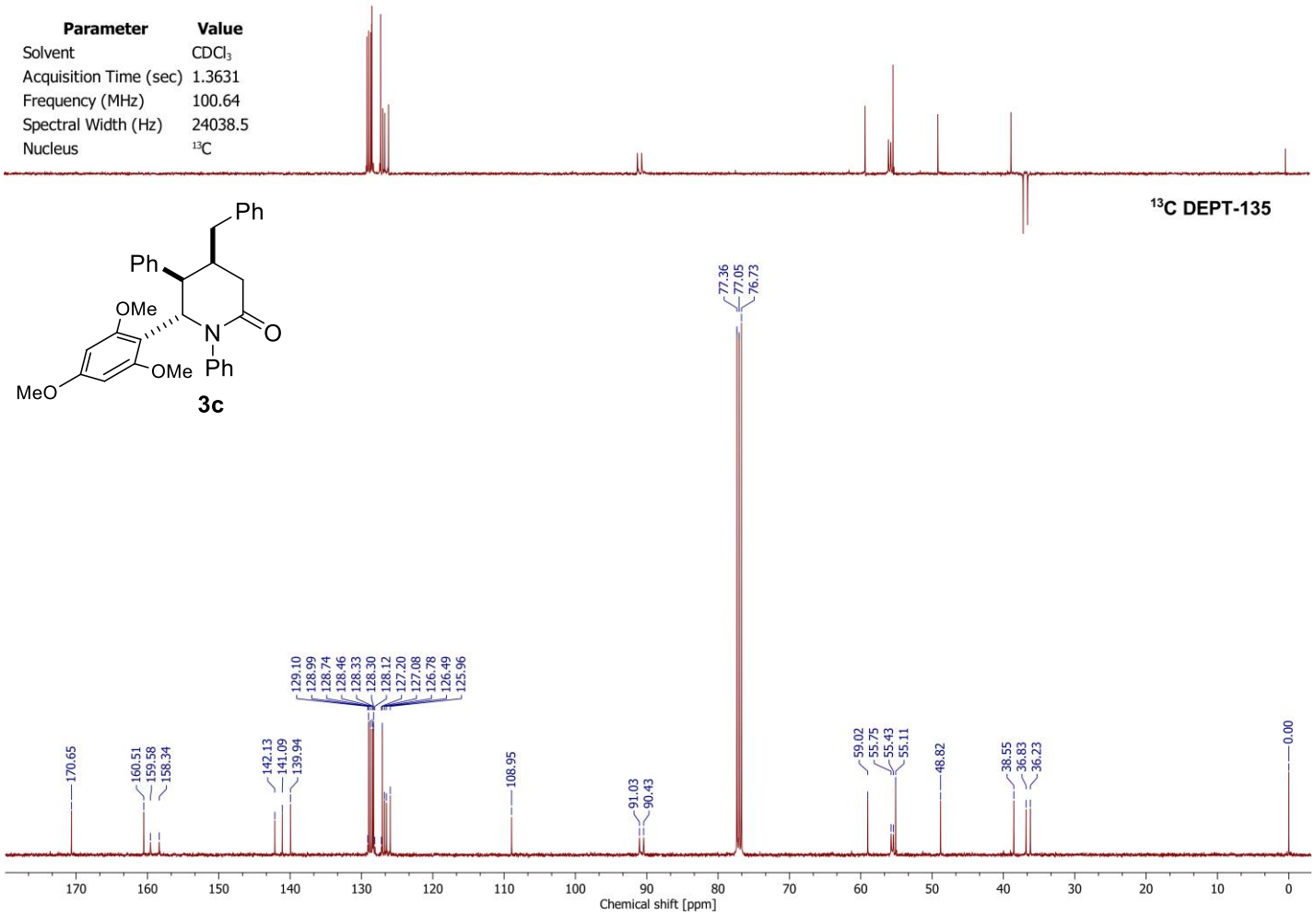


3b

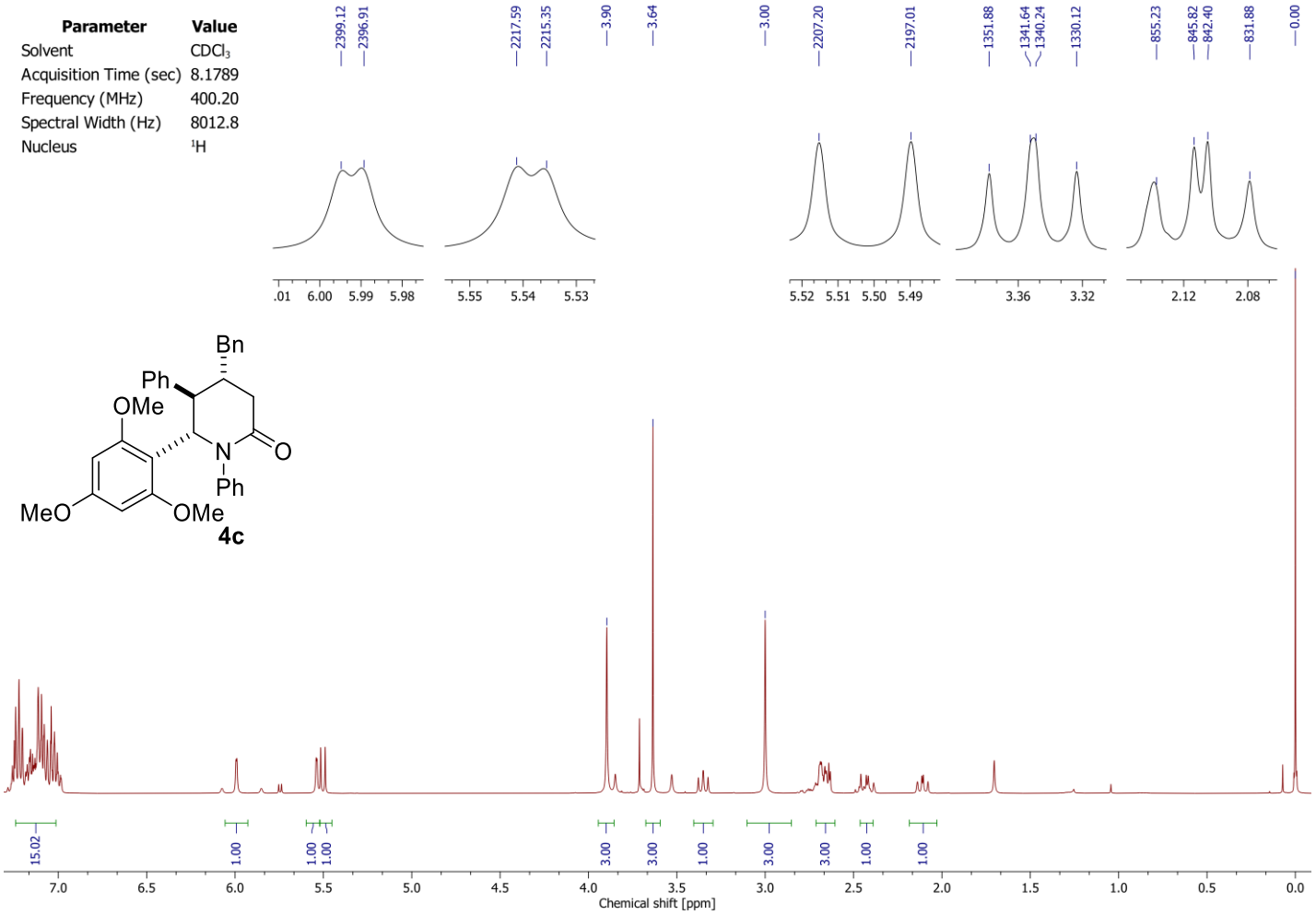

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
5.98
5.80
3.83
3.68
3.52
2193.85
2187.28
2182.97
2176.48
0.00
50 5.48 5.46 5.44
OMe
MeO
OMe
N
O
Ph
4b
2.00
3.00
2.00
3.00
1.00
1.00
1.00
3.00
3.00
3.00
3.00
2.00
2.00
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
OMe
MeO
OMe
N
O
Ph
4b
77.39
77.27
77.07
76.75
129.19
129.10
128.43
128.37
127.99
127.13
126.77
126.22
126.16
126.06
170.40
160.50
159.28
158.08
141.13
139.44
109.27
90.90
90.68
90.09
55.88
55.60
55.32
55.15
55.10
54.40
54.29
42.54
39.76
34.97
34.03
0.00
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical shift [ppm]

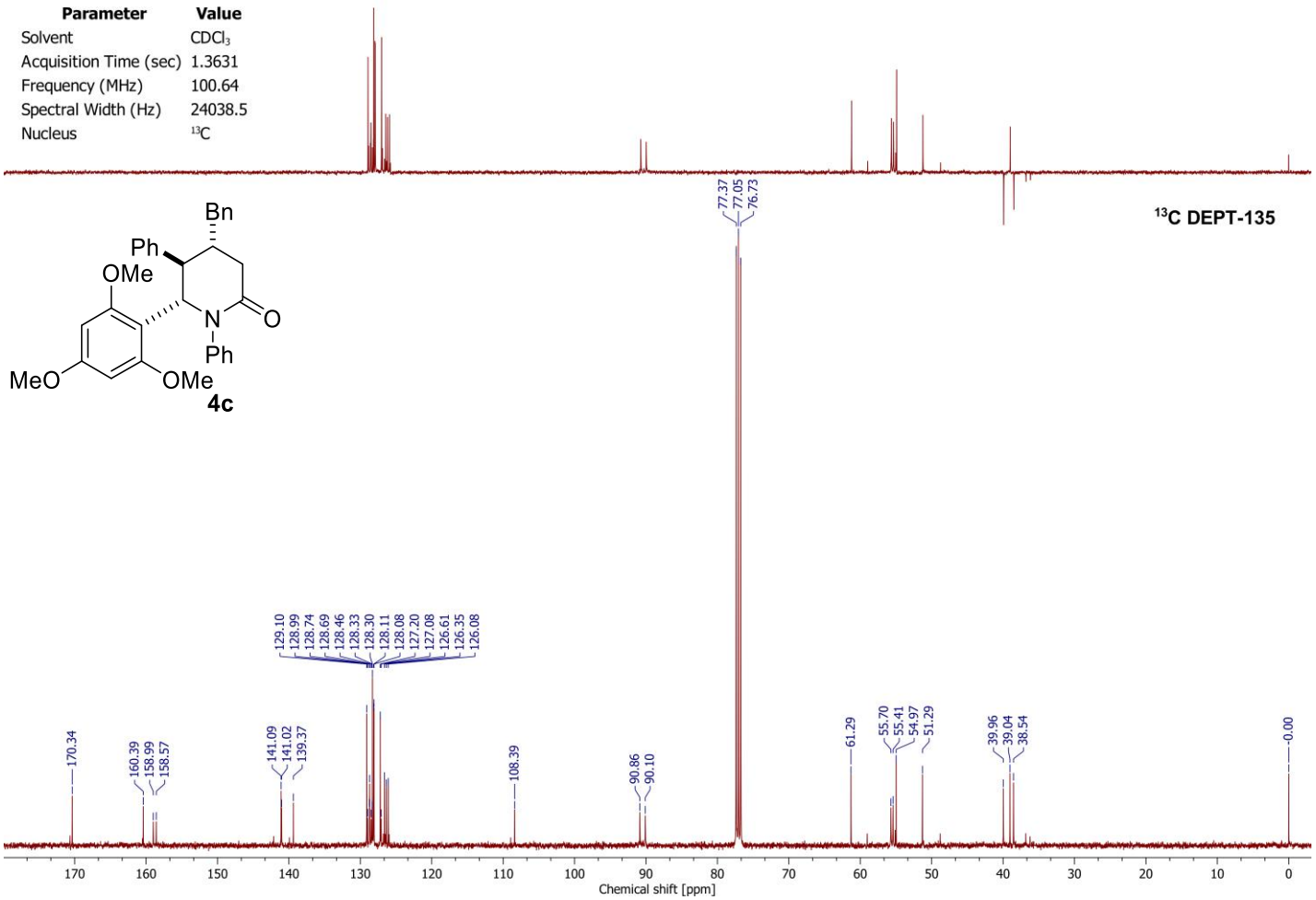

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 4.0894
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
6.08
5.85
3.85
3.71
3.53
2302.81
2296.50
1120.59
1116.78
1107.40
1103.62
0.00
5.76
5.74
2.80
2.78
2.76
Ph
Ph
OMe
N
O
OMe
Ph
MeO
3c
2.00
2.00
7.02
2.00
1.00
1.00
1.00
3.00
4.01
3.00
1.00
2.00
2.00
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
Ph
Ph
OMe
N
O
OMe
Ph
MeO
3c
77.36
77.05
76.73
129.10
128.99
128.74
128.46
128.33
128.30
128.12
127.20
127.08
126.78
126.49
125.96
170.65
160.51
159.58
158.34
142.13
141.09
139.94
108.95
91.03
90.43
59.02
55.75
55.43
55.11
48.82
38.55
36.83
36.23
0.00
Chemical shift [ppm]

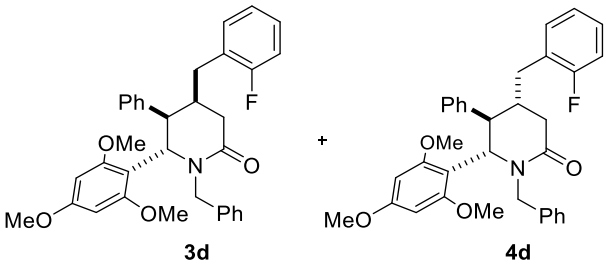
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

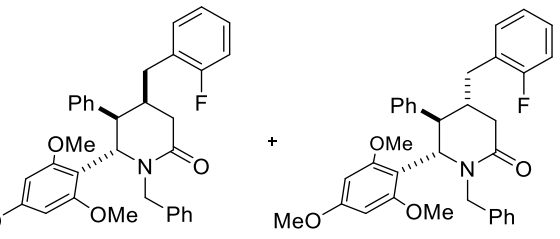


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



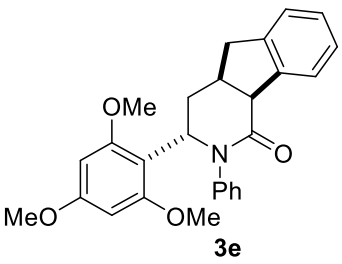
3d + **4d**

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



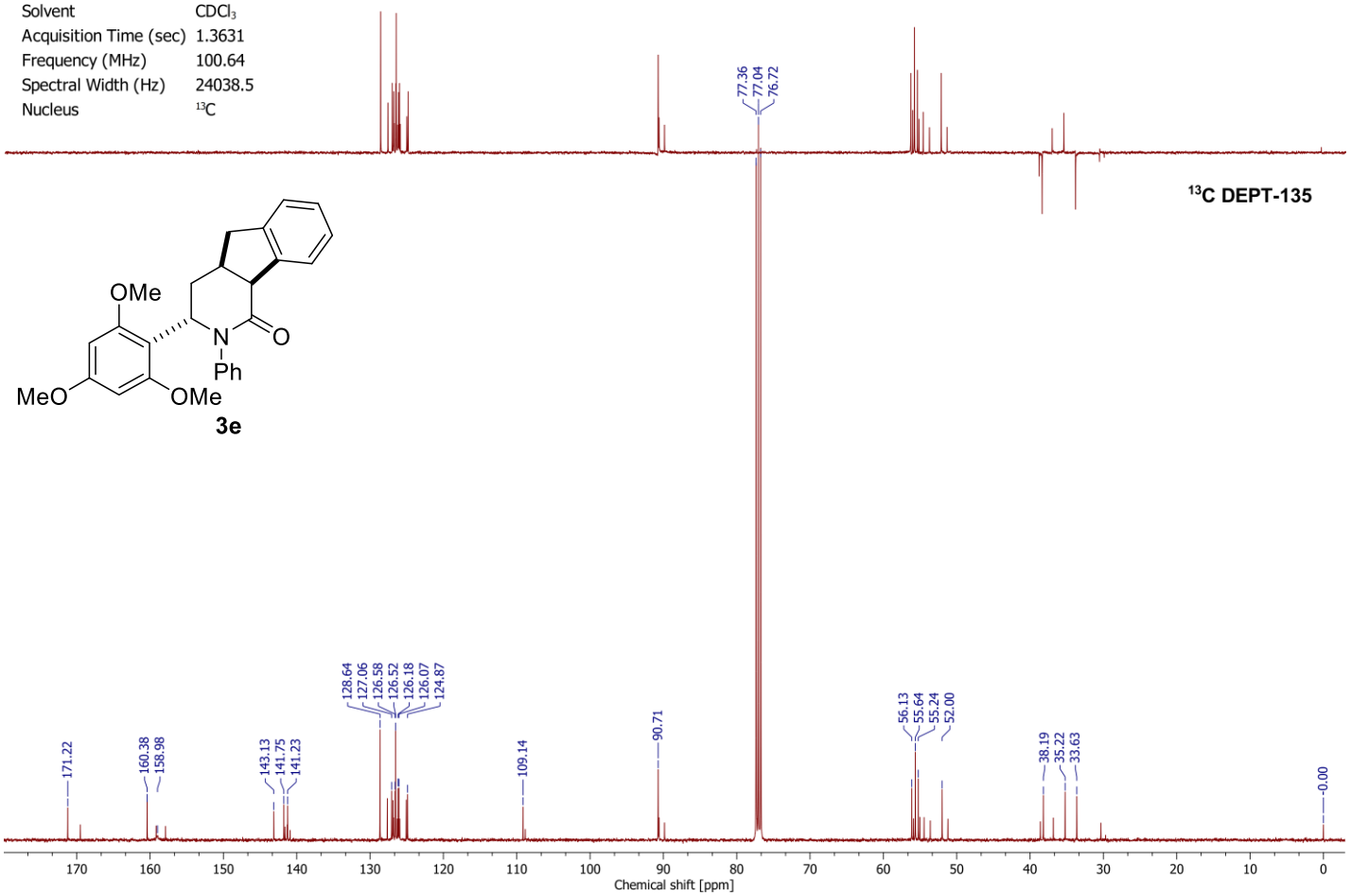
3d + **4d**

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



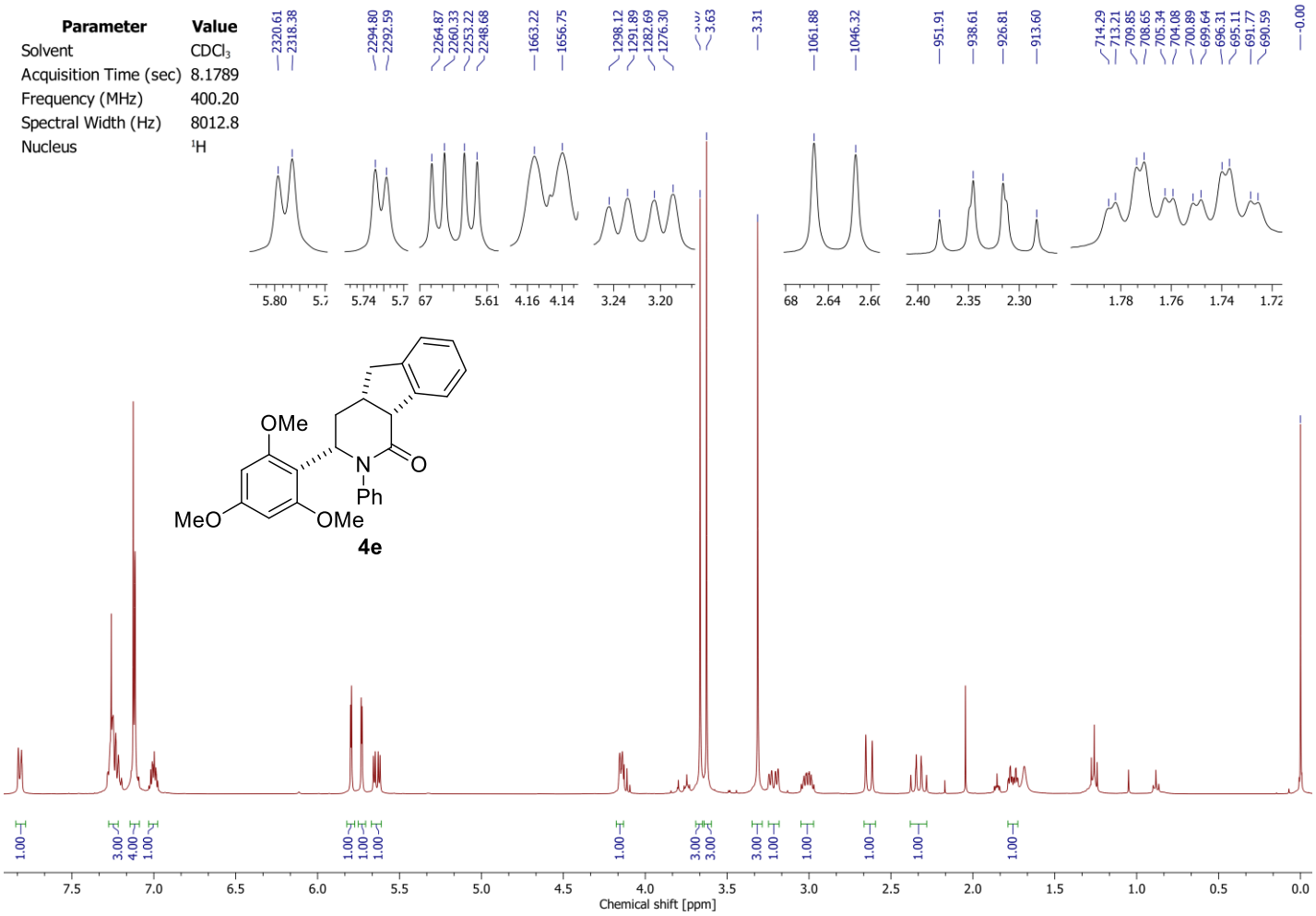
3e

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



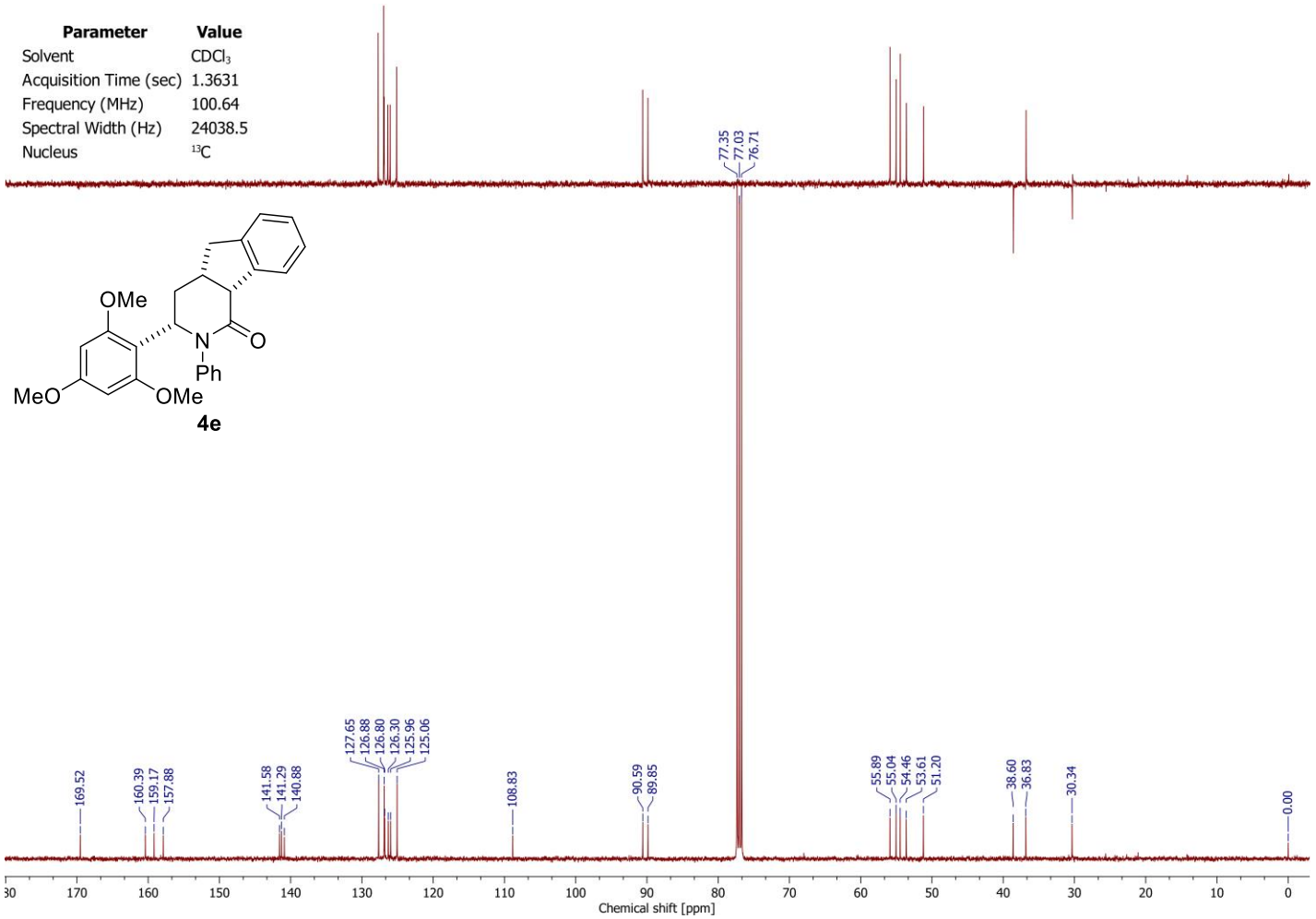
3e

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

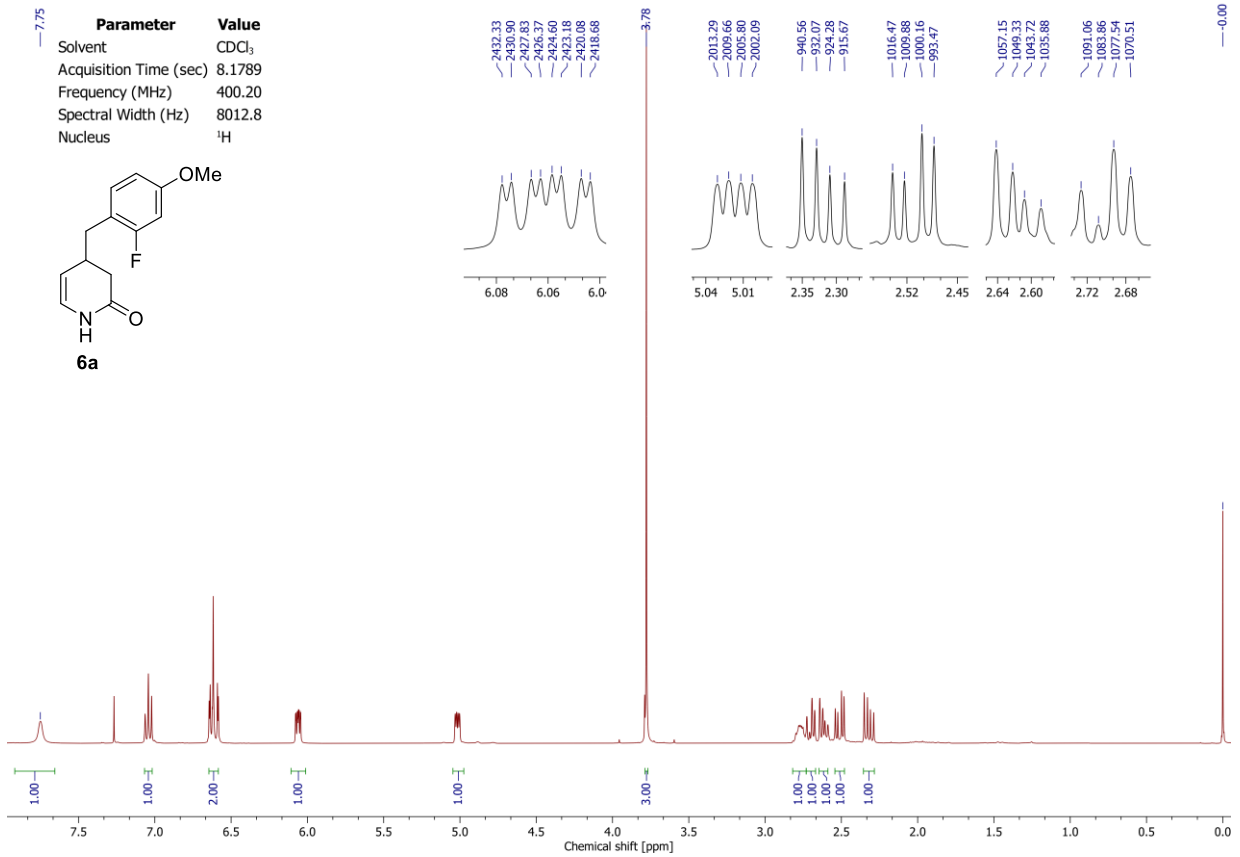


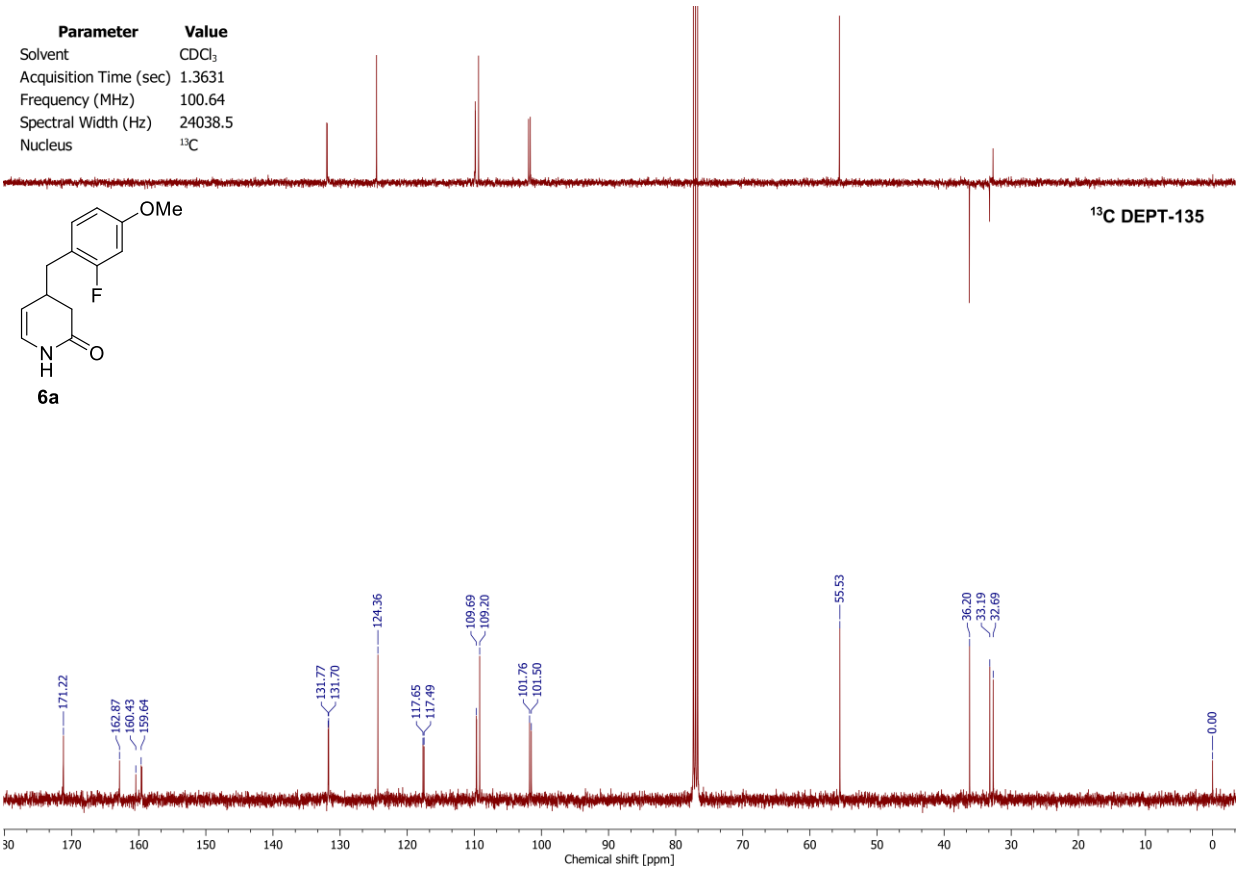
4e

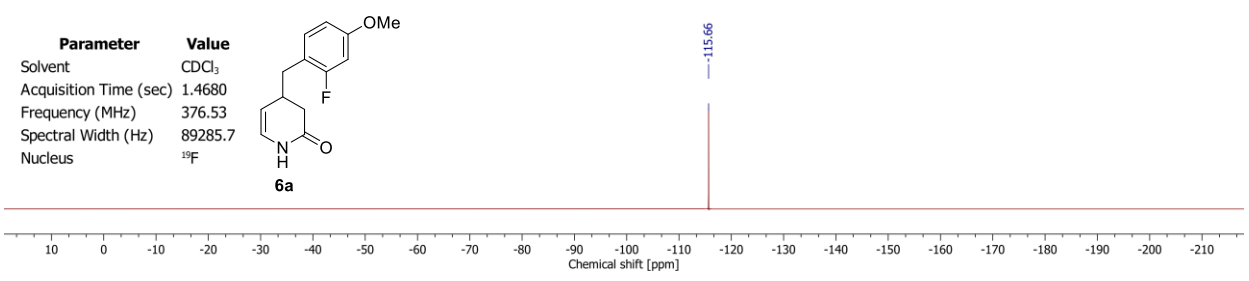
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



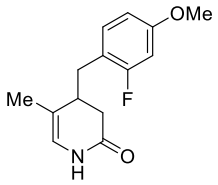
4e


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
OMe
F
N
H
O
6a
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
OMe
F
N
H
O
6a
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.4680
Frequency (MHz) 376.53
Spectral Width (Hz) 89285.7
Nucleus 19F
OMe
F
N
H
O
6a
Chemical shift [ppm]

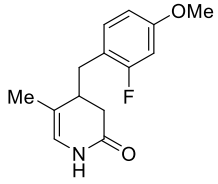
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



6b

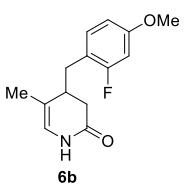
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

^{13}C DEPT-135



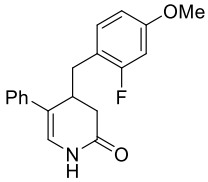
6b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.4680
Frequency (MHz)	376.53
Spectral Width (Hz)	89285.7
Nucleus	^{19}F



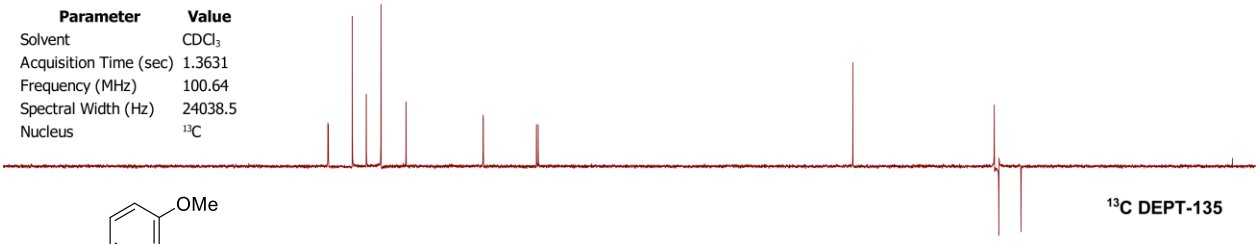
6b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

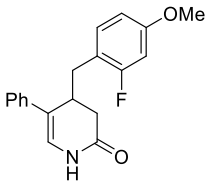


6c

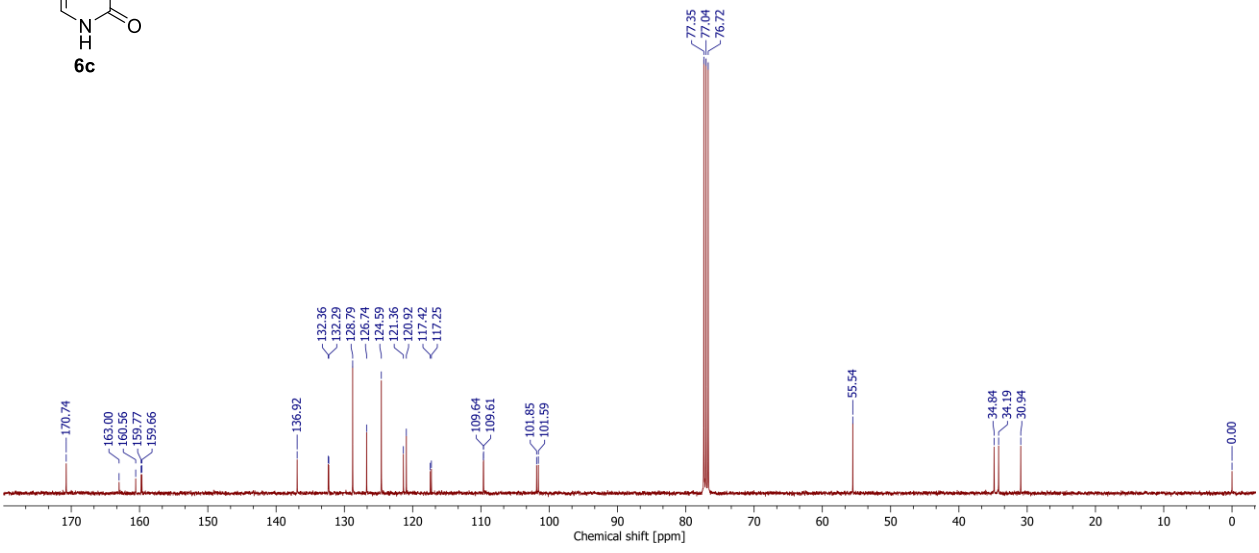
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



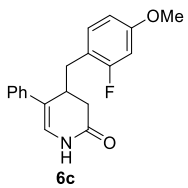
^{13}C DEPT-135



6c

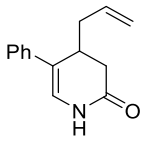


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.4680
Frequency (MHz)	376.53
Spectral Width (Hz)	89285.7
Nucleus	^{19}F



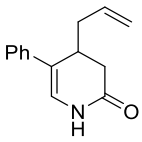
6c

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



6d

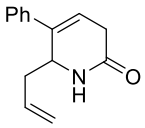
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



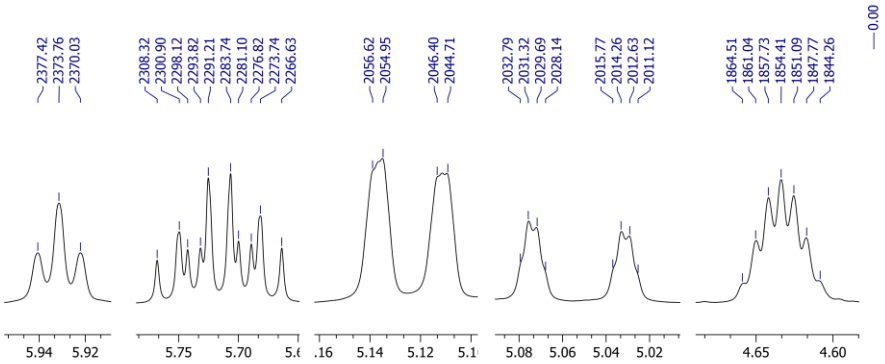
6d

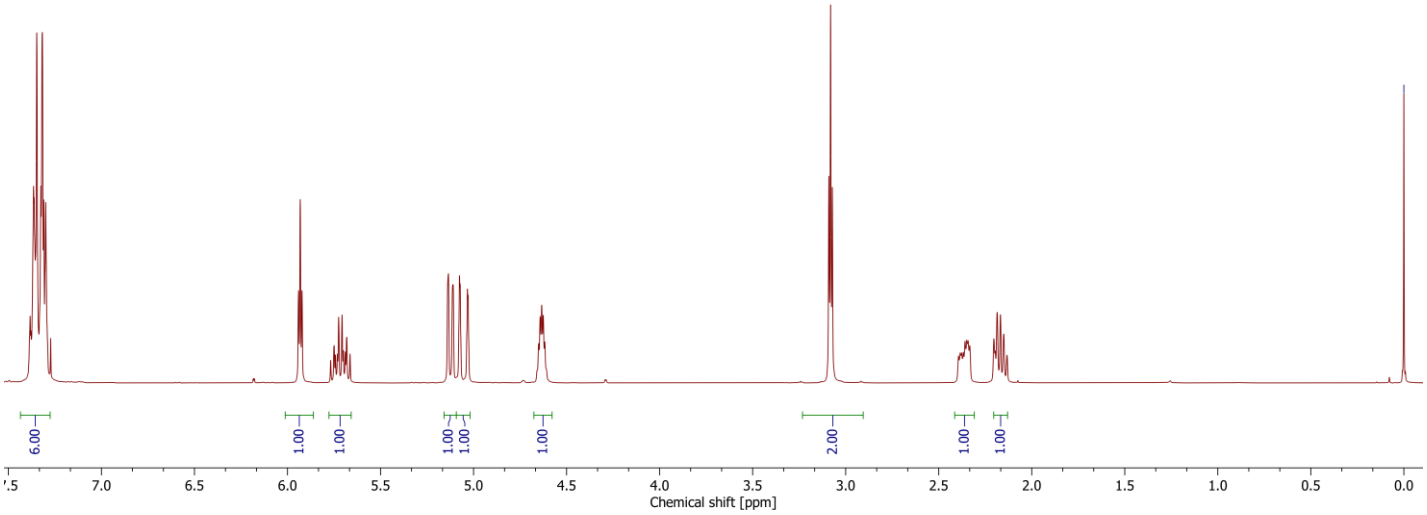
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

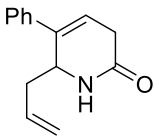


6d-isomer-6

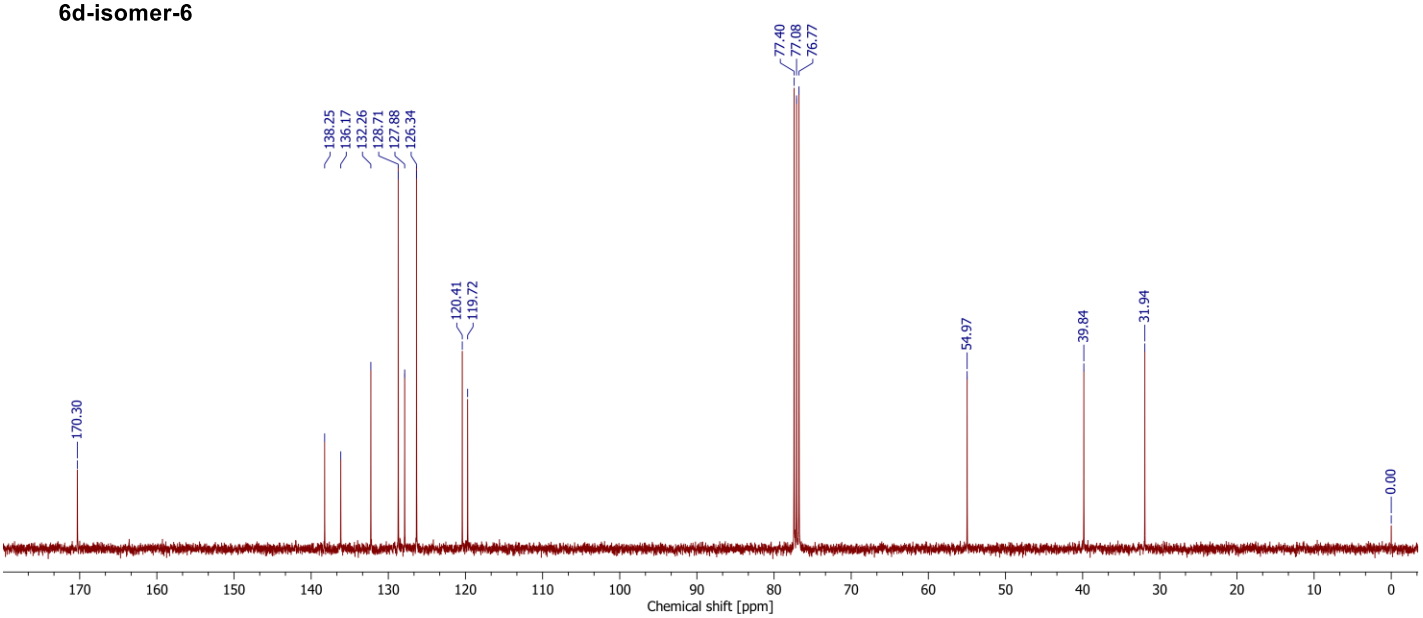




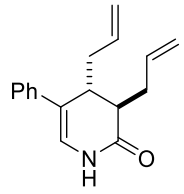
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



6d-isomer-6

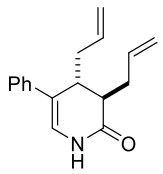


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



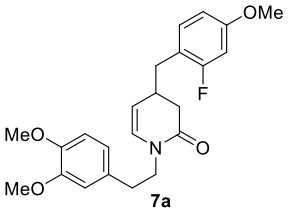
6e

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



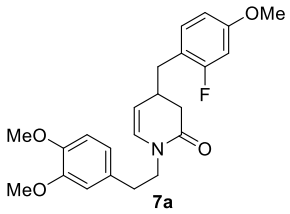
6e

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



7a

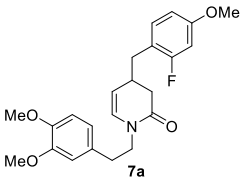
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



7a

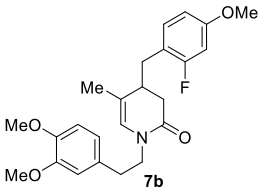
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.4680
Frequency (MHz)	376.53
Spectral Width (Hz)	89285.7
Nucleus	^{19}F



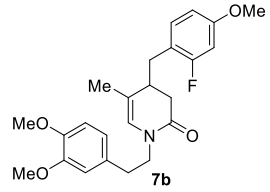
7a

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



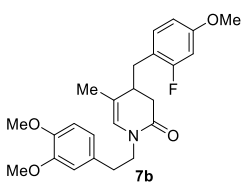
7b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

