Supporting Information

Pd-Catalyzed α-Selective C(sp^3)-H Acetoxylation of Amides through an Unusual Cyclopalladation Mechanism

Meining Wang,[†,ϕ] Yang Yang,[‡,ϕ] Zhoulong Fan,[†] Zhen Cheng,[ʃ,*] Weiliang Zhu, [‡,*] and Ao Zhang[†,*]

[†]CAS Key Laboratory of Receptor Research, and Synthetic Organic & Medicinal Chemistry Laboratory (SOMCL), Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences, Shanghai 201203, China.

[‡]Drug Discovery and Design Center, Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences, Shanghai 201203, China.

[ʃ]Department of Radiology, School of Medicine, Stanford University, Stanford, California, 94305-5484.

1. General information

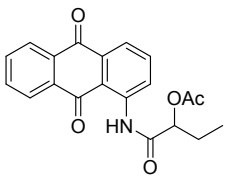
All reactions were performed in glassware containing a Teflon-coated stir bar. All solvents and chemical reagents were obtained from commercial sources and used without further purifications. ^{1}H and ^{13}C NMR spectra were recorded with tetramethylsilane as an internal reference. High-resolution mass spectrometry (HRMS) analysis was recorded by electron ionization (EI-TOF). Flash column chromatography on silica gel (200-300 mesh) was used for the routine purification of reaction products. The column output was monitored by TLC on silica gel (100-200 mesh) precoated on plates (15×50 mm), and spots were visualized by UV light at 254 or 365 nm.

2. General procedure for preparation of N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)amides 1

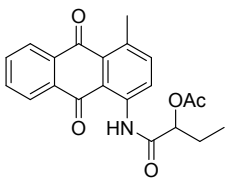
To the solution of 1-amino anthraquinoneand triethylamine (2 equiv) in dichloromethane was added dropwise acyl chlorides (2 equiv) at 0 °C. The resulting mixture was then stirred at room temperature for 1-5 h, and then quenched with water. The organic layer was concentrated, and the residue was purified by column chromatography to give the N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)amides **1**.

3. General procedure for the screening of directing group

A solution of amides **1** (0.1 mmol), $Pd(OAc)_2$ (0.1 equiv) and $PhI(OAc)_2$ (3 equiv) in AcOH-Ac_2O (50:1, 0.5 mL) was stirred in sealed tube at 120 °C for 12 h. The reaction was then cooled to room temperature, concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products **2**.



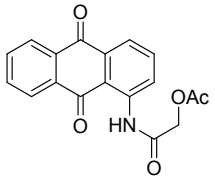
1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxobutan-2-yl acetate (2ae). Yellow solid, 27 mg (76%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 12.84 (s, 1H), 9.18 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.30 (m, 2H), 8.10 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.80 (m, 3H), 5.34 (dd, *J* = 7.1, 4.7 Hz, 1H), 2.46 (s, 3H), 2.05 (m, 1H), 1.06 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.7, 182.1, 169.8(2), 140.7, 135.4, 134.0, 133.8, 133.6, 133.4, 132.3, 126.9, 126.6, 125.6, 122.5, 117.8, 74.8, 24.9, 20.6, 8.9. **EI-MS (m/z)**: 351 (M^+); **HRMS** (EI): calcd for $C_{20}H_{17}NO_5$ (M^+), 351.1107; found, 351.1100.



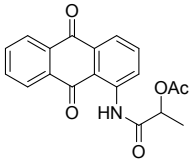
1-((4-Methyl-9,10-dioxo-9,10-dihydroanthracen-1-yl)amino)-1-oxobutan-2-yl acetate (2af). Yellow solid, 6 mg (16%). **^{1}H NMR**(400 MHz, $CDCl_3$) δ 13.03 (s, 1H), 9.07 (d, *J* = 8.8 Hz, 1H), 8.26 (m, 2H), 7.81 (m, 2H), 7.62 (d, *J* = 8.8 Hz, 1H), 5.36 (dd, *J* = 7.3, 4.5 Hz, 1H), 2.82 (s, 3H), 2.49 (s, 3H), 2.05 (m, 2H), 1.08 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR**(126 MHz, $CDCl_3$) δ 187.9, 185.0, 170.3(2), 140.4, 140.0, 137.7, 134.5, 133.9, 133.7, 133.3, 131.5, 126.9, 126.8, 125.7, 119.3, 75.3, 25.4, 23.8, 21.1, 9.4. **ESI-MS (m/z)**: 388 (M+Na); **HRMS** (EI): calcd for $C_{21}H_{19}NO_5Na$ (M+Na), 388.1161; found, 388.1163.

4. General procedure for preparation of 2

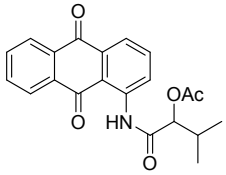
A solution of amides **1** (0.1 mmol), $Pd(OAc)_2$ (0.1 equiv), $PhI(OAc)_2$ (5 equiv) and LiOAc (2 equiv) in DCE (0.5 mL) was stirred in sealed tube at 120 °C for 12 h. The reaction was then cooled to room temperature, concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products **2**.



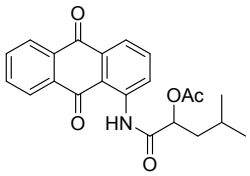
2-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-2-oxoethyl acetate (2ba). Yellow solid, 30 mg (92%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 12.85 (s, 1H), 9.12 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.25 (m, 2H), 8.06 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.78 (m, 3H), 4.79 (s, 2H), 2.45 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 187.1, 182.5, 169.9, 167.3, 140.9, 135.9, 134.5, 134.3, 134.0, 133.8, 132.7, 127.3, 127.1, 126.0, 123.1, 118.1, 63.0, 20.8. **EI-MS (m/z)**: 323 (M^+); **HRMS** (EI): calcd for $C_{18}H_{13}NO_5$ (M^+), 323.0794; found, 323.0788.



1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxopropan-2-yl acetate (2bb). Yellow solid, 28 mg (82%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.85 (s, 1H), 9.12 (d, *J* = 8.1 Hz, 1H), 8.24 (m, 2H), 8.05 (d, *J* = 7.3 Hz, 1H), 7.77 (m, 3H), 5.43 (q, *J* = 6.8 Hz, 1H), 2.46 (s, 3H), 1.65 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.0, 182.4, 170.7, 169.9, 141.1, 135.8, 134.4, 134.2, 133.9, 133.8, 132.7, 127.3, 127.0, 126.0, 122.9, 118.1, 70.7, 21.1, 17.9. **EI-MS (m/z)**: 337(M^+); **HRMS** (EI): calcd for $C_{19}H_{15}NO_5$ (M^+), 337.0950; found, 337.0956.

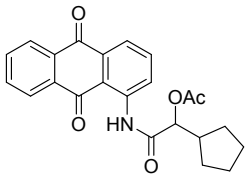


1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-3-methyl-1-oxobutan-2-yl acetate (2bc). Yellow solid, 19 mg (52%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 12.77 (s, 1H), 9.16 (d, *J* = 7.9 Hz, 1H), 8.26 (m, 2H), 8.07 (d, *J* = 6.9 Hz, 1H), 7.78 (m, 3H), 5.26 (d, *J* = 3.9 Hz, 1H), 2.44 (m, 4H), 1.05 (m, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.2, 182.5, 170.4, 169.9, 141.0, 135.8, 134.4, 134.3, 134.0, 133.9, 132.7, 127.3, 127.0, 126.1, 122.9, 118.2, 78.3, 30.9, 21.0, 18.9, 16.9. **EI-MS (m/z)**: 365(M^+); **HRMS** (EI): calcd for $C_{21}H_{19}NO_5$ (M^+), 365.1263; found, 365.1259.

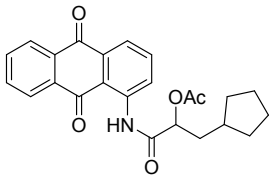


1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-4-methyl-1-oxopentan-2-yl acetate (2bd). Yellow solid, 22 mg (59%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.84 (s, 1H), 9.17 (d, *J* = 8.4 Hz, 1H), 8.30 (m, 2H), 8.10 (d, *J* = 7.6 Hz, 1H), 7.81 (m, 3H), 5.43 (dd, *J* = 8.7, 4.3 Hz, 1H), 2.48 (s, 3H), 1.89 (m, 3H), 1.03 (m, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.2, 182.5, 170.8, 170.3, 141.2, 135.8, 134.4, 134.3, 134.0, 133.8, 132.7, 127.3, 127.1, 126.1, 122.9, 118.2, 73.1, 41.0, 24.7, 23.1, 21.7, 21.1. **EI-MS (m/z)**: 379(M^+); **HRMS** (EI): calcd for $C_{22}H_{21}NO_5$ (M^+), 379.1420; found, 379.1417.

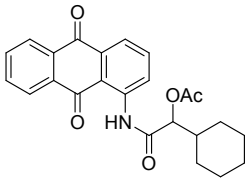
1-Cyclopentyl-2-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)-2-oxoethyl acetate (2be). Yellow



solid, 21 mg (53%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.80 (s, 1H), 9.19 (d, *J* = 8.5 Hz, 1H), 8.31 (m, 2H), 8.11 (d, *J* = 7.5 Hz, 1H), 7.80 (m, 3H), 5.32 (d, *J* = 5.5 Hz, 1H), 2.60 (m, 1H), 2.46 (s, 3H), 1.83 (m, 2H), 1.71 (m, 2H), 1.56 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.2, 182.6, 170.4, 170.2, 141.2, 135.8, 134.4, 134.3, 134.0, 133.9, 132.7, 127.3, 127.1, 126.1, 122.9, 118.2, 76.7, 41.8, 28.7, 27.6, 25.4, 25.2, 21.0. **EI-MS (m/z)**: 391(M^+); **HRMS** (EI): calcd for $C_{23}H_{21}NO_5$ (M^+), 391.1420; found, 391.1422.

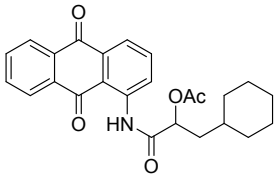


3-Cyclopentyl-1-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxopropan-2-yl acetate (2bf). Yellow solid, 27 mg (66%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.83 (s, 1H), 9.15 (d, *J* = 8.4 Hz, 1H), 8.27 (m, 2H), 8.07 (d, *J* = 7.5 Hz, 1H), 7.78 (m, 3H), 5.40 (t, *J* = 6.2 Hz, 1H), 2.48 (s, 3H), 2.02 (m, 3H), 1.87 (m, 2H), 1.65 (m, 2H), 1.57 (m, 2H), 1.24 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.1, 182.5, 170.6, 170.2, 141.1, 135.8, 134.4, 134.2, 133.9, 133.8, 132.7, 127.3, 127.0, 126.0, 122.9, 118.1, 74.1, 38.2, 36.5, 33.0, 32.4, 25.1, 25.0, 21.1. **EI-MS (m/z)**: 405(M^+); **HRMS** (EI): calcd for $C_{24}H_{23}NO_5$ (M^+), 405.1576; found, 405.1578.

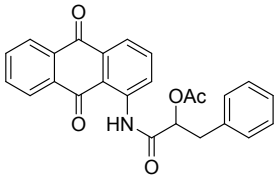


1-Cyclohexyl-2-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)-2-oxoethyl acetate (2bg). Yellow solid, 28 mg (68%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.78 (s, 1H), 9.19 (d, *J* = 8.3 Hz, 1H), 8.28 (m, 2H), 8.08 (d, *J* = 7.6 Hz, 1H), 7.78 (m, 3H), 5.26 (d, *J* = 4.0 Hz, 1H), 2.48 (s, 3H), 2.13 (m, 1H), 1.75 (m, 5H), 1.28 (m, 5H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.1, 182.5, 170.3, 169.9, 141.0, 135.8, 134.4, 134.2, 133.9, 133.8, 132.7, 127.3, 127.0, 126.0, 122.9, 118.1, 78.1, 40.4, 29.3, 27.2, 26.1, 25.9, 21.0. **EI-MS (m/z)**: 405(M^+); **HRMS** (EI): calcd for $C_{24}H_{23}NO_5$ (M^+), 405.1576; found, 405.1576.

3-Cyclohexyl-1-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxopropan-2-yl acetate (2bh).

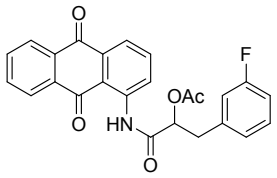


Yellow solid, 26 mg (62%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.80 (s, 1H), 9.14 (d, *J* = 8.5 Hz, 1H), 8.27 (m, 2H), 8.06 (d, *J* = 7.6 Hz, 1H), 7.78 (m, 3H), 5.44 (dd, *J* = 8.7, 4.7 Hz, 1H), 2.47 (s, 3H), 1.90 (m, 3H), 1.72 (m, 4H), 1.51 (m, 1H), 1.23 (m, 3H), 1.02 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.1, 182.4, 170.9, 170.3, 141.2, 135.8, 134.4, 134.2, 133.9, 133.8, 132.7, 127.3, 127.0, 126.1, 122.9, 118.1, 72.6, 39.7, 34.0, 33.7, 32.3, 26.4, 26.2, 26.0, 21.1. **EI-MS (m/z)**: 419(M^+); **HRMS** (EI): calcd for $C_{25}H_{25}NO_5$ (M^+), 419.1733; found, 419.1734.

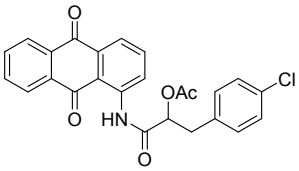


1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxo-3-phenylpropan-2-yl acetate (2bi). Yellow solid, 26 mg (63%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.77 (s, 1H), 9.18 (d, *J* = 8.5 Hz, 1H), 8.28 (m, 2H), 8.11 (d, *J* = 7.6 Hz, 1H), 7.81 (m, 3H), 7.26 (m, 5H), 5.62 (dd, *J* = 8.4, 4.1 Hz, 1H), 3.43 (dd, *J* = 14.3, 4.0 Hz, 1H), 3.24 (dd, *J* = 14.3, 8.4 Hz, 1H), 2.39 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.0, 182.5, 169.9, 169.5, 140.9, 136.0, 135.8, 134.4, 134.2, 134.0, 133.8, 132.7,

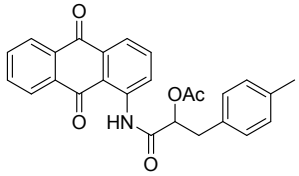
129.5, 128.4, 127.3, 127.1, 126.9, 126.1, 123.0, 118.3, 74.7, 38.1, 20.9. **EI-MS (m/z)**: 413(M^+); **HRMS** (EI): calcd for $C_{25}H_{19}NO_5$ (M^+), 413.1263; found, 413.1243.



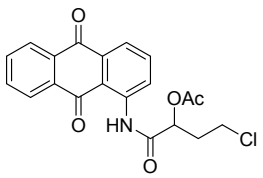
1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-3-(3-fluorophenyl)-1-oxopropan-2-yl acetate(2bj). Yellow solid, 20 mg (47%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.80 (s, 1H), 9.17 (d, *J* = 8.4 Hz, 1H), 8.31 (m, 2H), 8.13 (d, *J* = 7.6 Hz, 1H), 7.83 (m, 3H), 7.25 (m, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 9.7 Hz, 1H), 6.93 (m, 1H), 5.62 (dd, *J* = 8.1, 4.1 Hz, 1H), 3.42 (dd, *J* = 14.3, 4.0 Hz, 1H), 3.25 (dd, *J* = 14.3, 8.2 Hz, 1H), 2.42 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 187.1, 182.5, 169.8, 169.2, 162.8 (d, J = 245.9 Hz), 140.8, 138.5 (d, J = 7.3 Hz), 135.9, 134.5, 134.3, 134.0, 133.8, 132.8, 129.9 (d, J = 8.2 Hz), 127.4, 127.1, 126.1, 125.2 (d, J = 2.6 Hz), 123.2, 118.3, 116.5(d, J = 21.3 Hz), 114.0 (d, J = 21.0 Hz), 74.3, 37.8, 21.0. **EI-MS (m/z)**: 431(M^+); **HRMS** (EI): calcd for $C_{25}H_{18}FNO_5$ (M^+), 431.1169; found, 431.1160.



3-(4-Chlorophenyl)-1-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxopropan-2-yl acetate (2bk). Yellow solid, 23 mg (51%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.78 (s, 1H), 9.16 (d, *J* = 8.5 Hz, 1H), 8.30 (m, 2H), 8.13 (d, *J* = 7.6 Hz, 1H), 7.83 (m, 3H), 7.26 (m, 4H), 5.60 (dd, *J* = 7.9, 4.2 Hz, 1H), 3.39 (dd, *J* = 14.3, 4.2 Hz, 1H), 3.24 (dd, *J* = 14.3, 7.9 Hz, 1H), 2.41 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 187.1, 182.6, 169.8, 169.3, 140.8, 135.9, 134.5(2), 134.3, 134.1, 133.8, 132.9, 132.8, 130.9, 128.6, 127.4, 127.1, 126.1, 123.2, 118.4, 74.3, 37.4, 21.0. **EI-MS (m/z)**: 447(M^+); **HRMS** (EI): calcd for $C_{25}H_{18}ClNO_5$ (M^+), 447.0874; found, 447.0874.

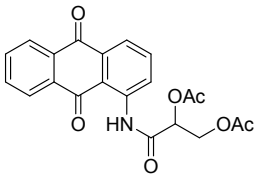


1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxo-3-*p*-tolylpropan-2-yl acetate (2bl). Yellow solid, 26 mg (61%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 12.72 (s, 1H), 9.14 (d, *J* = 8.5 Hz, 1H), 8.25 (m, 2H), 8.08 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.79 (m, 3H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.06 (d, *J* = 7.8 Hz, 2H), 5.54 (dd, *J* = 8.2, 4.1 Hz, 1H), 3.34 (dd, *J* = 14.2, 4.1 Hz, 1H), 3.16 (dd, *J* = 14.3, 8.2 Hz, 1H), 2.35 (s, 3H), 2.24 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 187.0, 182.6, 169.9, 169.7, 141.0, 136.5, 135.8, 134.5, 134.3, 134.0, 133.9, 132.9, 132.8, 129.4, 129.2, 127.4, 127.1, 126.2, 123.1, 118.3, 74.9, 37.7, 21.1, 21.0. **EI-MS (m/z)**: 426([M-H]$^+$); **HRMS** (EI): calcd for $C_{26}H_2NO_5$ ([M-H]$^+$), 426.1336; found, 426.1338.

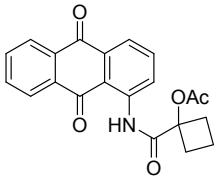


4-Chloro-1-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)-1-oxobutan-2-yl acetate (2bm). Yellow solid, 27 mg (69%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 12.89 (s, 1H), 9.11 (d, *J* = 8.4 Hz, 1H), 8.26 (m, 2H), 8.08 (d, *J* = 7.6 Hz, 1H), 7.78 (m, 3H), 5.53 (dd, *J* = 8.0, 4.4 Hz, 1H), 3.68 (dd, *J* = 9.6, 4.1 Hz, 2H), 2.47 (m, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 187.3, 182.5, 169.9, 169.3, 140.9, 135.9, 134.6, 134.3, 134.0, 133.8, 132.8, 127.4, 127.1, 126.1, 123.2, 118.3, 71.6, 40.1, 34.9, 21.0. **EI-MS (m/z)**: 385(M^+); **HRMS** (EI): calcd for $C_{20}H_{16}ClNO_5$ (M^+), 385.0717; found,

385.0717.



3-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-3-oxopropane-1,2-diyl diacetate (2bn). Yellow solid, 31 mg (78%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 12.94 (s, 1H), 9.11 (d, *J* = 8.5 Hz, 1H), 8.25 (m, 2H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.77 (m, 3H), 5.61 (m, 1H), 4.68 (dd, *J* = 12.1, 2.7 Hz, 1H), 4.52 (dd, *J* = 12.1, 4.8 Hz, 1H), 2.47 (s, 3H), 2.04 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.2, 182.4, 170.5, 169.7, 167.1, 140.7, 135.9, 134.6, 134.3(2), 133.8, 132.7, 127.3, 127.1, 126.0, 123.3, 118.3, 72.0, 63.2, 20.9, 20.7. **EI-MS (m/z)**: 395(M^+); **HRMS** (EI): calcd for $C_{21}H_{17}NO_7$ (M^+), 395.1005; found, 395.1004.

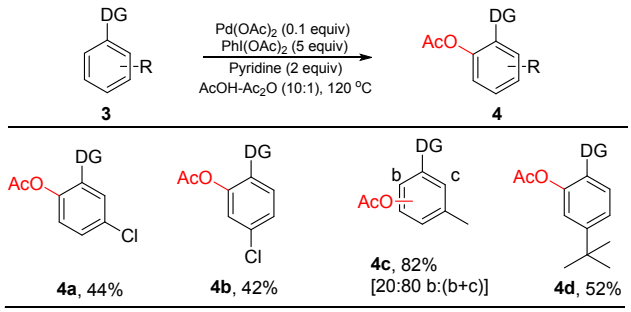


1-(9,10-Dioxo-9,10-dihydroanthracen-1-ylcarbamoyl)cyclobutyl acetate (2bo). Yellow solid, 12 mg (32%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.64 (s, 1H), 9.20 (d, *J* = 8.5 Hz, 1H), 8.27 (m, 2H), 8.06 (d, *J* = 7.6 Hz, 1H), 7.79 (m, 3H), 2.88 (m, 2H), 2.48 (m, 2H), 2.35 (s, 3H), 2.10 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.3, 182.5, 171.7, 170.1, 141.8, 135.8, 134.4, 134.2, 133.9(2), 132.7, 127.3, 127.0, 126.1, 122.6, 118.1, 81.0, 32.1, 21.4, 14.5. **EI-MS (m/z)**: 363(M^+); **HRMS** (EI): calcd for $C_{21}H_{17}NO_5$ (M^+), 363.1107; found, 363.1105.

5. General procedure for preparation of 4

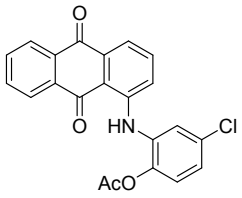
Encouraged by the successful acetoxylation of α-C(sp^3)-H bonds, we further expanded the reaction protocol to the *ortho* C(sp^2)-H bond activation. As shown in Scheme S1, with the assistance of 1-aminoanthraquinone as the BDG, substrates **3** took part in the C-H activation/acetoxylation smoothly and yielded the corresponding mono-acetoxylated products **4a**, **4b**, and **4d** in moderate yields, except for **4c** which gave a mixture of products in 82% total yield due to the existence of two asymmetric *ortho* C(sp^2)-H bonds.

Scheme S1. Acetoxylation of *ortho* C(sp^2)-H bonds[a,b]

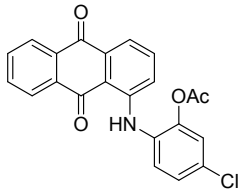


[a]The reaction were performed with N-anthraquinon-1-ylanilines **3** (0.1 mmol), $Pd(OAc)_2$ (0.1 equiv), $PhI(OAc)_2$ (5 equiv) and pyridine (2 equiv) in AcOH-Ac_2O (10:1, 0.5 mL) in a sealed tube at 120 °C for 12 h. [b]Isolated yields were listed.

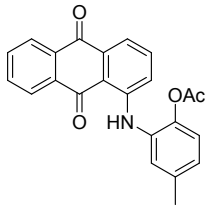
A solution of **3** (0.1 mmol), $Pd(OAc)_2$ (0.1 equiv), $PhI(OAc)_2$ (5 equiv)and pyridine (2 equiv) in AcOH-AcO_2 (10:1, 0.5 mL) was stirred in sealed tube at 120 °C for 12 h. The reaction was then cooled to room temperature, concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products **4**.



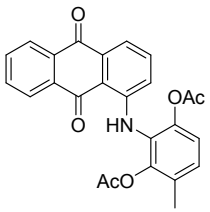
4-Chloro-2-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)phenyl acetate (4a). Red solid, 17 mg (44%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 11.28 (s, 1H), 8.25 (m, 2H), 7.74 (m, 3H), 7.48 (t, *J* = 7.2 Hz, 2H), 7.39 (d, *J* = 2.2 Hz, 1H), 7.21 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 1H), 2.36 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.7, 183.2, 168.7, 148.4, 143.8, 138.3, 135.2, 134.7, 134.6, 134.2, 133.6, 133.0, 127.7, 127.0, 126.9, 125.3, 124.5, 123.1, 119.8, 118.5, 114.6, 20.7. **EI-MS (m/z)**: 391(M^+); **HRMS** (EI): calcd for $C_{22}H_{14}ClNO_4$ (M^+), 391.0611; found, 391.0612.



5-Chloro-2-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)phenyl acetate (4b). Red solid, 16 mg (42%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 11.32 (s, 1H), 8.33 (d, *J* = 7.6 Hz, 1H), 8.27 (d, *J* = 7.1 Hz, 1H), 7.76 (m, 3H), 7.51 (m, 2H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.30 (d, *J* = 2.4 Hz, 1H), 7.05 (dd, *J* = 8.7, 2.4 Hz, 1H), 2.31 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.2, 184.8, 170.6, 149.6, 148.9, 136.5, 136.2, 136.1, 135.6, 135.0, 134.5, 130.8, 128.5, 128.3, 126.7, 125.3, 122.4, 121.3, 119.9, 116.5, 22.5. **EI-MS (m/z)**: 391(M^+); **HRMS** (EI): calcd for $C_{22}H_{14}ClNO_4$ (M^+), 391.0611; found, 391.0607.

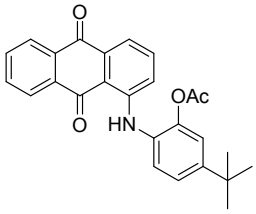


2-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-4-methylphenyl acetate (4c). Red solid, 6 mg (16%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 11.28 (s, 1H), 8.30 (d, *J* = 7.4 Hz, 1H), 8.26 (d, *J* = 7.6 Hz, 1H), 7.74 (m, 3H), 7.47 (m, 2H), 7.15 (m, 2H), 7.04 (d, *J* = 8.2 Hz, 1H), 2.33 (s, 3H), 2.19 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.5, 183.5, 169.4, 149.4, 146.5, 137.1, 135.0, 134.8, 134.6, 134.1, 133.4, 133.1, 131.7, 126.9(2), 123.0, 122.8, 120.1, 117.8, 114.1, 20.9, 16.4. **EI-MS (m/z)**: 371(M^+); **HRMS** (EI): calcd for $C_{23}H_{17}NO_4$ (M^+), 371.1158; found, 371.1158.



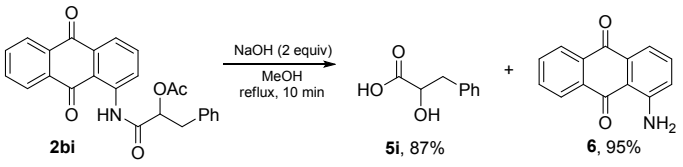
2-(9,10-Dioxo-9,10-dihydroanthracen-1-ylamino)-4-methyl-1,3-phenylene diacetate (4c'). Red solid, 28 mg (66%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 11.30 (s, 1H), 8.26 (m, 2H), 7.73 (m, 3H), 7.52 (m, 2H), 7.03 (d, *J* = 8.8 Hz, 2H), 2.32 (s, 3H), 2.28 (s, 3H), 2.21 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.6, 183.4, 168.3, 168.2, 148.7, 143.0, 137.9, 137.4, 135.1, 134.7, 134.6, 134.1, 133.4(2), 133.0, 127.0, 126.9, 123.5, 120.1, 118.2, 116.4, 114.4, 20.7, 20.4, 16.4. **EI-MS (m/z)**: 429(M^+); **HRMS** (EI): calcd for $C_{25}H_{19}NO_6$ (M^+), 429.1212; found, 429.1206.

