

Supporting Information

Catalytic Cascade Reaction To Access Cyclopentane-Fused Heterocycles: Expansion of Pd-TMM Cycloaddition

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Acknowledgment We acknowledge the Korea Basic Science Institute (KBSI) for the HRMS and X-ray analysis.

I. General Methods

Unless otherwise stated, all commercial reagents including catalysts and solvents were used without additional purification. The pyridinium zwitterions and quinolinium zwitterions were prepared according to reported procedure.^{S1} Analytical thin layer chromatography (TLC) was performed on Merck pre-coated silica gel 60 F254 plates. Visualization on TLC was achieved by use of UV light (254 nm). Flash column chromatography was undertaken on silica gel (Merck Kiesel gel 60 F254 230-400 mesh). ¹H NMR was recorded on Bruker DPX FT (300 and 400 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). ¹³C NMR was recorded on Bruker FT AM 400 (100 MHz) and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-d. Infrared spectra were recorded on a JASCO FT/IR-460 plus FT-IR spectrometer. Frequencies are given in reciprocal centimeters (cm-1) and only selected absorbance is reported. High resolution mass spectra were obtained from the Korea Basic Science Institute (Daegu) by EI method.

II. Experimental Procedure

II-1. General procedure for the optimization studies (Table 1 and Table S1)

To a test tube with a triangular-shaped stir bar were added pyridinium zwitterion (**1a**, 0.1 mmol), 3-acetoxy-2-trimethylsilylmethyl-1-propene (**2**, 2.0 equiv), Pd(PPh₃)₄ catalyst, and solvent (1.0 mL) under N₂ atmospheric conditions. The reaction mixture was stirred at room temperature for 2 h, filtered through a pad of celite and then washed with CH₂Cl₂ (10 mL x 3). Organic solvents were removed under reduced pressure. The NMR yield of desired product **3a** was determined by integration using an internal standard (CH₂Br₂).

7-methylene-3,5-diphenyl-1-tosyl-5,5a,6,7,8,9a-hexahydro-1H-cyclopenta[d]imidazo[1,2-a]pyridine (3a): air/moisture sensitive compound; yellow oil (2.1 mg, Isolated yield 4%); R_f = 0.4 (hexane/EtOAc = 6:1); ¹H NMR (400 MHz, CDCl₃) δ 7.50-7.48 (m, 2H), 7.44-7.40 (m, 4H), 7.40-7.35 (m, 2H), 7.22-7.18 (m, 1H), 7.14-7.10 (m, 2H), 6.94-6.91 (m, 2H), 6.84 (d, *J* = 8.12 Hz, 2H), 6.35-6.33 (m, 1H); 6.11(s, 1H), 4.93 (d, *J* = 25.8 Hz, 2H), 4.15-4.12 (m, 1H), 4.02-3.95 (m, 1H), 3.03-2.97 (m, 1H), 2.82-2.71 (m, 3H), 2.25 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 149.9, 142.2, 138.7, 136.8, 131.7, 128.9, 128.8, 128.6, 128.5, 128.1, 127.4, 127.0, 126.0, 123.0, 106.9, 106.9, 103.4, 85.8, 44.1, 40.6, 35.2, 32.1, 21.3.

Table S1. Optimization Studies.

entry	solvent	x mol % [Pd]	yield (%) ^a
1	DME	10	4
2	CH ₂ Cl ₂	10	27
3	CHCl ₃	10	56
4	1,4-Dioxane	10	65

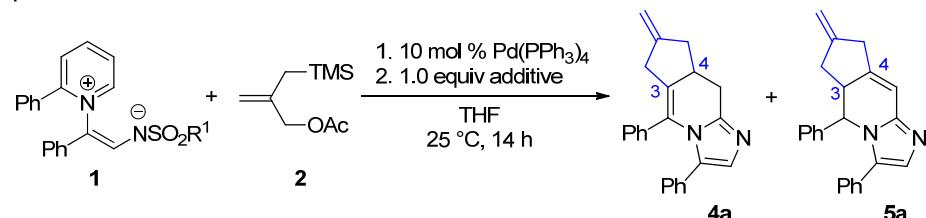
5	Benzene	10	55
6	THF	10	96
7	THF	5	51 ^b

^a NMR yields of **3a**. ^b 5 mol % Pd(PPh₃)₄ was used as a catalyst.

II-2. General procedure for the optimization studies (Table S2)

To a test tube with a triangular-shaped stir bar were added pyridinium zwitterion (**1**, 0.1 mmol), 3-acetoxy-2-trimethylsilylmethyl-1-propene (**2**, 2.0 equiv), Pd(PPh₃)₄ (10 mol %), and THF (1.0 mL) under N₂ atmospheric conditions. The reaction mixture was stirred at room temperature for 2 h, and then added the indicated acid. The reaction mixture was stirred for 12 h more, and the reaction was quenched with H₂O. The mixture was extracted with CH₂Cl₂; the organic phases were combined, dried over MgSO₄. Organic solvents were removed under reduced pressure. The NMR yield of desired product **4a** and **5a** were determined by integration using an internal standard (CH₂Br₂).

Table S2. Optimization Studies.



entry	additive	R ¹	yield (%) ^{a,b}
1	Et ₃ N	p-CH ₃ C ₆ H ₄	<1
2	K ₂ CO ₃	p-CH ₃ C ₆ H ₄	<1
3	TsOH	p-CH ₃ C ₆ H ₄	15 (20)
4	CF ₃ CO ₂ H	p-CH ₃ C ₆ H ₄	0 (20)
5	HCO ₂ H	p-CH ₃ C ₆ H ₄	40 (20)
6	CH ₃ CO ₂ H	p-CH ₃ C ₆ H ₄	40 (20)
7	CH ₃ CO ₂ H (2.0 equiv)	p-CH ₃ C ₆ H ₄	78 (20)
8	CH ₃ CO ₂ H (2.0 equiv)	p-CF ₃ C ₆ H ₄	72 (13)
9	CH ₃ CO ₂ H (2.0 equiv)	p-MeOC ₆ H ₄	58 (18)

^a NMR yields of **4a**. ^b NMR yields of **5a** in parentheses.

II-3. Procedure for the Pd(0)-catalyzed cycloaddition of pyridinium zwitterion and TMM (Scheme 2)

To a test tube with a triangular-shaped stir bar were added pyridinium zwitterion (**1**, 0.1 mmol), 3-acetoxy-2-trimethylsilylmethyl-1-propene (**2**, 2.0 equiv), Pd(PPh₃)₄ (10 mol %), and THF (1.0 mL) under N₂ atmospheric conditions. The reaction mixture was stirred at room temperature for 2 h, and then added the acetic acid (2.0 equiv). The reaction mixture was stirred for 2 h more at 50 °C, and the reaction was quenched with H₂O. The mixture was extracted with CH₂Cl₂; the organic phases were combined, dried over MgSO₄. Organic solvents were removed under reduced pressure. The organic residue was purified by chromatography on silica gel to give the desired product **4** and **5**.

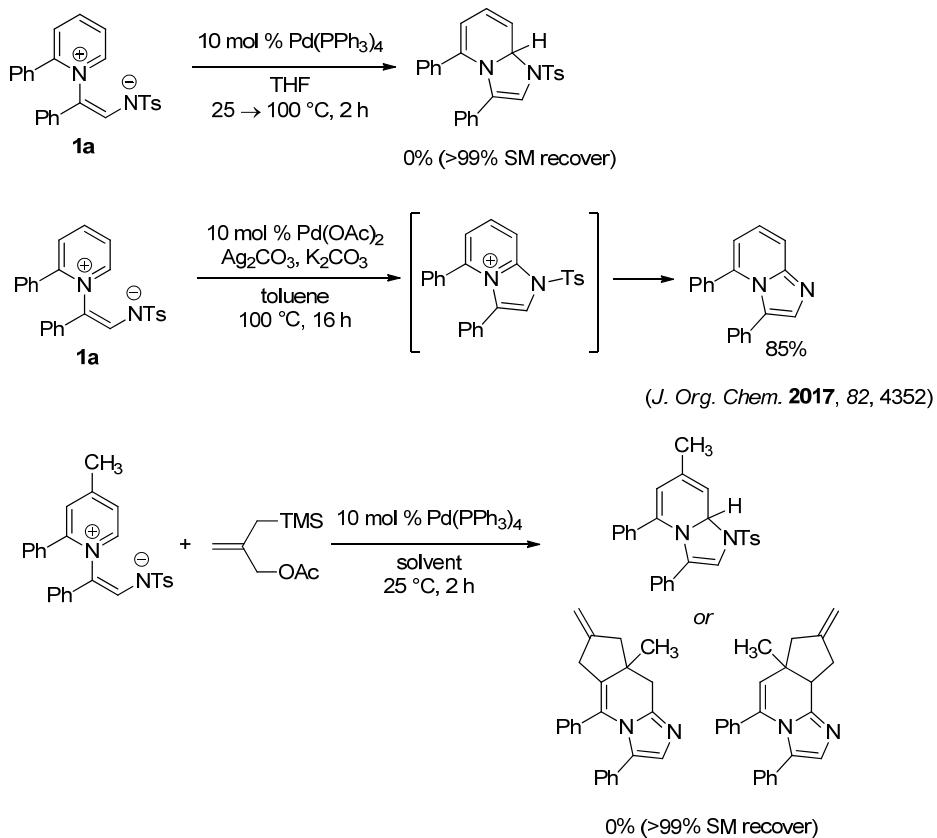
II-4 Representative procedure for the cycloaddition between 1.0 mmol scale of pyridinium zwitterion (**1a**) and Pd-TMM

To a 50 mL round bottom flask with a stir bar were added pyridinium zwitterion (**1a**, 1.0 mmol), 3-acetoxy-2-trimethylsilylmethyl-1-propene (**2**, 2.0 equiv), Pd(PPh₃)₄ (10 mol %), and THF (5.0 mL) under N₂ atmospheric conditions. The reaction mixture was stirred at 30 °C for 1.5 h, and then added the acetic acid (2.0 equiv). The reaction mixture was stirred for 2 h more at 50 °C, and the reaction was quenched with H₂O. The mixture was extracted with CH₂Cl₂; the organic phases were combined, dried over MgSO₄. Organic solvents were removed under reduced pressure. The organic residue was purified by chromatography on silica gel to give the desired product **4a** in 67% (217.3mg).

II-5. Procedure for the Pd(0)-catalyzed cycloaddition of 3-substituted pyridinium zwitterion and TMM (Scheme 3)

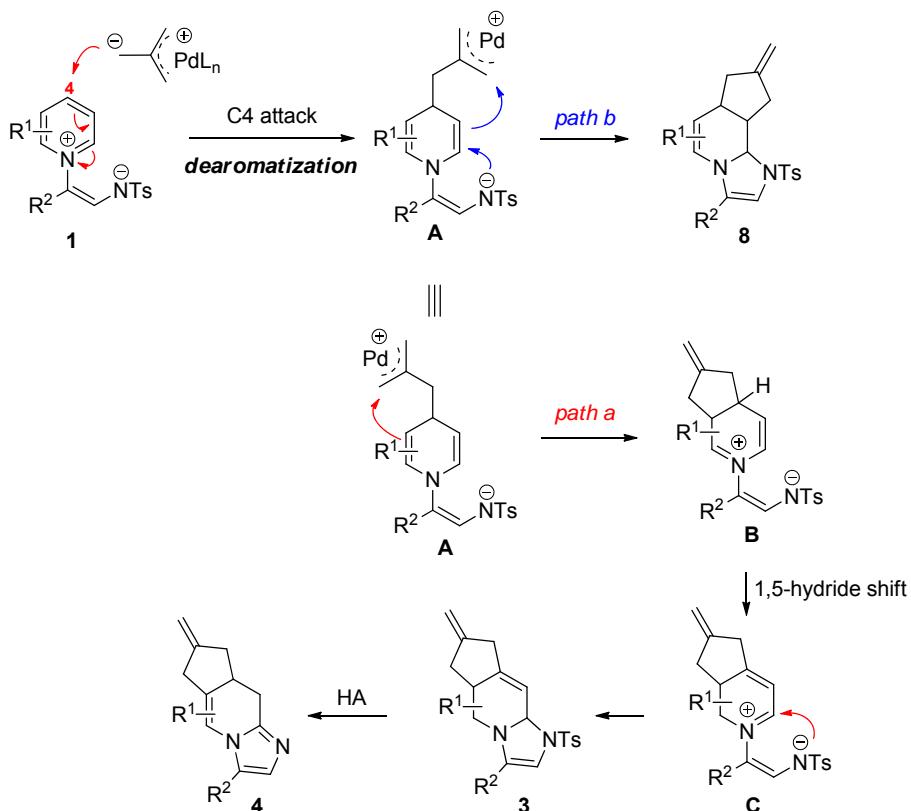
To a test tube with a triangular-shaped stir bar were added 3-substituted pyridinium zwitterion (**7**, 0.1 mmol), 3-acetoxy-2-trimethylsilylmethyl-1-propene (**2**, 2.0 equiv), Pd(PPh₃)₄ (10 mol %), and THF (1.0 mL) under N₂ atmospheric conditions. The reaction mixture was stirred at 80 °C for 5 h, and the reaction was quenched with H₂O. The mixture was extracted with CH₂Cl₂; the organic phases were combined, dried over MgSO₄. Organic solvents were removed under reduced pressure. The organic residue was purified by chromatography on silica gel to give the desired product **9**.

II-6. Background reactions for mechanistic insight

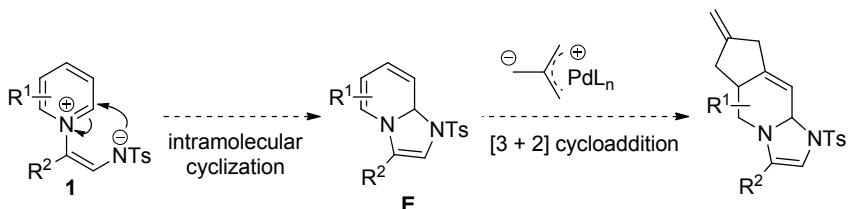


Scheme S1. Experimental Mechanism Studies

A. Dearomative [3 + 2] cycloaddition of pyridinium zwitterion and Pd-TMM: major pathway



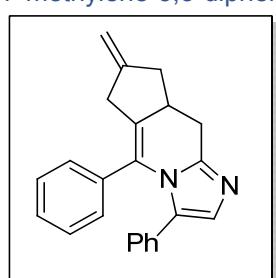
B. Cascade reaction via intramolecular cyclization/[3 + 2] cycloaddition



Scheme S2. Possible Reaction Mechanism

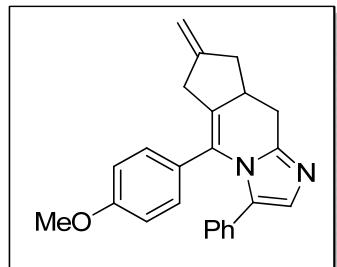
III. Spectroscopic data

7-methylene-3,5-diphenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (**4a**):



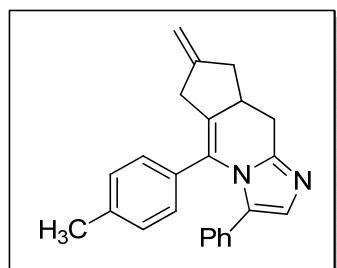
Red solid (23.4 mg, 72%); m.p. 95.8–99.2 °C; $R_f = 0.2$ (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.91–6.81 (m, 11H), 4.82 (d, $J = 24.7$ Hz, 2H), 3.40 (d, $J = 21.0$ Hz, 1H), 3.24–3.16 (m, 2H), 2.99 (d, $J = 21.0$ Hz, 1H), 2.83 (q, $J = 8.1$ Hz, 1H), 2.59 (t, $J = 16.5$ Hz, 1H), 2.22–2.16 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.8, 147.4, 133.9, 133.4, 131.1, 130.4, 128.8, 128.0, 127.4, 127.3, 126.8, 126.3, 107.2, 38.8, 38.6, 36.7, 30.9; IR (liquid) ν 3057.6, 2924.5, 2853.2, 1669.1, 1605.5, 1517.7, 1481.1, 1445.4, 1384.6, 1137.8, 891.9 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{23}\text{H}_{20}\text{N}_2$ [M^+]: 324.1626, found: 324.1626.

5-(4-methoxyphenyl)-7-methylene-3-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4b**):**



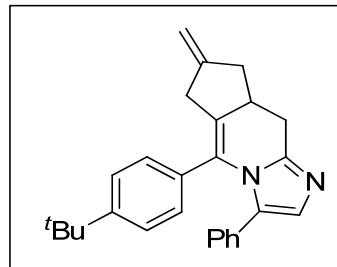
Red solid (28.2mg, 80%); m.p. 99.7-100.2 °C; R_f = 0.3 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.89-6.84 (m, 8H), 6.41 (d, J = 7.4 Hz, 2H), 4.81 (d, J = 23.8 Hz, 2H), 3.54 (s, 3H), 3.36 (d, J = 20.9, 1H), 3.23-3.15 (m, 2H), 2.98 (d, J = 20.9 Hz, 1H), 2.84-2.78 (m, 1H), 2.58(t, J = 16.5 Hz, 1H), 2.21-2.15 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.5, 149.0, 147.3, 132.0, 131.1, 130.5, 129.9, 128.6, 128.1, 127.2, 126.8, 126.3, 126.1, 112.8, 107.0, 55.0, 38.9, 38.5, 36.7, 30.9; IR (liquid) ν 3073.0, 2956.3, 2836.8, 1668.1, 1608.3, 1512.9, 1482.0, 1445.4, 1385.6, 1138.8, 894.8 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}$ [M^+]: 354.1732, found: 354.1730.

7-methylene-3-phenyl-5-(p-tolyl)-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4c**):**



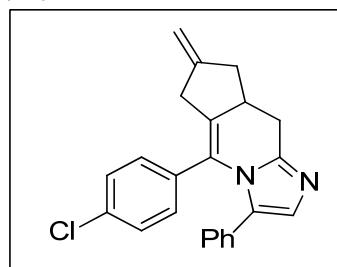
Red solid (18.8mg, 56%); m.p. 99.3-101.3 °C; R_f = 0.3 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.90-6.81 (m, 8H), 6.69-6.68 (m, 2H), 4.81 (d, J = 24.4 Hz, 2H), 3.41-3.36 (m, 1H), 3.23-3.16 (m, 2H), 2.99 (d, J = 20.8 Hz, 1H), 2.85-2.79 (m, 1H), 2.58 (t, J = 16.4 Hz, 1H), 2.21-2.15 (m, 1H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.0, 147.3, 137.1, 132.6, 131.2, 131.0, 130.5, 128.9, 128.5, 128.1, 128.0, 127.2, 126.8, 126.0, 107.1, 38.9, 38.6, 36.7, 30.9, 20.9; IR (liquid) ν 3055.7, 2920.7, 1668.1, 1606.4, 1514.8, 1482.0, 1446.4, 1386.6, 1138.8, 894.8 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2$ [M^+]: 338.1783, found: 338.1781.

5-(4-(tert-butyl)phenyl)-7-methylene-3-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4d**):**



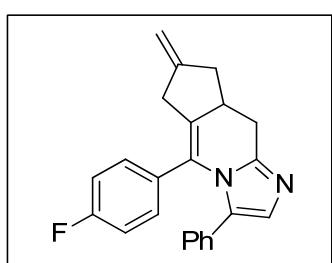
Red solid (23.0mg, 60%); m.p. 93.1-98.6 °C; R_f = 0.3 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.86-6.79 (m, 10H), 4.84 (d, J = 24.2Hz, 2H), 3.44-3.38 (m, 1H), 3.27-3.17 (m, 2H), 3.05 (d, J = 21.1 Hz, 1H), 2.88-2.81 (m, 1H), 2.61 (t, J = 16.7 Hz, 1H), 2.23-2.18 (m, 1H), 1.07 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 150.3, 149.1, 147.2, 132.4, 131.4, 130.7, 130.6, 129.0, 128.6, 128.4, 127.2, 126.6, 126.2, 124.3, 107.1, 39.1, 38.6, 36.7, 34.3, 30.9; IR (liquid) ν 3073.0, 3053.7, 3033.5, 2961.2, 2902.3, 2866.7, 1668.1, 1606.4, 1516.7, 1383.7, 1267.9 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{27}\text{H}_{28}\text{N}_2$ [M^+]: 380.2252, found: 380.2252.

5-(4-chlorophenyl)-7-methylene-3-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4e**):**



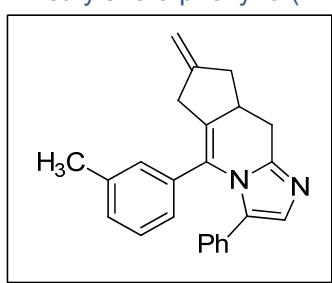
Red oil (28.7mg, 80%); R_f = 0.2 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.99-6.95 (m, 10H), 4.91 (d, J = 25.8 Hz, 2H), 3.47-3.41 (m, 1H), 3.34-3.28 (m, 2H), 3.04 (d, J = 21.0 Hz 1H), 2.96-2.89 (m, 1H), 2.67 (t, J = 16.7 Hz, 1H), 2.31-2.25 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.6, 147.3, 134.2, 133.2, 132.5, 131.1, 130.3, 129.9, 128.3, 127.9, 127.7, 127.6, 126.8, 126.7, 107.5, 38.9, 38.8, 36.8, 30.8; IR (solid) ν 1645.9, 1515.8, 1481.1, 1385.6, 1140.7, 1091.5, 816.7, 758.9 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{23}\text{H}_{19}\text{ClN}_2$ [M^+]: 358.1237, found: 358.1235.

5-(4-fluorophenyl)-7-methylene-3-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (**4f**):



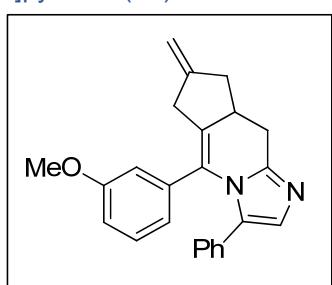
Red solid (24.6 mg, 72%); m.p. 115.0-119.5 °C; R_f = 0.3 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.90-6.87 (m, 8H), 6.62-6.58 (m, 2H), 4.85 (d, J = 25.5 Hz, 2H), 3.39-3.34 (m, 1H), 3.27-3.17 (m, 2H), 2.97 (d, J = 21.0 Hz, 1H), 2.88-2.82 (m, 1H), 2.60 (t, J = 16.7, 1H), 2.24-2.19 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.8, 160.4, 148.7, 147.3, 133.5, 131.1, 130.4, 130.3, 130.1, 130.1, 128.2, 128.0, 127.5, 126.9, 126.6, 114.6, 114.4, 107.4, 38.9, 38.7, 36.7, 30.8; IR (liquid) ν 3073.0, 2924.5, 2853.2, 1669.1, 1604.5, 1509.0, 1482.0, 1446.4, 1385.6, 1138.8, 894.8 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{23}\text{H}_{19}\text{FN}_2$ [M+]: 342.1532, found: 342.1530.

7-methylene-3-phenyl-5-(m-tolyl)-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (**4g**):



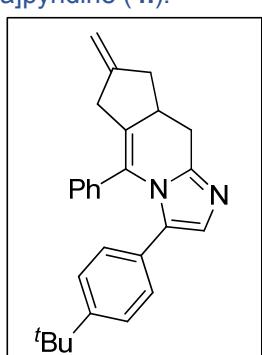
Red oil (20.2 mg, 60%); R_f = 0.2 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.89-6.79 (m, 8H), 6.64-6.62 (m, 2H), 4.81 (d, J = 22.7 Hz, 2H), 3.41-3.35 (m, 1H), 3.23-3.15 (m, 2H), 3.00 (d, J = 20.8 Hz, 1H), 2.85-2.78 (m, 1H), 2.57 (t, J = 16.5 Hz, 1H), 2.20-2.15 (m, 1H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.0, 147.3, 136.9, 133.7, 132.9, 131.3, 130.7, 129.0, 128.0, 127.4, 127.1, 126.7, 126.3, 107.2, 38.9, 38.6, 36.8, 30.9, 21.0; IR (liquid) ν 3056.6, 2954.1, 2855.1, 1669.1, 1605.5, 1518.7, 1482.0, 1446.4, 1386.6, 1138.8, 886.1 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2$ [M+]: 338.1783, found: 338.1781.

5-(3-methoxyphenyl)-7-methylene-3-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (**4h**):



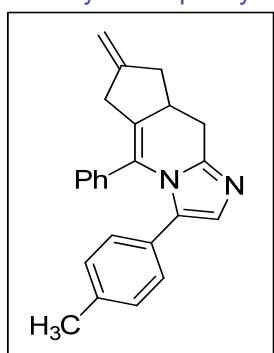
Red solid (21.7 mg, 61%); m.p. 71.6-79.4 °C; R_f = 0.2 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.92-6.87 (m, 7H), 6.66-6.53 (m, 1H), 6.41-6.39 (m, 2H), 4.83 (d, J = 22.7 Hz, 2H), 3.51 (s, 3H), 3.40 (d, J = 21.0 Hz, 1H), 3.24-3.19 (m, 2H), 3.03 (d, J = 21.0 Hz, 1H), 2.86-2.80 (m, 1H), 2.59 (t, J = 16.5 Hz, 1H), 2.22-2.16 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.5, 148.8, 147.3, 135.1, 133.4, 131.2, 130.5, 128.6, 128.4, 127.9, 127.2, 126.7, 126.3, 107.2, 55.0, 38.8, 38.6, 36.8, 30.8; IR (liquid) ν 3073.0, 2956.3, 2834.9, 1669.1, 1600.6, 1518.7, 1488.8, 1447.3, 1386.6, 1151.3, 885.2 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}$ [M+]: 354.1732, found: 354.1732.

3-(4-(tert-butyl)phenyl)-7-methylene-5-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (**4i**):



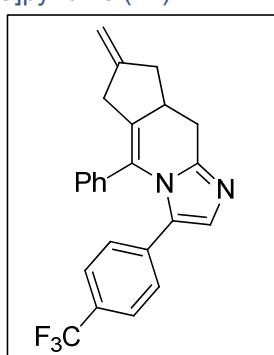
Red solid (19.9 mg, 52%); m.p. 94.7-96.0 °C; R_f = 0.3 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.93-6.75 (m, 10H), 4.83 (d, J = 26.4 Hz, 2H), 3.41-3.35 (m, 1H), 3.26-3.18 (m, 2H), 2.99 (d, J = 21.0 Hz, 1H), 2.87-2.80 (m, 1H), 2.60 (t, J = 16.5 Hz, 1H), 2.23-2.17 (m, 1H), 1.09 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.1, 148.9, 146.9, 133.9, 133.0, 131.3, 129.1, 128.8, 128.3, 127.5, 127.3, 127.2, 126.2, 124.1, 107.1, 39.1, 38.7, 36.7, 34.2, 30.9, 30.9; IR (liquid) ν 3058.6, 2961.2, 2904.3, 2866.7, 1669.1, 1617.9, 1523.5, 1493.6, 1445.4, 1378.9, 1362.5, 1182.2, 1136.8, 893.8 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{27}\text{H}_{28}\text{N}_2$ [M+]: 380.2252, found: 380.2255.

7-methylene-5-phenyl-3-(p-tolyl)-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4j):



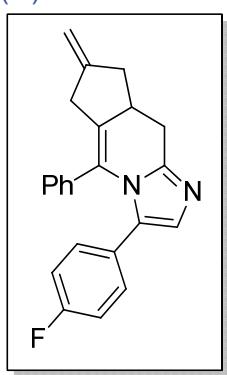
Red solid (13.9 mg, 41%); m.p. 98.3-99.9 °C; R_f = 0.3 (hexane/Acetone = 2:1); ^1H NMR (400 MHz, CDCl_3) δ 6.91-6.77 (m, 8H), 6.66 (d, J = 7.9 Hz, 2H), 4.83 (d, J = 24.6 Hz, 2H), 3.43-3.38 (m, 1H), 3.24-3.18 (m, 2H), 3.00 (d, J = 20.8 Hz, 1H), 2.86-2.80 (m, 1H), 2.59 (t, J = 16.4 Hz, 1H), 2.22-2.17 (m, 1H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.0, 147.1, 135.9, 134.0, 133.4, 131.3, 129.0, 128.6, 128.0, 127.9, 127.6, 127.4, 127.2, 126.5, 107.2, 38.9, 38.7, 36.8, 30.9, 20.9; IR (liquid) ν 3056.6, 3027.7, 2954.4, 2922.6, 2854.1, 1698.0, 1668.1, 1560.1, 1493.6, 1445.4, 1383.7, 1182.2, 1137.8, 892.9 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2$ [M^+]: 338.1783, found: 338.1780.

7-methylene-5-phenyl-3-(4-(trifluoromethyl)phenyl)-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4k):



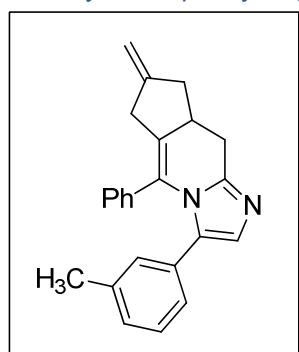
Red oil (33.2 mg, 85%); R_f = 0.3 (hexane/Acetone = 2:1); ^1H NMR (400 MHz, CDCl_3) δ 7.11-6.88 (m, 10H), 4.84 (d, J = 25.0 Hz, 2H), 3.45-3.39 (m, 1H), 3.28-3.19 (m, 2H), 3.01 (d, J = 21.1 Hz, 1H), 2.89-2.82 (m, 1H), 2.61 (t, J = 16.8 Hz, 1H), 2.24-2.18 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.6, 148.2, 134.1, 134.1, 133.8, 133.7, 129.8, 128.5, 128.2, 128.1, 127.9, 127.8, 127.7, 127.6, 125.2, 124.2, 124.1, 124.1, 122.5, 107.4, 38.9, 38.6, 36.7, 30.8; IR (liquid) ν 3058.6, 2891.7, 2853.2, 1671.0, 1653.7, 1618.9, 1523.5, 1493.6, 1445.4, 1416.5, 1382.7, 1164.8, 1123.3, 892.9 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{19}\text{F}_3\text{N}_2$ [M^+]: 392.1500, found: 392.1502.

3-(4-fluorophenyl)-7-methylene-5-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4l):



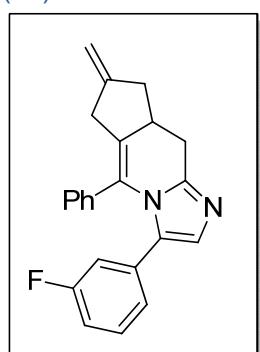
Red solid (20.8 mg, 61%); m.p. 132.0-138.4 °C; R_f = 0.4 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.93-6.83 (m, 8H), 6.59-6.54 (m, 2H), 4.84 (d, J = 25.5 Hz, 2H), 3.43-3.37 (m, 1H), 3.26-3.17 (m, 2H), 3.00 (d, J = 21.0 Hz, 1H), 2.89-2.82 (m, 1H), 2.61 (t, J = 16.5 Hz, 1H), 2.24-2.19 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.6, 160.1, 148.8, 147.4, 133.9, 133.7, 130.2, 129.9, 129.8, 128.8, 127.7, 127.6, 126.8, 126.7, 126.7, 114.4, 114.2, 107.3, 39.0, 38.7, 36.8, 30.9; IR (solid) ν 3073.0, 2956.3, 2836.8, 1608.3, 1512.6, 1385.6, 1249.7, 1176.4, 1249.7, 756.9 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{23}\text{H}_{20}\text{FN}_2$ [M^+]: 343.1609, found: 343.1605.