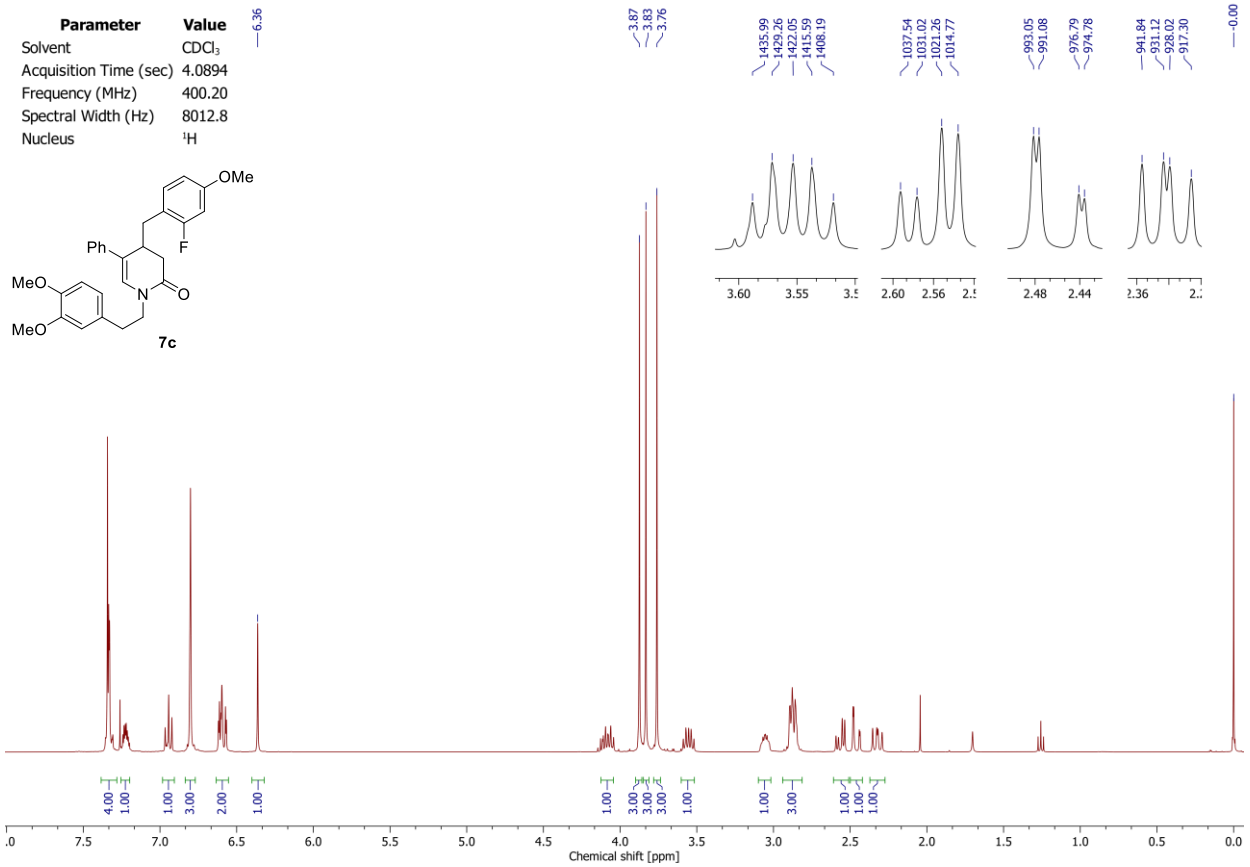


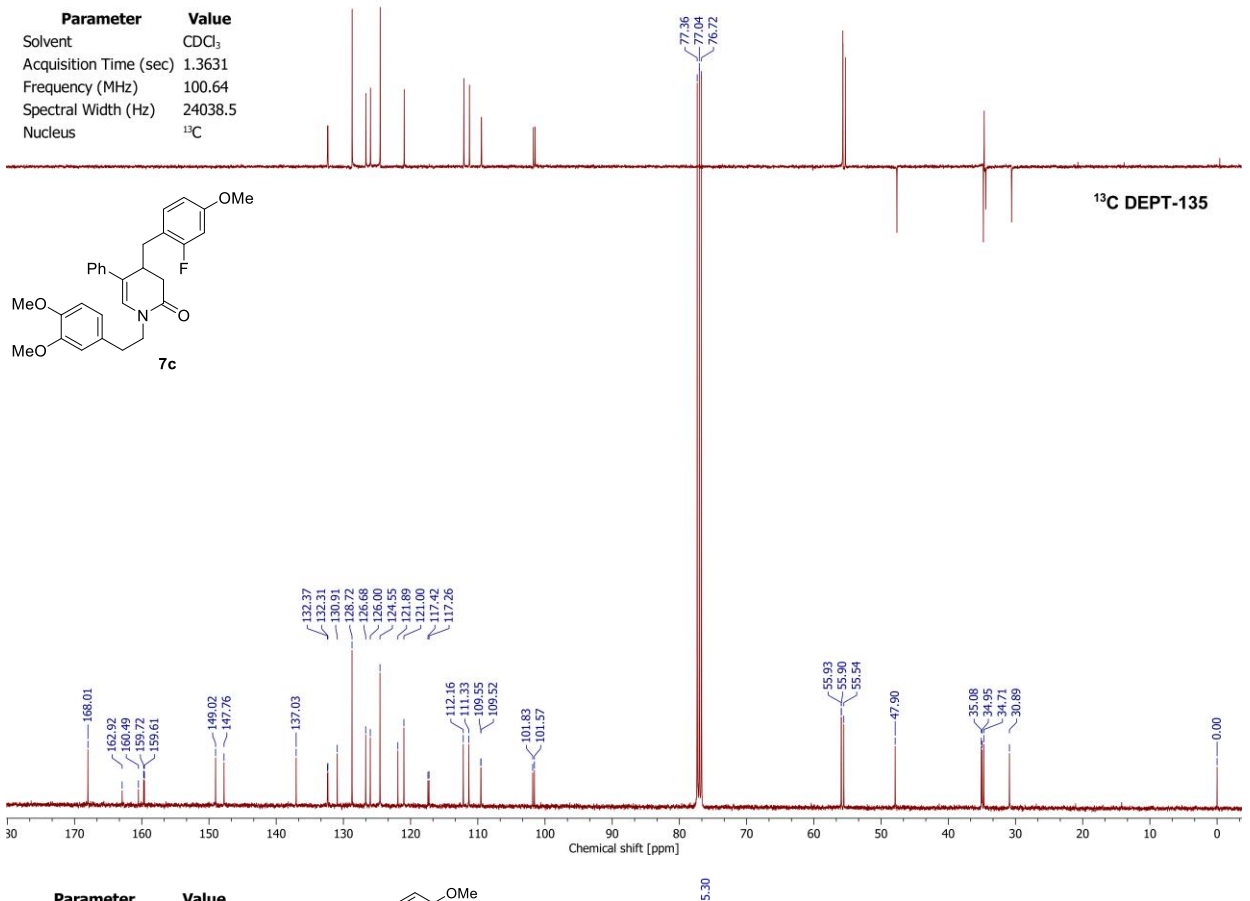
7b

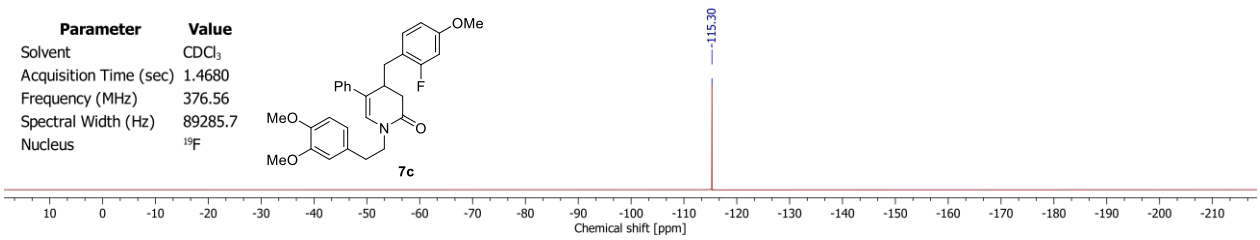
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.4680
Frequency (MHz)	376.53
Spectral Width (Hz)	89285.7
Nucleus	^{19}F

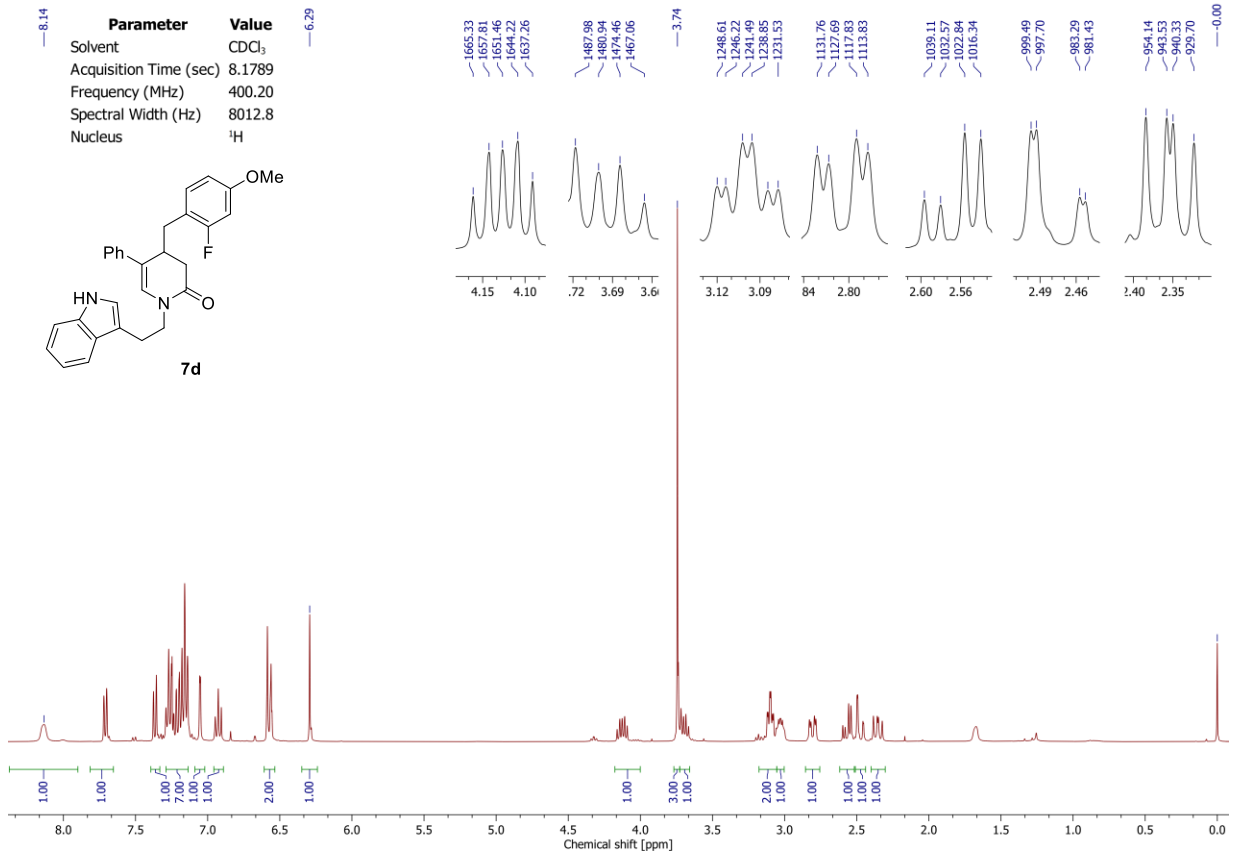


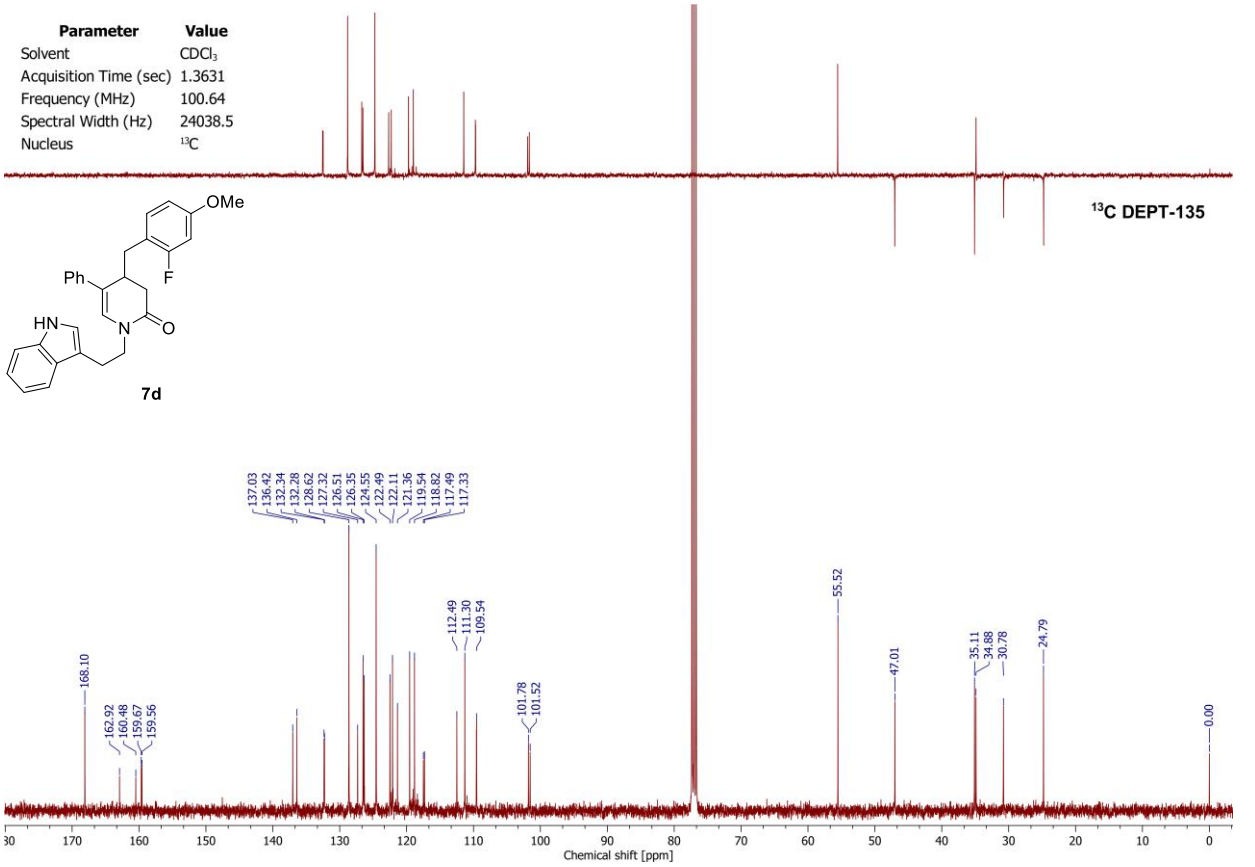
7b

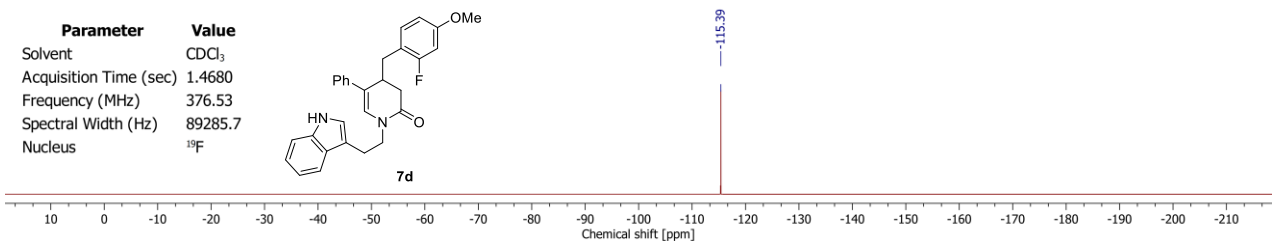

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 4.0894
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
7c
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
7c
Chemical shift [ppm]

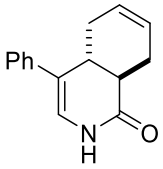

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.4680
Frequency (MHz) 376.56
Spectral Width (Hz) 89285.7
Nucleus 19F
7c
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
OMe
Ph
F
HN
N
O
7d
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
OMe
Ph
F
HN
N
O
7d
Chemical shift [ppm]

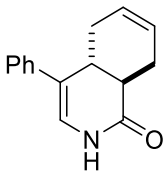

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.4680
Frequency (MHz) 376.53
Spectral Width (Hz) 89285.7
Nucleus 19F
OMe
Ph
F
HN
N
O
7d
Chemical shift [ppm]

Parameter	Value
Solvent	DMSO
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

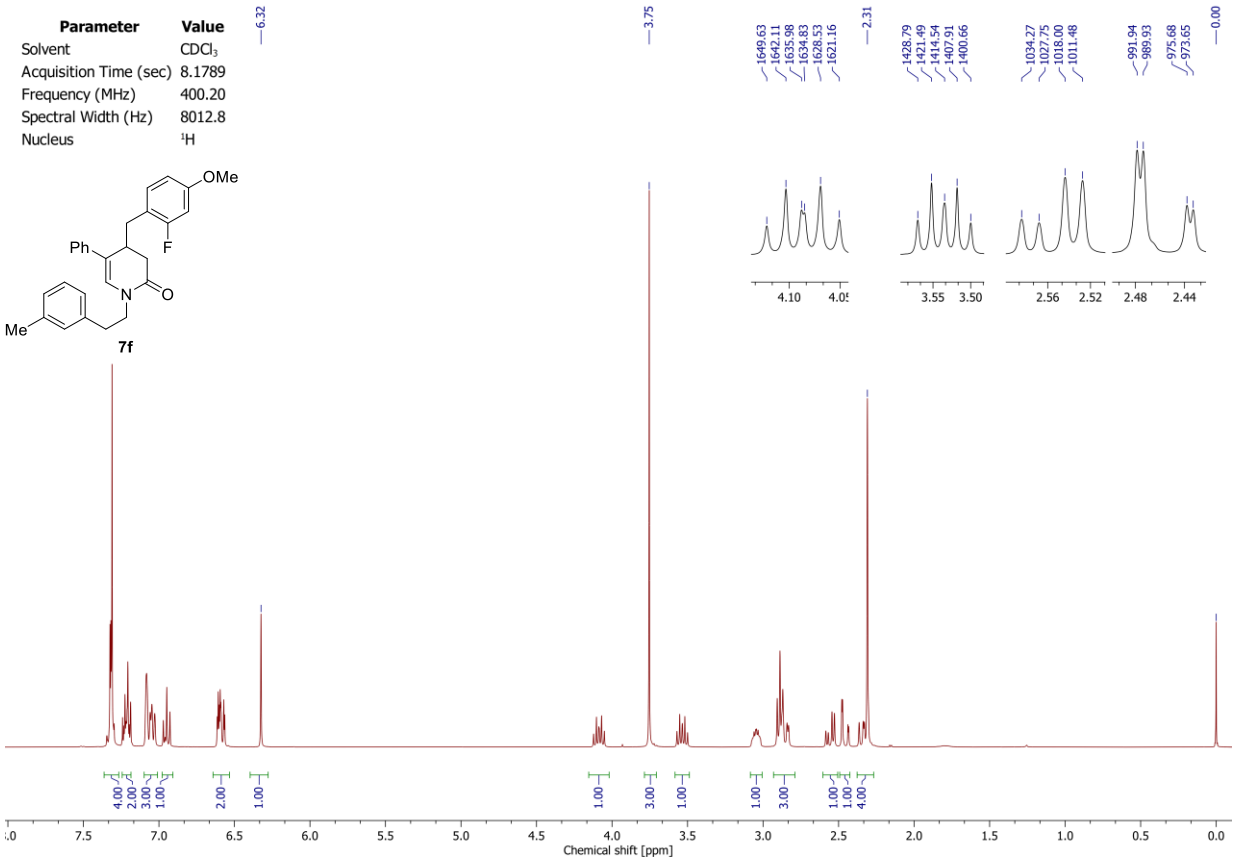


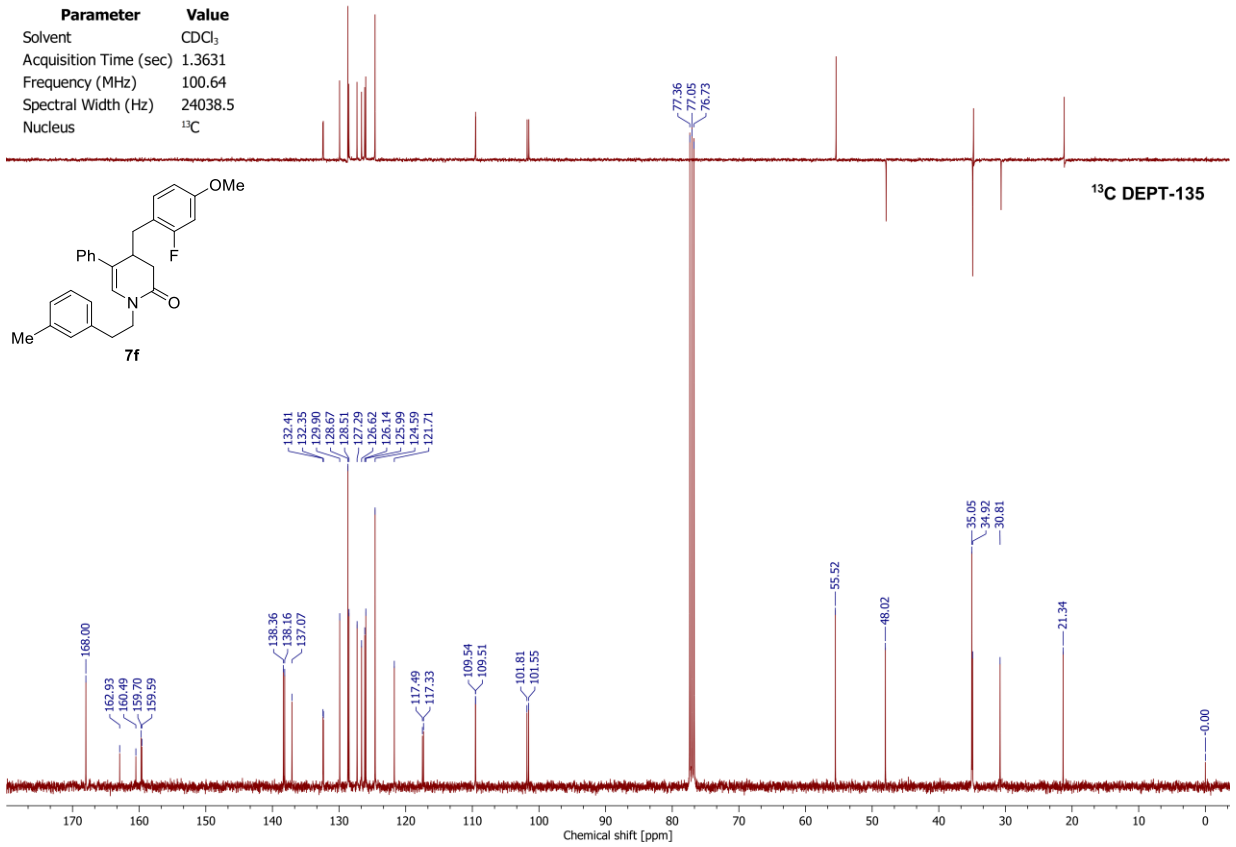
7e

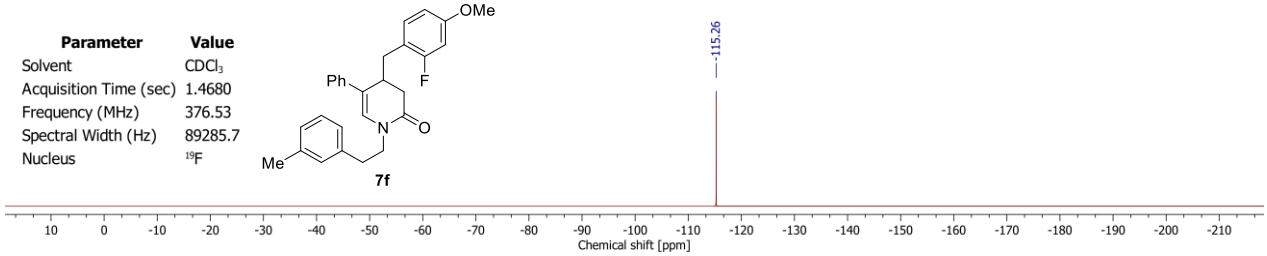
Parameter	Value
Solvent	DMSO
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



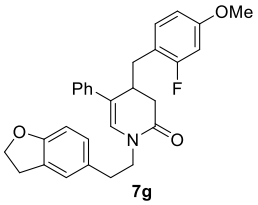
7e


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
OMe
Ph
F
N
O
Me
7f
Chemical shift [ppm]


Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
OMe
Ph
F
N
O
Me
7f
Chemical shift [ppm]

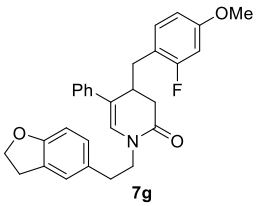

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.4680
Frequency (MHz) 376.53
Spectral Width (Hz) 89285.7
Nucleus 19F
OMe
Ph
F
N
O
Me
7f
Chemical shift [ppm]

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



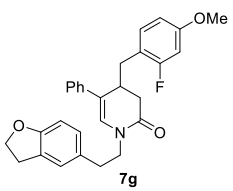
7g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



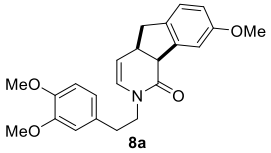
7g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.4680
Frequency (MHz)	376.53
Spectral Width (Hz)	89285.7
Nucleus	^{19}F



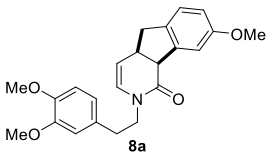
7g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



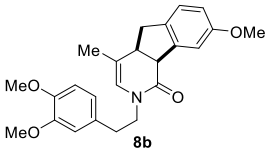
8a

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



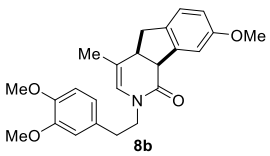
8a

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



8b

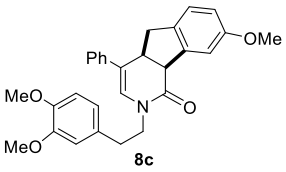
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



8b

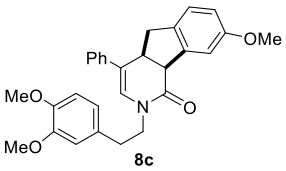
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



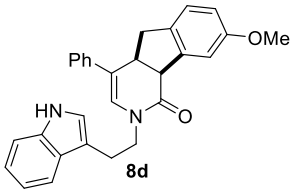
8c

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



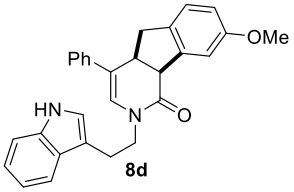
8c

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



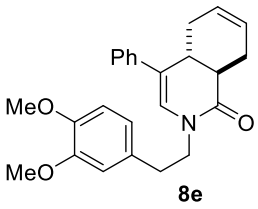
8d

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



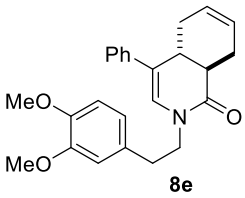
8d

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



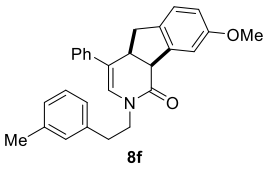
8e

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



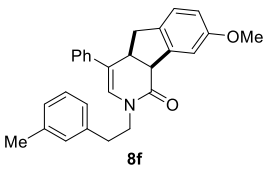
8e

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



8f

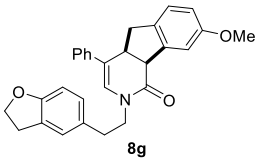
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



8f

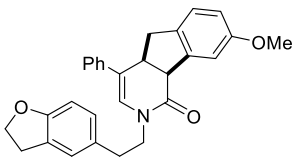
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



8g

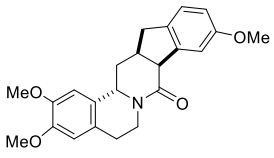
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



8g

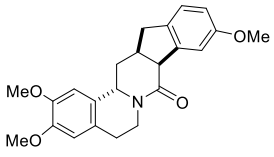
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



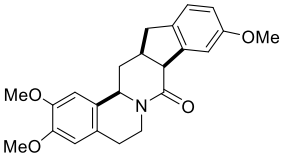
9a

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



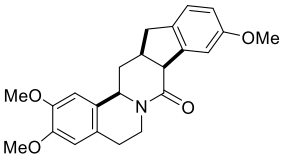
9a

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



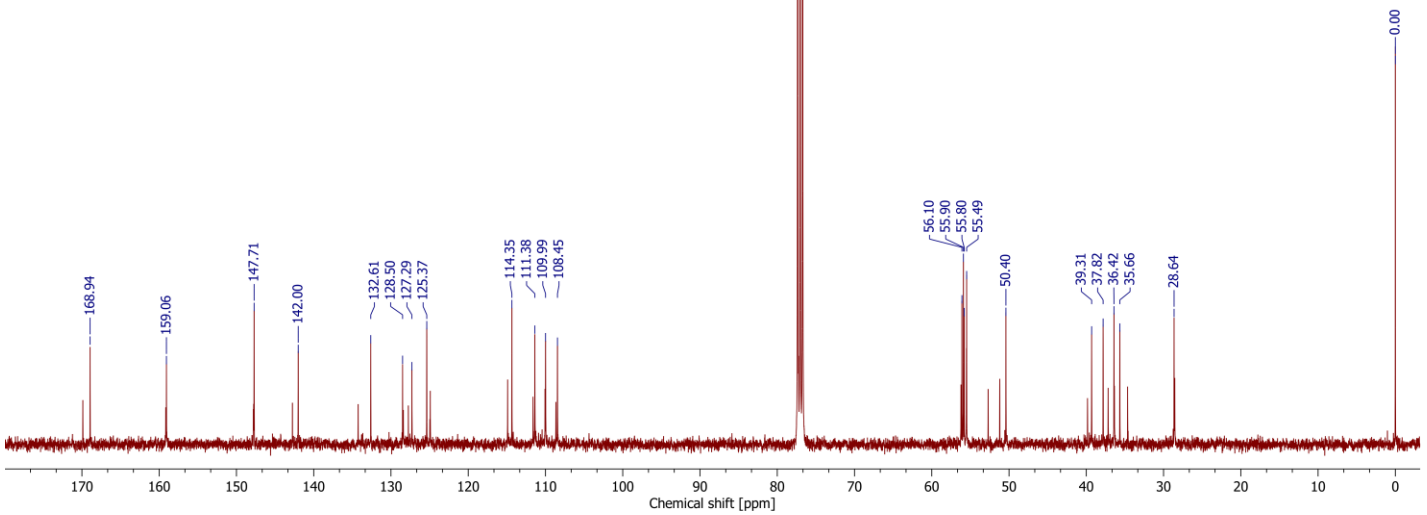
10a

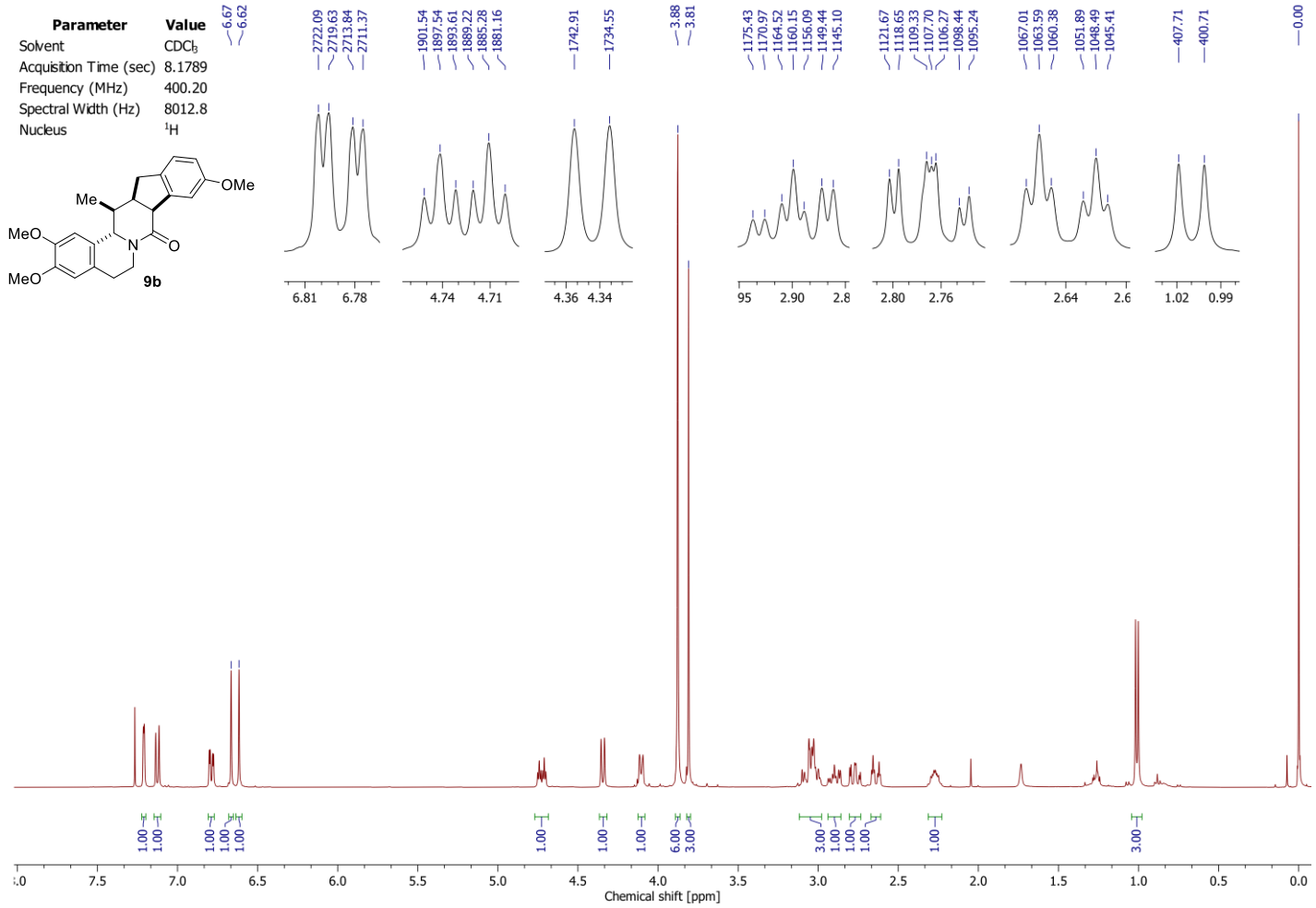
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

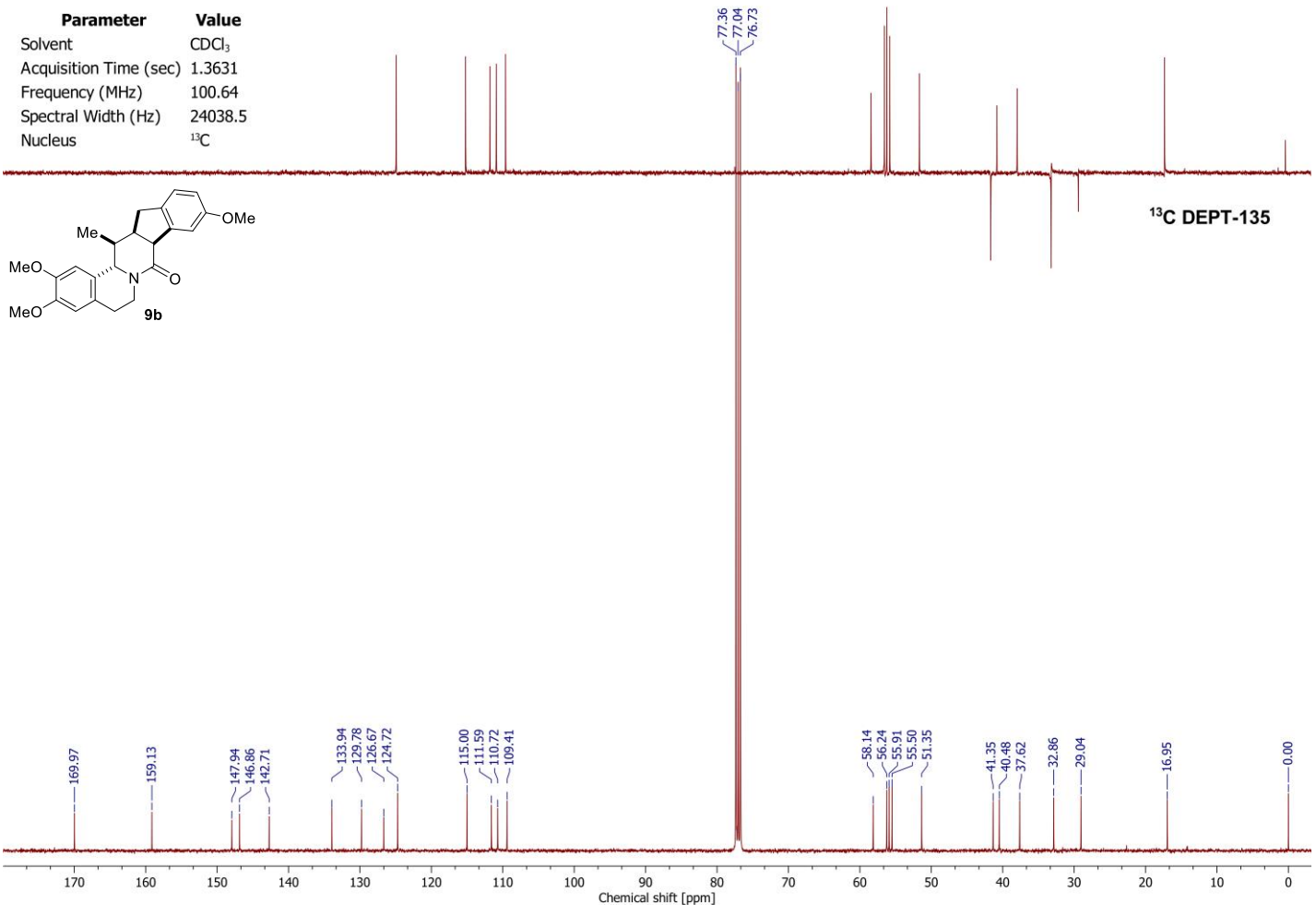


10a

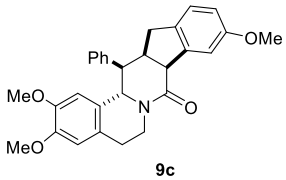
^{13}C DEPT-135




Parameter Value
Solvent CDCl3
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
9b
Chemical shift [ppm]

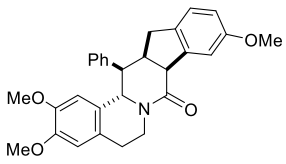

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
9b
Chemical shift [ppm]

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



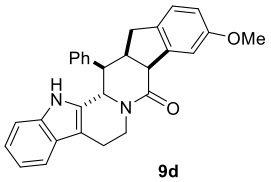
9c

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



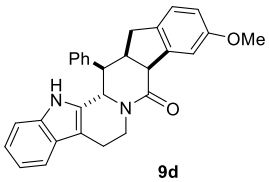
9c

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

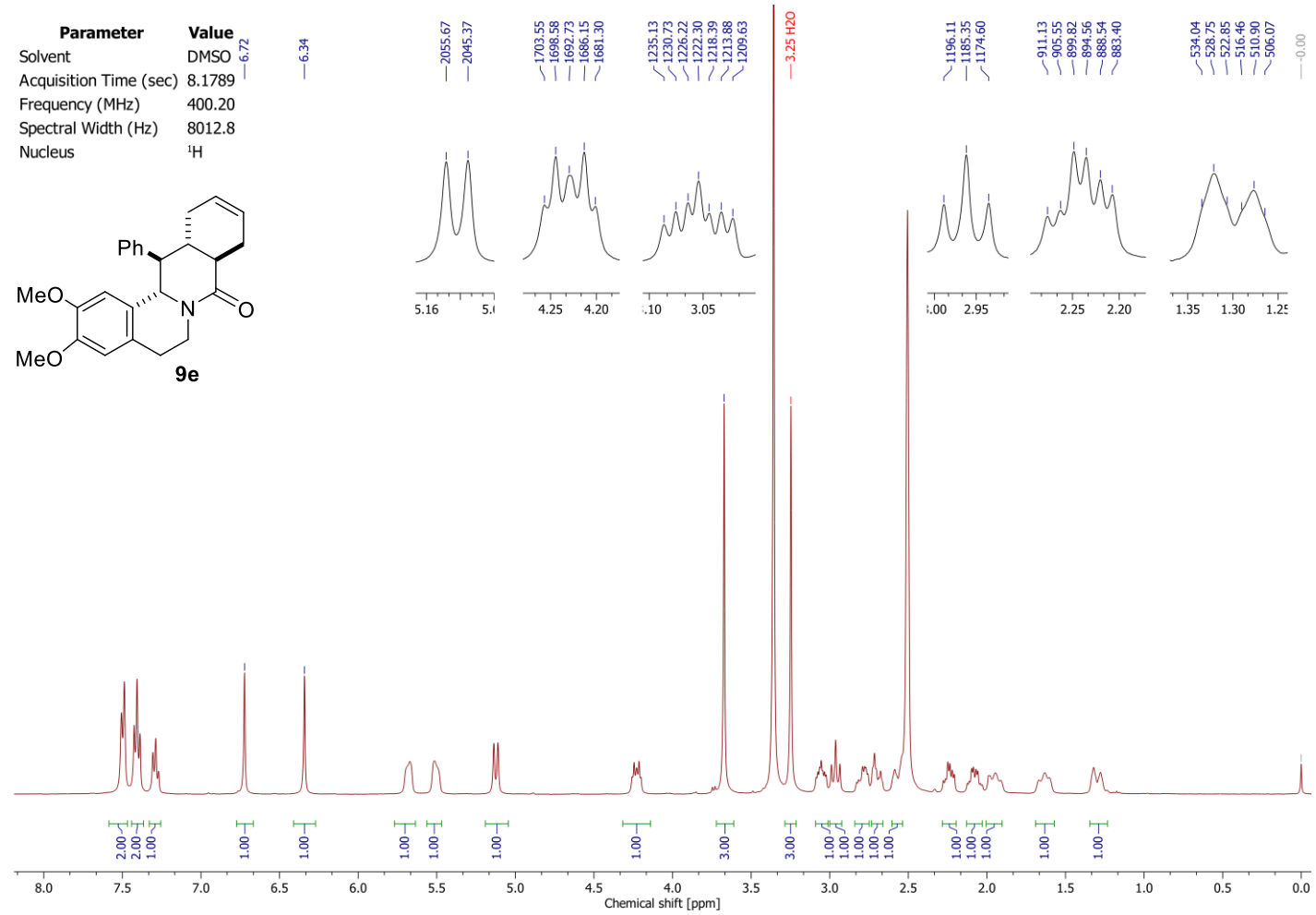


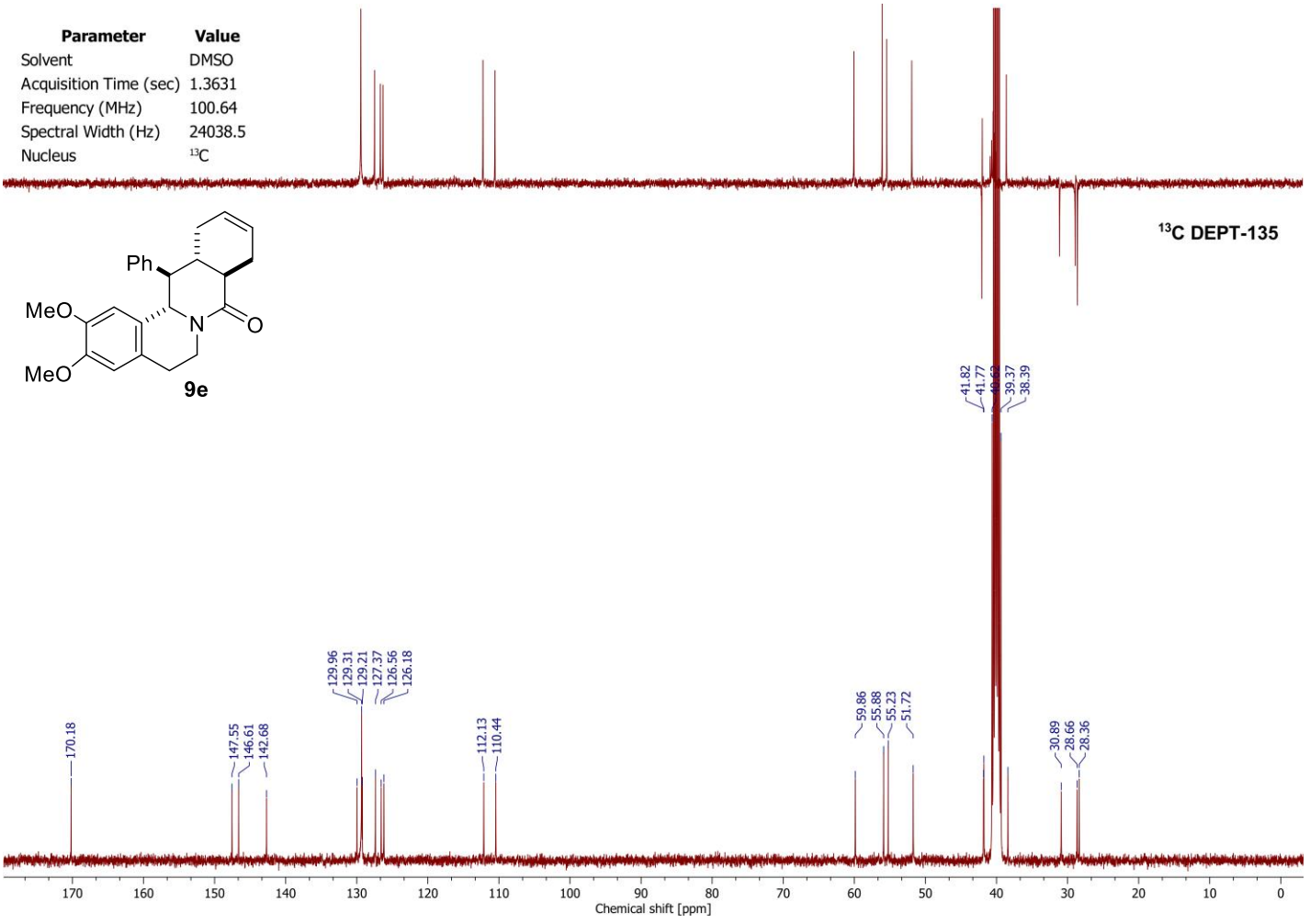
9d

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.63
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

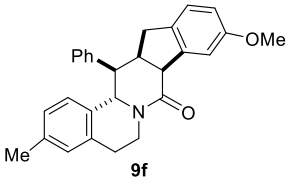


9d


Parameter Value
Solvent DMSO
Acquisition Time (sec) 8.1789
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
6.72
6.34
2055.67
2045.37
1703.55
1698.58
1692.73
1686.15
1681.30
1235.13
1230.73
1226.22
1222.30
1218.39
1213.88
1209.63
3.25 H2O
1196.11
1185.35
1174.60
911.13
905.55
899.82
894.56
888.54
883.40
534.04
528.75
522.85
516.46
510.90
506.07
-0.00
Ph
MeO
MeO
N
O
9e
2.00
2.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
3.00
3.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
Chemical shift [ppm]

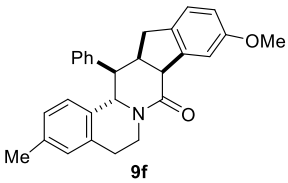

Parameter Value
Solvent DMSO
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
Ph
MeO
MeO
N
O
9e
41.82
41.77
39.37
38.39
129.96
129.31
129.21
127.37
126.56
126.18
170.18
147.55
146.61
142.68
112.13
110.44
59.86
55.88
55.23
51.72
30.89
28.66
28.36
Chemical shift [ppm]

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



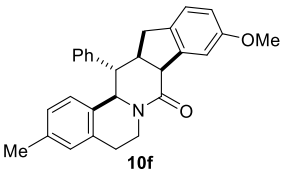
9f

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



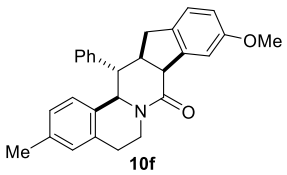
9f

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



10f

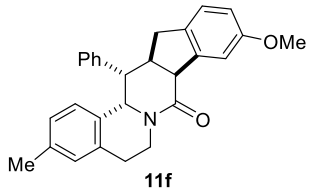
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



10f

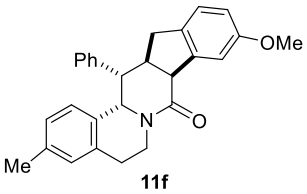
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



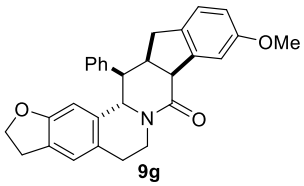
11f

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



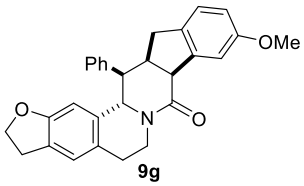
11f

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



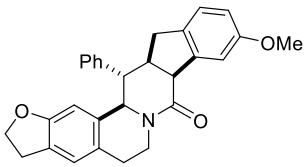
9g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