5-*tert*-Butyl-2-(9,10-dioxo-9,10-dihydroanthracen-1-ylamino)phenyl acetate (4d). Red solid, 21 mg (52%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 11.07 (s, 1H), 8.32 (d, *J* = 7.3 Hz, 1H), 8.25 (d, *J* = 7.7 Hz, 1H),



7.74 (m, 3H), 7.47 (m, 1H), 7.34 (m, 3H), 7.19 (d, *J* = 1.8 Hz, 1H), 2.22 (s, 3H), 1.34 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.5, 183.5, 169.2, 150.0, 149.1, 144.7, 134.9, 134.8, 134.5, 134.1, 133.3, 133.1, 129.1, 127.0, 126.8, 125.4, 123.7, 120.4, 120.2, 117.9, 114.3, 34.7, 31.3, 20.8. **EI-MS (m/z)**: 413(M^+); **HRMS** (EI): calcd for $C_{26}H_{23}NO_4$ (M^+), 413.1627; found, 413.1629.

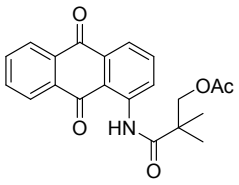
6. Removal of directing group



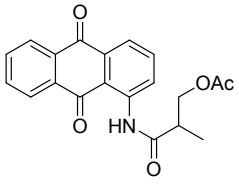
A solution of **2bi** (50mg, 0.12 mmol) and NaOH (20mg, 0.5 mmol) in MeOH (5 ml) was refluxed for 10 min and then concentrated in vacuum. The residue was dissolved in water and washed with ethyl acetate for two times. Concentration of the combined ethyl acetate layer gave 1-aminoanthraquinone**6** in 95% yield. Proper PH adjustment of the aqueous phase (2-3), followed by extraction with ethyl acetate and concentration, gave product **5i** in 87% yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.27 (m, 5H), 5.99 (m, 2H), 4.49 (m, 1H), 3.18 (d, J = 13.4 Hz, 1H), 2.97 (dd, J = 13.7, 6.7 Hz, 1H).

7. General procedure for preparation of 7

A solution of amides **1** (0.1 mmol), $Pd(OAc)_2$ (0.1 equiv), $PhI(OAc)_2$ (5equiv) and LiOAc (2 equiv) in DCE (0.5 mL) was stirred in sealed tube at 120 ^{o}C for 12 h. The reaction was then cooled to room temperature, concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products **7**.

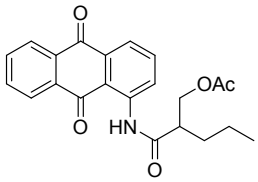


3-((9,10-Dioxo-9,10-dihydroanthracen-1-yl)amino)-2,2-dimethyl-3-oxopropyl acetate (7a). Yellow solid, 14 mg (37%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 12.61 (s, 1H), 9.18 (d, *J* = 8.6 Hz, 1H), 8.29 (m, 2H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.78 (m, 3H), 4.25 (s, 2H), 2.05 (s, 3H), 1.46 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.4, 182.8, 175.8, 171.0, 142.1, 135.9, 134.5, 134.4, 134.0(2), 132.8, 127.4, 127.1, 126.3, 122.7, 118.0, 70.4, 44.2, 22.8, 20.9. **EI-MS (m/z)**: 365(M^+); **HRMS** (EI): calcd for $C_{21}H_{19}NO_5$ (M^+), 365.1263; found, 365.1262.



3-((9,10-Dioxo-9,10-dihydroanthracen-1-yl)amino)-2-methyl-3-oxopropyl acetate (7b). Yellow solid, 15 mg (41%). **^{1}H NMR**(400 MHz, $CDCl_3$) δ 12.51 (s, 1H), 9.18 (d, *J* = 8.5 Hz, 1H), 8.30 (m, 2H), 8.10 (d, *J* = 7.6 Hz, 1H), 7.82 (m, 3H), 4.35 (m, 2H), 2.99 (m, 1H), 2.09 (s, 3H), 1.40 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR**(126 MHz, $CDCl_3$) δ 187.3, 182.6, 173.6, 170.8, 141.9, 135.8, 134.4, 134.3, 133.9(2), 132.8,

127.3, 127.1, 126.2, 122.7, 117.7, 65.9, 42.6, 20.9, 14.3. **EI-MS (m/z)**: 351(M^+); **HRMS** (EI): calcd for $C_{20}H_{17}NO_5$ (M^+), 351.1107; found, 365.1118.



2-((9,10-Dioxo-9,10-dihydroanthracen-1-yl)carbamoyl)pentyl acetate (7c). Yellow solid, 13 mg (33%). **^{1}H NMR**(300 MHz, $CDCl_3$) δ 12.46 (s, 1H), 9.17 (dd, *J* = 8.5, 1.0 Hz, 1H), 8.28 (m, 2H), 8.07 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.80 (m, 3H), 4.31 (m, 2H), 2.82 (m, 1H), 2.02 (s, 3H), 1.79 (m, 1H), 1.60 (m, 1H), 1.45 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR**(126 MHz, $CDCl_3$) δ187.4, 182.7, 173.5, 170.9, 141.9, 135.9, 134.5, 134.4, 134.0(2), 132.8, 127.4, 127.1, 126.3, 122.8, 117.8, 65.2, 48.6, 31.4, 20.9, 20.5, 14.0. **EI-MS (m/z)**: 379(M^+); **HRMS** (EI): calcd for $C_{22}H_{21}NO_5$ (M^+), 379.1420; found, 379.1408.

8. Computational methods

Gaussian 09[1] was performed at the B3LYP[2] level of density functional theory (DFT) for geometry optimizations. A combined basis set was applied in which Pd was described by the LANL2DZ basis set and 6-31(d) was used for C, H, O, N.[3] Frequency calculations were performed for all stationary points to determine them either as local minima or transition states and to obtain the thermochemical corrections to Gibbs free energies (Table S1). Each transition structure contained one imaginary frequency, exhibiting atom displacements consistent with the anticipated reaction pathway. For each saddle point, intrinsic reaction coordinate (IRC) analysis[4] was carried out to confirm whether it connected the correct configurations of reactant and product on the potential energy surface. Solvent effects in dichloroethane solvent (ε = 10.125) were evaluated by structure optimizations and frequency calculations in the solvent utilizing the self-consistent reaction field method[5] with CPCM solvation model.[6] The solvation single-point energies with Gibbs free energy corrections were used to describe the reaction energetics throughout the study.

Different initial conformations have been investigated to obtain the geometry of intermediate A at the energy minimum. Careful examination of the optimized geometry of **A** has revealed a distance of 2.36Å between the α-C(sp^3)-H and oxygen atom of acetic acid moiety (Figure S1a), which is reasonable for the proton abstraction. However, there will be too much steric hindrance for the β-C(sp^3)-H to approach the same oxygen atom by a near dihedral 180-degree rotation of the bond C(O)-C(α). In addition, there is an energy barrier of about 1.3 kcal/mol between the optimized orientation of **1a** and the configuration **of 1a'** (Figure S1b, S1c), thus disfavoring an effective β-selective C-H activation.

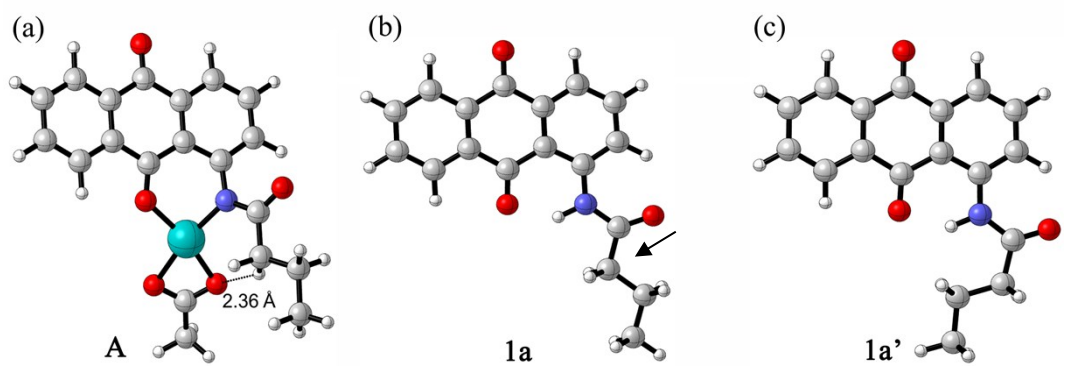


Figure S1. Optimized geometry of **A**, **1a** and **1a'**.

9. Calculated energies and cartesiancoordinates for the relevant intermediates and transition states

Table S1. Calculated energy values

Species	E[a,b]	ZPE[a,c]	H_{298}[a,d]	G_{298}[a,e]	Frequency[a,f]
$Pd(OAc)_2$	-583.7295404	-583.625871	-583.614194	-583.664888	
$PhI(OAc)_2$	-699.899216	-699.706441	-699.688281	-699.755715	
PhI	-243.024598	-242.934338	-242.92749	-242.966125	
AcOH	-229.087810	-229.026009	-229.020473	-229.053384	
1a	-975.439368	-975.146486	-975.127045	-975.195211	
E	-1559.150962	-1558.753632	-1558.721439	-1558.821112	
A	-1330.066707	-1329.733358	-1329.707398	-1329.790467	
TS (A-B)	-1330.025984	-1329.697685	-1329.672435	-1329.753629	-1395.77
B	-1330.058712	-1329.72574	-1329.699747	-1329.78312	
C	-1786.984071	-1786.548256	-1786.511759	-1786.619792	
D	-1787.050730	-1786.611509	-1786.575172	-1786.68522	
2ea	-1203.323902	-1202.988574	-1202.964711	-1203.044943	
TS (A-B')	-1330.021880	-1329.693417	-1329.668377	-1329.74897	-1408.15
B'	-1330.065631	-1329.732065	-1329.706559	-1329.787843	
C'	-1786.996898	-1786.560407	-1786.524172	-1786.630607	
D'	-1787.050730	-1786.611509	-1786.575172	-1786.68522	
7d	-1203.323902	-1202.988574	-1202.964711	-1203.044943	

[a]With B3LYP functional; 6-31(d)for C,H,O,N and LANL2DZ for Pd

[b]Electronic energies (Gibss free energy in a. u.)

[c]Sum of electronic and zero-point energies(Gibss free energy in a. u.)

[d]Sum of electronic and thermal enthalpies(Gibss free energy in a. u.)

[e]Sum of electronic and thermal free energies(Gibss free energy in a. u.)

[f]The only imaginary frequency of transition state

Cartesian coordinates

$Pd(OAc)_2$:

0 1 (charge, spin multiplicity)

C	-2.19951713	-1.86428369	0.52422447
O	-1.00305452	-2.17743381	0.19681937
O	-2.41360374	-0.63528978	0.80754452
C	1.37931939	1.46293824	0.40837695
O	0.18270917	1.77560663	0.73581171
O	1.59390487	0.23406384	0.12503487
Pd	-0.40987819	-0.20090758	0.46626161
C	2.46544427	2.48948745	0.33122830
H	3.44270739	2.01176586	0.42904080
H	2.41550345	2.99122040	-0.64238459
H	2.32354510	3.24349890	1.10961996
C	-3.28613440	-2.89031987	0.60128430
H	-3.14467538	-3.64422563	-0.17729500
H	-3.23635527	-3.39229054	1.57478019
H	-4.26317690	-2.41212419	0.50359730

$PhI(OAc)_2$:

0 1 (charge, spin multiplicity)

C	2.41965386	-1.82648443	0.18349676
O	1.59607556	-1.48374127	-0.79581437
O	2.21058737	-1.64633170	1.37755031
C	3.68796464	-2.47505683	-0.34841834
H	4.20762064	-1.78197911	-1.01780267
H	4.34231972	-2.74689470	0.48153060
H	3.43581155	-3.36686300	-0.93079032
I	-0.37708076	-0.70814211	-0.21878250
O	-2.19977917	0.44564595	0.23203811
C	-3.23449948	-0.36727547	0.24251036
O	-3.14132522	-1.57794252	0.03969805
C	-4.54868416	0.33365369	0.52965855
H	-4.50174247	0.82632057	1.50599928
H	-4.73004086	1.10816349	-0.22219902
H	-5.36522589	-0.38993549	0.51994351
C	0.51108014	1.23953956	-0.07429373
C	0.15310040	2.19761406	-1.01852392
C	1.41053756	1.48571998	0.95846078
C	0.73091899	3.46589159	-0.91562513

H	-0.55559968	1.97709907	-1.80820679
C	1.98033082	2.76039830	1.03671665
H	1.67550788	0.70930681	1.66613089
C	1.64130066	3.74527114	0.10664279
H	0.46793976	4.22991063	-1.64095386
H	2.68663178	2.97700138	1.83254796
H	2.08736882	4.73272851	0.17774744

PhI:

0 1 (charge, spin multiplicity)

I	1.56868546	-0.00000045	-0.00001140
C	-0.58522687	-0.00000181	0.00006912
C	-1.26513163	-1.21743393	0.00008732
C	-1.26510647	1.21740844	0.00000998
C	-2.66360587	-1.20824141	-0.00004694
H	-0.72570688	-2.15820138	0.00004270
C	-2.66358823	1.20825854	0.00001959
H	-0.72581356	2.15826049	0.00020327
C	-3.36370181	0.00000100	-0.00005014
H	-3.20047943	-2.15274294	0.00001239
H	-3.20041602	2.15277884	-0.00011019
H	-4.44974831	-0.00001606	-0.00007761

AcOH:

0 1 (charge, spin multiplicity)

C	-0.09185722	0.12250219	-0.00065308
O	-0.64371908	1.20424192	0.00016580
O	-0.77940488	-1.04332913	0.00007972
H	-1.72853277	-0.81373068	0.00043437
C	1.39636407	-0.11143734	0.00011351
H	1.68292783	-0.69260602	0.88260553
H	1.68380348	-0.69212159	-0.88240799
H	1.91975203	0.84476684	0.00064128

1a:

0 1 (charge, spin multiplicity)

C	2.23126198	-1.19353106	-0.00002917
C	0.42848437	0.62007250	-0.00008089
C	1.45859564	1.59812453	-0.00004370
C	2.90479764	1.22167583	-0.00003376
C	3.24744382	-0.22117977	0.00001233

C	-0.93085040	1.06060226	-0.00007524
C	1.15860927	2.95720954	-0.00000634
C	-0.17339002	3.37096548	-0.00000667
C	-1.20613424	2.44452001	-0.00004223
H	1.97361832	3.67148608	0.00001765
H	-0.41239524	4.43046109	0.00001416
H	-2.23783717	2.76331935	-0.00004231
N	-1.95469334	0.11573456	-0.00012915
C	-3.32554650	0.30000012	0.00012625
O	-3.87765419	1.39517115	0.00034158
C	-4.09956292	-1.01544852	0.00014203
H	-3.78693037	-1.60114654	-0.87606773
H	-3.78718461	-1.60091605	0.87660078
C	-5.61740938	-0.82497091	-0.00009112
H	-5.90557846	-0.23246634	0.87619724
H	-5.90534303	-0.23269589	-0.87661567
C	-6.37052211	-2.15846167	-0.00002183
H	-7.45407794	-1.99636096	-0.00019264
H	-6.12217489	-2.75692997	-0.88517677
H	-6.12241863	-2.75669708	0.88535895
C	4.59099701	-0.61321775	0.00009913
C	4.92476493	-1.96524963	0.00015292
H	5.96811610	-2.26639347	0.00022404
C	3.91498240	-2.93475729	0.00011546
H	4.17439892	-3.98928376	0.00016128
C	2.57579088	-2.55130249	0.00001986
H	1.78346805	-3.29137998	-0.00001906
H	5.35676159	0.15497298	0.00012360
O	3.78257228	2.08254813	-0.00004718
C	0.79006311	-0.81573520	-0.00014676
O	-0.06056012	-1.71983082	-0.00029089
H	-1.60868584	-0.84511519	-0.00024898

E:

0 1 (charge, spin multiplicity)

C	-0.62681697	2.20326321	0.70926683
C	1.55023265	1.45690135	-0.38134794
C	1.89775236	2.82415723	-0.56641743
C	0.95981811	3.92747579	-0.19874169
C	-0.28237282	3.55868538	0.52160794

C	2.50721016	0.45158160	-0.73705329
C	3.12707026	3.18914736	-1.10041150
C	4.04139158	2.20059138	-1.46972662
C	3.73499745	0.85965922	-1.29855803
H	3.34563494	4.24171018	-1.23591696
H	4.99253565	2.47626206	-1.91438419
H	4.43606482	0.11182967	-1.64127829
N	2.21466898	-0.89707614	-0.56856412
C	3.00675662	-2.01988893	-0.32018255
O	2.44095994	-3.10523479	-0.26449258
C	4.49931357	-1.87573713	-0.07245253
H	5.01100684	-1.86082795	-1.04542097
H	4.71350338	-0.91318102	0.40526726
C	5.05898025	-3.03015438	0.77019205
H	4.55047786	-3.04560595	1.74223523
H	4.81697269	-3.97870300	0.28031977
Pd	-2.09272657	-0.99310320	-0.31107870
O	-3.77702708	-1.87420733	-1.14123663
C	-3.43552776	-1.47389670	-2.31335037
C	-4.29219069	-1.75818708	-3.50559417
O	-2.34989708	-0.80645960	-2.40123494
C	6.57190978	-2.91088688	0.97540029
H	6.94961004	-3.74191436	1.58127416
H	7.10558059	-2.92621409	0.01707353
H	6.83475159	-1.97736668	1.48789170
C	-1.09439701	4.56741454	1.04565203
C	-2.22914852	4.23931446	1.78630343
H	-2.85428790	5.02585210	2.19774467
C	-2.54756093	2.89722829	2.01469330
H	-3.41328714	2.63854121	2.61660926
C	-1.75679656	1.88129561	1.47787280
H	-1.99882313	0.84506485	1.68445911
H	-0.81384230	5.60087101	0.87435008
H	-5.09979759	-1.01808371	-3.55048837
H	-4.74412838	-2.74935646	-3.41734864
H	-3.70058841	-1.68777040	-4.42069863
O	1.23328648	5.09930413	-0.44398528
C	0.20262605	1.13818417	0.11042102
O	-0.22333138	-0.04330188	0.00681481

C	-1.69750861	-2.33956289	2.16258157
O	-2.37172362	-1.33061449	1.65516609
O	-0.93481614	-3.06500847	1.52757962
C	-1.96536042	-2.52975914	3.64926604
H	-1.70680322	-1.61908573	4.19945395
H	-3.03010980	-2.72275011	3.81726468
H	-1.37745489	-3.36759376	4.02864793
H	1.22384381	-1.10617712	-0.48290189

A:

0 1 (charge, spin multiplicity)

C	-2.70183871	-0.92607579	0.71513001
C	-1.20103868	0.63323938	-0.61461902
C	-2.35440772	1.16226573	-1.25782018
C	-3.72037594	0.62667679	-0.97624276
C	-3.84973399	-0.38458234	0.10291494
C	0.06569208	1.26524933	-0.81508122
C	-2.25093438	2.22752163	-2.14363299
C	-1.00011020	2.80185079	-2.39330927
C	0.12945587	2.33515889	-1.74029215
H	-3.14780964	2.59233469	-2.63035599
H	-0.90800081	3.61538604	-3.10653658
H	1.09601591	2.77678551	-1.95217149
N	1.20547124	0.84564201	-0.14944258
C	2.15473715	1.65952658	0.43143066
O	3.20279757	1.17757849	0.86865028
C	1.87290778	3.15420123	0.62383993
H	2.38281604	3.70330619	-0.18023248
H	0.80613617	3.37634963	0.52633536
C	2.39307332	3.65669457	1.98000293
H	1.88397972	3.11089211	2.78548786
H	3.45644213	3.41149561	2.06321519
Pd	1.52510319	-1.14360804	-0.05016866
O	3.43697954	-1.53196974	-0.82529952
C	3.28106848	-2.78948292	-0.63449513
C	4.38338142	-3.75613300	-0.94692540
O	2.16881757	-3.17888169	-0.14213163
C	2.17886253	5.16241093	2.16045542
H	2.55537696	5.49822036	3.13338737

H	2.70272979	5.73355088	1.38387628
H	1.11519925	5.42548113	2.10548873
C	-5.11881448	-0.81449913	0.50128143
C	-5.25090756	-1.76306712	1.51420657
H	-6.23883646	-2.08733310	1.82665985
C	-4.11165625	-2.29931093	2.12543445
H	-4.21457321	-3.03821843	2.91403034
C	-2.84162935	-1.89264252	1.72181939
H	-1.95438562	-2.31223553	2.18184677
H	-5.98838819	-0.39377579	0.00819883
H	5.03231454	-3.85351418	-0.06843286
H	4.98764216	-3.38810887	-1.77942483
H	3.96946663	-4.73965128	-1.18071220
O	-4.70361617	1.03998773	-1.58534655
C	-1.35532335	-0.52521108	0.25832392
O	-0.39793090	-1.25011919	0.64021081

TS (A-B) :

0 1 (charge, spin multiplicity)

N	-1.25377337	-1.60527042	-1.00039154
C	-0.07410314	-2.30507735	-1.14345762
O	1.06563349	-1.94848521	-0.87128835
C	-0.40462470	-3.67219408	-1.75940370
H	0.22621490	-4.40119081	-1.23041574
H	0.99493709	-3.41738657	-3.35920013
C	-0.06859619	-3.67900240	-3.26646502
H	-1.42253214	-4.62024665	-1.49858908
H	-0.62932087	-2.87950375	-3.76579059
Pd	-2.54986753	-3.03187743	-1.35155064
O	-3.82201121	-4.66924554	-1.67918692
C	-3.21910073	-5.78553000	-1.57838220
C	-4.03017750	-7.05372238	-1.70536269
O	-1.96451060	-5.88636409	-1.39555269
C	-0.32122352	-5.00750214	-3.98521937
H	-1.38546508	-5.26273537	-4.00213653
H	0.02662774	-4.94427323	-5.02235110
H	0.21313918	-5.83223354	-3.50003545
H	-3.78378623	-7.53854881	-2.65662795
H	-3.76241692	-7.74722070	-0.90341437

H	-5.09947504	-6.84029985	-1.67672540
C	-1.48530039	-0.33875530	-0.53188097
C	-2.81601451	0.18251093	-0.34246081
C	-0.37311506	0.50329955	-0.24593032
C	-4.04217500	-0.57553988	-0.58363678
C	-2.94342372	1.53547987	0.11700278
C	-0.54557210	1.79633299	0.19997786
H	0.61564403	0.09109819	-0.38750550
C	-5.36767302	0.07085211	-0.39571417
C	-4.26816799	2.19000353	0.33944054
C	-1.83198730	2.31850228	0.38199736
H	0.32535109	2.41050221	0.40926656
C	-6.53436677	-0.66318533	-0.66361726
C	-5.48268562	1.39925845	0.05093562
H	-1.98537772	3.33310085	0.72981171
C	-7.78704372	-0.07995484	-0.48895378
H	-6.44850628	-1.68662169	-1.00787230
C	-6.74432435	1.97795789	0.22683182
C	-7.89539615	1.24229648	-0.04235650
H	-8.68177921	-0.65742921	-0.70084735
H	-6.79876542	3.00361807	0.57497738
H	-8.87357543	1.69336904	0.09406438
O	-4.10951384	-1.78406665	-0.94732638
O	-4.34486101	3.34880004	0.74461758

B:

0 1 (charge, spin multiplicity)

C	2.25188937	-3.78444887	0.33742976
C	3.29952156	-2.86148364	0.24730818
C	0.60921079	-1.97563239	0.16287095
C	0.94259165	-3.35514162	0.30014409
C	5.08343228	1.71459321	-0.10384820
H	6.08296058	1.29907323	-0.03532219
C	4.87602826	3.08645807	-0.21319165
C	3.57119985	3.58669460	-0.30290052
C	2.48252583	2.71826140	-0.28357597
H	2.46655898	-4.84422290	0.44181266
H	4.33534358	-3.17712021	0.28426617
H	0.12512407	-4.05896156	0.37154329

H	5.72310497	3.76572873	-0.22923356
H	3.40402689	4.65637555	-0.38801934
H	1.47108778	3.09980111	-0.35523618
O	0.39008195	1.01297606	-0.31790175
O	5.36328947	-1.07603756	0.08159172
C	-2.98188107	-1.36760757	0.16012271
H	-3.39740713	-1.24327951	1.16882108
C	-1.86132218	-2.40122229	0.17045495
O	-1.97062490	-3.62150450	0.11273296
N	-0.71397565	-1.62062177	0.18446131
Pd	-1.57890966	0.12615329	-0.13179835
O	-2.73150847	1.93624276	-0.44892476
C	-3.20731471	2.56172936	0.50595832
O	-3.07860429	2.15468780	1.76144638
C	-3.98522151	3.83159640	0.34694311
H	-3.98722826	4.13902962	-0.69831498
H	-5.01323775	3.67169363	0.68905557
H	-3.54746692	4.61561841	0.97207003
C	-4.07657782	-1.61027020	-0.87295570
H	-4.50500828	-2.60698981	-0.68422686
H	-3.63619280	-1.65688564	-1.87793416
C	-5.19937519	-0.56883635	-0.84849253
H	-4.82152644	0.42589345	-1.10677057
H	-5.98803153	-0.82809449	-1.56413887
H	-5.65795336	-0.50766030	0.14656856
C	4.22197190	-0.61686381	0.03619571
C	1.48928768	0.43235450	-0.15092382
C	2.68032639	1.33341257	-0.16926109
C	3.99179209	0.83786318	-0.07957206
C	3.02510487	-1.50910406	0.10780579
C	1.67973523	-1.01397033	0.04462010
H	-2.56510268	1.31009230	1.75420502

C:

0 1 (charge, spin multiplicity)

N	-0.44553011	1.71646669	-0.69950829
C	-1.54534241	2.47623258	-1.02289056
O	-1.62864659	3.66038897	-1.31613181
C	-2.72618633	1.52548199	-0.93839412