7-methylene-5-phenyl-3-(m-tolyl)-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4m):



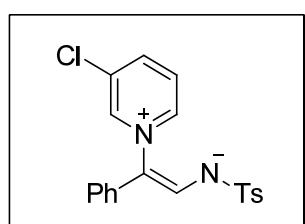
Red solid (23.3 mg, 69%); m.p. 77.3-78.9 °C; R_f = 0.4 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.99-6.94 (m, 6H), 6.87-6.84 (m, 2H), 6.73-6.72 (m, 2H), 4.91 (d, J = 24.8 Hz, 2H), 3.52-3.46 (m, 1H), 3.34-3.25 (m, 2H), 3.08 (d, J = 20.7 Hz, 1H), 2.95-2.89 (m, 1H), 2.68 (t, J = 16.5 Hz, 1H), 2.31-2.25 (m, 1H), 2.08 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.0, 147.3, 136.6, 134.1, 133.5, 131.4, 130.2, 129.2, 129.0, 128.6, 127.4, 127.3, 127.1, 126.5, 125.0, 107.2, 39.0, 38.7, 36.8, 30.9, 21.0; IR (liquid) ν 3055.7, 2954.4, 2918.7, 2890.8, 2857.0, 1670.1, 1608.3, 1516.7, 1493.6, 1445.4, 1380.8, 1136.8, 887.1 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2$ [M^+]: 338.1783, found: 338.1779.

3-(3-fluorophenyl)-7-methylene-5-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4n):



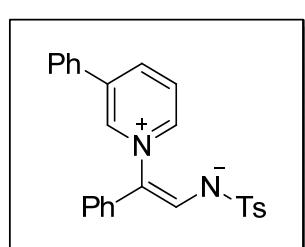
Red solid (23.2 mg, 68%); m.p. 80.1-82.7 °C; R_f = 0.4 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 6.98-6.80 (m, 7H), 6.71 (d, J = 7.7 Hz, 1H), 6.59-6.50 (m, 2H), 4.83 (d, J = 24.4 Hz, 2H), 3.41 (d, J = 21.0 Hz, 1H), 3.25-3.18 (m, 2H), 3.01 (d, J = 21.0 Hz, 1H), 2.87-2.81 (m, 1H), 2.59 (t, J = 16.6 Hz, 1H), 2.23-2.17 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.8, 160.4, 148.7, 147.8, 133.9, 133.8, 132.6, 132.5, 129.9, 129.9, 128.9, 128.8, 128.6, 128.4, 127.6, 127.5, 127.3, 123.6, 123.6, 115.0, 114.8, 113.2, 113.0, 107.3, 38.8, 38.6, 36.7, 30.8; IR (liquid) ν 3061.4, 2923.6, 2853.2, 1670.1, 1615.1, 1585.2, 1517.7, 1483.9, 1446.4, 1385.6, 1185.0, 1136.8, 898.7 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{23}\text{H}_{19}\text{FN}_2$ [M^+]: 342.1532, found: 342.1533.

(Z)-(2-(3-chloropyridin-1-iom-1-yl)-2-phenylvinyl)(tosyl)amide (7a):



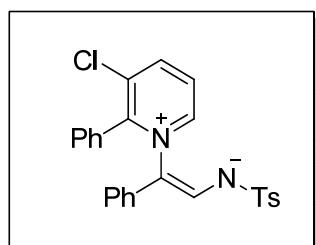
Red solid; (20.3 mg, 53%); m.p. 74-76.1 °C; R_f = 0.4 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, CDCl_3) δ 8.95 (d, J = 6.2 Hz, 1H), 8.90 (s, 1H), 7.95 (d, J = 8.3 Hz, 1H), 7.88 (s, 1H), 7.78 (d, J = 8.2 Hz, 2H), 7.69 (t, J = 7.3 Hz, 1H), 7.32 (t, J = 7.6 Hz, 2H), 7.24-7.20 (m, 3H), 7.11 (d, J = 7.24 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.1, 142.8, 142.2, 141.9, 140.7, 139.9, 136.2, 134.8, 129.6, 129.4, 129.1, 127.5, 126.6, 125.9, 125.1, 115.8, 21.3; IR (liquid) ν 3052.8, 1614.1, 1586.2, 1474.3, 1444.4, 1433.8, 1257.4, 1132.9, 1082.8 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{20}\text{H}_{18}\text{ClN}_2\text{O}_2\text{S}$ [$M+1$]: 385.0774, found: 385.0772.

(Z)-(2-phenyl-2-(3-phenylpyridin-1-iom-1-yl)vinyl)(tosyl)amide (7b):



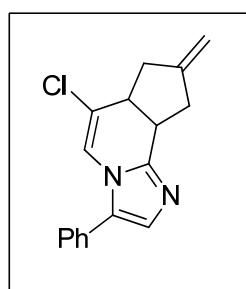
Red solid; (75.0 mg, 88%); m.p. 97-109 °C; R_f = 0.4 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, CDCl_3) δ 8.94 (s, 1H), 8.56 (d, J = 6.1 Hz, 1H), 8.31 (d, J = 8.1 Hz, 1H), 7.96 (s, 1H), 7.86-7.82 (m, 1H), 7.78 (d, J = 8.1 Hz, 2H), 7.52-7.44 (m, 5H), 7.30-7.28 (m, 2H), 7.20-7.13 (m, 3H), 7.06 (d, J = 7.4 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 144.6, 143.3, 142.8, 140.6, 140.3, 140.1, 139.9, 136.5, 133.1, 130.2, 129.6, 129.1, 128.9, 127.5, 127.1, 125.8, 125.7, 123.4, 117.4, 21.3; IR (liquid) ν 3059.5, 2982.4, 2922.6, 1590.0, 1479.1, 1445.4, 1421.3, 1288.2, 1246.8, 1132.9, 1083.8 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_2\text{S}$ [$M+1$]: 427.1477, found: 427.1475.

(Z)-(2-(3-chloro-2-phenylpyridin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (**7d**):



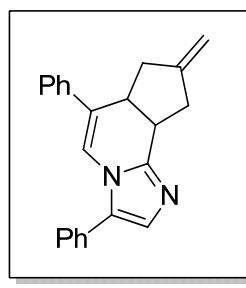
Red solid; (32.2 mg, 70%); m.p. 136-148 °C; R_f = 0.4 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, CDCl_3) δ 8.54-8.51 (m, 2H), 8.02 (dd, J = 4.8 Hz, 1H), 7.74 (d, J = 8.2 Hz, 2H), 7.67 (s, 1H), 7.33-7.21 (m, 5H), 7.04-6.98 (m, 4H), 6.93-6.89 (m, 1H), 6.76-6.75 (m, 1H), 6.44-6.42 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 156.3, 149.6, 145.6, 143.2, 140.2, 139.9, 136.7, 136.0, 130.8, 129.0, 128.4, 128.3, 128.0, 127.6, 127.3, 125.9, 124.7, 121.1, 118.7, 21.3; IR (liquid) ν 3058.6, 2986.2, 2921.6, 1590.0, 1494.6, 1446.4, 1341.3, 1296.9, 1243.9, 1132.0, 1083.8 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{26}\text{H}_{22}\text{ClN}_2\text{O}_2\text{S}$ [$M+1$]: 461.1088, found: 461.1085.

6-chloro-8-methylene-3-phenyl-7,8,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine (**9a**):



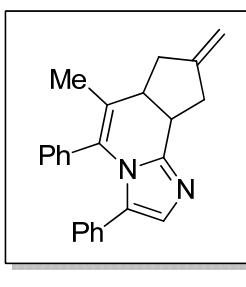
yellow oil (20.1 mg, 71%); R_f = 0.3 (hexane/EtOAc = 1:1); ^1H NMR (400 MHz, CDCl_3) δ 7.48-7.44 (m, 2H), 7.41-7.37 (m, 1H), 7.36-7.33 (m, 2H), 7.02 (s, 1H), 6.93 (m, 1H), 4.98-4.95 (m, 2H), 3.75-3.70 (m, 1H), 3.19 (q, J = 8.1 Hz, 1H), 3.05-2.99 (m, 1H), 2.94-2.83 (m, 2H), 2.60-2.54 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.8, 145.1, 130.5, 128.9, 128.7, 128.6, 128.2, 127.0, 124.9, 118.6, 107.3, 44.1, 38.6, 38.1, 37.8; IR (liquid) ν 3073.0, 2922.6, 2851.2, 1737.6, 1659.4, 1605.5, 1510.9, 1480.1, 1447.3, 1409.7, 1260.3 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{17}\text{H}_{16}\text{ClN}_2$ [$M+1$]: 283.0998, found: 283.0997.

8-methylene-3,6-diphenyl-7,8,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine (**9b**):



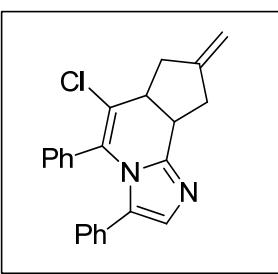
yellow oil (24.9 mg, 77%); R_f = 0.2 (hexane/EtOAc = 3:1); ^1H NMR (400 MHz, CDCl_3) δ 7.47-7.25 (m, 10H), 7.10 (d, J = 9.3 Hz, 2H), 4.96 (d, J = 34.2 Hz, 2H), 3.68-3.65 (m, 1H), 3.38-3.31 (m, 2H), 2.95-2.89 (m, 2H), 2.36-2.29 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.1, 146.1, 137.8, 130.9, 129.3, 128.9, 128.7, 128.6, 128.1, 127.9, 127.6, 127.3, 125.3, 117.3, 106.9, 40.9, 39.2, 38.4, 37.1; IR (liquid) ν 3056.6, 3034.4, 2921.6, 2851.2, 1736.6, 1643.1, 1604.5, 1509.9, 1480.1, 1447.3, 1410.7, 1262.2, 1143.6 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{23}\text{H}_{21}\text{N}_2$ [$M+1$]: 325.1698, found: 325.1699.

6-methyl-8-methylene-3,5-diphenyl-7,8,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine (**9c**):



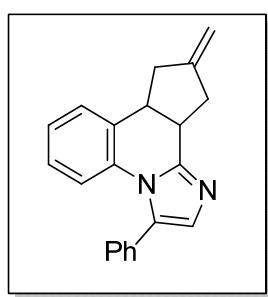
Red oil (24.2 mg, 71%); R_f = 0.3 (hexane/EtOAc = 3:1); ^1H NMR (400 MHz, CDCl_3) δ 6.88-6.77 (m, 11H), 4.90 (d, J = 19.3 Hz, 2H), 3.52-3.48 (m, 1H), 3.29 (d, J = 16.6 Hz, 1H), 2.84-2.67 (m, 3H), 2.25-2.19 (m, 1H), 1.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.5, 148.2, 133.8, 131.7, 130.9, 130.4, 130.1, 129.0, 128.1, 127.4, 127.1, 126.3, 123.9, 106.9, 45.0, 38.2, 37.3, 37.2, 19.1; IR (liquid) ν 3058.6, 3030.6, 2981.4, 2920.7, 2854.1, 1733.7, 1716.3, 1480.1, 1445.4, 1399.1, 1352.8, 1178.3, 1073.2, 889.0 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{24}\text{H}_{22}\text{N}_2$ [$M+1$]: 338.1783, found: 338.1779.

6-chloro-8-methylene-3,5-diphenyl-7,8,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine (9d)



Pale yellow solid (35.4 mg, 99%); m.p. 61-64.1 °C; R_f = 0.4 (hexane/EtOAc = 3:1); ^1H NMR (400 MHz, CDCl_3) δ 6.98-6.84 (m, 11H), 5.00(d, J = 12.0 Hz, 2H), 3.76-3.71(m, 1H), 3.30-3.18 (m, 2H), 2.96-2.86 (m, 2H), 2.57-2.44 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 147.5, 146.9, 132.1, 131.8, 131.7, 130.2, 129.0, 128.7, 128.3, 127.4, 127.2, 126.6, 123.5, 107.6, 46.5, 38.8, 37.1, 37.0; IR (liquid) ν 3058.6, 3030.6, 2924.6, 2851.2, 1737.6, 1659.5, 1603.5, 1513.9, 1481.1, 1445.4, 1389.5, 1264.1 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{23}\text{H}_{20}\text{ClN}_2$ [$M+1$]: 359.1310, found: 359.1310.

10-methylene-3-phenyl-9,10,11,11a-tetrahydro-8bH-cyclopenta[c]imidazo[1,2-a]quinoline (9e):



Pale brown oil (17.5 mg, 58%); R_f = 0.4 (hexane/EtOAc = 4:1); ^1H NMR (400 MHz, CDCl_3) δ 7.42-7.31 (m, 6H), 7.11-7.07 (m, 2H), 6.99 (td, J = 3.43 Hz, 1H), 6.84-6.82 (m, 1H), 4.97 (d, J = 23.5 Hz, 2H), 3.56-3.52 (m, 1H), 3.45-3.38 (m, 1H), 3.34 (d, J = 16.7 Hz, 1H), 2.94-2.86 (m, 1H), 2.81-2.75 (m, 1H), 2.45-2.37 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 148.8, 148.3, 133.6, 131.1, 130.5, 130.4, 129.9, 129.0, 128.9, 128.6, 127.9, 126.9, 125.2, 119.3, 107.3, 43.0, 38.8, 38.7, 37.4; IR (liquid) ν 3072.1, 3048.9, 2914.9, 2841.6, 1658.5, 1603.5, 1493.6, 1461.8, 1390.4, 1267.0, 1147.4 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{21}\text{H}_{19}\text{N}_2$ [$M+1$]: 299.1546, found: 299.1543.

IV. Computational details

All calculations were performed using density functional theory (DFT)^{S2} as implemented in the Jaguar 9.1 suite of ab initio quantum chemistry programs.^{S3} Geometry optimizations were performed with the B3LYP-D3^{S4} functional using the 6-31G** basis set.^{S5} Palladium was represented using the Los Alamos LACVP basis set^{S6} that includes relativistic core potentials. More accurate single point energies were computed from the optimized geometries using Dunning's correlation-consistent triple- ζ basis set, cc-pVTZ(-f)^{S7} that includes a double set of polarization functions. Vibrational frequencies computed at the B3LYP-D3/6-31G** level of theory were used to derive zero point energy and vibrational entropy corrections from unscaled frequencies. Solvation energies were evaluated by a self-consistent reaction field (SCRF) approach^{S8} with the dielectric constant $\epsilon = 7.6$ using the optimized gas phase structures. The calculations were carried out using a minimally simplified model where the methyl group on the tosyl group was removed. This slight modification is not expected to have any notable impact on the conclusions of this work.

IV-1. Energy profile of the early stage of the [3+2] cycloaddition process

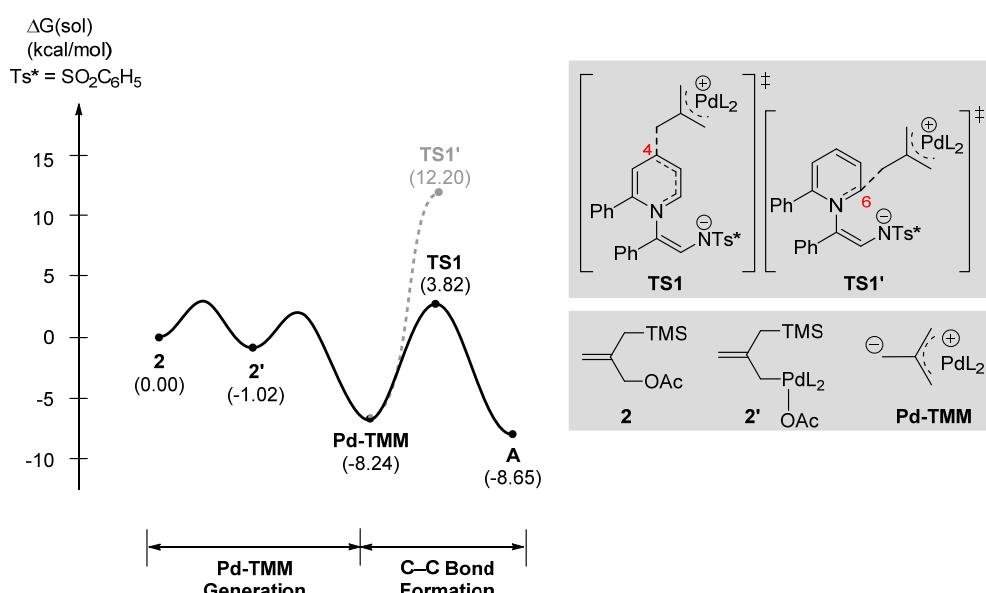


Figure S1. Energy profile of the Pd-TMM generation and the regio-selective coupling of Pd-TMM with pyridinium zwitterion

The reactive intermediate **Pd-TMM** is generated by liberating the silyl acetate in **2'**, which is derived from the oxidative addition of the silyl-substituted allyl acetate (**2**) to Pd(0). Next, the dearomatization of the pyridinium zwitterion (**1a**) by the nucleophilic attack of Pd-TMM occurs smoothly, traversing the transition state **TS1** at 3.8 kcal/mol. The analogous attack at the C6 position was kinetically highly disfavored. We located a transition state at 12.2 kcal/mol (**TS1'**), which was 8.4 kcal/mol higher in energy than **TS1**. This result is in good agreement with aforementioned rationale based on the MO-diagrams of the pyridinium zwitterion. Since the LUMO of the pyridinium zwitterion is

partially localized at the C4 position, the C4-carbon is the most nucleophilic site and it is for that reason that the C–C bond formation at the C4-position is most preferred.

IV-2. DFT-optimized structure's energy components

Table S3. Computed energy components for DFT-optimized structures.

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal/mol)	G(solv)/(kcal/mol)
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
PdL₂	-59864.743	345.59	225.19	-9.04
2	-21605.858	158.93	133.06	-8.31
2'	-81471.742	506.67	293.645	-13.47
TMS-OAc	-17359.942	102.53	108.33	-7.56
TS1'	-108281.633	647.73	359.164	-17.9
Pd-TMM	-64111.023	401.05	239.751	-11.73
Pyridinium Zwitterion (1)	-44170.174	246.16	168.004	-21.66
E	-44169.832	246.84	166.60	-12.23
Intra-TS	-44169.559	245.80	168.10	-15.13
TS1	-108281.528	647.39	358.990	-28.41
A	-108281.838	649.31	357.566	-36.08
TS2	-108281.859	649.499	357.111	-19.36
TS3	-108281.453	649.026	358.471	-22.50
B	-108282.578	650.648	352.401	-18.83
C	-108282.612	650.38	351.918	-25.32
TS4	-108282.517	650.41	345.858	-23.51
3	-108282.753	652.787	351.901	-18.42

IV-3. Cartesian coordinates of the optimized geometries

Table S4. Cartesian Coordinates of the Optimized Geometries.

PdL2	C	-0.806659400	-5.104610920	0.388933539
	C	3.098929167	-1.736091375	1.691012263
	C	5.832359314	-1.351727962	1.185290813
Pd	C	4.065374374	-2.322735786	2.522964478
P	C	3.519407749	-0.945835769	0.611423016
P	C	4.877838135	-0.760941982	0.354994535
C	C	5.423841476	-2.129623652	2.270549297
C	C	1.197083712	-2.339362144	3.745682716
C	C	1.074356079	-2.802573681	6.513962269
C	C	1.196499228	-1.265481591	4.651165962
C	C	1.126977682	-3.647531509	4.244922638

C	1.061419249	-3.875274420	5.621724129	Si	2.208741903	3.156787395	2.857747316
C	1.144580483	-1.495102763	6.024657249	C	3.686210871	4.063265324	3.612208843
C	-3.639481544	-1.031094551	1.329154491	H	3.358774900	4.818387985	4.335355759
C	-5.329732895	-3.147919178	0.572797656	H	4.352312565	3.368821144	4.136319160
C	-4.750115395	-1.372175813	2.115312099	H	4.275796413	4.573762417	2.842555046
C	-3.384057999	-1.768865108	0.161929652	C	1.201055169	2.296595097	4.200772285
C	-4.225712299	-2.814772844	-0.216550499	H	0.397253811	1.703889728	3.752252102
C	-5.587372780	-2.424851656	1.738912106	H	1.824374437	1.620579481	4.796569347
C	-2.808001280	0.570052624	3.570213079	H	0.746140659	3.021518230	4.884595394
C	-3.209846497	0.812678039	6.339976788	C	1.103437901	4.381399632	1.930643320
C	-3.620898962	1.590321183	4.082610607	H	1.647816062	4.907784939	1.138166904
C	-2.196154594	-0.325279593	4.464076519	H	0.246854842	3.871121883	1.476613760
C	-2.399261236	-0.208472684	5.836734295	H	0.708861291	5.139743805	2.616192818
C	-3.816833019	1.710199714	5.461146832	=====	=====	=====	=====
C	-3.241261721	1.816702604	1.000930667	2'	=====	=====	=====
C	-4.281229496	4.186010361	-0.093528785	C	12.154064178	7.385988235	11.027726173
C	-2.408321619	2.921717167	0.768359125	C	12.315397263	5.910259724	11.096685410
C	-4.600260258	1.908027530	0.664847672	H	12.267953873	5.409826756	10.123595238
C	-5.114491940	3.085438251	0.118854336	H	11.763829231	5.371845245	11.867217064
C	-2.925810575	4.101329803	0.233188719	C	13.375308037	7.798480034	10.286358833
H	-0.102984399	-6.950037956	-0.482198924	H	13.405653954	7.489047527	9.237248421
H	-1.210860252	-3.182284832	1.267697692	H	13.748729706	8.814101219	10.428418159
H	2.944265127	-4.234684467	0.864020526	C	11.324075699	8.159918785	11.757891655
H	2.295869350	-6.380483627	-0.176449716	H	10.552651405	7.719357967	12.384416580
H	-1.859457850	-5.339438438	0.255470902	H	11.409315109	9.243446350	11.751089096
H	6.890976906	-1.199925065	0.992521942	Pd	14.403020859	6.313076496	11.418336868
H	3.755409956	-2.925663710	3.371378422	P	14.699259758	4.575868130	13.043489456
H	2.772310495	-0.469810933	-0.019612756	P	16.571985245	7.235682964	11.157738686
H	5.191022396	-0.146837920	-0.484961927	C	17.489597321	7.659007549	12.693959236
H	6.163781166	-2.585102797	2.923494816	C	16.668190002	8.795285225	10.187599182
H	1.023590803	-2.982628107	7.584511757	C	17.700267792	6.137284279	10.198398590
H	1.214251757	-0.247492477	4.270315170	C	14.854950905	2.887591600	12.322829247
H	1.119750738	-4.489411831	3.5593477868	C	13.231729507	4.486300945	14.148292542
H	1.001444817	-4.893985271	5.995923996	C	16.090520859	4.614648342	14.253984451
H	1.143702745	-0.653174698	6.711625576	C	16.725692749	7.921199322	13.840204239
H	-5.979870796	-3.969427347	0.284758747	C	17.343759537	8.292906761	15.033567429
H	-4.955671310	-0.821090102	3.028258801	C	18.733156204	8.402164459	15.095072746
H	-2.506632566	-1.531952143	-0.434816152	C	19.502456665	8.138087273	13.960031509
H	-4.011195660	-3.376805067	-1.121644855	C	18.885520935	7.769075871	12.765708923
H	-6.440541267	-2.681501389	2.361486912	C	17.103338242	10.009585381	10.732878685
H	-3.362254620	0.911619663	7.411556721	C	17.109148026	11.169558525	9.954012871
H	-4.100436687	2.2944655542	3.409845591	C	16.686225891	11.127723694	8.626464844
H	-1.5444980645	-1.104860425	4.079577446	C	16.248254776	9.919586182	8.076579094
H	-1.908946037	-0.907088637	6.509298801	C	16.232330322	8.764107704	8.852581978
H	-4.445346832	2.508806705	5.846728802	C	17.401590347	4.768870831	10.112835884
H	-4.684436321	5.101481915	-0.517552733	C	18.248111725	3.896882057	9.427244186
H	-1.349887490	2.847360611	1.007922769	C	19.396793365	4.384804726	8.803483963
H	-5.257289410	1.059033990	0.829306662	C	19.687593460	5.750320435	8.854655266
H	-6.168615818	3.143057585	-0.139562592	C	18.843124390	6.622098923	9.541175842
H	-2.269480944	4.950564861	0.063256979	C	15.543285370	1.843431592	12.959237099
=====	=====	=====	C	15.640775681	0.590988398	12.352427483	
2	=====	=====	C	15.053021431	0.367044479	11.106034279	
C	1.779155016	1.168060541	0.846091390	C	14.366044044	1.400550961	10.466075897
C	1.049527049	0.131745130	1.272445202	C	14.269412994	2.654947042	11.068111420
H	0.248951957	-0.280786902	0.670536041	C	12.512335777	5.666648865	14.394254684
H	1.245629787	-0.324659675	2.238292456	C	11.429057121	5.659922123	15.272770882
C	1.552945733	1.809762478	-0.502457023	C	11.046502113	4.475491047	15.904669762
H	1.484645367	2.898920774	-0.384002656	C	11.749720573	3.295168877	15.654649734
H	2.425409317	1.609615445	-1.143532753	C	12.839155197	3.299608946	14.783250809
C	2.872900248	1.822006106	1.654466033	C	15.889040947	4.793708324	15.629439354
H	3.396589756	1.073665977	2.261046648	C	16.978271484	4.880362511	16.499200821
H	3.630584717	2.275687933	1.000442505	C	18.279651642	4.788791656	16.009023666
O	0.365033329	1.294422626	-1.106592059	C	18.490549088	4.608001709	14.640192986
C	-0.095335014	1.760914803	-2.299319506	C	17.407150269	4.524810791	13.770910263
O	-1.094679236	1.270217538	-2.764427900	H	13.381020546	2.377461672	14.595029831
C	0.675920904	2.882813931	-2.968917608	H	11.449609756	2.369014502	16.137529373
H	1.717432737	2.599833727	-3.150942087	H	10.197104454	4.469187260	16.582485199
H	0.188316345	3.106877565	-3.916613579	H	10.876163483	6.578632832	15.447185516
H	0.682945848	3.781557560	-2.343438625	H	12.771940231	6.582575798	13.869318008

H	16.013444901	2.012663126	13.923107147	C	11.502411842	11.755865097	15.153226852
H	16.179285049	-0.209311485	12.853096962	H	11.612154961	12.564023018	14.436144829
H	15.134022713	-0.608269155	10.633740425	C	11.907454491	11.944513321	16.472320557
H	13.910553932	1.233649969	9.493825912	H	12.353487968	12.892627716	16.763195038
H	13.749262810	3.466099501	10.566547394	C	11.713195801	10.942140579	17.425867081
H	14.882145882	4.867353439	16.026329041	H	12.010616302	11.098609924	18.459245682
H	16.804628372	5.021945953	17.562770844	C	11.113215446	9.742565155	17.033224106
H	19.126070023	4.864608765	16.686120987	H	10.953461647	8.949915886	17.760725021
H	19.500782013	4.547802448	14.245536804	C	10.727706909	9.542645454	15.711483955
H	17.590566635	4.395808220	12.709001541	H	10.282377243	8.595664978	15.423671722
H	19.061851501	7.686070919	9.551297188	N	9.523326874	9.361812592	13.057061195
H	20.570196152	6.138652802	8.353413582	C	9.851299286	8.266733170	12.262381554
H	20.056190491	3.708053589	8.266889572	H	10.493456841	8.490999222	11.425169945
H	17.999372482	2.840365887	9.376482010	C	8.947505951	7.178604603	12.210737228
H	16.494977951	4.385043621	10.568447113	H	9.208212852	6.347069740	11.565053940
H	17.440914154	10.054066658	11.763251305	C	7.808225632	7.171097279	12.972482681
H	17.448434830	12.105812073	10.389200211	H	7.128197193	6.324544430	12.943147659
H	16.692468643	12.031040192	8.022679329	C	7.478827000	8.315911293	13.737835884
H	15.911253929	9.880168915	7.044359684	H	6.531378269	8.390697479	14.257869720
H	15.876751900	7.830816269	8.424838066	C	8.322252274	9.403388023	13.749330521
H	19.495527267	7.556152344	11.894152641	C	7.920719624	10.659947395	14.419700623
H	20.585603714	8.216051102	14.005780220	C	7.984072208	11.880995750	13.730032921
H	19.216640472	8.683872223	16.026611328	H	8.385486603	11.903634071	12.721936226
H	16.740472794	8.481093407	15.916921616	C	7.540361404	13.050481796	14.339598656
H	15.644892693	7.815545082	13.794866562	H	7.589431763	13.990717888	13.797241211
				C	7.032240391	13.017988205	15.641391754
				H	6.692947388	13.934463501	16.116609573
				C	6.965400696	11.806915283	16.330102921

TMS-OAc

O	3.008249044	2.428082228	1.697381020	C	7.407114983	10.632530212	15.722049713
C	3.548862696	1.187861443	1.795838952	H	7.383345127	9.691729546	16.263940811
O	3.916970730	0.602891266	0.807535768	H	10.204736710	13.885307312	5.823249817
C	3.628359795	0.595538974	3.191423416	C	11.997910500	6.346618652	12.285237312
H	2.622335911	0.467860252	3.602918148	C	12.189599991	5.036904335	12.865036964
H	4.123394489	-0.373777241	3.138177633	H	11.690950394	4.184544086	12.398992538
H	4.183820248	1.252837062	3.867399216	H	12.326107025	4.959336758	13.941740036
Si	2.545608521	3.667812824	2.764249563	C	12.176265717	6.263085365	10.840919495
C	4.059458256	4.283351421	3.696006536	H	11.634503365	5.470253468	10.321963310
H	3.806947470	5.176347256	4.279397964	H	12.308635712	7.177389622	10.264068604
H	4.456865788	3.538838387	4.393342495	C	11.955683708	7.537186146	13.011101723
H	4.859724045	4.554926872	2.999915600	H	12.002480507	7.496397018	14.095160484
C	1.219607353	3.057877302	3.953403950	H	12.349490166	8.439329147	12.562491417
H	0.404914290	2.562686920	3.414373636	Pd	13.966638565	5.307524204	11.557192802
H	1.612335920	2.356746435	4.696107388	P	15.544346809	4.808964729	13.274076462
H	0.788534462	3.906179428	4.497999668	P	15.297780037	5.992392540	9.738582611
C	1.866267920	4.993472576	1.628931522	C	16.300798416	7.444192410	10.217393875
H	2.627249241	5.318518162	0.912403405	C	14.399053574	6.476546288	8.208064079
H	1.010441422	4.616820812	1.059816122	C	16.447885513	4.722113132	9.075294495
H	1.536885858	5.870388031	2.197304010	C	15.311076164	3.314778328	14.314551353
				C	15.231518745	6.244765759	14.377996445
				C	17.363618851	4.808855534	12.998025894
				C	15.636591911	8.678635597	10.337192535

TS1'