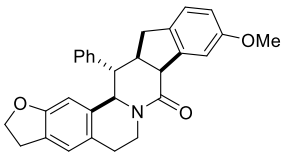
9g

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H



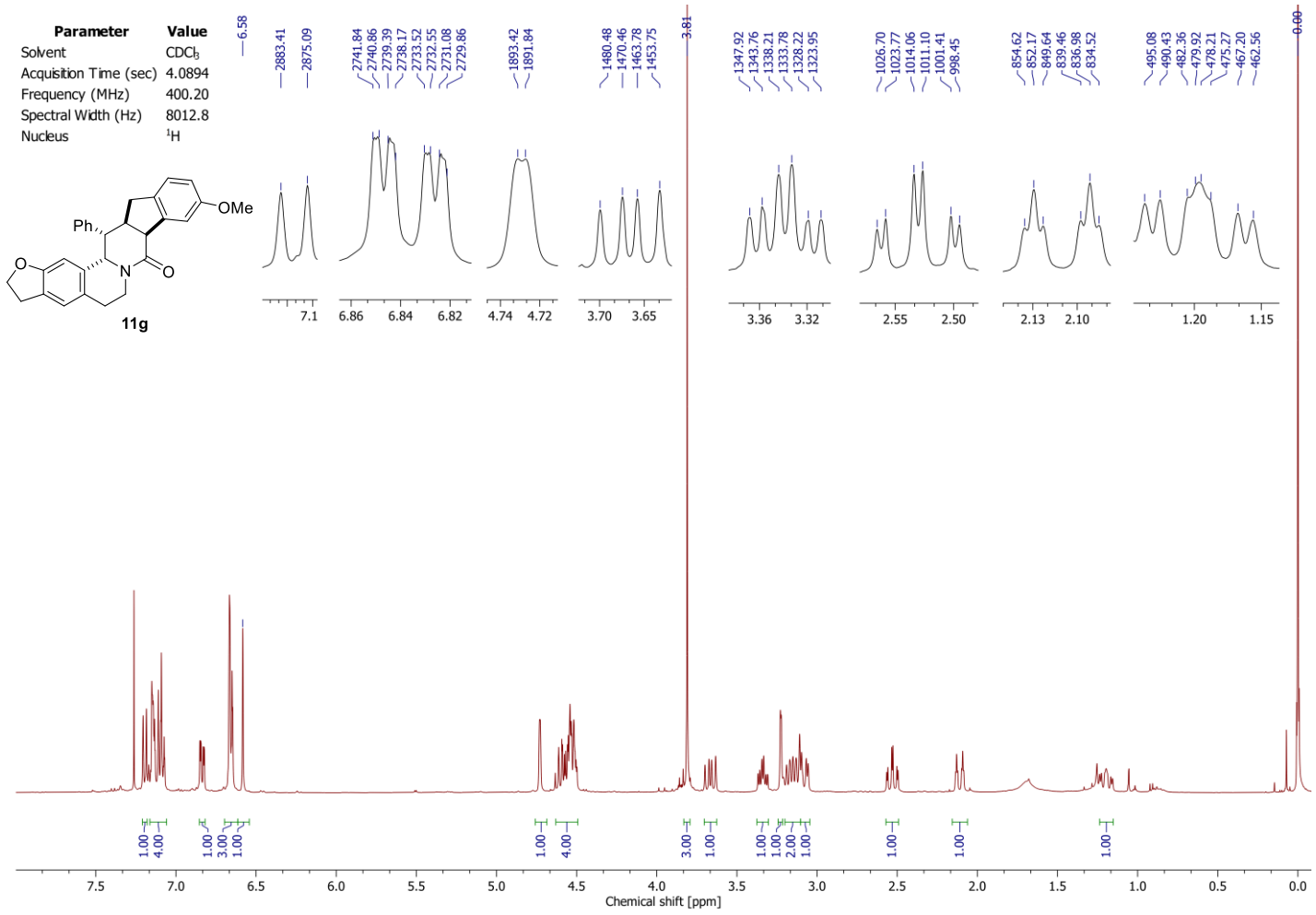
10g

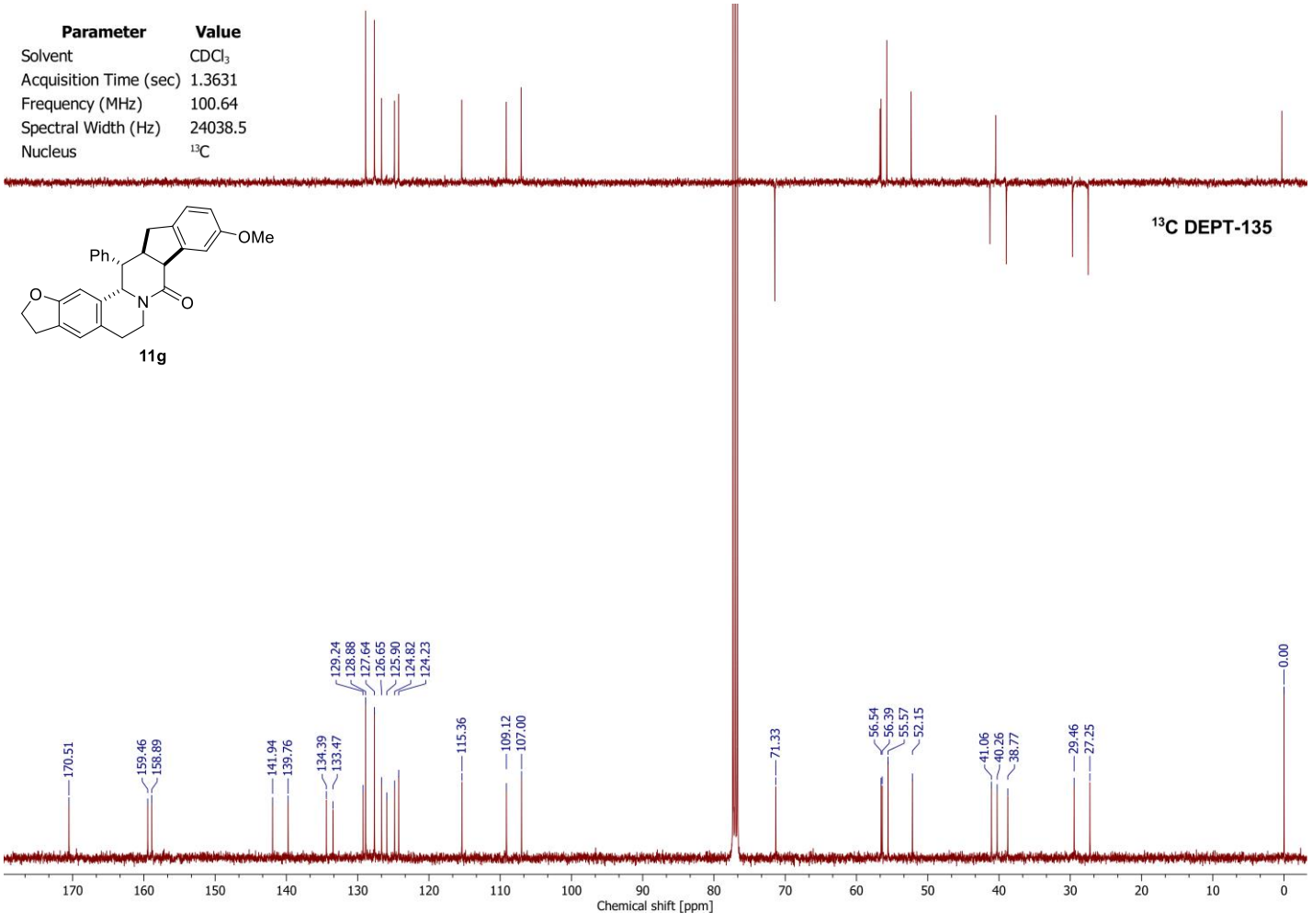
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



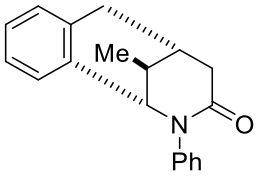
10g

^{13}C DEPT-135

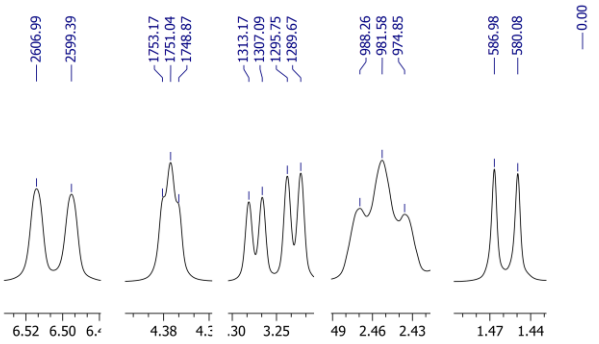

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 4.0894
Frequency (MHz) 400.20
Spectral Width (Hz) 8012.8
Nucleus 1H
OMe
Ph
O
N
O
11g
Chemical shift [ppm]

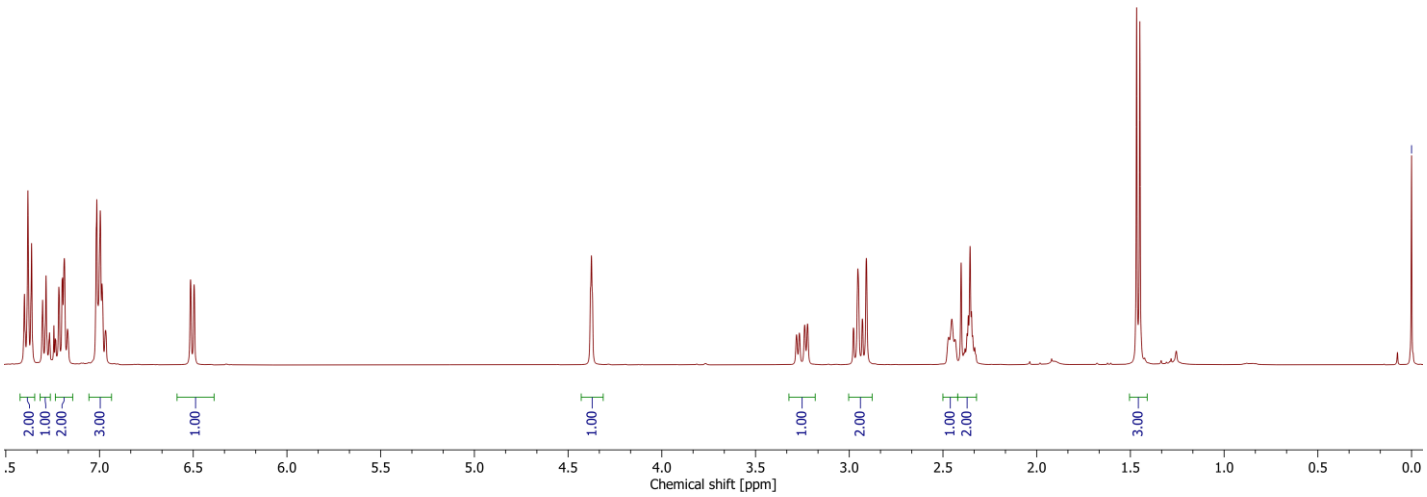

Parameter Value
Solvent CDCl3
Acquisition Time (sec) 1.3631
Frequency (MHz) 100.64
Spectral Width (Hz) 24038.5
Nucleus 13C
13C DEPT-135
OMe
Ph
O
N
O
11g
Chemical shift [ppm]

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

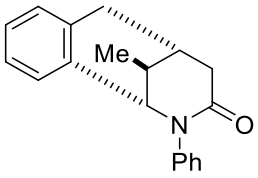


12a

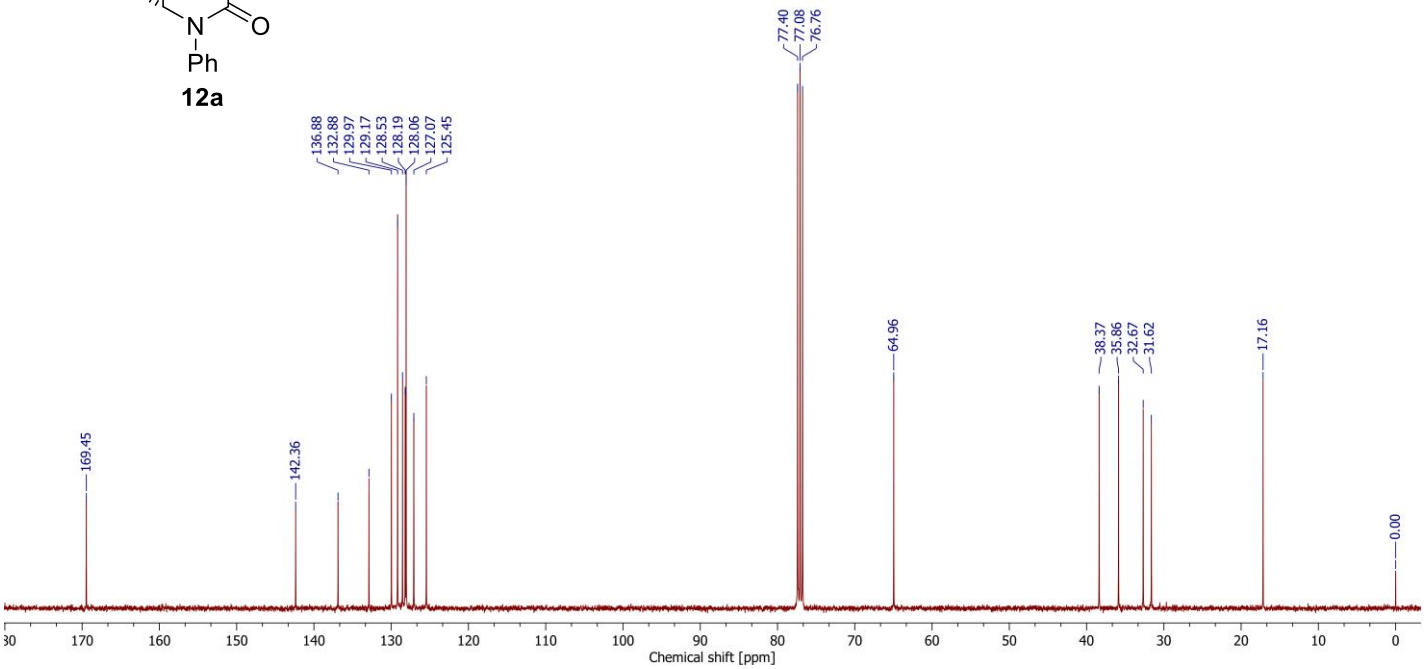




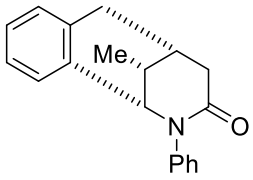
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



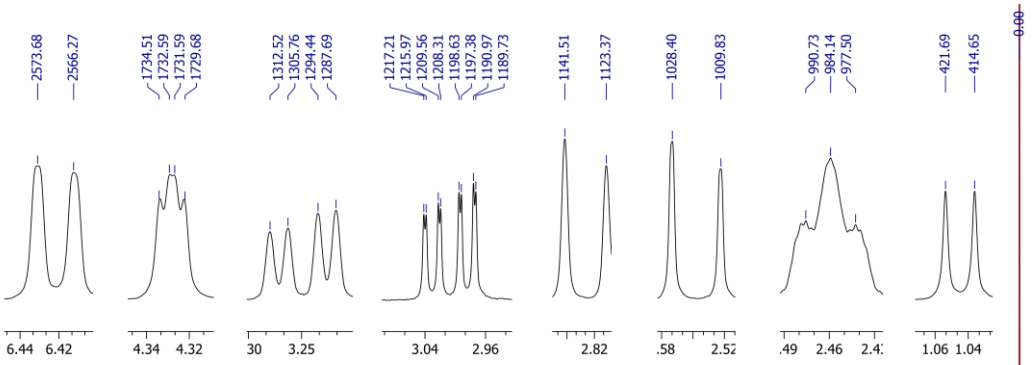
12a

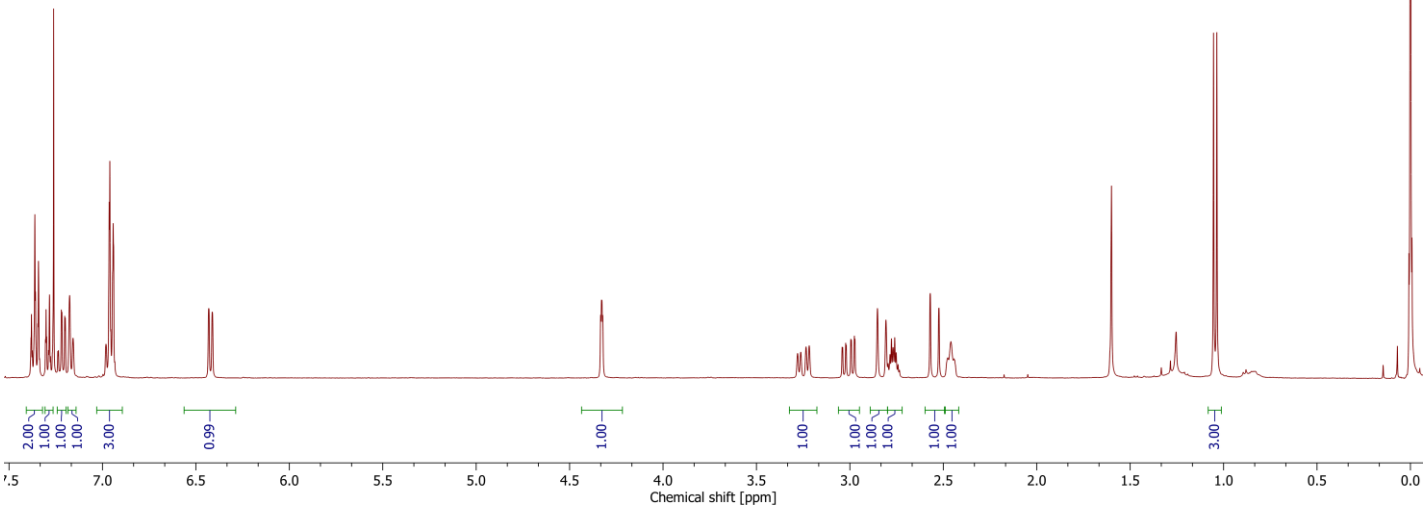


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H

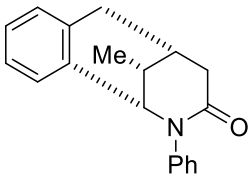


13a

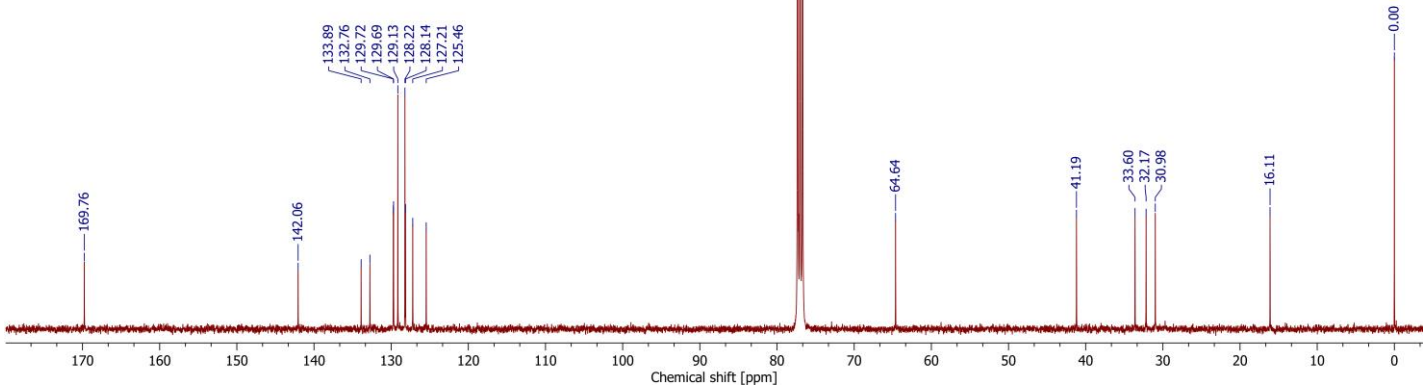




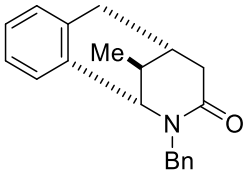
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



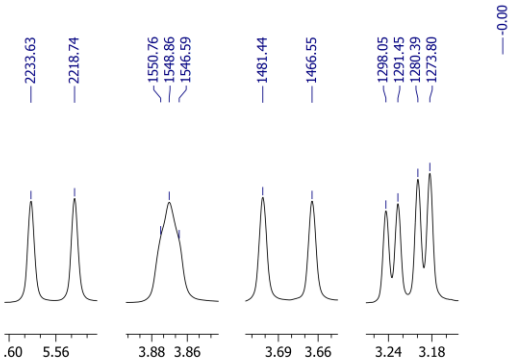
13a

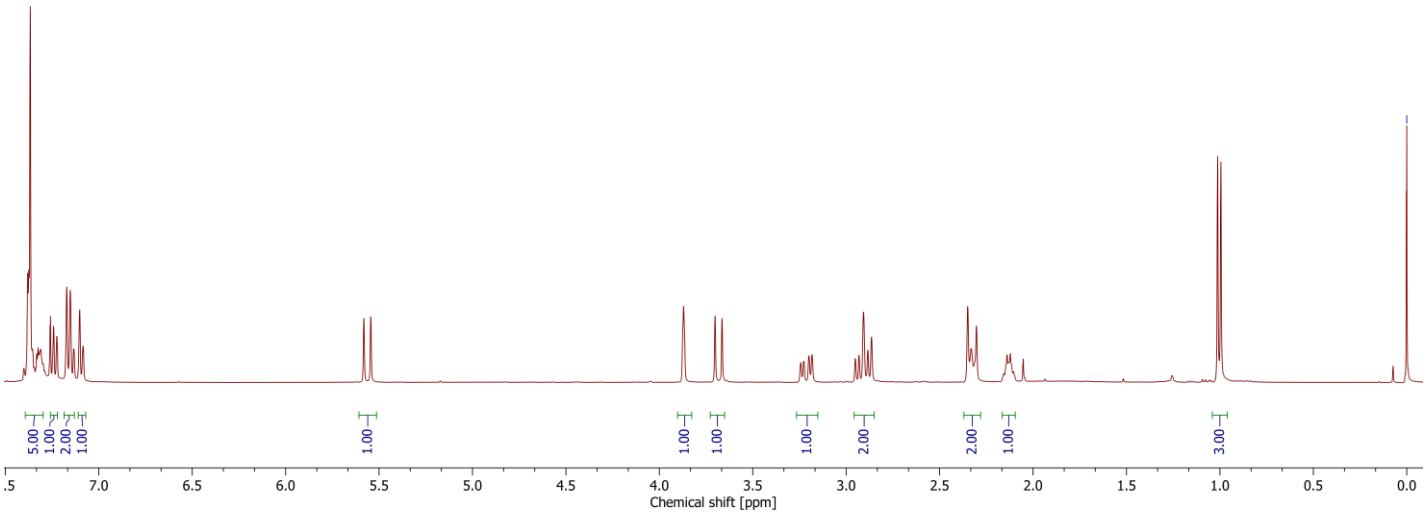


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

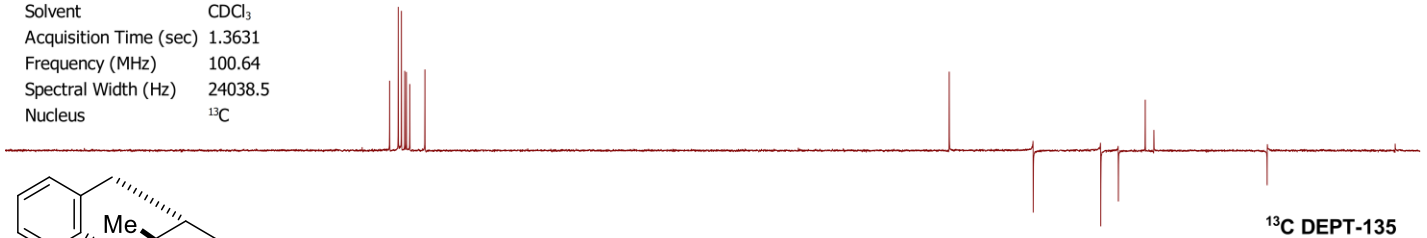


12b

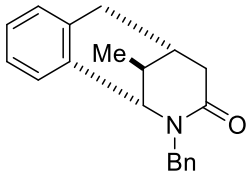




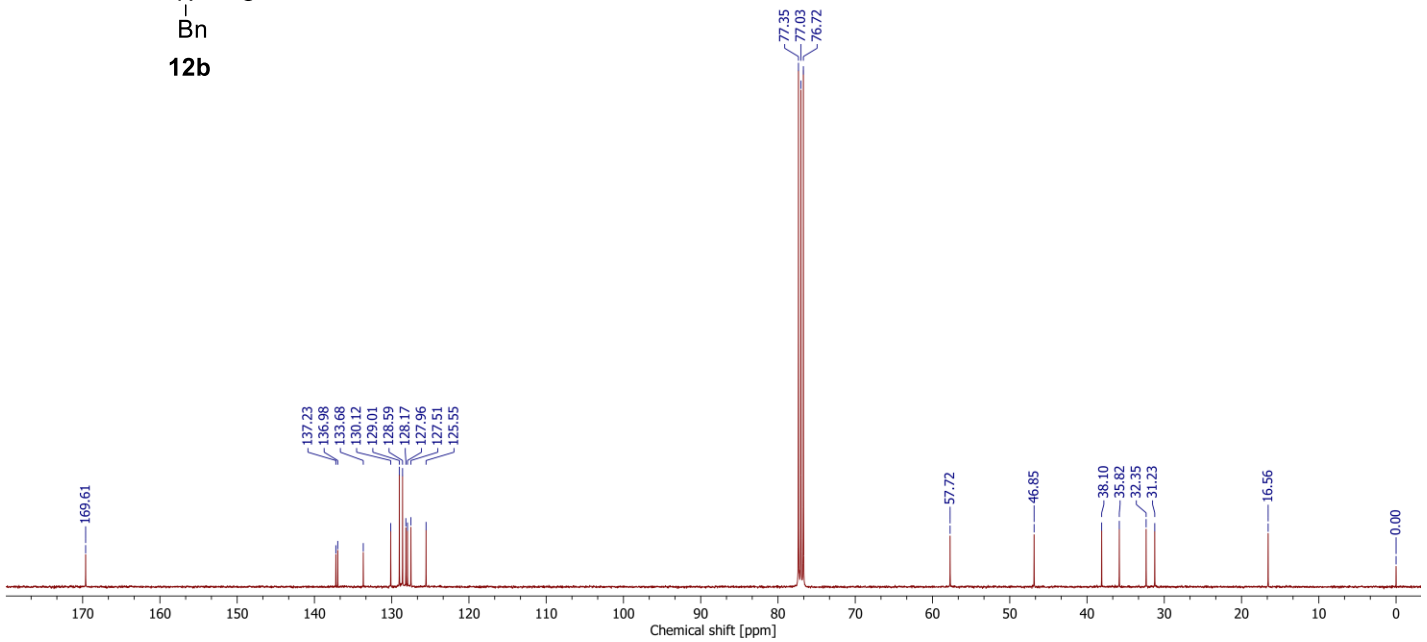
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



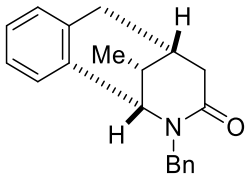
^{13}C DEPT-135



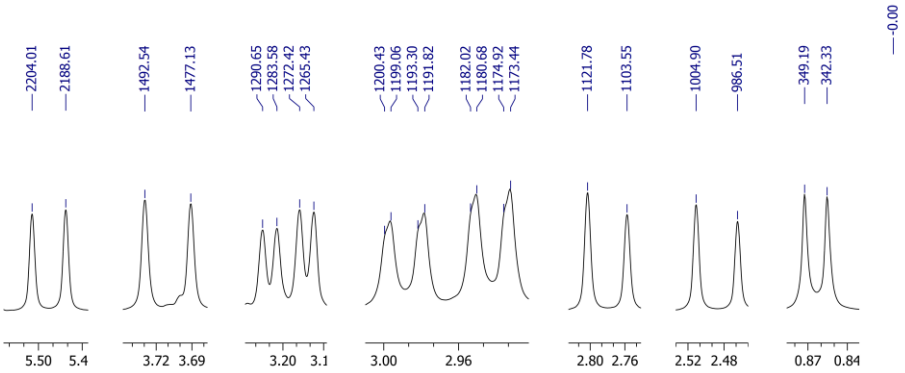
12b

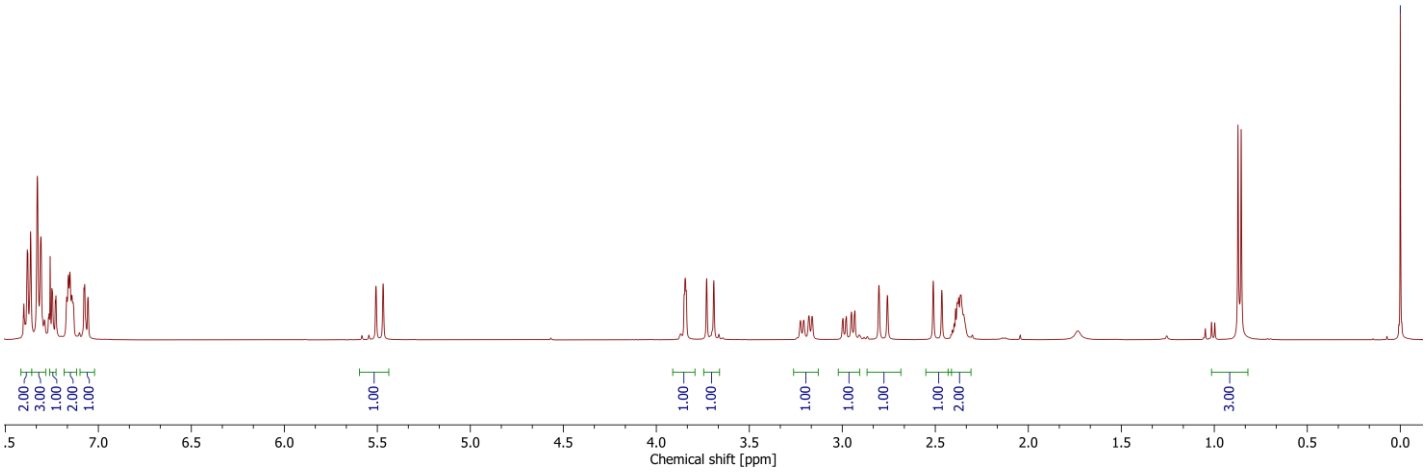


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H

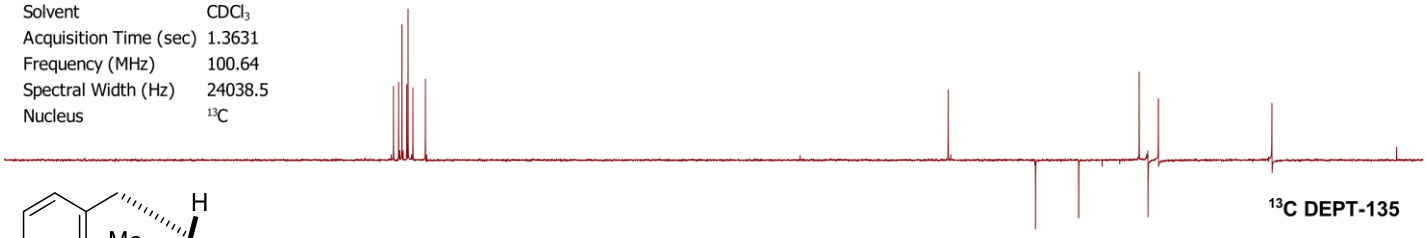


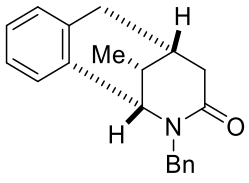
13b





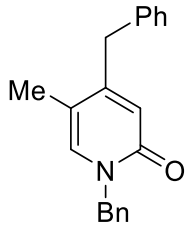
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C





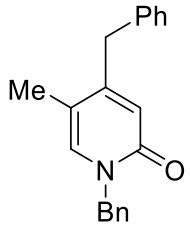
13b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



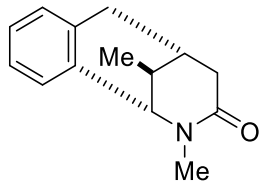
14b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



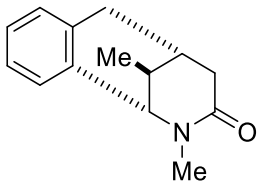
14b

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

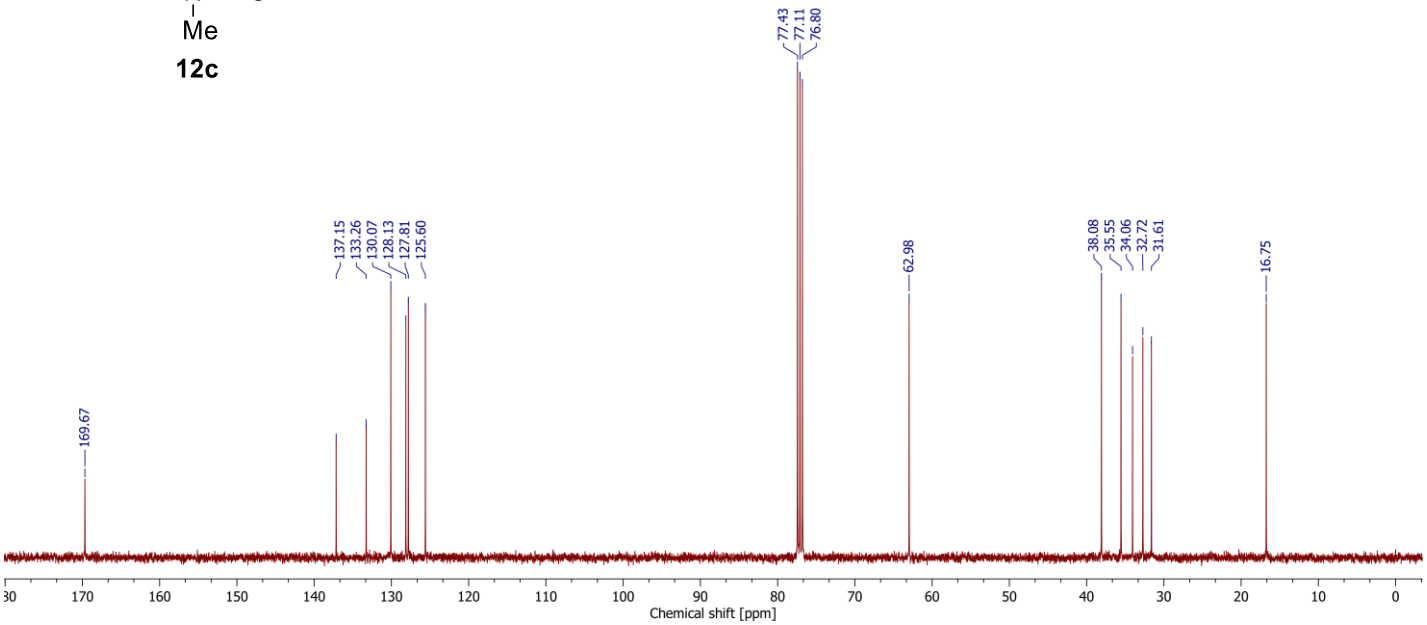


12c

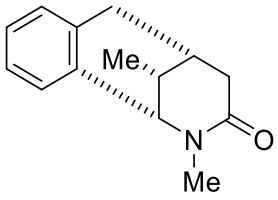
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



12c

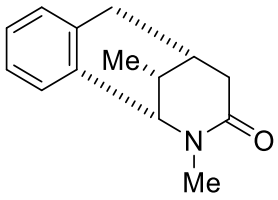


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



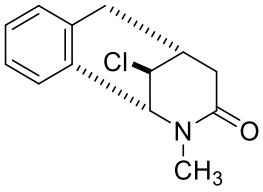
13c

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



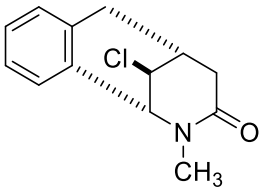
13c

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



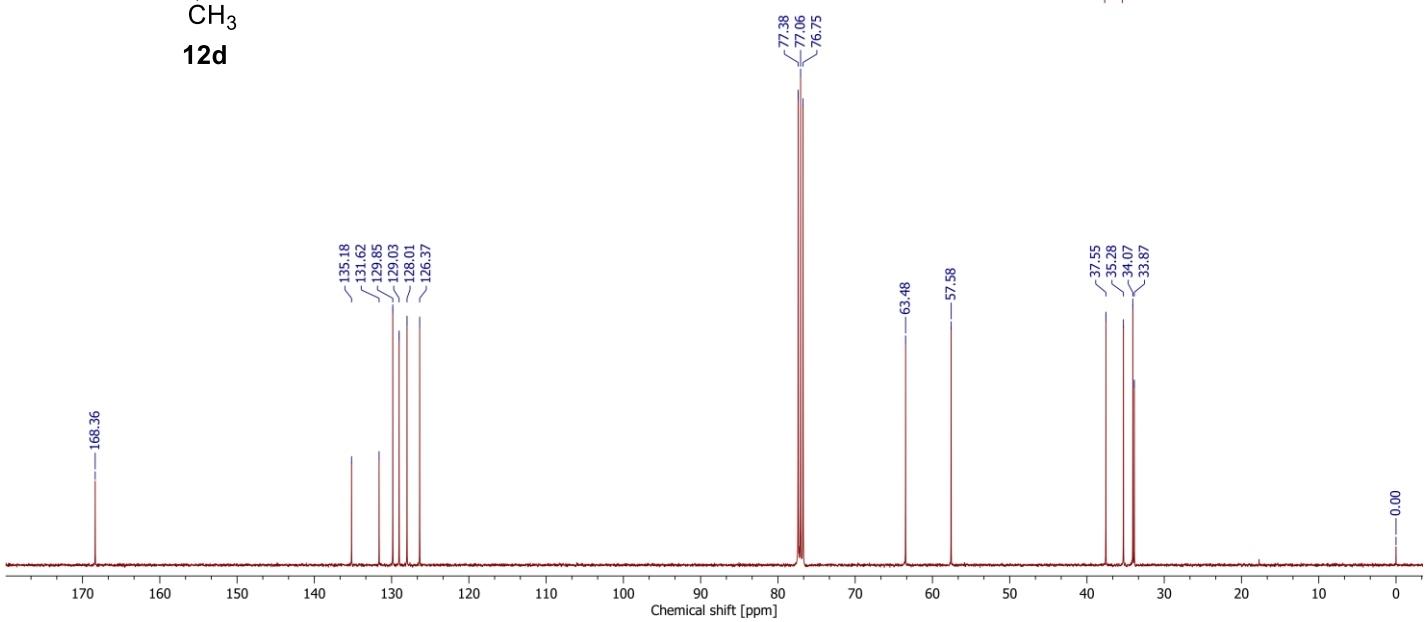
12d

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

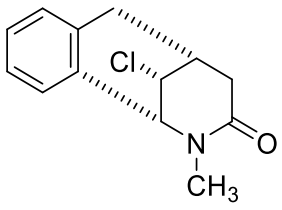


12d

^{13}C DEPT-135

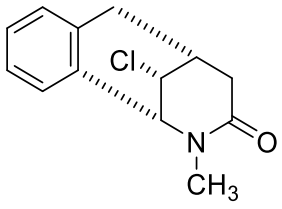


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

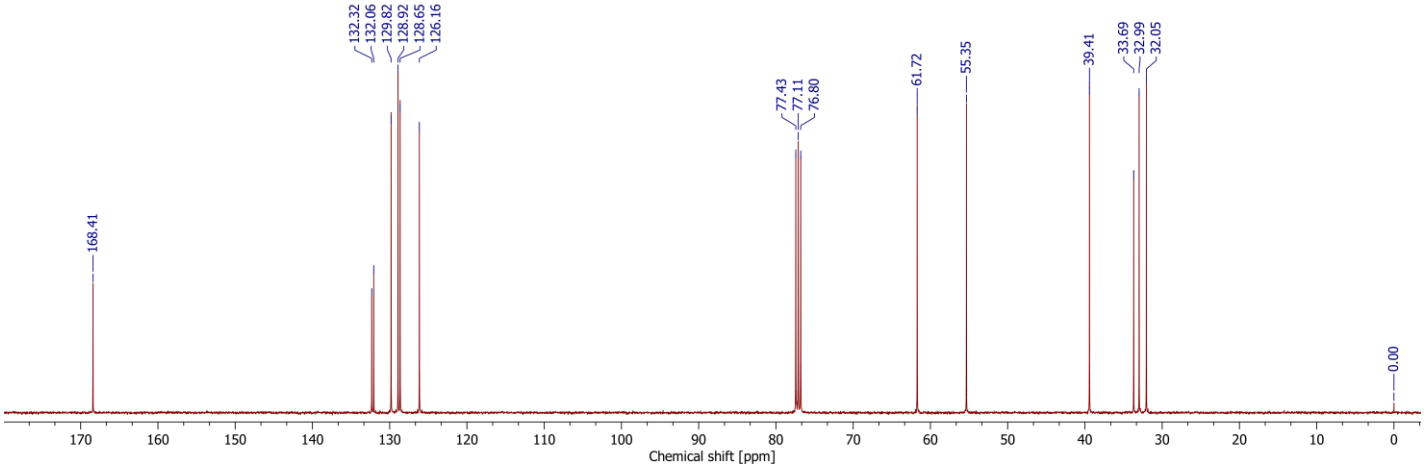


13d

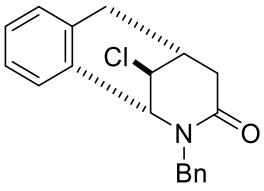
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



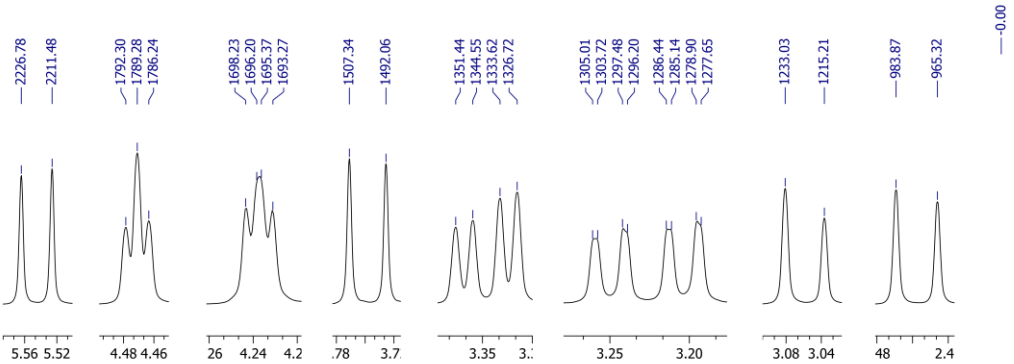
13d

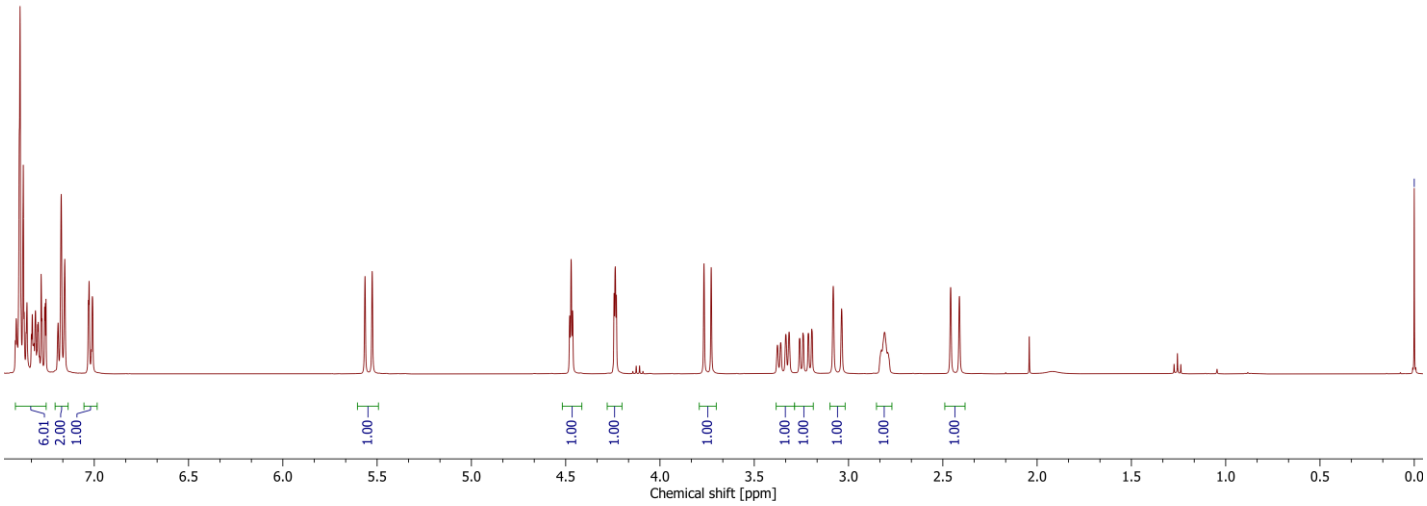


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H

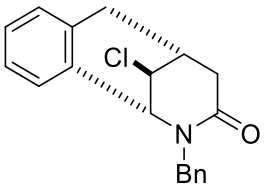


12e





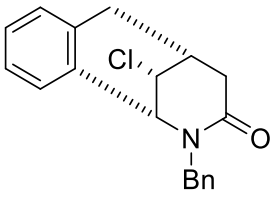
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



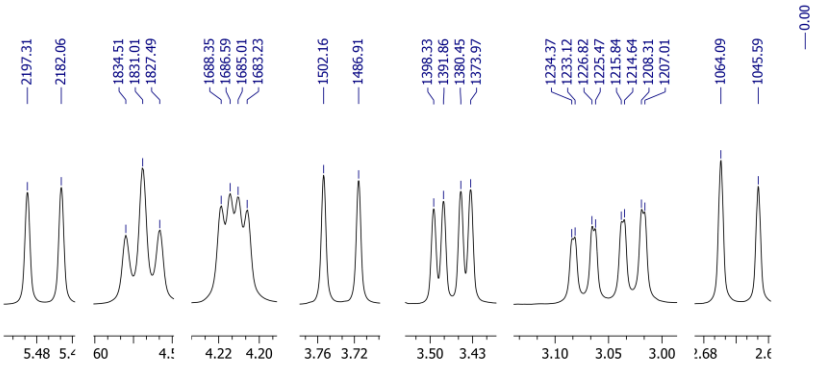
12e

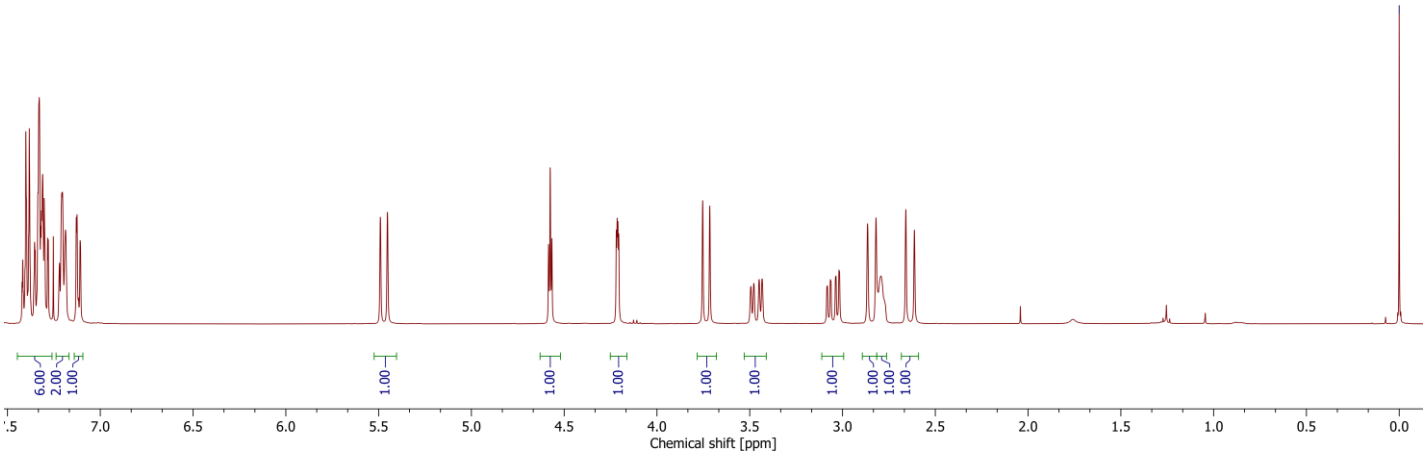
^{13}C DEPT-135

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

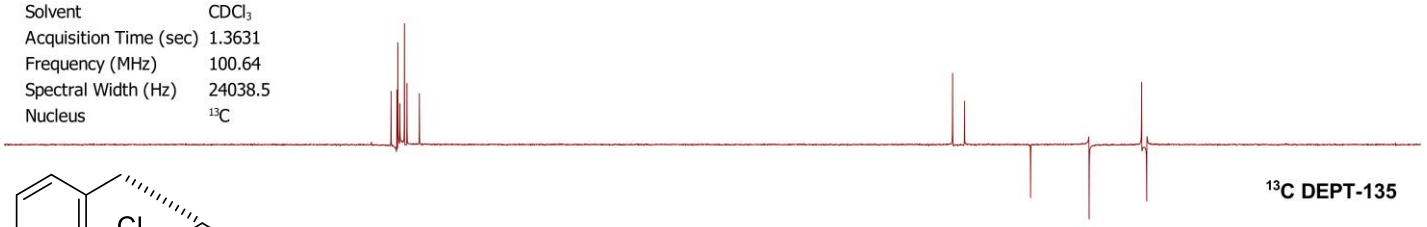


13e

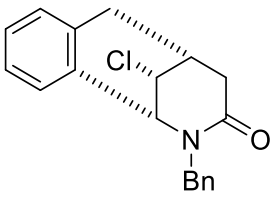




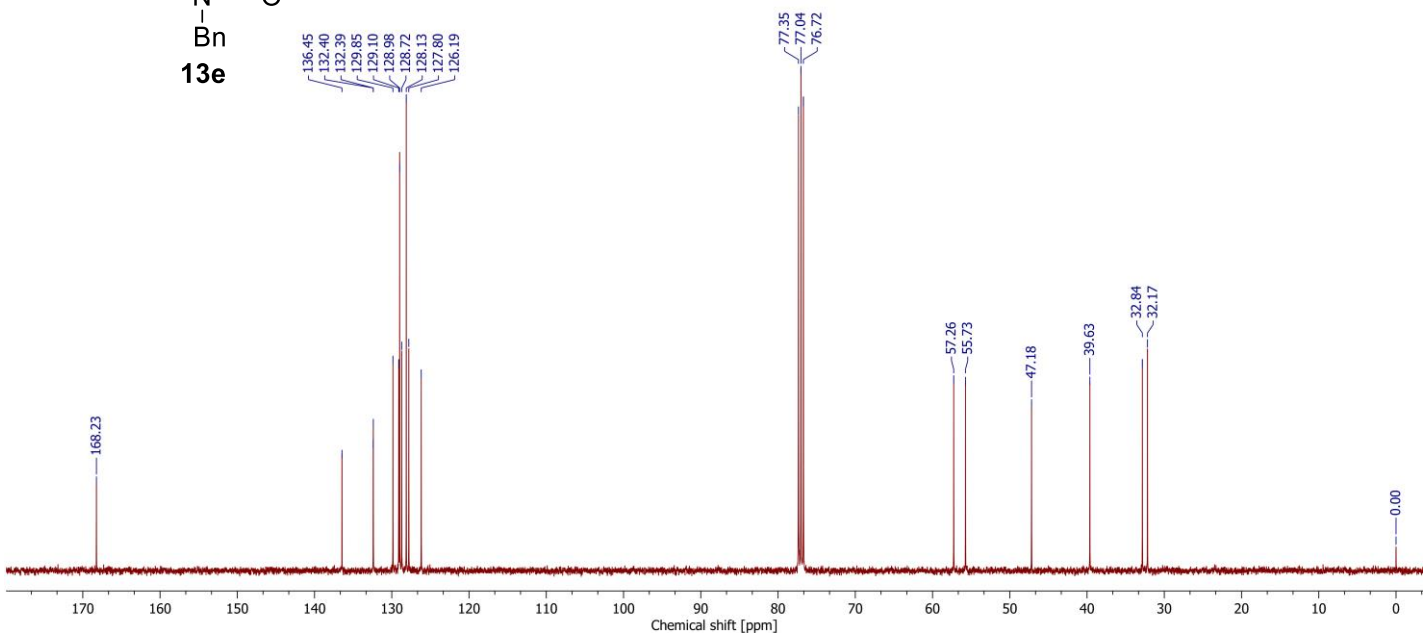
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