H	-2.95852232	1.04475452	-1.89055345
H	-4.23396818	2.90594865	-0.56696236
C	-3.91653835	1.94717752	-0.12354145
H	-3.60280572	2.17479714	0.89961764
Pd	-1.40424062	0.05853767	-0.14419253
O	-2.74925364	-1.47641284	0.48436515
O	-1.63612755	-3.41340059	0.13076644
H	-1.06743712	-2.91855317	-0.59190734
C	-5.08342028	0.95701856	-0.14195434
H	-4.79836470	0.00809304	0.32106074
H	-5.93546878	1.36671624	0.41026249
H	-5.41276321	0.75210871	-1.16747534
C	0.84580022	2.11833442	-0.38151458
C	1.90871940	1.20854716	-0.06726888
C	1.13475692	3.50638123	-0.43661159
C	1.74084469	-0.24673792	0.12991723
C	3.21860143	1.74480451	0.11817148
C	2.41157640	3.98959131	-0.21095145
H	0.32909718	4.18407719	-0.67874643
C	2.94362120	-1.12110115	0.14759090
C	4.41632699	0.87950286	0.36399282
C	3.46077264	3.11190219	0.05814176
H	2.59007819	5.05979053	-0.25441691
C	2.77659676	-2.51081243	0.06042917
C	4.23545588	-0.58573680	0.28289361
H	4.47158034	3.46716546	0.21898195
C	3.88853258	-3.34982675	0.10121431
H	1.77829219	-2.91572902	-0.05463946
C	5.34569920	-1.43456901	0.34356790
C	5.17354482	-2.81384553	0.24863037
H	3.75469873	-4.42427419	0.01988501
H	6.33086970	-0.99617939	0.46015560
H	6.03628720	-3.47199167	0.28690764
O	0.64772976	-0.81681257	0.31351377
O	5.51878752	1.37497466	0.58532647
O	-1.53849338	1.35045275	3.80263712
C	-1.39283559	0.56769635	2.86873816
O	-1.63845382	1.00289005	1.64221169
C	-0.99281226	-0.87468376	3.11047738

H	-0.49617080	-0.94477857	4.08049866
H	-1.89968084	-1.48805465	3.14918874
H	-0.33974545	-1.27015746	2.33104024
C	-0.69925699	-1.60298146	-2.55206409
O	-1.28547066	-0.53164250	-2.13536830
O	-0.36684001	-2.58095933	-1.85048351
C	-0.39479980	-1.60312674	-4.03842788
H	0.49396043	-0.98677078	-4.21677802
H	-0.19786574	-2.61990417	-4.38246016
H	-1.22256758	-1.16410443	-4.60076981
C	-3.62307490	-3.49545548	1.41003943
H	-4.14944322	-4.17879501	0.73511707
H	-3.11018755	-4.10483052	2.16045067
H	-4.33734811	-2.82675524	1.88976081
C	-2.60901527	-2.71319392	0.62256449

D:

0 1 (charge, spin multiplicity)

C	1.70088590	-3.76092318	-1.24236990
C	2.92030873	-3.08056510	-1.30829433
C	0.62732952	-1.81736519	-0.23461160
C	0.58096423	-3.14863568	-0.69749964
C	5.73054187	0.77661378	-0.00386895
H	6.59778903	0.25279142	-0.39087442
C	5.85756320	2.00365140	0.64579926
C	4.72096884	2.66484947	1.12541131
C	3.45759950	2.10445687	0.94952854
H	1.62790852	-4.77943342	-1.61173616
H	3.81082704	-3.55408616	-1.70535488
H	-0.35479021	-3.68597202	-0.62581647
H	6.83984211	2.44703603	0.77750938
H	4.82041106	3.61988286	1.63185046
H	2.57099503	2.61610804	1.30607007
O	1.00519707	1.06729745	0.23317885
O	5.32289108	-1.66280573	-1.36236890
C	-2.29468658	-1.20766046	2.12829335
H	-2.20351123	-1.60801126	3.14045344
C	-1.15257047	-1.89140746	1.35595810
O	-0.86247350	-3.03857242	1.71439251
N	-0.50559695	-1.22798780	0.34778131

Pd	-0.89701494	0.59341875	-0.40340587
O	-2.18615415	0.23400973	2.20994240
C	-1.26105050	0.73060481	3.06815310
O	-0.50551913	0.03171645	3.71323691
C	-1.29805671	2.23816428	3.09390429
H	-2.32357351	2.59641754	3.22237952
H	-0.66688710	2.60556436	3.90410501
H	-0.92684940	2.62841883	2.13948196
C	-3.69341977	-1.50697201	1.57166528
H	-3.76823614	-1.08942007	0.56365399
H	-4.40321119	-0.95765354	2.20246072
C	-4.05389574	-2.99640113	1.57110108
H	-3.99550847	-3.42247771	2.57945996
H	-5.07843679	-3.13149336	1.20806965
H	-3.38681110	-3.57708681	0.92708590
C	4.34719050	-1.11722973	-0.85320116
C	1.98362618	0.28988762	0.07945471
C	3.32462932	0.86204785	0.31256125
C	4.47023968	0.19447338	-0.16503546
C	3.00648521	-1.77129650	-0.84851744
C	1.85587658	-1.10538301	-0.34381596
C	-2.12621289	3.21427090	-1.39422652
C	-2.76907931	-0.62928013	-2.26246147
O	-3.31085600	2.65604413	-1.44841554
O	-1.07944295	2.60138686	-1.11093856
O	-2.75245977	0.12351531	-1.16551515
O	-1.76841125	-1.06839316	-2.81225341
C	-4.17702103	-0.90533672	-2.76394557
H	-4.73831249	-1.46504914	-2.00803610
H	-4.71309786	0.03346187	-2.93883045
H	-4.13776773	-1.48182654	-3.68965722
C	-2.10660827	4.68023546	-1.71285103
H	-2.85408839	5.19927384	-1.10549160
H	-1.11565810	5.09488896	-1.52972956
H	-2.37875248	4.82270939	-2.76430510
H	-3.23223378	1.65622303	-1.30740762

2ea:

0 1 (charge, spin multiplicity)

C	0.51675203	3.60896751	0.42916218
C	1.82354477	3.12234561	0.42573577
C	-0.34545435	1.39757032	-0.08926246
C	-0.55627217	2.76584337	0.17545463
C	5.06962067	-0.58928624	-0.05132207
H	5.87013131	0.11559313	0.14561046
C	5.33527446	-1.93634306	-0.28494134
C	4.28224570	-2.82354023	-0.53661001
C	2.96771471	-2.36296404	-0.55421246
H	0.32924542	4.65967582	0.62963300
H	2.66963037	3.77074489	0.62103741
H	-1.56869409	3.14171766	0.17731377
H	6.35935335	-2.29724922	-0.27167712
H	4.48855611	-3.87393363	-0.71909902
H	2.14248194	-3.03846547	-0.74926662
O	0.38357829	-1.37709666	-0.58760555
O	4.39682952	2.10683540	0.40198786
C	-3.61449000	-0.44465567	-0.69615803
H	-3.54586095	-0.52783364	-1.78703414
C	-2.76230254	0.77743240	-0.29187512
O	-3.28011518	1.85309736	-0.01945493
N	-1.41016254	0.53626564	-0.35801771
O	-2.99856273	-1.68828194	-0.26226741
C	-2.80992467	-1.87837599	1.07013968
O	-3.10916078	-1.05550087	1.91028226
C	-2.15151866	-3.20786142	1.32957132
H	-1.13032495	-3.18102147	0.93311820
H	-2.12342534	-3.40050307	2.40242392
H	-2.68754572	-4.01010689	0.81449816
C	-5.09012203	-0.33533620	-0.29703646
H	-5.16739943	0.03822297	0.72656500
H	-5.49572185	-1.35381591	-0.30737948
C	-5.90234085	0.54604678	-1.25369417
H	-5.85529763	0.16517409	-2.28128336
H	-6.95508321	0.56107250	-0.95182709
H	-5.53262333	1.57470196	-1.25128837
C	3.48108252	1.31628896	0.18440141
C	1.27654359	-0.54783347	-0.34883099
C	2.69154406	-1.00988610	-0.31937683

C	3.75130525	-0.12009162	-0.06669905
C	2.05842882	1.77462550	0.16827991
C	0.98593136	0.88173136	-0.09256278
H	-1.11221309	-0.41832625	-0.56973729

TS (A-B') :

0 1 (charge, spin multiplicity)

N	-0.98796076	-1.47978940	-0.76505799
C	0.25692245	-1.92050674	-0.33780472
O	1.04830810	-1.26141596	0.33378639
C	0.55817744	-3.35292215	-0.73975999
H	1.64471534	-3.42443580	-0.87956876
H	0.31507355	-3.99929005	0.11415844
C	-0.17340779	-3.84875341	-1.99512889
H	-1.30962324	-4.63814746	-2.05135205
H	0.16965182	-4.89022755	-2.09628786
Pd	-2.20091187	-2.93042148	-1.47088020
O	-3.63565814	-4.29169514	-2.14604066
C	-3.21754325	-5.45131202	-2.45442881
C	-4.22079717	-6.48120292	-2.91737929
O	-1.99248755	-5.77275524	-2.39944489
C	0.21829420	-3.14613037	-3.30097602
H	1.28796546	-3.29686497	-3.50509796
H	-0.34240580	-3.55908997	-4.14671846
H	0.03339729	-2.06855336	-3.27013783
H	-4.02361578	-6.72499811	-3.96680925
H	-4.09604235	-7.40011885	-2.33711753
H	-5.24118943	-6.11034323	-2.81547414
C	-1.36386718	-0.14957018	-0.68206613
C	-2.72231632	0.28797691	-0.52457301
C	-0.35967833	0.85595224	-0.78064817
C	-3.85926127	-0.61868526	-0.52122150
C	-2.98696591	1.68791061	-0.37211177
C	-0.65493595	2.19978968	-0.68023182
H	0.66181569	0.54545158	-0.94135046
C	-5.19556631	-0.14085282	-0.09053736
C	-4.35738801	2.21517483	-0.10004577
C	-1.96976225	2.62394098	-0.45260404
H	0.14262769	2.93020626	-0.77984841

C	-6.23606971	-1.06356520	0.09568034
C	-5.44438816	1.23010820	0.10150516
H	-2.21689021	3.67364130	-0.34640313
C	-7.50048482	-0.62274591	0.47984022
H	-6.04250541	-2.11865836	-0.05817013
C	-6.72064991	1.66601079	0.47267770
C	-7.74563476	0.74291415	0.66686632
H	-8.29771125	-1.34396759	0.63196886
H	-6.88753247	2.72950289	0.60504935
H	-8.73374288	1.08296087	0.96183166
O	-3.81884805	-1.82103355	-0.89482764
O	-4.57013853	3.42336471	-0.01274390

B' :

0 1 (charge, spin multiplicity)

N	0.85289178	1.67296611	-0.28081951
C	1.67043512	2.65766811	-0.82253422
O	1.31938892	3.80077310	-1.11760861
C	3.08131204	2.15367265	-1.09406635
H	3.13185160	1.89497916	-2.16196666
H	3.77827310	2.99160609	-0.95096614
C	3.45132169	0.93454152	-0.24519228
H	3.62869817	1.24742475	0.79243624
Pd	1.71745449	-0.14735689	-0.18790331
O	2.63978251	-2.10449905	-0.04624911
C	2.92331780	-2.59101021	1.05452569
C	3.48377803	-3.97007319	1.22071865
O	2.76181895	-1.92975502	2.19299321
H	2.39523484	-1.03712688	1.97833226
C	4.65770458	0.17495060	-0.78005272
H	5.52347629	0.85068658	-0.86824776
H	4.95338559	-0.64825672	-0.12219192
H	4.46718982	-0.23964181	-1.77754521
H	2.82702698	-4.55661828	1.87091823
H	3.57841105	-4.45401071	0.24922242
H	4.46268479	-3.91079377	1.70734884
C	-0.42989998	1.94421416	0.17719639
C	-1.50339553	0.98570914	0.18100476
C	-0.70719554	3.24062962	0.69703571
C	-1.35332889	-0.42559923	-0.19444839

C	-2.80369068	1.41592566	0.60306959
C	-1.96097750	3.60526341	1.14486826
H	0.10135599	3.95490038	0.73898504
C	-2.56607841	-1.24735979	-0.46143402
C	-4.00477659	0.52964641	0.53739483
C	-3.02384082	2.69999645	1.07947974
H	-2.11641845	4.60164200	1.54870880
C	-2.42376312	-2.51215069	-1.05083838
C	-3.84580861	-0.79916495	-0.09418737
H	-4.02253795	2.97183496	1.40035709
C	-3.54409084	-3.30752491	-1.28123575
H	-1.43368597	-2.85705106	-1.32594658
C	-4.96572022	-1.61035239	-0.31086588
C	-4.81750960	-2.85926456	-0.90848874
H	-3.42635293	-4.28040413	-1.74917527
H	-5.93970664	-1.24301815	-0.00598465
H	-5.68768576	-3.48475736	-1.08381127
O	-0.25976484	-1.02679983	-0.28101469
O	-5.09886397	0.90377482	0.95901902

C' :

0 1 (charge, spin multiplicity)

N	-0.47715182	-1.70663290	-0.67592313
C	-1.28722531	-2.53470513	-1.43600950
O	-0.86685219	-3.41192698	-2.18301219
C	-2.77333860	-2.24163994	-1.25670860
H	-3.13232485	-1.63592677	-2.09479508
H	-3.30947468	-3.19992872	-1.29997450
C	-3.04892769	-1.57087992	0.07163856
H	-2.71997274	-2.17956594	0.91432138
Pd	-1.45470231	-0.17569132	0.16197181
O	-2.57558725	1.46011835	0.96040570
O	-0.98330364	2.73558883	1.92986433
H	-0.50316108	1.84745330	2.12983320
C	-4.39324335	-0.94061946	0.29160524
H	-5.14202976	-1.74811034	0.23510834
H	-4.46913825	-0.49068026	1.28492353
H	-4.61925705	-0.19216706	-0.46862607
C	0.86082648	-1.99318628	-0.38736363

C	1.89423054	-1.01356099	-0.26423832
C	1.20990648	-3.35539102	-0.21967650
C	1.65231101	0.44445976	-0.26556656
C	3.23666614	-1.45828069	-0.08785654
C	2.51728210	-3.75619454	-0.00324223
H	0.42579465	-4.09799899	-0.27772557
C	2.79739815	1.36719155	-0.48565330
C	4.39535885	-0.51170818	-0.08008934
C	3.54001799	-2.80904210	0.04583814
H	2.73989841	-4.81087066	0.12726102
C	2.54807476	2.72071408	-0.75058151
C	4.12353503	0.91340295	-0.37869662
H	4.57461020	-3.09727632	0.19023416
C	3.61099884	3.60437826	-0.92653834
H	1.52240574	3.06508703	-0.81825195
C	5.18595789	1.81019528	-0.53572283
C	4.93115850	3.15059915	-0.81706610
H	3.41221546	4.64915735	-1.14536086
H	6.20003491	1.43872699	-0.43548699
H	5.75665010	3.84364037	-0.94844688
O	0.54272308	0.96012370	-0.05459236
O	5.53890901	-0.91288431	0.12430897
O	-3.77256192	1.35050992	-1.81905657
C	-2.64670203	1.19947705	-2.28062556
O	-1.64329165	0.54090141	-1.74408293
C	-2.24502455	1.78819300	-3.63343596
H	-3.11638107	2.24175000	-4.11013544
H	-1.46896763	2.54796070	-3.49151645
H	-1.82934679	1.01038209	-4.28128804
C	-0.33592414	-0.50515280	2.89660179
O	-1.08795212	-1.04975077	1.99410524
O	0.12479692	0.65119980	2.87270681
C	-0.00993748	-1.43373134	4.05290941
H	0.68345775	-2.20798252	3.70639585
H	0.45171112	-0.87241700	4.86676667
H	-0.91572688	-1.93463212	4.40547962
C	-3.05149309	3.75873066	1.37787584
H	-3.77880351	3.66784855	0.57050839
H	-3.58756655	3.81873768	2.33240493

H	-2.45720141	4.66823434	1.26626181
C	-2.15792301	2.55104555	1.40221770

D' :

0 1 (charge, spin multiplicity)

N	-0.51218747	0.22356475	-1.34358519
C	-1.20145691	1.30214486	-1.85145006
O	-0.75376934	2.01739690	-2.75463814
C	-2.55228196	1.65436727	-1.23806318
H	-3.26558544	1.71757044	-2.06863355
H	-2.91726898	0.89642983	-0.54511688
C	-2.50815849	3.02713675	-0.56478320
H	-2.07181442	3.75892435	-1.24763177
Pd	-1.01673882	-0.81445761	0.29888290
O	-1.34803618	-1.84537501	2.14084765
O	-3.58992699	-2.07967586	2.02952322
H	-3.44833500	-1.76569858	1.07737723
C	-3.87071346	3.49991001	-0.07283271
H	-4.29548504	2.78715510	0.64269755
H	-3.78291507	4.47657483	0.41181892
H	-4.56203196	3.59645714	-0.91696856
C	0.72211283	-0.11925507	-1.90687546
C	1.89291354	-0.32273680	-1.12092954
C	0.82841188	-0.25378280	-3.30977227
C	1.87572546	-0.22942831	0.33640810
C	3.13269954	-0.58679797	-1.77143255
C	2.03257124	-0.56950042	-3.91753420
H	-0.06296651	-0.11403321	-3.90712925
C	3.14508986	-0.08141430	1.07767711
C	4.41250711	-0.67194411	-1.01021212
C	3.19346694	-0.72464698	-3.15184641
H	2.07357535	-0.69028216	-4.99586801
C	3.12720005	0.23520296	2.44416840
C	4.37488562	-0.31802405	0.43210909
H	4.14934136	-0.94457292	-3.61311599
C	4.32310945	0.33693408	3.15158452
H	2.17707010	0.40344366	2.93799065
C	5.56758470	-0.23449550	1.15610101
C	5.54387539	0.09993596	2.50915236

H	4.30451036	0.59655183	4.20551074
H	6.50179739	-0.43226919	0.64195039
H	6.47363601	0.17393816	3.06491466
O	0.82703948	-0.29245178	1.03165924
O	5.46653227	-0.97672838	-1.56317850
O	-1.02827582	5.07890249	0.45278733
C	-0.92263709	3.98559110	0.97421311
O	-1.60097708	2.88966913	0.57186878
C	-0.03567700	3.66610885	2.15398836
H	0.60451781	4.52109396	2.37476287
H	-0.65517100	3.44123653	3.02944006
H	0.57353346	2.78144378	1.94617827
C	-2.92826523	-2.30415328	-1.33393728
O	-2.87442763	-1.38047683	-0.37855317
O	-1.94800162	-2.83284664	-1.83887880
C	-4.35375899	-2.63795636	-1.74294988
H	-4.87107404	-1.73231239	-2.07571802
H	-4.34941423	-3.37704154	-2.54574946
H	-4.90934310	-3.03487394	-0.88612128
C	-2.50993400	-2.75284120	4.02926673
H	-1.52744290	-2.73332078	4.50017948
H	-3.22589868	-2.17770254	4.62450523
H	-2.87720836	-3.78325965	3.97687440
C	-2.43626807	-2.18246605	2.64342240

7d :

0 1 (charge, spin multiplicity)

N	-0.88120920	0.14496596	-0.69716229
C	-2.21830538	0.33580129	-0.96479725
O	-2.77342218	1.42845021	-1.02413452
C	-2.97480999	-0.96614317	-1.22622665
H	-2.94918050	-1.15057038	-2.30835920
H	-2.48045708	-1.81708430	-0.74492910
C	-4.43051322	-0.88394118	-0.78183563
H	-4.88666351	0.02325413	-1.18049534
H	-0.53603488	-0.81561128	-0.66506420
C	-5.24755292	-2.11117210	-1.16562846
H	-4.81519683	-3.02060723	-0.73442688
H	-6.27584511	-2.00695724	-0.80811199
H	-5.27298919	-2.22217670	-2.25500780

C	0.12438479	1.08787059	-0.47815547
C	1.45812409	0.63814438	-0.23692320
C	-0.14733647	2.47101661	-0.48946046
C	1.81212082	-0.80046686	-0.20946352
C	2.47077705	1.60869994	-0.01784264
C	0.86859973	3.39143595	-0.27134664
H	-1.16109208	2.79584340	-0.67143611
C	3.22710984	-1.18701344	0.04805910
C	3.89171610	1.22308786	0.24000506
C	2.17652043	2.96929937	-0.03570899
H	0.63480833	4.45190721	-0.28570121
C	3.56383759	-2.54643929	0.07456191
C	4.22682769	-0.22127853	0.26312679
H	2.97807442	3.67820552	0.13579024
C	4.87936826	-2.93833596	0.31182697
H	2.78429877	-3.28119371	-0.09246430
C	5.54653286	-0.62184745	0.50088093
C	5.87283694	-1.97554299	0.52516445
H	5.13286127	-3.99409700	0.33093999
H	6.30005793	0.14111557	0.66382200
H	6.89779364	-2.28307889	0.70981062
O	0.97474565	-1.69802895	-0.39317585
O	4.75446829	2.07856261	0.42692164
O	-6.31802704	0.43893920	0.66385954
C	-5.38706043	-0.06132996	1.26447162
O	-4.39269762	-0.75654442	0.67120227
C	-5.17803432	0.00534414	2.75792680
H	-6.00025065	0.55285806	3.21972731
H	-5.12373620	-1.00504159	3.17573224
H	-4.22938159	0.50430826	2.98111676

10. References

1. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J.

Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

2. Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

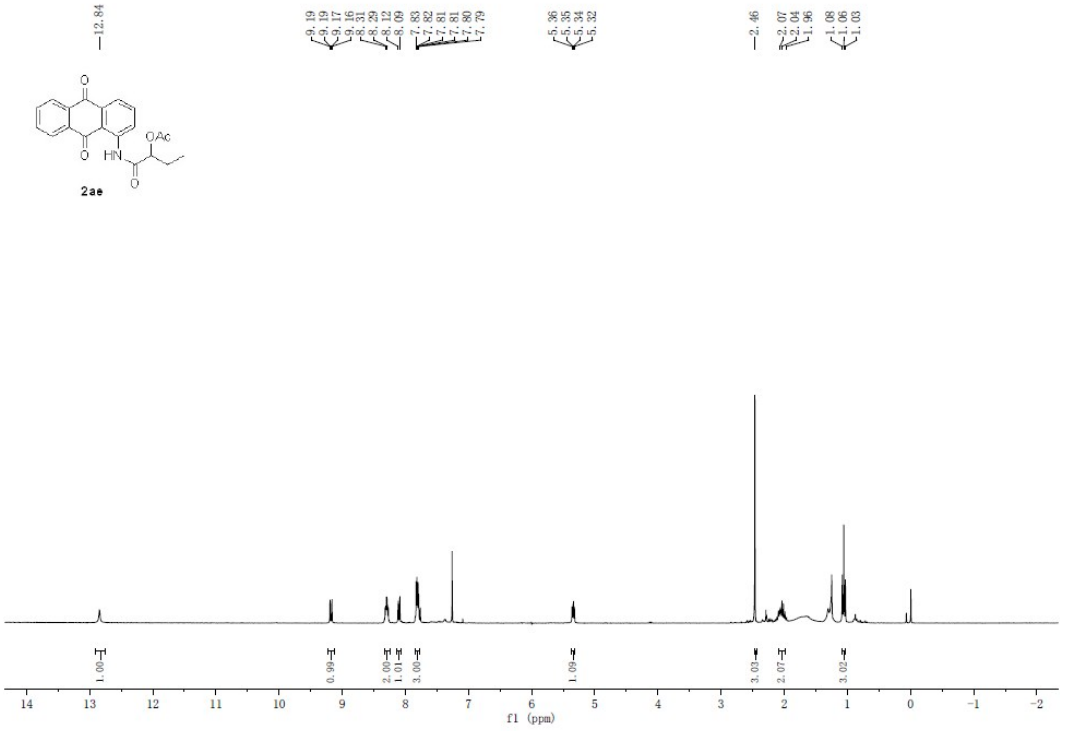
3. Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 299.

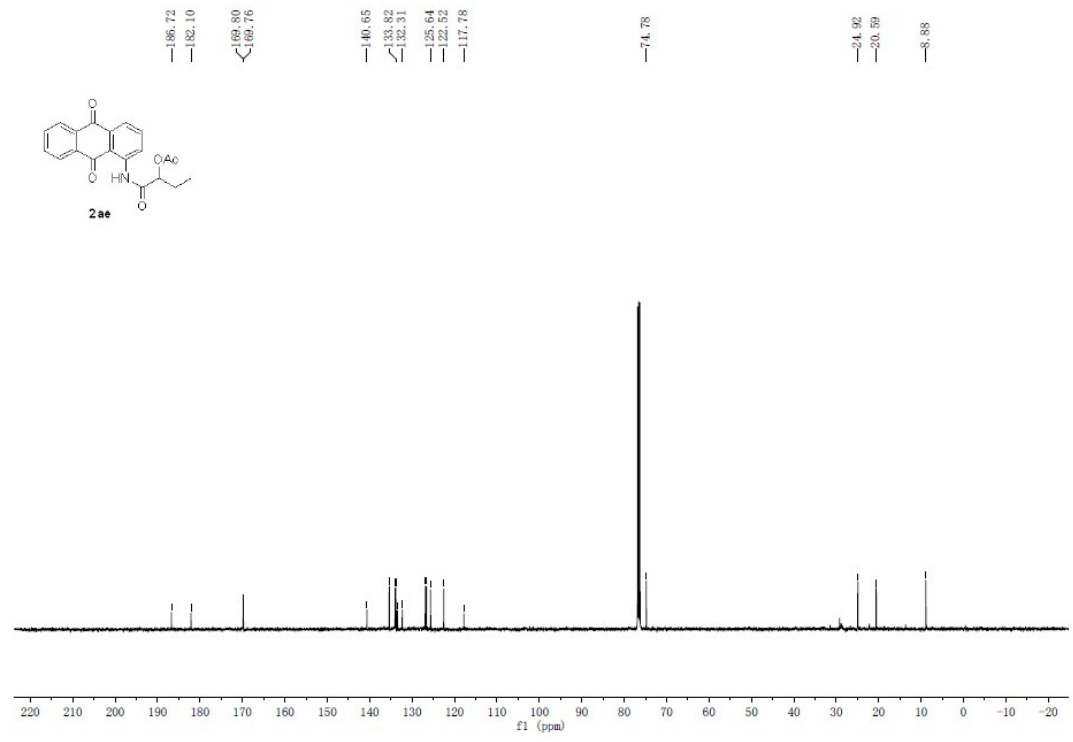
4. Hratchian, H. P.; Schlegel, H. B. in *Theory and Applications of Computational Chemistry:The First 40 Years*, Ed. Dykstra, C. E.; Frenking, G.; Kim, K. S.; Scuseria G., Elsevier:Amsterdam, **2005**, 195–249.