S	12.370831490	10.726560593	9.983386993	C	16.303844452	9.791844368	10.846568108
O	12.673181534	9.408224106	9.366802216	C	17.635213852	9.682081223	11.260725975
O	13.524980545	11.468089104	10.555193901	C	18.292524338	8.453979492	11.160743713
C	11.681323051	11.734938622	8.670252800	C	17.632955551	7.336390972	10.644273758
C	10.552842140	11.279690742	7.983202934	C	14.750804901	7.576582909	7.416340828
H	10.102070808	10.331602097	8.256846428	C	14.050323486	7.848108768	6.240067959
C	10.023231506	12.060579300	6.959249496	C	13.004998207	7.019320965	5.832296371
H	9.143488884	11.719294548	6.420155525	C	12.656491280	5.914309025	6.612990379
C	10.621500969	13.279729843	6.623733997	C	13.344192505	5.649034977	7.795293808
C	11.750240326	13.720012665	7.315410614	C	16.133937836	3.372098923	9.284475327
H	12.214466095	14.667140007	7.053972721	C	16.933801651	2.364096165	8.743157387
C	12.287149429	12.946826935	8.347194672	C	18.063787460	2.695502281	7.992744446
H	13.161264420	13.266356468	8.904518127	C	18.373205185	4.039539814	7.765533447
N	11.112556458	10.553015709	10.997616768	C	17.564790726	5.046753407	8.292081833
C	11.350445747	10.793566704	12.305689812	C	16.210054398	2.995078087	15.345335960
H	12.252600670	11.338670731	12.593229294	C	16.005931854	1.863052130	16.132604599
C	10.561103821	10.329522133	13.328918457	C	14.906346321	1.031926155	15.897613525
C	10.919895172	10.543297768	14.736402512	C	14.015279770	1.337482333	14.868152618
				C	14.216658592	2.472219467	14.078652382

C	15.435251236	7.530213833	13.842826843	C	16.248254776	9.919586182	8.076579094
C	15.031379700	8.661572456	14.546424866	C	16.232330322	8.764107704	8.852581978
C	14.404901505	8.530532837	15.787939072	C	17.401590347	4.768870831	10.112835884
C	14.217499733	7.259306908	16.332544327	C	18.248111725	3.896882057	9.427244186
C	14.630034447	6.119369030	15.637062073	C	19.396793365	4.384804726	8.803483963
C	18.237689972	5.723706245	13.599918365	C	19.687593460	5.750320435	8.854655266
C	19.600370407	5.703434944	13.292969704	C	18.843124390	6.622098923	9.541175842
C	20.106866837	4.776059628	12.381013870	C	15.543285370	1.843431592	12.959237099
C	19.243911743	3.846529484	11.792499542	C	15.640775681	0.590988398	12.352427483
C	17.885967255	3.861116171	12.103693962	C	15.053021431	0.367044479	11.106034279
H	14.461138725	5.136310577	16.066642761	C	14.366044044	1.400550961	10.466075897
H	13.729204178	7.151159763	17.297607422	C	14.269412994	2.654947042	11.068111420
H	14.040830612	9.408223152	16.314712524	C	12.512335777	5.666648865	14.394254684
H	15.174117088	9.642407417	14.101737022	C	11.429057121	5.659922123	15.272770882
H	15.879454613	7.648806095	12.860850334	C	11.046502113	4.475491047	15.904669762
H	17.071649551	3.631954432	15.526903152	C	11.749720573	3.295168877	15.654649734
H	16.706703186	1.627351642	16.929014206	C	12.839155197	3.299608946	14.783250809
H	14.749875069	0.149189070	16.511465073	C	15.889040947	4.793708324	15.629439354
H	13.161857605	0.692812920	14.675698280	C	16.978271484	4.880362511	16.499200821
H	13.525147438	2.712361336	13.276847839	C	18.279651642	4.788791656	16.009023666
H	17.855194092	6.467470169	14.291027069	C	18.490549088	4.608001709	14.640192986
H	20.264230728	6.424837112	13.762193680	C	17.407150269	4.524810791	13.770910263
H	21.164489746	4.774711609	12.132284164	H	13.381020546	2.377461672	14.595029831
H	19.620046616	3.121602535	11.076052666	H	11.449609756	2.369014502	16.137529373
H	17.225719452	3.143608332	11.629118919	H	10.197104454	4.469187260	16.582485199
H	17.807842255	6.087998867	8.101476669	H	10.876163483	6.578632832	15.447185516
H	19.244268417	4.304694653	7.172297955	H	12.771940231	6.582575798	13.869318008
H	18.692985535	1.912967205	7.577740669	H	16.013444901	2.012663126	13.923107147
H	16.679294586	1.321946263	8.917204857	H	16.179285049	-0.209311485	12.853096962
H	15.268382072	3.114894867	9.891052246	H	15.134022713	-0.608269155	10.633740425
H	15.554656029	8.237090111	7.722972393	H	13.910553932	1.233649969	9.493825912
H	14.319639206	8.717674255	5.647009850	H	13.749262810	3.466099501	10.566547394
H	12.459115982	7.237057209	4.918488026	H	14.882145882	4.867353439	16.026329041
H	11.839697838	5.265335560	6.308006763	H	16.804628372	5.021945953	17.562770844
H	13.056448936	4.800598145	8.410597801	H	19.126070023	4.864608765	16.686120987
H	18.152082443	6.385107517	10.603190422	H	19.500782013	4.547802448	14.245536804
H	19.320301056	8.351159096	11.498111725	H	17.590566635	4.395808220	12.709001541
H	18.154478073	10.546492577	11.666164398	H	19.061851501	7.686070919	9.551297188
H	15.757426262	10.727637291	10.918388367	H	20.570196152	6.138652802	8.353413582
H	14.596993446	8.782302856	10.039171219	H	20.056190491	3.708053589	8.266889572
H	17.999372482			H	17.999372482	2.840365887	9.376482010
H	16.494977951			H	16.494977951	4.385043621	10.568447113
Pd-TMM				H	17.440914154	10.054066658	11.763251305
C	12.154064178	7.385988235	11.027726173	H	17.448434830	12.105812073	10.389200211
C	12.315397263	5.910259724	11.096685410	H	16.692468643	12.031040192	8.022679329
H	12.267953873	5.409826756	10.123595238	H	15.911253929	9.880168915	7.044359684
H	11.763829231	5.371845245	11.867217064	H	15.876751900	7.830816269	8.424838066
C	13.375308037	7.798480034	10.286358833	H	19.495527267	7.556152344	11.894152641
H	13.405653954	7.489047527	9.237248421	H	20.585603714	8.216051102	14.005780220
H	13.748729706	8.814101219	10.428418159	H	19.216640472	8.683872223	16.026611328
C	11.324075699	8.159918785	11.757891655	H	16.740472794	8.481093407	15.916921616
H	10.552651405	7.719357967	12.384416580	H	15.644892693	7.815545082	13.794866562
H	11.409315109	9.243446350	11.751089096	===== Pyridinium-Zwitterion =====			
Pd	14.403020859	6.313076496	11.418336868	S	11.804778099	10.003917694	17.656282425
P	14.699259758	4.575868130	13.043489456	O	12.866579056	9.025971413	17.926286697
P	16.571985245	7.235682964	11.157738686	O	10.717187881	10.205290794	18.638784409
C	17.489597321	7.659007549	12.693959236	C	12.595900536	11.611374855	17.431213379
C	16.668190002	8.795285225	10.187599182	C	13.852528572	11.675332069	16.823923111
C	17.700267792	6.137284279	10.198398590	H	14.369013786	10.754400253	16.572334290
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C	13.231729507	4.486300945	14.148292542	H	15.398394585	12.983543396	16.092454910
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C	18.733156204	8.402164459	15.095072746	C	11.908932686	12.771162987	17.793489456
C	19.502456665	8.138087273	13.960031509	H	10.943525314	12.685507774	18.281887054
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C	17.103338242	10.009585381	10.732878685	C	9.968310356	10.072339058	15.899958611

H	9.330366135	10.419911385	16.716260910	H	8.644911766	7.339219093	11.221608162
C	9.411224365	10.034482956	14.636755943	C	9.885438919	9.044146538	10.880040169
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H	7.930705070	11.945858002	15.868943214	H	10.906230927	10.989773750	10.755764961
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H	5.720522881	12.786742210	15.201317787	C	10.533338547	11.992086411	13.180421829
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H	4.636464596	11.971980095	13.110897064	H	12.617528915	11.779360771	12.698026657
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C	7.491325378	10.115266800	13.036786079	C	11.200916290	14.590718269	13.993330956
H	7.971926212	9.355018616	12.426157951	H	11.460415840	15.594386101	14.318019867
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C	10.579396248	8.178746223	13.635257721	H	9.106577873	14.801918983	14.467195511
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C	11.313395500	7.579819679	12.632176399	H	8.518684387	12.516292572	13.735975266
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C	11.716349602	8.350280762	11.537620544	=====			
H	12.270790100	7.900640965	10.720138550	Intra-TS			
C	11.429228783	9.710666656	11.527528763	=====			
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C	10.740837097	10.298886299	12.588895798	O	4.880490780	9.095190048	13.750585556
C	10.587792397	11.763747215	12.697291374	O	6.071399689	8.135344505	11.694195747
C	11.138273239	12.423439980	13.808632851	C	6.207371235	10.737228394	12.178037643
H	11.629799843	11.850439072	14.589065552	C	5.633014679	11.806227684	12.868317604
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C	10.430091858	14.540088654	12.879611969	H	5.397247791	13.945386887	12.928681374
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H	9.391339302	14.450434685	10.991648674	H	7.790068626	12.418922424	9.695009232
C	9.969419479	12.494709969	11.677927971	C	6.979352951	10.942871094	11.033910751
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=====			C	7.754498005	9.603492737	14.740663528	
E			H	7.004285336	9.866332054	15.480122566	
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S	6.163805962	8.971087456	12.751505852	C	9.752335548	10.645583153	15.940015793
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C	6.358774185	10.688748360	12.263879776	C	9.718069077	11.939733505	17.997924805
C	5.843398094	11.685635567	13.096854210	H	9.154603958	12.489743233	18.746438980
H	5.302544117	11.407793045	13.994315147	C	11.107275009	11.829257011	18.110128403
C	6.011566162	13.021297455	12.732355118	H	11.628249168	12.286034584	18.946062088
H	5.610117435	13.807261467	13.365269661	C	11.816875458	11.130819321	17.132562637
C	6.694993973	13.346437454	11.557692528	H	12.896935463	11.037739754	17.204261780
C	7.202396870	12.337999344	10.735681534	C	11.148418427	10.543162346	16.060964584
H	7.731945515	12.593890190	9.823263168	H	11.706540108	9.996377945	15.307509422
C	7.032141209	10.998391151	11.082240105	N	9.756813049	9.663172722	13.597456932
H	7.413897991	10.200239182	10.457804680	C	9.250588417	8.460471153	13.112531662
N	7.562002659	8.528475761	13.668289185	H	9.261034966	7.658328533	13.842089653
C	7.767913342	9.304450035	14.850231171	C	9.465104103	8.125977516	11.736160278
H	7.047969341	9.260834694	15.652441025	H	9.120441437	7.159690857	11.389989853
C	8.938700676	9.982551575	14.810630798	C	10.071569443	9.027365685	10.912534714
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C	8.747519493	11.448960304	16.811239243	C	10.459812164	10.303850174	11.408367157
H	7.670877934	11.462324142	16.668415070	H	10.878651619	11.055860519	10.751400948
C	9.321935654	12.153932571	17.865209579	C	10.230963707	10.634622574	12.717421532
H	8.687265396	12.698994637	18.558042526	C	10.463184357	12.018125534	13.198588371
C	10.709676743	12.174565315	18.021980286	C	11.758315086	12.547450066	13.215869904
H	11.157910347	12.733330727	18.838283539	H	12.594915390	11.917643547	12.929376602
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H	12.598179817	11.493304253	17.234655380	H	12.982150078	14.265752792	13.638462067
C	10.946036339	10.766215324	16.071018219	C	10.892212868	14.666034698	13.989764214
H	11.572448730	10.227668762	15.368041992	H	11.059116364	15.692055702	14.304820061
N	9.594375610	9.711454391	13.570796967	C	9.596273422	14.146148682	13.954648018
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H	9.390449524	7.643229485	13.665919304	C	9.378579140	12.828752518	13.560191154
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C	6.152482986	13.030729294	10.479211807	C	18.207710266	7.575875759	12.408456802	
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H	3.318233013	11.209014893	10.060294151	C	18.153709412	5.286711693	11.633419037	
C	3.910609245	12.181277275	11.894011497	C	16.398679733	3.119624853	14.612096786	
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H	4.747718334	13.261814117	13.564160347	C	18.248552322	1.830538154	15.478816032	
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H	6.742878437	14.041664124	12.280675888	C	18.573591232	4.148758888	14.871491432	
N	8.707084656	12.362394333	9.860825539	C	11.718787193	3.537481308	16.590852737	
C	9.537742615	12.558208466	10.892813683	C	10.993837357	2.351099730	16.688508987	
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H	14.677009583	11.188793182	13.330598831	C	15.517813683	5.672355652	19.134603500	
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H	11.874839783	11.740713120	9.163193703	H	9.715436935	10.048002243	16.243844986	
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H	12.892999649	9.832378387	7.894403934	H	13.041708946	8.298566818	14.177734375	
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H	10.317609787	7.215006828	10.149584770	H	10.912549019	1.490593553	13.399127007	
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C	8.076396942	8.085190773	13.523668289	H	18.648485184	0.893073320	15.855917931	
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H	9.379487991	13.316970825	12.679244995	C	11.579568863	1.656242013	16.123558044	
C	10.816476822	11.801275253	12.311805725	C	11.475171089	2.276586056	14.876291275	
C	11.561783791	11.951323509	13.550273895	C	11.977289200	3.564149618	14.692628860	
C	11.075350761	12.707055092	14.654565274	C	11.850634575	8.390310287	15.439646721	
H	10.095067024	13.166911125	14.597997665	C	10.888521194	9.290868759	15.896136284	
C	11.815664291	12.857723236	15.822215080	C	9.810024261	8.833641052	16.656045914	
H	11.398126602	13.448013306	16.635257721	C	9.690238953	7.475430489	16.956087112	
C	13.068468094	12.247816086	15.977636337	C	10.670902252	6.577563286	16.536079407	
H	13.635526657	12.363579750	16.896738052	C	14.133108139	7.442849636	17.695146561	
C	13.562202454	11.493381500	14.911072731	C	15.012056351	7.700207710	18.750131607	
H	14.534556389	11.007927895	14.992901802	C	16.068513870	6.830395222	19.022302628	
C	12.834510803	11.345133781	13.731444359	C	16.234447479	5.688899994	18.233608246	
H	13.267271996	10.775943756	12.916993141	C	15.364251137	5.431525230	17.177368164	
N	11.326359749	10.850854874	11.353080750	H	10.590006828	5.530488968	16.808633804	
C	12.355288506	11.257902145	10.504650116	H	8.842051506	7.112628460	17.530460358	
H	12.554098129	12.323597908	10.530996323	H	9.058651924	9.539244652	16.999841690	
C	13.010960579	10.398976326	9.703554153	H	10.977726936	10.339429855	15.642778397	
H	13.766672134	10.754254341	9.011604309	H	12.674632072	8.765949249	14.838253021	
C	12.737895012	8.927492142	9.868260384	H	13.137279510	4.140555859	17.842811584	
H	13.016733170	8.358253479	8.972768784	H	12.257777214	1.859390259	18.160938263	
C	11.276142120	8.773156166	10.188318253	H	11.191864967	0.651522756	16.267164230	
H	10.729281425	7.893565178	9.870337486	H	11.004109383	1.758318901	14.045584679	
C	10.671267509	9.661869049	11.016260147	H	11.895998001	4.037361622	13.718627930	
C	9.324877739	9.377179146	11.573288918	H	13.320366859	8.135574341	17.505029678	
C	8.229465485	9.206380844	10.719233513	H	14.864025116	8.587924004	19.359729767	
H	8.357481956	9.380666733	9.655879021	H	16.752902985	7.036177635	19.840381622	
C	6.978378296	8.874051094	11.235866547	H	17.051044464	4.999451637	18.431682587	
H	6.128748894	8.784189224	10.567018509	H	15.513882637	4.537407875	16.582023621	
C	6.806737423	8.709963799	12.611029625	H	18.953962326	3.848264933	13.820739746	
H	5.826089382	8.466164589	13.012210846	H	19.355936050	1.584426522	14.713289261	
C	7.895876884	8.874835014	13.468316078	H	17.461000443	0.211009488	15.553587914	
H	7.777693272	8.746098518	14.541313171	H	15.140953064	1.131820083	15.477780342	
C	9.145875931	9.211225510	12.950733185	H	14.742129326	3.390667200	14.598259926	
H	9.988222122	9.355222702	13.613658905	H	18.194664001	7.663945198	12.513480186	
H	3.247599602	10.198510170	10.013786316	H	19.430368423	7.884616852	10.388678551	
C	13.377177238	6.940318584	11.341522217	H	19.465034485	6.009052753	8.754411697	
C	12.281093597	6.509779930	12.134595871	H	18.249277115	3.899919033	9.277224541	
H	11.882615089	5.506444454	11.991759300	H	17.007097244	3.673766851	11.395752907	
H	11.599181175	7.236205578	12.561926842	H	18.985198975	5.5465557903	15.289577484	
C	14.337894440	5.955005646	11.026453972	H	19.941030502	7.266726971	16.766201019	
H	14.043122292	4.912981033	10.900577545	H	18.745916367	9.417568207	17.131113052	
H	15.273137093	6.239500046	10.555068970	H	16.577632904	9.834969521	15.977276802	
C	13.627480507	8.386843681	11.066020966	H	15.618448257	8.116539001	14.489752769	
H	13.346095085	8.985434532	11.936557770	<hr/>				
H	14.686850548	8.565123558	10.848686218	<hr/>				
Pd	14.174282074	6.016552925	13.241497040	TS2				
P	13.205220222	5.961285591	15.446112633	S	13.743391037	11.290513039	14.803094864	
P	16.467952728	5.510851383	13.611421585	O	14.124094009	10.044038773	15.511057854	
C	17.235086441	6.711444378	14.772929192	O	13.351364136	12.456337929	15.626374245	
C	17.513486862	5.653489113	12.107213020	C	15.204939842	11.757642746	13.862830162	
C	16.823034286	3.810382843	14.202163696	C	15.935027122	10.764916420	13.203607559	
C	12.588785172	4.252099037	15.753757477	H	15.648835182	9.724720955	13.306168556	
C	11.766323090	7.034007549	15.785815239	C	17.032325745	11.128957748	12.427851677	
C	14.304266930	6.307760239	16.887866974	H	17.594118118	10.361914635	11.903036118	
C	16.571966171	7.931771755	14.978109360	C	17.403129578	12.473409653	12.323905945	
C	17.113502502	8.902882576	15.820130348	C	16.674768448	13.454264641	12.998512268	
C	18.326623917	8.666748047	16.467588425	H	16.969020844	14.497881889	12.926025391	
C	18.996765137	7.457345486	16.263141632	C	15.566464424	13.099761009	13.770778656	
C	18.457548141	6.485223770	15.421957016	H	14.986118317	13.842387199	14.308663368	
C	18.202375412	6.837352753	11.809530258					

N	12.665143013	10.908256531	13.636510849	C	12.524780273	3.634600639	16.999416351
C	11.632000923	11.766971588	13.443273544	C	12.065782547	2.317110062	17.051454544
H	11.432091713	12.537211418	14.191766739	C	11.539426804	1.708932400	15.911315918
C	10.813448906	11.710422516	12.342487335	C	11.471088409	2.425964355	14.714931488
C	9.597736359	12.484822273	12.118552208	C	11.934741974	3.739455938	14.660396576
C	8.917347908	13.112823486	13.183984756	C	11.523543358	8.425069809	15.633543968
H	9.283762932	12.993929863	14.198861122	C	10.508251190	9.276279449	16.073833466
C	7.765523911	13.858736992	12.961209297	C	9.474181175	8.780544281	16.869274139
H	7.265797138	14.329841614	13.804280281	C	9.462795258	7.430599213	17.233322144
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H	6.325825214	14.555110931	11.506144524	C	13.856835365	7.437299252	18.027612686
C	7.881524563	13.349726677	10.613835335	C	14.694859505	7.631401062	19.127696991
H	7.479899883	13.428700447	9.606470108	C	15.753552437	6.758385181	19.375648499
C	9.043689728	12.613582611	10.829165459	C	15.976253510	5.685528278	18.509300232
H	9.534241676	12.131900787	9.988967896	C	15.146369934	5.491419315	17.408462524
N	11.268921852	10.822558403	11.289236069	H	10.499647141	5.549405575	17.151826859
C	12.351879120	11.285552979	10.508951187	H	8.655593872	7.038094997	17.846435547
H	12.478535652	12.360202789	10.551143646	H	8.681921005	9.442559242	17.209449768
C	13.092625618	10.456965446	9.767230034	H	10.536401749	10.324533463	15.789319038
H	13.871635437	10.850343704	9.122968674	H	12.322905540	8.821840286	15.020103455
C	12.957487106	8.980369568	9.981434822	H	12.932519913	4.094573021	17.893375397
H	13.252540588	8.414669037	9.091683388	H	12.118462563	1.767213702	17.987497330
C	11.517487526	8.626431465	10.370259285	H	11.184383392	0.682768464	15.954020500
H	10.970789909	7.885045052	9.794672966	H	11.061727524	1.960533738	13.822233200
C	10.748328209	9.599573135	11.042493820	H	11.887833595	4.290745735	13.724277496
C	9.415529251	9.227705956	11.571618080	H	13.054111481	8.141619682	17.840549469
C	8.418976784	8.793605804	10.687129974	H	14.519435883	8.477656364	19.786355972
H	8.610413551	8.800001144	9.617565155	H	16.406991959	6.916739464	20.229120255
C	7.182146072	8.377697945	11.176681519	H	16.807823181	5.007150173	18.678766251
H	6.408594131	8.057991028	10.483950615	H	15.342090544	4.657793522	16.741630554
C	6.938313961	8.371887207	12.551467896	H	18.992164612	4.195155621	13.574189186
H	5.975742817	8.040250778	12.931289673	H	19.535139084	1.852146387	14.149114609
C	7.934285164	8.788429260	13.435845375	H	17.766324997	0.333159298	15.007335663
H	7.767085552	8.770395279	14.508889198	H	15.433748245	1.172753334	15.270318031
C	9.164774895	9.221387863	12.948945999	H	14.889163017	3.508652687	14.684111595
H	9.937520027	9.541115761	13.632928848	H	18.058788300	8.158389091	13.110456467
H	18.262372971	12.754606247	11.720660210	H	19.276315689	8.825285912	11.071202278
C	13.338891029	7.217692375	11.577666283	H	19.385656357	7.294253349	9.112547874
C	11.963338852	7.332334518	11.978932381	H	18.274744034	5.067952633	9.232120514
H	11.295042038	6.475456238	11.912907600	H	17.057275772	4.393878460	11.270777702
H	11.721739769	8.041469574	12.759856224	H	18.919044495	5.612562656	15.511291504
C	13.994046211	6.021776199	11.277775764	H	19.807746887	7.140311718	17.229267120
H	13.446594238	5.079792976	11.236867905	H	18.559219360	9.199660301	17.849334717
H	14.950344086	6.045687199	10.763124466	H	16.373575211	9.706759453	16.712368011
C	13.896937370	8.547377586	11.179413795	H	15.486745834	8.190060616	15.044621468
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H	14.949742317	8.511902809	10.885179520	TS3	=====	=====	=====
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P	16.425971985	5.768650532	13.790180206	O	18.988807678	9.628807068	6.999083996
C	17.146490097	6.796821117	15.131575584	C	17.478120804	10.819691658	5.191088676
C	17.466915131	6.227453709	12.339891434	C	16.511241913	10.748573303	4.186024189
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C	12.470435143	4.361750126	15.800872803	C	16.278812408	11.867054939	3.386321306
C	11.543153763	7.084551811	16.037767410	H	15.528789520	11.822912216	2.600583315
C	14.069704056	6.358844280	17.158864975	C	17.008884430	13.042414665	3.591807365
C	16.446508408	7.956630230	15.492594719	C	17.979883194	13.097884178	4.594525337
C	16.953205109	8.824982643	16.459203720	H	18.554256439	14.008580208	4.747273445
C	18.164455414	8.537373432	17.086559296	C	18.219120026	11.9983411789	5.401625633
C	18.866415024	7.374835014	16.738197327	H	18.973562241	11.997912407	6.181868553
C	18.365526199	6.511601925	15.764307022	N	16.402383804	9.550654411	7.303491592
C	18.096858978	7.479463100	12.263969421	C	16.625890732	10.144037247	8.489665031
C	18.782066345	7.857620716	11.107537270	H	17.635965347	10.474164009	8.741417885
C	18.849359512	6.997877598	10.009580612	C	15.669063568	10.329614639	9.462052345
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C	17.536331177	5.368968487	11.229512215	C	16.916276932	12.076968193	10.736146927
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C	15.575984955	11.469544411	13.091668129	C	16.763170242	7.272743225	17.669828415
H	15.058499336	11.216473579	14.012609482	C	17.391538620	6.081547737	18.030395508
C	15.285143852	10.766421318	11.923044205	C	16.899862289	4.866949081	17.546863556
H	14.525655746	9.993731499	11.948167801	C	15.783641815	4.847340107	16.715131760
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C	12.928444862	7.879934788	8.961772919	H	13.023705482	10.695339203	14.029557228
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C	11.950436592	8.517448425	9.947610855	H	13.240597725	5.240173817	18.109424591
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H	14.488077164	11.946514130	7.597083092	H	18.265735626	6.098723412	18.675519943
C	14.176185608	13.992511749	8.199733734	H	17.387884140	3.933301210	17.813737869
H	14.714301109	14.400010109	7.347707748	H	15.409098625	3.895618439	16.350318909
C	13.616544724	14.849055290	9.152464867	H	19.003215790	4.212397099	11.978043556
H	13.724503517	15.925665855	9.047116280	H	19.866575241	1.960407495	12.538393021
C	12.925100327	14.318783760	10.242500305	H	18.465616226	0.378459305	13.847432137
H	12.497127533	14.979999542	10.991763115	H	16.191875458	1.059258223	14.588895798
C	12.801694870	12.936657906	10.384688377	H	15.329498291	3.316541195	14.024217606
H	12.297060013	12.514302254	11.249463081	H	18.151908875	7.730382442	11.241959572
H	16.823305130	13.912922859	2.966903925	H	18.759481430	8.063697815	8.865070343
C	12.730528831	6.644959927	11.303126335	H	18.041252136	6.448867321	7.152565956
C	11.997292519	5.661338329	11.961819649	H	16.767093658	4.406315804	7.826561451
H	12.037148476	4.621045589	11.639870644	H	16.135877609	4.066721916	10.192004204
H	11.156611443	5.945932865	12.588013649	H	18.755310059	5.299181938	14.534546852
C	13.739545822	6.380797386	10.308014870	H	20.050834656	6.972220421	15.799064636
H	13.777757645	5.414914131	9.808585167	H	19.504957199	9.389441490	15.606855392
H	14.684544563	6.896311760	10.354014397	H	17.609365463	10.115657806	14.154184341
C	12.389488220	8.099589348	11.401844978	H	16.298692703	8.451287270	12.915840149
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H	13.278052330	8.682053566	11.651782990	B			
Pd	14.081455231	5.696207523	12.890974045	S	14.215910912	11.958630562	14.006085396
P	13.689895630	5.942768097	15.227165222	O	14.854455948	11.019075394	14.953226089
P	16.456172943	5.595738411	12.598052979	O	13.951803207	13.340312004	14.460562706
C	17.440217972	6.753038406	13.626592636	C	15.294568062	12.023882866	12.565706253
C	17.097103119	5.873719692	10.888967514	C	16.091705322	10.921360970	12.254519463
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C	12.583413124	4.768824100	16.105333328	C	16.816198349	10.919566154	11.061694145
C	12.862757683	7.580390930	15.421236038	H	17.436281204	10.061918259	10.818294525
C	15.132597923	6.041801453	16.362314224	C	16.745389938	12.013808250	10.194360733
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C	18.922584534	8.653421402	15.058676720	C	15.232892036	13.132287025	11.720530510
C	19.233255386	7.297922611	15.161444664	H	14.621649742	13.984259605	12.003002167
C	18.500267029	6.349723816	14.447181702	N	12.910052299	11.230036736	13.346194267
C	17.846395493	6.994498253	10.505828857	C	11.736351967	11.889970779	13.284674644
C	18.197681427	7.184573174	9.166219711	H	11.527835846	12.742757797	13.934316635
C	17.806285858	6.261935711	8.195987701	C	10.780634880	11.469126701	12.387042999
C	17.074365616	5.131945610	8.575616837	C	9.365442276	11.798698425	12.326766014
C	16.718938828	4.940507889	9.908147812	C	8.691437721	12.286228180	13.465420723
C	16.329299927	3.022711515	13.715694427	C	9.230880737	12.383138657	14.402407646
C	16.813686371	1.751636624	14.027449608	C	7.337454796	12.602118492	13.414580345
C	18.088862611	1.369710207	13.609739304	H	6.842803478	12.972789764	14.308959007
C	18.877075195	2.258620262	12.874085426	C	6.605377197	12.411150932	12.240010262
C	18.394311905	3.528141022	12.561830521	H	5.543438435	12.638061523	12.209560394
C	12.562923431	4.644975185	17.504528046	C	7.254945755	11.910401344	11.110184669
C	11.683534622	3.755516529	18.120231628	H	6.699748516	11.752329826	10.188830376
C	10.815002441	2.979758024	17.348428726	C	8.614313126	11.614478111	11.148611069
C	10.832076073	3.092482567	15.957539558	H	9.103989601	11.237802505	10.254216194
C	11.714923859	3.978641033	15.339072227	N	11.322772980	10.528703690	11.408453941
C	13.314627647	8.648822784	14.625306129	C	12.280304909	11.114554405	10.518488884
C	12.682769775	9.891184807	14.674057007	H	12.281860352	12.193606377	10.557266235
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C	9.986031532	8.716351509	12.273480415	H	13.666159630	7.027560711	18.282886505	
C	8.888310432	8.019279480	11.745360374	H	14.906572342	5.845227718	20.046495438	
H	8.794301033	7.887608528	10.671048164	H	15.779572487	3.548868179	19.655225754	
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C	8.025010109	7.695387363	13.977006912	H	19.196453094	5.058231831	14.899973869	
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C	9.131651878	8.362564087	14.505762100	H	18.794851303	0.776487529	14.939414024	
H	9.249677658	8.472910881	15.577758789	H	16.420137405	0.998210669	14.228321075	
C	10.111121178	8.874958038	13.661095619	H	15.434578896	3.254974842	13.884062767	
H	10.978745461	9.375793457	14.070508003	H	18.087472916	8.500684738	14.199645042	
H	17.310234070	12.008896828	9.265990257	H	19.607479095	9.495332718	12.544767380	
C	13.439481735	6.991255760	11.352569580	H	20.083459854	8.322865486	10.399166107	
C	11.977016449	6.919328213	10.893266678	H	19.006181717	6.120435238	9.944646835	
H	11.862389565	6.184131145	10.087572098	H	17.479536057	5.119255066	11.602466583	
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C	14.362028122	5.954531193	11.228466034	H	17.956417084	6.785717010	18.882850647	
H	14.027578354	4.941646099	11.002968788	H	17.001756668	9.080384254	18.924121857	
H	15.399326324	6.174661160	10.988537788	H	15.807940483	9.954872131	16.896236420	
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C	16.684375763	6.875710487	15.725839615	C	13.652371407	8.821431160	6.366744041	
C	17.653818130	6.741065979	13.019835472	C	14.621026993	8.923815727	7.366114140	
C	17.232542038	4.307938576	14.409016609	H	14.788993835	9.883026123	7.844765663	
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C	16.913221359	8.468734741	18.029825211	C	13.422401428	7.613936424	5.704406738	
C	17.4545559326	7.183233738	18.004230499	H	12.680109978	7.574849606	4.913093567	
C	17.343305588	6.388432026	16.861785889	N	11.453632355	10.119460106	7.114732742	
C	18.272645950	7.974714279	13.269067764	C	10.246741295	9.721337318	6.711204052	
C	19.140741348	8.537656784	12.329555511	H	10.019138336	9.660332680	5.644020557	
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C	9.505012512	4.413147449	13.968073845	H	7.067414284	9.309111595	9.158757210	
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C	14.022493362	6.020909786	18.095296860	C	11.280400276	7.960752487	10.135219574	
C	14.730447769	5.349199772	19.095554352	H	11.936901093	8.095276833	9.259997368	
C	15.224248886	4.063723564	18.875795364	C	9.839233398	7.940236568	9.657027245	
C	15.004819870	3.447550058	17.640529633	C	9.572540283	6.750773907	8.770969391	
C	14.294443130	4.115116119	16.645402908	H	10.434872627	6.449128628	7.708024025	
H	10.797412872	6.617865086	17.549932480	H	11.269974709	7.103252888	7.478141785	