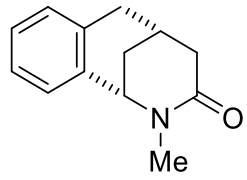
^{13}C DEPT-135



13e

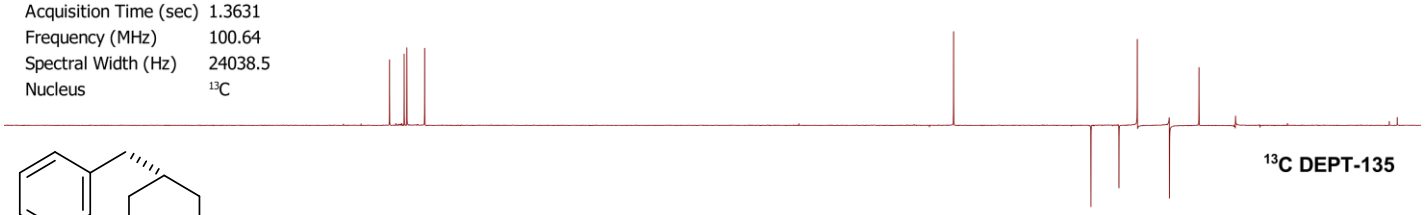


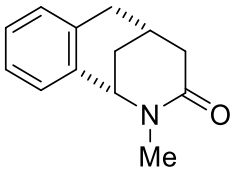
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H



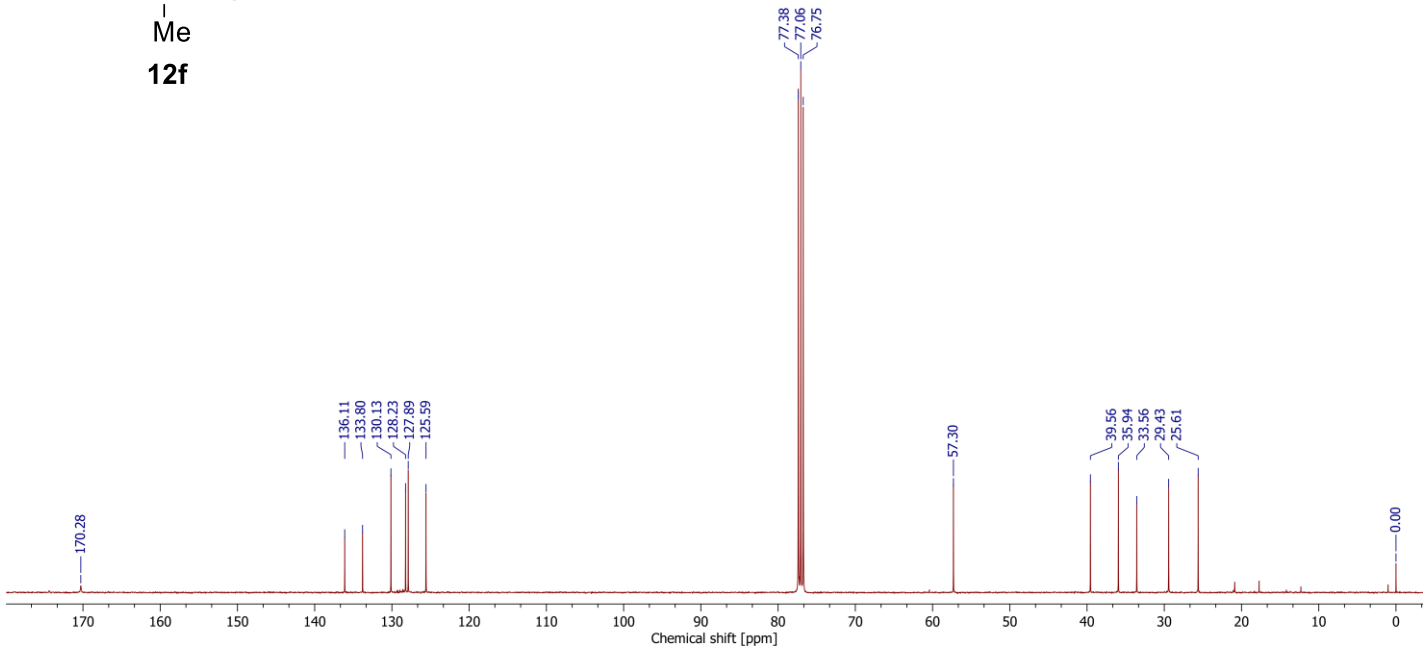
12f

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

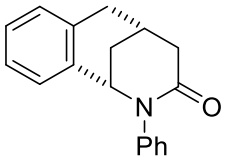




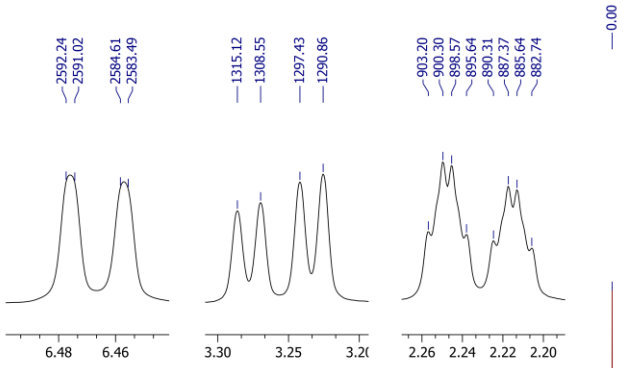
12f

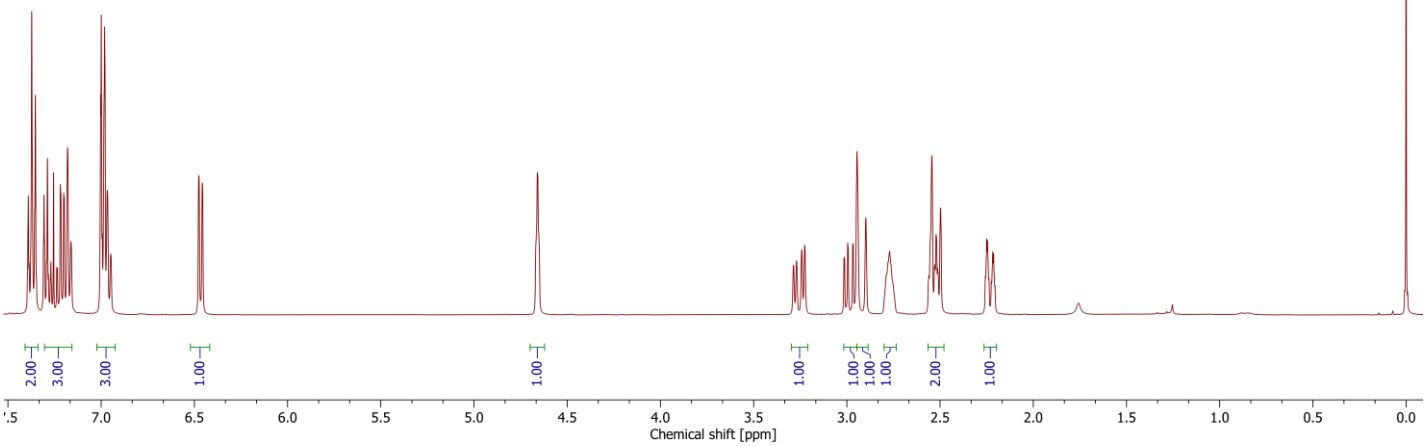


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^{1}H

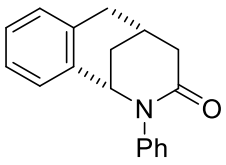


12g

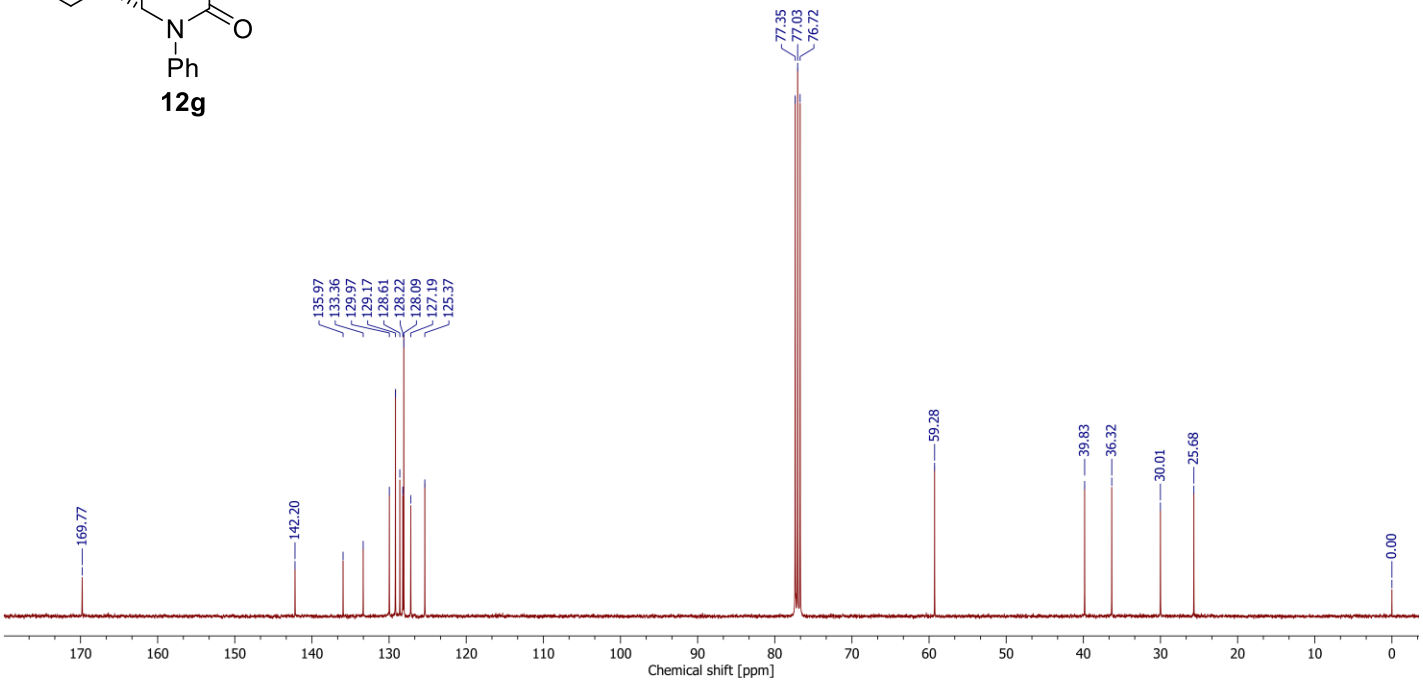




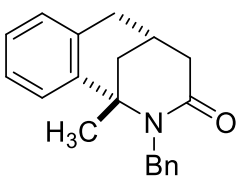
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C



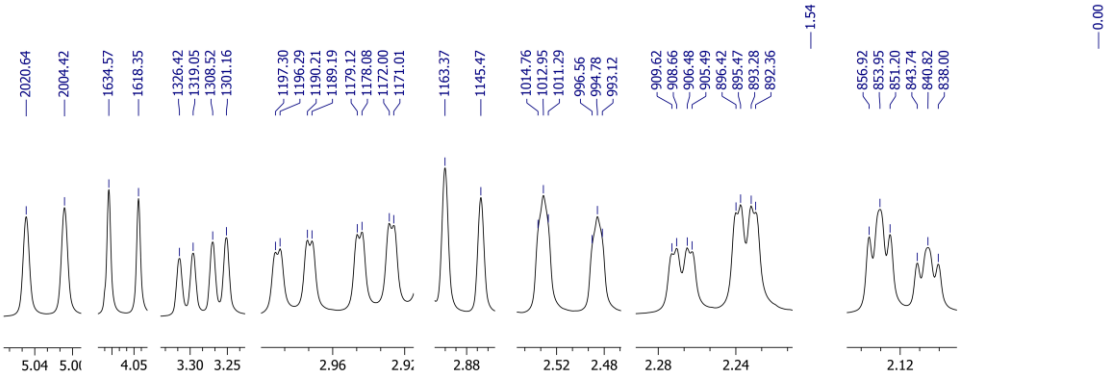
12g

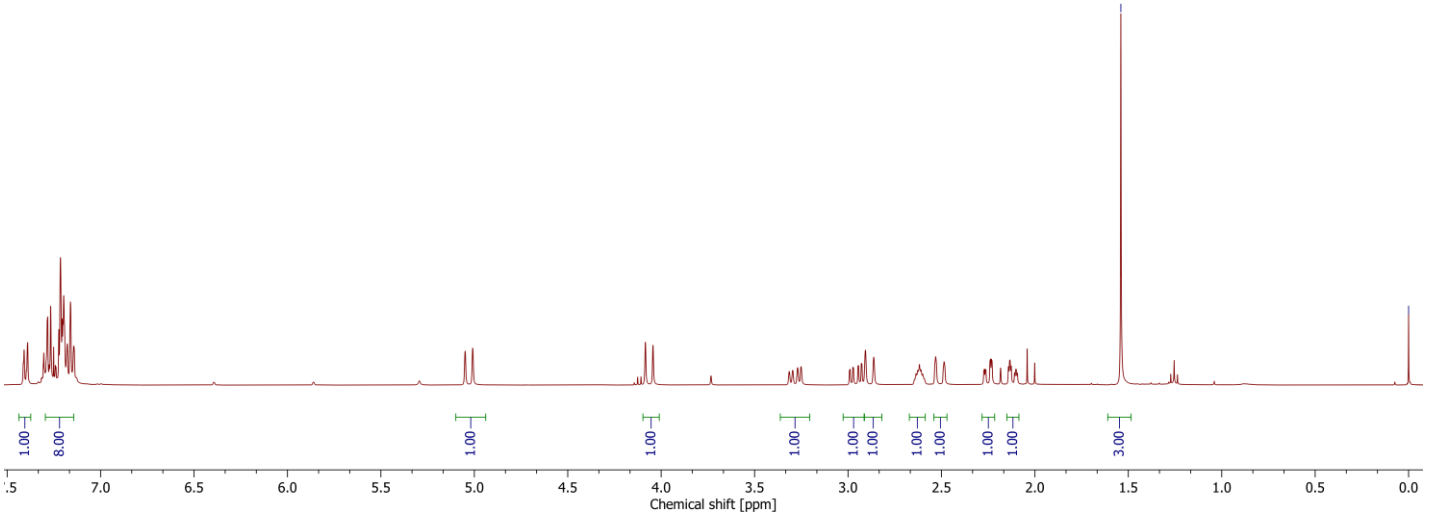


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H

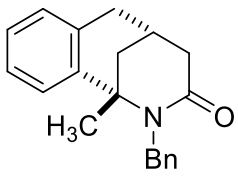


12h



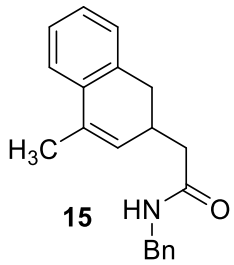


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

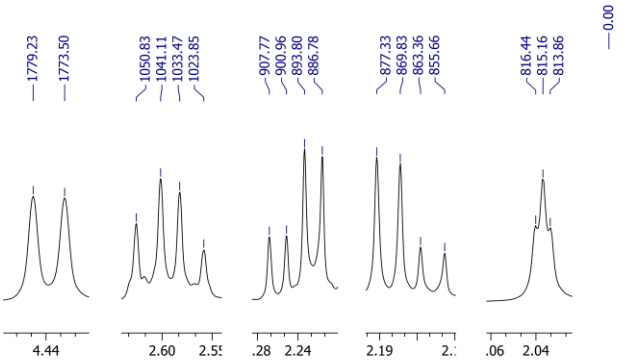


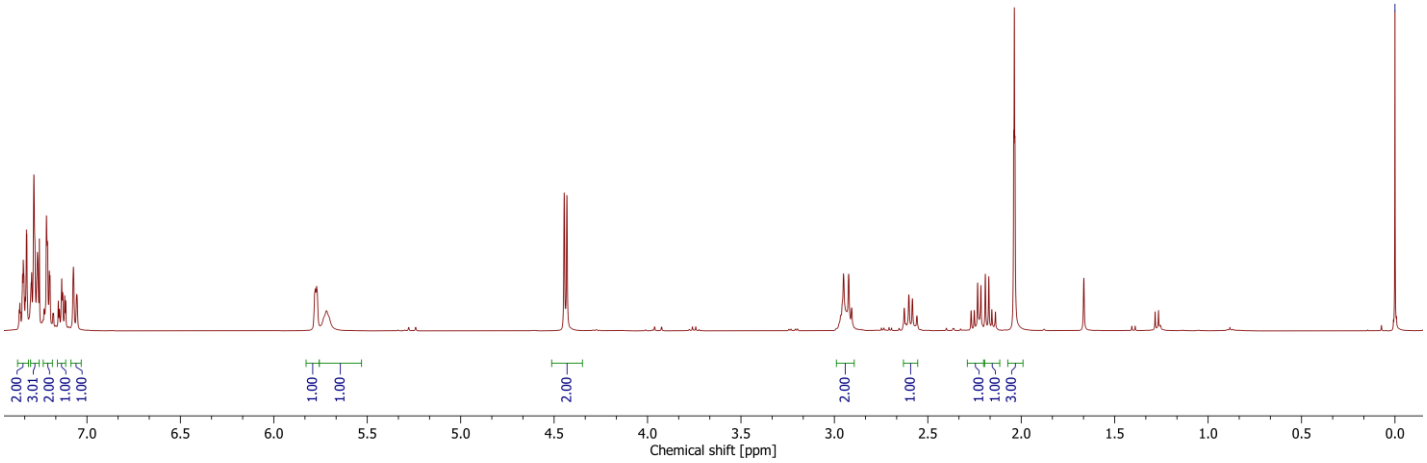
12h

Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	4.0894
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H

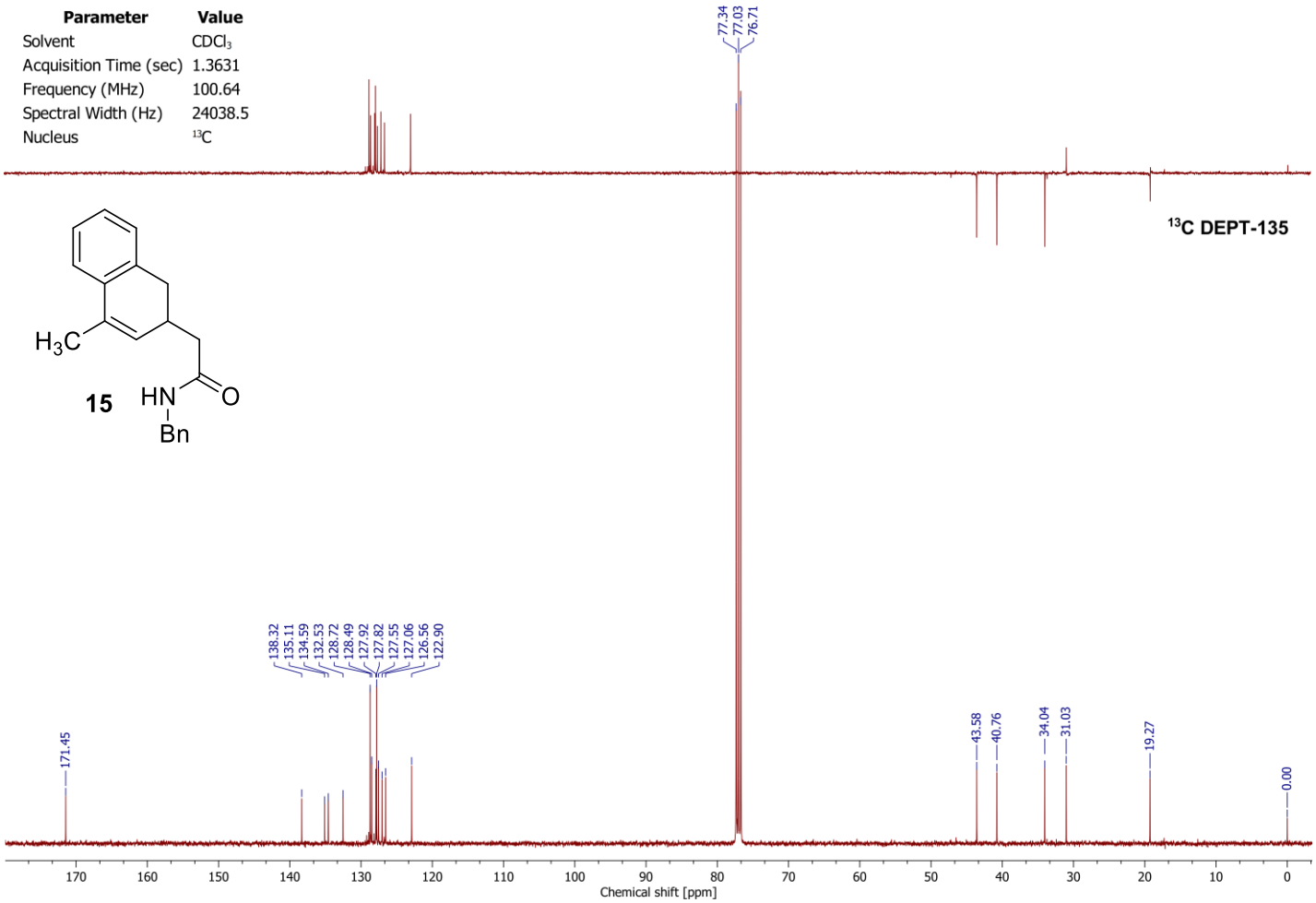


15

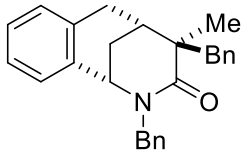




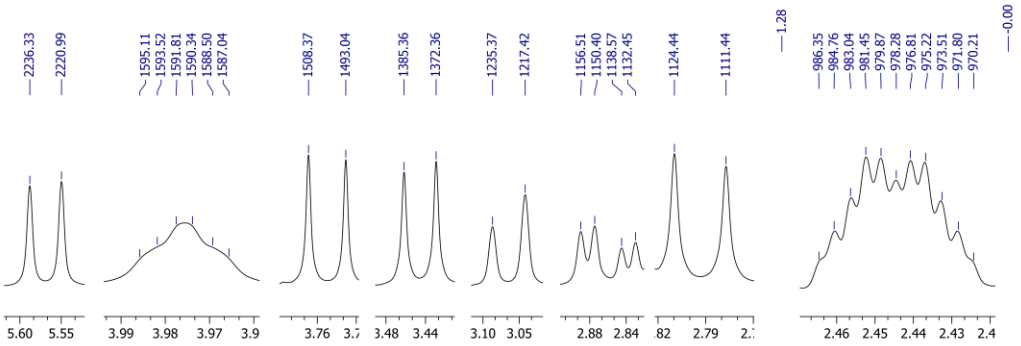
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

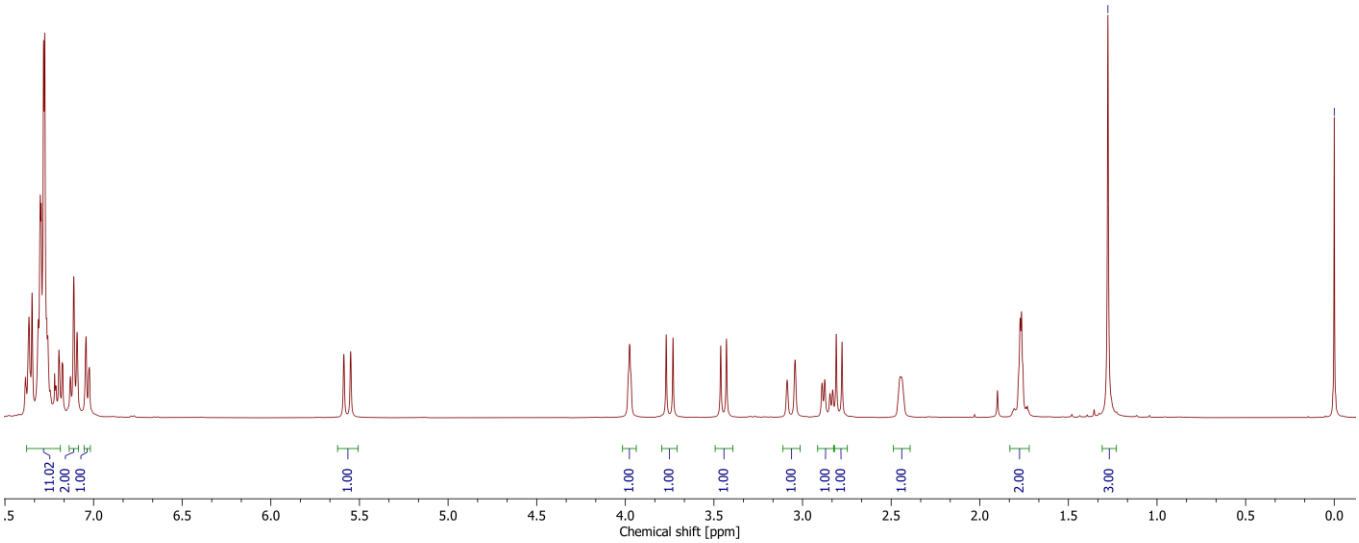


Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	8.1789
Frequency (MHz)	400.20
Spectral Width (Hz)	8012.8
Nucleus	^1H

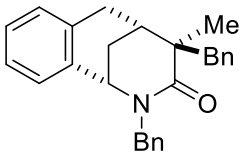


12i

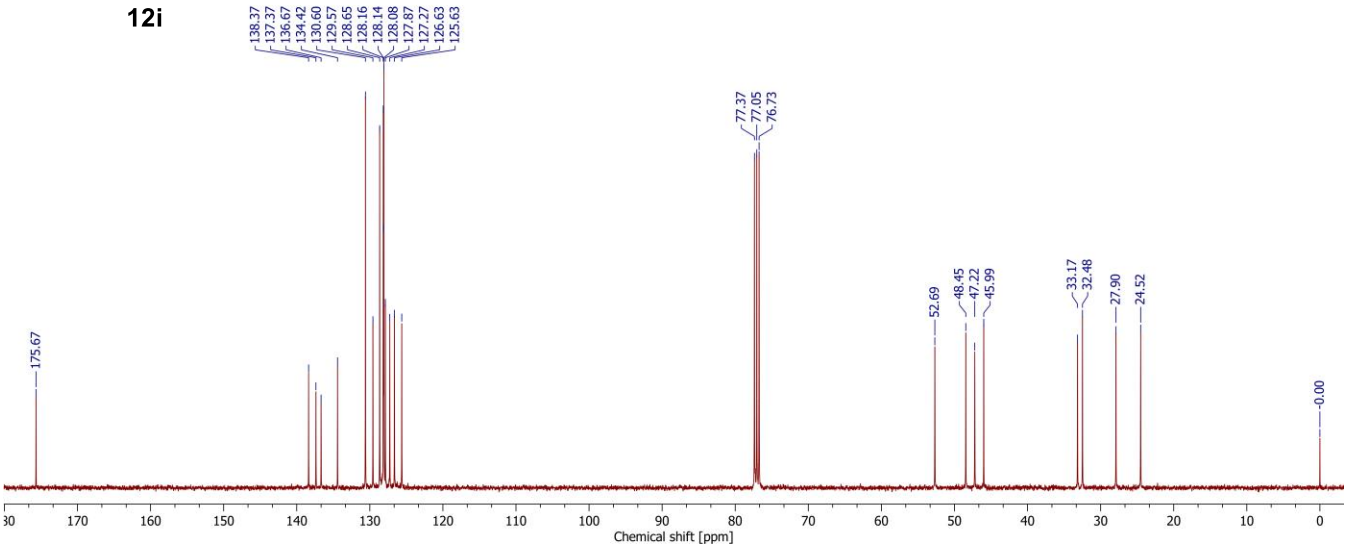




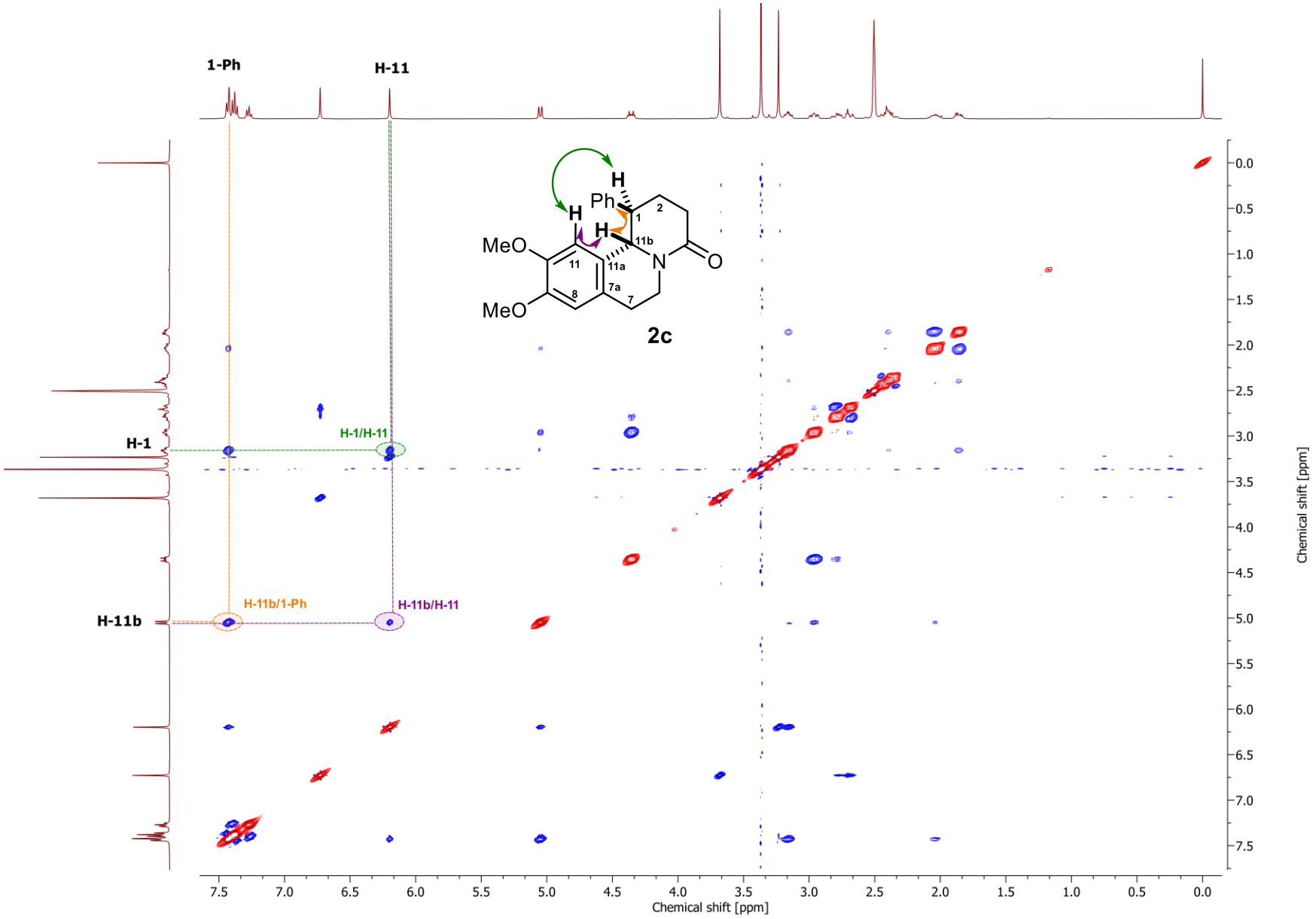
Parameter	Value
Solvent	$CDCl_3$
Acquisition Time (sec)	1.3631
Frequency (MHz)	100.64
Spectral Width (Hz)	24038.5
Nucleus	^{13}C

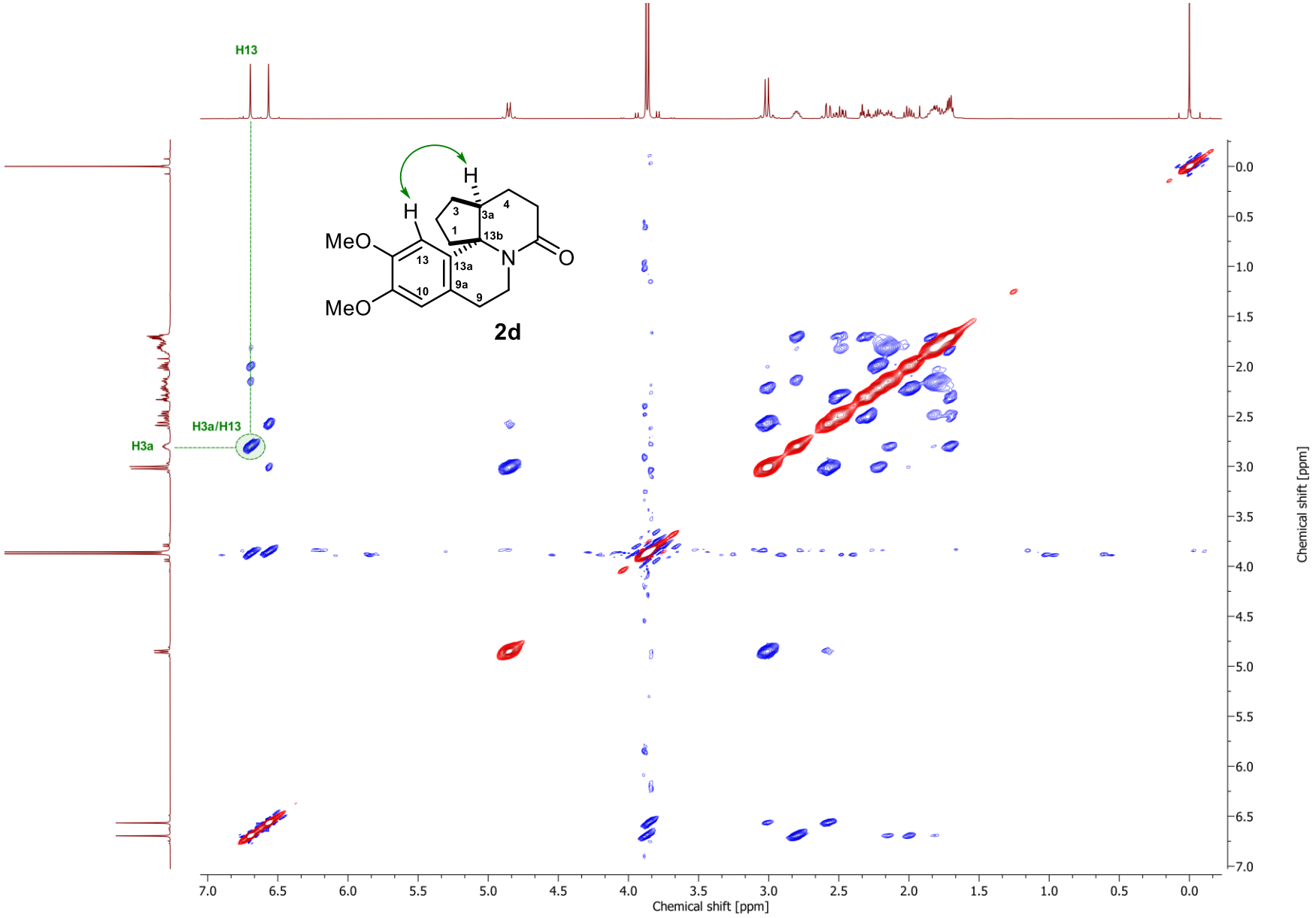


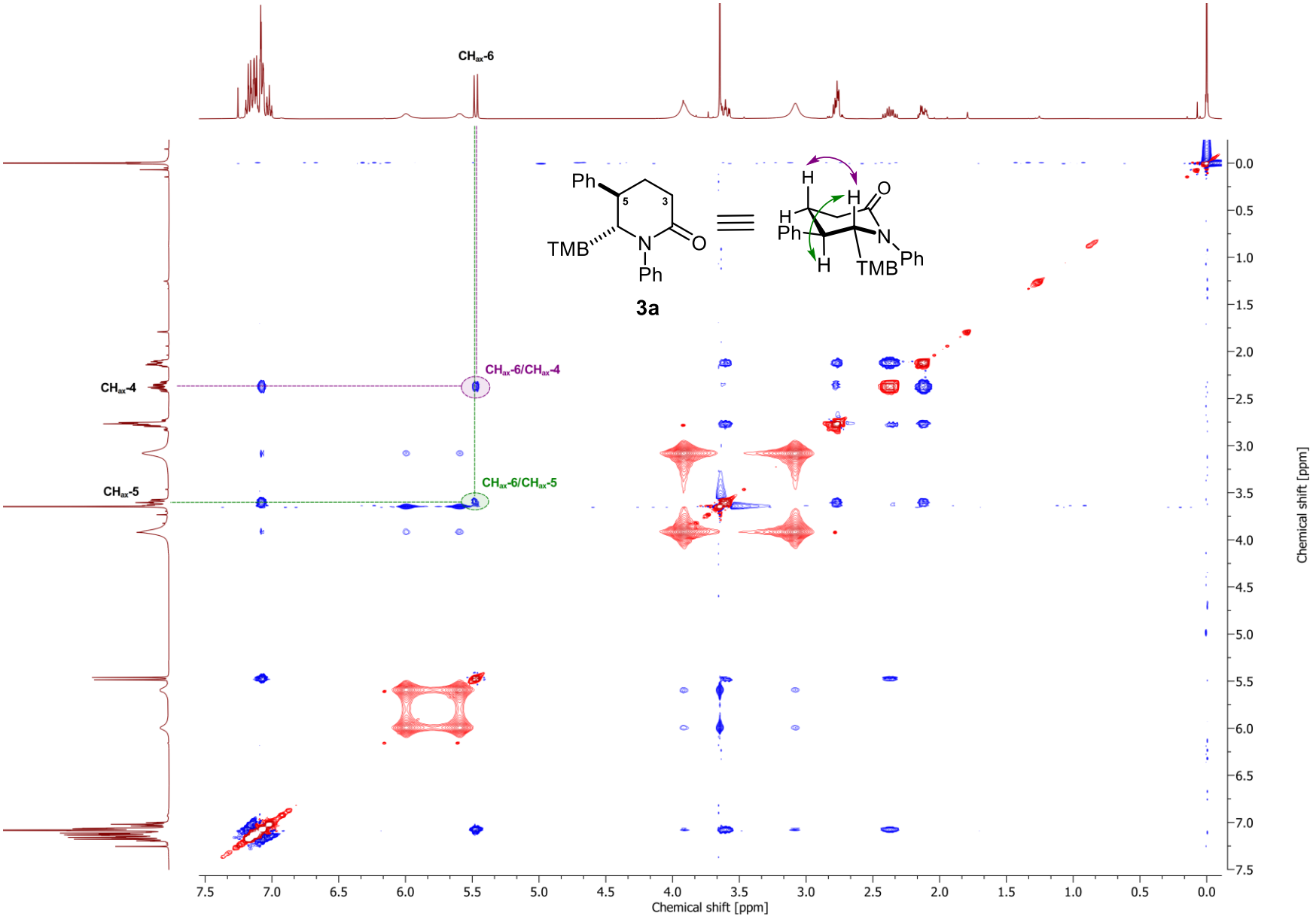
12i

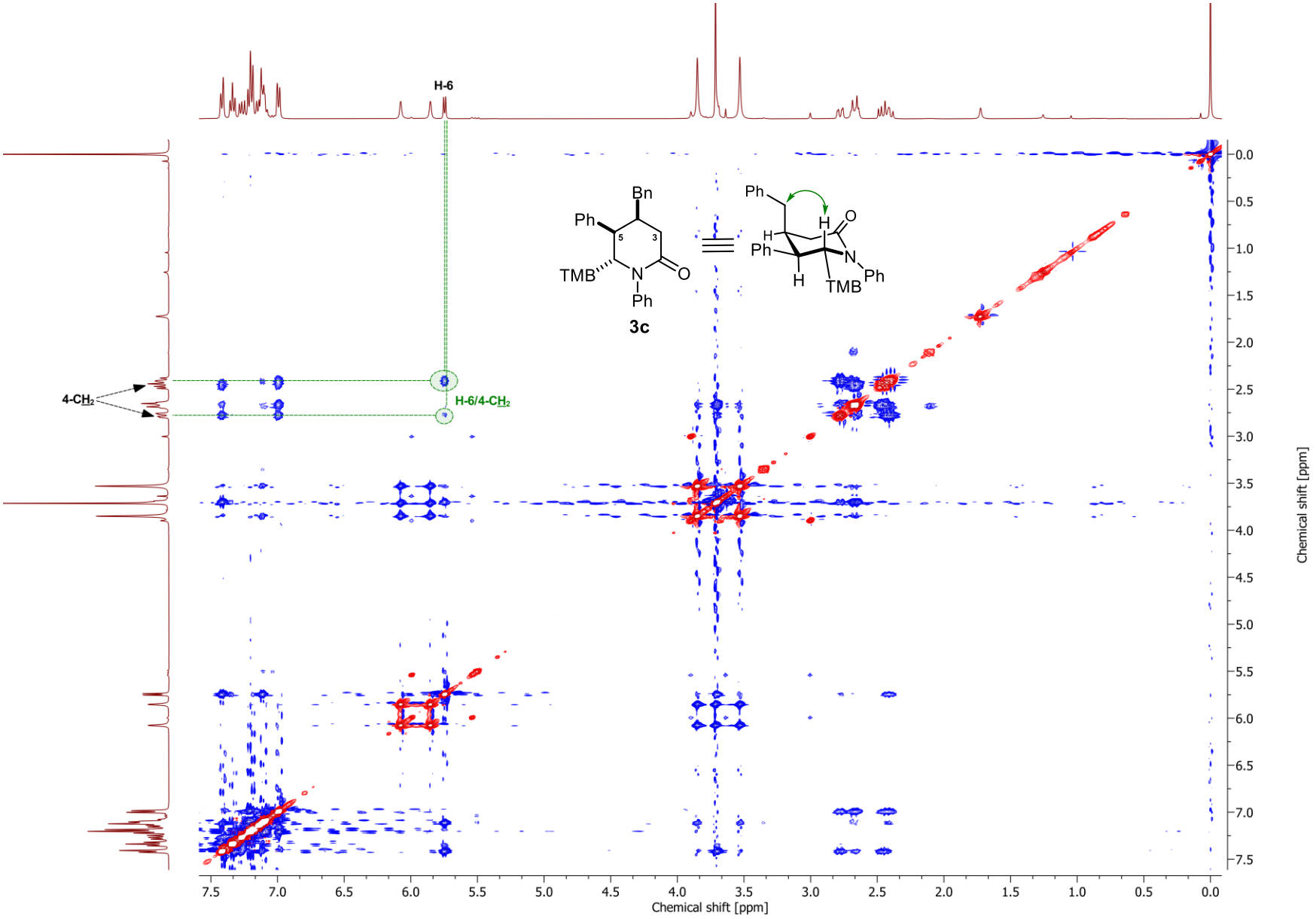


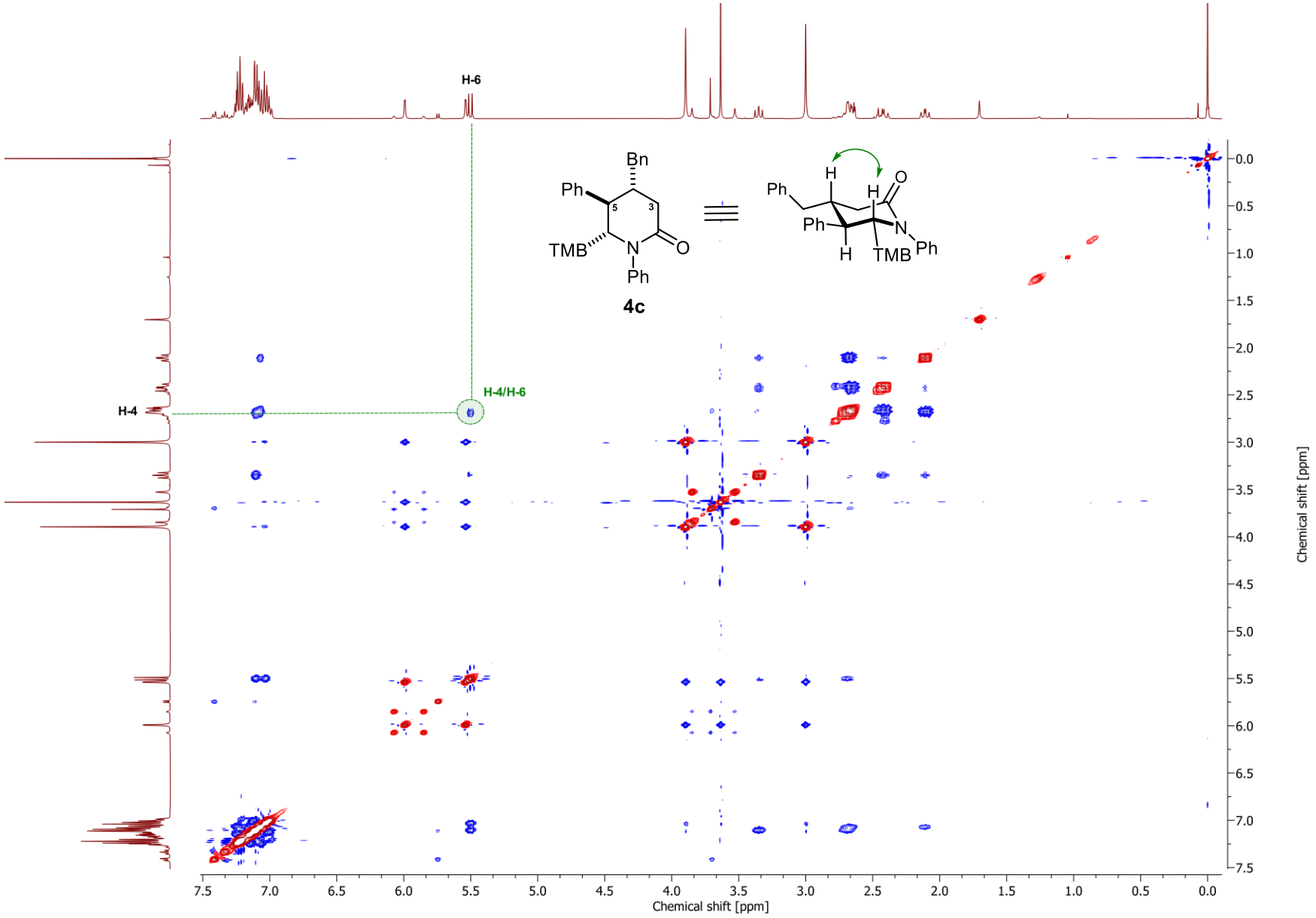
12. $^{1}H,^{1}H$ NOESY spectra for selected compounds

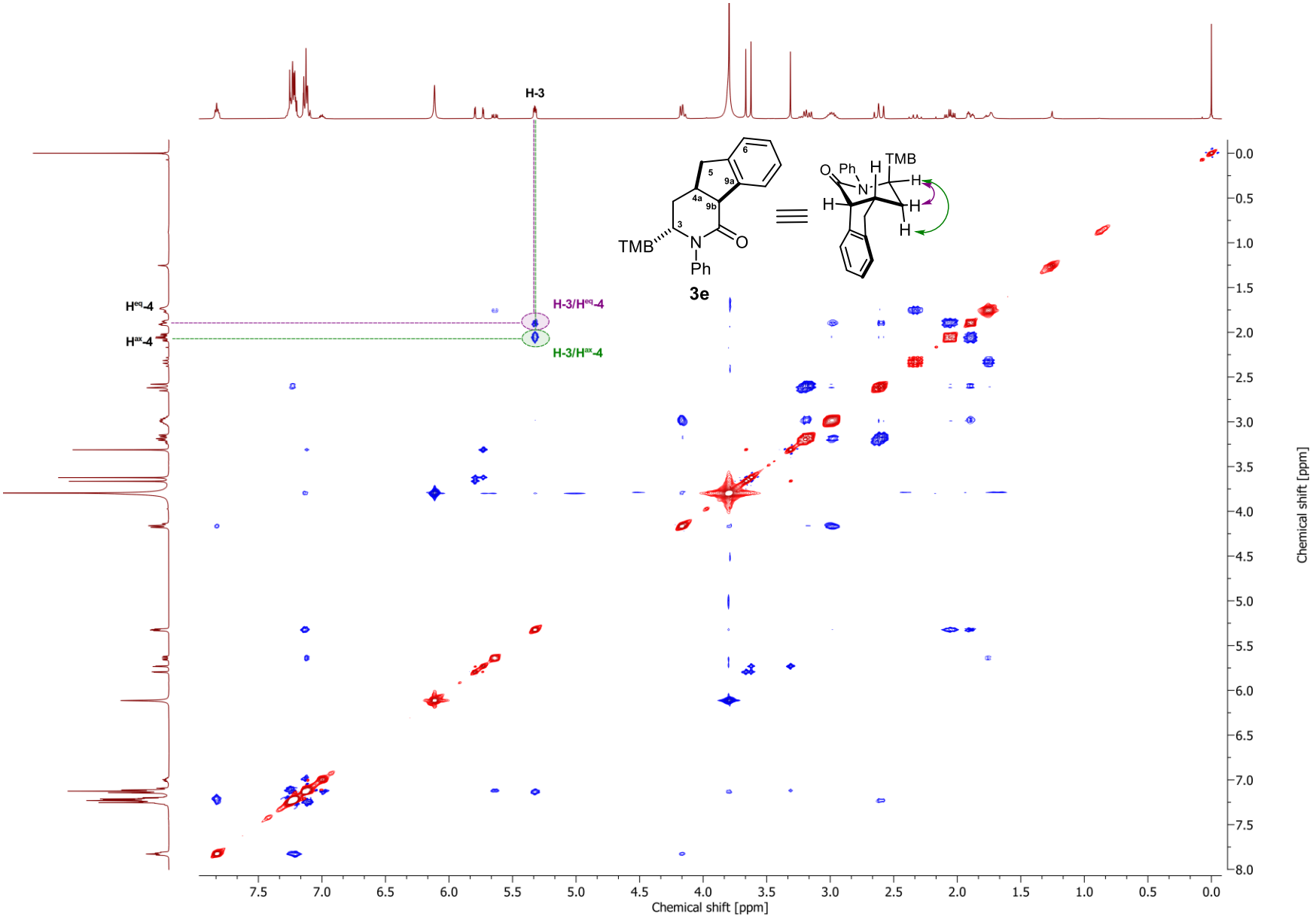

1-Ph
H-11
H-1
H-11b
H-1/H-11
H-11b/1-Ph
H-11b/H-11
MeO
MeO
Ph
H
H
H
1
2
11
11a
11b
7a
7
8
N
O
2c
Chemical shift [ppm]
Chemical shift [ppm]