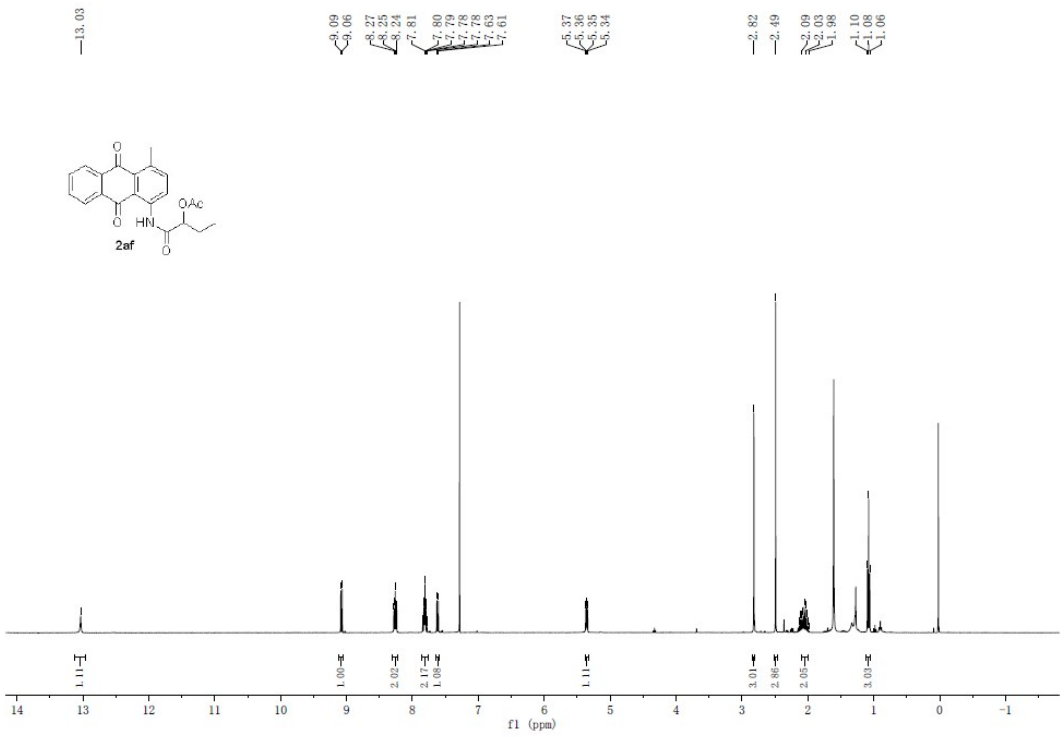
5. Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. J. *Comput. Chem.* **2003**, *24*, 669.

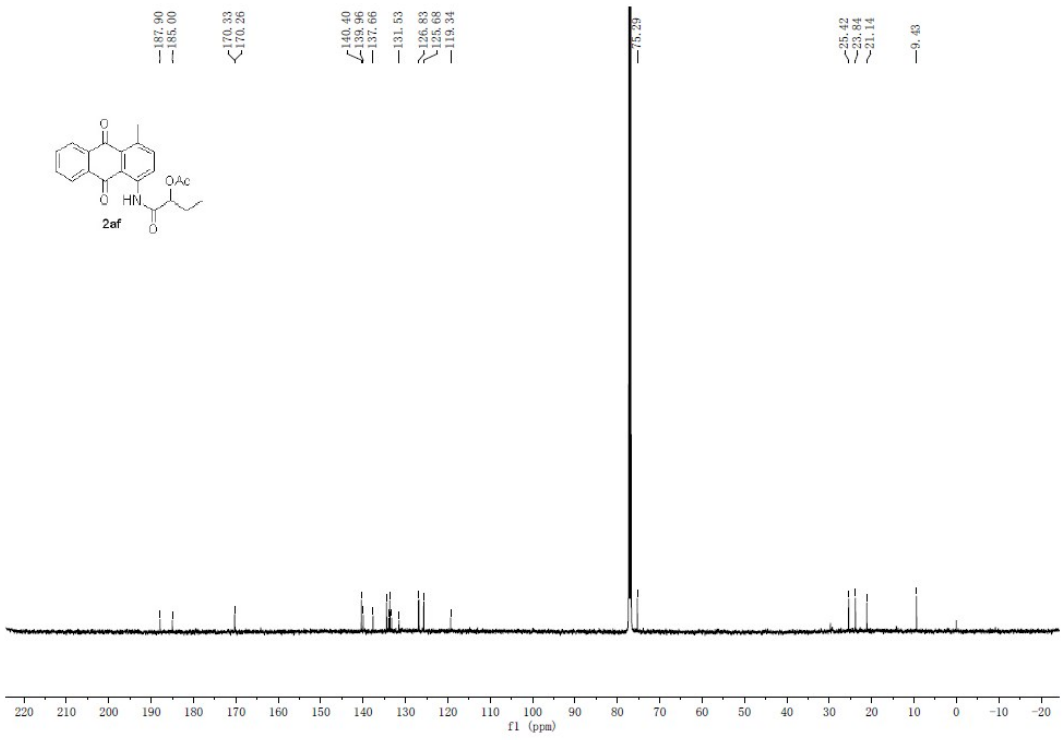
6. Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999.

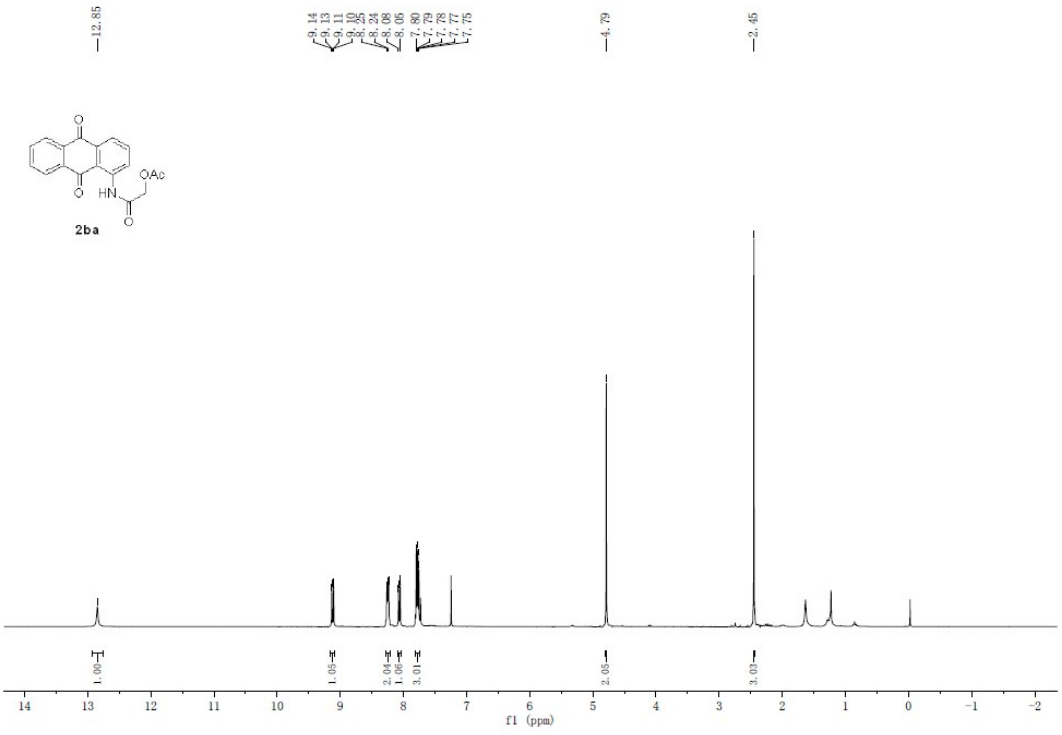
11. NMR Spectra of New Compounds

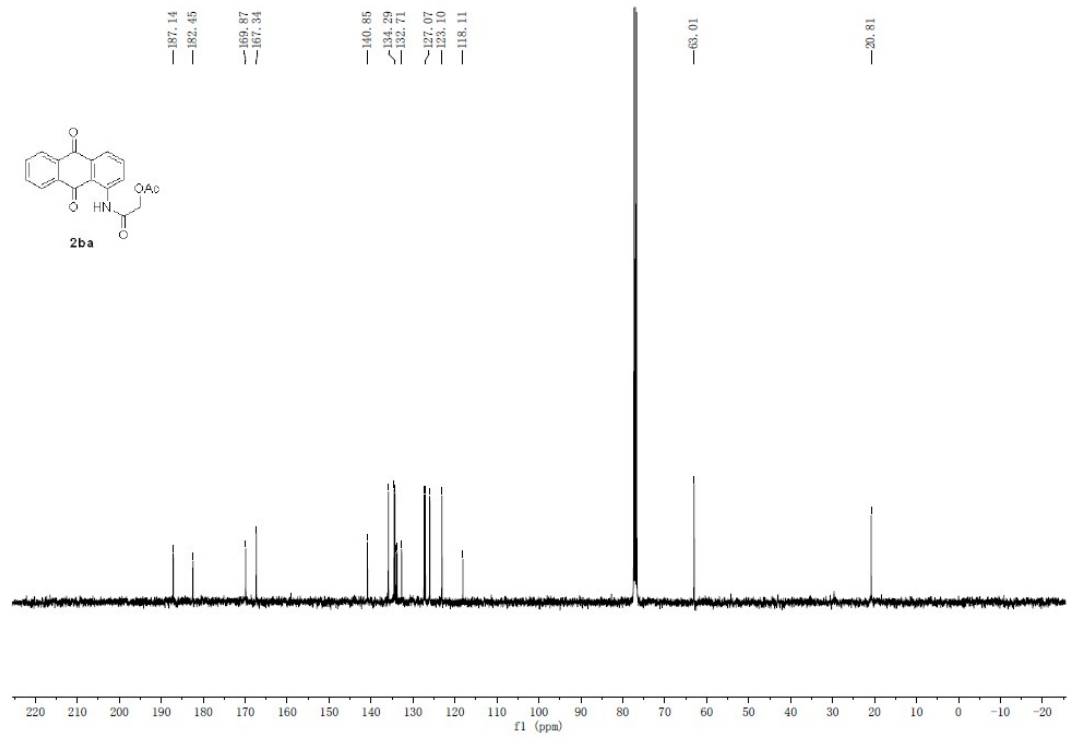


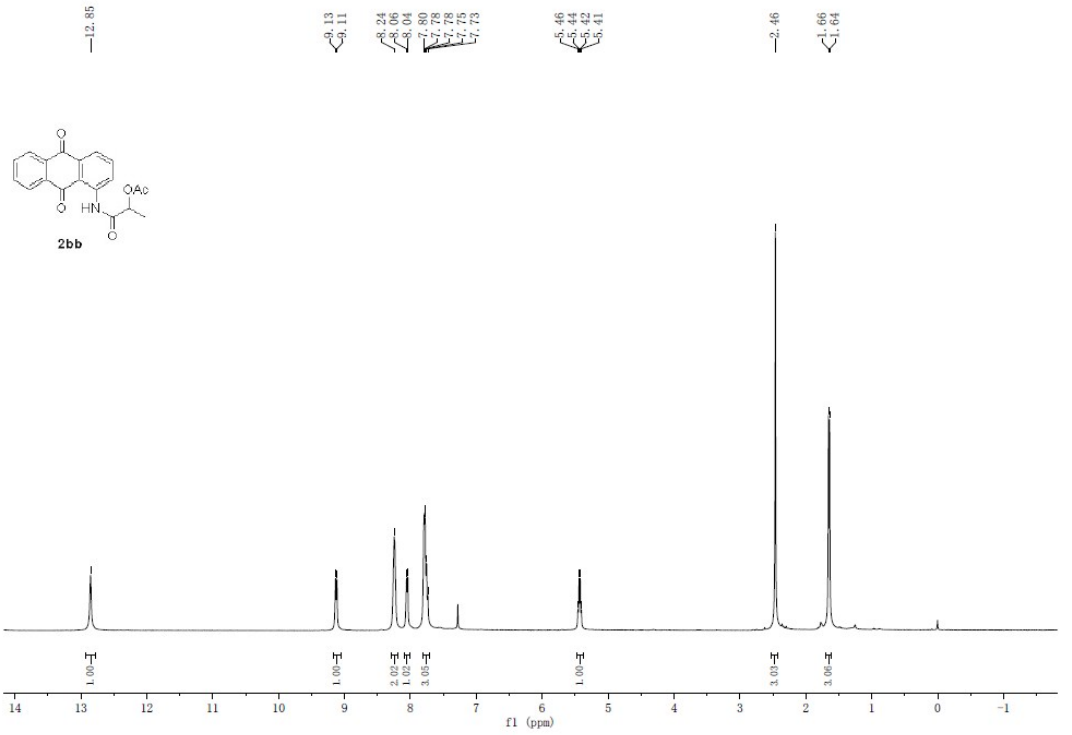


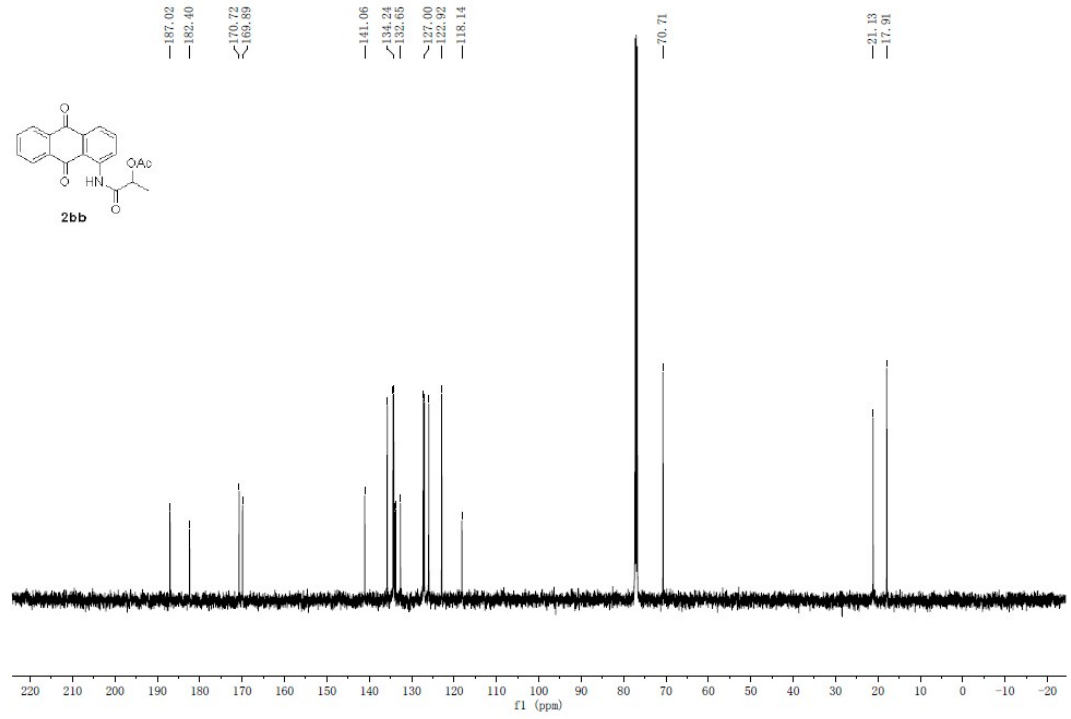

13.03
9.09
9.06
8.27
8.25
8.24
7.81
7.80
7.79
7.78
7.78
7.63
7.61
5.37
5.36
5.35
5.34
2.82
2.49
2.09
2.03
1.98
1.10
1.08
1.06
OAc
HN
O
2af
1.11
1.00
2.02
2.17
1.08
1.11
3.01
2.86
2.05
3.03
f1 (ppm)

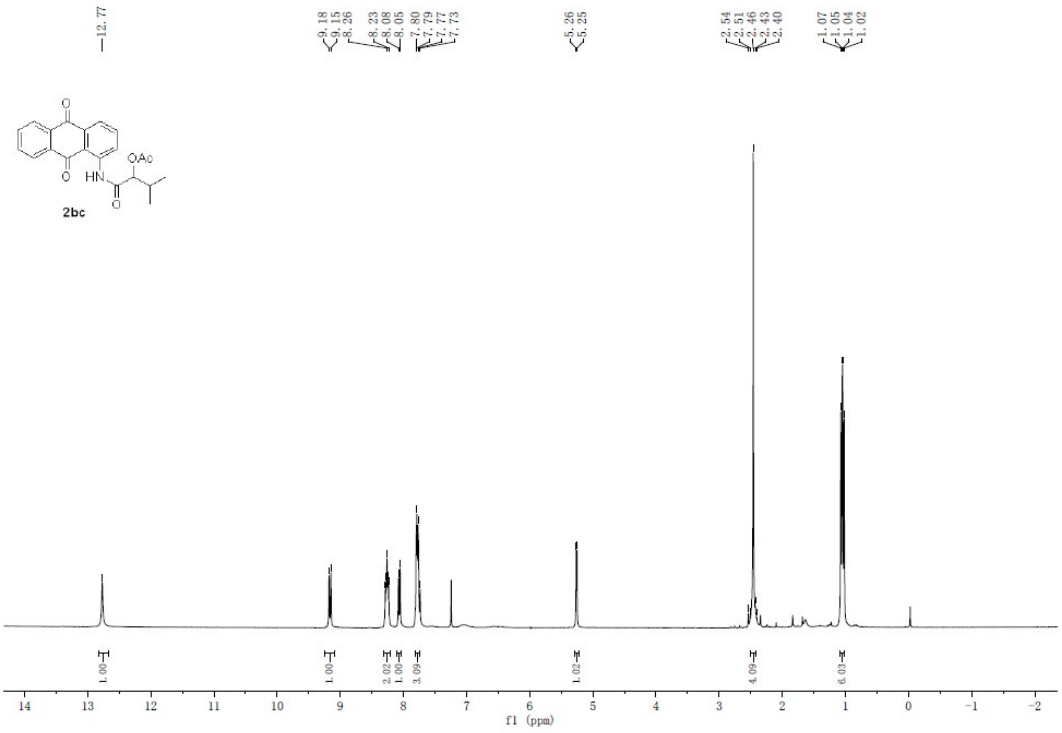

187.90
185.60
170.33
170.26
140.40
139.96
137.66
131.53
126.83
125.68
119.34
75.29
25.42
23.84
21.14
9.43
OAc
HN
O
2af
f1 (ppm)

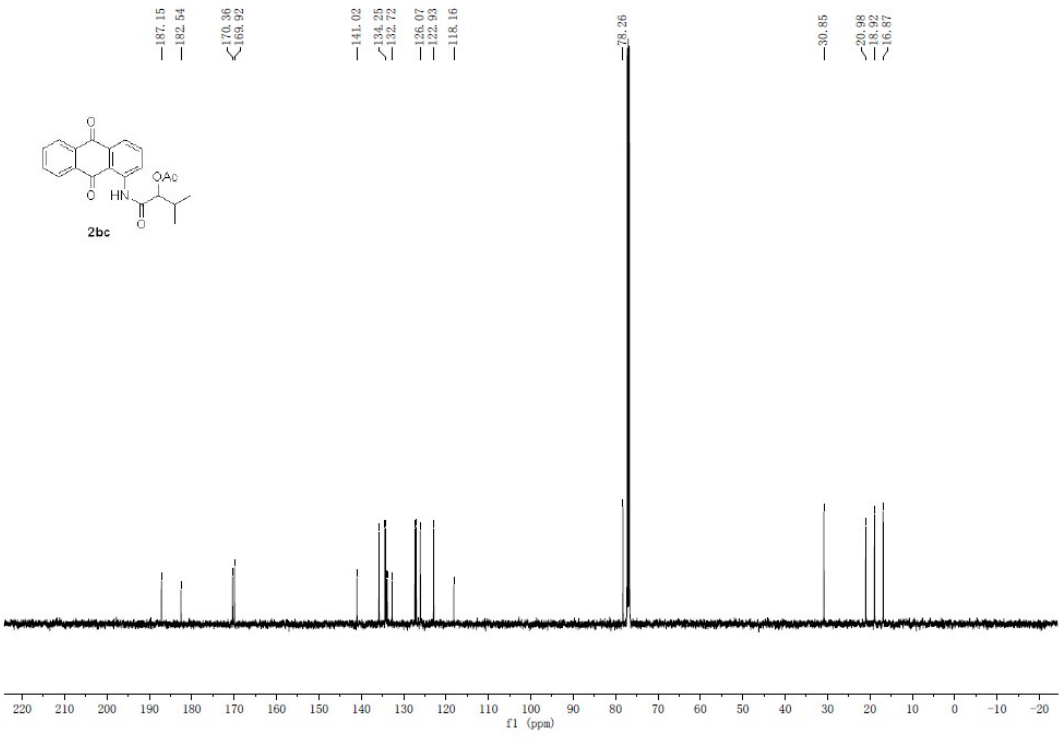

12.85
9.14
9.13
9.11
9.10
8.25
8.24
8.06
8.05
7.80
7.79
7.78
7.77
7.75
4.79
2.45
OAc
HN
O
2ba
1.00
1.05
2.04
1.06
3.01
2.05
3.03
f1 (ppm)

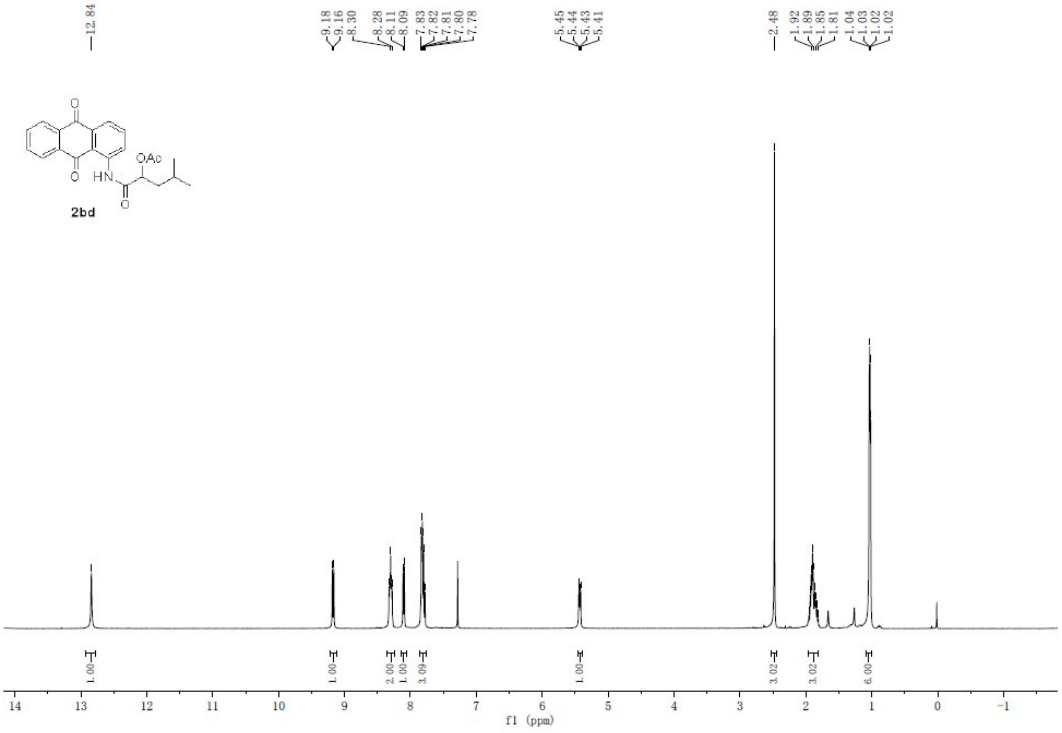

187.14
182.45
169.87
167.34
140.85
134.29
132.71
127.07
123.10
118.11
63.01
20.81
OAc
HN
O
2ba
f1 (ppm)

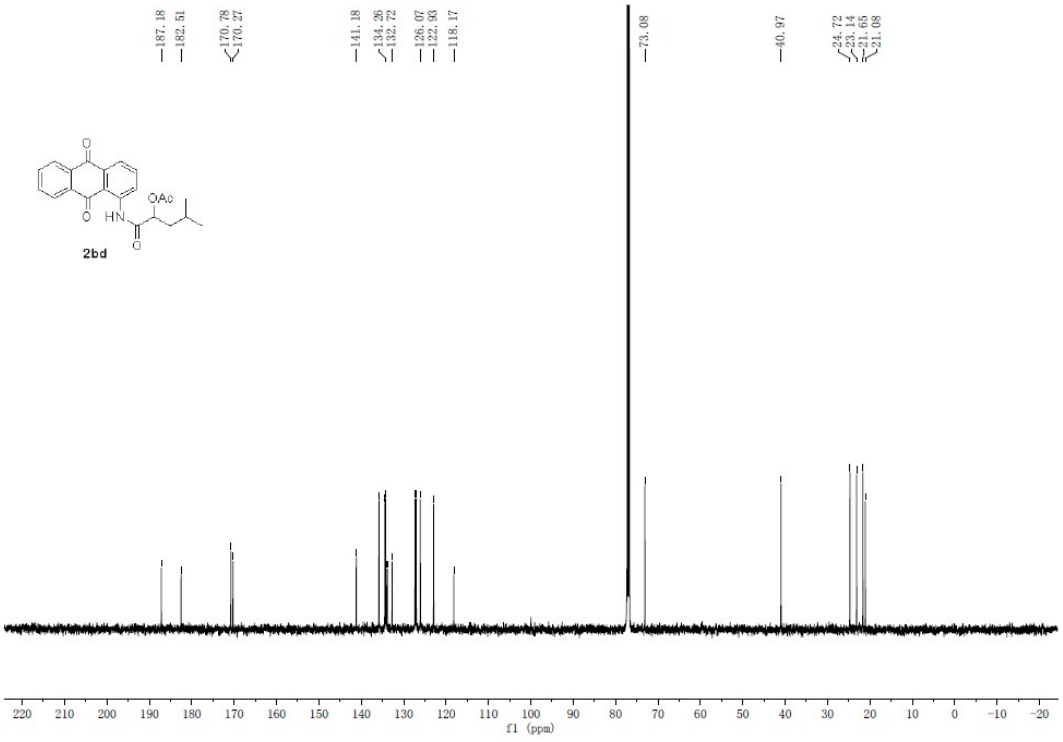

12.85
9.13
9.11
8.24
8.06
8.04
7.80
7.78
7.75
7.73
5.46
5.44
5.42
5.41
2.46
1.66
1.64
OAc
HN
O
2bb
1.00
1.00
2.02
1.02
3.05
1.00
3.03
3.06
f1 (ppm)

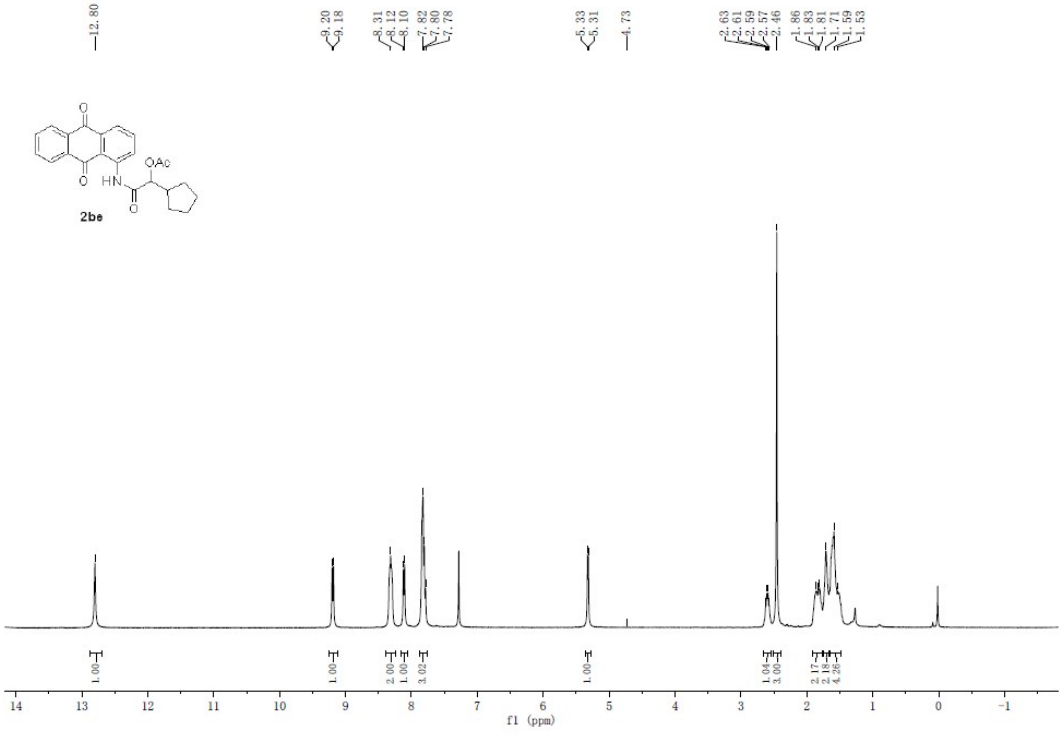

187.02
182.40
170.72
169.89
141.06
134.24
132.65
127.00
122.92
118.14
70.71
21.13
17.91
OAc
HN
O
2bb
f1 (ppm)

