

Palladium-catalyzed and ligand-controlled divergent cycloadditions of vinylidenecyclopropane-diester with *para*-quinone methides enabled by zwitterionic π -propargyl palladium species

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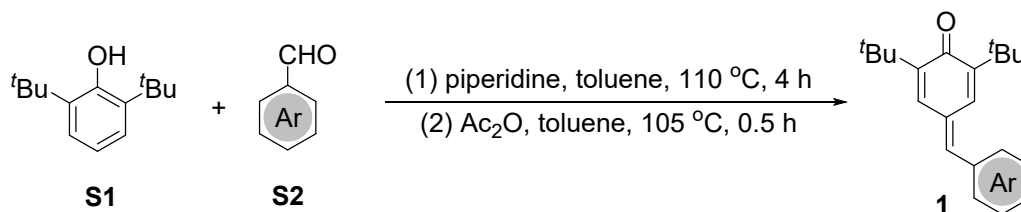
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(A) General Information

Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. Proton nuclear magnetic resonance (^1H NMR) spectra, carbon nuclear magnetic resonance (^{13}C NMR) spectra fluorine nuclear magnetic resonance (^{19}F NMR) were recorded at 400 MHz, 100 MHz and 376 MHz, respectively. ^1H NMR spectrum uses TMS ($\delta = 0.00$ ppm) as internal standard, ^{13}C NMR spectrum uses CDCl_3 ($\delta = 77.00$ ppm) as internal standard. Data are presented as follows: chemical shift (ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad, hept = heptet), coupling constants in Hertz (Hz) and integration. IR spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in cm^{-1} . High Resolution Mass Spectra (HRMS) were recorded by ESI and MALDI method. The employed solvents were dry up by standard methods when necessary. Commercially obtained reagents were used without further purification. Petroleum ether refers to the fraction with boiling point in the range 60-90 $^\circ\text{C}$. For thin-layer chromatography (TLC), silica gel plates (Huanghai GF254) were used. Column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

The preparation of *para*-quinone methides (*p*-QMs) **1**,¹ vinylidenecyclopropane-diester **2**,² and compounds **1a-1u**,^{1,3-6,8} **1y**,⁴ **1aa**,^{4,7} **1af**,⁸ **1ag**⁸ have been reported in the previous literature.

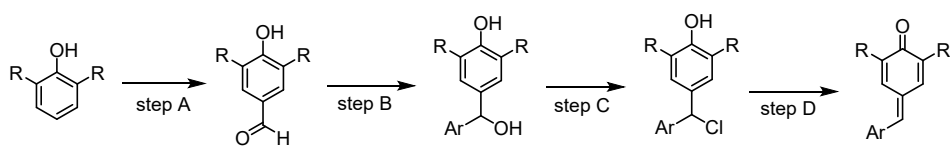
(B) General Procedure for the Preparation of *para*-Quinone Methides 1a-1u.¹



General procedure for the synthesis of *p*-QMs 1a~1u from phenols and aldehydes.

A solution of phenols (5.0 mmol, 1.0 equiv) and the corresponding aldehydes (5.0 mmol, 1.0 equiv) in toluene (20 mL) was heated to reflux. Piperidine (10.0 mmol, 2.0 equiv 1.0 mL) was dropwise added within 1.0 h. The reaction mixture was continued to reflux for 6-15 h. After cooling just below the boiling point of the reaction mixture, acetic anhydride (10.0 mmol, 2.0 equiv, 0.51 g) was added and stirring was continued for 15 min. Then, the reaction mixture was cooled to room temperature and the organic phases were removed under reduced pressure. The crude products were purified by a flash column chromatography on silica gel and further recrystallized from *n*-hexane, affording the desired *p*-QMs.

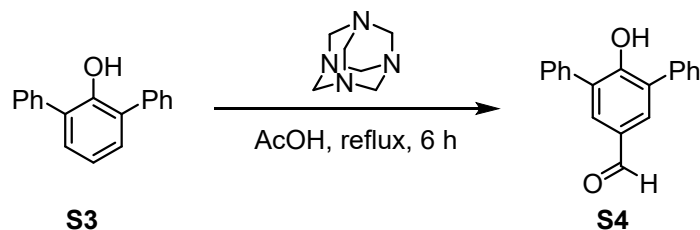
(C) General Procedure for the Preparation of *para*-Quinone Methides **1y-1ag**.⁴



substrate	R	Ar
1y	Ph	C ₆ H ₅
1z	Ph	4-F-C ₆ H ₄
1aa	Ph	4-OMe-C ₆ H ₄
1ab	Ph	4-Me-C ₆ H ₄
1ac	Ph	4- ^t Bu-C ₆ H ₄
1ad	Ph	2-Me-C ₆ H ₄
1ae	Ph	3-Cl-C ₆ H ₄
1af	ⁱ Pr	C ₆ H ₅
1ag	Me	C ₆ H ₅

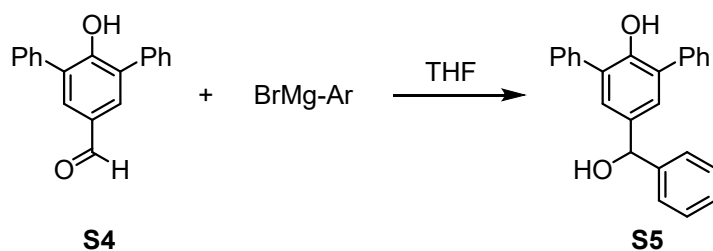
All the above substrates were synthesized by this method; here, phenyl substrate (**1y**) was used as an example.

Step A:⁵



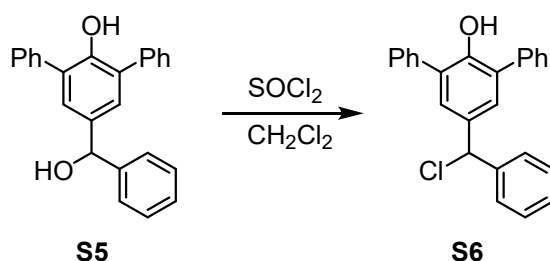
A stirred mixture of **S3** (5.0 g, 20 mmol, 1.0 equiv) and hexamethylenetetramine (5.5 g, 39 mmol, 2.0 equiv) was treated dropwise with AcOH (45 mL). After 20 min, H₂O (10 mL) was added, and the mixture was heated to reflux. Distillate was removed until the reaction pot temperature was at 114 °C. Reflux was then maintained for 6 h. Then cooled mixture was treated with H₂O (20 mL), and the precipitated product was filtered and washed with H₂O. Recrystallization from EtOH gave 3.0 g (55%) of **S4**.

Step B:



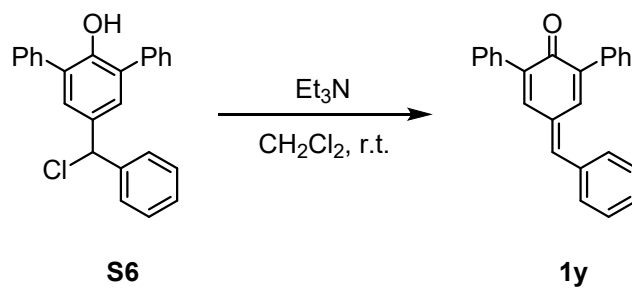
Phenylmagnesium bromide (6.0 mL, 2.4 equiv) (2.0 M, THF) was added dropwise to a solution of the adequate compound **S4** (1.37 g, 5.0 mmol, 1.0 equiv) in dry THF (20 mL). After stirring for 12 h, the reaction mixture was hydrolyzed with saturated aqueous NH_4Cl solution (25 mL). The aqueous phase was washed with diethyl ether. Then the combined organic layers were dried over anhydrous MgSO_4 and the solvent was evaporated under reduced pressure. Crude products with low solubility in *n*-pentane were suspended in *n*-pentane. After 1.0 h of stirring, the purified product was isolated by filtration. Crude products with high solubility in Et_2O were crystallized from diethyl ether/*n*-pentane.

Step C:



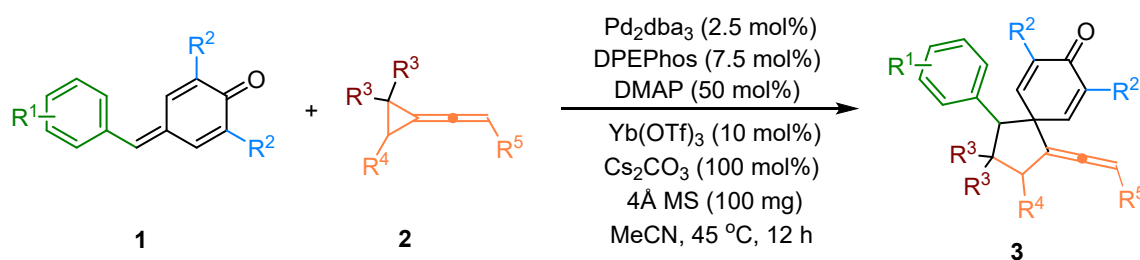
Under an atmosphere of dry N_2 , SOCl_2 (1.2 equiv) was added dropwise to a solution of compound **S5** (1.0 mmol, 1.0 equiv) in dry CH_2Cl_2 (20 mL) at 0 °C. After stirring at room temperature for 8-12 h, the solvent was removed under reduced pressure. Because the products were formed nearly quantitatively, they were used for the following step without further purification.

Step D:

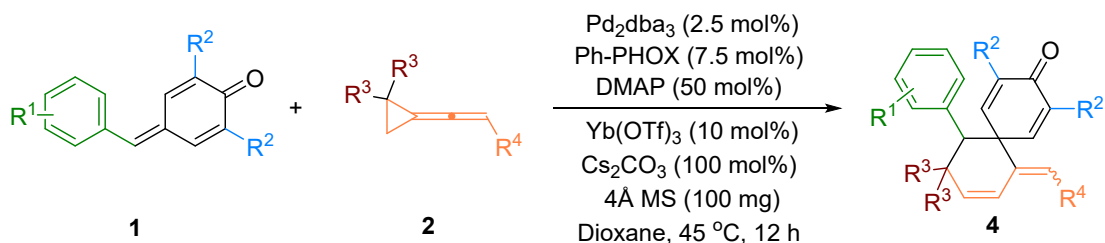


Under an atmosphere of dry N_2 , the **S6** (dried in the previous step) was dissolved in dry CH_2Cl_2 (20 mL) and 1.3 equiv of NEt_3 were added. After stirring for 2-3 h, diethyl ether was added. The resulting precipitate was filtered off and dried under reduced pressure, the residue was purified by a flash alkaline column chromatography to afford the desired product.

(D) General Procedure for the Synthesis of Compounds 3 and 4

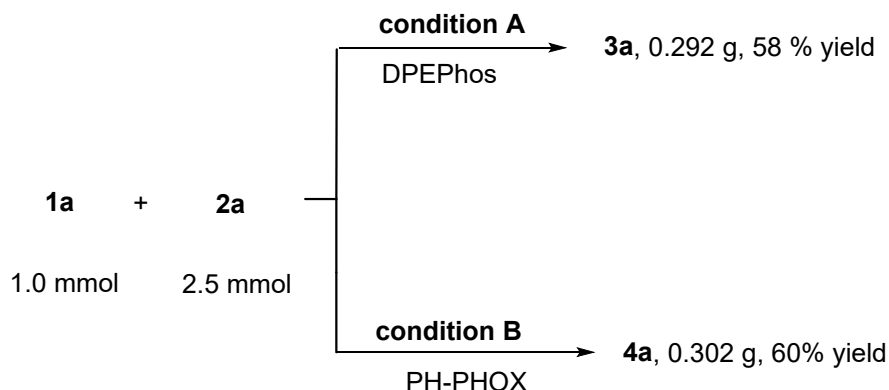


Tris(dibenzylideneacetone)dipalladium (0.0023 g, 0.002 mmol, 2.5 mol%), 4Å MS (100 mg) and DPEphos (0.0040 g, 0.007 mmol, 7.5 mol%) were added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in MeCN (degassed) (1.5 mL) for 30 minutes. After that, **1** (0.1 mmol), **2** (0.25 mmol), Yb(OTf)₃ (0.0062 g, 0.01 mmol, 10 mol%), DMAP (0.0061 g, 0.05 mmol, 50 mol%) and Cs₂CO₃ (0.1 mmol, 1.0 equiv) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and the residue was purified by a column chromatography to afford the desired product **3**.



Tris(dibenzylideneacetone)dipalladium (0.002 mmol, 2.5 mol%), 4Å MS (100 mg) and Ph-PHOX (0.007 mmol, 7.5 mol%) was added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in 1,4-dioxane (degassed) (1.5 mL) for 30 minutes. After that, **1** (0.1 mmol), **2** (0.25 mmol), Yb(OTf)₃ (0.0062 g, 0.01 mmol, 10 mol%), DMAP (0.05 mmol, 50 mol%) and Cs₂CO₃ (0.1 mmol, 1.0 equiv.) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and the residue was purified by a column chromatography to afford the desired product **4**.

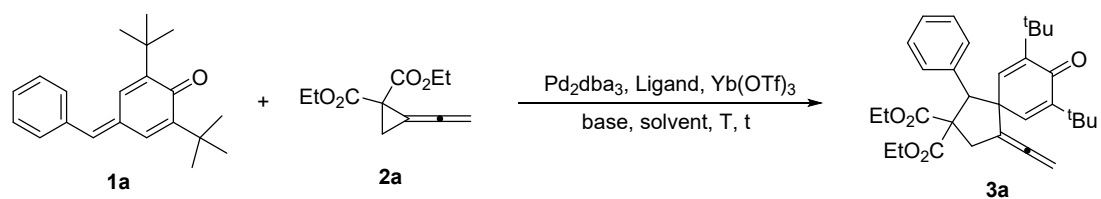
(E) The General Procedure for the Scale-up Synthesis of Compounds **3a** and **4a**



Tris(dibenzylideneacetone)dipalladium (0.023 g, 0.02 mmol, 2.5 mol%), 4Å MS (1.0 g) and DPEphos (0.040 g, 0.07 mmol, 7.5 mol%) was added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in MeCN (degassed) (15 mL) for 30 minutes. After that, **1a** (0.294 g, 1.0 mmol), **2a** (430 μ L, 2.5 mmol), Yb(OTf)₃ (0.062 g, 0.1 mmol, 10 mol%), DMAP (0.061 g, 0.5 mmol, 50 mol%) and Cs₂CO₃ (0.325 g, 1.0 mmol, 1.0 equiv.) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and the residue was purified by a column chromatography to afford the desired product **3a**.

Tris(dibenzylideneacetone)dipalladium (0.023 g, 0.02 mmol, 2.5 mol%), 4Å MS (1.0 g) and Ph-PHOX (0.030 g, 0.07 mmol, 7.5 mol%) was added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in 1,4-dioxane (degassed) (15 mL) for 30 minutes. After that, **1a** (0.294 g, 1.0 mmol), **2a** (430 μ L, 2.5 mmol), Yb(OTf)₃ (0.062 g, 0.1 mmol, 10 mol%), DMAP (0.061 g, 0.5 mmol, 50 mol%) and Cs₂CO₃ (0.325 g, 1.0 mmol, 1.0 equiv.) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and the residue was purified by a column chromatography to afford the desired product **4a**.

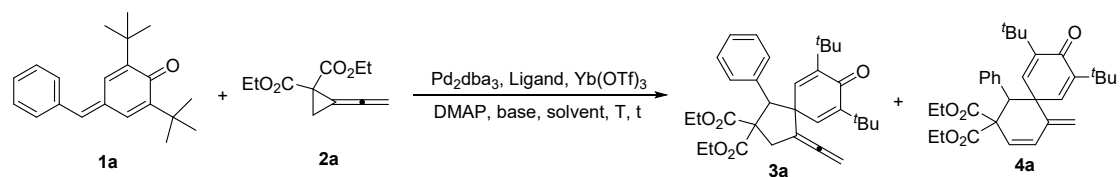
(F) Optimization of Reaction Conditions



entry ^a	2a (equiv)	[Pd]	ligand	solvent	base	DMAP (mol%)	T °C	t (h)	yield ^b (%)
1	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	40	22	29
2	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	45	22	46
3	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	50	22	36
4	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	55	22	31
5	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	60	22	28
6	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	65	22	24
7	1.0	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	45	12	11
8	2.0	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	45	12	44
9	3.0	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	-	45	12	27
10	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	30	45	12	64
11	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	50	45	12	68
12	2.5	Pd ₂ dba ₃	DPEphos	THF	Cs ₂ CO ₃	70	45	12	52
13	2.5	Pd ₂ dba ₃	DPEphos	Acetone	Cs ₂ CO ₃	50	45	12	51
14	2.5	Pd ₂ dba ₃	DPEphos	Dioxane	Cs ₂ CO ₃	50	45	12	45
15	2.5	Pd ₂ dba ₃	DPEphos	MeCN	Cs ₂ CO ₃	50	45	12	85
16	2.5	Pd ₂ dba ₃	DPEphos	Toluene	Cs ₂ CO ₃	50	45	12	27
17	2.5	Pd ₂ dba ₃	DPEphos	DCE	Cs ₂ CO ₃	50	45	12	44
18	2.5	Pd ₂ dba ₃	DPEphos	DMF	Cs ₂ CO ₃	50	45	12	57
19	2.5	Pd ₂ dba ₃	DPEphos	DMSO	Cs ₂ CO ₃	50	45	12	82
20	2.5	Pd ₂ dba ₃	Binap	MeCN	Cs ₂ CO ₃	50	45	12	55
21	2.5	Pd ₂ dba ₃	dppe	MeCN	Cs ₂ CO ₃	50	45	12	trace
22	2.5	Pd ₂ dba ₃	Xantphos	MeCN	Cs ₂ CO ₃	50	45	12	32
23	2.5	Pd ₂ dba ₃	DPEphos	MeCN	DBU	50	45	12	54
24	2.5	Pd ₂ dba ₃	DPEphos	MeCN	TEA	50	45	12	20
25	2.5	Pd ₂ dba ₃	DPEphos	MeCN	KH ₂ PO ₄	50	45	12	trace
26	2.5	Pd(OAc) ₂	DPEphos	MeCN	Cs ₂ CO ₃	50	45	12	77
27	2.5	Pd(PPh ₃) ₄	DPEphos	MeCN	Cs ₂ CO ₃	50	45	12	79

(a) Reaction conditions: a solution of **1a** (0.1 mmol) and **2a** (0.25 mmol), [Pd] (5.0 mol%), ligand (7.5 mol%), 4Å MS (100 mg), Yb(OTf)₃ (10.0 mol%) and base (0.1 mmol) in solvent (1.5 mL) was heated at 45 °C for 12 h. (b) isolated yield.

Scheme S1. Optimization of the reaction conditions for the synthesis of **3a**



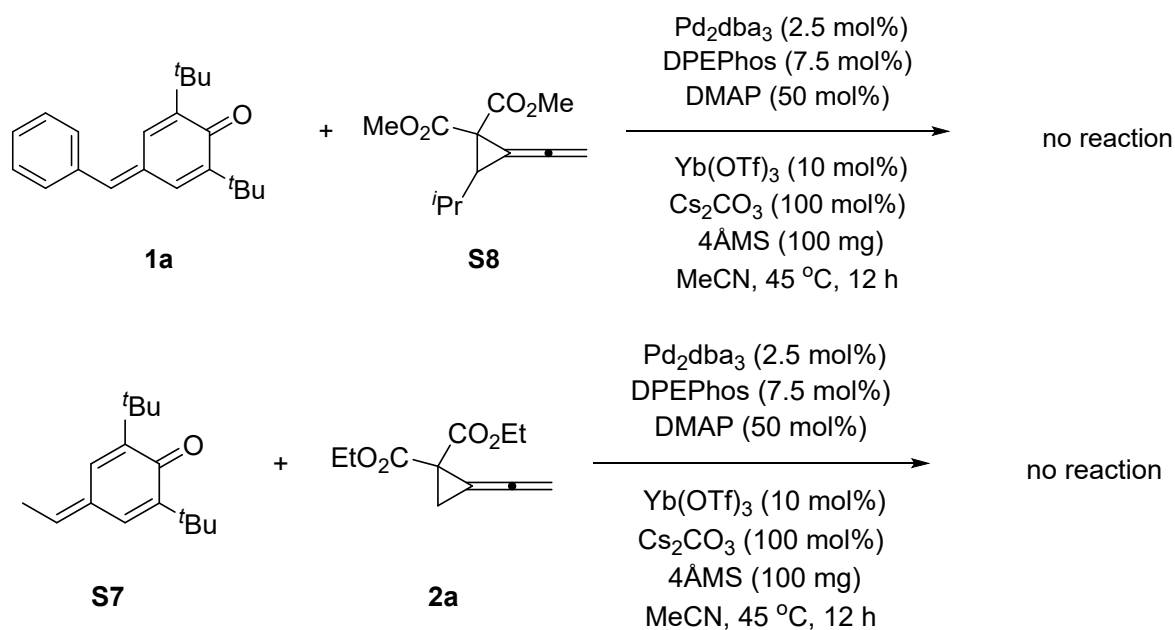
entry ^a	2a (equiv)	solvent	base	T (°C)	t (h)	total yield ^b (%)	3a:4a , yield ^b (%)
1	2.5	THF	Cs ₂ CO ₃	45	12	84	21 : 63
2	2.5	MeCN	Cs ₂ CO ₃	45	12	88	24 : 64
3	2.5	1,4-dioxane	Cs ₂ CO ₃	45	12	97	23 : 74
4	2.5	DMF	Cs ₂ CO ₃	45	12	91	24 : 67
5	2.5	DCM	Cs ₂ CO ₃	45	12	95	28 : 67
6	2.5	Toluene	Cs ₂ CO ₃	45	12	91	35 : 56
7	2.5	DMSO	Cs ₂ CO ₃	45	12	73	26 : 47
8	2.5	DCE	Cs ₂ CO ₃	45	12	34	7 : 27
9	2.5	1,4-dioxane	Cs ₂ CO ₃	55	12	91	28 : 63
10	2.5	1,4-dioxane	Cs ₂ CO ₃	65	12	85	27 : 58

(a) Reaction conditions: a solution of **1a** (0.1 mmol) and **2a** (0.25 mmol), [Pd] (5.0 mol%), PH-PHOX (7.5 mol%), Yb(OTf)₃ (10.0 mol%), 4Å MS (100 mg), DMAP (50 mol%) and base (0.1 mmol) in solvent (1.5 mL). (b) yields were determined by ¹H NMR using dibromomethane as an internal standard.

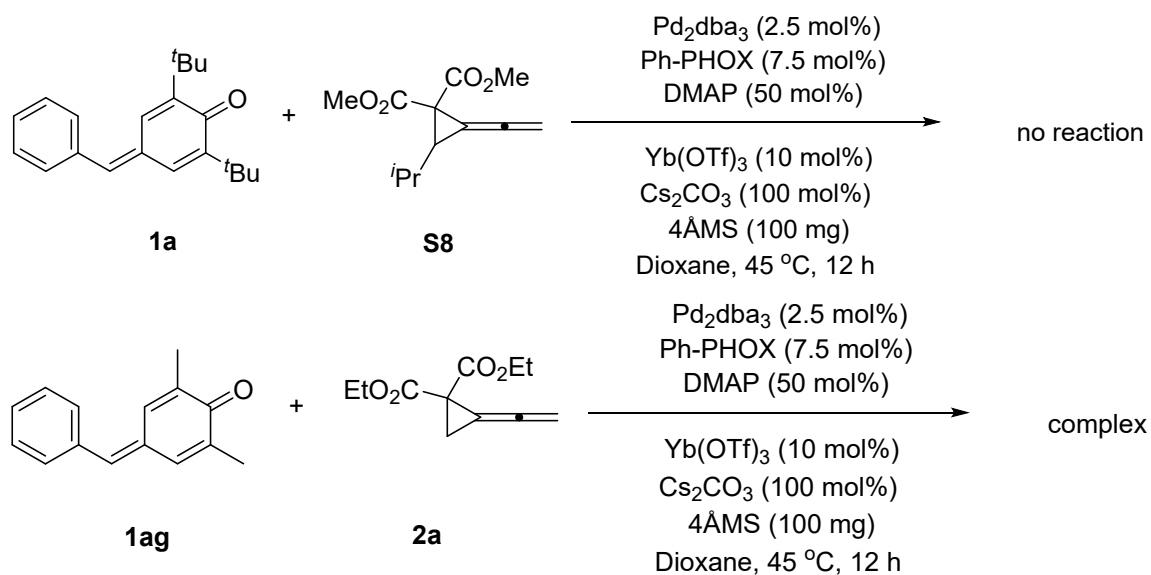
Scheme S2. Optimization of the reaction conditions for the synthesis of **4a**

(G) Reaction of Unreactive Substrate

DPEphos as ligand:

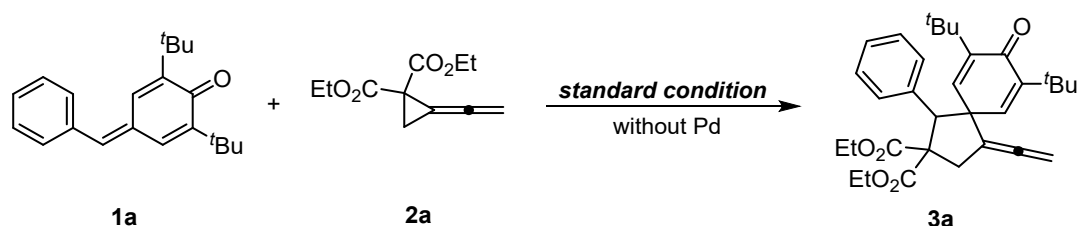


Ph-PHOX as ligand:

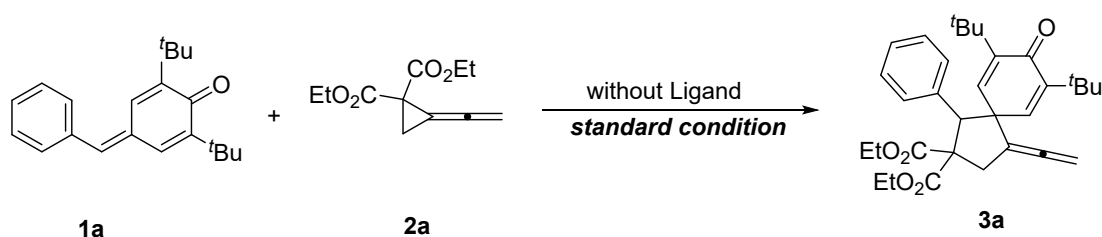


Scheme S3. Reactions that fail to obtain the target product

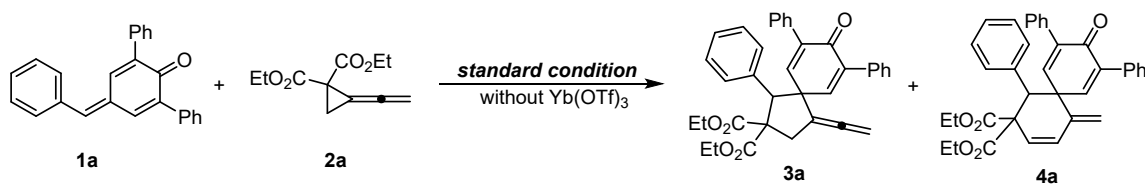
(H) Control Experiments



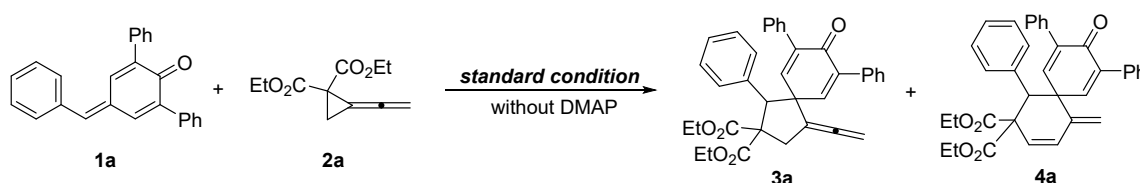
4Å MS (100 mg) and DPEphos (0.004 g, 0.007 mmol, 7.5 mol%) was added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in MeCN (degassed) (1.5 mL) for 30 minutes. After that, **1a** (0.029 g, 0.1 mmol), **2a** (43 μL, 0.25 mmol), Yb(OTf)₃ (0.006 g, 0.01 mmol, 10 mol%), DMAP (0.006 g, 0.05 mmol, 50 mol%) and Cs₂CO₃ (0.1 mmol, 1.0 equiv) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Trace of the desired product **3a** was generated through TLC detection.



Tris(dibenzylideneacetone)dipalladium (0.002 g, 0.002 mmol, 2.5 mol%) and 4Å MS (100 mg) was added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in MeCN (degassed) (1.5 mL) for 30 minutes. After that, **1a** (0.029 g, 0.1 mmol), **2a** (43 μL, 0.25 mmol), Yb(OTf)₃ (0.006 g, 0.01 mmol, 10 mol%), DMAP (0.006 g, 0.05 mmol, 50 mol%) and Cs₂CO₃ (0.033 g, 0.1 mmol, 1.0 equiv.) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and **3a** was afforded by a column chromatography in the yield of 14%.

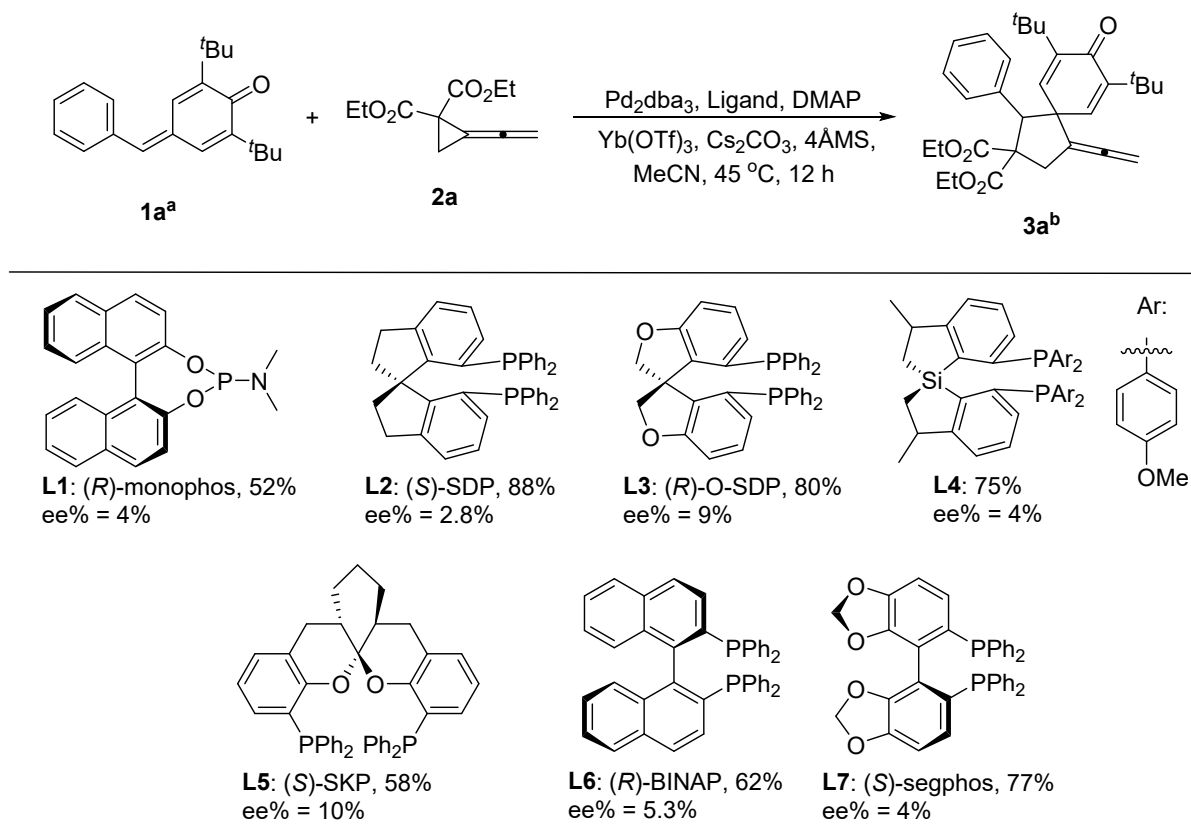


Tris(dibenzylideneacetone)dipalladium (0.002 g, 0.002 mmol, 2.5 mol%), PH-PHOX (0.030 g, 0.07 mmol, 7.5 mol%) and 4Å MS (100 mg) were added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in 1,4-dioxane (degassed) (1.5 mL) for 30 minutes. After that, **1a** (0.029 g, 0.1 mmol), **2a** (43 μL, 0.25 mmol), DMAP (0.006 g, 0.05 mmol, 50 mol%) and Cs₂CO₃ (0.033 g, 0.1 mmol, 1.0 equiv) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and **3a** : **4a** was afforded by ¹H NMR using dibromomethane as an internal standard in the yield of 20 : 48.



Tris(dibenzylideneacetone)dipalladium (0.002 g, 0.002 mmol, 2.5 mol%), PH-PHOX (0.030 g, 0.07 mmol, 7.5 mol%) and 4Å MS (100 mg) were added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in 1,4-dioxane (degassed) (1.5 mL) for 30 minutes. After that, **1a** (0.029 g, 0.1 mmol), **2a** (43 μL, 0.25 mmol), Yb(OTf)₃ (0.006 g, 0.01 mmol, 10 mol%) and Cs₂CO₃ (0.033 g, 0.1 mmol, 1.0 equiv) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and **3a** : **4a** was afforded by ¹H NMR using dibromomethane as an internal standard in the yield of 14 : 32.

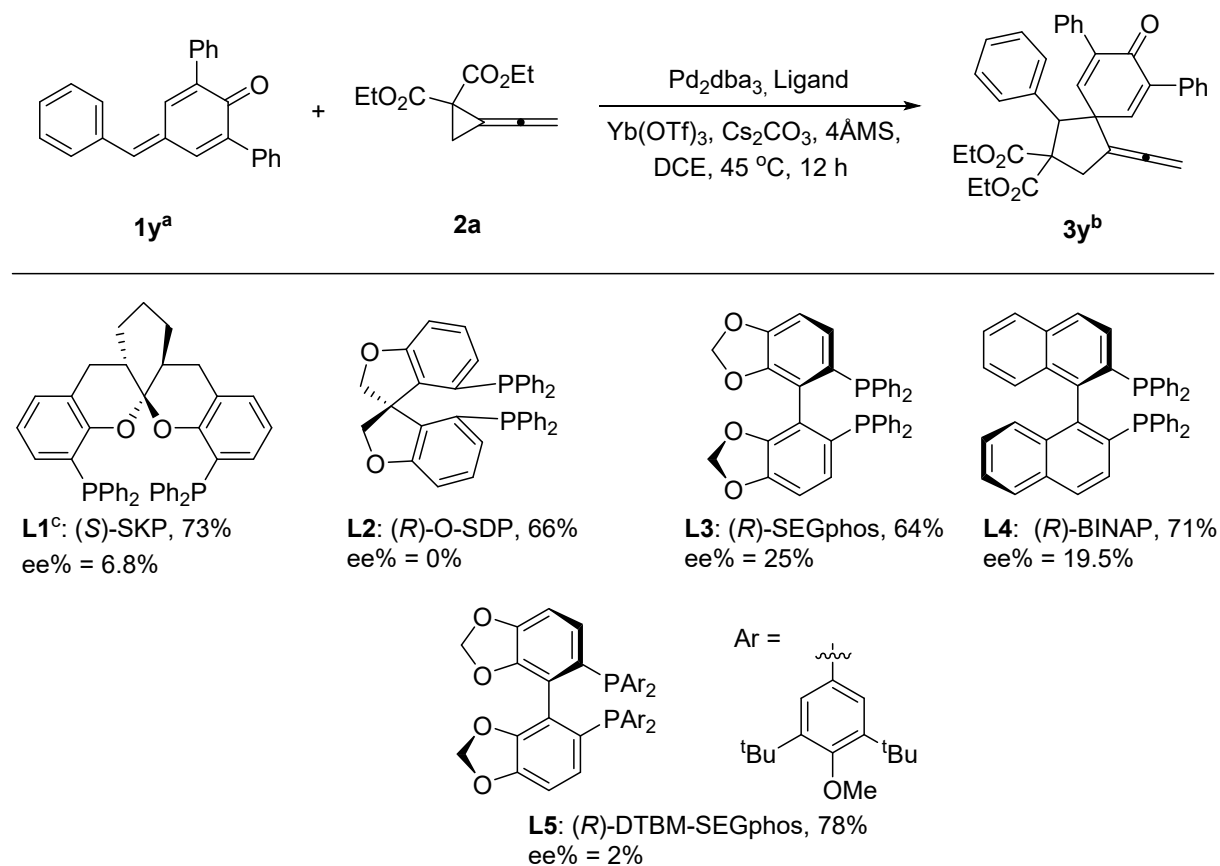
(I) Asymmetric Variant



(a) Reaction conditions: a solution of **1a** (0.1 mmol) and **2a** (0.2 mmol), Pd₂dba₃ (2.5 mol%), ligand (7.5 mol%), Yb(OTf)₃ (10.0 mol%), 4Å MS (100 mg), DMAP (50.0 mol%) and base (0.1 mmol) in solvent (1.5 mL) was heated at 45 °C for 12 h. (b) isolated yield.

Scheme S4. Optimization of asymmetric synthesis of **3a**

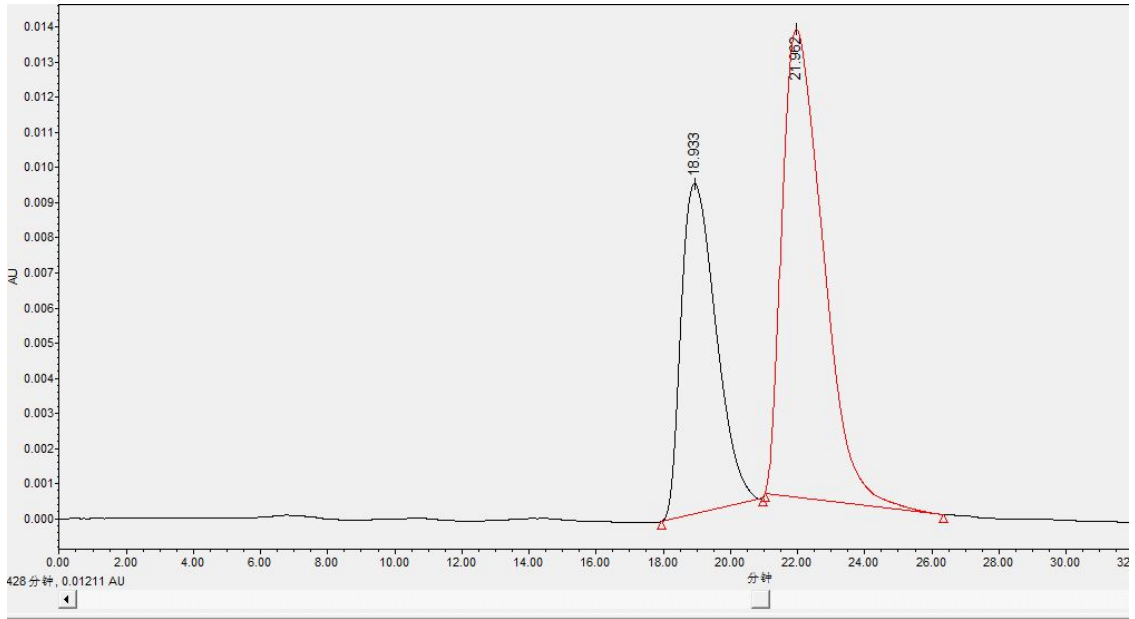
Tris(dibenzylideneacetone)dipalladium (0.002 g, 0.002 mmol, 2.5 mol%) and ligand (0.007 mmol, 7.5 mol%) were added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in MeCN (degassed) (1.5 mL) for 30 min. After that, **1a** (0.029 g, 0.1 mmol), **2a** (43 μL, 0.25 mmol), Yb(OTf)₃ (0.006 g, 0.01 mmol, 10 mol%), DMAP (0.006 g, 50 mol%) and Cs₂CO₃ (0.033 g, 0.1 mmol, 1.0 equiv) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and **3a** was afforded by a column chromatography. The ee was determined by HPLC using a Chiralpak OD-H column [*n*-hexane/*i*-PrOH (99 : 1)]; flow rate 0.7 mL/min.



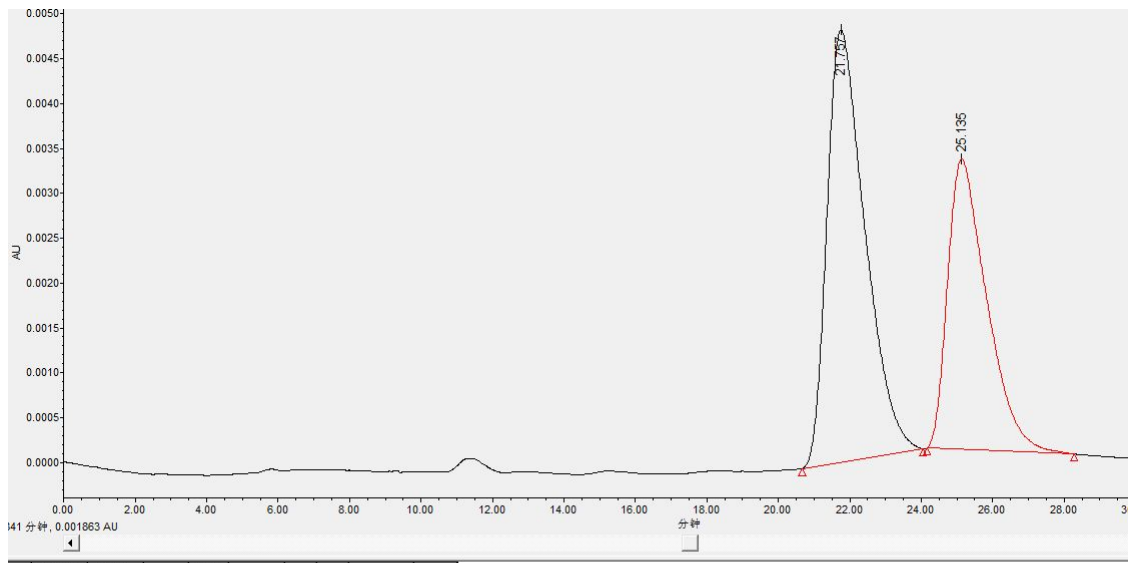
(a) Reaction conditions: a solution of **1a** (0.1 mmol) and **2a** (0.2 mmol), Pd₂dba₃ (2.5 mol%), ligand (7.5 mol%), Yb(OTf)₃ (10.0 mol%), 4Å MS (100 mg) and base (0.1 mol) in solvent (1.5 mL) was heated at 45 °C for 12 h. (b) isolated yield. (c) DMF as solvent.

Scheme S5. Optimization of asymmetric synthesis of **3y**

Tris(dibenzylideneacetone)dipalladium (0.002 g, 0.002 mmol, 2.5 mol%) and ligand (0.007 mmol, 7.5 mol%) were added to an oven dried 10 mL sealed tube equipped with a magnetic stirring bar under argon atmosphere. The resulting catalyst system was stirred in solvent (degassed) (1.5 mL) for 30 min. After that, **1y** (0.033 g, 0.1 mmol), **2a** (43 μL, 0.25 mmol), Yb(OTf)₃ (0.006 g, 0.01 mmol, 10 mol%) and Cs₂CO₃ (0.033 g, 0.1 mmol, 1.0 equiv) were added under argon atmosphere. The reaction mixture was stirred at 45 °C for 12 h. The reaction solution was filtered through a pad of celite to remove insoluble solids. Then, the solvent was evaporated under vacuum and **3y** was afforded by a column chromatography. The ee was determined by HPLC using a Chiralpak IC column [*n*-hexane/*i*-PrOH (60 : 4)]; flow rate 0.7 mL/min.

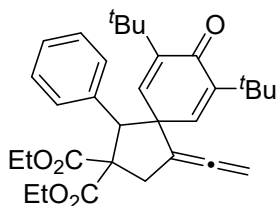


名称	保留时间 (分钟)	面积 (微伏秒)	% 面积	高度 (微伏)	积分类型	含量	单位	峰类型	峰代码
	18.933	681170	37.60	9406	bb			未知	
	21.962	1130257	62.40	13336	bb			未知	



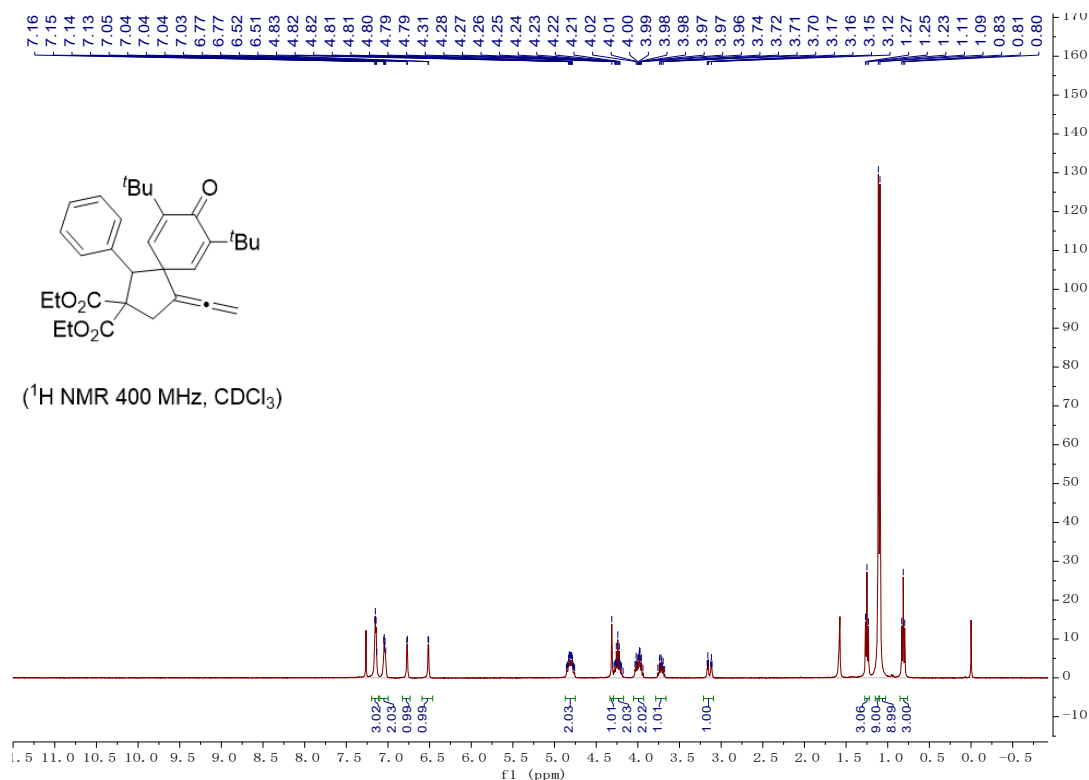
名称	保留时间 (分钟)	面积 (微伏秒)	% 面积	高度 (微伏)	积分类型	含量	单位	峰类型	峰代码
	21.757	356298	59.22	4819	bb			未知	
	25.135	245385	40.78	3238	bb			未知	

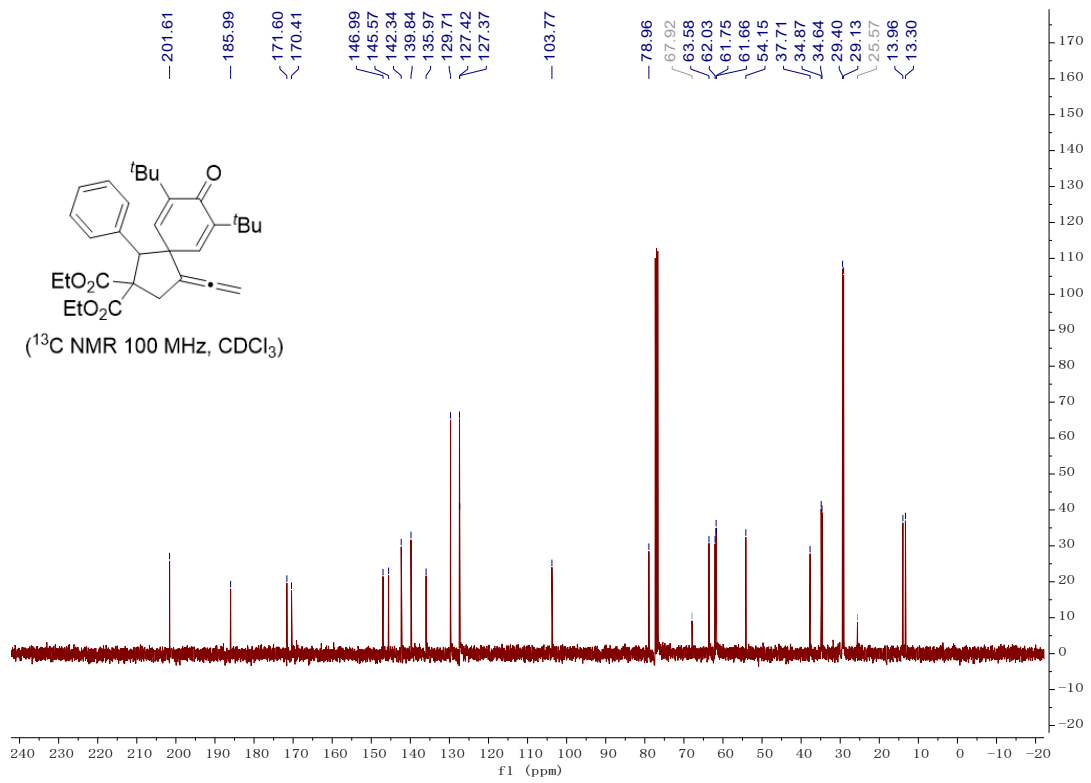
(J) Characterization Data of Substrates and Products

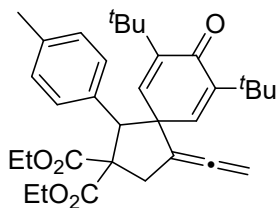


diethyl 7,9-di-tert-butyl-8-oxo-1-phenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate

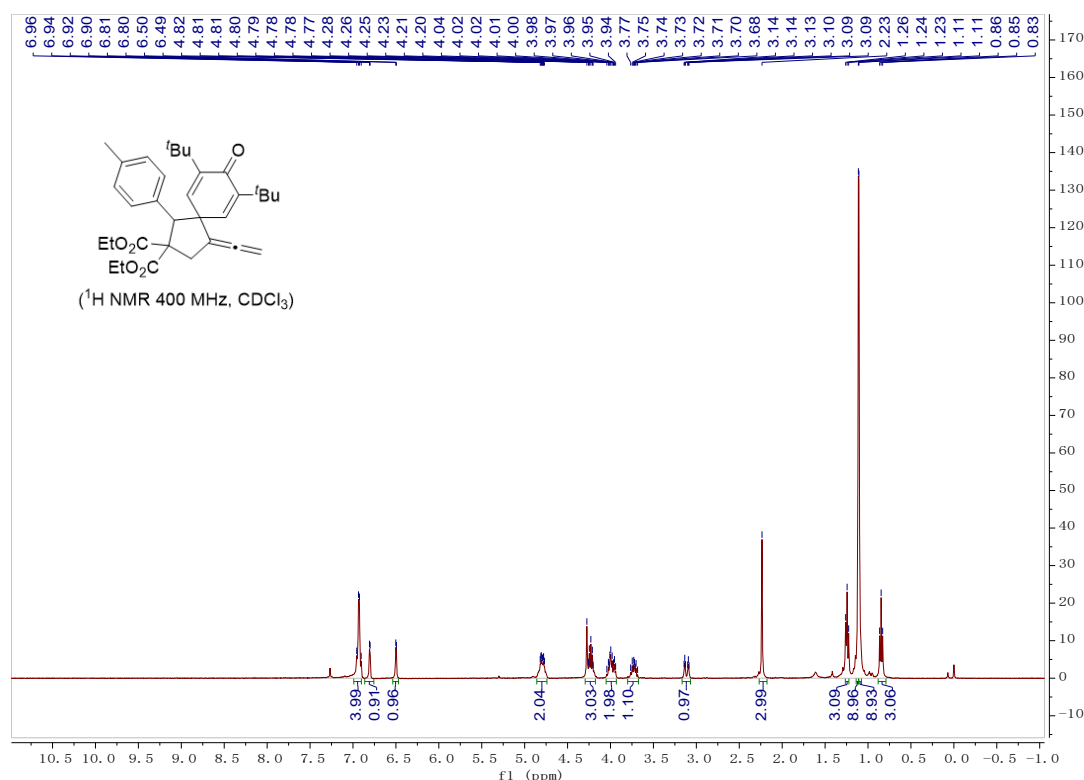
(3a): Yield: 0.0428 g, 85%, a colorless solid, m.p: 92-94 °C; Eluent: PE/EA = 30/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.15 (m, 3H), 7.10 - 7.00 (m, 2H), 6.77 (d, *J* = 3.0 Hz, 1H), 6.52 (d, *J* = 3.0 Hz, 1H), 4.87 - 4.75 (m, 2H), 4.31 (s, 1H), 4.29 - 4.17 (m, 2H), 4.05 - 3.93 (m, 2H), 3.72 (dq, *J* = 10.8, 7.2 Hz, 1H), 3.14 (dt, *J* = 17.0, 3.0 Hz, 1H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 9H), 1.09 (s, 9H), 0.81 (t, *J* = 7.2 Hz, 3H); ¹³C{¹H}-NMR (100 MHz, CDCl₃, TMS) δ 201.6, 186.0, 171.6, 170.4, 147.0, 145.6, 142.3, 139.8, 136.0, 129.7, 127.4, 127.4, 103.8, 79.0, 67.9, 63.6, 62.0, 61.8, 61.7, 54.2, 37.7, 34.9, 34.6, 29.4, 29.1, 25.6, 14.0, 13.3; IR (neat): ν 2956.66, 2904.17, 2865.03, 1959.67, 1725.12, 1658.92, 1636.96, 1455.82, 1253.79, 1095.86, 822.02, 700.60 cm⁻¹; HRMS (ESI-TOF) Calcd for C₃₂H₄₁O₅ [M+H]⁺ : 505.2949, found: 505.2946.

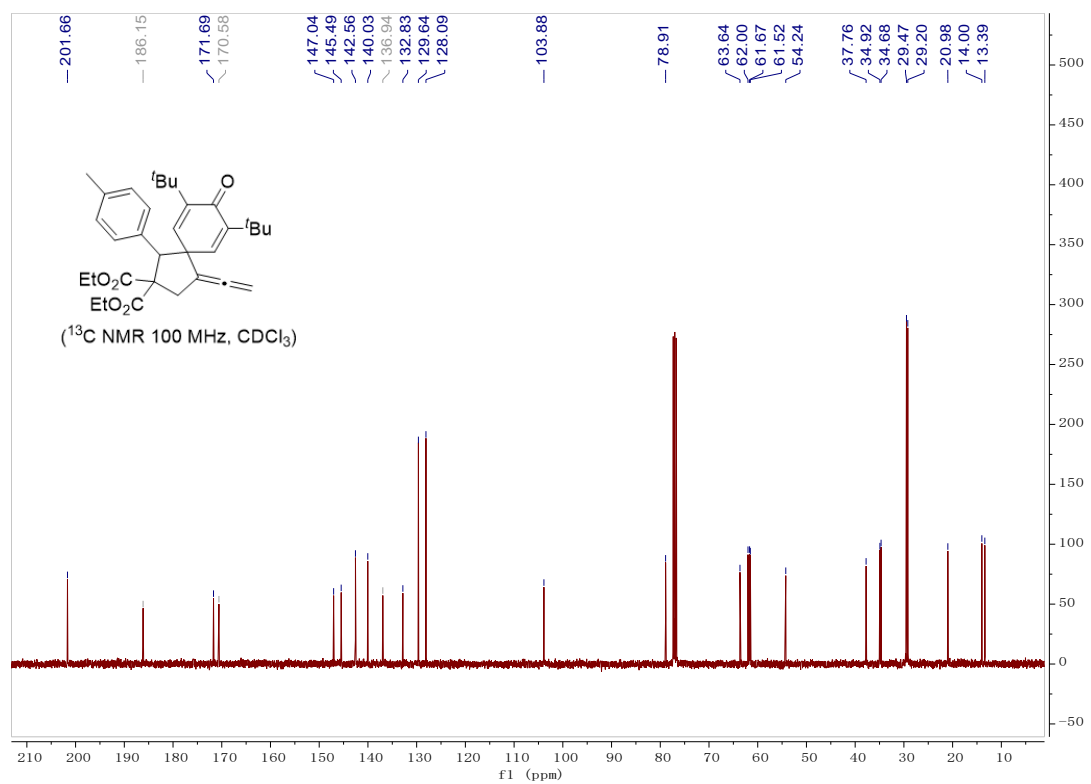


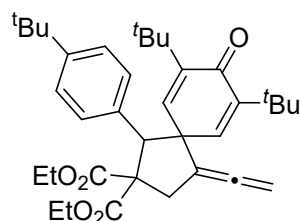




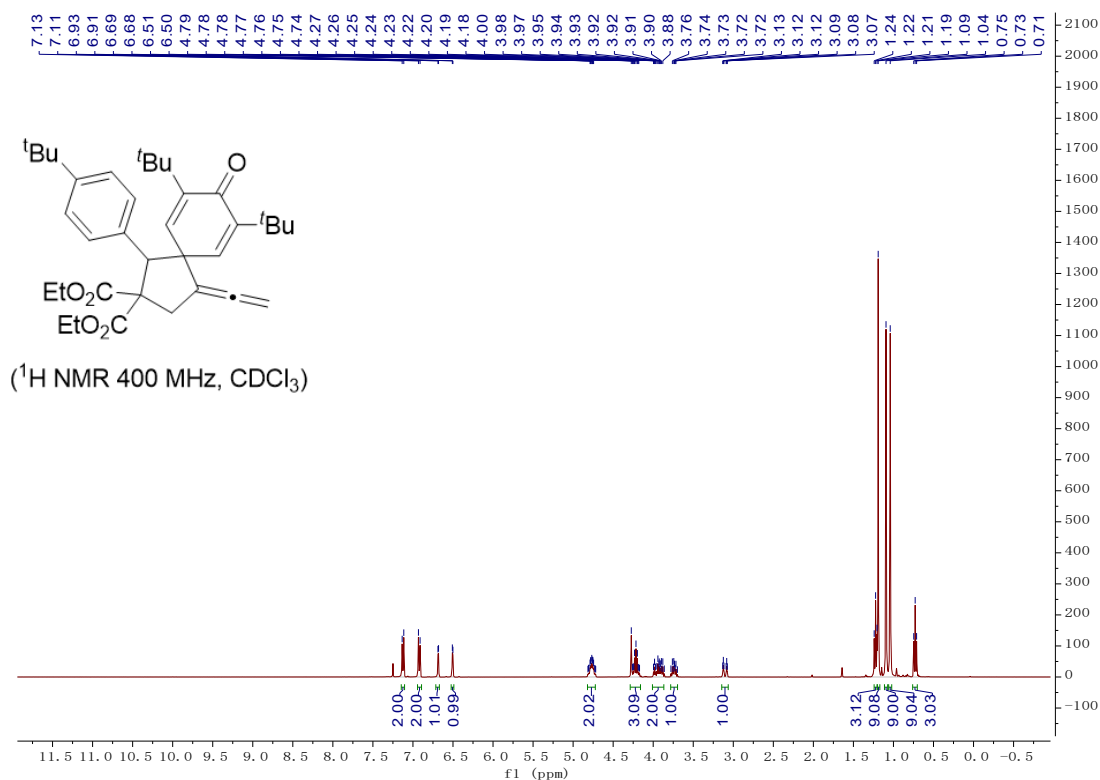
diethyl 7,9-di-*tert*-butyl-8-oxo-1-(*p*-tolyl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3b): Yield: 0.0368 g, 71%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 6.99 – 6.90 (m, 4H), 6.80 (d, $J = 3.0$ Hz, 1H), 6.50 (d, $J = 3.0$ Hz, 1H), 4.86 – 4.74 (m, 2H), 4.29 – 4.18 (m, 3H), 4.05 – 3.93 (m, 2H), 3.72 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.11 (dt, $J = 17.0, 3.2$ Hz, 1H), 2.23 (s, 3H), 1.24 (t, $J = 7.2$ Hz, 3H), 1.11 (s, 9H), 1.11 (s, 9H), 0.85 (t, $J = 7.2$ Hz, 3H); ^{13}C $\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.7, 186.2, 171.7, 170.6, 147.0, 145.5, 142.6, 140.0, 136.94, 132.8, 129.6, 128.1, 103.9, 78.9, 63.6, 62.0, 61.7, 61.5, 54.2, 37.8, 35.0, 34.7, 29.5, 29.2, 21.0, 14.0, 13.4; IR (neat): ν 2956.29, 2867.08, 1962.33, 1724.69, 1659.33, 1637.13, 1515.72, 1388.83, 1366.05, 1253.44, 1218.82, 1033.90, 882.33 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_5$ $[\text{M}+\text{H}]^+$: 519.3105, found: 519.3106.

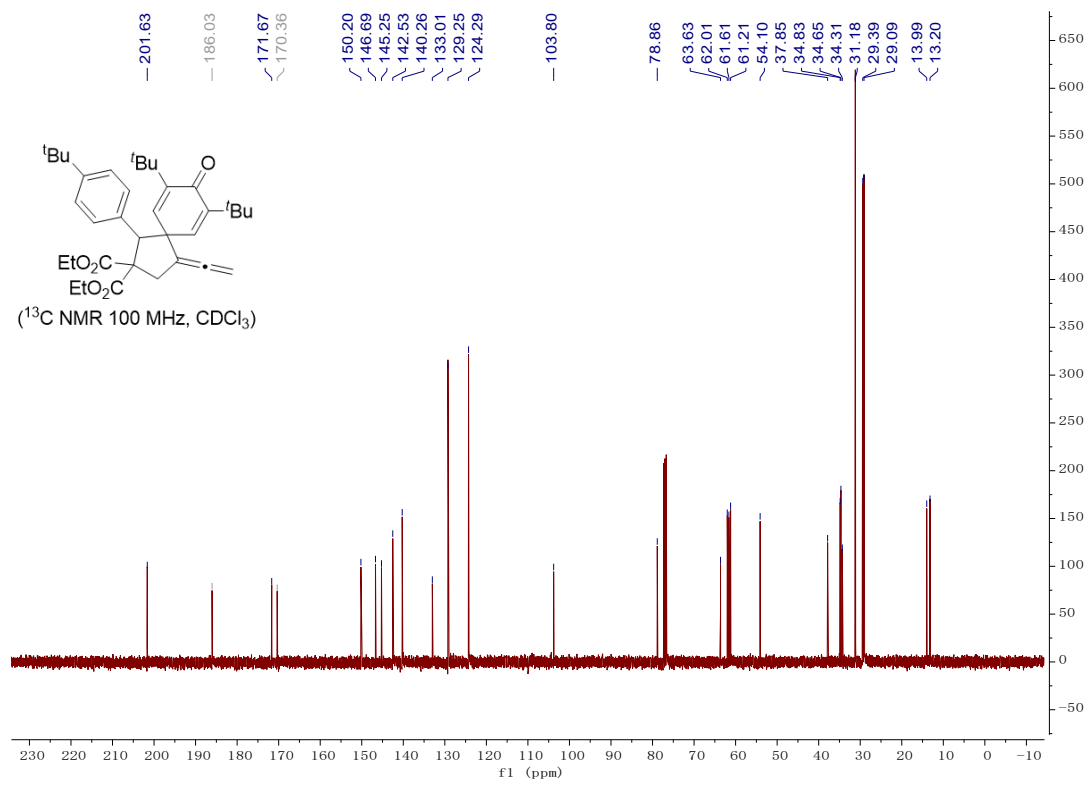


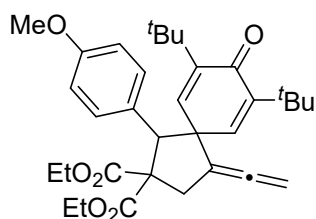




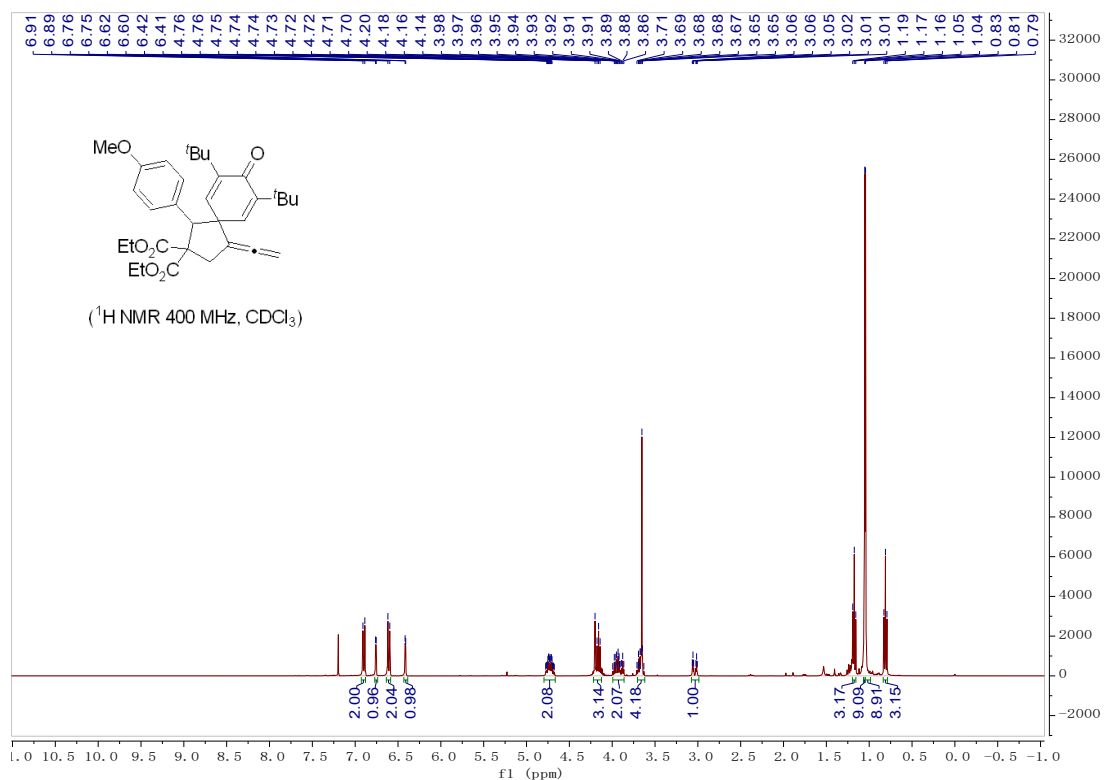
diethyl 7,9-di-*tert*-butyl-1-(4-(*tert*-butyl)phenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3c): Yield: 0.0409 g, 73%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.12 (d, $J = 8.2$ Hz, 2H), 6.92 (d, $J = 8.2$ Hz, 2H), 6.68 (d, $J = 2.8$ Hz, 1H), 6.50 (d, $J = 2.8$ Hz, 1H), 4.82 – 4.72 (m, 2H), 4.29 – 4.16 (m, 3H), 4.01 – 3.87 (m, 2H), 3.74 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.10 (dt, $J = 16.8, 3.2$ Hz, 1H), 1.22 (t, $J = 7.2$ Hz, 3H), 1.19 (s, 9H), 1.09 (s, 9H), 1.04 (s, 9H), 0.73 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 186.0, 171.7, 170.4, 150.2, 146.7, 145.3, 142.5, 140.3, 133.0, 129.3, 124.3, 103.8, 78.9, 63.6, 62.0, 61.6, 61.2, 54.1, 37.9, 34.8, 34.7, 34.3, 31.2, 29.4, 29.1, 14.0, 13.2; IR (neat): ν 2957.90, 2906.78, 2865.03, 1962.28, 1726.50, 1659.23, 1636.95, 1366.10, 1253.47, 1030.84, 857.90, 732.29 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{36}\text{H}_{49}\text{O}_5$ $[\text{M}+\text{H}]^+$: 561.3575, found: 561.3571.

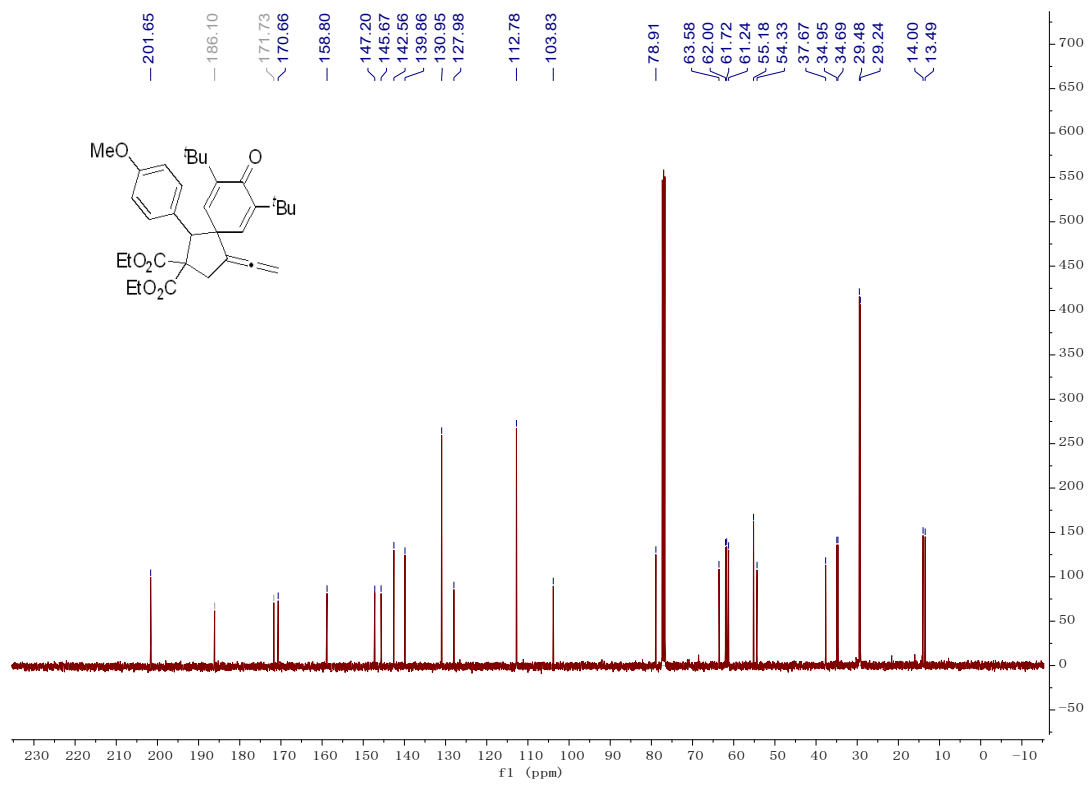


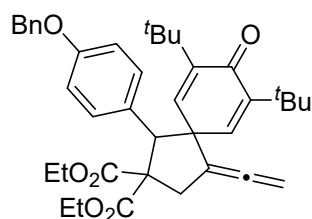




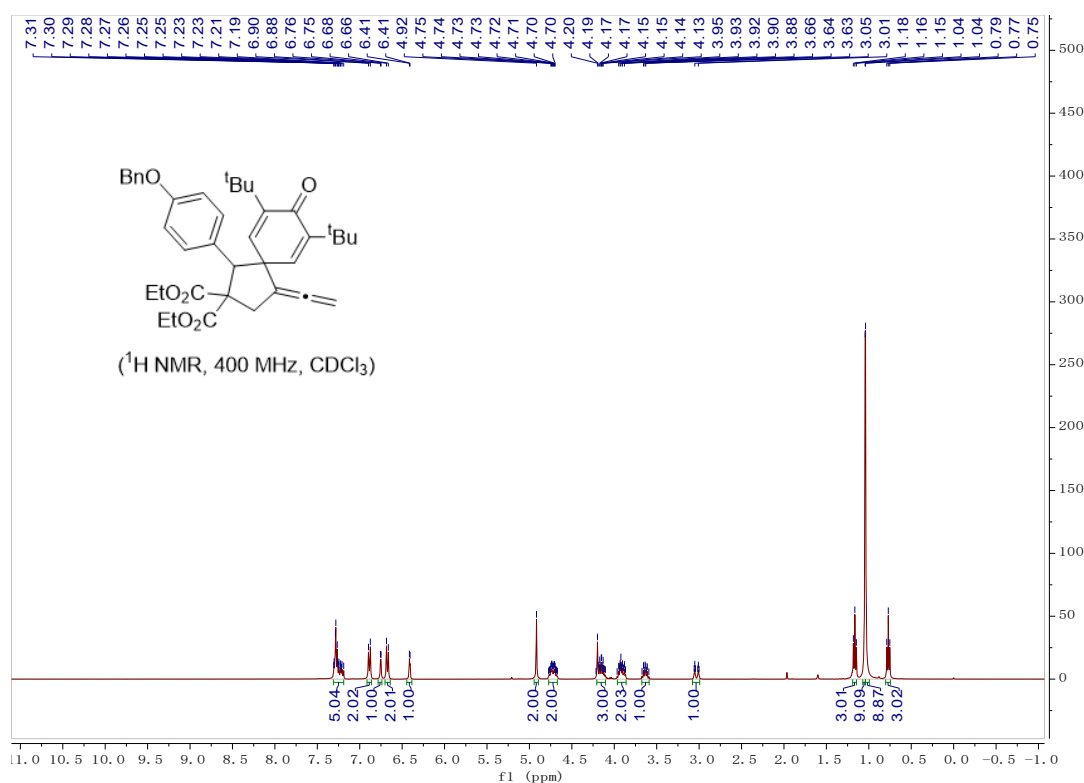
diethyl 7,9-di-*tert*-butyl-1-(4-methoxyphenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3d): Yield: 0.0395 g, 74%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 6.90 (d, $J = 8.8$ Hz, 2H), 6.76 (d, $J = 3.0$ Hz, 1H), 6.61 (d, $J = 8.8$ Hz, 2H), 6.41 (d, $J = 3.0$ Hz, 1H), 4.80 – 4.66 (m, 2H), 4.22 – 4.12 (m, 3H), 3.99 – 3.86 (m, 2H), 3.70 – 3.62 (m, 4H), 3.04 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.17 (t, $J = 7.2$ Hz, 3H), 1.05 (s, 9H), 1.04 (s, 9H), 0.81 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 186.1, 171.7, 170.7, 158.8, 147.2, 145.7, 142.6, 139.9, 131.0, 128.0, 112.8, 103.8, 78.9, 63.6, 62.0, 61.7, 61.2, 55.2, 54.3, 37.7, 35.0, 34.7, 29.5, 29.2, 14.0, 13.5; IR (neat): ν 2956.61, 2906.54, 2861.68, 1961.68, 1724.22, 1659.01, 1636.98, 1514.39, 1463.12, 1366.76, 1294.99, 1250.67, 1180.00, 1131.10, 822.19, 732.10 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_6$ $[\text{M}+\text{H}]^+$: 535.3054, found: 535.3066.