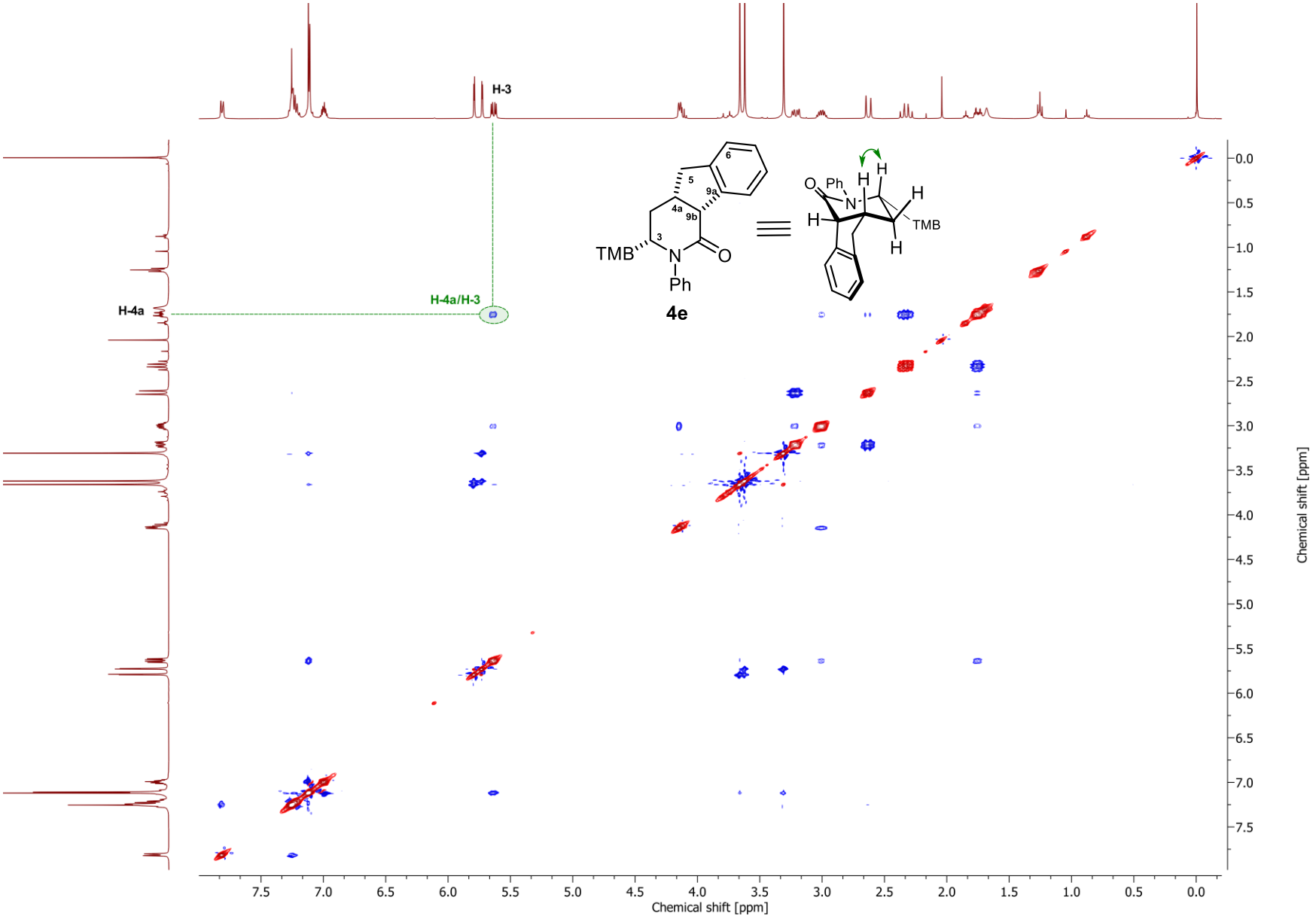

H13
H3a/H13
H3a
MeO
MeO
2d
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]

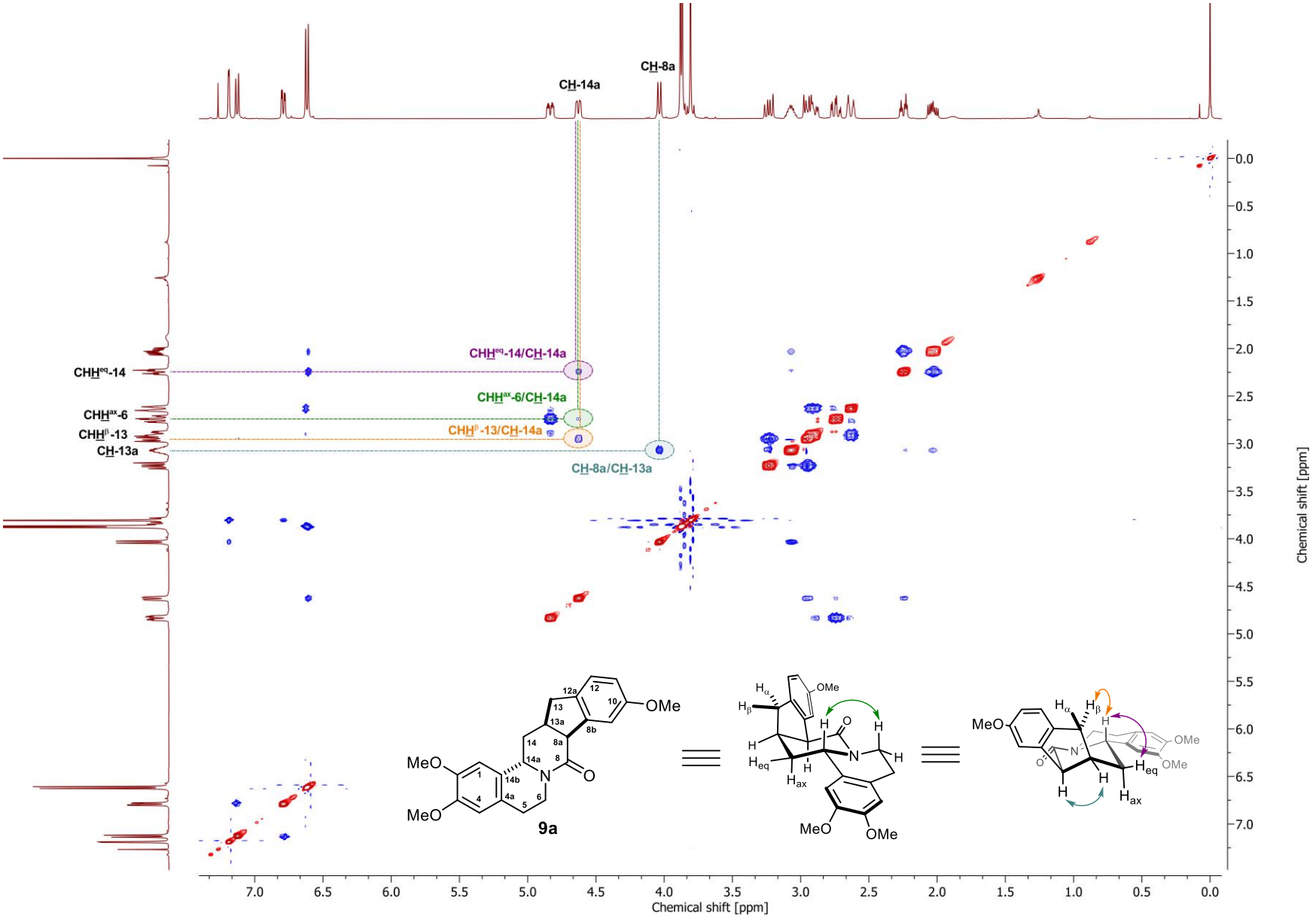

CHax-6
CHax-4
CHax-5
CHax-6/CHax-4
CHax-6/CHax-5
Ph
TMB
N
O
Ph
3a
H
H
O
H
Ph
H
TMB
N
Ph
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]
Chemical shift [ppm]

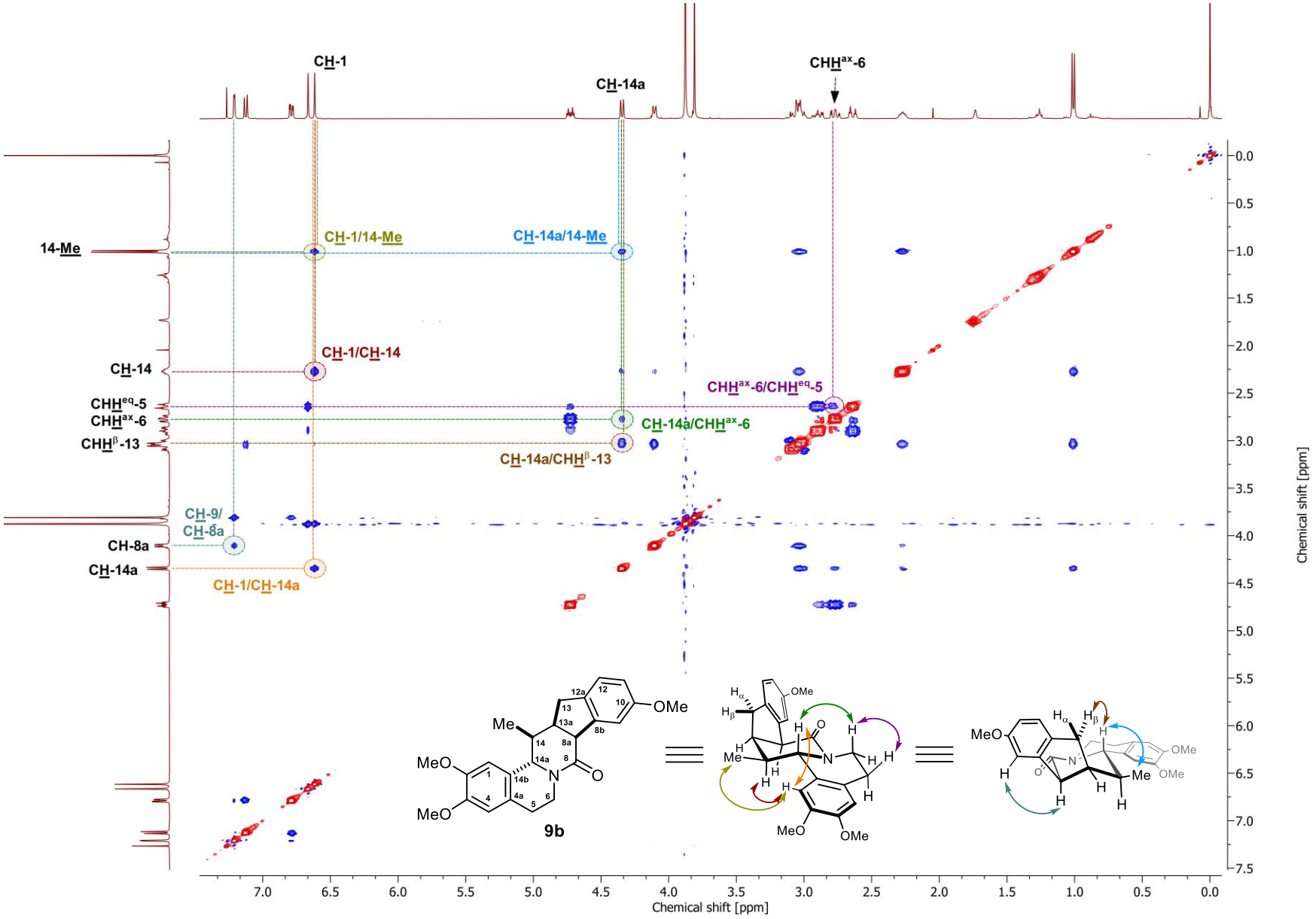

H-6
4-CH2
H-6/4-CH2
Bn
Ph
TMB
N
O
Ph
3c
Ph
H
O
H
Ph
N
Ph
H
TMB
Chemical shift [ppm]
Chemical shift [ppm]

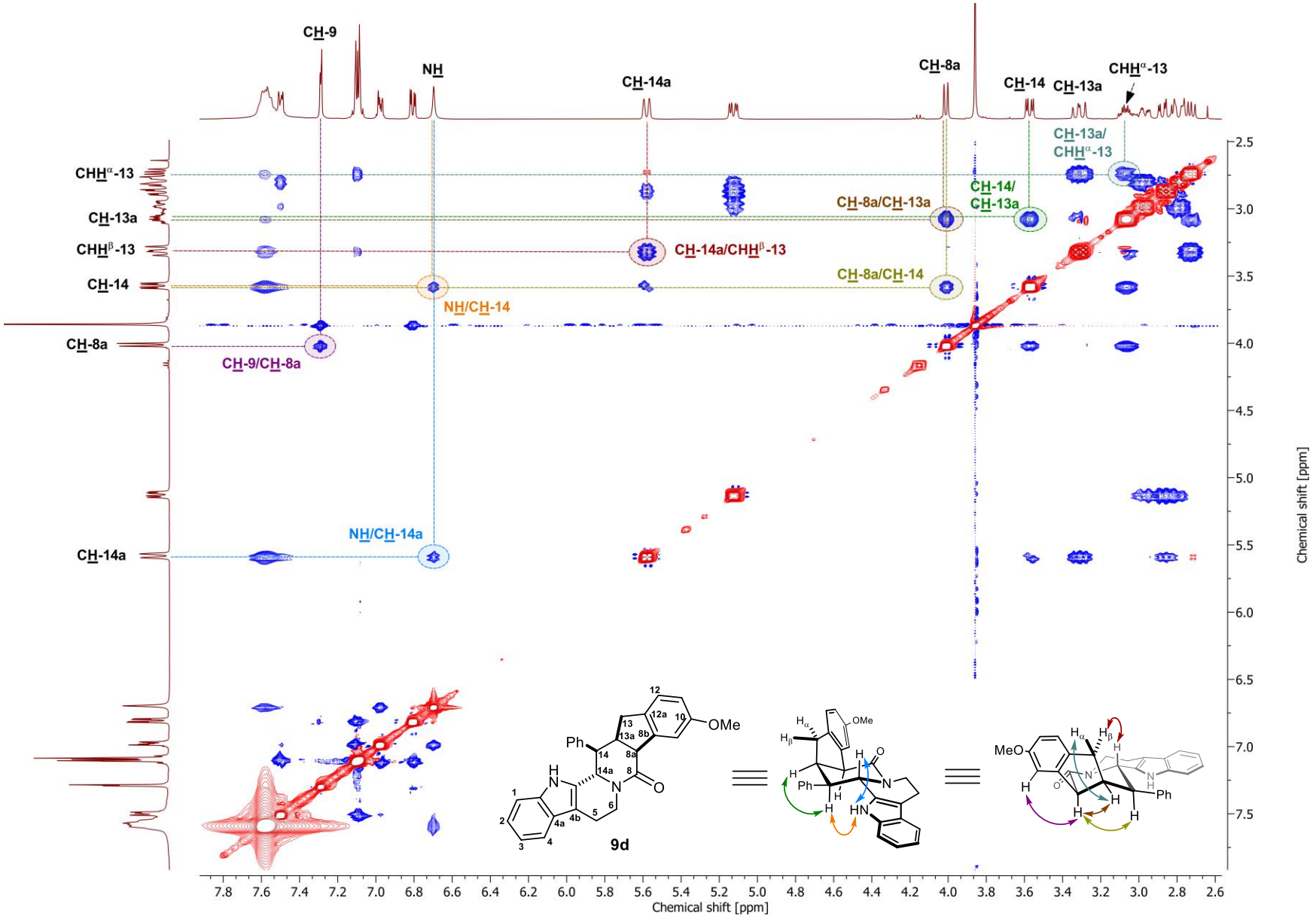

H-6
H-4
H-4/H-6
Bn
Ph
TMB
N
O
Ph
4c
H
H
O
Ph
Ph
N
Ph
H
TMB
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift [ppm]
Chemical shift [ppm]

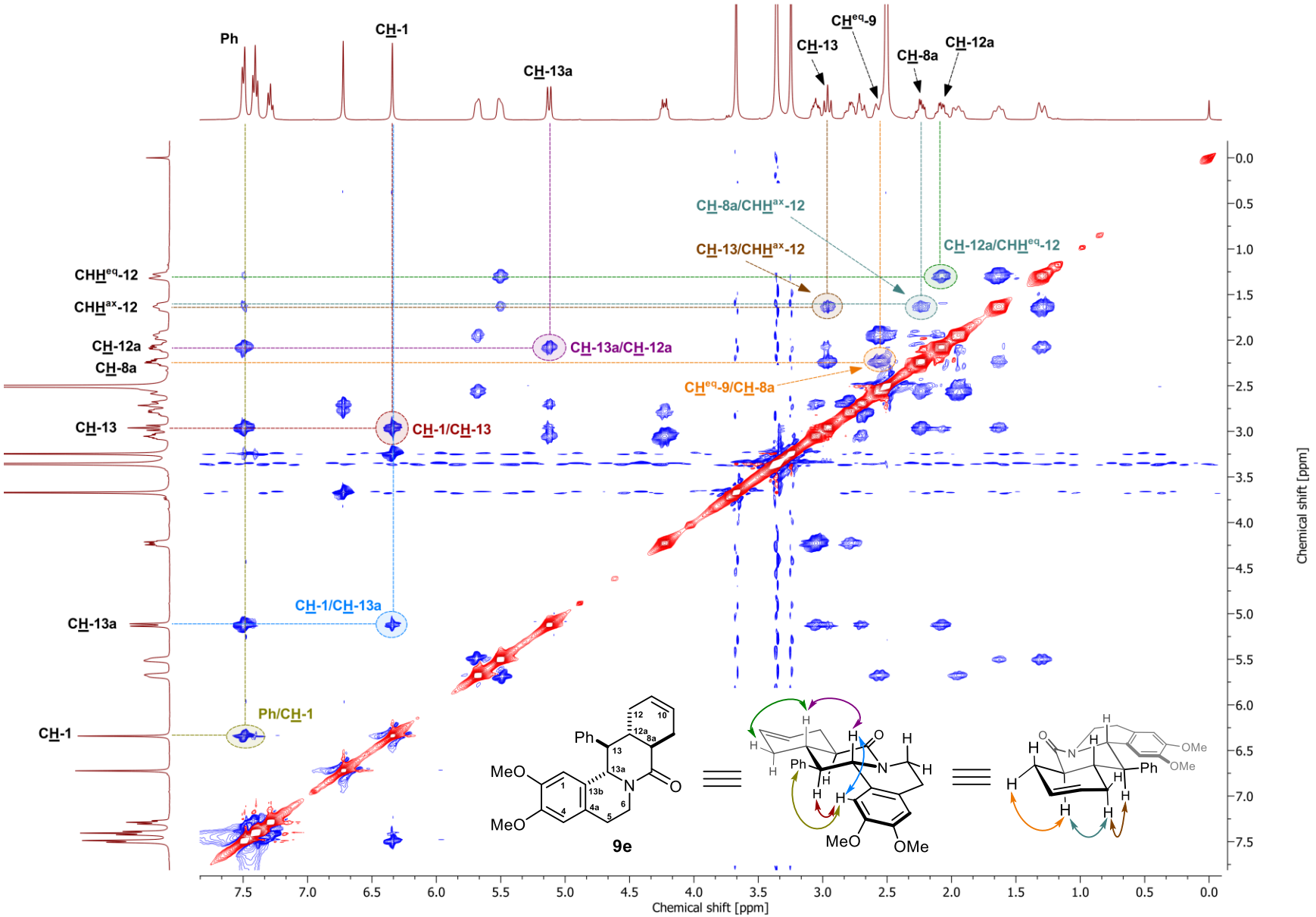

H-3
H-3/H^eq-4
H-3/H^ax-4
H^eq-4
H^ax-4
TMB
Ph
3e
Chemical shift [ppm]
Chemical shift [ppm]

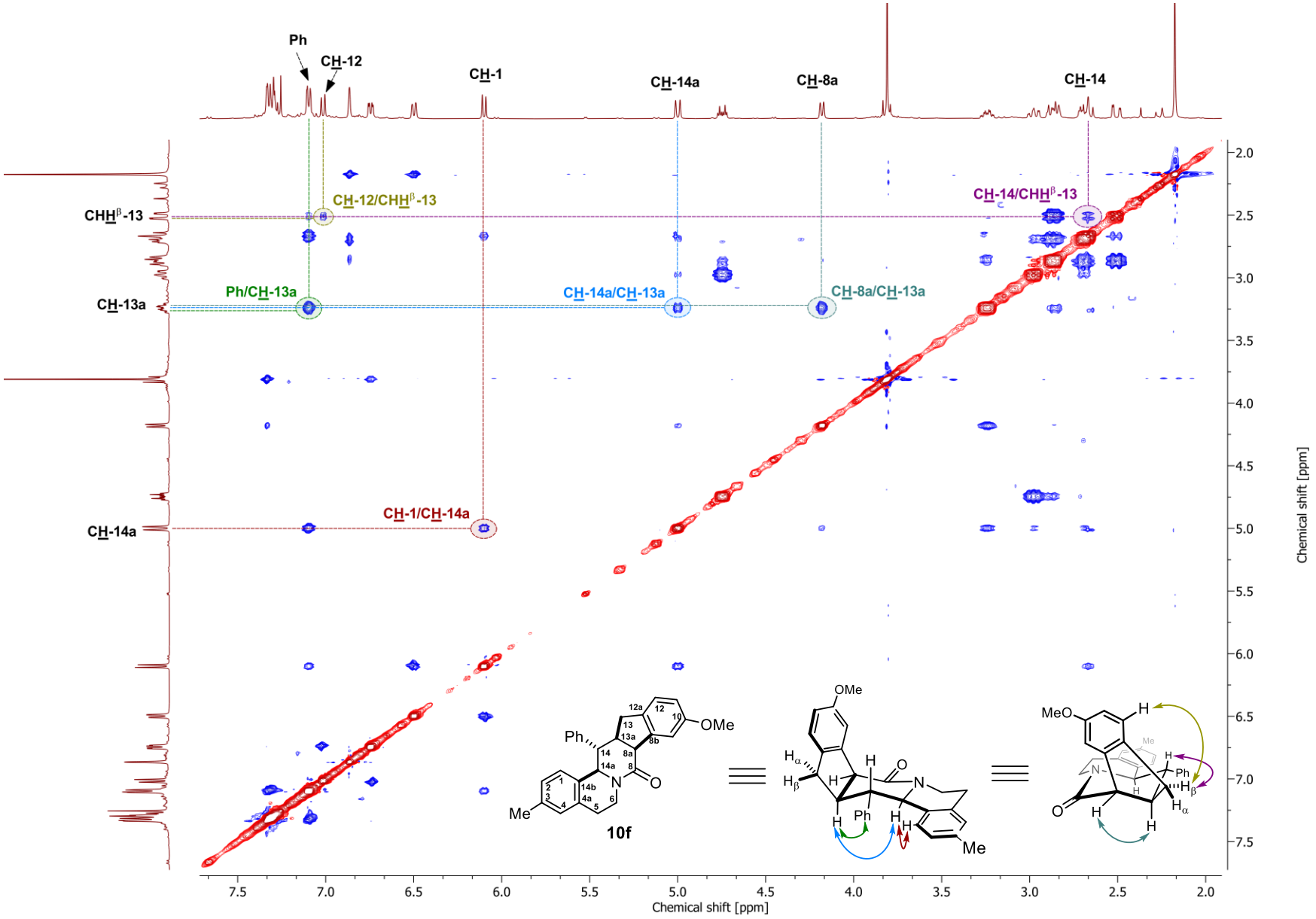

H-3
H-4a
H-4a/H-3
TMB
Ph
4e
Chemical shift [ppm]
Chemical shift [ppm]

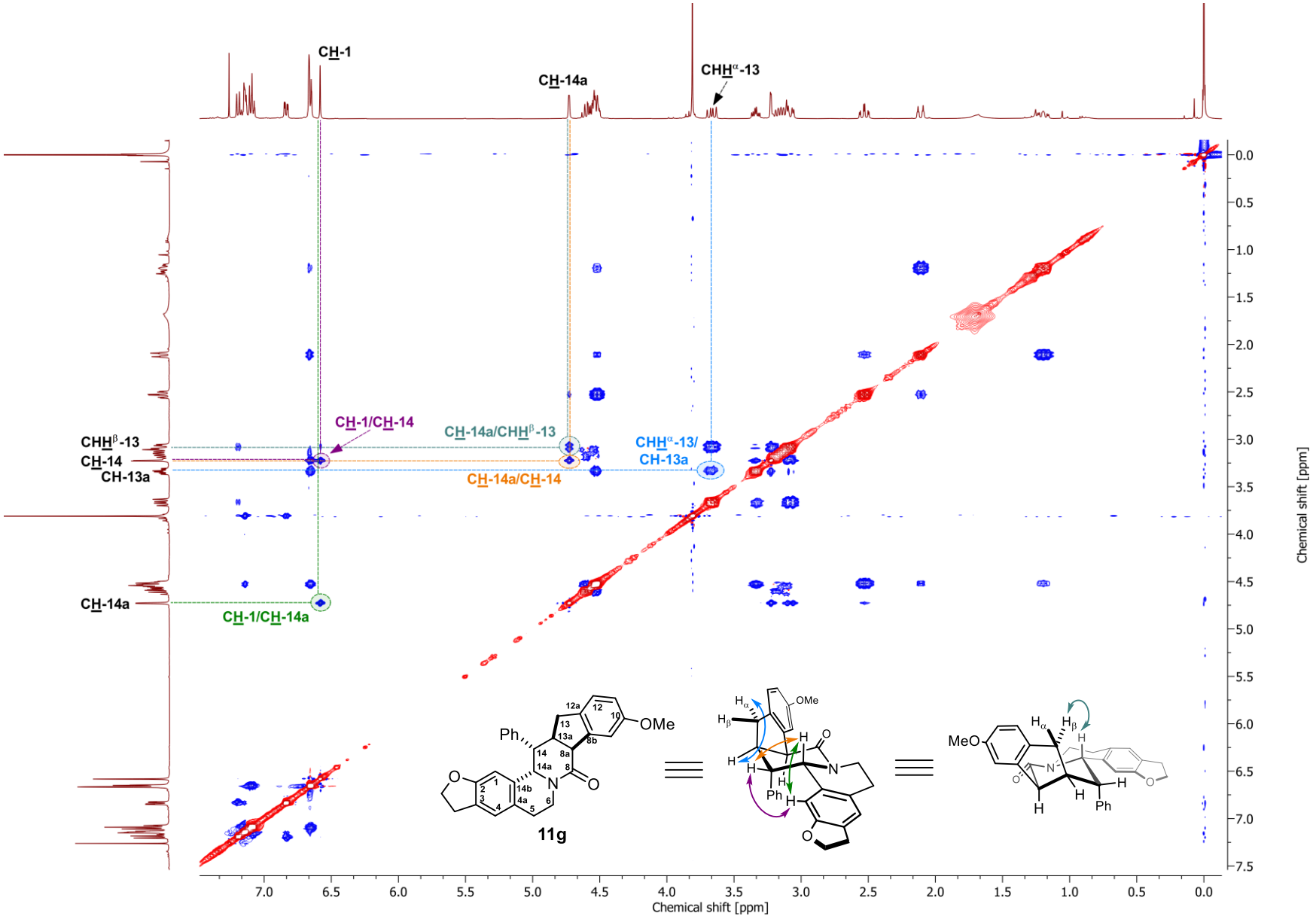

CH-14a
CH-8a
CHH^eq-14/CH-14a
CHH^ax-6/CH-14a
CHH^β-13/CH-14a
CH-8a/CH-13a
CHH^eq-14
CHH^ax-6
CHH^β-13
CH-13a
MeO
MeO
OMe
9a
Chemical shift [ppm]
Chemical shift [ppm]

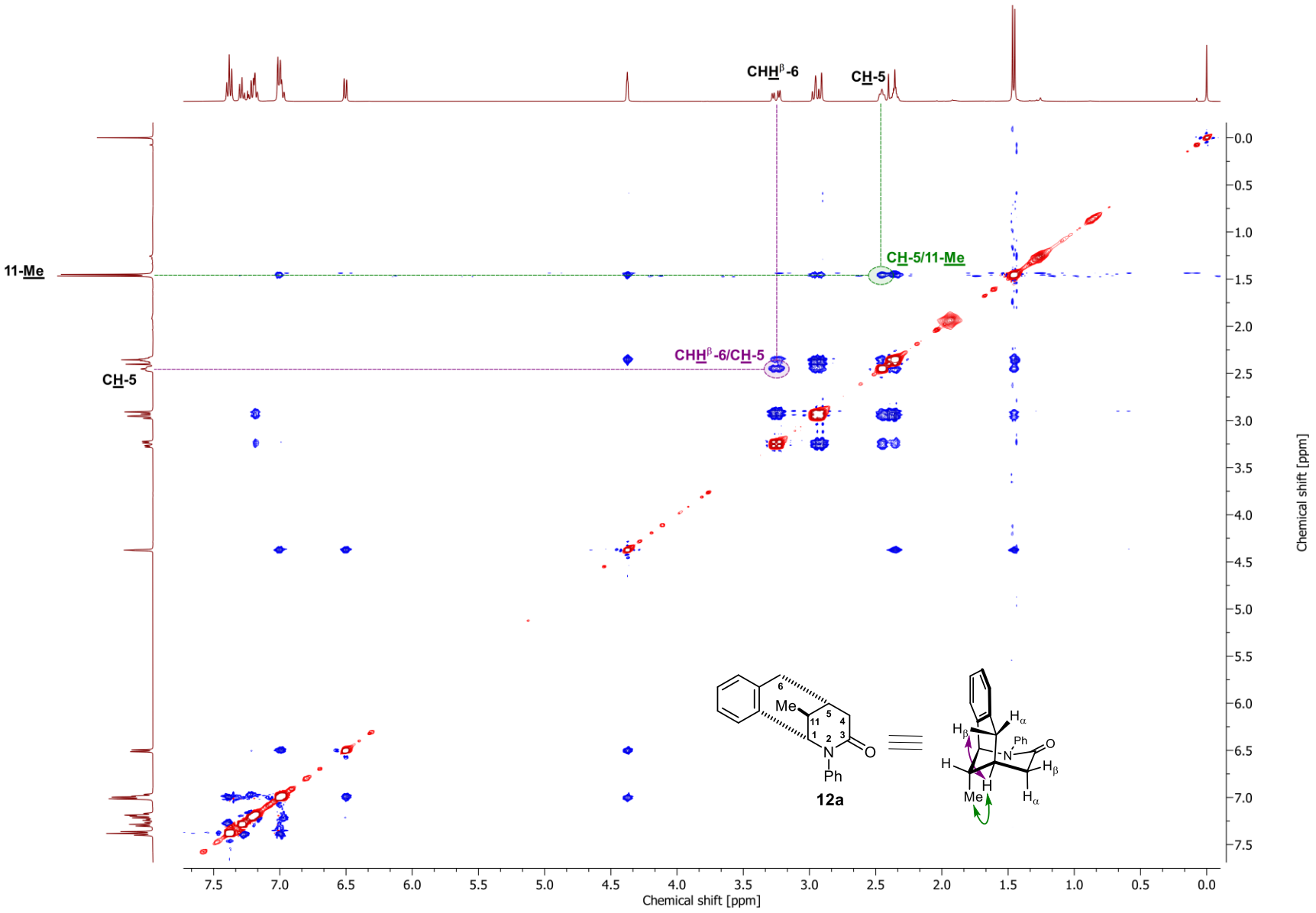

CH-1
CH-14a
CHHax-6
14-Me
CH-1/14-Me
CH-14a/14-Me
CH-1/CH-14
CH-14
CHHeq-5
CHHax-6
CHHβ-13
CHHax-6/CHHeq-5
CH-14a/CHHax-6
CH-14a/CHHβ-13
CH-9/
CH-8a
CH-8a
CH-14a
CH-1/CH-14a
9b
Chemical shift [ppm]
Chemical shift [ppm]

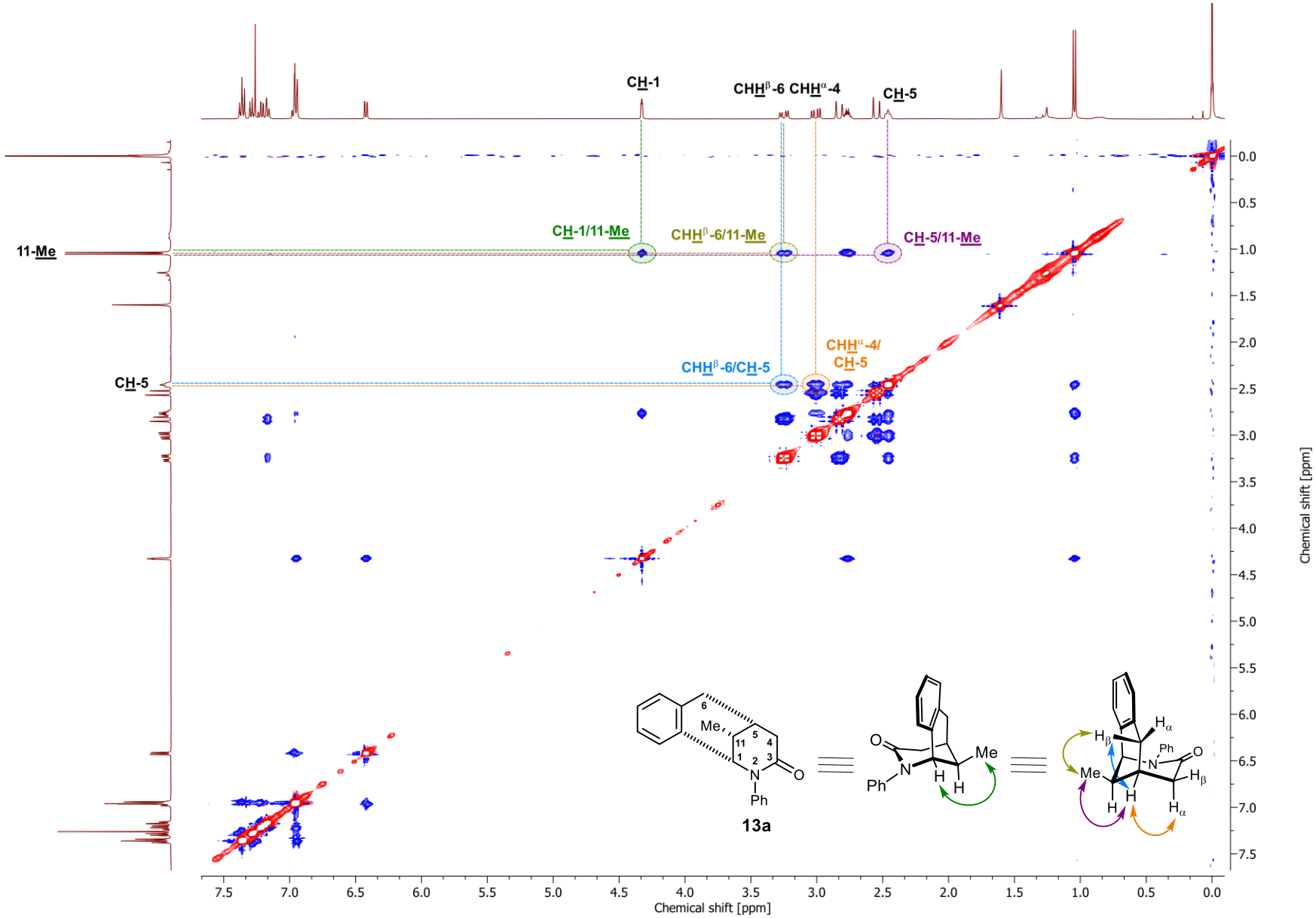

CH-9
NH
CH-14a
CH-8a
CH-14
CH-13a
CHHα-13
CH-13a/
CHHα-13
CHHα-13
CH-13a
CHHβ-13
CH-14
CH-8a
CH-14a
CH-8a/CH-13a
CH-14/
CH-13a
CH-14a/CHHβ-13
CH-8a/CH-14
NH/CH-14
CH-9/CH-8a
NH/CH-14a
9d
Chemical shift [ppm]
Chemical shift [ppm]

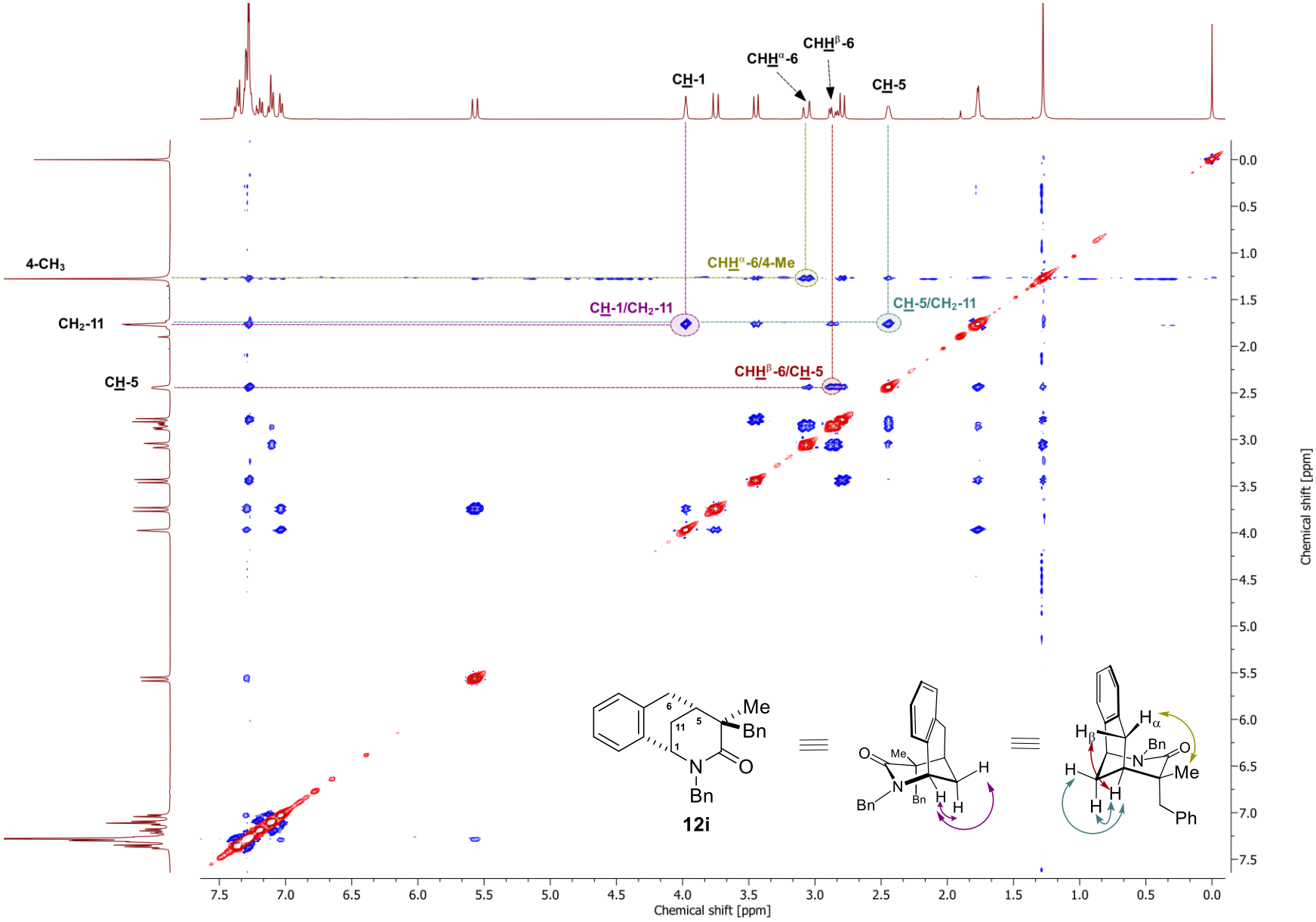

Ph
CH-1
CH-13a
CH-13
CHeq-9
CH-8a
CH-12a
CH-8a/CHHax-12
CH-13/CHHax-12
CH-12a/CHHeq-12
CHHeq-12
CHHax-12
CH-12a
CH-8a
CH-13a/CH-12a
CHeq-9/CH-8a
CH-13
CH-1/CH-13
CH-1/CH-13a
CH-13a
Ph/CH-1
CH-1
MeO
MeO
OMe
OMe
9e
Chemical shift [ppm]
Chemical shift [ppm]


Ph
CH-12
CH-1
CH-14a
CH-8a
CH-14
CHHβ-13
CH-13a
CH-14a
CH-12/CHHβ-13
Ph/CH-13a
CH-14a/CH-13a
CH-8a/CH-13a
CH-14/CHHβ-13
CH-1/CH-14a
10f
Chemical shift [ppm]
Chemical shift [ppm]


CH-1
CH-14a
CHHα-13
CHHβ-13
CH-14
CH-13a
CH-14a
CH-1/CH-14
CH-14a/CHHβ-13
CHHα-13/
CH-13a
CH-14a/CH-14
CH-1/CH-14a
11g
Chemical shift [ppm]
Chemical shift [ppm]

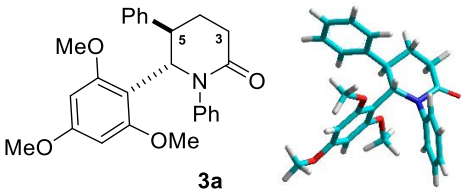

CHH$^{\beta}$-6
CH-5
11-Me
CH-5/11-Me
CHH$^{\beta}$-6/CH-5
CH-5
Me
Ph
12a
Chemical shift [ppm]
Chemical shift [ppm]


CH-1
CHHβ-6 CHHα-4
CH-5
11-Me
CH-5
CH-1/11-Me
CHHβ-6/11-Me
CH-5/11-Me
CHHβ-6/CH-5
CHHα-4/
CH-5
Me
Ph
13a
Hα
Hβ
Chemical shift [ppm]
Chemical shift [ppm]


CH-1
CHHα-6
CHHβ-6
CH-5
4-CH3
CH2-11
CH-5
CHHα-6/4-Me
CH-1/CH2-11
CH-5/CH2-11
CHHβ-6/CH-5
Me
Bn
N
O
Bn
12i
Chemical shift [ppm]
Chemical shift [ppm]

13. Computational results

Compound **3a**



3a

HyperChem, Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 160
in which
Number of Alpha Electrons = 80
Number of Beta Electrons = 80
Charge on the System = 0
Total Orbitals = 151

Energy=-6272.176049 kcal/mol Gradient=0.027885 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -111428.7909618 (kcal/mol)
Total Energy = -177.573059536 (a.u.)
Binding Energy = -6272.1760488 (kcal/mol)
Isolated Atomic Energy = -105156.6149130 (kcal/mol)
Electronic Energy = -1070440.8592002 (kcal/mol)
Core-Core Interaction = 959012.0682383 (kcal/mol)
Heat of Formation = -71.0460488 (kcal/mol)
Gradient = 0.0278849 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.044548	-3.20494	-0.72084	0.55880	12.01100
2	6	0.040908	-1.80122	-1.18955	0.09969	12.01100
3	7	0.001529	-1.77939	-1.73032	-1.30603	14.00700
4	6	0.254217	-2.75510	-1.32452	-2.26583	12.01100
5	6	-0.119598	-4.07359	-0.76698	-1.77863	12.01100
6	6	-0.103987	-3.89566	0.08296	-0.54000	12.01100
7	8	-0.371341	-2.51918	-1.50760	-3.45200	15.99900
8	6	-0.073764	-3.08670	0.11832	1.80358	12.01100
10	6	-0.184441	-1.24793	-2.22443	1.05583	12.01100
14	6	0.163804	-0.13856	-1.91354	1.86912	12.01100
15	6	0.164309	-1.79306	-3.51922	1.19486	12.01100

16	6	-0.263128	-1.27361	-4.44703	2.10358	12.01100
17	6	0.164878	-0.18221	-4.08988	2.90112	12.01100
18	6	-0.298520	0.39506	-2.82540	2.78890	12.01100
19	8	-0.193384	0.44531	-0.67494	1.66748	15.99900
20	8	-0.187311	0.23260	-5.08209	3.76344	15.99900
21	8	-0.193614	-2.91562	-3.82186	0.44357	15.99900
22	6	0.045769	-3.07933	-5.17516	0.08571	12.01100
23	6	0.050828	1.32681	-4.80072	4.60116	12.01100
24	6	0.047019	1.17586	-0.13630	2.74413	12.01100
25	6	-0.102133	-2.61068	1.42983	1.73319	12.01100
26	6	-0.092182	-3.46415	-0.40726	3.03997	12.01100
27	6	-0.103054	-3.35833	0.36795	4.19012	12.01100
28	6	-0.106348	-2.87841	1.67061	4.11452	12.01100
29	6	-0.100829	-2.50573	2.20137	2.88351	12.01100
47	6	-0.044714	-0.43791	-2.04073	-1.80718	12.01100
48	6	-0.098586	0.52414	-1.04171	-1.98717	12.01100
49	6	-0.074243	-0.13609	-3.37071	-2.11456	12.01100
50	6	-0.102279	1.12803	-3.69464	-2.59534	12.01100
51	6	-0.100560	2.08787	-2.70376	-2.76875	12.01100
52	6	-0.098093	1.78465	-1.38072	-2.46494	12.01100
32	1	0.034053	-2.99163	-5.85746	0.94457	1.00800
33	1	0.031954	-2.35516	-5.46441	-0.68497	1.00800
34	1	0.050727	-4.09408	-5.19486	-0.31836	1.00800
35	1	0.028031	1.12391	-3.96842	5.28507	1.00800
36	1	0.029596	2.24302	-4.59763	4.03472	1.00800
37	1	0.051522	1.43276	-5.73159	5.16480	1.00800
38	1	0.030973	1.90211	-0.84672	3.16643	1.00800
39	1	0.032656	0.50459	0.21065	3.53717	1.00800
40	1	0.051225	1.69195	0.70948	2.28371	1.00800
41	1	0.110136	-2.33325	1.84321	0.75300	1.00800
42	1	0.111158	-3.83996	-1.43516	3.10681	1.00800
43	1	0.102974	-3.65568	-0.05068	5.15714	1.00800
44	1	0.102497	-2.79710	2.27886	5.02103	1.00800
45	1	0.102568	-2.13246	3.22853	2.81955	1.00800
46	1	0.060761	-3.30969	1.00228	-0.76164	1.00800
9	1	0.093277	-3.84197	-1.61100	0.78998	1.00800
11	1	0.078467	-1.13782	-0.28202	0.10302	1.00800
12	1	0.078392	-4.75773	-1.61647	-1.57615	1.00800
13	1	0.079747	-4.55504	-0.17829	-2.58471	1.00800
30	1	0.140238	-1.72742	-5.44765	2.18451	1.00800
31	1	0.136842	1.26614	-2.52930	3.39393	1.00800
53	1	0.063456	-4.88098	0.43952	-0.18143	1.00800
54	1	0.106811	0.29698	0.00596	-1.75781	1.00800
55	1	0.112113	-0.89129	-4.15623	-1.98610	1.00800
56	1	0.101322	1.36542	-4.73471	-2.84131	1.00800
57	1	0.100920	3.08107	-2.96398	-3.14839	1.00800
58	1	0.100980	2.53969	-0.60076	-2.60666	1.00800

ATOMIC GRADIENTS

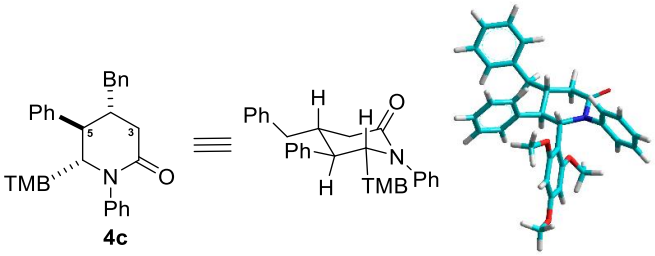
Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.01464	-0.01081	0.00435