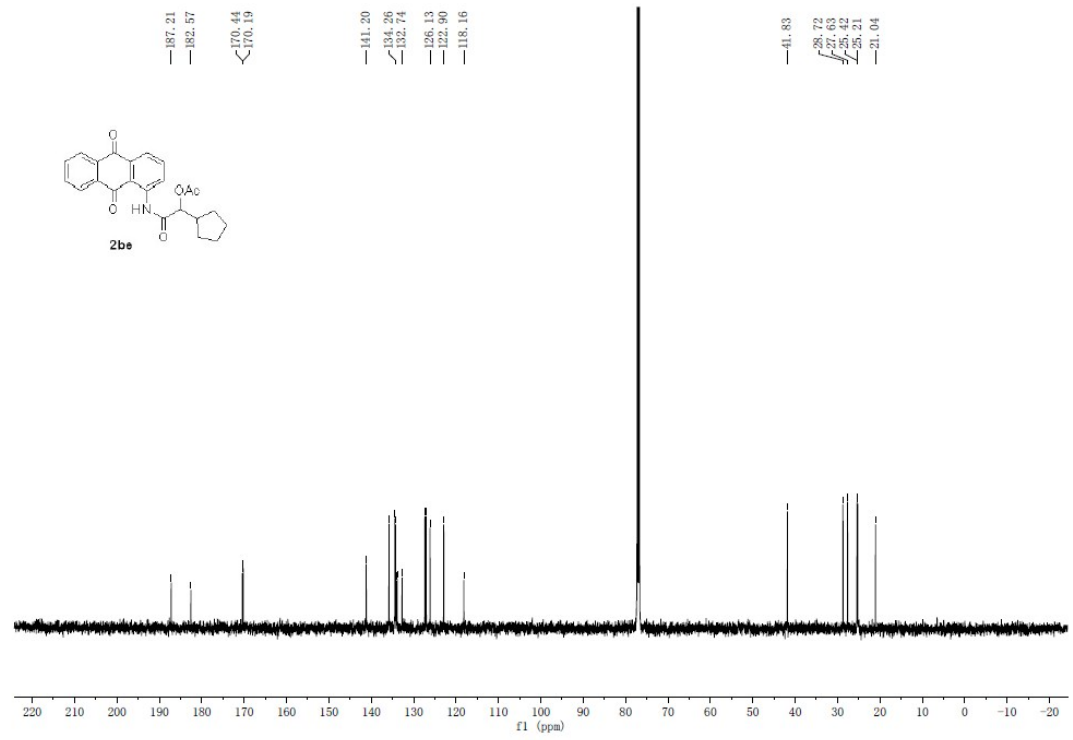

12.77
9.18
9.15
8.26
8.23
8.08
8.05
7.80
7.79
7.77
7.73
5.26
5.25
2.54
2.51
2.46
2.43
2.40
1.07
1.05
1.04
1.02
OAc
HN
O
2bc
1.00
1.00
2.02
1.00
3.09
1.02
4.09
6.03
f1 (ppm)

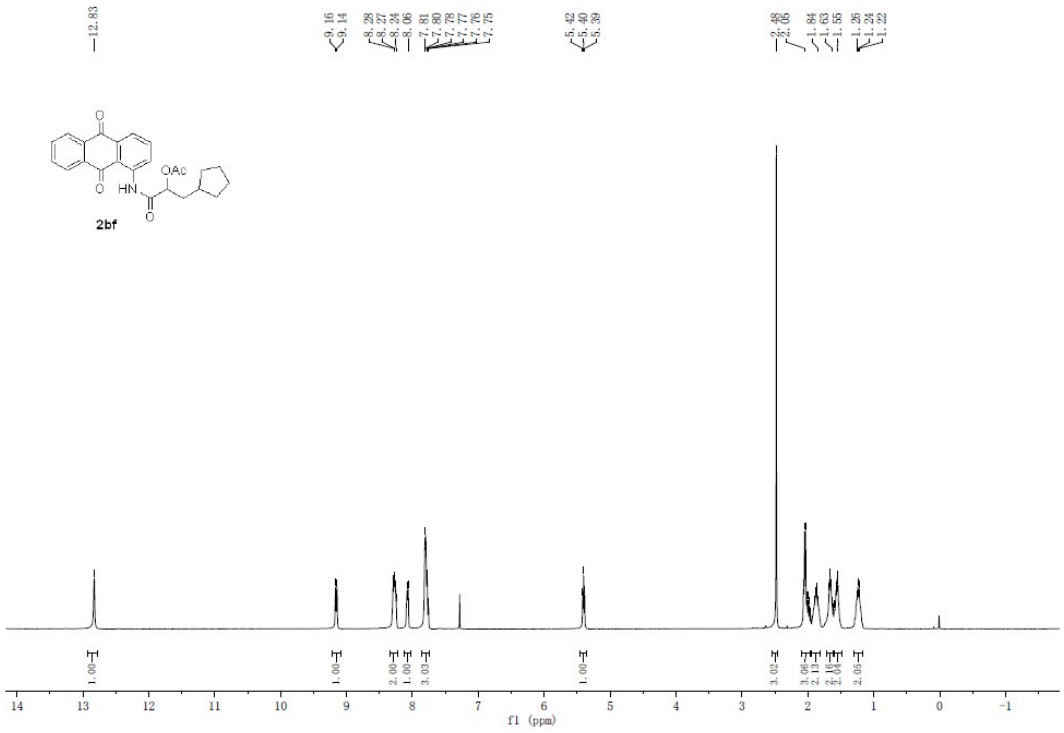

187.15
182.54
170.36
169.92
141.02
134.25
132.72
126.07
122.93
118.16
78.26
30.85
20.98
18.92
16.87
OAc
HN
O
2bc
f1 (ppm)

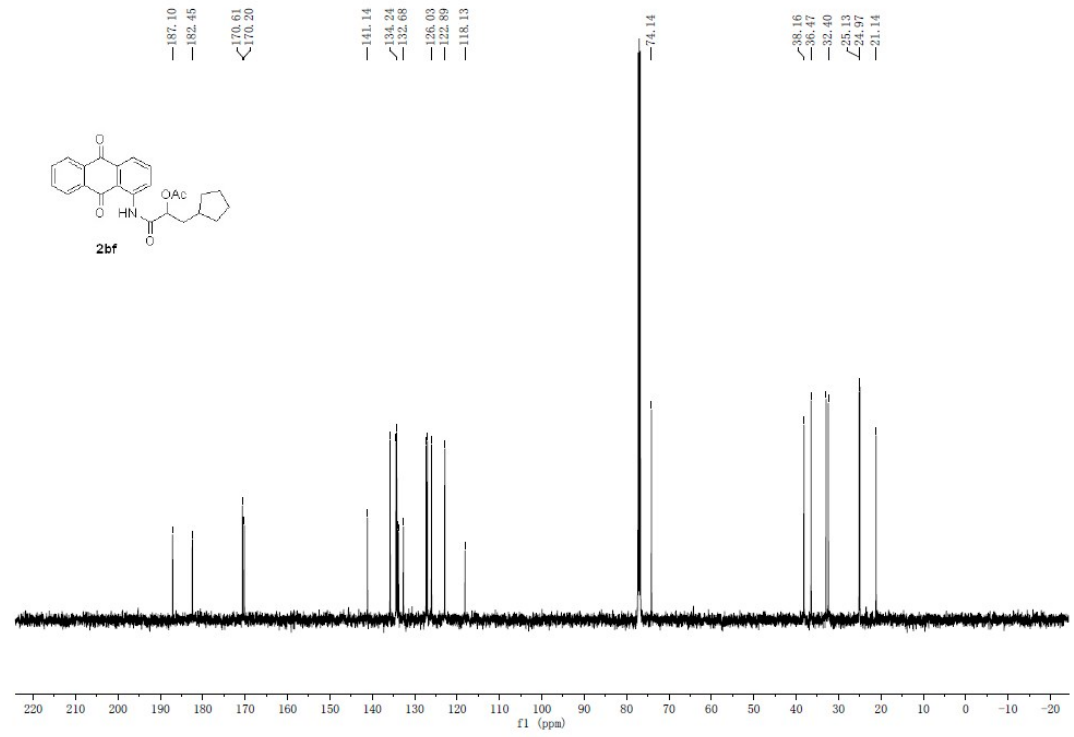

12.84
9.18
9.16
8.30
8.28
8.11
8.09
7.83
7.82
7.81
7.80
7.78
5.45
5.44
5.43
5.41
2.48
1.92
1.89
1.85
1.81
1.04
1.03
1.02
1.02
OAc
HN
O
2bd
1.00
1.00
2.00
1.00
3.09
1.00
3.02
3.02
6.00
f1 (ppm)

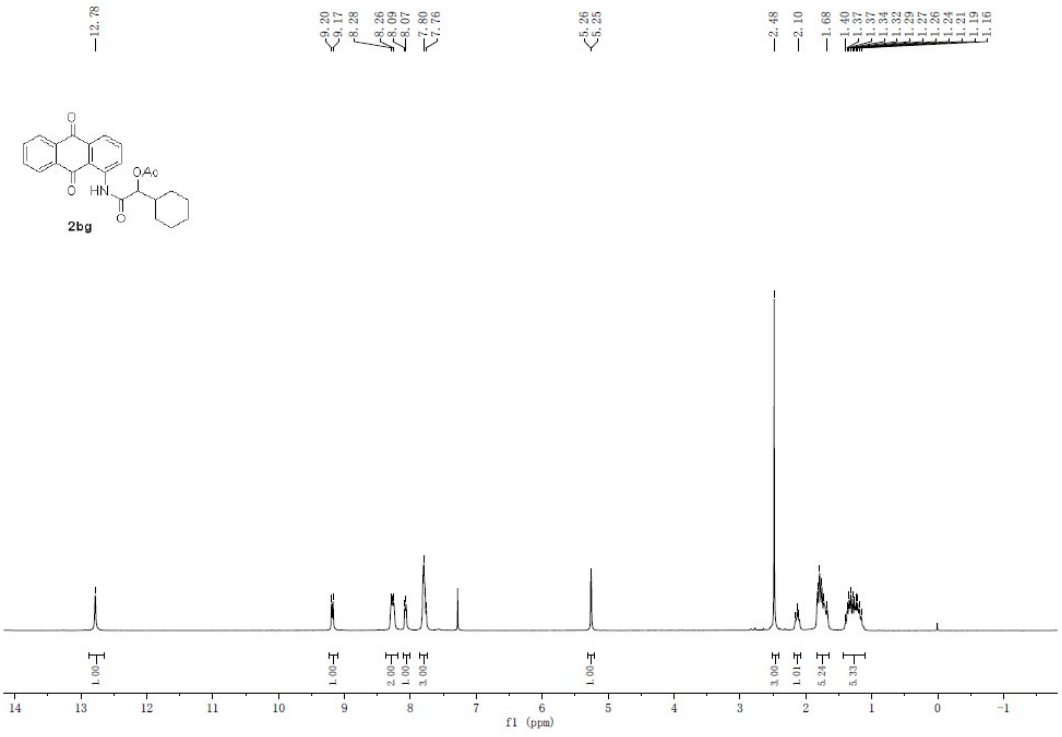

187.18
182.51
170.78
170.27
141.18
134.26
132.72
126.07
122.93
118.17
73.08
40.97
24.72
23.14
21.65
21.08
OAc
HN
O
2bd
f1 (ppm)

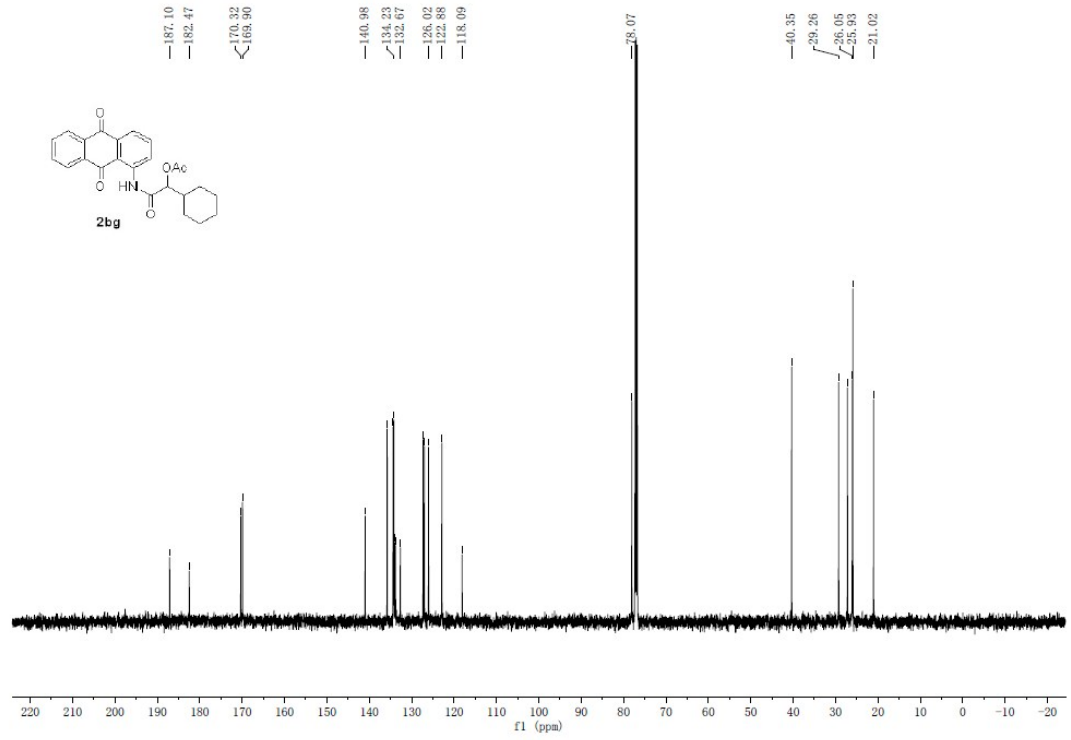

12.80
9.20
9.18
8.31
8.12
8.10
7.82
7.80
7.78
5.33
5.31
4.73
2.63
2.61
2.59
2.57
2.46
1.86
1.83
1.81
1.71
1.59
1.53
OAc
HN
O
2be
1.00
1.00
2.00
1.00
3.02
1.00
1.04
3.00
2.17
2.18
4.28
f1 (ppm)

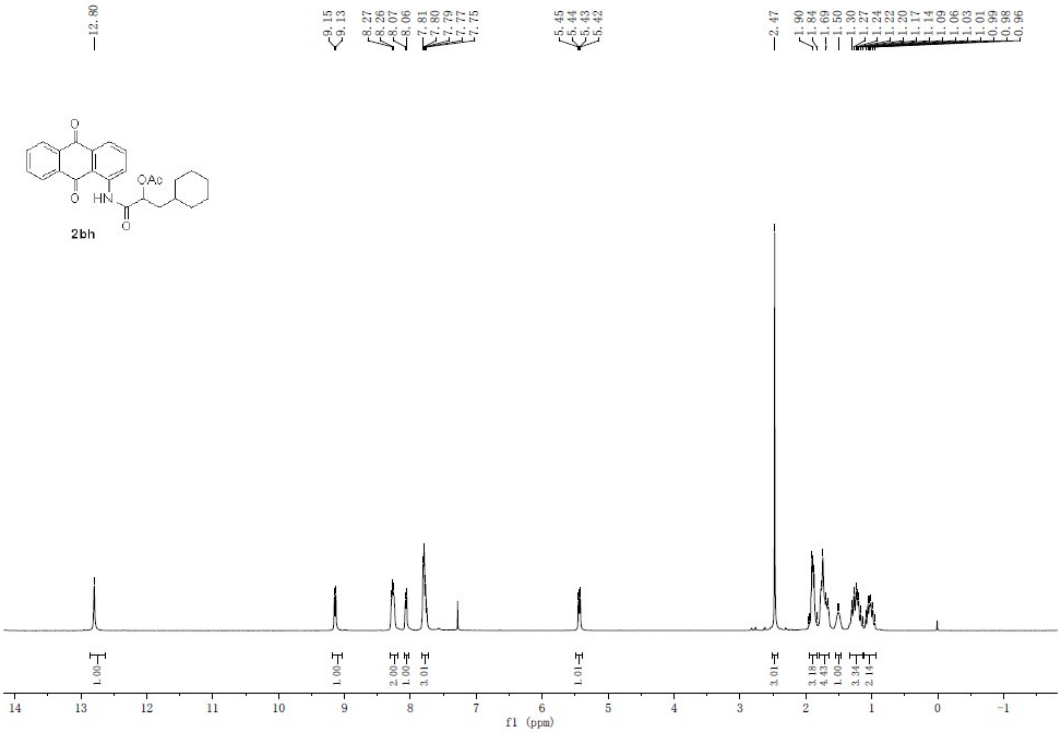

187.21
182.57
170.44
170.19
141.20
134.26
132.74
126.13
122.90
118.16
41.83
28.72
27.63
25.42
25.21
21.04
OAc
HN
O
2be
f1 (ppm)

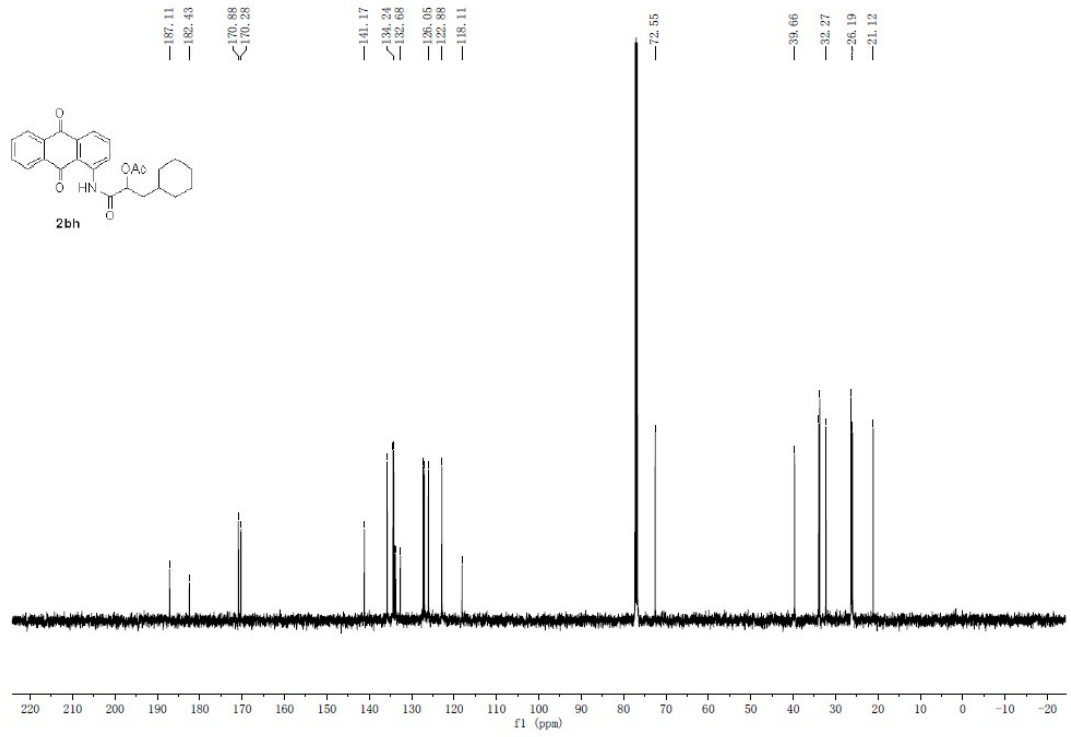

12.83
9.16
9.14
8.28
8.27
8.24
8.06
7.81
7.80
7.78
7.77
7.76
7.75
5.42
5.40
5.39
2.48
2.46
1.84
1.63
1.55
1.26
1.24
1.22
OAc
HN
O
2bf
1.00
1.00
2.00
1.00
3.03
1.00
3.02
3.06
2.19
2.14
2.05
f1 (ppm)

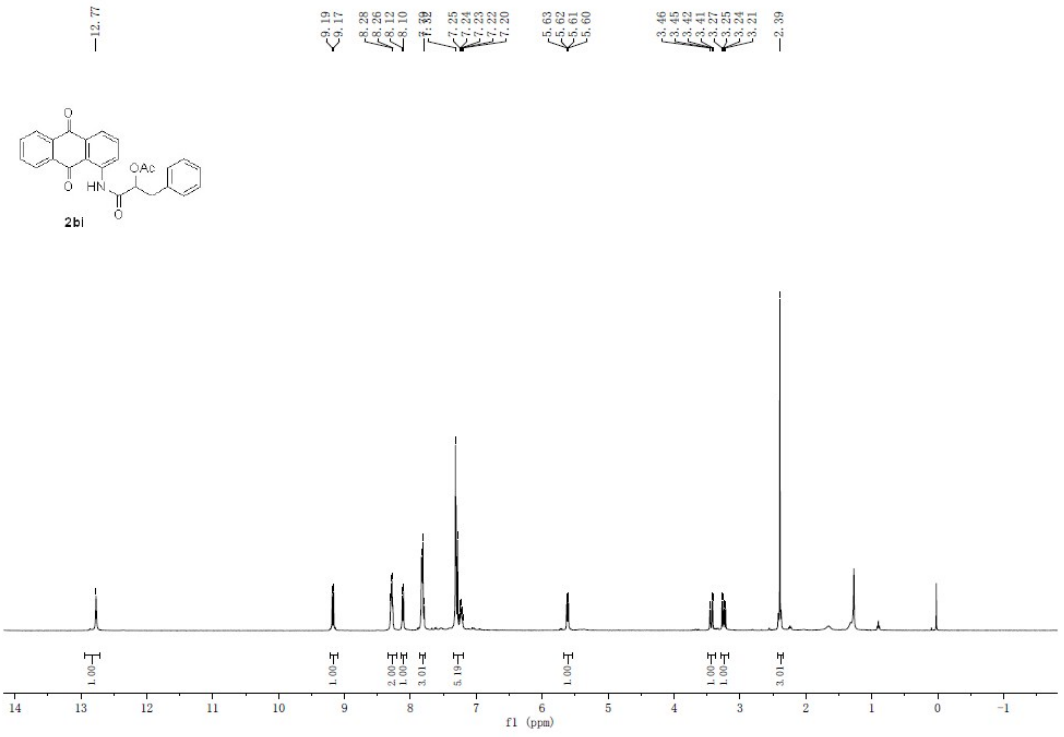

187.10
182.45
170.61
170.20
141.14
134.24
132.68
126.03
122.89
118.13
74.14
38.16
36.47
32.40
25.13
24.97
21.14
OAc
HN
O
2bf
f1 (ppm)

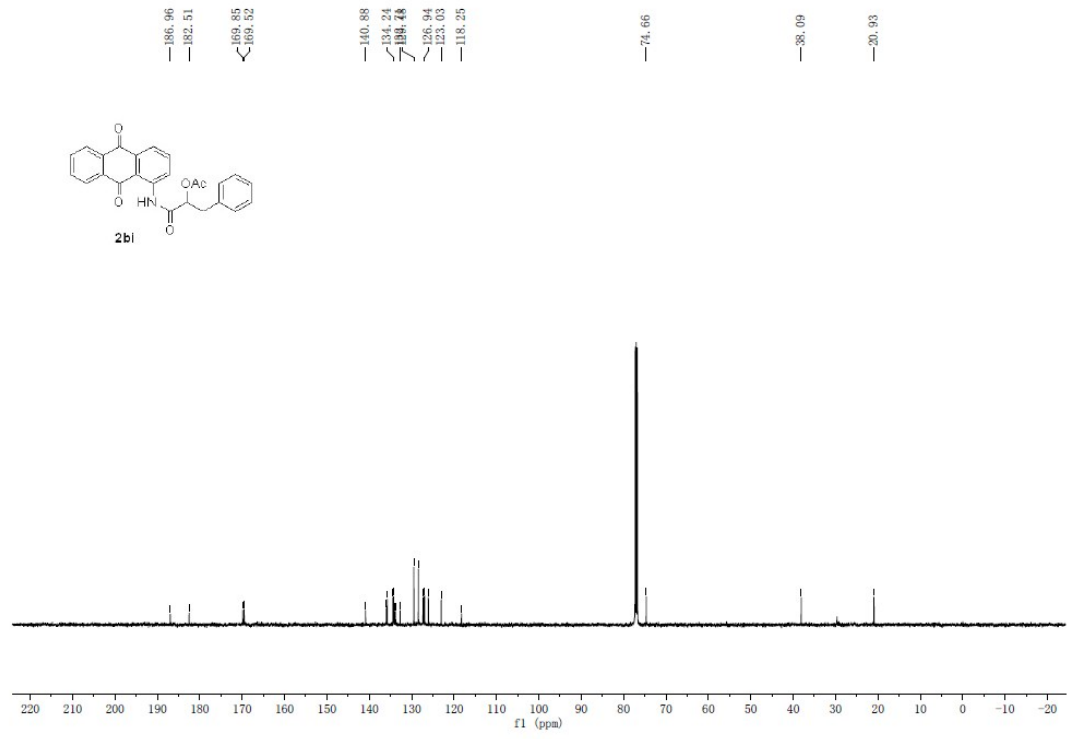

12.78
9.20
9.17
8.28
8.26
8.09
8.07
7.80
7.76
5.26
5.25
2.48
2.10
1.68
1.40
1.37
1.37
1.34
1.32
1.29
1.27
1.26
1.24
1.21
1.19
1.16
OAc
HN
O
2bg
1.00
1.00
2.00
1.00
3.00
1.00
3.00
1.01
5.24
5.33
f1 (ppm)