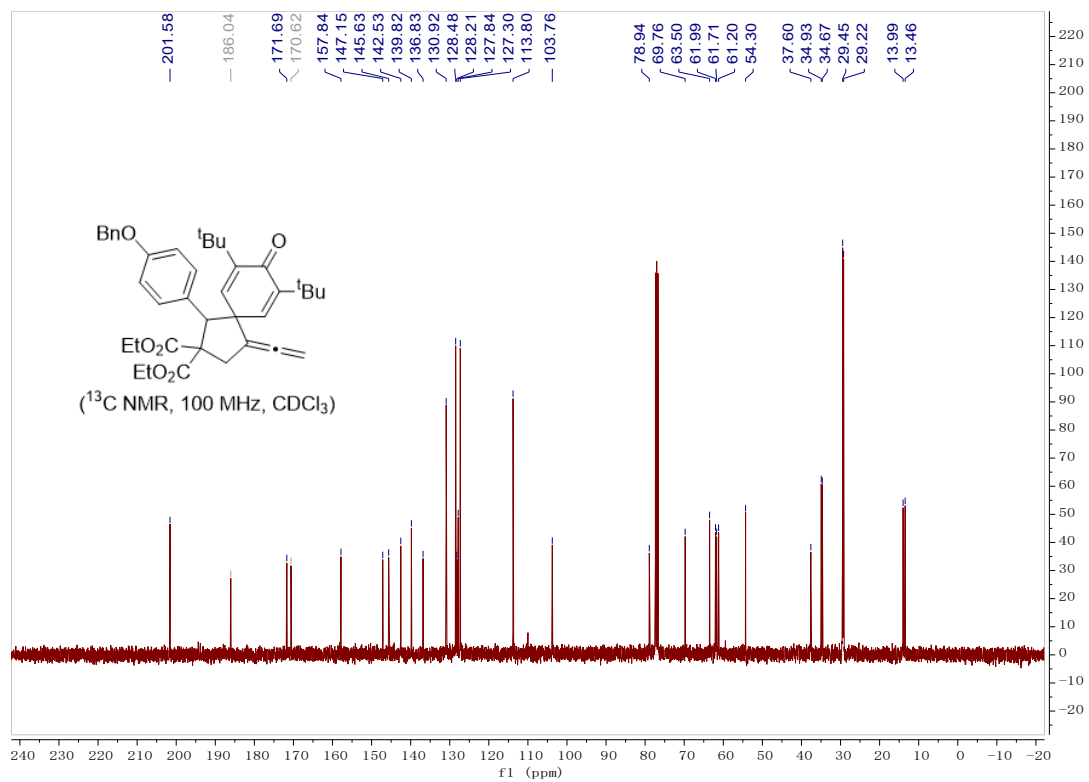


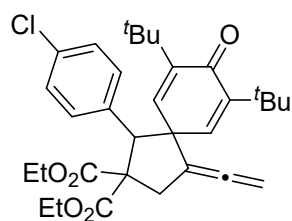




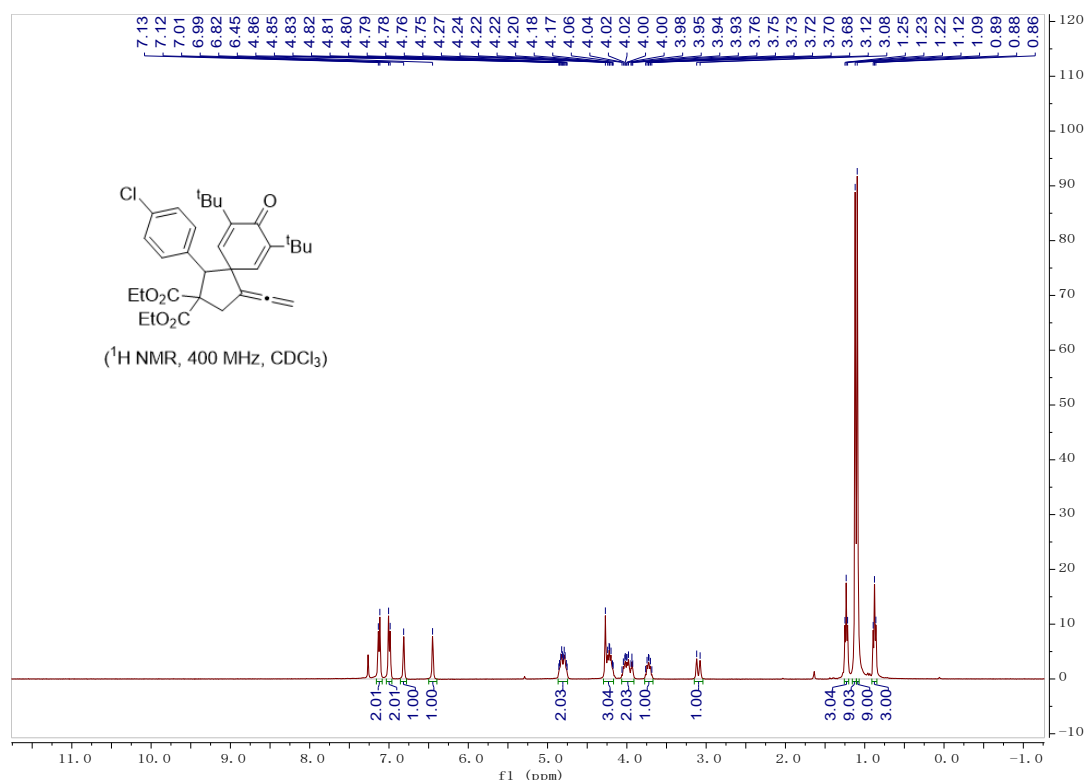
diethyl 1-(4-(benzyloxy)phenyl)-7,9-di-*tert*-butyl-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3e): Yield: 0.0439 g, 72%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.31 – 7.19 (m, 5H), 6.89 (d, $J = 8.8$ Hz, 2H), 6.75 (d, $J = 3.0$ Hz, 1H), 6.67 (d, $J = 8.8$ Hz, 2H), 6.41 (d, $J = 3.0$ Hz, 1H), 4.92 (s, 2H), 4.77 – 4.67 (m, 2H), 4.21 – 4.10 (m, 3H), 3.96 – 3.86 (m, 2H), 3.63 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.03 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.16 (t, $J = 7.2$ Hz, 3H), 1.05 (s, 9H), 1.04 (s, 9H), 0.77 (t, $J = 7.2$ Hz, 3H); ^{13}C $\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 186.0, 171.7, 170.6, 157.8, 147.2, 145.6, 142.5, 139.8, 136.8, 130.9, 128.5, 128.2, 127.8, 127.3, 113.8, 103.8, 78.9, 69.7, 63.5, 62.0, 61.7, 61.2, 54.3, 37.6, 34.9, 34.7, 29.5, 29.2, 14.0, 13.5; IR (neat): ν 2961.66, 2906.86, 2865.11, 1962.33, 1724.41, 1658.73, 1636.64, 1511.58, 1366.70, 1251.45, 1179.23, 910.46, 731.45 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{39}\text{H}_{47}\text{O}_6$ $[\text{M}+\text{H}]^+$: 611.3367, found: 611.3362.

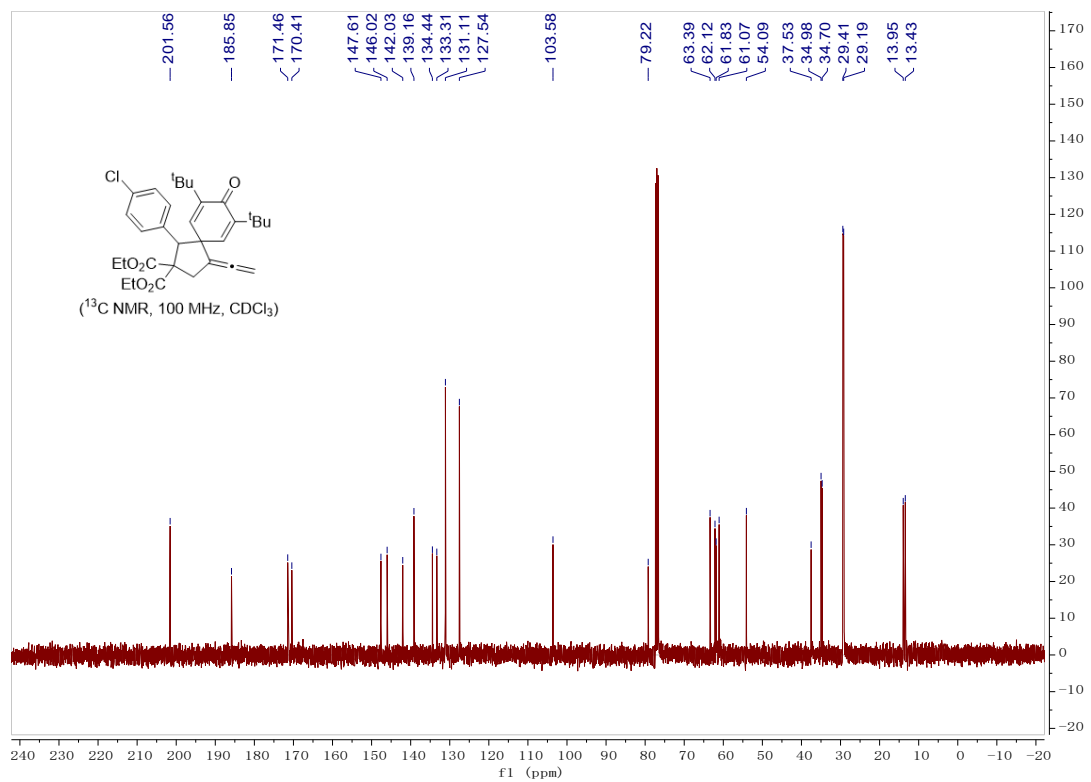


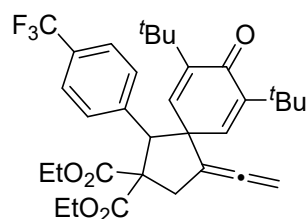




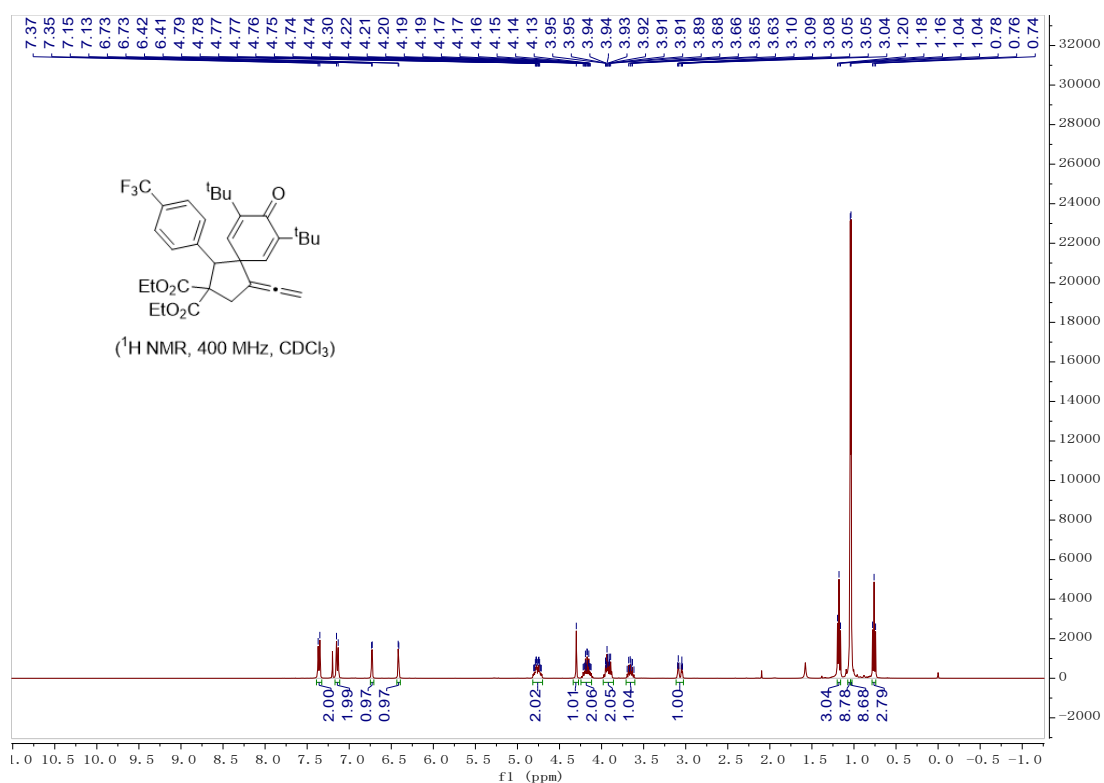
diethyl 7,9-di-*tert*-butyl-1-(4-chlorophenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3f): Yield: 0.0367 g, 68%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.12 (d, $J = 7.6$ Hz, 2H), 7.00 (d, $J = 8.0$ Hz, 2H), 6.82 (s, 1H), 6.45 (s, 1H), 4.87 – 4.75 (m, 2H), 4.29 – 4.17 (m, 3H), 4.07 – 3.91 (m, 2H), 3.78 – 3.67 (m, 1H), 3.10 (d, $J = 17.4$ Hz, 1H), 1.23 (t, $J = 6.8$ Hz, 3H), 1.12 (s, 9H), 1.09 (s, 9H), 0.88 (t, $J = 6.8$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 185.9, 171.5, 170.4, 147.6, 146.0, 142.0, 139.2, 134.4, 133.3, 131.1, 127.5, 103.5, 79.2, 63.4, 62.1, 61.8, 61.1, 54.1, 37.5, 35.0, 34.7, 29.4, 29.2, 14.0, 13.4; IR (neat): ν 2957.75, 2906.78, 2862.42, 1959.67, 1725.17, 1659.31, 1637.69, 1493.19, 1252.87, 1158.69, 909.24, 731.30 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{32}\text{H}_{40}\text{ClO}_5\text{Na}[\text{M}+\text{Na}]^+$: 561.2378, found: 561.2375.

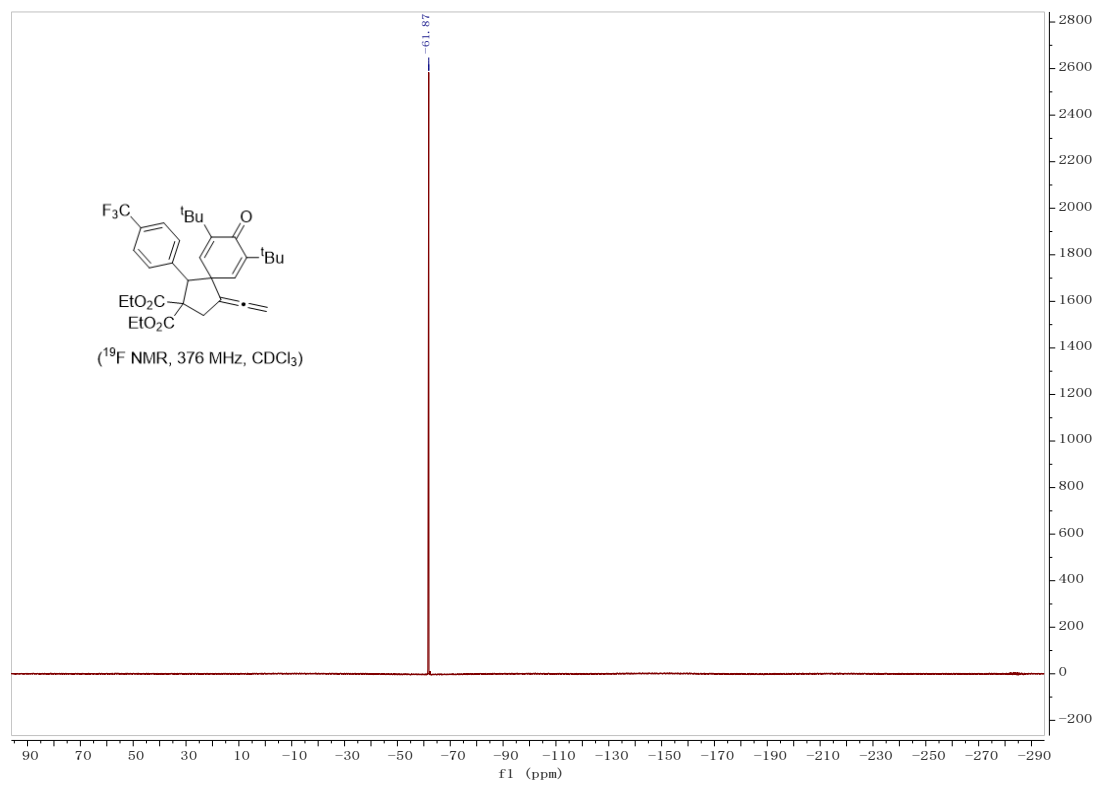
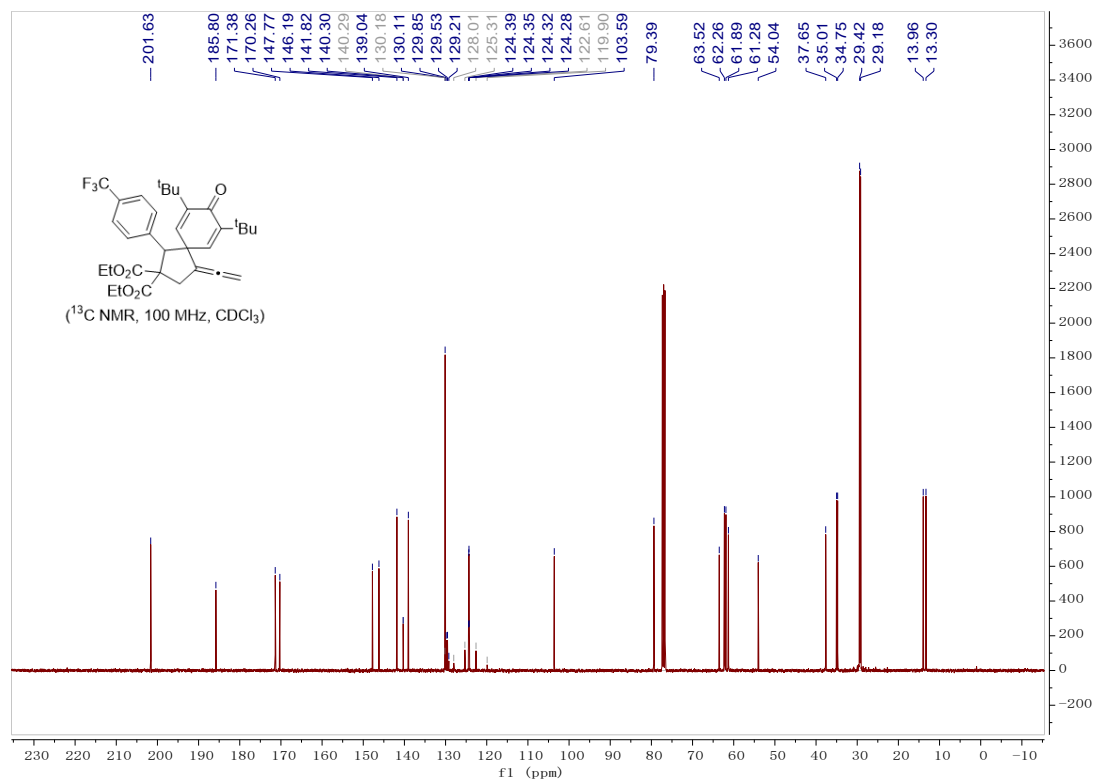


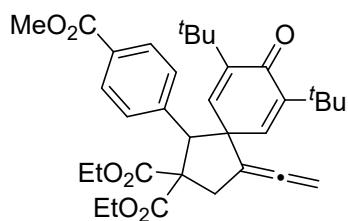




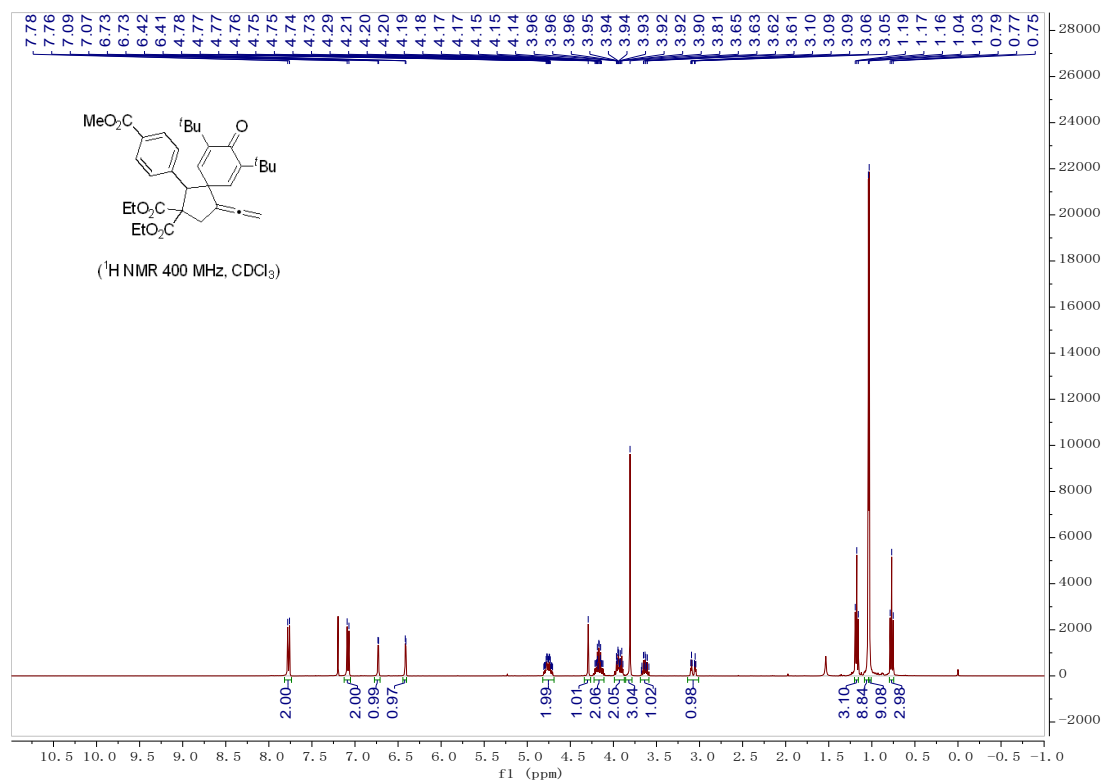
diethyl 7,9-di-*tert*-butyl-8-oxo-1-(4-(trifluoromethyl)phenyl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3g): Yield: 0.0389 g, 68%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.36 (d, $J = 8.2$ Hz, 2H), 7.14 (d, $J = 8.2$ Hz, 2H), 6.73 (d, $J = 3.0$ Hz, 1H), 6.41 (d, $J = 3.0$ Hz, 1H), 4.76 (m, 2H), 4.30 (s, 1H), 4.23 – 4.11 (m, 2H), 3.99 – 3.86 (m, 2H), 3.66 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.07 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.18 (t, $J = 7.2$ Hz, 3H), 1.04 (s, 9H), 1.03 (s, 9H), 0.76 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 185.8, 171.4, 170.3, 147.8, 146.2, 141.8, 140.3, 139.0, 130.1, 129.6 (q, $J = 32.6$ Hz), 124.3 (q, $J = 3.8$ Hz), 123.9 (q, $J = 272$ Hz), 103.6, 79.4, 63.5, 62.2, 61.9, 61.3, 54.0, 37.7, 35.0, 34.7, 29.4, 29.2, 14.0, 13.3; ^{19}F NMR (376 MHz, CDCl_3) δ -61.87; IR (neat): ν 2958.45, 2914.69, 2865.11, 1964.94, 1715.71, 1660.15, 1638.34, 1618.94, 1389.96, 1325.53, 1165.09, 1096.83, 1070.22, 1033.48, 822.12 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{40}\text{F}_3\text{O}_5$ $[\text{M}+\text{H}]^+$: 573.2824, found: 573.2822.

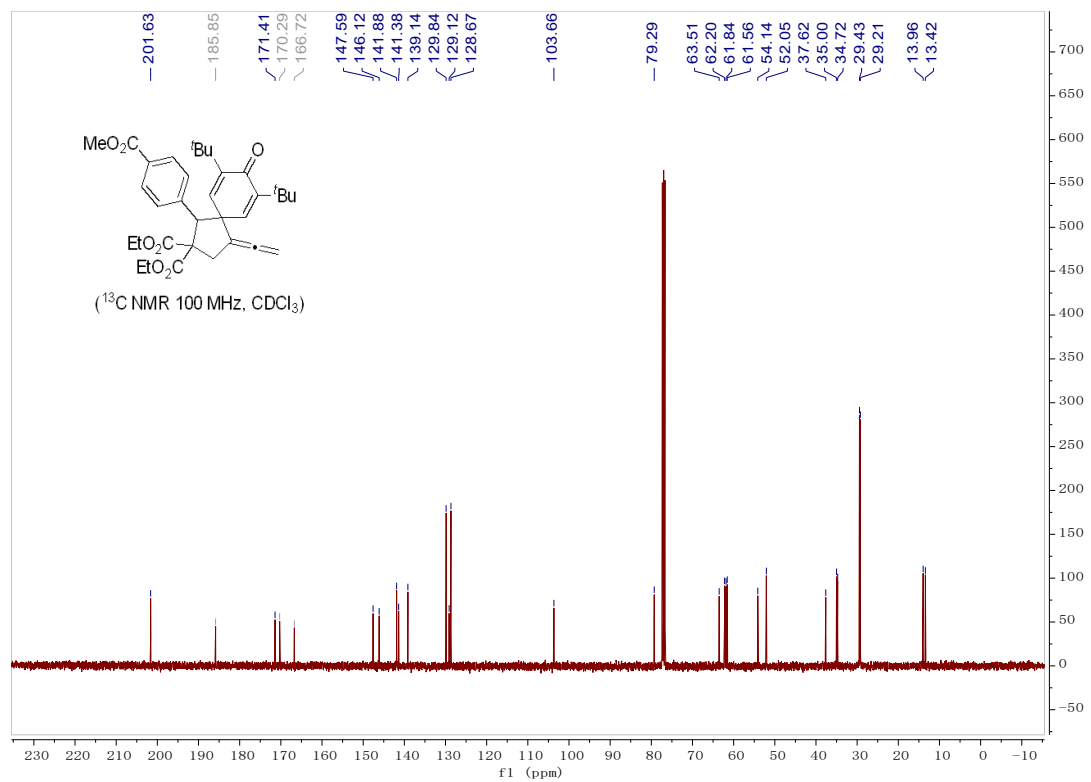


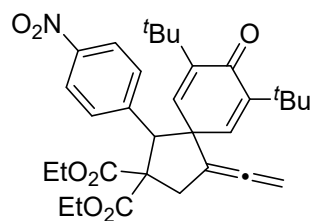




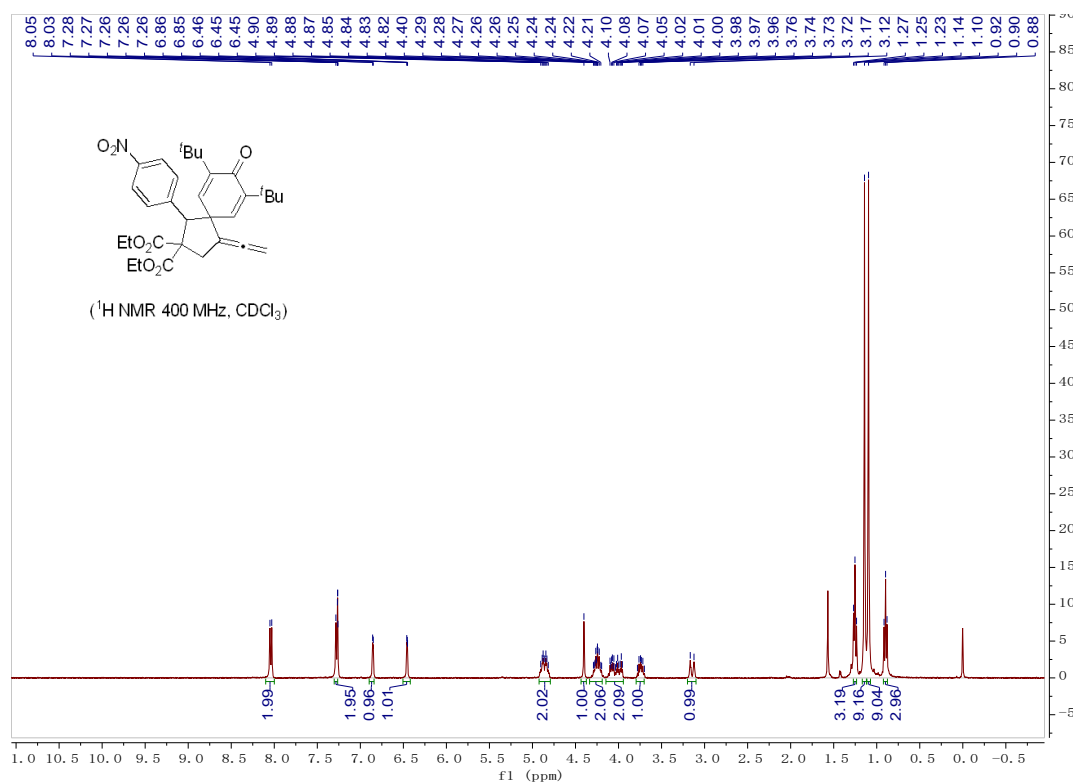
diethyl 7,9-di-*tert*-butyl-1-(4-(methoxycarbonyl)phenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3h): Yield: 0.0416 g, 74%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.77 (d, $J = 8.4$ Hz, 2H), 7.08 (d, $J = 8.4$ Hz, 2H), 6.73 (d, $J = 3.0$ Hz, 1H), 6.41 (d, $J = 3.0$ Hz, 1H), 4.82 – 4.69 (m, 2H), 4.29 (s, 1H), 4.22 – 4.11 (m, 2H), 3.99 – 3.87 (m, 2H), 3.81 (s, 3H), 3.63 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.07 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.17 (t, $J = 7.2$ Hz, 3H), 1.04 (s, 9H), 1.03 (s, 9H), 0.77 (t, $J = 7.2$ Hz, 3H); ^{13}C $\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 185.9, 171.4, 170.3, 166.7, 147.6, 146.1, 141.9, 141.4, 139.1, 129.8, 129.1, 128.7, 103.7, 79.3, 63.5, 62.2, 61.8, 61.6, 54.1, 52.1, 37.6, 35.0, 34.7, 29.4, 29.2, 14.0, 13.4; IR (neat): ν 2955.71, 2904.25, 2867.72, 1959.72, 1722.03, 1659.67, 1637.97, 1611.21, 1366.19, 1278.24, 1254.33, 1219.08, 1108.80 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{34}\text{H}_{43}\text{O}_7$ $[\text{M}+\text{H}]^+$: 563.3003, found: 563.3003.

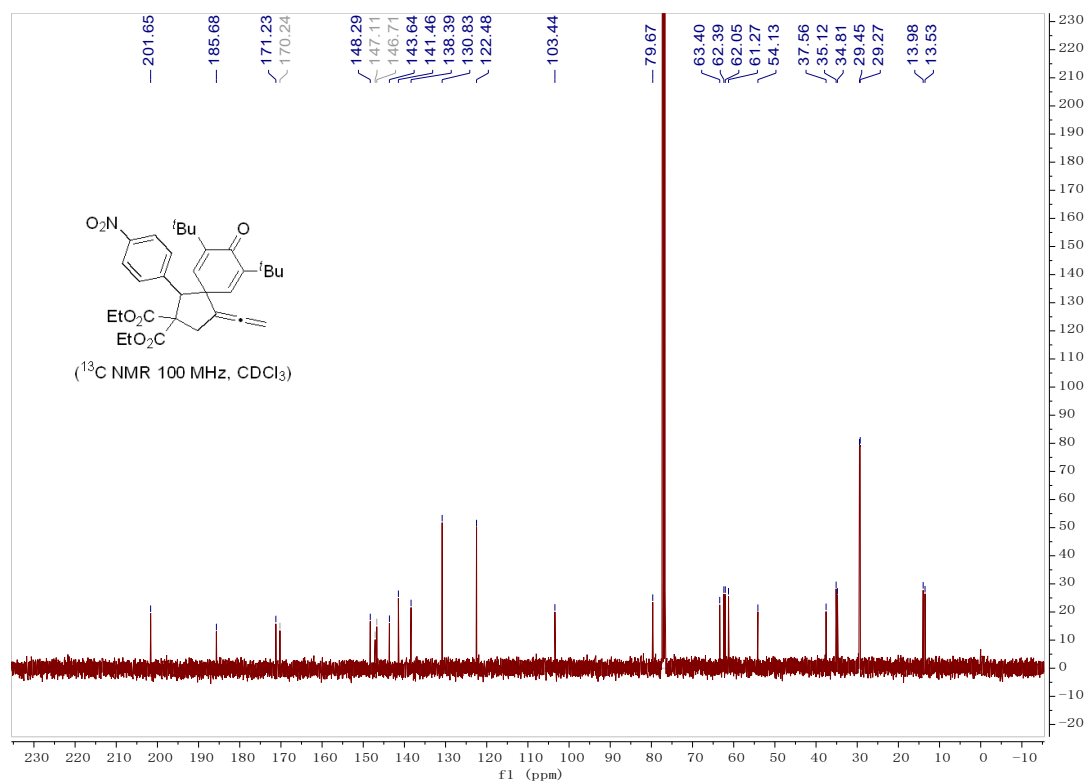


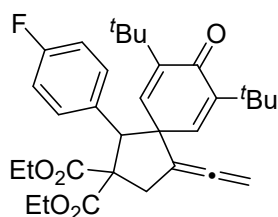




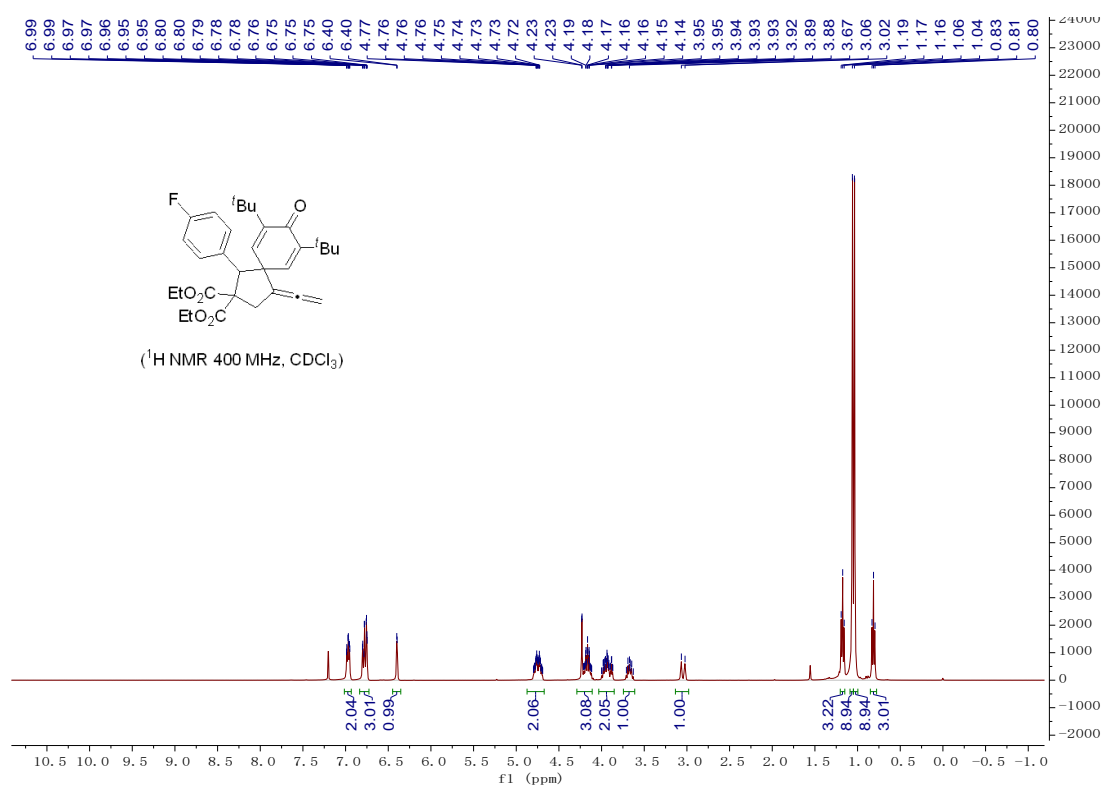
diethyl 7,9-di-*tert*-butyl-1-(4-nitrophenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3i): Yield: 0.0234 g, 42%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 8.04 (d, $J = 8.2$ Hz, 2H), 7.30 – 7.26 (m, 2H), 6.85 (d, $J = 3.0$ Hz, 1H), 6.50 – 6.42 (m, 1H), 4.92 – 4.79 (m, 2H), 4.40 (s, 1H), 4.34 – 4.19 (m, 2H), 4.15 – 3.94 (m, 2H), 3.80 – 3.70 (m, 1H), 3.14 (d, $J = 17.2$ Hz, 1H), 1.25 (t, $J = 7.0$ Hz, 3H), 1.14 (s, 9H), 1.10 (s, 9H), 0.90 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.7, 185.7, 171.2, 170.2, 148.3, 147.1, 146.7, 143.6, 141.5, 138.4, 130.8, 122.5, 103.4, 79.7, 63.4, 62.4, 62.0, 61.3, 54.1, 37.6, 35.1, 34.8, 29.4, 29.3, 14.0, 13.5; IR (neat): ν 2957.82, 2862.51, 1964.94, 1725.64, 1715.35, 1659.96, 1523.15, 1346.94, 1255.85, 1219.70, 1110.56, 882.15, 857.82 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{32}\text{H}_{40}\text{NO}_7$ $[\text{M}+\text{H}]^+$: 550.2799, found: 550.2793.

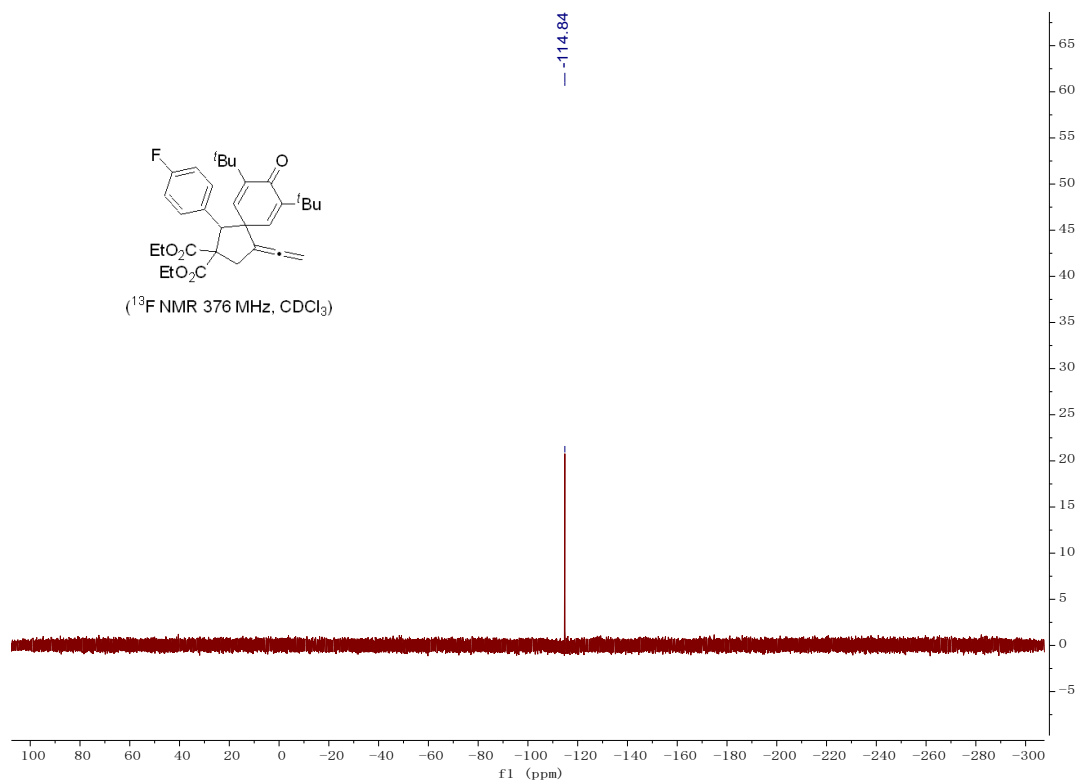
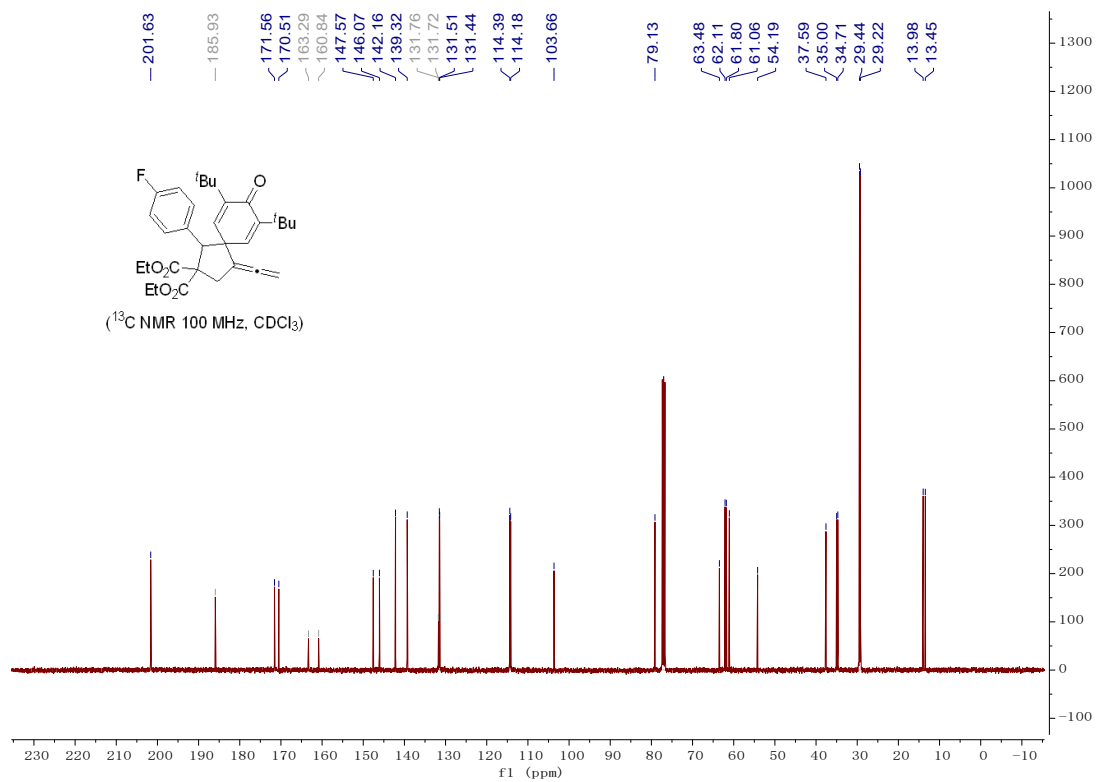


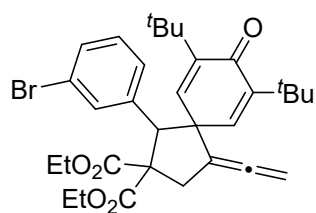




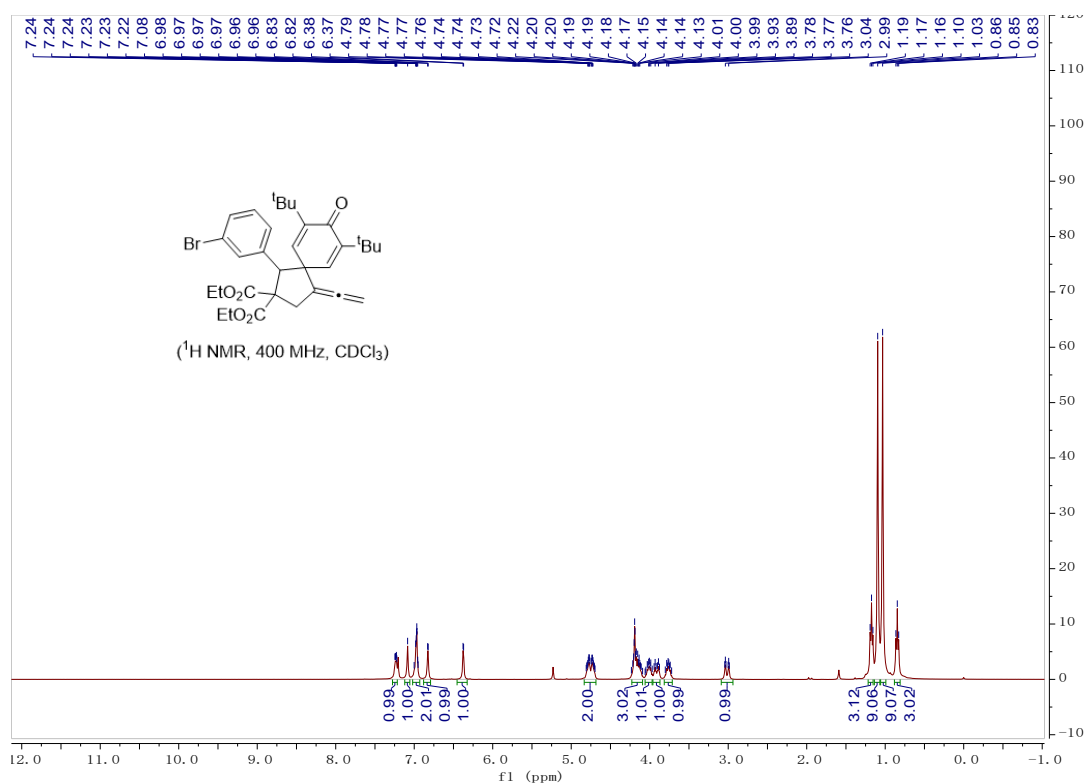
diethyl 7,9-di-*tert*-butyl-1-(4-fluorophenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3j): Yield: 0.0376 g, 72%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.01 – 6.93 (m, 2H), 6.84 – 6.73 (m, 3H), 6.53 – 6.32 (m, 1H), 4.87 – 4.67 (m, 2H), 4.29 – 4.11 (m, 3H), 4.03 – 3.85 (m, 2H), 3.67 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.04 (d, $J = 17.2$ Hz, 1H), 1.17 (t, $J = 7.0$ Hz, 3H), 1.06 (s, 9H), 1.04 (s, 9H), 0.81 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 185.9, 171.6, 170.5, 162.1 (d, $J = 246.6$ Hz), 147.6, 146.1, 142.2, 139.3, 131.7 (d, $J = 3.4$ Hz), 131.5 (d, $J = 8.0$ Hz), 114.3 (d, $J = 21.4$ Hz), 103.7, 79.1, 63.5, 62.1, 61.8, 61.1, 54.2, 37.6, 35.0, 34.7, 29.4, 29.2, 14.0, 13.5; ^{19}F NMR (376 MHz, CDCl_3) δ -114.84; IR (neat): ν 2957.85, 2904.25, 2859.90, 1962.33, 1724.69, 1659.60, 1638.09, 1252.83, 1228.13, 1207.17, 1161.92, 1130.87, 1096.98, 1034.38, 882.02 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{32}\text{H}_{40}\text{FO}_5$ $[\text{M}+\text{H}]^+$: 523.2854, found: 523.2857.

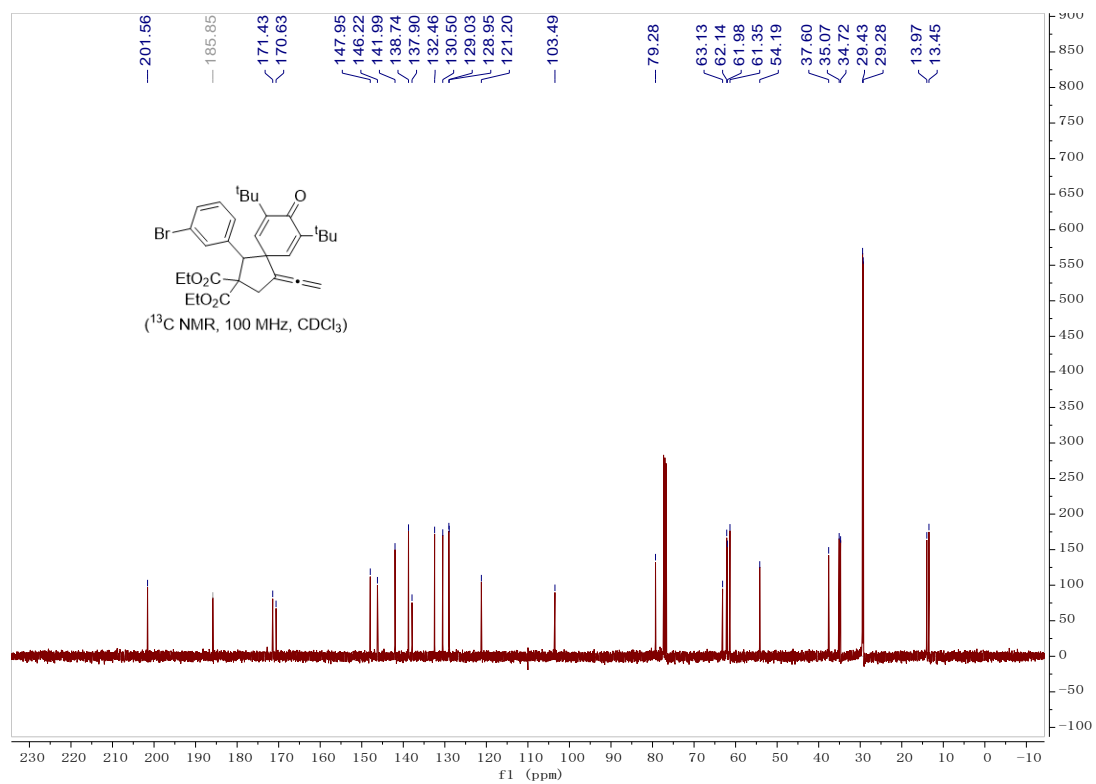


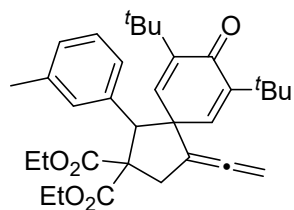




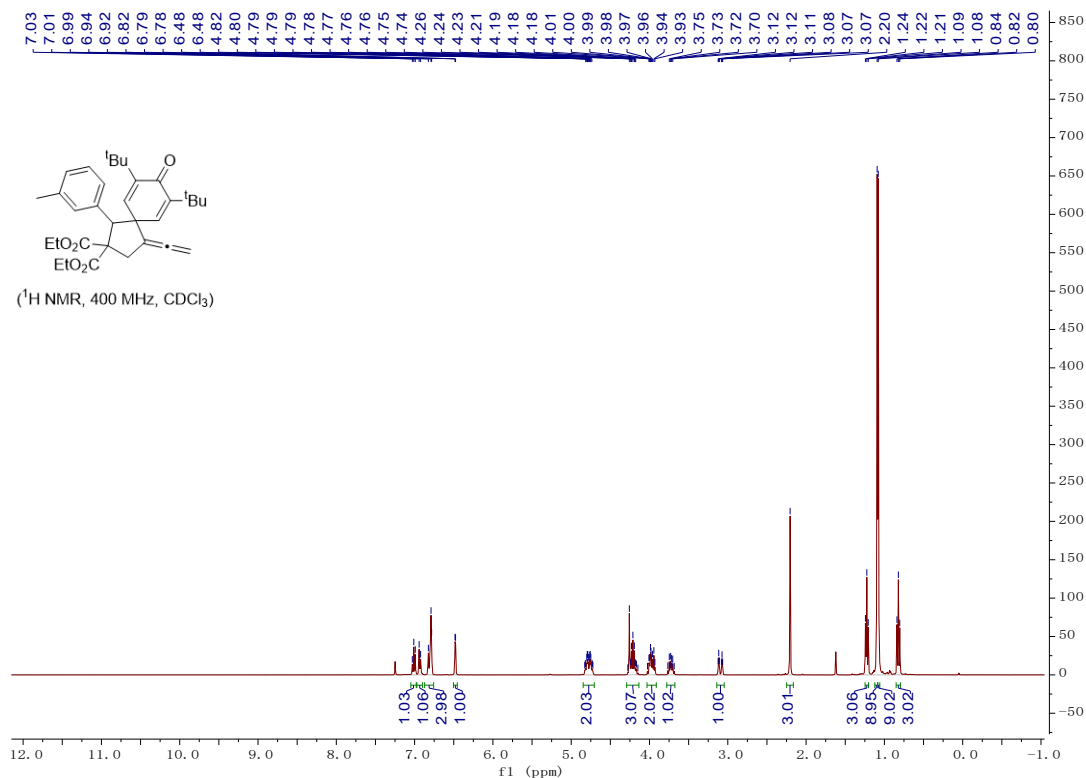
diethyl 1-(3-bromophenyl)-7,9-di-*tert*-butyl-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3k): Yield: 0.0442 g, 76%, a pale yellow solid, m.p. 100-102 °C; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.28 – 7.20 (m, 1H), 7.08 (s, 1H), 7.02 – 6.93 (m, 2H), 6.83 (d, $J = 2.8$ Hz, 1H), 6.37 (d, $J = 2.8$ Hz, 1H), 4.83 – 4.68 (m, 2H), 4.23 – 4.09 (m, 3H), 4.06 – 3.97 (m, 1H), 3.91 (dt, $J = 17.0, 5.2$ Hz, 1H), 3.76 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.02 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.17 (t, $J = 7.2$ Hz, 3H), 1.10 (s, 9H), 1.03 (s, 9H), 0.85 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 185.9, 171.4, 170.6, 147.9, 146.2, 142.0, 138.7, 137.9, 132.5, 130.5, 129.0, 128.9, 121.2, 103.5, 79.3, 63.1, 62.1, 62.0, 61.4, 54.2, 37.6, 35.1, 34.7, 29.4, 29.3, 14.0, 13.5; IR (neat): ν 2957.06, 2909.39, 2865.03, 1962.28, 1724.48, 1659.34, 1638.14, 1365.87, 1261.71, 1218.85, 881.41, 858.40, 698.49 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{32}\text{H}_{40}\text{BrO}_5$ $[\text{M}+\text{H}]^+$: 583.2054, found: 583.2052.

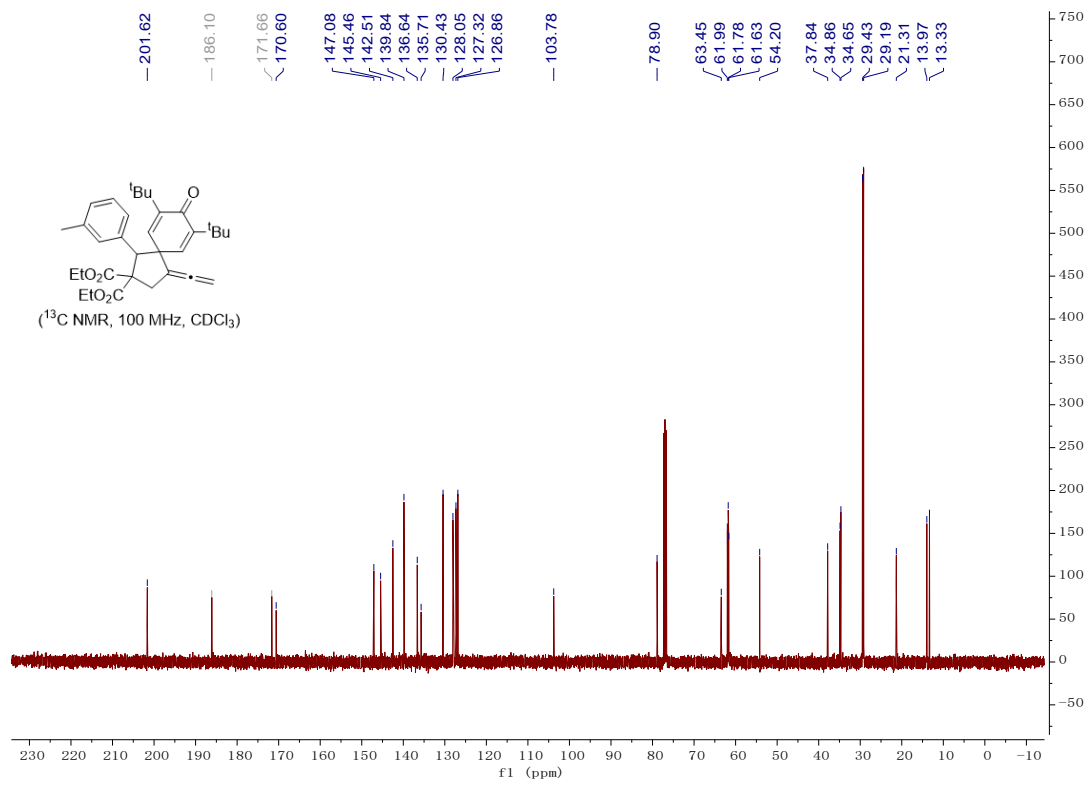


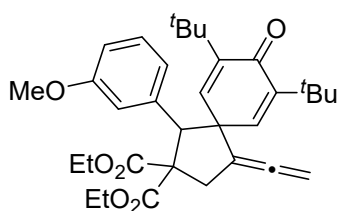




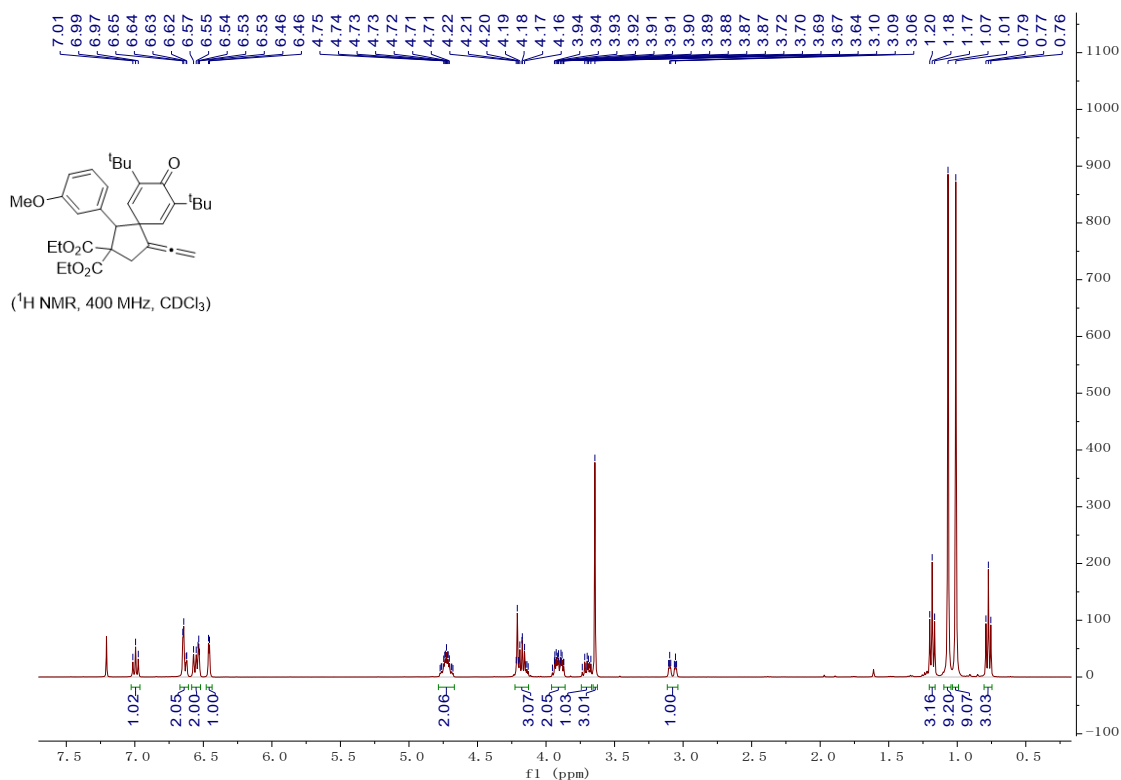
diethyl 7,9-di-*tert*-butyl-8-oxo-1-(*m*-tolyl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (31): Yield: 0.0363 g, 70%, a pale yellow solid, m.p. 108-110 °C; Eluent: PE/EA = 30/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.01 (t, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.87 – 6.76 (m, 3H), 6.48 (d, *J* = 2.8 Hz, 1H), 4.85 – 4.71 (m, 2H), 4.29 – 4.14 (m, 3H), 4.03 – 3.91 (m, 2H), 3.73 (dq, *J* = 10.8, 7.2 Hz, 1H), 3.09 (dt, *J* = 17.0, 3.2 Hz, 1H), 2.20 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H), 1.09 (s, 9H), 1.08 (s, 9H), 0.82 (t, *J* = 7.2 Hz, 3H); ¹³C{¹H}-NMR (100 MHz, CDCl₃, TMS) δ 201.6, 186.1, 171.7, 170.6, 147.1, 145.5, 142.5, 139.8, 136.6, 135.7, 130.4, 128.0, 127.3, 126.8, 103.8, 78.9, 63.5, 62.0, 61.8, 61.6, 54.2, 37.8, 34.9, 34.7, 29.4, 29.2, 21.3, 14.0, 13.3; IR (neat): ν 2956.67, 2865.03, 1967.50, 1725.27, 1658.92, 1638.07, 1453.53, 1366.12, 1255.84, 1096.61, 858.20, 780.35 cm⁻¹; HRMS (ESI-TOF) Calcd for C₃₃H₄₃O₅ [M+H]⁺ : 519.3105, found: 519.3102.

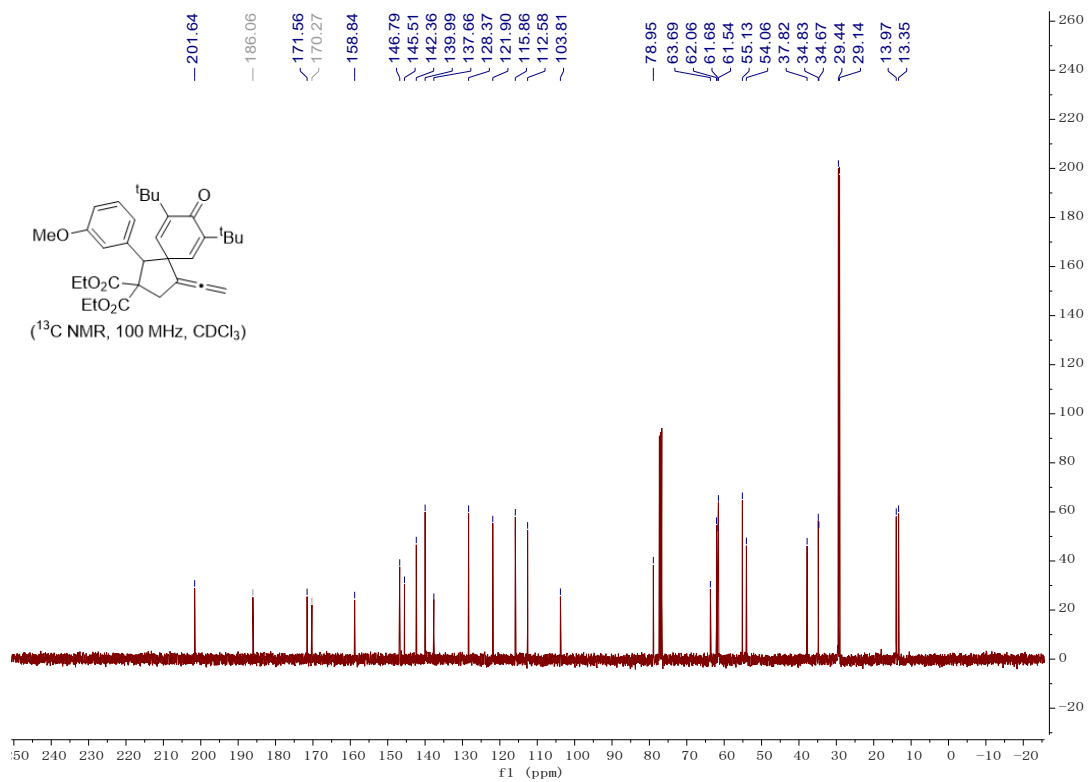


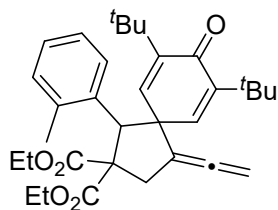




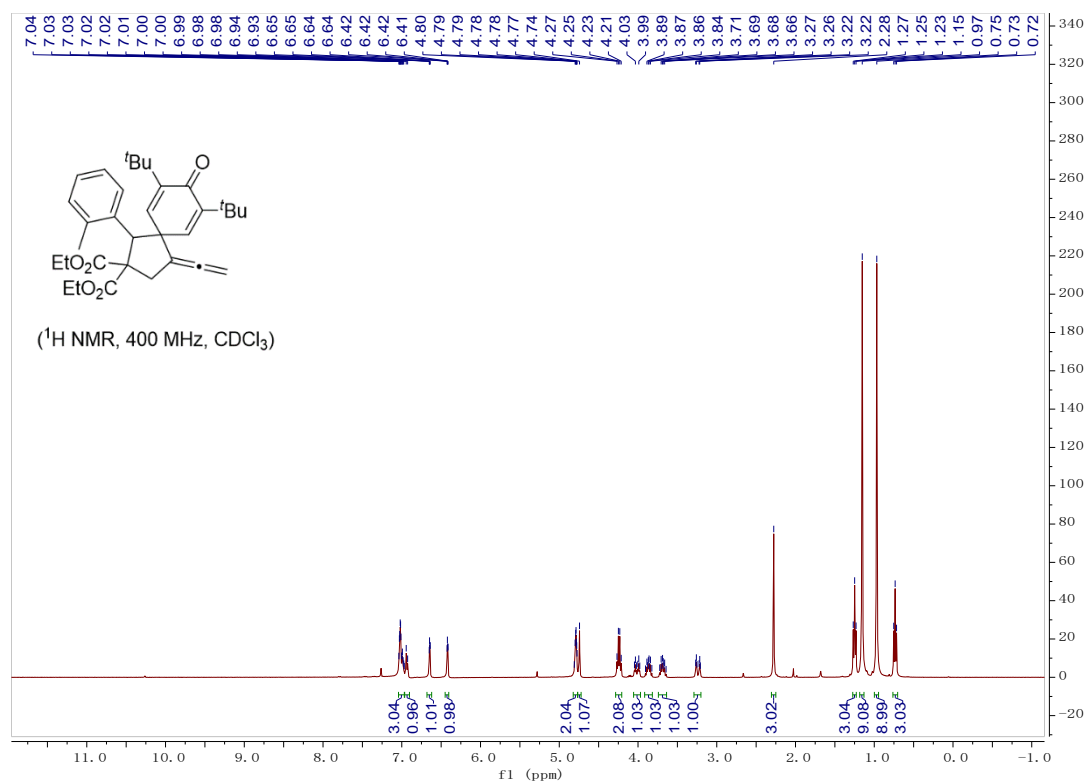
diethyl 7,9-di-*tert*-butyl-1-(3-methoxyphenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3m): Yield: 0.0443 g, 83%, a pale yellow solid, m.p. 118-120 °C; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 6.99 (t, $J = 8.0$ Hz, 1H), 6.63 (dd, $J = 9.2, 2.4$ Hz, 2H), 6.59 – 6.51 (m, 2H), 6.46 (d, $J = 2.8$ Hz, 1H), 4.79 – 4.67 (m, 2H), 4.23 – 4.13 (m, 3H), 3.96 – 3.86 (m, 2H), 3.74 – 3.67 (m, 1H), 3.64 (s, 3H), 3.08 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.18 (t, $J = 7.2$ Hz, 3H), 1.07 (s, 9H), 1.01 (s, 9H), 0.77 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 186.1, 171.6, 170.3, 158.8, 146.8, 145.5, 142.4, 140.0, 137.7, 128.4, 121.9, 115.8, 112.6, 103.8, 78.9, 63.7, 62.1, 61.7, 61.5, 55.1, 54.1, 37.8, 34.8, 34.7, 29.4, 29.1, 14.0, 13.4; IR (neat): ν 2956.33, 2906.54, 2867.29, 1967.29, 1725.75, 1658.76, 1638.12, 1366.54, 1256.49, 1157.56, 858.67, 700.88 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_6$ $[\text{M}+\text{H}]^+$: 535.3053, found: 535.3054.

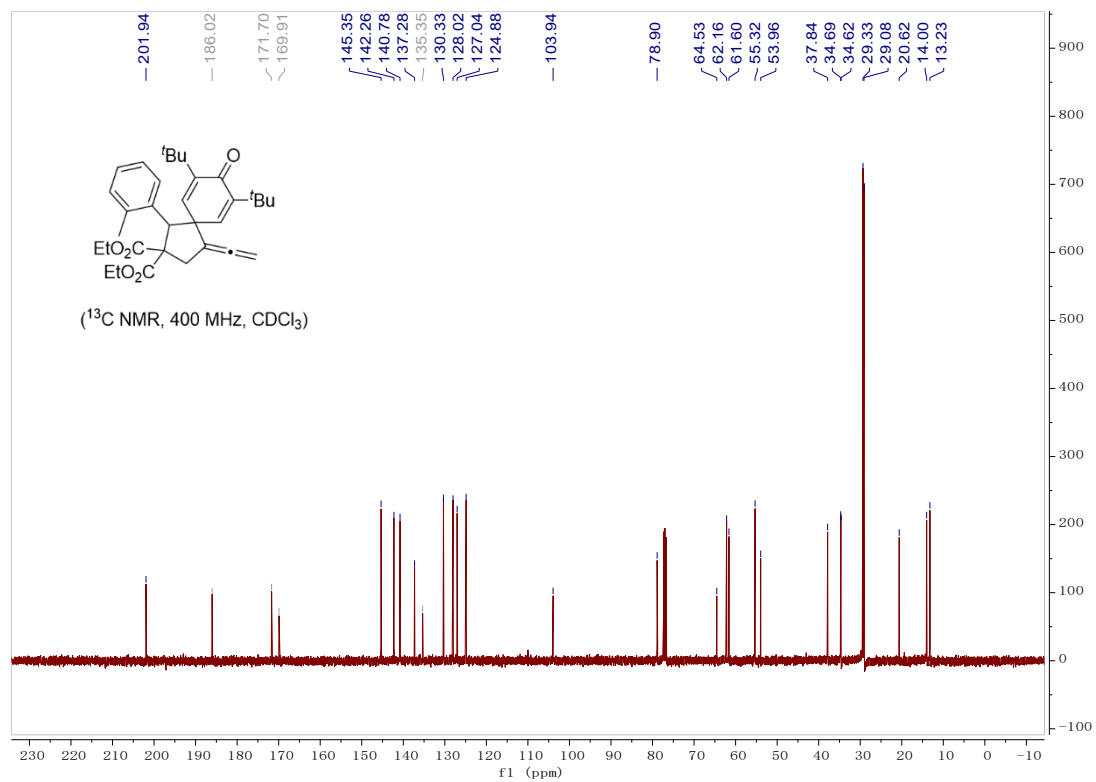


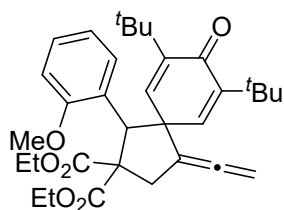




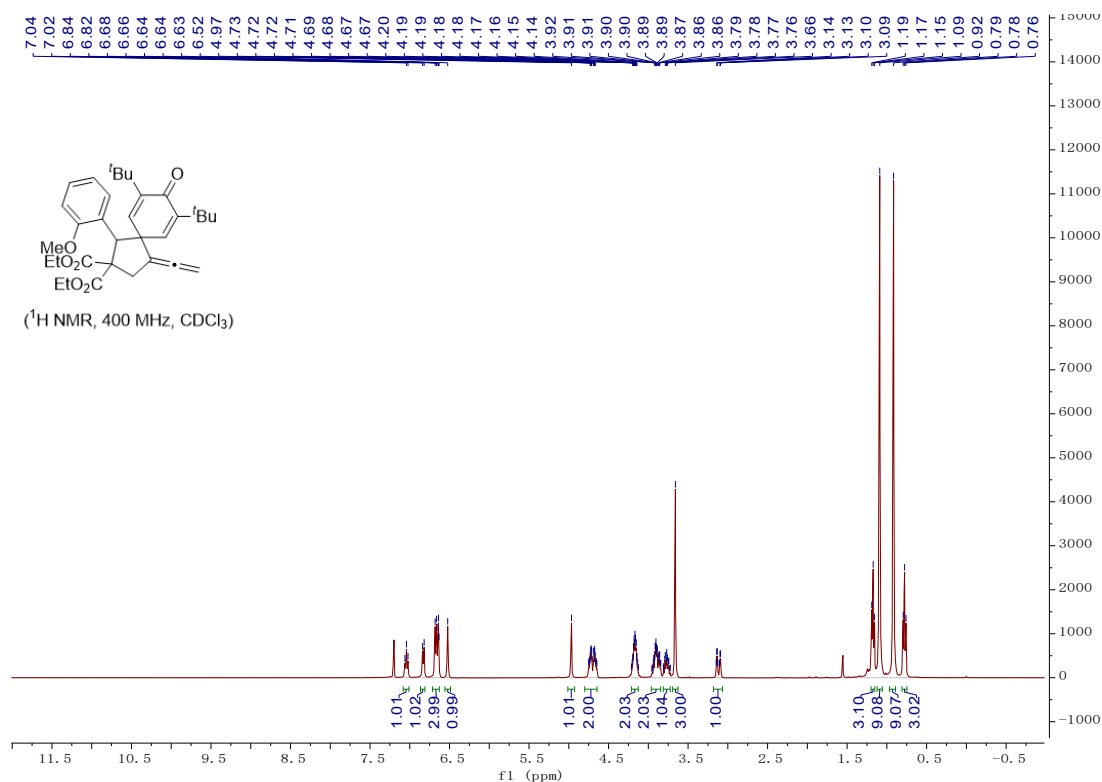
diethyl 7,9-di-*tert*-butyl-8-oxo-1-(*o*-tolyl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3n): Yield: 0.0373 g, 72%, a pale yellow solid, m.p. 119-121 °C; Eluent: PE/EA = 30/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.04 – 6.97 (m, 3H), 6.93 (d, *J* = 7.2 Hz, 1H), 6.68 - 6.62 (m, 1H), 6.45 - 6.40 (m, 1H), 4.82 – 4.77 (m, 2H), 4.74 (s, 1H), 4.24 (q, *J* = 7.2 Hz, 2H), 4.01 (dt, *J* = 17.2, 5.0 Hz, 1H), 3.86 (dq, *J* = 10.8, 7.2 Hz, 1H), 3.68 (dq, *J* = 10.8, 7.2 Hz, 1H), 3.24 (dt, *J* = 17.2, 3.4 Hz, 1H), 2.28 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 3H), 1.15 (s, 9H), 0.97 (s, 9H), 0.73 (t, *J* = 7.2 Hz, 3H); ¹³C {¹H}-NMR (100 MHz, CDCl₃, TMS) δ 201.9, 186.0, 171.7, 169.9, 145.4, 142.3, 140.8, 137.3, 135.4, 130.3, 128.0, 127.0, 124.9, 103.9, 78.9, 64.5, 62.2, 61.6, 55.3, 53.9, 37.8, 34.7, 34.6, 29.3, 29.1, 20.6, 14.0, 13.2; IR (neat): ν 2956.69, 2906.78, 2865.03, 1959.67, 1730.82, 1658.78, 1637.57, 1366.11, 1251.87, 1203.89, 811.73, 731.10 cm⁻¹; HRMS (ESI-TOF) Calcd for C₃₃H₄₃O₅ [M+H]⁺ : 519.3105, found: 519.3102.

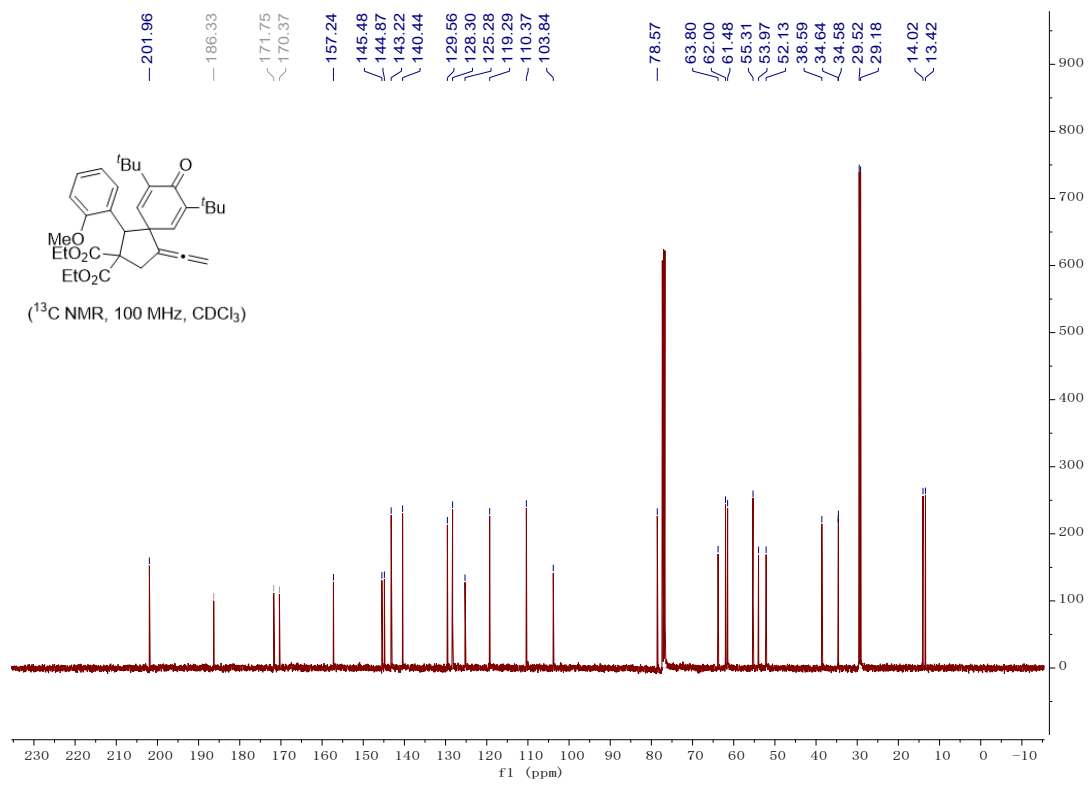


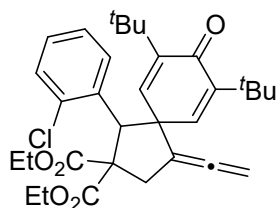




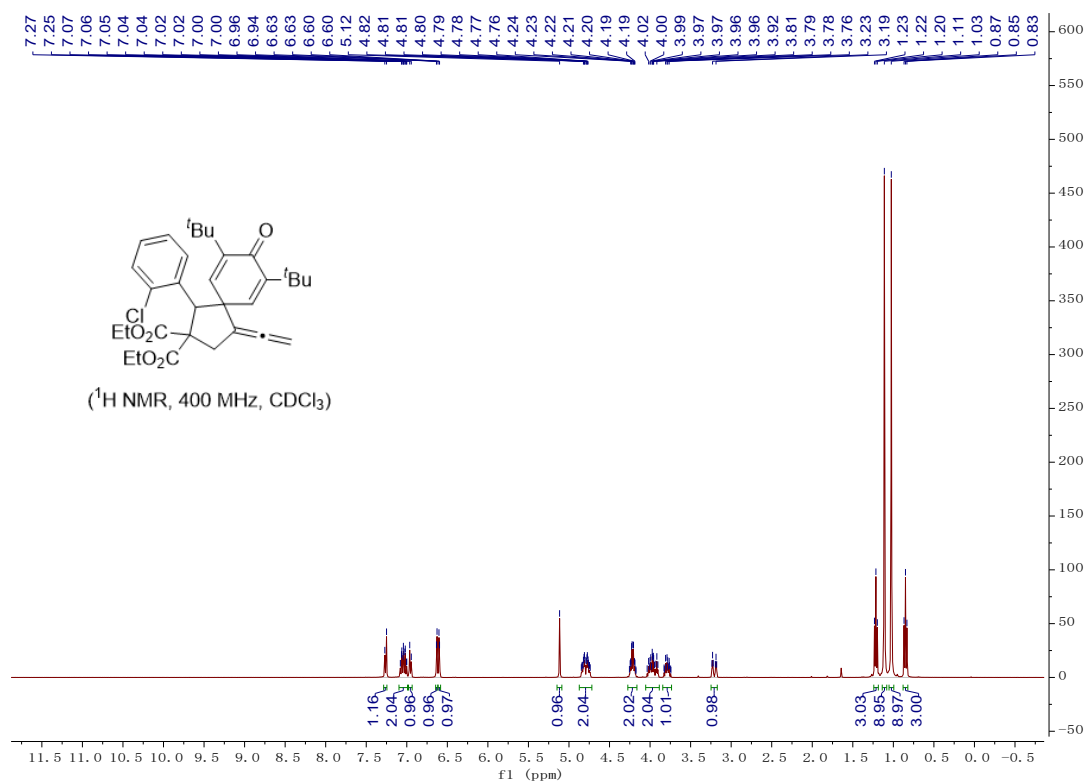
diethyl 7,9-di-*tert*-butyl-1-(2-methoxyphenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (30): Yield: 0.0336 g, 63%, a pale yellow solid, m.p. 104-106 °C; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.04 (t, $J = 7.8$ Hz, 1H), 6.83 (d, $J = 7.8$ Hz, 1H), 6.71 – 6.63 (m, 3H), 6.52 (s, 1H), 4.97 (s, 1H), 4.80 – 4.64 (m, 2H), 4.24 – 4.11 (m, 2H), 3.96 – 3.84 (m, 2H), 3.81 – 3.72 (m, 1H), 3.66 (s, 3H), 3.18 – 3.07 (m, 1H), 1.17 (t, $J = 7.2$ Hz, 3H), 1.09 (s, 9H), 0.92 (s, 9H), 0.78 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 202.0, 186.3, 171.7, 170.4, 157.2, 145.5, 144.9, 143.2, 140.4, 129.6, 128.3, 125.3, 119.3, 110.4, 103.8, 78.6, 63.8, 62.0, 61.5, 55.3, 54.0, 52.1, 38.60, 34.6, 34.6, 29.5, 29.2, 14.0, 13.4; IR (neat): ν 2956.15, 2912.08, 2865.11, 1959.72, 1730.86, 1658.87, 1636.39, 1365.30, 1247.86, 1219.26, 822.29, 755.22 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_6$ $[\text{M}+\text{H}]^+$: 535.3054, found: 535.3051.

