

Supporting Information

Remote-stereocontrolled (3+2)-annulation of pyrrolidinone-based MBH carbonates with 2-arylideneindane-1,3-diones

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A: General Information

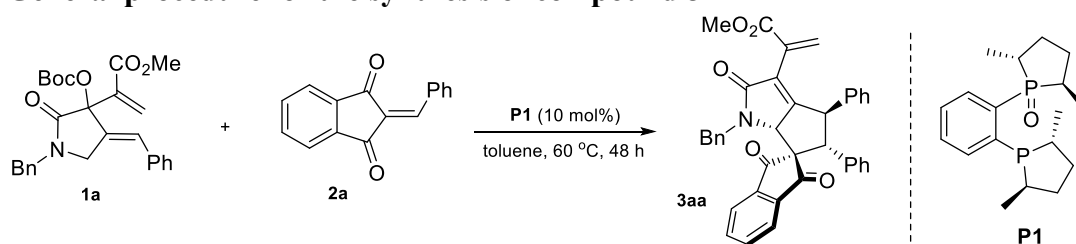
All chemicals were used without further purification as commercially available unless otherwise noted. Thin-layer chromatography (TLC) was performed on silica gel plates (60F-254) using UV-light (254 and 365 nm). Flash chromatography was conducted on silica gel (300 or 400 mesh). NMR spectra were recorded on a Bruker-400/500/600 MHz spectrometer. High resolution mass spectral (HRMS) analyses were measured on a Thermo Scientific Orbitrap Fusion mass spectrometer using ESI and quadrupole technology. Chemical shift is reported in ppm and coupling constants are given in Hz.

B: General Procedure

General procedure for the synthesis of compounds **1** and **2**

Substrates **1** and **2** were prepared following the literature procedures¹⁻².

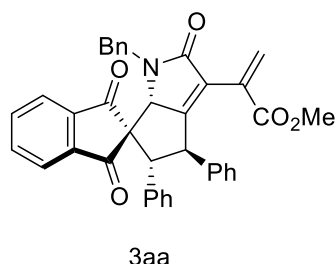
General procedure for the synthesis of compound **3**



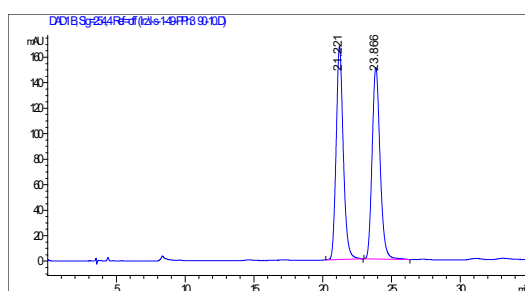
To a solution of toluene (1.0 mL) were added pyrrolidone-based MBH carbonate **1** (0.075 mmol, 1.5 eq), 2-arylideneindane-1,3-dione **2** (0.05 mmol, 1.0 eq) and catalyst **P1** (10 mol%). The reaction mixture was stirred at 60 °C for 48 h under Ar atmosphere. The solvent was removed under vacuum and the residue was purified by flash chromatography (petroleum ether/ethyl acetate = 2/1) to provide product **3**.

C: Characterization Data

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4,5-diphenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (**3aa**)

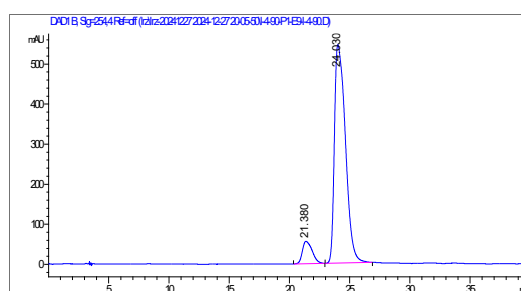


Light yellow solid, 29.1 mg, 99% yield, mp: 104.6-106.2 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.56 (m, 1H), 7.54 – 7.48 (m, 2H), 7.47 – 7.42 (m, 1H), 7.23 – 7.16 (m, 3H), 7.04 – 7.00 (m, 2H), 6.94 (d, *J* = 12.9 Hz, 6H), 6.87 (t, *J* = 7.7 Hz, 2H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.48 (d, *J* = 1.4 Hz, 1H), 6.08 (d, *J* = 1.4 Hz, 1H), 5.13 (d, *J* = 1.7 Hz, 1H), 4.80 (dd, *J* = 10.4, 1.6 Hz, 1H), 4.53 (d, *J* = 15.0 Hz, 1H), 4.10 (d, *J* = 15.0 Hz, 1H), 3.89 (d, *J* = 10.4 Hz, 1H), 3.52 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.9, 196.6, 173.0, 166.2, 160.6, 142.3, 141.4, 140.6, 136.3, 135.7, 135.1, 134.2, 131.8, 130.9, 129.0, 128.8, 128.5, 128.4, 128.1, 127.7, 127.5, 127.2, 122.9, 122.8, 77.5, 77.2, 76.8, 70.8, 65.1, 64.5, 52.1, 46.9, 46.8. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₃₀NO₅⁺ 580.2118; Found 580.2120. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 2.138 min, *t*_R (major) = 24.03 min, 83% ee. [α]_D²⁵ = -114.35 (c = 0.20, DCM).



Racemic

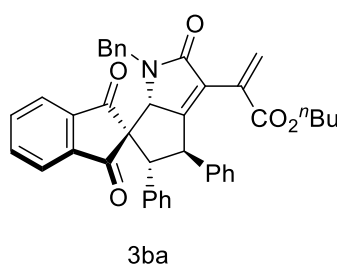
#	Time	Area	Height	Width	Area%	Symmetry
1	21.221	6020.7	167.6	0.5371	49.883	0.822
2	23.866	6049	150.4	0.6191	50.117	0.825



Chiral

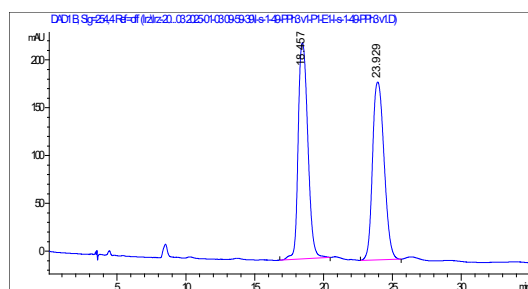
#	Time	Area	Height	Width	Area%	Symmetry
1	21.38	3146	55.9	0.771	8.353	0.56
2	24.03	34518.7	545.4	0.8824	91.647	0.445

Butyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4,5-diphenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (**3ba**)



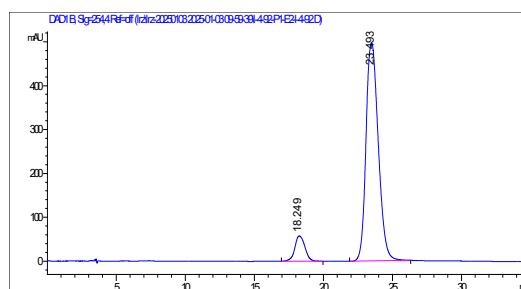
Light yellow solid, 30.6 mg, 98% yield, mp: 107.2-108.3 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.56 (m, 1H), 7.53 – 7.49 (m, 2H), 7.45 – 7.42 (m, 1H), 7.21 – 7.16 (m, 3H), 7.04 – 7.01 (m, 2H), 6.97 (d, *J* = 3.3 Hz, 5H), 6.92 (d, *J* = 7.2 Hz, 2H), 6.88 (s, 1H), 6.86 – 6.83 (m, 1H), 6.76 (d, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 1.4 Hz, 1H), 5.97 (d, *J* = 1.4 Hz, 1H), 5.10 (d, *J* = 1.6 Hz, 1H), 4.86 (dd, *J* = 10.5, 1.6 Hz, 1H), 4.55 (d, *J* = 15.0 Hz, 1H), 4.13 (d, *J* = 10.8 Hz, 1H), 4.08 (d, *J* = 14.8 Hz, 1H), 3.97 (d, *J* = 10.8 Hz, 1H), 3.

89 (d, $J = 10.5$ Hz, 1H), 1.64 – 1.57 (m, 2H), 1.40 – 1.34 (m, 2H), 0.93 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 200.0, 196.5, 173.1, 165.7, 160.6, 141.4, 140.8, 136.4, 135.7, 135.0, 134.4, 132.4, 130.4, 129.0, 128.6, 128.5, 128.3, 128.0, 127.7, 127.4, 127.3, 122.8, 77.5, 77.2, 76.8, 70.9, 65.2, 65.1, 64.4, 46.9, 46.7, 30.7, 19.3, 14.0. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{41}\text{H}_{36}\text{NO}_5^+$ 622.2588; Found 622.2590. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 18.249 min, t_R (major) = 23.493 min, 8% ee. $[\alpha]_{\text{D}}^{25} = -111.23$ ($c = 0.23$, DCM).



Racemic

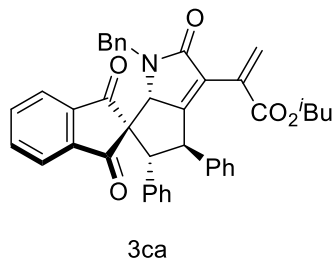
#	Time	Area	Height	Width	Area%	Symmetry
1	18.457	10976.4	225.9	0.7689	50.323	0.736
2	23.929	10835.4	185.9	0.9119	49.677	0.774



Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	18.249	2944.1	57.7	0.7635	8.753	0.793
2	23.493	30692.3	498	0.947	91.247	0.786

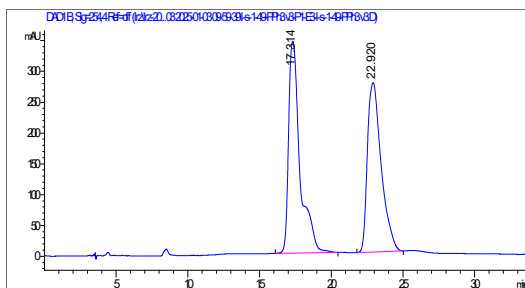
Isobutyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4,5-diphenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl) acrylate (**3ca**)



3ca

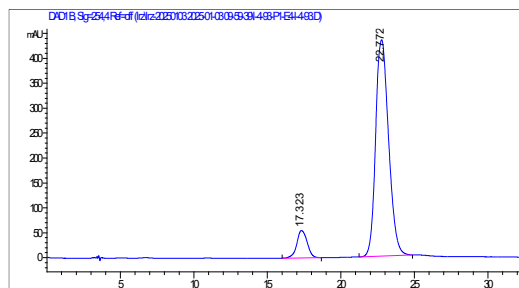
Light yellow solid, 26.2 mg, 84% yield, mp: 108.1-109.4 °C. ^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.60 – 7.57 (m, 1H), 7.54 – 7.49 (m, 2H), 7.46 – 7.43 (m, 1H), 7.18 (t, $J = 7.1$ Hz, 3H), 7.02 (dd, $J = 7.7, 1.8$ Hz, 2H), 7.00 – 6.95 (m, 5H), 6.93 (d, $J = 6.8$ Hz, 2H), 6.89 (s, 1H), 6.85 (s, 1H), 6.77 (d, $J = 7.3$ Hz, 1H), 6.41 (d, $J = 1.5$ Hz, 1H), 5.97 (d, $J = 1.4$ Hz, 1H), 5.09 (d, $J = 1.6$ Hz, 1H),

4.88 (dd, $J = 10.4, 1.6$ Hz, 1H), 4.50 (d, $J = 15.0$ Hz, 1H), 4.10 (d, $J = 15.0$ Hz, 1H), 3.96 – 3.88 (m, 2H), 3.78 (dd, $J = 10.6, 6.7$ Hz, 1H), 1.94 (dt, $J = 13.4, 6.7$ Hz, 1H), 0.93 (dd, $J = 6.7, 4.2$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 200.0, 196.4, 173.1, 165.6, 160.6, 142.4, 141.5, 140.8, 136.4, 135.7, 135.1, 134.4, 132.5, 130.3, 129.1, 129.0, 128.6, 128.5, 128.3, 128.0, 127.7, 127.4, 127.2, 122.9, 122.8, 77.5, 77.2, 76.8, 71.4, 70.9, 65.2, 64.2, 46.9, 46.6, 27.8, 19.3. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{41}\text{H}_{36}\text{NO}_5^+$ 622.2588; Found 622.2588. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 17.323 min, t_R (major) = 22.772 min, 82% ee. $[\alpha]_{\text{D}}^{25} = -111.31$ ($c = 0.21$, DCM).



Racemic

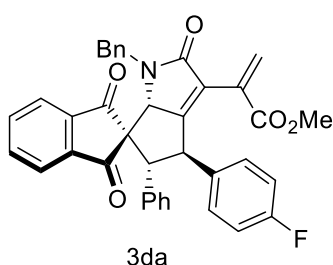
#	Time	Area	Height	Width	Area%	Symmetry
1	17.314	18927.7	343.8	0.8283	50.813	0.511
2	22.92	18322.2	274.7	0.99	49.187	0.647



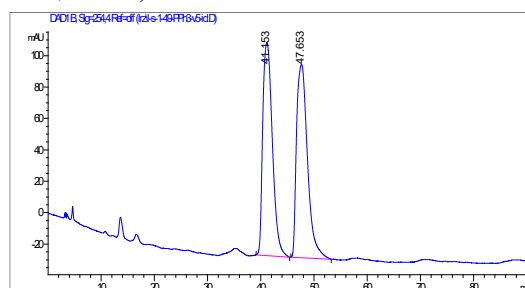
Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	17.323	2709.7	54.9	0.7514	9.262	0.841
2	22.772	26546.5	434.1	0.9355	90.738	0.807

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(4-fluorophenyl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3*da*)

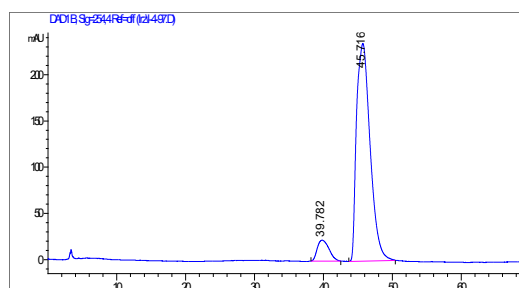


Light yellow solid, 18.9 mg, 63% yield, mp: 113.4-114.2 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.57 (m, 1H), 7.55 – 7.49 (m, 2H), 7.47 – 7.42 (m, 1H), 7.01 – 6.90 (m, 10H), 6.88 (dd, *J* = 8.2, 1.4 Hz, 3H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.49 (d, *J* = 1.3 Hz, 1H), 6.12 (d, *J* = 1.4 Hz, 1H), 5.10 (d, *J* = 1.6 Hz, 1H), 4.80 (dd, *J* = 10.4, 1.6 Hz, 1H), 4.51 (d, *J* = 15.0 Hz, 1H), 4.10 (d, *J* = 15.1 Hz, 1H), 3.82 (d, *J* = 10.4 Hz, 1H), 3.57 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 199.8, 196.6, 172.9, 166.0, 161.9 (*J* = 245.7 Hz), 160.2, 142.3, 141.4, 136.4, 136.3 (*J* = 3.8 Hz), 135.8, 135.2, 134.0, 131.7, 131.0, 129.0 (*J* = 8.8 Hz), 128.9, 128.6, 128.5, 128.4, 128.3, 128.2, 127.8, 122.9, 122.8, 115.9 (*J* = 21.4 Hz), 70.6, 65.0, 64.5, 52.2, 46.8, 46.1. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₂₉FN₂O₅⁺ 598.2024; Found 598.2029. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t_R* (minor) = 39.782 min, *t_R* (major) = 45.716 min, 84% ee. [α]_D²⁵ = -121.16 (c = 0.23, DCM).



Racemic

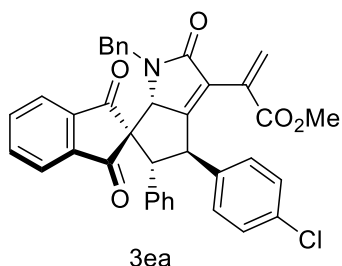
#	Time	Area	Height	Width	Area%	Symmetry
1	41.153	17027.9	135.8	1.4969	49.163	0.75
2	47.653	17607.4	123.2	1.6898	50.837	0.777



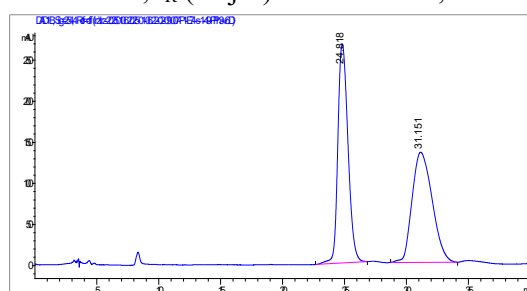
Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	39.782	2661.1	22.5	1.389	7.660	0.648
2	45.716	32080.2	235.3	1.6726	92.340	0.811

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(4-chlorophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6a-hexahydro-1H-spiro[cyclopenta[b]pyrrole-6,2'-inden]-3-yl)acrylate (3ea)

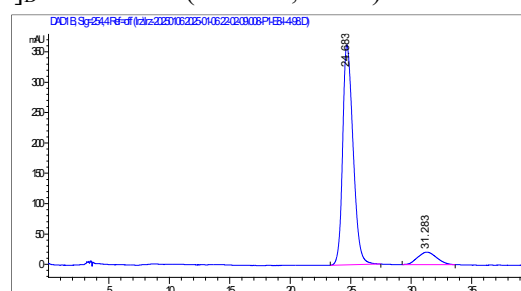


Light yellow solid, 17.8 mg, 58% yield, mp: 116.5-117.3 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.56 (m, 1H), 7.55 – 7.49 (m, 2H), 7.47 – 7.43 (m, 1H), 7.18 (d, *J* = 8.3 Hz, 2H), 6.98 – 6.91 (m, 8H), 6.87 (t, *J* = 7.6 Hz, 2H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.50 (d, *J* = 1.3 Hz, 1H), 6.14 (d, *J* = 1.3 Hz, 1H), 5.09 (d, *J* = 1.6 Hz, 1H), 4.80 (dd, *J* = 10.5, 1.6 Hz, 1H), 4.52 (d, *J* = 15.0 Hz, 1H), 4.10 (d, *J* = 15.0 Hz, 1H), 3.81 (d, *J* = 10.5 Hz, 1H), 3.57 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.8, 196.6, 172.8, 166.0, 159.9, 142.3, 141.4, 139.1, 136.3, 135.8, 135.2, 133.9, 133.1, 131.7, 131.1, 129.1, 129.0, 128.8, 128.7, 128.5, 128.4, 128.3, 128.2, 127.8, 122.9, 122.8, 77.5, 77.2, 76.8, 70.7, 65.0, 64.4, 52.2, 46.9, 46.3. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₂₉ClNO₅⁺ 614.1729; Found 614.1730. HPLC conditions: Daicel Chiralpak IA-3 column, *n*-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t_R* (minor) = 31.283 min, *t_R* (major) = 24.683 min, 81% ee. [α]_D²⁵ = -101.00 (*c* = 0.22, DCM).



Racemic

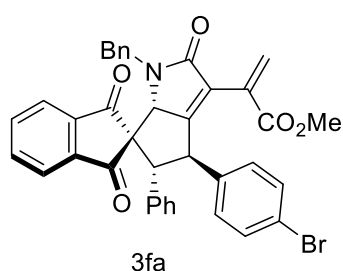
#	Time	Area	Height	Width	Area%	Symmetry
1	24.818	15186.8	267	0.8877	50.079	0.742
2	31.151	15138.8	134.2	1.356	49.921	0.729



Chiral

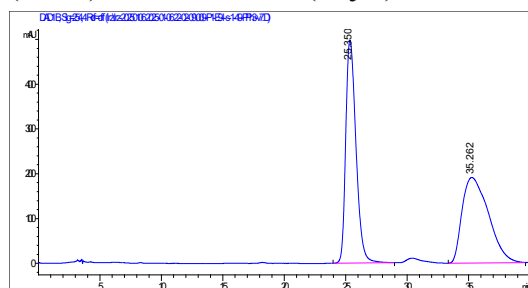
#	Time	Area	Height	Width	Area%	Symmetry
1	24.683	21713.8	362.5	0.9149	90.605	0.652
2	31.283	2251.6	20.7	1.2836	9.395	0.894

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(4-bromophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6a-hexahydro-1H-spiro[cyclopenta[b]pyrrole-6,2'-inden]-3-yl)acrylate (3fa)



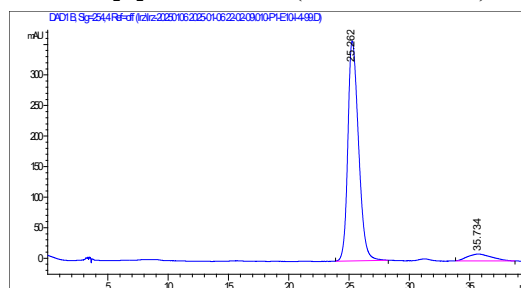
Light yellow solid, 16.9 mg, 51% yield, mp: 138.1-139.6 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.56 (m, 1H), 7.54 – 7.49 (m, 2H), 7.46 – 7.43 (m, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 6.98 – 6.90 (m, 8H), 6.89 – 6.85 (m, 3H), 6.77 (d, *J* = 7.2 Hz, 1H), 6.50 (d, *J* = 1.4 Hz, 1H), 6.14 (d, *J* = 1.3 Hz, 1H), 5.08 (d, *J* = 1.6 Hz, 1H), 4.78 (dd, *J* = 10.5, 1.6 Hz, 1H), 4.52 (d, *J* = 15.0 Hz, 1H), 4.09 (d, *J* = 15.1 Hz, 1H), 3.80 (d, *J* = 10.5 Hz, 1H), 3.57 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.7, 196.6, 172.8, 166.0, 159.8, 142.3, 141.4, 139.6, 136.3, 135.8,

135.2, 133.9, 132.1, 131.7, 131.2, 129.2, 129.0, 128.7, 128.5, 128.4, 128.3, 128.2, 127.8, 122.9, 122.8, 121.2, 77.5, 77.2, 76.8, 70.7, 65.0, 64.3, 52.2, 46.9, 46.4. HRMS (ESI) m/z : $[M+H]^+$ Calcd for $C_{38}H_{29}BrNO_5^+$ 658.1224; Found 658.1230. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 35.734 min, t_R (major) = 25.262 min, 87% ee. $[\alpha]_D^{25}$ = -90.90 (c = 0.24, DCM).



Racemic

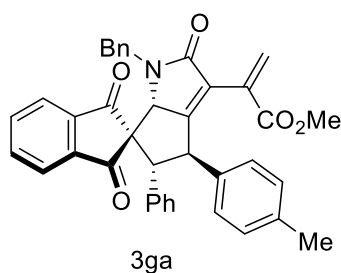
#	Time	Area	Height	Width	Area%	Symmetry
1	25.35	28856.7	497.6	0.8946	50.368	0.662
2	35.262	28435	190.8	1.7522	49.632	0.565



Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	25.262	22111.5	360.1	0.9383	93.490	0.662
2	35.734	1539.8	11.2	1.6149	6.510	0.788

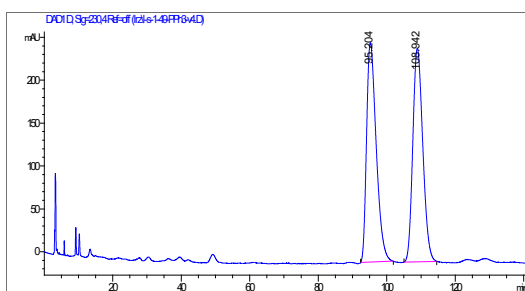
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-5-phenyl-4-(*p*-tolyl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ga)



Light yellow solid, 26.1 mg, 88% yield, mp: 105.7-106.7 °C.

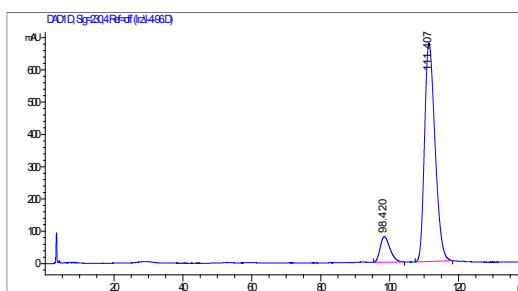
1H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.55 (m, 1H), 7.53 – 7.48 (m, 2H), 7.46 – 7.41 (m, 1H), 7.01 (d, J = 7.8 Hz, 2H), 6.96 – 6.84 (m, 11H), 6.75 (t, J = 7.3 Hz, 1H), 6.46 (d, J = 1.4 Hz, 1H), 6.05 (d, J = 1.4 Hz, 1H), 5.12 (d, J = 1.6 Hz, 1H), 4.77 (dd, J = 10.4, 1.6 Hz, 1H), 4.54 (d, J = 15.0 Hz, 1H), 4.09 (d, J

= 15.0 Hz, 1H), 3.87 (d, J = 10.4 Hz, 1H), 3.57 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.0, 196.7, 173.0, 166.2, 161.0, 142.3, 141.4, 137.6, 136.9, 136.4, 135.7, 135.0, 134.4, 131.9, 130.8, 129.6, 128.6, 128.5, 128.4, 128.3, 128.2, 128.0, 127.7, 127.3, 122.9, 122.8, 77.5, 77.2, 76.8, 70.8, 65.1, 64.6, 52.1, 46.9, 46.4, 21.1. HRMS (ESI) m/z : $[M+H]^+$ Calcd for $C_{39}H_{32}NO_5^+$ 594.2275; Found 594.2275. HPLC conditions: Daicel Chiralpak IC-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 230 nm, retention time: t_R (minor) = 98.42 min, t_R (major) = 111.407 min, 80% ee. $[\alpha]_D^{25}$ = -108.71 (c = 0.23, DCM)



Racemic

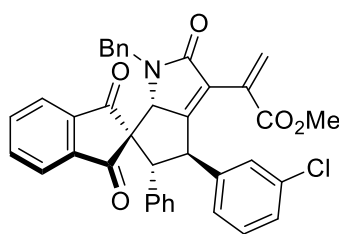
#	Time	Area	Height	Width	Area%	Symmetry
1	95.204	50021.9	256.1	2.2908	49.883	0.611
2	108.94	50256.3	248.9	2.3613	50.117	0.818



Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	98.42	15697.6	79.4	2.3177	9.922	0.684
2	111.407	142517.2	677	2.47	90.078	0.703

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(3-chlorophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ha)

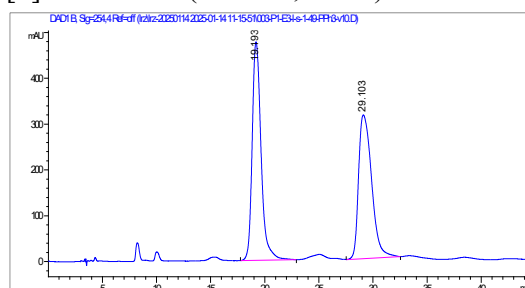


3ha

Light yellow solid, 22.3 mg, 73% yield, mp: 120.7-121.1 °C.

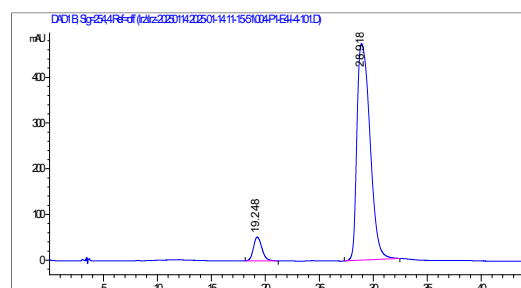
¹H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.56 (m, 1H), 7.53 – 7.49 (m, 2H), 7.45 – 7.42 (m, 1H), 7.16 – 7.12 (m, 2H), 7.04 (t, *J* = 1.9 Hz, 1H), 6.98 – 6.91 (m, 7H), 6.89 – 6.84 (m, 3H), 6.76 (d, *J* = 7.3 Hz, 1H), 6.53 (d, *J* = 1.4 Hz, 1H), 6.16 (d, *J* = 1.3 Hz, 1H), 5.11 (d, *J* = 1.6 Hz, 1H), 4.79 (dd, *J* = 10.4,

1.6 Hz, 1H), 4.57 (d, *J* = 15.0 Hz, 1H), 4.08 (d, *J* = 15.1 Hz, 1H), 3.85 (d, *J* = 10.5 Hz, 1H), 3.57 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.7, 196.6, 172.8, 166.0, 159.6, 142.5, 142.3, 141.4, 136.3, 135.8, 135.2, 134.7, 133.8, 131.6, 131.3, 130.2, 129.1, 128.7, 128.5, 128.4, 128.3, 128.2, 127.8, 127.6, 127.5, 125.8, 122.9, 122.8, 77.5, 77.2, 76.8, 70.7, 64.9, 64.3, 52.2, 46.9, 46.4. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₂₉ClNO₅⁺ 614.1729; Found 614.1733. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 19.248 min, *t*_R (major) = 28.918 min, 87% ee. [α]_D²⁵ = -98.00 (c = 0.23, DCM).