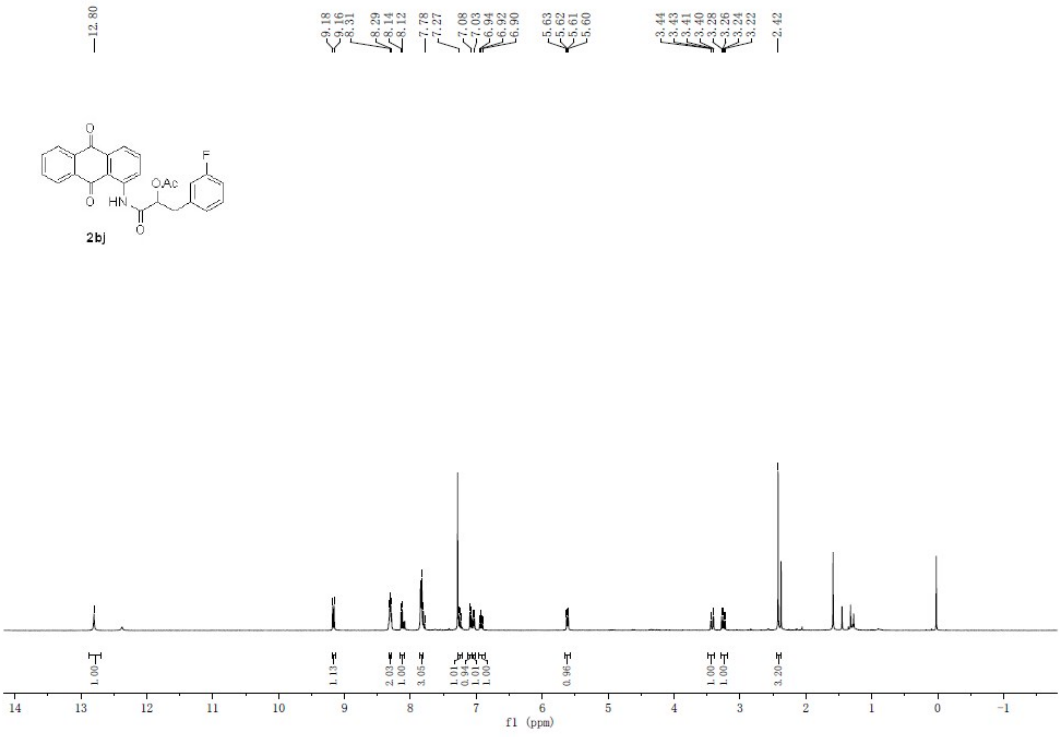

187.10
182.47
170.32
169.90
140.98
134.23
132.67
126.02
122.88
118.09
78.07
40.35
29.26
26.05
25.93
21.02
OAc
HN
O
2bg
f1 (ppm)

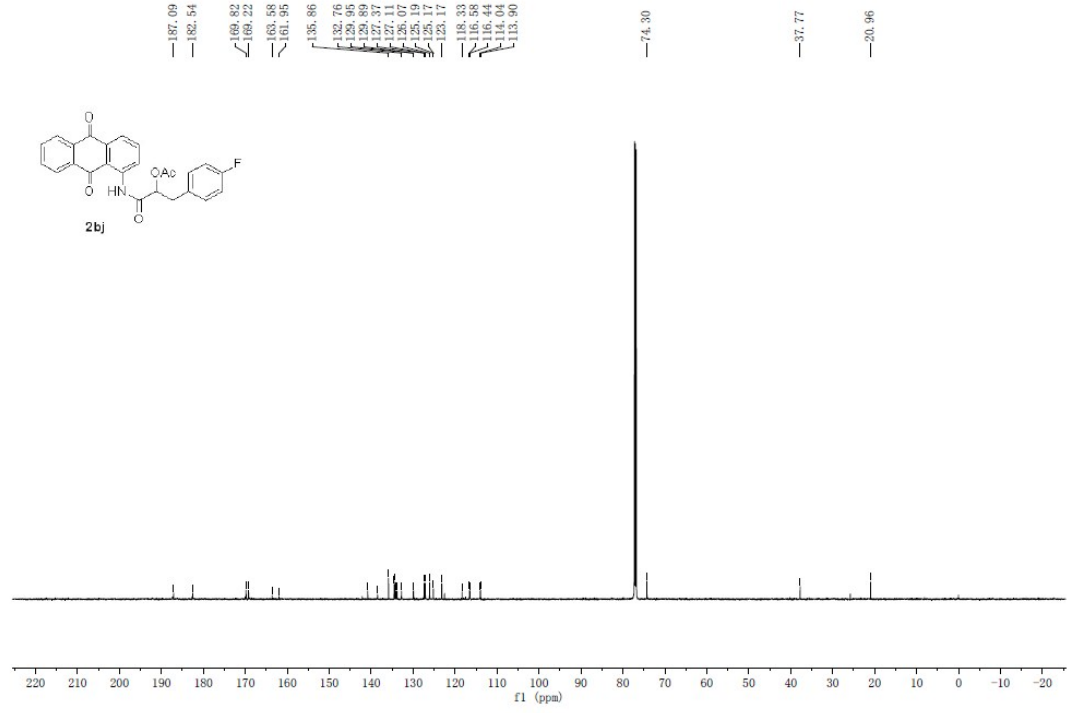

12.80
9.15
9.13
8.27
8.26
8.07
8.06
7.81
7.80
7.79
7.77
7.75
5.45
5.44
5.43
5.42
2.47
1.90
1.84
1.69
1.50
1.30
1.27
1.24
1.22
1.20
1.17
1.14
1.09
1.06
1.03
1.01
0.99
0.98
0.96
OAc
HN
O
2bh
1.00
1.00
2.00
1.00
3.01
1.01
3.01
3.18
4.43
1.00
3.34
2.14
f1 (ppm)

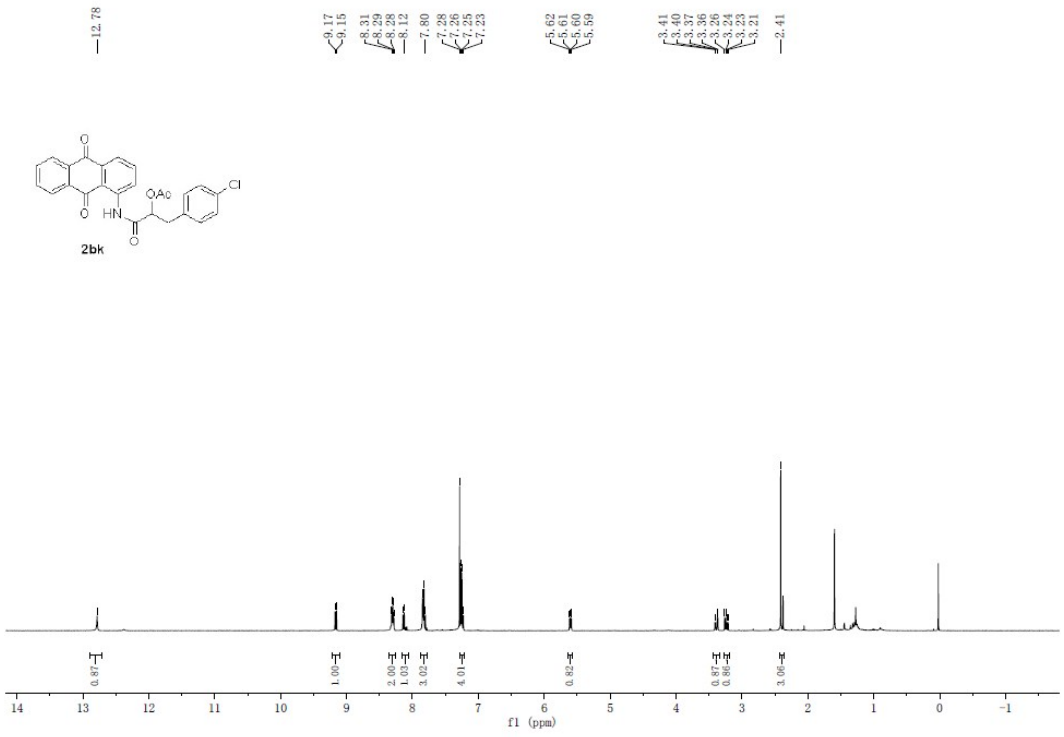

187.11
182.43
170.88
170.28
141.17
134.24
132.68
126.05
122.88
118.11
72.55
39.66
32.27
26.19
21.12
OAc
HN
O
2bh
f1 (ppm)

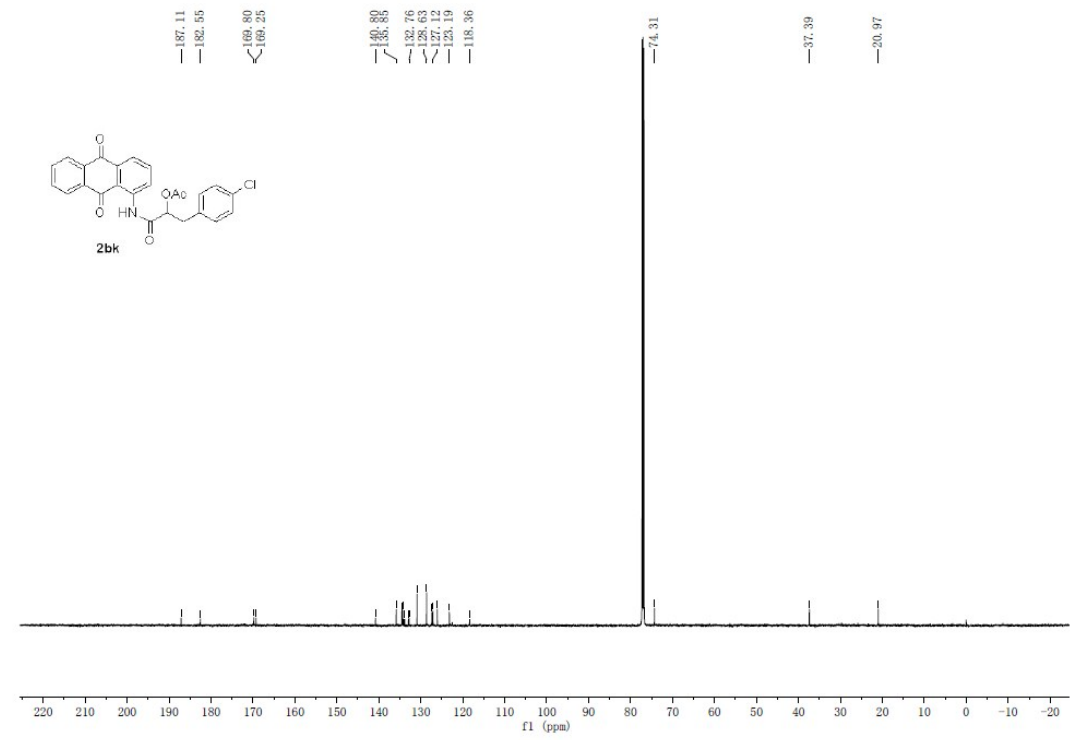

12.77
9.19
9.17
8.28
8.26
8.12
8.10
7.39
7.37
7.25
7.24
7.23
7.22
7.20
5.63
5.62
5.61
5.60
3.46
3.45
3.42
3.41
3.27
3.25
3.24
3.21
2.39
OAc
HN
O
2bi
1.00
1.00
2.00
1.00
3.01
5.19
1.00
1.00
1.00
3.01
f1 (ppm)

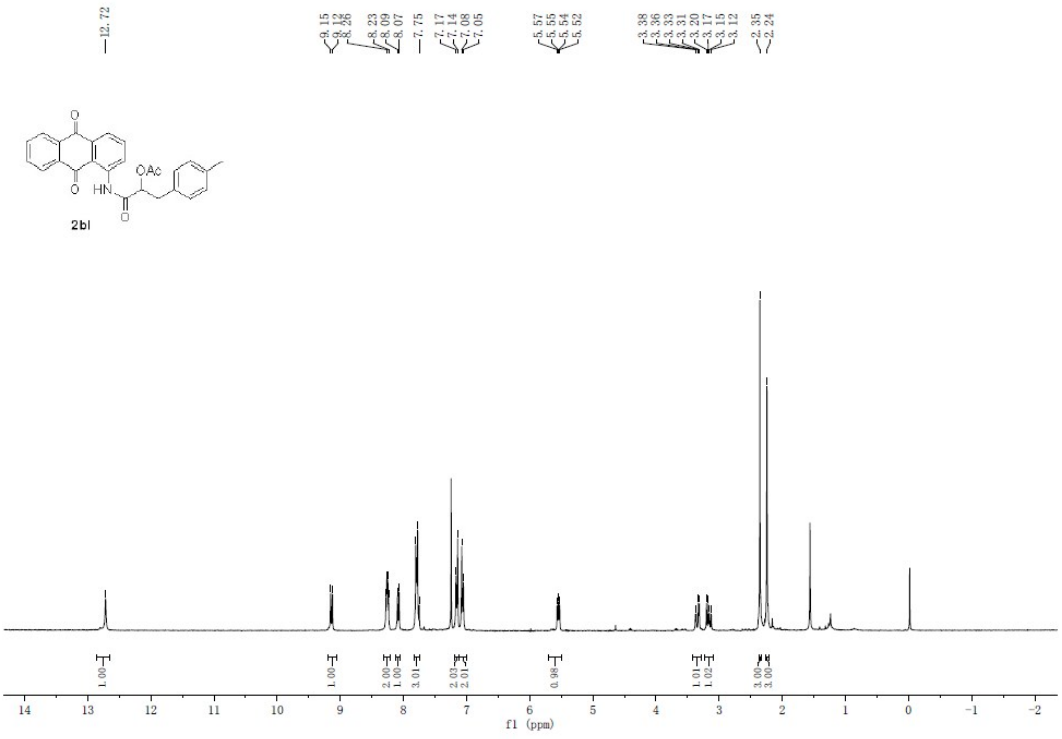

186.96
182.51
169.85
169.52
140.88
134.24
126.94
123.03
118.25
74.66
38.09
20.93
OAc
HN
O
2bi
f1 (ppm)

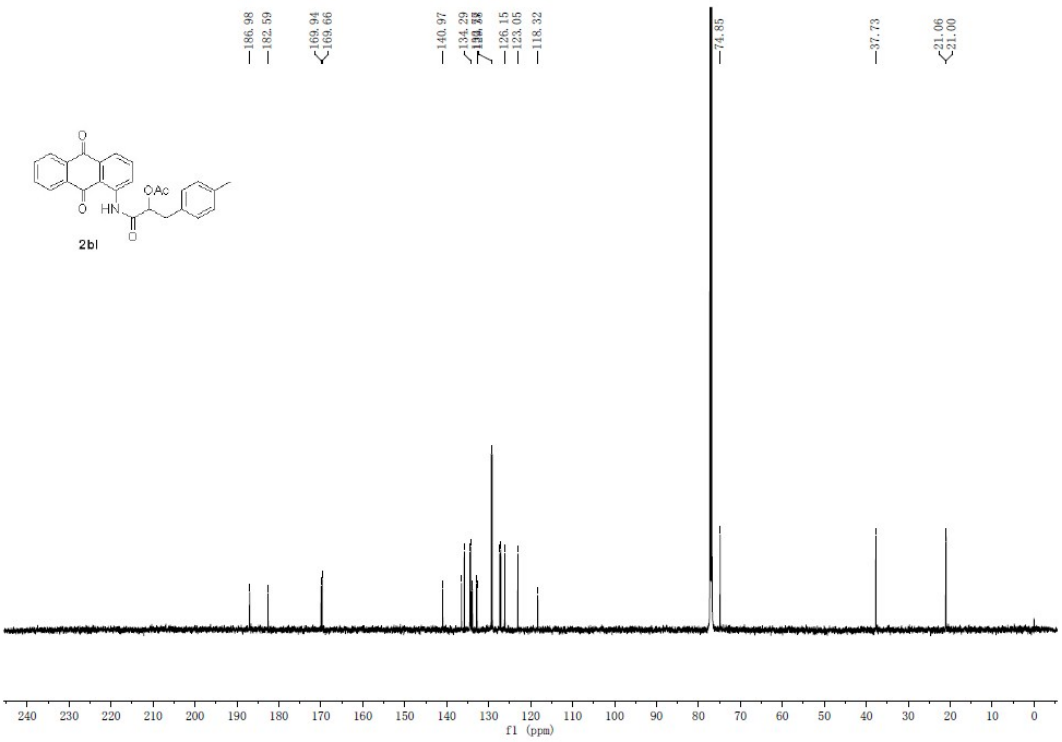

12.80
9.18
9.16
8.31
8.29
8.14
8.12
7.78
7.27
7.08
7.03
6.94
6.92
6.90
5.63
5.62
5.61
5.60
3.44
3.43
3.41
3.40
3.28
3.26
3.24
3.22
2.42
O
O
HN
OAc
F
O
2bj
1.00
1.13
2.03
1.00
3.05
1.01
0.94
1.02
1.00
0.90
1.00
1.00
3.20
f1 (ppm)

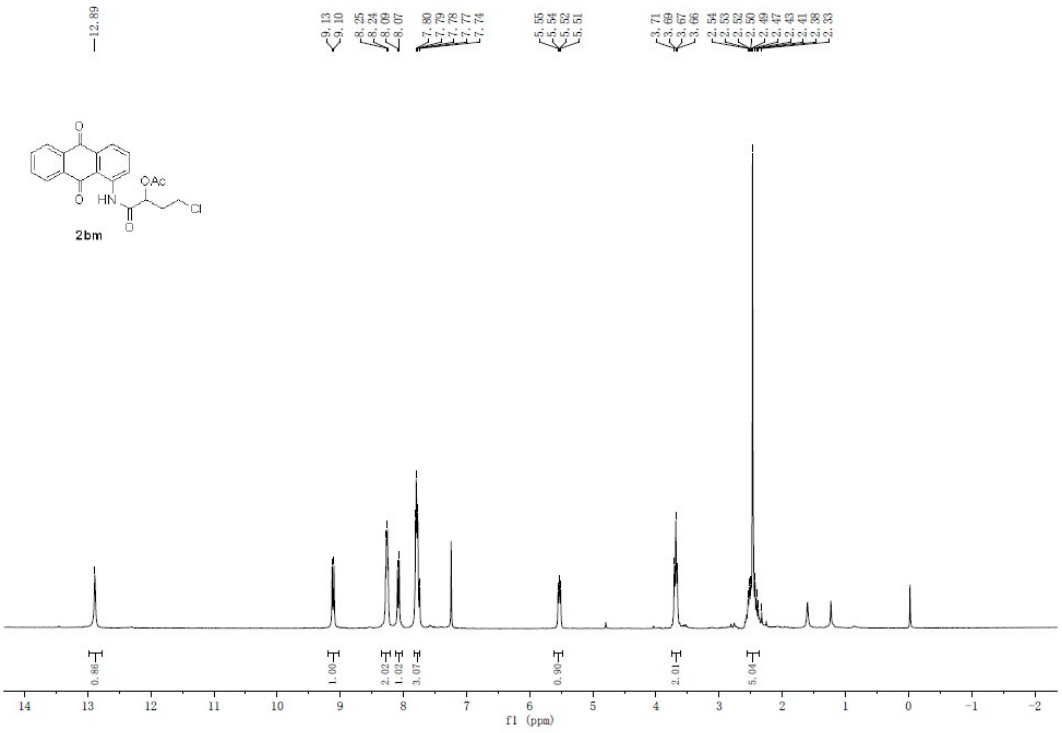

187.09
182.54
169.82
169.22
163.58
161.95
135.86
132.76
129.95
129.89
127.37
127.11
126.07
125.19
125.17
123.17
118.33
116.58
116.44
114.04
113.90
74.30
37.77
20.96
O
O
HN
OAc
F
O
2bj
f1 (ppm)

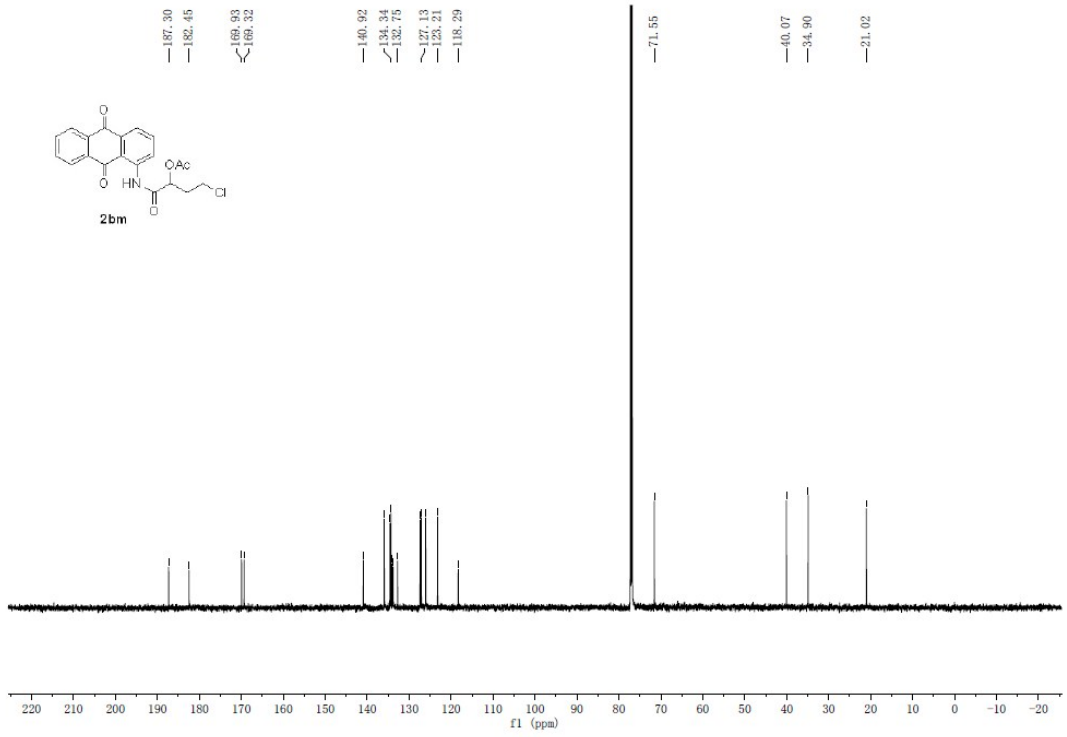

12.78
9.17
9.15
8.31
8.29
8.28
8.12
7.80
7.28
7.26
7.25
7.23
5.62
5.61
5.60
5.59
3.41
3.40
3.37
3.36
3.26
3.24
3.23
3.21
2.41
OAc
HN
Cl
2bk
0.87
1.00
2.00
1.03
3.02
4.01
0.82
0.87
0.86
3.06
f1 (ppm)

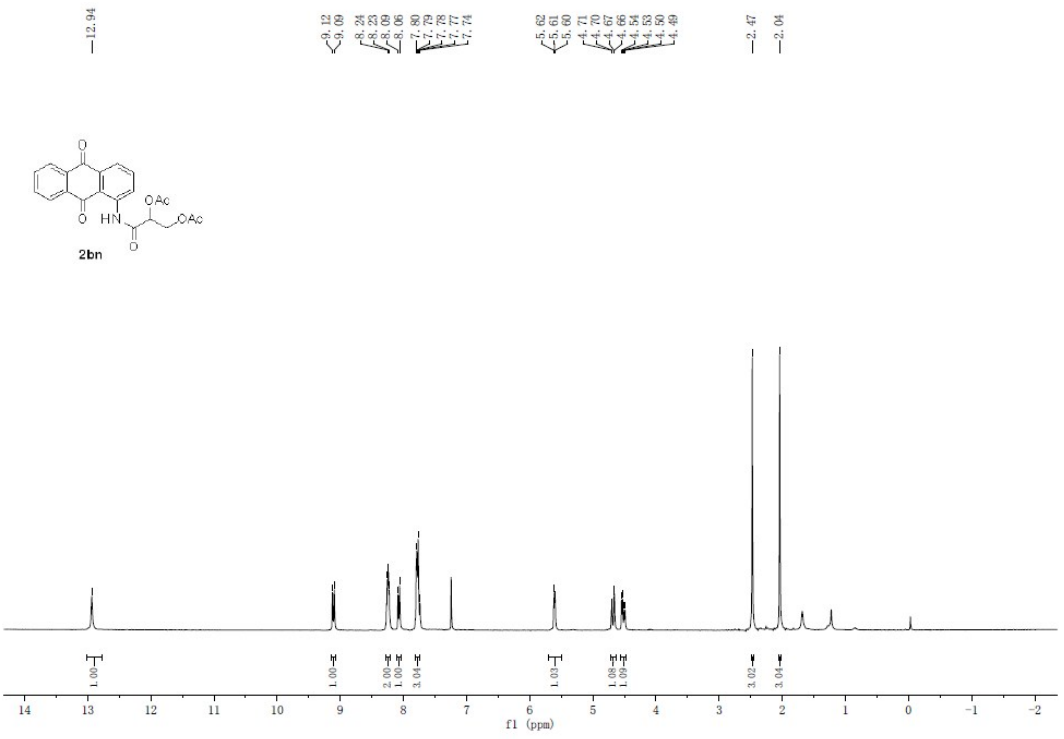

187.11
182.55
169.80
169.25
140.80
135.85
132.76
128.63
127.12
123.19
118.36
74.31
37.39
20.97
OAc
HN
Cl
2bk
f1 (ppm)

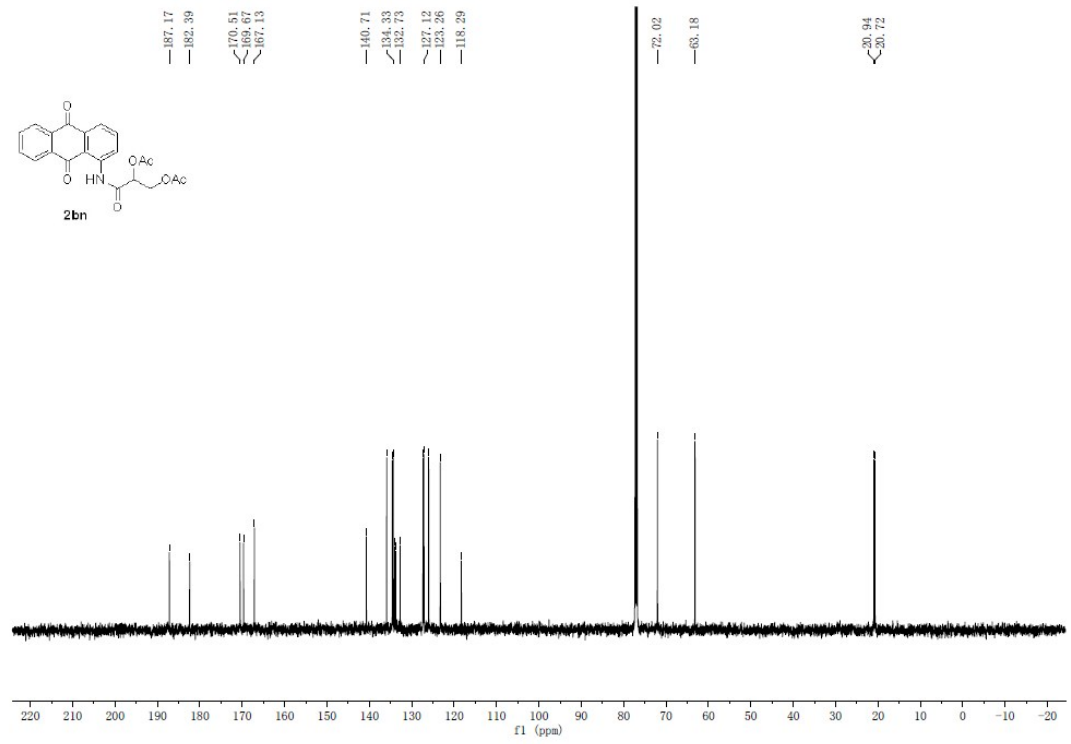

12.72
9.15
9.12
8.26
8.23
8.09
8.07
7.75
7.17
7.14
7.08
7.05
5.57
5.55
5.54
5.52
3.38
3.36
3.33
3.31
3.20
3.17
3.15
3.12
2.35
2.24
OAc
HN
O
2bl
1.00
1.00
2.00
1.00
3.01
2.03
2.01
0.98
1.01
1.02
3.00
3.00
f1 (ppm)