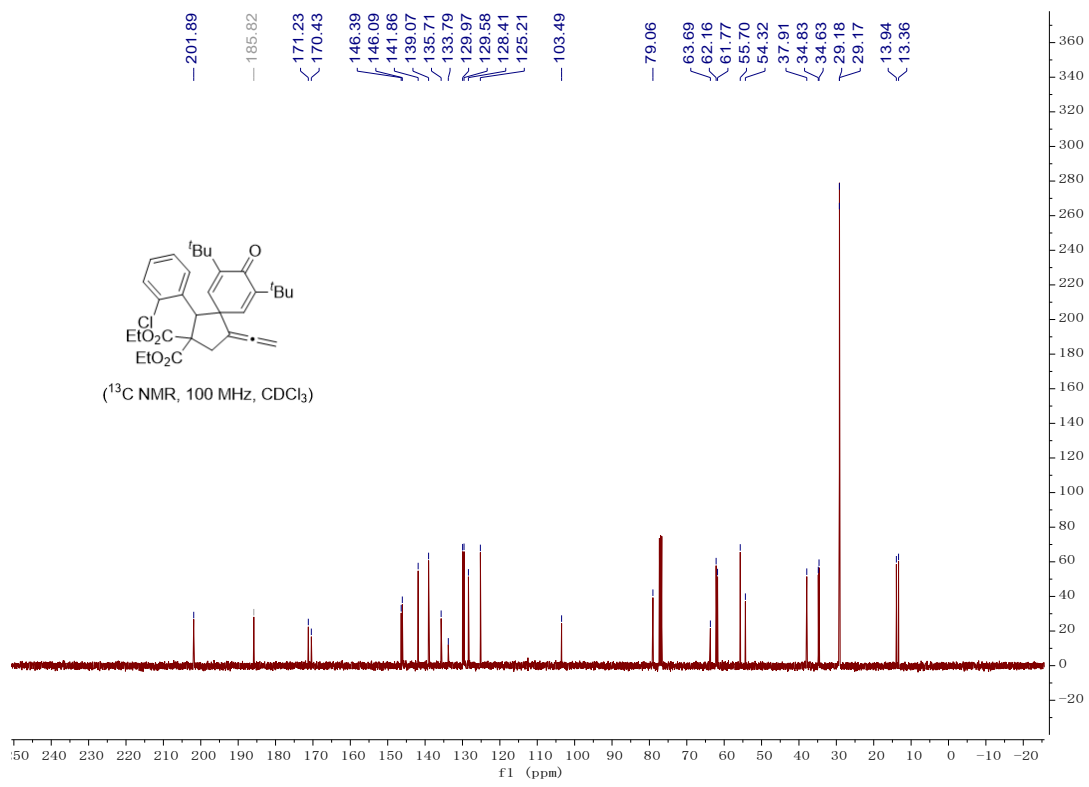


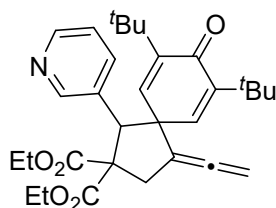




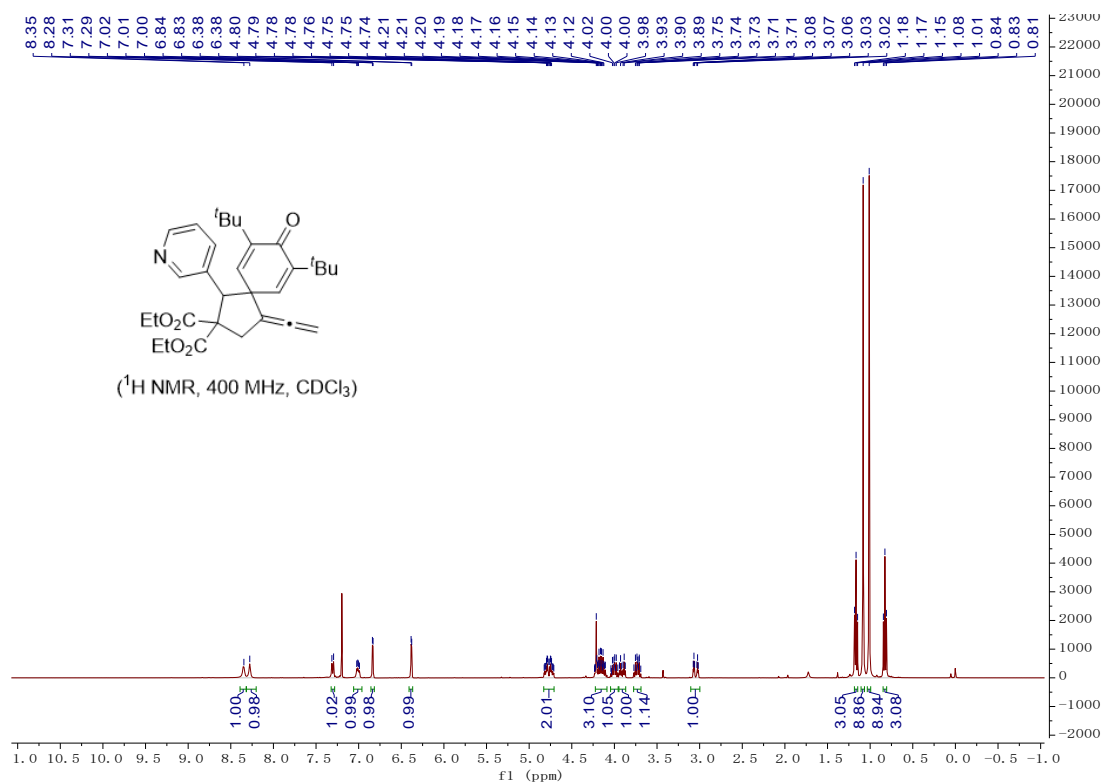
diethyl 7,9-di-*tert*-butyl-1-(2-chlorophenyl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3p): Yield: 0.0457 g, 85%, a pale yellow solid, m.p. 140-146 °C; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.26 (d, $J = 8.4$ Hz, 1H), 7.10 – 6.99 (m, 2H), 6.95 (d, $J = 7.8$ Hz, 1H), 6.63 (d, $J = 2.8$ Hz, 1H), 6.60 (d, $J = 2.8$ Hz, 1H), 5.12 (s, 1H), 4.87 – 4.72 (m, 2H), 4.27 – 4.16 (m, 2H), 4.05 – 3.89 (m, 2H), 3.79 (dq, $J = 10.6, 7.2$ Hz, 1H), 3.21 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.22 (t, $J = 7.2$ Hz, 3H), 1.11 (s, 9H), 1.03 (s, 9H), 0.85 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.89, 185.82, 171.23, 170.43, 146.39, 146.09, 141.86, 139.07, 135.71, 133.79, 129.97, 129.58, 128.41, 125.21, 103.49, 79.06, 63.69, 62.16, 61.77, 55.70, 54.32, 37.91, 34.83, 34.63, 29.18, 29.17, 13.94, 13.36; IR (neat): ν 3000.71, 2958.08, 2909.39, 2865.03, 1964.89, 1713.25, 1659.63, 1437.88, 1219.70, 1030.84, 882.16, 759.66 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{32}\text{H}_{40}\text{ClO}_5$ $[\text{M}+\text{H}]^+$: 539.2559, found: 539.2558.

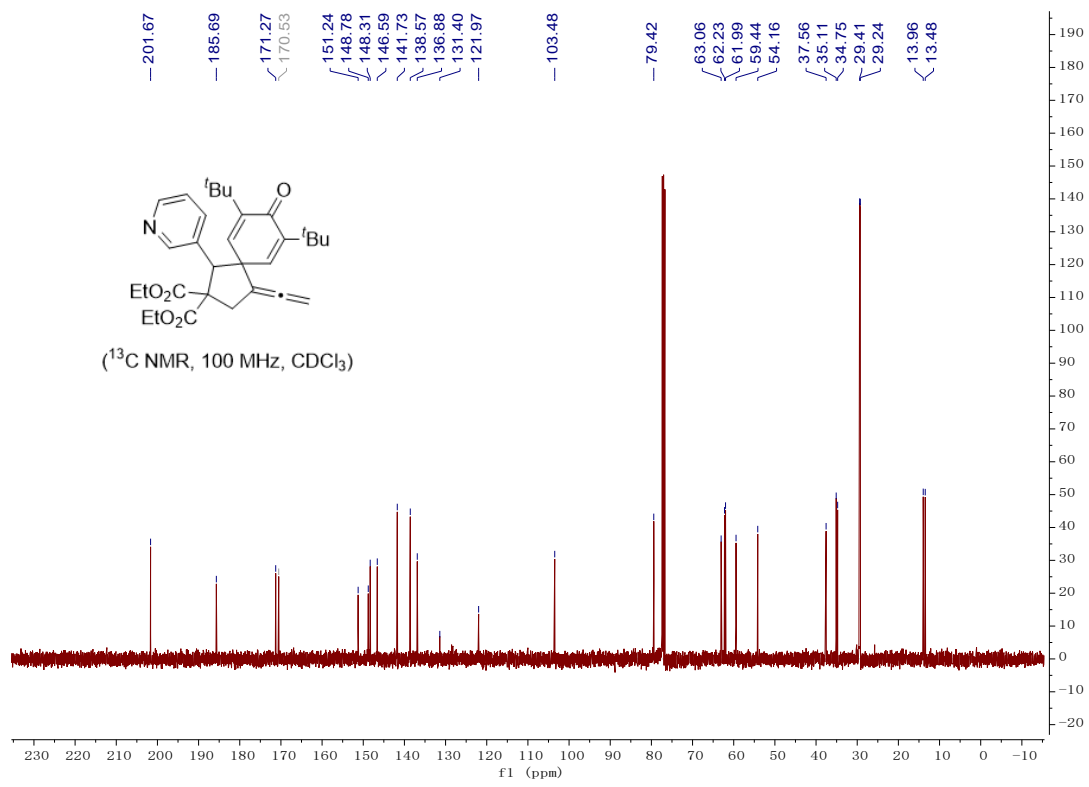


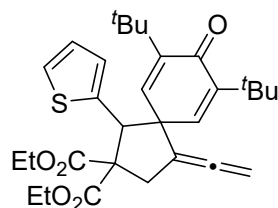




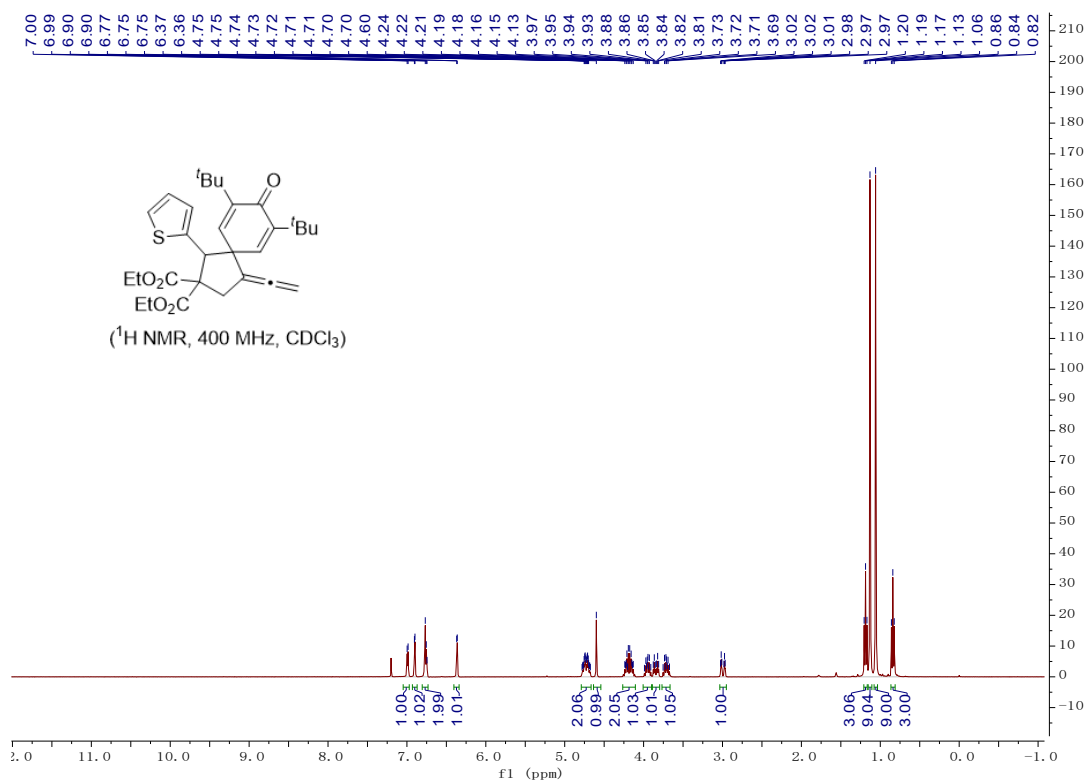
diethyl 7,9-di-*tert*-butyl-8-oxo-1-(pyridin-3-yl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3q): Yield: 0.0328 g, 65%, a colorless oil; Eluent: PE/EA = 4/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 8.35 (s, 1H), 8.28 (s, 1H), 7.30 (d, $J = 8.0$ Hz, 1H), 7.06 – 6.96 (m, 1H), 6.83 (d, $J = 3.0$ Hz, 1H), 6.38 (d, $J = 3.0$ Hz, 1H), 4.83 – 4.71 (m, 2H), 4.22 – 4.09 (m, 3H), 4.05 – 3.96 (m, 1H), 3.91 (dt, $J = 17.0, 5.2$ Hz, 1H), 3.77 – 3.69 (m, 1H), 3.05 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.17 (t, $J = 7.2$ Hz, 3H), 1.08 (s, 9H), 1.01 (s, 9H), 0.83 (t, $J = 7.2$ Hz, 3H); ^{13}C $\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.7, 185.7, 171.3, 170.5, 151.2, 148.8, 148.3, 146.6, 141.7, 138.6, 136.9, 131.4, 122.0, 103.5, 79.4, 63.1, 62.2, 62.0, 59.4, 54.2, 37.3, 35.1, 34.8, 29.4, 29.2, 14.0, 13.5; IR (neat): ν 2957.20, 2912.00, 2862.42, 1957.06, 1725.40, 1659.38, 1637.83, 1461.36, 1257.33, 1098.68, 1026.85, 732.13, 714.80 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{31}\text{H}_{40}\text{NO}_5$ $[\text{M}+\text{H}]^+$: 506.2901, found: 506.2898.

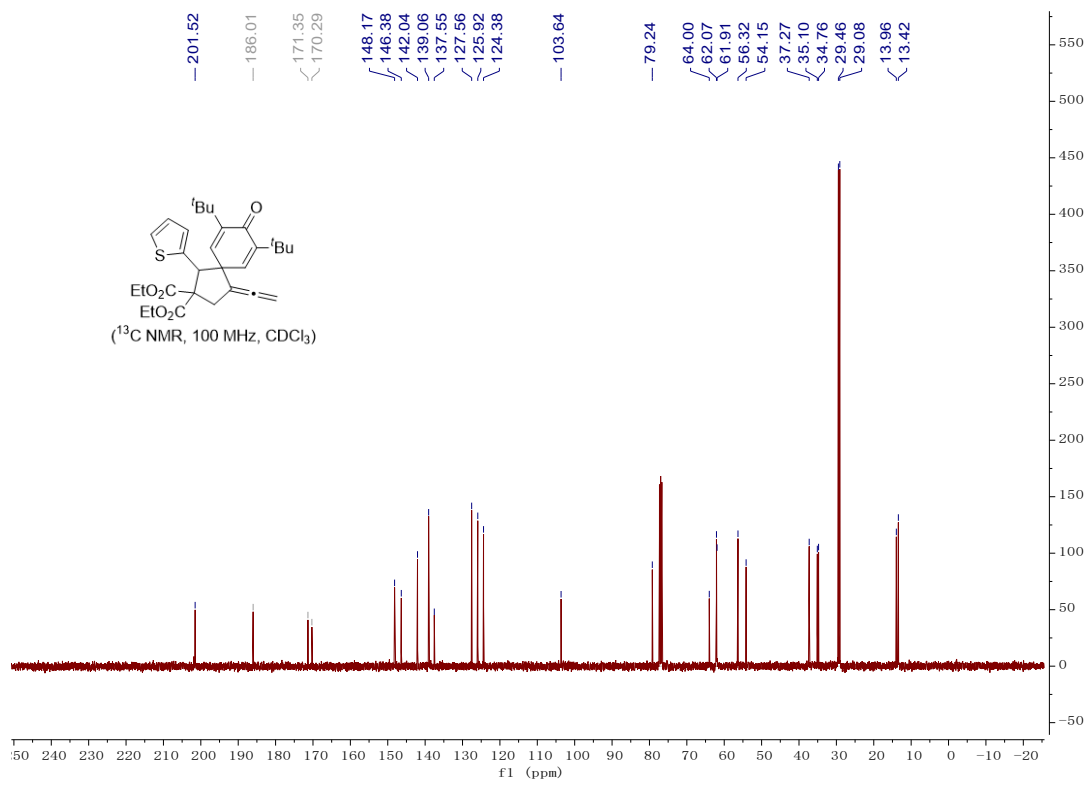


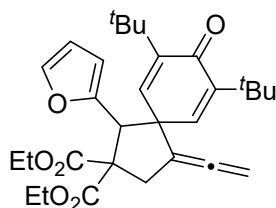




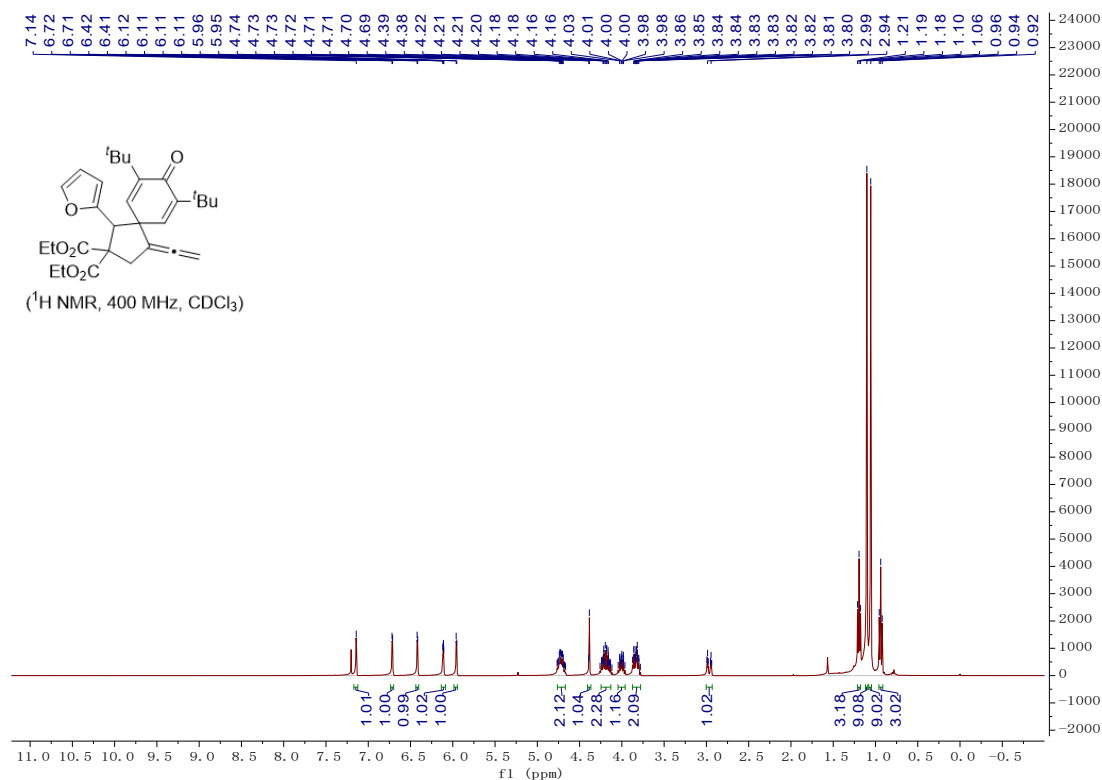
diethyl 7,9-di-*tert*-butyl-8-oxo-1-(thiophen-2-yl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3r): Yield: 0.0377 g, 74%, a pale yellow solid, m.p. 92-94 °C; Eluent: PE/EA = 30/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 6.99 (d, *J* = 4.8 Hz, 1H), 6.90 (d, *J* = 2.8 Hz, 1H), 6.81 – 6.73 (m, 2H), 6.37 (d, *J* = 2.8 Hz, 1H), 4.79 – 4.67 (m, 2H), 4.60 (s, 1H), 4.26 – 4.10 (m, 2H), 4.01 – 3.90 (m, 1H), 3.84 (dt, *J* = 16.8, 5.2 Hz, 1H), 3.71 (dq, *J* = 10.8, 7.2 Hz, 1H), 3.00 (dt, *J* = 16.8, 3.2 Hz, 1H), 1.19 (t, *J* = 7.2 Hz, 3H), 1.13 (s, 9H), 1.06 (s, 9H), 0.84 (t, *J* = 7.2 Hz, 3H); ¹³C{¹H}-NMR (100 MHz, CDCl₃, TMS) δ 201.5, 186.0, 171.4, 170.3, 148.2, 146.4, 142.0, 139.1, 137.6, 127.6, 125.9, 124.4, 103.6, 79.2, 64.0, 62.1, 61.9, 56.3, 54.2, 37.3, 35.1, 34.8, 29.5, 29.1, 14.0, 13.4; IR (neat): ν 2957.00, 2909.39, 2865.03, 1962.28, 1724.08, 1658.99, 1637.99, 1258.43, 1207.00, 1178.16, 1034.15, 856.58 cm⁻¹; HRMS (ESI-TOF) Calcd for C₃₀H₃₉O₅S [M+H]⁺ : 511.2513, found: 511.2511.

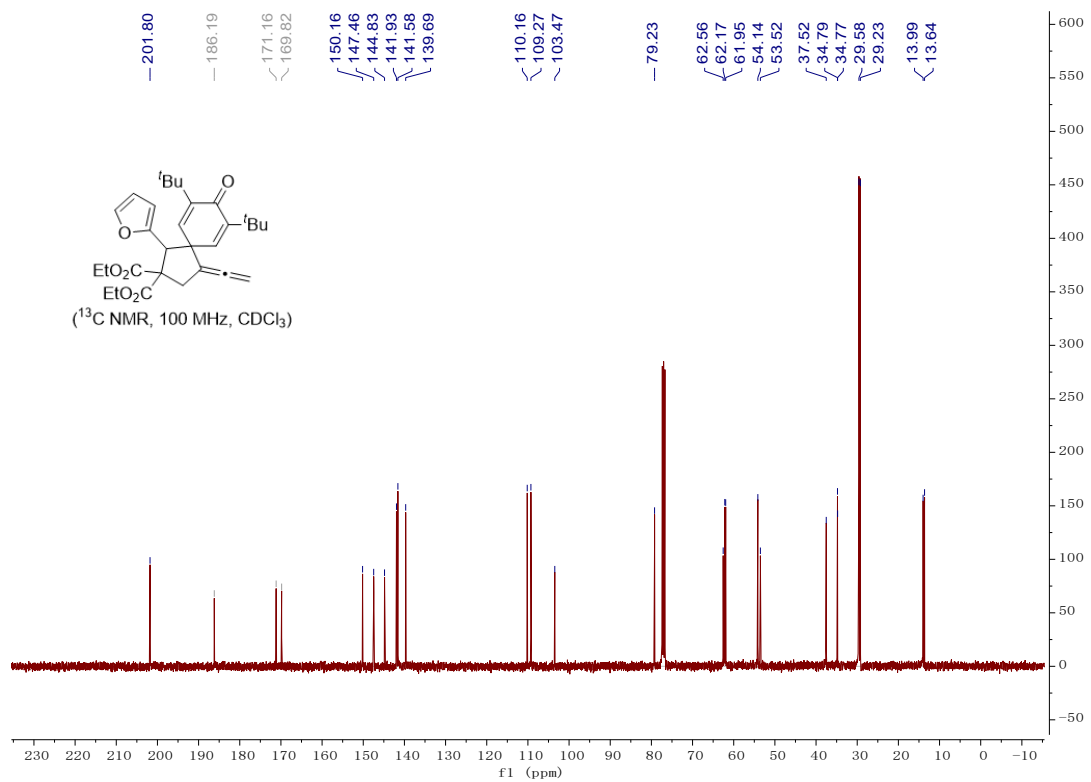


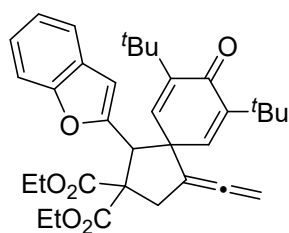




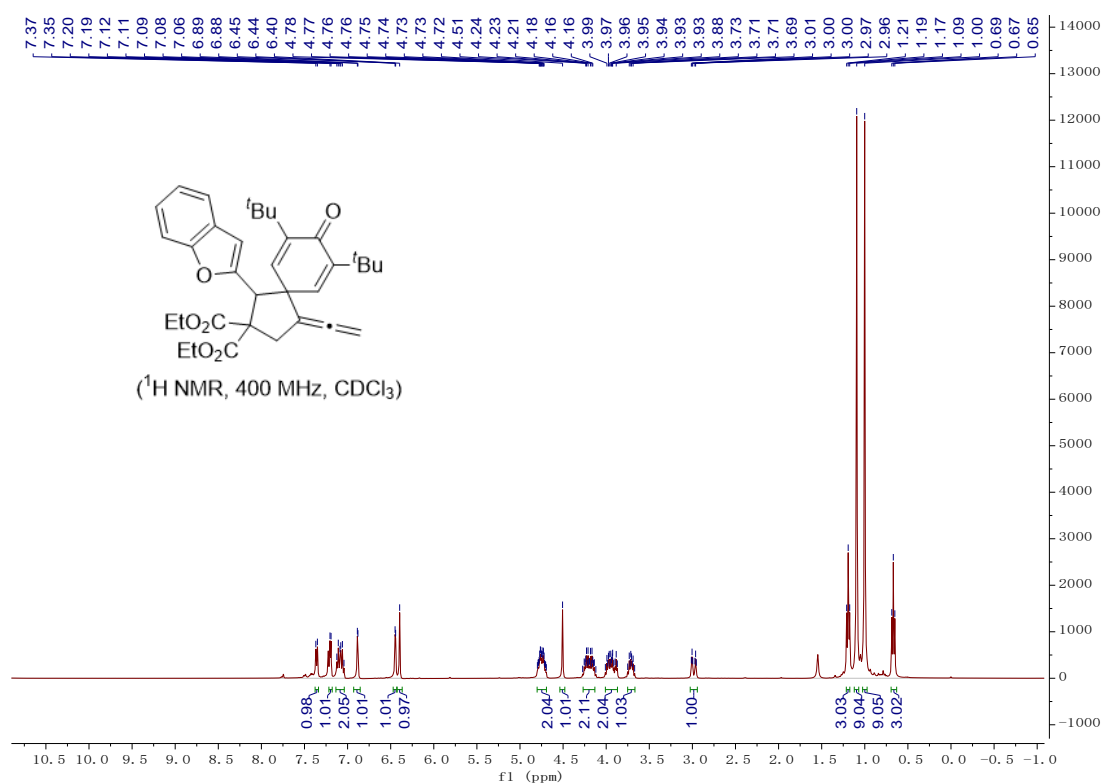
diethyl 7,9-di-*tert*-butyl-1-(furan-2-yl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3s): Yield: 0.0371 g, 75%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.14 (s, 1H), 6.72 (d, $J = 3.0$ Hz, 1H), 6.42 (d, $J = 3.0$ Hz, 1H), 6.14 – 6.09 (m, 1H), 5.96 (d, $J = 3.2$ Hz, 1H), 4.76 – 4.67 (m, 2H), 4.38 (s, 1H), 4.25 – 4.13 (m, 2H), 4.05 – 3.96 (m, 1H), 3.87 – 3.78 (m, 2H), 2.97 (dt, $J = 16.6, 3.2$ Hz, 1H), 1.19 (t, $J = 7.2$ Hz, 3H), 1.10 (s, 9H), 1.06 (s, 9H), 0.94 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.8, 186.2, 171.2, 169.8, 150.2, 147.5, 144.8, 141.9, 141.6, 139.7, 110.2, 109.3, 103.5, 79.2, 62.6, 62.2, 61.9, 54.1, 53.5, 37.5, 34.79, 34.77, 29.6, 29.2, 14.0, 13.6; IR (neat): ν 2956.93, 2904.17, 2862.42, 1962.28, 1729.19, 1659.52, 1638.45, 1366.43, 1258.09, 1198.95, 1012.24, 882.53, 731.89 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{30}\text{H}_{39}\text{O}_6$ $[\text{M}+\text{H}]^+$: 495.2741, found: 495.2739.

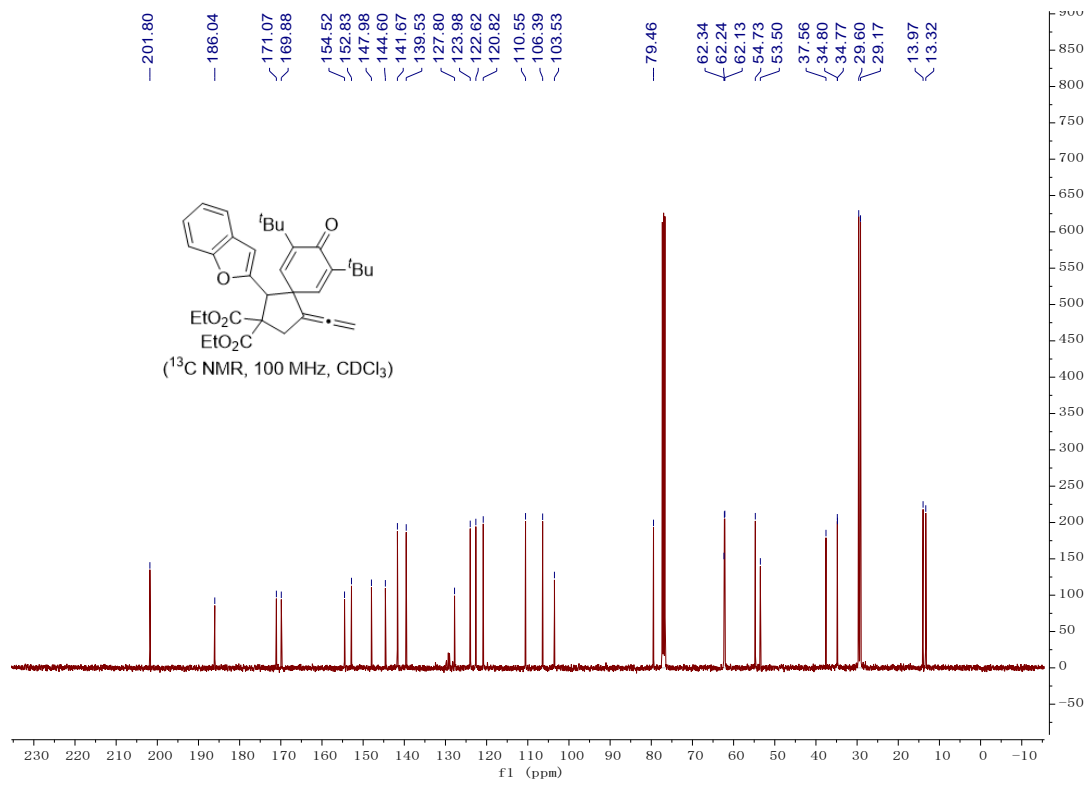


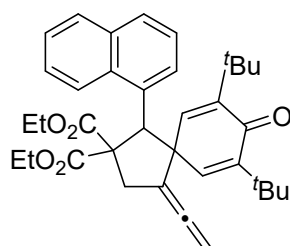




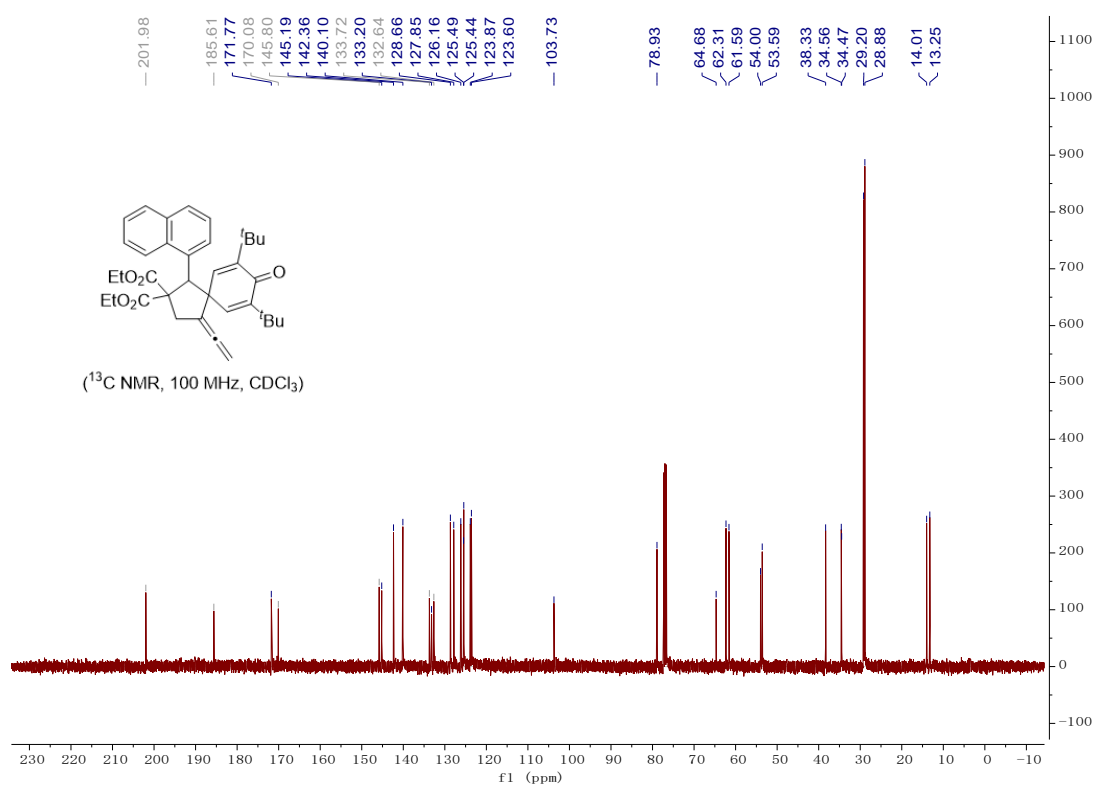
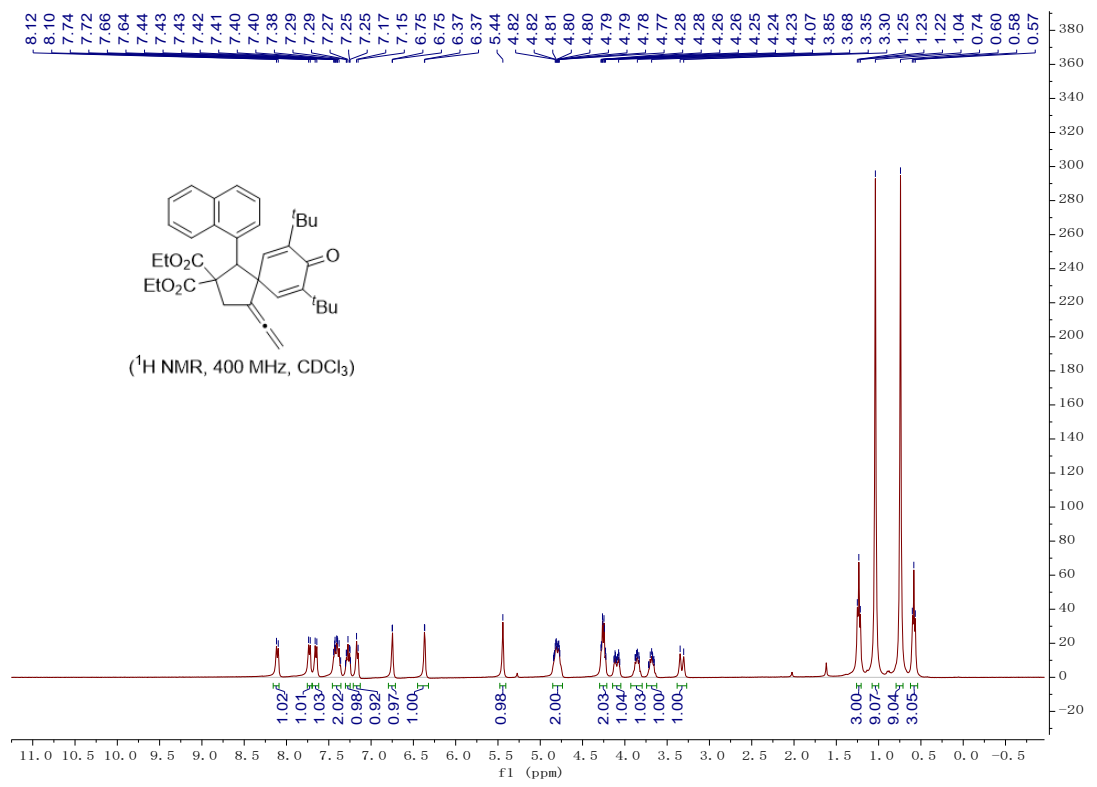
diethyl 1-(benzofuran-2-yl)-7,9-di-*tert*-butyl-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3t): Yield: 0.0370 g, 68%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.36 (d, $J = 7.2$ Hz, 1H), 7.20 (d, $J = 5.0$ Hz, 1H), 7.14 – 7.04 (m, 2H), 6.88 (d, $J = 2.6$ Hz, 1H), 6.45 (d, $J = 2.6$ Hz, 1H), 6.40 (s, 1H), 4.80 – 4.69 (m, 2H), 4.51 (s, 1H), 4.27 – 4.13 (m, 2H), 4.01 – 3.87 (m, 2H), 3.71 (dq, $J = 10.8, 7.2$ Hz, 1H), 2.98 (dt, $J = 16.6, 3.2$ Hz, 1H), 1.19 (t, $J = 7.2$ Hz, 3H), 1.09 (s, 9H), 1.00 (s, 9H), 0.67 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.8, 186.0, 171.1, 169.9, 154.5, 152.8, 148.0, 144.6, 141.7, 139.5, 127.8, 124.0, 122.6, 120.8, 110.6, 106.4, 103.5, 79.5, 62.3, 62.2, 62.1, 54.7, 53.5, 37.6, 34.80, 34.77, 29.6, 29.2, 14.0, 13.3; IR (neat): ν 2956.78, 2862.42, 2257.11, 1962.28, 1729.32, 1659.79, 1637.98, 1454.89, 1253.04, 1191.13, 882.34, 734.25 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{34}\text{H}_{41}\text{O}_6$ $[\text{M}+\text{H}]^+$: 545.2898, found: 545.2897.

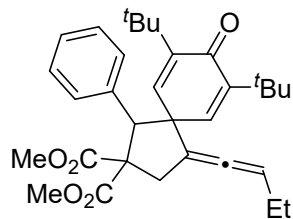




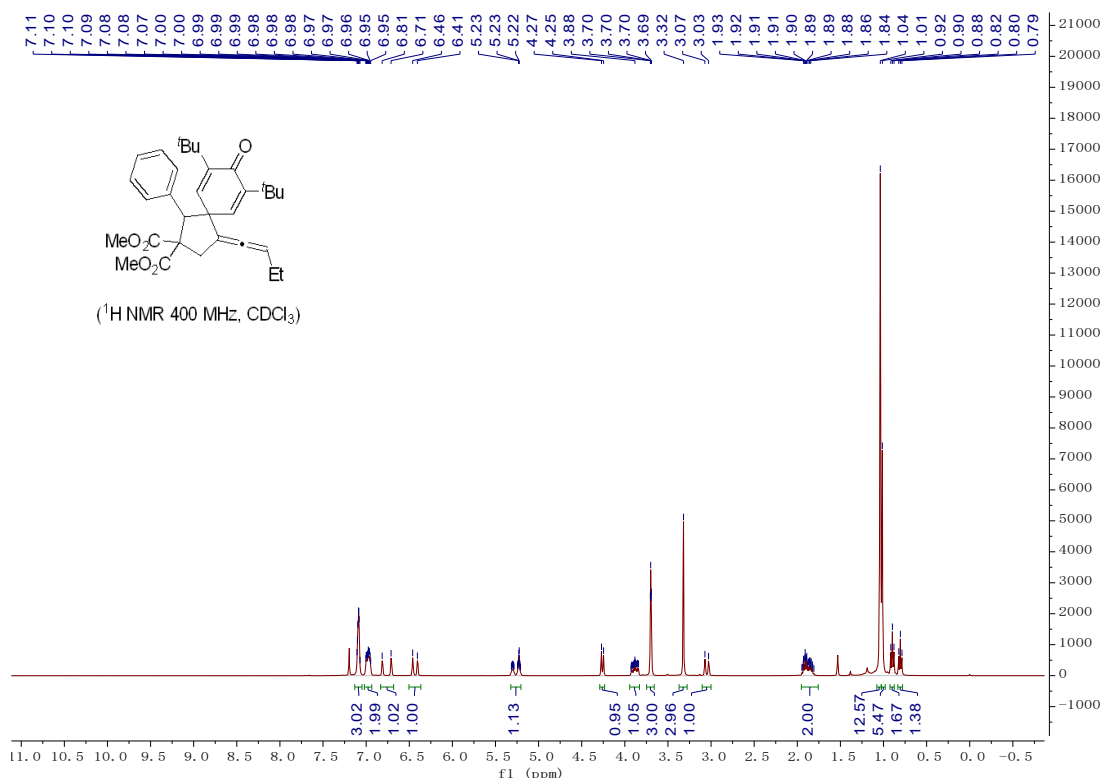


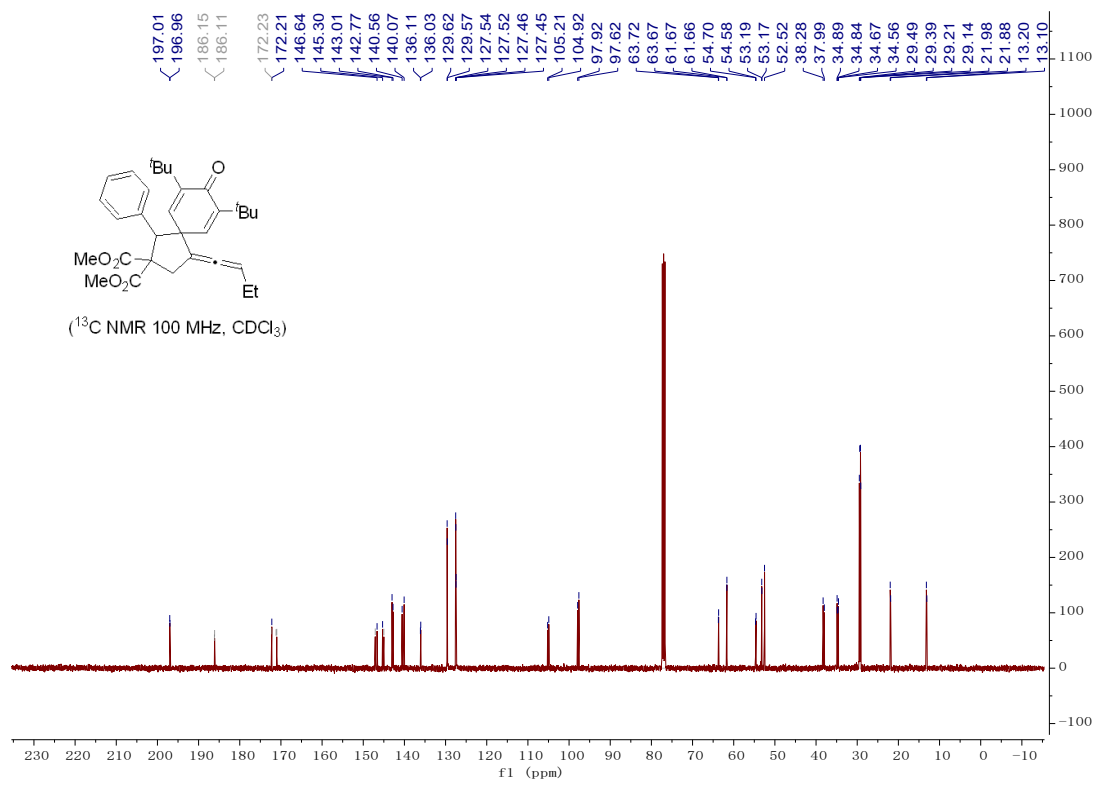
diethyl 7,9-di-tert-butyl-1-(naphthalen-1-yl)-8-oxo-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3u): Yield: 0.0460 g, 83%, a colorless solid, m.p. 165-167 °C; Eluent: PE/EA = 30/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 8.11 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.36 (m, 2H), 7.30 – 7.25 (m, 1H), 7.16 (d, *J* = 7.4 Hz, 1H), 6.80 – 6.71 (m, 1H), 6.41 – 6.33 (m, 1H), 5.44 (s, 1H), 4.85 – 4.74 (m, 2H), 4.30 – 4.21 (m, 2H), 4.14 – 4.05 (m, 1H), 3.93 – 3.80 (m, 1H), 3.74 – 3.62 (m, 1H), 3.33 (d, *J* = 16.8 Hz, 1H), 1.23 (t, *J* = 7.0 Hz, 3H), 1.04 (s, 9H), 0.74 (s, 9H), 0.58 (t, *J* = 7.0 Hz, 3H); ¹³C{¹H}-NMR (100 MHz, CDCl₃, TMS) δ 202.0, 185.6, 171.8, 170.1, 145.8, 145.2, 142.4, 140.1, 133.7, 133.2, 132.6, 128.7, 127.9, 126.2, 125.5, 125.4, 123.9, 123.6, 103.7, 78.9, 64.7, 62.3, 61.6, 54.0, 53.6, 38.3, 34.6, 34.5, 29.2, 28.9, 14.0, 13.3; IR (neat): ν 2956.13, 2918.47, 2865.03, 1962.28, 1731.30, 1659.24, 1638.37, 1458.75, 1259.48, 1200.44, 1158.69, 882.11, 781.50 cm⁻¹; HRMS (ESI-TOF) Calcd for C₃₆H₄₃O₅ [M+H]⁺ : 555.3105, found: 555.3103.

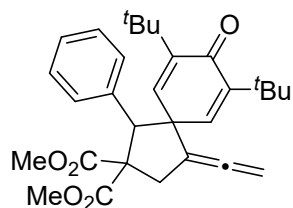




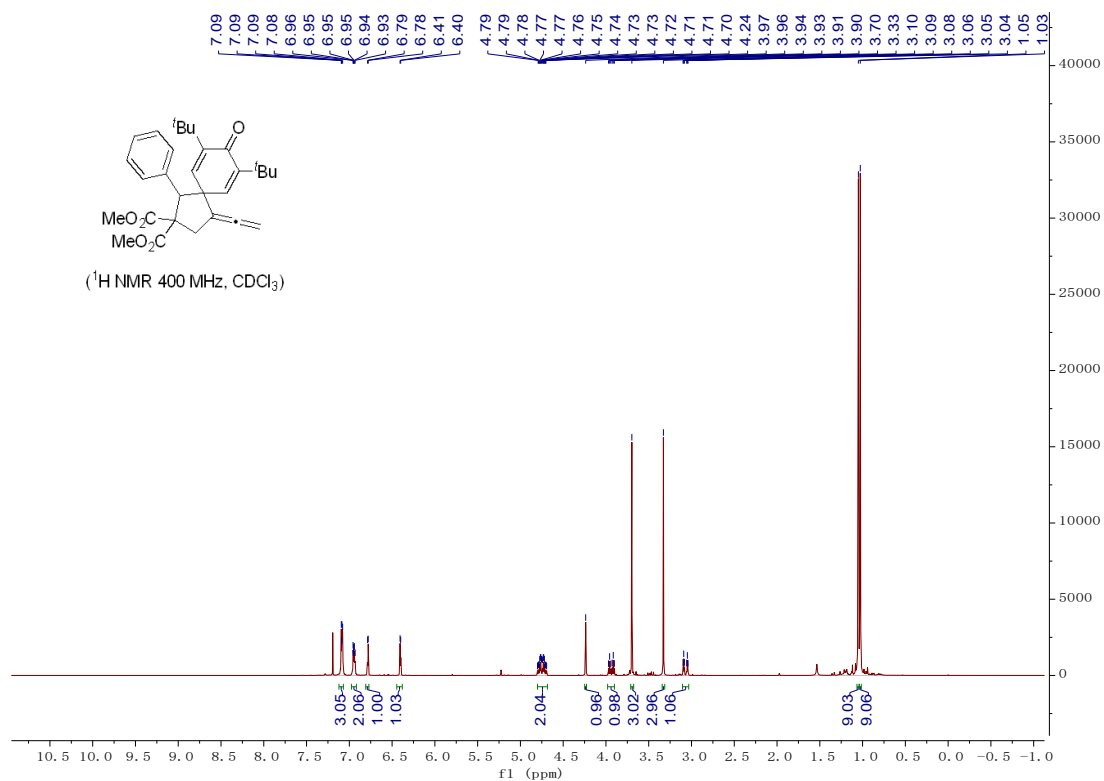
dimethyl 4-(but-1-en-1-ylidene)-7,9-di-*tert*-butyl-8-oxo-1-phenylspiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3v): Yield: 0.0151 g, 30%, dr = 2.3:1, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.13 – 7.05 (m, 3H), 7.02 – 6.93 (m, 2H), 6.83 – 6.68 (m, 1H), 6.50 – 6.38 (m, 1H), 5.32 – 5.21 (m, 1H), 4.29 – 4.23 (m, 1H), 3.94 – 3.83 (m, 1H), 3.75 – 3.66 (m, 3H), 3.32 (s, 3H), 3.05 (d, $J = 17.0$ Hz, 1H), 1.95 – 1.76 (m, 2H), 1.04 (s, 12.5H), 1.01 (s, 5.5H), 0.90 (t, $J = 7.4$ Hz, 1.7H), 0.80 (t, $J = 7.4$ Hz, 1.3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 197.01, 196.96, 186.15, 186.11, 172.23, 172.21, 171.18, 171.01, 147.08, 146.64, 145.30, 144.99, 143.01, 142.77, 140.56, 140.07, 136.11, 136.03, 129.62, 129.57, 127.54, 127.52, 127.46, 127.45, 105.21, 104.92, 97.92, 97.62, 63.72, 63.67, 61.67, 61.66, 54.70, 54.58, 53.19, 53.17, 52.52, 38.28, 37.99, 34.89, 34.84, 34.67, 34.56, 29.49, 29.39, 29.21, 29.14, 21.98, 21.88, 13.20, 13.10; IR (neat): ν 2954.53, 1970.11, 1729.64, 1685.31, 1636.79, 1455.76, 1434.40, 1253.22, 1201.20, 1163.19, 1030.84, 909.46, 878.22, 732.96 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{32}\text{H}_{41}\text{O}_5$ $[\text{M}+\text{H}]^+$: 505.2959, found: 505.2949.

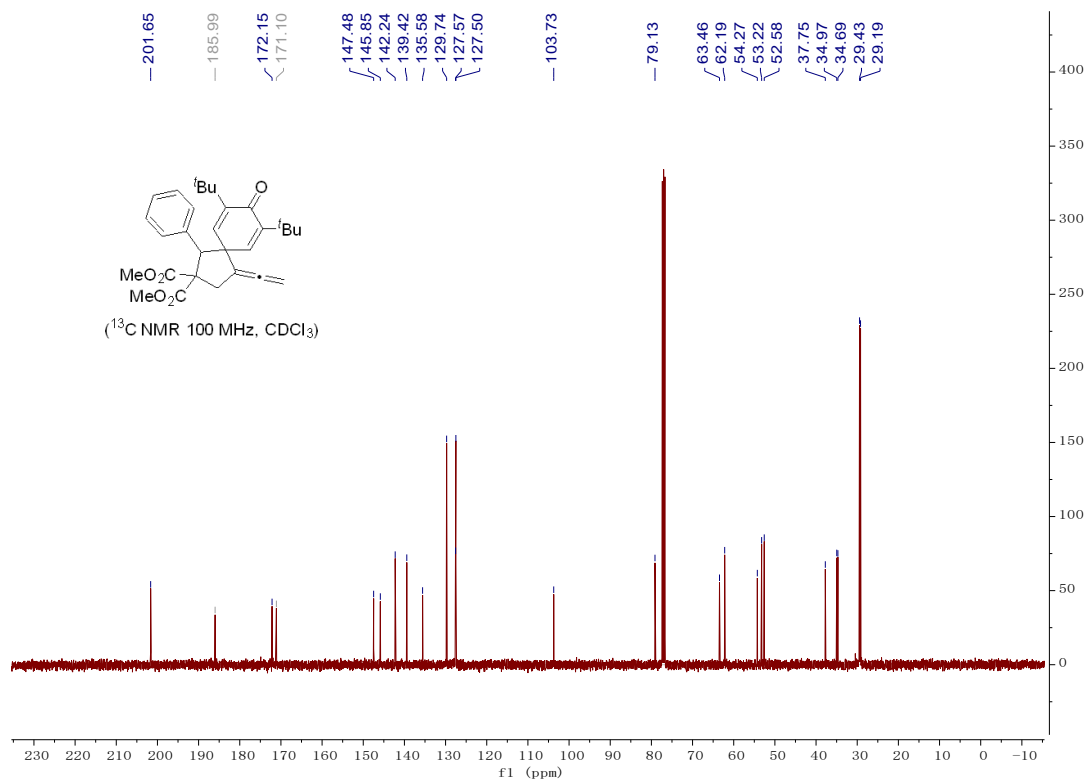


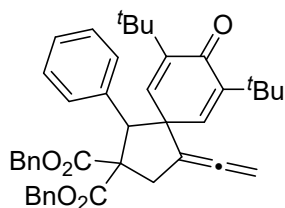




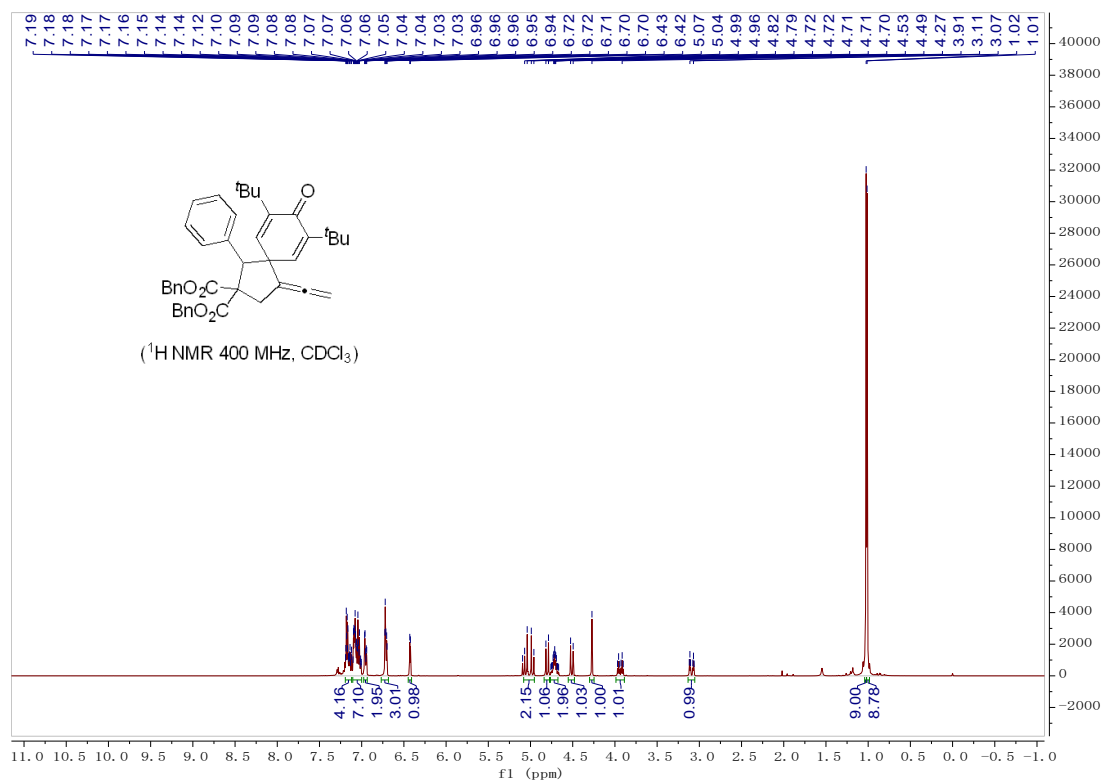
dimethyl 7,9-di-*tert*-butyl-8-oxo-1-phenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3w): Yield: 0.0301 g, 63%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.12 – 7.07 (m, 3H), 6.98 – 6.92 (m, 2H), 6.78 (d, $J = 3.0$ Hz, 1H), 6.40 (d, $J = 3.0$ Hz, 1H), 4.80 – 4.68 (m, 2H), 4.24 (s, 1H), 3.94 (dt, $J = 17.0, 5.2$ Hz, 1H), 3.70 (s, 3H), 3.33 (s, 3H), 3.07 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.05 (s, 9H), 1.03 (s, 9H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 186.0, 172.2, 171.1, 147.5, 145.8, 142.2, 139.4, 135.6, 129.7, 127.6, 127.5, 103.7, 79.1, 63.5, 62.2, 54.3, 53.2, 52.6, 37.8, 35.0, 34.7, 29.4, 29.2; IR (neat): ν 3003.40, 2954.39, 2862.51, 1959.72, 1728.95, 1713.95, 1659.38, 1637.21, 1455.76, 1357.94, 1254.89, 1219.27, 1165.25, 1088.97, 877.42 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{30}\text{H}_{37}\text{O}_5$ $[\text{M}+\text{H}]^+$: 477.2636, found: 477.2634.

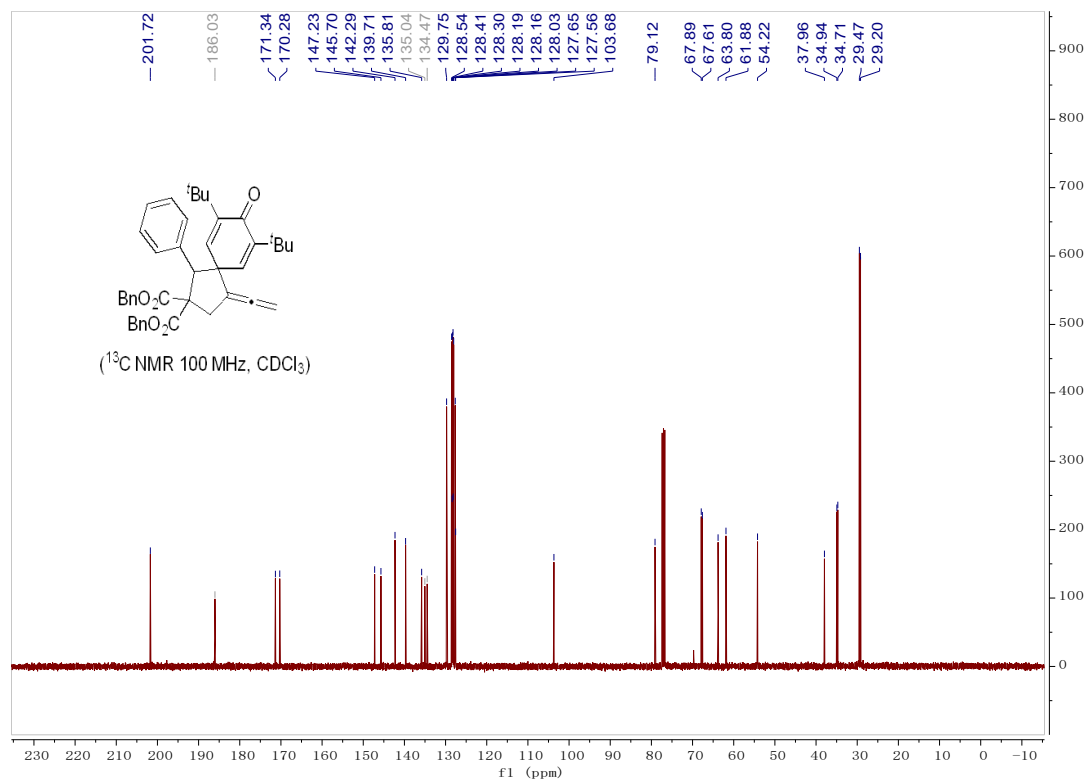


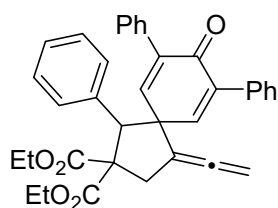




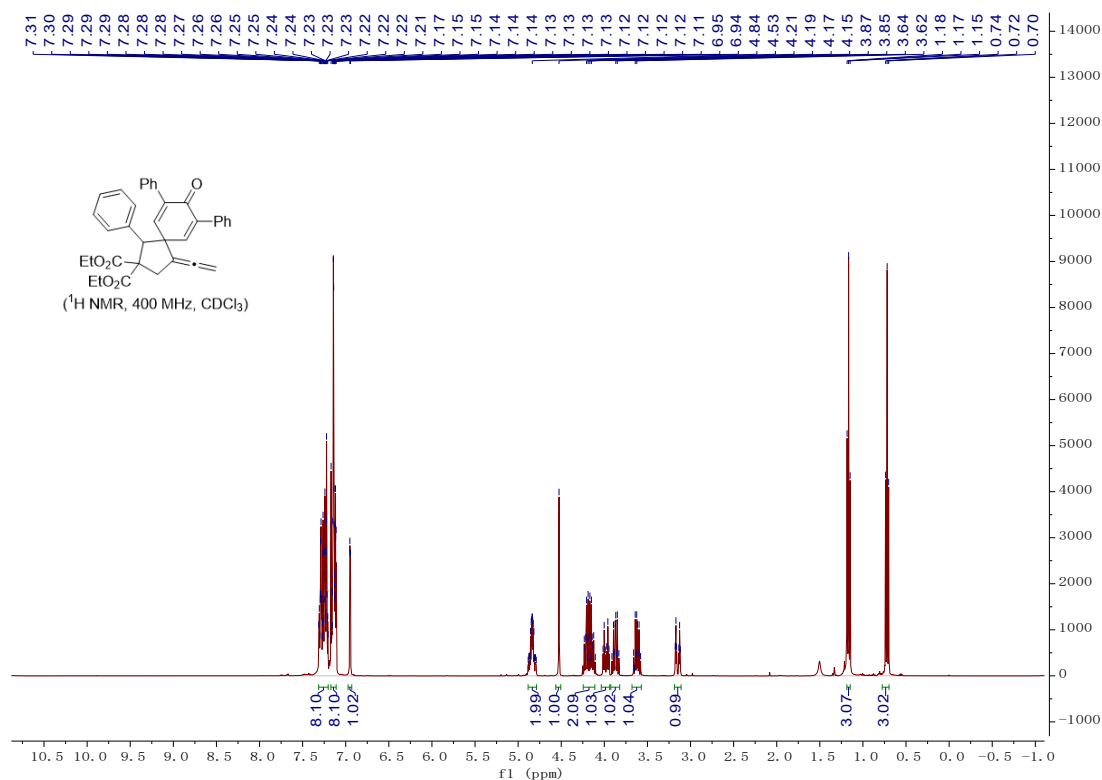
dibenzyl 7,9-di-*tert*-butyl-8-oxo-1-phenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3x): Yield: 0.0490 g, 78%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.19 – 7.12 (m, 4H), 7.11 – 7.00 (m, 7H), 6.98 – 6.93 (m, 2H), 6.77 – 6.68 (m, 3H), 6.43 (d, $J = 3.0$ Hz, 1H), 5.08 – 4.95 (m, 2H), 4.80 (d, $J = 12.4$ Hz, 1H), 4.76 – 4.67 (m, 2H), 4.51 (d, $J = 12.4$ Hz, 1H), 4.27 (s, 1H), 3.94 (dt, $J = 17.0, 5.2$ Hz, 1H), 3.09 (dt, $J = 17.0, 3.0$ Hz, 1H), 1.02 (s, 9H), 1.01 (s, 9H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.7, 186.0, 171.3, 170.3, 147.2, 145.7, 142.3, 139.7, 135.8, 135.0, 134.5, 129.8, 128.5, 128.4, 128.3, 128.19, 128.16, 128.0, 127.65, 127.56, 103.7, 79.1, 67.9, 67.6, 63.8, 61.9, 54.2, 38.0, 34.9, 34.7, 29.5, 29.2; IR (neat): ν 3003.40, 2959.05, 2865.11, 1962.33, 1711.81, 1659.34, 1358.94, 1220.12, 1163.54, 1131.12, 1090.95, 907.46, 868.96 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{42}\text{H}_{45}\text{O}_5$ $[\text{M}+\text{H}]^+$: 629.3262, found: 629.3265.

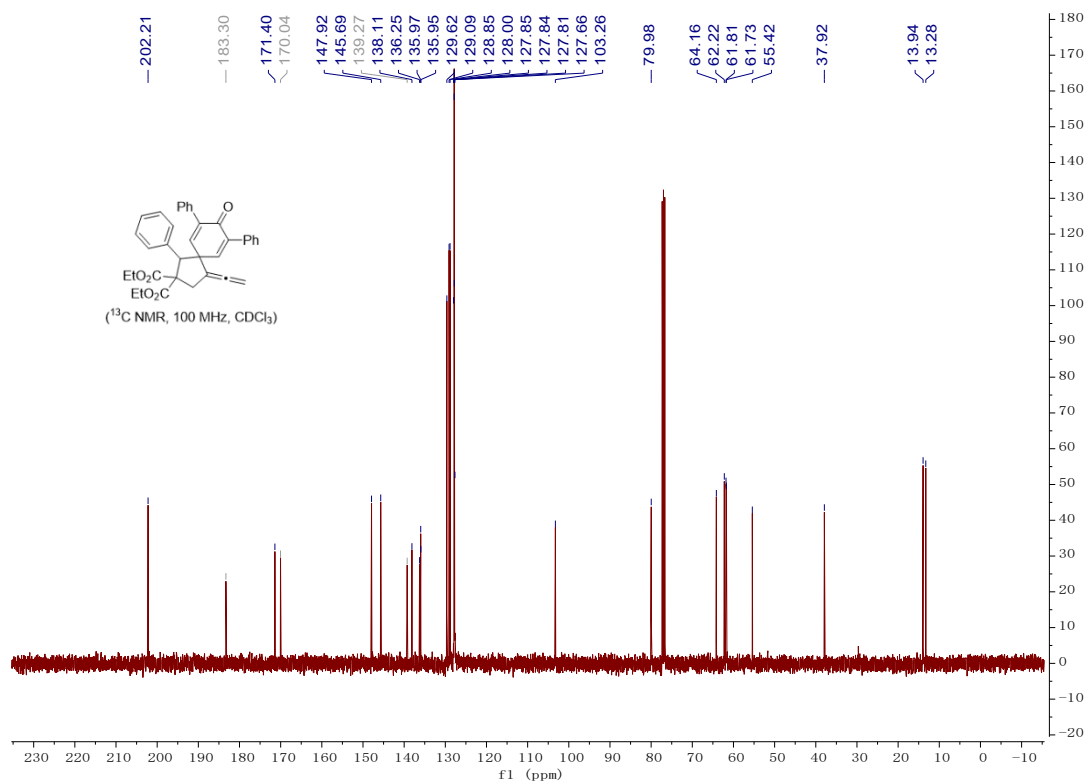


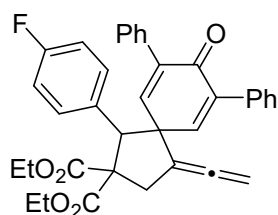




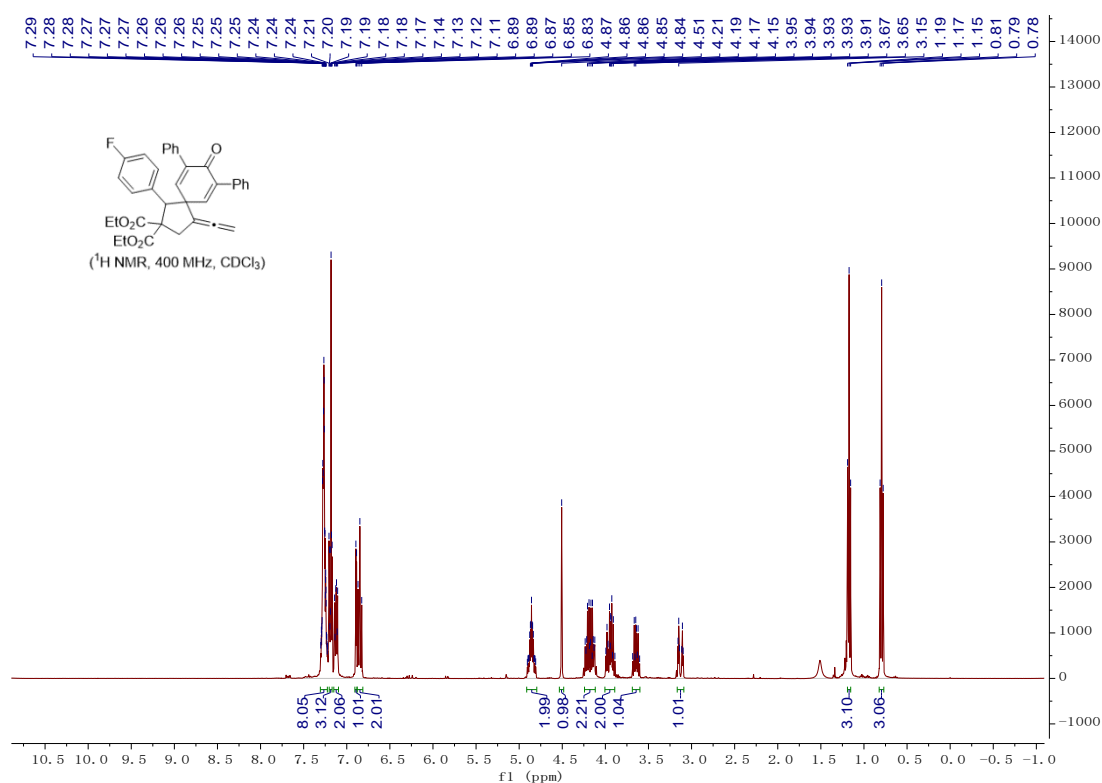
diethyl 8-oxo-1,7,9-triphenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3y): Yield: 0.0392 g, 72%, a yellow oil; Eluent: PE/EA = 10/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.31 – 7.20 (m, 8H), 7.17 – 7.11 (m, 8H), 6.95 (d, $J = 3.2$ Hz, 1H), 4.88 – 4.79 (m, 2H), 4.53 (s, 1H), 4.25 – 4.11 (m, 2H), 3.98 (dt, $J = 17.0, 5.2$ Hz, 1H), 3.87 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.62 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.15 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.17 (t, $J = 7.2$ Hz, 3H), 0.72 (t, $J = 7.2$ Hz, 3H); ^{13}C $\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 202.2, 183.3, 171.4, 170.0, 147.9, 145.7, 139.3, 138.1, 136.3, 135.97, 135.95, 129.6, 129.1, 128.9, 128.0, 127.85, 127.84, 127.81, 127.7, 103.3, 80.0, 64.2, 62.2, 61.8, 61.7, 55.4, 37.9, 14.0, 13.3; IR (neat): ν 3055.50, 2979.92, 2927.65, 1962.28, 1723.67, 1659.37, 1495.37, 1259.67, 1206.13, 909.52, 859.10, 696.30 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{36}\text{H}_{33}\text{O}_5$ $[\text{M}+\text{H}]^+$: 545.2323, found: 545.2321.