C	10.215906143	5.317217350	6.927687168	H	15.626970291	1.757339001	16.439975739	
H	10.890309334	5.097515583	6.104539394	H	14.421772957	3.159347534	14.815397263	
C	9.138250351	4.471282959	7.202634335	H	18.951295853	4.331692696	14.634449959	
H	8.967366219	3.589243889	6.591401100	H	19.583026886	1.954484940	14.880926132	
C	8.280458450	4.763858795	8.262737274	H	18.148029327	0.173354581	13.909152985	
H	7.436536789	4.114780426	8.479136467	H	16.068298340	0.787651956	12.690236092	
C	8.499371529	5.899392605	9.043085098	H	15.417317390	3.178069353	12.477324486	
H	7.820193768	6.137475491	9.857733727	H	19.509901047	6.599902630	13.170787811	
H	15.702404022	5.696628571	7.352089882	H	21.048265457	7.048153400	11.291999817	
C	13.019351006	7.390930653	11.593993187	H	20.268503189	6.789379597	8.945549965	
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H	12.037627220	5.895971298	10.310563087	H	16.378637314	5.652173042	10.381832123	
H	11.052384377	6.451006889	11.678704262	H	16.904821396	5.014336109	16.137668610	
C	14.283371925	7.265468121	10.990245819	H	17.383417130	6.410151958	18.096408844	
H	14.413473129	6.575510502	10.160128593	H	17.954469681	8.822561264	17.821044922	
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C	12.530165672	8.752429008	12.103301048	H	17.544519424	8.410765648	13.562778473	
H	12.004931450	8.658670425	13.065097809	H	9.163238525	7.921713829	10.521017075	
H	13.330709457	9.484146118	12.249703407	<hr/>				
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C	11.528602600	4.887042999	14.785565376	C	12.568732262	10.163456917	6.772363663	
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C	13.974952698	4.734827995	16.217704773	H	14.046580315	11.041774750	8.054567337	
C	17.519607544	7.965058804	14.553325653	C	14.610883713	9.051155090	7.395173073	
C	17.791816711	8.756266594	15.668235779	H	15.548791885	9.036396980	7.942563057	
C	17.748874664	8.204205513	16.951837540	C	14.233233452	7.943005562	6.632868290	
C	17.436954498	6.852613926	17.105657578	C	13.026834488	7.955582142	5.925737381	
C	17.169731140	6.055612087	15.991319656	H	12.738540649	7.097525597	5.324698448	
C	19.156810760	6.485624790	12.150259018	C	12.189360619	9.069592476	5.990481377	
C	20.026533127	6.738318920	11.088801384	H	11.256323814	9.107436180	5.436846256	
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C	18.277999878	6.187674046	9.518339890	C	9.377693176	10.263779640	7.935138226	
C	17.403375626	5.950248241	10.578082085	H	8.842839241	10.398615837	6.996617317	
C	16.334403992	2.903426170	12.994043350	C	8.942313194	9.338233948	8.857061386	
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C	11.085017204	4.424468040	13.539730072	H	5.449462891	7.175530434	10.999608994	
C	13.971857071	8.131712914	16.004503250	C	7.090012550	8.184832573	10.047158241	
C	13.821100235	9.409635544	16.537124634	H	7.616138935	8.371363640	10.979366302	
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C	14.800871849	4.360473633	18.470539093	H	12.298599243	10.957696915	11.358504295	
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H	10.685189247	7.302626610	15.664629936	C	10.566257477	7.759284496	10.058349609	
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H	12.425401688	10.939265251	17.157159805	C	10.011068344	6.568908691	7.888422966	
H	14.706508636	9.991690636	16.778823853	H	10.465446472	7.386900902	7.339970112	
H	14.969581604	7.741780758	15.831814766	C	9.482505798	5.478564739	7.202495098	
H	11.075051308	4.983957767	16.895282745	H	9.528600693	5.451043606	6.116893768	
H	8.888099670	3.846207142	16.678878784	C	8.897918701	4.421429157	7.904647350	
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H	12.996412277	5.968410015	9.239665985	H	17.835174561	5.471685410	10.593474388	
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Pd	15.143639565	6.012388706	12.245529175	=====				
P	13.335249901	5.748897552	13.785779953	3				
P	17.101070404	5.302879810	13.364554405	=====				
C	17.366977692	6.422289848	14.805644035	S	10.009830475	12.140092850	13.228218079	
C	18.750442505	5.330547810	12.529847145	O	9.775999069	10.692667961	13.088653564	
C	17.079408646	3.602717638	14.082207680	O	8.985339165	13.082511902	12.764664650	
C	12.047709465	4.540777206	13.251642227	C	10.392593384	12.475489616	14.946235657	
C	12.441548347	7.341059208	14.017063141	C	10.349230766	11.431753159	15.869050026	
C	13.546511650	5.170376778	15.530384064	H	10.118724823	10.428481102	15.528081894	
C	18.045431137	7.636975288	14.605914116	C	10.617646217	11.706850052	17.210550308	
C	18.114931107	8.587946892	15.622712135	H	10.589372635	10.902911186	17.940355301	
C	17.503612518	8.346078873	16.855421066	C	10.926369667	13.008728981	17.612392426	
C	16.825716019	7.144750118	17.062654495	C	10.960483551	14.044913292	16.673860550	
C	16.755355835	6.190052986	16.047327042	H	11.197113037	15.057451248	16.988079071	
C	19.965993881	5.254027843	13.228464127	C	10.688357353	13.784059525	15.331565857	
C	21.177795410	5.245529652	12.539424896	H	10.710857391	14.574718475	14.589101791	
C	21.194322586	5.315968990	11.141980171	N	11.467091560	12.669314384	12.451064110	
C	19.989490509	5.394195557	10.443797112	C	11.279449463	12.796304703	11.028122902	
C	18.775039673	5.402508736	11.132586479	H	10.665108681	13.592397690	10.635502815	
C	16.295114517	2.641606808	13.426836014	C	11.996707916	11.871202469	10.359049797	
C	16.234333038	1.328144789	13.895954132	C	12.093648911	11.706095695	8.904706955	
C	16.952493668	0.958415389	15.035532951	C	13.316078186	11.365476608	8.305685997	
C	17.738601685	1.907881021	15.693806648	H	14.184638977	11.214295387	8.936841011	
C	17.808105469	3.217214108	15.216890335	C	13.403211594	11.204236031	6.926137924	
C	10.896136284	4.293393135	14.018367767	H	14.352235794	10.926174164	6.476055622	
C	9.964574814	3.341509342	13.609333992	C	12.274589539	11.390385628	6.124000072	
C	10.178399086	2.611256123	12.436107635	H	12.342182159	11.256672859	5.047651768	
C	11.326499939	2.835648775	11.677404404	C	11.056812286	11.740194321	6.710566044	
C	12.257440567	3.793852806	12.084754944	H	10.173249245	11.878103256	6.093090534	
C	13.209020615	8.431917191	14.466804504	C	10.965014458	11.893286705	8.092415810	
C	12.631879807	9.691331863	14.620491982	H	10.012450218	12.131714821	8.556408882	
C	11.283730507	9.890027046	14.308386803	N	12.708859444	11.009613037	11.262066841	
C	10.519341469	8.820226669	13.845805168	C	12.703775406	11.794802666	12.503096581	
C	11.092078209	7.554463863	13.704213142	H	13.503446579	12.538943291	12.381703377	
C	13.299319267	5.956849098	16.662759781	C	12.947366714	11.029695511	13.754162788	
C	13.529487610	5.447006702	17.942977905	H	13.340496063	11.579499245	14.604944229	
C	14.008154869	4.147939205	18.110664368	C	12.772300720	9.712665558	13.790493965	
C	14.237336159	3.348534822	16.986946106	H	11.061514854	9.711028099	11.034658432	
C	14.005102158	3.854731321	15.711108208	C	12.212201118	8.907063484	12.650151253	
H	10.477427483	6.730536938	13.357802391	H	11.174708366	8.690468788	12.933953285	
H	9.474538803	8.968324661	13.584958076	C	12.130108333	9.622788429	11.259037018	
H	10.837771416	10.875062943	14.415349007	C	12.772291183	8.782547951	10.168437958	
H	13.237473488	10.520564079	14.976453781	C	14.163271904	8.745686531	10.012388229	
H	14.263469696	8.288793564	14.695016861	H	14.777102470	9.390189171	10.629962921	
H	10.739437103	4.839202404	14.944881439	C	14.752101898	7.898585320	9.077608109	
H	9.075743675	3.162748098	14.208717346	H	15.834363937	7.871777534	8.988425255	
H	9.452627182	1.866823554	12.119601250	C	13.957736969	7.074721813	8.274472237	
H	11.495828629	2.272195816	10.764296532	H	14.418172836	6.409853935	7.549001217	
H	13.154398918	3.970901012	11.496237755	C	12.570377350	7.115664959	8.414229393	
H	12.932700157	6.972000599	16.555992126	H	11.939879417	6.489926338	7.787475109	
H	13.331486702	6.072071075	18.810226440	C	11.983467102	7.963766575	9.357995033	
H	14.192190170	3.757296085	19.107799530	H	10.900831223	7.992419243	9.461463928	
H	14.611858368	2.334924936	17.098722458	H	11.138830185	13.217796326	18.657047272	
H	14.195376396	3.224195004	14.849525452	C	13.182268143	7.392446518	14.260276794	
H	18.409637451	3.947627306	15.749549866	C	12.770759583	6.260879040	14.959299088	
H	18.297307968	1.629290342	16.583608627	H	12.389978409	5.384150505	14.438557625	
H	16.897916794	-0.060030874	15.410294533	H	12.478165627	6.354592800	16.003231049	
H	15.615330696	0.598709702	13.380384445	C	13.006684303	7.584262371	12.755740166	
H	15.707937241	2.940323591	12.561441422	H	12.498515129	6.741476059	12.277434349	
H	19.965391159	5.212594986	14.314026833	H	13.967393875	7.708945274	12.256892204	
H	22.111690521	5.187210560	13.092546463	C	13.123962402	8.778911591	14.923002243	

H	12.336693764	8.797973633	15.690619469	C	18.995229721	1.882825136	14.992346764
H	14.045530319	9.081772804	15.428983688	C	18.664876938	1.537204027	13.679794312
Pd	14.970190048	6.092981815	14.733797073	C	17.468631744	2.001695156	13.123951912
P	15.788008690	4.309084892	16.070610046	C	16.620719910	2.816674232	13.873617172
P	16.766807556	6.695714951	13.251709938	H	15.843563080	3.778571606	19.058885574
C	18.530851364	6.585087776	13.803958893	H	17.192098618	4.770696163	20.872856140
C	16.782127380	8.397603989	12.525320053	H	18.927410126	6.474061012	20.360513687
C	16.708681107	5.625298977	11.743876457	H	19.301155090	7.179154396	17.993402481
C	14.652015686	3.093909740	16.871215820	H	17.930435181	6.222933769	16.193338394
C	16.792285919	4.923564434	17.490522385	H	16.062412262	1.462251306	17.014953613
C	16.950437546	3.178336859	15.189717293	H	14.494536400	-0.058641184	18.165115356
C	19.189916611	5.346975327	13.886081696	H	12.181765556	0.689614236	18.688360214
C	20.457393646	5.249383450	14.460107803	H	11.450076103	2.978791952	18.044645309
C	21.094997406	6.382164001	14.967961311	H	13.027724266	4.498869896	16.881080627
C	20.453735352	7.620184422	14.883986473	H	18.422908783	2.981070518	16.754590988
C	19.186761856	7.722240448	14.307581902	H	19.923213959	1.525573969	15.431979179
C	16.191463470	9.427045822	13.266595840	H	19.335723877	0.915409386	13.093361855
C	16.227357864	10.746674538	12.811645508	H	17.20777023	1.758283496	12.097723007
C	16.854948044	11.050717354	11.604564667	H	15.715126991	3.210971594	13.421569824
C	17.451280594	10.029864311	10.857254028	H	18.815698624	5.653072357	11.259404182
C	17.418962479	8.714085579	11.314926147	H	18.587699890	4.248315334	9.249746323
C	15.453190804	5.145198345	11.338217735	H	16.351879120	3.401422262	8.554342270
C	15.323728561	4.357302189	10.194711685	H	14.339566231	4.009505272	9.893669128
C	16.450258255	4.021821499	9.441036224	H	14.573551178	5.388339043	11.926430702
C	17.704071045	4.497968197	9.831678391	H	15.695235252	9.184089661	14.198987007
C	17.832466125	5.296011448	10.969531059	H	15.749961853	11.527971268	13.394760132
C	15.054890633	1.799988270	17.238100052	H	16.873044968	12.074514389	11.240824699
C	14.169162750	0.940594673	17.887413025	H	17.936750412	10.260747910	9.912534714
C	12.870348930	1.361257911	18.182474136	H	17.879995346	7.930301189	10.722389221
C	12.460076332	2.644911051	17.821485519	H	18.707143784	8.694686890	14.252777100
C	13.344740868	3.503135204	17.167226791	H	20.940460205	8.514192581	15.265942574
C	17.771215439	5.894086838	17.212867737	H	22.079023361	6.303450584	15.421733856
C	18.543567657	6.438485622	18.235717773	H	20.935533524	4.275729656	14.518441200
C	18.334796906	6.040862560	19.558807373	H	18.713203430	4.449784756	13.510479927
C	17.360462189	5.084678860	19.845788956				
C	16.594711304	4.524670124	18.819820404				
C	18.144981384	2.698053598	15.743500710				

IV-4. Vibrational frequencies of the optimized geometries

Table S5. Vibrational Frequencies (in cm⁻¹) of the Optimized Geometries

PdL2							1014.14	1014.18	1014.42	1050.60	1051.92	1052.12
8.93	17.87	19.56	30.50	31.16	36.59		1111.29	1112.09	1113.26	1114.05	1114.53	1116.49
37.29	45.79	49.64	50.89	53.28	54.01		1116.78	1119.69	1120.47	1195.59	1195.79	1196.22
60.70	63.06	66.33	67.17	73.91	96.18		1196.38	1196.86	1197.21	1220.10	1220.53	1220.93
102.74	160.06	185.83	193.86	207.80	212.50		1221.97	1222.29	1223.38	1324.35	1324.98	1327.07
217.38	221.63	224.29	252.68	253.85	260.72		1327.66	1329.39	1329.84	1361.44	1361.88	1362.20
261.65	269.05	270.12	406.99	408.46	410.13		1362.78	1362.82	1363.37	1474.15	1475.19	1475.30
411.76	412.91	415.86	431.90	433.05	437.41		1475.71	1476.02	1477.04	1523.33	1524.02	1524.39
444.87	446.83	452.54	510.06	511.96	515.20		1524.81	1524.89	1525.18	1625.34	1626.35	1626.86
517.72	518.59	541.72	630.68	631.08	631.28		1627.18	1627.47	1628.30	1643.43	1644.22	1644.50
631.81	632.09	632.80	697.58	699.57	708.15		1645.20	1645.40	1646.38	3168.93	3169.85	3171.41
708.76	709.47	710.74	712.18	712.77	713.11		3171.88	3172.29	3172.62	3176.56	3176.57	3177.97
713.96	714.21	714.93	761.61	763.40	765.71		3178.70	3180.82	3183.99	3187.13	3187.32	3187.38
766.38	767.18	767.62	865.27	867.56	869.39		3188.17	3189.13	3192.53	3196.73	3197.22	3197.38
869.63	871.33	874.19	935.65	938.98	939.56		3197.95	3198.53	3201.05	3203.84	3203.96	3204.22
940.63	941.12	943.13	979.88	982.27	983.06		3204.37	3205.01	3205.81			
983.60	985.75	987.88	1000.56	1001.99	1004.46		2					
1004.88	1005.21	1007.00	1013.32	1013.68	1013.88							

20.03	31.50	36.22	94.34	109.12	137.37		3205.53	3206.66	3208.05	3210.97	3213.03	3214.13
150.69	160.68	172.22	173.28	182.58	192.58		3215.55	3218.00	3220.79			
215.67	218.72	232.91	250.65	301.57	359.17							
458.62	491.03	520.16	570.63	583.66	610.20							
663.95	688.13	692.77	693.37	696.92	740.22							
795.69	825.54	848.77	878.25	880.21	892.99							
904.44	923.09	984.80	1027.71	1039.53	1059.38							
1099.00	1130.69	1193.46	1267.75	1285.70	1294.19							
1304.62	1306.20	1315.46	1405.44	1432.33	1452.66							
1467.33	1470.23	1472.56	1474.89	1480.74	1481.67							
1483.94	1489.68	1499.62	1512.58	1724.97	1857.33							
2997.87	3025.85	3033.72	3036.06	3039.61	3053.15							
3057.85	3081.81	3109.88	3114.49	3115.13	3116.33							
3117.10	3121.39	3125.62	3165.82	3181.16	3264.88							
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2'												
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25.27	29.13	41.45	43.96	47.05	50.72		-183.64	2.28	14.35	18.34	18.57	22.13
54.18	56.95	60.36	61.72	63.50	66.93		24.59	27.03	29.44	34.26	36.89	38.41
71.49	73.68	75.25	76.81	84.31	94.00		42.39	46.94	47.95	49.54	49.91	53.78
97.98	105.29	109.53	150.54	157.76	176.36		55.48	58.15	61.14	62.06	67.81	69.33
188.80	198.56	208.23	216.01	221.72	234.21		71.51	74.60	76.20	82.01	86.83	87.93
239.03	254.13	257.14	259.29	261.24	278.37		91.05	96.55	100.66	104.42	109.86	124.36
280.14	364.00	380.93	408.47	409.36	412.51		126.41	136.20	147.29	162.82	169.41	171.61
416.43	419.17	422.80	431.96	433.59	443.11		182.34	187.58	194.01	195.16	198.06	207.02
445.95	450.51	455.26	458.81	476.33	506.60		218.30	223.57	228.21	229.78	237.17	245.10
507.98	521.34	523.24	529.59	538.42	610.66		248.51	250.62	255.48	258.12	261.69	279.67
630.95	632.10	633.13	633.55	633.73	634.96		286.64	309.53	311.75	332.59	338.23	347.73
673.39	699.28	701.77	709.02	710.38	711.28		356.41	366.80	386.33	398.34	403.74	407.04
711.77	715.39	716.11	716.63	718.45	718.99		410.92	411.52	413.83	416.77	417.88	421.52
720.93	737.78	760.66	764.15	764.63	765.55		424.24	425.56	428.51	434.70	442.18	444.03
767.58	771.50	772.52	779.25	864.58	866.82		446.33	455.54	461.80	471.51	480.75	492.73
868.01	875.07	876.68	880.57	884.61	935.45		498.35	502.81	506.91	521.45	524.72	529.93
937.24	941.60	949.58	951.49	955.10	964.96		530.57	540.59	548.42	558.12	580.61	609.97
979.82	981.28	983.45	988.69	992.93	994.33		622.01	626.83	626.99	628.13	628.27	629.50
998.10	999.74	1003.27	1003.81	1006.63	1010.41		629.71	631.59	632.00	632.65	633.16	639.12
1011.38	1012.60	1015.64	1015.68	1016.57	1017.26		661.07	694.67	698.52	702.31	706.38	707.01
1018.93	1019.69	1030.86	1051.48	1052.54	1054.03		708.67	710.66	711.00	711.84	712.71	715.65
1054.77	1055.22	1055.88	1103.28	1112.65	1113.68		716.41	718.03	719.80	720.38	721.95	728.50
1115.43	1115.49	1116.81	1117.17	1118.01	1118.63		729.58	743.00	752.42	758.38	762.38	765.41
1120.62	1120.86	1122.42	1124.44	1199.13	1199.22		767.10	768.07	769.19	769.79	771.31	776.47
1199.41	1199.91	1200.05	1200.56	1221.67	1224.16		779.48	792.68	800.30	830.20	854.07	859.42
1225.46	1225.82	1227.08	1229.33	1282.31	1323.62		859.82	862.61	863.94	865.87	868.59	870.78
1325.02	1328.63	1330.82	1333.66	1333.98	1362.68		871.22	875.64	900.34	911.07	913.69	934.48
1365.65	1366.51	1367.09	1367.73	1369.60	1433.17		935.11	936.98	940.20	942.15	944.15	945.21
1455.72	1475.33	1475.64	1476.73	1479.14	1479.46		949.80	957.52	965.49	969.28	970.77	973.17
1479.72	1487.21	1524.99	1526.41	1527.05	1528.26		974.99	978.29	980.28	982.26	983.89	985.86
1529.03	1530.50	1627.19	1627.85	1629.18	1630.64		986.13	988.90	989.87	997.40	1000.53	1000.85
1630.93	1631.07	1645.77	1646.05	1646.78	1647.91		1002.31	1003.08	1003.68	1006.34	1008.07	1008.75
1648.91	1649.35	1676.64	3058.28	3068.50	3137.05		1009.28	1012.65	1013.56	1014.05	1014.28	1014.50
3153.62	3162.18	3174.43	3175.74	3175.83	3176.32		1015.11	1015.73	1017.24	1020.52	1039.59	1047.15
3177.37	3177.47	3179.55	3181.84	3186.26	3186.53		1047.39	1049.57	1049.71	1050.43	1051.13	1051.87
3187.36	3188.96	3190.48	3191.63	3194.91	3196.44		1053.01	1054.05	1060.19	1067.11	1072.35	1082.76
3197.66	3199.62	3199.75	3203.61	3205.00	3205.48		1093.98	1108.70	1110.28	1110.38	1111.60	1113.94

1115.79	1116.07	1116.96	1117.34	1118.50	1119.13		1199.41	1199.91	1200.05	1200.56	1221.67	1224.16
1120.44	1122.54	1123.86	1125.76	1126.43	1134.26		1225.46	1225.82	1227.08	1229.33	1282.31	1323.62
1150.19	1195.08	1195.50	1196.36	1196.83	1197.19		1325.02	1328.63	1330.82	1333.66	1333.98	1362.68
1197.77	1198.04	1198.13	1198.86	1201.70	1212.05		1365.65	1366.51	1367.09	1367.73	1369.60	1433.17
1220.33	1220.79	1221.37	1222.70	1224.02	1225.35		1455.72	1475.33	1475.64	1476.73	1479.14	1479.46
1225.67	1226.18	1242.86	1272.61	1294.72	1322.18		1479.72	1487.21	1524.99	1526.41	1527.05	1528.26
1325.09	1326.84	1327.37	1328.60	1331.55	1331.58		1529.03	1530.50	1627.19	1627.85	1629.18	1630.64
1335.21	1336.52	1340.09	1345.36	1348.56	1351.67		1630.93	1631.07	1645.77	1646.05	1646.78	1647.91
1362.26	1362.69	1363.84	1365.86	1366.06	1368.45		1648.91	1649.35	1676.64	3058.28	3068.50	3137.05
1368.97	1372.24	1379.72	1385.29	1422.51	1457.66		3153.62	3162.18	3174.43	3175.74	3175.83	3176.32
1471.13	1473.20	1475.48	1477.62	1478.76	1480.63		3177.37	3177.47	3179.55	3181.84	3186.26	3186.53
1484.20	1487.04	1489.05	1491.47	1492.86	1506.81		3187.36	3188.96	3190.48	3191.63	3194.91	3196.44
1524.11	1525.11	1525.82	1526.34	1527.60	1528.54		3197.66	3199.62	3199.75	3203.61	3205.00	3205.48
1532.13	1539.60	1542.38	1556.03	1596.15	1616.77		3205.53	3206.66	3208.05	3210.97	3213.03	3214.13
1622.98	1625.25	1626.62	1627.96	1628.71	1629.50		3215.55	3218.00	3220.79			
1630.33	1633.88	1643.11	1643.57	1644.20	1644.77							
1645.01	1645.88	1647.83	1648.03	1655.84	1661.02							
1665.48	3093.13	3100.71	3113.75	3163.82	3165.50							
3166.30	3171.76	3172.60	3174.30	3175.07	3175.86		8.16	22.33	34.80	37.83	47.82	48.37
3176.44	3176.90	3177.12	3178.06	3181.95	3183.36		58.86	68.17	70.51	88.70	110.20	149.38
3185.20	3186.28	3186.92	3187.81	3188.04	3189.61		178.50	186.78	201.45	215.05	248.33	265.70
3189.86	3190.32	3190.40	3192.91	3193.76	3194.89		293.79	304.73	306.86	317.49	349.64	367.63
3196.74	3197.24	3197.84	3198.15	3198.64	3200.71		375.59	414.62	415.16	416.33	452.82	470.28
3201.71	3202.26	3202.75	3203.06	3203.76	3205.15		486.36	507.30	532.97	545.92	556.88	576.51
3206.27	3208.50	3210.57	3211.11	3212.67	3213.29		607.26	619.28	627.66	628.87	634.25	644.61
3215.09	3215.95	3216.24	3217.78	3220.28	3227.17		655.85	702.17	709.07	714.17	717.64	740.54
3227.89	3254.55	3265.28					755.84	766.50	767.69	775.07	790.69	804.44
							829.12	845.67	864.72	870.37	899.02	903.80
							938.34	944.03	965.45	973.78	977.51	987.00
							989.87	990.12	1001.72	1002.68	1009.08	1012.34
Pd-TMM												
25.27	29.13	41.45	43.96	47.05	50.72		1012.64	1014.91	1019.28	1038.07	1047.83	1061.84
54.18	56.95	60.36	61.72	63.50	66.93		1068.55	1082.14	1088.18	1105.63	1116.76	1119.79
71.49	73.68	75.25	76.81	84.31	94.00		1131.48	1135.43	1170.23	1194.27	1195.76	1197.16
97.98	105.29	109.53	150.54	157.76	176.36		1199.20	1209.24	1222.44	1226.68	1285.80	1299.18
188.80	198.56	208.23	216.01	221.72	234.21		1302.05	1304.29	1325.15	1333.64	1335.60	1336.53
239.03	254.13	257.14	259.29	261.24	278.37		1346.42	1358.76	1369.87	1372.94	1401.79	1470.14
280.14	364.00	380.93	408.47	409.36	412.51		1483.49	1491.57	1493.38	1518.23	1522.44	1540.51
416.43	419.17	422.80	431.96	433.59	443.11		1548.37	1603.74	1607.04	1623.78	1634.98	1637.42
445.95	450.51	455.26	458.81	476.33	506.60		1641.71	1657.97	1659.46	1671.41	3114.71	3165.36
507.98	521.34	523.24	529.59	538.42	610.66		3171.23	3175.95	3181.46	3182.69	3184.71	3190.32
630.95	632.10	633.13	633.55	633.73	634.96		3195.23	3198.13	3198.37	3206.14	3206.27	3208.07
673.39	699.28	701.77	709.02	710.38	711.28		3212.11	3212.92	3214.08	3229.53	3234.55	3267.15
711.77	715.39	716.11	716.63	718.45	718.99							
720.93	737.78	760.66	764.15	764.63	765.55		E					
767.58	771.50	772.52	779.25	864.58	866.82							
868.01	875.07	876.68	880.57	884.61	935.45		18.13	26.71	45.91	54.28	67.28	67.60
937.24	941.60	949.58	951.49	955.10	964.96		81.99	88.75	98.89	110.66	122.02	179.93
979.82	981.28	983.45	988.69	992.93	994.33		188.86	221.84	233.49	239.44	245.57	265.31
998.10	999.74	1003.27	1003.81	1006.63	1010.41		286.20	304.33	311.38	350.26	374.70	402.57
1011.38	1012.60	1015.64	1015.68	1016.57	1017.26		416.54	417.29	420.85	425.41	460.51	474.41
1018.93	1019.69	1030.86	1051.48	1052.54	1054.03		500.93	536.44	550.42	570.90	573.60	601.27
1054.77	1055.22	1055.88	1103.28	1112.65	1113.68		620.39	627.04	628.36	630.32	644.17	664.15
1115.43	1115.49	1116.81	1117.17	1118.01	1118.63		682.24	697.89	708.61	711.01	717.23	725.20
1120.62	1120.86	1122.42	1124.44	1199.13	1199.22		732.27	762.93	769.86	770.95	793.42	806.52