2	6	-0.01668	-0.01589	-0.02458
3	7	0.07593	-0.00089	0.01628
4	6	-0.10521	0.01466	0.03820
5	6	0.03911	0.00191	0.00116
6	6	-0.01780	0.02473	-0.00993
7	8	0.00174	0.00142	-0.04057
8	6	0.00964	-0.04428	0.02366
10	6	0.03256	-0.04265	-0.01254
14	6	-0.02011	-0.08805	0.05087
15	6	0.01801	0.03789	0.02039
16	6	0.04982	0.02167	0.06273
17	6	-0.03854	0.04045	-0.05496
18	6	-0.05496	0.04251	-0.01195
19	8	0.02279	0.05600	-0.02456
20	8	-0.00760	-0.01020	0.07931
21	8	-0.04192	-0.00342	0.00190
22	6	0.02269	-0.00714	-0.02278
23	6	-0.01209	0.00253	0.00807
24	6	0.00547	-0.00289	-0.00405
25	6	-0.03707	0.03304	0.03828
26	6	-0.02830	0.01177	-0.05682
27	6	0.06264	0.01269	0.02789
28	6	-0.03976	-0.03616	-0.00066
29	6	0.05337	-0.03288	-0.03483
47	6	-0.04214	-0.03406	0.00558
48	6	0.02282	-0.04194	-0.00102
49	6	0.01520	0.03323	-0.01550
50	6	0.01122	-0.00164	-0.05688
51	6	-0.05263	-0.00866	0.01607
52	6	-0.02108	0.01361	-0.00750
32	1	0.02227	-0.02085	-0.00091
33	1	0.04571	-0.02520	-0.03299
34	1	0.02298	0.02071	0.00232
35	1	-0.00698	0.00087	-0.00420
36	1	-0.01794	0.00604	0.01796
37	1	-0.00668	0.03556	0.01389
38	1	-0.00263	0.01402	-0.02873
39	1	-0.00051	-0.01729	-0.03175
40	1	0.00412	0.02150	0.03084
41	1	0.01276	0.00855	-0.00204
42	1	0.01720	-0.01545	0.00235
43	1	-0.00652	-0.02122	-0.00160
44	1	0.00776	-0.00686	0.01968
45	1	-0.01437	0.00579	0.00539
46	1	0.02573	-0.00250	0.03546
9	1	-0.01042	0.01708	0.00045
11	1	0.03115	-0.00391	0.00947
12	1	0.02334	0.00506	-0.03344
13	1	-0.00486	0.00151	-0.01096
30	1	-0.00739	0.01491	0.00481
31	1	-0.00632	0.01200	0.00391
53	1	0.00730	-0.01112	0.01347

54	1	0.00572	0.01833	0.00920
55	1	-0.04086	0.00382	-0.03117
56	1	-0.02535	0.00776	-0.02590
57	1	0.00321	-0.00911	0.00133
58	1	-0.00016	-0.02651	0.01754

Dipole (Debyes)	x	y	z	Total
Point-Chg.	0.786	-0.216	4.235	4.313
sp Hybrid	0.713	0.426	0.695	1.083
pd Hybrid	0.000	0.000	0.000	0.000
Sum	1.499	0.210	4.930	5.158

Compound **4c**



Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 194
in which
Number of Alpha Electrons = 97
Number of Beta Electrons = 97
Charge on the System = 0
Total Orbitals = 185

Starting PM3 calculation with 185 orbitals

Energy=-7755.279949 kcal/mol Gradient=0.030956 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -132676.2787903 (kcal/mol)
Total Energy = -211.433082503 (a.u.)
Binding Energy = -7755.2799493 (kcal/mol)
Isolated Atomic Energy = -124920.9988410 (kcal/mol)
Electronic Energy = -1431119.4910750 (kcal/mol)
Core-Core Interaction = 1298443.2122847 (kcal/mol)
Heat of Formation = -45.3079493 (kcal/mol)
Gradient = 0.0309561 (kcal/mol/Ang)

MOLECULAR POINT GROUP
C1
NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	-0.043417	-2.92212	-0.27603	0.69677	12.01100
2	6	0.038099	-1.41685	-0.41302	0.34617	12.01100
3	7	0.003119	-1.12649	-0.44194	-1.12913	14.00700
4	6	0.253842	-2.01913	0.17612	-2.05263	12.01100
5	6	-0.128413	-3.46922	0.33113	-1.66072	12.01100
6	6	-0.071662	-3.63672	0.74650	-0.20309	12.01100
7	8	-0.370322	-1.60103	0.48523	-3.15986	15.99900
8	6	-0.045914	0.30192	-0.42398	-1.45704	12.01100
9	6	-0.068714	-3.06165	0.09737	2.15126	12.01100
11	6	-0.182819	-0.84293	-1.65170	1.00300	12.01100
15	6	-0.059977	-5.13859	0.84044	0.12521	12.01100
16	6	0.162969	0.10357	-1.52948	2.04064	12.01100
17	6	0.163757	-1.21394	-2.96398	0.63534	12.01100
18	6	-0.262395	-0.69546	-4.08872	1.28477	12.01100
19	6	0.164329	0.22069	-3.91847	2.32747	12.01100
20	6	-0.295866	0.63110	-2.64191	2.70922	12.01100
21	8	-0.195117	0.55163	-0.25054	2.32501	15.99900
22	8	-0.187305	0.64877	-5.09810	2.89771	15.99900
23	8	-0.193823	-2.17008	-3.10094	-0.35630	15.99900
24	6	0.045829	-2.10406	-4.27771	-1.12883	12.01100
25	6	0.050580	1.56308	-5.01164	3.96301	12.01100
26	6	0.045475	0.99477	-0.01526	3.64114	12.01100
27	6	-0.090813	-2.54920	1.29710	2.65111	12.01100
28	6	-0.098379	-3.72294	-0.77417	3.02004	12.01100
29	6	-0.105372	-3.86167	-0.45403	4.36609	12.01100
30	6	-0.106514	-3.34359	0.73880	4.85769	12.01100
31	6	-0.102240	-2.68858	1.61355	3.99746	12.01100
48	6	-0.075027	0.85457	-1.55511	-2.06482	12.01100
49	6	-0.095531	1.10269	0.68869	-1.18068	12.01100
50	6	-0.097857	2.45380	0.65935	-1.50635	12.01100
51	6	-0.099684	3.00697	-0.46684	-2.10669	12.01100
52	6	-0.102791	2.20761	-1.56975	-2.38593	12.01100
59	6	-0.076729	-5.52380	2.13572	0.76474	12.01100
60	6	-0.105366	-5.31623	3.34481	0.09715	12.01100
61	6	-0.098836	-5.69891	4.54358	0.68687	12.01100
62	6	-0.106895	-6.29692	4.54510	1.94305	12.01100
63	6	-0.099669	-6.51115	3.34371	2.60917	12.01100
64	6	-0.097258	-6.12566	2.14266	2.02409	12.01100
39	1	0.051547	1.71767	-6.06269	4.22161	1.00800
40	1	0.031267	1.70546	-0.77602	3.99708	1.00800
41	1	0.034046	0.14647	0.04407	4.33202	1.00800
42	1	0.050583	1.48696	0.95665	3.55755	1.00800
43	1	0.109779	-2.03501	1.99733	1.98107	1.00800
44	1	0.109240	-4.13243	-1.71789	2.64003	1.00800
45	1	0.102860	-4.38006	-1.14445	5.03927	1.00800
46	1	0.102469	-3.45372	0.99068	5.91721	1.00800
47	1	0.102969	-2.28546	2.55739	4.37884	1.00800
12	1	0.079380	-0.89818	0.49986	0.74849	1.00800
13	1	0.080717	-3.98476	-0.63238	-1.85562	1.00800
14	1	0.081833	-3.95707	1.07549	-2.32375	1.00800

10	1	0.092971	-3.42468	-1.26487	0.53971	1.00800
32	1	0.140142	-1.01325	-5.09674	0.97385	1.00800
53	1	0.111931	0.22788	-2.42662	-2.29213	1.00800
54	1	0.106584	0.67811	1.58452	-0.71291	1.00800
55	1	0.101258	3.08320	1.52917	-1.29236	1.00800
56	1	0.100979	4.07117	-0.48320	-2.36281	1.00800
57	1	0.101388	2.64307	-2.45360	-2.86327	1.00800
58	1	0.081036	-3.16571	1.75111	-0.05672	1.00800
33	1	0.136763	1.36565	-2.48397	3.51427	1.00800
34	1	0.034320	-2.04778	-5.18959	-0.51551	1.00800
35	1	0.031813	-1.24837	-4.24543	-1.81327	1.00800
36	1	0.050427	-3.04168	-4.24953	-1.68878	1.00800
37	1	0.028392	1.15089	-4.46985	4.82220	1.00800
38	1	0.029585	2.51253	-4.55513	3.66016	1.00800
65	1	0.065371	-5.43802	-0.00743	0.77660	1.00800
66	1	0.062716	-5.74814	0.72947	-0.79592	1.00800
67	1	0.107942	-4.85206	3.34388	-0.89631	1.00800
68	1	0.102558	-5.53053	5.48864	0.16035	1.00800
69	1	0.102344	-6.59865	5.48978	2.40641	1.00800
70	1	0.102104	-6.98202	3.34081	3.59757	1.00800
71	1	0.109392	-6.28705	1.19854	2.55818	1.00800

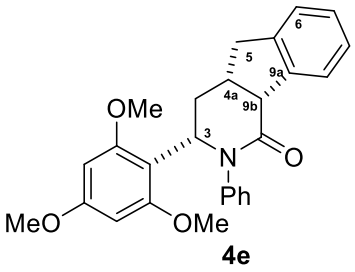
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.00688	0.00121	-0.00451
2	6	0.00256	-0.01038	-0.00805
3	7	0.06107	0.07556	0.00455
4	6	-0.01540	-0.03992	-0.02526
5	6	0.01572	-0.01449	-0.05414
6	6	-0.00806	0.01611	-0.00090
7	8	-0.00254	-0.00332	-0.02477
8	6	-0.01961	-0.06618	-0.02806
9	6	0.01852	0.01785	-0.02243
11	6	-0.00449	0.02965	-0.00539
15	6	-0.01924	0.00905	-0.02788
16	6	0.02216	-0.04513	0.04029
17	6	-0.01993	-0.01738	-0.01975
18	6	-0.00803	-0.01529	0.02422
19	6	0.00421	0.00403	0.01976
20	6	-0.03839	0.06027	-0.03874
21	8	0.02669	0.03014	-0.00659
22	8	-0.02554	0.01642	0.01813
23	8	0.02251	0.00787	-0.00451
24	6	0.00659	-0.02709	0.01259
25	6	-0.02113	-0.00926	0.00594
26	6	-0.00239	-0.00412	0.01642
27	6	-0.00581	0.05364	0.04816
28	6	-0.01271	0.00277	-0.03529
29	6	0.02063	0.07113	0.01967
30	6	0.00490	-0.01475	-0.00673
31	6	0.00426	0.02338	-0.08262

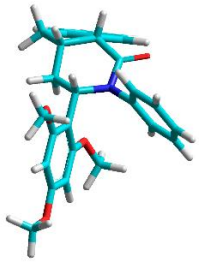
48	6	0.05451	0.01819	-0.02288
49	6	-0.00523	0.04078	-0.00192
50	6	0.04587	-0.00564	-0.00884
51	6	-0.01570	-0.03639	0.00739
52	6	-0.01807	0.01599	0.02775
59	6	-0.00236	0.02287	-0.01538
60	6	-0.02684	0.04955	0.07880
61	6	-0.00537	-0.07250	0.07509
62	6	0.02350	-0.07005	-0.00971
63	6	-0.04366	-0.03188	0.07110
64	6	-0.01871	-0.09073	-0.00344
39	1	-0.03040	0.00781	0.01737
40	1	-0.01254	-0.01646	0.00865
41	1	-0.00418	0.01469	0.00893
42	1	-0.01196	0.00578	-0.01943
43	1	-0.00116	0.02235	-0.03399
44	1	0.01068	0.03066	0.01017
45	1	0.01385	0.03912	-0.00939
46	1	0.01181	0.04221	-0.01236
47	1	-0.00785	0.03411	-0.02327
12	1	0.00106	0.00098	-0.02057
13	1	0.01887	0.03156	-0.01765
14	1	-0.00898	-0.01943	-0.02318
10	1	0.00729	0.02909	-0.00612
32	1	-0.01559	0.00479	0.01441
53	1	-0.01349	-0.02960	-0.01180
54	1	0.01954	-0.00248	-0.01566
55	1	0.00180	-0.03146	-0.01220
56	1	0.02471	-0.02015	-0.00080
57	1	0.00904	-0.02589	0.01200
58	1	-0.01300	-0.02698	-0.04819
33	1	0.01466	0.01633	-0.01387
34	1	-0.00481	-0.02388	-0.01041
35	1	0.01044	0.00678	0.01632
36	1	-0.01318	-0.02611	0.02752
37	1	-0.01314	0.00345	0.01585
38	1	-0.01900	0.01114	0.01606
65	1	-0.02228	0.03195	-0.02061
66	1	-0.00256	0.07063	-0.05870
67	1	0.04084	0.01903	0.00745
68	1	0.04121	0.04514	0.07949
69	1	0.00168	-0.07877	0.11747
70	1	-0.01138	-0.08797	0.02839
71	1	-0.02330	-0.07034	-0.03400

Dipole (Debyes)	x	y	z	Total
Point-Chg.	0.283	-1.777	4.019	4.403
sp Hybrid	0.494	0.215	0.902	1.050
pd Hybrid	0.000	0.000	0.000	0.000
Sum	0.777	-1.561	4.921	5.221

Compound



4e



HyperChem log start -- Thu Oct 01 04:01:29 2020.
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PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 164
in which
Number of Alpha Electrons = 82
Number of Beta Electrons = 82
Charge on the System = 0
Total Orbitals = 155

Starting PM3 calculation with 155 orbitals
Energy=-6441.205822 kcal/mol Gradient=0.025971 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -114162.8957653 (kcal/mol)
Total Energy = -181.930132344 (a.u.)
Binding Energy = -6441.2058223 (kcal/mol)
Isolated Atomic Energy = -107721.6899430 (kcal/mol)
Electronic Energy = -1093005.2936271 (kcal/mol)
Core-Core Interaction = 978842.3978618 (kcal/mol)
Heat of Formation = -69.1858223 (kcal/mol)
Gradient = 0.0259709 (kcal/mol/Ang)

MOLECULAR POINT GROUP
C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.122159	-0.18189	1.18447	1.01414	12.01100
2	6	0.040137	-0.57019	-0.26582	1.30046	12.01100
3	7	0.011091	0.00971	-1.19363	0.27155	14.00700
4	6	0.265266	1.30684	-0.92656	-0.25980	12.01100
5	6	-0.042778	1.99846	0.40850	-0.03378	12.01100

6	6	-0.072103	1.32763	1.36399	0.98365	12.01100
7	8	-0.375219	1.83524	-1.81274	-0.91898	15.99900
8	6	-0.041771	-0.37525	-2.59951	0.41826	12.01100
11	6	-0.191904	-2.07514	-0.39087	1.37630	12.01100
13	6	-0.078231	2.15294	1.24686	-1.27116	12.01100
14	6	-0.047295	1.67389	2.78757	0.48972	12.01100
17	6	-0.090187	1.98897	2.60735	-0.95791	12.01100
18	6	-0.073650	2.45161	0.85312	-2.56456	12.01100
19	6	-0.106812	2.57730	1.83738	-3.54783	12.01100
20	6	-0.101534	2.41250	3.18185	-3.23766	12.01100
21	6	-0.090660	2.11648	3.58123	-1.93280	12.01100
28	6	0.159549	-2.69354	-0.65859	2.61366	12.01100
29	6	-0.302387	-4.08028	-0.80875	2.74254	12.01100
30	6	0.168806	-4.88127	-0.68019	1.60814	12.01100
31	6	-0.267931	-4.31405	-0.38371	0.36481	12.01100
32	6	0.173350	-2.92744	-0.23344	0.25994	12.01100
33	8	-0.198144	-1.85931	-0.70633	3.71806	15.99900
34	6	0.048637	-2.32024	-1.43810	4.82952	12.01100
35	8	-0.186957	-6.25311	-0.80980	1.58241	15.99900
36	6	0.050964	-6.89902	-1.13850	2.78779	12.01100
37	8	-0.181361	-2.33452	0.13398	-0.93104	15.99900
38	6	0.041811	-3.04193	-0.15520	-2.11424	12.01100
39	6	-0.071852	-1.06720	-3.21578	-0.62859	12.01100
40	6	-0.101568	-1.44524	-4.54914	-0.51168	12.01100
41	6	-0.101225	-1.13918	-5.26754	0.63865	12.01100
42	6	-0.100613	-0.44692	-4.65414	1.67750	12.01100
43	6	-0.108527	-0.05950	-3.32341	1.57302	12.01100
22	1	0.059913	2.55028	3.19839	1.02542	1.00800
23	1	0.065463	0.84749	3.50416	0.65156	1.00800
24	1	0.128685	2.58341	-0.20703	-2.81134	1.00800
25	1	0.102388	2.80848	1.54129	-4.57645	1.00800
26	1	0.100596	2.51369	3.93801	-4.02304	1.00800
27	1	0.105440	1.98415	4.63912	-1.68614	1.00800
12	1	0.069823	-0.12368	-0.55671	2.28946	1.00800
10	1	0.087558	-0.61748	1.53619	0.05650	1.00800
9	1	0.066607	-0.62215	1.83270	1.79807	1.00800
15	1	0.092442	3.02916	0.16524	0.32985	1.00800
16	1	0.068366	1.74198	1.18847	2.00294	1.00800
44	1	0.136513	-4.50862	-1.01728	3.73508	1.00800
45	1	0.141187	-4.94956	-0.26039	-0.52660	1.00800
46	1	0.030697	-2.26445	-2.51529	4.63909	1.00800
47	1	0.031972	-3.34794	-1.17354	5.12002	1.00800
48	1	0.050925	-1.61554	-1.15147	5.61369	1.00800
49	1	0.028473	-6.77287	-0.36260	3.55176	1.00800
50	1	0.028798	-6.57033	-2.10538	3.18604	1.00800
51	1	0.051778	-7.94702	-1.19562	2.48128	1.00800
52	1	0.034781	-4.09735	0.15271	-2.07296	1.00800
53	1	0.030887	-2.98446	-1.22499	-2.34679	1.00800
54	1	0.054815	-2.50024	0.42691	-2.86361	1.00800
55	1	0.116082	-1.30496	-2.65661	-1.54224	1.00800
56	1	0.101915	-1.98336	-5.03461	-1.33234	1.00800
57	1	0.101454	-1.43873	-6.31684	0.72510	1.00800

58	1	0.100568	-0.19989	-5.22265	2.57988	1.00800
59	1	0.107133	0.49073	-2.85486	2.39740	1.00800

ATOMIC GRADIENTS

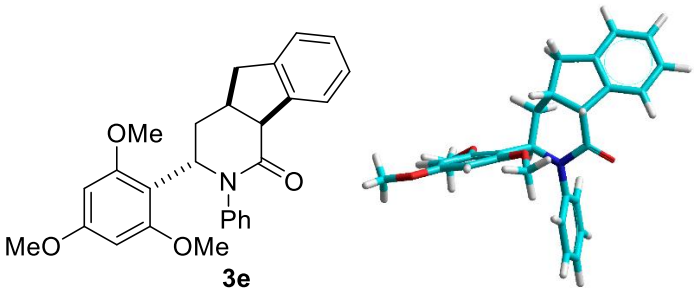
Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.02498	0.03440	-0.00287
2	6	0.00091	0.06291	-0.00125
3	7	0.00484	0.00481	0.00494
4	6	0.01469	-0.01172	-0.00506
5	6	-0.00508	-0.03814	0.08203
6	6	-0.00826	-0.01056	0.03916
7	8	0.01809	0.00310	-0.00884
8	6	0.04704	-0.03392	-0.00877
11	6	0.00206	-0.01691	0.00096
13	6	-0.00460	-0.02341	0.01195
14	6	-0.01562	-0.01057	0.10397
17	6	-0.01233	0.00542	0.00532
18	6	-0.03356	-0.03590	-0.02652
19	6	-0.04144	-0.01075	-0.01723
20	6	-0.05127	-0.00952	-0.01725
21	6	-0.03386	0.00644	-0.00916
28	6	-0.00021	0.03328	-0.00433
29	6	0.00072	0.00220	0.00097
30	6	-0.00245	0.02561	-0.04469
31	6	0.00032	-0.01259	0.00344
32	6	0.01290	0.03486	0.00214
33	8	-0.02165	0.00389	0.00212
34	6	-0.01796	0.01817	0.01312
35	8	0.00439	-0.01542	-0.01227
36	6	0.00660	-0.01466	-0.01301
37	8	0.01973	0.01784	0.01343
38	6	0.02694	0.01124	0.01380
39	6	0.00383	-0.01000	0.00509
40	6	0.02466	-0.02603	-0.00071
41	6	-0.02193	-0.00667	-0.00069
42	6	0.00925	-0.02539	-0.01341
43	6	-0.00286	-0.03481	0.01733
22	1	0.03102	0.00872	-0.01814
23	1	0.01214	-0.01801	0.02600
24	1	-0.01880	-0.09773	-0.02723
25	1	-0.03272	-0.03479	-0.06939
26	1	-0.04166	0.03814	-0.05589
27	1	-0.03702	0.07858	0.02596
12	1	0.02575	0.00124	-0.01927
10	1	0.01316	0.02528	0.03596
9	1	0.02676	-0.03657	0.00375
15	1	0.02784	0.01027	-0.00429
16	1	0.01187	-0.00624	-0.00288
44	1	-0.01629	0.01373	-0.02471
45	1	0.01970	-0.00463	-0.01039
46	1	-0.04070	0.01347	0.03878

47	1	-0.01325	0.01687	0.02975
48	1	-0.00047	0.04664	-0.02385
49	1	-0.00855	-0.02057	-0.01319
50	1	0.01088	-0.01194	-0.03256
51	1	-0.00124	-0.02228	0.01082
52	1	0.03266	0.01802	0.03388
53	1	0.01614	0.01005	0.00263
54	1	0.03569	0.01272	0.01134
55	1	0.03537	0.01432	-0.00806
56	1	0.01609	0.02063	-0.00850
57	1	-0.03272	0.03325	-0.01087
58	1	-0.02587	-0.00318	-0.02558
59	1	0.00537	-0.02319	0.00221

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-3.178	0.981	2.308	4.049
sp Hybrid	-0.330	-0.282	1.083	1.167
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-3.508	0.699	3.391	4.929

HyperChem log stop -- Thu Oct 01 04:07:10 2020.

Compound **3e**



3e

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 164
in which
Number of Alpha Electrons = 82
Number of Beta Electrons = 82
Charge on the System = 0
Total Orbitals = 155

Starting PM3 calculation with 155 orbitals
Energy=-6440.423192 kcal/mol Gradient=0.016234 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -114162.1131351 (kcal/mol)

Total Energy = -181.928885143 (a.u.)
Binding Energy = -6440.4231921 (kcal/mol)
Isolated Atomic Energy = -107721.6899430 (kcal/mol)
Electronic Energy = -1085630.3233886 (kcal/mol)
Core-Core Interaction = 971468.2102536 (kcal/mol)
Heat of Formation = -68.4031921 (kcal/mol)
Gradient = 0.0162341 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.113992	-0.09463	1.14304	0.72502	12.01100
2	6	0.035240	-0.35465	-0.29489	1.17947	12.01100
3	7	0.006878	0.31996	-1.28776	0.28985	14.00700
4	6	0.274505	1.24311	-0.87507	-0.71458	12.01100
5	6	-0.033092	1.97985	0.44756	-0.56932	12.01100
6	6	-0.074048	1.37324	1.43183	0.46410	12.01100
7	8	-0.380534	1.48468	-1.67507	-1.60874	15.99900
8	6	-0.045126	-0.44517	-2.51735	0.07394	12.01100
11	6	-0.182316	-0.03996	-0.48380	2.64965	12.01100
12	6	-0.082563	2.08713	1.25199	-1.83389	12.01100
13	6	-0.048896	1.54302	2.84471	-0.13607	12.01100
16	6	-0.090093	1.85411	2.61249	-1.57472	12.01100
17	6	-0.070567	2.41567	0.83008	-3.11249	12.01100
18	6	-0.108925	2.49361	1.78151	-4.13161	12.01100
19	6	-0.100739	2.25494	3.12607	-3.87367	12.01100
20	6	-0.094466	1.93343	3.55553	-2.58548	12.01100
27	6	-0.101647	-1.63532	-2.50970	-0.66102	12.01100
28	6	-0.098319	-2.34156	-3.69416	-0.83446	12.01100
29	6	-0.100218	-1.86824	-4.88039	-0.28292	12.01100
30	6	-0.101940	-0.68301	-4.88582	0.44402	12.01100
31	6	-0.076894	0.03419	-3.70805	0.62653	12.01100
38	6	0.149428	-1.05867	-0.20594	3.58870	12.01100
39	6	0.164981	1.19443	-0.91770	3.17628	12.01100
40	6	-0.261477	1.38702	-1.11418	4.54924	12.01100
41	6	0.162314	0.34145	-0.85088	5.43742	12.01100
42	6	-0.297591	-0.88569	-0.38427	4.96602	12.01100
43	8	-0.196719	-2.23735	0.31086	3.07658	15.99900
44	6	0.049056	-3.39570	0.14987	3.86095	12.01100
45	8	-0.186652	0.65228	-1.08262	6.76019	15.99900
46	6	0.050929	-0.35401	-0.85183	7.71542	12.01100
47	8	-0.193352	2.24920	-1.07859	2.29728	15.99900
48	6	0.045011	3.21350	-2.04751	2.64009	12.01100
33	1	0.102192	-3.27081	-3.69307	-1.41344	1.00800
34	1	0.101781	-2.42690	-5.81086	-0.42617	1.00800
35	1	0.101820	-0.30863	-5.82148	0.87190	1.00800
36	1	0.112504	0.97323	-3.71974	1.19400	1.00800
37	1	0.080016	-1.45589	-0.48622	1.05448	1.00800
22	1	0.063425	0.64075	3.47163	-0.00656	1.00800
23	1	0.131314	2.60343	-0.22923	-3.32364	1.00800

24	1	0.102506	2.74627	1.45987	-5.14733	1.00800
25	1	0.100373	2.31979	3.85687	-4.68621	1.00800
26	1	0.105020	1.74715	4.61332	-2.37662	1.00800
9	1	0.071777	-0.48242	1.84131	1.49356	1.00800
14	1	0.095264	3.01728	0.17682	-0.24775	1.00800
15	1	0.083216	1.93117	1.35475	1.42640	1.00800
10	1	0.062258	-0.68462	1.35057	-0.19228	1.00800
21	1	0.060656	2.37029	3.39292	0.35282	1.00800
32	1	0.108808	-2.01112	-1.58272	-1.10986	1.00800
49	1	0.140712	2.36249	-1.46811	4.91985	1.00800
50	1	0.136744	-1.71616	-0.14593	5.64864	1.00800
51	1	0.031154	-3.25315	0.47254	4.90308	1.00800
52	1	0.030576	-3.73766	-0.89056	3.84919	1.00800
53	1	0.052059	-4.11793	0.79539	3.35563	1.00800
54	1	0.028391	-1.22854	-1.49476	7.56240	1.00800
55	1	0.028758	-0.66854	0.19791	7.74341	1.00800
56	1	0.052116	0.14812	-1.11762	8.64964	1.00800
57	1	0.031034	2.81414	-3.05971	2.50713	1.00800
58	1	0.034457	3.58763	-1.93354	3.66850	1.00800
59	1	0.052890	4.01021	-1.85435	1.91752	1.00800

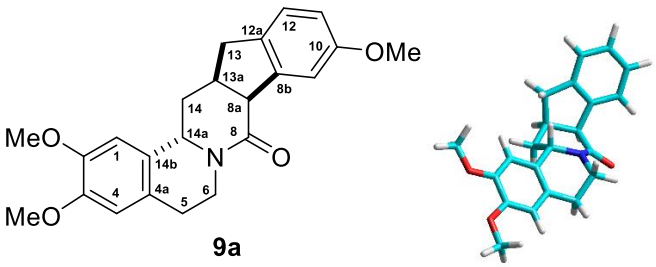
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	-0.00102	-0.00046	-0.00438
2	6	0.00438	0.00713	0.01801
3	7	-0.00353	0.01215	-0.01748
4	6	-0.00064	-0.03988	0.00092
5	6	0.00763	0.02517	-0.02493
6	6	0.01013	-0.01727	0.00804
7	8	-0.00051	0.01083	0.01389
8	6	-0.00055	-0.01553	-0.02160
11	6	0.01022	-0.00817	0.00850
12	6	0.00574	-0.01552	0.01916
13	6	0.00952	-0.03302	-0.04049
16	6	-0.02377	-0.01483	0.04226
17	6	-0.01781	-0.03655	0.00370
18	6	0.00979	-0.00980	-0.04269
19	6	-0.01773	0.02434	-0.02941
20	6	-0.00707	0.02290	0.00562
27	6	0.00912	0.00310	0.00108
28	6	0.00643	-0.01490	-0.02249
29	6	-0.00144	0.01001	0.00191
30	6	-0.00429	-0.01152	-0.02054
31	6	-0.01166	0.00949	0.00784
38	6	-0.00430	-0.00471	-0.02658
39	6	0.00969	-0.00476	-0.00290
40	6	0.01058	-0.00040	0.00694
41	6	0.00253	0.00777	-0.00078
42	6	0.01140	0.00008	0.00750
43	8	0.00317	-0.01209	-0.00454
44	6	0.00077	0.01988	0.01728

45	8	-0.00854	0.02073	0.00324
46	6	-0.01838	0.00044	0.00991
47	8	-0.00761	0.00350	0.01388
48	6	0.00770	-0.00329	0.00005
33	1	0.01273	0.00401	-0.01184
34	1	0.01136	0.00810	-0.01749
35	1	0.01093	0.00499	-0.01058
36	1	0.00835	0.00040	-0.00097
37	1	-0.00696	0.00878	-0.00339
22	1	-0.02962	-0.00536	0.01574
23	1	-0.01193	-0.01912	-0.00634
24	1	-0.01510	0.00940	0.01074
25	1	-0.00888	-0.00618	0.02360
26	1	-0.02456	0.00449	0.01295
9	1	-0.00765	0.00710	-0.02218
14	1	0.00969	-0.01712	0.00043
15	1	0.01326	-0.00880	0.02311
10	1	0.02080	-0.01311	-0.01885
21	1	0.00062	0.02019	0.02127
32	1	0.02928	0.00229	-0.03478
49	1	-0.00819	-0.00209	0.01060
50	1	-0.00982	-0.00364	0.00297
51	1	0.03647	0.06177	-0.00747
52	1	-0.00684	0.02958	0.06473
53	1	0.00348	0.00995	0.00177
54	1	-0.00674	-0.00804	0.00654
55	1	-0.03482	-0.01011	0.01908
56	1	-0.00730	-0.00669	0.00419
57	1	0.01157	-0.00586	0.00034
58	1	0.01326	-0.00273	-0.00365
59	1	0.00662	0.00295	-0.01143

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-1.630	0.789	4.123	4.504
sp Hybrid	-0.809	0.193	0.567	1.007
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-2.439	0.982	4.690	5.377

Compound **9a**



9a

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES
UHF Calculation:
Singlet state calculation
Number of electrons = 134
in which
Number of Alpha Electrons = 67
Number of Beta Electrons = 67
Charge on the System = 0
Total Orbitals = 127

Starting PM3 calculation with 127 orbitals
Energy=-5319.977913 kcal/mol Gradient=0.391836 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -92337.8710323 (kcal/mol)
Total Energy = -147.149745849 (a.u.)
Binding Energy = -5319.9779133 (kcal/mol)
Isolated Atomic Energy = -87017.8931190 (kcal/mol)
Electronic Energy = -773932.7546351 (kcal/mol)
Core-Core Interaction = 681594.8836028 (kcal/mol)
Heat of Formation = -70.3749133 (kcal/mol)
Gradient = 0.3918358 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1
NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.119337	-1.61400	-0.29400	0.45300	12.01100
2	6	0.012680	-0.16600	-0.77900	0.60600	12.01100
3	7	-0.056809	0.68200	-0.31600	-0.54200	14.00700
4	6	0.269550	0.15900	0.70700	-1.39400	12.01100
5	6	-0.040598	-0.80900	1.74000	-0.82500	12.01100
6	6	-0.075361	-1.66600	1.22000	0.35500	12.01100
7	8	-0.378096	0.56900	0.78700	-2.54400	15.99900
8	6	-0.063661	1.61100	-1.32800	-1.10400	12.01100
10	6	-0.091176	-0.16900	-2.27000	0.82700	12.01100
13	6	-0.087890	-0.05800	2.90800	-0.25600	12.01100
15	6	-0.055040	-1.13700	1.91700	1.62900	12.01100
16	6	-0.072033	0.91900	-2.65500	-1.38400	12.01100
19	6	-0.061181	0.30000	-3.16700	-0.12800	12.01100
20	6	-0.154345	-0.68100	-2.75100	2.04000	12.01100
21	6	0.058406	-0.76000	-4.12000	2.27800	12.01100
22	6	0.067174	-0.31000	-5.03400	1.28600	12.01100
23	6	-0.157625	0.22600	-4.54600	0.09700	12.01100
27	8	-0.166347	-1.24700	-4.69900	3.43300	15.99900
28	8	-0.166682	-0.44300	-6.36900	1.60900	15.99900
30	6	-0.082516	-0.26200	3.01500	1.12800	12.01100
33	6	-0.090277	0.32100	4.04200	1.85200	12.01100
34	6	-0.096711	1.11500	4.96700	1.17300	12.01100
35	6	-0.105275	1.31700	4.86100	-0.19900	12.01100
36	6	-0.069663	0.72900	3.82700	-0.93000	12.01100
42	6	0.046991	-1.78800	-3.84200	4.40700	12.01100

43	6	0.046975	-0.00200	-7.31000	0.66200	12.01100
18	1	0.060814	2.41600	-1.46100	-0.35400	1.00800
9	1	0.067548	-2.21000	-0.63500	1.32300	1.00800
29	1	0.121102	0.60000	-5.22700	-0.67800	1.00800
14	1	0.072177	-2.72600	1.52700	0.18800	1.00800
31	1	0.068165	-0.54200	1.20900	2.24800	1.00800
32	1	0.063199	-1.95400	2.29300	2.26900	1.00800
11	1	0.082248	0.27400	-0.27800	1.51500	1.00800
12	1	0.096603	-1.46800	2.08600	-1.65600	1.00800
17	1	0.088770	2.09600	-0.93800	-2.02100	1.00800
24	1	0.064561	1.65500	-3.38000	-1.78500	1.00800
37	1	0.106214	0.16000	4.12600	2.93100	1.00800
38	1	0.101877	1.58400	5.78600	1.72900	1.00800
39	1	0.104000	1.94400	5.59600	-0.71500	1.00800
40	1	0.120149	0.88800	3.73900	-2.01100	1.00800
41	1	0.068306	-2.09100	-0.75200	-0.43600	1.00800
25	1	0.069507	0.14300	-2.55000	-2.16800	1.00800
26	1	0.119107	-1.01600	-2.02900	2.79600	1.00800
44	1	0.026108	-2.64000	-3.26300	4.03100	1.00800
45	1	0.026440	-1.03800	-3.16100	4.82800	1.00800
46	1	0.053458	-2.12300	-4.54800	5.17100	1.00800
47	1	0.027797	1.07400	-7.23200	0.46500	1.00800
48	1	0.027609	-0.55500	-7.24500	-0.28200	1.00800
49	1	0.053088	-0.22400	-8.25700	1.16200	1.00800

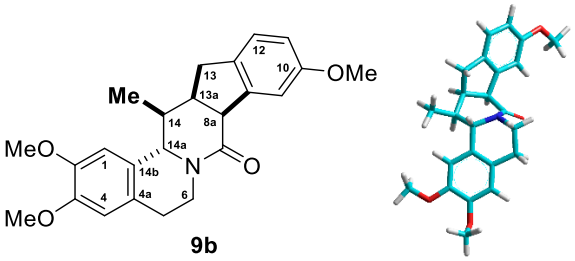
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	-0.43962	-0.49817	-0.30956
2	6	-0.18334	0.28361	0.42084
3	7	-0.18982	0.19632	0.01647
4	6	0.07443	0.09758	-0.14234
5	6	-0.51527	0.22638	-0.65861
6	6	0.90237	-0.00037	0.57186
7	8	-0.16500	0.02455	0.34238
8	6	0.78993	-0.19680	0.35584
10	6	0.76964	-0.71132	-1.32095
13	6	0.17620	-0.24042	-0.23341
15	6	0.24538	-0.04563	-0.06201
16	6	-0.70530	-0.09181	-0.35335
19	6	-0.38774	1.47579	0.64408
20	6	-0.53208	0.30125	0.82353
21	6	0.25125	-0.69247	0.10020
22	6	-0.83994	-0.07643	1.38034
23	6	0.57718	-0.46275	-0.98005
27	8	0.19611	0.10154	-0.58825
28	8	0.12570	0.15725	-0.12995
30	6	-0.22251	0.14251	-0.13759
33	6	0.55489	0.46395	0.06928
34	6	-0.61863	-0.59650	0.47591
35	6	0.10065	0.08868	-0.35684
36	6	-0.38065	-0.31319	0.70217

42	6	-0.44343	-0.62250	0.56350
43	6	-0.33298	-0.26991	-0.33787
18	1	-0.29547	0.09542	-0.26757
9	1	0.25422	0.11407	-0.16842
29	1	0.00884	-0.03727	-0.01316
14	1	-0.59465	0.14287	-0.18777
31	1	-0.10262	0.08002	-0.12964
32	1	0.02928	0.01686	-0.02192
11	1	0.05181	0.01778	-0.13736
12	1	0.38127	-0.18323	0.40675
17	1	-0.02813	0.03531	-0.03047
24	1	0.07511	-0.00079	-0.08466
37	1	-0.01580	0.01622	-0.03563
38	1	0.13065	0.22491	0.13046
39	1	0.11971	0.12755	-0.13027
40	1	0.04521	-0.02243	-0.50449
41	1	0.08060	0.11800	0.24285
25	1	0.43963	-0.10390	0.32833
26	1	0.07344	-0.13080	-0.14546
44	1	-0.11784	0.06780	-0.08507
45	1	0.27553	0.31794	0.10109
46	1	0.07347	0.30329	-0.37482
47	1	0.22977	0.12981	-0.02363
48	1	0.13829	0.02971	0.21960
49	1	-0.05975	-0.10027	0.05566

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-0.752	-0.549	2.300	2.481
sp Hybrid	-0.452	-0.144	-0.209	0.519
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.203	-0.693	2.090	2.510

Compound **9b**



9b

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 152
in which

Number of Alpha Electrons = 76
Number of Beta Electrons = 76
Charge on the System = 0
Total Orbitals = 143
Starting PM3 calculation with 143 orbitals

Energy=-5968.619459 kcal/mol Gradient=0.029129 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -105995.0843120 (kcal/mol)
Total Energy = -168.913897877 (a.u.)
Binding Energy = -5968.6194590 (kcal/mol)
Isolated Atomic Energy = -100026.4648530 (kcal/mol)
Electronic Energy = -940514.2553124 (kcal/mol)
Core-Core Interaction = 834519.1710003 (kcal/mol)
Heat of Formation = -109.2694590 (kcal/mol)
Gradient = 0.0291287 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.074375	-1.31514	-0.19676	1.39760	12.01100
2	6	0.020600	0.06748	-0.89329	1.37535	12.01100
3	7	-0.074136	1.04521	-0.18259	0.49275	14.00700
4	6	0.277889	0.53054	0.48234	-0.67910	12.01100
5	6	-0.042591	-0.63064	1.43962	-0.46121	12.01100
6	6	-0.069687	-1.32116	1.25100	0.90873	12.01100
7	8	-0.357095	1.08813	0.35076	-1.75597	15.99900
8	6	-0.059857	2.32932	-0.91580	0.37138	12.01100
9	6	-0.124613	-1.92181	-0.24271	2.79706	12.01100
10	6	-0.073083	-0.02566	-2.37365	1.03731	12.01100
13	6	-0.055309	-0.09804	2.84521	-0.39230	12.01100
15	6	-0.041477	-0.67333	2.28911	1.85378	12.01100
16	6	-0.079126	2.15743	-2.28967	-0.25369	12.01100
19	6	-0.083801	0.96975	-3.01306	0.28910	12.01100
20	6	-0.185883	-1.09144	-3.13308	1.53079	12.01100
21	6	0.073600	-1.19609	-4.49761	1.25919	12.01100
22	6	0.028009	-0.20098	-5.12790	0.47890	12.01100
23	6	-0.093378	0.87510	-4.38021	0.01069	12.01100
27	8	-0.174398	-2.20323	-5.31952	1.72298	15.99900
28	8	-0.193644	-0.32293	-6.45436	0.07625	15.99900
30	6	-0.117423	-0.12329	3.32081	0.92640	12.01100
33	6	-0.055468	0.31953	4.59971	1.22494	12.01100
34	6	-0.138361	0.78983	5.40757	0.19303	12.01100
35	6	0.085569	0.80920	4.92415	-1.12485	12.01100
36	6	-0.145884	0.36206	3.63002	-1.43569	12.01100
39	8	-0.190322	1.29202	5.83504	-2.04481	15.99900
42	6	0.048393	-3.31575	-4.70393	2.32345	12.01100
43	6	0.055252	0.24369	-7.37254	0.98558	12.01100
50	6	0.049349	1.39316	5.41314	-3.38233	12.01100

11	1	0.079369	0.52233	-0.82728	2.39852	1.00800
31	1	0.070217	0.13723	1.84675	2.46507	1.00800
32	1	0.058871	-1.40576	2.71173	2.56539	1.00800
17	1	0.077409	3.04016	-0.30036	-0.21413	1.00800
18	1	0.057907	2.74757	-0.99246	1.39543	1.00800
24	1	0.064207	3.07483	-2.88913	-0.08715	1.00800
25	1	0.081509	2.04845	-2.20738	-1.35549	1.00800
37	1	0.105502	0.29838	4.96968	2.25476	1.00800
38	1	0.119516	1.14370	6.42169	0.41213	1.00800
26	1	0.131571	-1.85589	-2.64614	2.15577	1.00800
40	1	0.131241	0.37913	3.23107	-2.45649	1.00800
41	1	0.074776	-1.98679	-0.76348	0.70233	1.00800
14	1	0.069166	-2.39446	1.54144	0.78533	1.00800
12	1	0.094940	-1.35703	1.32396	-1.29886	1.00800
44	1	0.024240	-3.05652	-4.19854	3.26175	1.00800
45	1	0.053269	-3.96777	-5.55779	2.52709	1.00800
46	1	0.029831	-3.81801	-3.99743	1.65257	1.00800
47	1	0.029389	-0.24957	-7.34518	1.96339	1.00800
48	1	0.019567	1.31966	-7.20824	1.11383	1.00800
49	1	0.045813	0.06357	-8.33423	0.49886	1.00800
29	1	0.119784	1.65425	-4.86630	-0.59066	1.00800
51	1	0.050914	-1.28652	0.26222	3.53844	1.00800
52	1	0.046415	-2.06973	-1.27657	3.14636	1.00800
53	1	0.046048	-2.90317	0.25018	2.81752	1.00800
54	1	0.027606	0.41565	5.17291	-3.81654	1.00800
55	1	0.032959	2.06921	4.55844	-3.50107	1.00800
56	1	0.049214	1.81345	6.29548	-3.87254	1.00800

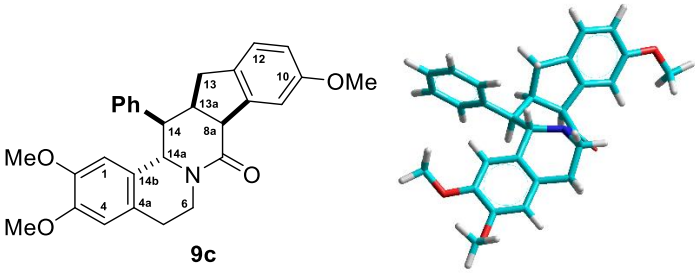
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.01200	-0.00899	0.00578
2	6	0.00353	-0.00319	0.00186
3	7	0.00481	-0.02344	0.01378
4	6	0.06650	-0.00663	-0.10349
5	6	0.01311	0.01109	0.00610
6	6	-0.00247	0.02283	-0.01438
7	8	-0.04938	0.01281	0.10251
8	6	-0.00392	0.01038	-0.00874
9	6	-0.00701	-0.00567	0.00671
10	6	0.05400	0.00613	-0.01748
13	6	-0.03317	-0.03574	0.14425
15	6	0.01064	0.00787	-0.01983
16	6	0.01501	0.00770	-0.00067
19	6	-0.03684	-0.04777	0.00206
20	6	-0.01191	-0.07536	-0.01537
21	6	0.01425	0.04885	-0.00059
22	6	-0.00137	0.05467	0.02110
23	6	-0.00897	0.03890	0.02449
27	8	0.04716	-0.01152	-0.02606
28	8	-0.00366	-0.02376	-0.02498
30	6	-0.01324	-0.08124	-0.06053

33	6	0.00193	0.03472	0.04324
34	6	0.00258	0.00475	-0.06871
35	6	0.01714	0.07712	0.07696
36	6	0.01221	-0.02677	-0.14657
39	8	-0.00971	-0.01679	-0.01623
42	6	-0.03045	0.04220	0.00845
43	6	-0.00940	0.00785	0.01732
50	6	-0.00967	0.01652	0.00920
11	1	0.00119	0.00094	0.00176
31	1	0.00603	0.00043	0.00243
32	1	-0.00431	0.00064	0.00646
17	1	0.00541	0.00032	0.00698
18	1	0.00333	-0.00053	0.01474
24	1	-0.00475	0.00529	0.00473
25	1	0.00831	-0.00402	0.01791
37	1	0.00144	-0.00313	-0.01103
38	1	-0.00362	-0.00216	-0.00369
26	1	-0.00208	0.00070	0.00585
40	1	0.00217	0.01147	0.04036
41	1	0.00031	-0.00037	0.00191
14	1	0.00686	-0.00164	0.00259
12	1	-0.00213	-0.00550	-0.00224
44	1	-0.00337	-0.00741	-0.01694
45	1	-0.01091	-0.00465	-0.00801
46	1	0.00295	-0.00458	0.00422
47	1	-0.01318	-0.00756	-0.00910
48	1	-0.01505	-0.01176	0.00776
49	1	-0.00746	-0.00711	-0.01010
29	1	0.00130	0.00316	-0.00500
51	1	0.00779	0.00363	0.00194
52	1	0.00766	0.00250	-0.00105
53	1	0.00187	0.00157	0.00392
54	1	-0.01568	-0.00443	-0.00583
55	1	-0.00649	-0.00148	-0.00306
56	1	-0.01133	-0.00185	-0.00767

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-1.015	0.358	2.951	3.142
sp Hybrid	-0.347	-0.692	-0.020	0.774
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.362	-0.334	2.932	3.250

Compound **9c**



9c

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 174
in which
Number of Alpha Electrons = 87
Number of Beta Electrons = 87
Charge on the System = 0
Total Orbitals = 165

Starting PM3 calculation with 165 orbitals

Energy=-6892.493836 kcal/mol Gradient=0.665784 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -120347.2867453 (kcal/mol)
Total Energy = -191.785585483 (a.u.)
Binding Energy = -6892.4938363 (kcal/mol)
Isolated Atomic Energy = -113454.7929090 (kcal/mol)
Electronic Energy = -1172347.0606393 (kcal/mol)
Core-Core Interaction = 1051999.7738940 (kcal/mol)
Heat of Formation = -74.4898363 (kcal/mol)
Gradient = 0.6657837 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	-0.030316	-1.53243	-0.22745	1.07444	12.01100
2	6	0.016683	-0.14199	-0.90684	1.13385	12.01100
3	7	-0.072434	0.84068	-0.25477	0.20962	14.00700
4	6	0.275795	0.33271	0.47966	-0.92155	12.01100
5	6	-0.043388	-0.75218	1.50763	-0.64469	12.01100
6	6	-0.069220	-1.50469	1.25368	0.68054	12.01100
7	8	-0.358952	0.84760	0.34747	-2.02008	15.99900
8	6	-0.059761	2.06856	-1.06421	0.01094	12.01100
9	6	-0.078519	-2.30493	-0.33535	2.36800	12.01100
10	6	-0.073136	-0.24108	-2.40827	0.91626	12.01100
13	6	-0.055071	-0.11433	2.85466	-0.44422	12.01100
15	6	-0.043123	-0.88609	2.21462	1.72052	12.01100
16	6	-0.079228	1.76792	-2.41155	-0.62273	12.01100
19	6	-0.086729	0.65246	-3.10095	0.08742	12.01100
20	6	-0.186043	-1.21633	-3.13215	1.61310	12.01100
21	6	0.075184	-1.33888	-4.51560	1.46066	12.01100
22	6	0.025755	-0.46360	-5.19790	0.58185	12.01100
23	6	-0.093022	0.52811	-4.48383	-0.08790	12.01100
27	8	-0.173255	-2.26959	-5.30380	2.10386	15.99900
28	8	-0.193217	-0.62969	-6.54750	0.28897	15.99900