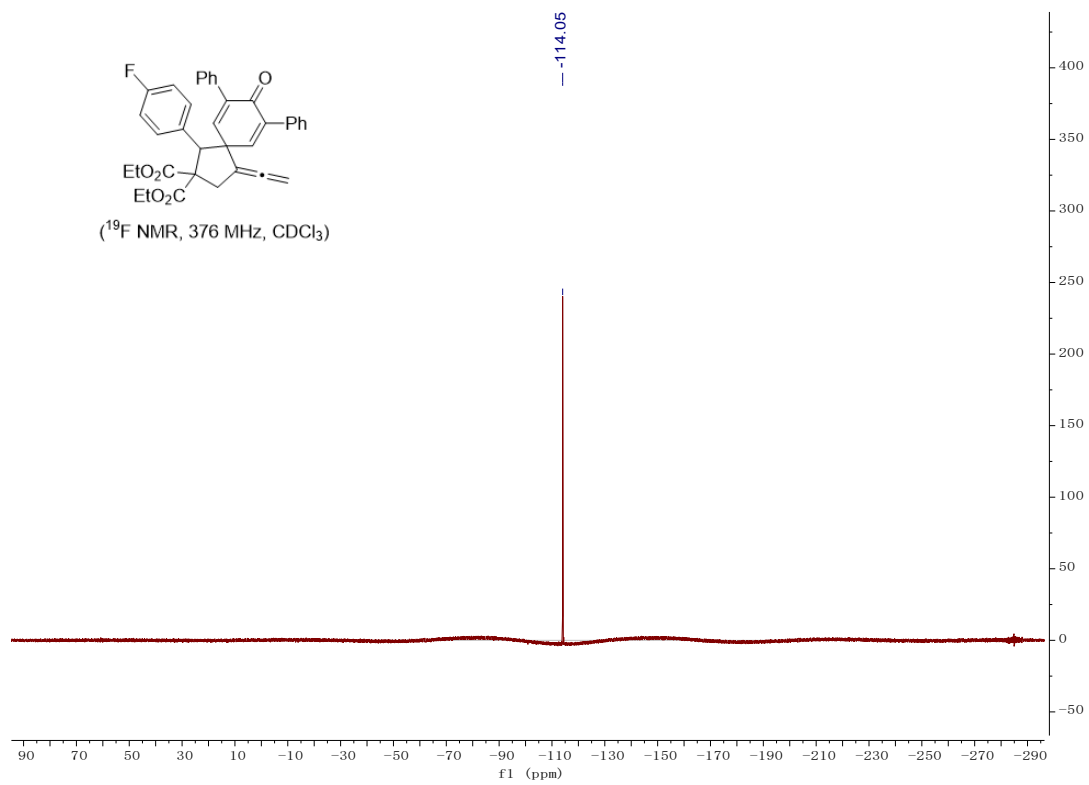
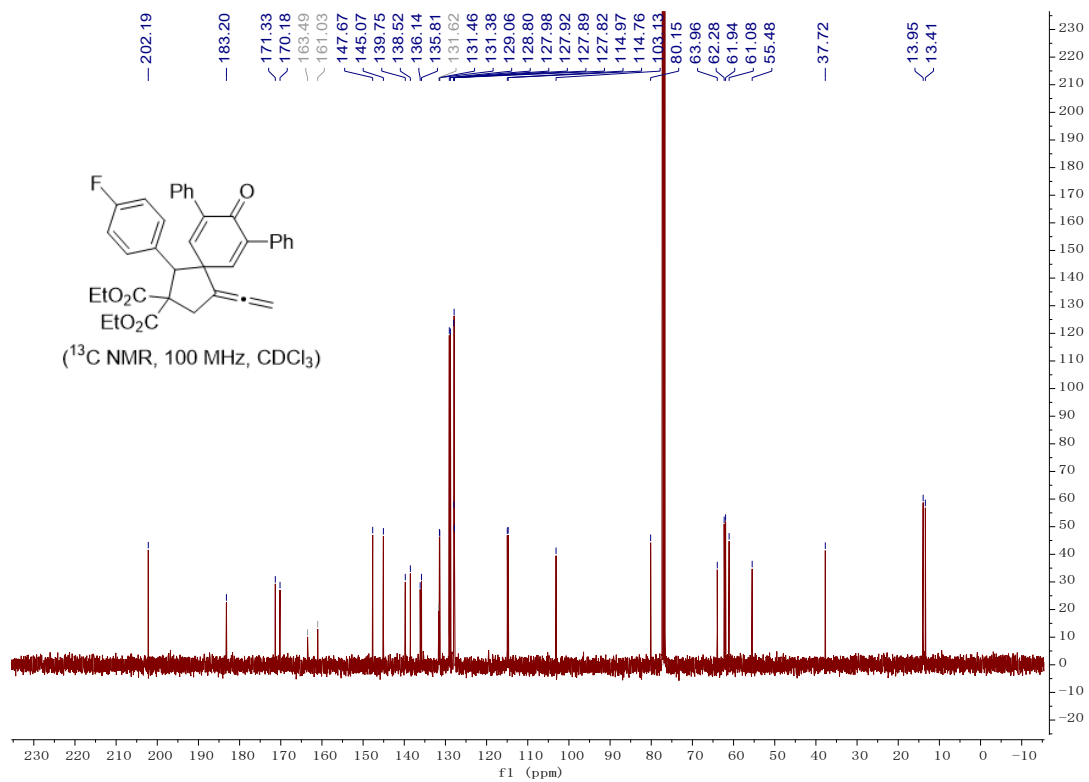


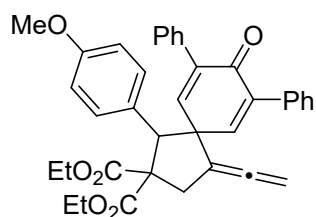




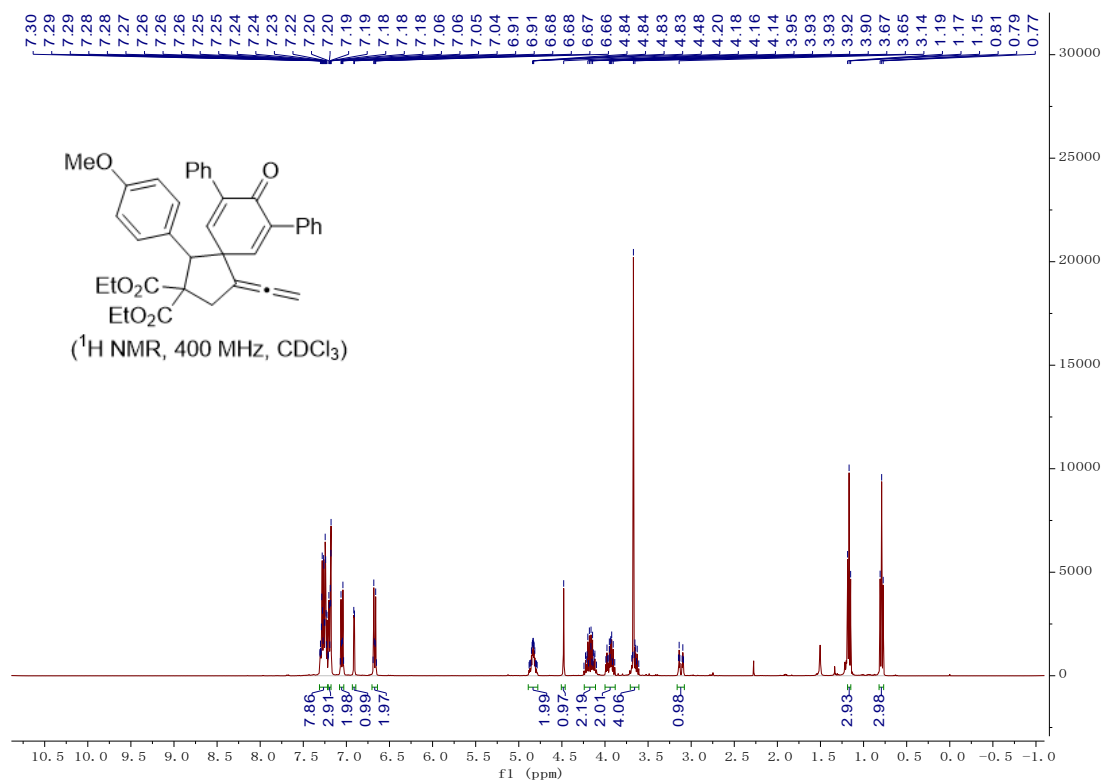
diethyl 8-oxo-1,7,9-triphenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3z): Yield: 0.0298 g, 53%, a yellow solid, m.p. 170-172 °C; Eluent: PE/EA = 10/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.31 – 7.23 (m, 8H), 7.20 – 7.17 (m, 3H), 7.15 – 7.10 (m, 2H), 6.89 (d, *J* = 3.2 Hz, 1H), 6.85 (t, *J* = 8.6 Hz, 2H), 4.91 – 4.80 (m, 2H), 4.51 (s, 1H), 4.24 – 4.12 (m, 2H), 4.01 – 3.89 (m, 2H), 3.64 (dq, *J* = 10.8, 7.2 Hz, 1H), 3.13 (dt, *J* = 17.2, 3.2 Hz, 1H), 1.17 (t, *J* = 7.2 Hz, 3H), 0.79 (t, *J* = 7.2 Hz, 3H); ¹³C {¹H}-NMR (100 MHz, CDCl₃, TMS) δ 202.2, 183.2, 171.3, 170.2, 162.3 (d, *J* = 246.0 Hz), 147.7, 145.1, 139.8, 138.5, 136.1, 135.8, 131.6 (d, *J* = 3.0 Hz), 131.4 (d, *J* = 7.2 Hz), 129.1, 128.8, 127.98, 127.92, 127.89, 127.8, 114.90 (d, *J* = 21.0 Hz), 103.1, 80.2, 64.0, 62.3, 61.9, 61.1, 55.5, 37.7, 14.0, 13.4; ¹⁹F NMR (376 MHz, CDCl₃) δ -114.05; IR (neat): ν 2979.84, 2922.52, 1959.72, 1724.65, 1660.08, 1636.14, 1510.18, 1262.18, 1226.07, 1162.33, 1017.79, 697.87 cm⁻¹; HRMS (ESI-TOF) Calcd for C₃₆H₃₂O₅F [M+H]⁺ : 563.2228, found: 563.2227.

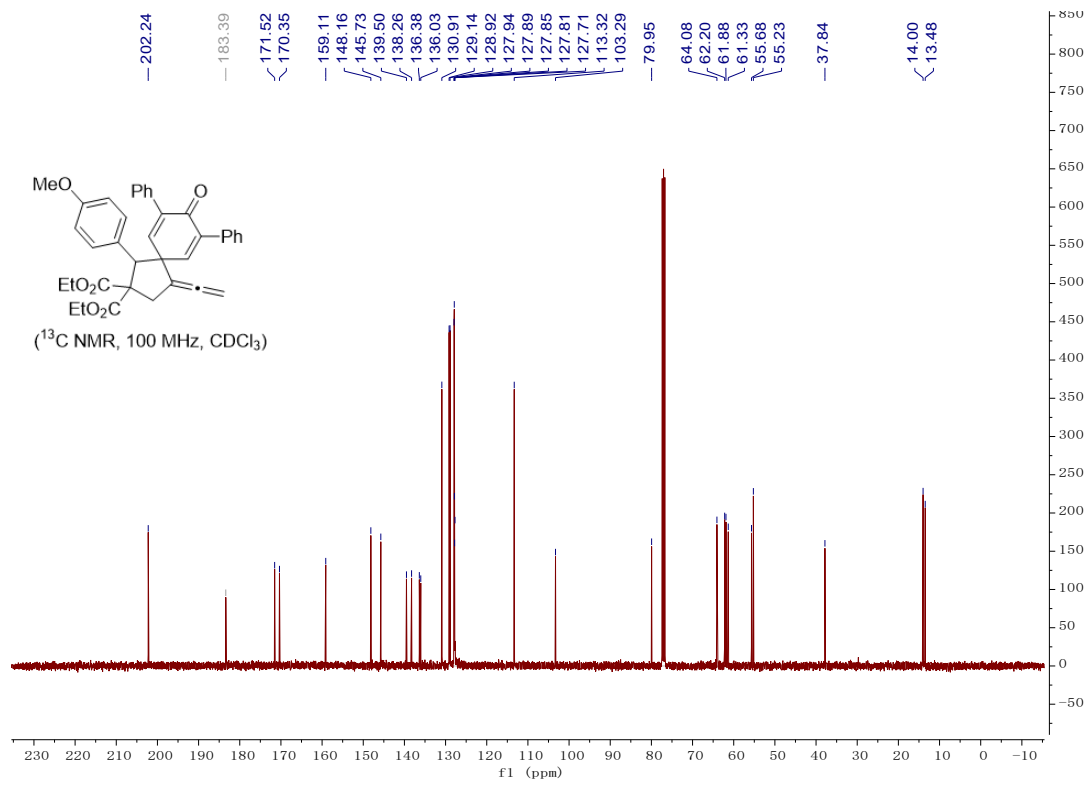


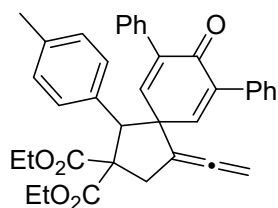




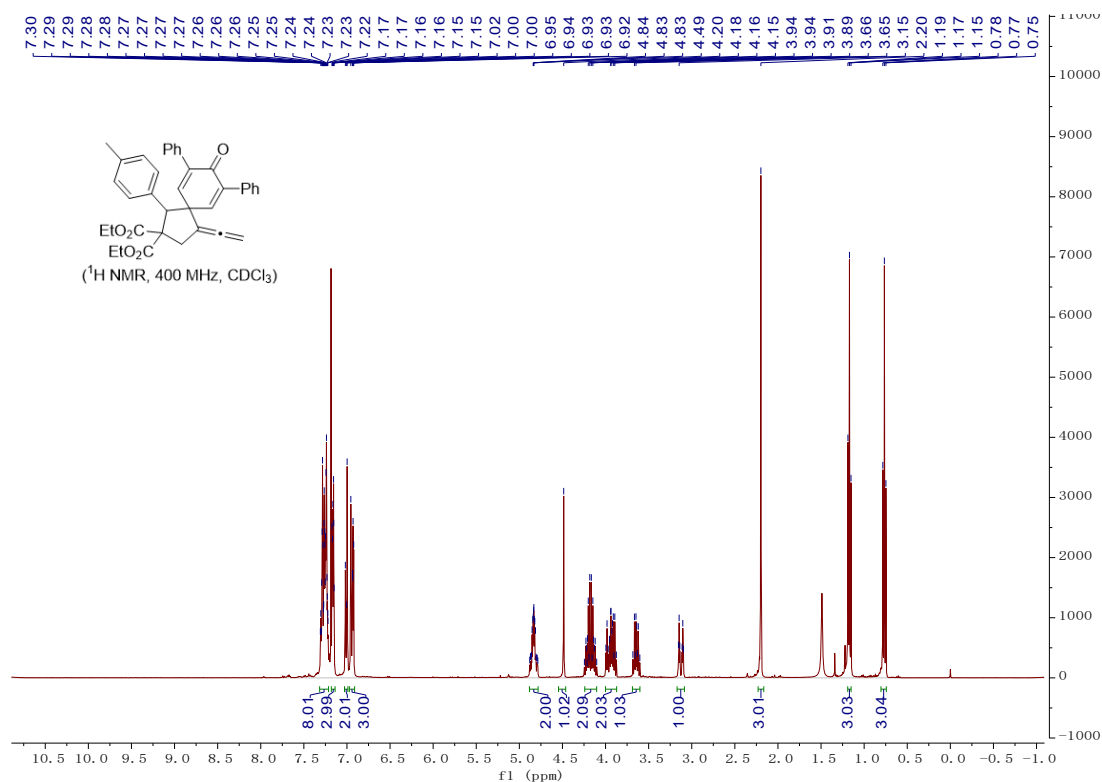
diethyl 1-(4-methoxyphenyl)-8-oxo-7,9-diphenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3aa): Yield: 0.0390 g, 68%, a yellow oil; Eluent: PE/EA = 10/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.31 – 7.22 (m, 8H), 7.21 – 7.18 (m, 3H), 7.08 – 7.03 (m, 2H), 6.91 (d, $J = 3.2$ Hz, 1H), 6.70 – 6.64 (m, 2H), 4.89 – 4.78 (m, 2H), 4.48 (s, 1H), 4.24 – 4.11 (m, 2H), 4.00 – 3.88 (m, 2H), 3.71 – 3.61 (m, 4H), 3.12 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.16 (t, $J = 7.2$ Hz, 3H), 0.79 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 202.2, 183.4, 171.5, 170.4, 159.1, 148.2, 145.7, 139.5, 138.3, 136.4, 136.0, 130.9, 129.1, 128.9, 127.9, 128.0, 127.9, 127.8, 127.7, 113.3, 103.3, 80.0, 64.1, 62.2, 61.9, 61.3, 55.7, 55.2, 37.8, 14.0, 13.5; IR (neat): ν 3058.11, 2982.53, 2927.65, 2831.12, 1957.06, 1722.81, 1659.26, 1637.71, 1514.10, 1251.85, 1206.41, 1180.90, 727.44, 696.72 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{37}\text{H}_{35}\text{O}_6$ $[\text{M}+\text{H}]^+$: 575.2428, found: 575.2424.

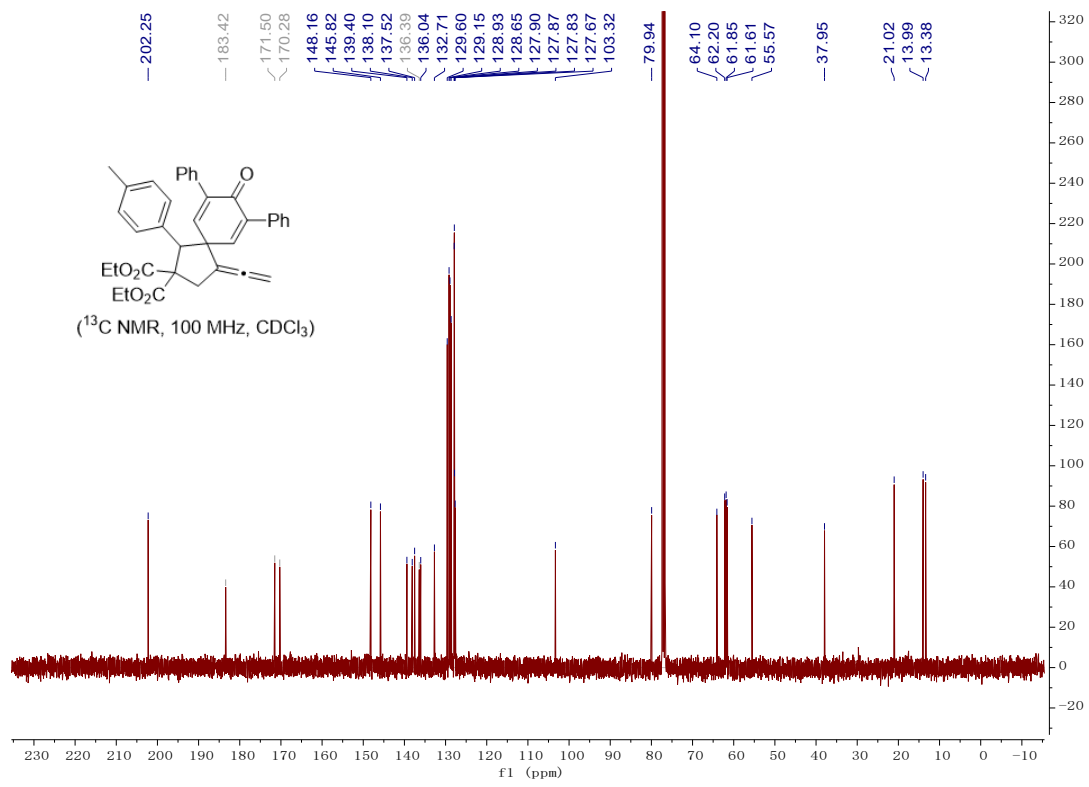


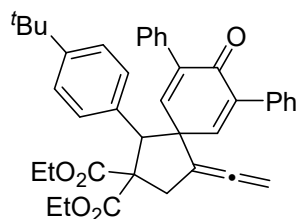




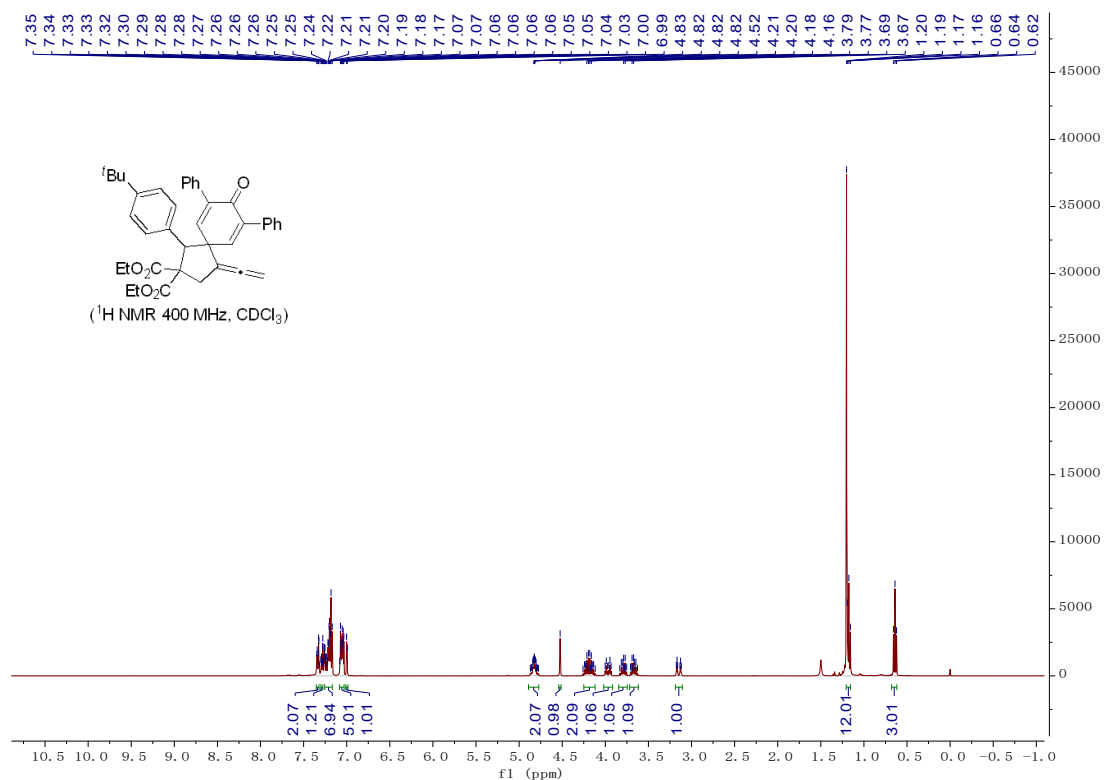
diethyl 8-oxo-7,9-diphenyl-1-(p-tolyl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3ab): Yield: 0.0262 g, 47%, a yellow solid, m.p. 126-128 °C; Eluent: PE/EA = 10/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.32 – 7.21 (m, 8H), 7.18 – 7.14 (m, 3H), 7.03 – 6.99 (m, 2H), 6.97 – 6.91 (m, 3H), 4.88 – 4.78 (m, 2H), 4.49 (s, 1H), 4.24 – 4.10 (m, 2H), 4.00 – 3.87 (m, 2H), 3.64 (dq, *J* = 10.8, 7.2 Hz, 1H), 3.13 (dt, *J* = 17.0, 3.2 Hz, 1H), 2.20 (s, 3H), 1.17 (t, *J* = 7.2 Hz, 3H), 0.77 (t, *J* = 7.2 Hz, 3H); ¹³C {¹H}-NMR (100 MHz, CDCl₃, TMS) δ 202.3, 183.4, 171.5, 170.3, 148.2, 145.8, 139.4, 138.1, 137.5, 136.4, 136.0, 132.7, 129.6, 129.2, 128.9, 128.7, 127.9, 127.9, 127.8, 127.7, 103.3, 79.9, 64.1, 62.2, 61.9, 61.6, 55.6, 38.0, 21.0, 14.0, 13.4; IR (neat): ν 3058.11, 2979.92, 2919.83, 1962.28, 1723.08, 1659.52, 1638.16, 1455.28, 1364.21, 1259.00, 1219.79, 793.40, 697.14 cm⁻¹; HRMS (ESI-TOF) Calcd for C₃₇H₃₅O₅ [M+H]⁺ : 559.2479, found: 559.2478.

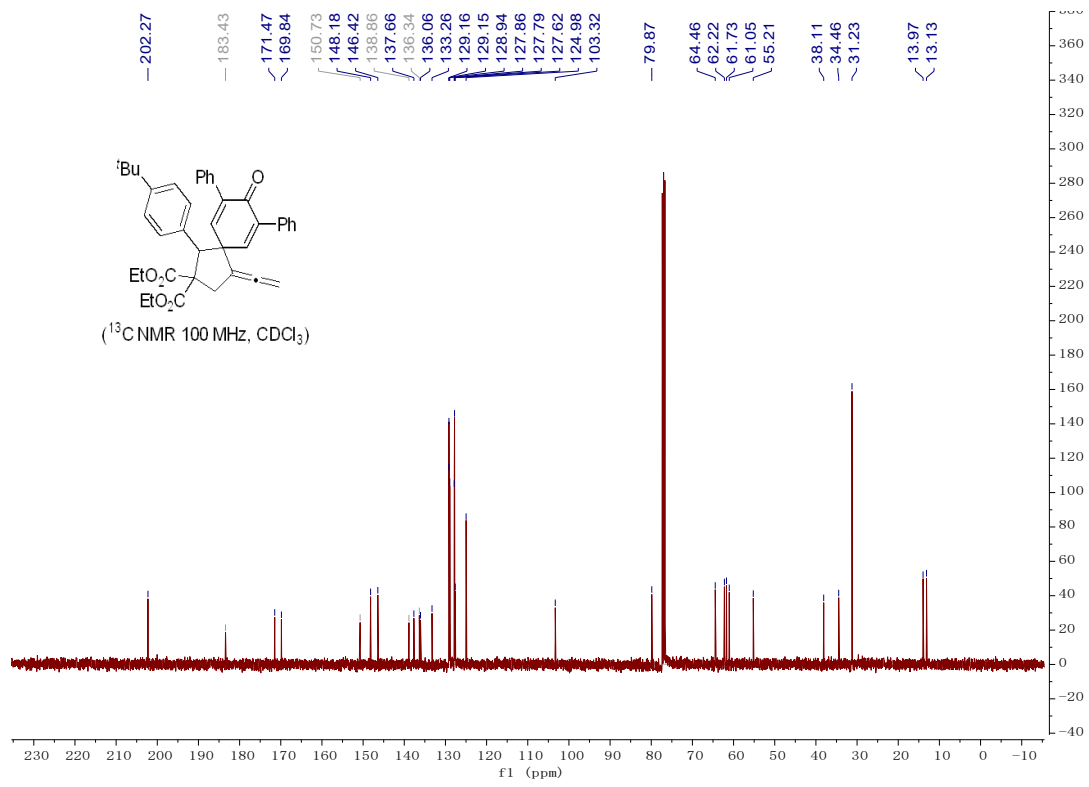


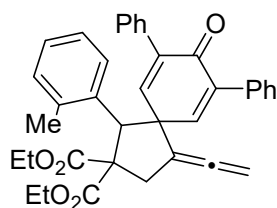




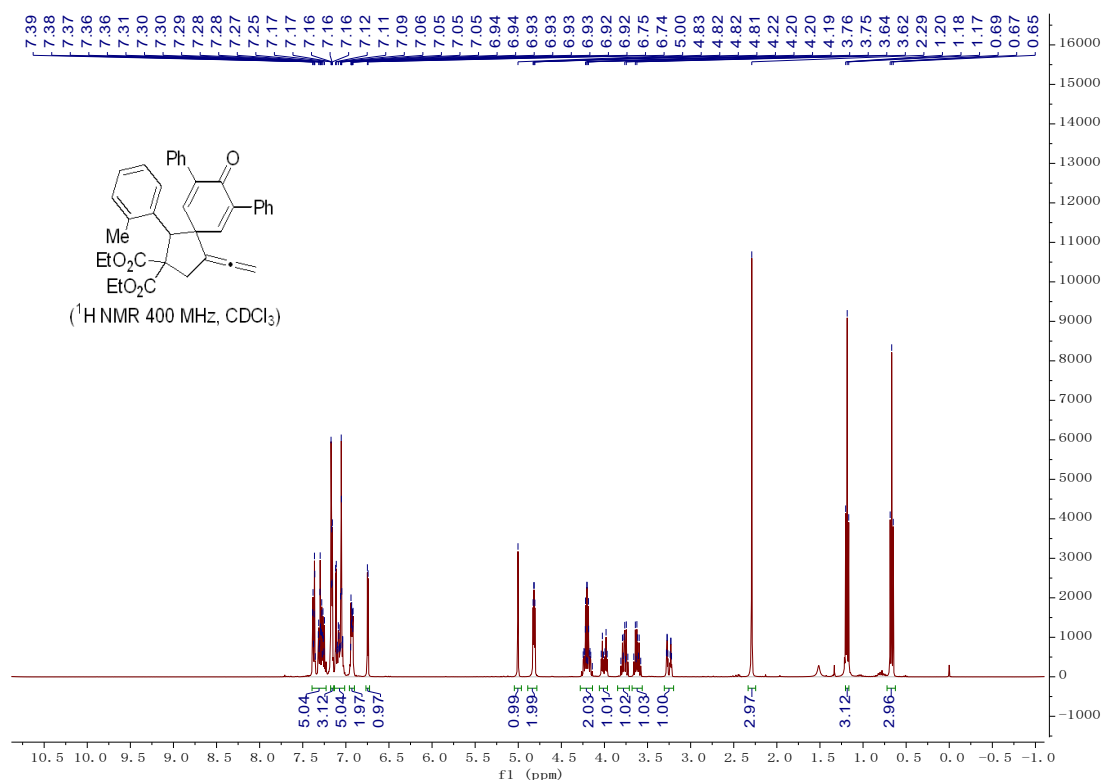
diethyl 1-(4-(*tert*-butyl)phenyl)-8-oxo-7,9-diphenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3ac): Yield: 0.0390 g, 65%, a yellow oil; Eluent: PE/EA = 10/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.35 – 7.17 (m, 10H), 7.08 – 7.03 (m, 5H), 7.00 (d, $J = 3.2$ Hz, 1H), 4.89 – 4.77 (m, 2H), 4.52 (s, 1H), 4.25 – 4.12 (m, 2H), 3.97 (dt, $J = 17.0, 5.2$ Hz, 1H), 3.84 – 3.75 (m, 1H), 3.72 – 3.62 (m, 1H), 3.15 (dt, $J = 17.0, 3.0$ Hz, 1H), 1.21 – 1.16 (m, 12H), 0.64 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 202.3, 183.4, 171.5, 169.8, 150.7, 148.2, 146.4, 138.9, 137.7, 136.3, 136.1, 133.3, 129.2, 129.1, 128.9, 127.9, 127.8, 127.6, 125.0, 103.3, 79.9, 64.5, 62.2, 61.7, 61.1, 55.2, 38.1, 34.5, 31.2, 14.0, 13.1; IR (neat): ν 3058.11, 2979.92, 2919.83, 1962.28, 1723.08, 1659.52, 1638.16, 1455.28, 1364.21, 1259.00, 1219.79, 793.40, 697.14 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{40}\text{H}_{41}\text{O}_5$ $[\text{M}+\text{H}]^+$: 601.2949, found: 601.2947.

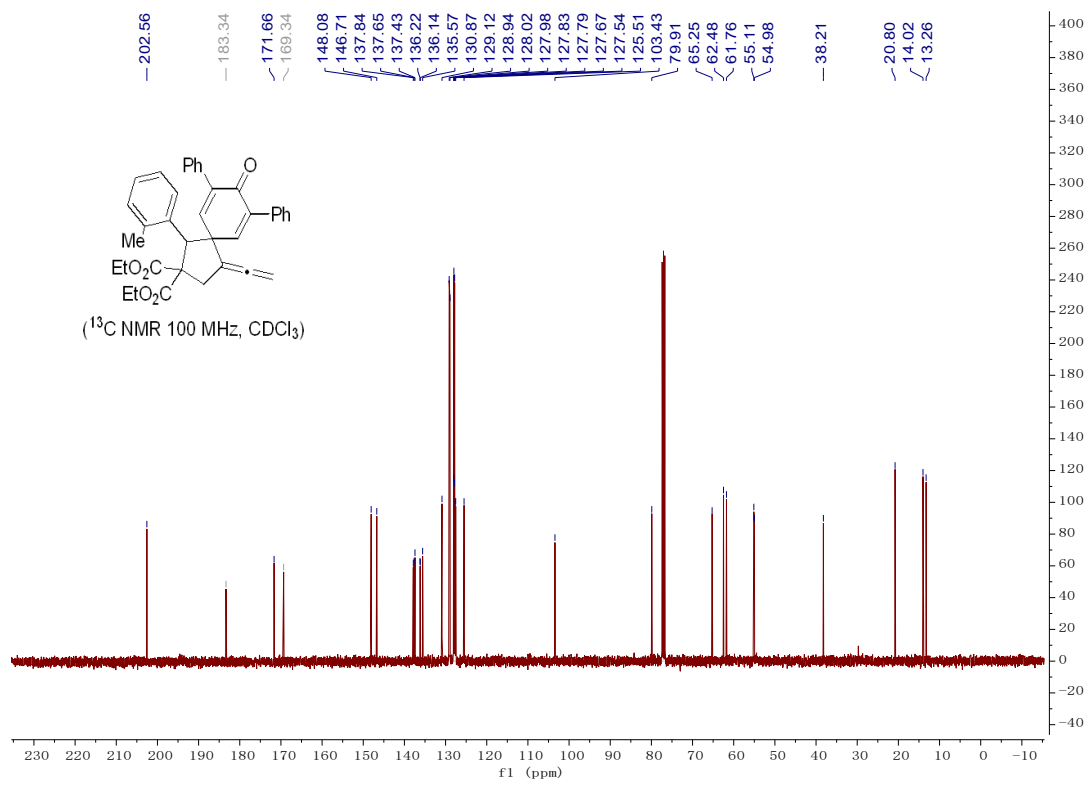


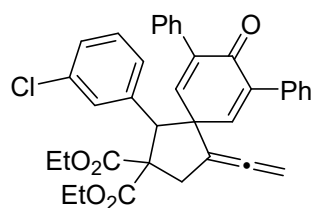




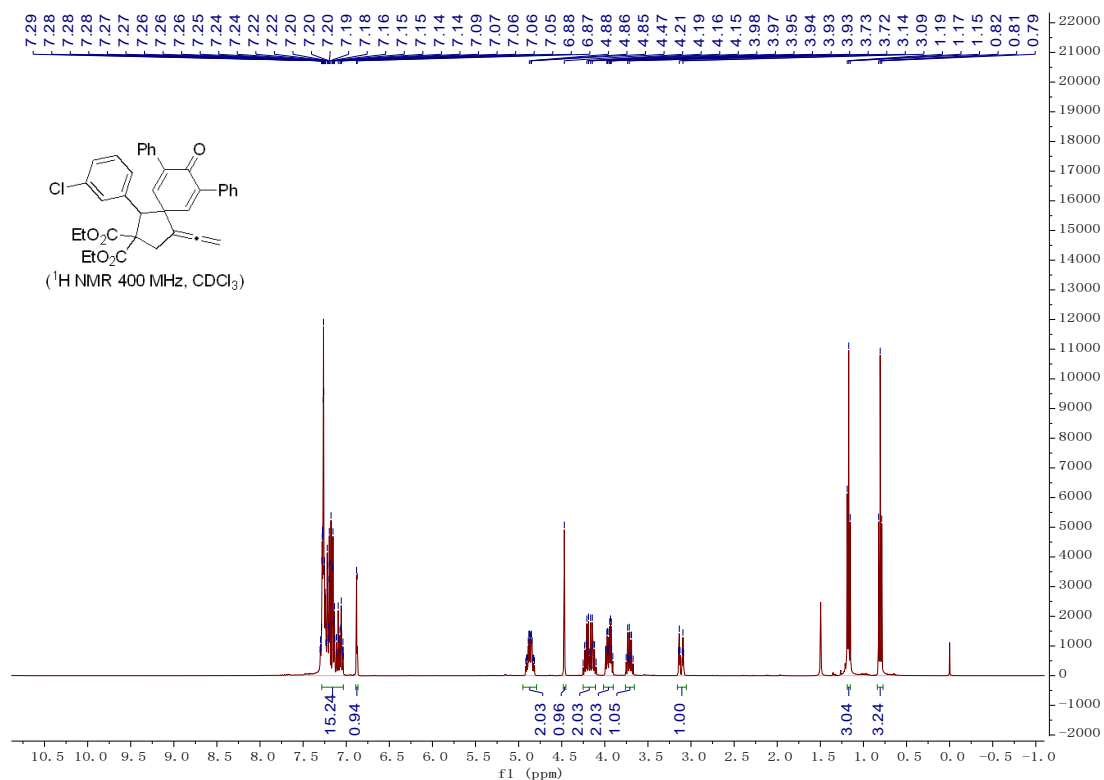
diethyl 8-oxo-7,9-diphenyl-1-(o-tolyl)-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3ad): Yield: 0.0390 g, 76%, a yellow solid, m.p. 147-149 °C; Eluent: PE/EA = 10/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.39 – 7.23 (m, 5H), 7.18 – 7.14 (m, 3H), 7.13 – 7.01 (m, 5H), 6.96 – 6.90 (m, 2H), 6.75 (d, $J = 3.2$ Hz, 1H), 5.00 (s, 1H), 4.82 (dd, $J = 5.0, 3.2$ Hz, 2H), 4.28 – 4.14 (m, 2H), 4.00 (dt, $J = 17.2, 5.0$ Hz, 1H), 3.77 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.62 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.31 – 3.20 (m, 1H), 2.29 (s, 3H), 1.18 (t, $J = 7.2$ Hz, 3H), 0.67 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 202.6, 183.3, 171.7, 169.3, 148.1, 146.7, 137.8, 137.6, 137.4, 136.2, 136.1, 135.6, 130.9, 129.1, 128.9, 128.02, 127.98, 127.83, 127.79, 127.7, 127.5, 125.5, 103.4, 79.9, 65.3, 62.5, 61.8, 55.1, 55.0, 38.2, 20.8, 14.0, 13.3; IR (neat): ν 3024.19, 2979.84, 2930.34, 1959.67, 1728.21, 1659.42, 1638.38, 1493.91, 1445.36, 1367.43, 1256.40, 1118.03, 861.45, 697.28 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{37}\text{H}_{35}\text{O}_5$ $[\text{M}+\text{H}]^+$: 559.2479, found: 559.2477.

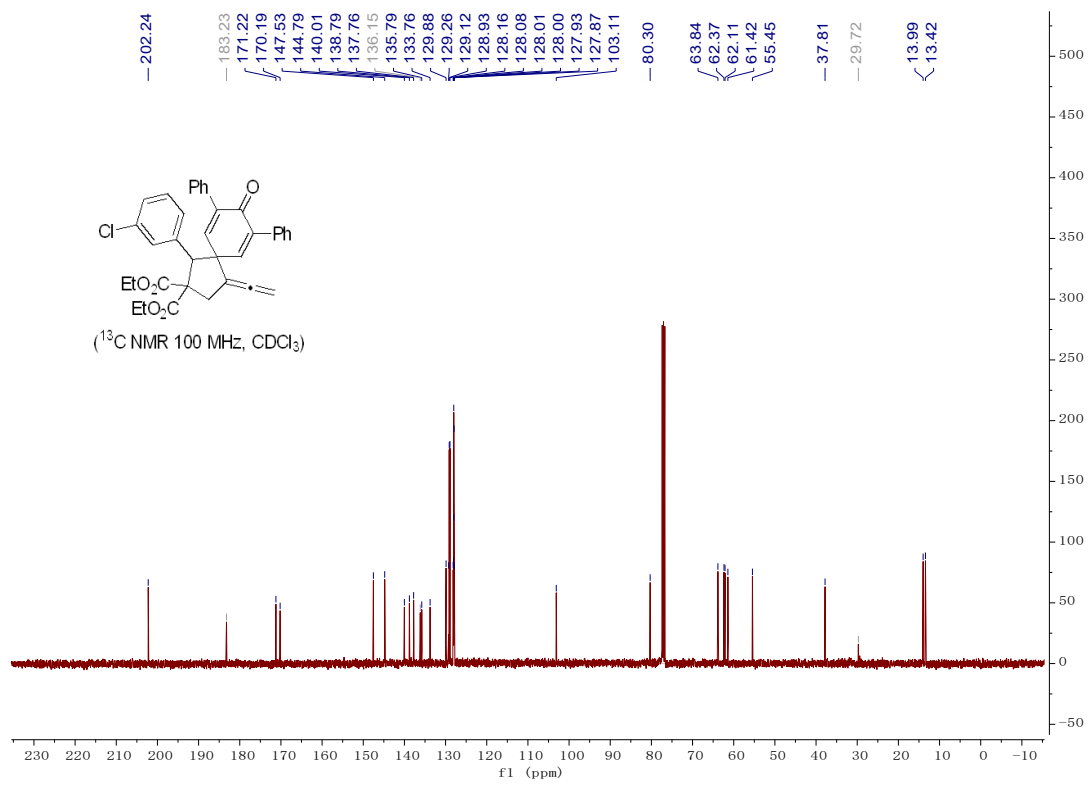


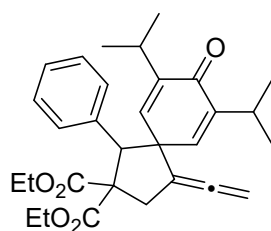




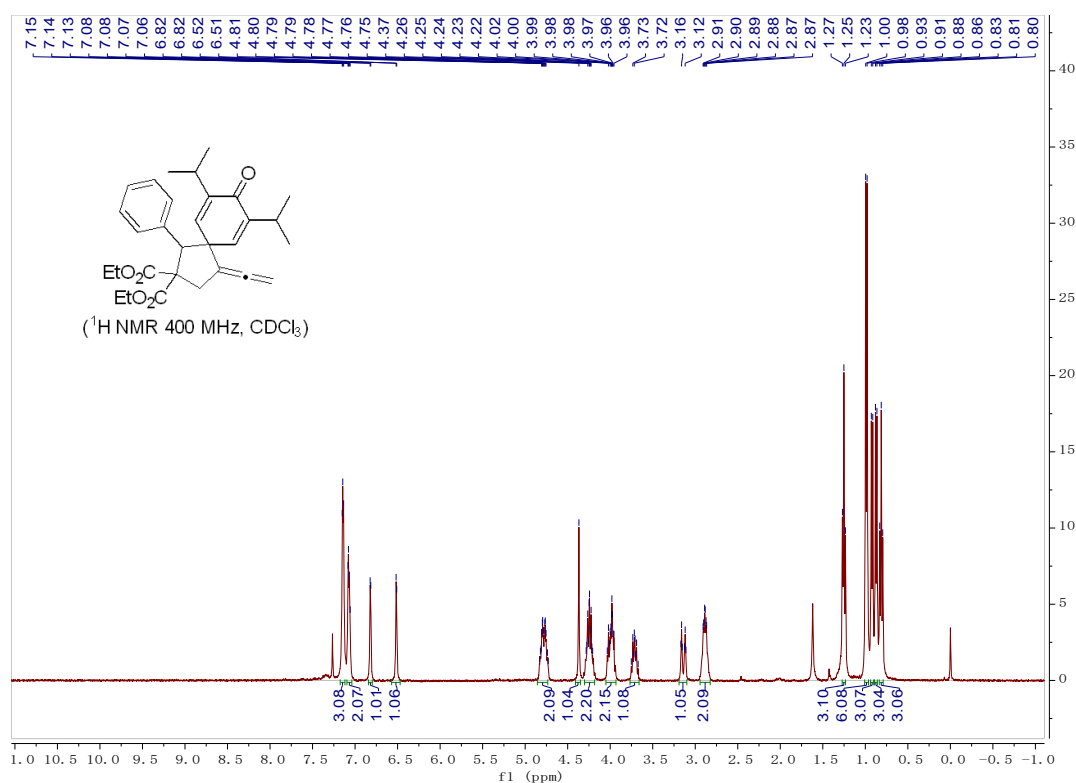
diethyl 1-(3-chlorophenyl)-8-oxo-7,9-diphenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3ae): Yield: 0.0393 g, 68%, a yellow solid, m.p. 143-145 °C; Eluent: PE/EA = 10/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.28 – 7.04 (m, 15H), 6.88 (d, $J = 3.2$ Hz, 1H), 4.96 – 4.78 (m, 2H), 4.47 (s, 1H), 4.27 – 4.09 (m, 2H), 4.02 – 3.88 (m, 2H), 3.71 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.12 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.18 (d, $J = 7.2$ Hz, 3H), 0.81 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 202.2, 183.2, 171.2, 170.2, 147.5, 144.8, 140.0, 138.8, 137.8, 136.2, 135.8, 133.8, 129.9, 129.3, 129.1, 128.9, 128.2, 128.1, 128.01, 128.00, 127.93, 127.87, 103.1, 80.3, 63.8, 62.4, 62.1, 61.4, 55.5, 37.8, 14.0, 13.4; IR (neat): ν 3052.89, 2982.53, 2927.65, 1957.11, 1723.45, 1659.96, 1638.91, 1568.34, 1262.24, 1219.53, 1113.19, 1012.57, 858.78, 696.57 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{36}\text{H}_{32}\text{ClO}_5$ $[\text{M}+\text{H}]^+$: 579.1933, found: 579.1930.

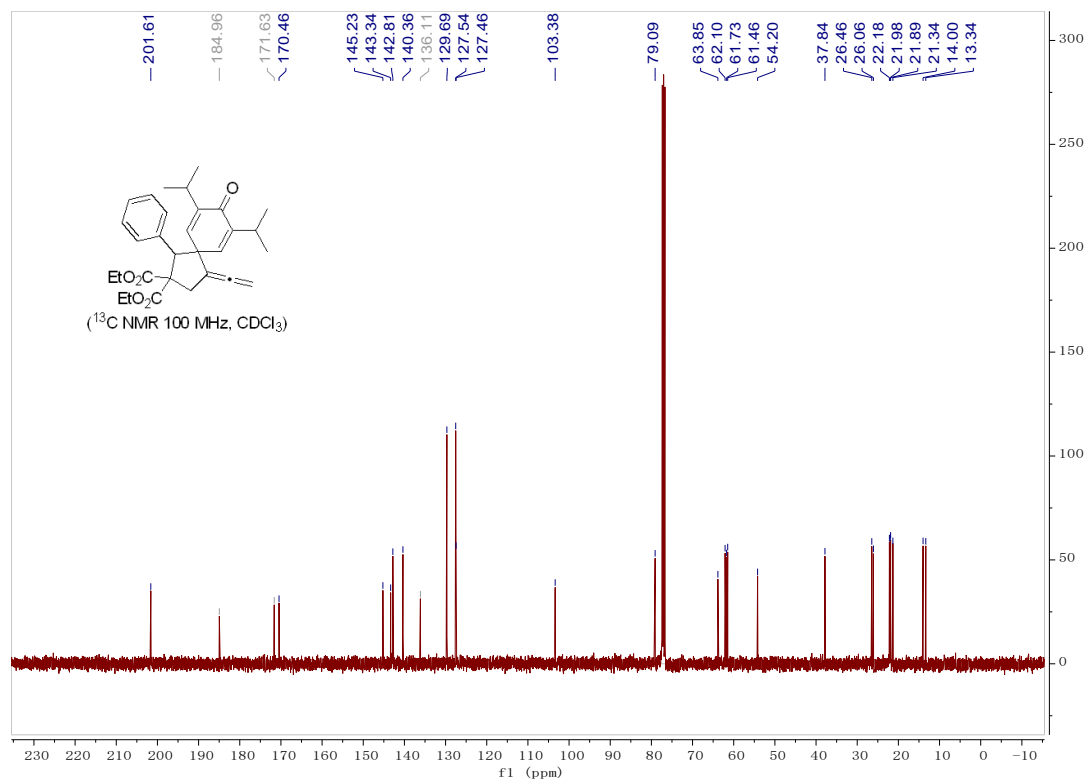


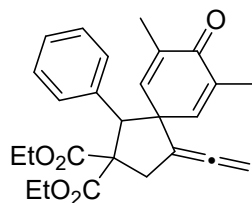




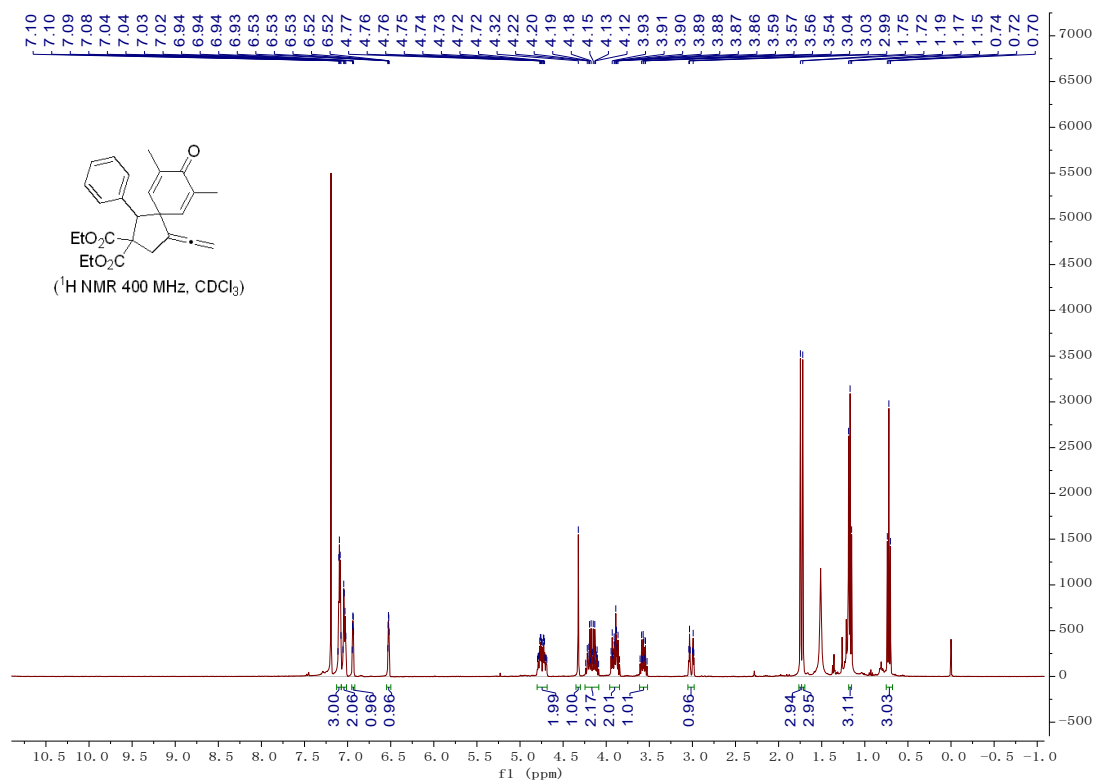
diethyl 7,9-diisopropyl-8-oxo-1-phenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3af): Yield: 0.0190 g, 40%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.17 – 7.12 (m, 3H), 7.10 – 7.04 (m, 2H), 6.82 (d, $J = 3.0$ Hz, 1H), 6.51 (d, $J = 3.0$ Hz, 1H), 4.86 – 4.73 (m, 2H), 4.37 (s, 1H), 4.30 – 4.18 (m, 2H), 4.05 – 3.93 (m, 2H), 3.71 (dq, $J = 10.6, 7.2$ Hz, 1H), 3.14 (dt, $J = 17.0, 3.2$ Hz, 1H), 2.94 – 2.82 (m, 2H), 1.25 (t, $J = 7.2$ Hz, 3H), 0.99 (d, $J = 6.8$ Hz, 6H), 0.92 (d, $J = 6.8$ Hz, 3H), 0.87 (d, $J = 6.8$ Hz, 3H), 0.81 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.6, 185.0, 171.6, 170.5, 145.2, 143.3, 142.8, 140.4, 136.1, 129.7, 127.54, 127.46, 103.4, 79.1, 63.9, 62.1, 61.7, 61.5, 54.2, 37.8, 26.5, 26.1, 22.2, 22.0, 21.9, 21.3, 14.0, 13.3; IR (neat): ν 2959.53, 2925.04, 2867.64, 1959.72, 11725.28, 1636.06, 1463.07, 1253.83, 1204.04, 1090.85, 1009.96, 754.26, 700.72 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{30}\text{H}_{37}\text{O}_5$ $[\text{M}+\text{H}]^+$: 477.2636, found: 477.2628.

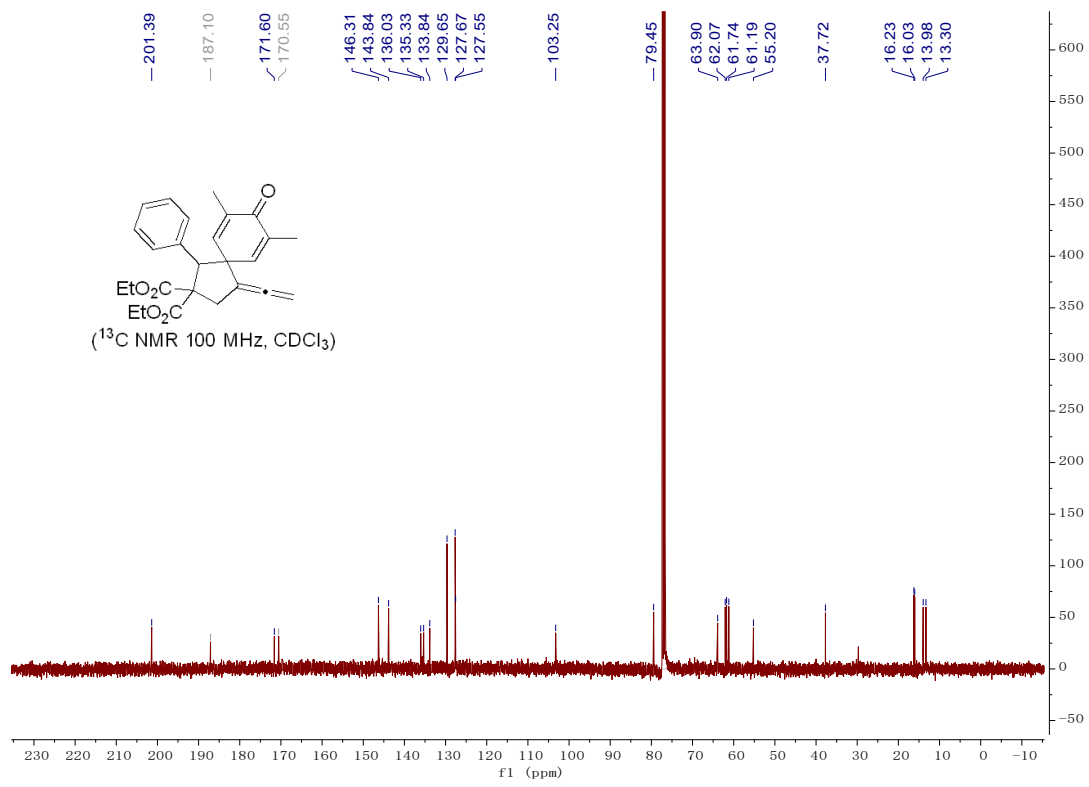


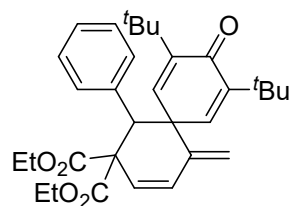




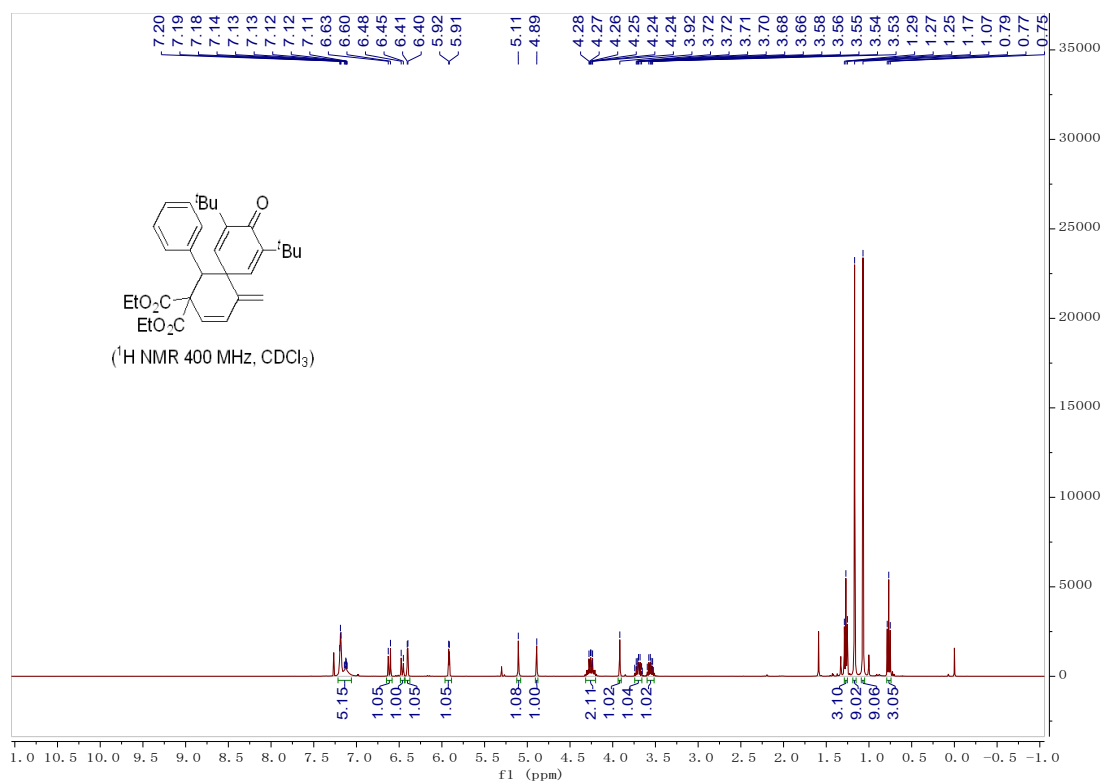
diethyl 7,9-dimethyl-8-oxo-1-phenyl-4-vinylidenespiro[4.5]deca-6,9-diene-2,2-dicarboxylate (3ag): Yield: 0.0096 g, 23%, a colorless oil; Eluent: PE/EA = 30/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.13 – 7.07 (m, 3H), 7.07 – 7.01 (m, 2H), 6.95 – 6.92 (m, 1H), 6.56 – 6.51 (m, 1H), 4.80 – 4.69 (m, 2H), 4.32 (s, 1H), 4.25 – 4.09 (m, 2H), 3.96 – 3.85 (m, 2H), 3.57 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.01 (dt, $J = 17.0, 3.2$ Hz, 1H), 1.75 (s, 3H), 1.72 (s, 3H), 1.16 (t, $J = 7.2$ Hz, 3H), 0.72 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 201.4, 187.1, 171.6, 170.5, 146.3, 143.8, 136.0, 135.3, 133.8, 129.6, 127.7, 127.6, 103.3, 79.5, 63.9, 62.1, 61.7, 61.2, 55.2, 37.7, 16.2, 16.0, 14.0, 13.3; IR (neat): ν 2961.57, 2923.21, 2846.77, 1962.28, 1723.49, 1668.21, 1637.59, 1453.53, 1370.04, 1252.80, 1204.80, 1113.31, 1034.36, 939.52, 700.55 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{26}\text{H}_{29}\text{O}_5$ $[\text{M}+\text{H}]^+$: 421.2010, found: 421.2008.

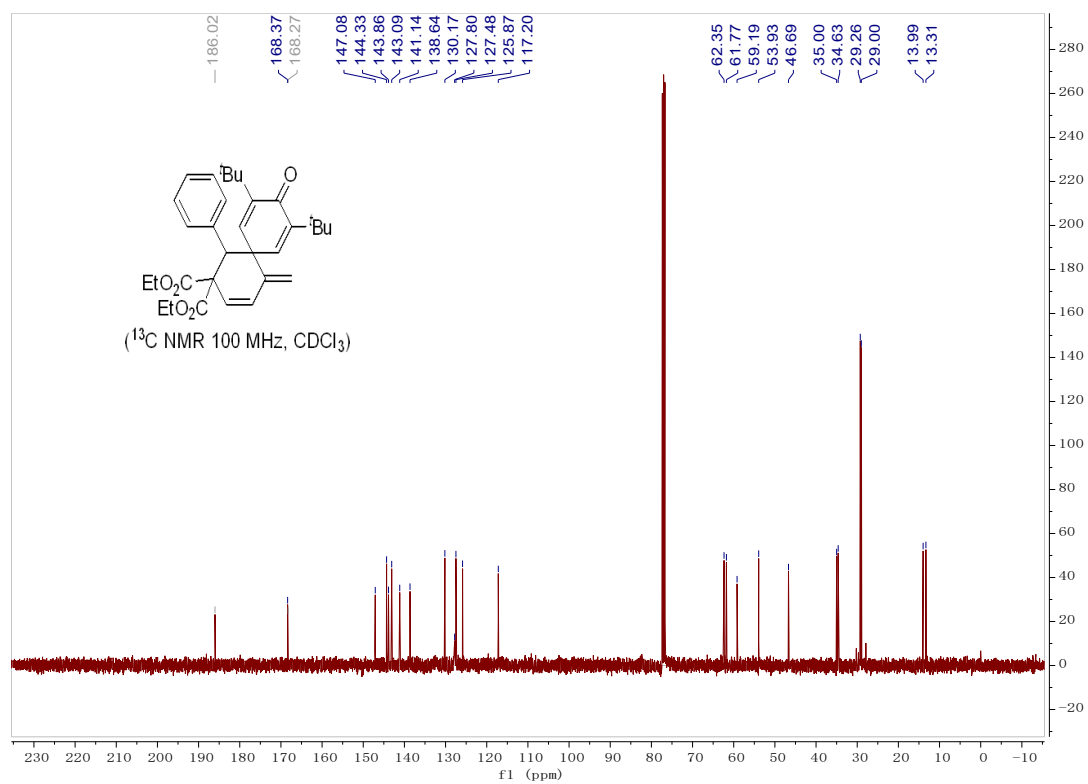


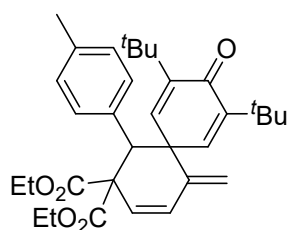




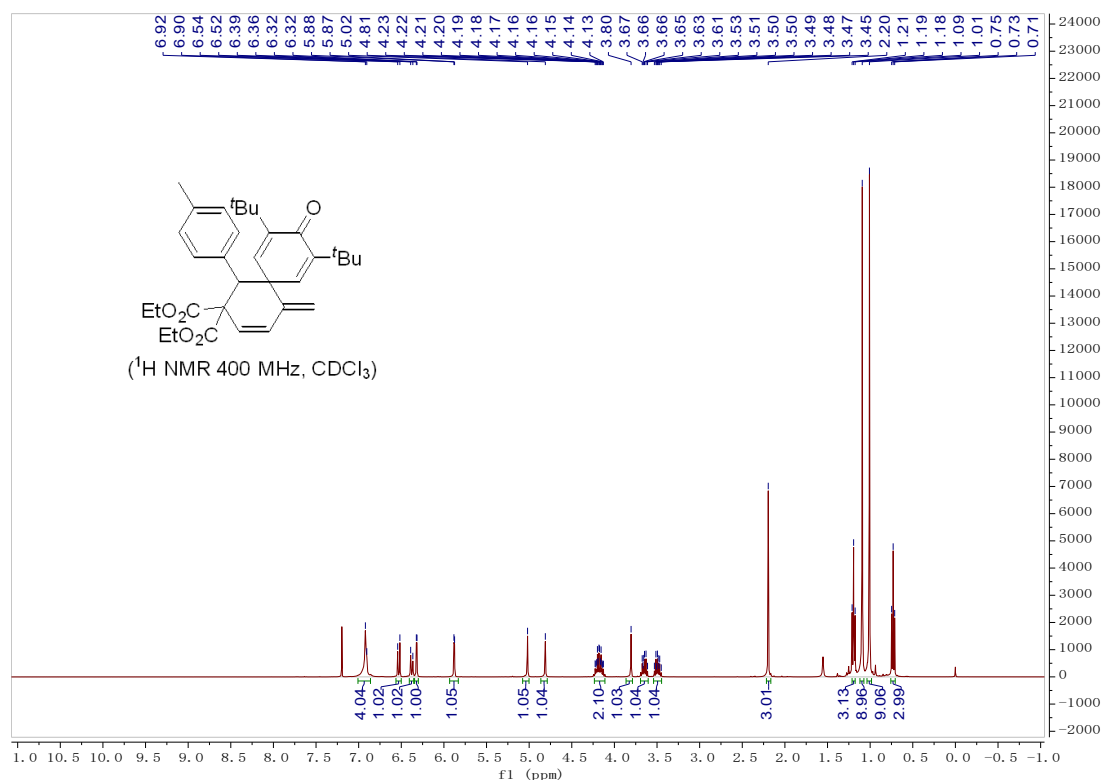
diethyl 8,10-di-*tert*-butyl-5-methylene-9-oxo-1-phenylspiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4a): Yield: 74%, a pale yellow solid, m.p. 117-119 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.22 – 7.06 (m, 5H), 6.61 (d, $J = 10.2$ Hz, 1H), 6.46 (d, $J = 10.2$ Hz, 1H), 6.40 (d, $J = 3.2$ Hz, 1H), 5.92 (d, $J = 3.2$ Hz, 1H), 5.11 (s, 1H), 4.89 (s, 1H), 4.32 – 4.20 (m, 2H), 3.92 (s, 1H), 3.74 – 3.66 (m, 1H), 3.60 – 3.52 (m, 1H), 1.27 (t, $J = 7.2$ Hz, 3H), 1.17 (s, 9H), 1.07 (s, 9H), 0.77 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) 186.0, 168.4, 168.3, 147.1, 144.3, 143.9, 143.1, 141.1, 138.6, 130.2, 127.8, 127.5, 125.9, 117.2, 62.4, 61.8, 59.2, 53.9, 46.7, 35.0, 34.6, 29.3, 29.0, 14.0, 13.3; IR (neat): ν 2995.58, 2957.60, 2906.86, 2865.11, 1736.30, 1715.05, 1658.45, 1388.35, 1232.46, 1182.75, 1117.73, 1061.27, 714.94 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{32}\text{H}_{41}\text{O}_5$ $[\text{M}+\text{H}]^+$: 505.2949, found: 505.2946.

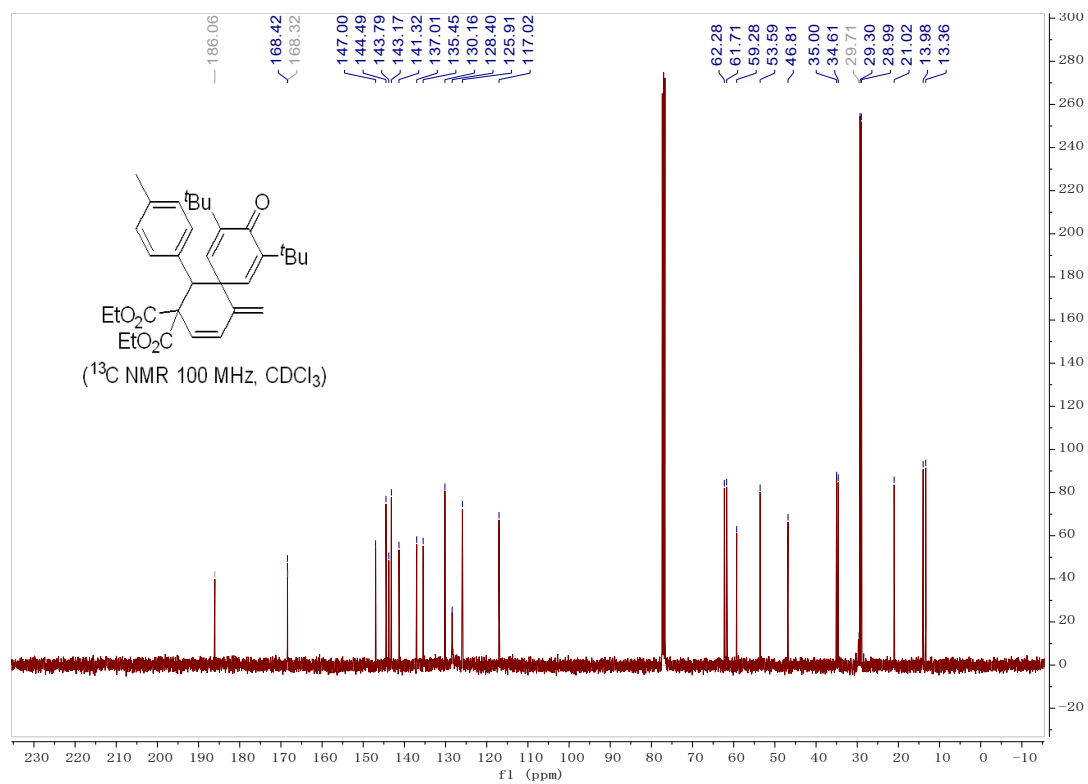


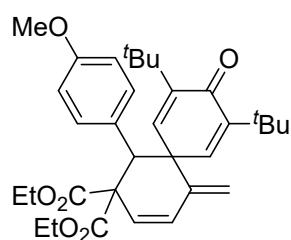




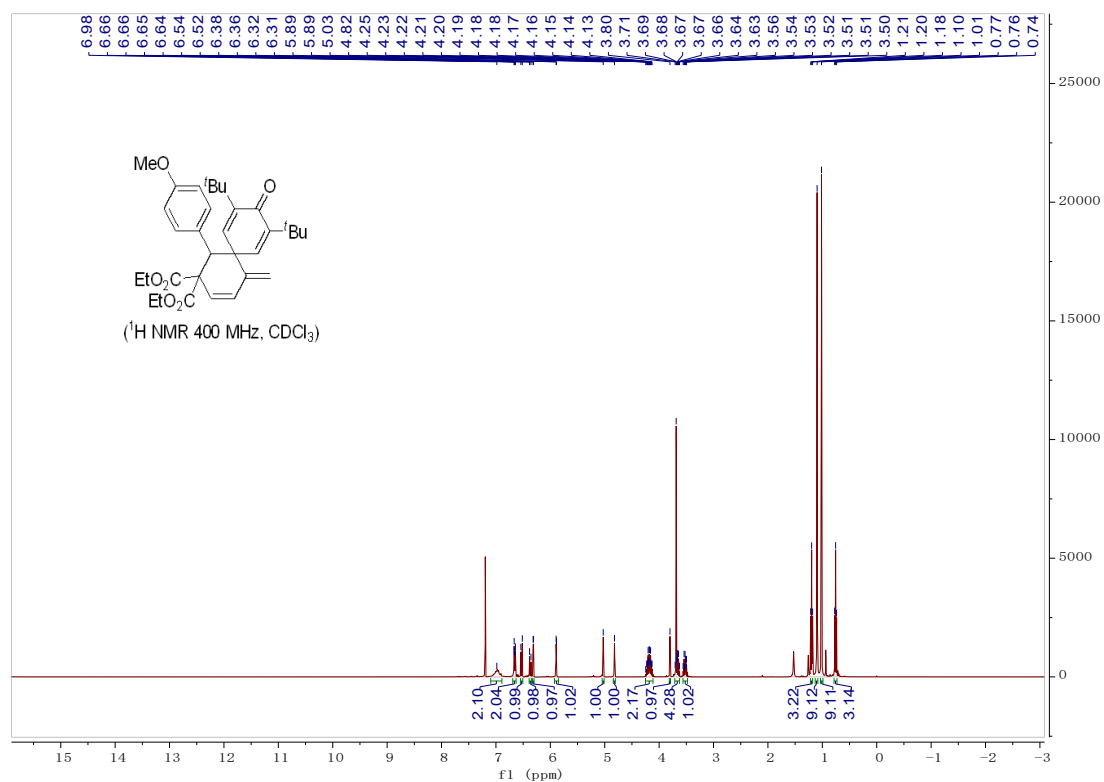
diethyl 8,10-di-*tert*-butyl-5-methylene-9-oxo-1-(*p*-tolyl)spiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4b): Yield: 60%, a pale yellow solid, m.p. 120-122 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.01 – 6.86 (m, 4H), 6.53 (d, $J = 10.2$ Hz, 1H), 6.38 (d, $J = 10.2$ Hz, 1H), 6.32 (d, $J = 3.0$ Hz, 1H), 5.88 (d, $J = 3.0$ Hz, 1H), 5.02 (s, 1H), 4.81 (s, 1H), 4.23 – 4.11 (m, 2H), 3.80 (s, 1H), 3.69 – 3.60 (m, 1H), 3.49 (dq, $J = 10.8, 7.2$ Hz, 1H), 2.20 (s, 3H), 1.19 (t, $J = 7.2$ Hz, 3H), 1.09 (s, 9H), 1.01 (s, 9H), 0.73 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.1, 168.4, 168.3, 147.0, 144.5, 143.8, 143.2, 141.3, 137.0, 135.4, 130.2, 128.4, 125.9, 117.0, 62.3, 61.7, 59.3, 53.6, 46.8, 35.0, 34.6, 29.7, 29.3, 29.0, 21.0, 14.0, 13.4; IR (neat): ν 2996.26, 2957.10, 2864.49, 1736.51, 1716.03, 1658.55, 1637.58, 1388.56, 1365.12, 1232.21, 1181.87, 1034.91, 948.75, 727.76 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_5$ $[\text{M}+\text{H}]^+$: 519.3105, found: 519.3106.

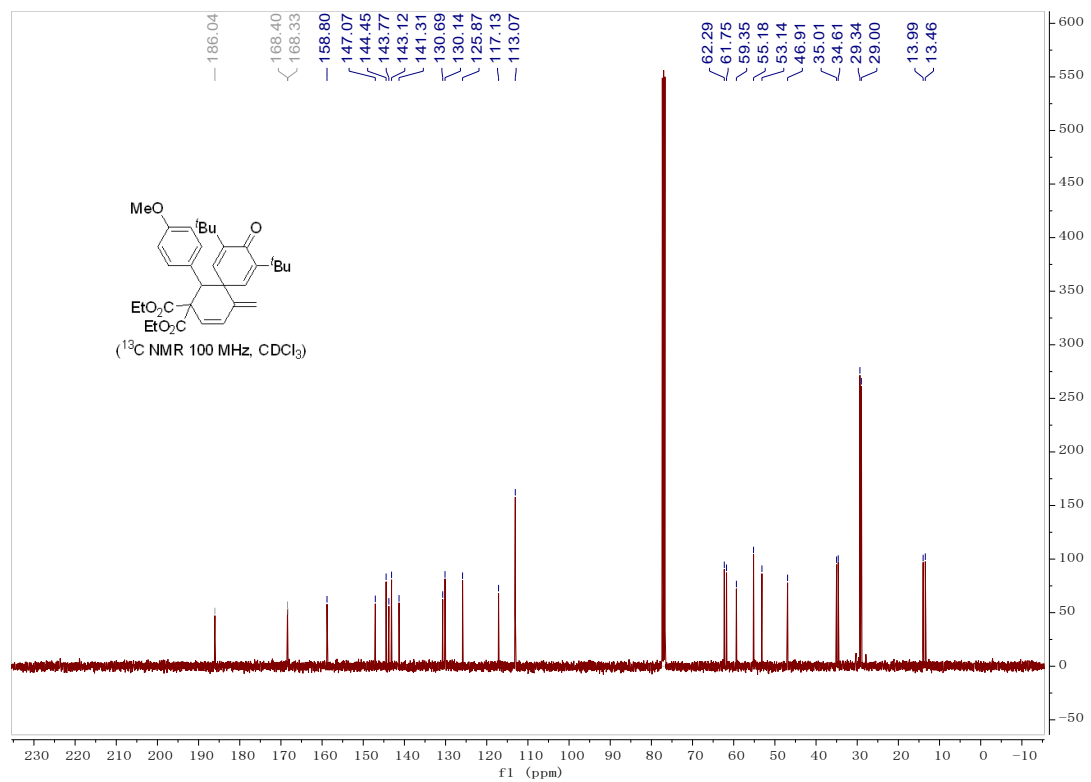


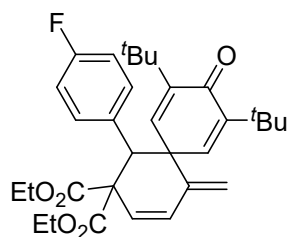




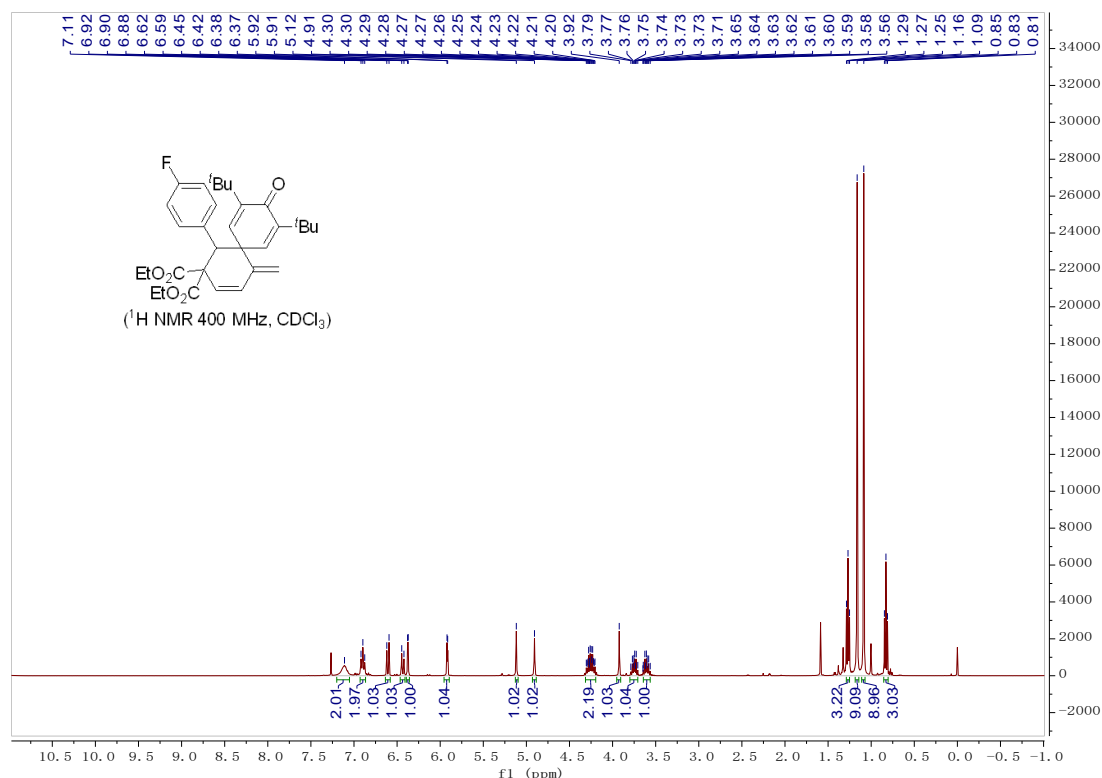
diethyl 8,10-di-*tert*-butyl-1-(4-methoxyphenyl)-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4c): Yield: 57%, a pale yellow solid, m.p. 158-160 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 6.98 (s, 2H), 6.69 – 6.63 (m, 2H), 6.53 (d, $J = 10.2$ Hz, 1H), 6.37 (d, $J = 10.2$ Hz, 1H), 6.31 (d, $J = 3.0$ Hz, 1H), 5.89 (d, $J = 3.0$ Hz, 1H), 5.03 (s, 1H), 4.82 (s, 1H), 4.25 – 4.11 (m, 2H), 3.80 (s, 1H), 3.71 – 3.62 (m, 4H), 3.56 – 3.48 (m, 1H), 1.20 (t, $J = 7.2$ Hz, 3H), 1.10 (s, 9H), 1.01 (s, 9H), 0.76 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.4, 168.3, 158.8, 147.1, 144.4, 143.8, 143.1, 141.3, 130.7, 130.1, 125.9, 117.1, 113.1, 62.3, 61.7, 59.3, 55.2, 53.1, 46.9, 35.0, 34.6, 29.3, 29.0, 14.0, 13.5; IR (neat): ν 2957.34, 2901.64, 2865.11, 1736.11, 1716.07, 1658.30, 1512.70, 1279.36, 1250.67, 1180.06, 1061.53, 1036.34, 876.06, 735.86 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_6$ $[\text{M}+\text{H}]^+$: 535.3054, found: 535.3051.