814.35	822.19	859.35	862.47	865.82	920.03	252.94	254.69	257.70	259.68	261.19	279.89
933.39	939.80	944.40	965.85	977.90	982.92	281.08	299.68	307.81	314.88	322.47	347.54
985.97	988.47	999.15	1000.47	1007.11	1013.00	358.22	362.02	376.67	382.95	405.96	408.24
1015.80	1017.17	1017.83	1050.08	1050.84	1052.57	411.31	413.34	414.34	416.66	419.40	423.57
1062.29	1078.29	1090.22	1113.26	1114.38	1116.04	424.73	425.00	427.44	433.28	440.20	441.46
1130.99	1142.00	1155.96	1195.73	1195.83	1197.34	448.74	459.85	462.39	467.28	470.30	487.58
1198.68	1215.64	1217.44	1218.81	1224.30	1279.64	499.88	501.49	505.09	516.51	524.05	531.39
1312.53	1329.64	1333.26	1336.09	1343.89	1346.59	536.38	541.36	541.80	563.56	574.82	608.76
1350.04	1365.26	1368.04	1368.51	1390.30	1443.10	611.04	618.49	623.85	624.53	626.92	627.85
1452.92	1487.18	1488.42	1490.13	1520.80	1539.40	628.00	628.86	631.07	632.83	633.34	639.18
1539.96	1620.65	1630.36	1638.29	1641.00	1643.21	646.35	694.02	695.70	696.35	702.93	704.62
1659.82	1663.00	1665.88	1704.45	2958.83	3176.58	707.61	708.55	710.44	711.19	712.01	712.41
3178.11	3183.35	3184.97	3186.30	3186.39	3195.76	713.51	714.44	714.91	716.45	720.08	721.10
3196.64	3197.06	3205.40	3205.89	3209.01	3213.88	724.76	729.74	753.42	759.14	761.63	763.16
3225.87	3227.23	3232.18	3240.24	3243.60	3286.72	764.29	766.34	767.28	768.95	770.64	771.15
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Intra-TS											
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-264.09	21.13	30.47	33.53	47.34	54.87	875.94	777.94	787.26	801.16	821.11	852.03
64.10	64.76	80.81	92.65	103.28	127.70	862.62	864.18	864.98	865.14	870.79	873.17
147.22	192.30	212.18	220.68	248.26	259.63	873.50	877.91	878.82	897.44	901.54	930.36
263.71	300.37	306.98	335.62	351.93	376.40	935.04	936.00	936.39	938.77	944.68	946.73
398.03	412.70	414.56	415.96	424.22	474.90	949.97	954.19	956.24	961.65	968.03	971.55
489.74	519.80	538.58	553.81	568.20	585.99	979.04	980.65	980.68	981.16	983.85	985.37
604.95	625.88	627.39	629.61	635.56	640.83	988.81	988.87	992.70	994.88	996.24	997.18
662.58	700.63	707.12	710.62	717.26	720.45	998.18	1000.26	1001.24	1004.67	1004.91	1006.70
726.18	762.40	771.13	771.70	777.04	785.08	1006.91	1008.60	1012.01	1012.95	1013.36	1013.70
819.47	849.62	858.61	862.40	865.19	883.80	1014.14	1014.35	1015.40	1016.98	1018.13	1026.66
919.16	938.20	942.07	969.98	975.26	979.94	1030.51	1044.59	1046.11	1049.12	1049.34	1052.18
986.46	993.96	994.44	1002.26	1005.06	1012.94	1052.67	1053.92	1054.05	1060.83	1066.33	1070.89
1013.93	1016.56	1019.67	1049.43	1054.79	1060.92	1082.74	1106.32	1109.67	1110.23	1113.18	1113.96
1078.78	1083.33	1100.45	1109.32	1114.59	1115.66	1114.41	1115.29	1115.63	1116.88	1117.77	1118.85
1137.06	1142.46	1174.22	1195.68	1196.66	1196.80	1119.16	1119.27	1121.02	1124.94	1126.99	1131.84
1202.04	1210.58	1215.23	1217.00	1224.66	1279.19	1167.81	1186.84	1194.40	1195.07	1198.64	1199.21
1290.47	1315.60	1321.96	1332.10	1338.75	1339.87	1199.50	1200.03	1200.20	1200.44	1201.53	1210.29
1347.88	1353.72	1364.06	1364.97	1369.87	1456.01	1219.19	1222.04	1224.74	1225.53	1227.68	1228.83
1481.76	1485.42	1488.34	1489.02	1520.57	1537.85	1229.58	1230.24	1287.81	1289.31	1304.51	1319.44
1540.67	1601.32	1613.51	1634.49	1636.21	1640.80	1324.05	1325.32	1326.18	1329.32	1329.92	1330.20
1643.71	1661.56	1662.42	1676.18	3176.81	3179.31	1334.40	1335.95	1336.08	1336.42	1344.21	1358.51
3181.48	3183.48	3188.49	3188.98	3192.48	3194.08	1360.68	1362.45	1364.07	1366.17	1367.22	1369.64
3195.57	3198.70	3200.30	3204.10	3205.09	3208.00	1370.86	1372.66	1373.54	1389.79	1428.40	1460.73
3209.78	3219.59	3226.04	3230.02	3230.33	3239.65	1472.89	1474.46	1475.36	1476.34	1477.58	1478.45
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TS1											
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-76.85	4.48	13.43	16.12	20.09	21.57	1665.62	3103.62	3106.50	3114.59	3142.49	3159.99
22.65	27.26	31.67	32.80	37.24	38.18	3168.30	3169.13	3172.69	3173.08	3173.12	3175.48
41.88	44.11	46.94	51.24	54.56	57.56	3175.72	3178.30	3179.03	3179.32	3180.12	3181.00
59.47	61.24	62.99	65.43	69.40	72.01	3182.49	3187.28	3187.79	3188.12	3191.02	3191.63
75.41	78.51	83.03	84.15	89.69	92.77	3192.16	3193.60	3196.79	3198.02	3198.74	3199.62
96.04	101.05	103.08	109.07	111.45	113.38	3200.55	3200.72	3203.29	3203.29	3203.48	3205.75
123.62	138.82	149.37	157.90	164.60	181.86	3206.29	3206.48	3208.96	3209.61	3211.38	3211.92
185.31	191.00	194.42	199.13	200.37	204.92	3212.04	3213.67	3213.99	3216.36	3217.05	3219.90
210.86	211.30	218.30	232.10	238.45	247.42	3221.29	3221.87	3226.07	3227.02	3234.26	3245.59

3250.11	3262.28	3263.25					1530.81	1534.43	1540.22	1540.70	1597.63	1602.04	
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A							1624.43	1624.64	1626.48	1627.49	1627.70	1628.21	
							1630.09	1640.29	1641.50	1643.45	1643.61	1644.85	
							1645.37	1645.46	1645.58	1646.25	1654.28	1666.10	
4.59	13.57	15.48	17.78	23.13	24.84		1702.75	3036.37	3051.86	3117.34	3118.14	3126.30	
30.44	32.08	35.92	36.27	40.00	41.78		3139.38	3139.56	3164.68	3165.48	3169.06	3171.93	
46.69	48.21	49.81	52.67	54.33	55.76		3177.52	3177.66	3178.15	3179.56	3181.19	3181.52	
58.43	60.95	63.04	66.73	69.69	78.60		3182.08	3184.64	3185.65	3186.48	3187.39	3187.97	
81.50	82.83	86.91	88.70	93.20	98.90		3189.69	3191.21	3192.52	3192.92	3194.48	3198.13	
101.27	104.52	112.60	113.93	122.65	137.59		3198.36	3199.36	3201.32	3201.58	3202.67	3202.95	
140.11	144.38	156.95	179.37	182.35	186.04		3206.08	3207.71	3208.36	3210.09	3210.43	3211.67	
200.61	203.77	206.35	207.51	209.21	218.00		3212.83	3213.54	3214.48	3215.30	3215.49	3216.14	
220.68	228.94	231.05	239.26	253.55	257.42		3216.81	3216.92	3217.09	3224.64	3225.49	3239.79	
258.74	261.77	264.98	269.18	279.00	282.31		3249.92	3252.00	3257.65				
295.87	299.27	305.53	316.07	323.84	341.35								
353.79	378.94	399.80	405.63	406.65	406.83	TS2							
409.24	410.98	412.96	414.33	417.87	420.94								
424.31	431.37	432.84	444.72	445.48	452.93		-387.57	8.12	10.16	12.99	20.76	22.45	
459.25	463.04	467.82	483.86	491.31	497.32		26.80	27.21	31.39	35.34	39.00	39.71	
499.96	504.69	520.63	522.79	531.26	531.99		42.00	42.91	44.50	47.04	50.46	52.71	
541.00	544.35	554.93	572.43	607.10	619.75		57.04	59.07	62.09	65.39	68.89	70.36	
626.27	629.83	630.13	630.45	631.15	632.67		74.62	76.10	79.50	83.47	85.73	89.39	
632.77	633.29	633.73	645.83	650.24	660.15		91.23	95.41	98.89	101.77	112.26	118.84	
691.58	696.79	699.30	700.82	705.14	706.36		124.44	144.57	153.50	161.18	169.39	181.45	
706.59	707.04	708.33	709.98	710.93	712.85		187.17	198.43	201.00	202.28	205.68	209.15	
714.04	715.33	715.88	719.19	720.78	721.77		214.63	224.19	229.19	235.16	243.96	254.01	
747.84	751.16	759.30	761.62	762.38	764.17		258.18	261.48	264.02	269.76	274.46	278.92	
764.59	765.59	767.56	772.23	772.31	774.48		282.44	300.06	310.10	321.62	335.09	360.44	
779.17	787.36	806.18	836.90	853.86	858.69		366.74	384.95	402.13	404.68	411.61	412.47	
861.84	862.25	867.28	868.18	871.14	873.64		413.55	414.11	415.70	419.08	420.08	421.45	
877.73	878.91	900.18	920.19	931.51	933.93		422.51	429.53	429.80	436.80	445.67	446.25	
937.58	939.57	940.34	943.64	944.18	945.50		459.28	461.97	468.39	492.75	497.37	499.91	
947.93	950.60	957.00	961.20	967.69	968.39		503.58	510.85	516.78	521.48	528.94	534.73	
973.72	977.52	978.03	982.41	985.06	987.36		539.09	551.31	554.81	585.27	602.46	626.65	
987.64	988.83	992.08	993.25	995.15	998.50		628.45	629.11	629.82	630.18	630.61	631.33	
1000.19	1006.78	1007.65	1009.57	1010.68	1011.70		632.17	632.69	633.44	640.17	660.03	668.86	
1012.47	1012.89	1013.31	1014.08	1014.61	1015.70		695.29	696.59	697.43	704.32	705.28	708.09	
1016.39	1018.75	1020.15	1022.08	1045.41	1048.53		708.18	709.66	711.88	712.04	712.83	714.96	
1051.05	1052.55	1052.84	1053.10	1053.40	1053.73		717.45	717.83	718.98	719.99	720.46	737.50	
1053.98	1057.09	1060.70	1072.49	1077.64	1106.32		747.60	757.77	761.58	764.72	765.80	766.50	
1109.39	1110.52	1110.57	1112.25	1114.32	1114.42		770.11	772.02	772.27	777.06	789.74	797.43	
1115.37	1116.92	1118.13	1118.73	1119.65	1120.80		810.69	840.28	844.31	845.82	859.94	865.17	
1121.27	1122.98	1132.33	1150.86	1171.39	1189.48		866.25	867.93	870.28	877.03	877.62	881.14	
1193.15	1193.59	1194.55	1199.22	1200.17	1200.24		891.96	899.73	917.54	932.29	932.85	935.92	
1200.78	1201.12	1204.90	1209.81	1215.07	1221.55		937.83	938.90	940.77	944.07	946.71	949.41	
1223.15	1225.50	1225.93	1226.41	1227.60	1233.54		953.81	955.09	958.45	975.22	976.78	977.42	
1270.41	1271.85	1281.82	1297.87	1309.37	1321.95		979.28	981.44	984.38	985.22	986.09	986.33	
1322.52	1329.36	1330.05	1331.36	1332.42	1333.78		991.87	993.08	996.46	996.93	1002.23	1003.74	
1333.92	1336.22	1338.55	1341.72	1361.18	1362.55		1006.33	1006.59	1008.57	1009.89	1012.20	1012.66	
1362.81	1364.10	1364.32	1365.53	1367.43	1369.60		1013.48	1014.10	1014.65	1014.79	1016.03	1017.20	
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630.82	631.48	632.25	633.73	650.06	670.91		80.23	84.36	85.69	90.23	94.43	96.53	
688.58	695.53	696.47	701.26	705.35	708.28		100.26	104.77	109.68	117.48	125.10	129.51	
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766.77	767.79	772.51	779.39	780.48	799.61		257.08	261.62	265.65	273.82	277.36	281.24	
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225.20	228.11	229.17	243.26	249.95	255.80	3209.10	3209.21	3210.26	3211.25	3216.40	3216.82
256.64	258.09	259.68	277.65	278.74	284.70	3222.46	3234.38	3236.91			
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628.42	630.46	630.82	631.01	632.62	632.87	82.16	86.62	89.20	93.85	96.58	99.69
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847.15	850.86	853.35	858.16	863.09	865.09	402.13	409.97	412.83	413.43	413.90	414.39
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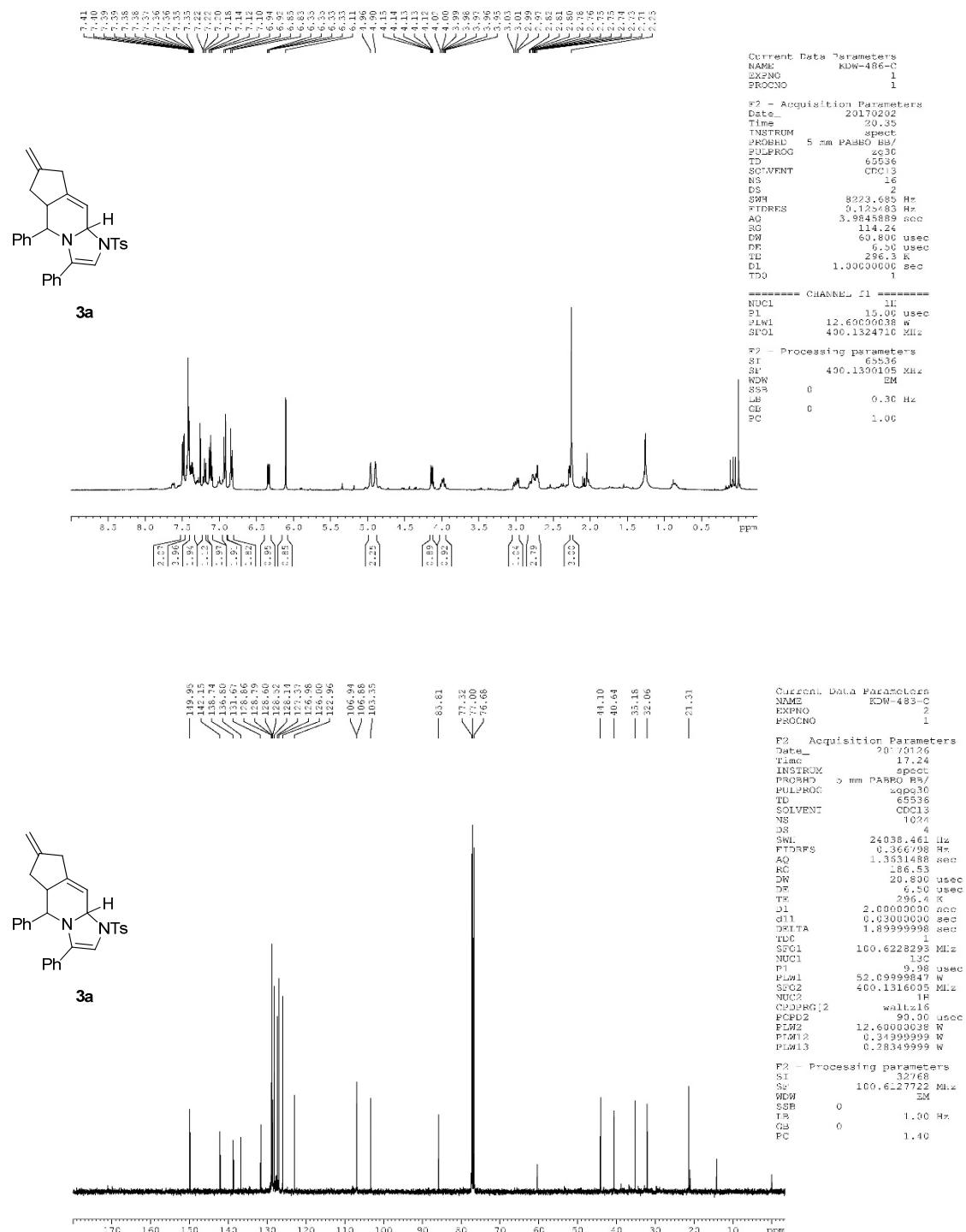
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1001.34	1003.04	1004.10	1005.04	1005.16	1006.56		1508.47	1523.69	1524.74	1525.13	1526.21	1526.40
1007.58	1008.69	1012.34	1013.06	1014.49	1014.59		1527.07	1527.92	1538.76	1540.02	1564.80	1622.53
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V. References

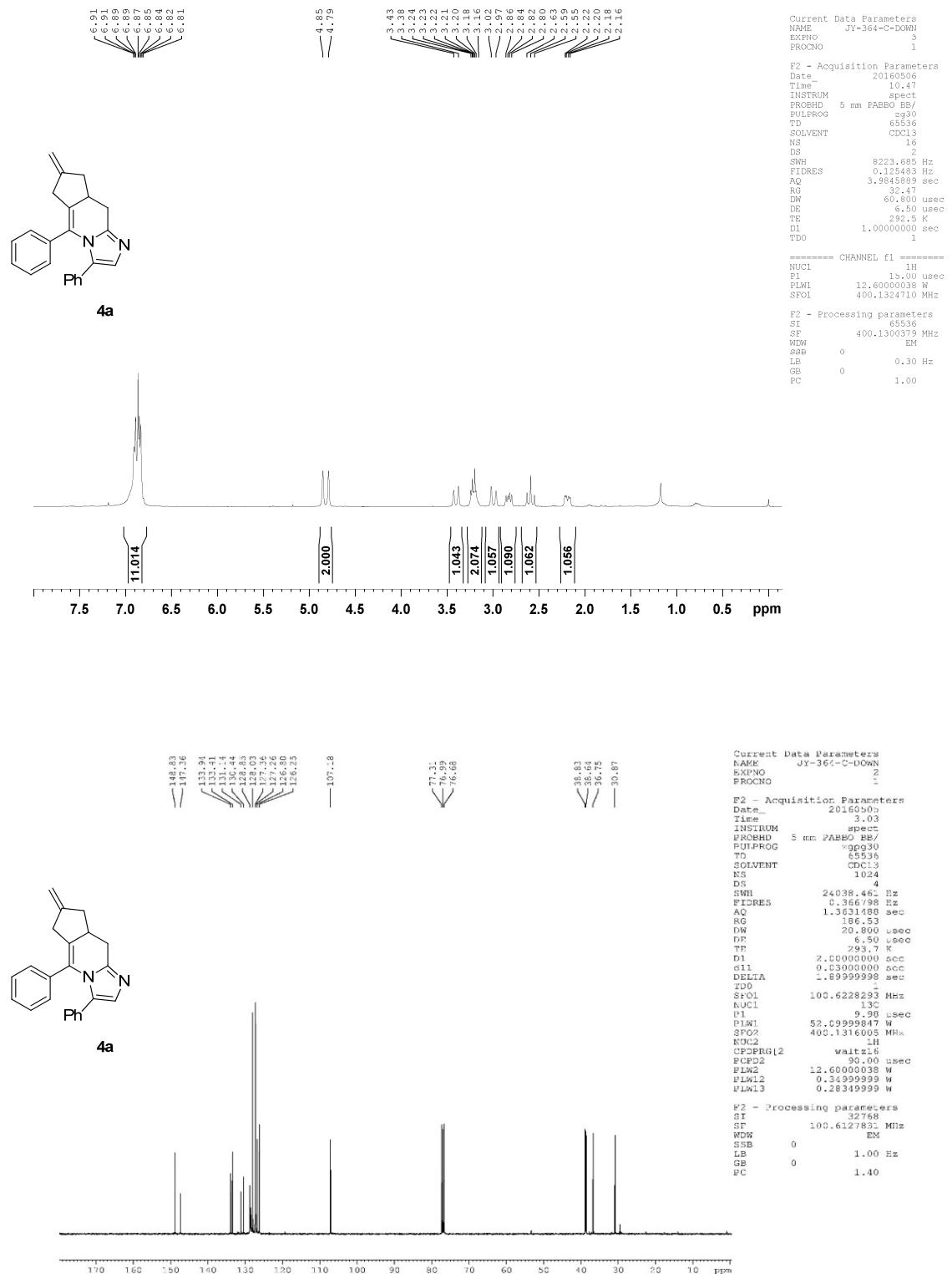
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VI. Copies of Spectral Data of Compounds