30	6	-0.115951	-0.19217	3.24777	0.89978	12.01100
33	6	-0.055665	0.33301	4.46324	1.31376	12.01100
34	6	-0.137990	0.93932	5.29084	0.37191	12.01100
35	6	0.085331	1.00997	4.89083	-0.97354	12.01100
36	6	-0.147699	0.48026	3.66190	-1.40047	12.01100
39	8	-0.190035	1.63068	5.81205	-1.79466	15.99900
42	6	0.044139	-3.08534	-4.68887	3.07049	12.01100
43	6	0.055216	0.05413	-7.40397	1.17775	12.01100
50	6	0.049246	1.77917	5.47376	-3.15133	12.01100
54	6	-0.103921	-3.70092	-0.39701	2.31275	12.01100
55	6	-0.097933	-4.44725	-0.45838	3.48371	12.01100
56	6	-0.103770	-3.80998	-0.45832	4.72035	12.01100
57	6	-0.095206	-2.42197	-0.39932	4.78293	12.01100
58	6	-0.110945	-1.67319	-0.33859	3.61343	12.01100
24	1	0.064837	2.67967	-3.04156	-0.60748	1.00800
25	1	0.081709	1.50063	-2.29639	-1.69394	1.00800
37	1	0.105880	0.27064	4.76741	2.36323	1.00800
38	1	0.119577	1.36002	6.25444	0.68193	1.00800
26	1	0.137604	-1.89149	-2.59486	2.29487	1.00800
40	1	0.131634	0.53418	3.32885	-2.44349	1.00800
41	1	0.081004	-2.11784	-0.76281	0.28145	1.00800
14	1	0.072933	-2.57027	1.56049	0.53218	1.00800
12	1	0.095478	-1.45838	1.52832	-1.50761	1.00800
44	1	0.029137	-2.50554	-4.25645	3.89442	1.00800
45	1	0.052020	-3.68234	-5.53023	3.43317	1.00800
46	1	0.031431	-3.74065	-3.92265	2.63943	1.00800
47	1	0.028927	-0.30283	-7.30365	2.20865	1.00800
48	1	0.019242	1.13737	-7.23994	1.14839	1.00800
49	1	0.045607	-0.18859	-8.39618	0.78944	1.00800
29	1	0.119547	1.21809	-5.01032	-0.75965	1.00800
51	1	0.027966	0.81386	5.35280	-3.65650	1.00800
52	1	0.032616	2.38503	4.57127	-3.29288	1.00800
53	1	0.049296	2.30436	6.34530	-3.55144	1.00800
11	1	0.084042	0.29546	-0.75264	2.16115	1.00800
31	1	0.068729	-0.16799	1.69847	2.38755	1.00800
32	1	0.064050	-1.65632	2.65594	2.37906	1.00800
17	1	0.078326	2.78773	-0.48673	-0.60235	1.00800
18	1	0.058454	2.53181	-1.18813	1.01046	1.00800
59	1	0.110435	-4.20994	-0.39278	1.34133	1.00800
60	1	0.106183	-5.54008	-0.50476	3.43070	1.00800
61	1	0.106246	-4.39996	-0.50403	5.64150	1.00800
62	1	0.106193	-1.91571	-0.39933	5.75387	1.00800
63	1	0.118075	-0.57295	-0.30317	3.65438	1.00800

ATOMIC GRADIENTS

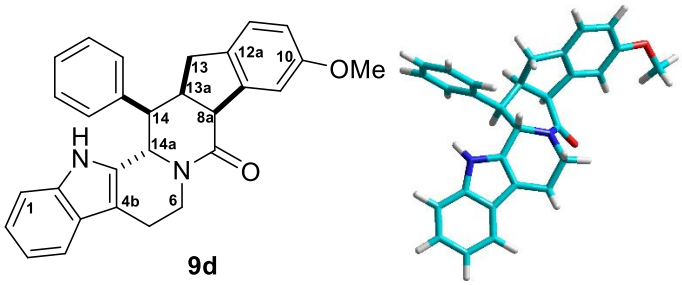
Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.00403	-0.01707	0.02432
2	6	-0.03200	-0.02543	-0.09145
3	7	-0.00933	-0.00967	-0.01057
4	6	0.03848	0.02825	-0.04668
5	6	0.01335	0.01962	0.03729

6	6	0.01254	0.03267	-0.05817
7	8	-0.01892	-0.00096	0.04873
8	6	-0.00608	-0.00187	-0.02642
9	6	0.11432	-0.01425	-0.10292
10	6	-0.64784	3.48331	0.97996
13	6	-0.51710	-1.37711	-0.82568
15	6	0.01578	0.04159	-0.10671
16	6	-0.08358	-0.08188	0.20435
19	6	2.81945	0.87284	-2.07718
20	6	-1.46858	1.63566	1.60198
21	6	-2.49509	-1.58257	1.90109
22	6	-0.24578	-3.42801	-0.43431
23	6	1.98704	-1.10561	-1.90072
27	8	0.21671	0.10702	-0.16152
28	8	-0.01929	0.21879	-0.01714
30	6	-0.71027	-0.95506	1.31757
33	6	0.00701	0.57853	1.47207
34	6	0.51161	1.31264	0.80895
35	6	0.69783	0.82148	-1.42182
36	6	0.00996	-0.51113	-1.31351
39	8	-0.03426	-0.01608	0.10149
42	6	0.05483	0.00231	0.00563
43	6	-0.00476	0.08010	0.03998
50	6	-0.02834	-0.02819	0.05256
54	6	-0.09245	0.01844	-0.16368
55	6	-0.14328	-0.01304	-0.01933
56	6	-0.02334	0.00190	0.08465
57	6	0.01763	-0.01273	0.02840
58	6	0.06208	0.03105	0.01657
24	1	-0.03711	-0.03343	-0.01244
25	1	-0.09164	-0.05716	-0.01318
37	1	0.01929	-0.00786	0.01649
38	1	0.02224	0.02347	0.00795
26	1	-0.01948	0.03085	0.08706
40	1	0.00912	-0.00602	-0.03130
41	1	0.00280	-0.00224	-0.03153
14	1	-0.00811	-0.00310	-0.01729
12	1	0.01801	0.03148	-0.00665
44	1	0.04433	-0.02952	0.01772
45	1	0.04765	-0.00734	0.04430
46	1	0.01770	-0.02159	0.06544
47	1	0.00504	-0.00370	0.02213
48	1	-0.00947	0.00614	-0.00341
49	1	-0.01715	0.00249	-0.00449
29	1	-0.00478	-0.00775	-0.03039
51	1	-0.00370	0.01635	0.03776
52	1	-0.01633	0.01241	0.02241
53	1	0.00197	0.01667	-0.00030
11	1	0.01296	-0.03189	0.01365
31	1	0.01099	0.00035	-0.01774
32	1	0.00038	0.01872	0.00516
17	1	-0.00253	-0.01301	-0.01965

18	1	0.01252	-0.02615	-0.01321
59	1	0.00610	0.00454	-0.01523
60	1	0.00005	-0.00373	-0.03254
61	1	-0.02040	-0.01966	-0.02829
62	1	-0.01088	0.00559	0.00068
63	1	0.00804	-0.00042	-0.01093

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-0.774	0.517	3.263	3.393
sp Hybrid	-0.341	-0.586	-0.035	0.679
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.116	-0.069	3.228	3.416

Compound **9d**



9d

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 164
in which
Number of Alpha Electrons = 82
Number of Beta Electrons = 82
Charge on the System = 0
Total Orbitals = 158

Starting PM3 calculation with 158 orbitals

Energy=-6641.143364 kcal/mol Gradient=0.037641 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -109481.2116436 (kcal/mol)
Total Energy = -174.469394718 (a.u.)
Binding Energy = -6641.1433636 (kcal/mol)
Isolated Atomic Energy = -102840.0682800 (kcal/mol)
Electronic Energy = -1061475.7009313 (kcal/mol)
Core-Core Interaction = 951994.4892877 (kcal/mol)
Heat of Formation = 14.4366364 (kcal/mol)
Gradient = 0.0376407 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.038514	-1.71856	1.90656	0.50502	12.01100
2	6	0.051238	-1.27018	0.43538	0.64263	12.01100
3	7	-0.067610	-0.48230	-0.04887	-0.54179	14.00700
4	6	0.273318	-0.54250	0.72322	-1.75308	12.01100
5	6	-0.044584	-0.38169	2.23354	-1.63762	12.01100
6	6	-0.067398	-0.71035	2.78948	-0.23158	12.01100
7	8	-0.361273	-0.60694	0.15666	-2.83263	15.99900
8	6	-0.094500	-2.04780	2.53223	1.83686	12.01100
10	6	-0.253852	-2.45126	-0.45799	0.87236	12.01100
13	6	-0.052109	1.06192	2.59977	-1.83824	12.01100
15	6	-0.042155	0.64449	3.01533	0.47459	12.01100
16	6	-0.056834	-0.39779	-1.53274	-0.65100	12.01100
17	6	-0.117874	-2.67734	-1.66180	0.23025	12.01100
18	6	-0.043365	-1.75438	-2.22501	-0.77281	12.01100
19	6	-0.107721	-1.34724	2.20390	2.99912	12.01100
20	6	-0.092934	-1.65402	2.82396	4.20460	12.01100
21	6	-0.098620	-2.66354	3.77896	4.26024	12.01100
22	6	-0.097044	-3.36645	4.11101	3.10668	12.01100
23	6	-0.103890	-3.06176	3.49206	1.89991	12.01100
33	6	-0.115941	1.63790	3.04138	-0.63794	12.01100
34	6	-0.056781	2.96359	3.44302	-0.59369	12.01100
35	6	-0.148660	1.79212	2.55945	-3.01191	12.01100
36	6	0.081888	3.13490	2.96725	-2.95848	12.01100
37	6	-0.134614	3.72131	3.40402	-1.76236	12.01100
42	8	-0.192362	3.96293	3.02516	-4.06513	15.99900
44	7	0.280993	-3.46590	-0.25763	1.84451	14.00700
45	6	-0.072173	-3.90880	-2.21182	0.72976	12.01100
46	6	-0.161202	-4.40989	-1.30057	1.69913	12.01100
47	6	-0.101118	-5.61567	-1.53669	2.37417	12.01100
48	6	-0.087081	-6.29905	-2.69495	2.06277	12.01100
49	6	-0.128695	-5.80593	-3.60886	1.11136	12.01100
50	6	-0.046695	-4.61899	-3.38359	0.44334	12.01100
56	6	0.044376	3.55227	2.29121	-5.19493	12.01100
9	1	0.078076	-2.65295	1.91339	-0.11649	1.00800
14	1	0.073426	-1.19341	3.78975	-0.36018	1.00800
11	1	0.085761	-0.57172	0.33903	1.52260	1.00800
24	1	0.057680	0.12995	-1.87281	0.26277	1.00800
38	1	0.067556	0.88297	2.20568	1.19171	1.00800
39	1	0.063903	0.65041	3.95425	1.05761	1.00800
40	1	0.105898	3.40873	3.78793	0.34485	1.00800
41	1	0.134544	1.34539	2.22049	-3.95862	1.00800
25	1	0.077944	0.25321	-1.79124	-1.50869	1.00800
43	1	0.119704	4.77060	3.72030	-1.74584	1.00800
26	1	0.073700	-2.18229	-2.09747	-1.78791	1.00800
27	1	0.063821	-1.64122	-3.31682	-0.62578	1.00800
28	1	0.118962	-0.55431	1.44066	2.94670	1.00800
29	1	0.107645	-1.09801	2.55898	5.11006	1.00800
30	1	0.107142	-2.90417	4.26885	5.20943	1.00800

31	1	0.106922	-4.16090	4.86370	3.14703	1.00800
32	1	0.109958	-3.61416	3.76473	0.99259	1.00800
51	1	0.077867	-3.68631	0.63630	2.20909	1.00800
52	1	0.106701	-5.99788	-0.82885	3.11571	1.00800
53	1	0.099262	-7.24742	-2.91501	2.56419	1.00800
54	1	0.101785	-6.38333	-4.51555	0.90289	1.00800
55	1	0.105753	-4.22978	-4.09325	-0.29331	1.00800
12	1	0.095444	-1.02148	2.71784	-2.41256	1.00800
57	1	0.036327	2.47721	2.39057	-5.40806	1.00800
58	1	0.029390	3.79741	1.23068	-5.07310	1.00800
59	1	0.048615	4.14536	2.72784	-6.00182	1.00800

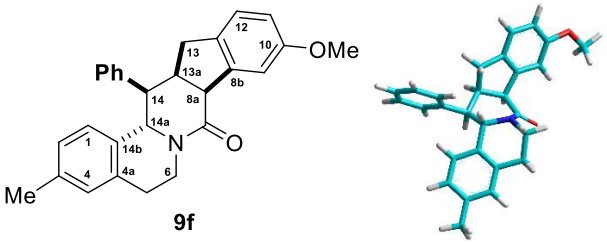
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.04107	0.04824	-0.02020
2	6	-0.05143	-0.01667	-0.03406
3	7	0.05887	0.01039	0.04250
4	6	-0.02991	0.02096	0.02385
5	6	0.00775	-0.02807	0.01655
6	6	0.02334	-0.00192	0.01917
7	8	0.02085	-0.04280	-0.01993
8	6	-0.03944	0.00970	0.02767
10	6	0.08591	0.16124	0.06068
13	6	0.01855	0.00544	-0.01093
15	6	0.01362	-0.01524	0.00659
16	6	-0.03188	-0.02904	0.01526
17	6	-0.03621	-0.18384	-0.10411
18	6	-0.01333	-0.02624	0.00266
19	6	-0.00780	0.00513	-0.03363
20	6	-0.01718	0.03140	0.02818
21	6	-0.01700	0.02314	-0.00684
22	6	0.00563	0.00055	-0.01042
23	6	0.03991	-0.01383	0.00582
33	6	-0.05797	-0.02729	0.03806
34	6	-0.00785	-0.00676	0.03816
35	6	-0.00554	0.00475	0.03260
36	6	-0.00811	-0.00996	-0.01033
37	6	-0.00226	0.00900	-0.02826
42	8	0.02432	0.03342	-0.02616
44	7	-0.01541	0.04173	0.04075
45	6	0.06225	0.03027	-0.03015
46	6	-0.03891	0.00130	0.00571
47	6	0.06021	0.15958	0.04543
48	6	-0.09508	-0.10996	-0.01414
49	6	-0.08983	0.01136	0.03874
50	6	0.08233	-0.07627	-0.10348
56	6	-0.00668	0.02782	-0.02375
9	1	-0.00677	0.00043	-0.00717
14	1	0.02113	-0.02895	0.00009
11	1	0.00326	-0.02371	0.03302
24	1	0.01299	-0.01246	0.03376

38	1	-0.00130	0.00514	-0.01779
39	1	0.01383	-0.03968	-0.01151
40	1	0.00631	-0.00704	-0.00813
41	1	-0.01063	-0.00098	-0.02402
25	1	0.00971	-0.01508	-0.00059
43	1	0.03606	0.00888	-0.01054
26	1	0.01033	0.00271	0.03328
27	1	-0.00705	-0.00190	0.01834
28	1	0.01069	-0.01370	0.00194
29	1	-0.00591	0.00605	0.00082
30	1	0.00218	-0.00432	-0.03391
31	1	0.01677	-0.01059	-0.01276
32	1	0.00816	-0.01463	-0.00576
51	1	-0.00828	0.02220	0.00184
52	1	-0.01782	0.00014	0.00908
53	1	-0.02784	-0.00705	0.00118
54	1	-0.01968	-0.01714	-0.02342
55	1	0.00936	0.01685	0.04205
12	1	0.00640	-0.02605	0.00858
57	1	-0.01511	0.03830	-0.01380
58	1	-0.00422	0.03342	-0.02970
59	1	-0.01537	0.04165	0.00315

Dipole (Debyes)	x	y	z	Total
Point-Chg.	0.024	1.791	2.906	3.413
sp Hybrid	-1.203	0.105	-0.254	1.234
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.179	1.895	2.652	3.466

Compound **9f**



9f

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 156
in which
Number of Alpha Electrons = 78
Number of Beta Electrons = 78
Charge on the System = 0
Total Orbitals = 151

Starting PM3 calculation with 151 orbitals
Energy=-6435.624497 kcal/mol Gradient=0.431782 Symmetry=C1

ENERGIES AND GRADIENT

Total Energy	= -103377.3577462 (kcal/mol)
Total Energy	= -164.742285574 (a.u.)
Binding Energy	= -6435.6244972 (kcal/mol)
Isolated Atomic Energy	= -96941.7332490 (kcal/mol)
Electronic Energy	= -982463.9520988 (kcal/mol)
Core-Core Interaction	= 879086.5943526 (kcal/mol)
Heat of Formation	= -11.8324972 (kcal/mol)
Gradient	= 0.4317825 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1
NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.030388	-1.53971	-0.19101	1.08981	12.01100
2	6	0.019257	-0.15325	-0.87809	1.13931	12.01100
3	7	-0.072866	0.83348	-0.22044	0.22423	14.00700
4	6	0.276437	0.32816	0.50715	-0.91152	12.01100
5	6	-0.043648	-0.75857	1.53477	-0.63839	12.01100
6	6	-0.068298	-1.50853	1.28823	0.69054	12.01100
7	8	-0.361128	0.84504	0.37063	-2.00878	15.99900
8	6	-0.058940	2.07121	-1.01864	0.04421	12.01100
9	6	-0.078127	-2.30121	-0.29844	2.39006	12.01100
10	6	-0.110878	-0.25855	-2.37425	0.90169	12.01100
13	6	-0.055158	-0.12134	2.88340	-0.44647	12.01100
15	6	-0.043293	-0.88508	2.25278	1.72404	12.01100
16	6	-0.084013	1.79664	-2.37786	-0.57581	12.01100
19	6	-0.054706	0.66652	-3.06992	0.10894	12.01100
20	6	-0.101960	-1.26634	-3.10676	1.53762	12.01100
21	6	-0.106329	-1.37600	-4.48122	1.37513	12.01100
22	6	-0.065945	-0.46773	-5.16688	0.56765	12.01100
23	6	-0.109373	0.55178	-4.45210	-0.05787	12.01100
28	6	-0.115073	-0.19574	3.28325	0.89574	12.01100
31	6	-0.056046	0.32821	4.50211	1.30132	12.01100
32	6	-0.138063	0.93223	5.32483	0.35375	12.01100
33	6	0.084711	1.00164	4.91684	-0.98936	12.01100
34	6	-0.147874	0.47089	3.68580	-1.40840	12.01100
37	8	-0.190259	1.62043	5.83372	-1.81705	15.99900
40	6	0.049246	1.78800	5.47795	-3.16701	12.01100
44	6	-0.103692	-3.69760	-0.35653	2.34696	12.01100
45	6	-0.096810	-4.43401	-0.42164	3.52391	12.01100
46	6	-0.102323	-3.78624	-0.42888	4.75484	12.01100
47	6	-0.093935	-2.39770	-0.37310	4.80549	12.01100
48	6	-0.108575	-1.65910	-0.30857	3.62988	12.01100
55	6	-0.064950	-0.57118	-6.63563	0.37560	12.01100
11	1	0.084321	0.28655	-0.73968	2.16769	1.00800
17	1	0.077421	2.78867	-0.43954	-0.56949	1.00800
18	1	0.058711	2.52679	-1.12487	1.04929	1.00800
35	1	0.105934	0.26698	4.81262	2.34902	1.00800

36	1	0.119364	1.35226	6.29068	0.65748	1.00800
24	1	0.065359	2.71310	-2.99939	-0.52883	1.00800
38	1	0.131325	0.52263	3.34733	-2.44973	1.00800
39	1	0.079726	-2.13442	-0.72422	0.30217	1.00800
25	1	0.081020	1.55600	-2.27894	-1.65494	1.00800
41	1	0.027770	0.82981	5.34900	-3.68365	1.00800
42	1	0.032593	2.39692	4.57465	-3.28911	1.00800
43	1	0.049044	2.31719	6.34507	-3.57139	1.00800
26	1	0.121957	-1.98797	-2.59487	2.18823	1.00800
27	1	0.109657	1.27677	-4.98375	-0.68637	1.00800
14	1	0.072270	-2.57361	1.59752	0.54393	1.00800
29	1	0.069444	-0.16367	1.73869	2.38913	1.00800
30	1	0.064100	-1.65198	2.69621	2.38504	1.00800
49	1	0.108597	-4.21521	-0.34786	1.38024	1.00800
50	1	0.105002	-5.52722	-0.46729	3.48024	1.00800
51	1	0.105386	-4.36810	-0.47954	5.68085	1.00800
52	1	0.105347	-1.88294	-0.38056	5.77185	1.00800
53	1	0.117003	-0.55872	-0.27675	3.66300	1.00800
54	1	0.107630	-2.17754	-5.02699	1.88581	1.00800
12	1	0.094833	-1.46665	1.54969	-1.49981	1.00800
56	1	0.046987	0.36689	-7.13508	0.65292	1.00800
57	1	0.048005	-0.77526	-6.87673	-0.67637	1.00800
58	1	0.044196	-1.37418	-7.07855	0.97938	1.00800

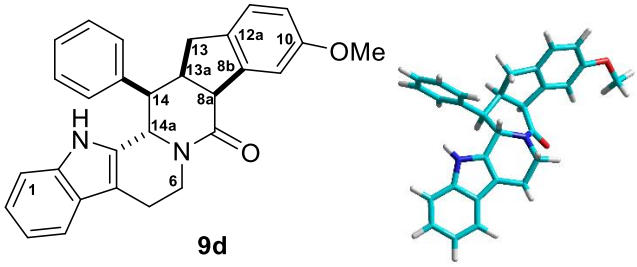
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.02550	-0.03804	-0.05004
2	6	-0.04042	-0.03006	-0.00849
3	7	-0.01509	0.01835	-0.02267
4	6	-0.02134	0.03754	0.08395
5	6	0.05105	0.01609	0.04219
6	6	0.00777	0.02252	0.00477
7	8	0.03590	0.02463	-0.06364
8	6	0.00992	-0.02792	-0.04044
9	6	-0.08467	0.00293	-0.02472
10	6	0.06313	1.75916	0.23023
13	6	-0.56103	-1.38627	-0.72248
15	6	0.00318	0.07467	-0.10299
16	6	-0.07843	-0.04518	0.05967
19	6	1.30828	0.70416	-0.82603
20	6	-1.01237	0.57207	0.90235
21	6	-1.12077	-0.64359	0.77548
22	6	-0.13139	-1.73521	-0.20013
23	6	1.03613	-0.72468	-0.91298
28	6	-0.68245	-0.95374	1.31011
31	6	-0.00094	0.62372	1.40701
32	6	0.51108	1.34431	0.87065
33	6	0.68969	0.76507	-1.46983
34	6	0.04017	-0.43506	-1.36220
37	8	-0.03068	-0.03077	0.08493
40	6	-0.00036	0.01221	0.02936

44	6	0.07519	-0.00971	-0.02835
45	6	-0.00984	-0.01072	0.06934
46	6	-0.04532	-0.00372	-0.08000
47	6	0.06701	0.00976	-0.04697
48	6	-0.00659	-0.00740	0.08441
55	6	0.02188	0.05858	0.03398
11	1	0.00095	-0.02821	-0.04114
17	1	-0.02182	-0.02341	-0.00811
18	1	-0.00592	-0.01399	-0.03893
35	1	0.00304	0.01382	0.01017
36	1	0.00994	0.01424	0.00519
24	1	-0.01738	-0.01285	-0.03866
38	1	0.01336	0.01885	-0.01265
39	1	0.00974	0.01695	0.00971
25	1	-0.05259	-0.01602	-0.00762
41	1	0.01527	0.02008	0.00481
42	1	-0.00303	0.00719	-0.00320
43	1	0.00793	-0.00465	-0.00164
26	1	0.00514	-0.00177	0.04244
27	1	-0.02416	-0.03643	-0.01272
14	1	-0.00197	0.00361	0.01146
29	1	0.02382	0.02661	-0.00055
30	1	0.00504	0.03493	0.00181
49	1	-0.00562	-0.01008	-0.00604
50	1	-0.01113	-0.02159	-0.00897
51	1	-0.01904	-0.00561	-0.00633
52	1	-0.01833	0.00851	-0.01181
53	1	-0.04212	0.02282	-0.00498
54	1	-0.00468	-0.00464	0.04661
12	1	-0.02047	0.04277	-0.00884
56	1	0.01220	-0.00636	0.02095
57	1	0.03242	0.00323	0.02559
58	1	0.00523	-0.01172	0.00700

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-1.055	-0.507	2.033	2.346
sp Hybrid	-0.381	-0.966	-0.462	1.137
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.436	-1.474	1.571	2.589

Compound **9d**



9d

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 164
in which
Number of Alpha Electrons = 82
Number of Beta Electrons = 82
Charge on the System = 0
Total Orbitals = 158
Starting PM3 calculation with 158 orbitals
Energy=-6641.143364 kcal/mol Gradient=0.037641 Symmetry=C1
MOLECULAR POINT GROUP C1

ENERGIES AND GRADIENT
Total Energy = -109481.2116436 (kcal/mol)
Total Energy = -174.469394718 (a.u.)
Binding Energy = -6641.1433636 (kcal/mol)
Isolated Atomic Energy = -102840.0682800 (kcal/mol)
Electronic Energy = -1061475.7009313 (kcal/mol)
Core-Core Interaction = 951994.4892877 (kcal/mol)
Heat of Formation = 14.4366364 (kcal/mol)
Gradient = 0.0376407 (kcal/mol/Ang)

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.038514	-1.71856	1.90656	0.50502	12.01100
2	6	0.051238	-1.27018	0.43538	0.64263	12.01100
3	7	-0.067610	-0.48230	-0.04887	-0.54179	14.00700
4	6	0.273318	-0.54250	0.72322	-1.75308	12.01100
5	6	-0.044584	-0.38169	2.23354	-1.63762	12.01100
6	6	-0.067398	-0.71035	2.78948	-0.23158	12.01100
7	8	-0.361273	-0.60694	0.15666	-2.83263	15.99900
8	6	-0.094500	-2.04780	2.53223	1.83686	12.01100
10	6	-0.253852	-2.45126	-0.45799	0.87236	12.01100
13	6	-0.052109	1.06192	2.59977	-1.83824	12.01100
15	6	-0.042155	0.64449	3.01533	0.47459	12.01100
16	6	-0.056834	-0.39779	-1.53274	-0.65100	12.01100
17	6	-0.117874	-2.67734	-1.66180	0.23025	12.01100
18	6	-0.043365	-1.75438	-2.22501	-0.77281	12.01100
19	6	-0.107721	-1.34724	2.20390	2.99912	12.01100
20	6	-0.092934	-1.65402	2.82396	4.20460	12.01100
21	6	-0.098620	-2.66354	3.77896	4.26024	12.01100
22	6	-0.097044	-3.36645	4.11101	3.10668	12.01100
23	6	-0.103890	-3.06176	3.49206	1.89991	12.01100
33	6	-0.115941	1.63790	3.04138	-0.63794	12.01100
34	6	-0.056781	2.96359	3.44302	-0.59369	12.01100
35	6	-0.148660	1.79212	2.55945	-3.01191	12.01100
36	6	0.081888	3.13490	2.96725	-2.95848	12.01100

37	6	-0.134614	3.72131	3.40402	-1.76236	12.01100
42	8	-0.192362	3.96293	3.02516	-4.06513	15.99900
44	7	0.280993	-3.46590	-0.25763	1.84451	14.00700
45	6	-0.072173	-3.90880	-2.21182	0.72976	12.01100
46	6	-0.161202	-4.40989	-1.30057	1.69913	12.01100
47	6	-0.101118	-5.61567	-1.53669	2.37417	12.01100
48	6	-0.087081	-6.29905	-2.69495	2.06277	12.01100
49	6	-0.128695	-5.80593	-3.60886	1.11136	12.01100
50	6	-0.046695	-4.61899	-3.38359	0.44334	12.01100
56	6	0.044376	3.55227	2.29121	-5.19493	12.01100
9	1	0.078076	-2.65295	1.91339	-0.11649	1.00800
14	1	0.073426	-1.19341	3.78975	-0.36018	1.00800
11	1	0.085761	-0.57172	0.33903	1.52260	1.00800
24	1	0.057680	0.12995	-1.87281	0.26277	1.00800
38	1	0.067556	0.88297	2.20568	1.19171	1.00800
39	1	0.063903	0.65041	3.95425	1.05761	1.00800
40	1	0.105898	3.40873	3.78793	0.34485	1.00800
41	1	0.134544	1.34539	2.22049	-3.95862	1.00800
25	1	0.077944	0.25321	-1.79124	-1.50869	1.00800
43	1	0.119704	4.77060	3.72030	-1.74584	1.00800
26	1	0.073700	-2.18229	-2.09747	-1.78791	1.00800
27	1	0.063821	-1.64122	-3.31682	-0.62578	1.00800
28	1	0.118962	-0.55431	1.44066	2.94670	1.00800
29	1	0.107645	-1.09801	2.55898	5.11006	1.00800
30	1	0.107142	-2.90417	4.26885	5.20943	1.00800
31	1	0.106922	-4.16090	4.86370	3.14703	1.00800
32	1	0.109958	-3.61416	3.76473	0.99259	1.00800
51	1	0.077867	-3.68631	0.63630	2.20909	1.00800
52	1	0.106701	-5.99788	-0.82885	3.11571	1.00800
53	1	0.099262	-7.24742	-2.91501	2.56419	1.00800
54	1	0.101785	-6.38333	-4.51555	0.90289	1.00800
55	1	0.105753	-4.22978	-4.09325	-0.29331	1.00800
12	1	0.095444	-1.02148	2.71784	-2.41256	1.00800
57	1	0.036327	2.47721	2.39057	-5.40806	1.00800
58	1	0.029390	3.79741	1.23068	-5.07310	1.00800
59	1	0.048615	4.14536	2.72784	-6.00182	1.00800

ATOMIC GRADIENTS

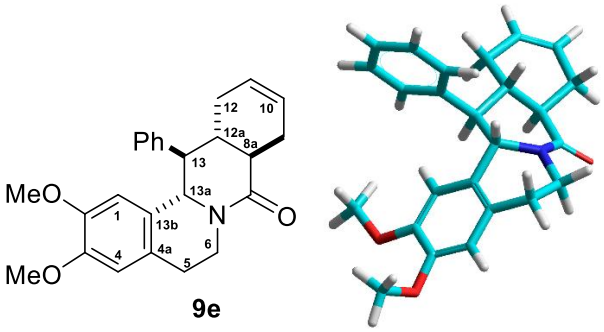
Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.04107	0.04824	-0.02020
2	6	-0.05143	-0.01667	-0.03406
3	7	0.05887	0.01039	0.04250
4	6	-0.02991	0.02096	0.02385
5	6	0.00775	-0.02807	0.01655
6	6	0.02334	-0.00192	0.01917
7	8	0.02085	-0.04280	-0.01993
8	6	-0.03944	0.00970	0.02767
10	6	0.08591	0.16124	0.06068
13	6	0.01855	0.00544	-0.01093
15	6	0.01362	-0.01524	0.00659
16	6	-0.03188	-0.02904	0.01526

17	6	-0.03621	-0.18384	-0.10411
18	6	-0.01333	-0.02624	0.00266
19	6	-0.00780	0.00513	-0.03363
20	6	-0.01718	0.03140	0.02818
21	6	-0.01700	0.02314	-0.00684
22	6	0.00563	0.00055	-0.01042
23	6	0.03991	-0.01383	0.00582
33	6	-0.05797	-0.02729	0.03806
34	6	-0.00785	-0.00676	0.03816
35	6	-0.00554	0.00475	0.03260
36	6	-0.00811	-0.00996	-0.01033
37	6	-0.00226	0.00900	-0.02826
42	8	0.02432	0.03342	-0.02616
44	7	-0.01541	0.04173	0.04075
45	6	0.06225	0.03027	-0.03015
46	6	-0.03891	0.00130	0.00571
47	6	0.06021	0.15958	0.04543
48	6	-0.09508	-0.10996	-0.01414
49	6	-0.08983	0.01136	0.03874
50	6	0.08233	-0.07627	-0.10348
56	6	-0.00668	0.02782	-0.02375
9	1	-0.00677	0.00043	-0.00717
14	1	0.02113	-0.02895	0.00009
11	1	0.00326	-0.02371	0.03302
24	1	0.01299	-0.01246	0.03376
38	1	-0.00130	0.00514	-0.01779
39	1	0.01383	-0.03968	-0.01151
40	1	0.00631	-0.00704	-0.00813
41	1	-0.01063	-0.00098	-0.02402
25	1	0.00971	-0.01508	-0.00059
43	1	0.03606	0.00888	-0.01054
26	1	0.01033	0.00271	0.03328
27	1	-0.00705	-0.00190	0.01834
28	1	0.01069	-0.01370	0.00194
29	1	-0.00591	0.00605	0.00082
30	1	0.00218	-0.00432	-0.03391
31	1	0.01677	-0.01059	-0.01276
32	1	0.00816	-0.01463	-0.00576
51	1	-0.00828	0.02220	0.00184
52	1	-0.01782	0.00014	0.00908
53	1	-0.02784	-0.00705	0.00118
54	1	-0.01968	-0.01714	-0.02342
55	1	0.00936	0.01685	0.04205
12	1	0.00640	-0.02605	0.00858
57	1	-0.01511	0.03830	-0.01380
58	1	-0.00422	0.03342	-0.02970
59	1	-0.01537	0.04165	0.00315

Dipole (Debyes)	x	y	z	Total
Point-Chg.	0.024	1.791	2.906	3.413
sp Hybrid	-1.203	0.105	-0.254	1.234
pd Hybrid	0.000	0.000	0.000	0.000

Sum -1.179 1.895 2.652 3.466

Compound **9e**



HyperChem log start -- Mon Sep 21 06:29:24 2020.
Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:
Singlet state calculation
Number of electrons = 150
in which
Number of Alpha Electrons = 75
Number of Beta Electrons = 75
Charge on the System = 0
Total Orbitals = 143

Energy=-6024.712408 kcal/mol Gradient=0.507064 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -101943.7364288 (kcal/mol)
Total Energy = -162.457664864 (a.u.)
Binding Energy = -6024.7124078 (kcal/mol)
Isolated Atomic Energy = -95919.0240210 (kcal/mol)
Electronic Energy = -944068.1902365 (kcal/mol)
Core-Core Interaction = 842124.4538077 (kcal/mol)
Heat of Formation = -54.0314078 (kcal/mol)
Gradient = 0.5070639 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.039928	-1.51045	0.03125	0.51854	12.01100
2	6	0.008830	-1.69136	1.56123	0.62793	12.01100
3	7	-0.065587	-0.66058	2.25127	1.47039	14.00700
4	6	0.259118	0.16397	1.50900	2.36750	12.01100
5	6	-0.093003	0.45436	0.04760	2.06961	12.01100
6	6	-0.070009	-0.03972	-0.37223	0.68351	12.01100
7	8	-0.375572	0.67210	2.10457	3.30840	15.99900

8	6	-0.077281	-2.03918	-0.46421	-0.80578	12.01100
10	6	-0.075593	-3.08353	1.95979	1.05219	12.01100
13	6	-0.064626	0.15086	-1.88264	0.52490	12.01100
14	6	-0.055387	-0.95854	3.67048	1.83796	12.01100
15	6	-0.096196	-3.32283	3.33019	1.23650	12.01100
16	6	-0.056186	-2.16015	4.25125	1.10219	12.01100
17	6	-0.102005	-1.71830	0.18971	-1.99698	12.01100
18	6	-0.091228	-2.19237	-0.28807	-3.21227	12.01100
19	6	-0.100758	-2.99624	-1.42294	-3.24845	12.01100
20	6	-0.098240	-3.32776	-2.07440	-2.06545	12.01100
21	6	-0.108749	-2.85365	-1.59821	-0.84806	12.01100
31	6	-0.081089	-4.59678	3.79197	1.55842	12.01100
32	6	0.030801	-5.65094	2.88231	1.70009	12.01100
33	6	-0.051858	1.95469	-0.23303	2.18847	12.01100
35	6	-0.152818	1.50275	-2.33229	0.94675	12.01100
36	6	-0.144216	2.31302	-1.59098	1.70344	12.01100
43	6	0.066796	-5.40931	1.49908	1.54335	12.01100
44	6	-0.164781	-4.12057	1.04960	1.23043	12.01100
45	8	-0.176235	-6.47207	0.64556	1.77182	15.99900
46	6	0.041272	-6.39403	-0.61813	1.15295	12.01100
47	8	-0.193379	-6.88266	3.37457	2.11766	15.99900
48	6	0.055281	-7.82828	3.49101	1.07690	12.01100
30	1	0.105788	-3.11857	-2.11922	0.08086	1.00800
9	1	0.081905	-2.11427	-0.45572	1.33369	1.00800
11	1	0.086428	-1.52285	1.99792	-0.40043	1.00800
12	1	0.089687	-0.08847	-0.55387	2.84220	1.00800
34	1	0.083827	0.56685	0.14668	-0.10025	1.00800
22	1	0.063285	-0.04467	4.25360	1.60772	1.00800
23	1	0.070948	-1.12247	3.75844	2.93375	1.00800
37	1	0.067278	-0.02790	-2.16978	-0.53105	1.00800
38	1	0.058311	-0.60711	-2.43493	1.11944	1.00800
39	1	0.075807	2.27603	-0.11399	3.24241	1.00800
40	1	0.065924	2.53661	0.51156	1.60750	1.00800
41	1	0.100789	1.80469	-3.32993	0.60904	1.00800
42	1	0.101666	3.30429	-1.95791	1.99233	1.00800
24	1	0.062875	-1.93910	4.40867	0.02623	1.00800
25	1	0.066709	-2.39107	5.25436	1.51169	1.00800
26	1	0.114768	-1.10541	1.10268	-1.94833	1.00800
27	1	0.105551	-1.93427	0.23162	-4.14073	1.00800
28	1	0.105493	-3.36970	-1.80071	-4.20578	1.00800
29	1	0.104116	-3.96341	-2.96570	-2.09085	1.00800
49	1	0.120460	-4.77399	4.86430	1.70786	1.00800
50	1	0.134004	-3.92706	-0.03479	1.12707	1.00800
51	1	0.052727	-7.16528	-1.19149	1.67233	1.00800
52	1	0.027666	-6.62909	-0.54203	0.08564	1.00800
53	1	0.031338	-5.41012	-1.09874	1.27122	1.00800
54	1	0.046371	-8.70982	3.87478	1.59649	1.00800
55	1	0.019314	-7.50183	4.20180	0.30939	1.00800
56	1	0.029589	-8.05576	2.52697	0.60854	1.00800

ATOMIC GRADIENTS

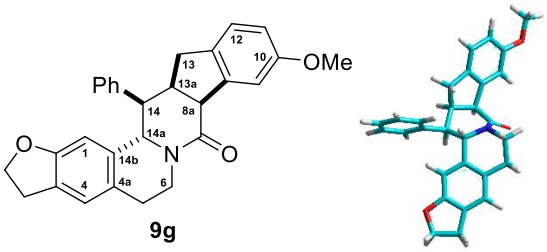
Atom Z Gradients(kcal/mol/Angstrom)

		x	y	z
1	6	0.01777	0.07693	-0.01452
2	6	0.04251	-0.08056	0.08694
3	7	-0.13371	-0.00255	-0.15935
4	6	0.02685	-0.08282	0.02804
5	6	0.02629	-0.05990	0.02537
6	6	-0.04084	0.04026	-0.06915
7	8	0.06963	0.04829	0.07038
8	6	-0.08911	-0.15577	0.11548
10	6	2.33385	-1.27388	-0.66369
13	6	0.00818	-0.03393	0.01405
14	6	-0.05174	0.01104	0.03309
15	6	1.64436	1.99901	-0.22382
16	6	0.06593	0.04999	0.12205
17	6	-0.03010	-0.00643	-0.14728
18	6	0.05190	0.08727	0.05385
19	6	-0.07815	-0.08700	0.07904
20	6	0.00527	0.02381	-0.10236
21	6	0.08909	0.10295	0.09763
31	6	-0.27796	2.30595	0.26030
32	6	-2.48287	1.33502	0.57929
33	6	0.07611	-0.00822	0.02221
35	6	-0.01181	-0.04516	-0.06528
36	6	0.09851	0.06936	0.06953
43	6	-2.00974	-2.29935	0.12217
44	6	0.52703	-2.24860	-0.21604
45	8	0.17448	0.25436	-0.01727
46	6	-0.04482	-0.03229	-0.01220
47	8	0.10235	0.00271	-0.04522
48	6	0.07440	-0.02468	-0.04076
30	1	0.00716	-0.00103	0.01322
9	1	0.00562	-0.02582	0.01697
11	1	-0.02631	0.00660	0.00306
12	1	0.02613	0.01088	-0.01100
34	1	-0.01324	0.00251	0.02278
22	1	0.01997	0.01987	0.00225
23	1	0.01536	0.01630	0.01165
37	1	0.01423	0.00531	-0.01717
38	1	0.03939	0.00609	-0.00155
39	1	0.00806	-0.01431	-0.06156
40	1	-0.00518	-0.01280	-0.00514
41	1	0.01281	-0.00692	-0.00802
42	1	-0.01916	0.02064	-0.03730
24	1	-0.06279	0.00278	0.03749
25	1	0.01199	-0.03145	0.03331
26	1	0.00385	0.01241	0.00548
27	1	-0.04499	-0.01903	0.04830
28	1	-0.03332	-0.00263	0.02416
29	1	-0.01686	-0.02582	0.02592
49	1	-0.01183	0.07546	0.01102
50	1	-0.00575	-0.01439	0.04519
51	1	0.01727	0.02586	-0.06061

52	1	-0.02214	-0.01595	-0.04158
53	1	-0.01163	0.00166	-0.03887
54	1	-0.03460	-0.00795	0.00121
55	1	-0.04292	-0.00219	0.00194
56	1	-0.01479	0.00810	-0.02362

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-0.968	-1.604	-4.022	4.437
sp Hybrid	-0.451	-0.493	-0.242	0.710
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.419	-2.096	-4.264	4.959

Compound **9g**



9g

Single Point, SemiEmpirical,PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 166
in which
Number of Alpha Electrons = 83
Number of Beta Electrons = 83
Charge on the System = 0
Total Orbitals = 159

Starting PM3 calculation with 159 orbitals
Energy=-6693.100054 kcal/mol Gradient=0.542003 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -112872.4241947 (kcal/mol)
Total Energy = -179.873635247 (a.u.)
Binding Energy = -6693.1000537 (kcal/mol)
Isolated Atomic Energy = -106179.3241410 (kcal/mol)
Electronic Energy = -1082903.9967977 (kcal/mol)
Core-Core Interaction = 970031.5726030 (kcal/mol)
Heat of Formation = -38.8590537 (kcal/mol)
Gradient = 0.5420031 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1
NET CHARGES AND COORDINATES
Atom Z Charge Coordinates(Angstrom) Mass
x y z

1	6	-0.029327	-2.37413	-0.93090	-1.58435	12.01100
2	6	0.012835	-1.73260	-1.35289	-0.23966	12.01100
3	7	-0.075643	-0.37465	-0.75178	-0.05301	14.00700
4	6	0.276128	0.38294	-0.41678	-1.23401	12.01100
5	6	-0.043084	-0.32022	0.44814	-2.26785	12.01100
6	6	-0.068268	-1.86099	0.39679	-2.15252	12.01100
7	8	-0.354000	1.55872	-0.72917	-1.32075	15.99900
8	6	-0.079834	-3.88164	-0.84902	-1.52245	12.01100
10	6	-0.069861	-1.73423	-2.86234	-0.06195	12.01100
12	6	-0.059172	0.35522	-1.33514	1.09873	12.01100
13	6	-0.059189	0.01179	1.89219	-2.01011	12.01100
14	6	-0.043768	-2.27934	1.66474	-1.37583	12.01100
15	6	-0.108078	-4.56081	-0.46910	-0.36328	12.01100
16	6	-0.093976	-5.94712	-0.36869	-0.35930	12.01100
17	6	-0.101182	-6.67009	-0.64698	-1.51393	12.01100
18	6	-0.095220	-6.00188	-1.02927	-2.67251	12.01100
19	6	-0.102236	-4.61579	-1.13068	-2.67884	12.01100
20	6	-0.097543	-0.64340	-3.54062	0.50451	12.01100
21	6	-0.078790	0.59352	-2.82603	0.93650	12.01100
22	6	-0.137337	-2.88939	-3.57965	-0.42043	12.01100
23	6	0.082566	-2.89420	-4.95060	-0.22199	12.01100
24	6	-0.159657	-1.79330	-5.63876	0.32539	12.01100
25	6	-0.048158	-0.66665	-4.93510	0.69229	12.01100
26	8	-0.185630	-3.95552	-5.78399	-0.52735	15.99900
27	6	0.051476	-3.56245	-7.12528	-0.16831	12.01100
28	6	-0.057439	-2.12660	-7.08992	0.40135	12.01100
46	6	-0.113972	-1.10647	2.57645	-1.50119	12.01100
47	6	-0.053287	-1.03147	3.92279	-1.19458	12.01100
48	6	-0.180537	0.17310	4.59946	-1.40044	12.01100
49	6	0.084787	1.27938	3.91380	-1.91138	12.01100
50	6	-0.105089	1.21276	2.53952	-2.22497	12.01100
55	8	-0.187093	2.51784	4.47297	-2.16027	15.99900
57	6	0.050610	2.67343	5.84650	-1.90614	12.01100
34	1	0.104921	-6.56811	-1.25268	-3.58274	1.00800
35	1	0.108665	-4.09572	-1.43116	-3.59640	1.00800
36	1	0.079832	1.39569	-3.01819	0.19336	1.00800
37	1	0.062993	0.96391	-3.24675	1.89286	1.00800
38	1	0.140825	-3.76987	-3.07513	-0.83841	1.00800
39	1	0.110191	0.19802	-5.44829	1.12718	1.00800
40	1	0.050443	-3.65384	-7.72699	-1.08679	1.00800
41	1	0.050273	-4.31165	-7.47986	0.55777	1.00800
42	1	0.066220	-1.42569	-7.70488	-0.19106	1.00800
43	1	0.065695	-2.07754	-7.47043	1.43728	1.00800
44	1	0.095775	0.01521	0.13982	-3.28574	1.00800
45	1	0.072456	-2.28306	0.48169	-3.18514	1.00800
11	1	0.085875	-2.34237	-0.92621	0.60666	1.00800
9	1	0.080554	-2.10677	-1.72423	-2.33120	1.00800
29	1	0.057827	-0.25658	-1.12498	1.99903	1.00800
30	1	0.077415	1.31150	-0.79223	1.23134	1.00800
31	1	0.115950	-3.98498	-0.26118	0.55216	1.00800
51	1	0.069870	-2.49402	1.44664	-0.31120	1.00800
52	1	0.063851	-3.20060	2.11320	-1.79042	1.00800

53	1	0.105212	-1.90288	4.45356	-0.79854	1.00800
54	1	0.115120	0.22920	5.66614	-1.15605	1.00800
32	1	0.104834	-6.46832	-0.07123	0.55647	1.00800
56	1	0.134529	2.08455	2.00170	-2.61606	1.00800
33	1	0.105072	-7.76191	-0.56792	-1.51078	1.00800
58	1	0.027321	2.52892	6.09415	-0.84800	1.00800
59	1	0.026964	2.00809	6.46255	-2.52227	1.00800
60	1	0.050285	3.71465	6.01902	-2.19178	1.00800

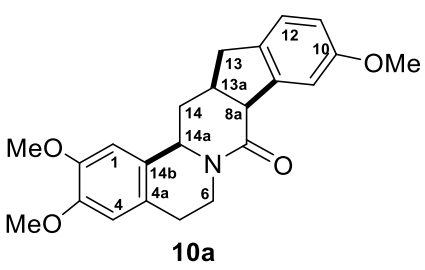
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.07021	-0.06294	0.01786
2	6	0.01370	-0.08619	-0.01752
3	7	-0.03485	-0.02330	0.01812
4	6	-0.07245	0.02655	0.00047
5	6	-0.02942	0.04299	0.01902
6	6	-0.01764	0.04420	-0.00426
7	8	0.12353	-0.05748	-0.02581
8	6	0.03527	0.00417	-0.04416
10	6	-1.01156	2.93534	-0.93948
12	6	-0.00002	0.03930	0.00533
13	6	-0.11209	-0.98250	-0.18758
14	6	0.04511	0.01366	-0.03157
15	6	-0.05686	0.00160	0.02726
16	6	-0.01812	0.02586	0.00109
17	6	-0.03725	-0.00618	-0.02345
18	6	-0.06841	0.04531	0.02694
19	6	0.00677	-0.00533	0.01582
20	6	2.78527	0.57801	1.06915
21	6	-0.17036	0.02503	0.03335
22	6	-1.61827	1.64192	-0.85949
23	6	-1.98629	-1.65926	-0.55381
24	6	-0.27671	-2.64771	0.26203
25	6	2.12465	-0.95238	1.00173
26	8	0.09041	0.09806	0.02931
27	6	0.01622	0.04881	0.02543
28	6	-0.01977	0.14794	-0.01995
46	6	-0.85055	-0.65012	0.11231
47	6	-0.48565	0.73960	0.33866
48	6	-0.44902	0.86209	0.35639
49	6	1.05482	0.27661	-0.22327
50	6	0.81235	-0.36243	-0.33306
55	8	-0.01049	-0.03819	0.03107
57	6	-0.04274	-0.00689	0.00983
34	1	0.00744	0.00789	-0.01106
35	1	0.02752	-0.00814	-0.03107
36	1	0.00817	-0.06277	-0.08917
37	1	0.01716	-0.04751	0.01253
38	1	-0.01103	-0.00238	0.01424
39	1	0.04404	-0.02181	0.00489
40	1	-0.01510	-0.01138	0.00585