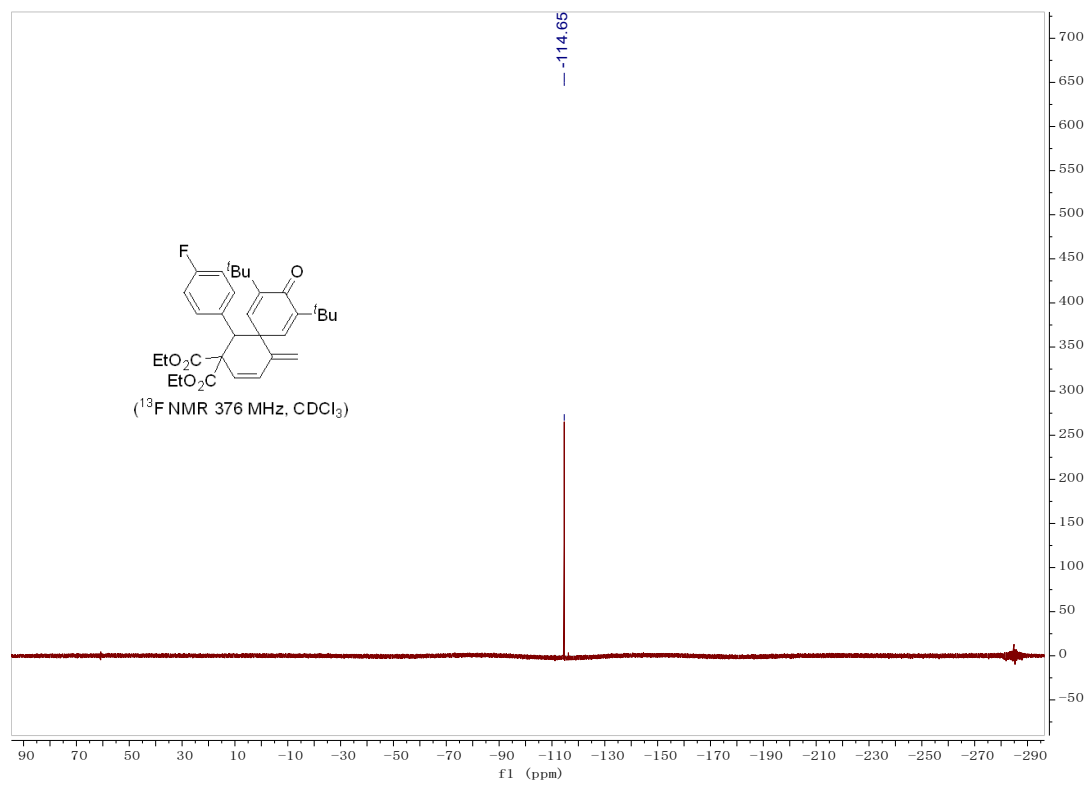
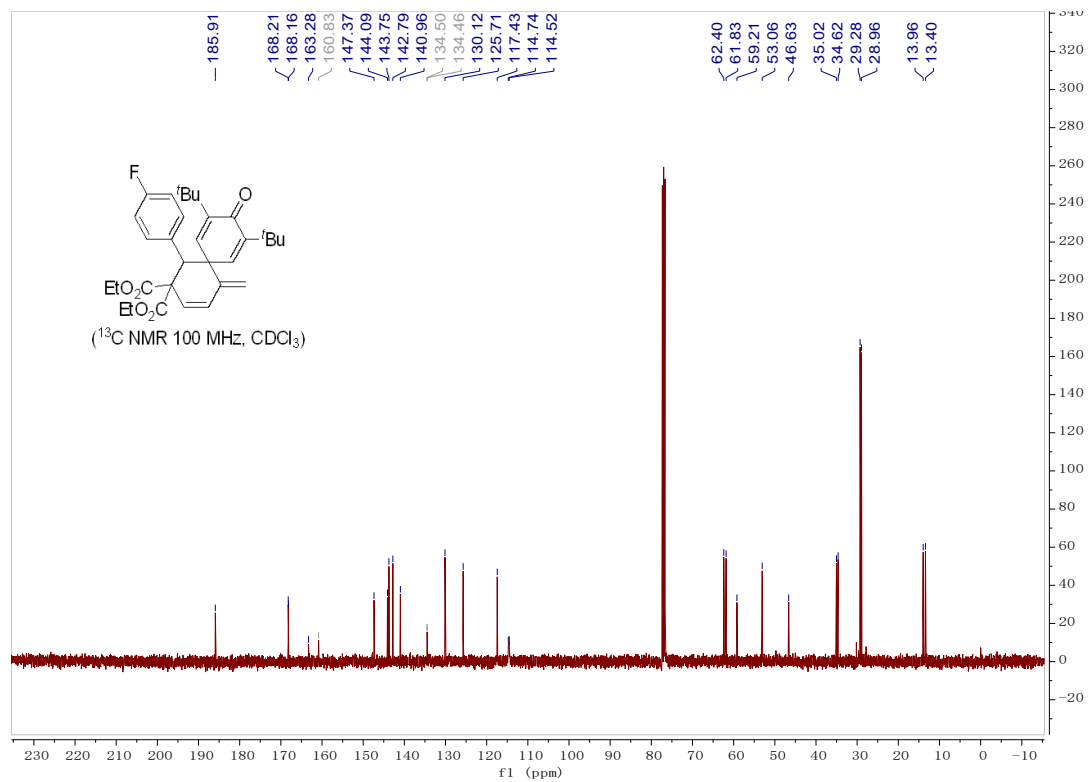


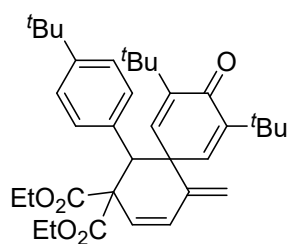




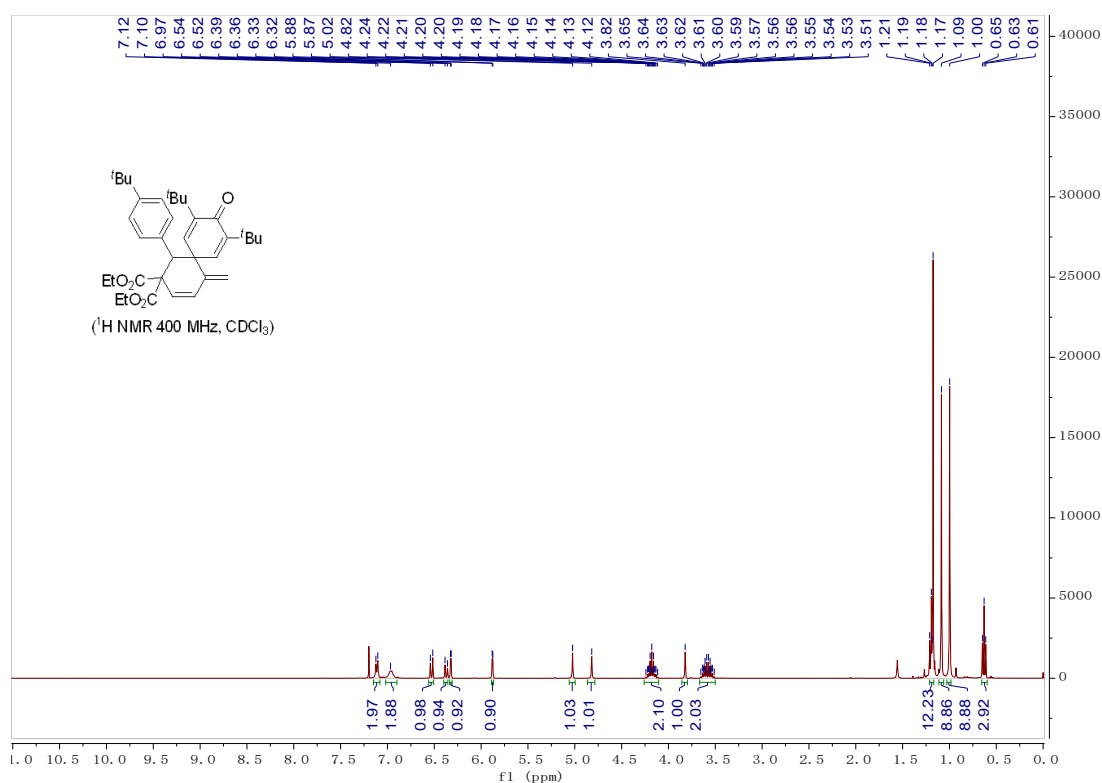
diethyl 8,10-di-*tert*-butyl-1-(4-fluorophenyl)-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4d): Yield: 70%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.11 (s, 2H), 6.90 (t, $J = 8.6$ Hz, 2H), 6.61 (d, $J = 10.2$ Hz, 1H), 6.43 (d, $J = 10.2$ Hz, 1H), 6.37 (d, $J = 3.0$ Hz, 1H), 5.92 (d, $J = 3.0$ Hz, 1H), 5.12 (s, 1H), 4.91 (s, 1H), 4.31 – 4.20 (m, 2H), 3.92 (s, 1H), 3.75 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.59 (dq, $J = 10.8, 7.2$ Hz, 1H), 1.28 (d, $J = 7.0$ Hz, 3H), 1.16 (s, 9H), 1.09 (s, 9H), 0.83 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.9, 168.21, 168.16, 162.1 (d, $J = 246$ Hz), 147.4, 144.1, 143.7, 142.8, 141.0, 134.5 (d, $J = 3.2$ Hz), 130.1, 125.7, 117.4, 114.6 (d, $J = 22$ Hz), 62.4, 61.8, 59.2, 53.1, 46.6, 35.0, 34.6, 29.3, 29.0, 14.0, 13.4; ^{19}F NMR (376 MHz, CDCl_3) δ -114.65; IR (neat): ν 2958.30, 2906.86, 2862.51, 1736.39, 1714.79, 1658.97, 1509.16, 1183.36, 1096.89, 1061.39, 840.57, 823.98, 784.70, 731.53 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{32}\text{H}_{40}\text{FO}_5$ $[\text{M}+\text{H}]^+$: 523.2854, found: 523.2848.

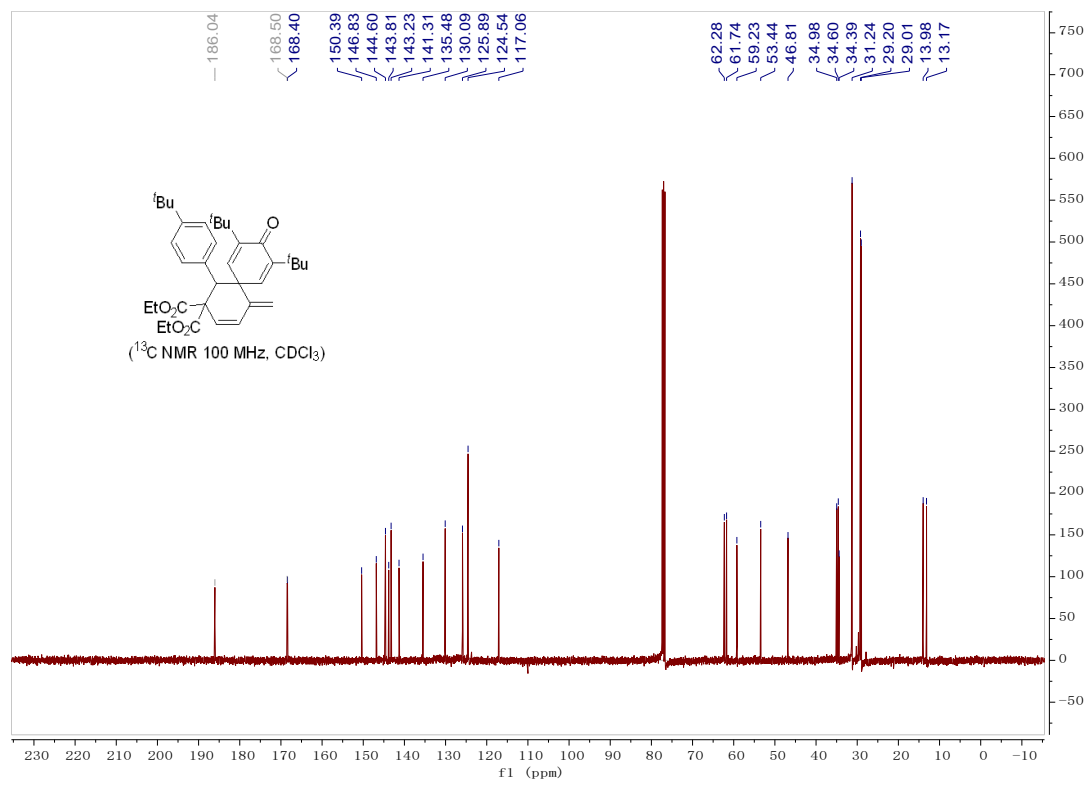


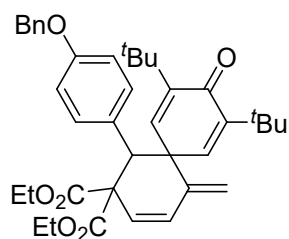




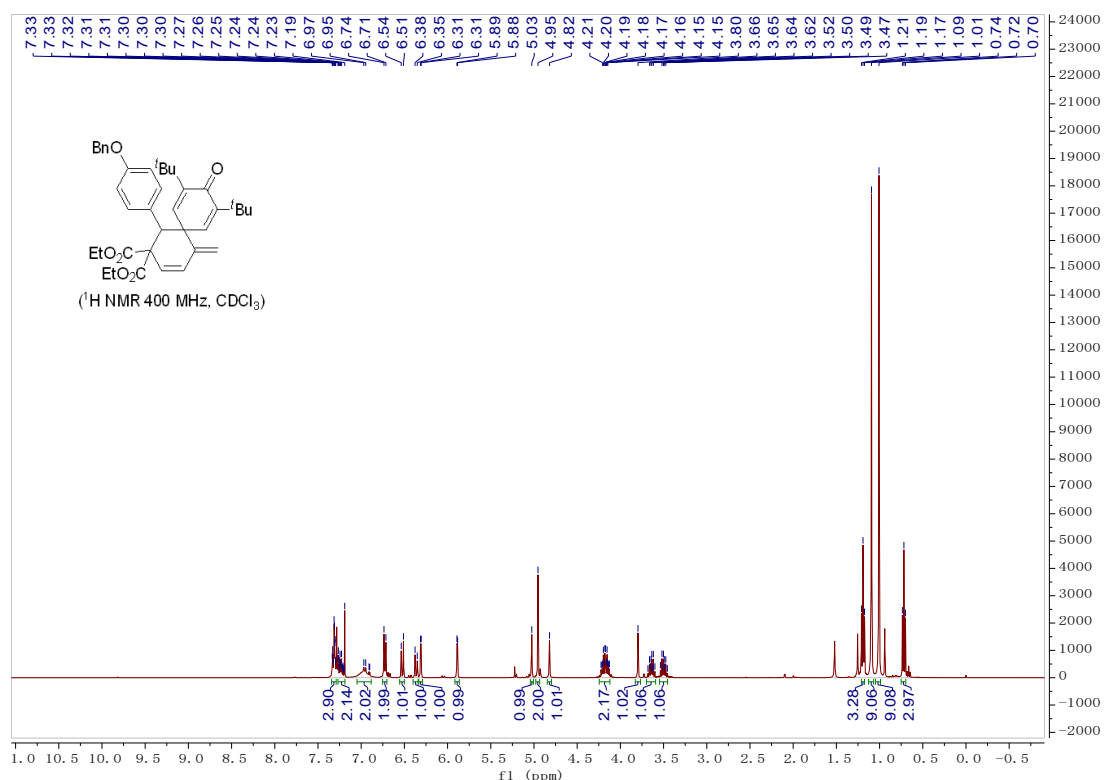
diethyl 8,10-di-*tert*-butyl-1-(4-(*tert*-butyl)phenyl)-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4e): Yield: 66%, a pale yellow solid, m.p. 132-134 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.11 (d, $J = 8.0$ Hz, 2H), 6.97 (s, 2H), 6.53 (d, $J = 10.2$ Hz, 1H), 6.37 (d, $J = 10.2$ Hz, 1H), 6.32 (d, $J = 3.0$ Hz, 1H), 5.88 (d, $J = 3.0$ Hz, 1H), 5.02 (s, 1H), 4.82 (s, 1H), 4.26 – 4.10 (m, 2H), 3.82 (s, 1H), 3.67 – 3.50 (m, 2H), 1.21 – 1.17 (m, 12H), 1.09 (s, 9H), 1.00 (s, 9H), 0.63 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.5, 168.4, 150.4, 146.8, 144.6, 143.8, 143.2, 141.3, 135.5, 130.1, 125.9, 124.5, 117.1, 62.3, 61.7, 59.2, 53.4, 46.8, 35.0, 34.6, 34.4, 31.2, 29.2, 29.0, 14.0, 13.2; IR (neat): ν 2957.70, 2906.86, 2867.72, 1736.29, 1716.39, 1658.76, 1637.72, 1388.85, 1364.85, 1183.08, 1061.67, 1034.86, 949.25 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{36}\text{H}_{49}\text{O}_5$ $[\text{M}+\text{H}]^+$: 561.3575, found: 561.3576.

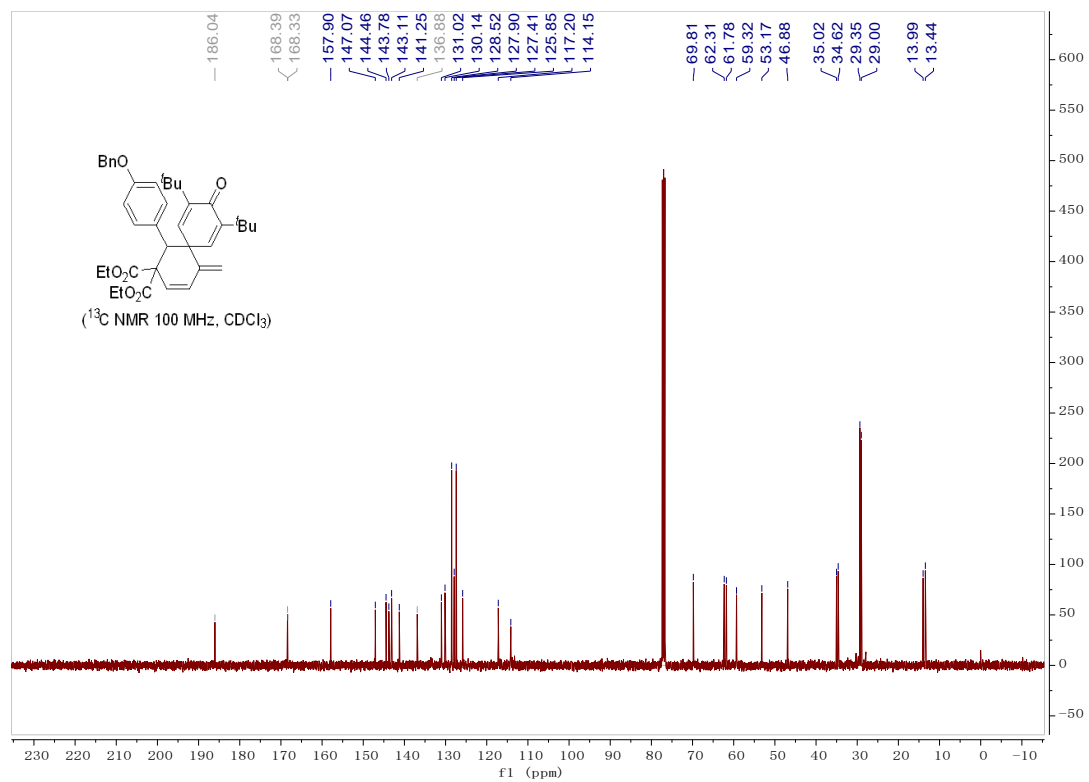


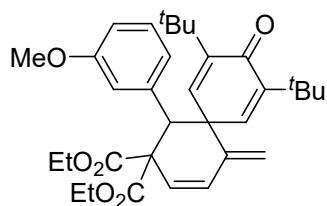




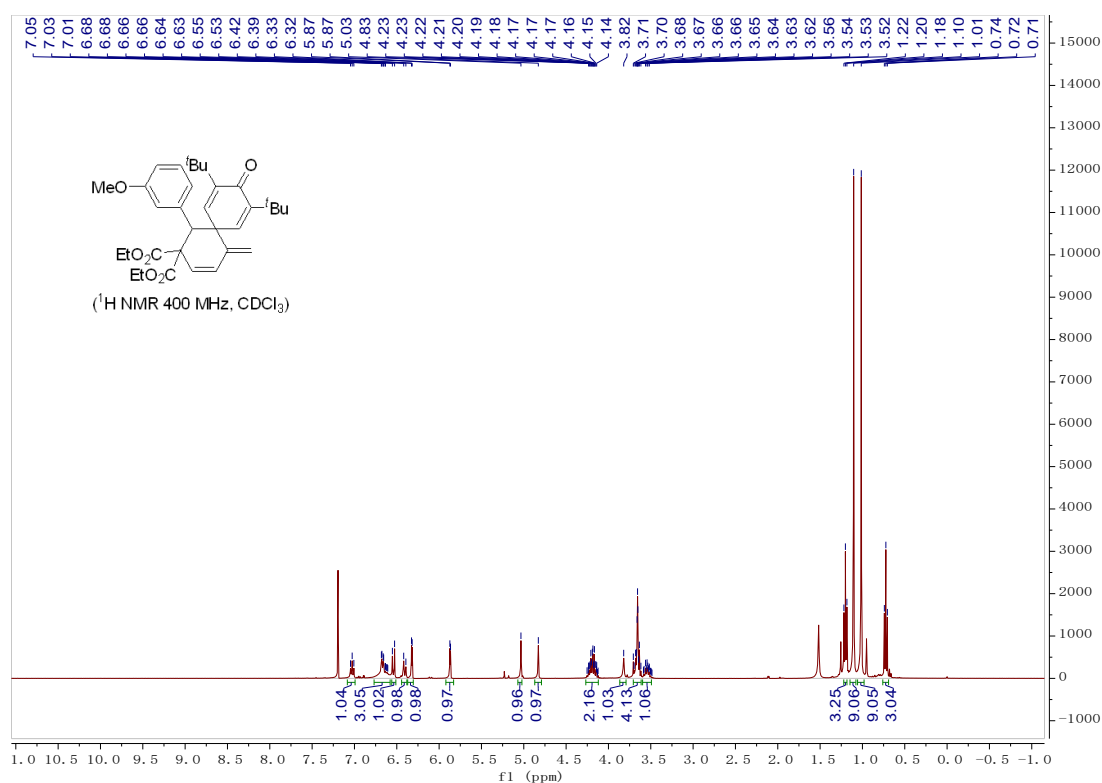
diethyl 1-(4-(benzyloxy)phenyl)-8,10-di-*tert*-butyl-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4f): Yield: 50%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.34 – 7.19 (m, 5H), 7.05 – 6.88 (m, 2H), 6.73 (d, $J = 9.0$ Hz, 2H), 6.52 (d, $J = 10.2$ Hz, 1H), 6.36 (d, $J = 10.2$ Hz, 1H), 6.31 (d, $J = 3.0$ Hz, 1H), 5.89 (d, $J = 3.0$ Hz, 1H), 5.03 (s, 1H), 4.95 (s, 2H), 4.82 (s, 1H), 4.24 – 4.12 (m, 2H), 3.80 (s, 1H), 3.64 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.50 (dq, $J = 10.8, 7.2$ Hz, 1H), 1.19 (t, $J = 7.0$ Hz, 3H), 1.09 (s, 9H), 1.01 (s, 9H), 0.72 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.4, 168.3, 157.9, 147.1, 144.5, 143.8, 143.1, 141.2, 136.9, 131.0, 130.1, 128.5, 127.9, 127.4, 125.8, 117.2, 114.2, 69.8, 62.3, 61.8, 59.3, 53.2, 46.9, 35.0, 34.6, 29.4, 29.0, 14.0, 13.4; IR (neat): ν 2957.46, 2909.47, 2857.29, 1735.77, 1714.06, 1658.09, 1510.32, 1363.96, 1220.79, 1179.93, 1061.44, 948.90, 875.89 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{39}\text{H}_{47}\text{O}_6$ $[\text{M}+\text{H}]^+$: 611.3367, found: 611.3370.

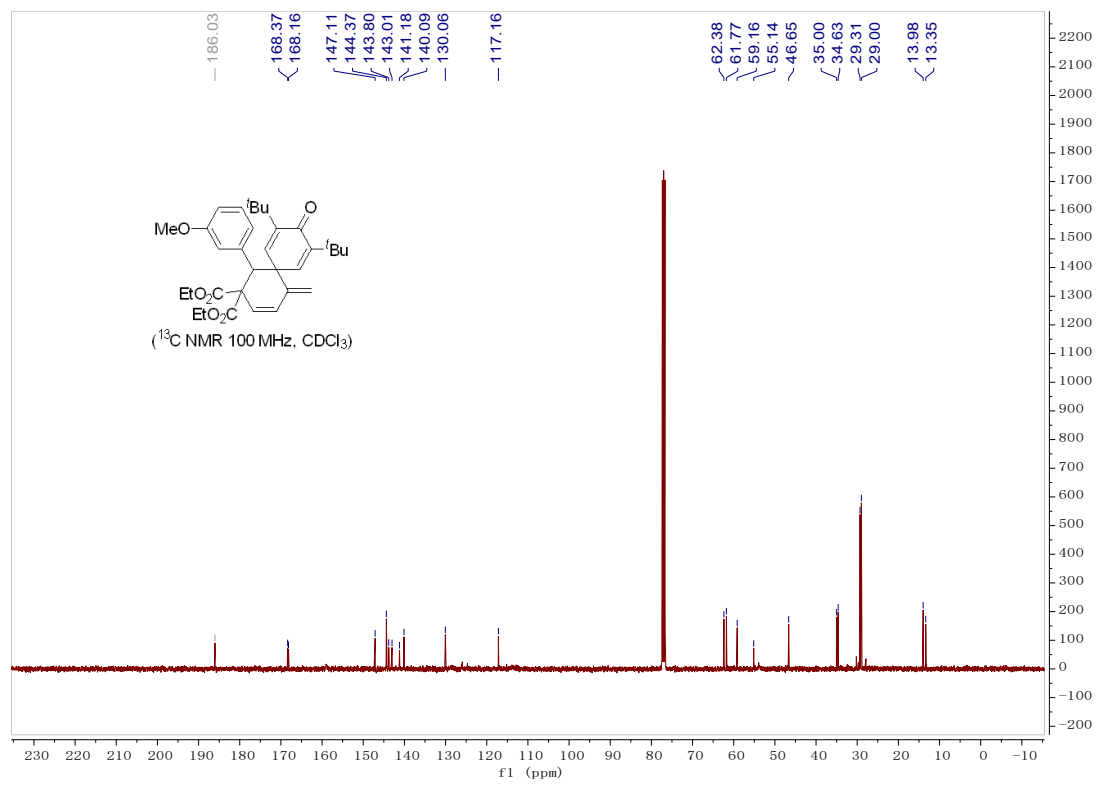


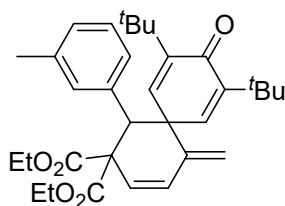




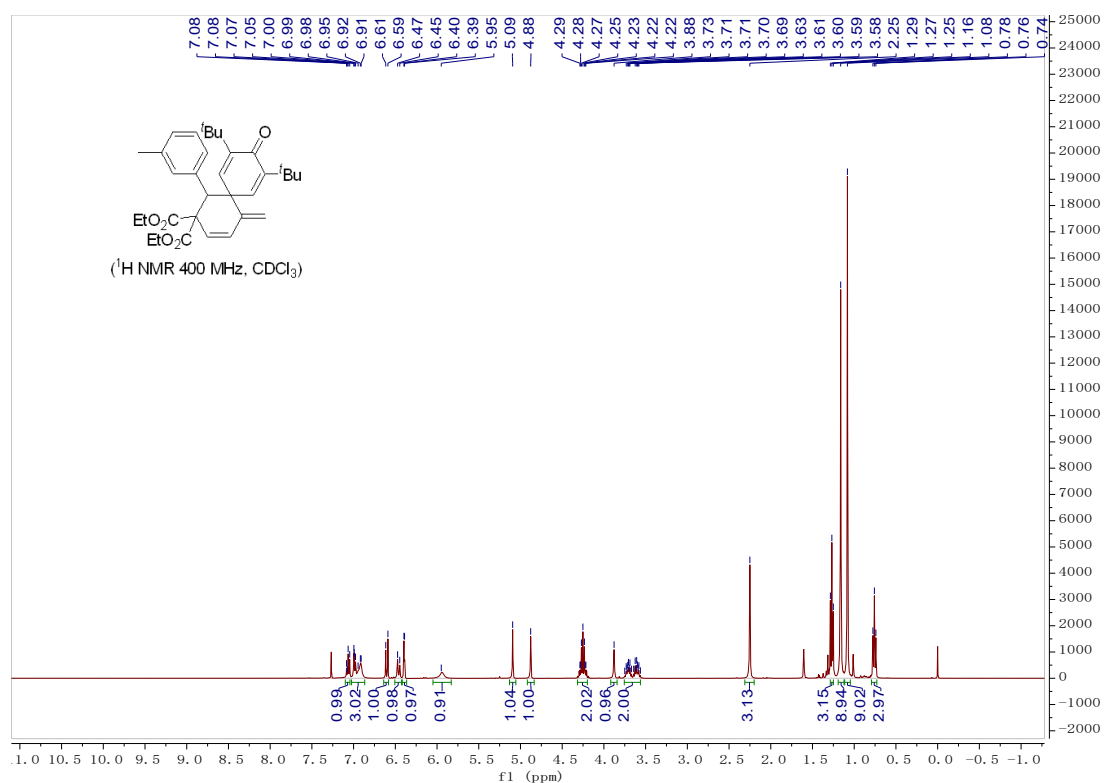
diethyl 8,10-di-*tert*-butyl-1-(3-methoxyphenyl)-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4g): Yield: 49%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.03 (t, $J = 7.8$ Hz, 1H), 6.77 – 6.58 (m, 3H), 6.54 (d, $J = 10.2$ Hz, 1H), 6.41 (d, $J = 10.2$ Hz, 1H), 6.32 (d, $J = 3.0$ Hz, 1H), 5.87 (d, $J = 3.0$ Hz, 1H), 5.03 (s, 1H), 4.83 (s, 1H), 4.27 – 4.12 (m, 2H), 3.82 (s, 1H), 3.71 – 3.61 (m, 4H), 3.60 – 3.49 (m, 1H), 1.20 (t, $J = 7.0$ Hz, 3H), 1.10 (s, 9H), 1.01 (s, 9H), 0.72 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.4, 168.2, 147.1, 144.4, 143.8, 143.0, 141.2, 140.1, 130.1, 117.2, 62.4, 61.8, 59.2, 55.1, 46.6, 35.0, 34.6, 29.3, 29.0, 14.0, 13.4; IR (neat): ν 2996.26, 2956.72, 2903.74, 2867.29, 1736.40, 1658.52, 1639.50, 1488.29, 1388.54, 1365.53, 1232.64, 1185.22, 1117.69, 1057.96, 719.26 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_6$ $[\text{M}+\text{H}]^+$: 535.3054, found: 535.3053.

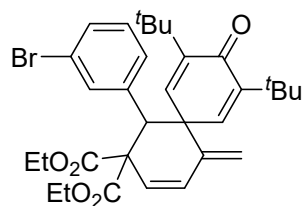




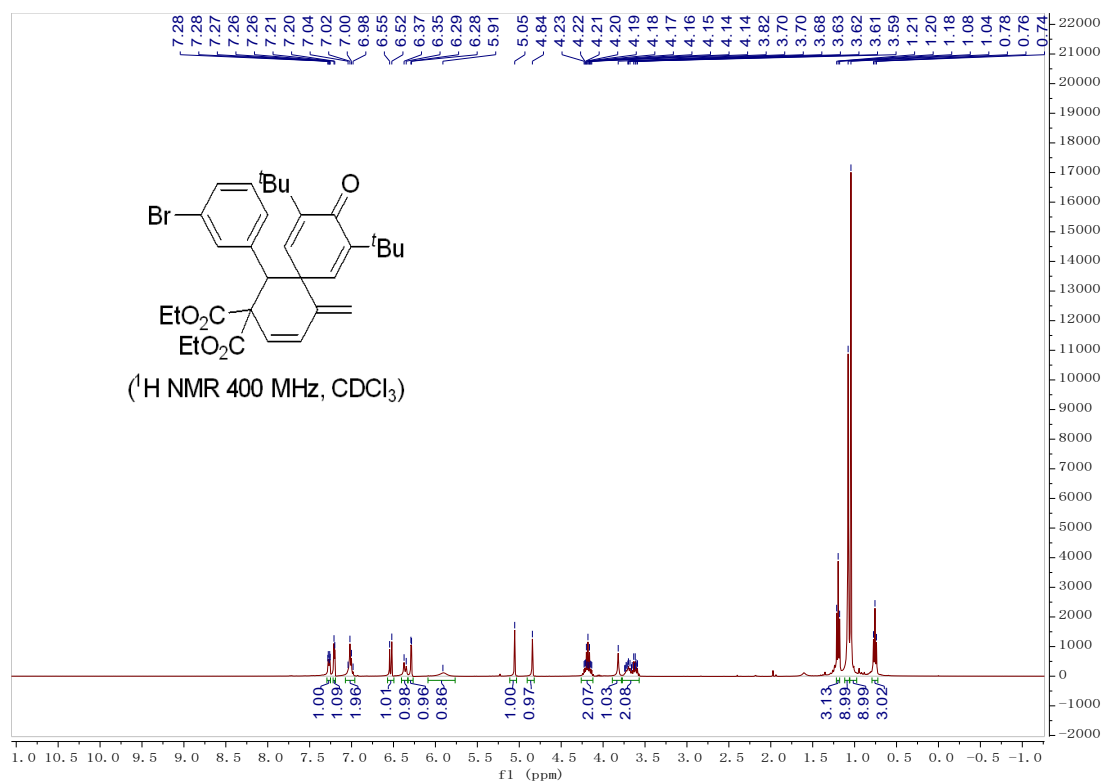


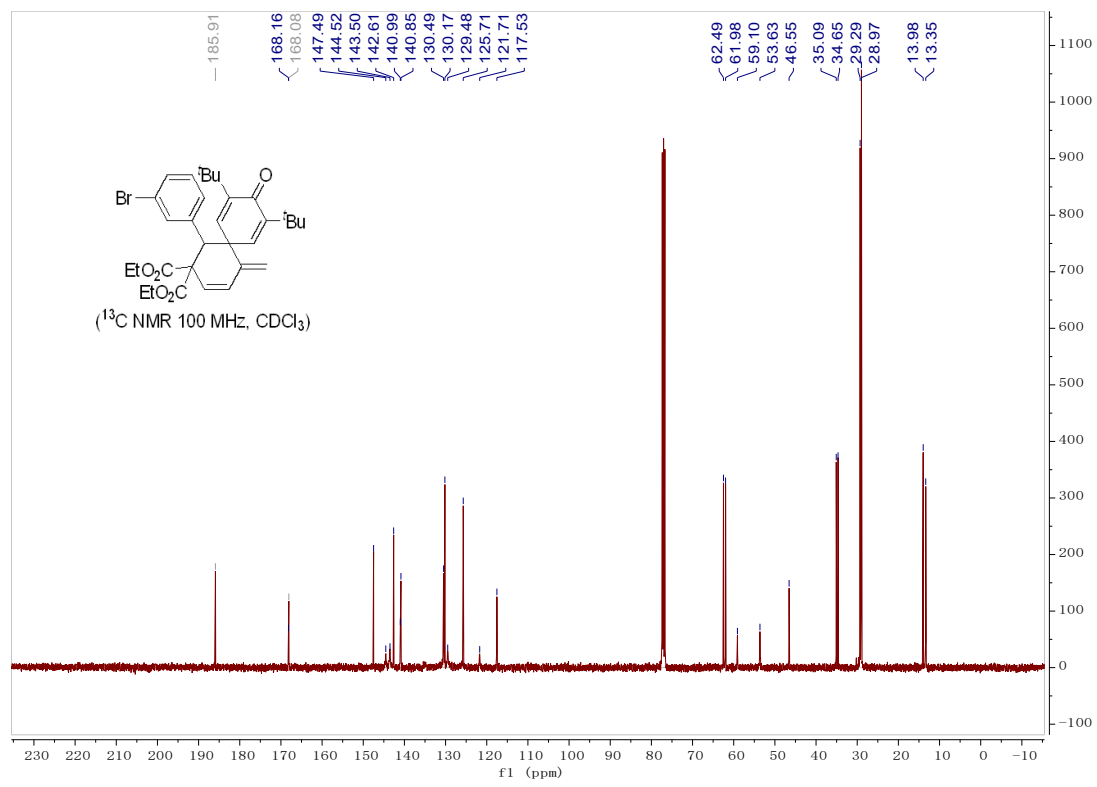
diethyl 8,10-di-*tert*-butyl-5-methylene-9-oxo-1-(*m*-tolyl)spiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4h): Yield: 52%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.07 (t, $J = 7.6$ Hz, 1H), 7.02 – 6.87 (m, 3H), 6.60 (d, $J = 10.2$ Hz, 1H), 6.46 (d, $J = 10.2$ Hz, 1H), 6.39 (d, $J = 3.0$ Hz, 1H), 5.95 (s, 1H), 5.09 (s, 1H), 4.88 (s, 1H), 4.32 – 4.20 (m, 2H), 3.88 (s, 1H), 3.76 – 3.56 (m, 2H), 2.25 (s, 3H), 1.27 (t, $J = 7.0$ Hz, 3H), 1.16 (s, 9H), 1.08 (s, 9H), 0.76 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.1, 168.4, 168.3, 146.9, 143.9, 143.2, 141.2, 138.5, 130.1, 128.0, 125.9, 117.0, 62.3, 61.7, 59.2, 46.7, 35.0, 34.6, 29.3, 29.0, 14.0, 13.3; IR (neat): ν 2957.08, 2903.74, 2864.49, 1736.86, 1658.35, 1636.16, 1486.10, 1388.58, 1232.27, 1185.28, 1118.08, 1061.86, 898.78 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_5$ $[\text{M}+\text{H}]^+$: 519.3105, found: 519.3102.

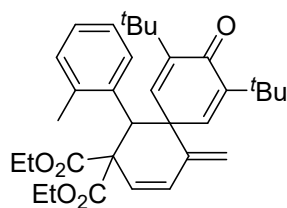




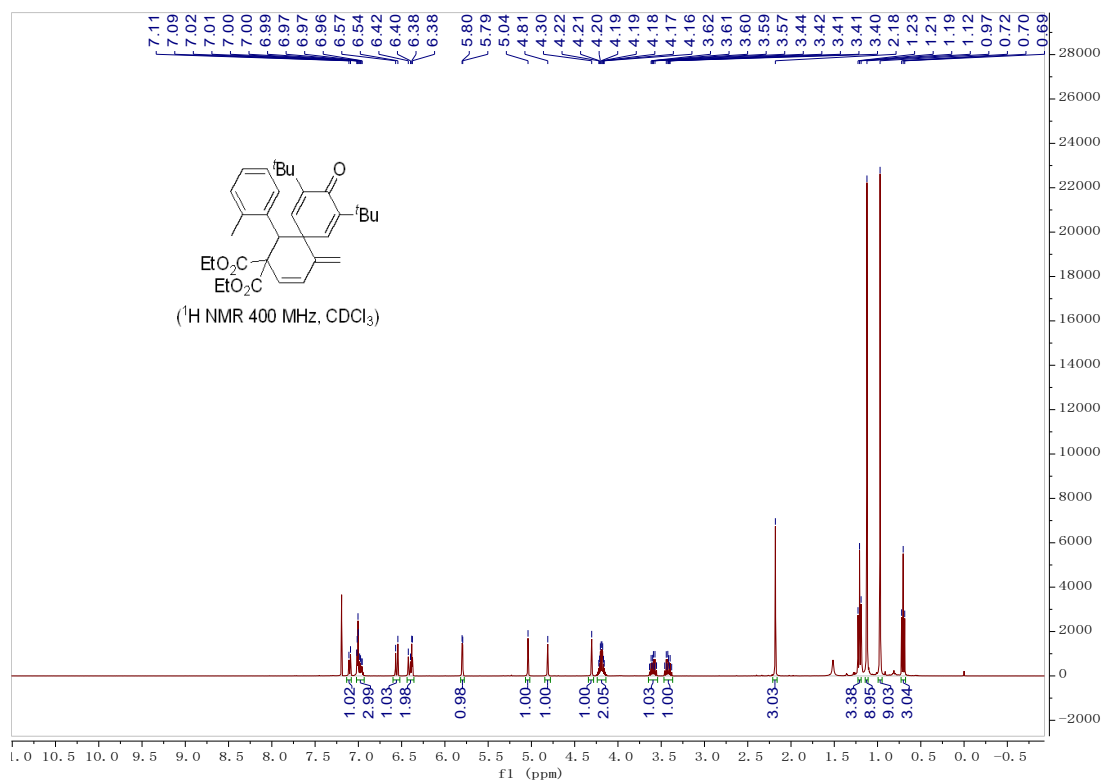
diethyl 1-(3-bromophenyl)-8,10-di-*tert*-butyl-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4i): Yield: 67%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.29 – 7.25 (m, 1H), 7.20 (d, $J = 3.6$ Hz, 1H), 7.07 – 6.96 (m, 2H), 6.53 (d, $J = 10.2$ Hz, 1H), 6.36 (d, $J = 10.2$ Hz, 1H), 6.29 (d, $J = 3.0$ Hz, 1H), 5.91 (s, 1H), 5.05 (s, 1H), 4.84 (s, 1H), 4.26 – 4.12 (m, 2H), 3.82 (s, 1H), 3.77 – 3.57 (m, 2H), 1.20 (t, $J = 7.0$ Hz, 3H), 1.08 (s, 9H), 1.04 (s, 9H), 0.76 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.9, 168.2, 168.1, 147.5, 144.5, 143.5, 142.6, 141.0, 140.8, 130.5, 130.2, 129.5, 125.7, 121.7, 117.5, 62.5, 62.0, 59.1, 53.6, 46.5, 35.1, 34.7, 29.3, 29.0, 14.0, 13.3; IR (neat): ν 2958.03, 2906.86, 2862.51, 1659.12, 1638.93, 1591.82, 1474.46, 1388.97, 1184.31, 1096.91, 1077.31, 1061.41 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{32}\text{H}_{40}\text{BrO}_5$ $[\text{M}+\text{H}]^+$: 583.2054, found: 583.2061.

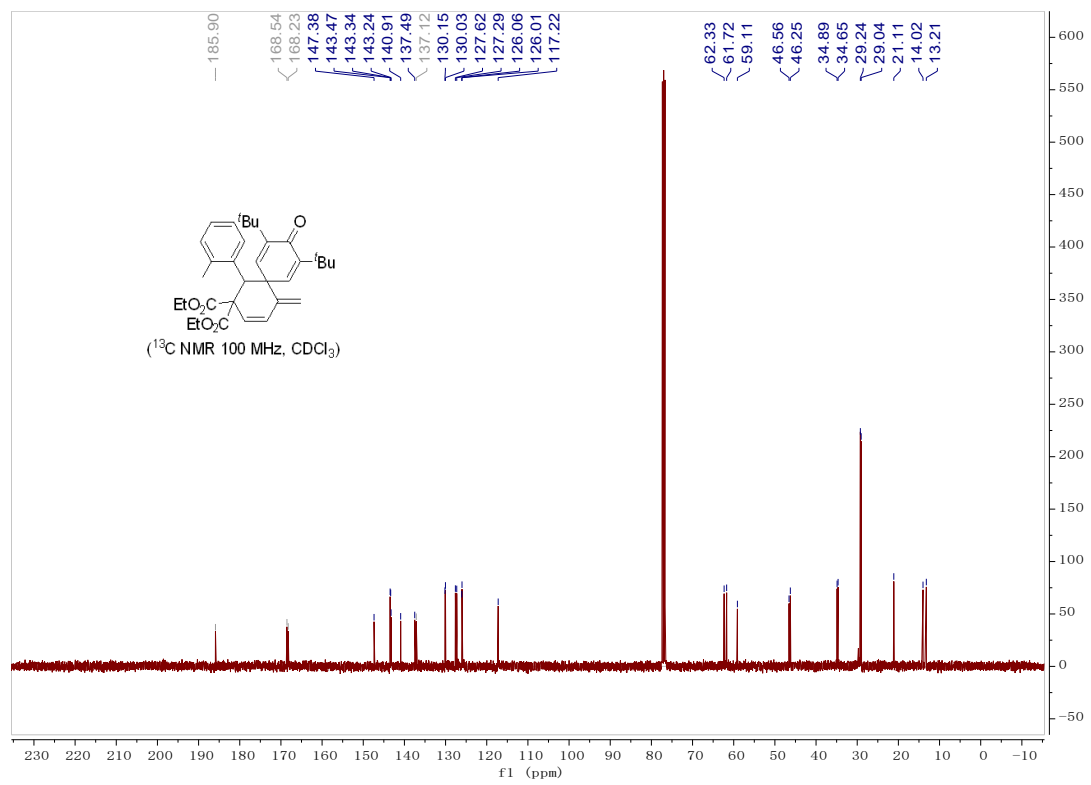


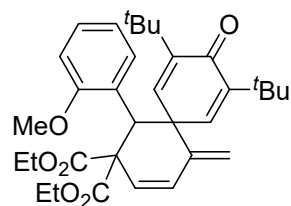




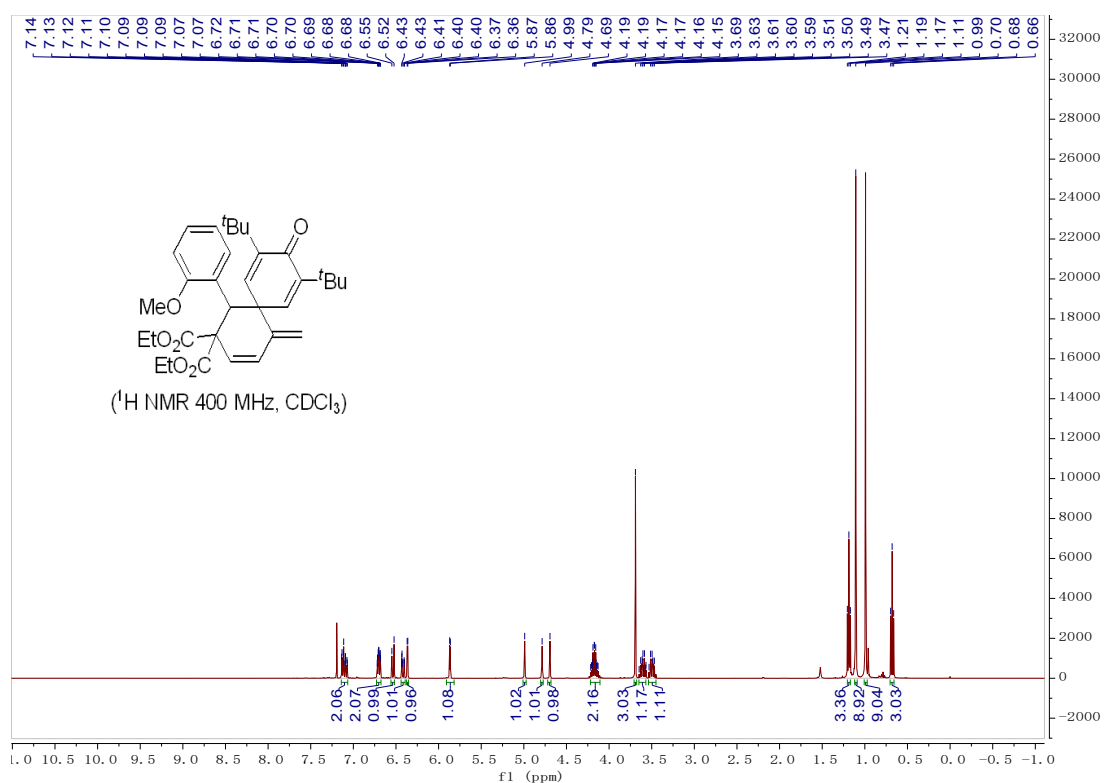
diethyl 8,10-di-*tert*-butyl-5-methylene-9-oxo-1-(*o*-tolyl)spiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4j): Yield: 37%, a pale yellow solid, m.p. 158-160 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.10 (d, $J = 7.2$ Hz, 1H), 7.02 – 6.93 (m, 3H), 6.56 (d, $J = 10.2$ Hz, 1H), 6.44 – 6.36 (m, 2H), 5.80 (d, $J = 3.0$ Hz, 1H), 5.04 (s, 1H), 4.81 (s, 1H), 4.30 (s, 1H), 4.24 – 4.14 (m, 2H), 3.59 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.42 (dq, $J = 10.8, 7.2$ Hz, 1H), 2.18 (s, 3H), 1.21 (t, $J = 7.0$ Hz, 3H), 1.12 (s, 9H), 0.97 (s, 9H), 0.70 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.9, 168.5, 168.2, 147.4, 143.5, 143.3, 143.2, 140.9, 137.5, 137.1, 130.2, 130.0, 127.6, 127.3, 126.1, 126.0, 117.2, 62.3, 61.7, 59.1, 46.6, 46.2, 34.9, 34.6, 29.2, 29.0, 21.1, 14.0, 13.2; IR (neat): ν 2957.61, 2867.29, 1737.48, 1658.31, 1637.36, 1486.21, 1389.19, 1234.68, 1188.05, 1095.99, 1060.41, 877.13 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_5$ $[\text{M}+\text{H}]^+$: 519.3105, found: 519.3101.

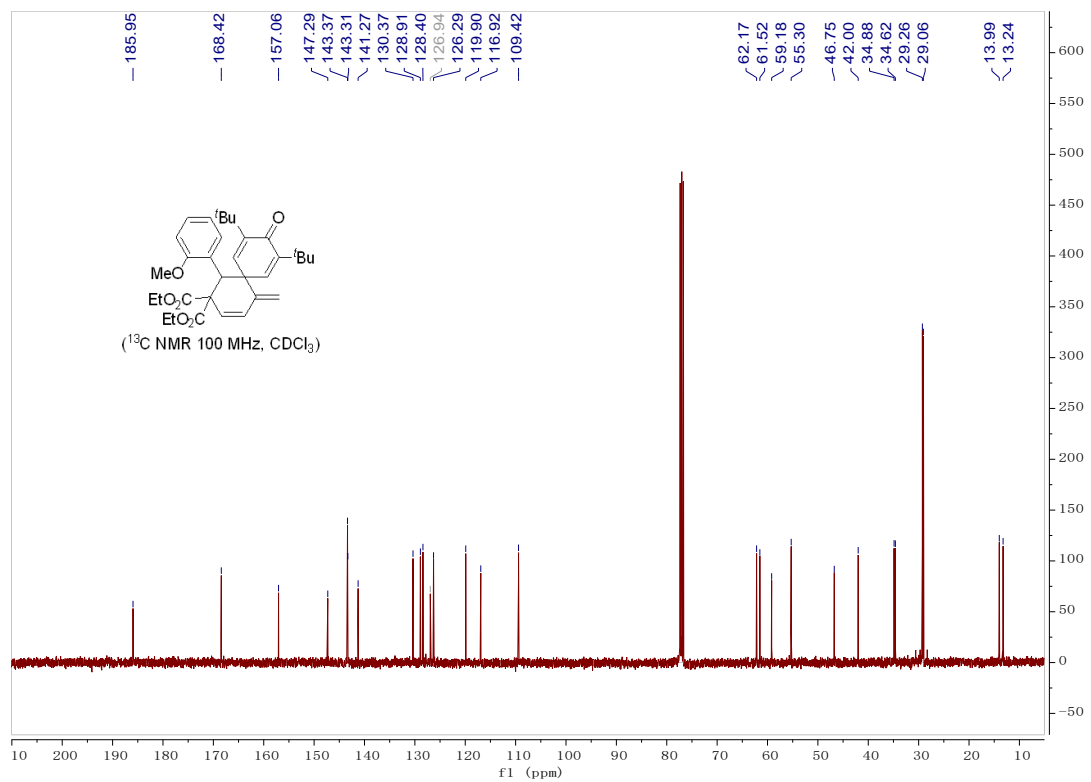


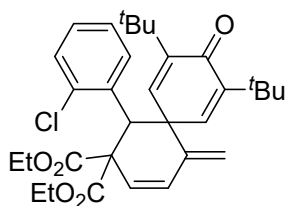




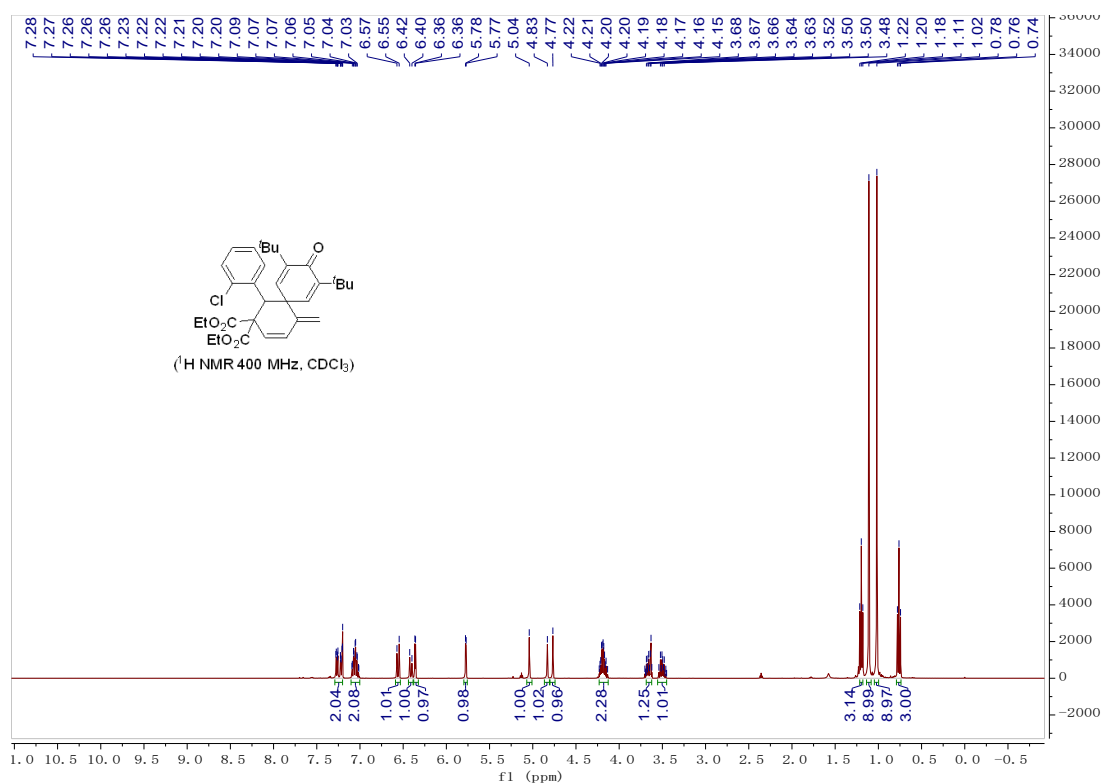
diethyl 8,10-di-tert-butyl-1-(2-methoxyphenyl)-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4k): Yield: 50%, a pale yellow solid, m.p. 149-151 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.14 – 7.07 (m, 2H), 6.73 – 6.68 (m, 2H), 6.54 (d, $J = 10.2$ Hz, 1H), 6.44 – 6.39 (m, 1H), 6.37 (d, $J = 3.0$ Hz, 1H), 5.87 (d, $J = 3.0$ Hz, 1H), 4.99 (s, 1H), 4.79 (s, 1H), 4.69 (s, 1H), 4.22 – 4.11 (m, 2H), 3.69 (s, 3H), 3.65 – 3.57 (m, 1H), 3.54 – 3.45 (m, 1H), 1.19 (t, $J = 7.0$ Hz, 3H), 1.11 (s, 9H), 0.99 (s, 9H), 0.68 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.9, 168.4, 157.1, 147.3, 143.4, 143.3, 141.3, 130.4, 128.9, 128.4, 126.9, 126.3, 119.9, 116.9, 109.4, 62.2, 61.5, 59.2, 55.3, 46.8, 42.0, 34.9, 34.6, 29.3, 29.1, 14.0, 13.2; IR (neat): ν 3004.67, 2956.77, 2912.15, 2861.68, 1735.68, 1715.26, 1657.98, 1634.51, 1491.63, 1245.04, 1058.50, 754.70 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{33}\text{H}_{43}\text{O}_6$ $[\text{M}+\text{H}]^+$: 535.3054, found: 535.3054.

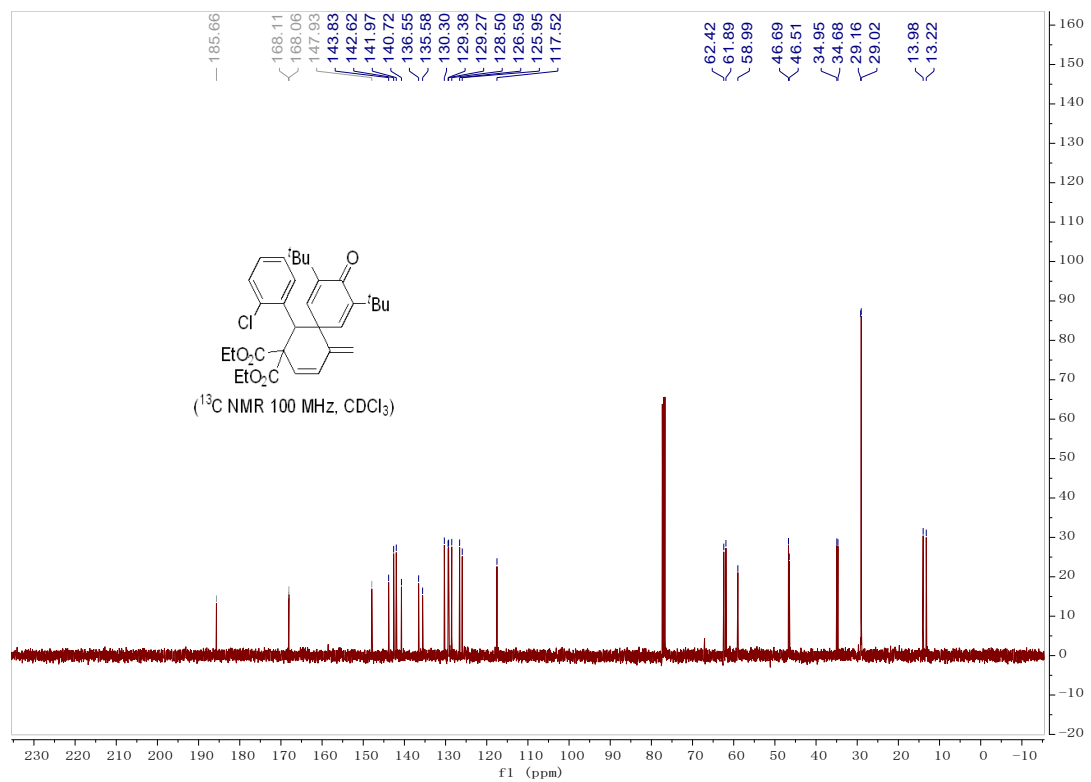


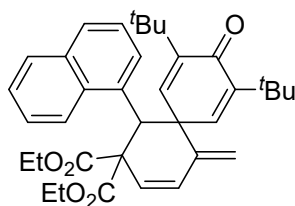




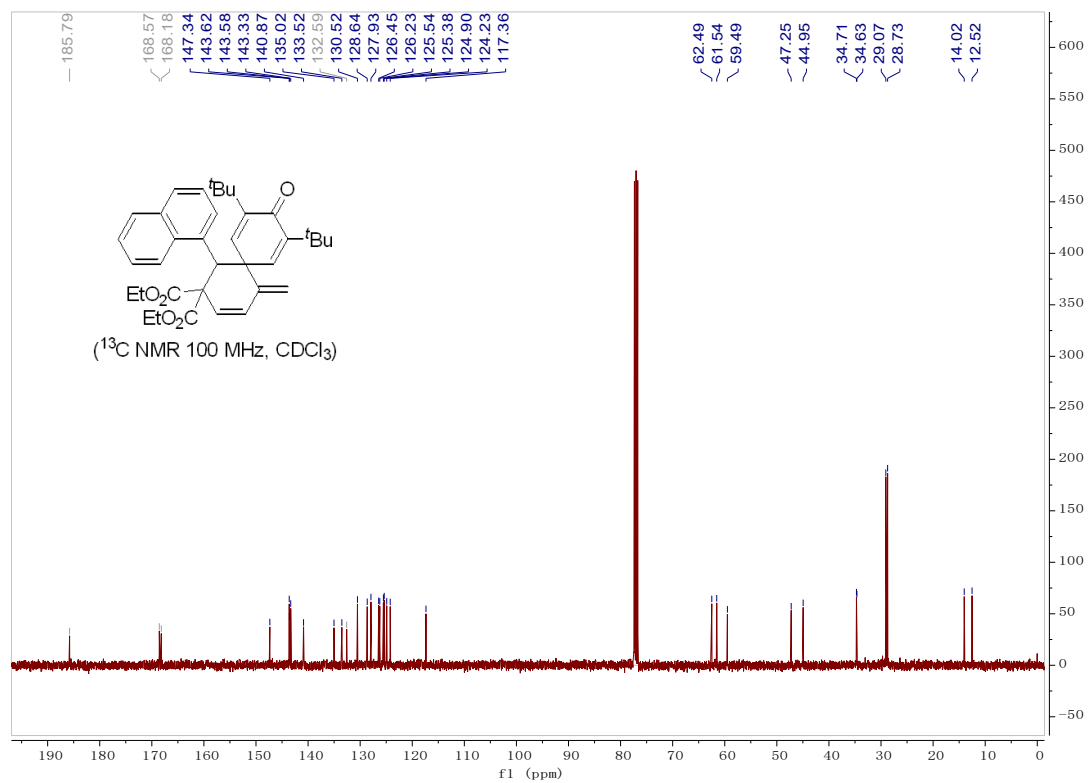
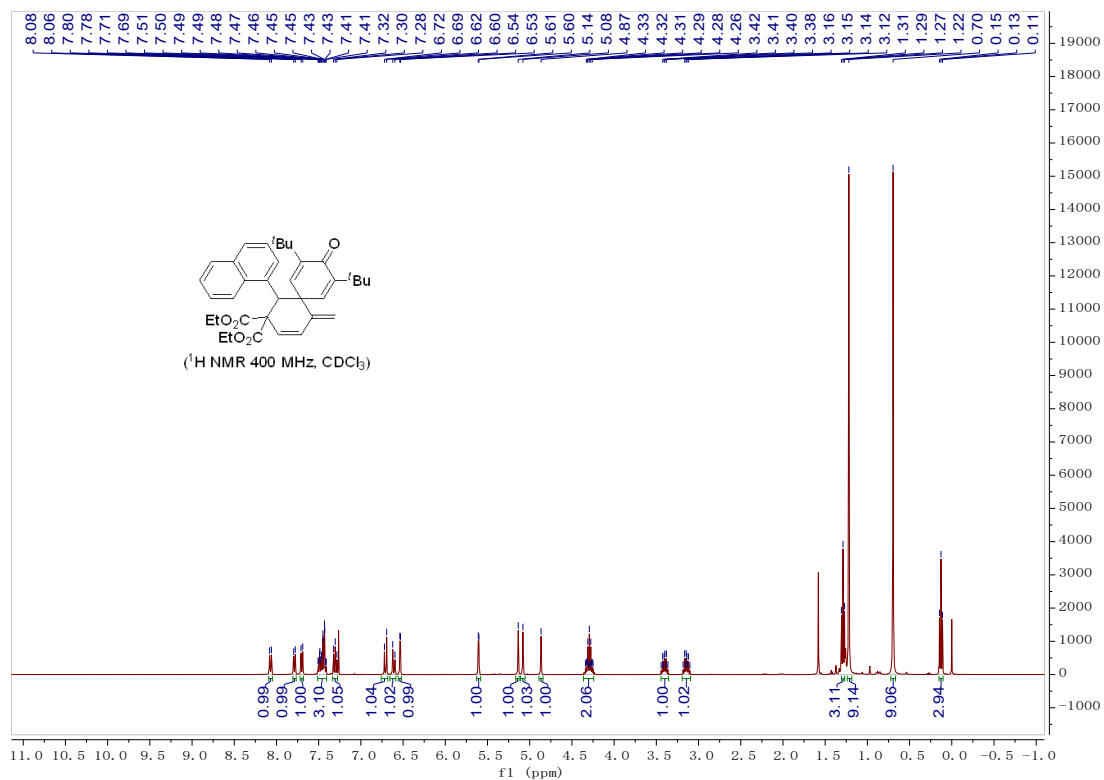
diethyl 8,10-di-*tert*-butyl-1-(2-chlorophenyl)-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4l): Yield: 70%, a pale yellow solid, m.p. 178-180 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.29 – 7.20 (m, 2H), 7.10 – 7.00 (m, 2H), 6.56 (d, $J = 10.2$ Hz, 1H), 6.41 (d, $J = 10.2$ Hz, 1H), 6.36 (d, $J = 3.0$ Hz, 1H), 5.77 (d, $J = 3.0$ Hz, 1H), 5.04 (s, 1H), 4.83 (s, 1H), 4.77 (s, 1H), 4.23 – 4.13 (m, 2H), 3.69 – 3.62 (m, 1H), 3.50 (dq, $J = 10.8, 7.2$ Hz, 1H), 1.20 (t, $J = 7.0$ Hz, 3H), 1.11 (s, 9H), 1.02 (s, 9H), 0.76 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.7, 168.11, 168.06, 147.9, 143.8, 142.6, 142.0, 140.7, 136.5, 135.6, 130.3, 129.4, 129.3, 128.5, 126.6, 125.9, 117.5, 62.4, 61.9, 59.0, 46.7, 46.5, 35.0, 34.7, 29.2, 29.0, 14.0, 13.2; IR (neat): ν 2957.67, 2920.56, 2861.68, 1732.83, 1655.84, 1633.73, 1387.22, 1364.19, 1238.51, 1196.34, 1097.14, 750.83 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{32}\text{H}_{40}\text{O}_5\text{Cl} [\text{M}+\text{H}]^+$: 539.2559, found: 539.2564.

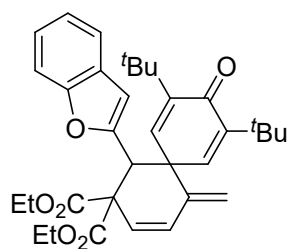




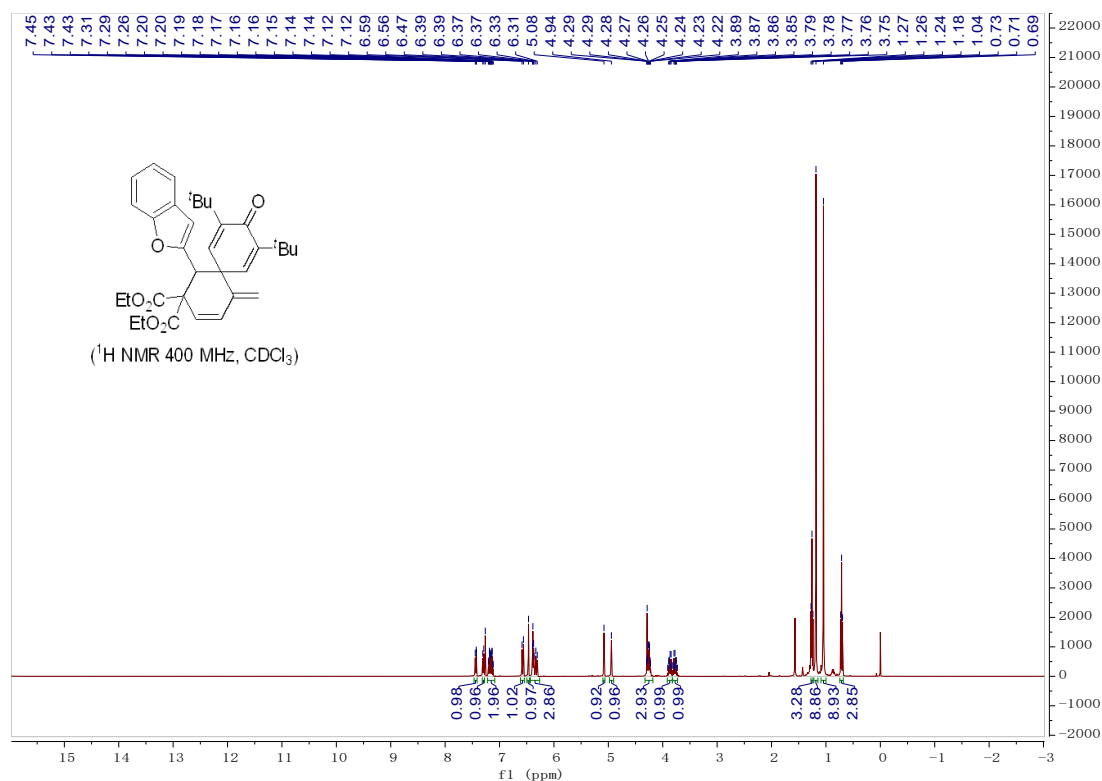


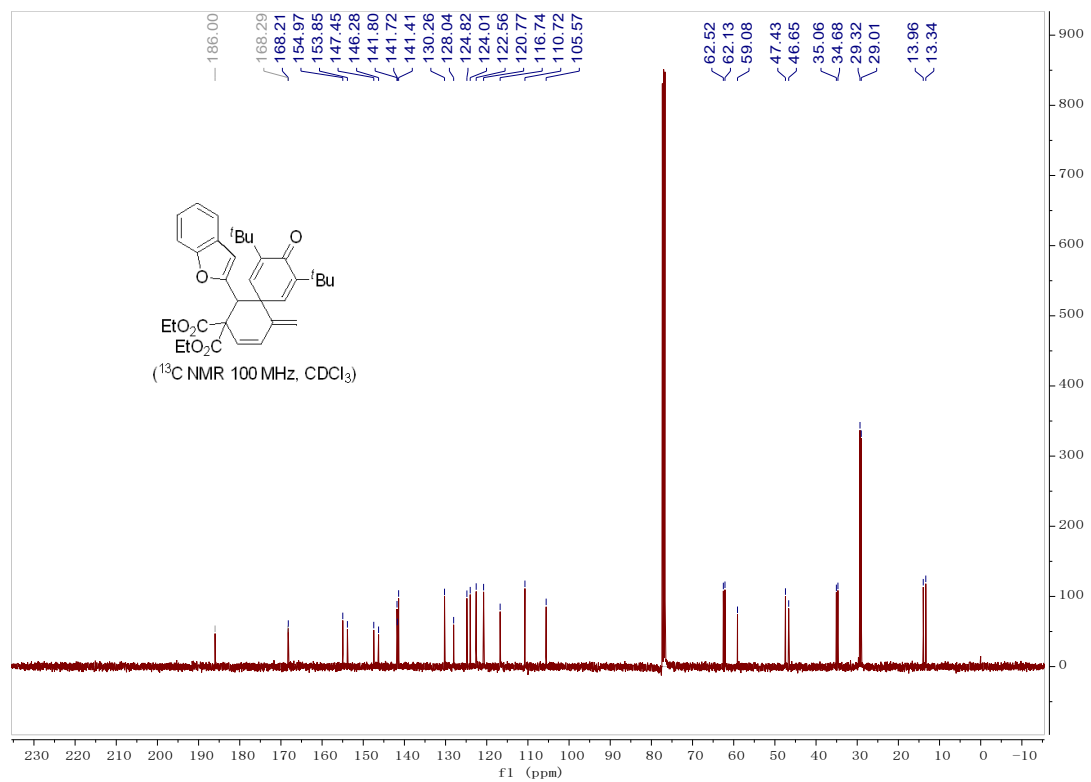
diethyl 8,10-di-*tert*-butyl-5-methylene-1-(naphthalen-1-yl)-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4m): Yield: 33%, a pale yellow solid, m.p. 181-183 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 8.07 (d, $J = 8.4$ Hz, 1H), 7.79 (d, $J = 7.2$ Hz, 1H), 7.70 (d, $J = 8.0$ Hz, 1H), 7.51 – 7.41 (m, 3H), 7.30 (t, $J = 7.8$ Hz, 1H), 6.71 (d, $J = 10.4$ Hz, 1H), 6.61 (d, $J = 10.4$ Hz, 1H), 6.53 (d, $J = 3.0$ Hz, 1H), 5.61 (d, $J = 3.0$ Hz, 1H), 5.14 (s, 1H), 5.08 (s, 1H), 4.87 (s, 1H), 4.36 – 4.24 (m, 2H), 3.40 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.14 (dq, $J = 10.8, 7.2$ Hz, 1H), 1.29 (t, $J = 7.0$ Hz, 3H), 1.22 (s, 9H), 0.70 (s, 9H), 0.13 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.8, 168.6, 168.2, 147.3, 143.62, 143.58, 143.3, 140.9, 135.0, 133.5, 132.6, 130.5, 128.6, 127.9, 126.4, 126.2, 125.5, 125.4, 124.9, 124.2, 117.4, 62.5, 61.5, 59.5, 47.2, 45.0, 34.7, 34.6, 29.1, 28.7, 14.0, 12.5; IR (neat): ν 2957.74, 2925.13, 1865.11, 1735.72, 1714.61, 1657.46, 1634.78, 1363.73, 1220.85, 1119.68, 1097.38, 798.03 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{36}\text{H}_{43}\text{O}_5$ $[\text{M}+\text{H}]^+$: 555.3105, found: 555.3106.

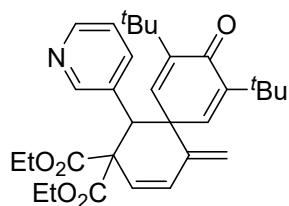




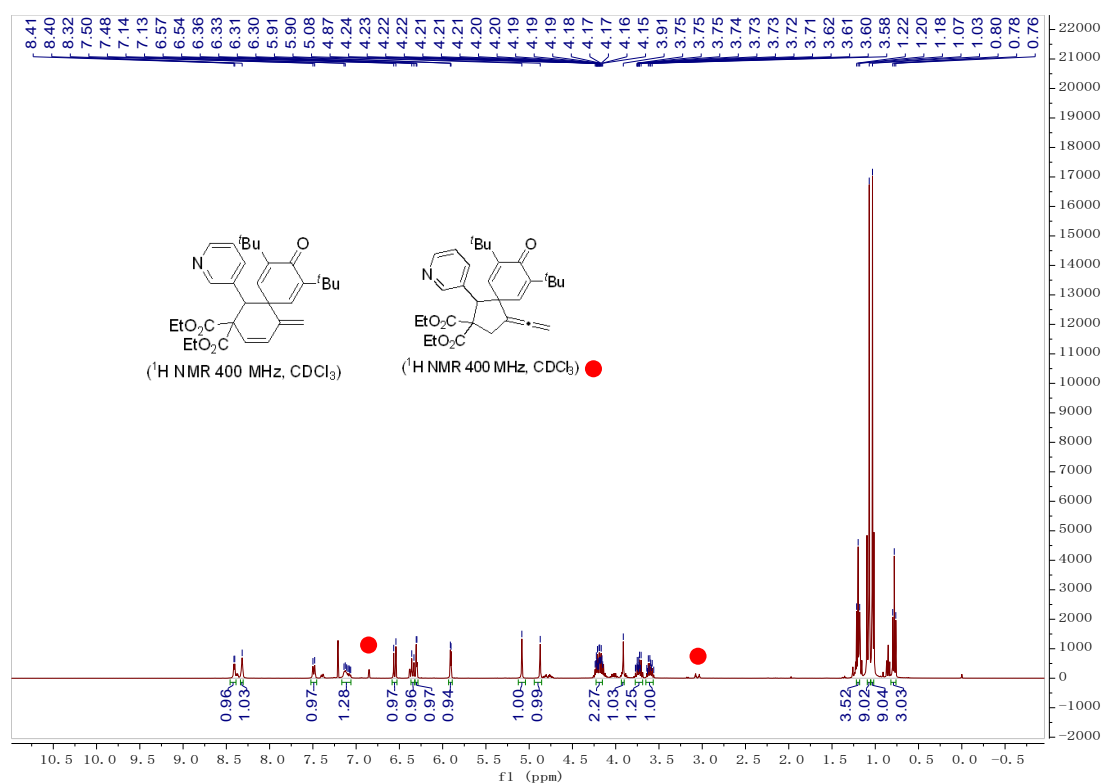
diethyl 1-(benzofuran-2-yl)-8,10-di-tert-butyl-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4n): Yield: 41%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.47 – 7.41 (m, 1H), 7.30 (d, $J = 8.2$ Hz, 1H), 7.22 – 7.09 (m, 2H), 6.57 (d, $J = 10.2$ Hz, 1H), 6.47 (s, 1H), 6.43 – 6.26 (m, 3H), 5.08 (s, 1H), 4.94 (s, 1H), 4.33 – 4.18 (m, 3H), 3.87 (dq, $J = 10.6, 7.0$ Hz, 1H), 3.77 (dq, $J = 10.6, 7.0$ Hz, 1H), 1.26 (t, $J = 7.0$ Hz, 3H), 1.18 (s, 9H), 1.04 (s, 9H), 0.71 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.3, 168.2, 155.0, 153.8, 147.4, 146.3, 141.8, 141.7, 141.4, 130.3, 128.0, 124.8, 124.0, 122.6, 120.8, 116.7, 110.7, 105.6, 62.5, 62.1, 59.1, 47.4, 46.6, 35.1, 34.7, 29.3, 29.0, 14.0, 13.3; IR (neat): ν 2998.18, 2958.05, 2865.11, 1728.71, 1714.38, 1660.28, 1638.88, 1454.34, 1364.47, 1252.77, 1189.47, 908.16, 752.15 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{34}\text{H}_{41}\text{O}_6$ $[\text{M}+\text{H}]^+$: 545.2898, found: 545.2895.