Racemic

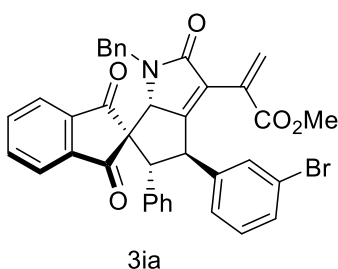
#	Time	Area	Height	Width	Area%	Symmetry
1	19.193	27258.5	477.1	0.8786	50.974	0.707
2	29.103	26216.5	313.6	1.3173	49.026	0.546



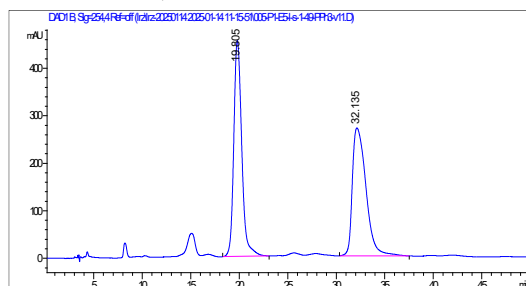
Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	19.248	2833.2	52	0.7859	6.649	0.779
2	28.918	39779.5	473.8	1.1696	93.351	0.528

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(3-bromophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ia)

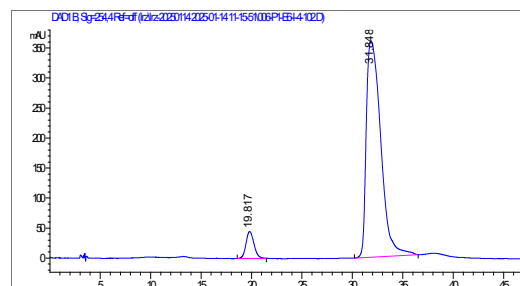


Light yellow solid, 26.4 mg, 80% yield, mp: 130.5-132.2 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.55 (m, 1H), 7.53 – 7.48 (m, 2H), 7.45 – 7.41 (m, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.20 (t, *J* = 1.8 Hz, 1H), 7.08 (d, *J* = 7.8 Hz, 1H), 6.98 – 6.91 (m, 7H), 6.86 (t, *J* = 7.6 Hz, 2H), 6.76 (s, 1H), 6.54 (d, *J* = 1.3 Hz, 1H), 6.17 (d, *J* = 1.4 Hz, 1H), 5.10 (d, *J* = 1.6 Hz, 1H), 4.78 (d, *J* = 11.7 Hz, 1H), 4.58 (d, *J* = 15.0 Hz, 1H), 4.07 (d, *J* = 15.1 Hz, 1H), 3.84 (d, *J* = 10.5 Hz, 1H), 3.57 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.7, 196.6, 172.8, 166.0, 159.5, 142.8, 142.3, 141.4, 136.3, 135.8, 135.2, 133.8, 131.6, 131.4, 130.5, 130.4, 130.3, 129.2, 128.7, 128.5, 128.4, 128.3, 127.8, 126.3, 123.0, 122.9, 77.5, 77.2, 76.8, 70.7, 64.9, 64.3, 52.2, 46.9, 46.3. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₂₉ClNO₅⁺ 658.1224; Found 658.1228. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 19.817 min, *t*_R (major) = 31.848 min, 87% ee. [α]_D²⁵ = -98.70 (c = 0.23, DCM).



Racemic

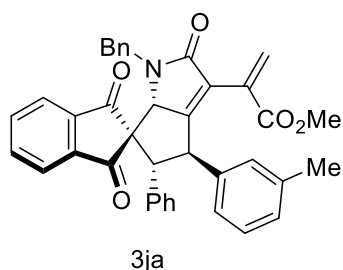
#	Time	Area	Height	Width	Area%	Symmetry
1	19.805	26003.9	454.8	0.8791	49.753	0.75
2	32.135	26262.3	269.3	1.3117	50.247	0.477



Chiral

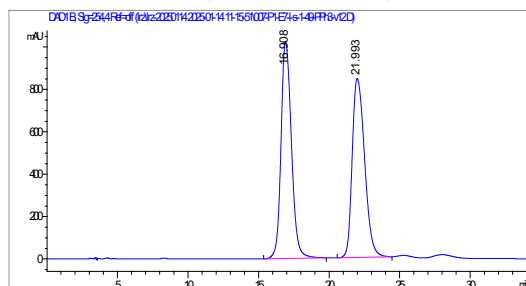
#	Time	Area	Height	Width	Area%	Symmetry
1	19.817	2463.1	44.9	0.7785	6.432	0.816
2	31.848	35831.9	360.4	1.3498	93.568	0.448

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-5-phenyl-4-(*m*-tolyl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ja)



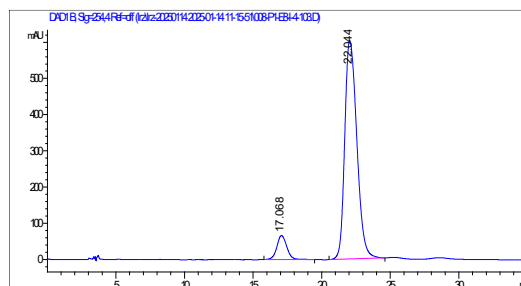
Light yellow solid, 26.4 mg, 89% yield, mp: 119.8-129.8 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.57 (ddt, *J* = 7.3, 3.4, 1.7 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.45 – 7.41 (m, 1H), 7.08 (s, 1H), 6.99 – 6.92 (m, 8H), 6.86 (t, *J* = 7.6 Hz, 3H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.75 (t, *J* = 7.3 Hz, 1H), 6.47 (d, *J* = 1.4 Hz, 1H), 6.05 (d, *J* = 1.4 Hz, 1H), 5.13 (d, *J* = 1.6 Hz, 1H), 4.75 (dd, *J* = 10.3, 1.6 Hz, 1H), 4.56 (d, *J* = 15.0 Hz, 1H), 4.08 (d, *J* = 15.0 Hz, 1H), 3.90 (d, *J* = 10.3 Hz, 1H), 3.54 (s, 3H), 2.24

(s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 200.0, 196.7, 173.0, 166.2, 160.9, 142.3, 141.4, 140.5, 138.6, 136.4, 135.7, 135.0, 134.3, 131.9, 130.9, 128.8, 128.7, 128.5, 128.4, 128.3, 128.1, 128.0, 127.7, 124.7, 122.9, 122.8, 77.5, 77.2, 76.8, 70.8, 65.1, 64.5, 52.1, 46.9, 46.6, 21.5. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{39}\text{H}_{32}\text{NO}_5^+$ 594.2275; Found 594.2277. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 17.068 min, t_R (major) = 22.044 min, 83% ee. $[\alpha]_D^{25}$ = -115.60 (c = 0.20, DCM).



Racemic

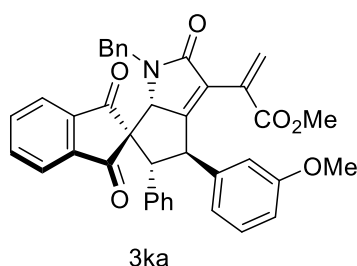
#	Time	Area	Height	Width	Area%	Symmetry
1	16.908	52387.8	1024.8	0.7864	50.319	0.729
2	21.993	51723.4	844.4	0.9566	49.681	0.659



Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	17.068	3343.5	66.2	0.7188	8.326	0.836
2	22.044	36811.9	602.6	0.9567	91.674	0.674

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(3-methoxyphenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ka)

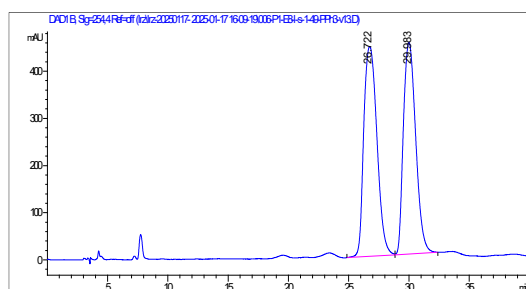


3ka

Light yellow solid, 19.8 mg, 65% yield, mp: 107.5-108.1 °C.

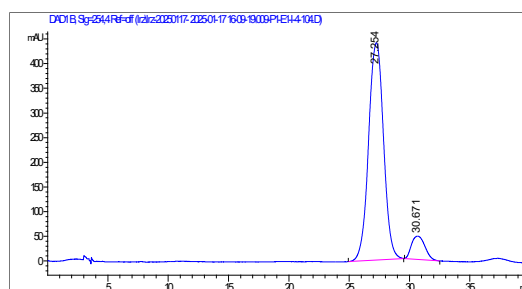
^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.59 – 7.56 (m, 1H), 7.53 – 7.48 (m, 2H), 7.46 – 7.42 (m, 1H), 7.12 (d, J = 7.9 Hz, 1H), 6.94 (d, J = 18.0 Hz, 7H), 6.86 (t, J = 7.6 Hz, 2H), 6.76 (d, J = 7.3 Hz, 1H), 6.71 (dd, J = 7.8, 2.4 Hz, 1H), 6.61 (d, J = 8.0 Hz, 1H), 6.53 (t, J = 2.1 Hz, 1H), 6.49 (d, J = 1.4 Hz, 1H),

6.09 (d, J = 1.3 Hz, 1H), 5.10 (d, J = 1.6 Hz, 1H), 4.78 (dd, J = 10.3, 1.6 Hz, 1H), 4.54 (d, J = 15.0 Hz, 1H), 4.09 (d, J = 15.0 Hz, 1H), 3.89 (d, J = 10.4 Hz, 1H), 3.66 (s, 3H), 3.59 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 199.9, 196.7, 173.0, 160.5, 159.9, 142.1, 136.4, 135.7, 135.1, 134.4, 131.9, 131.0, 130.0, 128.6, 128.4, 128.1, 127.7, 122.9, 122.8, 119.7, 113.4, 112.4, 77.5, 77.2, 76.8, 70.8, 65.1, 64.3, 55.3, 52.2, 46.9, 46.7. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{39}\text{H}_{32}\text{NO}_6^+$ 610.2224; Found 610.2229. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 30.671 min, t_R (major) = 27.254 min, 82% ee. $[\alpha]_D^{25}$ = -88.85 (c = 0.24, DCM).



Racemic

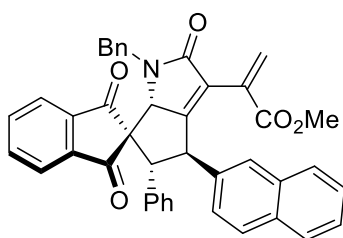
#	Time	Area	Height	Width	Area%	Symmetry
1	26.722	33749.5	444.9	0.931	51.508	0.709
2	29.983	31773.6	448.4	0.8587	48.492	0.722



Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	27.254	37910.2	441.1	1.0226	91.240	1.053
2	30.671	3639.9	47.1	0.9154	8.760	0.807

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(naphthalen-2-yl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3la)

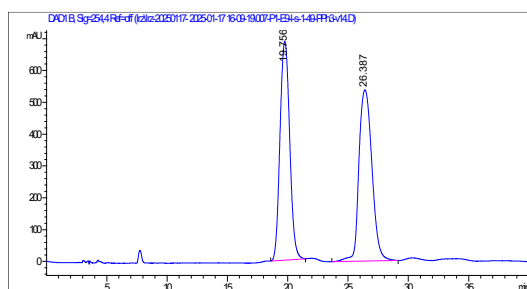


3la

Light yellow solid, 10.7 mg, 34% yield, mp: 113.1-114.2 °C. ¹H

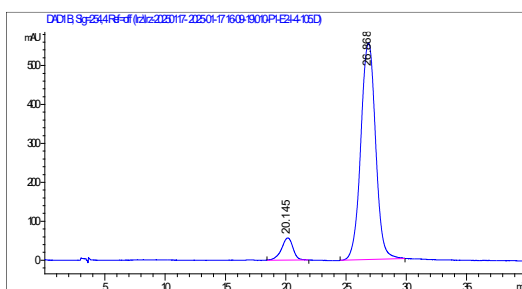
NMR (400 MHz, Chloroform-*d*) δ 7.77 – 7.74 (m, 1H), 7.70 (t, *J* = 8.1 Hz, 2H), 7.60 – 7.57 (m, 1H), 7.53 – 7.48 (m, 3H), 7.47 – 7.41 (m, 3H), 7.15 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.96 (d, *J* = 8.1 Hz, 7H), 6.88 (t, *J* = 7.6 Hz, 2H), 6.76 (t, *J* = 7.3 Hz, 1H), 6.45 (d, *J* = 1.4 Hz, 1H), 6.08 (d, *J* = 1.4 Hz, 1H), 5.22 (d, *J* = 1.6 Hz, 1H),

4.97 (dd, *J* = 10.4, 1.6 Hz, 1H), 4.60 (d, *J* = 15.0 Hz, 1H), 4.12 (d, *J* = 15.0 Hz, 1H), 3.98 (d, *J* = 10.4 Hz, 1H), 3.42 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 200.0, 196.7, 173.0, 166.1, 160.6, 142.4, 141.5, 138.0, 136.4, 135.7, 135.1, 134.2, 132.6, 131.8, 131.1, 129.1, 128.9, 128.6, 128.5, 128.4, 128.3, 128.1, 127.8, 127.7, 126.5, 126.3, 126.1, 125.5, 122.9, 122.8, 77.5, 77.2, 76.8, 70.9, 65.1, 64.5, 52.1, 47.0, 46.9. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₄₂H₃₂NO₅⁺ 630.2275; Found 630.2280. HPLC conditions: Daicel Chiralpak IA-3 column, *n*-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 20.145 min, *t*_R (major) = 26.868 min, 85% ee. [α]_D²⁵ = -108.20 (c = 0.20, DCM).



Racemic

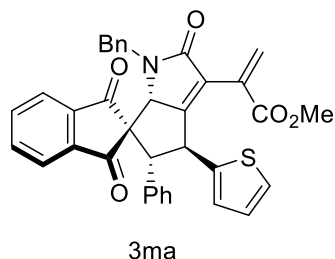
#	Time	Area	Height	Width	Area%	Symmetry
1	19.756	38284.8	687.1	0.7761	48.691	0.933
2	26.387	40342.5	538.5	0.8879	51.309	0.79



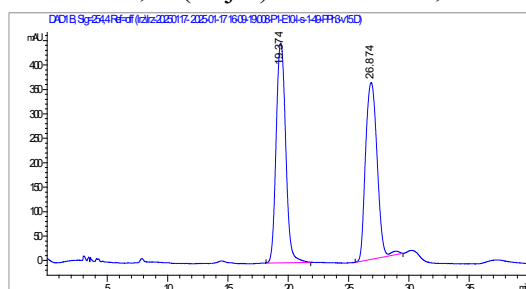
Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	20.145	3766.8	56.9	0.7837	7.355	1.089
2	26.868	47444.4	556.5	1.0122	92.645	1.066

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-5-phenyl-4-(thiophen-2-yl)-1',2,3',4,5,6a-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ma)

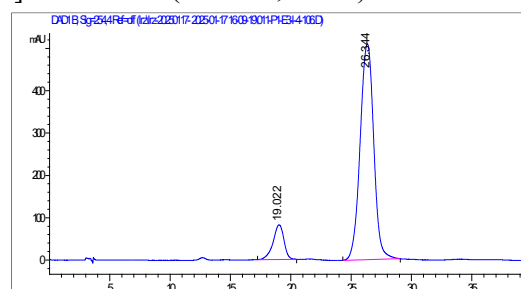


Light yellow solid, 11.3 mg, 38% yield, mp: 103.5-104.5 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.57 (m, 1H), 7.54 – 7.48 (m, 2H), 7.45 – 7.41 (m, 1H), 7.10 (d, *J* = 5.0 Hz, 1H), 7.00 (s, 5H), 6.91 (d, *J* = 7.2 Hz, 2H), 6.87 – 6.82 (m, 3H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.68 (d, *J* = 3.5 Hz, 1H), 6.57 (s, 1H), 6.25 (s, 1H), 5.15 (d, *J* = 10.4 Hz, 1H), 5.08 (d, *J* = 1.5 Hz, 1H), 4.57 (d, *J* = 15.1 Hz, 1H), 4.05 (d, *J* = 15.1 Hz, 1H), 3.98 (d, *J* = 10.4 Hz, 1H), 3.72 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 199.7, 196.5, 172.9, 166.1, 159.8, 142.5, 141.7, 140.1, 137.1, 136.3, 135.9, 135.3, 131.6, 131.2, 129.0, 128.8, 128.5, 128.4, 127.8, 127.6, 127.5, 127.1, 126.8, 125.3, 123.1, 123.0, 77.4, 77.2, 76.9, 70.5, 64.9, 59.2, 52.1, 49.4, 46.9. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₆H₂₈NO₅S⁺ 586.1683; Found 586.1686. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 19.022 min, *t*_R (major) = 26.344 min, 77% ee. [α]_D²⁵ = -61.30 (c = 0.20, DCM).



Racemic

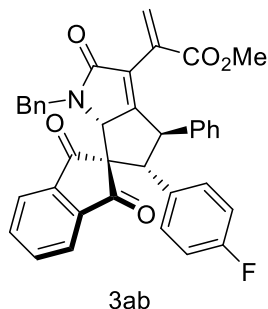
#	Time	Area	Height	Width	Area%	Symmetry
1	19.374	24700.7	449.5	0.725	50.563	0.872
2	26.874	24150.8	361.7	0.7739	49.437	0.921



Chiral

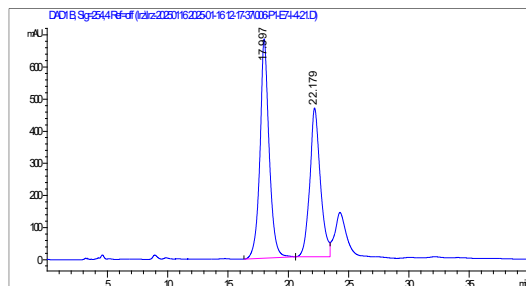
#	Time	Area	Height	Width	Area%	Symmetry
1	19.022	5124.3	81.8	0.7391	11.393	1.187
2	26.344	39853.4	509.4	0.9268	88.607	1.084

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-fluorophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6a-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ab)



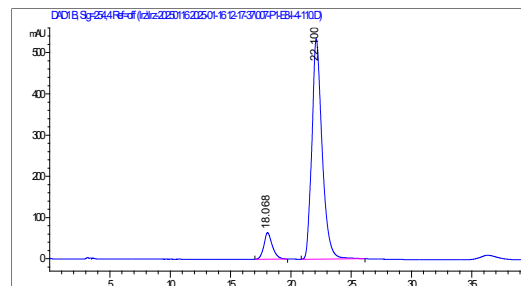
Light yellow solid, 21.7 mg, 73% yield, mp: 113.0-113.8 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.53 (m, 3H), 7.47 (dd, *J* = 6.0, 2.7 Hz, 1H), 7.23 – 7.18 (m, 3H), 7.02 – 6.98 (m, 2H), 6.96 – 6.90 (m, 4H), 6.87 (d, *J* = 7.8 Hz, 2H), 6.78 (d, *J* = 7.2 Hz, 1H), 6.67 (t, *J* = 8.6 Hz, 2H), 6.47 (d, *J* = 1.3 Hz, 1H), 6.07 (d, *J* = 1.3 Hz, 1H), 5.10 (d, *J* = 1.6 Hz, 1H), 4.73 (dd, *J* = 10.4, 1.6 Hz, 1H), 4.50 (d, *J* = 15.0 Hz, 1H), 4.10 (d, *J* = 15.0 Hz, 1H), 3.86 (d, *J* = 10.4 Hz, 1H), 3.52 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.8, 196.6, 172.9, 166.1, 162.3 (*J* = 257.6 Hz), 160.3, 142.3,

141.4, 140.5, 136.3, 136.0, 135.3, 131.8, 131.0, 130.3 ($J = 4.0$ Hz), 130.2, 129.0, 128.8, 128.4, 128.4, 127.8, 127.4, 127.4, 123.0, 122.9 ($J = 7.1$ Hz), 115.5 ($J = 21.2$ Hz), 77.5, 77.2, 76.8, 70.8, 65.0, 63.7, 52.1, 47.2, 46.9. HRMS (ESI) m/z : $[M+H]^+$ Calcd for $C_{38}H_{29}FNO_5^+$ 598.2024; Found 598.2028. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 18.068 min, t_R (major) = 22.1 min, 82% ee. $[\alpha]_D^{25} = -97.65$ ($c = 0.23$, DCM).



Racemic

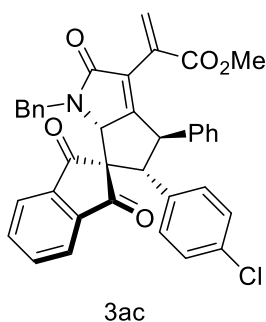
#	Time	Area	Height	Width	Area%	Symmetry
1	17.997	36107.7	683.1	0.7547	56.056	0.818
2	22.179	28306.4	463.8	0.866	43.944	0.809



Chiral

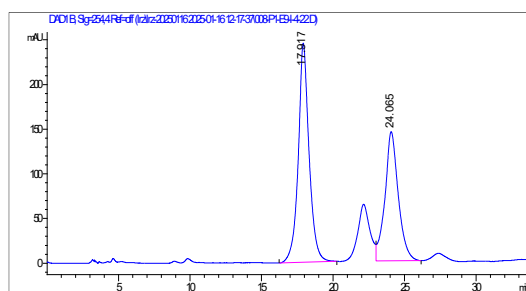
#	Time	Area	Height	Width	Area%	Symmetry
1	18.068	3149.7	64.6	0.6844	9.060	0.751
2	22.1	31612.9	534.3	0.8422	90.940	0.699

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-chlorophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ac)



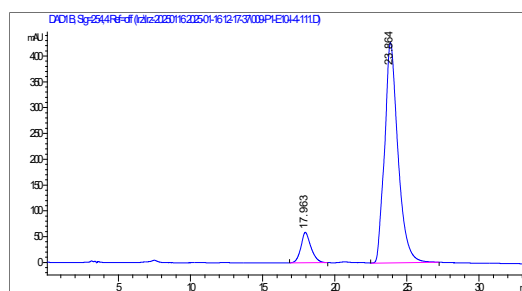
Light yellow solid, 24.6 mg, 80% yield, mp: 118.5-120.5 °C. 1H NMR (400 MHz, Chloroform-*d*) δ 7.63 – 7.55 (m, 3H), 7.50-7.47 (m, 3.1 Hz, 1H), 7.24 – 7.17 (m, 3H), 7.01 – 6.96 (m, 3H), 6.95 – 6.87 (m, 7H), 6.80 (t, $J = 6.9$ Hz, 1H), 6.47 (d, $J = 1.3$ Hz, 1H), 6.06 (d, $J = 1.3$ Hz, 1H), 5.09 (d, $J = 1.6$ Hz, 1H), 4.74 (dd, $J = 10.4, 1.6$ Hz, 1H), 4.45 (d, $J = 15.0$ Hz, 1H), 4.13 (d, $J = 15.1$ Hz, 1H), 3.86 (d, $J = 10.4$ Hz, 1H), 3.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.7, 196.5, 172.9,

166.1, 160.2, 142.2, 141.4, 140.4, 136.3, 136.1, 135.5, 134.0, 133.0, 131.7, 131.0, 129.9, 129.1, 128.9, 128.8, 128.4, 128.3, 127.8, 127.4, 123.1, 123.0, 77.5, 77.2, 76.8, 70.9, 65.0, 63.6, 52.1, 47.2, 46.9. HRMS (ESI) m/z : $[M+H]^+$ Calcd for $C_{38}H_{29}ClNO_5^+$ 614.1729; Found 614.1733. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, $\lambda = 254$ nm, retention time: t_R (minor) = 17.963 min, t_R (major) = 23.864 min, 81% ee. $[\alpha]_D^{25} = -100.28$ ($c = 0.21$, DCM).



Racemic

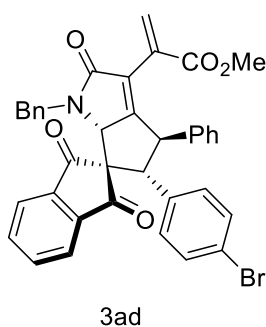
#	Time	Area	Height	Width	Area%	Symmetry
1	17.917	12881.3	245.5	0.7421	57.902	0.843
2	24.065	9365.4	144.6	0.9197	42.098	0.86



Chiral

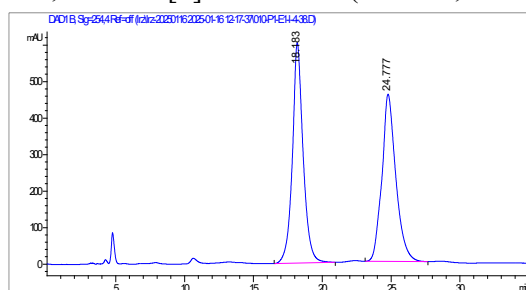
#	Time	Area	Height	Width	Area%	Symmetry
1	17.963	2869.4	59	0.6889	9.416	0.752
2	23.864	27605.1	426.7	0.9168	90.584	0.74

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-bromophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ad)



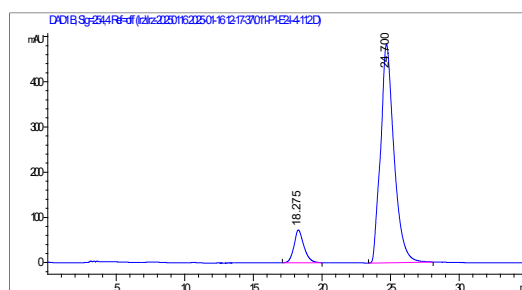
Light yellow solid, 31.0 mg, 94% yield, mp: 121.4-122.6 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 7.6 Hz, 1H), 7.83 (td, *J* = 7.4, 1.1 Hz, 1H), 7.75 (td, *J* = 7.4, 1.1 Hz, 1H), 7.67 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.33 (dd, *J* = 8.0, 6.6 Hz, 2H), 7.29 – 7.25 (m, 2H), 7.20 (d, *J* = 7.2 Hz, 2H), 7.14 – 7.06 (m, 3H), 6.95 (d, *J* = 8.2 Hz, 2H), 6.85 – 6.76 (m, 2H), 6.45 (d, *J* = 24.5 Hz, 2H), 4.89 (d, *J* = 15.1 Hz, 1H), 4.47 (d, *J* = 11.4 Hz, 1H), 4.25 (d, *J* = 15.1 Hz, 1H), 3.99 (d, *J* = 11.3 Hz, 1H),

3.87 (s, 3H), 3.77 (d, *J* = 19.5 Hz, 1H), 3.44 (d, *J* = 19.5 Hz, 1H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 200.3, 197.5, 168.1, 157.7, 142.9, 141.1, 140.1, 137.1, 136.4, 136.3, 135.0, 132.7, 131.3, 129.0, 128.9, 128.5, 127.9, 127.7, 127.6, 124.1, 123.7, 121.3, 61.9, 54.6, 53.5, 52.8, 52.5, 46.2, 29.8. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₂₉BrNO₅⁺ 658.1224; Found 658.1230. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 18.275 min, *t*_R (major) = 24.7 min, 80% ee. [α]_D²⁵ = -94.09 (c = 0.21, DCM).



Racemic

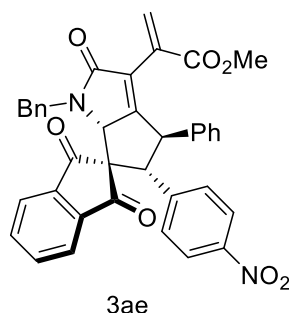
#	Time	Area	Height	Width	Area%	Symmetry
1	18.183	32647.9	603.7	0.7749	50.298	0.813
2	24.777	32261.2	458.3	0.9893	49.702	0.775



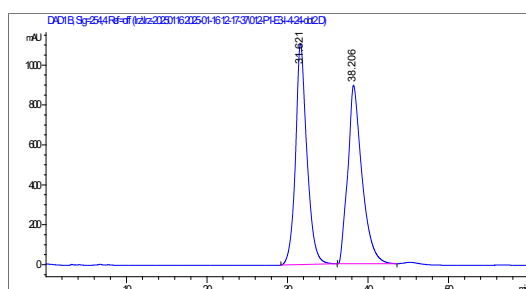
Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	18.275	3638.3	72.7	0.7122	9.956	0.746
2	24.7	32904.8	483.8	0.9494	90.044	0.747

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-nitrophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ae)

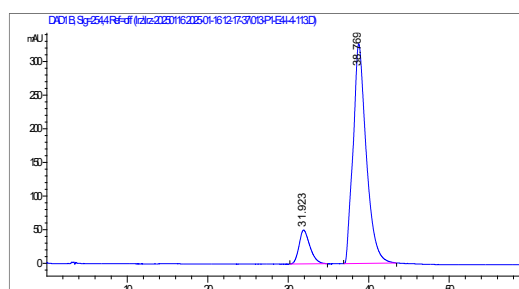


Light yellow solid, 20.0 mg, 64% yield, mp: 117.3-119.8 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 – 7.82 (m, 2H), 7.65 – 7.55 (m, 3H), 7.53 – 7.48 (m, 1H), 7.21 (dd, *J* = 16.0, 7.9 Hz, 5H), 7.02 – 6.97 (m, 2H), 6.96 – 6.87 (m, 4H), 6.83 (td, *J* = 5.8, 2.9 Hz, 1H), 6.48 (d, *J* = 1.3 Hz, 1H), 6.08 (d, *J* = 1.3 Hz, 1H), 5.11 (d, *J* = 1.6 Hz, 1H), 4.85 (dd, *J* = 10.3, 1.6 Hz, 1H), 4.41 (d, *J* = 15.1 Hz, 1H), 4.15 (d, *J* = 15.1 Hz, 1H), 3.99 (d, *J* = 10.4 Hz, 1H), 3.53 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.3, 196.1, 172.9, 166.0, 159.5, 147.6, 142.1, 142.0, 141.2, 140.1, 136.4, 136.2, 135.8, 131.6, 131.3, 129.7, 129.2, 129.1, 128.5, 128.3, 127.9, 127.7, 127.3, 123.8, 123.2, 123.1, 77.5, 77.2, 76.8, 71.1, 64.9, 63.4, 52.2, 47.3, 46.9. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₂₉N₂O₇⁺ 625.1969; Found 625.1974. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 31.923 min, *t*_R (major) = 38.769 min, 77% ee. [α]_D²⁵ = -94.09 (c = 0.21, DCM).