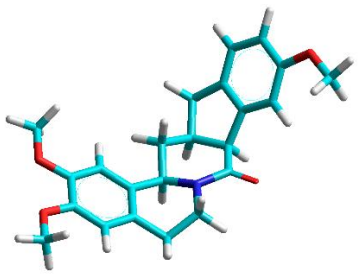
41	1	-0.01156	-0.00307	0.03513
42	1	0.00238	0.02311	0.00793
43	1	0.00920	0.03467	0.01672
44	1	0.01166	-0.00300	-0.02361
45	1	0.01377	0.01020	-0.00926
11	1	0.02809	-0.03371	-0.01813
9	1	-0.01062	0.01962	-0.01697
29	1	0.03148	-0.00828	-0.03027
30	1	0.01238	-0.02374	-0.01146
31	1	0.01842	0.00114	0.02044
51	1	0.00164	0.01893	-0.01382
52	1	-0.00282	-0.00499	-0.01741
53	1	-0.03051	-0.00116	0.01405
54	1	0.00349	0.01875	0.02445
32	1	0.01983	-0.00242	-0.02545
56	1	-0.00893	-0.00908	0.04819
33	1	0.07443	0.01220	-0.01134
58	1	-0.01252	0.04417	-0.01013
59	1	-0.00831	-0.01906	-0.01614
60	1	-0.02948	0.01567	-0.00690

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-2.204	0.608	0.931	2.468
sp Hybrid	-0.100	-0.693	0.062	0.702
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-2.304	-0.084	0.992	2.510

Compound **10a**



10a



Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 146
in which
Number of Alpha Electrons = 73
Number of Beta Electrons = 73
Charge on the System = 0
Total Orbitals = 137

Starting PM3 calculation with 137 orbitals

Energy=-5690.543565 kcal/mol Gradient=0.793462 Symmetry=C1

ENERGIES AND GRADIENT

Total Energy	= -102548.9804817 (kcal/mol)
Total Energy	= -163.422182537 (a.u.)
Binding Energy	= -5690.5435647 (kcal/mol)
Isolated Atomic Energy	= -96858.4369170 (kcal/mol)
Electronic Energy	= -873060.2276258 (kcal/mol)
Core-Core Interaction	= 770511.2471441 (kcal/mol)
Heat of Formation	= -106.2875647 (kcal/mol)
Gradient	= 0.7934618 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.124008	-1.78064	1.20887	-1.63485	12.01100
2	6	0.028225	-0.30387	0.83353	-1.52601	12.01100
3	7	-0.051662	0.18810	1.23917	-0.16893	14.00700
4	6	0.266431	-0.18320	2.51414	0.33320	12.01100
5	6	-0.040450	-1.32317	3.30961	-0.28783	12.01100
6	6	-0.071169	-1.94969	2.71805	-1.57663	12.01100
7	8	-0.394830	0.43463	2.93530	1.30583	15.99900
9	6	-0.087104	-0.05487	-0.62890	-1.77981	12.01100
10	6	-0.044289	-2.49841	3.51132	0.62877	12.01100
11	6	-0.039510	-3.44873	3.08602	-1.52156	12.01100
14	6	-0.132450	-3.70136	3.40527	-0.08769	12.01100
15	6	-0.055066	-4.92430	3.58942	0.53986	12.01100
16	6	-0.141925	-4.94674	3.87885	1.90175	12.01100
17	6	0.088036	-3.74045	3.98207	2.61439	12.01100
18	6	-0.152005	-2.49795	3.80572	1.98289	12.01100
23	8	-0.191186	-3.90976	4.27270	3.95401	15.99900
25	6	0.048906	-2.75675	4.31698	4.75823	12.01100
31	6	-0.053670	1.43100	0.59755	0.34539	12.01100
32	6	-0.070221	1.16416	-1.17466	-1.36773	12.01100
33	6	-0.059736	2.13500	-0.28017	-0.68053	12.01100
38	6	-0.153530	-0.98046	-1.42910	-2.45592	12.01100
39	6	0.059829	-0.70250	-2.77515	-2.69707	12.01100
40	6	0.065174	0.53295	-3.33106	-2.25990	12.01100
41	6	-0.150902	1.45895	-2.51994	-1.60117	12.01100
42	8	-0.166657	-1.53937	-3.64728	-3.36346	15.99900
43	6	0.047009	-2.84049	-3.19800	-3.64881	12.01100
44	8	-0.166187	0.71244	-4.66779	-2.54863	15.99900
45	6	0.046833	1.87566	-5.28379	-2.05475	12.01100
29	1	0.066534	-2.19657	0.80552	-2.58510	1.00800
30	1	0.061511	0.28079	1.39463	-2.30452	1.00800
12	1	0.093782	-0.90533	4.32131	-0.52099	1.00800
19	1	0.061594	-4.09800	2.26766	-1.88475	1.00800
20	1	0.059697	-3.67196	3.96309	-2.15784	1.00800
34	1	0.062603	1.12998	-0.00507	1.22629	1.00800
35	1	0.073799	2.14130	1.36592	0.71817	1.00800

36	1	0.061391	2.65162	0.33688	-1.44492	1.00800
37	1	0.064717	2.93133	-0.86182	-0.17534	1.00800
21	1	0.104608	-5.85716	3.50491	-0.02617	1.00800
22	1	0.119583	-5.90448	4.02348	2.41468	1.00800
13	1	0.068783	-1.47042	3.17407	-2.47383	1.00800
24	1	0.144230	-1.54912	3.88951	2.52827	1.00800
8	1	0.080572	-2.36859	0.72229	-0.82878	1.00800
26	1	0.048184	-3.17243	4.52468	5.74796	1.00800
27	1	0.032909	-2.21816	3.36230	4.76887	1.00800
28	1	0.030720	-2.07458	5.12196	4.46112	1.00800
46	1	0.126430	-1.92336	-0.96965	-2.79356	1.00800
47	1	0.120266	2.42077	-2.92039	-1.25731	1.00800
48	1	0.053139	-3.29673	-4.08652	-4.09397	1.00800
49	1	0.028880	-3.39197	-2.90206	-2.74879	1.00800
50	1	0.024189	-2.84633	-2.37326	-4.37139	1.00800
51	1	0.053010	1.74333	-6.31799	-2.38451	1.00800
52	1	0.026412	2.78842	-4.86455	-2.49422	1.00800
53	1	0.028570	1.94124	-5.24349	-0.96117	1.00800

ATOMIC GRADIENTS

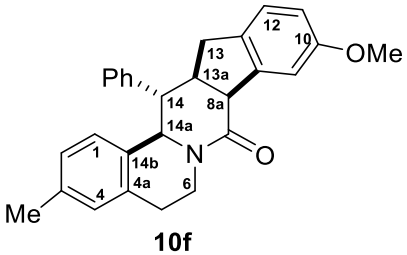
Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.00667	-0.00502	-0.00288
2	6	-0.03892	0.01155	0.13500
3	7	-0.02170	-0.02499	-0.07419
4	6	0.05730	0.08843	0.10364
5	6	-0.05184	-0.01627	0.00987
6	6	0.00937	0.01836	0.00472
7	8	-0.04902	-0.03235	-0.10254
9	6	-2.10854	3.25053	-0.09581
10	6	1.64464	-0.19553	-0.54570
11	6	0.04588	-0.00792	0.07085
14	6	-0.13202	-0.30102	-1.72863
15	6	-1.44994	-0.10242	-0.65559
16	6	-1.56540	0.18234	0.39602
17	6	0.31362	0.29397	1.72177
18	6	1.28310	0.14674	0.71557
23	8	-0.03478	-0.05254	-0.08398
25	6	-0.02177	-0.04216	-0.04222
31	6	0.02517	-0.02447	-0.03658
32	6	3.39079	0.82319	1.71387
33	6	-0.05475	-0.03068	0.02264
38	6	-2.34842	1.92013	-0.62987
39	6	-2.75380	-2.34002	-1.94478
40	6	0.86613	-3.91380	-0.66735
41	6	2.81246	-0.37722	1.22040
42	8	0.42462	0.35117	0.33500
43	6	-0.02920	0.02264	0.01630
44	8	-0.13747	0.50312	0.08399
45	6	-0.00125	0.01714	0.02744
29	1	0.00590	0.01612	0.01409
30	1	0.01099	-0.05894	-0.06008

12	1	0.00107	0.01749	0.01156
19	1	-0.01549	-0.00066	0.00524
20	1	-0.01943	0.02396	0.01612
34	1	0.00888	-0.00249	-0.01610
35	1	0.00790	-0.00294	-0.02317
36	1	0.00193	-0.03657	-0.05291
37	1	-0.00303	-0.01047	-0.01286
21	1	0.00893	-0.01552	-0.02541
22	1	-0.00696	-0.01917	0.00282
13	1	0.00953	0.00287	-0.00966
24	1	0.00805	-0.00669	0.00944
8	1	0.00686	0.02676	0.01707
26	1	0.01580	-0.02696	0.02984
27	1	-0.02324	-0.02564	0.01198
28	1	-0.02537	-0.03186	0.00365
46	1	-0.02395	0.04813	-0.01977
47	1	0.03109	0.00270	0.02803
48	1	-0.02380	0.00034	0.02150
49	1	-0.01064	-0.01715	0.01070
50	1	-0.00682	-0.01018	0.02721
51	1	-0.00429	-0.00268	0.03011
52	1	-0.02641	-0.01535	0.01734
53	1	-0.00845	-0.01800	-0.00368

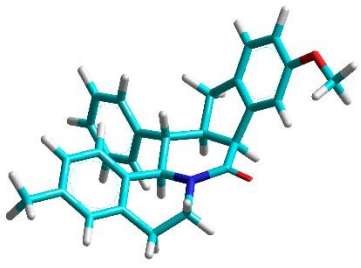
Dipole (Debyes)	x	y	z	Total
Point-Chg.	-0.088	-1.348	-1.946	2.369
sp Hybrid	0.626	0.448	-0.324	0.835
pd Hybrid	0.000	0.000	0.000	0.000
Sum	0.538	-0.900	-2.270	2.500

HyperChem log stop -- Fri Sep 25 04:31:39 2020.

Compound **10f**



10f



Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 156
in which
Number of Alpha Electrons = 78
Number of Beta Electrons = 78

Charge on the System = 0
Total Orbitals = 151

Starting PM3 calculation with 151 orbitals
Energy=-6433.889115 kcal/mol Gradient=0.375422 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -103375.6223643 (kcal/mol)
Total Energy = -164.739520067 (a.u.)
Binding Energy = -6433.8891153 (kcal/mol)
Isolated Atomic Energy = -96941.7332490 (kcal/mol)
Electronic Energy = -981120.5907371 (kcal/mol)
Core-Core Interaction = 877744.9683729 (kcal/mol)
Heat of Formation = -10.0971153 (kcal/mol)
Gradient = 0.3754216 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	-0.036546	-1.40270	1.57676	-1.91833	12.01100
2	6	0.021456	0.03941	1.04194	-1.82467	12.01100
3	7	-0.047790	0.75017	1.56693	-0.61314	14.00700
4	6	0.265321	0.48223	2.86043	-0.10426	12.01100
5	6	-0.042127	-0.64697	3.70828	-0.65004	12.01100
6	6	-0.072744	-1.44912	3.11198	-1.82937	12.01100
7	8	-0.393639	1.21219	3.26037	0.79789	15.99900
9	6	-0.088529	0.15576	-0.46625	-1.80818	12.01100
10	6	-0.045551	-1.68413	4.09771	0.36488	12.01100
11	6	-0.048536	-2.90387	3.60053	-1.62384	12.01100
14	6	-0.130177	-2.96490	4.04744	-0.20485	12.01100
15	6	-0.056528	-4.08680	4.40599	0.52811	12.01100
16	6	-0.140983	-3.92411	4.83651	1.84220	12.01100
17	6	0.086216	-2.63703	4.90286	2.40181	12.01100
18	6	-0.150011	-1.49842	4.52903	1.66904	12.01100
23	8	-0.191448	-2.62061	5.35270	3.70793	15.99900
25	6	0.048943	-1.36428	5.58761	4.29518	12.01100
29	6	-0.077301	-2.02123	1.19163	-3.24368	12.01100
31	6	-0.053553	2.10039	0.98746	-0.33167	12.01100
32	6	-0.074160	1.44926	-0.98997	-1.64573	12.01100
33	6	-0.063852	2.55180	-0.02753	-1.37453	12.01100
38	6	-0.085489	-0.90687	-1.35341	-1.96071	12.01100
39	6	-0.104984	-0.68212	-2.72586	-2.01002	12.01100
40	6	-0.067620	0.60962	-3.23896	-1.89653	12.01100
41	6	-0.097043	1.67699	-2.36099	-1.69678	12.01100
42	6	-0.065330	0.85369	-4.70091	-1.98919	12.01100
49	6	-0.104906	-3.32757	0.70058	-3.29929	12.01100
50	6	-0.106474	-1.30267	1.35788	-4.43040	12.01100
51	6	-0.091110	-1.88229	1.04836	-5.65394	12.01100
52	6	-0.101454	-3.18714	0.56801	-5.70371	12.01100
53	6	-0.096856	-3.90581	0.39242	-4.52641	12.01100

20	1	0.062143	-3.13968	4.44249	-2.30194	1.00800
21	1	0.104813	-5.08344	4.35534	0.07881	1.00800
34	1	0.068139	2.03935	0.51252	0.66856	1.00800
35	1	0.067245	2.85900	1.79491	-0.25036	1.00800
36	1	0.060344	2.84717	0.47083	-2.32113	1.00800
37	1	0.066950	3.46139	-0.54583	-1.01205	1.00800
22	1	0.119328	-4.79902	5.12548	2.43577	1.00800
13	1	0.072804	-1.04213	3.52285	-2.78493	1.00800
24	1	0.144725	-0.48916	4.56941	2.09855	1.00800
8	1	0.093504	-2.00439	1.14510	-1.07898	1.00800
26	1	0.047922	-1.63771	5.98435	5.27666	1.00800
43	1	0.118809	-1.93575	-0.98350	-2.05589	1.00800
44	1	0.109598	2.69357	-2.75359	-1.57412	1.00800
45	1	0.106717	-1.52975	-3.40815	-2.14121	1.00800
46	1	0.047953	1.12494	-4.97749	-3.01745	1.00800
47	1	0.045559	-0.03468	-5.28436	-1.71357	1.00800
48	1	0.045730	1.67605	-5.01774	-1.33414	1.00800
27	1	0.032853	-0.78145	4.66649	4.41134	1.00800
28	1	0.030454	-0.77616	6.32807	3.74064	1.00800
12	1	0.093405	-0.16650	4.65807	-0.99979	1.00800
30	1	0.066104	0.58052	1.39467	-2.75403	1.00800
19	1	0.071081	-3.65194	2.81388	-1.84189	1.00800
54	1	0.111209	-3.90158	0.55385	-2.37543	1.00800
55	1	0.111124	-0.26365	1.71723	-4.37151	1.00800
56	1	0.104628	-1.31027	1.18126	-6.57798	1.00800
57	1	0.105028	-3.64571	0.32551	-6.66781	1.00800
58	1	0.104634	-4.93103	0.00945	-4.56337	1.00800

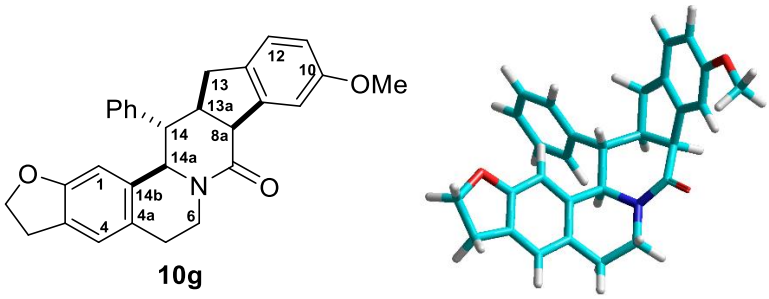
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	0.00828	0.00991	0.00067
2	6	-0.00079	0.01053	0.05702
3	7	-0.00904	-0.06986	-0.00249
4	6	0.00142	0.01681	0.08763
5	6	-0.03407	-0.03265	0.02949
6	6	0.01050	-0.00811	0.00869
7	8	-0.04887	-0.03292	-0.00250
9	6	-0.19021	1.11305	-0.02707
10	6	1.50947	-0.47905	-0.76684
11	6	0.05915	-0.02056	0.08103
14	6	-0.27485	-0.49316	-1.67698
15	6	-1.56171	0.01260	-0.41491
16	6	-1.55627	0.34831	0.55507
17	6	0.53958	0.58153	1.69228
18	6	1.40640	0.04716	0.59524
23	8	-0.04636	-0.00495	-0.07793
25	6	-0.00814	0.06762	-0.05086
29	6	-0.06194	-0.02874	0.02101
31	6	-0.03143	-0.02169	0.01832
32	6	0.90340	0.58407	0.12804
33	6	-0.03657	-0.01675	0.06060

38	6	-0.94244	0.17147	-0.08191
39	6	-0.90143	-0.45485	-0.14277
40	6	0.32410	-1.18198	-0.10402
41	6	0.90841	-0.34759	0.08179
42	6	-0.00517	0.05314	-0.03567
49	6	0.04630	0.01330	0.03074
50	6	0.00048	-0.00697	-0.04487
51	6	0.01936	0.02507	0.02416
52	6	-0.01067	-0.00856	0.02561
53	6	0.00123	0.00856	-0.04689
20	1	-0.00798	-0.01210	0.01237
21	1	-0.01448	-0.02866	0.02826
34	1	-0.01816	-0.02083	0.01050
35	1	-0.00464	-0.01939	0.01791
36	1	-0.01434	-0.00873	-0.00162
37	1	-0.00738	-0.01780	0.00790
22	1	-0.02035	0.00878	0.01196
13	1	0.00470	0.00374	0.00684
24	1	0.00604	-0.00401	0.02160
8	1	0.00492	-0.02485	-0.00789
26	1	0.01033	0.09899	-0.01994
43	1	-0.01174	0.00429	-0.00744
44	1	0.01199	-0.02090	-0.01020
45	1	-0.01860	-0.00710	-0.02962
46	1	0.02844	0.01238	-0.04128
47	1	0.02903	-0.01034	-0.05441
48	1	0.00755	0.00662	-0.04474
27	1	0.04022	0.09968	-0.00099
28	1	-0.01731	0.07570	-0.02555
12	1	0.00154	0.01137	0.01795
30	1	-0.01205	-0.01224	0.00798
19	1	-0.01633	-0.01722	0.05108
54	1	-0.02240	-0.00577	0.00567
55	1	-0.00024	0.01160	0.01244
56	1	0.00559	0.01714	0.01192
57	1	0.01267	0.00230	0.01024
58	1	0.00488	0.00259	-0.01262

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-0.494	-1.578	-2.582	3.066
sp Hybrid	0.492	0.091	-0.682	0.846
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-0.002	-1.487	-3.264	3.587

Compound **10g**



10g

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 166
in which
Number of Alpha Electrons = 83
Number of Beta Electrons = 83
Charge on the System = 0
Total Orbitals = 159

Starting PM3 calculation with 159 orbitals
Energy=-6692.805369 kcal/mol Gradient=0.506084 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -112872.1295105 (kcal/mol)
Total Energy = -179.873165638 (a.u.)
Binding Energy = -6692.8053695 (kcal/mol)
Isolated Atomic Energy = -106179.3241410 (kcal/mol)
Electronic Energy = -1091668.7163846 (kcal/mol)
Core-Core Interaction = 978796.5868741 (kcal/mol)
Heat of Formation = -38.5643695 (kcal/mol)
Gradient = 0.5060836 (kcal/mol/Ang)

MOLECULAR POINT GROUP
C1
NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.040569	-1.04706	1.85723	-2.34788	12.01100
2	6	0.014480	0.39404	1.30465	-2.39809	12.01100
3	7	-0.078014	1.36353	2.11018	-1.58406	14.00700
4	6	0.276336	0.87779	3.08837	-0.66203	12.01100
5	6	-0.044832	-0.28678	3.94853	-1.10299	12.01100
6	6	-0.065156	-1.06960	3.39395	-2.31851	12.01100
7	8	-0.376816	1.52086	3.29771	0.35737	15.99900
9	6	-0.063756	0.49879	-0.16885	-2.07106	12.01100
10	6	-0.048019	-1.34365	4.21841	-0.07044	12.01100
11	6	-0.053117	-2.50867	3.93002	-2.13286	12.01100
14	6	-0.130820	-2.60996	4.23645	-0.67771	12.01100

15	6	-0.056222	-3.75116	4.51433	0.05903	12.01100
16	6	-0.141691	-3.62691	4.77046	1.42243	12.01100
17	6	0.085930	-2.35862	4.74584	2.02579	12.01100
18	6	-0.150167	-1.19673	4.47628	1.28277	12.01100
23	8	-0.191347	-2.38243	5.01726	3.38010	15.99900
25	6	0.048930	-1.16884	4.91234	4.08306	12.01100
29	6	-0.078079	-1.82682	1.37873	-3.55024	12.01100
31	6	-0.054223	2.66131	1.45216	-1.24773	12.01100
32	6	-0.115925	1.79556	-0.70848	-2.00467	12.01100
33	6	-0.055639	2.93951	0.23863	-2.12316	12.01100
38	6	-0.120658	-0.61499	-0.99714	-1.88912	12.01100
39	6	0.086117	-0.37675	-2.34928	-1.67960	12.01100
40	6	-0.162283	0.91978	-2.89713	-1.63798	12.01100
41	6	-0.037098	2.01885	-2.07460	-1.79278	12.01100
42	6	-0.057863	0.81064	-4.36648	-1.40836	12.01100
45	8	-0.185938	-1.36935	-3.29517	-1.49715	15.99900
46	6	-0.102844	-3.12005	0.87346	-3.39247	12.01100
47	6	-0.105586	-1.27474	1.45165	-4.83085	12.01100
48	6	-0.092577	-2.00440	1.03567	-5.93741	12.01100
49	6	-0.101026	-3.29392	0.54001	-5.77458	12.01100
50	6	-0.095534	-3.84825	0.45756	-4.50189	12.01100
56	6	0.051745	-0.71839	-4.57172	-1.32673	12.01100
34	1	0.068266	2.68760	1.15223	-0.17800	1.00800
35	1	0.061645	3.44757	2.22138	-1.38119	1.00800
36	1	0.063667	3.08102	0.52503	-3.18569	1.00800
37	1	0.063732	3.89106	-0.23382	-1.80936	1.00800
22	1	0.119497	-4.51846	4.98923	2.02122	1.00800
13	1	0.077008	-0.63228	3.77485	-3.27088	1.00800
24	1	0.144349	-0.20086	4.46217	1.74354	1.00800
8	1	0.090308	-1.54512	1.48580	-1.41501	1.00800
26	1	0.048016	-1.47715	5.12486	5.11030	1.00800
43	1	0.137182	-1.64049	-0.60827	-1.92572	1.00800
44	1	0.110159	3.03655	-2.47622	-1.74728	1.00800
27	1	0.032933	-0.73475	3.90774	4.02017	1.00800
28	1	0.030279	-0.43234	5.65347	3.75146	1.00800
12	1	0.096501	0.15929	4.93768	-1.38069	1.00800
30	1	0.083221	0.76204	1.42310	-3.46003	1.00800
19	1	0.074921	-3.27947	3.20657	-2.46063	1.00800
20	1	0.062645	-2.67059	4.84632	-2.73158	1.00800
51	1	0.112129	-3.56607	0.80007	-2.39214	1.00800
52	1	0.112365	-0.24322	1.82010	-4.94026	1.00800
53	1	0.104120	-1.56128	1.09511	-6.93678	1.00800
54	1	0.104667	-3.86965	0.21106	-6.64571	1.00800
55	1	0.105104	-4.86057	0.06127	-4.37001	1.00800
21	1	0.105388	-4.73362	4.52956	-0.42297	1.00800
57	1	0.066355	1.32537	-4.67818	-0.48192	1.00800
58	1	0.065829	1.26779	-4.94632	-2.23011	1.00800
59	1	0.051285	-1.05648	-4.95999	-0.35264	1.00800
60	1	0.050686	-1.11436	-5.22547	-2.12045	1.00800

ATOMIC GRADIENTS

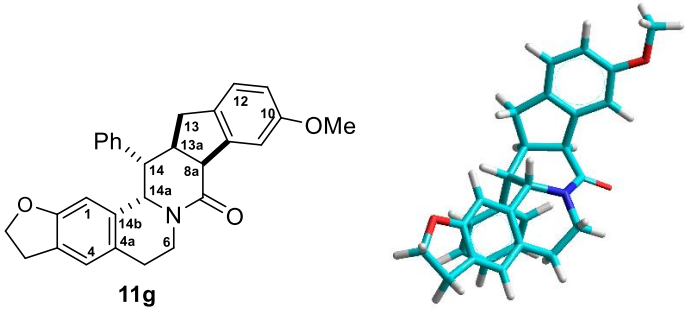
Atom Z Gradients(kcal/mol/Angstrom)

		x	y	z
1	6	0.00993	0.01757	0.01410
2	6	0.00789	-0.01059	0.01048
3	7	-0.02491	-0.00224	-0.04119
4	6	-0.06402	0.00318	-0.04233
5	6	-0.03316	0.01267	0.03614
6	6	0.02582	0.01615	0.00969
7	8	0.05521	0.03613	0.05955
9	6	-0.97443	2.11513	-0.34857
10	6	1.61349	-0.31201	-0.81487
11	6	0.05779	-0.00996	0.06166
14	6	-0.26038	-0.27627	-1.83609
15	6	-1.58460	0.06688	-0.47407
16	6	-1.64097	0.32087	0.48022
17	6	0.63236	0.26830	1.75871
18	6	1.38798	-0.01640	0.67837
23	8	-0.04637	-0.02755	-0.08413
25	6	-0.03181	-0.03141	-0.04327
29	6	0.03653	0.00270	-0.01567
31	6	-0.02970	-0.02575	0.02160
32	6	2.06494	0.84866	-0.23661
33	6	0.00326	-0.00744	0.11621
38	6	-1.67677	0.95327	-0.05950
39	6	-1.65698	-1.26045	0.24868
40	6	0.40139	-2.07202	0.31072
41	6	1.91509	-0.66626	0.02670
42	6	-0.05563	0.07303	-0.02663
45	8	0.08034	0.05065	-0.02310
46	6	-0.04177	-0.00451	0.00344
47	6	-0.01394	-0.01750	0.07065
48	6	-0.06021	-0.03200	0.00768
49	6	0.02573	-0.01892	0.01265
50	6	-0.01285	0.01052	0.08017
56	6	-0.02510	0.03735	-0.03694
34	1	0.01277	-0.00265	0.02058
35	1	0.00507	0.00118	0.01884
36	1	-0.02594	-0.03382	-0.00013
37	1	0.00824	-0.00713	0.01934
22	1	-0.01441	0.01366	-0.00809
13	1	0.00701	0.00741	-0.01732
24	1	0.01903	0.02190	0.00497
8	1	0.00672	0.03219	0.00553
26	1	-0.01037	-0.03720	0.00109
43	1	-0.03354	0.00229	0.00160
44	1	0.00792	0.00749	0.00593
27	1	-0.02927	-0.02851	-0.00354
28	1	-0.00737	-0.03942	0.02591
12	1	-0.01453	0.01781	0.01594
30	1	0.00112	-0.00635	-0.00016
19	1	0.00260	0.01929	-0.01065
20	1	-0.00304	0.03470	0.01479
51	1	-0.00752	0.01153	0.02913

52	1	-0.01505	-0.03003	0.00696
53	1	-0.01065	-0.05272	0.01012
54	1	-0.01937	-0.03766	0.03804
55	1	-0.02054	-0.01230	0.04353
21	1	0.01085	0.02988	-0.03388
57	1	0.01022	0.02172	-0.01849
58	1	0.01724	0.03125	-0.02760
59	1	0.00439	-0.01429	-0.03307
60	1	0.01428	0.00799	-0.03382

Dipole (Debyes)	x	y	z	Total
Point-Chg.	0.308	-1.687	-2.569	3.089
sp Hybrid	0.300	-0.725	0.143	0.798
pd Hybrid	0.000	0.000	0.000	0.000
Sum	0.608	-2.412	-2.426	3.475

Compound **11g**



11g

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 166
in which
Number of Alpha Electrons = 83
Number of Beta Electrons = 83
Charge on the System = 0
Total Orbitals = 159

Starting PM3 calculation with 159 orbitals
Energy=-6693.727176 kcal/mol Gradient=0.507860 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -112873.0513170 (kcal/mol)
Total Energy = -179.874634630 (a.u.)
Binding Energy = -6693.7271760 (kcal/mol)
Isolated Atomic Energy = -106179.3241410 (kcal/mol)
Electronic Energy = -1095662.1311751 (kcal/mol)
Core-Core Interaction = 982789.0798581 (kcal/mol)

Heat of Formation = -39.4861760 (kcal/mol)
Gradient = 0.5078605 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1
NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	-0.046013	-1.76918	-1.11442	-2.22145	12.01100
2	6	0.014234	-1.06169	-1.32532	-0.86133	12.01100
3	7	-0.040746	0.42597	-1.23981	-0.95272	14.00700
4	6	0.265479	0.98138	-0.37525	-1.93167	12.01100
5	6	-0.046608	0.09994	0.64181	-2.64391	12.01100
6	6	-0.074536	-1.38955	0.24496	-2.81965	12.01100
7	8	-0.386698	2.18889	-0.42589	-2.13897	15.99900
8	6	-0.078467	-1.60539	-2.24747	-3.20046	12.01100
9	6	-0.051872	-1.57401	-2.57601	-0.19647	12.01100
11	6	-0.061975	1.21984	-2.38435	-0.43562	12.01100
12	6	-0.053390	0.07570	1.95641	-1.92224	12.01100
13	6	-0.043584	-2.22953	1.38624	-2.19344	12.01100
14	6	-0.094325	-0.80912	-3.74782	-0.15322	12.01100
15	6	-0.074037	0.56415	-3.72585	-0.73038	12.01100
16	6	-0.128421	-2.86004	-2.53666	0.36832	12.01100
17	6	0.083335	-3.33561	-3.70671	0.94036	12.01100
18	6	-0.161273	-2.57796	-4.89583	0.97362	12.01100
19	6	-0.038777	-1.30830	-4.92168	0.43324	12.01100
20	8	-0.187069	-4.58037	-3.84202	1.52799	15.99900
21	6	0.052133	-4.68851	-5.20373	1.99343	12.01100
22	6	-0.058424	-3.38264	-5.95392	1.64960	12.01100
35	6	-0.126836	-1.24266	2.37949	-1.68847	12.01100
36	6	-0.051193	-1.49790	3.59180	-1.07057	12.01100
37	6	-0.181730	-0.42459	4.39701	-0.68490	12.01100
38	6	0.088577	0.88660	3.97217	-0.92611	12.01100
39	6	-0.109323	1.15530	2.73622	-1.55029	12.01100
44	8	-0.185800	2.02632	4.67801	-0.59488	15.99900
46	6	0.050213	1.86041	5.96222	-0.04814	12.01100
51	6	-0.096492	-2.62053	-3.20730	-3.27937	12.01100
52	6	-0.100409	-2.53037	-4.26022	-4.18129	12.01100
53	6	-0.101857	-1.42540	-4.36999	-5.01870	12.01100
54	6	-0.098255	-0.41370	-3.41957	-4.95000	12.01100
55	6	-0.107474	-0.50393	-2.36334	-4.04964	12.01100
34	1	0.079647	-1.60707	0.20193	-3.91374	1.00800
10	1	0.081305	-1.34236	-0.45635	-0.20683	1.00800
23	1	0.060204	1.31765	-2.23339	0.65872	1.00800
24	1	0.089563	2.24855	-2.36199	-0.84963	1.00800
25	1	0.074739	0.50494	-3.91236	-1.82361	1.00800
26	1	0.064581	1.18487	-4.54312	-0.31361	1.00800
40	1	0.062322	-2.88167	1.02881	-1.37180	1.00800
41	1	0.061476	-2.90464	1.84296	-2.94074	1.00800
42	1	0.104753	-2.52673	3.91803	-0.88890	1.00800
43	1	0.115725	-0.62975	5.35666	-0.19734	1.00800
27	1	0.124380	-3.45953	-1.61980	0.35546	1.00800
45	1	0.140248	2.18406	2.40239	-1.73551	1.00800

28	1	0.110941	-0.70209	-5.83341	0.45960	1.00800
47	1	0.026991	1.35299	5.93840	0.92326	1.00800
48	1	0.027558	1.32719	6.63944	-0.72544	1.00800
49	1	0.050949	2.89404	6.29579	0.07808	1.00800
50	1	0.082594	-2.86687	-1.06743	-1.98293	1.00800
29	1	0.050372	-5.57830	-5.62593	1.49929	1.00800
30	1	0.051618	-4.88563	-5.14243	3.07575	1.00800
31	1	0.066026	-3.55956	-6.82104	0.98822	1.00800
32	1	0.066931	-2.87542	-6.34595	2.54932	1.00800
33	1	0.098540	0.54829	0.81232	-3.65515	1.00800
56	1	0.110474	-3.49289	-3.13383	-2.61786	1.00800
57	1	0.103661	-3.33251	-5.00370	-4.23194	1.00800
58	1	0.104014	-1.35411	-5.19929	-5.72962	1.00800
59	1	0.106008	0.45870	-3.49845	-5.60725	1.00800
60	1	0.115992	0.29934	-1.61647	-4.01948	1.00800

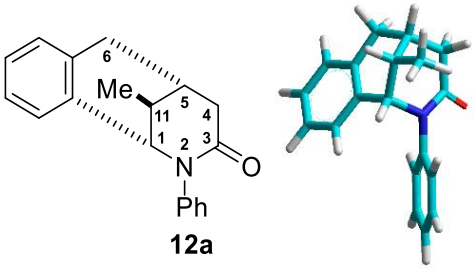
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	-0.00796	0.01234	0.06203
2	6	-0.02849	-0.07084	-0.02768
3	7	-0.01269	0.03284	0.05074
4	6	-0.08334	-0.03169	0.00058
5	6	0.02007	0.05517	0.05528
6	6	-0.01098	0.01812	0.04102
7	8	0.06179	0.00140	-0.00243
8	6	-0.06136	-0.00482	0.02642
9	6	0.07977	2.49852	-0.82705
11	6	-0.03005	0.00578	0.00323
12	6	0.05398	-1.24112	-0.63450
13	6	0.08758	0.06948	0.03902
14	6	2.29191	-0.90519	-0.77757
15	6	-0.05538	0.03854	0.14397
16	6	-0.76149	2.03380	-0.27018
17	6	-2.07162	-0.30219	1.00108
18	6	-0.96344	-1.82703	0.96446
19	6	1.41772	-1.65724	-0.11319
20	8	0.08798	-0.02411	-0.06583
21	6	0.01352	0.03806	-0.02407
22	6	0.00430	0.08947	-0.05227
35	6	-0.93404	-1.15810	-0.54026
36	6	-1.08834	0.85881	0.44754
37	6	-0.74309	0.99371	0.50978
38	6	1.30905	0.67906	0.28981
39	6	1.32568	-0.28505	-0.17541
44	8	-0.00826	-0.02775	-0.04012
46	6	0.00256	0.02671	-0.03479
51	6	0.02280	0.04187	0.02901
52	6	0.01967	-0.01719	-0.05379
53	6	-0.05913	-0.02335	0.02210
54	6	0.03181	0.05650	0.03265
55	6	0.05649	-0.04373	-0.02576

34	1	-0.00854	0.00037	-0.00975
10	1	-0.00113	-0.02704	0.02871
23	1	-0.02848	-0.00522	0.00186
24	1	-0.00147	0.00491	0.02228
25	1	-0.04302	-0.02028	-0.01419
26	1	0.00758	-0.02352	0.01047
40	1	0.02766	0.01412	0.01654
41	1	-0.00024	0.02720	0.04419
42	1	-0.02082	-0.01087	-0.01478
43	1	-0.01250	0.04579	0.01038
27	1	-0.01144	-0.00821	0.01659
45	1	0.02462	0.01726	-0.01015
28	1	0.00770	-0.04140	-0.02506
47	1	0.03596	0.03975	-0.05298
48	1	0.03095	0.00595	-0.02487
49	1	-0.00887	0.02187	-0.04702
50	1	-0.00384	-0.00043	0.00636
29	1	-0.00150	-0.02463	-0.01797
30	1	0.00230	-0.02356	-0.00997
31	1	0.02266	-0.00280	-0.04829
32	1	0.01888	-0.02519	-0.02222
33	1	-0.00595	-0.00650	0.00683
56	1	-0.01964	0.03025	0.01128
57	1	-0.01546	0.04429	-0.01625
58	1	-0.00631	0.04068	0.01258
59	1	0.00952	-0.00272	0.03147
60	1	0.03436	-0.00085	0.04013

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-2.576	-0.979	0.899	2.899
sp Hybrid	-0.708	-0.328	-0.126	0.790
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-3.284	-1.306	0.773	3.618

Compound **12a**



12a

Single Point, SemiEmpirical, PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 106

in which
Number of Alpha Electrons = 53
Number of Beta Electrons = 53
Charge on the System = 0
Total Orbitals = 103

Starting PM3 calculation with 103 orbitals

Energy=-4407.414202 kcal/mol Gradient=0.032336 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -69179.1446945 (kcal/mol)
Total Energy = -110.243970822 (a.u.)
Binding Energy = -4407.4142015 (kcal/mol)
Isolated Atomic Energy = -64771.7304930 (kcal/mol)
Electronic Energy = -554459.7360955 (kcal/mol)
Core-Core Interaction = 485280.5914009 (kcal/mol)
Heat of Formation = 1.9927985 (kcal/mol)
Gradient = 0.0323357 (kcal/mol/Ang)

MOLECULAR POINT GROUP C1

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom)			Mass
			x	y	z	
1	6	0.015061	-1.02413	1.96628	-0.17525	12.01100
2	6	-0.082498	-0.17242	3.24539	-0.15205	12.01100
3	7	-0.001586	-0.16776	0.76274	0.07861	14.00700
4	6	0.263932	1.05070	0.63245	-0.65894	12.01100
5	6	-0.122705	1.76344	1.90211	-1.08281	12.01100
6	6	-0.067090	0.87155	3.12730	-1.26607	12.01100
7	8	-0.366575	1.53908	-0.47503	-0.82512	15.99900
8	6	-0.055720	-0.89297	-0.41559	0.54214	12.01100
9	6	-0.084843	-1.26698	-1.45562	-0.31327	12.01100
10	6	-0.097943	-1.94921	-2.55381	0.20001	12.01100
11	6	-0.100903	-2.26165	-2.61828	1.55316	12.01100
12	6	-0.102812	-1.88921	-1.58173	2.40311	12.01100
13	6	-0.097202	-1.20509	-0.47942	1.90546	12.01100
14	6	-0.116708	-1.72899	1.87424	-1.50709	12.01100
16	6	-0.110652	0.43754	3.52979	1.20760	12.01100
19	6	-0.056358	0.16790	3.12770	-2.62641	12.01100
26	6	-0.053360	-1.13623	2.39848	-2.66080	12.01100
27	6	-0.079667	-2.98049	1.26096	-1.58829	12.01100
28	6	-0.109379	-3.63038	1.14974	-2.81073	12.01100
29	6	-0.087471	-3.03341	1.65245	-3.96291	12.01100
30	6	-0.110267	-1.79522	2.27560	-3.88753	12.01100
22	1	0.104284	-2.23750	-3.37269	-0.46736	1.00800
23	1	0.102967	-2.79676	-3.48646	1.95117	1.00800
24	1	0.102984	-2.12975	-1.63616	3.46985	1.00800
25	1	0.110769	-0.91076	0.33179	2.58208	1.00800
17	1	0.082841	2.33446	1.70787	-2.01401	1.00800
18	1	0.078424	2.52763	2.11240	-0.30497	1.00800

15	1	0.084156	-1.77703	1.99928	0.65245	1.00800
20	1	0.069238	1.53672	4.02541	-1.23048	1.00800
21	1	0.120040	-1.01386	-1.42168	-1.37961	1.00800
31	1	0.066963	0.84100	2.71135	-3.40382	1.00800
32	1	0.060722	-0.03031	4.17615	-2.93144	1.00800
33	1	0.110948	-3.44762	0.85759	-0.68178	1.00800
34	1	0.105990	-4.61004	0.66414	-2.86728	1.00800
35	1	0.103913	-3.54091	1.55965	-4.92872	1.00800
36	1	0.106770	-1.32796	2.67790	-4.79363	1.00800
37	1	0.076969	-0.85003	4.10076	-0.40117	1.00800
38	1	0.051196	1.13017	2.74238	1.53461	1.00800
39	1	0.043638	-0.34165	3.61830	1.97643	1.00800
40	1	0.041935	0.99948	4.47329	1.19451	1.00800

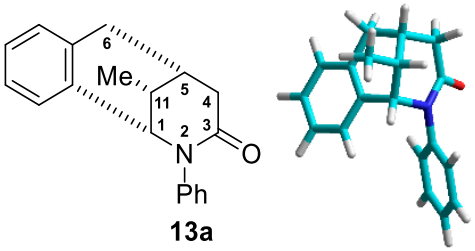
ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom)		
		x	y	z
1	6	-0.02533	0.00690	-0.00654
2	6	0.00294	-0.00030	0.01757
3	7	0.01086	0.02235	0.02251
4	6	0.01130	-0.07076	0.00133
5	6	0.02039	0.00861	0.02412
6	6	0.00238	0.01154	0.00656
7	8	-0.03525	0.05131	0.00113
8	6	-0.02111	-0.06046	-0.05580
9	6	0.00668	0.05655	0.04105
10	6	-0.04919	0.00919	0.03009
11	6	-0.01336	0.00956	-0.05273
12	6	0.03618	0.05273	0.00771
13	6	0.01075	-0.04317	0.00454
14	6	-0.02520	-0.02838	0.08205
16	6	0.00035	-0.00135	0.00292
19	6	-0.02135	0.00510	0.02098
26	6	0.04950	0.05166	-0.06985
27	6	0.01146	-0.00529	0.05785
28	6	-0.03822	-0.03280	-0.10129
29	6	-0.07582	-0.03772	-0.02844
30	6	0.06444	-0.00239	-0.01070
22	1	-0.02950	0.00236	0.02227
23	1	0.00502	0.00254	0.01199
24	1	0.07924	-0.02604	0.00267
25	1	0.05332	-0.01247	0.01998
17	1	-0.02079	0.02208	0.01055
18	1	0.03300	-0.04117	0.00232
15	1	-0.03409	0.04137	-0.02435
20	1	0.00198	0.00508	0.03210
21	1	-0.05856	-0.00182	-0.03483
31	1	-0.04519	0.00709	-0.01948
32	1	0.00563	0.01147	-0.02004
33	1	0.05474	0.00749	0.00218
34	1	-0.01479	-0.03628	-0.00866
35	1	0.00301	0.01746	-0.04632

36	1	0.04860	-0.01646	0.02470
37	1	0.00401	-0.01523	-0.01814
38	1	0.00132	0.00058	0.00163
39	1	-0.00441	0.01610	0.01353
40	1	-0.00493	0.01299	0.03283

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-1.413	2.808	0.331	3.161
sp Hybrid	-0.304	0.046	-0.520	0.604
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.717	2.854	-0.189	3.336

Compound **13a**



13a

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PM3
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
UHF Calculation:

Singlet state calculation
Number of electrons = 106
in which
Number of Alpha Electrons = 53
Number of Beta Electrons = 53
Charge on the System = 0
Total Orbitals = 103

Starting PM3 calculation with 103 orbitals

Energy=-4407.278198 kcal/mol Gradient=0.034747 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -69179.0086912 (kcal/mol)
Total Energy = -110.243754087 (a.u.)
Binding Energy = -4407.2781982 (kcal/mol)
Isolated Atomic Energy = -64771.7304930 (kcal/mol)
Electronic Energy = -554483.9032553 (kcal/mol)
Core-Core Interaction = 485304.8945641 (kcal/mol)
Heat of Formation = 2.1288018 (kcal/mol)

Gradient = 0.0347469 (kcal/mol/Ang)

MOLECULAR POINT GROUP
C1
NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
1	6	0.015733	-1.05029	2.02321	-0.14115	12.01100
2	6	-0.081202	-0.17119	3.28347	-0.07748	12.01100
3	7	-0.008829	-0.18165	0.83317	0.14716	14.00700
4	6	0.263211	1.05354	0.71668	-0.56920	12.01100
5	6	-0.122488	1.75602	1.99265	-0.99728	12.01100
6	6	-0.068037	0.84304	3.19772	-1.22204	12.01100
7	8	-0.363604	1.56128	-0.38458	-0.71401	15.99900
8	6	-0.055968	-0.89967	-0.35814	0.58935	12.01100
9	6	-0.085053	-1.28056	-1.37682	-0.28875	12.01100
10	6	-0.098430	-1.95709	-2.48833	0.20228	12.01100
11	6	-0.099898	-2.25511	-2.58833	1.55675	12.01100
12	6	-0.103485	-1.87474	-1.57392	2.42924	12.01100
13	6	-0.093566	-1.19733	-0.45751	1.95331	12.01100
14	6	-0.113009	-1.73142	1.90296	-1.48103	12.01100
17	6	-0.114310	-1.00147	4.55264	-0.11795	12.01100
20	6	-0.055914	0.16431	3.15655	-2.59175	12.01100
27	6	-0.051521	-1.12685	2.40823	-2.63617	12.01100
28	6	-0.080600	-2.97645	1.27613	-1.57005	12.01100
29	6	-0.109956	-3.60374	1.13017	-2.80036	12.01100
30	6	-0.087941	-2.99184	1.61177	-3.95395	12.01100
31	6	-0.110633	-1.76263	2.25103	-3.87148	12.01100
22	1	0.119145	-1.03860	-1.31384	-1.35629	1.00800
23	1	0.104258	-2.25267	-3.28923	-0.48342	1.00800
24	1	0.102961	-2.78518	-3.46731	1.93750	1.00800
25	1	0.103090	-2.10389	-1.65648	3.49673	1.00800
26	1	0.110699	-0.89712	0.33520	2.64846	1.00800
15	1	0.083615	-1.82135	2.06126	0.66920	1.00800
18	1	0.082789	2.35401	1.79233	-1.90983	1.00800
19	1	0.076317	2.49450	2.23183	-0.20388	1.00800
16	1	0.076654	0.39240	3.28354	0.89007	1.00800
21	1	0.068984	1.48587	4.11239	-1.19959	1.00800
32	1	0.067157	0.85992	2.73423	-3.34605	1.00800
33	1	0.062173	-0.04425	4.19487	-2.92476	1.00800
34	1	0.110898	-3.45656	0.88925	-0.66308	1.00800
35	1	0.105872	-4.57757	0.63371	-2.86245	1.00800
36	1	0.103941	-3.48111	1.48993	-4.92586	1.00800
37	1	0.106808	-1.28461	2.63980	-4.77786	1.00800
38	1	0.044206	-1.67944	4.60744	0.74390	1.00800
39	1	0.052952	-1.61828	4.61281	-1.02539	1.00800
40	1	0.042983	-0.36023	5.44350	-0.09485	1.00800

ATOMIC GRADIENTS

Atom	Z	Gradients(kcal/mol/Angstrom) x	y	z
1	6	0.01148	-0.00365	-0.01419

2	6	-0.00646	0.00628	0.00230
3	7	-0.01010	0.00614	0.04515
4	6	0.01722	-0.04385	-0.03059
5	6	0.00384	0.01040	0.01165
6	6	0.00784	0.00787	-0.00117
7	8	-0.01938	0.04498	0.00203
8	6	-0.03611	0.01830	0.08862
9	6	-0.07002	-0.07038	0.00961
10	6	0.00377	0.07392	-0.02995
11	6	-0.00195	0.04587	0.06318
12	6	0.01619	-0.06619	-0.02569
13	6	0.04460	-0.01494	-0.05835
14	6	-0.03790	-0.05572	0.10169
17	6	-0.00526	0.00117	-0.00032
20	6	-0.02810	-0.00158	0.00107
27	6	0.09344	0.05314	-0.05804
28	6	0.03615	-0.01500	0.05720
29	6	-0.04263	-0.01535	-0.06580
30	6	-0.06174	-0.06304	-0.05417
31	6	0.09092	0.04492	-0.05286
22	1	-0.06448	0.03267	0.00551
23	1	-0.07511	0.04311	-0.00406
24	1	0.00623	-0.00293	0.01072
25	1	0.06508	-0.03250	0.01889
26	1	0.05895	-0.02502	0.01659
15	1	-0.00694	0.00411	-0.00983
18	1	0.00175	-0.00181	0.01681
19	1	0.00600	0.00983	0.01283
16	1	0.00204	-0.00334	-0.00495
21	1	0.00109	0.00784	-0.00343
32	1	0.01037	0.02034	0.00220
33	1	-0.01892	-0.00074	0.00423
34	1	-0.00342	0.00204	-0.01115
35	1	0.00191	-0.01690	-0.02029
36	1	0.02600	-0.01839	-0.01548
37	1	0.00580	0.02428	-0.00118
38	1	-0.00915	-0.00963	0.00255
39	1	-0.01227	-0.00192	-0.00632
40	1	-0.00073	0.00568	-0.00502

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-1.493	2.797	0.240	3.179
sp Hybrid	-0.288	0.023	-0.546	0.618
pd Hybrid	0.000	0.000	0.000	0.000
Sum	-1.781	2.820	-0.306	3.349

14. References

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