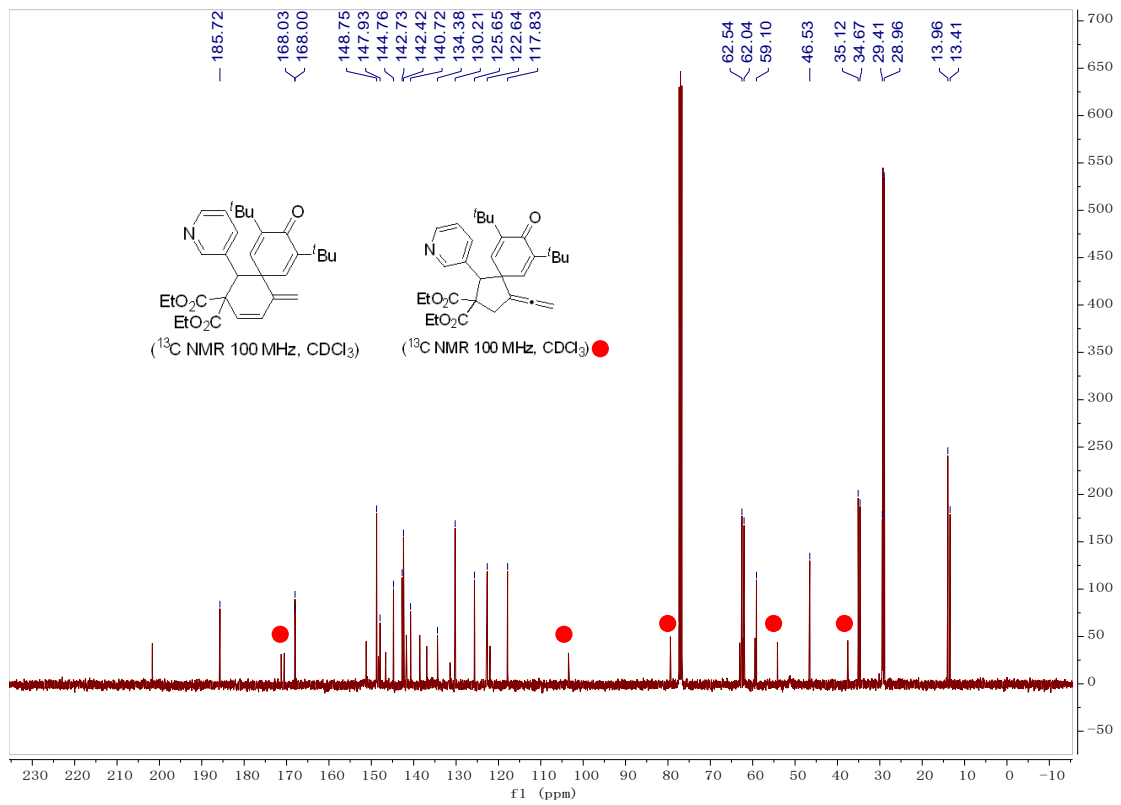


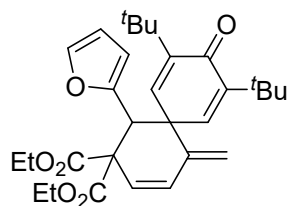




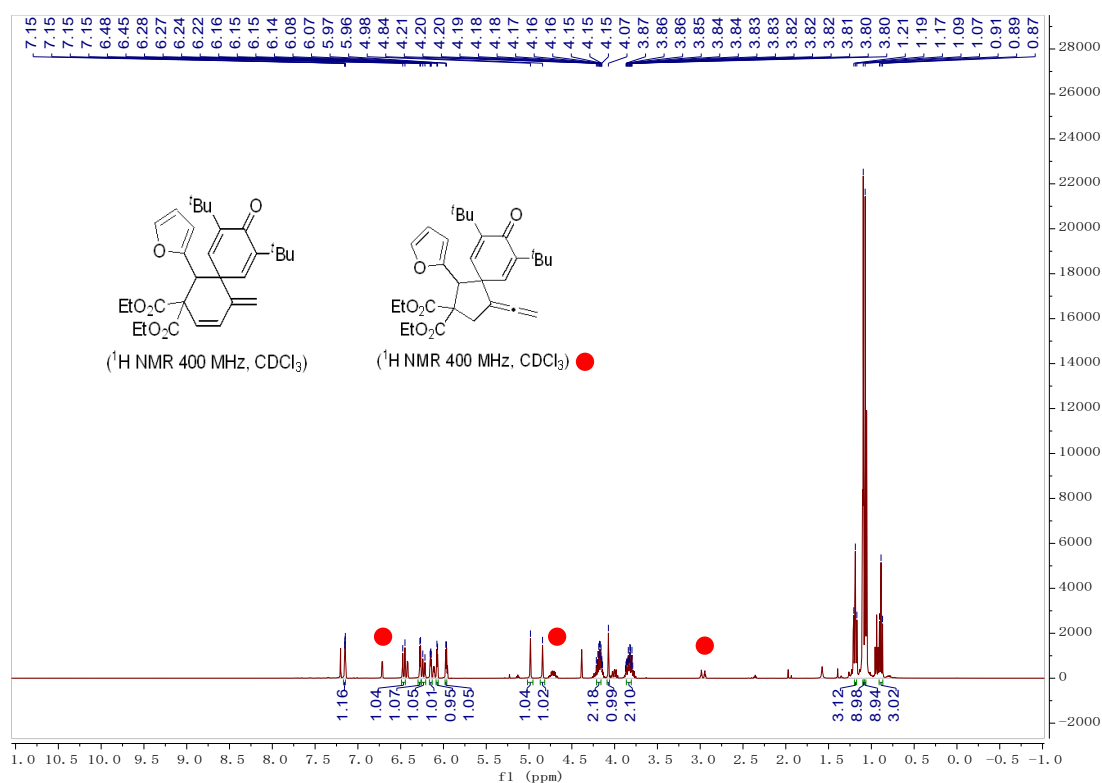
diethyl 8,10-di-*tert*-butyl-5-methylene-9-oxo-1-(pyridin-3-yl)spiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (40): Yield: 35%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. It contained some pentacyclic products ^1H NMR (400 MHz, CDCl_3 , TMS) δ 8.41 (d, $J = 3.8$ Hz, 1H), 8.32 (s, 1H), 7.49 (d, $J = 8.0$ Hz, 1H), 7.17 – 7.06 (m, 1H), 6.55 (d, $J = 10.2$ Hz, 1H), 6.34 (d, $J = 10.2$ Hz, 1H), 6.30 (d, $J = 3.0$ Hz, 1H), 5.91 (d, $J = 3.0$ Hz, 1H), 5.08 (s, 1H), 4.87 (s, 1H), 4.23 – 4.15 (m, 2H), 3.91 (s, 1H), 3.77 – 3.69 (m, 1H), 3.65 – 3.57 (m, 1H), 1.21 (t, $J = 7.0$ Hz, 3H), 1.07 (s, 9H), 1.03 (s, 9H), 0.78 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.7, 168.03, 168.00, 148.8, 147.9, 144.8, 142.7, 142.4, 140.7, 134.4, 130.2, 125.7, 122.6, 117.8, 62.5, 62.0, 59.1, 46.5, 35.1, 34.7, 29.4, 29.0, 14.0, 13.4; IR (neat): ν 2957.85, 2906.54, 2864.49, 1734.69, 1659.04, 1637.82, 1389.13, 1116.72, 1061.02, 948.10, 910.03, 30.88 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{31}\text{H}_{40}\text{NO}_5$ $[\text{M}+\text{H}]^+$: 506.2901, found: 506.2896.

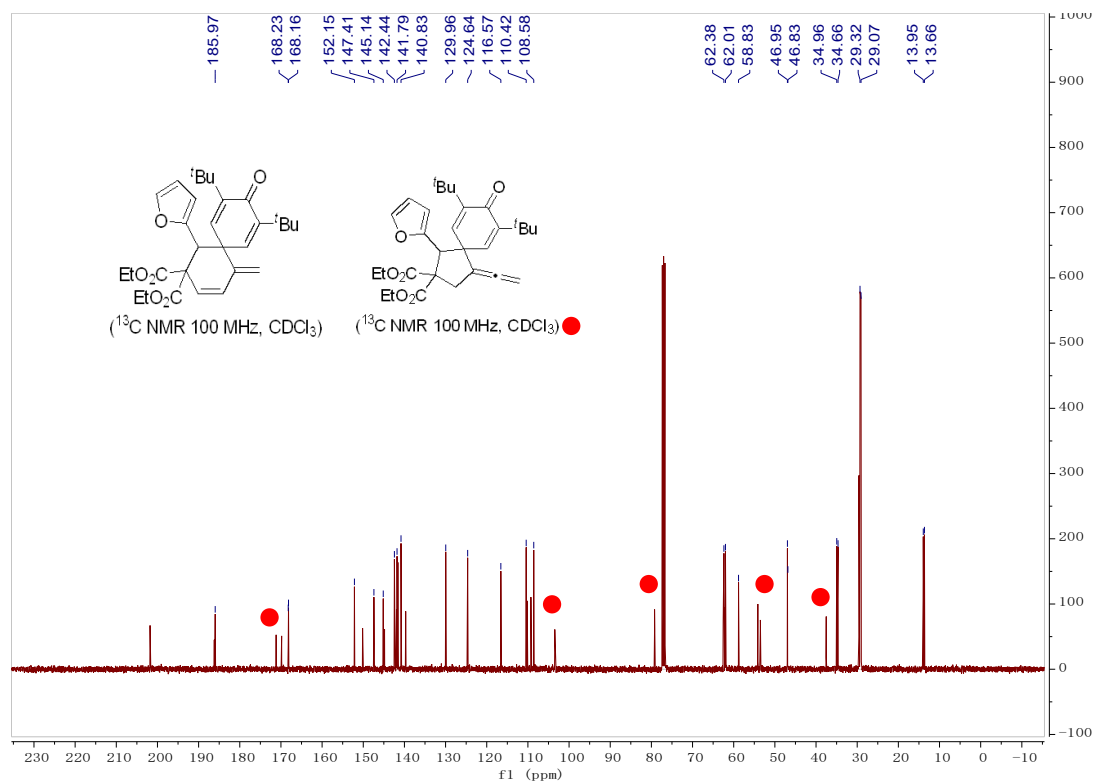


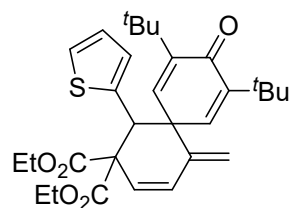




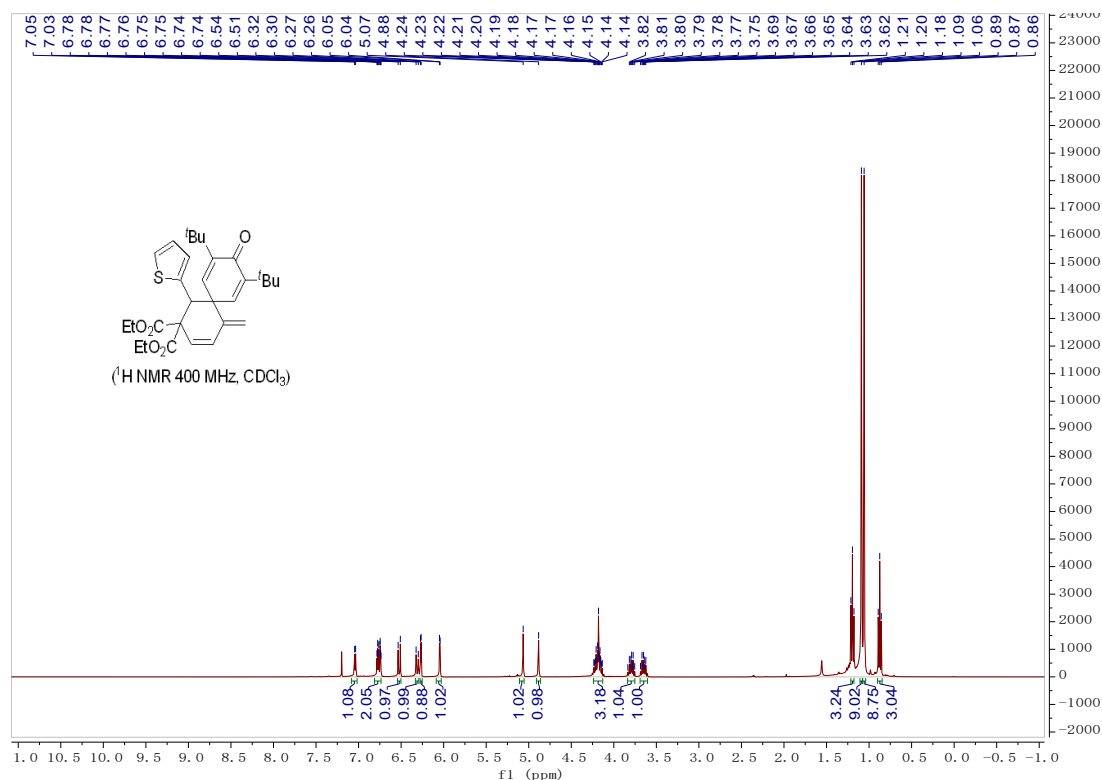
diethyl 8,10-di-*tert*-butyl-1-(furan-2-yl)-5-methylene-9-oxospiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4p): Yield: 55%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. It contained some pentacyclic products ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.17 – 7.14 (m, 1H), 6.46 (d, $J = 10.2$ Hz, 1H), 6.27 (d, $J = 3.0$ Hz, 1H), 6.23 (d, $J = 10.2$ Hz, 1H), 6.16 – 6.13 (m, 1H), 6.07 (d, $J = 3.0$ Hz, 1H), 5.98 – 5.96 (m, 1H), 4.98 (s, 1H), 4.84 (s, 1H), 4.21 – 4.16 (m, 2H), 4.07 (s, 1H), 3.86 – 3.81 (m, 2H), 1.19 (t, $J = 7.0$ Hz, 3H), 1.09 (s, 9H), 1.07 (s, 9H), 0.89 (t, $J = 7.0$ Hz, 3H); ^{13}C $\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.23, 168.16, 152.1, 147.4, 145.1, 142.4, 141.8, 140.8, 130.0, 124.6, 116.6, 110.4, 108.6, 62.4, 62.0, 58.8, 47.0, 46.8, 35.0, 34.7, 29.3, 29.1, 13.9, 13.7; IR (neat): ν 2957.39, 2903.74, 2864.49, 1731.65, 1659.48, 1637.88, 1499.21, 1388.81, 1366.02, 1255.67, 1189.83, 1034.24, 732.83 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{30}\text{H}_{39}\text{O}_6$ $[\text{M}+\text{H}]^+$: 495.2741, found: 495.2739.

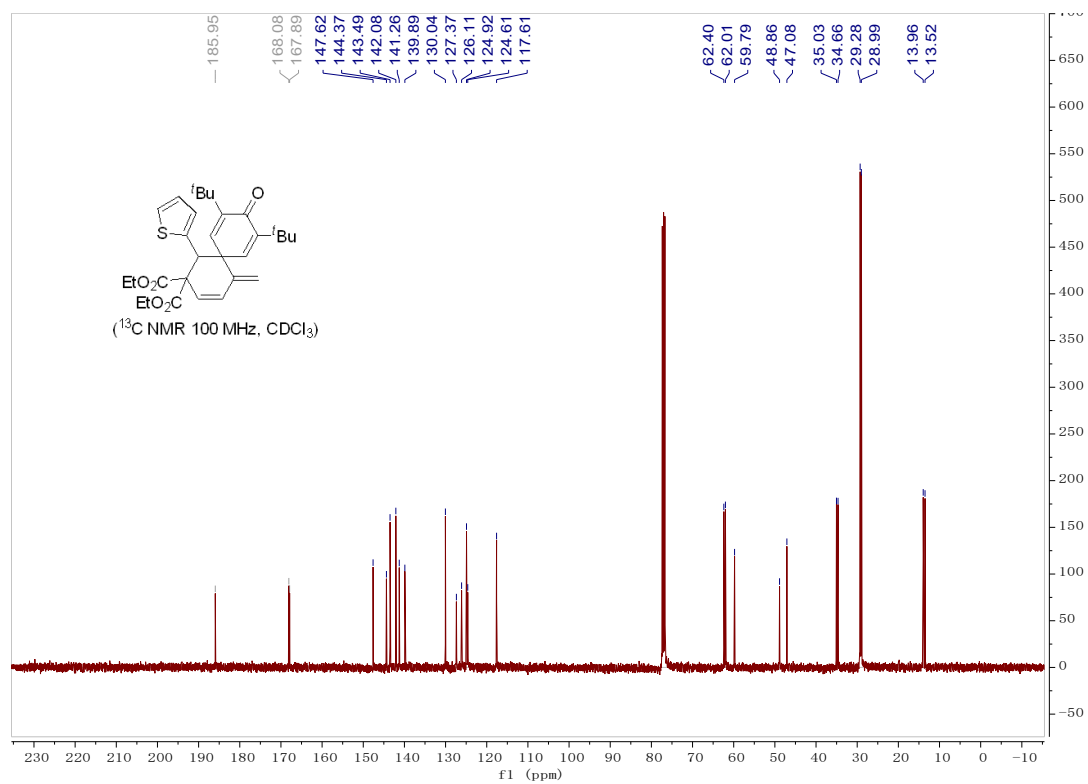


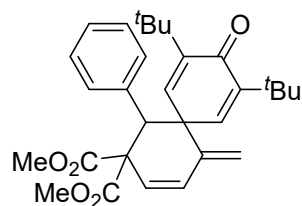




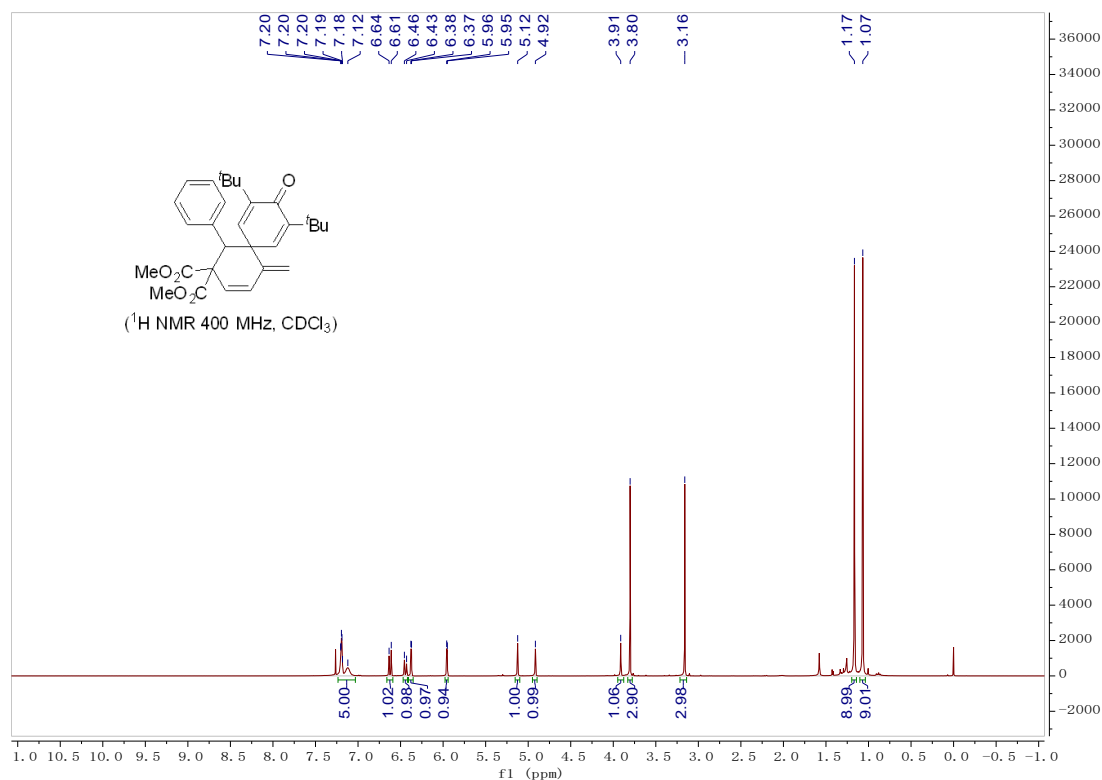
diethyl 8,10-di-*tert*-butyl-5-methylene-9-oxo-1-(thiophen-2-yl)spiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4p): Yield: 60%, a pale yellow solid, m.p. 150-152 °C; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.04 (d, $J = 4.8$ Hz, 1H), 6.81 – 6.74 (m, 2H), 6.52 (d, $J = 10.2$ Hz, 1H), 6.31 (d, $J = 10.2$ Hz, 1H), 6.27 (d, $J = 3.0$ Hz, 1H), 6.05 (d, $J = 3.0$ Hz, 1H), 5.07 (s, 1H), 4.88 (s, 1H), 4.24 – 4.13 (m, 3H), 3.79 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.69 – 3.60 (m, 1H), 1.20 (t, $J = 7.0$ Hz, 3H), 1.09 (s, 9H), 1.06 (s, 9H), 0.87 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.1, 167.9, 147.6, 144.4, 143.5, 142.1, 141.3, 139.9, 130.0, 127.4, 126.1, 124.9, 124.6, 117.6, 62.4, 62.0, 59.8, 48.9, 47.1, 35.0, 34.7, 29.3, 29.0, 14.0, 13.5; IR (neat): ν 3006.01, 2961.66, 2865.11, 1737.93, 1711.32, 1659.14, 1359.25, 1220.16, 1190.00, 10927, 1033.45, 904.12, 709.91 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{30}\text{H}_{39}\text{O}_5\text{S}$ $[\text{M}+\text{H}]^+$: 511.2513, found: 511.2513.

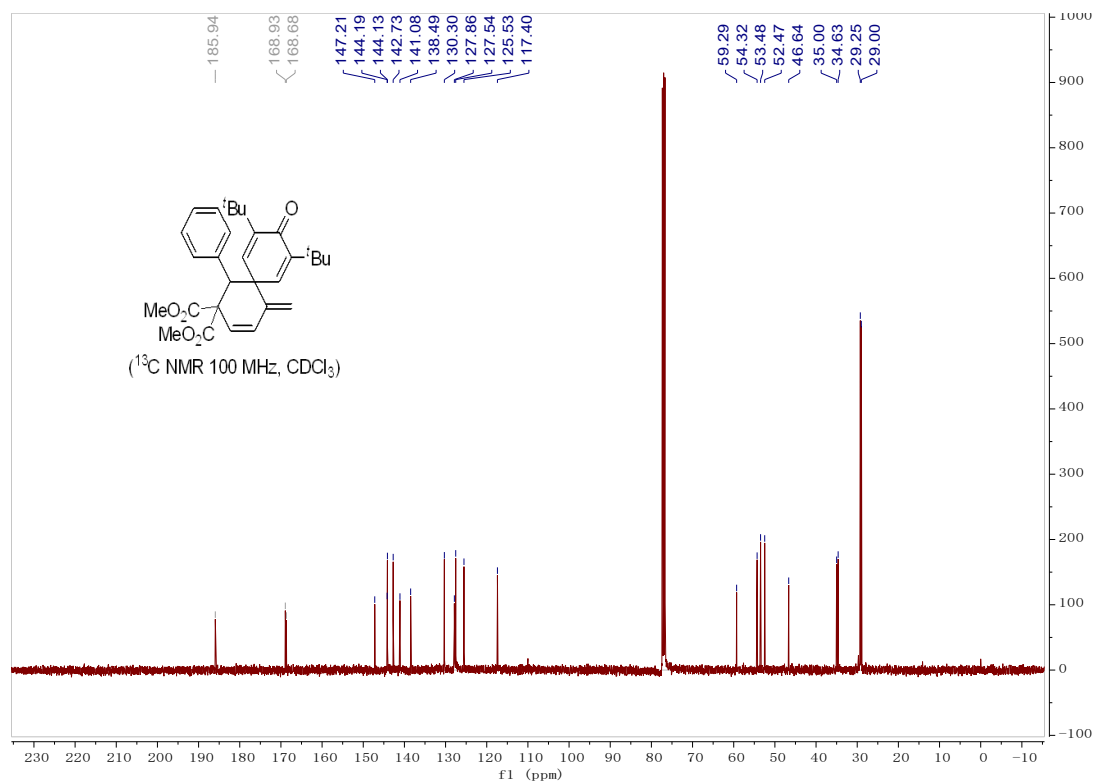


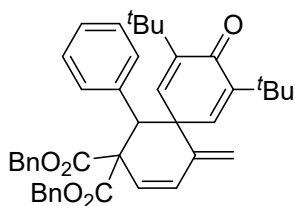




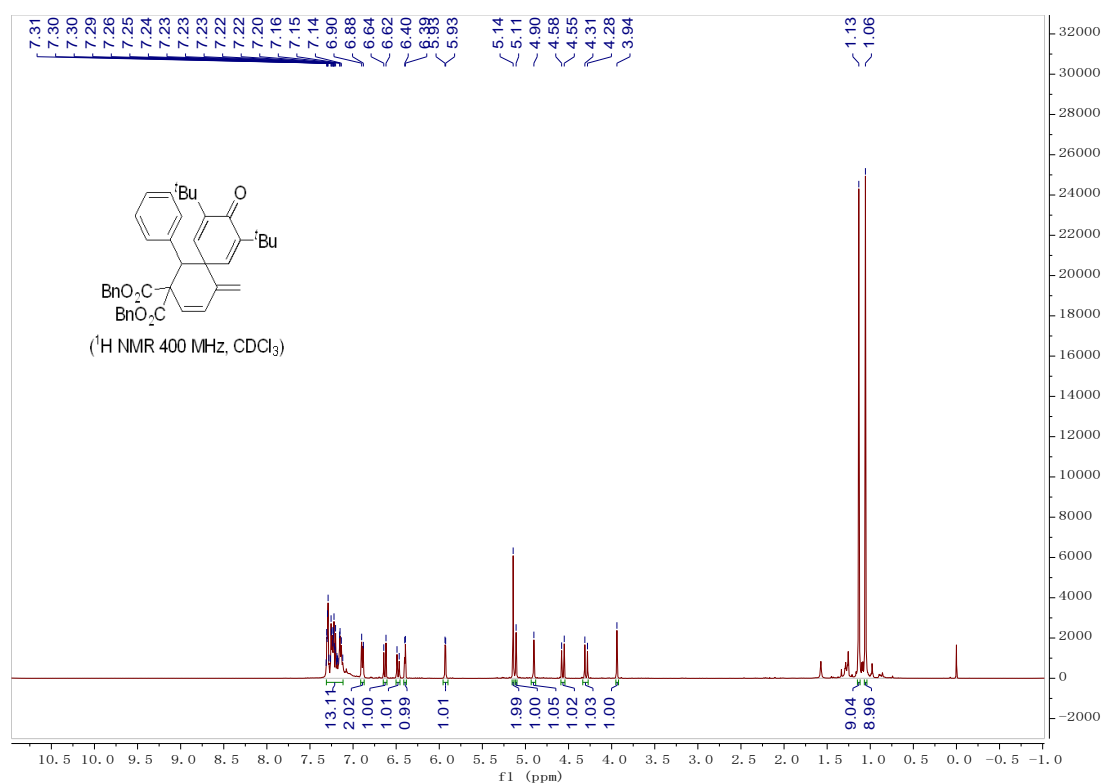
dimethyl 8,10-di-*tert*-butyl-5-methylene-9-oxo-1-phenylspiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4r): Yield: 27%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.24 – 7.03 (m, 5H), 6.62 (d, $J = 10.2$ Hz, 1H), 6.44 (d, $J = 10.2$ Hz, 1H), 6.38 (d, $J = 3.0$ Hz, 1H), 5.95 (d, $J = 3.0$ Hz, 1H), 5.12 (s, 1H), 4.92 (s, 1H), 3.91 (s, 1H), 3.80 (s, 3H), 3.16 (s, 3H), 1.17 (s, 9H), 1.07 (s, 9H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 185.9, 168.9, 168.7, 147.2, 144.2, 144.1, 142.7, 141.1, 138.5, 130.3, 127.9, 127.5, 125.5, 117.4, 59.3, 54.3, 53.5, 52.5, 46.6, 35.0, 34.6, 29.2, 29.0; IR (neat): ν 3000.79, 2954.59, 2862.51, 1740.97, 1714.69, 1658.50, 1635.53, 1454.86, 1433.05, 1364.34, 1251.39, 1179.72, 906.92 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{30}\text{H}_{37}\text{O}_5$ $[\text{M}+\text{H}]^+$: 477.2636, found: 477.2632.

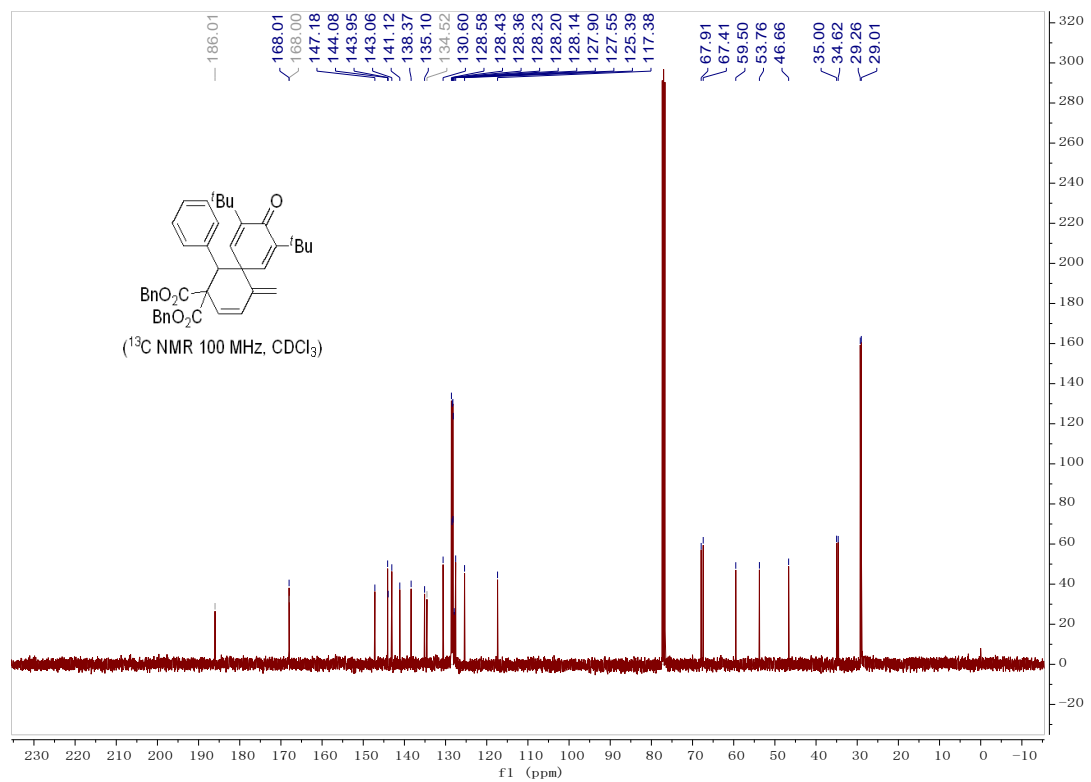


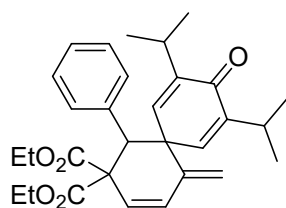




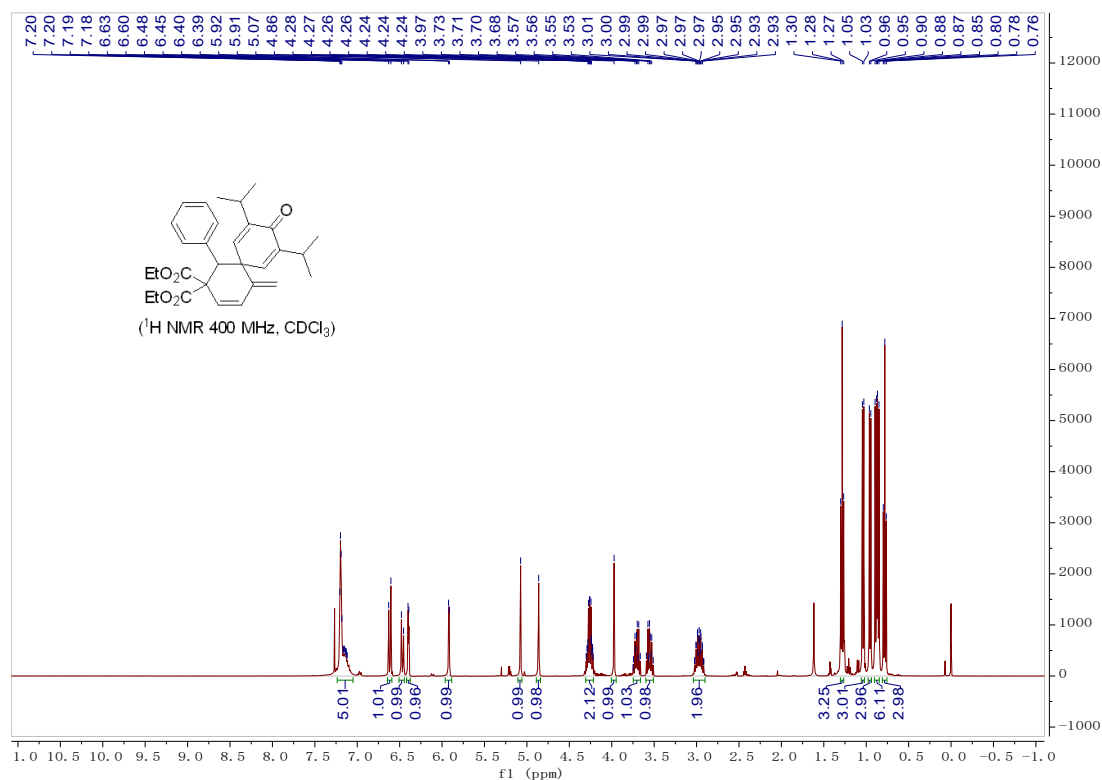
dibenzyl 8,10-di-tert-butyl-5-methylene-9-oxo-1-phenylspiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4s): Yield: 50%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.31 – 7.12 (m, 13H), 6.89 (d, $J = 8.0$ Hz, 2H), 6.63 (d, $J = 10.2$ Hz, 1H), 6.48 (d, $J = 10.2$ Hz, 1H), 6.40 (d, $J = 3.0$ Hz, 1H), 5.93 (d, $J = 3.0$ Hz, 1H), 5.14 (s, 2H), 5.11 (s, 1H), 4.90 (s, 1H), 4.57 (d, $J = 12.2$ Hz, 1H), 4.30 (d, $J = 12.2$ Hz, 1H), 3.94 (s, 1H), 1.13 (s, 9H), 1.06 (s, 9H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.0, 168.01, 168.00, 147.2, 144.1, 144.0, 143.1, 141.1, 138.4, 135.1, 134.5, 130.6, 128.6, 128.43, 128.36, 128.23, 128.20, 128.1, 127.9, 127.5, 125.4, 117.4, 67.9, 67.4, 59.5, 53.8, 46.7, 35.0, 34.6, 29.3, 29.0; IR (neat): ν 3003.40, 2959.05, 2865.11, 1711.81, 1659.34, 1637.01, 1358.94, 1220.12, 1163.54, 1131.12, 1090.95, 907.46, 698.96 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{42}\text{H}_{45}\text{O}_5$ $[\text{M}+\text{H}]^+$: 629.3262, found: 629.3263.

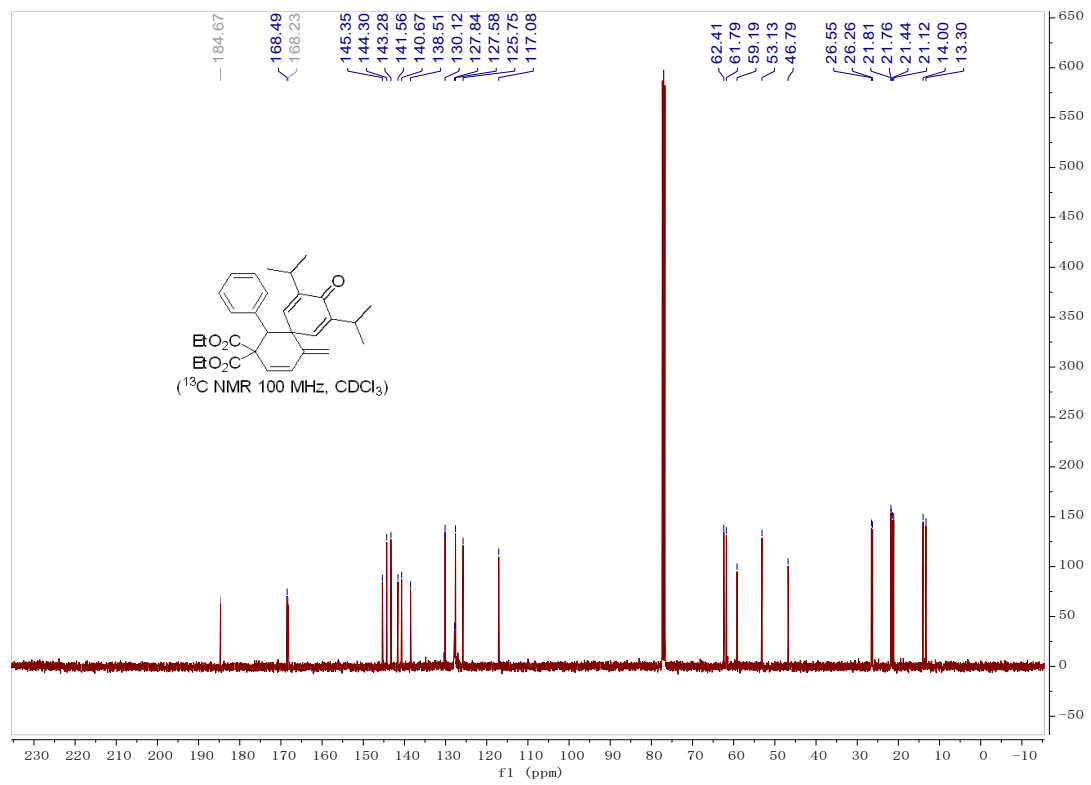


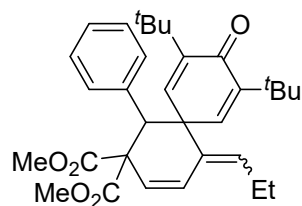




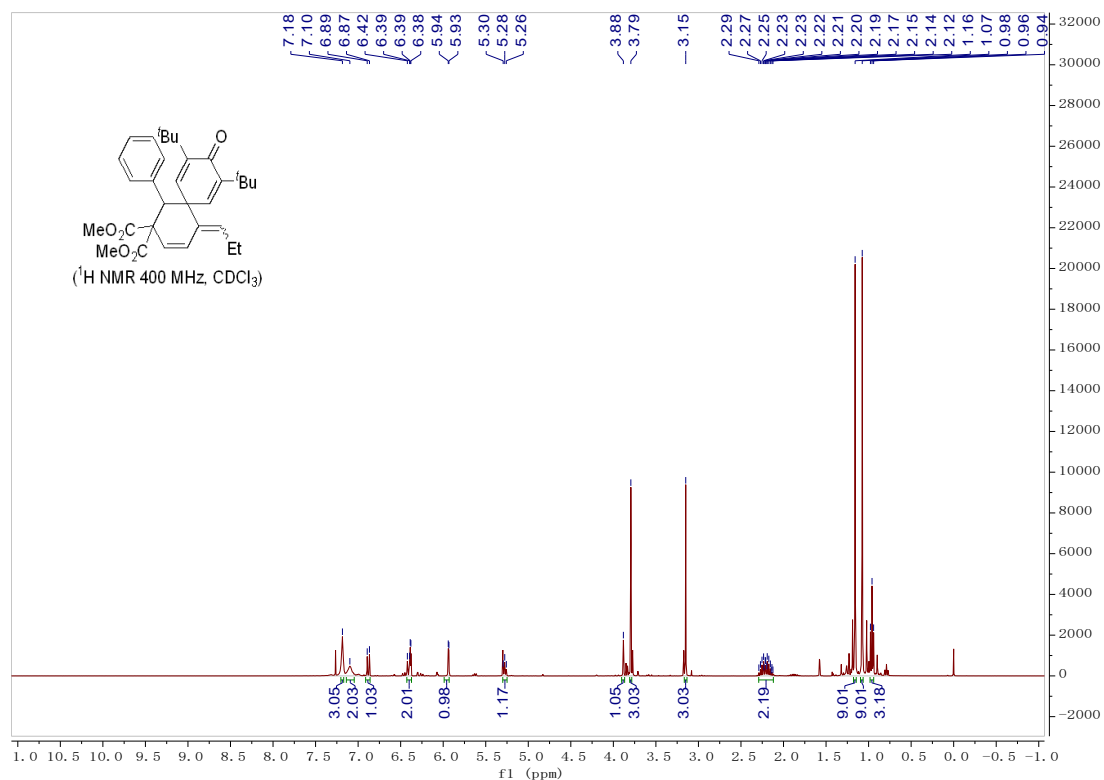
diethyl 8,10-diisopropyl-5-methylene-9-oxo-1-phenylspiro[5.5]undeca-3,7,10-triene-2,2-dicarboxylate (4t): Yield: 50%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.24 – 7.05 (m, 5H), 6.62 (d, $J = 10.2$ Hz, 1H), 6.47 (d, $J = 10.2$ Hz, 1H), 6.40 (d, $J = 3.8$ Hz, 1H), 5.92 (d, $J = 3.8$ Hz, 1H), 5.07 (s, 1H), 4.86 (s, 1H), 4.31 – 4.22 (m, 2H), 3.97 (s, 1H), 3.70 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.55 (dq, $J = 10.8, 7.2$ Hz, 1H), 3.04 – 2.90 (m, 2H), 1.28 (t, $J = 7.0$ Hz, 3H), 1.04 (d, $J = 6.8$ Hz, 3H), 0.95 (d, $J = 6.8$ Hz, 3H), 0.90 – 0.85 (m, 6H), 0.78 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 184.7, 168.5, 168.2, 145.4, 144.3, 143.3, 141.6, 140.7, 138.5, 130.1, 127.8, 127.6, 125.8, 117.1, 62.4, 61.8, 59.2, 53.1, 46.8, 26.6, 26.3, 21.81, 21.76, 21.4, 21.1, 14.0, 13.3; IR (neat): ν 2960.15, 2930.34, 2870.33, 1735.83, 1714.46, 1637.78, 1463.74, 1233.78, 1220.32, 1182.55, 1083.45, 1058.36 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{30}\text{H}_{37}\text{O}_5$ $[\text{M}+\text{H}]^+$: 477.2636, found: 477.2634.

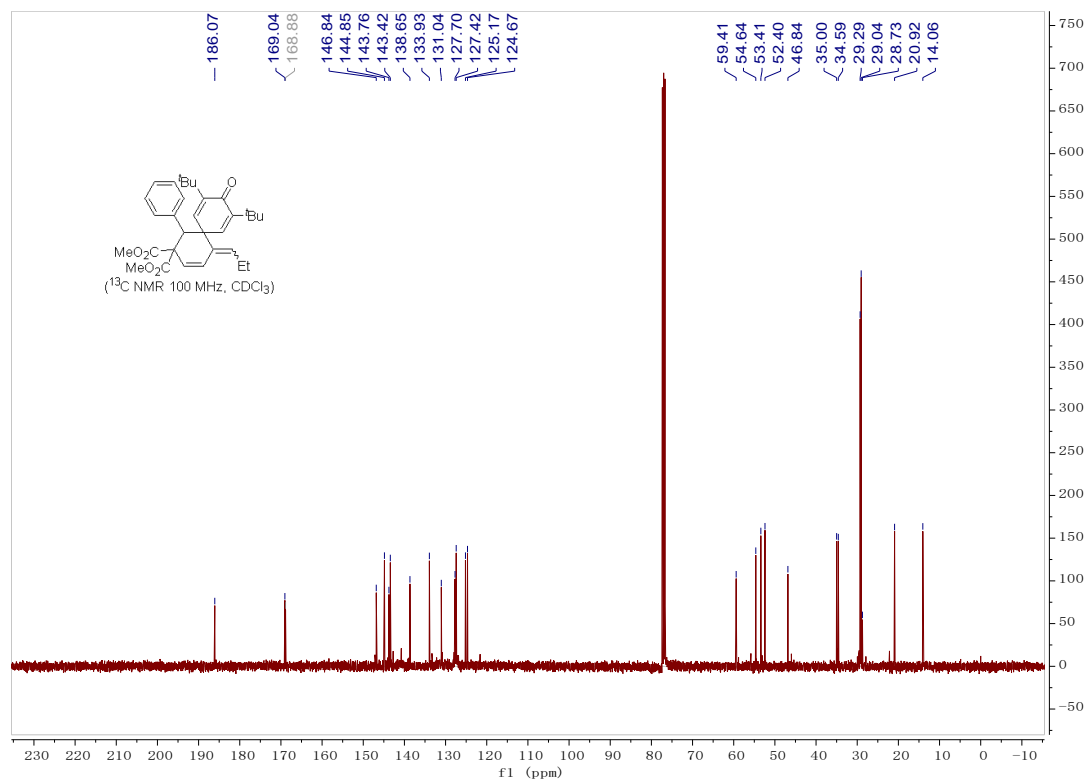


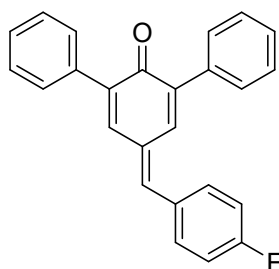




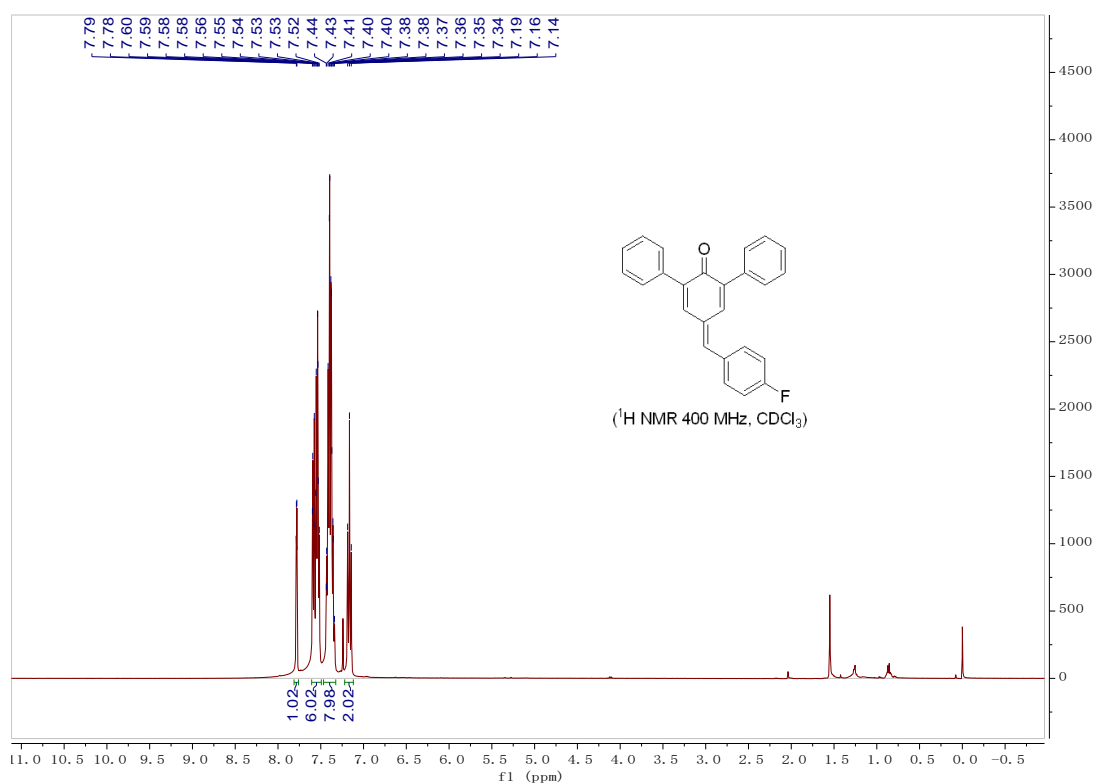
dimethyl 8,10-di-*tert*-butyl-9-oxo-1-phenyl-5-propylidene-2,2-dicarboxylate (4u): Yield: 44%, a colorless oil; Eluent: PE/EA = 30/1. Yield was determined by ^1H NMR using dibromomethane as an internal standard. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.18 (s, 3H), 7.10 (s, 2H), 6.88 (d, $J = 10.4$ Hz, 1H), 6.43 – 6.37 (m, 2H), 5.94 (d, $J = 3.0$ Hz, 1H), 5.28 (t, $J = 7.4$ Hz, 1H), 3.88 (s, 1H), 3.79 (s, 3H), 3.15 (s, 3H), 2.29 – 2.12 (m, 2H), 1.16 (s, 9H), 1.07 (s, 9H), 0.96 (t, $J = 7.4$ Hz, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 186.1, 169.0, 168.9, 146.8, 144.9, 143.8, 143.4, 138.7, 133.9, 131.0, 127.7, 127.4, 125.2, 124.7, 59.4, 54.6, 53.4, 52.4, 46.8, 35.0, 34.6, 29.3, 29.0, 28.7, 20.9, 14.1; IR (neat): ν 300.79, 2954.49, 2865.11, 1740.73, 1715.78, 1656.69, 1634.65, 1234.12, 1270, 1200.68, 1177.94, 1057.16, 914.75 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{32}\text{H}_{41}\text{O}_5$ $[\text{M}+\text{H}]^+$: 505.2949, found: 505.2948.

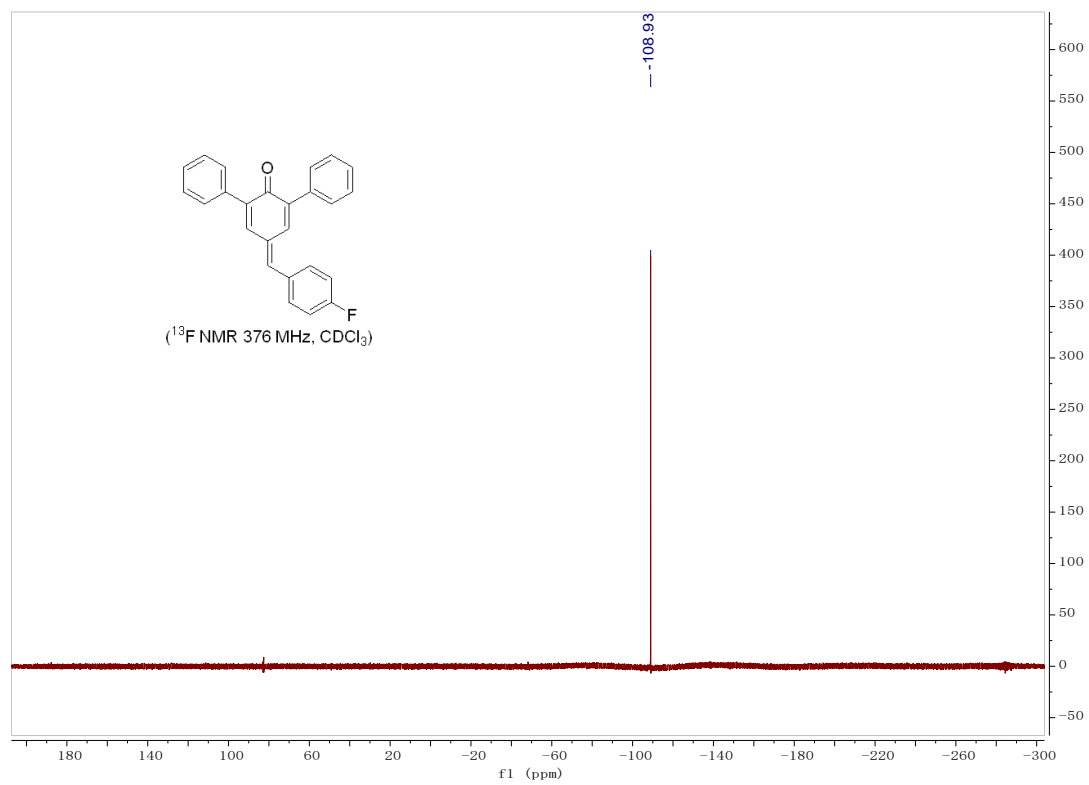
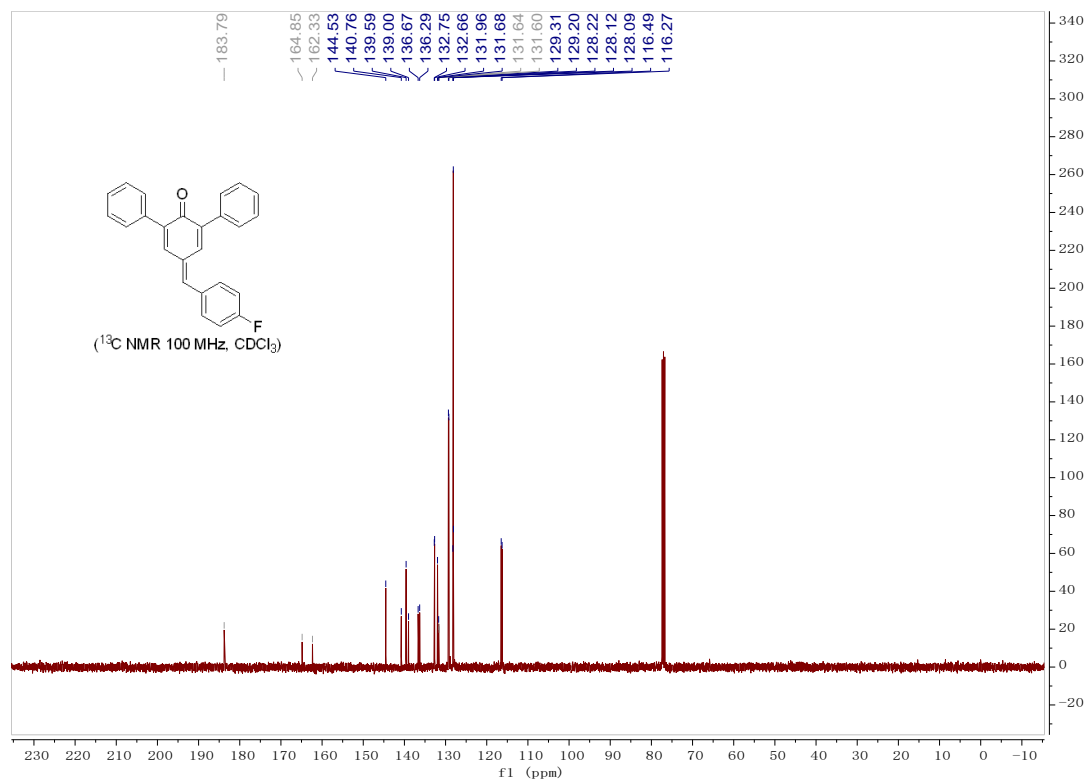


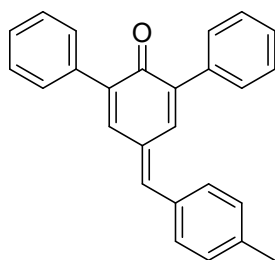




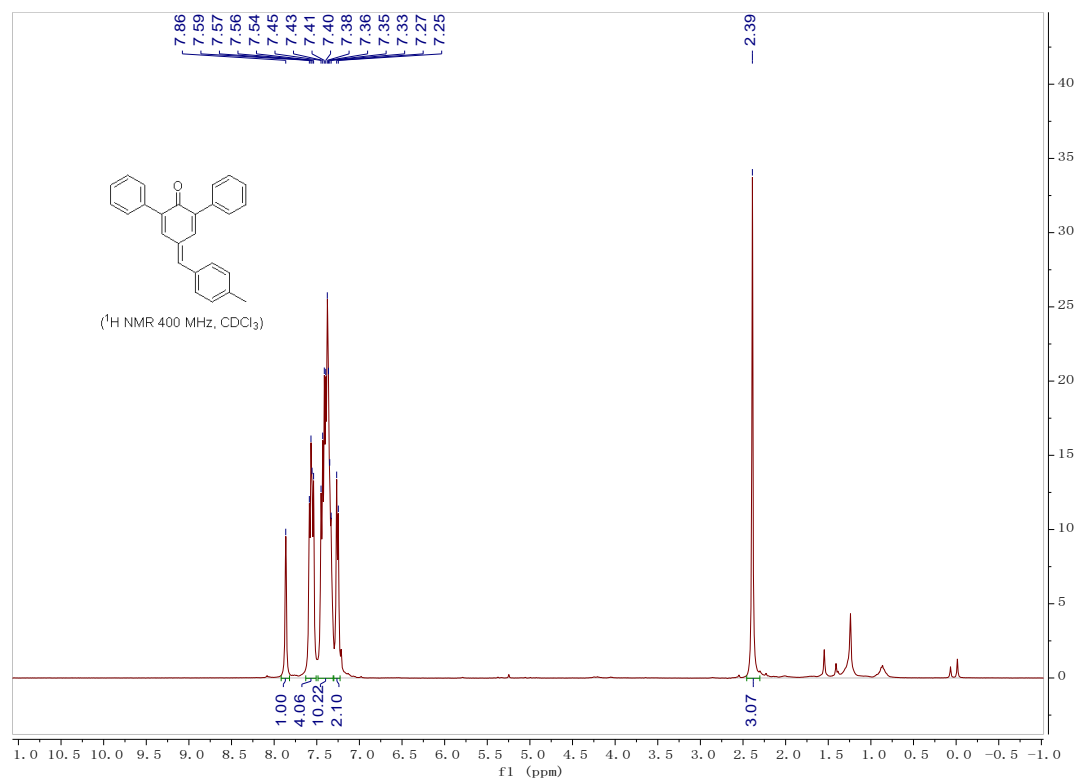
5'-(4-fluorobenzylidene)-[1,1':3',1''-terphenyl]-2'(5'*H*)-one (1z): Yield: 0.334 g, 95%, a yellow solid, m.p. 196-198 °C; Eluent: PE/DCM = 20/1. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.78 (d, *J* = 2.4 Hz, 1H), 7.61 – 7.49 (m, 6H), 7.47 – 7.32 (m, 8H), 7.16 (t, *J* = 8.6 Hz, 2H); ¹³C{¹H}-NMR (100 MHz, CDCl₃, TMS) δ 183.8, 163.6 (d, *J* = 253.0 Hz), 144.5, 140.8, 139.6, 139.0, 136.7, 136.3, 132.7 (d, *J* = 8.4 Hz), 132.0, 131.68, 131.66, 131.6 (d, *J* = 3.2 Hz), 129.3, 129.2, 128.2, 128.12, 128.09, 116.4 (d, *J* = 22.0 Hz); ¹⁹F NMR (376 MHz, CDCl₃) δ -108.93; IR (neat): ν 3055.59, 3032.10, 2956.44, 2852.07, 1712.58, 1504.64, 1461.68, 1225.86, 1157.99, 780.00, 697.62 cm⁻¹; HRMS (DART) Calcd for C₂₅H₁₈OF [M+H]⁺ : 353.1336, found: 353.1334.

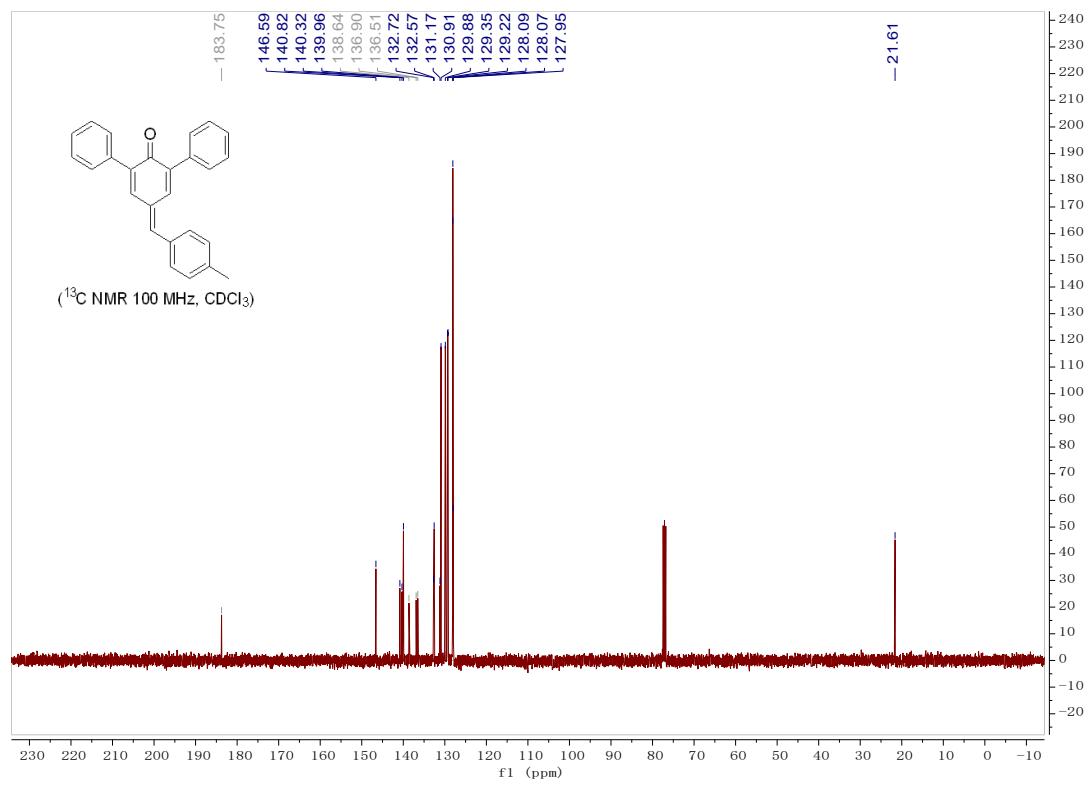


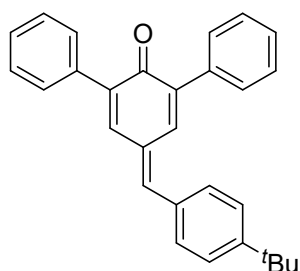




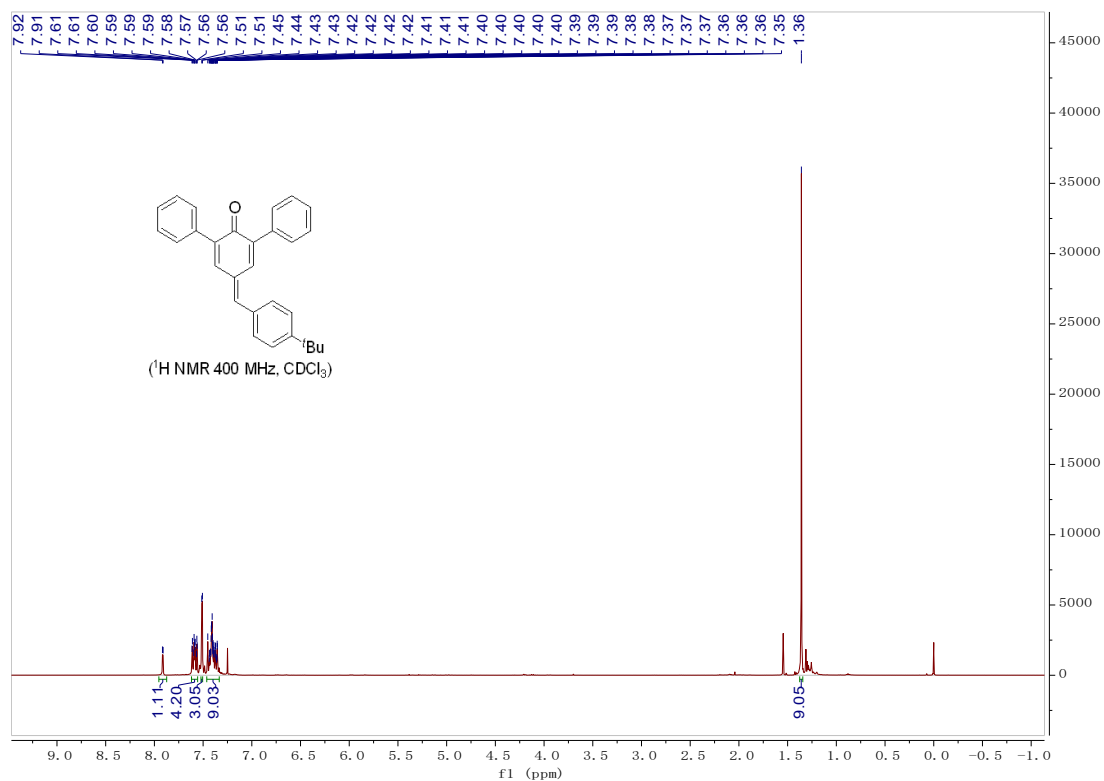
5'-(4-methylbenzylidene)-[1,1':3',1''-terphenyl]-2'(5'H)-one (1ab): Yield: 0.3483 g, 99%, a yellow solid, m.p. 155-157 °C; Eluent: PE/DCM = 20/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.86 (s, 1H), 7.63 – 7.52 (m, 4H), 7.46 – 7.31 (m, 10H), 7.25 (d, $J = 8.0$ Hz, 2H), 2.39 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 183.7, 146.6, 140.8, 140.3, 140.0, 138.6, 136.9, 136.5, 132.7, 132.6, 131.2, 130.9, 129.9, 129.4, 129.2, 128.09, 128.07, 128.0, 21.6; IR (neat): ν 3055.14, 3001.87, 2833.64, 1078.52, 1510.29, 1466.85, 1320.26, 1245.18, 1030.75, 837.26, 700.76 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{26}\text{H}_{21}\text{O}$ $[\text{M}+\text{H}]^+$: 349.1587, found: 349.1581.

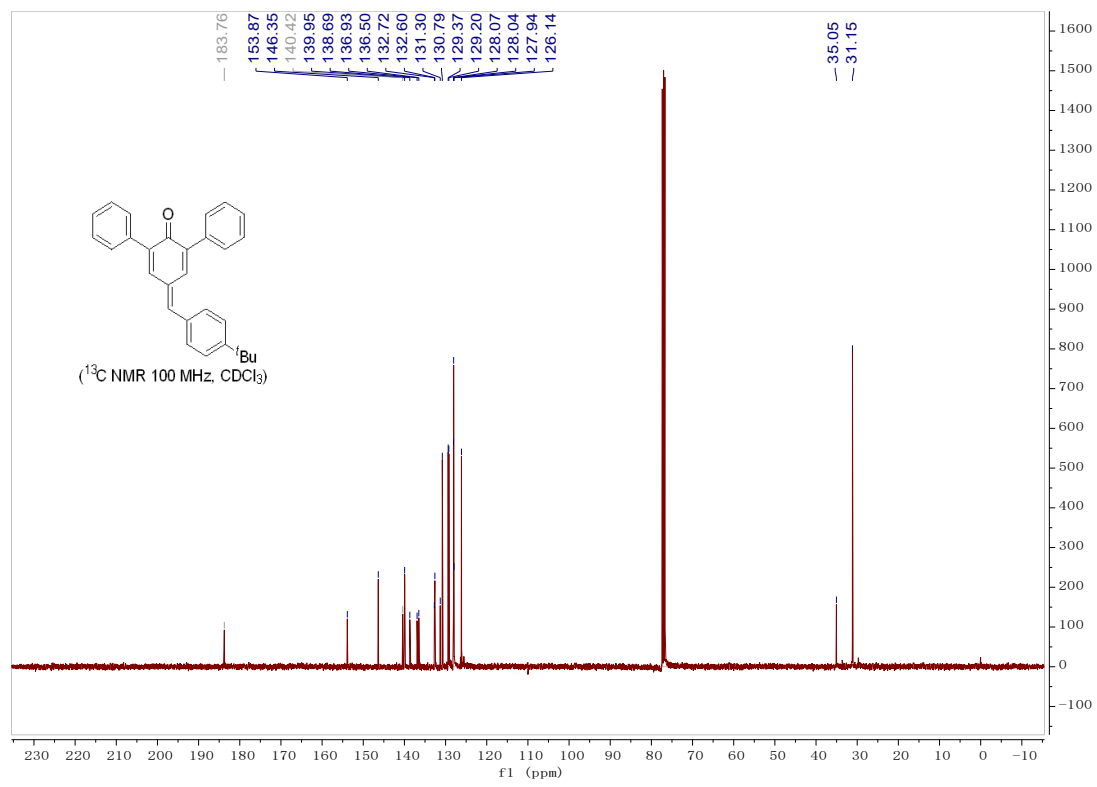


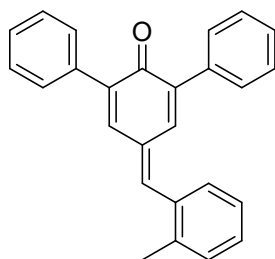




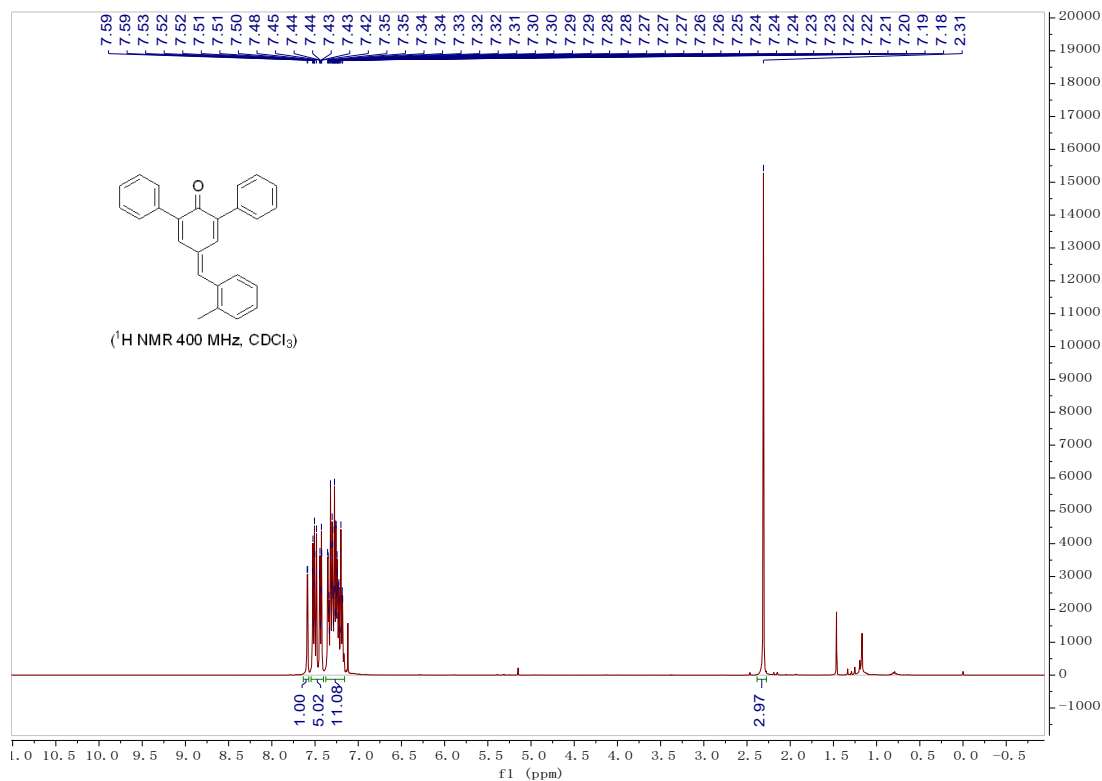
5'-(4-(tert-butyl)benzylidene)-[1,1':3',1''-terphenyl]-2'-(5'H)-one (1ac): Yield: 0.3702 g, 95%, a yellow solid, m.p. 163-165 °C; Eluent: PE/DCM = 20/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.91 (d, $J = 2.6$ Hz, 1H), 7.62 – 7.56 (m, 4H), 7.52 – 7.50 (m, 3H), 7.46 – 7.33 (m, 9H), 1.36 (s, 9H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 183.8, 153.9, 146.3, 140.4, 139.9, 138.7, 136.9, 136.5, 132.7, 132.6, 131.3, 130.8, 129.4, 129.2, 128.1, 128.0, 127.9, 126.1, 35.0, 31.1; IR (neat): ν 3058.20, 3029.50, 2961.09, 2867.27, 1711.64, 1620.78, 1598.78, 1542.43, 1493.01, 1361.13, 1334.11, 1156.91 cm^{-1} ; HRMS (DART) Calcd for $\text{C}_{29}\text{H}_{27}\text{O}$ $[\text{M}+\text{H}]^+$: 391.2056, found: 391.2055.