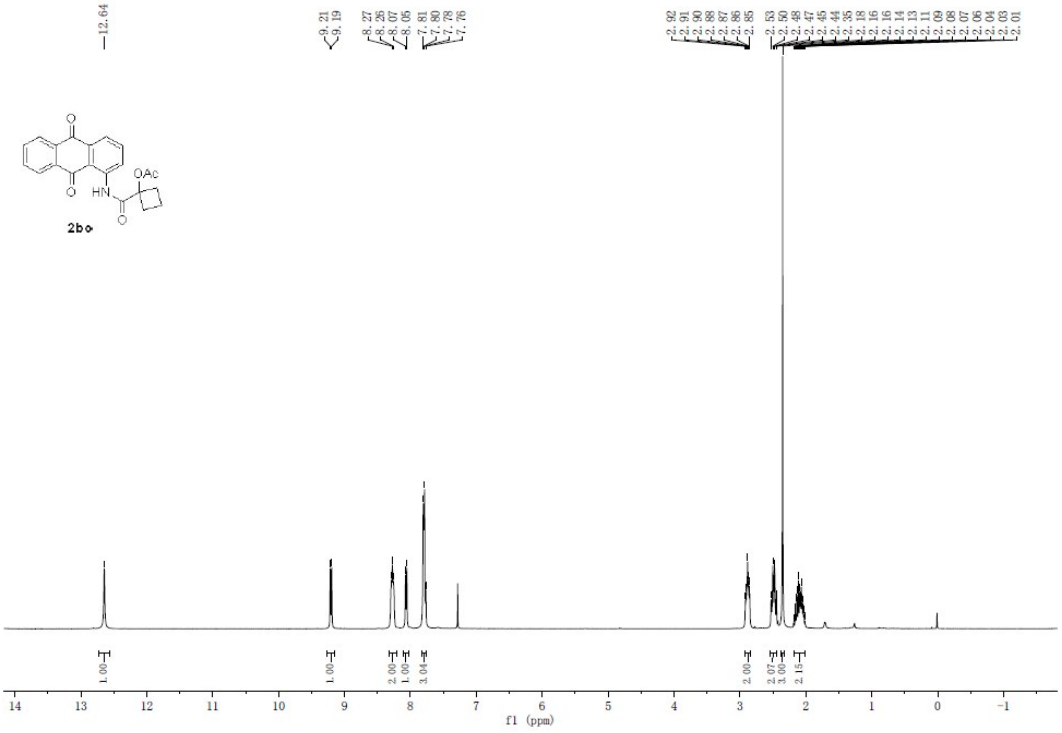

186.98
182.59
169.94
169.66
140.97
134.29
126.15
123.05
118.32
74.85
37.73
21.06
21.00
OAc
HN
O
2bl
f1 (ppm)

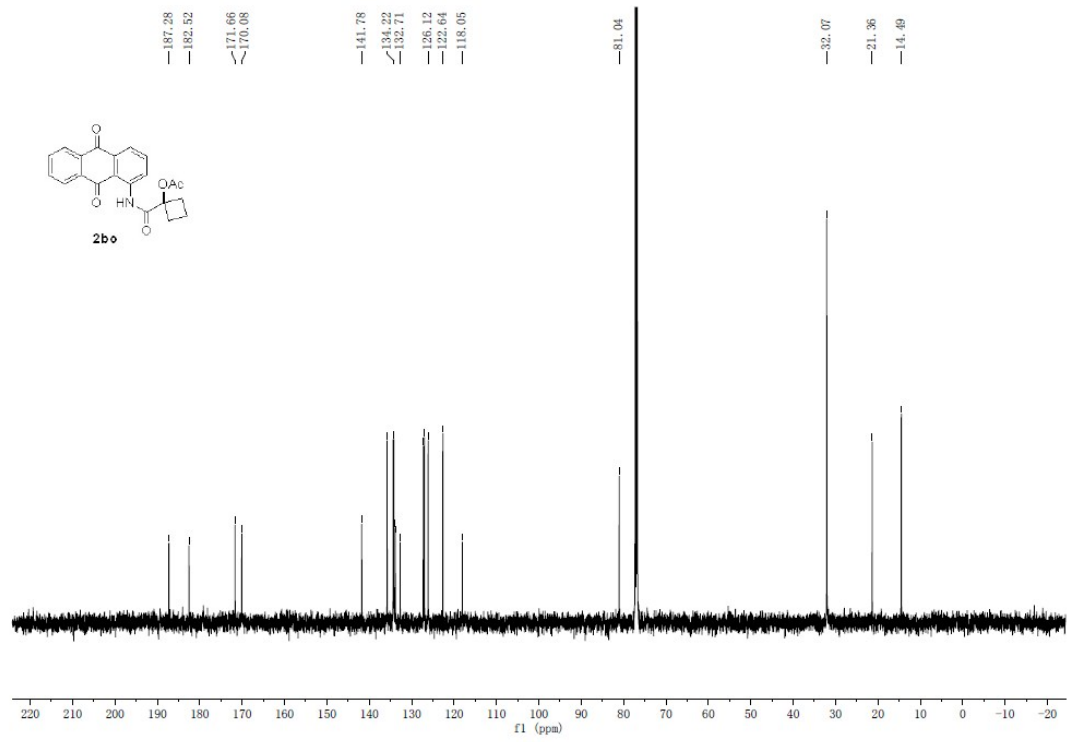

12.89
9.13
9.10
8.25
8.24
8.09
8.07
7.80
7.79
7.78
7.77
7.74
5.55
5.54
5.52
5.51
3.71
3.69
3.67
3.66
2.54
2.53
2.52
2.50
2.49
2.47
2.43
2.41
2.38
2.33
OAc
HN
O
Cl
2bm
0.88
1.00
2.02
1.02
3.07
0.90
2.01
5.04
f1 (ppm)

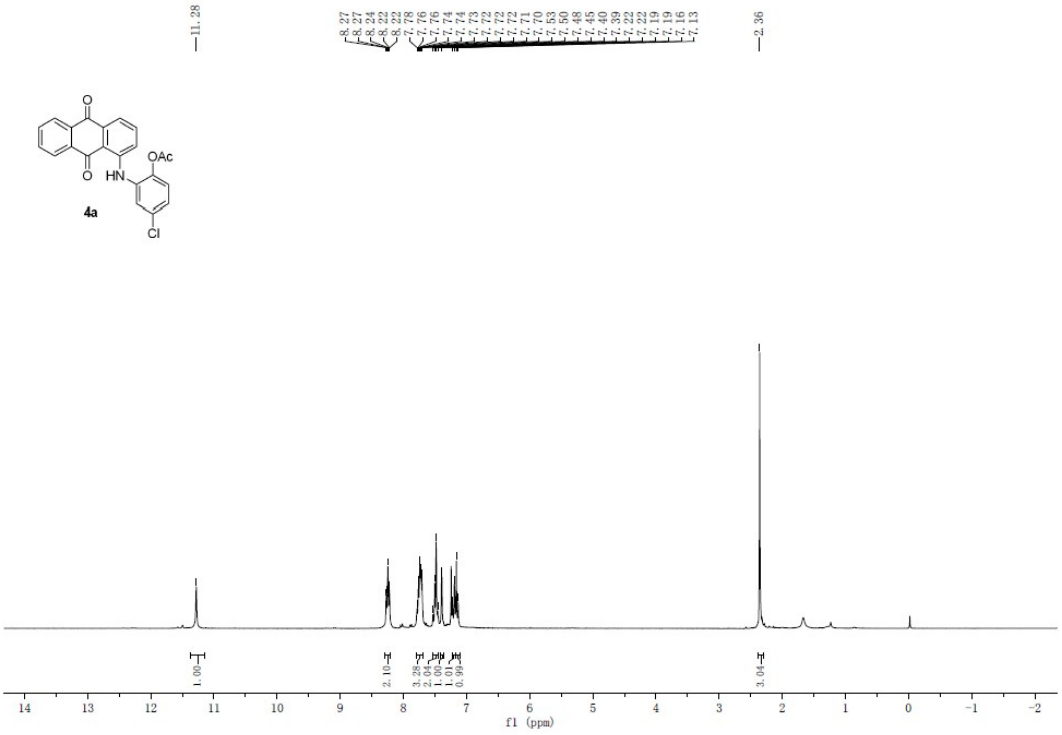

187.30
182.45
169.93
169.32
140.92
134.34
132.75
127.13
125.21
118.29
71.55
40.07
34.90
21.02
OAc
HN
O
Cl
2bm
f1 (ppm)

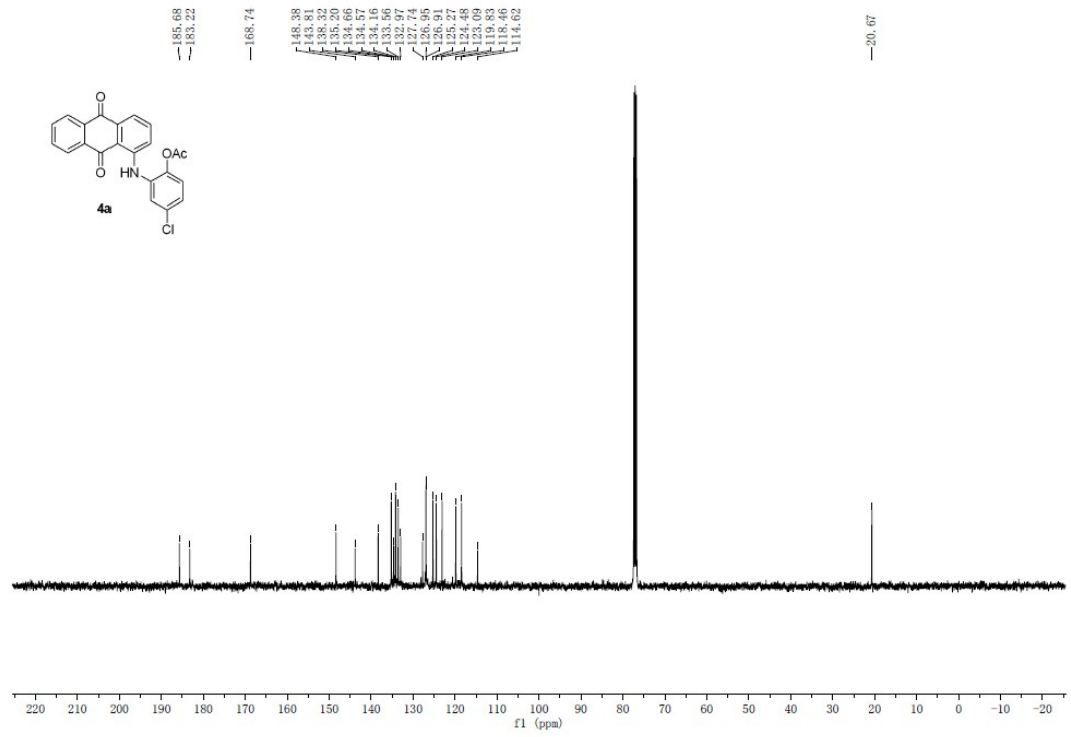

12.94
9.12
9.09
8.24
8.23
8.09
8.06
7.80
7.79
7.78
7.77
7.74
5.62
5.61
5.60
4.71
4.70
4.67
4.66
4.54
4.53
4.50
4.49
2.47
2.04
OAc
OAc
HN
O
O
O
2bn
1.00
1.00
2.00
1.00
3.04
1.03
1.08
1.09
3.02
3.04
f1 (ppm)

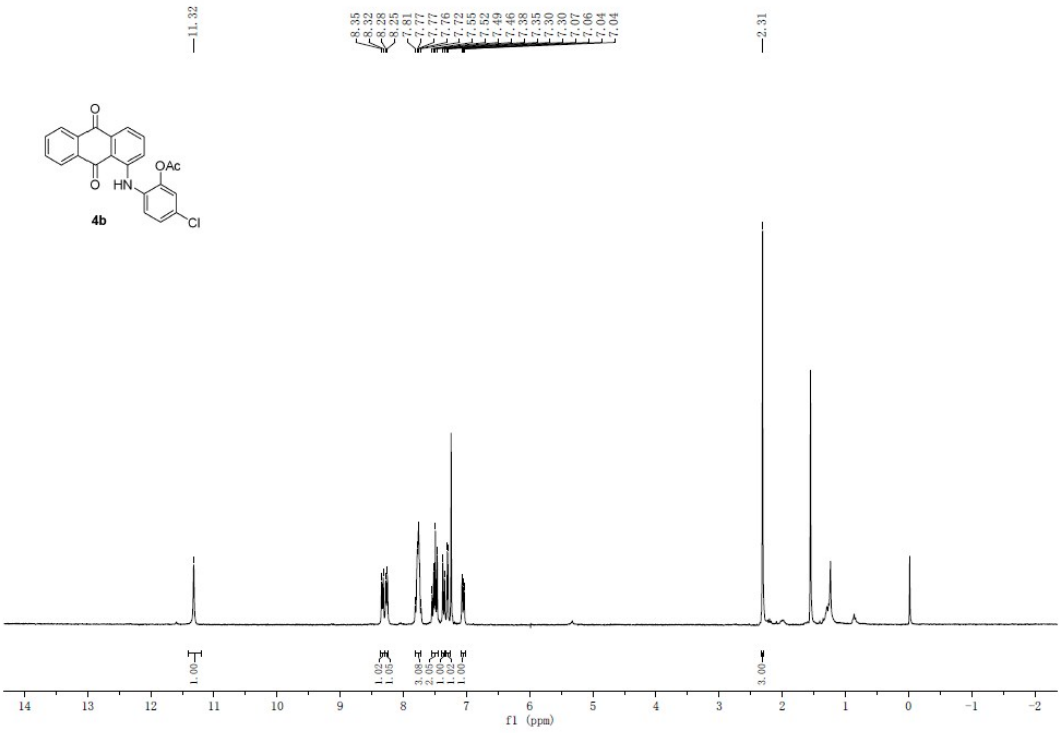

187.17
182.39
170.51
169.67
167.13
140.71
134.33
132.73
127.12
123.26
118.29
72.02
63.18
20.94
20.72
OAc
OAc
HN
O
O
O
2bn
f1 (ppm)

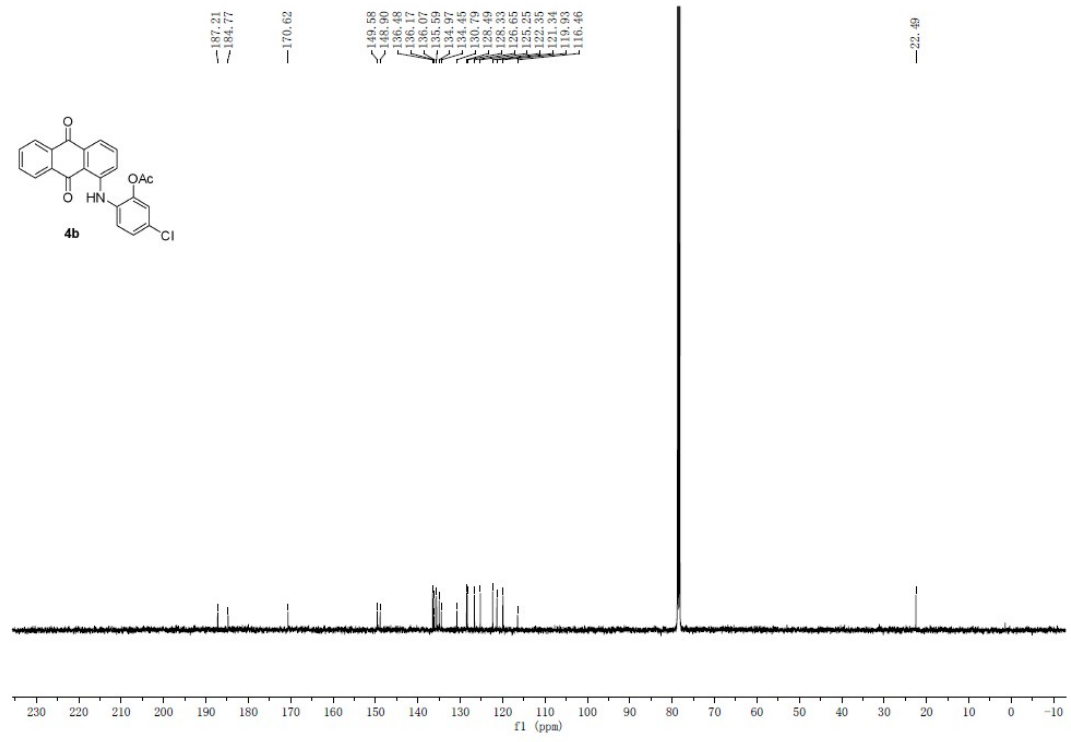

12.64
9.21
8.19
8.27
8.25
8.07
8.05
7.81
7.80
7.78
7.76
2.92
2.91
2.90
2.88
2.87
2.86
2.85
2.53
2.50
2.48
2.47
2.45
2.44
2.35
2.18
2.16
2.14
2.13
2.11
2.09
2.06
2.07
2.06
2.04
2.03
2.01
OAc
HN
O
2bo
1.00
1.00
2.00
1.00
3.04
2.00
2.07
3.00
2.15
f1 (ppm)

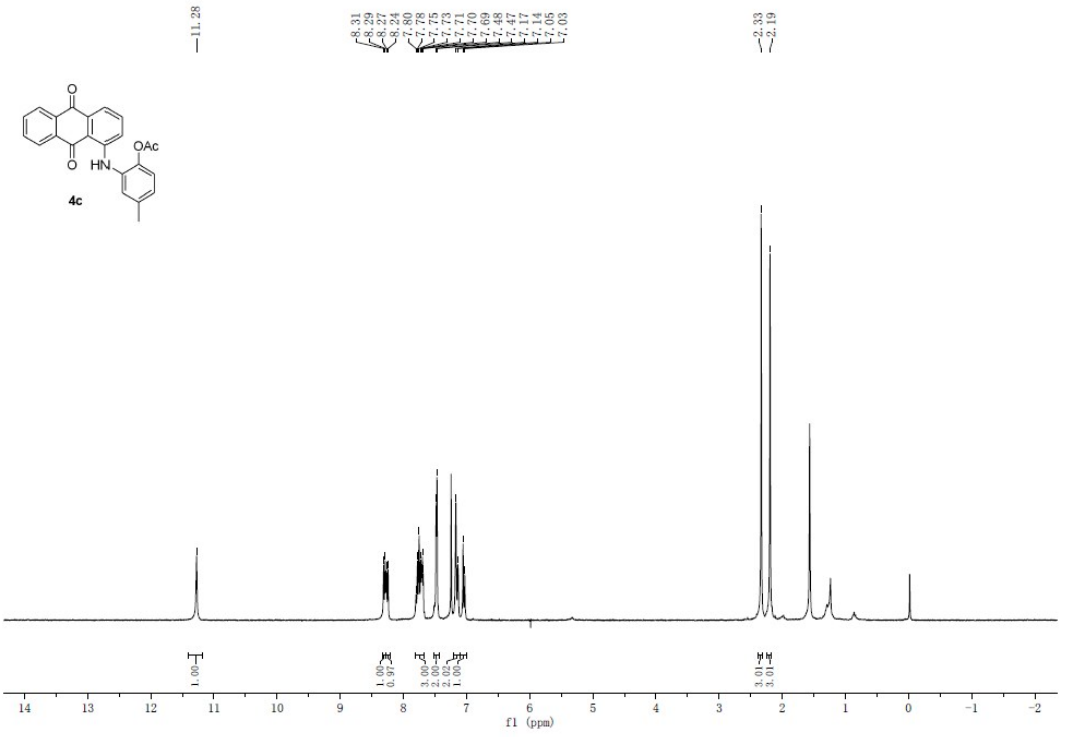

187.28
182.52
171.66
170.08
141.78
134.22
132.71
126.12
122.64
118.05
81.04
32.07
21.36
14.49
OAc
HN
O
2bo
f1 (ppm)

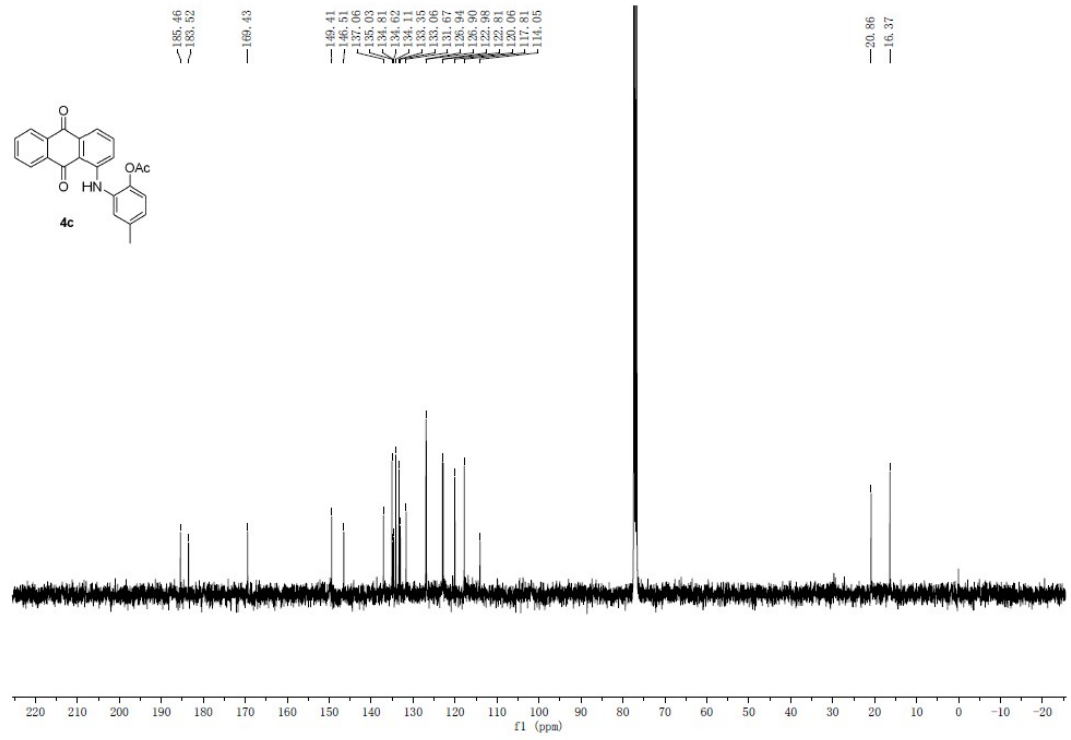

11.28
8.27
8.27
8.24
8.22
8.22
7.78
7.76
7.76
7.74
7.74
7.73
7.72
7.72
7.72
7.71
7.70
7.53
7.50
7.48
7.45
7.40
7.39
7.22
7.22
7.19
7.16
7.13
2.36
O
O
HN
OAc
Cl
4a
1.00
2.10
3.28
2.04
1.00
1.00
0.99
3.04
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2
f1 (ppm)

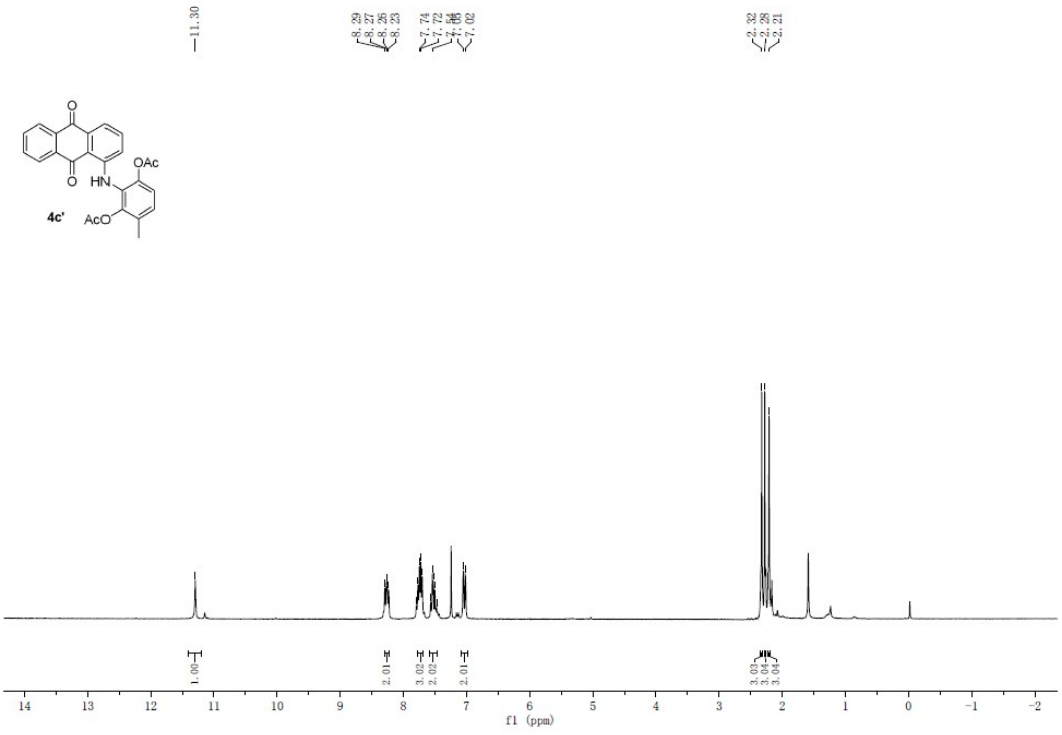

185.68
183.22
168.74
148.38
143.81
138.32
135.20
134.66
134.57
134.16
133.56
132.97
127.74
126.95
126.91
125.27
124.48
123.89
123.53
118.46
114.62
20.67
O
O
HN
OAc
Cl
4a
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)

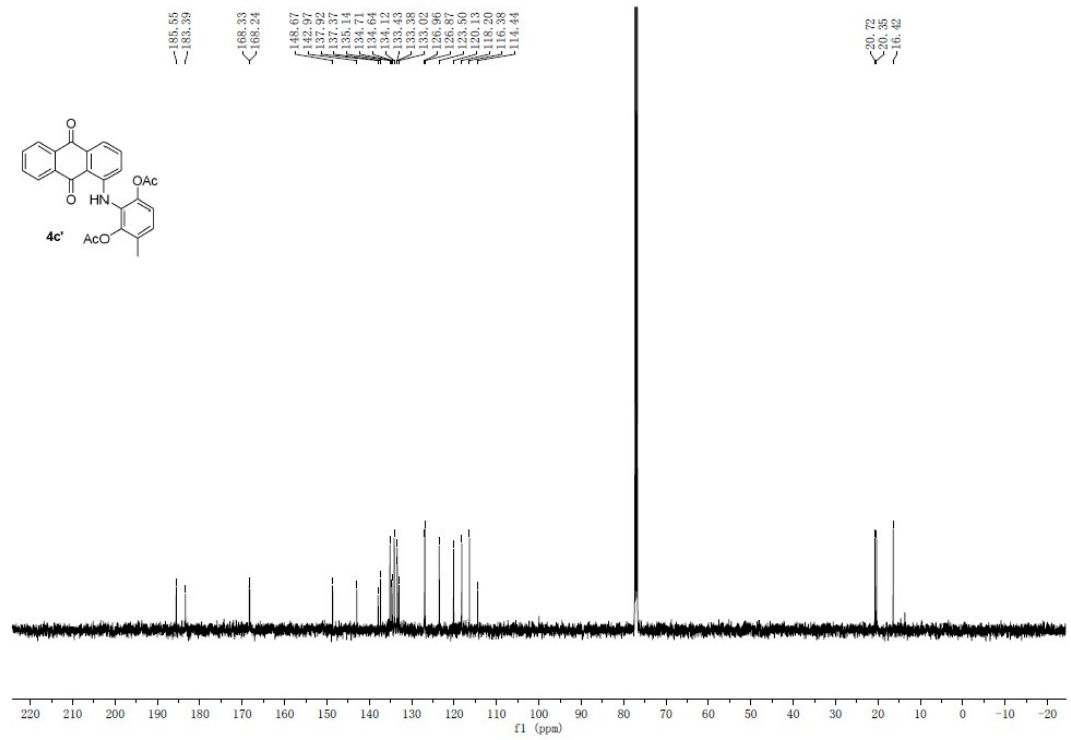

11.32
8.35
8.32
8.28
8.25
7.81
7.77
7.77
7.76
7.72
7.55
7.52
7.49
7.46
7.38
7.35
7.30
7.30
7.07
7.06
7.04
7.04
2.31
O
O
HN
OAc
Cl
4b
1.00
1.02
1.05
3.08
2.05
1.08
1.02
1.05
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2
f1 (ppm)