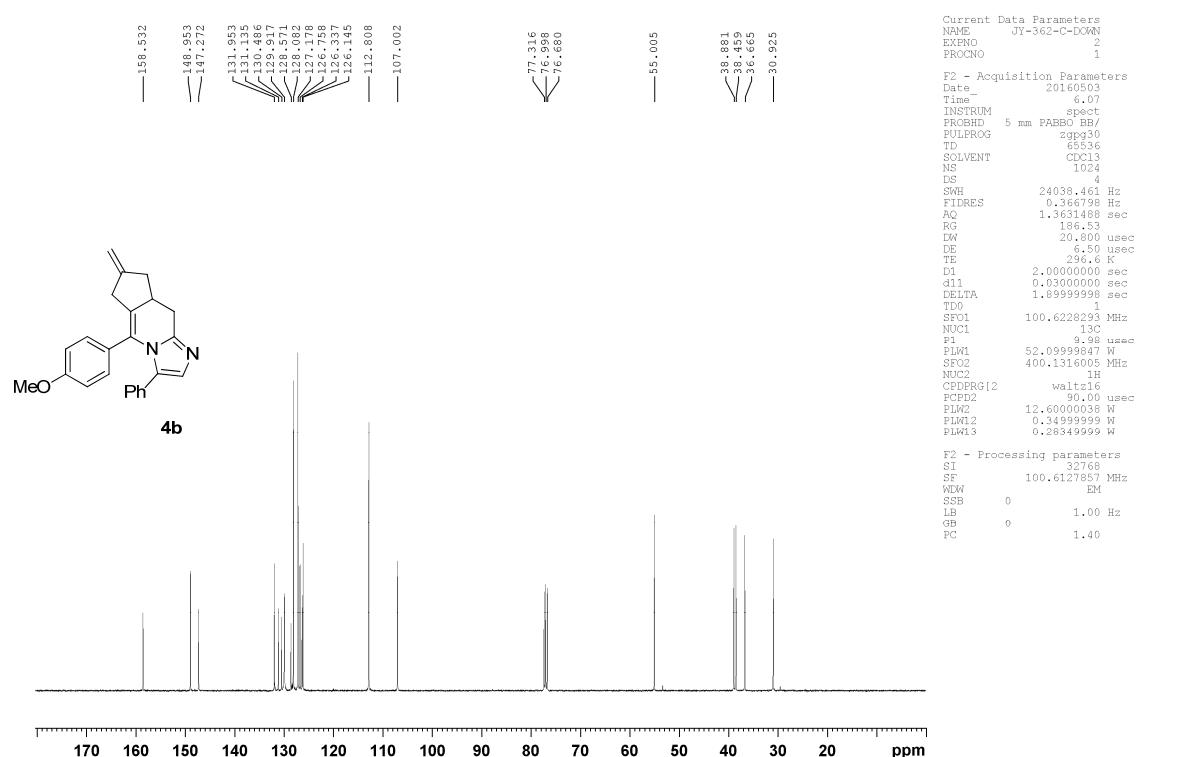
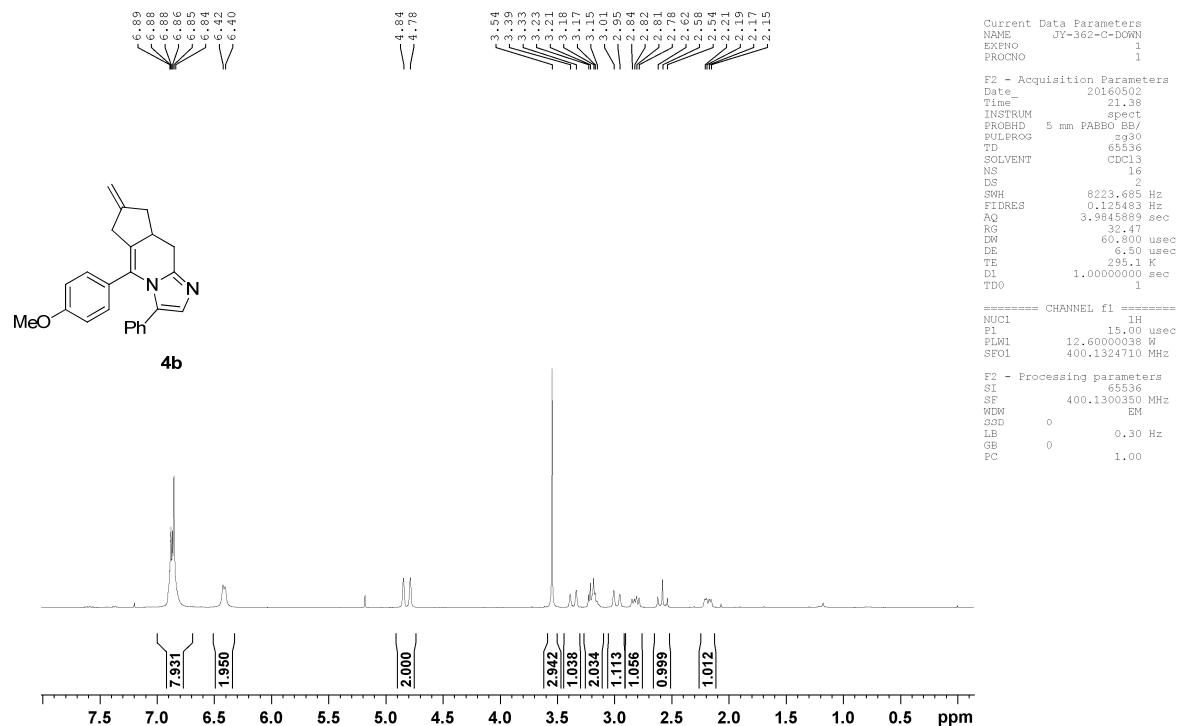
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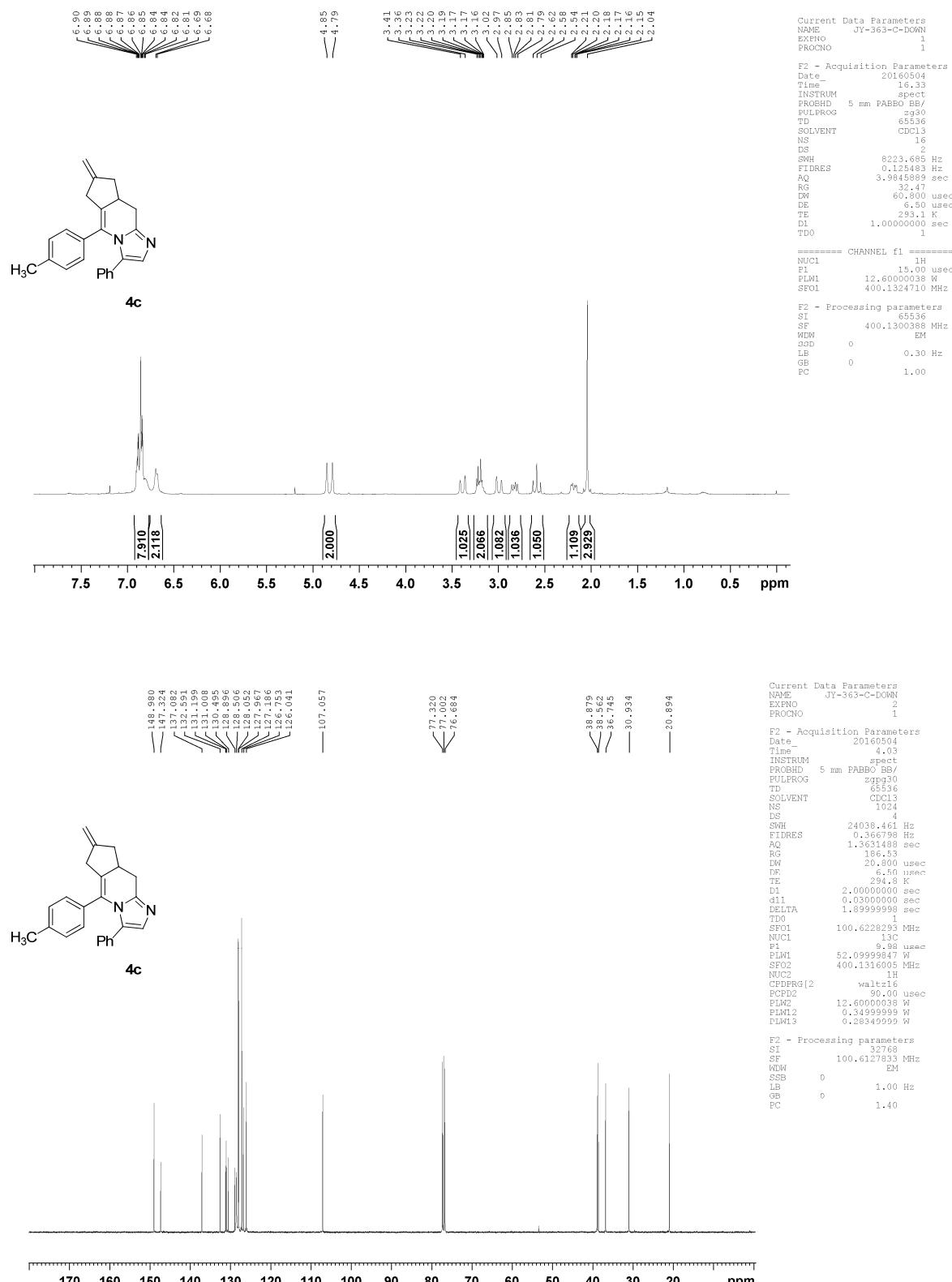
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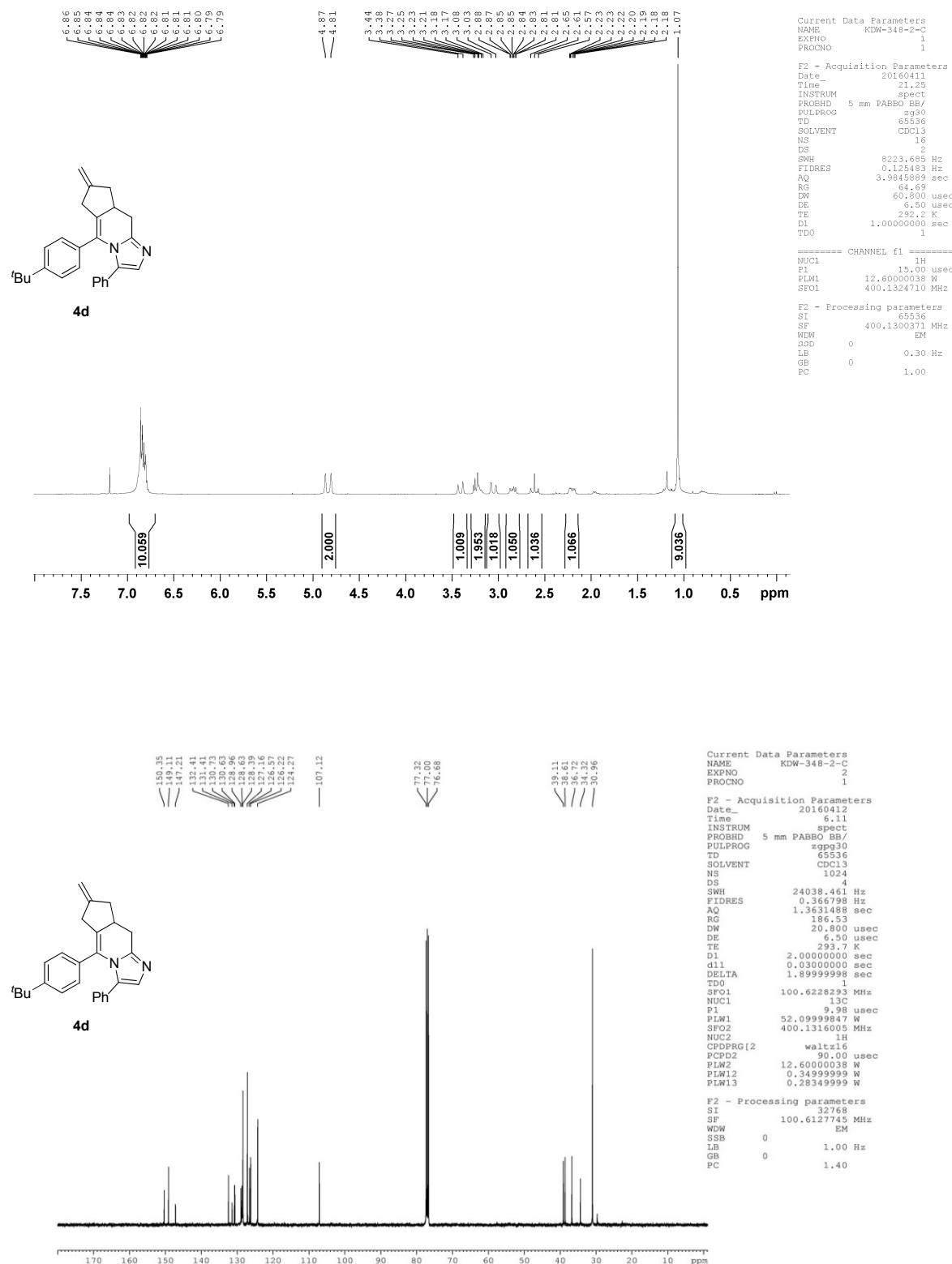
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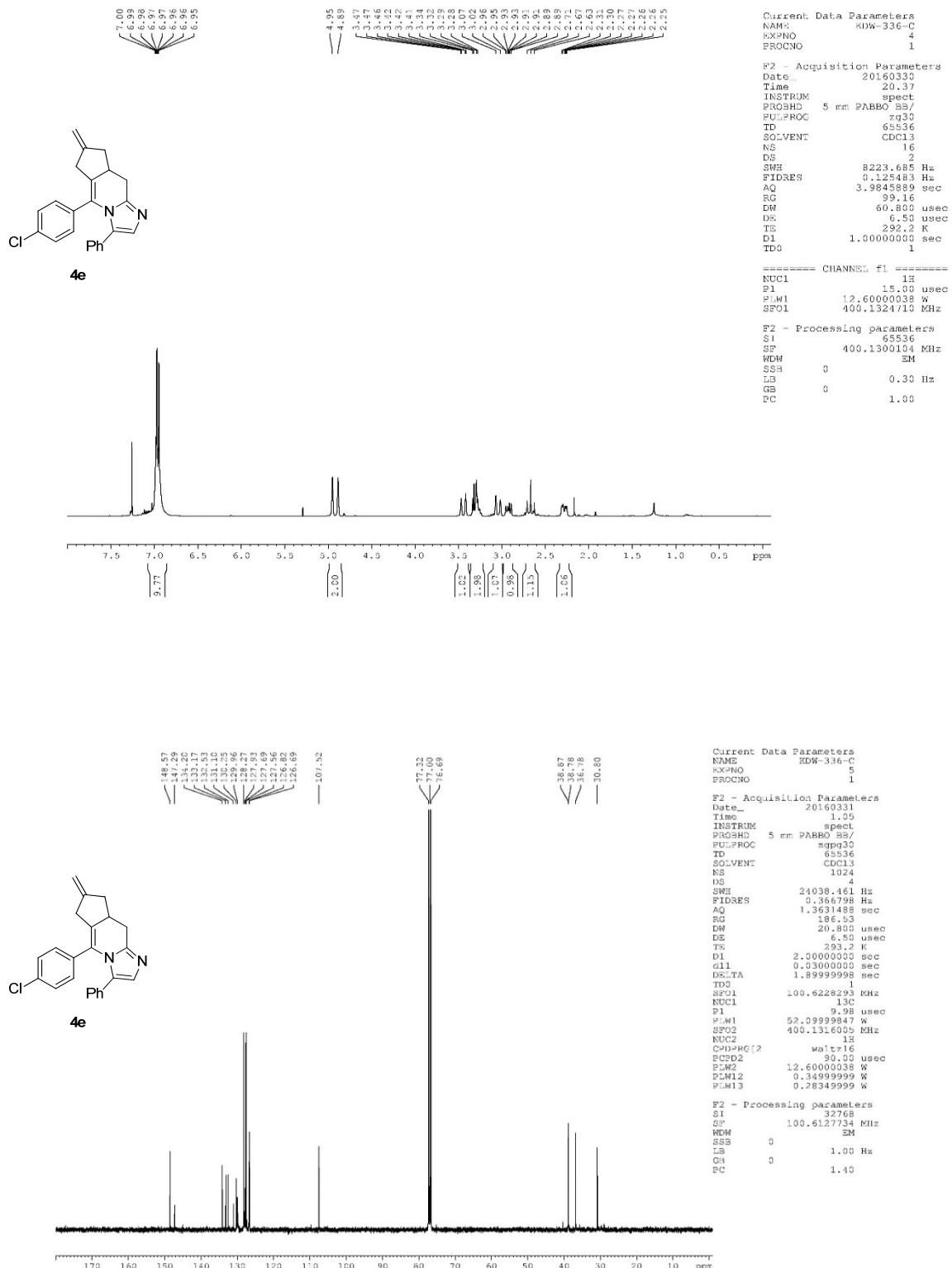
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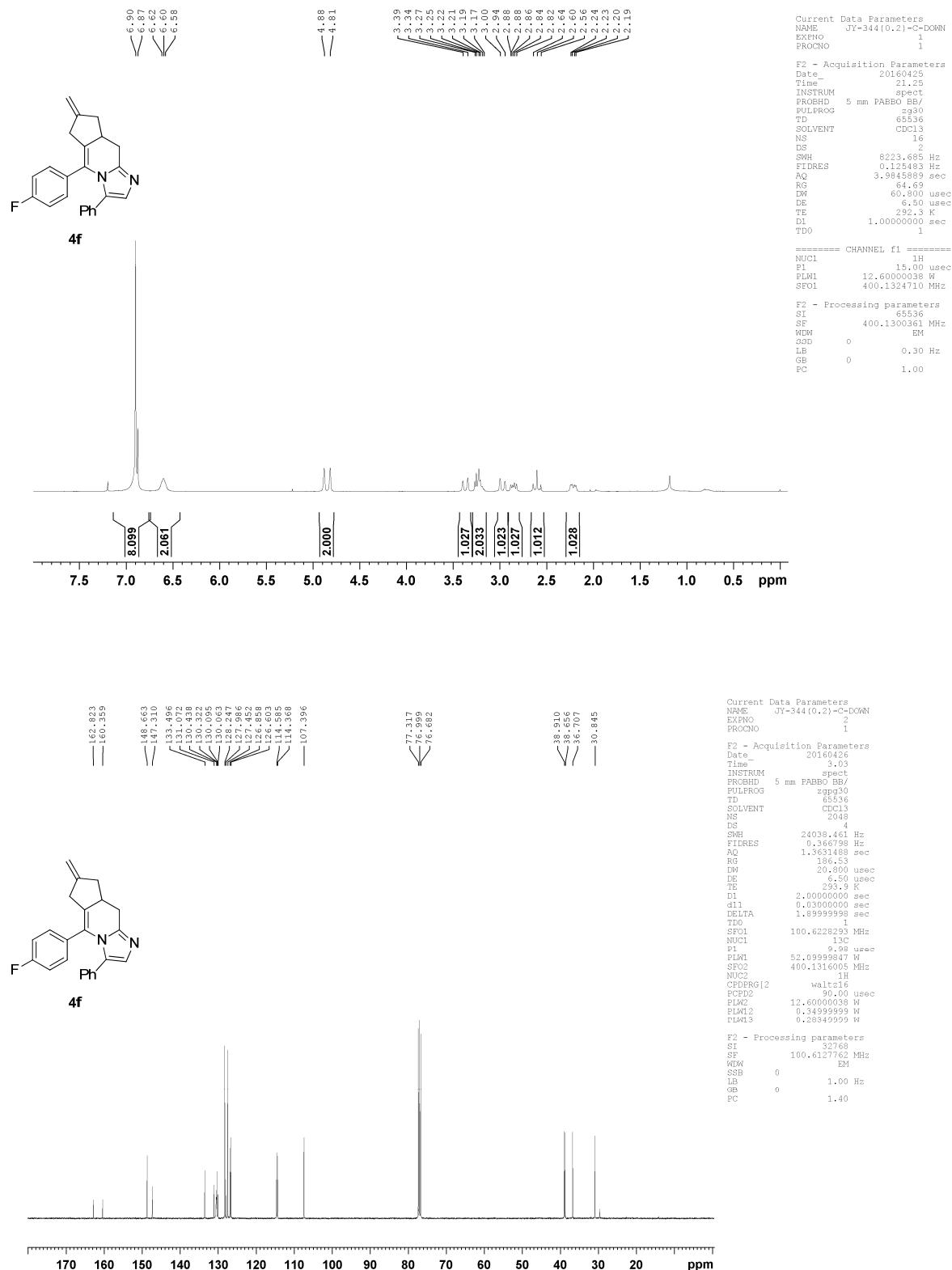
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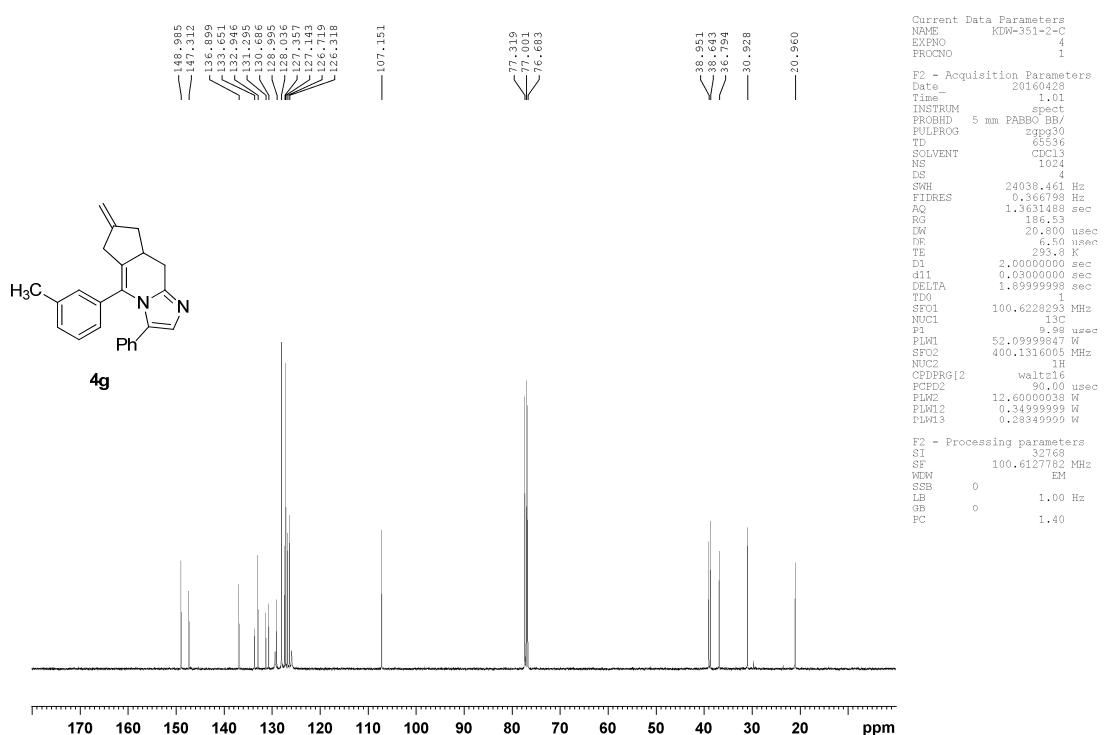
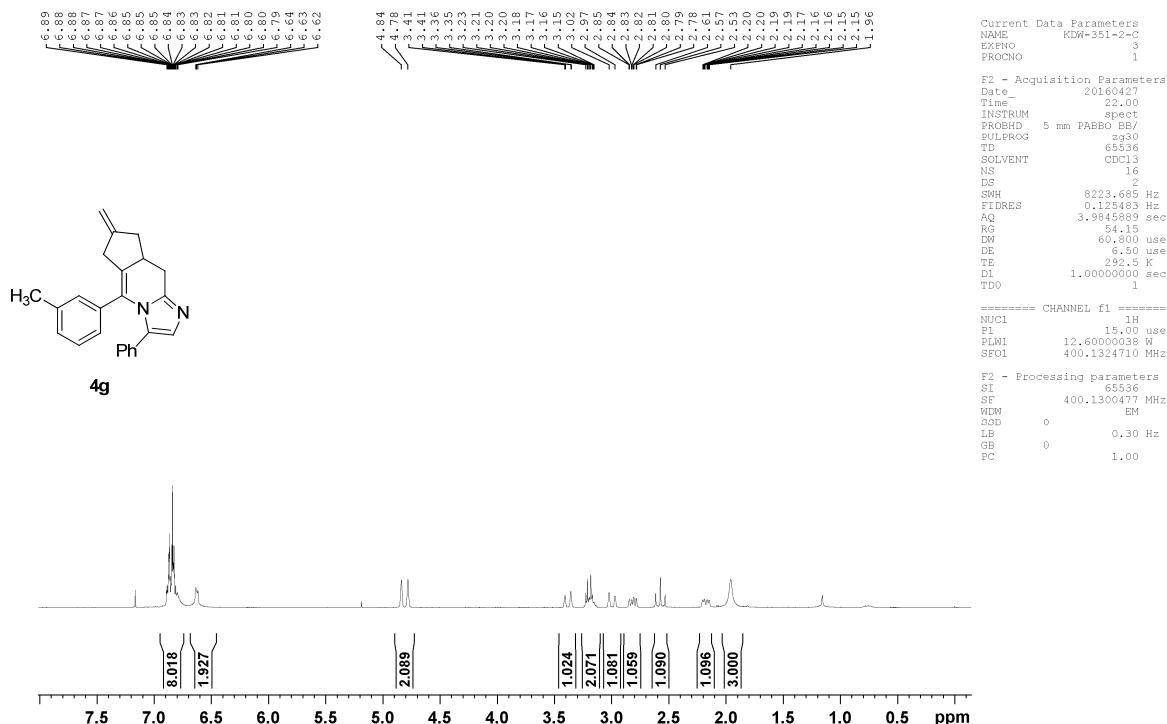
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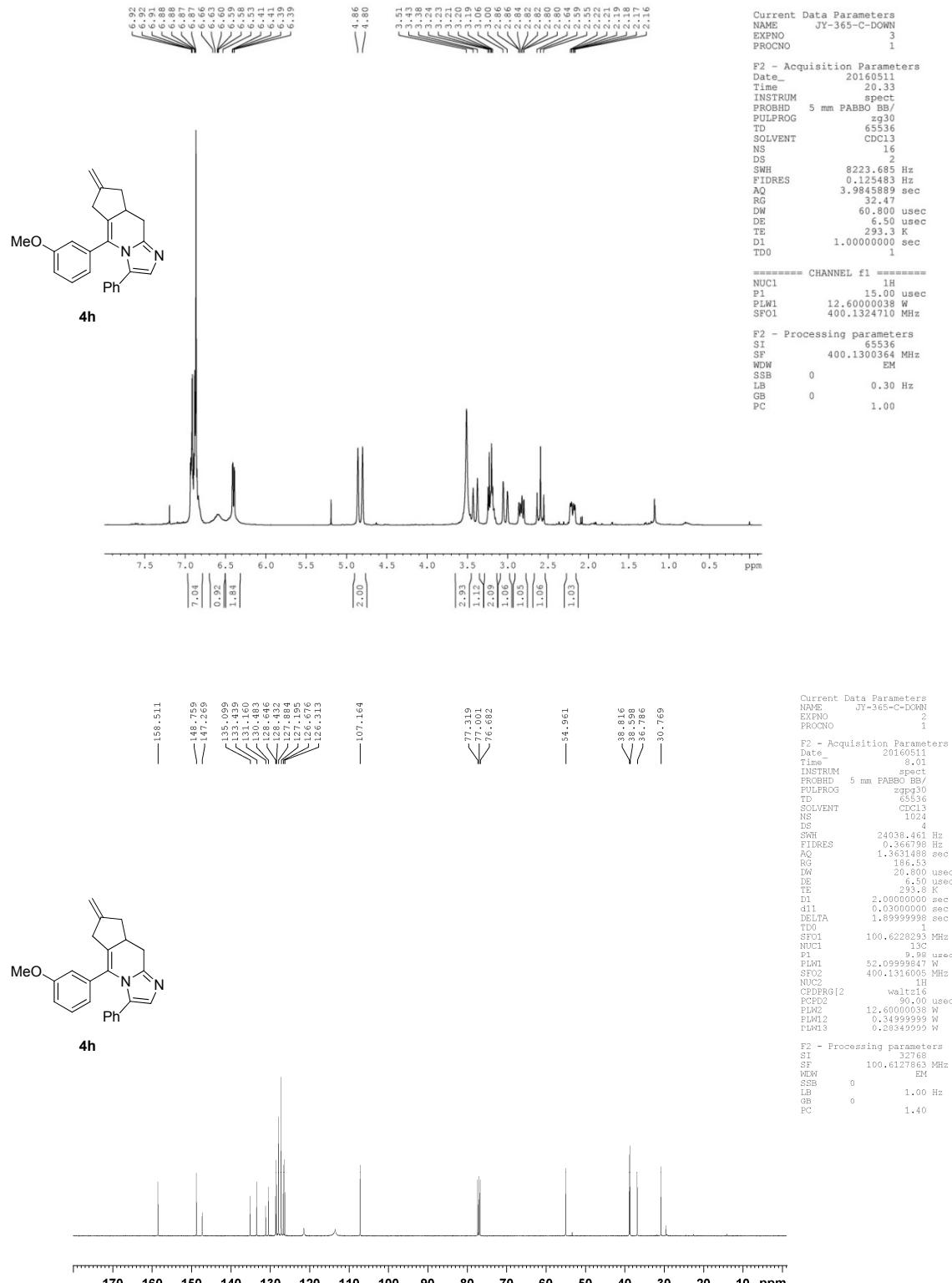
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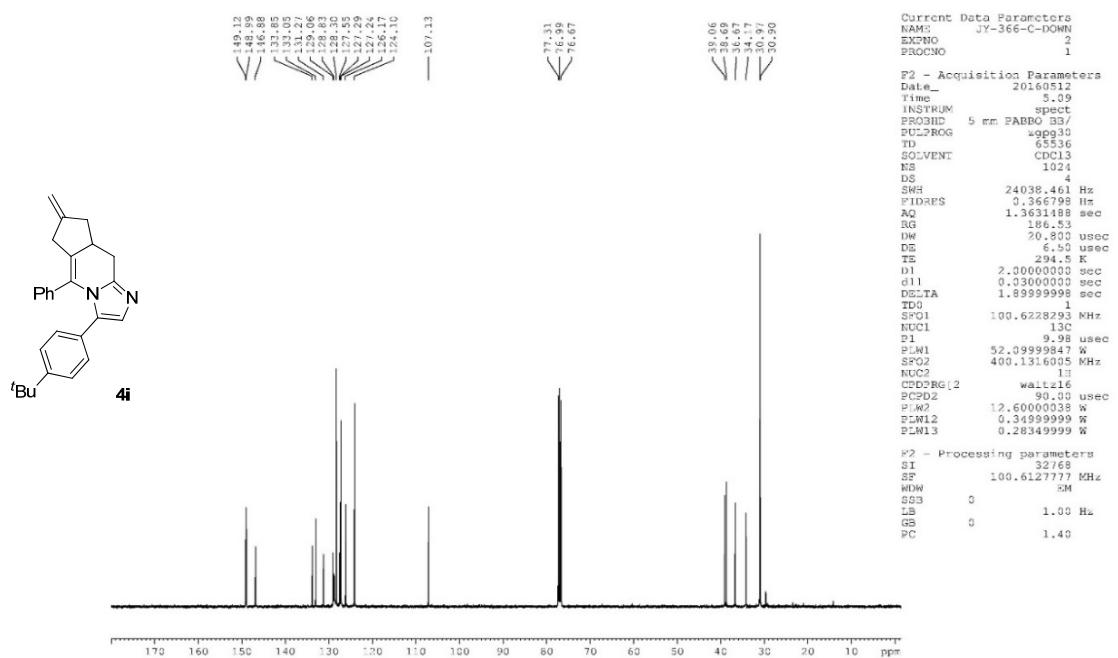
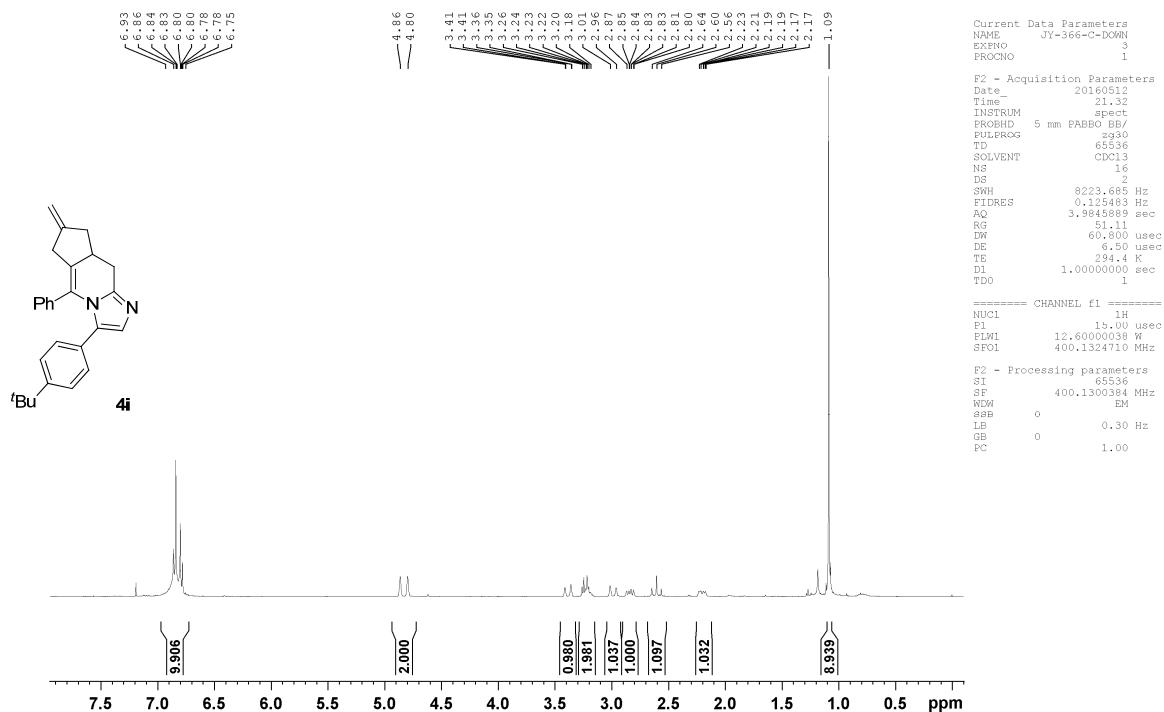
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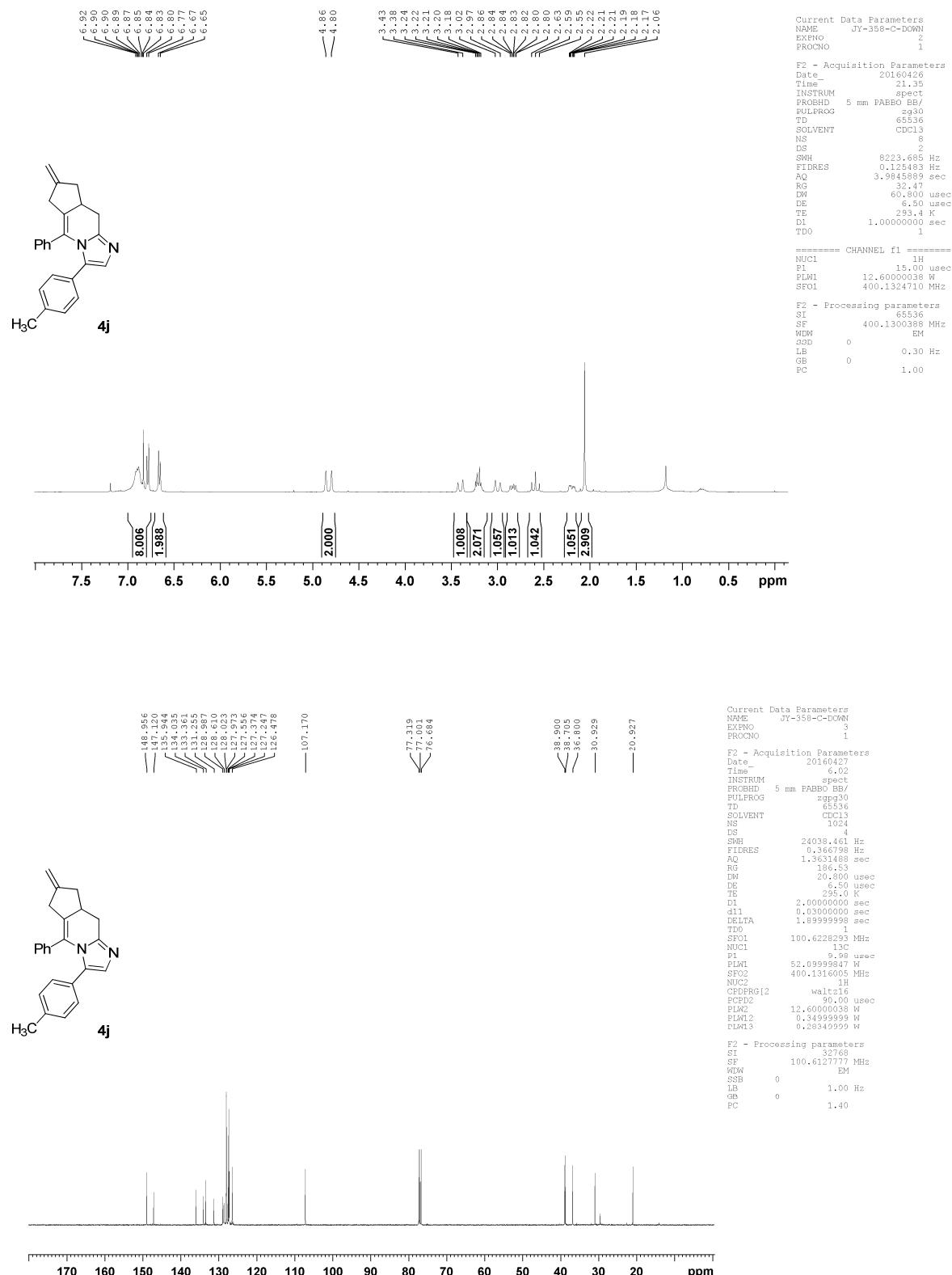
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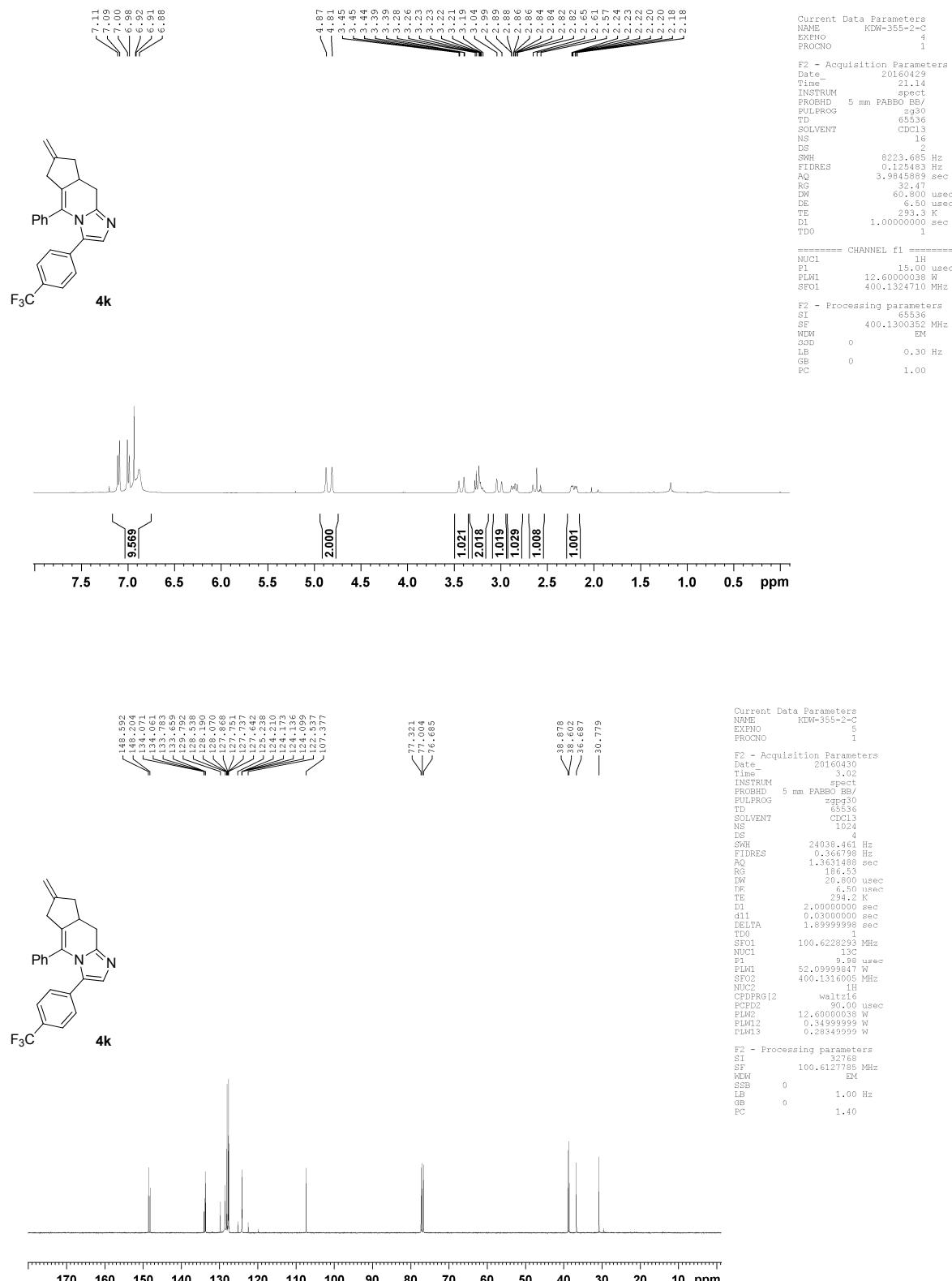
3-(4-(tert-butyl)phenyl)-7-methylene-5-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4i):