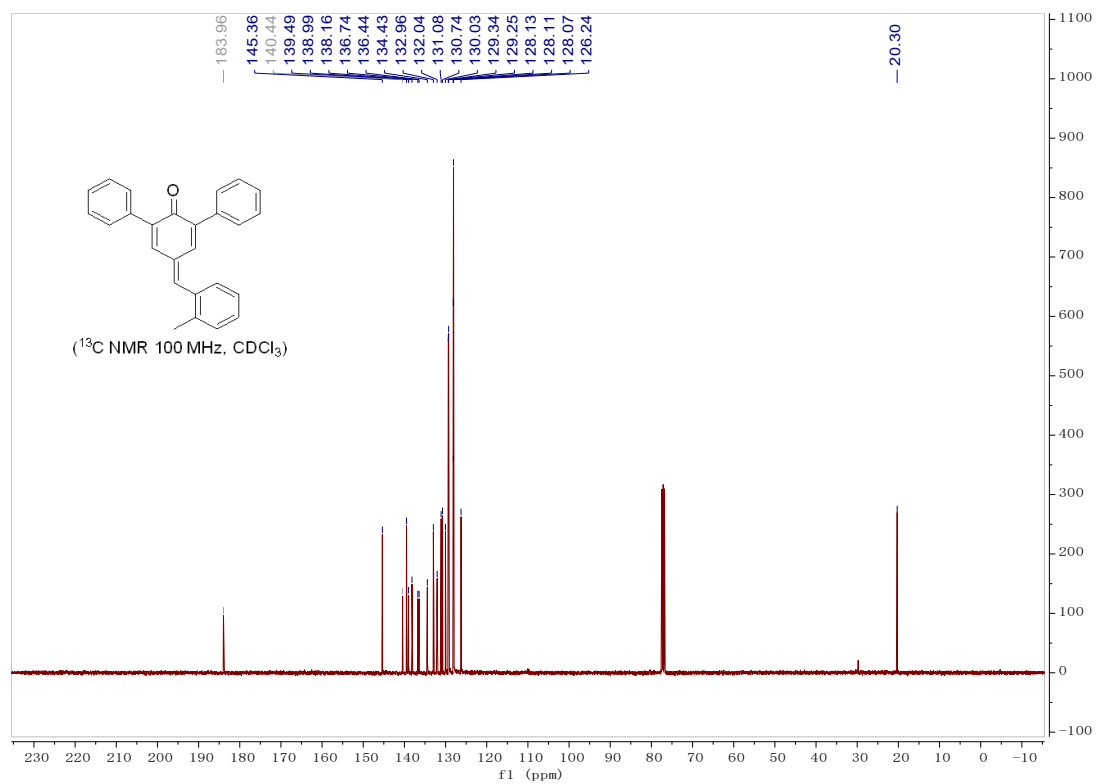


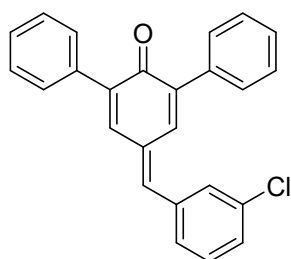




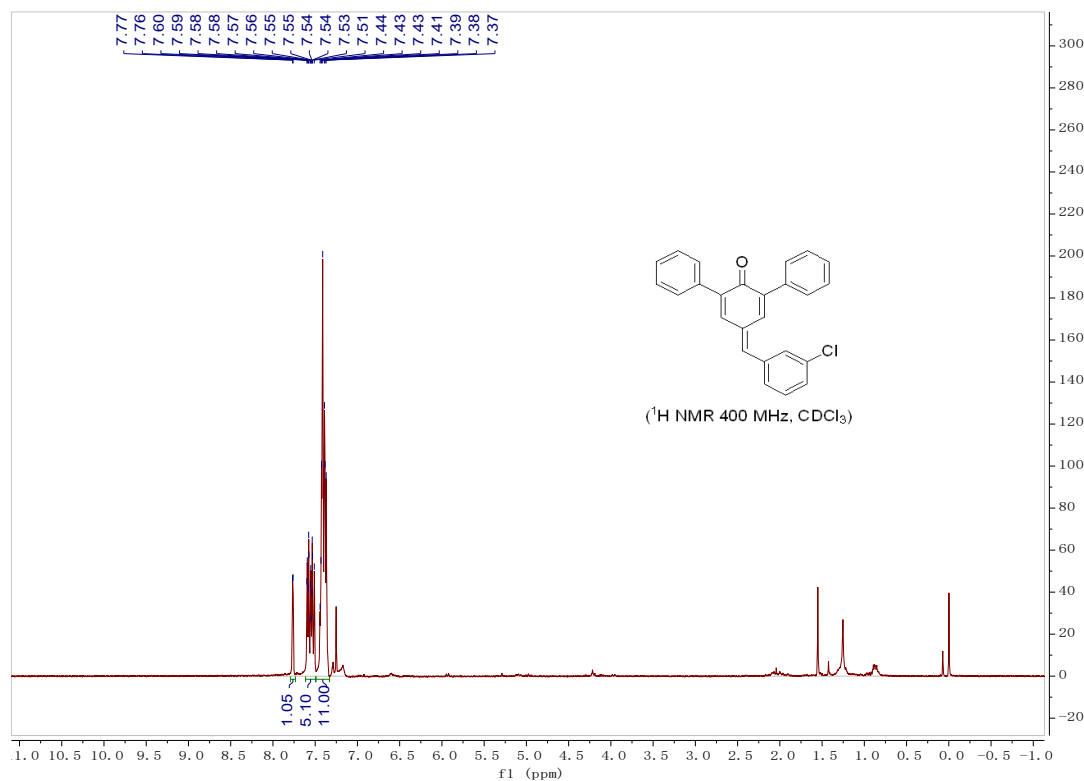
5'-(2-methylbenzylidene)-[1,1':3',1''-terphenyl]-2'(5'H)-one (1ad): Yield: 0.3130 g, 90%, a yellow solid, m.p. 183-185 °C; Eluent: PE/DCM = 20/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.59 (d, $J = 2.2$ Hz, 1H), 7.55 – 7.40 (m, 5H), 7.38 – 7.16 (m, 11H), 2.31 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 184.0, 145.4, 140.4, 139.5, 139.0, 138.2, 136.7, 136.4, 134.4, 133.0, 132.0, 131.1, 130.7, 130.0, 129.34, 129.25, 128.13, 128.13, 128.07, 126.2, 20.3; IR (neat): ν 3003.40, 2919.91, 1709.72, 1359.22, 1220.41, 1092.23, 905.45, 751.78, 699.71 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{26}\text{H}_{21}\text{O}$ $[\text{M}+\text{H}]^+$: 349.1587, found: 349.1588.

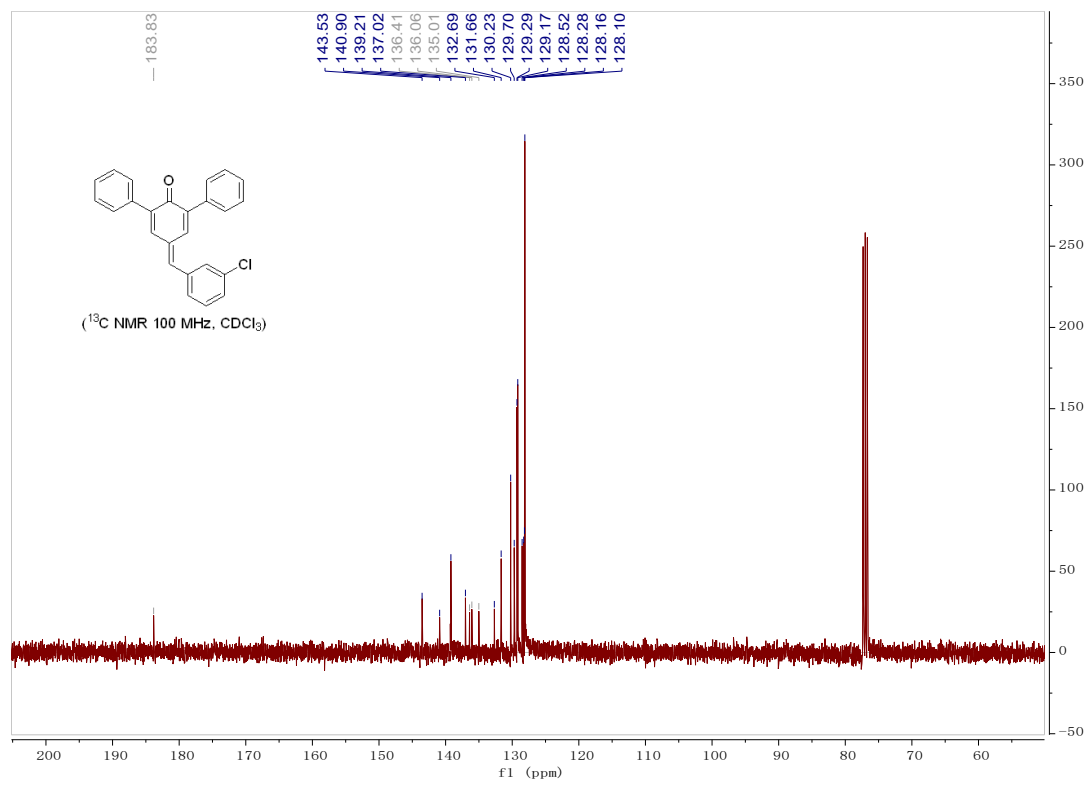






5'-(3-chlorobenzylidene)-[1,1':3',1''-terphenyl]-2'-(5'H)-one (1ae): Yield: 0.3665 g, 99%, a yellow solid, m.p. 135-137 °C; Eluent: PE/DCM = 20/1. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 7.76 (d, J = 2.4 Hz, 1H), 7.61 – 7.50 (m, 5H), 7.49 – 7.33 (m, 11H); ^{13}C $\{^1\text{H}\}$ -NMR (100 MHz, CDCl_3 , TMS) δ 183.8, 143.5, 140.9, 139.2, 137.0, 136.4, 136.1, 135.0, 132.7, 131.7, 130.2, 129.7, 129.3, 129.2, 128.5, 128.3, 128.2, 128.1; IR (neat): ν 3058.20, 3000.79, 2927.74, 1710.21, 1624.82, 1549.84, 1359.41, 1219.94, 1091.82, 728.78 cm^{-1} ; HRMS (ESI-TOF) Calcd for $\text{C}_{25}\text{H}_{18}\text{OCl}$ $[\text{M}+\text{H}]^+$: 369.1041, found: 369.1041.

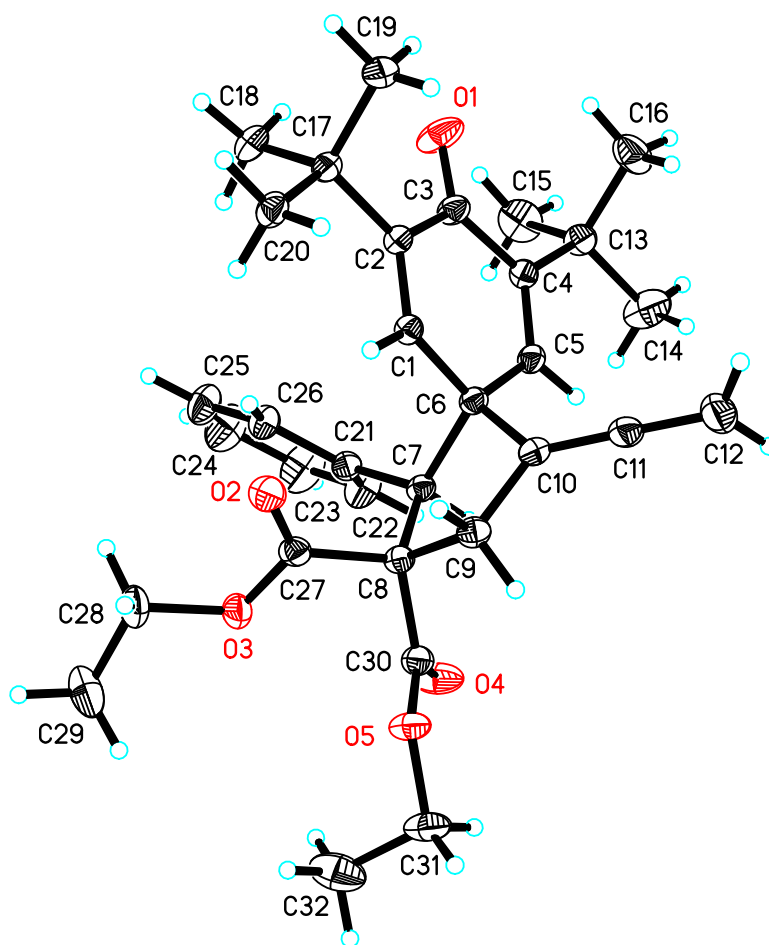




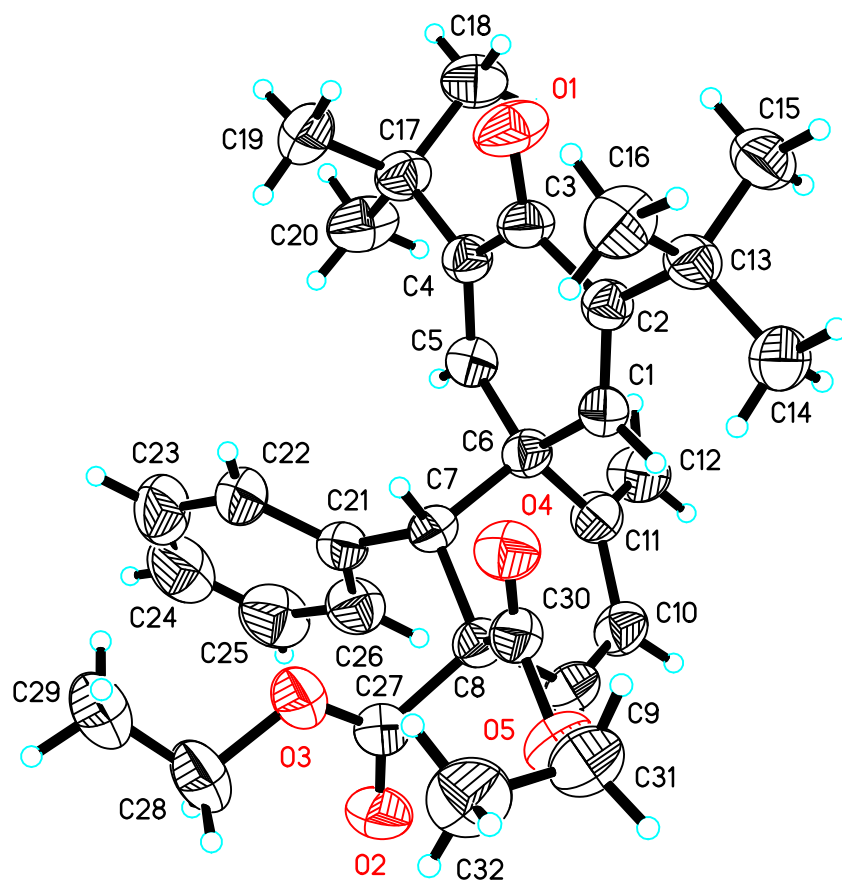
(K) X-ray Analysis

Single crystals suitable for XRD were obtained by evaporation experiment:

Compounds **3a** and **4a** (50 mg) were dissolved in 0.5 mL of ethyl acetate, and then 2.0 mL *n*-pentane was added, allowing this mixed solution evaporate slowly in a dry environment. Crystals were obtained in about 3-5 days with the evaporation of the solvent.



The crystal data of **3a** have been deposited in CCDC with number 2225338. Empirical Formula: $C_{32}H_{40}O_5$; Formula Weight: 504.64; Crystal Color, Habit: colorless, Crystal Dimensions: 0.200 x 0.150 x 0.120 mm³; Crystal System: Monoclinic; Lattice Parameters: $a = 11.9977(4)$ Å, $b = 16.6903(6)$ Å, $c = 14.9089(6)$ Å, $\alpha = 90^\circ$, $\beta = 95.2780(10)^\circ$, $\gamma = 90^\circ$, $V = 2972.78(19)$ Å³; Space group: P 21/n; $Z = 4$; $D_{calc} = 1.128$ g/cm³; $F_{000} = 1088$; Final R indices [$I > 2\sigma(I)$] $R1 = 0.0469$, $wR2 = 0.1106$.



The crystal data of **4a** have been deposited in CCDC with number 2288733. Empirical Formula: $C_{32}H_{40}O_5$; Formula Weight: 504.64; Crystal Color, Habit: colorless, Crystal Dimensions: 0.200 x 0.150 x 0.120 mm³; Crystal System: Monoclinic; Lattice Parameters: $a = 43.5637(17)$ Å, $b = 7.2829(3)$ Å, $c = 18.9126(9)$ Å, $\alpha = 90^\circ$, $\beta = 101.028(3)^\circ$, $\gamma = 90^\circ$, $V = 5889.6(4)$ Å³; Space group: $C 2/c$; $Z = 8$; $D_{calc} = 1.138$ g/cm³; $F_{000} = 2176$; Final R indices [$I > 2\sigma(I)$] $R1 = 0.0907$, $wR2 = 0.2674$.

(L) Computational Details

Computational methods

All DFT calculations were performed with Gaussian 16 program.⁷ The geometries of all minima and transition states have been optimized at B3LYP-D3BJ/6-31G(d,p) level of theory for all nonmetallic atom (H, C, N, O and P) and SDD level of theory for metallic atom Pd. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima or first-order saddle points on the respective potential energy surfaces. All transition states were characterized by one and only one imaginary frequency pertaining to the desired reaction coordinate. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The solvent effect was estimated by the SMD method in solvent. Solution-phase single point energy calculations were performed at B3LYP-D3BJ/def2tzvp level for all nonmetallic atom (H, C, N, O and P) and SDD level of theory for metallic atom Pd based on the gas phase optimized structures. The possible conformers for each species were searched manually, and the best conformer was used to calculate the reaction energy profile.

Scheme S6. DFT calculation of condition A

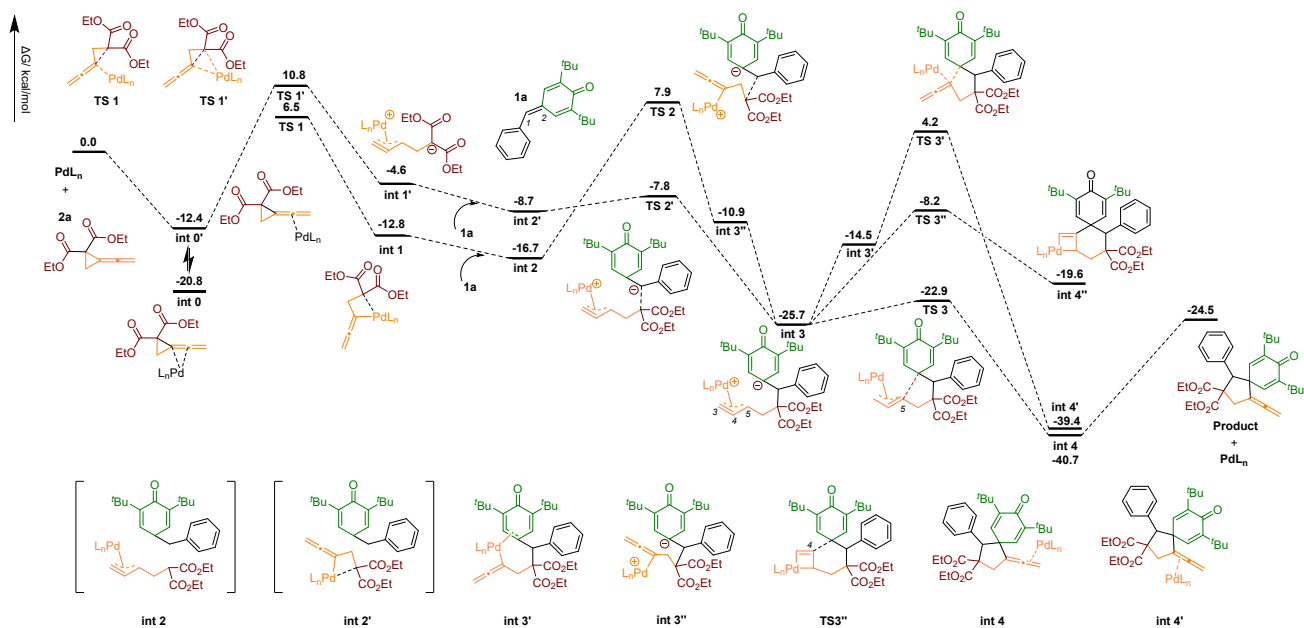


Table S1.^a DFT calculation of condition A

	G ₂₉₈ ^a	E _{tot} (E _h) ^a	E _{tot} (E _h), MeCN ^b
2a	-728.293025	-728.478677	-728.250554
PdL_n	-2274.356111	-2274.820264	-2274.01913
1a	-890.885923	-891.253567	-890.76864
Int0	-3002.686947	-3003.367641	-3002.333772
Int0'	-3002.665790	-3003.344893	-3002.318801
TS1'	-3002.645706	-3003.32554	-3002.282512
TS1	-3002.643654	-3003.320991	-3002.286923
Int1	-3002.656652	-3003.342003	-3002.31264
Int1'	-3002.688406	-3003.371298	-3002.323287
Int2	-3893.56723	-3894.644214	-3893.124442
Int2'	-3893.542652	-3894.621444	-3893.113558
Int2	-3893.56723	-3894.644214	-3893.124442
TS2'	-3893.532843	-3894.613863	-3893.114424
TS2	-3893.523696	-3894.600126	-3893.084666
Int3	-3893.555295	-3894.638822	-3893.145286
Int3'	-3893.553127	-3894.63469	-3893.125538
Int3''	-3893.539393	-3894.618019	-3893.116911
TS3	-3893.554606	-3894.636014	-3893.138876
TS3'	-3893.525662	-3894.604985	-3893.093456
TS3''	-3893.540689	-3894.624189	-3893.11743
Int4	-3893.596722	-3894.674873	-3893.163969
Int4''	-3893.560981	-3894.646356	-3893.137477
Int4'	-3893.592745	-3894.674534	-3893.16548
product	-1619.226011	-1619.809475	-1619.088461

(a) Calculated at B3LYP(D3BJ)/6-31g(d, p)/SDD

(b) Calculated at M06(D3)/def2-tzvp/SDD/SMD(MeCN)

Table S2.^a DFT calculation of **condition B**

	G ₂₉₈ ^a	E _{tot} (E _h) ^a	E _{tot} (E _h), MeCN ^b
PdL_n	-1641.213192	-1641.573248	-1640.949456
2a	-728.293025	-728.478677	-728.250554
PdL_n'	-1641.192612	-1641.547852	-1640.923591
1a	-890.885923	-891.253567	-890.760018
Int0-B	-2369.529803	-2370.104747	-2369.24523
Int0'-B	-3002.686947	-3003.367641	-3002.333772
TS1-B	-2369.503608	-2370.078741	-2369.207146
TS1'-B	-3002.643654	-3003.320991	-3002.286923
Int1-B	-2369.511324	-2370.085161	-2369.231233
Int1'-B	-2369.548067	-2370.123054	-2369.255667
Int2-B	-3260.398052	-3261.366103	-3260.032277
TS2-B	-3260.394131	-3261.365404	-3260.026845
Int2'-B	-3260.42540	-3261.391135	-3260.043886
TS2'-B	-3260.39728	-3261.368673	-3260.017819
Int3-B	-3260.415901	-3261.389292	-3260.05541
TS3-B	-3260.40402	-3261.377242	-3260.037122
Int4-B	-3260.426114	-3261.398654	-3260.061335
Int3'-B	-3260.434541	-3261.408725	-3260.062044
TS3'-B	-3260.409698	-3261.381823	-3260.036446
Int3''-B	-3260.40045	-3261.373556	-3260.028531
TS3''-B	-3260.404365	-3261.378592	-3260.029636
Int4'-B	-3260.445428	-3261.421604	-3260.085449
3a	-1619.226011	-1619.809475	-1619.075439
Int 4-B + HCO₃⁻	-3524.899536	-3525.894573	-3524.574875
TS7	-3524.847789	-3525.84534	-3524.533302
Int8	-3524.845958	-3525.84614	-3524.53696
Int8 - HCO₃⁻	-3260.890723	-3261.882732	-3260.554735
TS8	-3260.844384	-3261.829411	-3260.498278
Int9	-3260.862292	-3261.846277	-3260.509826
Int5	-3524.897648	-3525.888888	-3524.574006
TS5	-3524.891819	-3525.886195	-3524.563294
Int6	-3524.89424	-3525.891528	-3524.574728
TS6	-3524.884335	-3525.876999	-3524.549891
Int7	-3524.924819	-3525.91787	-3524.604498
4a	-1619.250687	-1619.837018	-1619.097054
PdLn + HCO₃⁻	-1905.690359	-1906.069186	-1905.473739
HCO₃⁻	-264.434189	-264.434743	-264.496322

(a) Calculated at B3LYP(D3BJ)/6-31g(d, p)/SDD

(b) Calculated at M06(D3)/def2-tzvp/SDD/SMD(1,4-dioxane)

Archive Entries

DFT calculation data of **condition A**

2a

1\1\GINC-OMC-1-821\Freq\RB3LYP\6-31G(d,p)\C11H14O4\SHIMGRP\15-Mar-2023
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Freq\1a_opt_freq\0,1\C,-0.0361470929,-0.0906203327,0.2023579826\C,-0
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0526756,2.0834631236\C,0.2675488934,2.5097533679,-0.2372482733\C,0.426
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76359\H,-0.4234902704,4.2199253867,-1.2252545306\C,1.1648362692,-0.945
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PdLn

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3\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP Fre
q\PdDPE2\0,1\O,-0.3536266864,-1.1711903569,1.2754674613\C,0.86887721
97,-1.697938007,1.6557873006\C,-0.6928845374,0.1310615184,1.5759374848
\C,2.0276929356,-1.4876152088,0.8818623859\C,0.8824811566,-2.521877378
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2.9258624446\C,-2.0526581279,2.0340426553,1.0200985899\C,-1.527807923,
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-1.8555712621,3.7392062169,2.3196977416\H,0.588420733,0.3268821335,3.2
855855565\H,-0.142654455,2.6545391645,3.7645643473\O,1.9826777152,-0.3

962318769,-0.6185573187\P,-2.0725906008,-0.1402277601,-0.8480120891\C,
2.1587201811,1.2537614236,0.1863872259\C,3.6465193602,-0.7118005484,-1
.3461793021\C,-3.1217457214,-1.5324488623,-0.2696647019\C,-3.296089281
6,1.0171472207,-1.5911225889\C,-3.7464550526,-1.5419423087,0.984394002
1\C,-3.2962914575,-2.6254620887,-1.128742001\C,-4.0968437741,-3.701949
7225,-0.7489808714\C,-4.5412517521,-2.6228220351,1.3669869683\C,-4.720
2476072,-3.7026249406,0.5004616416\H,-3.603854899,-0.7048583657,1.6606
950667\H,-2.7909826141,-2.6294636855,-2.0907185459\H,-4.2257986752,-4.
5440277073,-1.4226147449\H,-5.0195944271,-2.6224835004,2.3422846877\H,
-5.3372257274,-4.5445116338,0.8004939018\C,2.9742815508,1.4560715172,1
.3096372373\C,1.410479878,2.3260317042,-0.3142425615\C,1.4793598386,3.
5800688216,0.2922839692\C,2.2987533084,3.7750532264,1.404034283\C,3.04
75373471,2.7109078136,1.911556583\H,0.7517940257,2.1525350454,-1.16037
50014\H,0.8807866672,4.3991240149,-0.0945296538\H,2.3469522129,4.74970
6011,1.8808333049\H,3.6807767656,2.8562838245,2.7820872112\H,3.5387507
638,0.6261374638,1.7228374187\C,4.7489303718,0.1405135538,-1.205324198
4\C,3.7793923674,-1.8705152039,-2.1293130678\C,4.994433811,-2.18486986
33,-2.7324958489\C,5.9618912524,-0.1668003789,-1.8262141856\C,6.090401
9389,-1.3304404741,-2.5838810211\H,4.6620666819,1.0446581531,-0.613574
1062\H,2.9189054846,-2.5209864726,-2.2647752942\H,5.0838622599,-3.0881
072852,-3.3288783162\H,6.8076527952,0.5054831059,-1.7136933151\H,7.035
3047946,-1.5675885613,-3.0635993246\C,-2.8315086304,1.8938878064,-2.58
18075819\C,-4.6423795476,1.0747499872,-1.205165218\C,-5.5045116517,1.9
984330957,-1.7960629772\C,-3.6914600207,2.8247098997,-3.1643441986\C,-
5.0303882515,2.8771190822,-2.7726039525\H,-1.7914970321,1.8307635697,-
2.8924606264\H,-5.0151300405,0.3950147215,-0.4458972899\H,-6.547319800
2,2.032762508,-1.4939877039\H,-3.3201798424,3.4997677632,-3.9298846876
\H,-5.7041490835,3.5948327523,-3.2313175283\Pd,-0.0055284334,-0.554743
6786,-1.7198546938\

1a

1\1\GINC-OMC-1-823\Freq\RB3LYP\6-31G(d,p)\C21H26O1\SHIMGRP\12-Mar-2023
\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p)
Freq\|tBu\|0,1\C,-1.9790887033,0.4659820702,0.0592738551\C,-1.91638275
93,-1.0227800638,0.0178032087\C,-0.7012414366,-1.6164766211,-0.0572623
836\C,0.5453484547,-0.8784017412,-0.0790122614\C,0.4646266705,0.565930
6117,-0.1349711184\C,-0.7101946451,1.2388907627,-0.0787292571\H,-0.618
1052224,-2.6975195781,-0.0708189992\H,1.3903449399,1.1057151492,-0.271
3118489\C,-0.7810081114,2.7673593888,-0.1640759827\C,-3.2233004167,-1.
8213156892,0.0732249536\C,-1.3831235633,3.3327475228,1.1434393088\H,-2
.3931748641,2.957678886,1.3022207223\H,-1.4160972835,4.4265611162,1.09
17295315\H,-0.7645814112,3.0542938668,2.0035274125\C,-1.6528504088,3.1
879069279,-1.3693830146\H,-2.6710790117,2.815011083,-1.2663327163\H,-1
.2295250679,2.8036719684,-2.3036595059\H,-1.6848782866,4.2806383339,-1

.4382496622\C,0.6129407109,3.3911219839,-0.3500370006\H,1.2791736229,3
.1657010213,0.4894616071\H,0.5148924246,4.4790512445,-0.4083839785\H,1
.0947346232,3.0523951576,-1.2731288177\C,-4.125857448,-1.4285878408,-1
.1191139888\H,-4.3811020434,-0.3702082162,-1.0852763703\H,-5.051153850
6,-2.0141817599,-1.0902084645\H,-3.6228785835,-1.6396262634,-2.0689628
792\C,-3.9561795541,-1.5347045574,1.4040656019\H,-4.2048678625,-0.4780
761686,1.4936126761\H,-3.332202288,-1.8234442694,2.2567047654\H,-4.881
2687942,-2.1197812441,1.4496324994\C,-2.9669356357,-3.3357455503,-0.00
85649611\H,-2.4645604581,-3.6163131696,-0.9403385575\H,-3.9239063757,-
3.8647715438,0.0227894357\H,-2.3643933899,-3.6958464123,0.831912826\O,
-3.0636203466,1.0503733983,0.1816231985\C,1.7219389762,-1.5783245977,-
0.0802077073\C,3.0894628898,-1.0824302304,0.01757761\H,1.6370853848,-2
.6595922437,-0.1824342362\C,3.4478971129,0.053596529,0.7707864055\C,4.
771623728,0.4787035171,0.8284159743\C,5.7682388664,-0.221397168,0.1460
474601\C,4.1143189383,-1.7990751491,-0.6317568718\C,5.4348874301,-1.36
70899715,-0.579805146\H,2.6908989183,0.5747252707,1.3446103622\H,3.857
5567747,-2.6916282984,-1.1951625618\H,6.2064461032,-1.9259290046,-1.10
0141865\H,5.028703891,1.3517142313,1.4201852572\H,6.7997733619,0.11289
83113,0.1939444849\

Int0'

I\1\GINC-A01R06N08\Freq\RB3LYP\GenECP\C47H42O5P2Pd1\ACJSGGHI7X\14-Jan-
2024\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP
Freq\TS2\0,1\O,1.4295101608,0.0085308279,2.0873338295\C,2.4260922861
,0.9118740239,1.7758643747\C,1.7137809933,-1.3297027204,2.2990965009\C
,2.0119639621,2.0534419666,1.0654733416\C,3.7527603376,0.7214317633,2.
1484088648\C,4.6972064115,1.6953667182,1.823323026\C,2.9773620822,3.02
50220842,0.7747490644\C,4.3102439438,2.8524633171,1.1494966653\H,2.683
2602913,3.9135498604,0.2274233624\H,5.0437951053,3.613559279,0.9031640
374\H,5.7358487102,1.5426143249,2.0992312067\H,4.0409732356,-0.1846566
598,2.6684565707\C,1.7174027555,-2.219008888,1.2093939971\C,1.87488110
66,-1.7736725431,3.6083932973\C,2.0462036673,-3.1353194388,3.859075525
8\C,1.8928998591,-3.5828538648,1.4866882382\C,2.0532180154,-4.03899794
17,2.7957035473\H,1.8891635627,-4.2920159646,0.6666547598\H,2.18255923
06,-5.1004944355,2.9825784816\H,1.8421288556,-1.0465226423,4.412508474
8\H,2.1666802193,-3.4857582441,4.8792954739\O,0.3254298362,2.060999383
4,0.3299248594\O,1.4422501676,-1.5353886545,-0.481787514\C,-0.78940932
12,2.1180271236,1.7858711068\C,0.218895639,3.7672637442,-0.3520591387\
C,3.1424930509,-0.9184753845,-0.8465333406\C,1.3307596845,-3.04182099,
-1.5243515907\C,4.2875657454,-1.6127783125,-0.4300915154\C,3.292564584
,0.2810450723,-1.5527574988\C,4.5639819013,0.7843126667,-1.8297521304\
C,5.5570934834,-1.1125627211,-0.7108454238\C,5.6973593695,0.0894783285
,-1.4087222091\H,4.1824144315,-2.5409758564,0.1224987508\H,2.402904446
2,0.8237486704,-1.8600563609\H,4.6666895788,1.7252047739,-2.3617792397

\H,6.4373459088,-1.6568604595,-0.3809949287\H,6.6871986265,0.484350268
6,-1.6180854737\C,-0.3806532765,2.557160447,3.0517752872\C,-2.10503495
6,1.6714925407,1.6077201005\C,-3.0072358782,1.6760636792,2.6703714285\
C,-2.5967118727,2.1286571365,3.9255323108\C,-1.283335239,2.5647794189,
4.1156527492\H,-2.4034605215,1.3021594316,0.6326975635\H,-4.0084751728
,1.2870916786,2.5185838892\H,-3.293044668,2.1252525605,4.7590808113\H,
-0.9594246071,2.9052787839,5.0951026325\H,0.6450821958,2.8787010306,3.
2050011796\C,0.0687630055,4.9091119239,0.4474953155\C,0.2990810829,3.9
122814742,-1.7433414198\C,0.2489934772,5.1788053389,-2.3272518057\C,0.
0077545226,6.1735781902,-0.1369030371\C,0.1023809668,6.3107872649,-1.5
242211179\H,-0.00745502,4.8061112765,1.5251965871\H,0.3843466906,3.018
8171049,-2.3568857256\H,0.3131862121,5.2806466072,-3.4067331885\H,-0.1
142238295,7.0527479037,0.489218628\H,0.0541760926,7.2969002107,-1.9767
78643\C,0.2083947401,-3.8732241316,-1.3675875538\C,2.2304304011,-3.307
3974925,-2.5664881374\C,2.0149836334,-4.3854602941,-3.4274911203\C,0.0
064314627,-4.9568825564,-2.2181886476\C,0.9062910532,-5.2143452871,-3.
2556371305\H,-0.5101652027,-3.6852322311,-0.5787902952\H,3.1000778164,
-2.6748507083,-2.7052789222\H,2.7205811754,-4.5788101876,-4.2305464114
\H,-0.8634348957,-5.5904341033,-2.0726518352\H,0.7423948261,-6.0528439
986,-3.9260458984\Pd,-0.1212022327,0.2012426575,-1.0166441035\C,-3.271
3581572,-1.6215872556,-0.6461113377\C,-3.646027273,-2.284987408,-1.992
1063598\C,-2.4645252902,-1.4424267607,-1.8906424832\H,-4.5369258928,-1
.9064510368,-2.4898846116\H,-3.5123205508,-3.3645809143,-2.0110489958\
C,-1.440542919,-0.7887935404,-2.3645359382\C,-0.7226051227,-0.06951068
09,-3.2655254502\H,0.2445572804,-0.4072860998,-3.6279754903\H,-1.18510
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778821\C,-2.6863200615,-2.4898719703,0.429920903\O,-2.2379895857,-1.74
03607042,1.4419786334\O,-4.2345236333,0.483229322,-1.1080605394\O,-4.7
469210634,-0.4800400269,0.8753891816\O,-2.5666277292,-3.6991788501,0.3
601836031\C,-1.6659260864,-2.4335502722,2.5766659098\C,-1.5219997931,-
1.4142737217,3.6875625885\H,-0.7040512789,-2.8549783709,2.2771991993\H
, -2.3298374641,-3.2586968557,2.848937863\H,-0.8959405161,-0.5783901514
,3.3690077617\H,-1.0586582249,-1.8867609909,4.5587696865\H,-2.49798117
32,-1.0173376428,3.9757058341\C,-5.1218455716,1.5846631286,-0.80470523
27\C,-6.5678300048,1.2280292487,-1.1067705522\H,-4.7623816538,2.396248
2481,-1.4400874193\H,-4.9912834516,1.8638933288,0.2430193174\H,-6.6780
846222,0.910342575,-2.1477940851\H,-7.208624841,2.1006056223,-0.943746
7289\H,-6.9071937308,0.4237577347,-0.4503926789\

Int0

1\1\GINC-OMC-1-817\Freq\RB3LYP\GenECP\C47H42O5P2Pd1\SHIMGRP\13-Jan-202
4\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP Fre
q\TS2\0,1\O,-1.2309442812,0.0180074795,2.5027240362\C,-2.2971585642,
-0.8296087041,2.2763786401\C,-1.4114576602,1.3831111167,2.6365153048\C,

-1.9771877493,-2.0141663189,1.5918806468\C,-3.5911384004,-0.5542900118
,2.7033493623\C,-4.5967719164,-1.4900135118,2.45557514\C,-2.9997494477
,-2.9438374115,1.3748753478\C,-4.3025763627,-2.6870200911,1.8040883148
\H,-2.7758703011,-3.8635516985,0.8459472833\H,-5.0861491415,-3.4145965
448,1.618312856\H,-5.6120741562,-1.2764398539,2.774798437\H,-3.8076658
765,0.3819646976,3.2046051718\C,-1.357162309,2.1996147562,1.4943880788
\C,-1.522970354,1.9150940226,3.9174324349\C,-1.5943296768,3.2982986502
,4.0832142271\C,-1.4354076539,3.5856322418,1.6864031531\C,-1.551666576
1,4.1315692751,2.9655570486\H,-1.3907397747,4.2429048153,0.8262179831\
H,-1.6033930476,5.2090107339,3.0858124216\H,-1.5336707811,1.2376367694
,4.76465305\H,-1.6760451636,3.7195391771,5.0802126546\P,-0.3143416896,
-2.1165359276,0.8240686945\P,-1.1493834497,1.39847302,-0.1569040215\C,
0.8250588672,-2.2863994453,2.2563308638\C,-0.3276979631,-3.7830735025,
0.0622638805\C,-2.8664948662,0.8141921372,-0.4736811077\C,-1.014396705
6,2.8301708545,-1.3040129376\C,-3.9870467693,1.5449753307,-0.054464906
7\C,-3.0540255312,-0.3842659451,-1.1714541649\C,-4.3408746285,-0.85239
64663,-1.4375809647\C,-5.2719084719,1.0783560521,-0.321996551\C,-5.450
7156632,-0.1234660789,-1.0112755012\H,-3.8507130515,2.474956685,0.4883
029052\H,-2.1836217848,-0.9514342779,-1.4875545622\H,-4.4741568926,-1.
7909203595,-1.966970561\H,-6.1341182242,1.6485993655,0.011261607\H,-6.
4526995832,-0.4913731548,-1.2113243071\C,0.3723483412,-2.5818561689,3.
5494257975\C,2.1903105425,-2.0474624312,2.0461985925\C,3.0872603233,-2
.0896036074,3.1120786031\C,2.6292314866,-2.3759229217,4.3993047477\C,1
.2720890359,-2.6274606539,4.6148784957\H,2.5435589519,-1.7962628218,1.
0542594881\H,4.1332638509,-1.8631548565,2.9310747746\H,3.3245373939,-2
.3964822986,5.2335212178\H,0.9114978899,-2.8514802847,5.6148095798\H,-
0.6840017102,-2.7597032588,3.7243761527\C,-0.2031406547,-4.9589177168,
0.8151473131\C,-0.4739545918,-3.8696897002,-1.3285921098\C,-0.51159767
15,-5.1146718875,-1.9578040076\C,-0.2358273874,-6.2020768624,0.1848593
897\C,-0.3932865256,-6.2814607221,-1.201293974\H,-0.0734621238,-4.8965
019813,1.8911103353\H,-0.5305435787,-2.9546461884,-1.9115024579\H,-0.6
188825272,-5.171991615,-3.0368663671\H,-0.1345187623,-7.1091244118,0.7
734819141\H,-0.4142164016,-7.2508873098,-1.6902737399\C,0.0965288909,3
.6844039975,-1.1977630418\C,-1.9346061981,3.0365451803,-2.3405508757\C
, -1.7496915705,4.0780794887,-3.2519722555\C,0.2665579892,4.732162732,-
2.1010408741\C,-0.6528078088,4.9306284074,-3.133816472\H,0.8281105116,
3.5369645431,-0.4103247116\H,-2.796005735,2.3863340186,-2.4396428064\H
, -2.4698211831,4.2230740006,-4.0520336337\H,1.1261084529,5.3881039866,
-1.9990156216\H,-0.5130913934,5.7424102948,-3.8414674929\Pd,0.45651317
94,-0.3159753101,-0.4589183629\C,3.3118026095,1.073037045,-0.416038073
5\C,2.9240389653,1.5221056046,-1.8255538426\C,2.2750136301,0.326373693
4,-1.2688577487\H,3.6811026375,1.3917078653,-2.5939768952\H,2.35577633
11,2.4455811779,-1.8797094342\C,2.1300361652,-1.0417471125,-1.41422072
01\C,2.6452633979,-2.181211318,-1.8600113259\H,2.1337912549,-3.1317972

251,-1.7465421618\H,3.6113456092,-2.1891405583,-2.3639675887\C,4.60637
38718,0.3752477828,-0.1742696336\C,2.7474138736,1.800761193,0.77234206
49\O,2.5130146112,0.9375340566,1.7677991646\O,5.1154917478,-0.14548306
77,-1.3156650509\O,5.1435065647,0.2573579122,0.9112567518\O,2.48415640
5,2.9892491151,0.8145370446\C,1.9643186759,1.4421024168,3.002565983\C,
3.0855235797,1.7816514617,3.9682701799\H,1.344952135,0.6237763792,3.37
28184869\H,1.3382099468,2.3086929101,2.7849676076\H,3.722137204,0.9083
907106,4.1309212026\H,2.6677276786,2.097585741,4.9301206469\H,3.700178
0528,2.5947700523,3.5732394428\C,6.3387905175,-0.8993543164,-1.1773960
095\C,7.5519378387,0.0165427746,-1.1677128611\H,6.3449514181,-1.567214
0221,-2.0417744417\H,6.2849587851,-1.4918035471,-0.2611651364\H,7.5727
243866,0.6401637411,-2.0662827322\H,8.470553761,-0.5788637896,-1.13942
20693\H,7.5308670708,0.6624401366,-0.2873488357\

TS1'

1\1\GINC-OMC-1-818\Freq\RB3LYP\GenECP\C47H42O5P2Pd1\SHIMGRP\15-Feb-202

3\0\#p freq genecp b3lyp geom=check guess=read empiricaldispersion=gd
3bj\TS2\0,1\O,-0.8282408794,-1.5657594334,1.4632650095\C,-1.22082639
73,-2.6985840924,0.7836406803\C,-1.7306061836,-0.8154614045,2.19911368
31\C,-0.412391179,-3.0291908575,-0.3170134501\C,-2.3137783983,-3.47890
92203,1.1452794459\C,-2.6026607739,-4.6229838592,0.3995782595\C,-0.716
0554227,-4.1857891388,-1.0413010452\C,-1.8051051986,-4.9830404715,-0.6
857581955\H,-0.1041903844,-4.4523722955,-1.8960276547\H,-2.0325109244,
-5.875549435,-1.2596534781\H,-3.4589864385,-5.2318646142,0.6728769845\
H,-2.9347053781,-3.1872450987,1.9837701273\C,-2.2788940781,0.334133578
4,1.611635564\C,-1.9834474778,-1.161196415,3.5234465976\C,-2.832527405
3,-0.3623839209,4.2887839735\C,-3.1373344731,1.1141991206,2.3957136001
\C,-3.4139033823,0.7704086792,3.7188913938\H,-3.5846841255,2.003903265
5,1.9706786181\H,-4.0789333424,1.3955281082,4.3063536947\H,-1.50210997
99,-2.0409685963,3.9370202952\H,-3.0343803085,-0.6236795946,5.32268177
44\P,0.8667505205,-1.8148576732,-0.8039124613\P,-1.8185875458,0.734443
5478,-0.1277740312\C,2.0883473639,-1.8923420698,0.5598895172\C,1.68160
73432,-2.6295578619,-2.2311309788\C,-2.8472648154,-0.5175148565,-1.020
7014379\C,-2.7375918629,2.2833251184,-0.5255057505\C,-4.0542205063,-0.
9948078435,-0.4923025432\C,-2.4257193435,-0.9852752599,-2.2722489261\C
, -3.1803855125,-1.9255534436,-2.9724033432\C,-4.8089350792,-1.93538165
15,-1.190868127\C,-4.3711849301,-2.407993088,-2.4291109064\H,-4.398528
5443,-0.6381824985,0.4723739947\H,-1.4923708598,-0.6132806586,-2.68418
98101\H,-2.8325954014,-2.2872044221,-3.9355018453\H,-5.7369878388,-2.3
046018883,-0.7643798139\H,-4.9550812934,-3.1488902319,-2.9669680843\C,
2.2501660387,-3.0355896596,1.3560854476\C,2.8420436147,-0.7453510486,0.
.8430062937\C,3.751002417,-0.7360960751,1.9007181999\C,3.9148355095,-1
.8808976274,2.6813833928\C,3.1651678556,-3.0292019472,2.40812179\H,2.7
061150328,0.1595157978,0.262872181\H,4.2864127367,0.1837570181,2.10779

38615\H,4.6167032872,-1.8782796729,3.5104609303\H,3.2863853237,-3.9176
306425,3.0214192506\H,1.6488042952,-3.9190285925,1.1632906302\C,2.6536
722007,-3.6282379059,-2.0864688111\C,1.313380498,-2.214202609,-3.51913
88896\C,1.8945674353,-2.7977265222,-4.6446589476\C,3.2402097277,-4.205
7535322,-3.2127899121\C,2.8599543698,-3.79479961,-4.4920569462\H,2.958
3165929,-3.9431687024,-1.0939589903\H,0.5810510482,-1.419406844,-3.630
6314284\H,1.6032350559,-2.4671001099,-5.6371942227\H,3.9971338852,-4.9
749278056,-3.0913987576\H,3.320713695,-4.2441188236,-5.3666250927\C,-2
.5525773714,3.4603261577,0.2215125415\C,-3.5764936866,2.3246936816,-1.
6506726879\C,-4.2162502447,3.5087379092,-2.0174048402\C,-3.207619258,4
.63637397,-0.1428171574\C,-4.0390302646,4.66807865,-1.2630402295\H,-1.
8806536894,3.4453163361,1.0699484349\H,-3.7364118792,1.4324476066,-2.2
43653619\H,-4.8598142622,3.5189564703,-2.8922144813\H,-3.057806892,5.5
337734177,0.4505124341\H,-4.5423812533,5.587727925,-1.5461671655\Pd,0.
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96233,-1.3774309978\H,1.3495414784,4.5122788873,-1.088103948\H,-0.1285
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06674\C,2.7904413964,1.0671358058,-2.6625703178\H,2.6962966604,0.27755
3119,-3.4026690393\H,3.7998474473,1.3029579097,-2.3207835175\C,3.16100
34542,3.0330524917,0.3808525647\C,1.0202977632,2.427064072,1.609450228
5\O,1.8094315876,1.8523340803,2.548766252\O,3.5629224374,3.780911078,-
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4987514456,1.8580446734,4.6354778426\H,1.9335049022,0.3923249941,3.916
2931185\H,0.3992470175,0.4155880504,3.0270996004\H,1.2361625257,2.5114
979022,5.1117735387\H,0.0837513327,1.1895375865,5.3979854936\H,-0.3110
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7587\C,5.7214148544,4.7809142085,-0.1459533676\H,5.039656903,4.0019040
826,-2.0575991293\H,5.3589130415,2.7579473711,-0.8163524477\H,5.302809
6671,5.7823640001,-0.284059615\H,6.7786084466,4.8050095865,-0.43203184
95\H,5.6518582911,4.509689166,0.9094712697\

TS1

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2024\0\#p freq genecp b3lyp empiricaldispersion=gd3bj geom=check gues
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785032,0.339732945\C,-1.9129685799,-4.4664728635,-0.6985919699\C,0.220
5721168,-3.6020012375,-1.4281759576\C,-0.82961997,-4.5092175936,-1.574
9727808\H,1.0511471316,-3.6200621153,-2.1250357898\H,-0.8069671513,-5.
2366018904,-2.3802258702\H,-2.7428509179,-5.1554241624,-0.8196362242\H
, -2.7808935447,-3.4875699718,1.0258513063\C,-2.7074940006,-0.185697859

5,1.4513719885\C,-2.3384278946,-1.7194127299,3.3217416864\C,-3.4530876
014,-1.2030499161,3.9818913359\C,-3.8287989464,0.3096208112,2.13370625
62\C,-4.2009540862,-0.1904020813,3.3817041637\H,-4.4063144334,1.109619
237,1.6853374683\H,-5.0721612498,0.217148004,3.8850685355\H,-1.7281373
194,-2.5026584636,3.7588483384\H,-3.731788169,-1.5900242002,4.95698774
31\P,1.3856064564,-1.2384459007,-0.2977069152\P,-2.1187788797,0.504918
4883,-0.1589416401\C,2.3798140949,-1.6342917432,1.195067876\C,2.578279
7177,-1.6031327247,-1.6494018406\C,-2.8275676818,-0.710662487,-1.34694
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62167226,-1.1757558489\C,-2.063607991,-1.0827896533,-2.4586673085\C,-2
.565434115,-1.9961359137,-3.3864286596\C,-4.6054827541,-2.1764915087,-
2.1031461502\C,-3.8360075655,-2.5431838963,-3.2104372689\H,-4.69896443
27,-0.9888561293,-0.3112723191\H,-1.0661845838,-0.6676281604,-2.571376
8004\H,-1.9575438275,-2.2900671929,-4.2367140041\H,-5.5940694795,-2.60
37498047,-1.9614640669\H,-4.2245273296,-3.2590878387,-3.9288351569\C,2
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5011768927,0.2067003589,1.02181413\H,4.8614568033,-0.1951330471,3.0260
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61817,-2.6213878808,-1.5545131101\C,2.5311776229,-0.8130462677,-2.8048
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71962121,-2.6023589175\C,4.3714915809,-2.0595398625,-3.7553242828\H,3.
5894490426,-3.2285439174,-0.6560941174\H,1.8124054822,-0.0010893941,-2
.8621729605\H,3.3791252853,-0.4189526915,-4.7434050034\H,5.1732204674,
-3.6347775788,-2.5189220737\H,5.0705559464,-2.2341184605,-4.5679962662
\C,-3.0442847363,3.0534119217,0.4896016045\C,-4.1024581869,2.089439563
9,-1.4603496306\C,-4.8242110648,3.2709813897,-1.646931268\C,-3.7792270
693,4.2222955036,0.3086532339\C,-4.6698897855,4.3373854951,-0.76262918
74\H,-2.3325645231,2.9811727315,1.3061008548\H,-4.2385125156,1.2642747
612,-2.1499909109\H,-5.5113253417,3.3522025445,-2.4843526794\H,-3.6484
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1\H,-0.4812512575,4.2724865311,0.4884386535\C,0.57775288,2.6177081341,
-2.2482733821\C,0.8201959143,2.3652298902,-3.5167343416\H,0.1195229975
,1.8120652476,-4.1398390409\H,1.7351095261,2.714650432,-3.9957216118\C
,2.7286796011,2.9535791377,0.277538875\C,0.6765338687,2.3841935731,1.7
695878479\O,1.3912117047,1.3797235105,2.2927610864\O,3.062806083,3.613
7417682,-0.8594342343\O,3.557944332,2.4454450697,1.0098591428\O,-0.342
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0574\C,1.3641483779,1.3215526215,4.7259375123\H,1.1625911419,-0.330425

5724,3.328975509\H,-0.2532511401,0.7500628708,3.3901371245\H,2.4572694
617,1.2968341393,4.7362778338\H,0.9958057021,0.7595249037,5.5907808783
\H,1.0308729796,2.3583220967,4.8201636736\C,4.4344231107,3.4712684816,
-1.2870513691\C,4.6315417225,2.1486389338,-2.0126763726\H,5.0901956459
,3.5488136339,-0.4171404841\H,4.6032653879,4.3242310685,-1.9480478517\
H,4.4429934848,1.3070383536,-1.3423567835\H,5.6595499801,2.070139046,-
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Int1'

1\1\GINC-OMC-1-815\Freq\RB3LYP\GenECP\C47H42O5P2Pd1\SHIMGRP\07-Mar-202
3\0\#P Geom=AllCheck Guess=TChech SCRF=Check GenChk RB3LYP/GenECP Fre
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1,-2.7906253993,0.4351166532\C,-2.0086901214,-1.5882125279,2.171126754
7\C,0.1943484848,-2.6002677202,-0.4237192759\C,-1.9259965198,-3.674786
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226875,-3.3564967083,-1.5985765789\C,-0.7785704711,-4.2478538595,-1.91
40151457\H,1.0824783149,-3.2265120048,-2.2782093858\H,-0.7348633749,-4
.8152234318,-2.8380441082\H,-2.6741526565,-5.0750236219,-1.3064292173\
H,-2.7639340542,-3.777482646,0.8195615852\C,-2.7130486425,-0.523825744
1,1.5847234068\C,-2.4063381567,-2.1614737726,3.3760582027\C,-3.5442999
128,-1.68677896,4.0252893531\C,-3.8581350742,-0.0675090557,2.258722908
9\C,-4.2740869328,-0.6422491083,3.4594691398\H,-4.4225700092,0.7576506
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84091,-2.9679111491,3.7852142518\H,-3.8555108526,-2.1306569604,4.96564
98451\p,1.3380698512,-1.2303833212,0.0069065778\p,-2.1506544821,0.2738
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2.7661543258,-1.7098427733,-3.5161170735\C,-4.6761086434,-2.2100133938
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296559\H,-2.2260138939,-1.8250507472,-4.4508000926\H,-5.6277069929,-2.
7116071168,-1.9719768544\H,-4.4105467066,-2.9623358214,-4.1238328235\C
,2.0910965575,-3.177292254,1.9305406216\C,3.3544913389,-1.1089128846,1
.9360638008\C,4.1191775591,-1.5915195017,2.9983304271\C,3.8701415875,-
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90799087\H,2.5796646391,-0.1446749077,-4.6404606852\H,5.3972974035,-2.6338436474,-2.5495068277\H,4.6881065198,-1.4665221888,-4.6249392794\C,-2.697871398,2.8689476003,0.8250826828\C,-4.3891365442,1.9183867704,-0.6272560434\C,-5.1366777839,3.0944969104,-0.5206583304\C,-3.4526633388,4.0332763193,0.9356349172\C,-4.6724487748,4.15010206,0.2625558574\H,-1.7288759168,2.8089668655,1.3138472656\H,-4.7526274049,1.1029722667,-1.2420358839\H,-6.0776777232,3.1830699029,-1.0556453684\H,-3.0767547404,4.8571566757,1.5343758308\H,-5.2528284071,5.0645601986,0.3421760549\Pd,0.1179078015,0.8481265191,-0.2414383503\C,1.663703546,2.3949444879,0.0297141968\C,0.8371185326,3.4143929429,-0.7829570655\C,-0.2978819275,2.5668330084,-1.2581134189\H,1.4104881085,3.8563230268,-1.5994679338\H,0.48271552,4.2072349499,-0.1170356049\C,-1.1491477567,2.6294945118,-2.2256048645\C,-2.0770884367,2.653935268,-3.162384686\H,-3.0549567438,3.0899468282,-2.9721307661\H,-1.9020051603,2.2487942929,-4.1568300731\C,2.9757770999,1.9789817051,-0.4904197818\C,1.4160850135,2.480116408,1.4899542739\O,2.2213704004,1.7006148368,2.247984925\O,3.1384048354,2.3647697703,-1.7916617512\O,3.8528576567,1.3564761048,0.093159121\O,0.5273529385,3.1684738946,1.9902408559\C,1.926474486,1.6457754332,3.6566705037\C,2.5682996254,2.8052366791,4.4019286696\H,2.3376906691,0.6853744241,3.9759763783\H,0.8422211449,1.6416413614,3.7942136406\H,3.6459970978,2.8310130989,4.2149454854\H,2.4064330339,2.6961346555,5.4798373066\H,2.1296030191,3.7515063859,4.0782942468\C,4.3997659242,2.0203937689,-2.3952603631\C,5.4717549525,3.0407176486,-2.0452886148\H,4.1941674428,2.0065242737,-3.4679120014\H,4.6885010493,1.0184921413,-2.0739993527\H,5.1556577011,4.0488904535,-2.3298448146\H,6.4012043258,2.8074515217,-2.5759875894\H,5.6729979861,3.0219489772,-0.9719299441\

Int1

1\1\GINC-OMC-1-806\Freq\RB3LYP\GenECP\C47H42O5P2Pd1\SHIMGRP\07-Mar-2023\0\#P Geom=AllCheck Guess=TChef SCRF=Check GenChk RB3LYP/GenECP Freq\int1\0,1\O,2.0037238451,-2.3360275582,-0.6650990547\C,3.2919619844,-1.8671028367,-0.8578036782\C,1.6786965165,-2.6791301662,0.6490655963\C,3.6161541628,-0.5479296665,-0.4934372241\C,4.2365485296,-2.7182837637,-1.4232507358\C,5.5513186663,-2.278972503,-1.5822818439\C,4.9502229869,-0.1384758787,-0.635022182\C,5.912621399,-0.9974199781,-1.1656366538\H,5.2298675062,0.8687473346,-0.3491106116\H,6.9386047169,-0.6587149017,-1.2665347686\H,6.2917636558,-2.9427092192,-2.0172415575\H,3.9302995703,-3.7174594873,-1.7136737569\C,0.4205408008,-2.3030484893,1.1400036369\C,2.590909561,-3.3939523647,1.4243097879\C,2.2701314824,-3.722263188,2.7383533868\C,0.1342865646,-2.6325998209,2.4746639956\C,1.0431100319,-3.3291563018,3.2675295298\H,-0.8096051085,-2.323868999,2.902232865\H,0.7891895076,-3.5582851242,4.2972374129\H,3.5480773956,-3.6741633383,1.0007359634\H,2.9825992972,-4.274138901,3.3436342912\P,2.26619381,0.605612515,-0.0338803622\P,-0.7678208373,-1.3109806848,0.1214574025\

C,2.0072781825,0.4819919723,1.7651150983\C,3.0091826767,2.2680183473,-
0.2688774113\C,-1.4359880861,-2.4916975566,-1.1187369304\C,-2.16769199
5,-1.1456193401,1.284495813\C,-0.7300186264,-3.6048178228,-1.587784446
\C,-2.7036633305,-2.2020540082,-1.6501043347\C,-3.2486077825,-3.016889
7095,-2.6391435145\C,-1.2823328015,-4.4152261754,-2.5820473824\C,-2.53
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Int2'

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\C,-0.0850898747,2.3204777454,1.9919020429\C,0.2891163846,3.2117029713
,2.8886466827\H,0.4272915412,4.2556365333,2.6179496498\H,0.4617289842,
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, -2.7998783222,-0.0231063443\O,-1.0250698617,0.8508671265,-2.184973137

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4214335\H,-1.1014654122,-1.0682231206,-5.6502965589\H,-2.0059869551,-0
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.3934540145\H,-1.6480204244,-3.45324706,2.2343698944\H,-4.6265735285,-
2.7455867718,1.9517544504\H,-3.9833977826,-4.3137749532,2.4614007269\H
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TS2'

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TS2

1\1\GINC-A02R01N07\Freq\RB3LYP\GenECP\C68H68O6P2Pd1\ACJSGGHI7X\10-Jan-
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4.6605258861\H,0.6923890064,-1.2278154117,-5.5057260652\H,-0.704043186
4,-0.5928092723,-4.6145443529\C,-1.9179896809,-3.0175594675,2.36952023
64\C,-2.72265875,-4.2106896639,1.8822956238\H,-2.3230037266,-2.6120162
338,3.2993708615\H,-0.8664006463,-3.2759969854,2.5116160507\H,-3.77040
65228,-3.9398406658,1.7329741372\H,-2.6755900336,-5.0133747457,2.62616
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1\1\GINC-A04R05N06\Freq\RB3LYP\GenECP\C68H68O6P2Pd1\ACJSGGHI7X\06-Jan-
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87\C,-4.482360785,0.4213525602,1.3458601043\C,-5.2497095755,-1.0625044
596,3.1283808934\C,-6.15974499,-0.0933155803,3.5524744394\C,-5.4147368
406,1.3741818302,1.7815466287\C,-6.2502922066,1.1190143934,2.869386772
9\H,-5.4702386131,2.3291490051,1.272387132\H,-6.9618986303,1.873817831
2,3.1878918087\H,-6.7958208168,-0.2896302252,4.4096430894\H,-5.1592468
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633774,-0.7161364512\C,-3.2013130671,-3.6214602015,-1.5046922846\C,-4.
4954039684,-4.1098007308,-1.675204932\H,-2.4618038991,-3.8093239009,-2
.2716602091\H,-4.7383536949,-4.687039317,-2.5611128078\H,-5.911774143,
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\P,-3.2589636979,0.7900188526,0.0215920503\O,-1.169753758,-2.143470913
7,-0.128431869\C,-3.923686426,-0.0032597934,-1.4903582306\C,-3.5138114
305,2.5734197474,-0.3092421125\C,-0.4071517392,-3.2353051303,1.1520868
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69,-1.9104542867,0.7122075841\C,3.7714473625,-0.2102506749,2.362161764
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Int3'

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Int3''

1\1\GINC-A04R02N02\Freq\RB3LYP\GenECP\C68H68O6P2Pd1\ACJSGGHI7X\11-Jan-
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14490922\H,-5.8867414864,4.0562062868,1.0367452121\H,-5.6449369956,5.2

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49,2.3250226612,-4.5649707985\C,2.233846249,3.2723348074,-2.7346736848
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,3.0364047991,-1.4221112201,0.5680717721\O,1.9478798706,2.0918111269,-
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876\C,-1.6653439956,-4.7723233032,1.3456203917\H,-3.0551237956,-3.5000
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TS3

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TS3'

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0324,1.223445,0.169619\C,0,-6.516389,1.816125,-0.796476\C,0,-6.589545,
1.014222,-2.083902\H,0,-6.19093,2.841969,-0.985024\H,0,-7.476619,1.828
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,1.636414,4.17547\H,0,-3.730874,3.575213,4.797453\H,0,-3.775751,1.8471
7,5.217349\H,0,-4.905226,2.978249,5.986519\H,0,0.78109,-0.198676,-3.87
8895\H,0,-0.120794,-0.234638,-5.401777\H,0,0.131071,-1.737904,-4.48828
5\C,0,-2.544495,-1.110852,-4.389481\H,0,-3.504,-0.879751,-3.913677\H,0
,-2.411209,-2.192148,-4.404627\H,0,-2.589133,-0.745321,-5.421662\

TS3''

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011,1.9425660339,2.9039684135\C,-4.2195413524,1.7119298934,4.240886449
2\H,-3.8501438317,2.960477133,2.5373603644\H,-4.4478957188,2.552483565
6,4.8880628644\H,-4.4791817495,0.2274345927,5.7848589516\H,-3.89791732
86,-1.6771065989,4.2660153212\C,-3.5328235345,-2.3579609607,-0.3888964
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881036,-3.0932581364,-1.0577161634\H,-4.044500636,-3.0737636705,-2.351
465942\H,-6.4138558891,-3.4824239298,-1.8251585168\H,-5.7688940774,-2.
0115010638,2.1704553956\H,-7.2898153945,-2.9842453477,0.4515068219\O,-
2.941020809,1.1714405266,0.3281062429\O,-1.7440662764,-2.0261774188,-0
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74949,-4.5955309712\

Int4

1\1\GINC-A01R05N08\Freq\RB3LYP\GenECP\C68H68O6P2Pd1\ACJSGGHI7X\06-Jan-
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212\H,-5.7662893422,2.3856765775,1.6467612891\H,-7.3982316502,1.573999
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Int4''

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021204902,4.6119840721,2.9037516499\C,5.1607460215,4.7151326548,1.6566
657571\H,4.9361505597,5.2268148183,0.7212246836\H,5.9468802662,3.97459
96837,1.4712206027\H,5.5500478138,5.4475412403,2.3726971777\C,4.285092

5904,3.3926022434,3.5797573509\H,3.4264352285,2.9224834985,4.069817617
4\H,4.6674882654,4.1675190607,4.2512473833\H,5.0691997756,2.636941249,
3.4643001998\C,3.7010103163,-0.5997325872,0.6261209029\C,0.7488939721,
-1.0131843801,0.7914510316\C,2.984615786,-1.9760372642,0.7366786221\C,
1.5934004101,-2.0109930723,0.0575535628\H,1.6965392235,-1.789373628,-1
.0124473924\H,1.2088360986,-3.0258442705,0.1250827587\C,4.6514973648,-
0.4213560332,-0.5429980544\H,4.3001411701,-0.5254739478,1.5329780138\C
,5.7825456766,0.3824600002,-0.3506113839\C,4.4218588485,-0.9447664261,
-1.8234466881\C,5.2979280603,-0.671851307,-2.8747369326\C,6.6544918769
,0.6659050467,-1.4006024526\C,6.4153872581,0.1377988842,-2.6706639002\
H,7.0941085163,0.3526785386,-3.4904204541\H,5.1025035124,-1.093811169,
-3.8563161193\H,5.9691278225,0.8006682521,0.6340317627\H,7.5211973143,
1.29660124,-1.2262214077\H,3.5654945793,-1.582056273,-2.0069837105\C,3
.8795725265,-3.0950937104,0.201616738\C,2.756658585,-2.2610522573,2.24
07626174\C,1.2980025909,0.1597872212,1.1797457347\C,0.2707190335,1.015
8320922,1.7994019146\H,0.3876030677,2.0940156628,1.7359156432\H,-0.027
0462819,0.7064940405,2.8010556596\O,3.5957023529,-3.8510592185,-0.7023
357795\O,5.0429058038,-3.1240876687,0.8810269549\C,6.0517110951,-4.048
3788438,0.4104255576\C,6.8496154954,-3.4369464121,-0.7299786164\H,5.56
31177558,-4.9765378097,0.1051239701\H,6.6757103366,-4.2355310364,1.286
9091159\H,6.2149089098,-3.2844661065,-1.6046064676\H,7.6725419358,-4.1
042469904,-1.0068316577\H,7.2645218247,-2.4690942461,-0.4368399953\O,3
.1716640468,-1.5884216452,3.1602333244\O,2.03861683,-3.3871223096,2.38
96690268\C,1.5370614949,-3.6651304426,3.718049653\C,0.3506013171,-2.77
24553767,4.0441657463\H,1.2465426576,-4.7165759342,3.6743384043\H,2.35
07186187,-3.5364797342,4.4365295438\H,-0.4157295144,-2.8601332592,3.27
21354091\H,0.6620968573,-1.72803165,4.1051599653\H,-0.0777532318,-3.06
87509798,5.0080743128\H,0.3541791549,3.5599970834,-2.4418465029\H,1.24
53027,4.1413831568,-3.8571792744\H,1.598634891,4.8070247947,-2.2501374
723\C,3.7699804833,3.3069778079,-3.1092726292\H,4.5310042945,2.5276928
63,-2.9993400629\H,4.0898054405,4.1909314637,-2.5558973048\H,3.6979061
999,3.5706757291,-4.1706471957\

Product

```
1\1\GINC-OMC-1-822\SP\RB3LYP\def2TZVP\C32H40O5\SHIMGRP\16-Mar-2023\0\  
#p sp b3lyp/def2tzvp empiricaldispersion=gd3bj scrf=(smd,solvent=aceto  
nitrile)\product\0,1\C,0,3.263069,-0.397865,-0.183835\C,0,2.699299,0  
.542674,0.831696\C,0,1.404614,0.427482,1.167965\C,0,2.412557,-1.532022  
, -0.662951\C,0,1.129382,-1.589934,-0.269962\C,0,0.455445,-0.567574,0.5  
80602\H,0,0.971473,1.104865,1.892813\H,0,0.471527,-2.381078,-0.609288\  
C,0,3.606163,1.632264,1.417717\C,0,3.031877,-2.577475,-1.599223\O,0,4.  
412326,-0.252539,-0.607237\C,0,2.867071,2.470733,2.474623\C,0,4.839607  
,0.992254,2.091443\H,0,2.009222,2.998371,2.045941\H,0,3.550664,3.22369  
6,2.878006\H,0,2.517594,1.858042,3.312621\C,0,4.259503,-3.227754,-0.92
```

2819\H,0,5.02995,-2.487956,-0.708797\H,0,4.68314,-3.993249,-1.582025\H
,0,3.968508,-3.713811,0.014665\C,0,3.453789,-1.902802,-2.92411\H,0,4.1
98269,-1.127105,-2.74904\H,0,2.585467,-1.452697,-3.418202\H,0,3.876748
, -2.650814,-3.60382\C,0,2.030074,-3.695794,-1.933259\H,0,1.693814,-4.2
22373,-1.034107\H,0,2.512956,-4.427971,-2.587331\H,0,1.147601,-3.31512
, -2.457359\C,0,-0.670177,0.155653,-0.325451\C,0,-0.367867,-1.184991,1.
724908\C,0,-2.018104,-0.072834,0.431788\C,0,-1.628845,-0.375458,1.8952
61\H,0,-1.433203,0.574195,2.406233\H,0,-2.414039,-0.891402,2.447912\C,
0,-0.281487,1.565993,-0.700885\H,0,-0.737141,-0.416718,-1.249152\C,0,0
.396275,1.752345,-1.911112\C,0,-0.467,2.674524,0.136954\C,0,0.003682,3
.933093,-0.234501\C,0,0.881185,3.006392,-2.278527\C,0,0.684136,4.10400
7,-1.440751\H,0,1.058017,5.082938,-1.72383\H,0,-0.155523,4.779834,0.42
6182\H,0,0.559233,0.898293,-2.561933\H,0,1.41202,3.124753,-3.21801\H,0
, -0.982902,2.565637,1.083678\C,0,-3.006104,1.081385,0.316389\C,0,-2.70
0138,-1.326807,-0.139647\C,0,-0.042139,-2.272525,2.369043\C,0,0.299119
, -3.363419,3.000893\H,0,-0.00562,-4.345214,2.645428\H,0,0.904772,-3.33
2179,3.903835\O,0,-3.373739,1.780143,1.235142\O,0,-3.406655,1.215381,-
0.95975\C,0,-4.377802,2.256812,-1.224774\C,0,-5.782569,1.767626,-0.916
088\H,0,-4.247368,2.483688,-2.28426\H,0,-4.117888,3.134389,-0.629264\H
,0,-6.01043,0.864546,-1.489655\H,0,-6.513611,2.538269,-1.179885\H,0,-5
.882536,1.545995,0.148773\O,0,-2.205011,-2.117341,-0.91228\O,0,-3.9341
52,-1.454113,0.376672\C,0,-4.705958,-2.592635,-0.076666\C,0,-6.095779,
-2.448545,0.506733\H,0,-4.710512,-2.59582,-1.170093\H,0,-4.205926,-3.5
06551,0.257678\H,0,-6.564325,-1.521665,0.164558\H,0,-6.060815,-2.43400
5,1.599367\H,0,-6.720146,-3.289654,0.191506\H,0,4.532165,0.324219,2.90
352\H,0,5.474756,1.774457,2.521319\H,0,5.428675,0.422083,1.373881\C,0,
4.052084,2.588704,0.287254\H,0,3.181069,3.047787,-0.19054\H,0,4.628444
,2.057799,-0.469457\H,0,4.673976,3.388244,0.705507\

DFT calculation data of **condition B**

1b

1\1\GINC-OMC-1-821\Freq\RB3LYP\6-31G(d,p)\C11H14O4\SHIMGRP\15-Mar-2023
\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p)
Freq\|a_opt_freq\0,1\C,-0.0361470929,-0.0906203327,0.2023579826\C,-0
.0768257244,0.5907997647,1.5882653195\C,0.1170200923,1.389736574,0.382
8696507\H,0.7857299631,0.4157454384,2.2257603738\H,-1.0422180613,0.613
0526756,2.0834631236\C,0.2675488934,2.5097533679,-0.2372482733\C,0.426
9957457,3.6408925886,-0.8743666869\H,1.4174439663,4.040171376,-1.07787
76359\H,-0.4234902704,4.2199253867,-1.2252545306\C,1.1648362692,-0.945
78492,-0.0996360407\C,-1.3120817112,-0.5273090243,-0.4693894916\O,-2.3
853654591,-0.3449821699,0.3278336678\O,2.3119695443,-0.2873978366,0.16
49535224\O,1.110892462,-2.0953347855,-0.4709618538\O,-1.3718702167,-0.
9339658871,-1.6059773221\C,-3.6652890299,-0.6304991325,-0.2823843391\C
, -4.733024857,-0.322705741,0.7468236109\H,-3.677745537,-1.6792805865,-

0.5927556151\H,-3.7679110396,-0.0187296945,-1.1836637485\H,-4.60319286
66,-0.9406403185,1.6396386839\H,-5.7227866298,-0.5266580429,0.32766932
46\H,-4.6951276853,0.7286820781,1.0454315125\C,3.5238781125,-1.0573040
76,-0.0069107532\C,4.6850917763,-0.1471579062,0.3357933454\H,3.5674774
941,-1.4142090471,-1.0398805116\H,3.4790800702,-1.9363001085,0.6435051
888\H,4.701464532,0.725678667,-0.3224589009\H,5.6287164808,-0.68792692
72,0.2171789378\H,4.6150867791,0.20235762,1.3696734589\

PdL_n

1\1\GINC-OMC-1-812\Freq\RB3LYP\GenECP\C27H22N1O1P1Pd1\SHIMGRP\23-Aug-2
023\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP F
req\lezuolin\0,1\C,-1.2176142098,-2.4601602993,-1.9697650525\C,-1.538
4434931,-3.7908667466,-2.2324298405\C,-1.5615063843,-1.879062146,-0.74
30532353\C,-2.2175037945,-2.6511477789,0.2227491495\C,-2.5332602917,-3
.9847709782,-0.0390867321\C,-2.1966343711,-4.5560794553,-1.2673437702\
H,-0.6766931213,-1.8654751862,-2.7010429085\H,-1.265662053,-4.23401379
81,-3.1859057712\H,-3.0381947215,-4.5783282816,0.7176537025\H,-2.44022
11364,-5.5951496836,-1.4688630584\H,-2.4709936868,-2.2133263225,1.1832
155053\P,-1.135452551,-0.1138802157,-0.4799856653\C,-2.7269434901,0.74
26851663,-0.8478575983\C,-1.0433390228,0.0334298527,1.3724362528\C,-3.
9718861343,0.0999611829,-0.8826160661\C,-2.6637258828,2.1178693346,-1.
1214580814\C,-3.8221956237,2.8402300679,-1.400798447\C,-5.130137398,0.
8219391088,-1.1759741616\C,-5.0592142977,2.1921972672,-1.4302289263\H,
-4.035556648,-0.9642755096,-0.6842094769\H,-1.6942720947,2.6097752213,
-1.1214378766\H,-3.7589165328,3.9044735892,-1.6079501268\H,-5.96186454
5,2.7511481048,-1.658742794\H,-6.0886293324,0.311801854,-1.2060439804\
C,-2.1143301725,0.5993213581,2.0796578\C,0.1218207965,-0.3080540516,2.
105702645\C,0.1928784019,-0.044354724,3.4802721162\C,-0.8847946075,0.5
164440571,4.1585242999\C,-2.0446654428,0.830637879,3.4535073174\H,1.10
6931672,-0.2932541764,4.0077785443\H,-0.8178227747,0.7057785894,5.2252
201212\H,-2.897360603,1.2654736909,3.9665578299\H,-3.01652173,0.873228
8138,1.5468230373\C,1.2922963368,-0.9322767961,1.4717821499\O,2.515562
0425,-0.5473629324,1.9661282598\C,3.4871167325,-1.3541130124,1.2579457
001\N,1.2737303691,-1.7587149703,0.4991994183\C,2.6851626505,-1.949328
7869,0.0737954376\H,3.8546202055,-2.129021613,1.9387824302\H,4.3141101
105,-0.7089848544,0.9578931548\Pd,0.6751672254,0.6037098531,-1.6459123
024\H,2.8855820839,-3.0168740284,-0.0489260787\C,2.8684456223,-1.24752
87198,-1.2555442944\C,2.9053793469,-1.9624818228,-2.4437342133\C,2.847
2708893,0.1748628889,-1.2960927777\C,2.8697214282,-1.30208017,-3.68633
84109\H,2.9187372941,-3.0485514825,-2.410083636\C,2.8022535296,0.84426
68499,-2.5434130815\H,3.0033859779,0.7413450493,-0.3822806779\C,2.7919
124284,0.0821161058,-3.7388278536\H,2.8886003762,-1.8809080418,-4.6045
682472\H,2.9232600864,1.922744515,-2.589179162\H,2.7577454011,0.594149
2844,-4.6954786472\

PdL_n'