Racemic

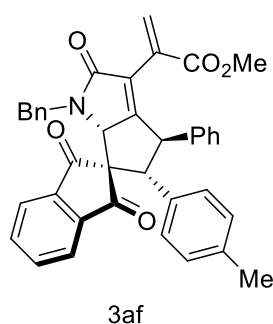
#	Time	Area	Height	Width	Area%	Symmetry
1	31.621	108826.6	1109.7	1.2662	49.854	0.747
2	38.206	109466.2	895.1	1.5668	50.146	0.652



Chiral

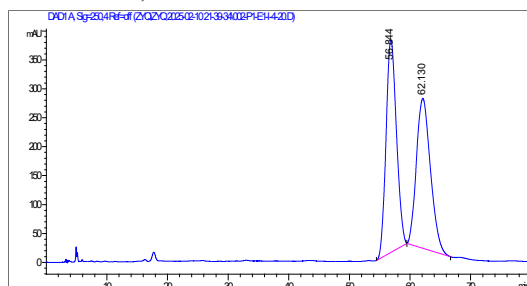
#	Time	Area	Height	Width	Area%	Symmetry
1	31.923	4748.1	50.5	1.1099	11.337	0.722
2	38.769	37132.2	326.6	1.5166	88.663	0.722

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4-phenyl-5-(*m*-tolyl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3af)



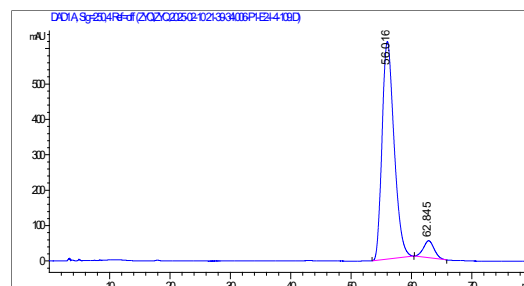
Light yellow solid, 22.6 mg, 76% yield, mp: 96.1-97.9 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.56 (m, 1H), 7.53 – 7.49 (m, 2H), 7.46 – 7.42 (m, 1H), 7.21-7.19 (m, 2H), 7.17 (d, *J* = 6.6 Hz, 1H), 7.05 – 7.01 (m, 2H), 6.93 (d, *J* = 7.6 Hz, 2H), 6.89 – 6.83 (m, 3H), 6.75 (dd, *J* = 12.3, 7.3 Hz, 4H), 6.47 (d, *J* = 1.2 Hz, 1H), 6.07 (s, 1H), 5.12 (d, *J* = 1.4 Hz, 1H), 4.76 (d, *J* = 10.4 Hz, 1H), 4.53 (d, *J* = 15.0 Hz, 1H), 4.10 (d, *J* = 15.1 Hz, 1H), 3.85 (d, *J* = 10.4 Hz, 1H), 3.51 (s, 3H), 2.05 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 200.0, 196.6, 173.0, 166.2, 160.7, 142.4, 141.5, 140.8,

138.1, 136.4, 135.7, 135.0, 134.1, 131.9, 130.9, 129.2, 129.0, 128.8, 128.5, 128.4, 127.7, 127.5, 127.2, 125.5, 122.8, 122.7, 77.5, 77.2, 76.8, 70.7, 65.1, 64.5, 52.1, 46.8, 46.7, 21.3. HRMS (ESI) m/z : $[M+H]^+$ Calcd for $C_{39}H_{32}NO_5^+$ 594.2275; Found 594.2278. HPLC conditions: Daicel Chiralpak IF-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 250 nm, retention time: t_R (minor) = 56.016 min, t_R (major) = 62.845 min, 87% ee. $[\alpha]_D^{25}$ = -93.19 (c = 0.24, DCM).



Racemic

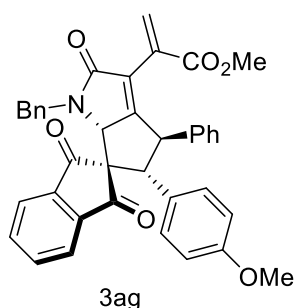
#	Time	Area	Height	Width	Area%	Symmetry
1	56.844	43810.1	367.2	1.4899	51.237	0.823
2	62.13	41694.3	259	1.9158	48.763	0.84



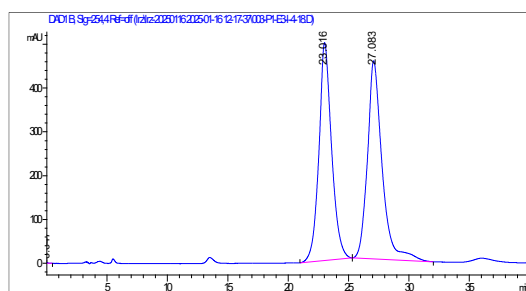
Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	56.016	85062.9	614.7	1.6305	93.390	0.759
2	62.845	6020.4	48.3	1.4792	6.610	0.923

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-methoxyphenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ag)

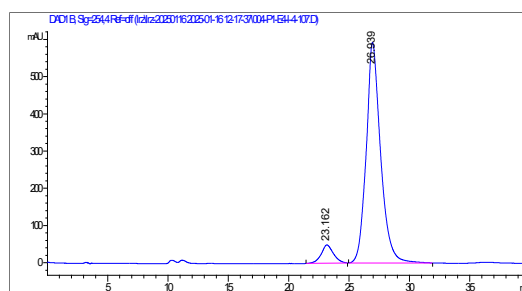


Light yellow solid, 27.7 mg, 91% yield, mp: 153.0-154.0 °C. 1H NMR (500 MHz, Chloroform-*d*) δ 7.93 (d, J = 7.7 Hz, 1H), 7.81 – 7.77 (m, 1H), 7.69 (t, J = 7.5 Hz, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.33 (t, J = 7.3 Hz, 2H), 7.26 (d, J = 14.7 Hz, 2H), 7.21 (d, J = 7.1 Hz, 2H), 7.07 (dd, J = 4.9, 1.9 Hz, 3H), 6.86 – 6.79 (m, 2H), 6.50 – 6.47 (m, 2H), 6.33 (d, J = 8.3 Hz, 2H), 4.89 (d, J = 15.1 Hz, 1H), 4.46 (d, J = 11.3 Hz, 1H), 4.26 (d, J = 15.1 Hz, 1H), 3.97 (d, J = 11.3 Hz, 1H), 3.87 (s, 3H), 3.77 (d, J = 19.5 Hz, 1H), 3.55 (s, 3H), 3.44 (d, J = 19.5 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.7, 198.0, 169.5, 168.2, 158.3, 157.9, 143.1, 141.3, 140.6, 137.1, 136.2, 136.1, 135.4, 132.5, 131.2, 128.9, 128.8, 128.5, 127.9, 127.6, 127.3, 126.5, 123.8, 123.4, 77.4, 77.2, 76.9, 62.3, 55.0, 54.9, 53.6, 52.8, 52.7, 46.1. HRMS (ESI) m/z : $[M+H]^+$ Calcd for $C_{39}H_{32}NO_6^+$ 610.2224; Found 610.2226. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 23.162 min, t_R (major) = 26.939 min, 87% ee. $[\alpha]_D^{25}$ = -90.27 (c = 0.22, DCM).



Racemic

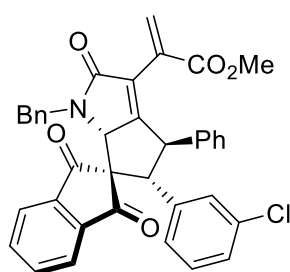
#	Time	Area	Height	Width	Area%	Symmetry
1	23.016	36271.6	497.4	1.0408	48.713	0.789
2	27.083	38188.7	452.3	1.191	51.287	0.689



Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	23.162	3441.7	49	0.9268	6.568	0.862
2	26.939	48955.2	592.1	1.1686	93.432	0.744

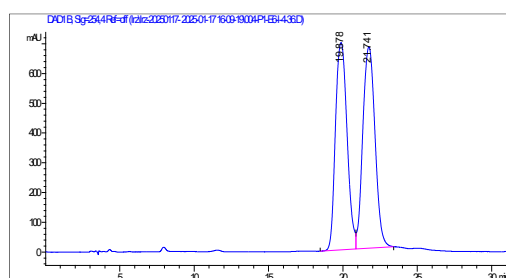
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(3-chlorophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ah)



3ah

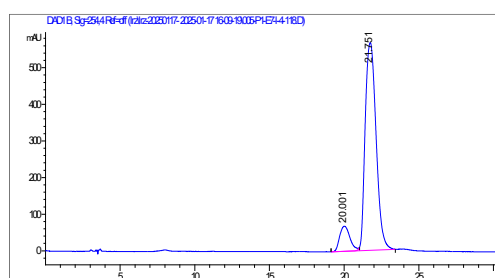
Light yellow solid, 17.0 mg, 55% yield, mp: 117.4-118.3 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.62 (q, *J* = 3.6 Hz, 1H), 7.59 – 7.54 (m, 2H), 7.51 – 7.48 (m, 1H), 7.21 (dd, *J* = 10.5, 6.9 Hz, 3H), 7.02 (d, *J* = 6.9 Hz, 2H), 6.95 – 6.87 (m, 8H), 6.78 (s, 1H), 6.48 (s, 1H), 6.06 (s, 1H), 5.10 (s, 1H), 4.74 (d, *J* = 10.4 Hz, 1H), 4.48 (d, *J* = 15.0 Hz, 1H), 4.12 (d, *J* = 15.0 Hz, 1H), 3.84 (d, *J* = 10.3 Hz, 1H), 3.52 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 199.6, 196.3, 172.9,

166.1, 160.1, 142.2, 140.4, 136.5, 136.3, 136.0, 135.4, 134.4, 131.7, 131.1, 129.9, 129.1, 128.7, 128.5, 128.4, 127.8, 127.5, 126.7, 123.1, 123.0, 77.5, 77.2, 76.8, 70.8, 64.9, 63.8, 52.1, 47.0, 46.9. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₈H₂₉ClNO₅⁺ 614.1729; Found 614.1734. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t_R* (minor) = 20.001 min, *t_R* (major) = 21.751 min, 80% ee. [α]_D²⁵ = -94.00 (c = 0.21, DCM).



Racemic

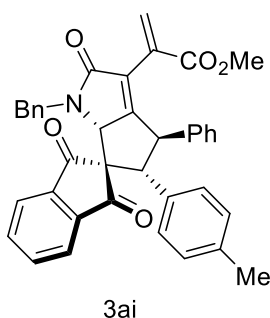
#	Time	Area	Height	Width	Area%	Symmetry
1	19.878	37882.5	697	0.7561	49.441	0.909
2	21.741	38739.7	677	0.7336	50.559	0.941



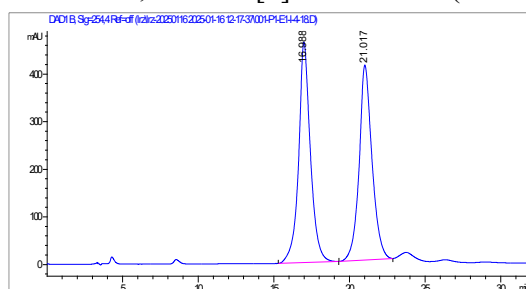
Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	20.001	3273.9	68.8	0.5734	10.245	0.754
2	21.751	28682.5	566.9	0.7363	89.755	1.381

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4-phenyl-5-(*p*-tolyl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ai)

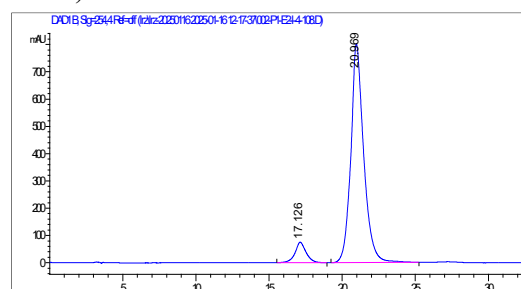


Light yellow solid, 27.1 mg, 91% yield, mp: 123.0-123.2 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.59-7.58 (m, 1H), 7.54 – 7.50 (m, 2H), 7.48 – 7.45 (m, 1H), 7.20 (dd, *J* = 8.1, 6.0 Hz, 2H), 7.18 – 7.15 (m, 1H), 7.03 – 7.00 (m, 2H), 6.95 – 6.89 (m, 3H), 6.89 – 6.82 (m, 4H), 6.80 – 6.75 (m, 3H), 6.47 (d, *J* = 1.4 Hz, 1H), 6.06 (d, *J* = 1.4 Hz, 1H), 5.11 (d, *J* = 1.6 Hz, 1H), 4.30 (dd, *J* = 142.9, 15.1 Hz, 2H), 3.86 (d, *J* = 10.4 Hz, 1H), 3.51 (s, 3H), 2.06 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 200.1, 196.8, 173.0, 166.2, 160.8, 142.4, 141.5, 140.7, 137.7, 136.4, 135.7, 135.1, 131.9, 131.2, 130.9, 129.2, 128.9, 128.8, 128.4, 128.3, 127.7, 127.5, 127.2, 122.9, 122.8, 77.5, 77.2, 76.8, 70.9, 65.1, 64.2, 52.1, 46.9, 46.8, 21.0. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₉H₃₂NO₅⁺ 594.2275; Found 594.2280. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: *t*_R (minor) = 17.126 min, *t*_R (major) = 20.969 min, 85% ee. [α]_D²⁵ = -113.14 (c = 0.21, DCM).



Racemic

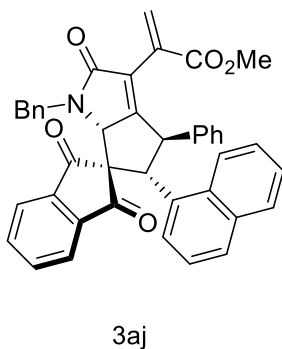
#	Time	Area	Height	Width	Area%	Symmetry
1	16.988	25061.7	463	0.7735	50.832	0.809
2	21.017	24241	409.6	0.8484	49.168	0.794



Chiral

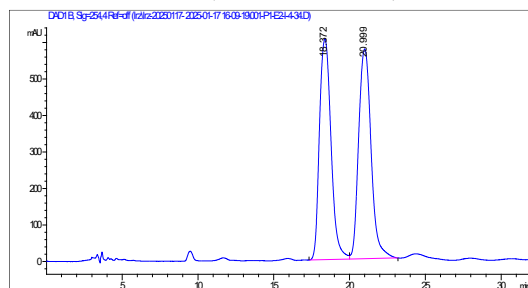
#	Time	Area	Height	Width	Area%	Symmetry
1	17.126	3996.6	75.6	0.741	7.532	0.858
2	20.969	49066.2	802.1	0.8677	92.468	0.727

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(naphthalen-1-yl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3aj)



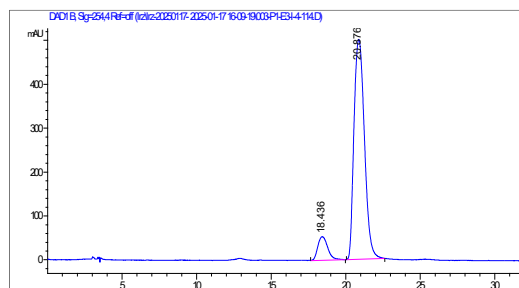
Light yellow solid, 21.3 mg, 68% yield, mp: 105.7-106.3 °C. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.4 Hz, 1H), 7.59 (d, *J* = 6.4 Hz, 1H), 7.52 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.45 (d, *J* = 8.1 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.32 – 7.26 (m, 3H), 7.25 – 7.22 (m, 2H), 7.16 – 7.10 (m, 3H), 7.03 (dd, *J* = 7.9, 1.8 Hz, 2H), 6.94 (d, *J* = 6.8 Hz, 2H), 6.85 (t, *J* = 7.6 Hz, 2H), 6.72 (t, *J* = 7.4 Hz, 1H), 6.52 (d, *J* = 1.4 Hz, 1H), 6.15 (d, *J* = 1.4 Hz, 1H), 5.37 – 5.32 (m, 1H), 4.98 (d, *J* = 1.9 Hz, 2H), 4.56 (d, *J* = 15.1 Hz, 1H), 4.15 (d, *J* = 15.1 Hz, 1H), 3.54 (s, 3H). ¹³C NMR

(101 MHz, CDCl₃) δ 200.1, 196.7, 172.9, 166.2, 160.6, 142.2, 141.2, 140.8, 136.3, 135.5, 134.8, 133.6, 131.9, 131.7, 131.0, 129.0, 128.6, 128.5, 128.4, 128.3, 127.7, 127.3, 127.2, 126.5, 126.4, 125.6, 125.0, 123.2, 122.7, 122.6, 77.5, 77.2, 76.8, 70.8, 65.2, 57.6, 52.1, 48.4, 46.8. HRMS (ESI) m/z : [M+H]⁺ Calcd for C₄₂H₃₂NO₅⁺ 630.2275; Found 630.2278. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 18.436 min, t_R (major) = 20.876 min, 81% ee. $[\alpha]_D^{25}$ = -240.73 (c = 0.22, DCM).



Racemic

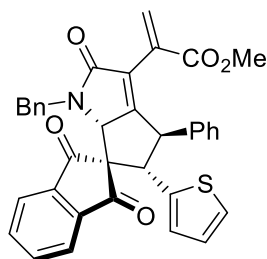
#	Time	Area	Height	Width	Area%	Symmetry
1	18.372	32058.5	605.4	0.6838	49.442	0.859
2	20.999	32781.5	574.6	0.7016	50.558	0.899



Chiral

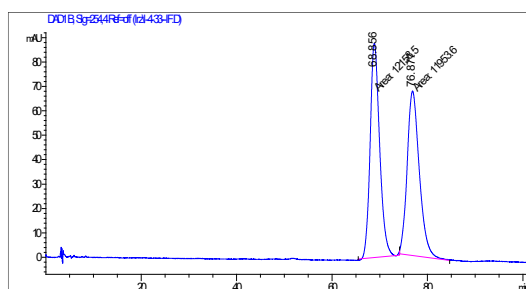
#	Time	Area	Height	Width	Area%	Symmetry
1	18.436	2490.8	53.6	0.5598	9.262	0.819
2	20.876	24402.5	500.9	0.7583	90.738	0.798

Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4-phenyl-5-(thiophen-2-yl)-1',2,3,3a,3',4,5,6a-octahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ak)



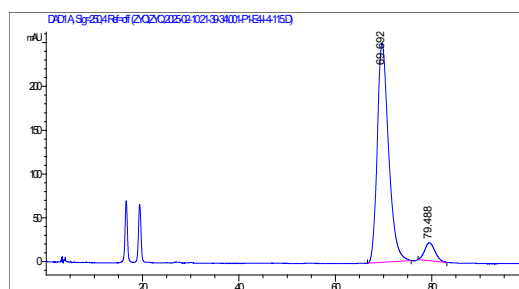
3ak

Light yellow solid, 8.5 mg, 29% yield, mp: 104.2-105.6 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.68 – 7.66 (m, 1H), 7.62 – 7.57 (m, 2H), 7.56 – 7.53 (m, 1H), 7.25 (dd, J = 8.1, 6.3 Hz, 4H), 7.22 – 7.18 (m, 1H), 7.10 – 7.07 (m, 2H), 6.95 – 6.86 (m, 5H), 6.80 (t, J = 7.2 Hz, 1H), 6.63 – 6.59 (m, 2H), 6.48 (d, J = 1.3 Hz, 1H), 6.05 (d, J = 1.3 Hz, 1H), 5.07 (d, J = 1.6 Hz, 1H), 4.65 (dd, J = 10.3, 1.6 Hz, 1H), 4.47 (d, J = 14.9 Hz, 1H), 4.17 – 4.11 (m, 2H), 3.51 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 199.7, 196.5, 172.9, 166.1, 159.8, 142.5, 141.7, 140.1, 137.1, 136.3, 135.9, 135.3, 131.6, 131.2, 129.0, 128.8, 128.5, 128.4, 127.8, 127.6, 127.5, 127.1, 126.8, 125.3, 123.1, 123.0, 77.4, 77.2, 76.9, 70.5, 64.9, 59.2, 52.1, 49.4, 46.9. HRMS (ESI) m/z : [M+H]⁺ Calcd for C₃₆H₂₈NO₅S⁺ 586.1683; Found 586.1686. HPLC conditions: Daicel Chiralpak IA-3 column, n-hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_R (minor) = 79.488 min, t_R (major) = 69.692 min, 86% ee. $[\alpha]_D^{25}$ = -81.66 (c = 0.21, DCM).



Racemic

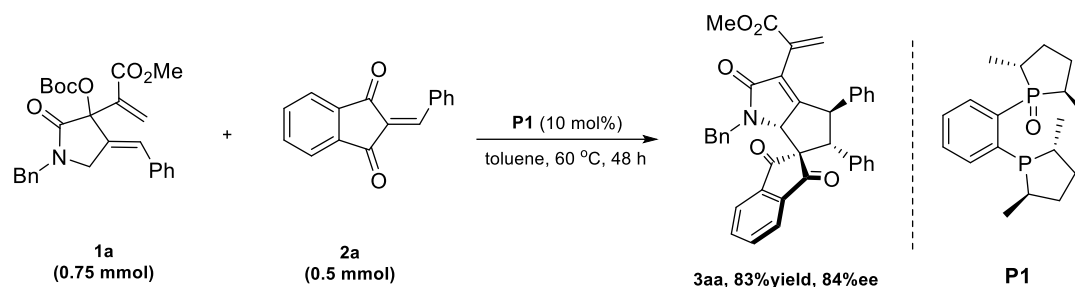
#	Time	Area	Height	Width	Area%	Symmetry
1	68.856	12158.5	87.9	2.3057	50.425	0.767
2	76.877	11953.6	67.5	2.9504	49.575	0.769



Chiral

#	Time	Area	Height	Width	Area%	Symmetry
1	69.692	40798.9	250.7	1.9109	93.085	0.725
2	79.488	3030.6	20.6	1.731	6.915	0.802

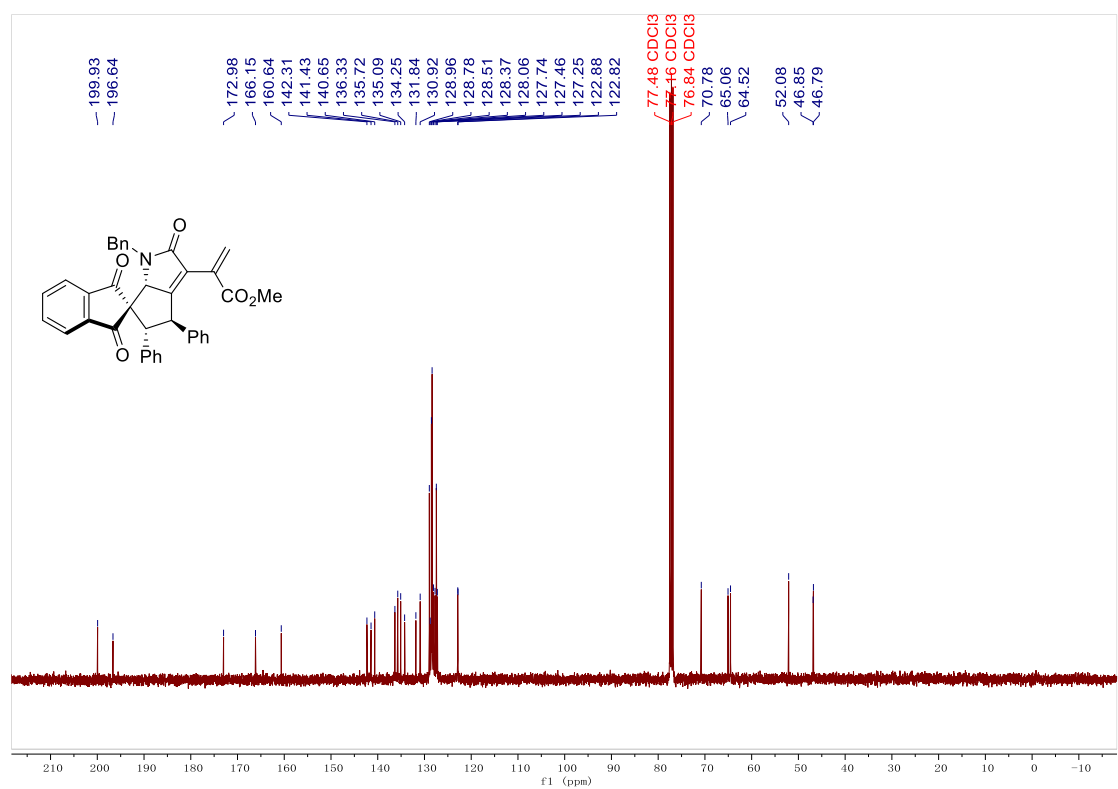
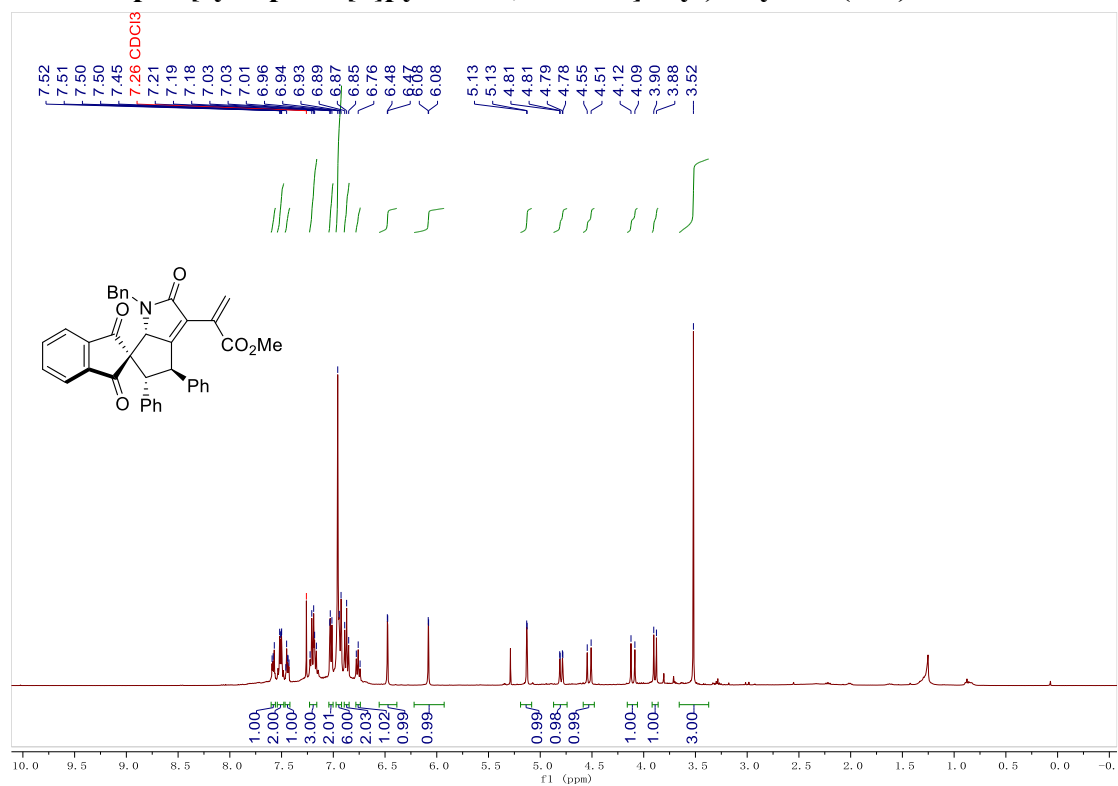
D: Large-scale Reaction



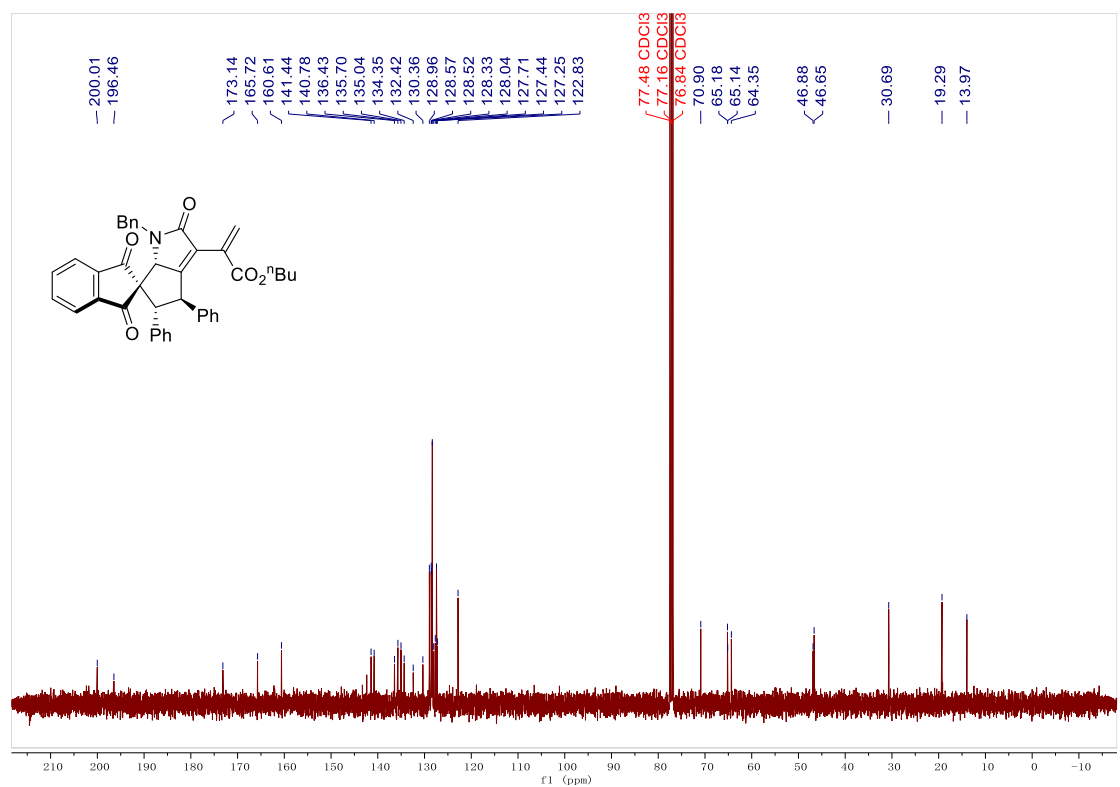
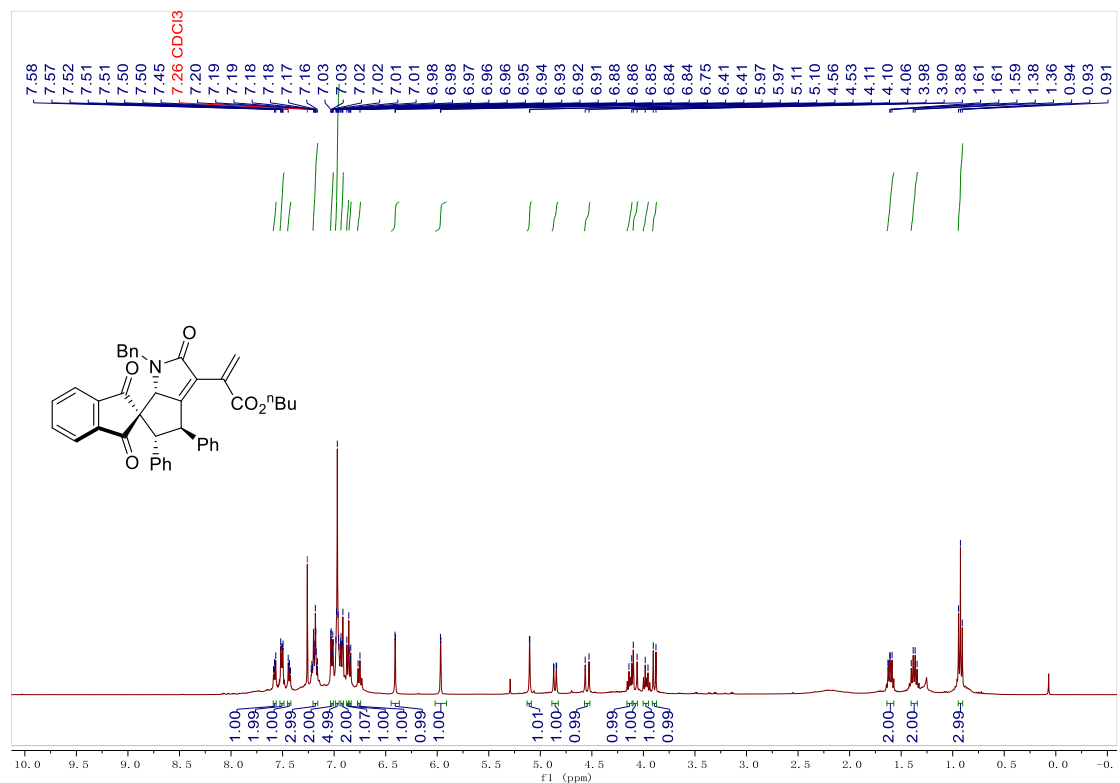
To a solution of toluene (5.0 mL) were added pyrrolidione-based MBH carbonate **1a** (0.75 mmol, 1.5 eq), 2-arylideneindane-1,3-dione **2a** (0.5 mmol, 1.0 eq) and catalyst **P1** (10 mol%). The reaction mixture was stirred at 60 °C for 48 h under Ar atmosphere. The solvent was removed under vacuum and the residue was purified by flash chromatography (petroleum ether/ethyl acetate = 2/1) to provide the desired product **3aa** (83% yield, 84% ee).

E: NMR Analysis

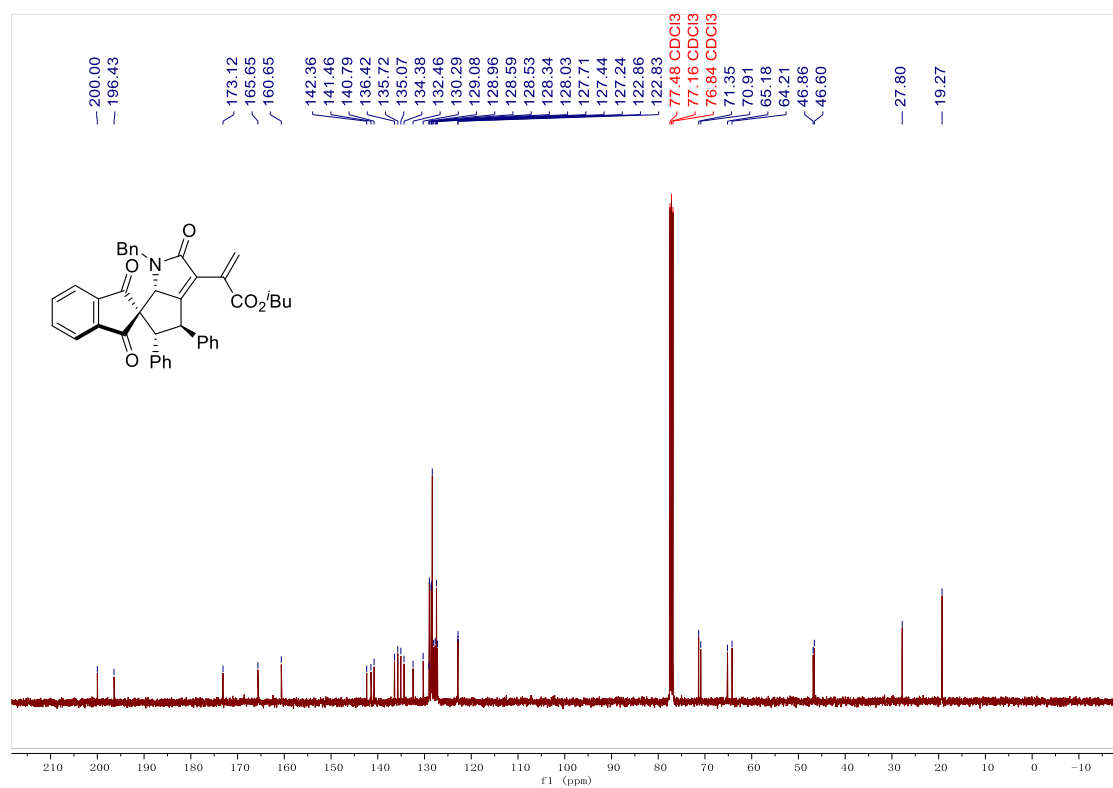
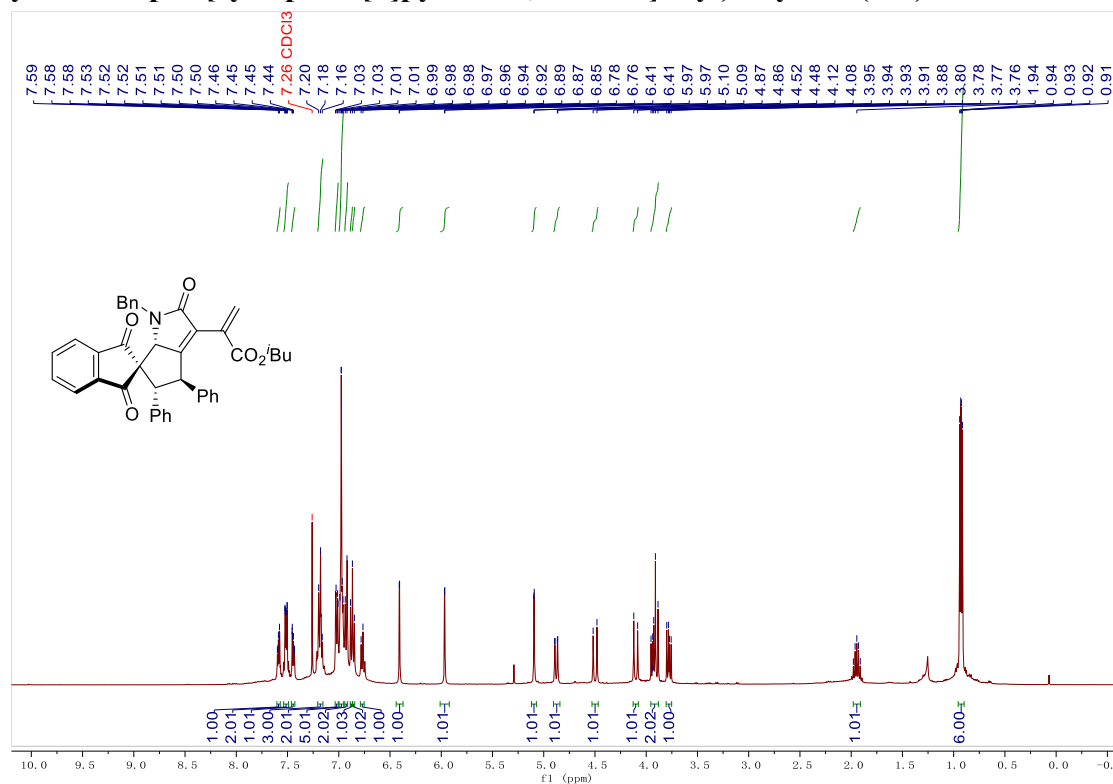
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4,5-diphenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3aa)



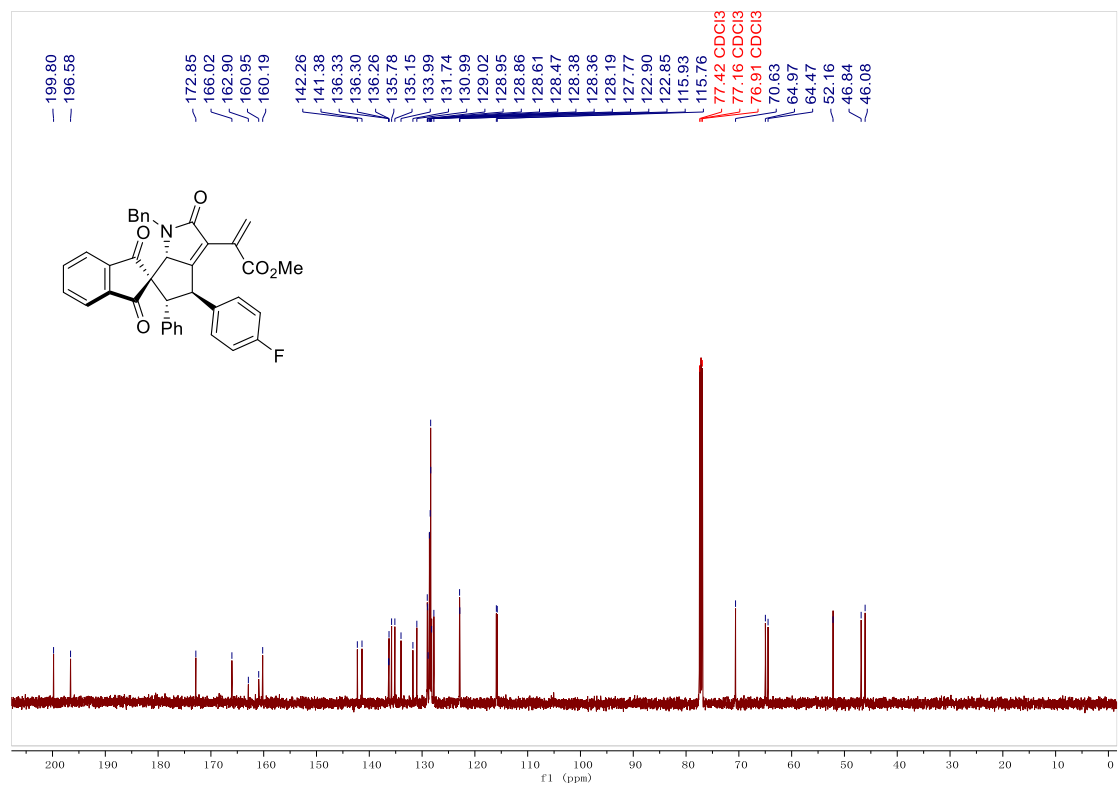
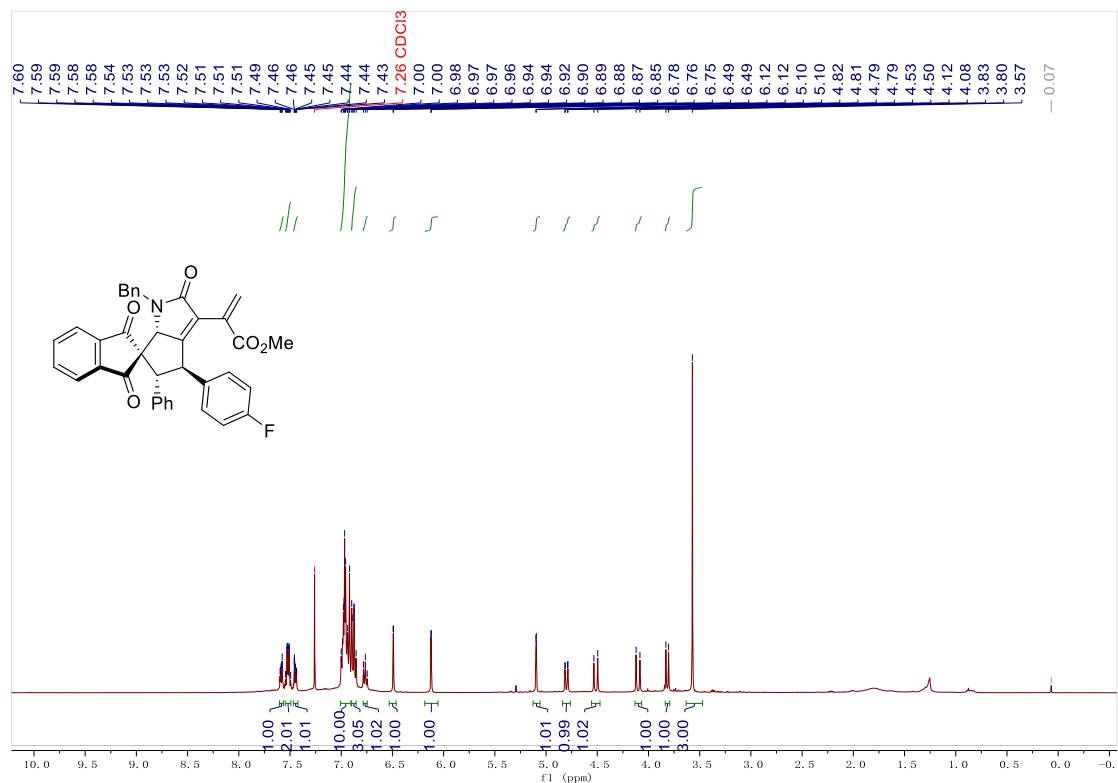
Butyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4,5-diphenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3*ba*)



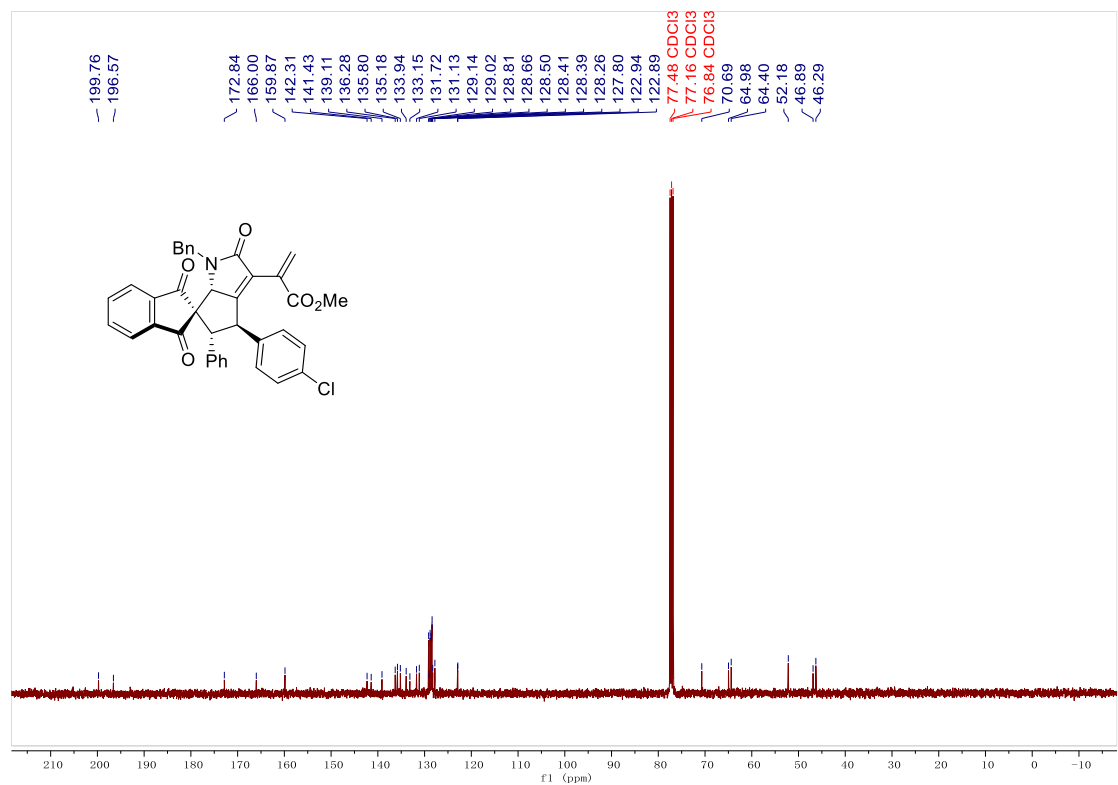
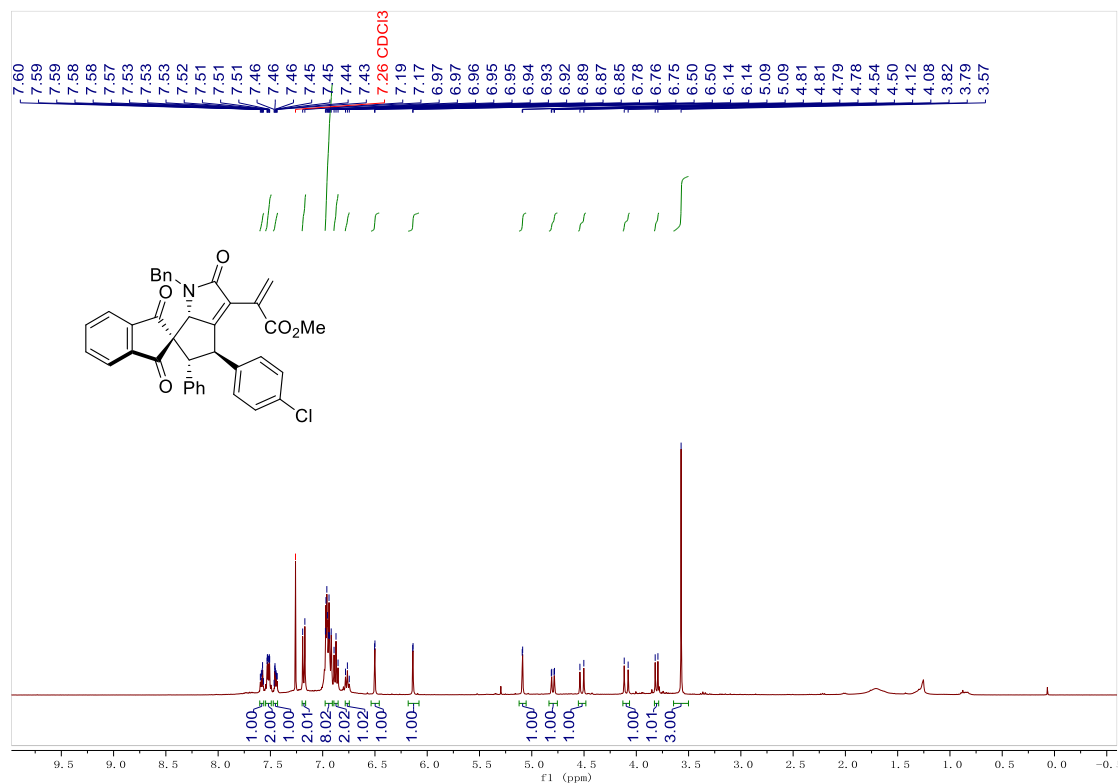
Isobutyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4,5-diphenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ca)



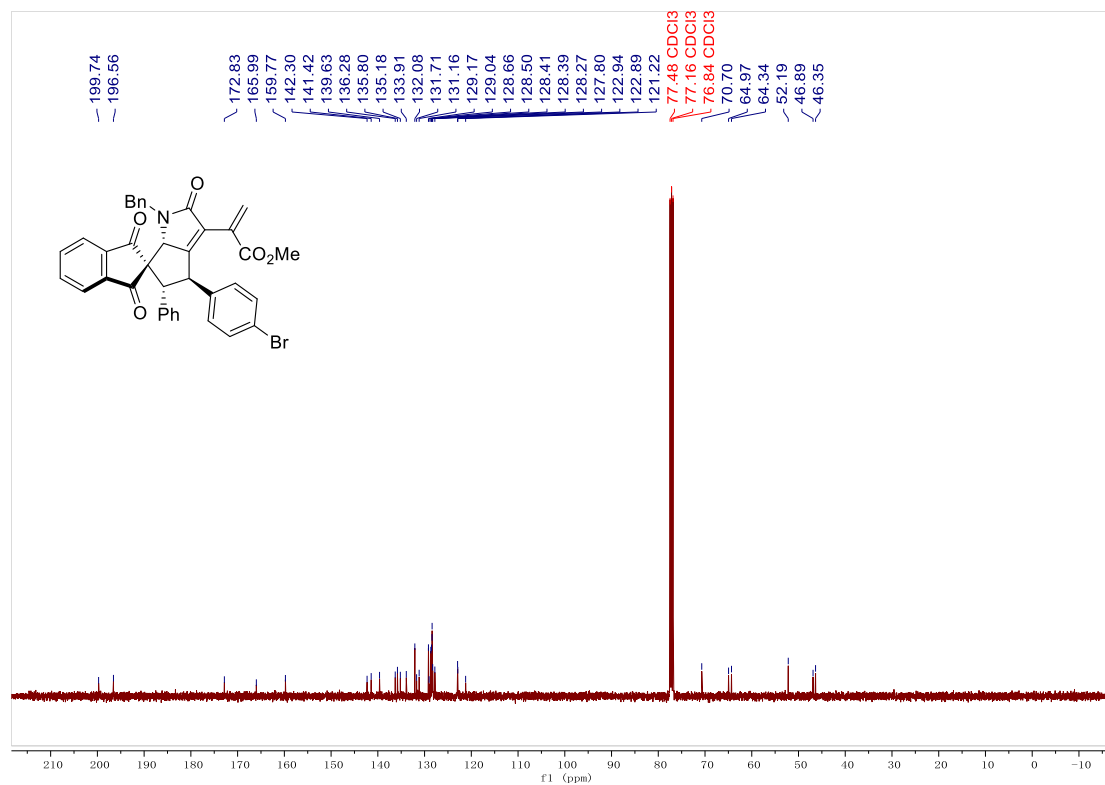
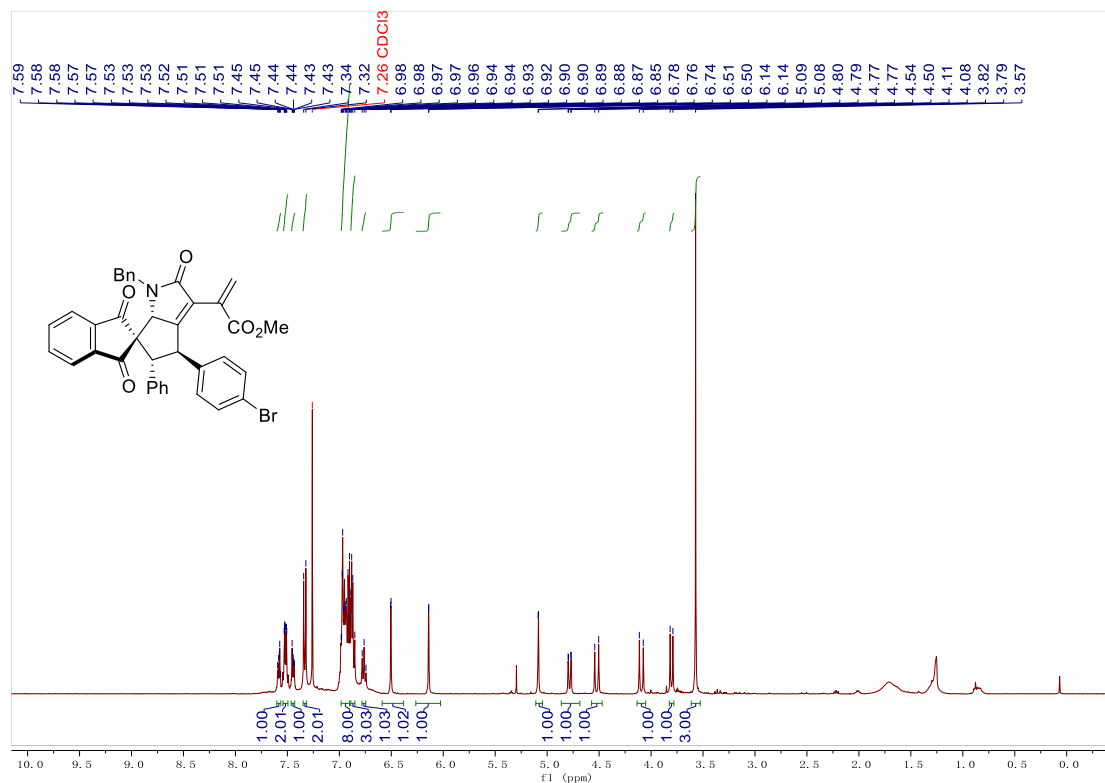
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(4-fluorophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3da)



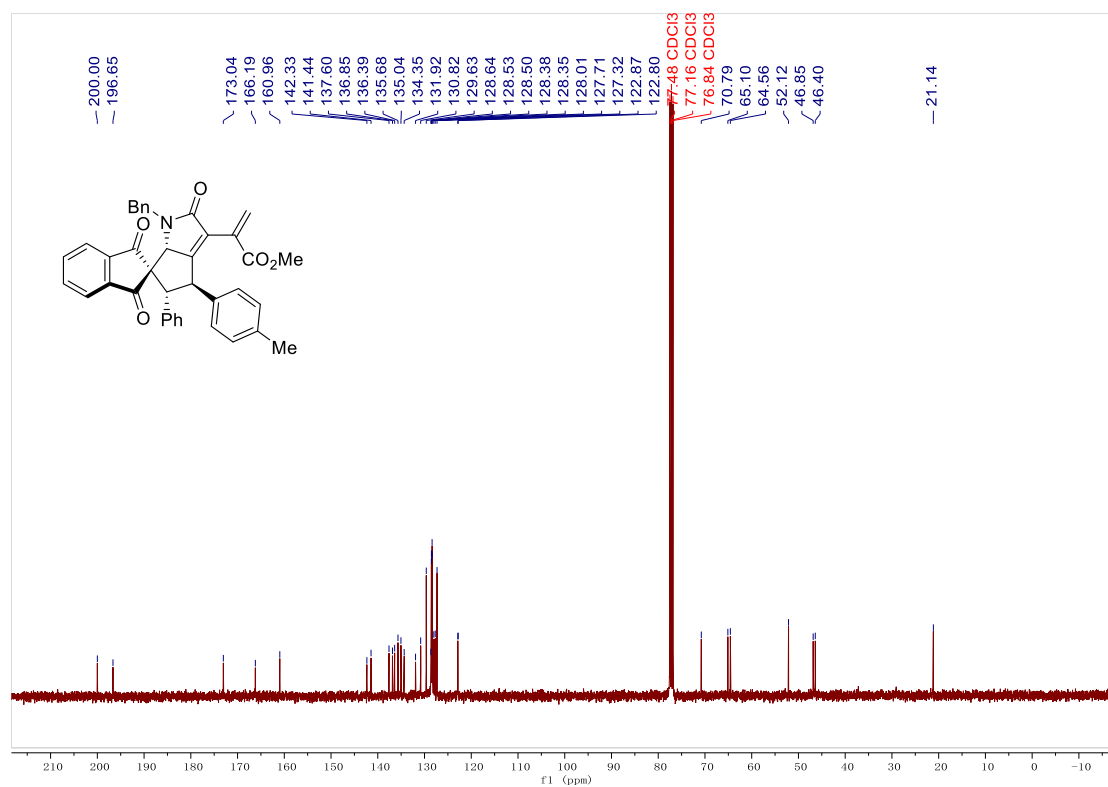
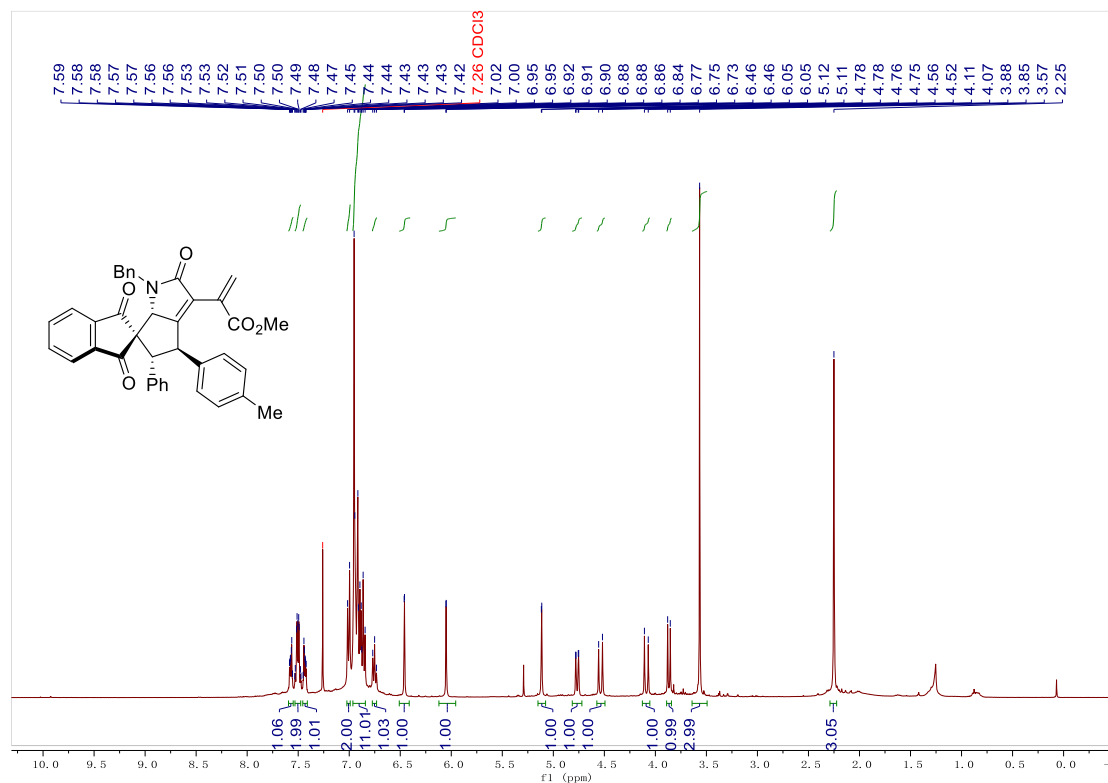
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(4-chlorophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ea)



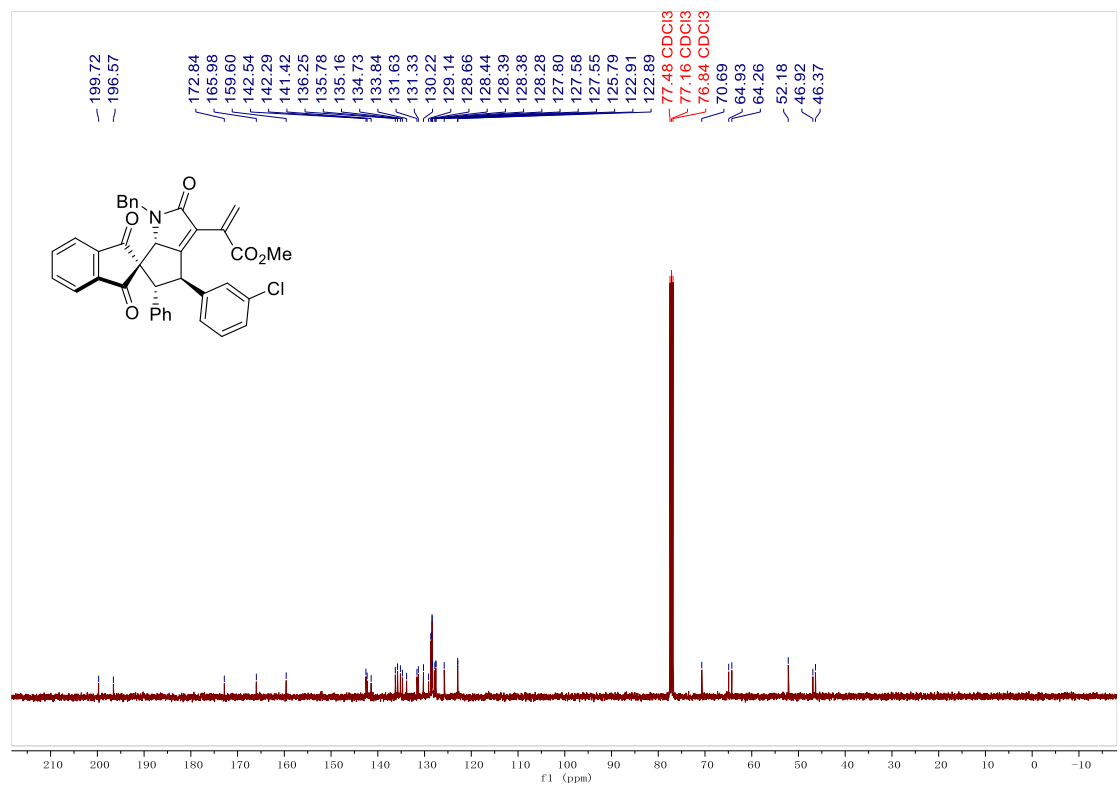
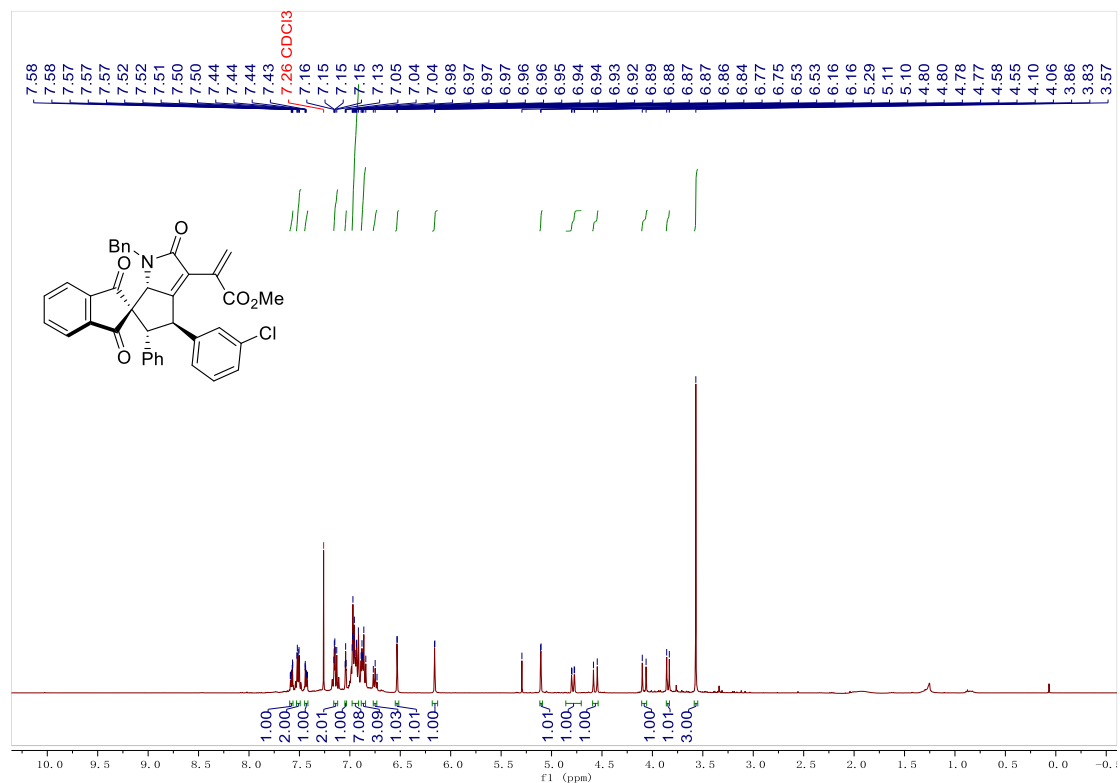
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(4-bromophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6a-hexahydro-1H-spiro[cyclopenta[b]pyrrole-6,2'-inden]-3-yl)acrylate (3fa)



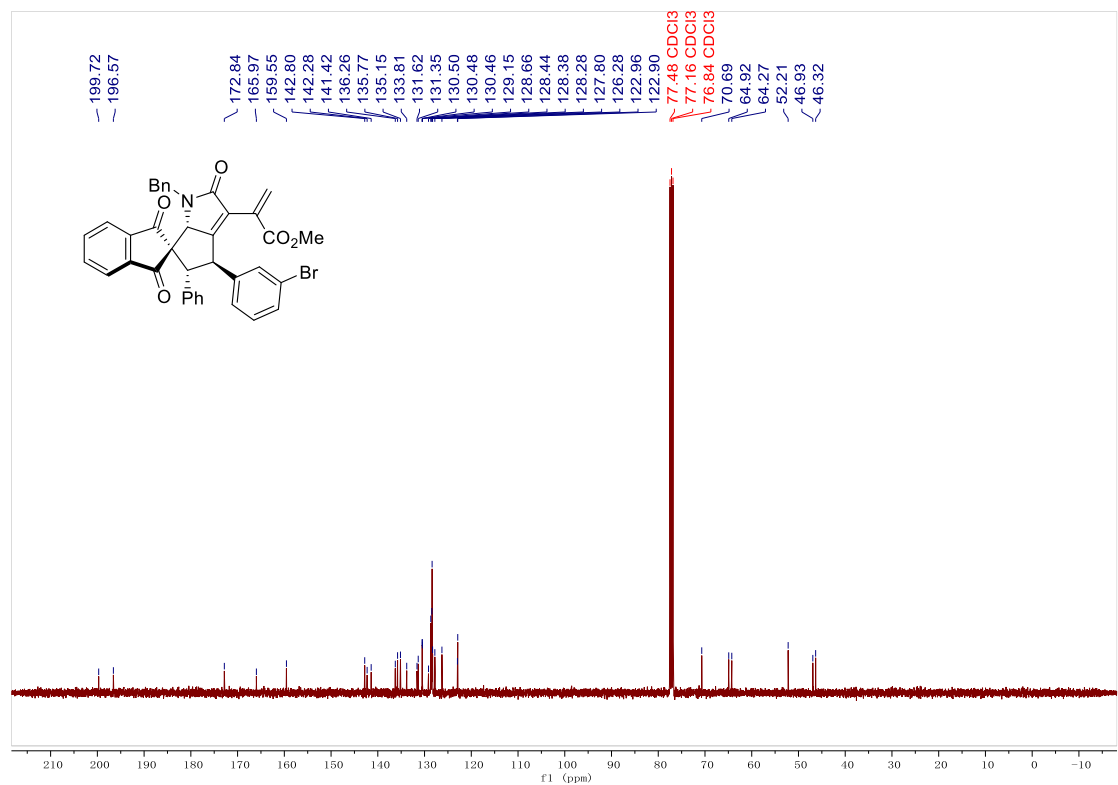
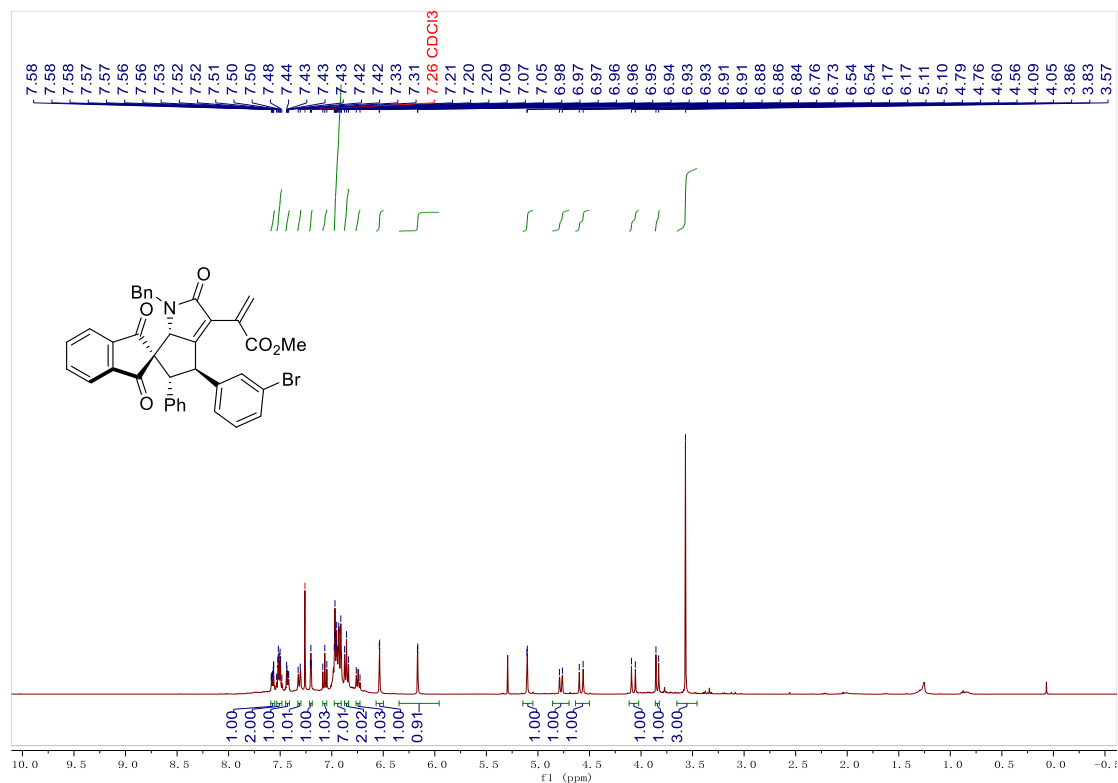
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-5-phenyl-4-(p-tolyl)-1',2,3',4,5,6a-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ga)



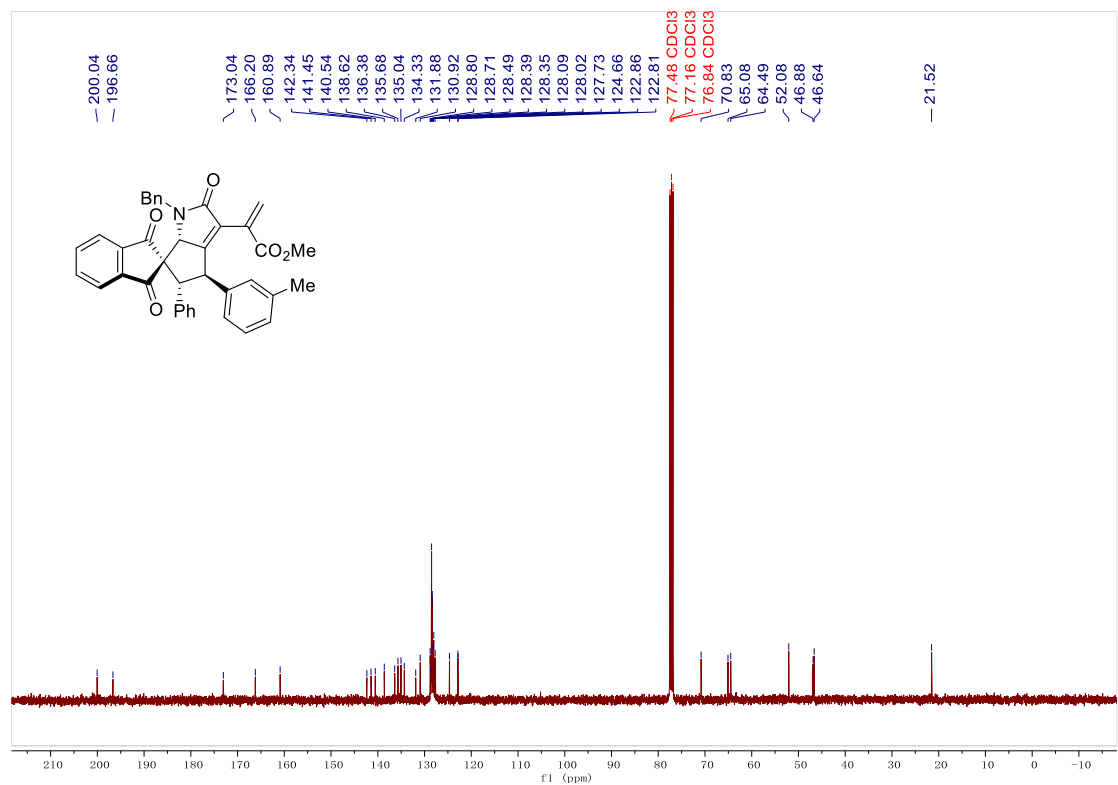
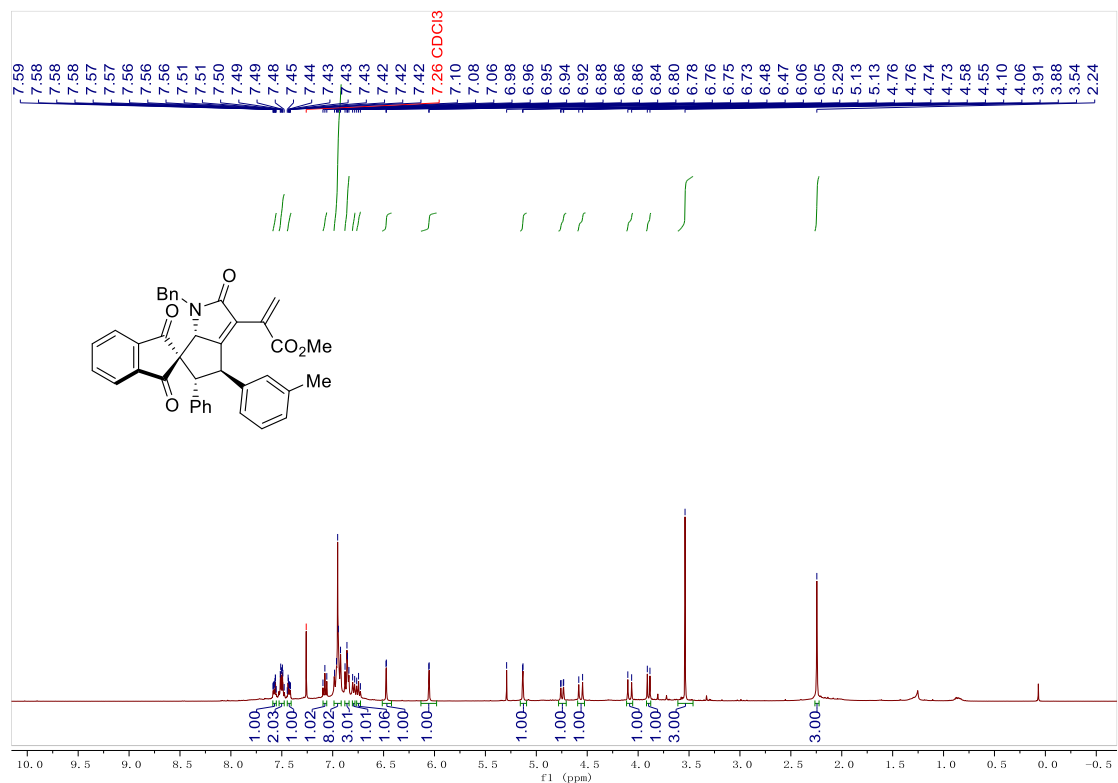
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(3-chlorophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ha)



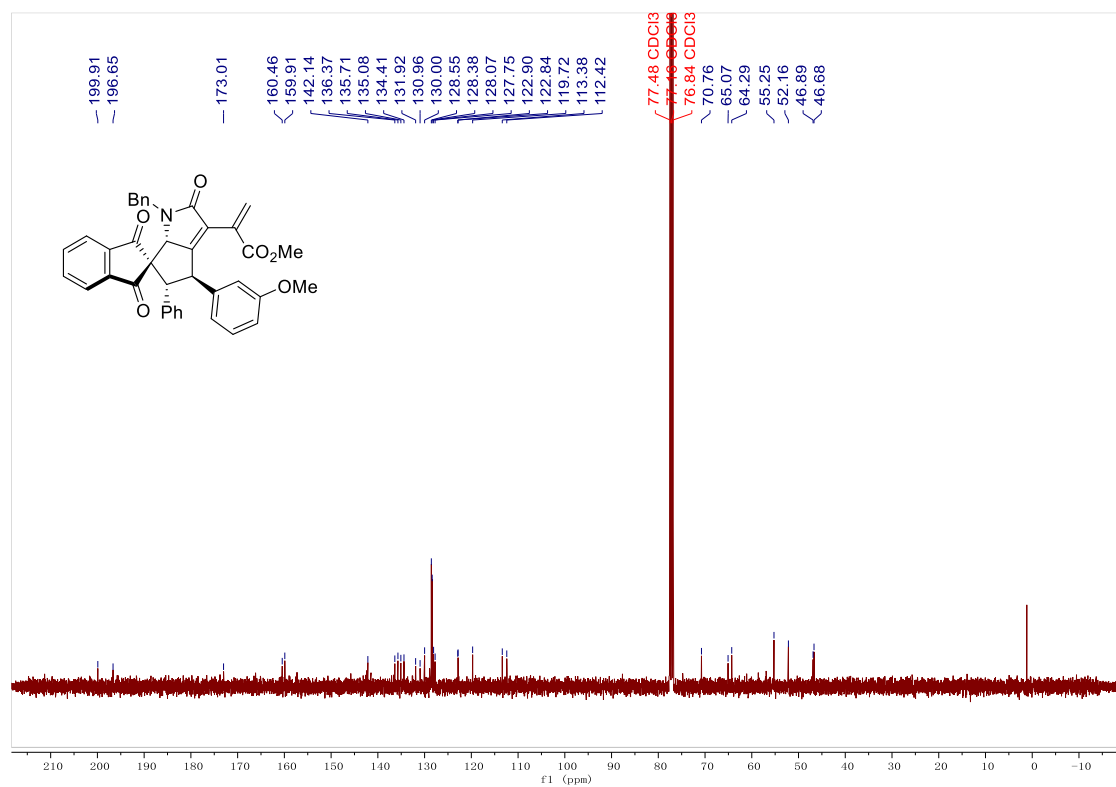
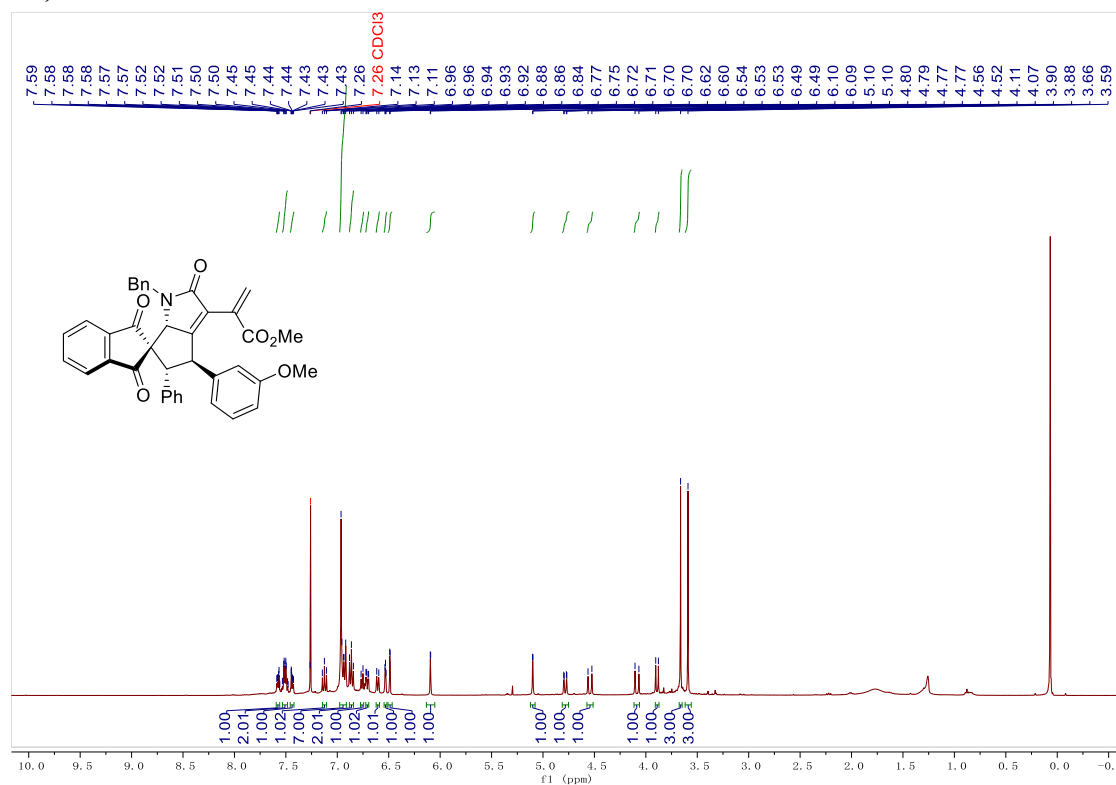
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(3-bromophenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ia)



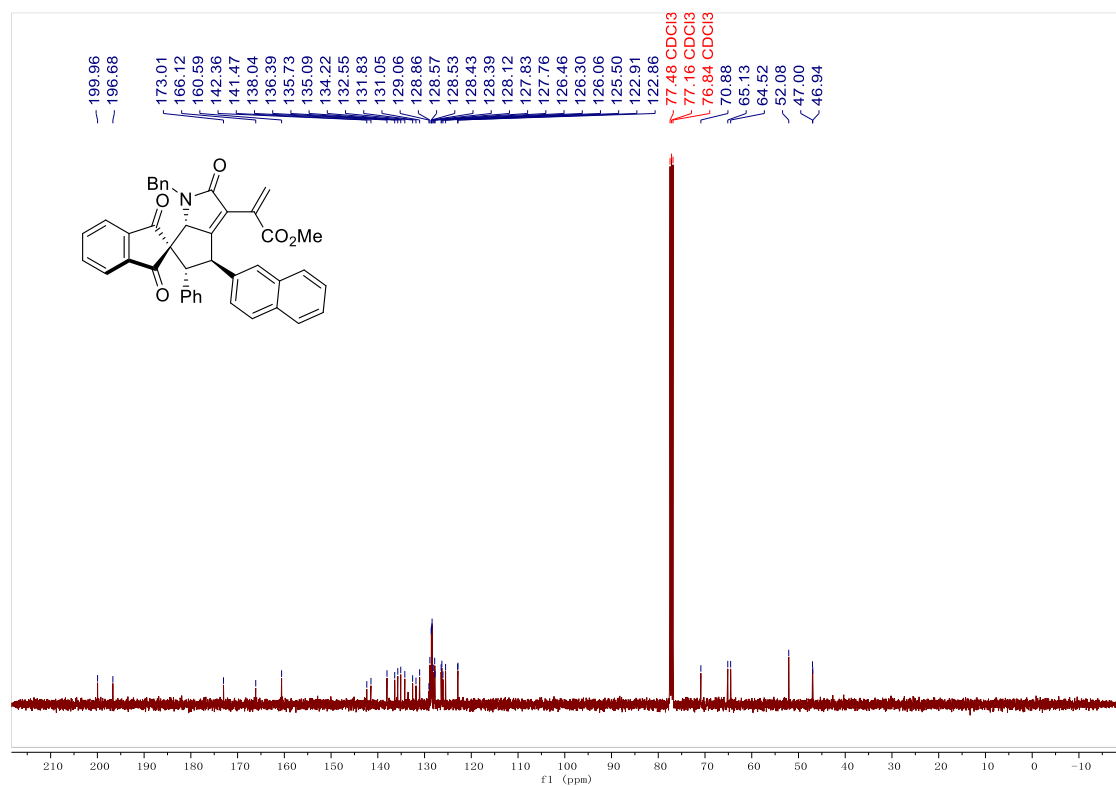
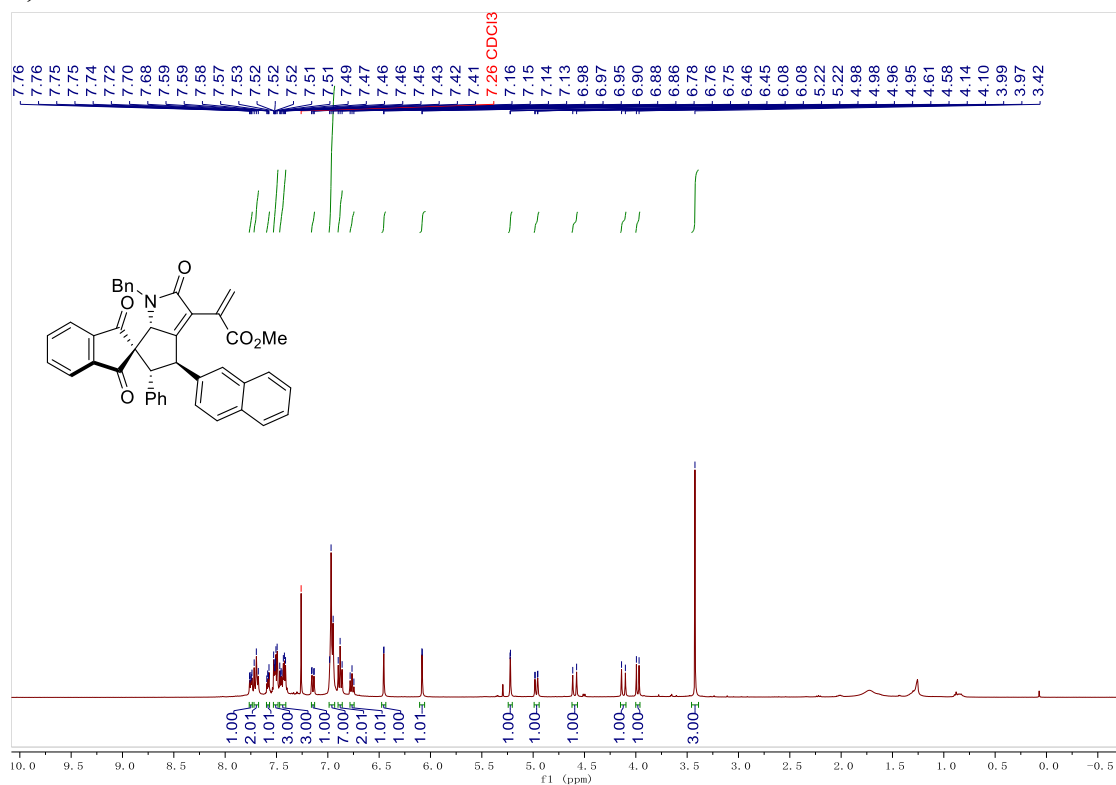
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-5-phenyl-4-(*m*-tolyl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ja)



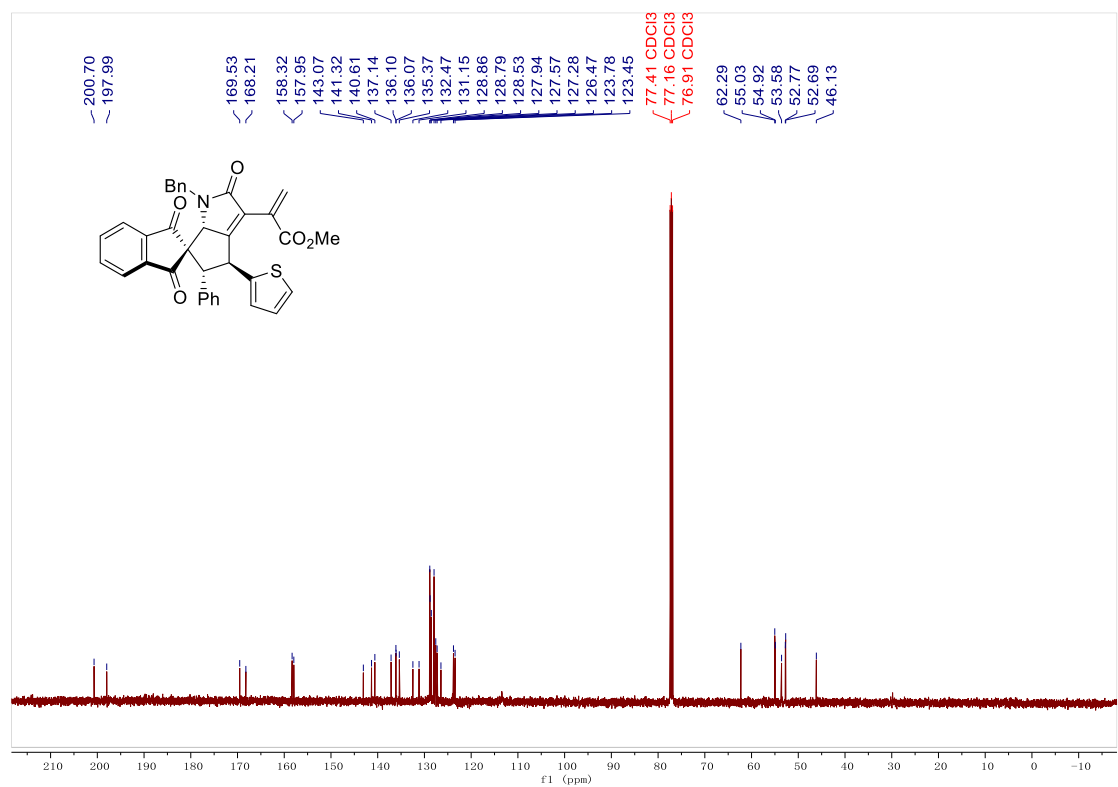
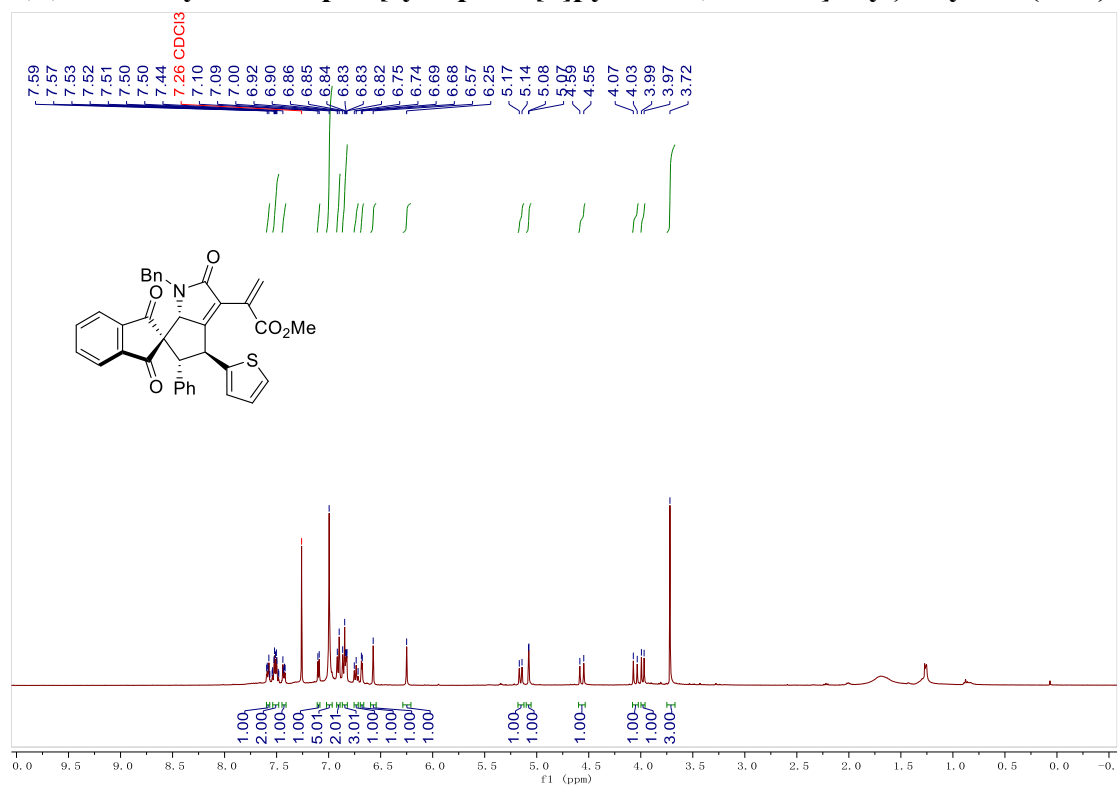
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(3-methoxyphenyl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6a-hexahydro-1H-spiro[cyclopenta[b]pyrrole-6,2'-inden]-3-yl)acrylate (3ka)



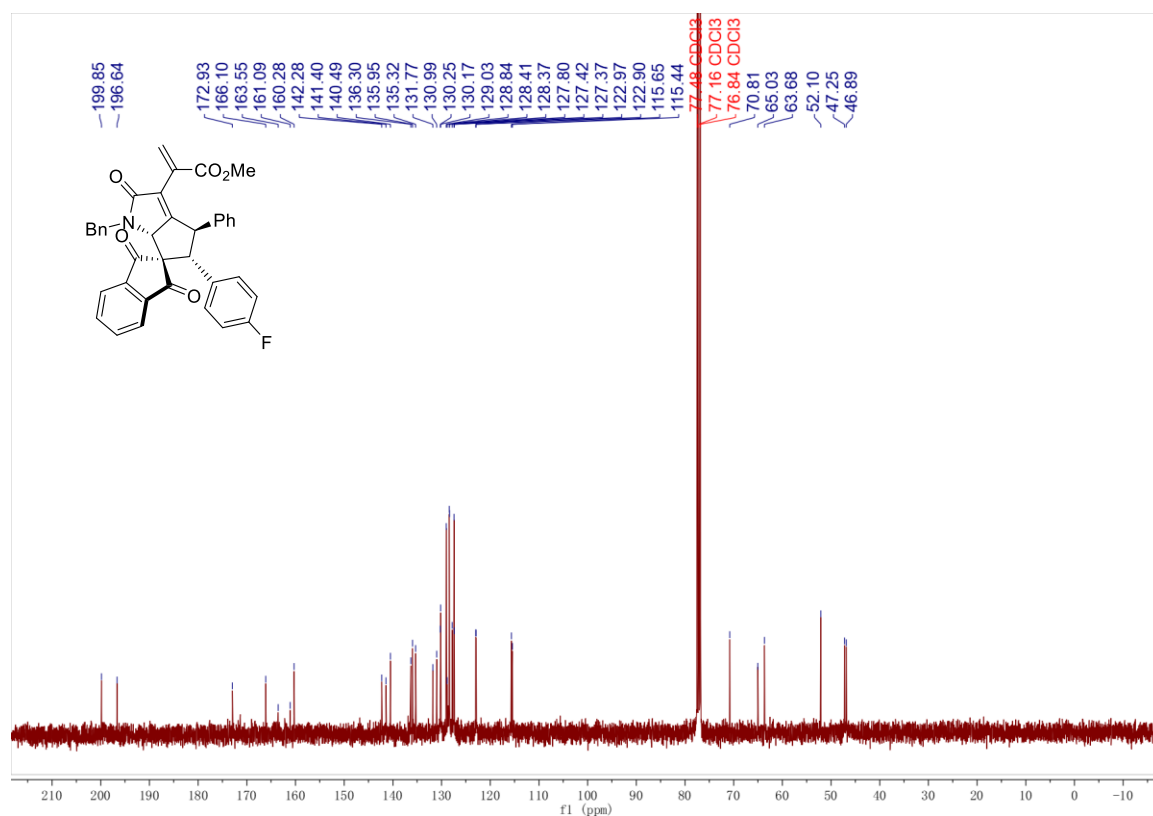
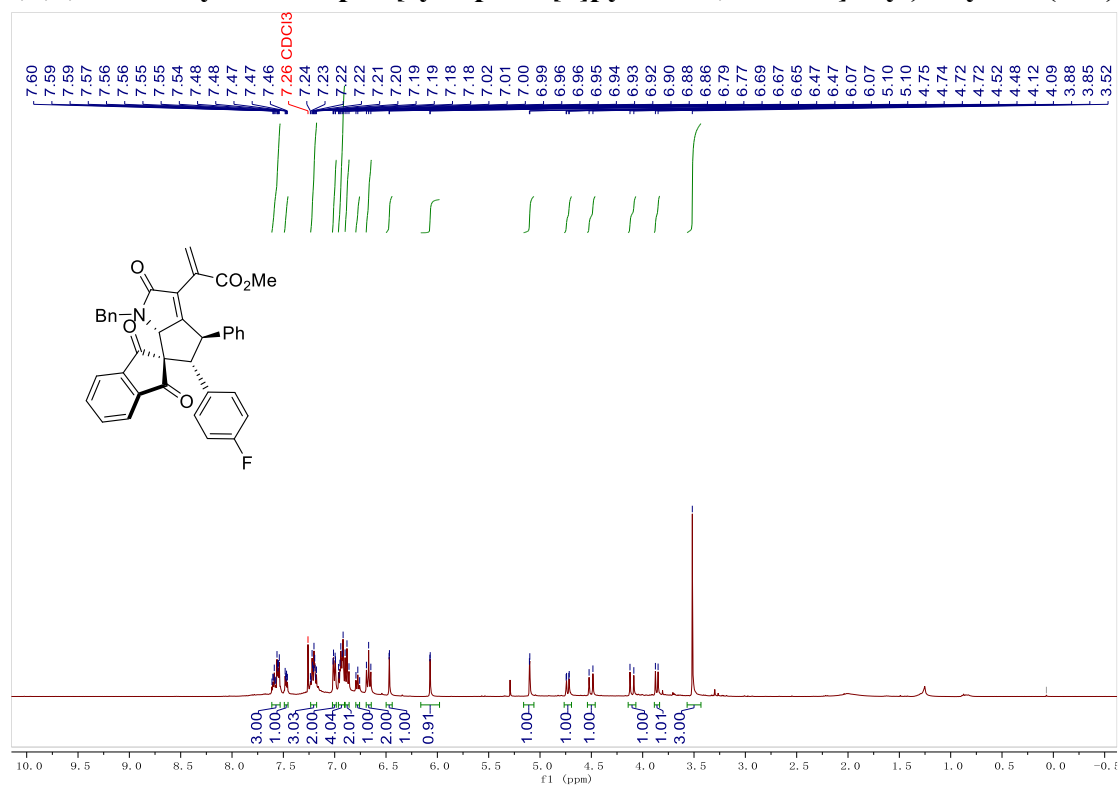
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-4-(naphthalen-2-yl)-1',2,3'-trioxo-5-phenyl-1',2,3',4,5,6a-hexahydro-1H-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (31a)



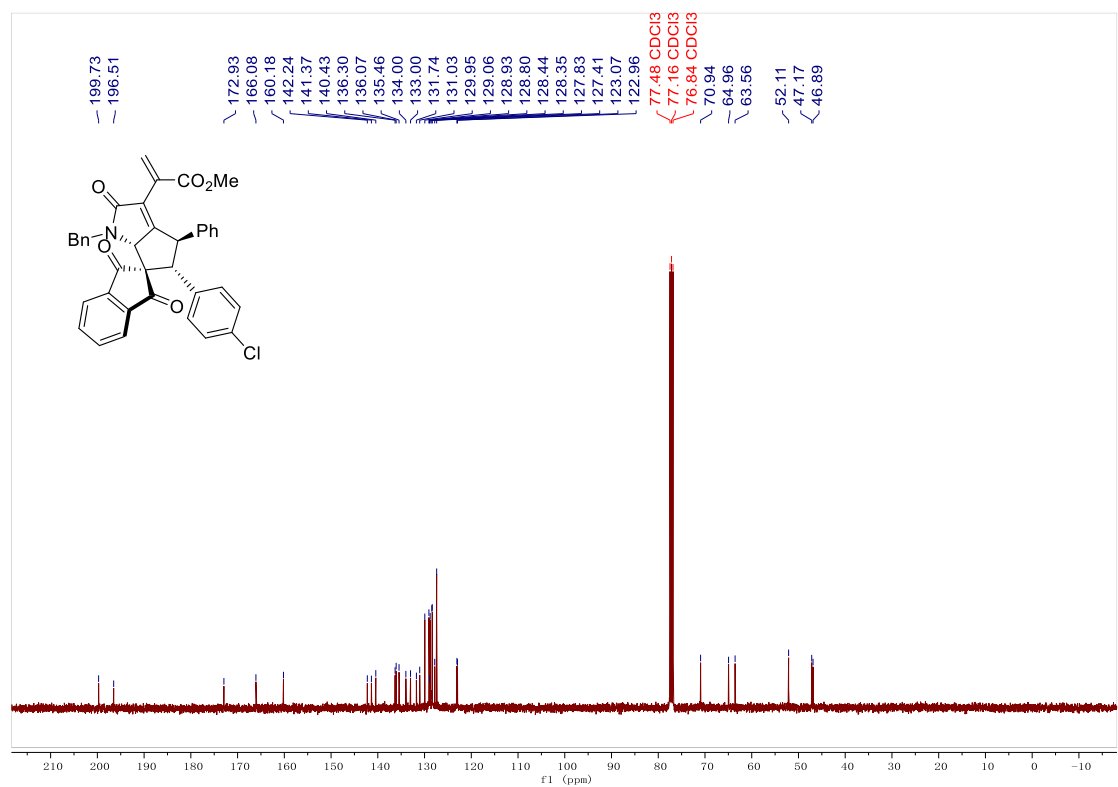
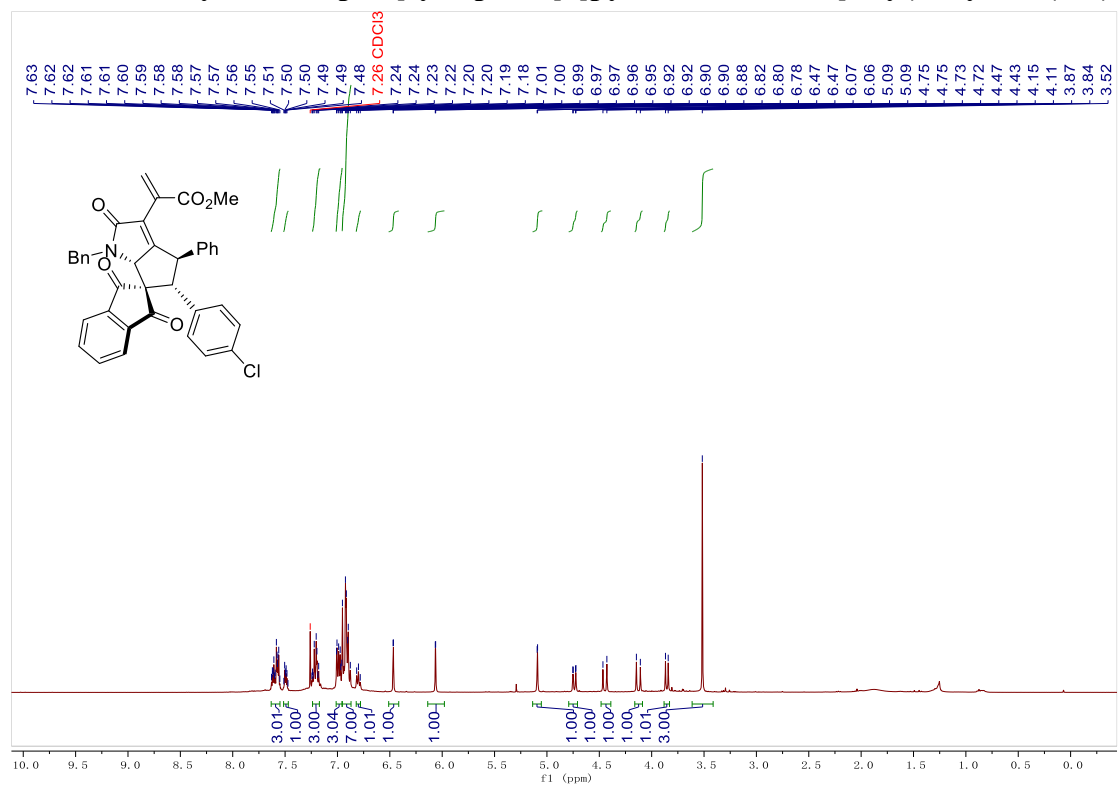
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-5-phenyl-4-(thiophen-2-yl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ma)



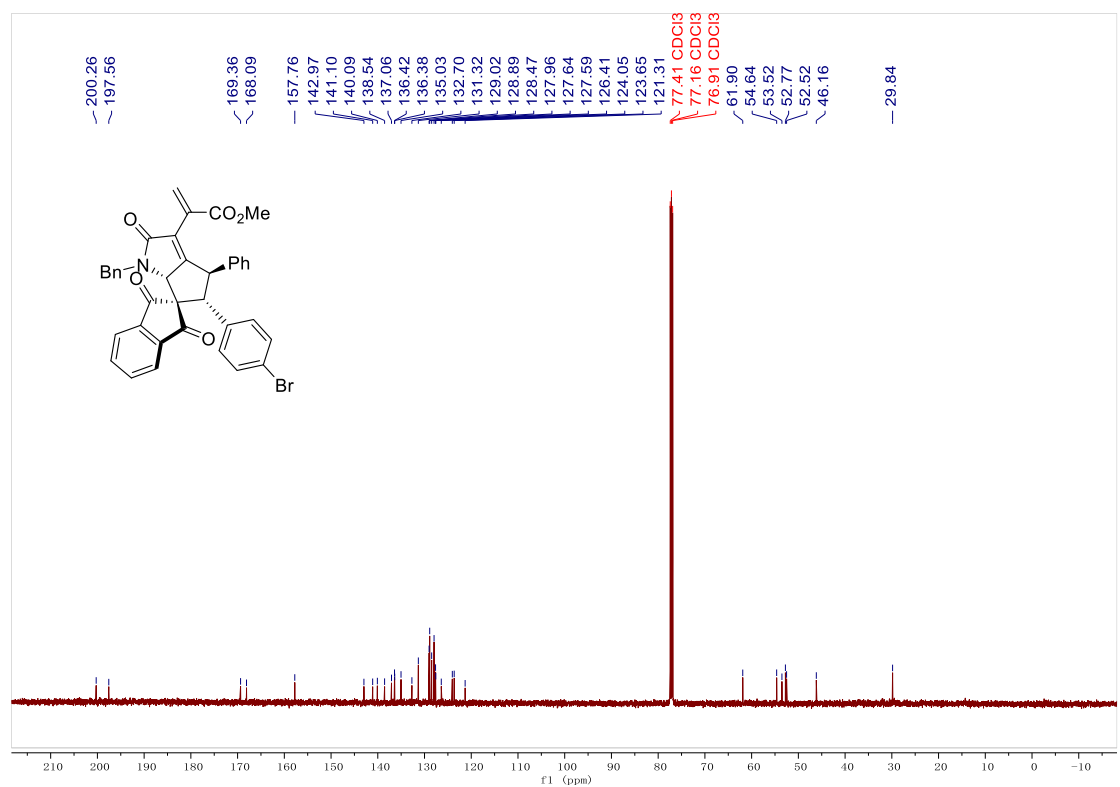
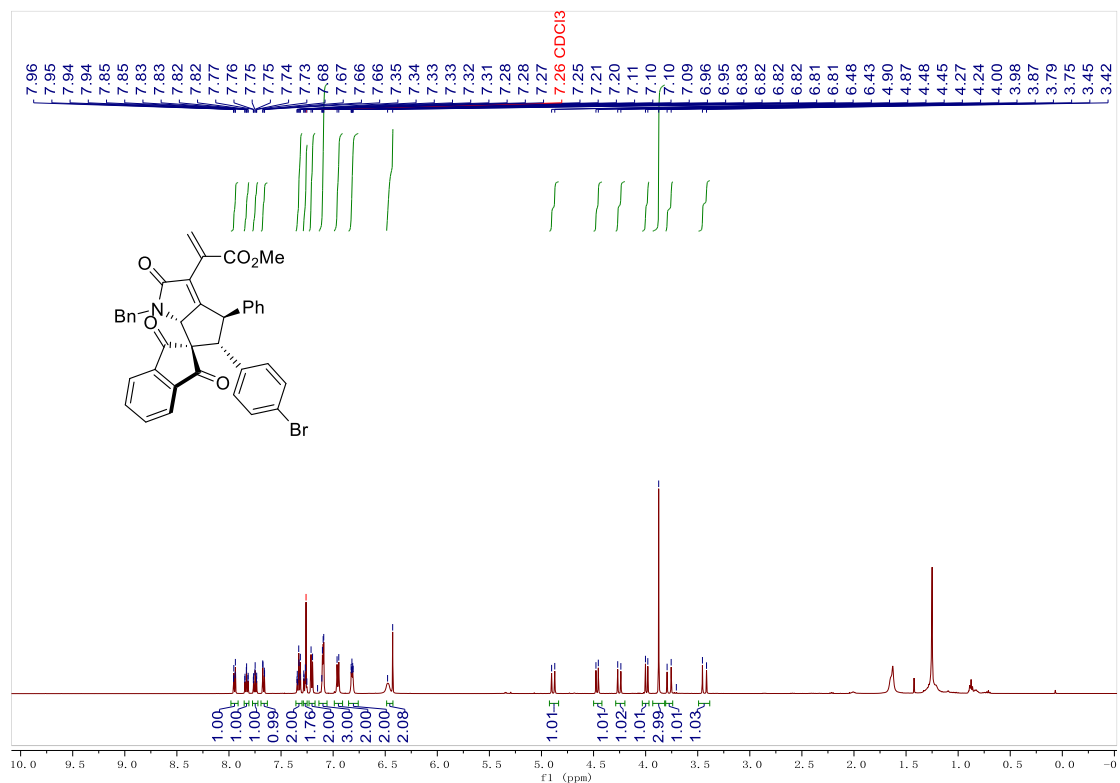
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-fluorophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ab)



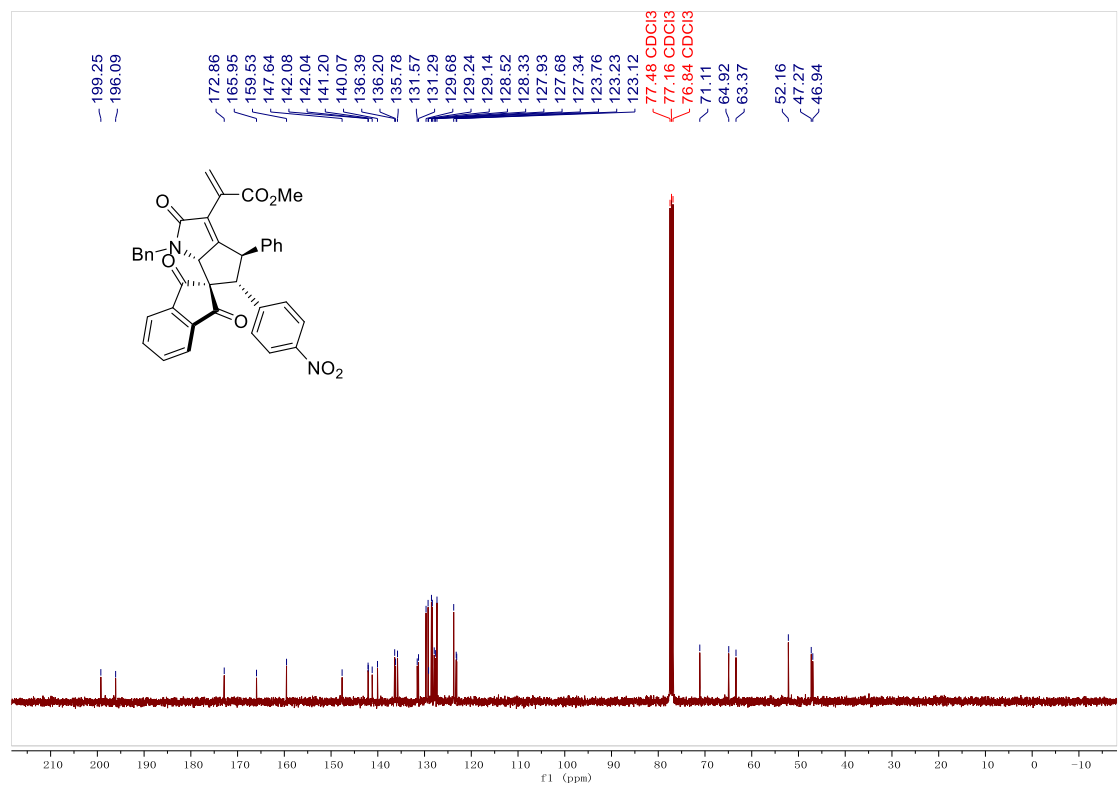
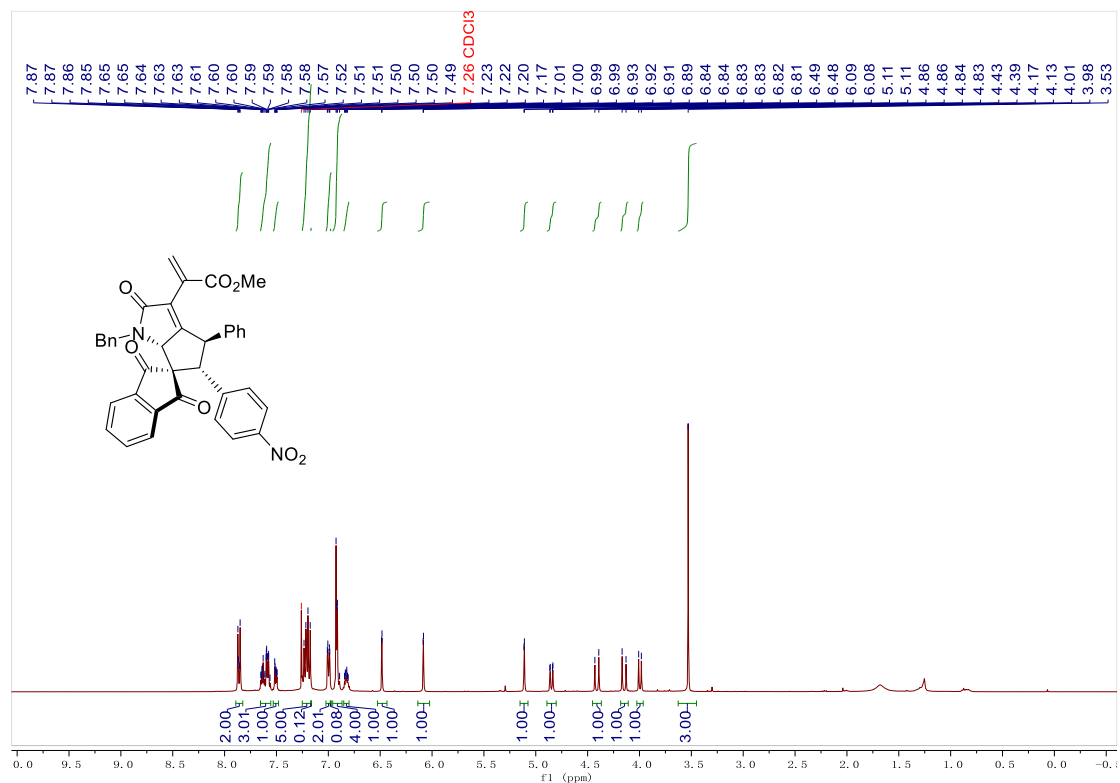
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-chlorophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3*ac*)



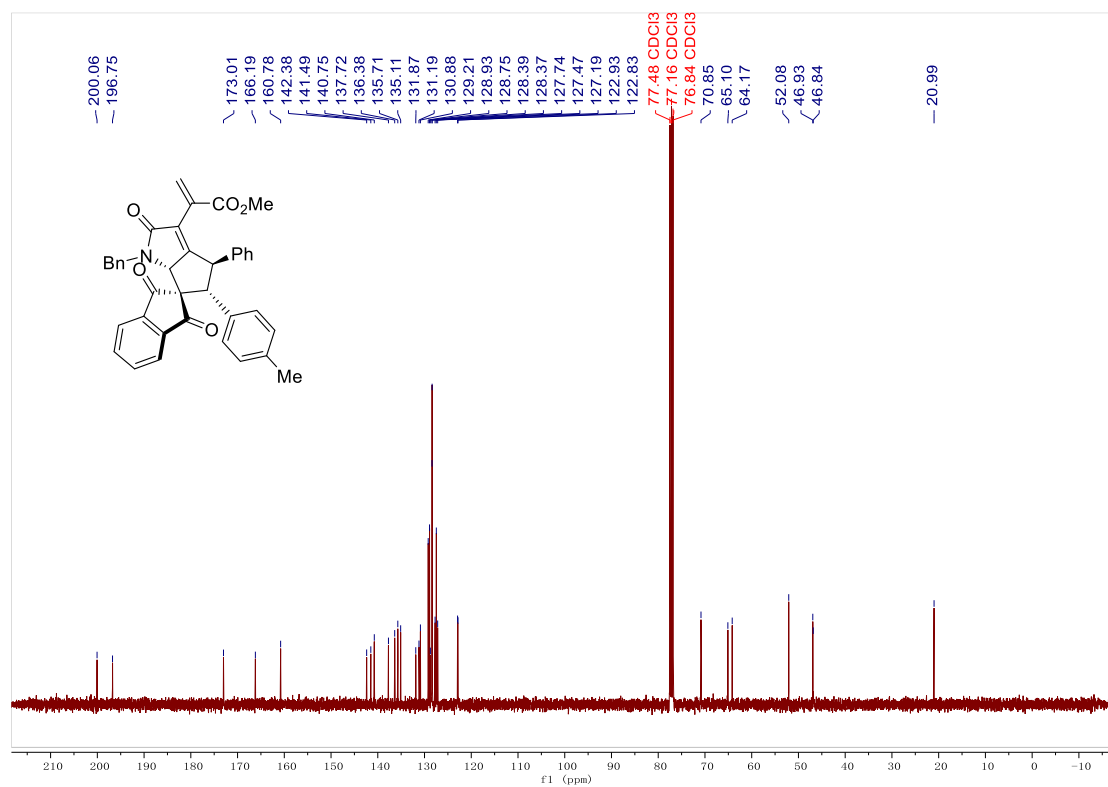
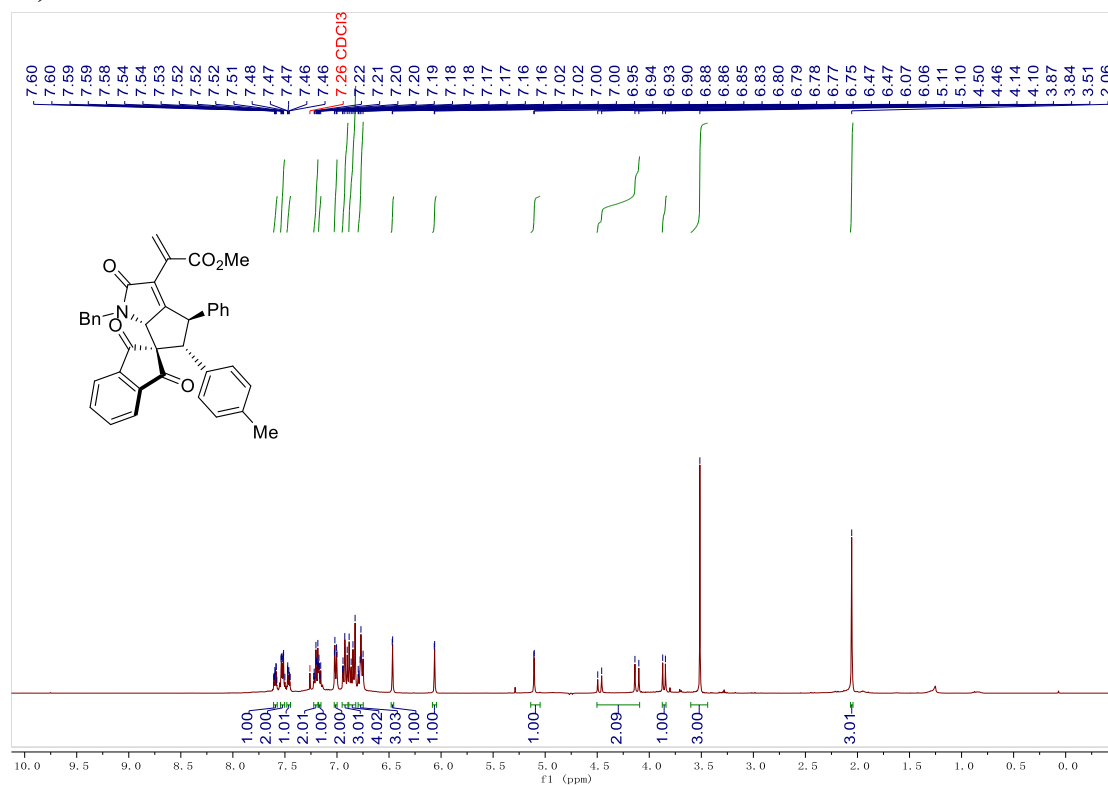
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-bromophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ad)



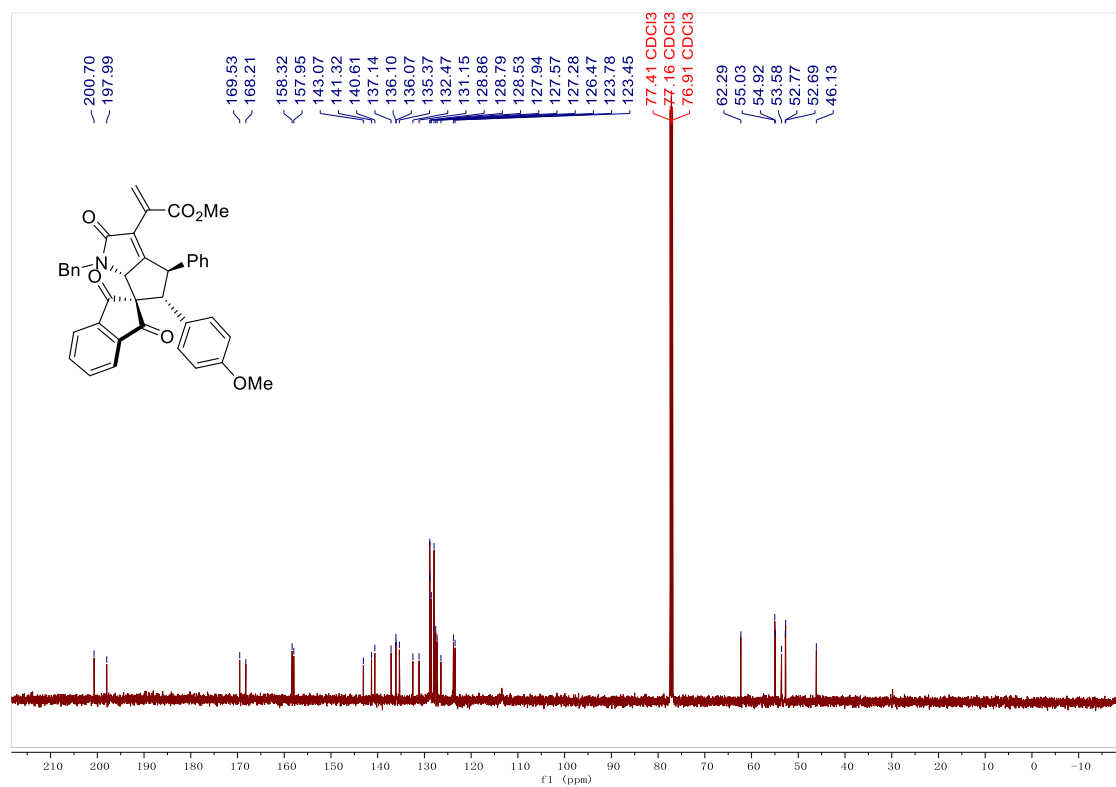
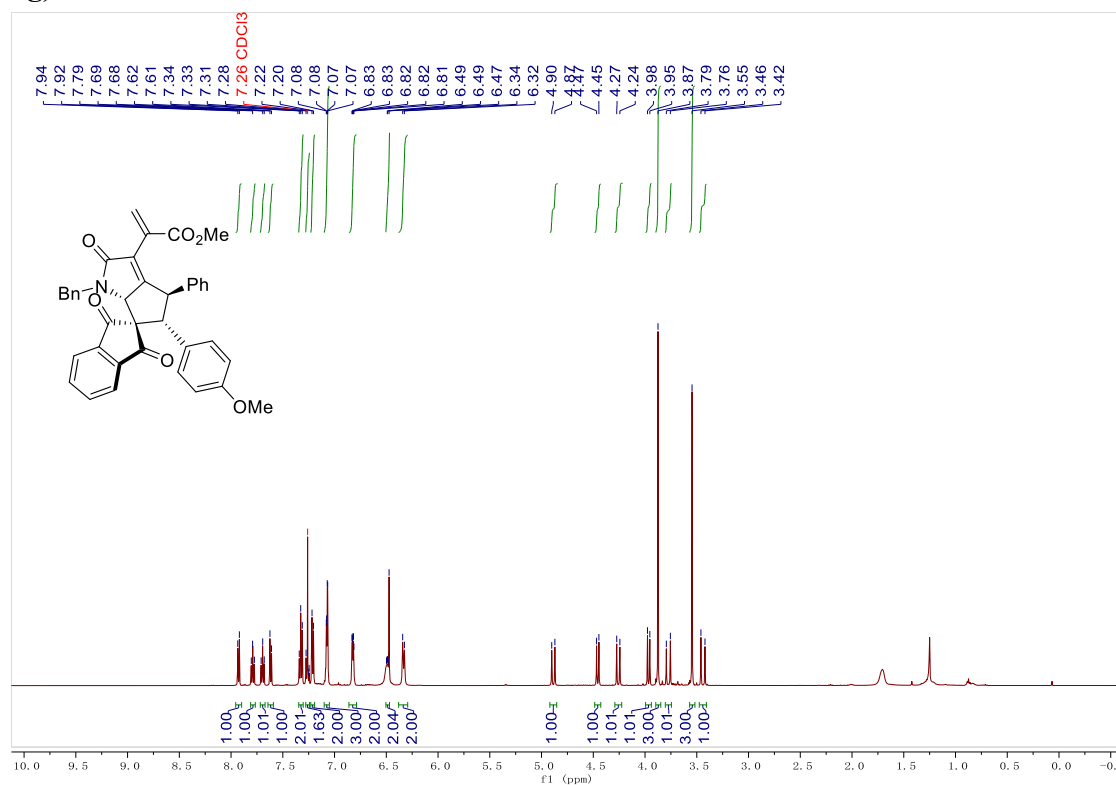
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-nitrophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ae)



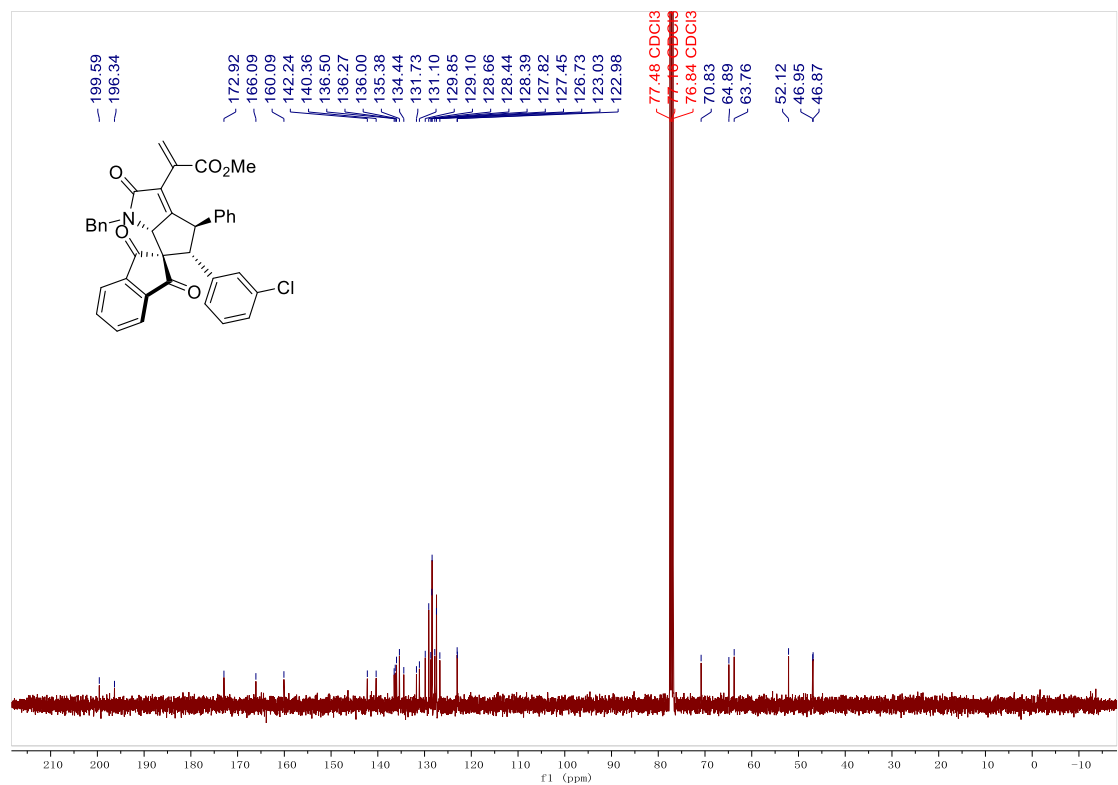
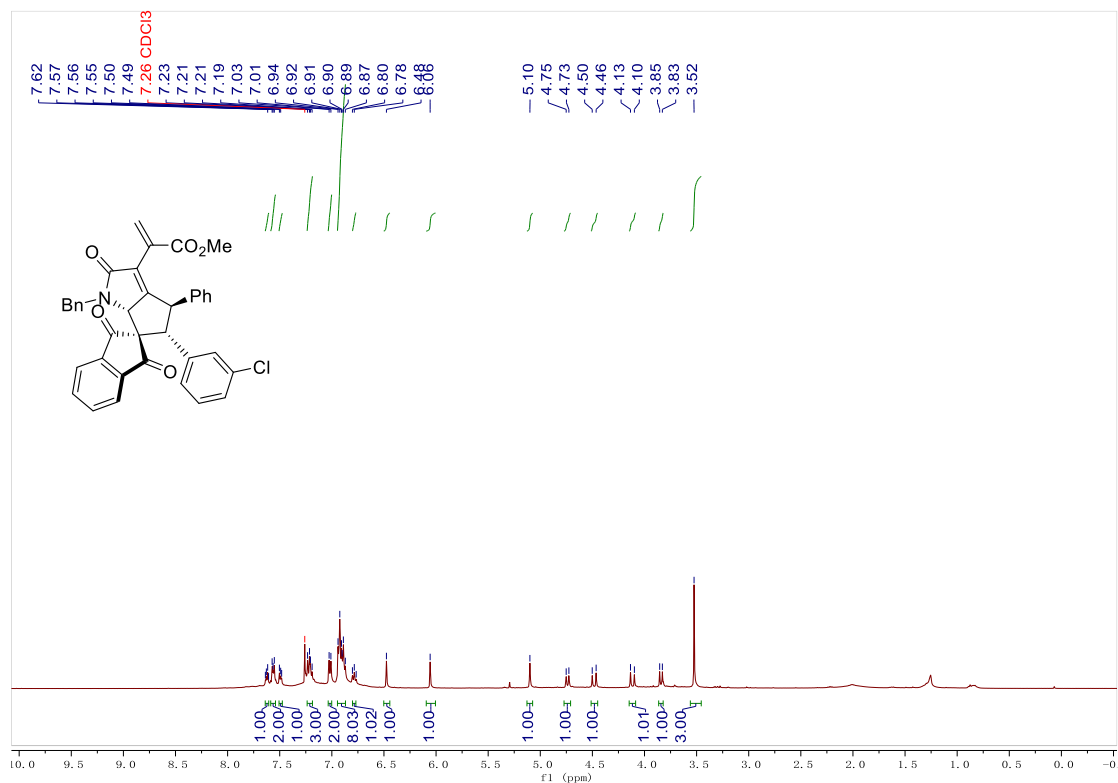
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-methoxyphenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6a-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3af)



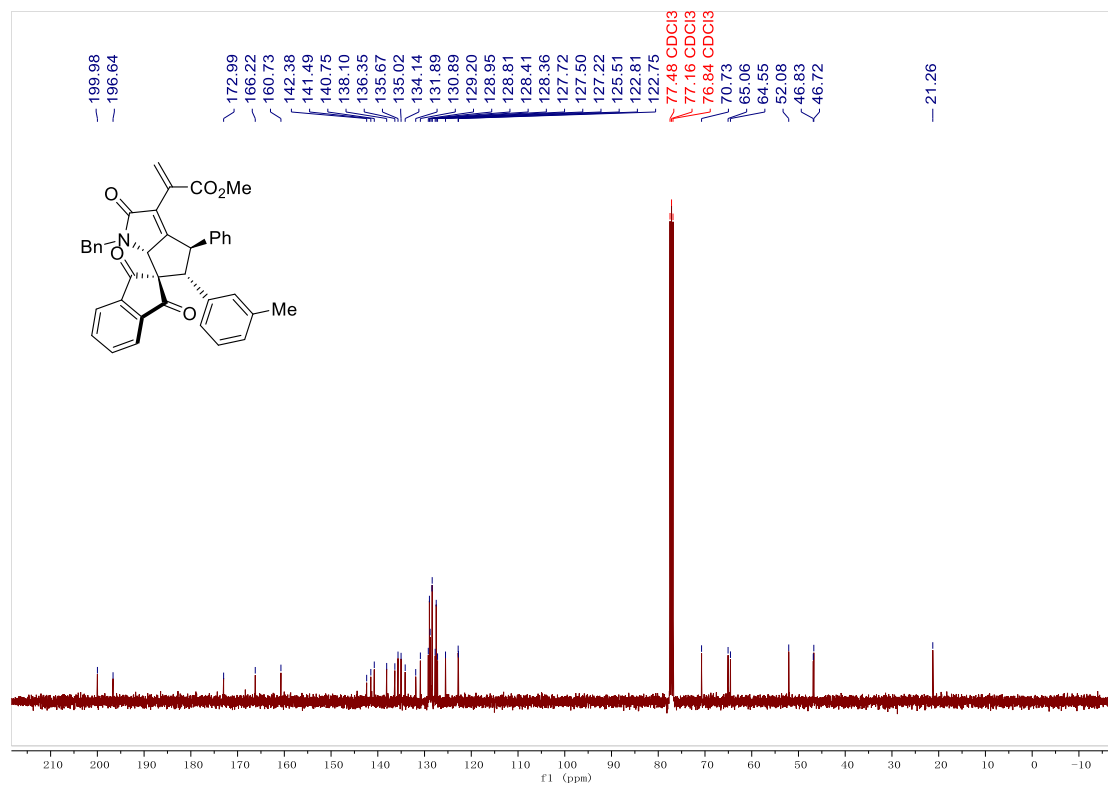
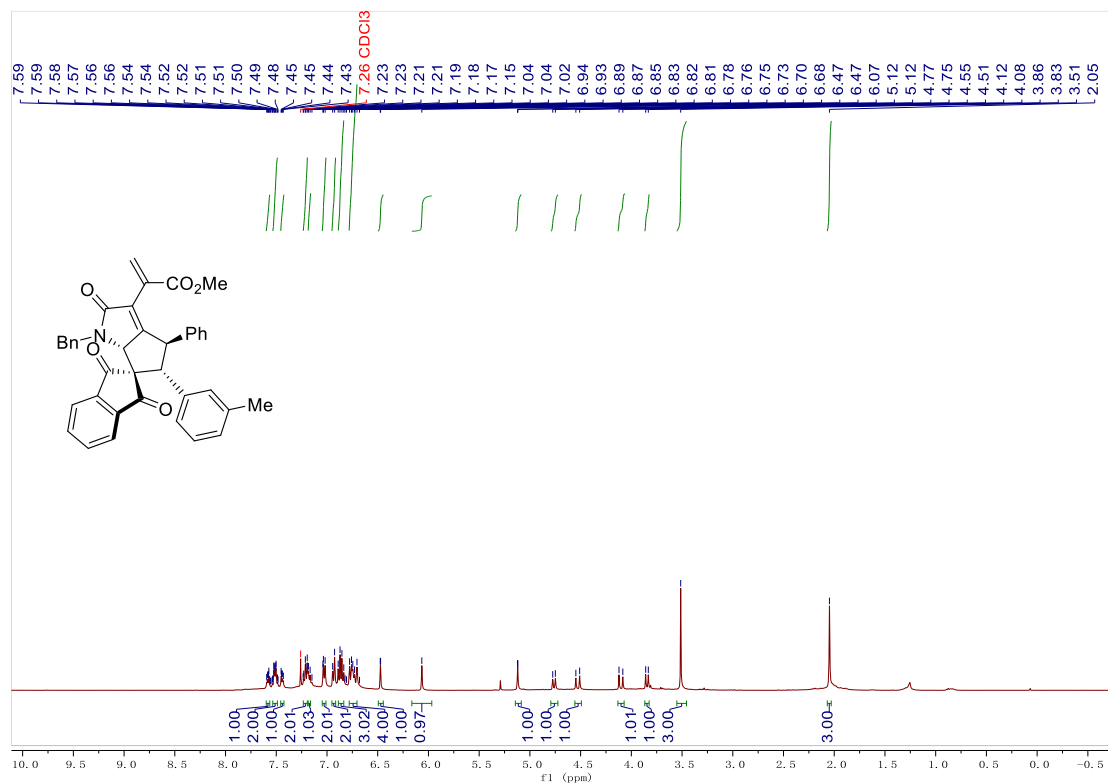
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(4-methoxyphenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ag)



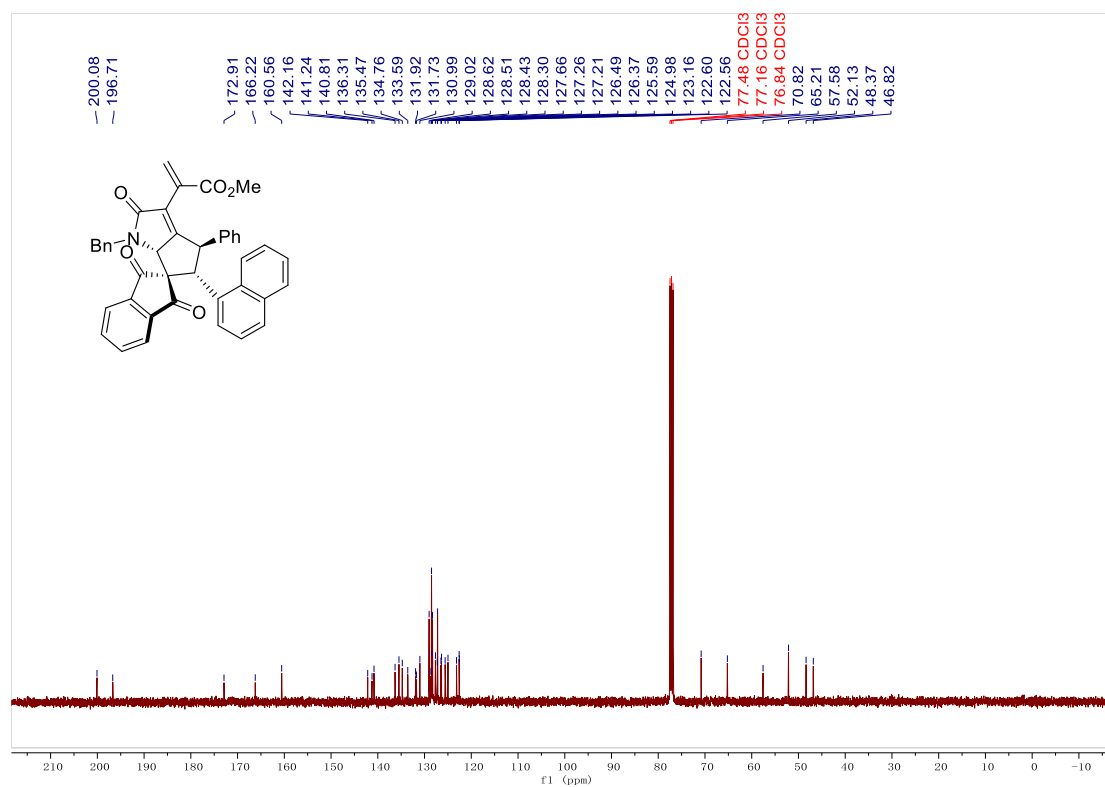
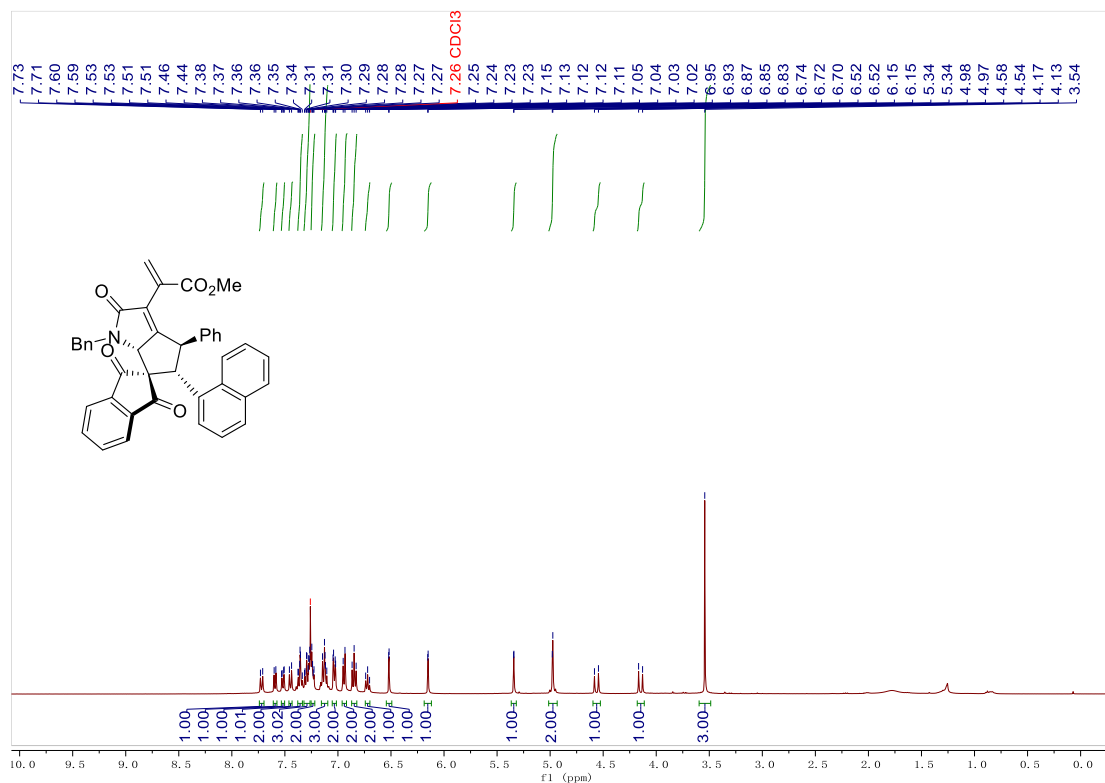
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(3-chlorophenyl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ah)



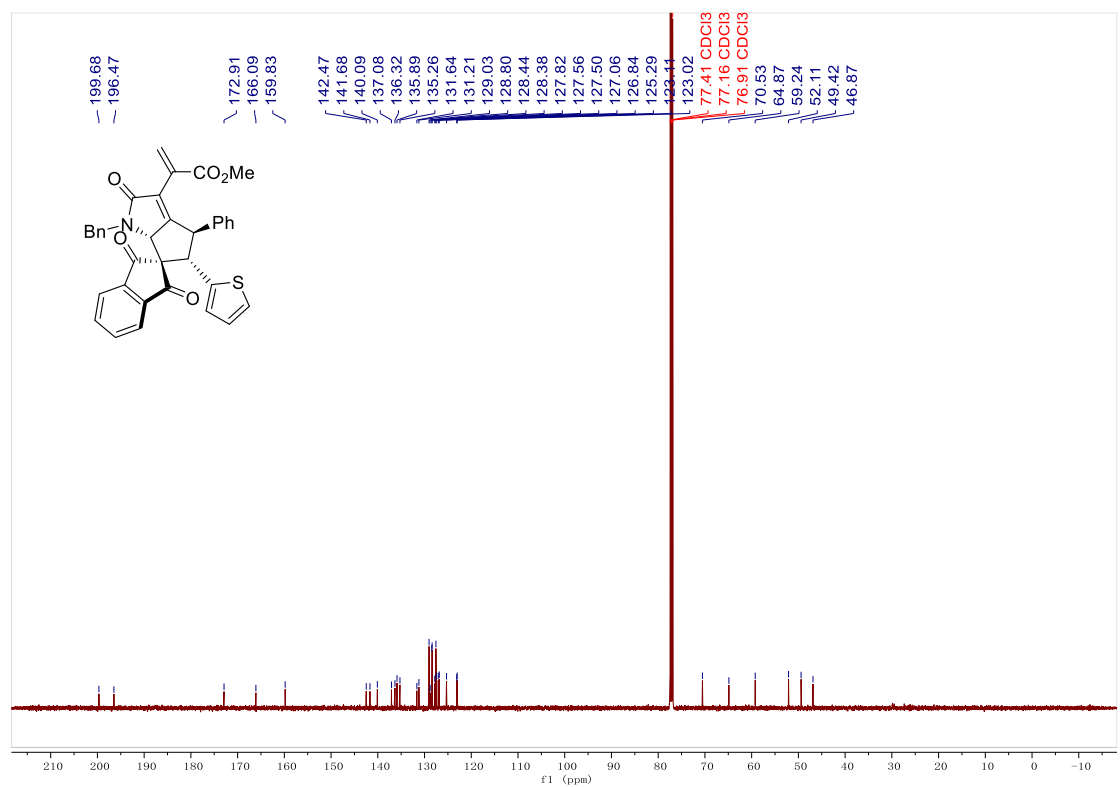
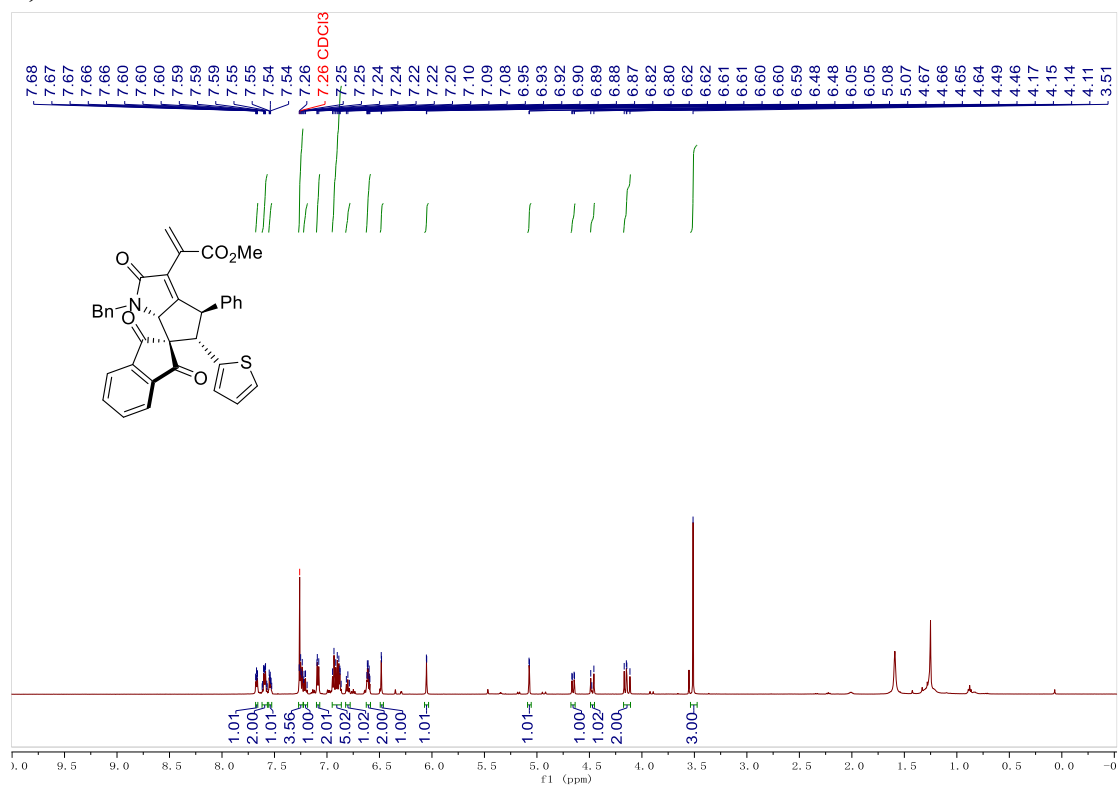
Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4-phenyl-5-(*p*-tolyl)-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3ai)



Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-5-(naphthalen-1-yl)-1',2,3'-trioxo-4-phenyl-1',2,3',4,5,6*a*-hexahydro-1*H*-spiro[cyclopenta[*b*]pyrrole-6,2'-inden]-3-yl)acrylate (3aj)



**Methyl 2-((4*R*,5*R*,6*aR*)-1-benzyl-1',2,3'-trioxo-4-phenyl-5-(thiophen-2-yl)-1',2,3,3a,3',4,5,6a-octahydro-1H-spiro[cyclopenta[b]pyrrole-6,2'-inden]-3-yl)acrylate (3a
k)**



E: Reference

- [1] R. Li, X. Chen, P. Li, Divergent annulations via organocatalysis: remote-controlled and switchable reactions of pyrrolidinone-based Morita-Baylis-Hillman carbonates with 2-arylideneindane-1,3-diones. *Org. Lett.*, 2025, **27**, 6872-6877.
- [2] N. Parui, P. Paul, Sk J. Ahashan, J. Dash, Regioselective and chemodivergent synthesis of 1,3-indandione-fused spirocyclopentenones and spiropyrrolidines. *J. Org. Chem.*, 2025, **90**, 26, 8886-8902.