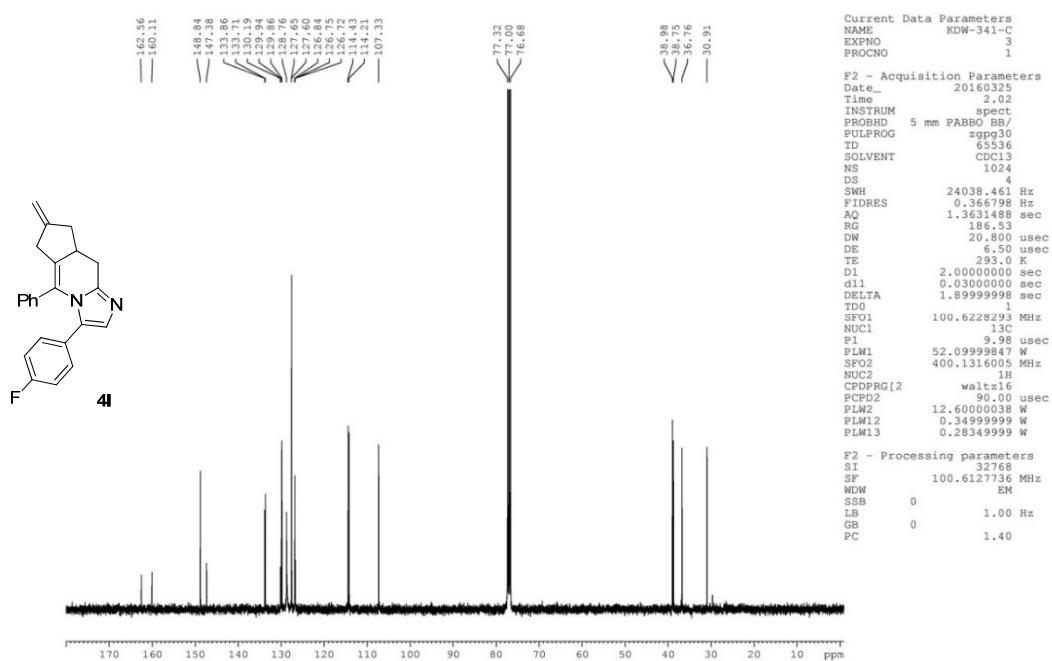
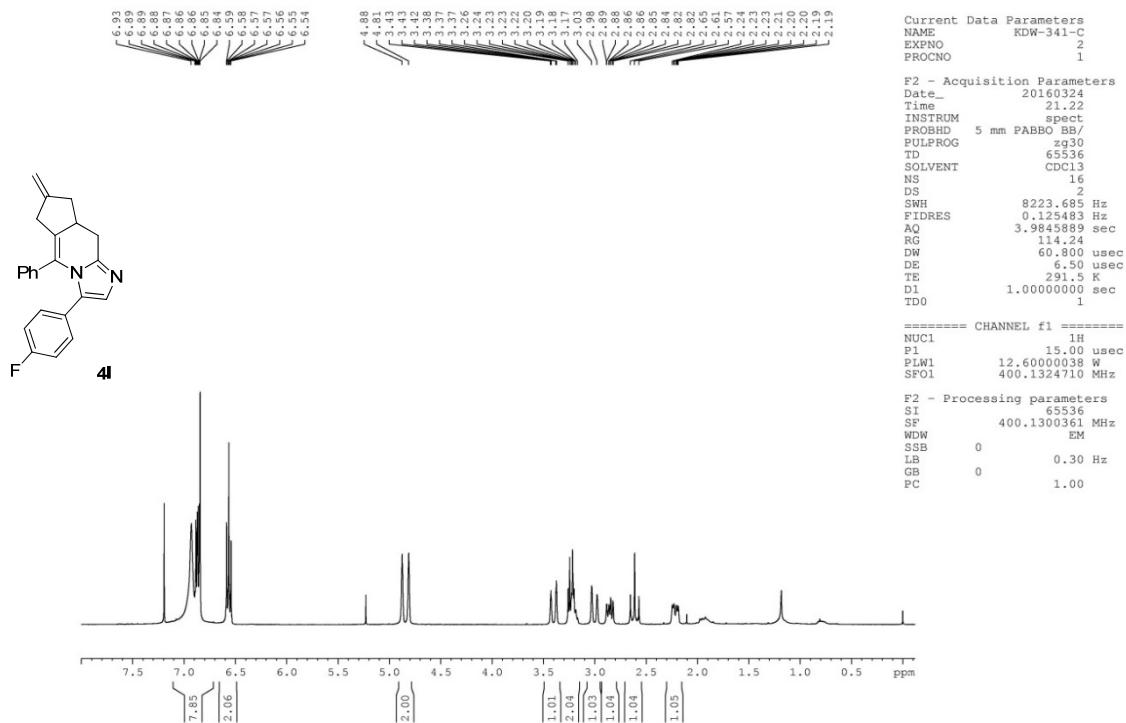
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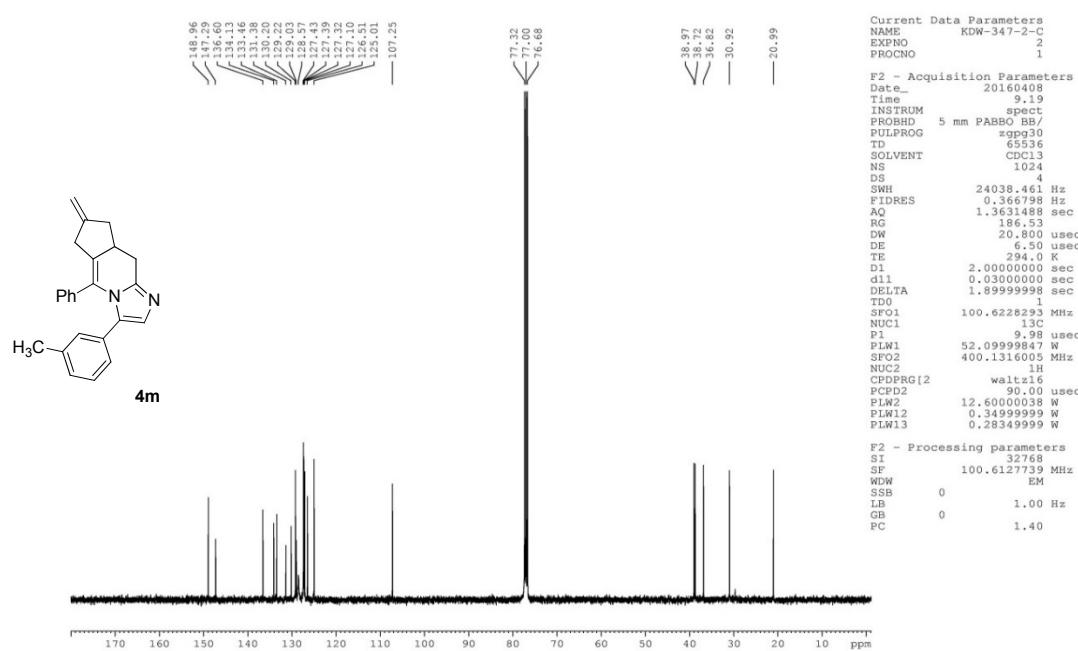
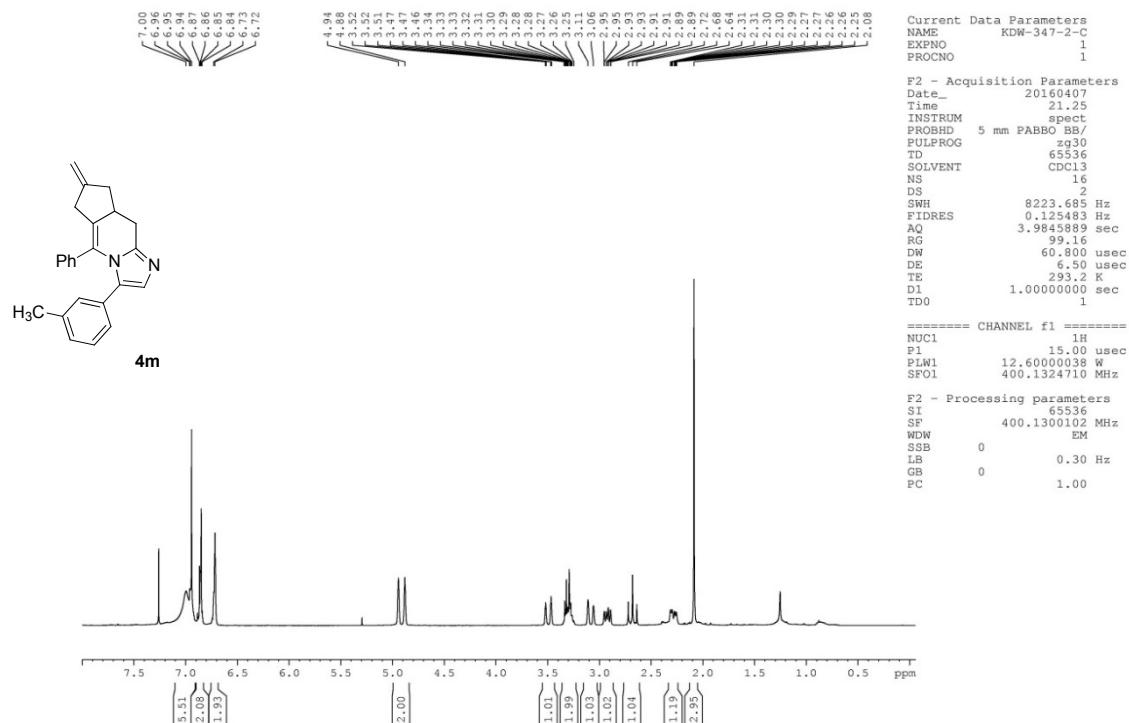
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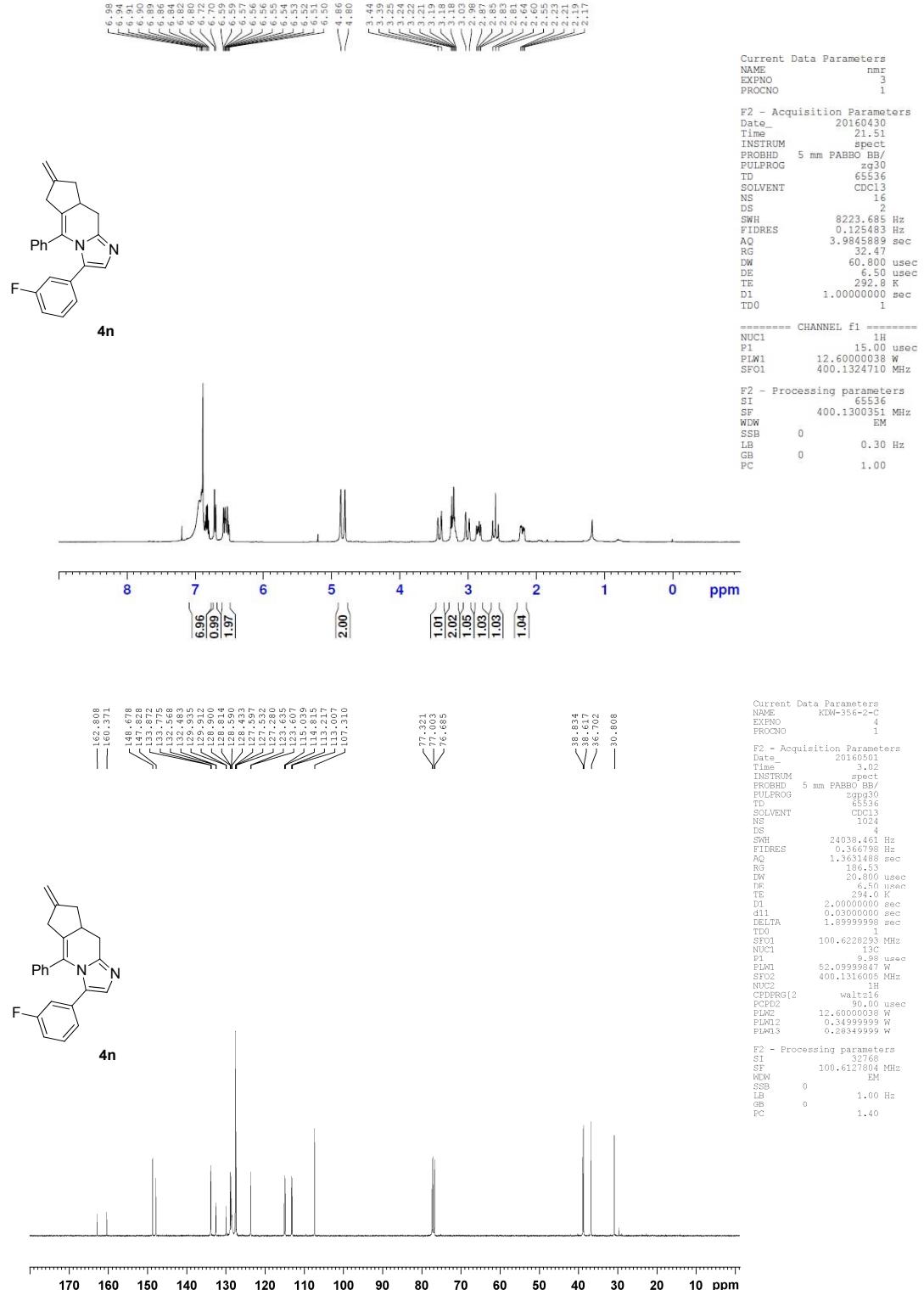
3-(4-fluorophenyl)-7-methylene-5-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4l):



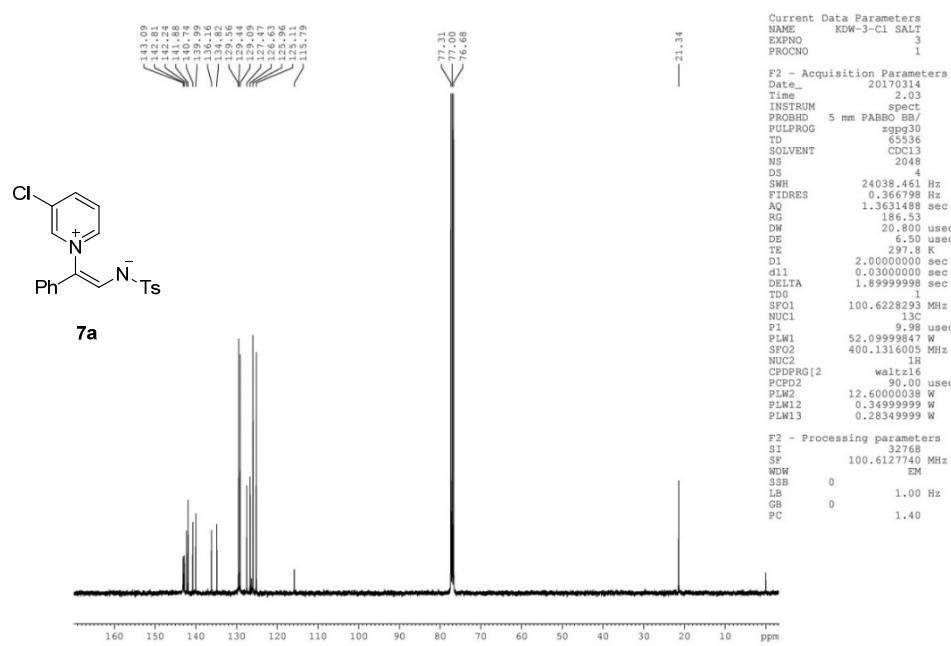
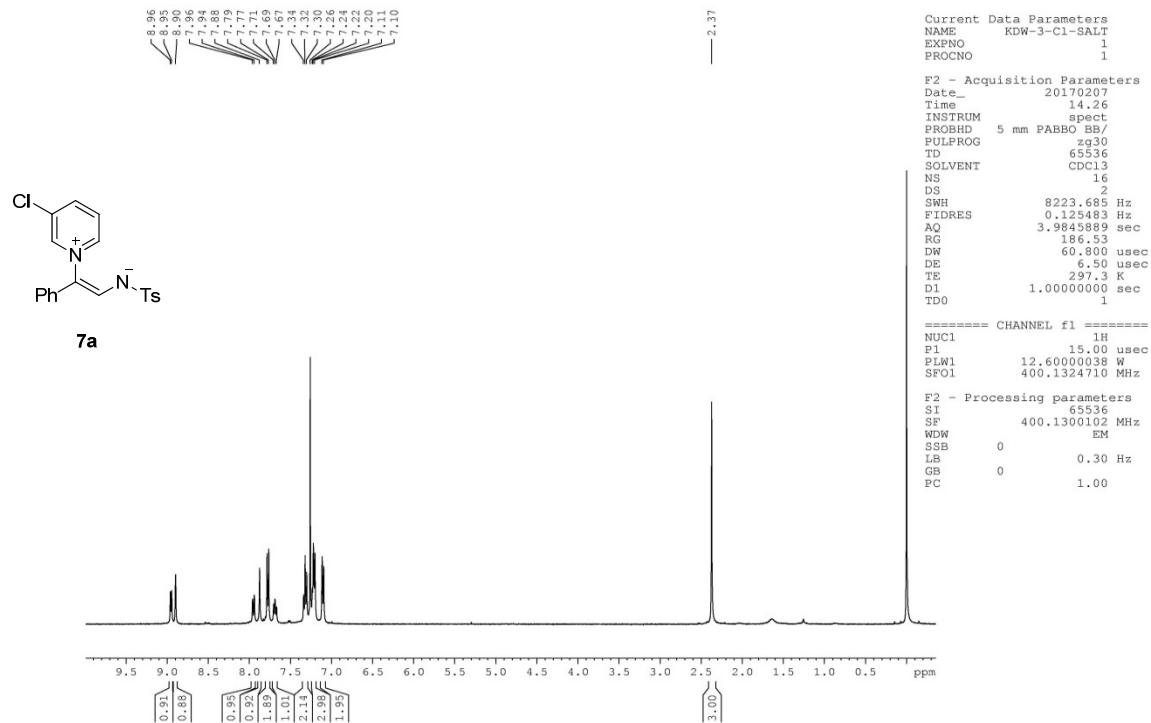
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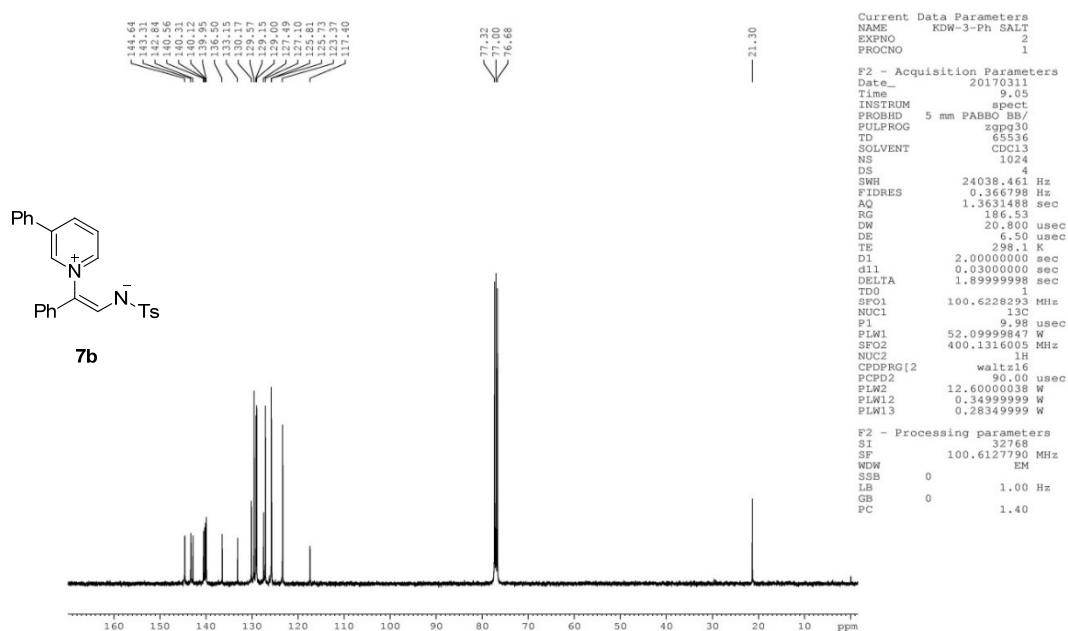
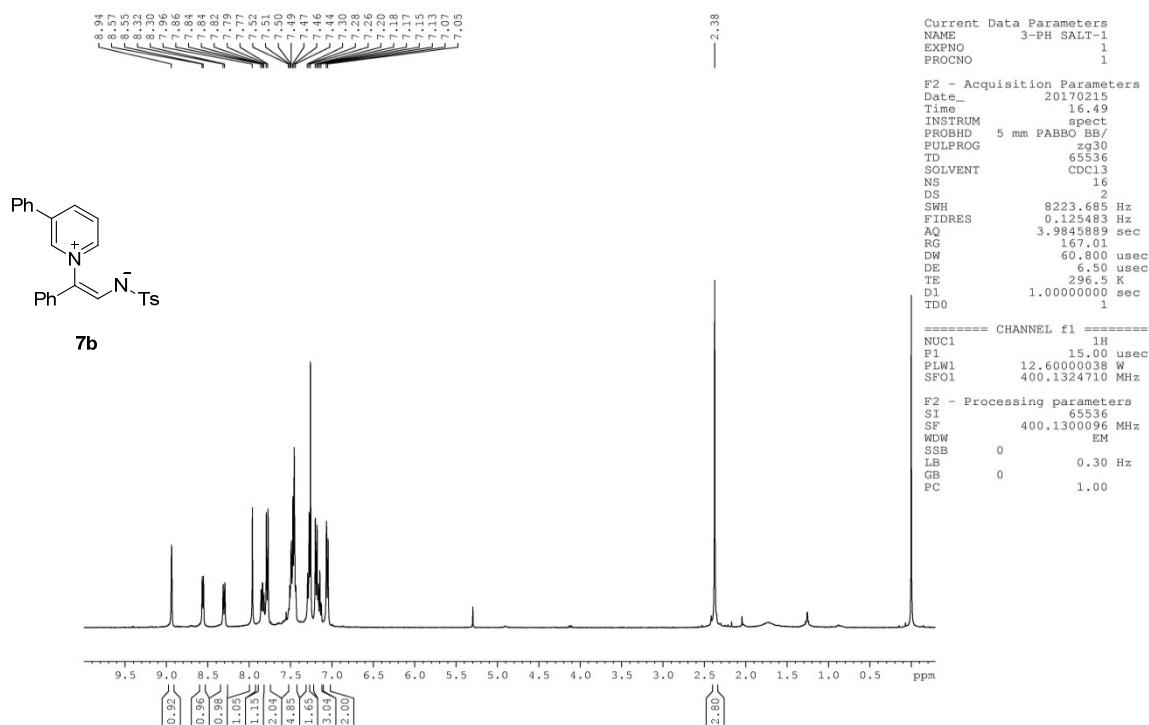
3-(3-fluorophenyl)-7-methylene-5-phenyl-7,8,8a,9-tetrahydro-6H-cyclopenta[d]imidazo[1,2-a]pyridine (4n):



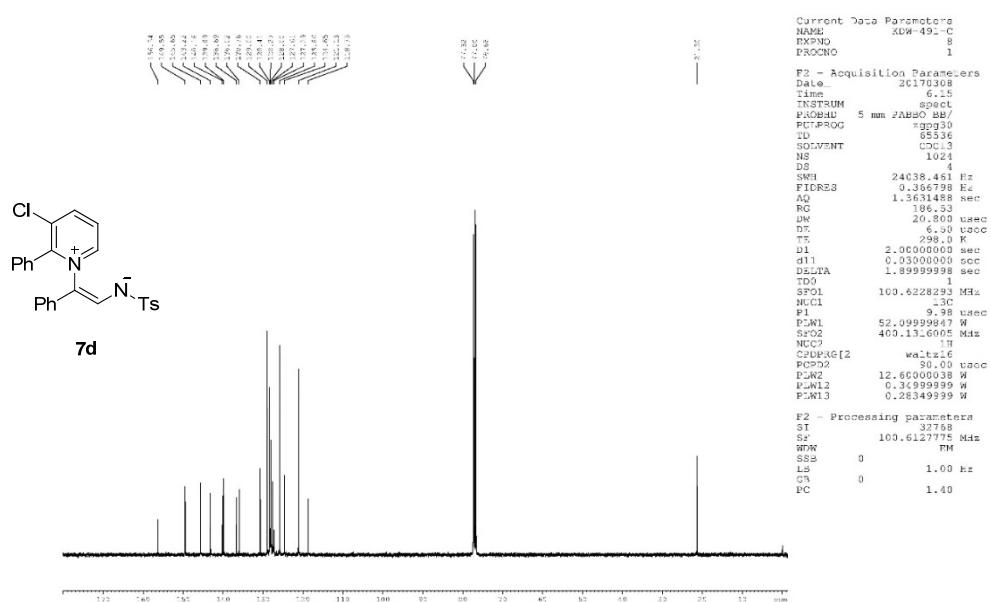
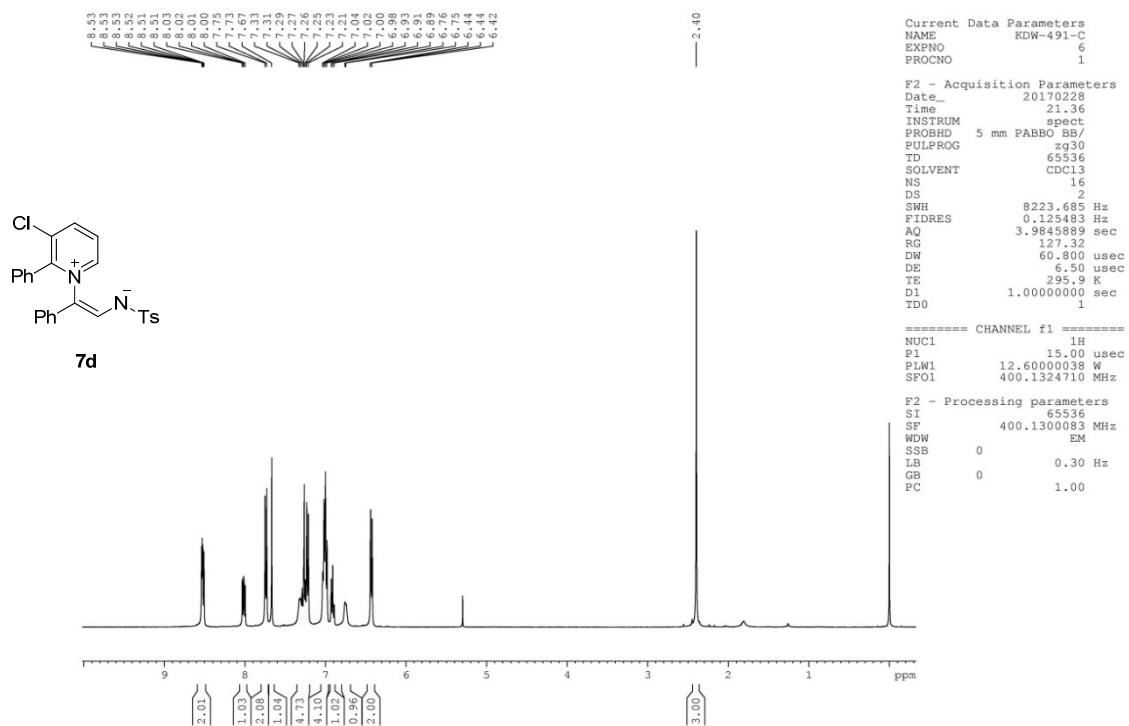
(Z)-(2-(3-chloropyridin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (7a):



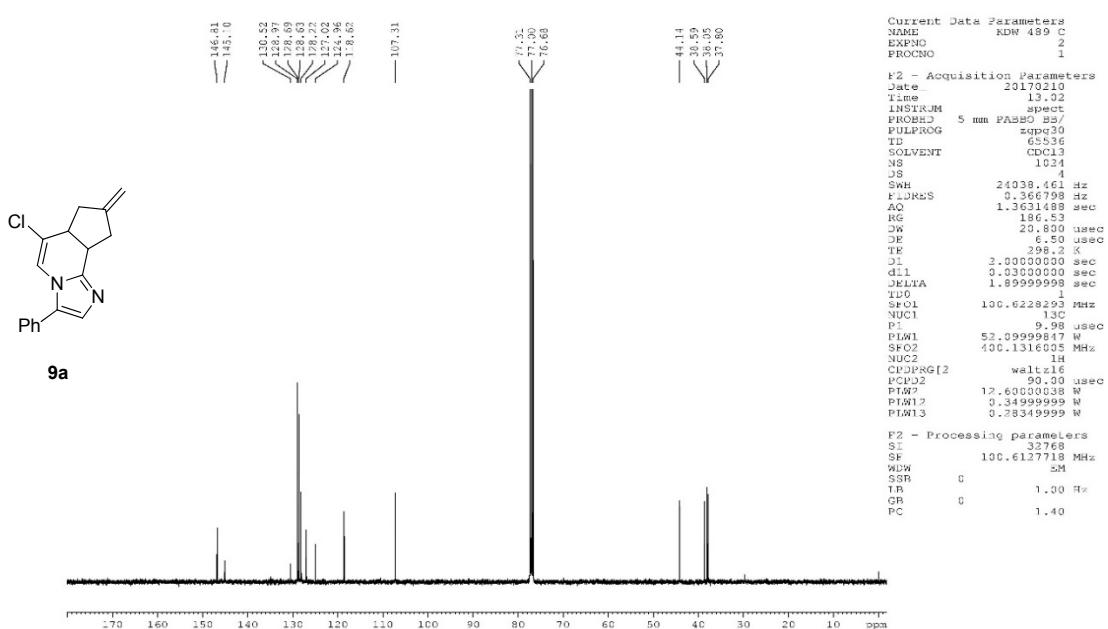
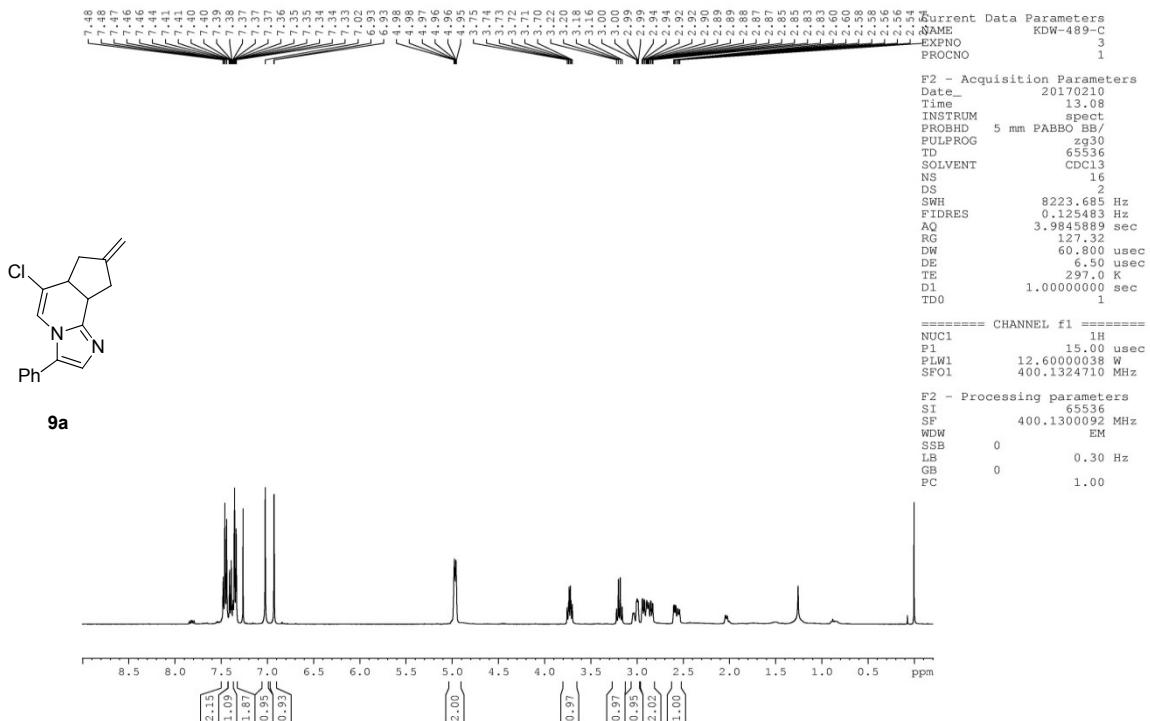
(Z)-(2-phenyl-2-(3-phenylpyridin-1-i um-1-yl)vinyl)(tosyl)amide (7b):