1\1\GINC-OMC-1-806\Freq\RB3LYP\GenECP\C27H22N1O1P1Pd1\SHIMGRP\27-Jul-2023\0\#P
Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP Freq\ezuolin\0,1\C,-2.6115769641,-0.0442822679,1.1606814973\C,-3.3115768089,-1.1772842822,0.7486160949\C,-1.7724532875,0.6409672566,0.2691698133\C,-1.6607359669,0.1759336782,-1.0489946251\C,-2.3697680623,-0.9527618931,-1.4640083206\C,-3.1941720371,-1.6326766662,-0.5665451977\H,-2.7173289511,0.3306371202,2.1747627587\H,-3.9561194335,-1.698815775,1.450307195\H,-2.2768266921,-1.3003202437,-2.4889835478\H,-3.746307011,-2.5097443131,-0.8912594296\H,-1.0204642892,0.6968147266,-1.753202726\H,-0.8845767526,2.1322569515,0.9010765268\C,0.7739857327,1.4469791089,1.3340387576\C,-0.5181061691,3.0025333197,-0.7151049804\C,1.2640562897,0.2186549773,0.8673697086\C,1.5664269272,2.2087532606,2.2054503683\C,2.833574917,1.7668338478,2.582229942\C,2.5247807159,-0.2320794392,1.2604542221\C,3.3141652853,0.5423018575,2.1126193036\H,0.6602260913,-0.3849678316,0.1981330298\H,1.17112116,3.1455106414,2.5905144651\H,3.4393813807,2.3691945993,3.2529781018\H,4.2953720137,0.1894228804,2.4162872334\H,2.8919141368,-1.1883171929,0.8984347445\C,0.7885160144,3.009885233,-1.2201324878\C,-1.5239788137,3.6504075241,-1.4862911226\C,-1.1895808204,4.2293720073,-2.7204991695\C,0.1201540149,4.228958784,-3.1927530779\C,1.1137239246,3.6225825768,-2.4314888553\H,-1.9766277223,4.6925303425,-3.3039658524\H,0.3547705326,4.6965368828,-4.1436358074\H,2.1424955254,3.6090378208,-2.7793800741\H,1.5710857426,2.5160601768,-0.6578165816\C,-2.9470474999,3.7934880128,-1.0998147458\O,-3.8295728484,3.7389649352,-2.1412492853\C,-5.1077662652,4.1650287838,-1.6092922714\N,-3.452728245,4.0200177781,0.0618644486\C,-4.9198315162,4.0562426674,-0.0779823541\H,-5.8820172435,3.5132055414,-2.0145429651\H,-5.286642552,5.1987401886,-1.9250331656\Pd,-2.2919816123,3.5250060367,1.8834911972\H,-5.306987641,3.0966110088,0.2890413432\C,-5.5652791775,5.1748328531,0.7019479328\C,-6.8860037086,5.0448461727,1.142512628\C,-4.8722104957,6.3632725758,0.9579489967\C,-7.5119178825,6.0900040833,1.8221682832\H,-7.4242720708,4.1182354291,0.9582447067\C,-5.4954235897,7.4061706528,1.6432396933\H,-3.8402526461,6.4539675972,0.6353985307\C,-6.8167119393,7.2737580695,2.0741207045\H,-8.5372011219,5.976699617,2.1614346167\H,-4.9464256795,8.321161211,1.8450058623\H,-7.299716188,8.0855773967,2.6094946563\

1a

1\1\GINC-OMC-1-823\Freq\RB3LYP\6-31G(d,p)\C21H26O1\SHIMGRP\12-Mar-2023\0\#P
Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq\tBu\0,1\C,-1.9790887033,0.4659820702,0.0592738551\C,-1.9163827593,-1.0227800638,0.0178032087\C,-0.7012414366,-1.6164766211,-0.0572623836\C,0.5453484547,-0.8784017412,-0.0790122614\C,0.4646266705,0.565930

6117,-0.1349711184\C,-0.7101946451,1.2388907627,-0.0787292571\H,-0.618
1052224,-2.6975195781,-0.0708189992\H,1.3903449399,1.1057151492,-0.271
3118489\C,-0.7810081114,2.7673593888,-0.1640759827\C,-3.2233004167,-1.
8213156892,0.0732249536\C,-1.3831235633,3.3327475228,1.1434393088\H,-2
.3931748641,2.957678886,1.3022207223\H,-1.4160972835,4.4265611162,1.09
17295315\H,-0.7645814112,3.0542938668,2.0035274125\C,-1.6528504088,3.1
879069279,-1.3693830146\H,-2.6710790117,2.815011083,-1.2663327163\H,-1
.2295250679,2.8036719684,-2.3036595059\H,-1.6848782866,4.2806383339,-1
.4382496622\C,0.6129407109,3.3911219839,-0.3500370006\H,1.2791736229,3
.1657010213,0.4894616071\H,0.5148924246,4.4790512445,-0.4083839785\H,1
.0947346232,3.0523951576,-1.2731288177\C,-4.125857448,-1.4285878408,-1
.1191139888\H,-4.3811020434,-0.3702082162,-1.0852763703\H,-5.051153850
6,-2.0141817599,-1.0902084645\H,-3.6228785835,-1.6396262634,-2.0689628
792\C,-3.9561795541,-1.5347045574,1.4040656019\H,-4.2048678625,-0.4780
761686,1.4936126761\H,-3.332202288,-1.8234442694,2.2567047654\H,-4.881
2687942,-2.1197812441,1.4496324994\C,-2.9669356357,-3.3357455503,-0.00
85649611\H,-2.4645604581,-3.6163131696,-0.9403385575\H,-3.9239063757,-
3.8647715438,0.0227894357\H,-2.3643933899,-3.6958464123,0.831912826\O,
-3.0636203466,1.0503733983,0.1816231985\C,1.7219389762,-1.5783245977,-
0.0802077073\C,3.0894628898,-1.0824302304,0.01757761\H,1.6370853848,-2
.6595922437,-0.1824342362\C,3.4478971129,0.053596529,0.7707864055\C,4.
771623728,0.4787035171,0.8284159743\C,5.7682388664,-0.221397168,0.1460
474601\C,4.1143189383,-1.7990751491,-0.6317568718\C,5.4348874301,-1.36
70899715,-0.579805146\H,2.6908989183,0.5747252707,1.3446103622\H,3.857
5567747,-2.6916282984,-1.1951625618\H,6.2064461032,-1.9259290046,-1.10
0141865\H,5.028703891,1.3517142313,1.4201852572\H,6.7997733619,0.11289
83113,0.1939444849\

Int0-B

1\1\GINC-OMC-1-816\Freq\RB3LYP\GenECP\C38H36N1O5P1Pd1\SHIMGRP\06-Oct-2
023\0\#P Geom=AllCheck Guess=TChef SCRF=Check GenChk RB3LYP/GenECP F
req\lezuolin\0,1\C,2.5262472174,-1.2646778844,2.384484141\C,2.8117006
541,-2.3347525011,3.2319105988\C,3.1907239891,-1.1367969275,1.15682505
11\C,4.1347728326,-2.1025240021,0.7832121467\C,4.4190003811,-3.1734790
071,1.6315130902\C,3.7587469421,-3.2902499299,2.8562306434\H,1.7683002
296,-0.5352370879,2.6553672336\H,2.2869731354,-2.4287688366,4.17790942
15\H,5.1504435033,-3.9190774193,1.3338600765\H,3.9760700317,-4.1276574
381,3.5125461215\H,4.6347035242,-2.0242724841,-0.1774856177\H,2.708170
9272,0.2609479959,0.0709361228\C,4.0777302784,1.4691773199,0.183455962
3\C,2.9197759812,-0.4744724315,-1.6237096548\C,5.3719038967,1.15481061
13,0.6197073118\C,3.7757238399,2.7886709868,-0.1891773777\C,4.76254288
33,3.7725741407,-0.1478080914\C,6.3528868189,2.1454056296,0.671618465\
C,6.0515987333,3.4524655569,0.2836452794\H,5.6098029471,0.1408761492,0
.9235110319\H,2.7636504445,3.0317101414,-0.5021808666\H,4.5221058585,4

.7902521431,-0.4405312203\H,6.8176519371,4.2210724158,0.325408489\H,7.3525640731,1.896609402,1.0155516785\C,3.9298333848,-0.0201595678,-2.4765586987\C,2.0204774987,-1.4593373766,-2.1175708342\C,2.1687660711,-1.9561240052,-3.4179195908\C,3.1778859373,-1.4804635477,-4.2522723776\C,4.0583227768,-0.5114613379,-3.7782561831\H,1.4787505023,-2.7168226727,-3.7642470274\H,3.2739759761,-1.8666538649,-5.2618697957\H,4.8525618083,-0.13508282,-4.4160295154\H,4.6270500128,0.7290855077,-2.1203121723\C,0.9573066657,-2.0300280123,-1.276588575\O,0.5049061959,-3.2670062208,-1.6112814398\C,-0.6101915695,-3.5111684536,-0.7021615011\N,0.4674448821,-1.5111764447,-0.2075732703\C,-0.2701560046,-2.5934419869,0.4809033711\H,-0.6231668065,-4.5763824198,-0.4759434497\H,-1.5360100196,-3.1935169495,-1.1914853882\Pd,0.4563616972,0.8159320917,-0.1296205471\H,0.4830352796,-3.0915991586,1.1134877361\C,-1.4273530025,-2.2271776974,1.3781457511\C,-1.7214635146,-0.915779854,1.7549961259\C,-2.2069711174,-3.2701048017,1.9000358859\C,-2.7944621408,-0.6412108158,2.6044610878\H,-1.1265333784,-0.0970544157,1.3605843162\C,-3.2670872248,-3.0022284205,2.7656375631\H,-1.9817231997,-4.3004075093,1.6354312674\C,-3.5668989963,-1.6840724503,3.1165093297\H,-3.0401057559,0.3920730735,2.8227138381\H,-3.8609738514,-3.8219764044,3.1594876464\H,-4.3999686917,-1.4720272249,3.7800263339\C,-2.6999679712,1.5892083573,-0.7054493107\C,-1.9996678463,2.0525936745,-1.9952746422\C,-1.20480788,1.8686835188,-0.7688940523\H,-2.2075660437,3.0677067304,-2.3206819691\H,-1.9556104212,1.2965556658,-2.7736140455\C,-0.307222597,2.6720523336,-0.0712437775\C,-0.0059018174,3.8571175573,0.445958449\H,0.937410261,4.0362987741,0.9534600679\H,-0.7030888357,4.6911948287,0.3873559765\C,-3.4697148456,2.5342216775,0.1601259076\C,-3.1415690329,0.1578676234,-0.7672494641\O,-4.3444930993,-0.0275580844,-0.2029658732\O,-3.763349792,3.691391643,-0.477396984\O,-3.7502087184,2.3213097325,1.3233342977\O,-2.5213350137,-0.7248829373,-1.3331179551\C,-4.8456665545,-1.3815795937,-0.2154702531\C,-6.1529073307,-1.377532816,0.5494965853\H,-4.1040861782,-2.0324055319,0.2513133312\H,-4.9736892981,-1.7000804629,-1.2553606868\H,-5.9878874474,-1.0420582218,1.5759735208\H,-6.5709904384,-2.3887053733,0.5769893895\H,-6.8824542487,-0.7126235216,0.0783228214\C,-4.4217137755,4.7015208038,0.3195842154\C,-3.4167274644,5.5291523232,1.1041701288\H,-5.1320927251,4.2109275875,0.9886443351\H,-4.9650126914,5.3103291994,-0.4068807001\H,-2.8620787381,4.8940365882,1.798159136\H,-3.9373559601,6.3020000464,1.6794866847\H,-2.7086382706,6.0209712343,0.430846464\

TS1-B

1\1\GINC-OMC-1-813\Freq\RB3LYP\GenECP\C38H36N1O5P1Pd1\SHIMGRP\08-Nov-2023\0\#p freq geneep b3lyp empiricdispersion=gd3bj geom=check guess =read\TS2\0,1\C,-2.4714846701,-1.0368433208,-2.91018547\C,-3.0468368627,-1.8873750851,-3.8532886687\C,-2.8079236574,-1.1486961425,-1.5534149567\C,-3.7286538268,-2.1272537475,-1.1578508622\C,-4.2972683539,-2.9

840195028,-2.101629706\C,-3.9577277186,-2.8661690963,-3.4503025523\H,-
1.7455562041,-0.2894702987,-3.2174865043\H,-2.7780074546,-1.7905503695
,-4.9010322172\H,-5.0082529653,-3.7405960259,-1.782721182\H,-4.4010133
612,-3.5332320027,-4.1836550362\H,-4.0030807072,-2.2190103162,-0.11215
55474\H,-2.0267624894,0.0123376193,-0.352497158\C,-3.2781053537,1.3578
576688,-0.2552487293\C,-2.1720214446,-0.9250514655,1.2142865564\C,-4.4
919080473,1.2772525487,-0.9569061622\C,-2.9912142888,2.5200557625,0.48
18447669\C,-3.910606633,3.5676927455,0.5227770381\C,-5.4008105273,2.33
4566443,-0.9180513954\C,-5.1146352415,3.4818351042,-0.177965308\H,-4.7
310380598,0.3921477108,-1.5335206967\H,-2.0575129538,2.5821426753,1.02
93842281\H,-3.6788108617,4.4570366332,1.1015295447\H,-5.8240486187,4.3
036935567,-0.1495594834\H,-6.3349222905,2.2574955097,-1.4668160615\C,-
2.9878989166,-0.4451506382,2.246579111\C,-1.421683949,-2.1117928143,1.
4407251111\C,-1.5451354749,-2.7777459474,2.674752247\C,-2.362547931,-2
.282161802,3.6822791021\C,-3.0829024354,-1.1065757353,3.4676366343\H,-
0.9739515268,-3.6827440188,2.8354367489\H,-2.4328272754,-2.8081960311,
4.6287758434\H,-3.7240353066,-0.7055641674,4.2466538425\H,-3.552272034
4,0.4653366487,2.0879383364\C,-0.4654971757,-2.6813130267,0.4801417169
\O,0.0660057636,-3.8804280377,0.8414581684\C,0.9998959675,-4.274106186
5,-0.1894901432\N,-0.0196248723,-2.1763903355,-0.623608132\C,1.0488883
762,-3.0530085207,-1.1454551717\H,0.6139283167,-5.1785165075,-0.667245
8863\H,1.9604075254,-4.4846336258,0.2837036903\Pd,0.2006514403,-0.0118
423256,-1.1206452285\H,0.7916243816,-3.3436205659,-2.1683038487\C,2.37
94621108,-2.3299740419,-1.1558009774\C,3.2741746501,-2.5239765942,-2.2
103455142\C,2.7316274075,-1.471584044,-0.1046583684\C,4.5100487108,-1.
8761238962,-2.2120258489\H,2.9996990684,-3.1759344858,-3.0361831226\C,
3.9641408725,-0.8193859019,-0.1054429528\H,2.0440687089,-1.2806147473,
0.7110425637\C,4.8550467143,-1.0251938105,-1.1598479207\H,5.1994179024
,-2.0309519843,-3.0369830538\H,4.1945736602,-0.1270557167,0.6974517503
\H,5.8132763726,-0.5156805749,-1.1686594828\C,1.5229402996,2.338361258
5,0.5765109743\C,0.7165015932,3.011240466,-0.5213664681\C,0.899316817,
1.8224423745,-1.3778741548\H,1.1808232157,3.9145227201,-0.9159525904\H
,-0.3154743413,3.1861855694,-0.2231970418\C,1.678495059,1.3115296227,-
2.3033303291\C,2.7115009909,0.9466258192,-3.056301822\H,2.609205878,0.
2538669962,-3.8866451485\H,3.714870425,1.3159967771,-2.8472305398\C,2.
9642514356,2.4803664409,0.6073606133\C,0.7894517388,1.6037926921,1.588
6762732\O,1.5105430806,0.6636884317,2.2560709104\O,3.41663847,3.235879
707,-0.4545774716\O,3.7408203667,2.062189541,1.4592876757\O,-0.4079074
75,1.7741539803,1.8379309429\C,0.8466491969,0.0216997878,3.3590796518\
C,1.5909675483,-1.2652269355,3.660256629\H,-0.1962240755,-0.1648661818
,3.1027020072\H,0.8648068909,0.70139761,4.2196303588\H,1.5068252834,-1
.9714855186,2.8289934201\H,1.1627221532,-1.7409830137,4.5482714842\H,2
.6513554847,-1.0710450941,3.8427977152\C,4.7905722998,3.6465507344,-0.
3868036965\C,5.7462919414,2.5831067153,-0.9059137203\H,5.0365270712,3.

9001606124,0.6479013189\H,4.8380576876,4.5503706485,-1.0008792372\H,5.
7012285339,1.7002981846,-0.2675943549\H,6.7722463445,2.9675089538,-0.9
00738588\H,5.495439626,2.2955809317,-1.931343463\

Int1-B

1\1\GINC-OMC-1-818\Freq\RB3LYP\GenECP\C38H36N1O5P1Pd1\SHIMGRP\06-Oct-2
023\0\#P Geom=AllCheck Guess=TChef SCRF=Check GenChk RB3LYP/GenECP F
req\ezulin\0,1\C,2.6157256004,-0.9786479066,2.219194408\C,2.9517738
351,-2.0792487743,3.0068459696\C,3.2436429385,-0.7824346071,0.98142576
39\C,4.2036078875,-1.7003809211,0.5342823053\C,4.5343396371,-2.8015816
185,1.3235383369\C,3.9099686921,-2.9907856308,2.5588238968\H,1.8442225
15,-0.2866598176,2.5436837257\H,2.452370419,-2.2318391392,3.958288997\
H,5.2737048139,-3.5146062888,0.9721998228\H,4.1646776469,-3.8529636126
,3.1674000777\H,4.6807555298,-1.5589859151,-0.4306292744\P,2.737871180
7,0.6516415991,-0.0253371835\C,4.0796393042,1.8770895048,0.1227279496\
C,2.8363743641,0.0537377058,-1.7800582455\C,5.2170029298,1.6475900469,
0.9070426163\C,3.9366398031,3.1058012661,-0.543571991\C,4.9241232454,4
.0812862487,-0.4377789396\C,6.1981779799,2.6341952404,1.0203398735\C,6
.0558147947,3.8479186372,0.3486337707\H,5.3359846976,0.7037210589,1.42
7113572\H,3.0564588117,3.2877639566,-1.1525116726\H,4.8082239957,5.025
1256958,-0.9613237745\H,6.8211864633,4.6124099731,0.4385703312\H,7.075
0829916,2.4504193636,1.6333509447\C,3.8338678356,0.5137124336,-2.64271
88053\C,1.868501752,-0.8516527311,-2.291271456\C,1.9235702672,-1.26316
50508,-3.6250630664\C,2.913346278,-0.7723005778,-4.4759522168\C,3.8698
725279,0.1098796536,-3.9811346331\H,1.1816296331,-1.9682673383,-3.9825
165\H,2.938440024,-1.0848307361,-5.5145838202\H,4.6529494468,0.4873698
704,-4.6313677989\H,4.5904928155,1.1954888422,-2.2731836983\C,0.869127
868,-1.4630609635,-1.4010909383\O,0.511112218,-2.7285315706,-1.6506482
619\C,-0.513353684,-3.0342141173,-0.6276145577\N,0.4122625507,-0.93903
24647,-0.3131259966\C,-0.1034187056,-2.0796379473,0.4977528988\H,-0.41
92711439,-4.0903606193,-0.3818308729\H,-1.4888587484,-2.7667578133,-1.
0463206354\Pd,0.5388948232,1.1689295727,0.050918854\H,0.7825347524,-2.
4934125137,1.0011909857\C,-1.133575848,-1.8031139821,1.5540170569\C,-1
.2259593861,-2.7067089485,2.6226075719\C,-2.0280509227,-0.7366462631,1
.4830033248\C,-2.2252865413,-2.5609093902,3.5824371378\H,-0.5182134197
, -3.530060095,2.6943611066\C,-3.0427262121,-0.5953111934,2.4330571112\
H,-1.9798119574,-0.0404268043,0.6592077592\C,-3.141277631,-1.509775205
3,3.4817203664\H,-2.294330396,-3.2700774184,4.4023479693\H,-3.78202848
56,0.1877844572,2.301732954\H,-3.9350684873,-1.4092056091,4.2159304156
\C,-3.6665063218,0.8101729225,-0.9434271004\C,-2.6125003648,1.53869900
44,-1.7420573618\C,-1.5463172041,2.1345413534,-0.9230907875\H,-3.03038
55067,2.3688156507,-2.3284814288\H,-2.1595460814,0.8264617376,-2.43871
95199\C,-0.8042097573,2.8861651595,-0.2706293746\C,0.3937734684,3.2278
888794,0.3938953015\H,1.1137828349,3.8382658531,-0.1475950031\H,0.3477

996903,3.4587814771,1.4583505489\C,-4.4853769024,1.5545455511,-0.04293
67982\C,-3.63799922,-0.6055019629,-1.0418994189\O,-4.6156553433,-1.251
0962744,-0.3381357788\O,-4.2573186051,2.9294517937,-0.2167751846\O,-5.
2753379756,1.1722576008,0.8198980938\O,-2.7905197886,-1.262798788,-1.6
864679891\C,-4.4999017761,-2.6677315842,-0.2448198017\C,-5.6376122837,
-3.1434890045,0.6410760308\H,-3.5318385786,-2.9331584326,0.1974502981\
H,-4.5408734625,-3.1195735497,-1.2431238206\H,-5.5585975708,-2.6847154
559,1.6302726872\H,-5.6053235143,-4.2326308712,0.7537572307\H,-6.60404
01646,-2.8639662965,0.2121619345\C,-4.8479376605,3.7783008123,0.765014
2166\C,-3.9582625463,3.8933601441,1.9980251033\H,-5.8315192842,3.38921
26161,1.0408006358\H,-4.9671046552,4.75103961,0.27652874\H,-3.86466138
95,2.916634981,2.4796201277\H,-4.3850408374,4.5966657702,2.7223953408\
H,-2.9586124792,4.2430394913,1.7196436239\

Int1'-B

1\GINC-OMC-1-824\Freq\RB3LYP\GenECP\C38H36N1O5P1Pd1\SHIMGRP\07-Oct-2
023\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP F
req\lezuolin\0,1\C,1.5520818031,-0.9603920131,2.5539090622\C,1.902105
7155,-1.8585851836,3.5623580898\C,2.0989084966,-1.0939019679,1.2693921
222\C,2.9920437392,-2.1403314034,1.0033448354\C,3.3350684776,-3.040742
1235,2.0118031272\C,2.7912991382,-2.9005212936,3.2907253895\H,0.845517
752,-0.1579633536,2.7480695845\H,1.4761419019,-1.7491782011,4.55512368
99\H,4.0242693587,-3.852475545,1.7994678721\H,3.0579940492,-3.60454461
83,4.0731654924\H,3.4106463502,-2.252440232,0.0079975999\H,1.560820483
2,0.1002405026,-0.0083621182\C,2.9270554076,1.2859316128,-0.2023221839
\C,1.6001474203,-0.9071028607,-1.5633439358\C,4.0699063827,1.251322188
2,0.6045903108\C,2.7781938447,2.3097148059,-1.1531945751\C,3.773416085
2,3.2715790645,-1.3028038699\C,5.0574198666,2.227229131,0.4599928912\C
,4.9123007101,3.2351609946,-0.4928463929\H,4.1876864187,0.4682646504,1
.3456798312\H,1.8784673504,2.3563373884,-1.756978998\H,3.652000996,4.0
594717607,-2.039614991\H,5.6809391442,3.9941896398,-0.6026569784\H,5.9
391903578,2.1976341889,1.0928442798\C,2.5437706726,-0.6761744821,-2.56
72537323\C,0.6366589247,-1.9236855228,-1.7714257758\C,0.6466407462,-2.
6794832023,-2.9475780093\C,1.5782365219,-2.413196496,-3.9492917499\C,2.
.5263678934,-1.4119412833,-3.7549866239\H,-0.0869643069,-3.4682523377,
-3.0702512442\H,1.5652660964,-2.9885818391,-4.8690542942\H,3.263364893
8,-1.2019006815,-4.5239416346\H,3.2970973281,0.0890463677,-2.425102377
6\C,-0.3419014007,-2.2634896634,-0.7263847884\O,-0.5723805655,-3.58580
18249,-0.5459652511\C,-1.584316249,-3.6687608804,0.4950710134\N,-0.935
0345821,-1.4519025778,0.0761749183\C,-1.5539585411,-2.2701309076,1.148
0646832\H,-1.3160142905,-4.4842249919,1.1658738077\H,-2.5496399907,-3.
8683662156,0.0199735257\Pd,-0.6376957356,0.7523536031,-0.0170816409\H,
-0.8455115027,-2.2583024515,1.9868122376\C,-2.906666036,-1.8384631874,
1.6416834866\C,-3.2154046246,-2.0017366935,2.9973923102\C,-3.890416427
6,-1.391274649,0.7564956429\C,-4.5038200403,-1.7424931687,3.4631221279

\H,-2.4450818747,-2.3395915947,3.6866913314\C,-5.1771038981,-1.1252951
553,1.2255637548\H,-3.6476338052,-1.2134249623,-0.2852673584\C,-5.4892
503066,-1.3102050373,2.5731123579\H,-4.7354933982,-1.8715513341,4.5161
593623\H,-5.9168067081,-0.7436976543,0.531979764\H,-6.4922227979,-1.10
11608831,2.9332371379\C,-2.3571442935,1.6952886992,-1.0090874554\C,-1.
6285280154,3.0624366819,-0.9618465644\C,-0.4557717985,2.7390437867,-0.
0910227395\H,-2.2570429023,3.8619094779,-0.5584322962\H,-1.3171862819,
3.3287977964,-1.9768791046\C,0.3753627447,3.4259695368,0.6246226674\C,
1.2580784624,4.0805140375,1.3510073966\H,2.2205207691,4.3806882476,0.9
411210666\H,1.0575406999,4.3517046165,2.385685266\C,-3.6420117372,1.64
31065959,-0.2894340402\C,-2.2412810856,0.9870031615,-2.3005432748\O,-2
.8347129293,-0.2444930906,-2.2947625903\O,-3.5343689126,2.2779938568,0
.9173439607\O,-4.690757647,1.1591562007,-0.6835955856\O,-1.6164188327,
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411,-3.7788545948\H,-3.2314555336,-0.5450988957,-4.307495789\H,-2.5976
552929,-2.8933774676,-2.4131752077\H,-3.1276539378,-3.0348250361,-4.09
93058477\H,-4.2314017325,-2.3822593336,-2.8714699718\C,-4.7084173248,2
.3759455391,1.7369777774\C,-4.3014022762,2.0953622656,3.1722967547\H,-
5.4547008053,1.6662460758,1.3782395265\H,-5.1133005024,3.389612621,1.6
271870679\H,-3.9146389448,1.0772762733,3.261973759\H,-5.1656923226,2.1
975789254,3.8375412867\H,-3.5266863198,2.7948347282,3.5003144878\

Int2-B

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03,2.1329051514,-2.3337084788\C,2.1917428316,1.369236717,-2.036453082\
C,1.7871292164,3.7047066547,-0.4549396131\C,2.7787875064,2.8253182493,
-0.1414681312\C,3.0341809285,1.6282360959,-0.9016227166\H,2.4418229754
,0.5193109524,-2.6534637868\H,3.4516702309,3.0134899759,0.686863491\C,
0.1629158402,1.7747364716,-3.4897706071\C,1.6593095331,5.0722807291,0.
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,1.6321486828,0.6962905902,-4.7153181611\H,-0.0571827226,0.3098484853,
-5.0676243559\H,0.7141018756,-0.3461859793,-3.6171027479\C,0.332874045
5,5.2016462329,1.0101761157\H,-0.5190896029,5.0688058148,0.347047167\H
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724568517,-1.5579267296\H,2.6706653127,6.1226345392,-1.396783653\H,1.6
611433912,7.1642179883,-0.378007121\C,2.809467699,5.3171171412,1.22460
13568\H,2.7988175256,4.5974231029,2.0485372918\H,2.7058093587,6.316651
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\C,3.9562458394,-1.291508993,-1.9063353558\C,4.6030470524,-2.267234619
2,-2.6604040536\C,6.7381136851,-1.25712791,-2.1666397932\C,5.990124678
7,-2.2473623467,-2.8085125535\H,6.4876519118,-3.011078678,-3.398976516
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96,-0.8903056129\H,7.8205627669,-1.2480941386,-2.252833411\H,2.8913059
194,-1.3601688767,-1.7323719857\C,3.7089826329,-1.7314088935,1.2795886
534\C,3.215056011,0.4301877205,2.4948614914\C,0.0268929056,1.159877159
7,1.1665048492\C,-0.978743798,2.0827174893,0.993097096\H,-1.4999173589
,2.4589436347,1.868898032\H,-0.993424729,2.7346055,0.1274456891\O,3.35
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70231,-2.9319333957,0.1549696868\H,6.250778697,-3.2340514903,3.1503060
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\C,1.0930616652,2.726901944,4.4099772713\H,3.0713015777,1.9115028077,4
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8,-1.150027022\C,0.152650255,-4.2104126579,0.0445747884\C,0.0711618797
,-2.6521826522,-1.8127699\C,1.1750105945,-3.2766308332,-2.3831324626\C
,1.2830109374,-4.8059094588,-0.514847876\C,1.7880511013,-4.3481499073,
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5,-1.7993804767,-2.304589256\H,1.5719623931,-2.9090765823,-3.324384523
3\H,2.6744697144,-4.8083839171,-2.150736591\H,1.7791493537,-5.61474906
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,-5.9569042405,-3.3419446422,-3.8012792132\H,-3.9506691591,-4.81086129
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27600352\Pd,-1.6564344873,-0.0134240548,0.5149813915\H,-4.4265514165,1
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TS2-B

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\C,1.2213437785,3.8355014799,-0.53448821\C,2.3140808276,3.0600413561,-
0.2453688459\C,2.624580671,1.8556388502,-0.9454757228\H,2.0678099679,0
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3475753\H,0.4859361017,-0.2988560383,-3.6872669394\C,-0.2809505088,5.2
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71044557\C,0.8967922022,6.2759144443,-0.9897705416\H,0.0572021027,6.05
34698649,-1.6491055925\H,1.8148835981,6.302683684,-1.5864117378\H,0.74
92176388,7.268966178,-0.5485831639\C,2.1801727345,5.5966105457,1.03710
54\H,2.2845203027,4.9097566165,1.8836493605\H,2.0071817976,6.597754698
9,1.4455230154\H,3.1311898365,5.615034064,0.4956544465\C,3.7496194878,
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031349637\C,-1.2531591525,2.0338578577,1.0229955546\H,-1.7420515607,2.
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7838443726,-2.3544424794,0.705385401\O,5.2787889893,-0.8940099233,1.58
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,-2.7256633386,2.8011064445\C,-1.2698724643,-3.4334078061,4.0020229577
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9492559,0.0621839197\Pd,-1.6007929085,-0.1285531597,0.4542694935\H,-4.
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7860631,-0.4841664808\C,-4.180326654,4.4666645813,1.5873927873\H,-4.57
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Int2'-B

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6842048967\C,6.4334588392,2.3632308365,-2.5060973891\H,6.2136747781,3.
4019292017,-2.2648589945\H,6.794822024,2.3062797544,-3.5391905325\H,7.
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117824\H,1.2862337031,4.2226944824,0.7591098499\C,4.483503264,5.117285
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TS2'-B

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Int3-B

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,0.127191532,3.5922430693,3.5338217655\H,-1.4701923787,4.1500762036,0.
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699628475,4.5742957151\H,0.746171989,4.1051825309,4.2628485328\H,-0.05
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999351\C,-4.7530453342,-0.1969675754,0.9211770547\C,-5.9235998328,-0.4
682711114,1.6499050045\C,-6.2789959153,0.3030802958,2.7514762756\C,-5.
4741333412,1.3740931891,3.1324799196\H,-6.5481079294,-1.2974693472,1.3
434105482\H,-7.1807205711,0.0661869875,3.3064544377\H,-5.7423702174,1.
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.4853680014,-1.079884214,-0.2317617206\O,-5.591088502,-1.6895485054,-0
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9,-1.3626777744,-0.8235028322\C,-3.6719025214,-2.2845402463,-1.9550431
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3.5633388556,-1.7012445012,-2.8769321919\C,-2.7793730542,-3.4956034255
, -2.0264998119\C,-2.4152657996,-4.0095374243,-3.2744112946\C,-2.334874
404,-4.1275800898,-0.8616170118\C,-1.6072339943,-5.1439859058,-3.35489
64547\H,-2.7534470488,-3.5148420113,-4.1821468473\C,-1.4997610117,-5.2
404988231,-0.9398012417\H,-2.5795731539,-3.7054415969,0.1070824942\C,-
1.1442924584,-5.7542260303,-2.188518287\H,-1.3197941183,-5.5350287411,
-4.3261125421\H,-1.0752125747,-5.6575805697,-0.035545084\H,-0.48038633
52,-6.6099752049,-2.2502465781\H,0.7017991447,2.2928950078,-0.32376689
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TS3-B

I\1\GINC-OMC-1-818\Freq\RB3LYP\GenECP\C59H62N1O6P1Pd1\SHIMGRP\05-Oct-2

023\0\#p freq genecp b3lyp empiricdispersion=gd3bj geom=check guess
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,0.8448624622\C,2.9110242691,0.5498658234,-0.0572237733\H,2.1254851573
,0.2768912813,-2.0355169555\H,3.8967466853,1.1602824246,1.7366296576\C
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708051962,-1.8343212987\C,2.840443362,-3.3461871461,0.6551310225\C,2.2
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7,-5.2370894385,0.1736885321\H,4.4933461801,-5.0501990805,3.2448275969
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\H,3.5086027053,3.3095410761,-3.8117776652\H,2.7409312633,4.6519934243
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Int4-B

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\C,4.4022690238,2.1841453997,5.2409687555\C,5.6109298427,2.7014075128,
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\C,8.538016977,3.1419238893,-5.0773603465\H,8.3571229226,2.6083460311,

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Int3'-B

1\1\GINC-OMC-1-822\Freq\RB3LYP\GenECP\C59H62N1O6P1Pd1\SHIMGRP\10-Nov-2023\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP Freq\TS2\0,1\C,1.4747151078,3.6045438958,-0.3809104215\C,1.3182174672,2.5870346447,-1.4610698223\C,1.8687568713,1.3099812957,-1.2776469338\C,2.1054717175,3.1711629595,0.8856454295\C,2.4397272949,1.8575648758,1.0403584967\C,2.2871348138,0.8529287685,0.0053930199\H,1.9371670869,0.6249208452,-2.1112685264\H,2.8713847281,1.5072310855,1.9666179134\C,0.8542164234,3.0593948021,-2.8476063348\C,2.4348006149,4.2091268936,1.966287942\O,1.1099121368,4.7839171006,-0.551993307\C,0.7779741865,1.8932939272,-3.8491436173\C,-0.5370893215,3.7258698206,-2.7709431124\H,1.762792734,1.4644076263,-4.0622100867\H,0.3641746567,2.2531045498,-4.7960543145\H,0.1321191137,1.0889810389,-3.4848104084\C,1.1635460754,4.9484371926,2.4322822239\H,0.6982061304,5.4563175475,1.5895156133\H,1.42214

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92\C,3.4326330958,5.2347322227,1.3795336888\H,3.0011012537,5.739736082
,0.5147327339\H,4.3584346328,4.7368327149,1.0715518037\H,3.6874801198,
5.9860090889,2.1358109018\C,3.0813158641,3.560656836,3.2023373324\H,2.
4177931764,2.8252321929,3.6696575161\H,3.2967027073,4.335938575,3.9443
887397\H,4.0243260344,3.060119715,2.9614234075\C,3.0979303348,-0.44639
79815,0.1823124843\C,0.1855971304,-0.5310823295,1.4208393772\C,2.45582
38517,-1.5732806649,1.0847934488\C,0.9290831577,-1.7554860301,0.973013
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178666,0.7581331117\C,4.902662596,-0.4715305009,-1.5504854695\C,2.9613
779337,-1.8216835862,-1.991588138\C,3.527228723,-2.2274147582,-3.20280
86121\C,5.4637219594,-0.8630201469,-2.7632886296\C,4.7764119566,-1.750
5944882,-3.5945622449\H,5.2126129796,-2.0670490295,-4.5374074589\H,2.9
78293094,-2.9161474631,-3.8351926631\H,5.4435365028,0.2106255512,-0.89
99900567\H,6.4384707733,-0.4832276516,-3.0551703737\H,1.9878073942,-2.
2044238458,-1.7165740039\C,3.1152772541,-2.923705882,0.7662842781\C,2.
7903197995,-1.2885929821,2.5652901098\C,-0.0964163627,-0.1975445937,2.
640918481\C,-0.4093221222,0.189444272,3.8607056187\H,0.2778117594,-2.5
485088533,5.0588834066\H,-1.381431472,-0.0267006267,4.2956730216\O,2.5
329099674,-3.9089760191,0.3667282302\O,4.4384382914,-2.8633151852,0.99
74118884\C,5.2074769656,-4.0412468916,0.6561104946\C,5.1592979226,-5.0
661020096,1.7766585109\H,6.2181291919,-3.6626186649,0.4921658667\H,4.8
162576897,-4.448823254,-0.2787890037\H,5.5069421439,-4.6267621324,2.71
6122759\H,5.8048682694,-5.9161628184,1.5331549493\H,4.1395423846,-5.43
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2517\C,1.2563915847,-2.8907455162,5.4054320806\H,3.3494742998,-2.34905
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3371,-3.9461185937,5.1433179546\H,0.2966659095,0.7513471873,4.46901983
04\H,1.2966774904,-2.7974825896,6.4951408912\H,-1.2919106148,3.0192589
882,-2.4193538407\H,-0.8359960972,4.0729336581,-3.766726935\H,-0.52126
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402,-2.7397981076\H,1.5785907488,4.4139590475,-4.3945016679\C,-2.78404
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7388\C,-3.3167159613,0.5813768535,-1.3598287079\C,-4.6451435286,0.1755
76307,-1.180855121\C,-5.4223739885,-0.1790204544,-2.2811328475\C,-4.88
16678612,-0.132385795,-3.5688179027\H,-1.7567178579,0.9436639138,-2.79
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.4983127488,-2.1334904551\H,-5.4875700326,-0.4158800734,-4.4240892415\
H,-5.0627601532,0.1215536878,-0.1808710687\H,-2.2809876055,1.110494645
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,0.3827440393,1.551289684\C,-3.8832669992,3.4189036762,-0.3943702448\C
,-1.8094598314,3.761367423,0.8036133807\C,-2.0902086522,5.1231348992,0

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,-0.8848232237,3.3681728164,1.211361693\H,-1.3844412215,5.7812152012,1
.3912251702\H,-3.471967939,6.6998958616,0.4046310781\H,-5.0662197812,5
.1782052387,-0.7466676802\C,-3.7105625893,1.2488869383,2.4598851483\C,
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,3.133920205\C,-4.1071078746,-0.5506835026,4.0175867278\C,-4.226459570
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H,-4.4927123577,-0.9156000352,4.9643834283\H,-4.7086901675,1.493286564
7,4.3481026236\H,-3.7881014345,2.3015894457,2.2197771895\C,-2.46192611
35,-2.0140557617,0.9868724674\O,-2.0438244716,-3.1897991224,1.55198147
56\C,-1.585131327,-4.0173724056,0.4464354083\N,-2.4660386286,-1.937527
2858,-0.2861715257\C,-2.1149658994,-3.2644280796,-0.8040880139\H,-2.00
92598551,-5.0141864754,0.5749653922\H,-0.4942523116,-4.0719029911,0.47
51385924\Pd,0.0345118449,0.8929116495,-0.004873144\H,-3.0582902773,-3.
7269009867,-1.1314074009\C,-1.2024990855,-3.2329354642,-2.0073991637\C
,-0.6689641327,-2.0314918797,-2.481530636\C,-0.9403810216,-4.418785478
7,-2.7039731595\C,0.086885195,-2.0131216192,-3.6547223137\H,-0.8590424
732,-1.1183889042,-1.930297287\C,-0.1730353552,-4.4032965129,-3.867100
4523\H,-1.3553960375,-5.3576375252,-2.3449332964\C,0.3299810522,-3.195
102164,-4.354384409\H,0.4969401411,-1.075721974,-4.0152003386\H,0.0190
064846,-5.3293928206,-4.4006356986\H,0.9089504284,-3.1759746655,-5.272
9177764\H,0.6568699577,-2.6046959056,1.600171017\H,0.6723313495,-2.011
9230018,-0.0546279795\

TS3'-B

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2\C,-0.372214099,3.700788423,0.1074056884\C,0.7672112579,3.0237054306,
0.4038835107\C,1.2184974804,1.8578220393,-0.319947424\H,1.0397213497,0
.9559582717,-2.2937584371\H,1.3611893705,3.2910099689,1.2678108778\C,-
1.2291608127,2.1040239525,-3.3813604834\C,-0.8519429936,4.8743516908,0
.9694848902\O,-2.2536347021,3.8904864426,-1.3399705956\C,-0.5142501659
,0.9994049159,-4.1741568887\C,-2.7296435682,1.7433461661,-3.3333200942
\H,0.5498982096,1.2080223857,-4.3258073079\H,-0.9776089407,0.902412900
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4\H,-2.5638993346,5.3513123858,2.2295520876\H,-2.1725360741,3.61994612
73,2.1746830884\C,-0.956986908,6.1548880581,0.1097265814\H,-1.65765023
1,6.0127368708,-0.7121788049\H,0.0225495605,6.4208953969,-0.3028561703
\H,-1.3003241068,6.9917187696,0.7285691416\C,0.1128513416,5.1641767071
,2.1318992911\H,0.2046214131,4.3091154163,2.8089437263\H,-0.2679948939

,6.0098397938,2.7130081154\H,1.1146874939,5.4286819901,1.7783140702\C,
2.7306562064,1.5252610795,-0.1964129703\C,0.5721246217,0.3171250255,0.
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92\C,3.3857588756,0.2107675912,-2.3086687179\C,4.0218633109,0.16094281
05,-3.5497650546\C,4.7015007737,2.4598895658,-3.308090891\C,4.67958241
91,1.2820005081,-4.0555763777\H,5.1692976622,1.2383067954,-5.023808797
9\H,3.9936067837,-0.7604309702,-4.1194068428\H,4.0995877466,3.42075283
57,-1.4797135918\H,5.2089482525,3.3411093349,-3.6893300144\H,2.8751792
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56,2.0741270736\C,-0.5474059979,1.2088751125,3.1516404156\H,1.25620699
63,-0.2613877391,4.6498709317\H,-1.4920218346,0.836374138,3.5371185386
\O,4.2707906227,-1.6482406584,0.206094739\O,5.3266524541,0.3296958528,
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1.0221934979,1.3416189447\H,7.2130335177,0.5618314071,-0.1523025556\H,
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2.2001440334\H,8.1782763782,-1.4119057539,1.0747974224\H,6.5520168203,
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5,-2.8430951787\H,-3.1317480851,1.6774032209,-4.3514858749\H,-3.291430
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-3.6228096401,-0.0285462092\C,-4.1977368008,-4.7142563026,-0.762319427
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,0.1967747293\C,-4.0394232094,1.4501812558,0.1358623123\C,-5.151374697
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,0.224153262\H,-3.0428695222,1.8727236884,0.0975786948\H,-5.0033726882
,3.3626145416,0.0189750248\H,-7.3038477669,2.3972698234,0.0524198819\H
, -7.6050883698,-0.0665916367,0.1543489124\C,-3.4260620051,-0.966899429

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123964753,0.9714981637\Pd,-0.9101238922,0.2215449421,-0.6599409007\H,0
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,-3.7062872794,-1.7767651988\C,0.8633286557,-2.3933592945,-3.632090206
8\H,-0.658529341,-2.4427224401,-2.101165175\C,2.9794834571,-3.38715911
77,-3.0370837433\H,3.1127817806,-4.210508008,-1.0600053995\C,2.1697472
702,-2.7452390457,-3.9743252133\H,0.2345124694,-1.8802457743,-4.351517
8354\H,4.0051656595,-3.6436742297,-3.2841251992\H,2.5537394693,-2.5142
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9839946,-1.146318298,-0.1191108543\

Int3''-B

1\1\GINC-A06R03N07\Freq\RB3LYP\GenECP\C59H62N1O6P1Pd1\ACJSGGHI7X\11-Ja
n-2024\0\#P Geom=AllCheck Guess=TChech SCRF=Check GenChk RB3LYP/GenEC
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,1.6610925785,1.3988413246\C,3.1968708605,0.4199689642,1.6056209147\C,
3.3787406295,-0.6724763877,0.7370386636\C,4.2569086762,-0.4940447202,-
0.3426623505\C,4.9016976355,0.7066522937,-0.6008965871\H,2.5816302839,
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,5.9075636174,0.8325574351,-1.7555304038\C,3.5734217748,2.8188813312,2
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7746798996\H,5.3241741542,2.8576682375,-2.2766916476\H,4.4724740875,1.
601812122,-3.2129382093\H,6.1620733926,1.9901877937,-3.5896166862\C,6.
0966670346,-0.4911799574,-2.5167736177\H,6.4598567112,-1.291983118,-1.
8638566387\H,6.8353332717,-0.3505801745,-3.3132983705\H,5.1658551788,-
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.6344711645,4.3537783944,0.8531031294\H,2.8718463623,4.8864117908,2.37
82912241\H,1.9897994681,3.8214115097,1.2673287375\C,4.9382785765,3.202
9494779,3.0016193746\H,5.6306146003,3.4794121055,2.2052690846\H,5.3581
075705,2.3583163437,3.5588759626\H,4.8284658419,4.048529906,3.69274750
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,1.6089140174,4.1273658618\O,5.1408446407,3.0100712928,-0.0233216872\C

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C,4.1440096225,-5.7746144137,-0.2937479908\C,3.3812655783,-4.256481301
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,-2.7931619024,-1.6303830914\H,3.1646134822,-4.0608224685,2.4699398125
\H,4.0406897146,-6.2692607807,1.8023958606\H,4.1189710883,-4.972276358
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,-2.0439237909,-0.3772357588,-0.521193063\H,-5.6479136531,-0.146457687
5,-0.0068961738\C,-4.6679214215,-1.9817538366,0.4658145853\C,-5.539882
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,-1.2499742,2.8186778516\O,0.490468988,-3.7200381799,-0.5715810301\O,-
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-0.7711471683,-5.3175565284,-1.8481069842\H,-0.2944035242,-5.439773163
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502,-4.7938507106,-1.6894368951\H,-0.9792355164,-6.3836965102,-1.98699
79143\H,-0.312592756,-4.9306761488,-2.7619390088\

TS3''-B

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\C,1.2015776188,3.2412954745,1.2311515704\C,2.3245152868,2.41023313,1.
1661453197\C,2.585939598,1.607170227,0.0658193477\H,2.1486571762,1.325
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39249,-3.7287452503\C,-1.3357393377,2.7198026361,-2.5324864252\H,1.880
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493235\H,0.7077599189,1.2540556894,-3.6055359161\C,-0.3898060919,4.282
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3\C,6.7366425226,-2.3130664518,0.5739492968\C,6.7381514122,-3.57866373
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72,-4.4048884263\H,1.76075714,-2.2138911509,0.3758300463\H,2.174875028
4,-1.3902866597,-1.093359384\

Int4'-B

1\1\GINC-OMC-1-820\Freq\RB3LYP\GenECP\C59H62N1O6P1Pd1\SHIMGRP\15-Nov-2
023\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/GenECP F
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0.8733863023\C,1.5721715794,0.8445370106,0.1912651231\H,1.2253076825,-
0.3842148808,-1.584479023\H,1.4272878881,2.2571364413,1.8325281089\C,-
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,0.2205389597\C,-5.1542898389,-4.5352780908,-0.8722070381\H,-3.0434712
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, -5.3115972282,3.0905318607,-1.7528080044\C,-7.0958590033,1.4877070249
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0801\H,-5.2422836345,1.979632123,3.9494316977\H,-5.0987525746,1.613735
3319,1.5157765714\C,-2.0803868356,-1.9053423001,2.0652430049\O,-1.8993
819331,-2.9469651524,2.9305810602\C,-0.858823929,-3.7670816761,2.33692
49888\N,-1.4762709128,-1.9934459398,0.9348879801\C,-0.9131976944,-3.36
84551975,0.8579287293\H,-1.0944777059,-4.8112099966,2.5397698679\H,0.0
924347429,-3.4891851421,2.8034492822\Pd,-1.2509784305,-0.178101108,-0.
5124169707\H,-1.6887161345,-3.9634245813,0.3505548688\C,0.3584476016,-
3.5049450818,0.0554852985\C,0.3819505033,-3.0169603956,-1.2565512418\C
,1.4820952858,-4.1793700684,0.5425084779\C,1.5146333745,-3.171481714,-
2.0536281403\H,-0.486354097,-2.48913886,-1.6375842136\C,2.6143173163,-
4.3468746635,-0.2584483118\H,1.4882648735,-4.5822747755,1.5503950704\C

,2.6379134503,-3.8374638716,-1.5556976455\H,1.518667822,-2.7669471481,
-3.0607844871\H,3.4839321384,-4.8600897765,0.1395766665\H,3.5280873167
,-3.9444278648,-2.1665413651\H,3.3369827959,-1.7940232961,1.5218846112
\H,2.8199192052,-1.621524484,-0.1571627447\

3a-B

1\1\GINC-OMC-1-821\Freq\RB3LYP\6-31G(d,p)\C32H40O5\SHIMGRP\15-Mar-2023

\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p)

Freq\product\0,1\C,3.2705074291,-0.3435813386,-0.2011075318\C,2.6963
890309,0.5716282761,0.8316229845\C,1.4058666912,0.428838594,1.17326554
96\C,2.4370466304,-1.4850770361,-0.6926012855\C,1.1573662448,-1.571253
1926,-0.2934444549\C,0.4707248713,-0.5736888108,0.5761866538\H,0.96523
93197,1.0876041005,1.9106513103\H,0.511387121,-2.3685654786,-0.6410464
997\C,3.5875845201,1.6679460503,1.4290228976\C,3.0689851806,-2.5053936
399,-1.6479764422\O,4.4145975987,-0.1718929004,-0.6286113397\C,2.84018
4194,2.4774339806,2.502549958\C,4.8358299552,1.039501367,2.0861705546\
H,1.9708396352,2.9964076481,2.0866405938\H,3.5129312384,3.2360626576,2
.9134821743\H,2.5062514007,1.8462276734,3.3331118727\C,4.3116070769,-3
.1442470474,-0.9882746318\H,5.0703260588,-2.3944215298,-0.7673578429\H
,4.7446415919,-3.8922525704,-1.6613066441\H,4.0345254107,-3.6493261496
,-0.0566488452\C,3.4714461478,-1.8036477534,-2.9648268355\H,4.20335281
17,-1.0178007224,-2.782171656\H,2.5925964414,-1.3613869589,-3.44725238
56\H,3.9033797645,-2.5338787931,-3.658092381\C,2.0848236574,-3.6358720
188,-1.9933328417\H,1.7629645711,-4.1816769715,-1.1003969503\H,2.57654
44891,-4.3496129108,-2.661055474\H,1.1928568146,-3.262820094,-2.506732
4804\C,-0.6725064708,0.1433208863,-0.3125958002\C,-0.3351087502,-1.222
482247,1.7155639923\C,-2.0118580859,-0.1199838442,0.4485438312\C,-1.60
89384376,-0.4377130317,1.9051014336\H,-1.4268516073,0.5074274792,2.429
2778449\H,-2.3818464673,-0.9755123977,2.4542235877\C,-0.3105321425,1.5
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0.3568745899,1.7819978198,-1.879814879\C,-0.5104008484,2.658124712,0.1
866957134\C,-0.0637913999,3.9301464314,-0.1682917833\C,0.8178118633,3.
0496859784,-2.2309101928\C,0.6065980993,4.1309944972,-1.3755641191\H,0
.961788419,5.1204377516,-1.6458786473\H,-0.2338386639,4.7639667388,0.5
059828715\H,0.5308591996,0.9407864168,-2.5443607912\H,1.3410643433,3.1
91379902,-3.1714172299\H,-1.0188452375,2.5260541167,1.1345034276\C,-3.
0203919972,1.0184313382,0.3560658561\C,-2.6753246509,-1.3769391253,-0.
1379989505\C,0.0131688238,-2.3137199997,2.3413784004\C,0.3769605927,-3
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.9871980515,-3.3796242661,3.8547217189\O,-3.394772846,1.696797825,1.28
72929109\O,-3.4305910695,1.1645679733,-0.9156689558\C,-4.4211841516,2.
1927648191,-1.1595501325\C,-5.8154383931,1.6745740607,-0.8505312069\H,
-4.3008436784,2.4377638829,-2.2161904025\H,-4.1730955864,3.0657009259,
-0.5522904576\H,-6.0309101544,0.7763716653,-1.4364130764\H,-6.56126058

52,2.4362252461,-1.0986054421\H,-5.9053771289,1.4352700552,0.211395300
3\O,-2.171034968,-2.1470273088,-0.925216685\O,-3.9039332804,-1.5334857
223,0.3831510206\C,-4.6584755551,-2.6783592239,-0.0830694784\C,-6.0471
867341,-2.5673063792,0.5101148645\H,-4.6693049024,-2.665205021,-1.1763
772534\H,-4.1407310098,-3.5883332204,0.2346545064\H,-6.5337219809,-1.6
43705743,0.1845830631\H,-6.0061541217,-2.5685658248,1.602634517\H,-6.6
586769312,-3.4143478697,0.1856688903\H,4.5447359393,0.3540875288,2.889
7454005\H,5.459786888,1.8261197973,2.5243011049\H,5.4305402287,0.49052
87227,1.3568272193\C,4.0102857469,2.6488838331,0.310696353\H,3.1286826
491,3.0998294659,-0.1552820169\H,4.5913818044,2.1395332724,-0.45712699
85\H,4.6206202642,3.452778446,0.7375415387\

Int4-B + HCO₃⁻

1\1\GINC-OMC-1-810\Freq\RB3LYP\GenECP\C60H63N1O9P1Pd1(1-)\SHIMGRP\14-N
ov-2023\0\#P Geom=AllCheck Guess=TCHECK SCRF=Check GenChk RB3LYP/GenE
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6857574226,-2.0775216694,-0.2685461034\C,-2.9559157702,-0.9701482135,-
0.5039920154\C,-3.9387118782,-1.3042586712,2.1546885501\C,-3.193009908
7,-0.2264824474,1.8517546076\C,-2.5537241808,0.0404386581,0.5260582913
\H,-2.5128432169,-0.8327933477,-1.4775149037\H,-2.9833444123,0.5145394
758,2.6085776313\C,-3.9501923943,-3.1169397668,-1.3686930999\C,-4.4961
330724,-1.5334085165,3.5670592232\O,-4.9713051467,-3.2780330227,1.3339
829939\C,-3.2473216723,-2.7426764853,-2.6857450098\C,-3.4074975585,-4.
4924438519,-0.9202678042\H,-3.5971904694,-1.7820120995,-3.0789979072\H
, -3.4714128085,-3.5052248175,-3.4390660808\H,-2.1610724117,-2.69134949
54,-2.5825866147\C,-3.9730653619,-2.878857884,4.1191896847\H,-4.293338
4867,-3.7066774215,3.4874585857\H,-4.3504275838,-3.0399397895,5.136671
8894\H,-2.8780335556,-2.8726097576,4.1598579887\C,-6.0408642898,-1.546
8001818,3.5293684826\H,-6.4031655862,-2.3406469391,2.8768101483\H,-6.4
215666652,-0.5874502968,3.1614166618\H,-6.4408705001,-1.704989887,4.53
85545206\C,-4.0565358413,-0.4246132974,4.5392472886\H,-2.9669528919,-0
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,1.3777996127,-2.4719317861\C,-3.0721952281,1.5154280253,-3.7630813799
\C,-5.1463513856,2.3429962612,-2.8552146118\C,-4.3644109663,2.00251350
76,-3.9608836085\H,-4.7643857562,2.1081346768,-4.9659694188\H,-2.43263
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831331679\C,-3.6995033,5.5833728546,-0.297268261\C,-3.0942321783,6.798
7834582,0.3875290207\H,-4.7814962397,5.5369190925,-0.1538256133\H,-3.4
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58157714\H,-3.5417215368,7.716556424,-0.0095151678\H,-2.0171878529,6.8
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83276738,-4.8407394202,-0.0165389655\C,-5.4689107577,-3.2079074033,-1.
6388092476\H,-5.853557817,-2.2390635584,-1.9771457494\H,-6.0117952566,
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,2.8579923569\C,3.9574837112,1.8557829927,1.1934254159\C,5.3061481016,
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.8540726645,3.5679390625,3.2298594466\H,2.0024233769,2.6836097115,1.59
78739035\H,2.8053720953,4.2317309123,3.3475216548\H,6.7978687993,2.707
7701946,2.8733305915\H,5.201131659,4.2340145682,4.0146753389\H,6.01508
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15\C,3.0769236517,4.0888688269,-2.6057969936\C,2.2355461806,3.62181173
5,-3.6195255056\H,4.0677013006,3.6250855202,-0.7492384931\H,1.67067191
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,1.9500549447,4.285000555,-4.431421788\H,3.4492437817,5.1095140057,-2.
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.4806734005,-0.2786297147\C,6.2375320772,-2.0824967565,-0.6914449536\C
,7.1377969091,-1.4126757745,-1.5109521336\C,6.8510467542,-0.1182107708
,-1.9402413095\H,6.4464005091,-3.0956474677,-0.3748283183\H,8.05281411
38,-1.9075297053,-1.8216967274\H,7.5385873474,0.4127619784,-2.59190331
7\H,5.4484066793,1.5039365438,-1.8580877182\C,4.1208232297,-2.34313541
68,0.5032232756\O,4.6701102865,-3.5292943147,0.8909057426\C,3.67447769
38,-4.1948392146,1.7036282715\N,2.8765371945,-2.1836220687,0.800272347
2\C,2.3688954771,-3.4716013586,1.3232011354\H,3.9507980765,-4.05321270
06,2.7552451623\H,3.6787242033,-5.2541686933,1.4485006503\Pd,1.5139329
348,-0.5433328678,0.551202241\H,1.7478184912,-3.2708024953,2.199490740
4\C,1.5547070352,-4.2292358335,0.2830248446\C,0.9823029528,-5.45603986
29,0.6490667193\C,1.3489431146,-3.7390534487,-1.0057380154\C,0.2293822

361,-6.1808951731,-0.2717358565\H,1.115479996,-5.8387365541,1.65979557
54\C,0.5714607414,-4.4482345726,-1.9265994595\H,1.7217166019,-2.766106
1208,-1.2929058555\C,0.0239179809,-5.6766624367,-1.5609214191\H,-0.216
4159571,-7.1273580076,0.0224394561\H,0.372065513,-3.9900895857,-2.8943
938056\H,-0.5905017139,-6.2292599391,-2.2658522618\H,-0.0796775507,-0.
6270746429,-1.7806124527\C,-0.1060158303,-1.1803178274,-3.6664997892\O
, -0.2386139484,0.0413919983,-3.9445553727\O,-0.0464516264,-2.192439240
8,-4.3748671267\O,0.0002561461,-1.4601073483,-2.2656275702\H,0.4652313
947,2.772732303,0.1086143485\H,-0.353399723,2.1076208824,-1.2621534259
\

TS7

1\1\GINC-OMC-1-816\Freq\RB3LYP\GenECP\C60H63N1O9P1Pd1(1-)\SHIMGRP\28-N
ov-2023\0\#p freq geneep b3lyp empiricaldispersion=gd3bj geom=check g
uess=read\TS2\ -1,1\C,-3.9691781064,-2.2856037919,0.7624984491\C,-4.0
09650855,-1.5850372762,-0.5389302812\C,-3.2887029031,-0.457777105,-0.7
022707376\C,-3.321252892,-1.5793202333,1.9136020336\C,-2.6012126509,-0.
.4672886946,1.6868645582\C,-2.3922531621,0.1651790488,0.3449105988\H,-
3.1497171837,-0.074782554,-1.7026612816\H,-2.1102469955,0.0376655957,2.
.5019333311\C,-4.7499682486,-2.2171406073,-1.7287964856\C,-3.477967115
3,-2.1713710628,3.3216231842\O,-4.4337520545,-3.4245779421,0.914906621
3\C,-4.8229919691,-1.2440192375,-2.922001157\C,-3.9646541434,-3.466248
5352,-2.1884216441\H,-5.3336235859,-0.312942664,-2.646121034\H,-5.4018
119895,-1.7179243053,-3.7236501827\H,-3.8296517236,-0.996673781,-3.313
821082\C,-2.7507692616,-3.5323156832,3.395093359\H,-3.1612288175,-4.22
27770857,2.6592681131\H,-2.8566377801,-3.9656508991,4.3976996162\H,-1.
6835838591,-3.4007164885,3.188375051\C,-4.9761869334,-2.3584379847,3.6
498696875\H,-5.4455002666,-3.0374056689,2.938816193\H,-5.4998468426,-1.
.3964307732,3.613703587\H,-5.0908383584,-2.768353942,4.6606316255\C,-2.
.8751101978,-1.2539541633,4.4000532538\H,-1.7936512653,-1.1360248926,4.
.2781481514\H,-3.0488734042,-1.6929275378,5.3883814509\H,-3.330316102,
-0.2579019531,4.3880068196\C,-2.5780018328,1.7400511105,0.4647540736\C
, -0.1525048483,0.6874320854,-0.8960010432\C,-1.241866938,2.5670900054,
0.400267257\C,-0.3665339512,2.1662548422,-0.8002320705\C,-3.5846324843
,2.3286195981,-0.5198780205\H,-2.9921117819,1.9198157618,1.4578894481\
C,-4.6909568169,3.0136970301,-0.0013426166\C,-3.4289474436,2.262608516
8,-1.9160417982\C,-4.3664958463,2.8689920212,-2.7508815084\C,-5.623444
1763,3.6252881788,-0.8398089874\C,-5.4612151684,3.5553656275,-2.222889
231\H,-6.1861769882,4.0233711677,-2.8836439868\H,-4.2363411099,2.78740
45588,-3.8256562536\H,-4.8178052577,3.0702165177,1.0765575425\H,-6.475
4124027,4.1470700133,-0.4114871893\H,-2.6187862743,1.6988674781,-2.377
832336\C,-1.6152403438,4.0533073451,0.2853659573\C,-0.3451984199,2.507
7205141,1.6403450521\C,-1.0290035829,-0.2111666817,-0.2713013989\C,-0.
5826061278,-1.549398541,-0.3045858712\H,-1.0529162053,-2.2852243292,0.

3383237618\H,-0.231633757,-1.9182944967,-1.2653920485\O,-1.4057412923,
4.7724869652,-0.6613306451\O,-2.2369978403,4.4620249534,1.4207418701\C
,-2.7152966494,5.8220156653,1.4204371299\C,-1.597217854,6.7972173796,1
.7541196265\H,-3.502192713,5.8349651097,2.1787628472\H,-3.1540755798,6
.0359345199,0.4428438732\H,-1.1328225282,6.5376453309,2.7101117753\H,-
1.994241119,7.8159095363,1.8245469519\H,-0.8331903441,6.7728170807,0.9
747063281\O,0.6563977556,3.1948276405,1.7331676682\O,-0.7494898707,1.6
644403139,2.6010389333\C,0.1365187907,1.4491571332,3.7253393744\C,0.94
13102282,0.1774572819,3.5145636801\H,0.7811935754,2.3228265899,3.83291
40174\H,-0.5256541365,1.3712810708,4.5914166271\H,1.5211627975,0.23482
30366,2.5884236106\H,0.28344169,-0.6922147792,3.4378431548\H,1.6304591
418,0.0295836199,4.3532313024\H,-2.9766911642,-3.1655122581,-2.5584256
462\H,-4.5054022235,-3.9572847102,-3.0084389904\H,-3.8613984961,-4.180
8897876,-1.3689013486\C,-6.1919592556,-2.5918507662,-1.3228271414\H,-6
.7419781227,-1.7038520035,-0.9868205292\H,-6.2045443106,-3.3326208928,
-0.5231373626\H,-6.7207530061,-3.00142366,-2.1916812798\C,3.6148153553
,2.1596569925,2.0516265042\C,4.3004942818,2.5938949601,3.1844039681\C,
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4168823,3.4571224145\H,2.6126317495,2.5273126659,1.8596461665\H,3.8229
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8,0.7543497771\H,3.2233810223,0.6570257119,-0.2683549902\C,3.087144952
7,2.06897272,-1.4192754868\C,4.4310041016,-0.4504433569,-1.1142818465\
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4.1236028353,3.5230672037,-0.2049045697\H,1.9386611322,0.8749452507,-2
.8527896793\H,1.5916030318,2.7240057955,-4.3964569182\H,2.460710136,5.
0061976587,-3.8777194932\H,3.7302540203,5.3919019842,-1.7761318356\C,5
.2896377119,0.0968911558,-2.075229692\C,4.5860818349,-1.8177866067,-0.
7692385822\C,5.6026992538,-2.5702807987,-1.3900341232\C,6.4353361956,-
2.0057468002,-2.3474435354\C,6.2766281832,-0.6646049366,-2.6967381269\
H,5.7147359859,-3.6124647176,-1.1205912558\H,7.1995205185,-2.613522684
3,-2.822146125\H,6.9166677818,-0.2100898661,-3.4469025489\H,5.17534319
01,1.1413430588,-2.340007594\C,3.7279932001,-2.5448123589,0.1765573446
\O,4.2186980339,-3.7566676282,0.5678524668\C,3.2867052579,-4.288105329
7,1.5337418381\N,2.5518666324,-2.2460329265,0.625409799\C,2.0130271856
,-3.4486851363,1.3047932824\H,3.7151414135,-4.1446808243,2.5327890878\
H,3.1494453007,-5.3503824086,1.3312206483\Pd,1.2991115778,-0.561884716
8,0.0766664286\H,1.5608391395,-3.1492466369,2.25375643\C,0.9678644289,
-4.1425648529,0.4521530206\C,-0.0746047944,-4.831002666,1.081926373\C,
0.9862004555,-4.0540669231,-0.9431655689\C,-1.0988578622,-5.4009217934
,0.3257040122\H,-0.1072862512,-4.8859727161,2.1675475779\C,-0.05606363

54,-4.5875216687,-1.7011631152\H,1.74356139,-3.4614437092,-1.444149157
4\C,-1.0956323806,-5.2671894167,-1.0639265173\H,-1.9242562594,-5.90013
64899,0.8241066443\H,-0.1089782653,-4.3553426381,-2.7591245567\H,-1.92
79172669,-5.6471587187,-1.6460205095\H,0.2425174627,0.2581703664,-1.94
63214159\C,-0.8383151312,-0.9310155114,-3.3362391302\O,-1.7574658741,-
0.031331708,-3.3303006142\O,-1.067404448,-2.17704594,-3.4480508414\O,0
.4262556502,-0.5268426733,-3.1370869538\H,0.5776757193,2.7086031439,-0
.7464344481\H,-0.8492211657,2.5096128265,-1.7179044704\

Int8

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9251904,-1.5413393419,-0.616302192\C,-3.2232732633,-0.4686548529,-0.77
6358599\C,-3.3624062774,-1.5677324696,1.8491124365\C,-2.5498949137,-0.
5222787075,1.6215663507\C,-2.3280570616,0.1282241747,0.2899084754\H,-3
.0253879298,-0.110852039,-1.7783848814\H,-2.0099166603,-0.0668180525,2
.4344353784\C,-4.7530948661,-2.1528919572,-1.8226767238\C,-3.576137748
6,-2.1355011128,3.2600531782\O,-4.6539513773,-3.297521032,0.8634445611
\C,-4.7199255646,-1.2030025469,-3.0365191402\C,-4.0193292781,-3.452823
544,-2.229383809\H,-5.1915330227,-0.2410895166,-2.8007337421\H,-5.288
604899,-1.6626080138,-3.8535531139\H,-3.700544951,-1.0145860041,-3.391
1930848\C,-3.0200114033,-3.5736329909,3.3443860474\H,-3.5199282667,-4.
2186769925,2.6231019335\H,-3.1673987258,-3.9771476745,4.3540091694\H,-
1.9478059486,-3.5751708494,3.1263770295\C,-5.0853310565,-2.1369634235,
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4,-1.1186819647,3.5530030215\H,-5.2463039754,-2.5257768683,4.605446026
7\C,-2.8617674947,-1.2916389597,4.3305383932\H,-1.7750445079,-1.300843
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9786\C,-0.1053464607,0.7158257757,-0.9353145487\C,-1.207144277,2.54142
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,0.1660893101\H,-0.1103681418,-1.8998096136,-1.3515166653\O,-1.3876123
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55\C,-2.7353316954,5.7456639657,1.5172576561\C,-1.6353404745,6.7260159
138,1.8927012775\H,-3.5305840331,5.7242982441,2.2665193506\H,-3.166286
6522,5.9820400158,0.5413924673\H,-1.1783353513,6.4450561299,2.84618774
23\H,-2.0481710503,7.7362585166,1.9884474699\H,-0.8621233906,6.7361066
654,1.1220705947\O,0.6818551901,3.1441495153,1.7745573148\O,-0.7408277
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\C,0.9651792124,0.1523601704,3.5487274572\H,0.7509188605,2.289214431,3
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77816107\H,6.2291215042,2.5113320985,4.2360341485\H,6.0485008669,0.160
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821,-2.9031899575\H,1.588451231,2.6146078241,-4.4481148613\H,2.3492907
47,4.9361569303,-3.9244217968\H,3.5756075233,5.3810626274,-1.808920448
8\C,5.257840796,0.0208432174,-2.1125659748\C,4.5720516718,-1.851761700
5,-0.7294278776\C,5.5931375404,-2.6186846462,-1.3317881882\C,6.4148071
152,-2.0841928201,-2.3130691526\C,6.2446807166,-0.7563454308,-2.713998
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9487,-2.7694640955\H,6.8757629667,-0.326656556,-3.4858465736\H,5.13609
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3406\O,4.1922495567,-3.7661757544,0.6349907816\C,3.2718557213,-4.26225
01801,1.6267696842\N,2.5502918377,-2.2257980892,0.7012231415\C,2.00441
38242,-3.4161089667,1.3954581398\H,3.7138650114,-4.0970226023,2.616938
5168\H,3.121495179,-5.3283174056,1.4549722986\Pd,1.3029479507,-0.54818
51642,0.1060061405\H,1.5583776982,-3.1057259203,2.3440055436\C,0.95054
25343,-4.1117294864,0.555285975\C,-0.1293672672,-4.7322933786,1.191595
8149\C,0.999470201,-4.0883873441,-0.8423939146\C,-1.1634718066,-5.2922
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3383349,-4.6127854655,-1.5972392445\H,1.7930253649,-3.5529920635,-1.35
2052429\C,-1.1302067758,-5.2182707902,-0.9529634242\H,-2.0169577155,-5

.7360467199,0.9438566558\H,-0.0726842109,-4.4330079689,-2.6661104612\H
,-1.9674986153,-5.5870263725,-1.5351126633\H,0.324253143,0.3698780544,
-1.9071263015\C,-0.7295729397,-0.9487709981,-3.3669668821\O,-1.6101948
081,-0.0031932203,-3.3908424648\O,-1.0656496602,-2.1854123274,-3.34635
0206\O,0.5447763034,-0.6276321884,-3.2796182705\H,0.6184468571,2.72940
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Int8 - CO₃⁻

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257274\C,-2.6530886831,-1.5443243437,1.720819381\C,-1.865031214,-0.571
3777731,1.2252647456\C,-2.1577074764,0.2394759263,-0.0121365259\H,-3.5
580422236,0.2071784819,-1.6909387928\H,-0.9788805299,-0.2769737326,1.7
690483951\C,-5.3736257659,-1.7326638427,-1.1689945994\C,-2.4377802765,
-2.1528342286,3.11846824\O,-4.5356080355,-2.9316840694,1.3190025299\C,
-5.5393733435,-0.8793367414,-2.4389703323\C,-5.2151346459,-3.208182139
1,-1.5997531662\H,-5.6716227018,0.1825354088,-2.2067647146\H,-6.428721
4287,-1.213349734,-2.9804795858\H,-4.6855496957,-0.9820490029,-3.11773
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270170499,-4.0209681757,2.5555445852\C,-3.6531744839,-1.7484353576,3.9
890413569\H,-4.5779786432,-2.1712979471,3.5963700583\H,-3.7487940726,-
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,-1.1773661598,-1.5879955427,3.7934367961\H,-0.2663973582,-1.818380679
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6\C,-0.0143922667,1.2320612237,-1.1428754833\C,-1.1900633241,2.5806998
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29\C,-4.6741220581,2.8471454869,-0.0585597932\C,-3.1160538153,2.697364
5296,-1.885363445\C,-4.0392399984,3.3220373175,-2.7231088408\C,-5.5993
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-1.3636055223\H,-0.0492486806,-1.1062533001,-2.4721914191\O,-1.1554667
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TS8

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2506\

Int9

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7994355,-3.6785860094,-0.4775374231\C,-0.1468003444,-4.1705743498,-0.5
461935617\C,1.8881061582,-3.4855953514,-1.6579454059\C,-0.7166512351,-
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,1.3160344698,-3.7933908271,-2.8908480345\H,2.8970434342,-3.0865781275
, -1.6192274127\C,0.0155088524,-4.3012079514,-2.9538915746\H,-1.7295846
163,-4.8731843248,-1.8220656169\H,1.8896155089,-3.639381625,-3.7988043
686\H,-0.4253874451,-4.549693125,-3.9142882291\H,0.2380260142,0.102464
5394,-2.2139141604\H,-0.0201149793,-1.2170084864,0.6800134171\H,0.6347
423546,2.0192872666,-0.7664775266\

Int5

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34636424,-1.8071689048\C,-2.5506903976,0.7000951142,-0.8123696252\H,-3
.0222508218,2.82561359,-0.7935682275\H,-2.3753560935,-1.3876165166,-1.
4486619577\C,-2.028502272,3.7888874229,-3.1672754621\C,-1.3241475696,-
1.2983511855,-3.9495330222\O,-0.9546357172,1.496083316,-4.5386608964\C
,-2.7126425981,4.7799192076,-2.210350943\C,-0.54057262,4.192525152,-3.
2875338747\H,-3.7722053025,4.5407782964,-2.0670770481\H,-2.6505141904,
5.7898445837,-2.629408045\H,-2.2278233165,4.7985970463,-1.2289383074\C
,0.2144438343,-1.2621032409,-4.1048590622\H,0.5342767502,-0.3073681067
,-4.5223133738\H,0.5448100799,-2.0710641494,-4.7679345645\H,0.69833119
51,-1.4046786258,-3.1347431755\C,-2.0017902664,-1.1692175225,-5.331566
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2.4066143638\H,-1.3883831244,-3.4585151916,-4.0542228218\H,-2.79208702
79,-2.7624552684,-3.2302610369\C,-3.7385206575,0.4900009968,0.17289242
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027,-0.4705866974\H,0.4048395312,0.4328321402,-1.3692285019\H,0.413797
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-4.8310519411,0.6711713507\H,-4.6687265357,-3.9500083526,-1.2896952816
\H,-2.9538269055,-4.0206095203,-0.8108515386\H,-5.3162543805,-4.614889
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,4.5565392581\H,5.5334526941,1.4004888756,2.7716054688\C,6.408116698,2
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111418351,-0.3340594113,-2.2611008798\H,-4.6578537345,-1.1397422739,-1
.9186265318\C,-7.5643132689,0.6127302116,-1.8855355101\H,-7.9957369216
,2.2503219997,-0.5486922551\H,-6.8172836614,-1.0182919334,-3.079649098
6\H,-8.5174208987,0.6689884524,-2.4040432428\O,1.3124840194,-0.1669112
214,3.3935595773\C,1.5778685996,-1.3237517892,3.8512181294\O,1.6585507
342,-2.3147601904,2.8472169703\O,1.7805166889,-1.6803881899,5.01151577
44\H,1.8322099501,-3.1254443684,3.3467085265\

TS5

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ec-2023\0\#p freq genecp b3lyp empiricaldispersion=gd3bj geom=check g
uess=read\TS2\1,1\C,3.9313491387,-2.8066832947,0.6134458911\C,2.629
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3820743849\H,0.8868152181,-1.5967050687,3.2884741131\H,0.6558493437,-3
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, -2.7405034851\C,2.194397825,0.7523444594,-0.0737585914\C,0.7356577736
,0.1568762975,-2.4634459562\C,2.4681124619,1.7424589382,-1.2456551578\
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74089938,-1.4287318737\C,6.363386554,3.5238962602,-2.0655519315\H,6.78
18524155,2.0323108266,-0.5339016236\H,6.3873690339,1.3528147202,-2.134
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10971,-2.9614548787\H,7.4136602172,3.6606403806,-2.3451376953\H,1.4254
452709,-4.9386518767,1.6411874939\H,1.9210189332,-5.1662027588,3.32721
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7,-3.6956185137,1.4942610307\C,-1.9495090057,0.6713167738,2.2064149726
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, -1.8137284875\H,-5.9679434861,4.7198447715,2.2604311645\H,-6.29345943
23,5.6563088916,-0.0217857365\H,1.8366584679,1.7640407357,-3.322071430
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,0.6045985183\C,4.1336043273,1.1367803916,3.7889203787\H,2.180831395,1
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Int6

1\1\GINC-OMC-1-801\Freq\RB3LYP\GenECP\C60H63N1O9P1Pd1(1-)\SHIMGRP\16-D
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.0673784396,-0.4015095104,-2.8048133535\H,-1.6832796674,-0.0602355193,
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5147889139\C,-0.7451757495,-3.6608717963,2.3804049731\H,-0.710049683,-
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TS6

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Int7

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4a

1\1\GINC-OMC-1-824\Freq\RB3LYP\6-31G(d,p)\C32H40O5\SHIMGRP\13-Nov-2023
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35,-0.5936227554,-3.7986625904\

PdLn+HCO₃⁻

1\1\GINC-OMC-1-816\Freq\RB3LYP\GenECP\C28H23N1O4P1Pd1(1-)\SHIMGRP\25-D
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HCO₃⁻

1\1\GINC-OMC-1-817\Freq\RB3LYP\6-31G(d,p)\C1H1O3(1-)\SHIMGRP\25-Dec-2023\0\#P Geom=AllCheck Guess=TChech SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq\zeuolin\ -1,1\C,-2.9199354702,-2.3816291951,0.0639137687\O,-4.1065075797,-2.4197965366,-0.2931400466\O,-2.0576125434,-3.2729019185,0.2578726275\O,-2.4174065816,-1.0401071934,0.309501425\H,-1.5071203251,-1.2440785464,0.5665086253\

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