F: Determination of the absolute configuration.

Computational details:

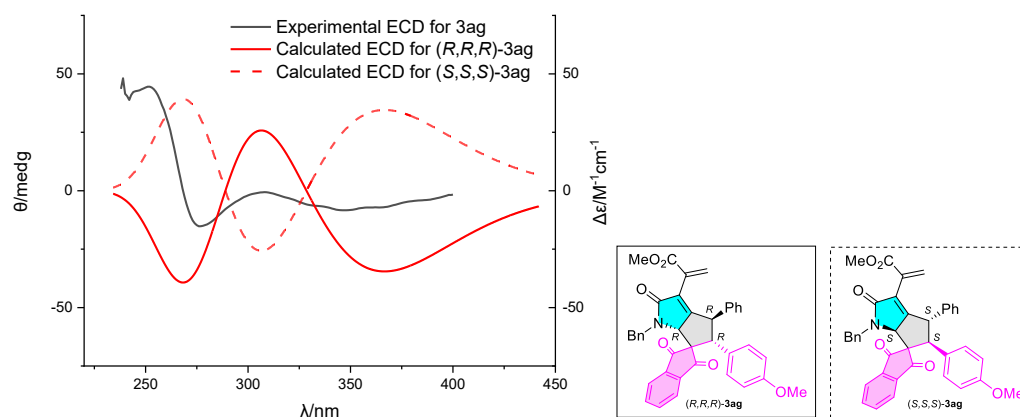
All calculations were performed using Gaussian 16, Revision A.03 package.¹ All of the intermediates were optimized by the DFT with the B3LYP-D3 functional.² For geometry optimizations, we employed 6-31G(d) basis sets for C, H, O, and N. All the stationary structures were characterized with no imaginary frequency. For single point energy calculation and time-dependent density functional theory (TD-DFT) calculation, we employed 6-311++G(d,p) basis sets for C, H, O, and N. The solvent effect of Dichloromethane was evaluated through the SMD method.³ All reported energies are free energies at a concentration of 1 M and a temperature of 298.15 K. ECD spectra of 107 were performed using Multiwfn 3.8.⁴

[1] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

[2] S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456-65.

[3] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B.*, **2009**, *113*, 6378.

[4] T. Lu, F. Chen, *J. Comput. Chem.*, **2012** *33*, 580.



Comparison of the calculated ECD spectrum of chiral compound **3ag**
with the experimental ECD spectrum of compound **3ag**

Cartesian coordinates of the optimized structures:

107-conformer 1

E = -2011.06960173 a.u.

O 1

C	2.43969100	-1.32411400	0.09064300
C	1.14479400	-0.83662300	0.31236200
C	0.88613700	0.53255800	0.35509100
C	1.95963300	1.40356100	0.16902900
C	3.25900900	0.91416700	-0.05463900
C	3.51383800	-0.45671000	-0.09704000
C	2.43400700	-2.80979500	0.08548800
C	0.20276600	-1.97011900	0.48319900
H	-0.12230400	0.89490000	0.52763800
H	1.79446700	2.47667000	0.19591200
H	4.07352400	1.61848900	-0.19628300
H	4.51061400	-0.84978800	-0.26921900
O	3.39222300	-3.53060000	-0.12248400
O	-0.99579100	-1.89792800	0.69081400
C	1.00316600	-3.26677700	0.38454600
C	0.40657600	-4.28500100	-0.64111600
C	0.93497100	-4.11921400	1.68233300
C	1.03934100	-5.66634900	-0.25339900
H	-0.65821500	-4.33711900	-0.38428600
C	1.39521200	-5.46203700	1.19840500
C	2.33156600	-5.95846000	2.02895900
C	2.57912500	-4.94037000	3.10783500
H	1.98558600	-5.78721800	-0.78993000
H	-0.11659800	-4.11891100	2.00881400
N	1.81731000	-3.82128200	2.77825600
O	3.31673200	-5.02334200	4.07878900
C	1.53913100	-2.76894200	3.74919700

H	2.39769700	-2.75596300	4.42519000
H	1.50335600	-1.80831700	3.22308500
C	0.25049500	-3.01040300	4.50553600
C	0.20566100	-3.99435200	5.50277600
C	-0.91669700	-2.31329400	4.17883000
C	-0.98828400	-4.26785600	6.16701200
H	1.11100200	-4.54416200	5.74530800
C	-2.11394600	-2.58849100	4.84361400
H	-0.89513200	-1.56346800	3.39250300
C	-2.15091900	-3.56411300	5.83956200
H	-1.01318000	-5.02993000	6.94094600
H	-3.01545600	-2.04329000	4.57860300
H	-3.08132900	-3.77889900	6.35782600
C	3.11325800	-7.18716000	1.88534200
C	4.39431800	-7.28996400	2.27498900
H	4.93972100	-8.21844600	2.14656800
H	4.90190400	-6.45781500	2.74818700
C	2.37667700	-8.38360000	1.36862700
O	1.22185500	-8.63656400	1.64058700
O	3.14423500	-9.16694400	0.58056500
C	2.47864500	-10.33824600	0.07961000
H	2.16273000	-10.98329000	0.90386600
H	1.60093200	-10.05078100	-0.50506900
H	3.21468400	-10.84500300	-0.54526300
C	0.50959200	-3.87455500	-2.08754400
C	-0.60200900	-3.31562700	-2.72211000
C	1.69821800	-3.99448200	-2.82756700
C	-0.55300600	-2.88427600	-4.04946300
H	-1.53015900	-3.20936800	-2.16678100
C	1.76344200	-3.57410200	-4.14863200
H	2.58720700	-4.40759400	-2.36388400
C	0.63777900	-3.01529400	-4.77089100
H	-1.44025400	-2.45936400	-4.50342800
H	2.67922900	-3.66743600	-4.72331200
O	0.80445300	-2.63498400	-6.07002300
C	-0.30782500	-2.07063600	-6.74278100
H	-0.64630500	-1.14612500	-6.25629800
H	0.03574900	-1.84238000	-7.75311700
H	-1.14748800	-2.77629100	-6.79485600
C	0.13562200	-6.82070200	-0.61917100
C	0.39118900	-7.56086800	-1.77650800
C	-0.97989000	-7.14178400	0.16084400
C	-0.44988700	-8.61200600	-2.14763800
H	1.25214600	-7.30939500	-2.39037400

C	-1.81922000	-8.19087300	-0.20430700
H	-1.17036200	-6.58874200	1.07648400
C	-1.55665500	-8.93057600	-1.35997400
H	-0.24037100	-9.17816700	-3.05122300
H	-2.67283400	-8.44014700	0.41948900
H	-2.21016800	-9.75111000	-1.64263600

107-conformer 2

E = -2011.06951777 a.u.

0 1

C	2.45102900	-1.35894100	0.04991600
C	1.15776500	-0.87182400	0.28178800
C	0.89686600	0.49716000	0.31586500
C	1.96662900	1.36855900	0.11122800
C	3.26454400	0.87967700	-0.12185000
C	3.52145200	-0.49104200	-0.15598300
C	2.44772700	-2.84465100	0.05576000
C	0.21975000	-2.00543800	0.47254700
H	-0.11046400	0.85901900	0.49561100
H	1.79959300	2.44152000	0.13071900
H	4.07623800	1.58436900	-0.27732200
H	4.51723800	-0.88366900	-0.33495500
O	3.40430200	-3.56553400	-0.15973800
O	-0.97621400	-1.93373200	0.69440900
C	1.02114500	-3.30156300	0.37446100
C	0.41856400	-4.32738300	-0.64051700
C	0.96649900	-4.14507700	1.67822500
C	1.05512900	-5.70528400	-0.24790200
H	-0.64476400	-4.37899400	-0.37737600
C	1.42345800	-5.49062500	1.19937100
C	2.36751500	-5.98082500	2.02483200
C	2.62480200	-4.95476700	3.09385400
H	1.99725300	-5.83010000	-0.79046200
H	-0.08189600	-4.14387300	2.01480900
N	1.85900700	-3.83866100	2.76366100
O	3.37223900	-5.03029800	4.05791700
C	1.58906200	-2.77975500	3.72989700
H	2.45445600	-2.76067500	4.39697200
H	1.54650300	-1.82302700	3.19723400
C	0.30858000	-3.01764800	4.50105500
C	0.27594800	-3.99322700	5.50695800
C	-0.86339600	-2.32588900	4.18011900
C	-0.91073700	-4.26384900	6.18523700
H	1.18492100	-4.53894300	5.74512300

C	-2.05337200	-2.59824300	4.85898100
H	-0.85142900	-1.58256100	3.38746300
C	-2.07820500	-3.56555800	5.86337300
H	-0.92620700	-5.01943200	6.96575500
H	-2.95872300	-2.05736300	4.59829200
H	-3.00296200	-3.77812600	6.39254600
C	3.14759300	-7.21081800	1.88356200
C	4.43244600	-7.31074400	2.26135400
H	4.97610900	-8.24068000	2.13613700
H	4.94489400	-6.47460400	2.72212900
C	2.40530500	-8.41165000	1.38548100
O	1.25256200	-8.66038400	1.66969100
O	3.16544800	-9.20441500	0.59940700
C	2.49472200	-10.38108700	0.11822700
H	2.18523400	-11.01583100	0.95283600
H	1.61231000	-10.09995800	-0.46243800
H	3.22510400	-10.89607700	-0.50658500
C	0.51401600	-3.92065500	-2.08898300
C	1.68267700	-4.06842200	-2.84171500
C	-0.59599500	-3.32541200	-2.70900000
C	1.75131500	-3.64542600	-4.17089300
H	2.56714300	-4.50491100	-2.39083900
C	-0.54385300	-2.89530200	-4.02753000
H	-1.51324900	-3.19596900	-2.14075600
C	0.63375900	-3.05479200	-4.77069900
H	2.67509100	-3.78015000	-4.72084900
H	-1.40313900	-2.43827300	-4.50730400
O	0.59044700	-2.60718800	-6.05839400
C	1.75588800	-2.75422500	-6.85093900
H	2.03724400	-3.80985000	-6.96161500
H	1.50763900	-2.34182000	-7.83034100
H	2.60401400	-2.19987800	-6.42746100
C	0.15004700	-6.86391400	-0.59655300
C	0.40206800	-7.61938700	-1.74466400
C	-0.96260300	-7.17531000	0.19147000
C	-0.43975900	-8.67566700	-2.09914100
H	1.26102100	-7.37580700	-2.36450100
C	-1.80262100	-8.22948800	-0.15691800
H	-1.15061800	-6.61005700	1.10014900
C	-1.54368500	-8.98425100	-1.30362800
H	-0.23330100	-9.25349100	-2.99603100
H	-2.65418500	-8.47066700	0.47279600
H	-2.19800600	-9.80843600	-1.57341800

107-conformer 3

E = -2011.07377662 a.u.

0 1

C	2.57317100	-1.53653300	0.01264600
C	1.30917400	-0.98103400	0.23867900
C	1.03176500	0.34299600	-0.09637400
C	2.05250100	1.09563300	-0.67447400
C	3.32283400	0.53734900	-0.90215900
C	3.59822500	-0.78450000	-0.55616900
C	2.58778500	-2.96663100	0.41510100
C	0.41027300	-2.00376700	0.82375000
H	0.04670900	0.75960000	0.08798500
H	1.86889900	2.12901400	-0.95450000
H	4.09833700	1.14940400	-1.35367600
H	4.57348700	-1.23019900	-0.72209500
O	3.54221900	-3.71910700	0.37786500
O	-0.72812500	-1.84327000	1.22745200
C	1.14940600	-3.34154600	0.79029000
C	0.51148100	-4.27707600	-0.31746200
C	0.96082700	-4.24997400	2.02727000
C	1.03651900	-5.71547700	0.02616200
H	-0.56227500	-4.26781500	-0.09576800
C	1.38092700	-5.58779000	1.48276300
C	2.27592100	-6.16414800	2.30002400
C	2.48311900	-5.25753500	3.48302400
H	1.96789500	-5.90997900	-0.51565200
H	-0.11341100	-4.19647100	2.27081400
N	1.75201900	-4.10776400	3.21633900
O	3.15111800	-5.45452700	4.48454100
C	1.64139700	-3.00795500	4.15154000
H	0.58372600	-2.77283300	4.32425600
H	2.07064000	-3.37034900	5.09142500
C	2.38115200	-1.77897400	3.66519600
C	1.73843000	-0.54525500	3.55042500
C	3.73135500	-1.88754600	3.30351100
C	2.43166000	0.57310600	3.08091100
H	0.68507100	-0.46377900	3.80674500
C	4.42222900	-0.77291100	2.83634200
H	4.22651200	-2.85199300	3.37217400
C	3.77361400	0.46058800	2.72217600
H	1.91747000	1.52454400	2.98022100
H	5.46564400	-0.86835700	2.54967100
H	4.31009900	1.32519500	2.34224300
C	3.06310300	-7.38151900	2.08989800

C	2.54755400	-8.51058900	1.57937000
H	3.17273500	-9.37884500	1.40517300
H	1.49476400	-8.58448100	1.32663700
C	4.52871200	-7.25369500	2.37269000
O	5.13223400	-6.20287300	2.35082400
O	5.11420000	-8.44866500	2.61161000
C	6.52921400	-8.38576800	2.83505100
H	7.04070900	-7.98104200	1.95716700
H	6.74983000	-7.75027700	3.69654100
H	6.84192000	-9.41331200	3.02319200
C	0.69464600	-3.80061500	-1.73444100
C	-0.33398500	-3.09008700	-2.35680400
C	1.89250700	-3.98233100	-2.44653900
C	-0.19408500	-2.56655900	-3.64366800
H	-1.26750000	-2.93305800	-1.82261300
C	2.04754200	-3.47220400	-3.72771100
H	2.72219100	-4.51104100	-1.98977400
C	1.00563100	-2.75758600	-4.33647400
H	-1.01846300	-2.02261400	-4.08890600
H	2.97153900	-3.61087800	-4.27947500
O	1.25760700	-2.29587800	-5.59416700
C	0.23426400	-1.56663300	-6.24988300
H	-0.02786900	-0.65499800	-5.69669800
H	0.63785700	-1.29375700	-7.22631200
H	-0.66922200	-2.17535900	-6.38695000
C	0.02286200	-6.77200600	-0.35874900
C	-0.03167300	-7.22836200	-1.68127600
C	-0.90223900	-7.26839300	0.56670300
C	-0.99051800	-8.16320200	-2.07000700
H	0.67938500	-6.84341800	-2.40690300
C	-1.85969800	-8.20741800	0.18072400
H	-0.86156300	-6.92672100	1.59761000
C	-1.90735000	-8.65697700	-1.13967100
H	-1.01869300	-8.50969000	-3.09937600
H	-2.56612200	-8.58860100	0.91288600
H	-2.65078100	-9.38946300	-1.44083800

107-conformer 4

E = -2011.07646623 a.u.

0 1

C	2.59643300	-1.53068000	0.03731900
C	1.32866700	-0.99004200	0.27862800
C	1.03088700	0.32935200	-0.05614000
C	2.03496800	1.09320100	-0.64869700

C	3.30938000	0.55042800	-0.89052100
C	3.60528300	-0.76713400	-0.54513300
C	2.63263200	-2.95780600	0.44683300
C	0.45068200	-2.02250900	0.87977700
H	0.04320200	0.73426000	0.13972400
H	1.83495700	2.12341000	-0.92908600
H	4.07134500	1.17074900	-1.35358800
H	4.58374100	-1.20082300	-0.72376300
O	3.60237500	-3.69343700	0.42606300
O	-0.68169100	-1.87419800	1.30380400
C	1.20204500	-3.35214700	0.82532600
C	0.55864000	-4.27146200	-0.29367200
C	1.04254700	-4.28454200	2.04695000
C	1.11104500	-5.70301200	0.00653300
H	-0.51176800	-4.28230200	-0.05535400
C	1.43507500	-5.61983900	1.47665200
C	2.33734200	-6.22390600	2.27095700
C	2.64564700	-5.29368000	3.41094500
H	2.06566500	-5.83443700	-0.51322900
H	-0.02210200	-4.23300100	2.32876600
N	1.87837800	-4.15678900	3.20774500
O	3.44109800	-5.44727200	4.32715000
C	1.77801800	-3.08626100	4.18003100
H	0.72212700	-2.90596400	4.41746400
H	2.27482000	-3.45462300	5.08310700
C	2.43175700	-1.80844300	3.69826400
C	1.70996000	-0.61755100	3.60113000
C	3.78255400	-1.82477700	3.32495300
C	2.32521900	0.54684500	3.13482000
H	0.65638900	-0.60595300	3.86811900
C	4.39586400	-0.66533700	2.85892500
H	4.33857200	-2.75541500	3.39130500
C	3.66740000	0.52415300	2.76065900
H	1.75009100	1.46414900	3.04883600
H	5.44091900	-0.68938100	2.56332100
H	4.14288400	1.42434400	2.38242600
C	3.06896800	-7.46665600	2.02194400
C	4.35142600	-7.64621200	2.37832800
H	4.85825900	-8.58210200	2.17030500
H	4.89649000	-6.87083600	2.90311600
C	2.27923600	-8.58950900	1.42543200
O	1.11421700	-8.81048300	1.68232900
O	3.01011000	-9.34773700	0.57951600
C	2.29267400	-10.44970000	-0.00029700

H	1.94883900	-11.13693100	0.77737500
H	1.42833900	-10.08290000	-0.56001300
H	3.00487900	-10.94325700	-0.66231100
C	0.71636500	-3.76008000	-1.70136500
C	-0.32569000	-3.04170900	-2.29115800
C	1.90648500	-3.91107100	-2.43247900
C	-0.20579600	-2.48087300	-3.56421900
H	-1.25394700	-2.90781900	-1.74171800
C	2.04251100	-3.36279900	-3.69993600
H	2.74598800	-4.44658200	-2.00218400
C	0.98746000	-2.64063800	-4.27583600
H	-1.04037100	-1.93251900	-3.98434600
H	2.96075000	-3.47805700	-4.26653500
O	1.22099200	-2.13985700	-5.52226100
C	0.18139700	-1.40664600	-6.14714400
H	-0.08591900	-0.51329900	-5.56715600
H	0.57053800	-1.10286700	-7.12032700
H	-0.71587700	-2.02302100	-6.29040500
C	0.16381300	-6.78040600	-0.46855000
C	0.41130300	-7.43668100	-1.67722600
C	-0.98149000	-7.11126500	0.26242700
C	-0.46781100	-8.41420900	-2.14779800
H	1.29657600	-7.17841200	-2.25244800
C	-1.85920300	-8.08716800	-0.20201400
H	-1.16517900	-6.62608000	1.21697100
C	-1.60506000	-8.74282900	-1.40915600
H	-0.26363100	-8.91581700	-3.08989000
H	-2.73634500	-8.34620500	0.38399800
H	-2.28840400	-9.50670400	-1.76934400

107-conformer 5

E = -2011.07375883 a.u.

0 1

C	2.62869500	-1.56809200	0.01323400
C	1.36795700	-0.99976700	0.22508800
C	1.10522300	0.32455300	-0.12038800
C	2.13766200	1.06472000	-0.69368900
C	3.40517000	0.49406400	-0.90587700
C	3.66557600	-0.82820000	-0.55003700
C	2.62641900	-2.99636100	0.42220100
C	0.45487800	-2.01090800	0.80840100
H	0.12203200	0.75067500	0.05147200
H	1.96531200	2.09757700	-0.98243300
H	4.19033300	1.09716200	-1.35285700

H	4.63861900	-1.28330900	-0.70333900
O	3.57382300	-3.75819800	0.39531100
O	-0.68454600	-1.83757400	1.20362200
C	1.18130300	-3.35586600	0.78673500
C	0.54693400	-4.29005800	-0.32494100
C	0.97190100	-4.25659500	2.02558000
C	1.04972700	-5.73291800	0.03274400
H	-0.52974200	-4.26693200	-0.11887600
C	1.38301300	-5.60113900	1.49149200
C	2.26430500	-6.18286600	2.31979900
C	2.47095000	-5.27213600	3.49972000
H	1.98308300	-5.94407700	-0.49918500
H	-0.10396100	-4.19109900	2.25878800
N	1.75360700	-4.11662800	3.22128400
O	3.12911500	-5.47077400	4.50748400
C	1.64578400	-3.01112900	4.15016400
H	0.58900900	-2.76484700	4.31223300
H	2.06308900	-3.37315600	5.09554000
C	2.40179500	-1.79176800	3.66461800
C	1.77164800	-0.55280200	3.53711500
C	3.75429000	-1.91474400	3.31643000
C	2.47963100	0.55654400	3.06825100
H	0.71668800	-0.46025300	3.78276000
C	4.45989300	-0.80903400	2.85002000
H	4.23978600	-2.88333100	3.39520900
C	3.82387300	0.42973500	2.72304300
H	1.97519500	1.51204700	2.95744900
H	5.50514400	-0.91554900	2.57408400
H	4.37196100	1.28732300	2.34375400
C	3.03885600	-7.41070500	2.12457400
C	2.51538100	-8.53613200	1.61400900
H	3.13174100	-9.41304400	1.45205200
H	1.46478300	-8.59853400	1.34932100
C	4.50262500	-7.29996400	2.42370400
O	5.12123500	-6.25808000	2.39662600
O	5.06823300	-8.50014500	2.68357700
C	6.48091100	-8.45427300	2.92502200
H	7.00962100	-8.06733100	2.04929700
H	6.69908600	-7.81155000	3.78175100
H	6.77664300	-9.48371400	3.12953100
C	0.75791700	-3.81847200	-1.74006500
C	1.94993300	-4.03210800	-2.43853400
C	-0.24670400	-3.06741200	-2.37014600
C	2.14399700	-3.51941700	-3.72277100

H	2.75880500	-4.58779200	-1.97636400
C	-0.06935400	-2.54656500	-3.64404500
H	-1.17995800	-2.88426400	-1.84400600
C	1.13189200	-2.76910900	-4.33134300
H	3.08277500	-3.70730600	-4.22987300
H	-0.84649600	-1.96647900	-4.13074900
O	1.21581900	-2.21983700	-5.57623500
C	2.41389400	-2.41509300	-6.30806700
H	2.60190900	-3.48042200	-6.49604100
H	2.27234800	-1.89978900	-7.25948400
H	3.27894300	-1.98483800	-5.78622500
C	0.02518500	-6.77866100	-0.35368300
C	-0.02869100	-7.23867300	-1.67498300
C	-0.90979900	-7.26138300	0.56902900
C	-0.99672100	-8.16329100	-2.06528000
H	0.68966800	-6.86371900	-2.39860600
C	-1.87643800	-8.19036500	0.18154900
H	-0.87002900	-6.91689400	1.59901200
C	-1.92347200	-8.64340500	-1.13762800
H	-1.02479000	-8.51220100	-3.09382800
H	-2.59073200	-8.56073100	0.91160500
H	-2.67434500	-9.36770800	-1.44006000

107-conformer 6

E = -2011.07640011 a.u.

0 1

C	2.67966300	-1.59427100	0.07528300
C	1.42027100	-1.02957300	0.30507200
C	1.15040400	0.29513500	-0.03223000
C	2.17426300	1.04016900	-0.61472300
C	3.44075300	0.47379000	-0.84365400
C	3.70839500	-0.84931400	-0.49637300
C	2.68452800	-3.02245800	0.48243200
C	0.51736700	-2.04537400	0.89763800
H	0.16834600	0.71819500	0.15299700
H	1.99586500	2.07358700	-0.89762900
H	4.21894600	1.08045900	-1.29786700
H	4.68057200	-1.30110200	-0.66445700
O	3.63958500	-3.77725800	0.46694600
O	-0.61497600	-1.87551300	1.31347800
C	1.24309600	-3.38926300	0.84778300
C	0.59601500	-4.29489300	-0.28094000
C	1.05211900	-4.31939000	2.06613600
C	1.11557900	-5.73721900	0.02518800

H	-0.47776400	-4.28451100	-0.05801300
C	1.42422700	-5.66162400	1.49907500
C	2.30498200	-6.28442500	2.30301400
C	2.61974900	-5.36095700	3.44674700
H	2.07364300	-5.88832900	-0.48247000
H	-0.01434000	-4.24704700	2.33629500
N	1.87754800	-4.20901000	3.23616500
O	3.40276200	-5.53065600	4.37087100
C	1.78939600	-3.13609400	4.20707800
H	0.73496500	-2.93196800	4.43111000
H	2.26642000	-3.51513900	5.11637100
C	2.47784400	-1.87360900	3.73324800
C	1.78472200	-0.66654100	3.62752900
C	3.83225000	-1.92098900	3.37587300
C	2.43192300	0.48332100	3.16841000
H	0.72860700	-0.63067600	3.88198000
C	4.47741700	-0.77603200	2.91715300
H	4.36603600	-2.86404600	3.44917700
C	3.77756100	0.42979000	2.81015600
H	1.87896700	1.41347500	3.07553900
H	5.52515900	-0.82401200	2.63418700
H	4.27794400	1.31879400	2.43761200
C	3.01309900	-7.54223500	2.06178700
C	4.28758200	-7.74870300	2.43202300
H	4.77657600	-8.69537600	2.23018300
H	4.84318100	-6.98465600	2.96236500
C	2.20613900	-8.64887500	1.45792700
O	1.03384000	-8.84435000	1.70181500
O	2.93021400	-9.42444700	0.62176300
C	2.19614900	-10.51302200	0.03742400
H	1.82899000	-11.19000000	0.81340600
H	1.34622600	-10.12995900	-0.53332200
H	2.90522600	-11.02401800	-0.61468000
C	0.78558300	-3.78080000	-1.68409700
C	1.96648600	-3.97349300	-2.40611600
C	-0.22489900	-3.00520100	-2.27351700
C	2.14541400	-3.41606900	-3.67382600
H	2.77950900	-4.54900000	-1.97655700
C	-0.06314400	-2.44021800	-3.53049300
H	-1.15022700	-2.83768800	-1.72848700
C	1.12803800	-2.64155900	-4.24142700
H	3.07609800	-3.58964700	-4.20060000
H	-0.84500400	-1.84138300	-3.98591900
O	1.19742800	-2.04763500	-5.46675400

C	2.38217400	-2.22576600	-6.22387400
H	2.55965700	-3.28532200	-6.45068800
H	2.22934600	-1.67757000	-7.15496300
H	3.25858600	-1.81911400	-5.70188700
C	0.15321600	-6.79639000	-0.46053100
C	0.40692900	-7.46566100	-1.66069500
C	-1.01081600	-7.09857700	0.25309900
C	-0.48462700	-8.42746700	-2.14015500
H	1.30717700	-7.22997700	-2.22220800
C	-1.90099300	-8.05884100	-0.22005500
H	-1.20053100	-6.60319100	1.20122300
C	-1.64068000	-8.72740000	-1.41876800
H	-0.27564900	-8.93914800	-3.07576800
H	-2.79320300	-8.29543100	0.35250900
H	-2.33407300	-9.47876700	-1.78592900