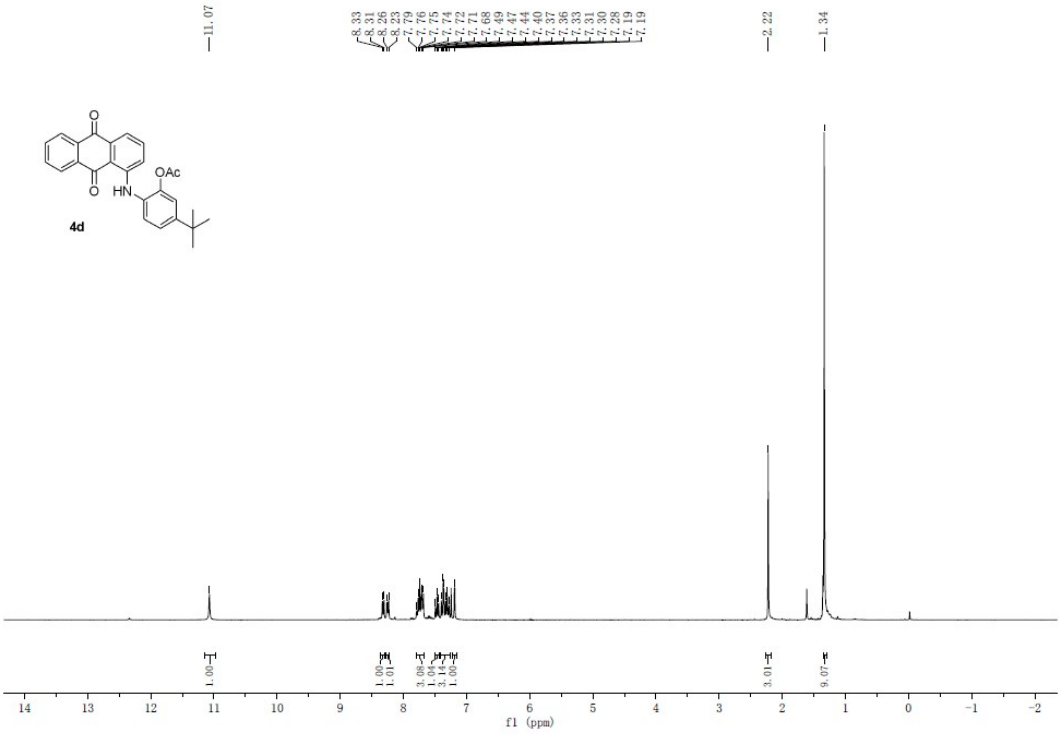

187.21
184.77
170.62
149.58
148.90
136.48
136.17
136.07
135.99
134.97
134.46
130.79
128.49
128.33
126.65
125.25
122.35
121.34
119.93
116.46
22.49
O
O
HN
OAc
Cl
4b
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

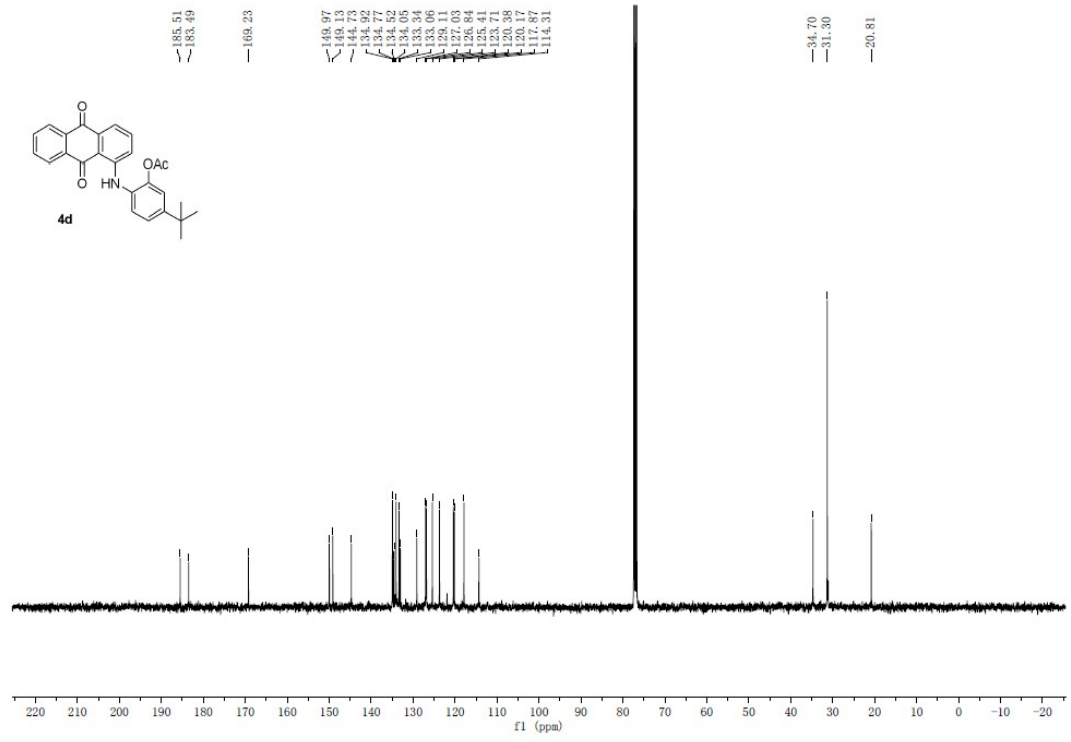

11.28
8.31
8.29
8.27
8.24
7.80
7.78
7.75
7.73
7.71
7.70
7.69
7.48
7.47
7.17
7.14
7.05
7.03
2.33
2.19
OAc
HN
O
O
4c
1.00
1.00
0.97
3.09
3.02
2.02
1.00
3.01
3.01
f1 (ppm)

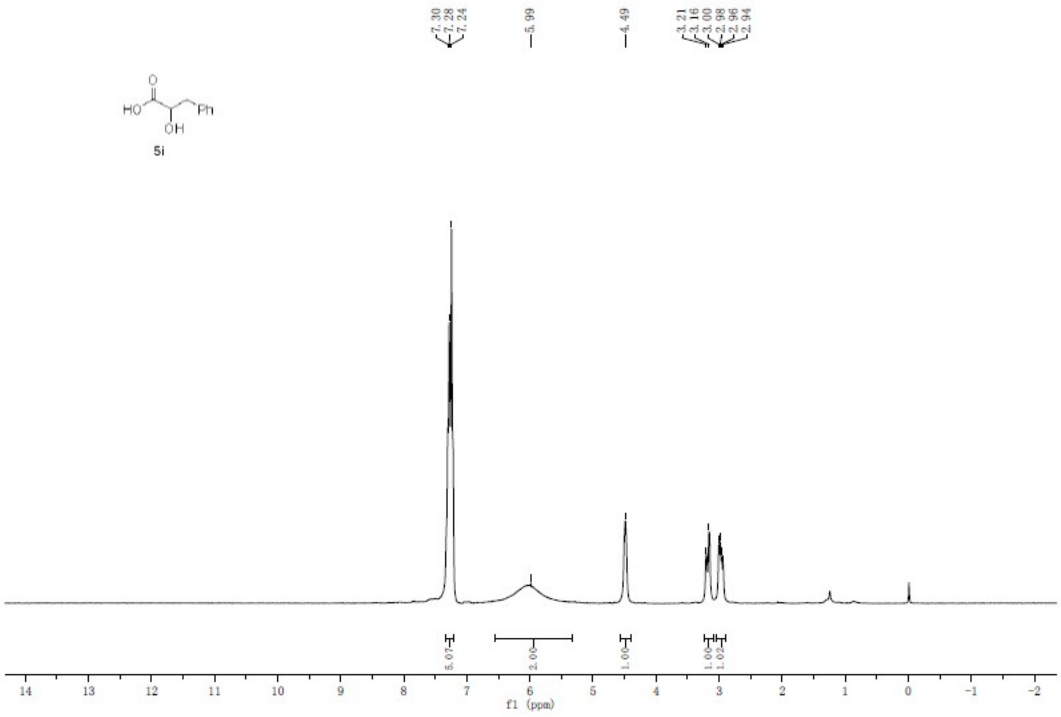

185.46
183.52
169.43
149.41
146.51
137.06
135.03
134.81
134.62
134.11
133.55
133.06
131.67
126.94
126.90
122.98
122.81
120.06
117.81
114.05
20.86
16.37
OAc
HN
O
O
4c
f1 (ppm)

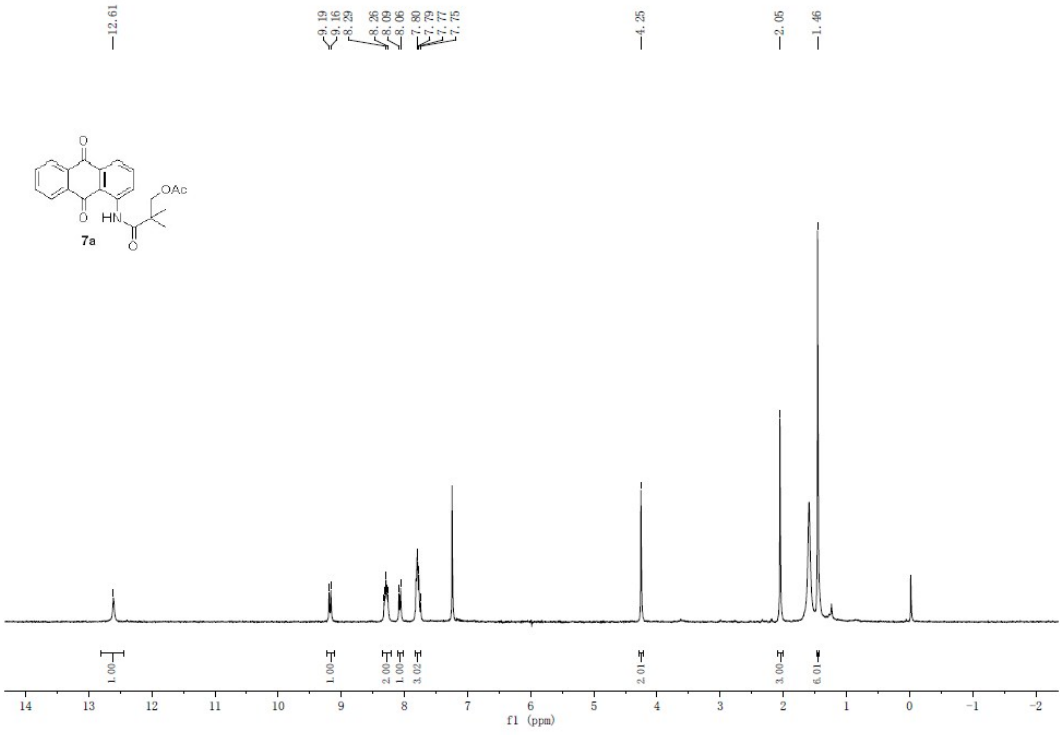

11.30
8.29
8.27
8.26
8.23
7.74
7.72
7.02
2.32
2.28
2.21
OAc
HN
AcO
4c'
1.00
2.01
3.02
2.02
2.01
3.03
3.04
3.04
f1 (ppm)

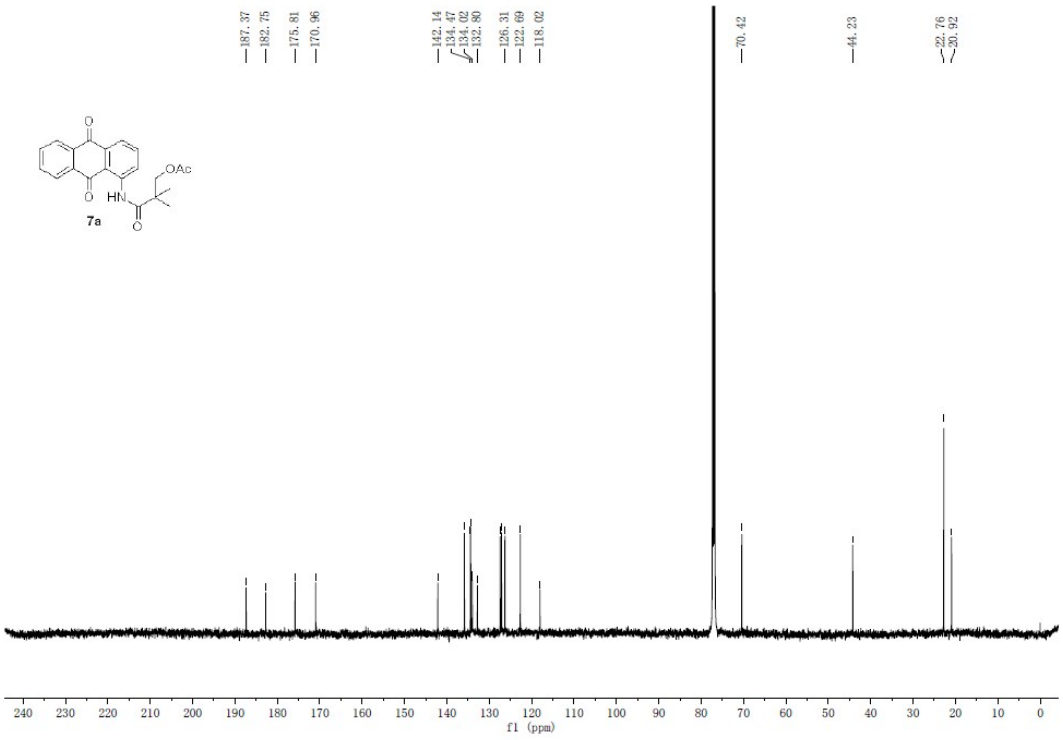

185.55
183.39
168.33
168.24
148.67
142.97
137.92
137.37
135.14
134.71
134.64
134.12
133.43
133.38
133.02
126.96
126.67
125.56
123.13
118.20
116.38
114.44
20.72
20.35
16.42
OAc
HN
AcO
4c'
f1 (ppm)

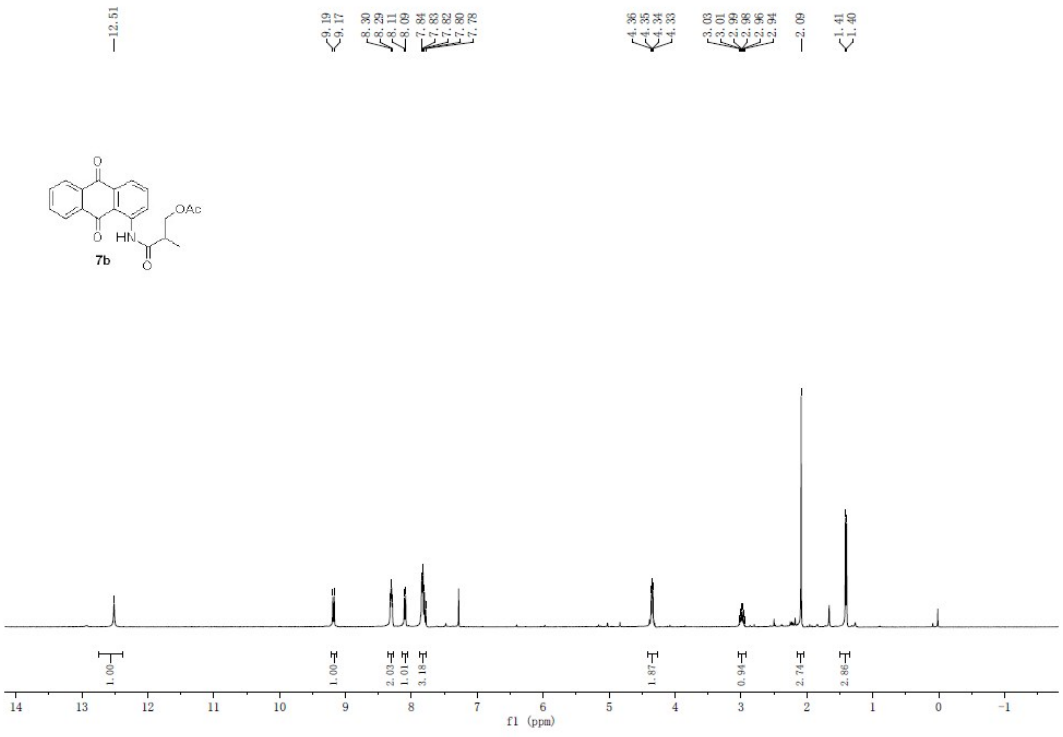

11.07
8.33
8.31
8.26
8.23
7.79
7.76
7.75
7.74
7.72
7.71
7.68
7.49
7.47
7.44
7.40
7.37
7.36
7.33
7.31
7.30
7.28
7.19
7.19
2.22
1.34
O
O
HN
OAc
4d
1.00
1.00
1.01
3.08
1.05
3.14
1.00
3.01
9.07
f1 (ppm)

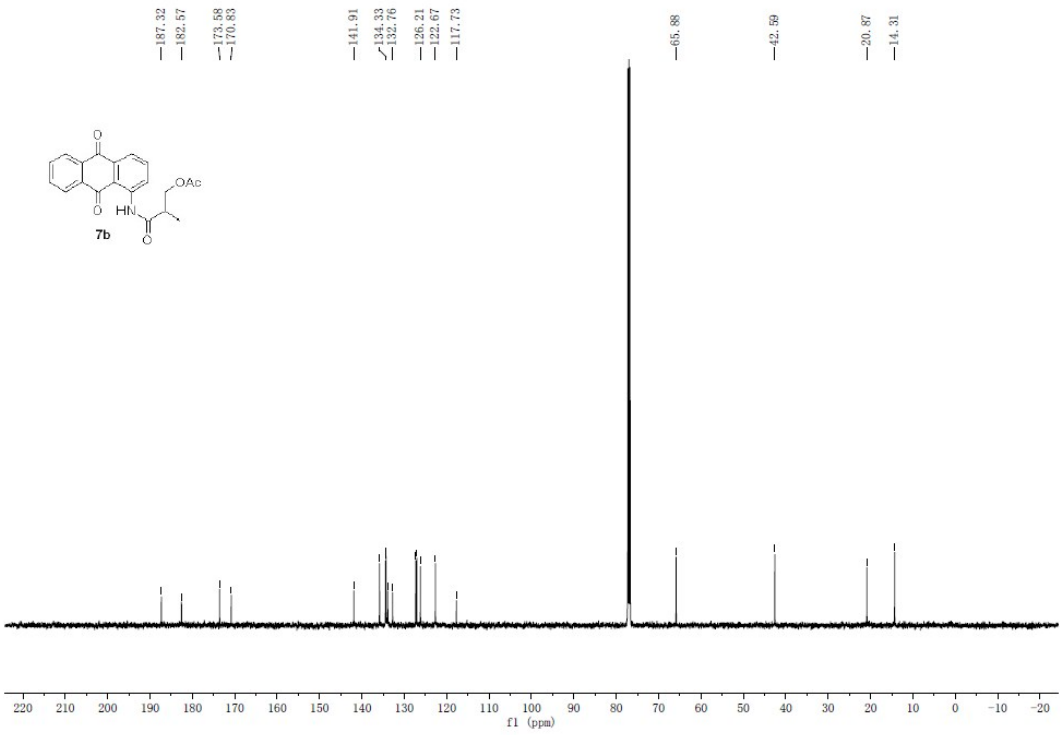

185.51
183.49
169.23
149.97
149.13
144.73
134.92
134.77
134.52
134.05
133.34
133.06
129.11
127.03
126.84
125.41
123.71
120.38
120.17
117.87
114.31
34.70
31.30
20.81
O
O
HN
OAc
4d
f1 (ppm)

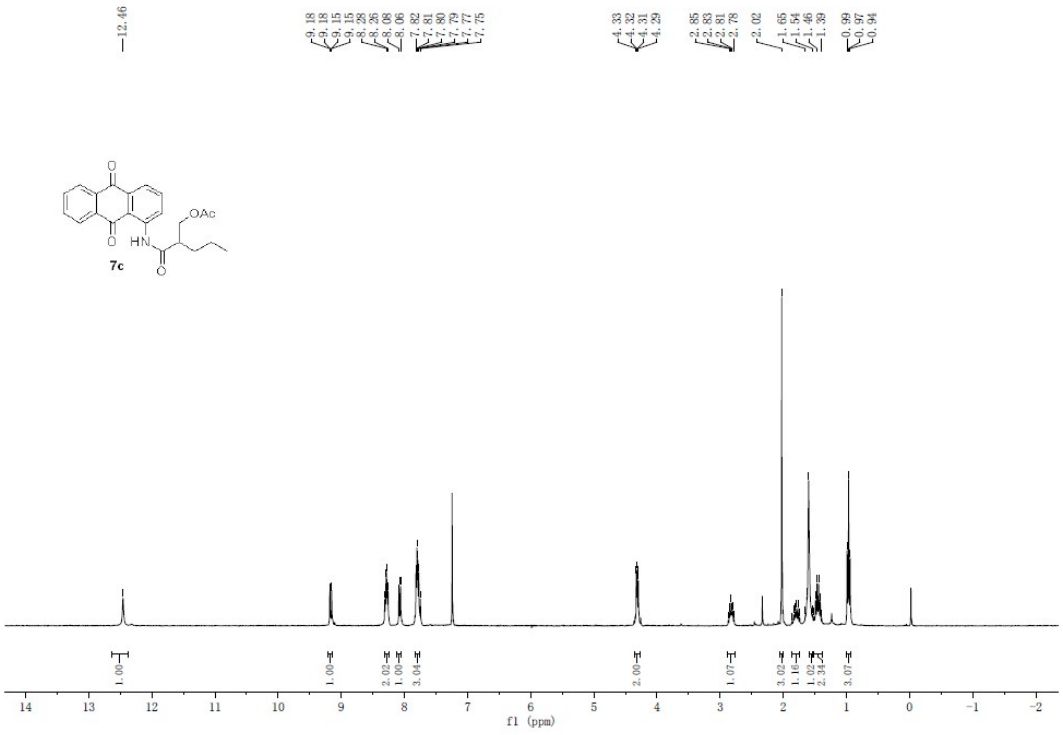

7.30
7.28
7.24
5.99
4.49
3.21
3.16
3.00
2.98
2.96
2.94
HO
O
OH
Ph
5i
6.07
2.00
1.00
1.00
1.03
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2
f1 (ppm)

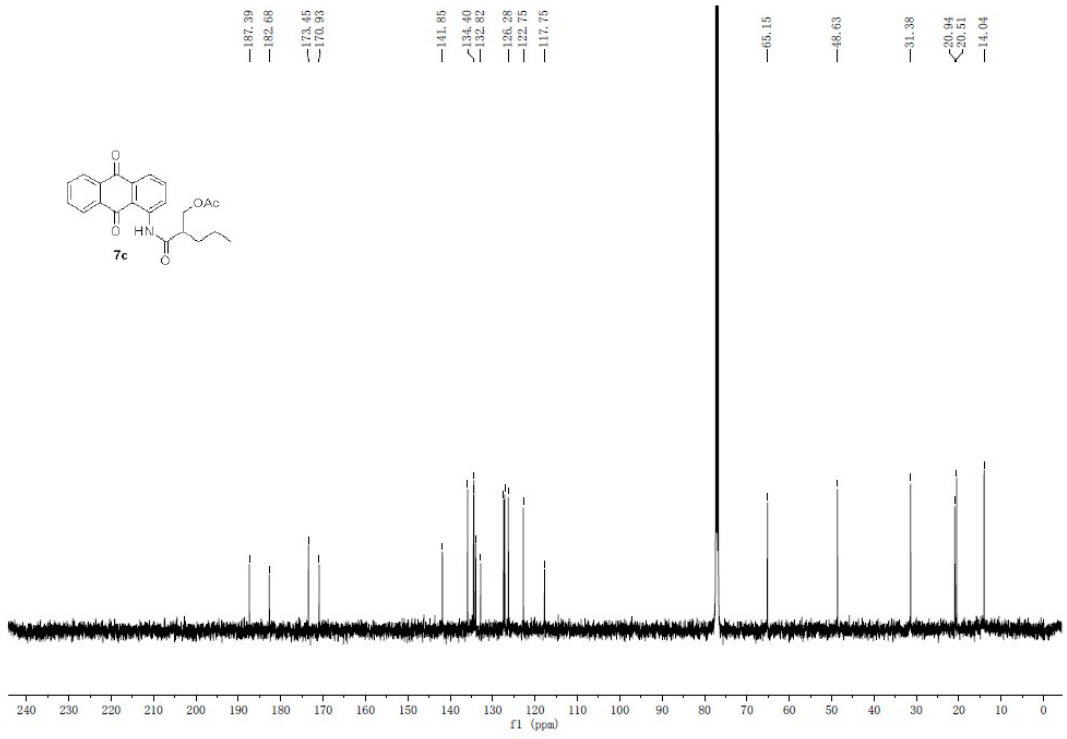

12.61
9.19
9.16
8.29
8.26
8.09
8.06
7.80
7.79
7.77
7.75
4.25
2.05
1.46
O
OAc
HN
O
O
7a
1.00
1.00
2.00
1.00
3.02
2.01
3.00
6.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2
f1 (ppm)


187.37
182.75
175.81
170.96
142.14
134.47
134.02
132.80
126.31
122.69
118.02
70.42
44.23
22.76
20.92
OAc
HN
7a
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


12.51
9.19
9.17
8.30
8.29
8.11
8.09
7.84
7.83
7.82
7.80
7.78
4.36
4.35
4.34
4.33
3.03
3.01
2.99
2.98
2.96
2.94
2.09
1.41
1.40
OAc
HN
7b
1.00
1.00
2.03
1.01
3.18
1.87
0.94
2.74
2.86
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)


187.32
182.57
173.58
170.83
141.91
134.33
132.76
126.21
122.67
117.73
65.88
42.59
20.87
14.31
OAc
HN
O
7b
f1 (ppm)


12.46
9.18
9.15
8.29
8.26
8.08
8.06
7.82
7.81
7.80
7.79
7.77
7.75
4.33
4.32
4.31
4.29
2.85
2.83
2.81
2.78
2.02
1.65
1.54
1.46
1.39
0.99
0.97
0.94
OAc
HN
O
7c
1.00
1.00
2.02
1.00
3.04
2.09
1.07
3.02
1.16
1.02
2.34
3.07
f1 (ppm)


187.39
182.68
173.45
170.93
141.85
134.40
132.82
126.28
122.75
117.75
65.15
48.63
31.38
20.94
20.51
14.04
OAc
HN
O
O
O
7c
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)