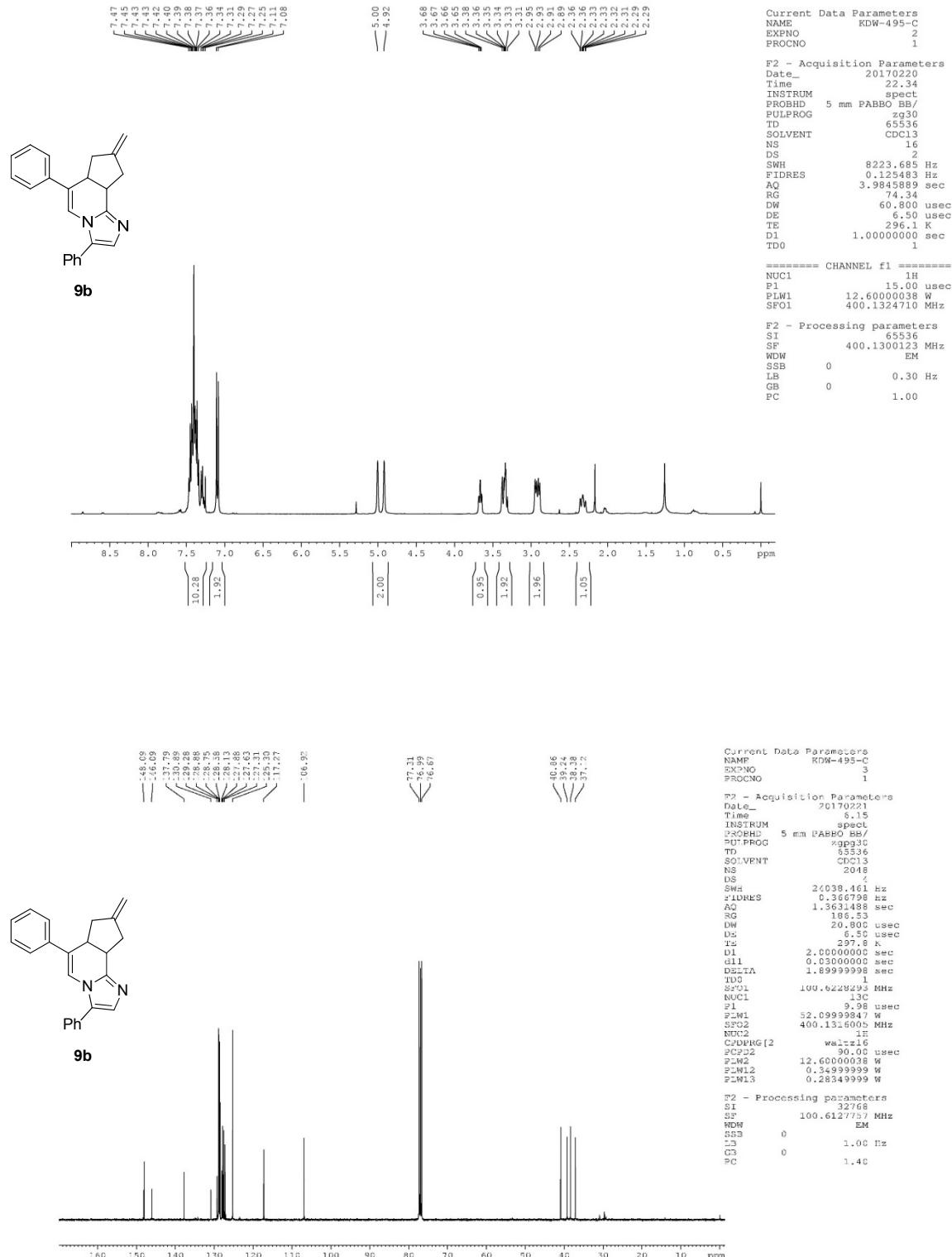
(Z)-(2-(3-chloro-2-phenylpyridin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (7d):



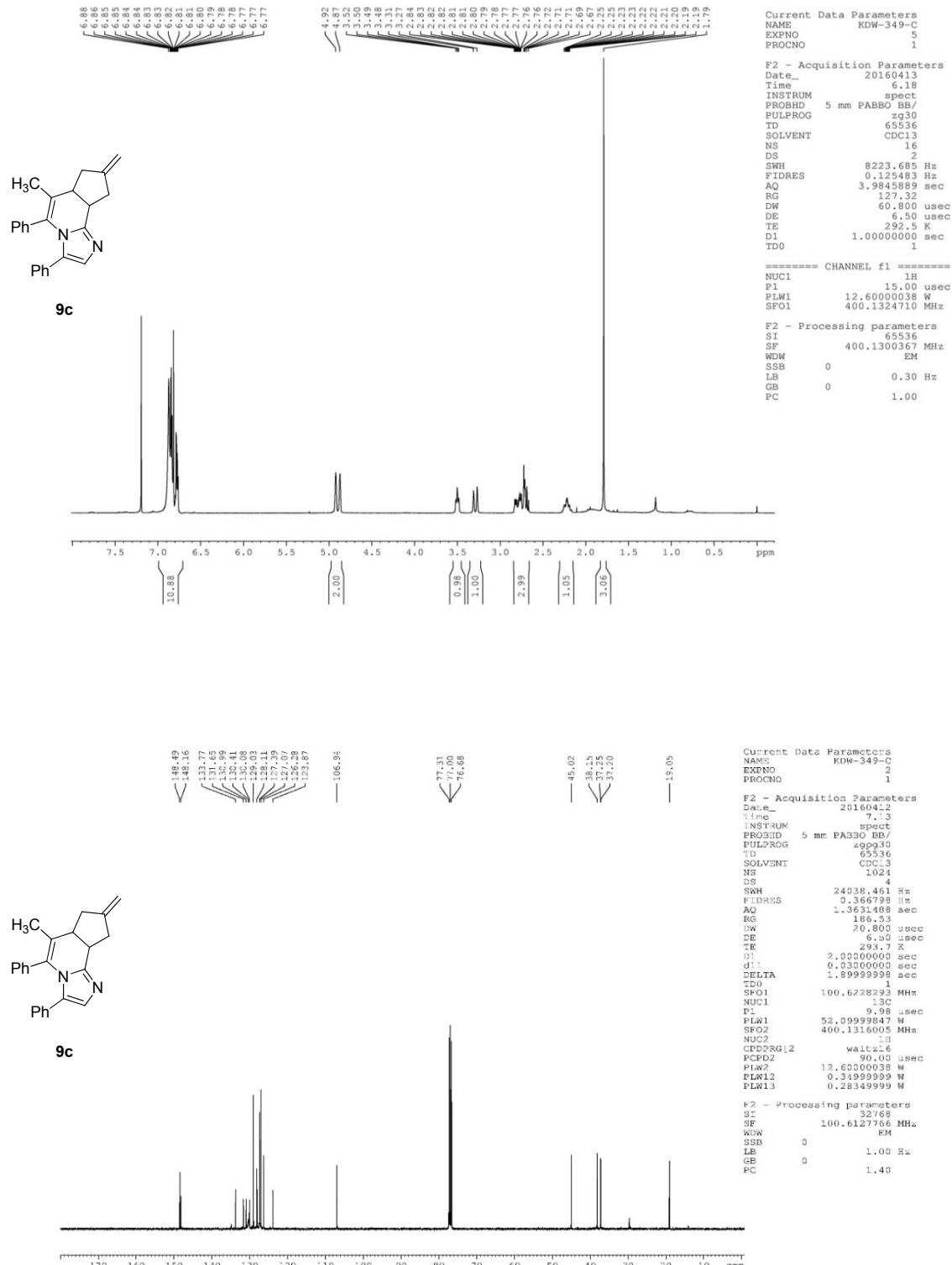
6-chloro-8-methylene-3-phenyl-7,8,9,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine (9a):



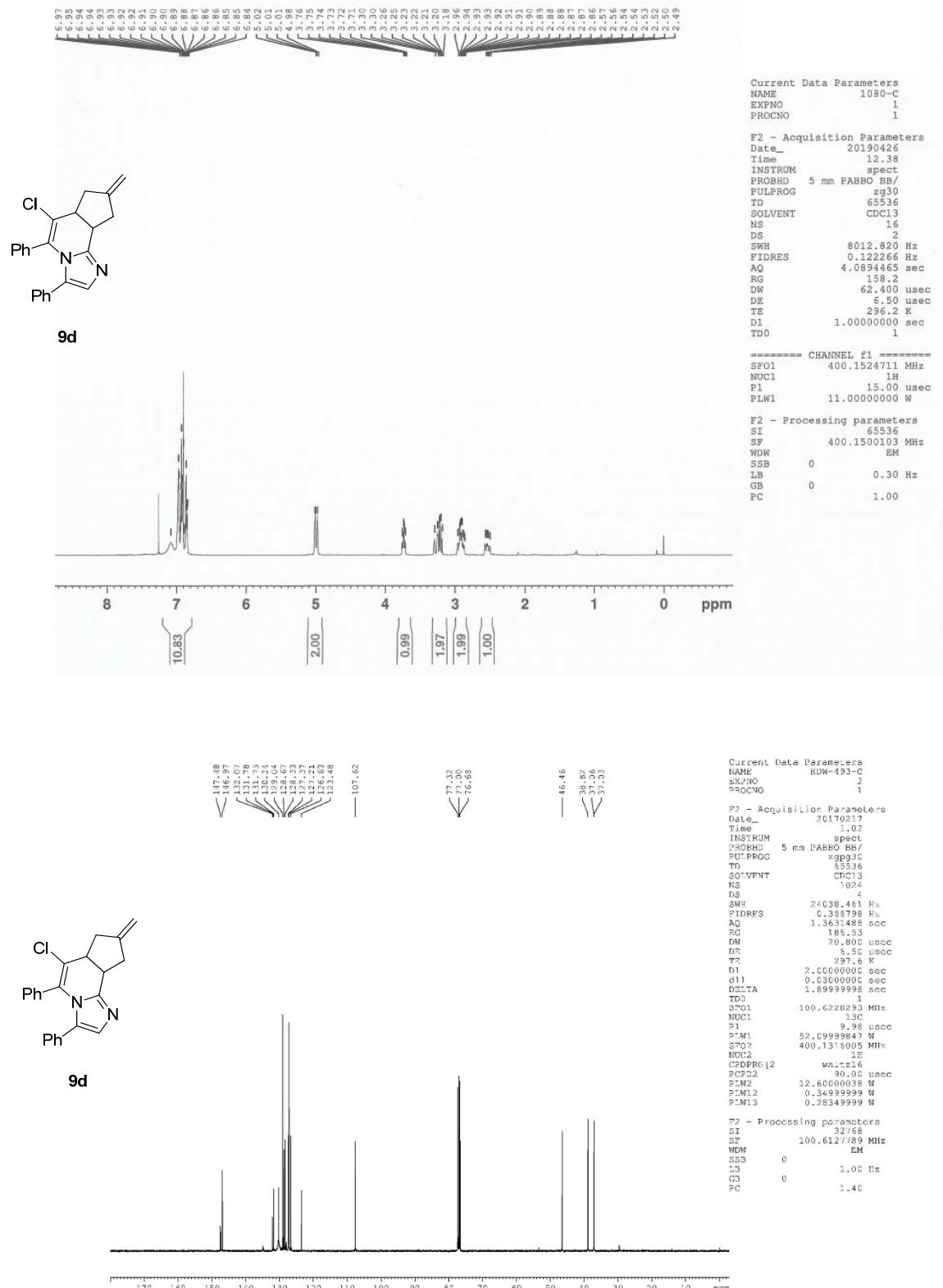
8-methylene-3,6-diphenyl-7,8,9,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine (9b):



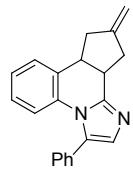
6-methyl-8-methylene-3,5-diphenyl-7,8,9,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine(9c):



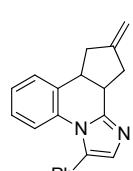
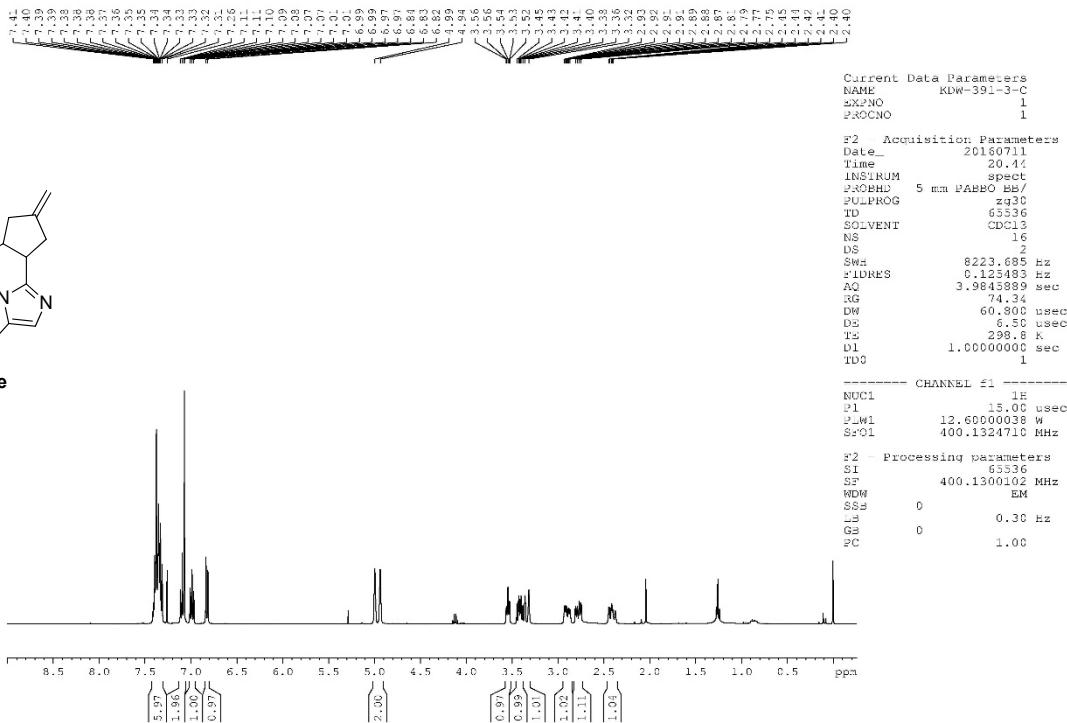
6-chloro-8-methylene-3,5-diphenyl-7,8,9,9a-tetrahydro-6aH-cyclopenta[c]imidazo[1,2-a]pyridine (9d):



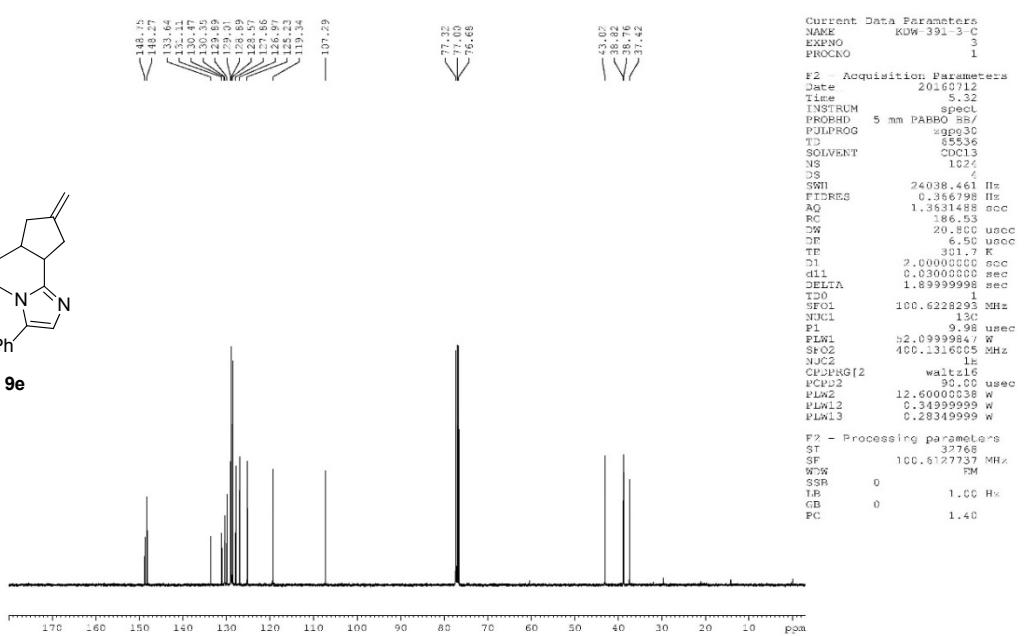
10-methylene-3-phenyl-9,10,11,11a-tetrahydro-8bH-cyclopenta[c]imidazo[1,2-a]quinoline (9e):



9e



9e



VII. Crystallographic Data (compound 4l)

Table 1. Crystal data and structure refinement for **4l**.

Identification code	4l	
Empirical formula	C ₂₃ H ₁₉ F N ₂	
Formula weight	342.40	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 18.4701(11) Å	α = 90°.
	b = 8.7574(6) Å	β = 97.799(3)°.
	c = 10.8753(8) Å	γ = 90°.
Volume	1742.8(2) Å ³	
Z	4	
Density (calculated)	1.305 Mg/m ³	
Absorption coefficient	0.084 mm ⁻¹	
F(000)	720	
Crystal size	0.22 x 0.15 x 0.10 mm ³	
Theta range for data collection	2.23 to 28.45°.	
Index ranges	-24<=h<=24, -11<=k<=11, -14<=l<=14	
Reflections collected	50521	
Independent reflections	4388 [R(int) = 0.0614]	
Completeness to theta = 28.45°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9916 and 0.9817	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4388 / 0 / 235	
Goodness-of-fit on F ²	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0472, wR2 = 0.1015	
R indices (all data)	R1 = 0.0792, wR2 = 0.1160	
Largest diff. peak and hole	0.212 and -0.164 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4I**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4303(1)	8431(3)	9155(2)	75(1)
C(2)	4111(1)	7219(2)	8460(2)	51(1)
C(3)	4445(1)	5653(2)	8601(2)	59(1)
C(4)	4165(1)	4761(2)	7423(2)	46(1)
C(5)	4015(1)	3073(2)	7629(2)	51(1)
C(6)	3520(1)	2418(2)	6571(2)	45(1)
N(1)	2994(1)	3324(1)	5923(1)	37(1)
C(7)	2914(1)	997(2)	5210(2)	53(1)
C(8)	2598(1)	2399(2)	5025(2)	40(1)
N(2)	3486(1)	1009(2)	6159(2)	57(1)
C(9)	2913(1)	4909(2)	6228(1)	33(1)
C(10)	3471(1)	5588(2)	6912(1)	37(1)
C(11)	3499(1)	7205(2)	7383(2)	50(1)
C(12)	2009(1)	2909(2)	4066(1)	38(1)
C(13)	1319(1)	2246(2)	3974(2)	46(1)
C(14)	758(1)	2725(2)	3088(2)	52(1)
C(15)	899(1)	3883(2)	2307(2)	52(1)
F(1)	344(1)	4405(1)	1453(1)	77(1)
C(16)	1571(1)	4543(2)	2347(2)	51(1)
C(17)	2129(1)	4041(2)	3224(1)	44(1)
C(18)	2196(1)	5639(2)	5838(1)	32(1)
C(19)	1569(1)	5041(2)	6218(1)	42(1)
C(20)	901(1)	5717(2)	5865(2)	55(1)
C(21)	847(1)	6982(2)	5123(2)	59(1)
C(22)	1463(1)	7598(2)	4736(2)	56(1)
C(23)	2142(1)	6937(2)	5102(1)	44(1)

Table 3. Bond lengths [Å] and angles [°] for **4I**.

C(1)-C(2)	1.323(3)	C(15)-F(1)	1.3653(19)
C(1)-H(1A)	0.9400	C(16)-C(17)	1.377(2)
C(1)-H(1B)	0.9400	C(16)-H(16)	0.9400
C(2)-C(3)	1.503(3)	C(17)-H(17)	0.9400
C(2)-C(11)	1.514(2)	C(18)-C(19)	1.384(2)
C(3)-C(4)	1.530(2)	C(18)-C(23)	1.387(2)
C(3)-H(3A)	0.9800	C(19)-C(20)	1.374(2)
C(3)-H(3B)	0.9800	C(19)-H(19)	0.9400
C(4)-C(10)	1.5108(19)	C(20)-C(21)	1.366(3)
C(4)-C(5)	1.527(2)	C(20)-H(20)	0.9400
C(4)-H(4)	0.9900	C(21)-C(22)	1.376(3)
C(5)-C(6)	1.484(2)	C(21)-H(21)	0.9400
C(5)-H(5A)	0.9800	C(22)-C(23)	1.389(2)
C(5)-H(5B)	0.9800	C(22)-H(22)	0.9400
C(6)-N(2)	1.312(2)	C(23)-H(23)	0.9400
C(6)-N(1)	1.3729(18)	C(2)-C(1)-H(1A)	120.0
N(1)-C(8)	1.396(2)	C(2)-C(1)-H(1B)	120.0
N(1)-C(9)	1.4402(18)	H(1A)-C(1)-H(1B)	120.0
C(7)-C(8)	1.363(2)	C(1)-C(2)-C(3)	126.80(17)
C(7)-N(2)	1.373(2)	C(1)-C(2)-C(11)	124.25(19)
C(7)-H(7)	0.9400	C(3)-C(2)-C(11)	108.95(15)
C(8)-C(12)	1.470(2)	C(2)-C(3)-C(4)	107.03(13)
C(9)-C(10)	1.327(2)	C(2)-C(3)-H(3A)	110.3
C(9)-C(18)	1.4795(18)	C(4)-C(3)-H(3A)	110.3
C(10)-C(11)	1.504(2)	C(2)-C(3)-H(3B)	110.3
C(11)-H(11A)	0.9800	C(4)-C(3)-H(3B)	110.3
C(11)-H(11B)	0.9800	H(3A)-C(3)-H(3B)	108.6
C(12)-C(17)	1.387(2)	C(10)-C(4)-C(5)	110.90(13)
C(12)-C(13)	1.392(2)	C(10)-C(4)-C(3)	103.70(14)
C(13)-C(14)	1.381(2)	C(5)-C(4)-C(3)	114.76(14)
C(13)-H(13)	0.9400	C(10)-C(4)-H(4)	109.1
C(14)-C(15)	1.371(3)	C(5)-C(4)-H(4)	109.1
C(14)-H(14)	0.9400	C(3)-C(4)-H(4)	109.1
C(15)-C(16)	1.364(2)	C(6)-C(5)-C(4)	111.39(13)
		C(6)-C(5)-H(5A)	109.3

C(4)-C(5)-H(5A)	109.3	C(12)-C(13)-H(13)	119.5
C(6)-C(5)-H(5B)	109.3	C(15)-C(14)-C(13)	117.99(15)
C(4)-C(5)-H(5B)	109.3	C(15)-C(14)-H(14)	121.0
H(5A)-C(5)-H(5B)	108.0	C(13)-C(14)-H(14)	121.0
N(2)-C(6)-N(1)	111.72(15)	C(16)-C(15)-F(1)	118.42(17)
N(2)-C(6)-C(5)	128.64(14)	C(16)-C(15)-C(14)	122.88(16)
N(1)-C(6)-C(5)	119.58(14)	F(1)-C(15)-C(14)	118.70(16)
C(6)-N(1)-C(8)	106.94(12)	C(15)-C(16)-C(17)	118.54(16)
C(6)-N(1)-C(9)	121.79(13)	C(15)-C(16)-H(16)	120.7
C(8)-N(1)-C(9)	131.25(12)	C(17)-C(16)-H(16)	120.7
C(8)-C(7)-N(2)	112.01(16)	C(16)-C(17)-C(12)	120.95(15)
C(8)-C(7)-H(7)	124.0	C(16)-C(17)-H(17)	119.5
N(2)-C(7)-H(7)	124.0	C(12)-C(17)-H(17)	119.5
C(7)-C(8)-N(1)	104.22(14)	C(19)-C(18)-C(23)	118.99(13)
C(7)-C(8)-C(12)	129.75(15)	C(19)-C(18)-C(9)	120.28(12)
N(1)-C(8)-C(12)	125.92(13)	C(23)-C(18)-C(9)	120.73(13)
C(6)-N(2)-C(7)	105.11(13)	C(20)-C(19)-C(18)	120.62(15)
C(10)-C(9)-N(1)	117.66(12)	C(20)-C(19)-H(19)	119.7
C(10)-C(9)-C(18)	124.34(13)	C(18)-C(19)-H(19)	119.7
N(1)-C(9)-C(18)	117.84(12)	C(21)-C(20)-C(19)	120.38(17)
C(9)-C(10)-C(11)	126.91(13)	C(21)-C(20)-H(20)	119.8
C(9)-C(10)-C(4)	123.14(14)	C(19)-C(20)-H(20)	119.8
C(11)-C(10)-C(4)	109.76(13)	C(20)-C(21)-C(22)	120.05(15)
C(10)-C(11)-C(2)	104.99(14)	C(20)-C(21)-H(21)	120.0
C(10)-C(11)-H(11A)	110.7	C(22)-C(21)-H(21)	120.0
C(2)-C(11)-H(11A)	110.7	C(21)-C(22)-C(23)	120.08(16)
C(10)-C(11)-H(11B)	110.7	C(21)-C(22)-H(22)	120.0
C(2)-C(11)-H(11B)	110.7	C(23)-C(22)-H(22)	120.0
H(11A)-C(11)-H(11B)	108.8	C(18)-C(23)-C(22)	119.87(16)
C(17)-C(12)-C(13)	118.50(15)	C(18)-C(23)-H(23)	120.1
C(17)-C(12)-C(8)	121.07(13)	C(22)-C(23)-H(23)	120.1
C(13)-C(12)-C(8)	120.42(14)		
C(14)-C(13)-C(12)	121.08(16)		
C(14)-C(13)-H(13)	119.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4I**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	58(1)	104(2)	60(1)	-21(1)	-4(1)	-18(1)
C(2)	38(1)	75(1)	42(1)	3(1)	5(1)	-13(1)
C(3)	39(1)	84(1)	51(1)	20(1)	-6(1)	-14(1)
C(4)	30(1)	60(1)	49(1)	18(1)	6(1)	4(1)
C(5)	40(1)	56(1)	56(1)	20(1)	9(1)	17(1)
C(6)	40(1)	40(1)	57(1)	16(1)	17(1)	14(1)
N(1)	37(1)	31(1)	44(1)	7(1)	11(1)	7(1)
C(7)	57(1)	32(1)	75(1)	1(1)	22(1)	5(1)
C(8)	44(1)	31(1)	49(1)	0(1)	19(1)	0(1)
N(2)	55(1)	38(1)	80(1)	13(1)	22(1)	15(1)
C(9)	35(1)	30(1)	34(1)	6(1)	8(1)	4(1)
C(10)	34(1)	42(1)	36(1)	9(1)	6(1)	2(1)
C(11)	48(1)	49(1)	49(1)	-3(1)	-4(1)	-5(1)
C(12)	46(1)	30(1)	41(1)	-7(1)	15(1)	-1(1)
C(13)	52(1)	38(1)	51(1)	-7(1)	19(1)	-5(1)
C(14)	46(1)	51(1)	60(1)	-18(1)	12(1)	-7(1)
C(15)	58(1)	50(1)	45(1)	-16(1)	-2(1)	3(1)
F(1)	75(1)	77(1)	71(1)	-10(1)	-22(1)	4(1)
C(16)	67(1)	44(1)	42(1)	-3(1)	5(1)	-6(1)
C(17)	51(1)	40(1)	43(1)	-3(1)	12(1)	-8(1)
C(18)	35(1)	28(1)	31(1)	-3(1)	1(1)	4(1)
C(19)	37(1)	42(1)	47(1)	0(1)	6(1)	5(1)
C(20)	37(1)	56(1)	71(1)	-9(1)	3(1)	6(1)
C(21)	47(1)	58(1)	68(1)	-13(1)	-14(1)	21(1)
C(22)	75(1)	35(1)	54(1)	1(1)	-12(1)	18(1)
C(23)	55(1)	31(1)	44(1)	3(1)	0(1)	5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4I**.

	x	y	z	U(eq)
H(1A)	4686	8360	9817	90
H(1B)	4057	9363	8986	90
H(3A)	4301	5141	9332	70
H(3B)	4979	5723	8702	70
H(4)	4522	4854	6826	56
H(5A)	4478	2510	7734	61
H(5B)	3792	2956	8392	61
H(7)	2759	125	4742	64
H(11A)	3034	7492	7659	60
H(11B)	3602	7917	6733	60
H(13)	1233	1458	4524	55
H(14)	293	2271	3023	62
H(16)	1652	5324	1788	61
H(17)	2597	4470	3252	53
H(19)	1599	4165	6722	50
H(20)	480	5307	6136	66
H(21)	388	7432	4877	71
H(22)	1425	8467	4224	68
H(23)	2564	7370	4850	52

Table 6. Torsion angles [°] for **4I**.

C(1)-C(2)-C(3)-C(4)	167.23(17)	C(9)-C(10)-C(11)-C(2)	159.55(14)
C(11)-C(2)-C(3)-C(4)	13.41(18)	C(4)-C(10)-C(11)-C(2)	-15.66(17)
C(2)-C(3)-C(4)-C(10)	-22.17(16)	C(1)-C(2)-C(11)-C(10)	-178.27(17)
C(2)-C(3)-C(4)-C(5)	-143.29(13)	C(3)-C(2)-C(11)-C(10)	1.11(18)
C(10)-C(4)-C(5)-C(6)	43.38(18)	C(7)-C(8)-C(12)-C(17)	-117.79(19)
C(3)-C(4)-C(5)-C(6)	160.46(13)	N(1)-C(8)-C(12)-C(17)	57.7(2)
C(4)-C(5)-C(6)-N(2)	150.80(16)	C(7)-C(8)-C(12)-C(13)	61.2(2)
C(4)-C(5)-C(6)-N(1)	-32.25(19)	N(1)-C(8)-C(12)-C(13)	-123.25(16)
N(2)-C(6)-N(1)-C(8)	-0.25(17)	C(17)-C(12)-C(13)-C(14)	-1.7(2)
C(5)-C(6)-N(1)-C(8)	-177.69(13)	C(8)-C(12)-C(13)-C(14)	179.21(14)
N(2)-C(6)-N(1)-C(9)	178.42(13)	C(12)-C(13)-C(14)-C(15)	-0.5(2)
C(5)-C(6)-N(1)-C(9)	1.0(2)	C(13)-C(14)-C(15)-C(16)	1.9(3)
N(2)-C(7)-C(8)-N(1)	-0.63(18)	C(13)-C(14)-C(15)-F(1)	-177.87(14)
N(2)-C(7)-C(8)-C(12)	175.64(14)	F(1)-C(15)-C(16)-C(17)	178.71(14)
C(6)-N(1)-C(8)-C(7)	0.52(16)	C(14)-C(15)-C(16)-C(17)	-1.1(3)
C(9)-N(1)-C(8)-C(7)	-177.98(14)	C(15)-C(16)-C(17)-C(12)	-1.2(2)
C(6)-N(1)-C(8)-C(12)	-175.94(14)	C(13)-C(12)-C(17)-C(16)	2.6(2)
C(9)-N(1)-C(8)-C(12)	5.6(2)	C(8)-C(12)-C(17)-C(16)	-178.35(14)
N(1)-C(6)-N(2)-C(7)	-0.13(18)	C(10)-C(9)-C(18)-C(19)	-118.13(16)
C(5)-C(6)-N(2)-C(7)	177.02(15)	N(1)-C(9)-C(18)-C(19)	57.21(18)
C(8)-C(7)-N(2)-C(6)	0.49(19)	C(10)-C(9)-C(18)-C(23)	61.11(19)
C(6)-N(1)-C(9)-C(10)	18.13(19)	N(1)-C(9)-C(18)-C(23)	-123.55(14)
C(8)-N(1)-C(9)-C(10)	-163.56(14)	C(23)-C(18)-C(19)-C(20)	0.4(2)
C(6)-N(1)-C(9)-C(18)	-157.53(13)	C(9)-C(18)-C(19)-C(20)	179.64(14)
C(8)-N(1)-C(9)-C(18)	20.8(2)	C(18)-C(19)-C(20)-C(21)	0.7(3)
N(1)-C(9)-C(10)-C(11)	-177.40(14)	C(19)-C(20)-C(21)-C(22)	-0.8(3)
C(18)-C(9)-C(10)-C(11)	-2.0(2)	C(20)-C(21)-C(22)-C(23)	-0.2(3)
N(1)-C(9)-C(10)-C(4)	-2.8(2)	C(19)-C(18)-C(23)-C(22)	-1.3(2)
C(18)-C(9)-C(10)-C(4)	172.56(13)	C(9)-C(18)-C(23)-C(22)	179.45(14)
C(5)-C(4)-C(10)-C(9)	-28.2(2)	C(21)-C(22)-C(23)-C(18)	1.2(2)
C(3)-C(4)-C(10)-C(9)	-151.84(14)		
C(5)-C(4)-C(10)-C(11)	147.25(14)		
C(3)-C(4)-C(10)-C(11)	23.58(16)		

Symmetry transformations used to generate equivalent atoms: