Supporting information

Iron-Catalyzed Asymmetric Csp^3–H/Csp^3–H Coupling: Improve the Chirality Induction by Mechanochemical Liquid-Assisted Grinding

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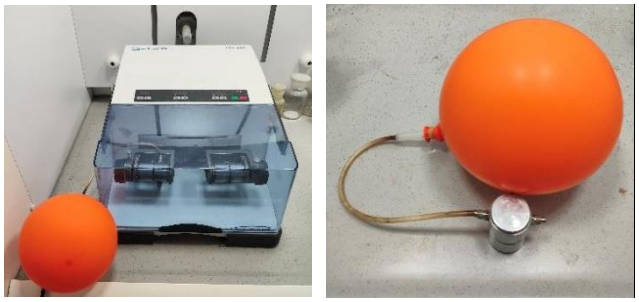
1. General information

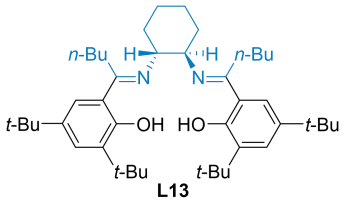
Unless otherwise stated, all reagents involving **L1~L8** and **L10~L12** were purchased from commercial suppliers and used without further purification. *β*-keto esters (**1**) were prepared according to the literature methods[1-3] (ref 1 for **1a~1e** and **1g**, ref 2 for **1f**, ref 3 for **1h~1m**). Glycine esters (**2**) were prepared according to the literature procedure[1]. All of the ball milling reactions were conducted in a Mixer mill (MM 400 RetschGmbh, Hann, Germany) with 25 mL stainless-steel vessels (equipped with gas inlet and outlet valve) with stainless-steel balls, if not mentioned otherwise. Reactions were monitored by Thin Layer Chromatography (TLC) using UV light (254 nm) for detection. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on Bruker 400, 500 or 600 MHz spectrometer in $CDCl_3$ with tetramethylsilane (TMS) as internal standard. Chemical shifts are reported in parts per million (ppm). The following abbreviations were used to explain multiplicities: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quadruplet, m = multiplet and the coupling constants (*J*) were reported in Hertz unit (Hz). Melting points were measured using an SRS OptiMelt MPA100 apparatus and were uncorrected. High Resolution Mass Spectrometry (HRMS) and Electrospray Ionization-Mass Spectrometry (ESI-MS) were recorded on an Agilent 6210 LC/TOFMS or Agilent 6550 QTOFMS. High Performance Liquid Chromatography (HPLC) were performed on SHIMADZU LC-20AT apparatus, using Daicel Chiralpak AD-H chiral column, eluted with a mixture of hexane and isopropyl alcohol. Optical Rotations were measured with Rudolph Autopol V polarimeter. X-ray crystallographic experiments were performed by the Crystallography Service of the Department of Chemistry, Zhejiang University.



Mixer mill and stainless-steel vessels equipped with gas inlet and outlet valve

2. General procedures for the synthesis of ligands

2.1 The synthesis of L13[4]



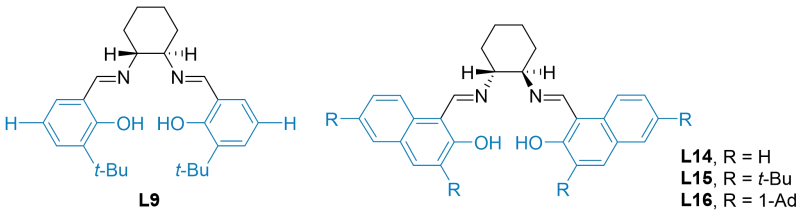
L13

Step1: Following a modified procedure from White et al[4]. To a solution of 3,5-di-*tert*-butylsalicylic acid (10.0 mmol, 1.0 equiv) in thionyl chloride (60.0 mmol, 6.0 equiv) at room temperature was added a catalytic amount (5 drops) of DMF and the mixture was stirred for 12 h. Excess thionyl chloride was removed under reduced pressure on a rotary evaporator and the residue was taken up into 25 mL of pyridine. To this mixture at 0 ℃ were added DMAP (0.5 mmol, 0.05 equiv) and Me_2NH (24.0 mmol, 2.4 equiv) and the reaction mixture was warmed to room temperature. Stirring was continued for an additional 3 h. The solution was poured into 300 mL of an ice-cold water containing 2N aqueous HCl (20 mL), at which time a white precipitate formed. The precipitate was filtered off and was crystallized from 100 mL of EtOH to give *N,N*-dimethyl-3,5-di-*tert*-butylsalicylamide as a yellowish solid (2.47 g, 89%, mp 123–124 ℃).

Step2: To a solution of the *n*-BuLi (7.56 mmol, 2.1 equiv) at 0 ℃ was added a solution of *N,N*-dimethyl-3,5-di-*tert*-butylsalicylamide (3.6 mmol, 1.0 equiv) in THF (20 mL) dropwise. After the addition was completed, the reaction mixture was warmed to room temperature and was stirred for 3 h. The mixture was added to 10% aqueous HCl (100 mL) and was extracted with EtOAc (2 × 25 mL). The organic layer was washed with brine (3 × 20 mL), dried (Na_2SO_4), and evaporated in vacuo, and the crude residue was purified by flash chromatography to obtain 2,4-di-*tert*-butyl-6-pentanoylphenol as a yellowish solid (836.4 mg, 80%, mp 62–63 ℃).

Step3: To a solution of (*R, R*)-1,2-diaminocyclohexane (0.76 mmol, 1.0 equiv) in EtOH (15 mL) was added a solution of 2,4-di-*tert*-butyl-6-pentanoylphenol (1.52 mmol, 2.0 equiv) in EtOH (5 mL). The suspension was refluxed for 6 h at which time a yellow precipitate had formed. The mixture was cooled to room temperature and the precipitate was filtered off. The crude solid was purified by flash chromatography on silica gel (5% EtOAc/hexanes) to give **L13** as an amorphous yellow solid (460.8 mg, 92%, mp 120–122 ℃).

2.2 Typical synthesis of L9 and L14~L16

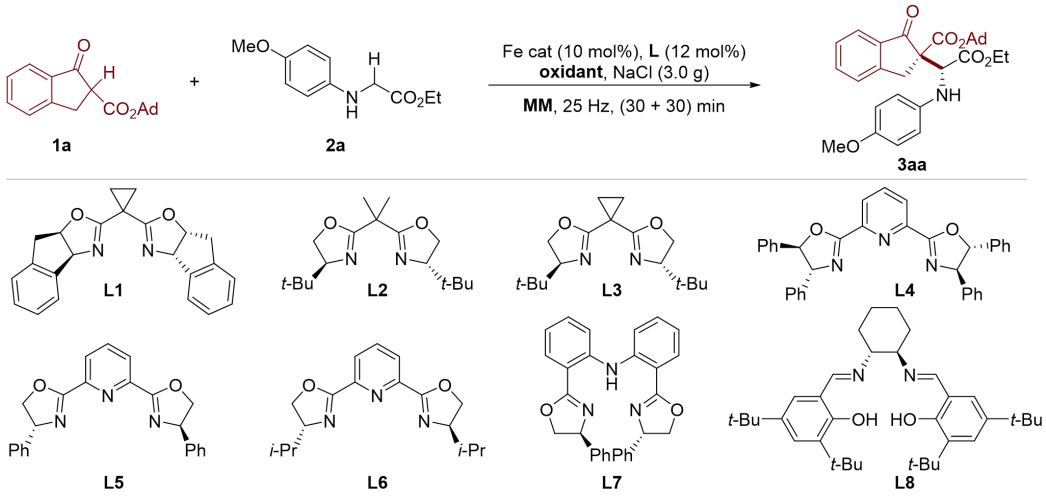


Typical synthesis of **L9** and **L14**~**L16.**[5a] Salicylaldehyde derivative (2.0 equiv) is added to a 0.2 M solution of (*R, R*)-1,2-diaminocyclohexane (1.0 equiv) in absolute ethanol. The mixture is heated to reflux for 6 h. After cooling down to room temperature, the reaction mixture was stored at -10 ℃ overnight. The resulting yellow crystalline solid was collected by filtration and washed with a small portion of cold ethanol.

3. Reaction optimization & typical procedures

3.1 Optimization of the reaction conditions

Table S1. Screening of chemical conditions[a]

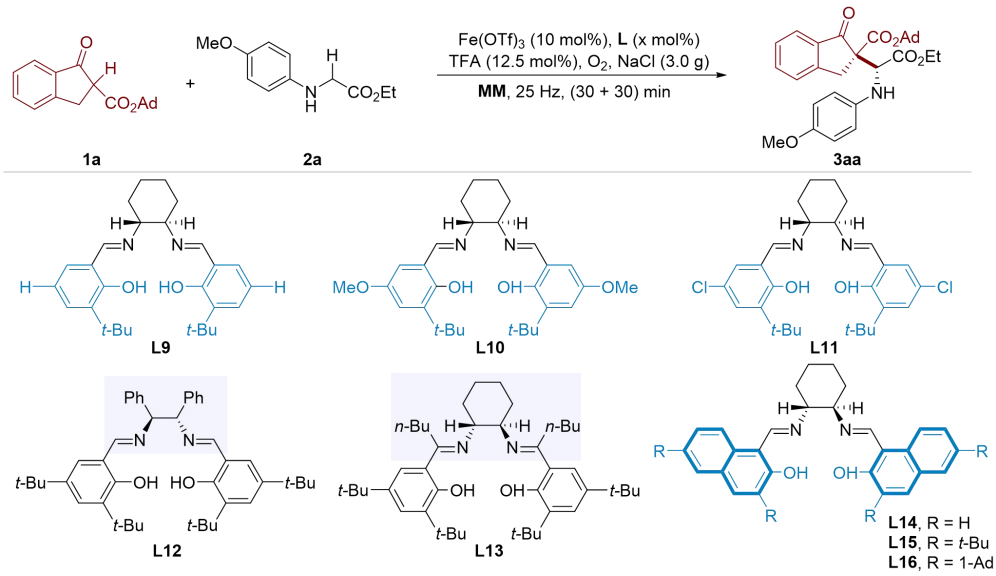


entry	catalyst	oxidant	L (mol%)	yield (%)[b]	*ee* (%)[b]	*dr*[b]
1	$Fe(OTf)_3$	O_2	–	18	_n.d.	_n.d.
2	$Fe(OTf)_3$	O_2	**L1**	9	<5	53:47
3	$Fe(OTf)_3$	O_2	**L2**	trace	_n.d.	_n.d.
4	$Fe(OTf)_3$	O_2	**L3**	trace	_n.d.	_n.d.
5	$Fe(OTf)_3$	O_2	**L4**	15	<5	50:50
6	$Fe(OTf)_3$	O_2	**L5**	21	<5	55:45
7	$Fe(OTf)_3$	O_2	**L6**	19	<5	50:50
8	$Fe(OTf)_3$	O_2	**L7**	trace	_n.d.	_n.d.
9	$Fe(OTf)_3$	O_2	**L8**	22	17	55:45
10[c]	$Fe(OTf)_3$	O_2	**L8**	49	23	60:40
11[d]	$Fe(OTf)_3$	O_2	**L8**	39	18	57:43
12[e]	$Fe(OTf)_3$	O_2	**L8**	36	11	53:47
13[f]	$Fe(OTf)_3$	O_2	**L8**	31	9	55:45
14[g]	$Fe(OTf)_3$	O_2	**L8**	24	20	63:27
15[c]	$FeCl_3$	O_2	**L8**	65	<5	55:45
16[c]	$FeBr_3$	O_2	**L8**	42	<5	61:39
17[c]	$Fe(NO_3)_3{\cdot}9H_2O$	O_2	**L8**	27	10	69:31
18[c]	$Fe(acac)_3$	O_2	**L8**	41	<5	50:50
19[c]	$Fe(OTf)_2$	O_2	**L8**	10	8	68:32
20[c]	$Fe(OTf)_3$	air	**L8**	_n.d.	_n.d.	_n.d.
21	$Fe(OTf)_3$	DDQ	**L8**	28	<5	50:50

22[h]	$Fe(OTf)_3$	DDQ	**L8**	35	<5	50:50
23	$Fe(OTf)_3$	BQ	**L8**	21	<5	50:50
25[c, i]	$Fe(OTf)_3$	O_2	**L8**	53	11	55:45
26[c, j]	$Fe(OTf)_3$	O_2	**L8**	trace	_n.d.	_n.d.

[a] Reaction conditions: $Fe(OTf)_3$ (10 mol %), **L** (12 mol%), NaCl (3.0 g) were pre-milled at 25 Hz for 30 min, using two stainless-steel balls (d_{MB} = 1.0 cm) in a 25 mL stainless vial, then, **1a** (0.2 mmol) and **2a** (0.2 mmol) and an oxidant were added and milled for another 30 min. [b] Yields are those of the isolated products, *ee* values were determined by HPLC, *dr* values were determined by ^{1}H NMR. [c] TFA (12.5 mol%) was added. [d] HOTf (12.5 mol%) was added. [e] $MeSO_3H$ (12.5 mol%) was added. [f] TCA (12.5 mol%) was added. [g] HOAc (12.5 mol%) was added. [h] DDQ were added in three portions. [i] Silica gel was used as milling auxiliary. [j] Anhydrous sodium sulfate was used as milling auxiliary. n.d. = not detected.

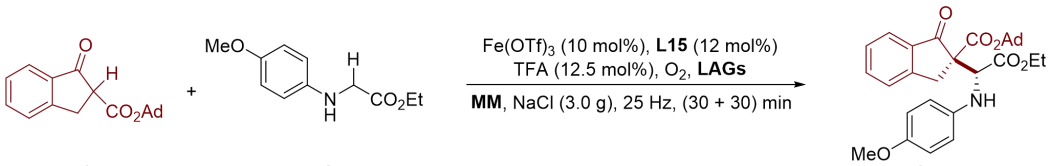
Table S2. Optimization of salen-type ligands[a]



entry	**L** (mol%)	yield (%)[b]	*ee* (%)[b]	*dr*[b]
1	**L9** (12)	52	<5	50:50
2	**L10** (12)	38	<5	50:50
3	**L11** (12)	33	<5	50:50
4	**L12** (12)	60	-20	50:50
5	**L13** (12)	38	<5	48:52
6	**L14** (12)	76	<5	57:43
7	**L15** (12)	65	46	68:32
8	**L15** (10)	66	42	65:35
9	**L15** (8)	68	38	60:40
10	**L15** (15)	65	45	70:30
11[c]	**L15** (12)	52	36	65:35
12[d]	**L15** (12)	48	20	60:40
13[e]	**L15** (12)	41	17	62:38
14[f]	**L15** (12)	32	37	66:34
15	**L16** (12)	45	15	65:35

[a] Reaction conditions: $Fe(OTf)_3$ (10 mol %), **L**, TFA (12.5 mol%) and NaCl (3.0 g) were pre-milled at 25 Hz for 30 min, using two stainless-steel balls (d_{MB} = 1.0 cm) in a 25 mL stainless vial, then, **1a** (0.2 mmol) and **2a** (0.2 mmol) were added and O_2 was filled in and milled for another 30 min. [b] Yields are those of the isolated products, *ee* values were determined by HPLC, *dr* values were determined by ^{1}H NMR. [c] HOTf (12.5 mol%) was added. [d] $MeSO_3H$ (12.5 mol%) was added. [e] TCA (12.5 mol%) was added. [f] HOAc (12.5 mol%) was added.

Table S3. Screening of LAGs[a]

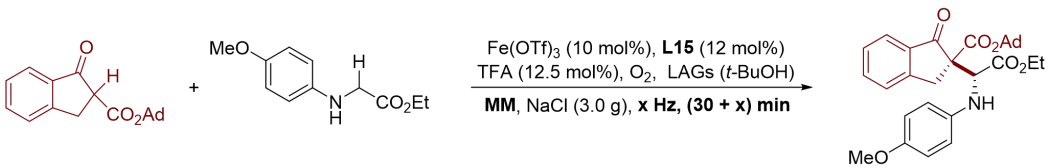


1a **2a** **3aa**

entry	LAGs (η)	yield (%)[b]	*ee* (%)[b]	*dr*[b]
1	–	65	46	68:32
2	EtOAc (0.77)	68	44	50:50
3	*n*-BuOAc (0.77)	67	57	50:50
4	*i*-PrOAc (0.77)	69	70	58:42
5	*t*-BuOAc (0.77)	69	75	66:34
6	MeOH (0.77)	50	<5	55:45
7	EtOH (0.77)	48	<5	55:45
8	*n*-BuOH (0.77)	66	60	60:40
9	*i*-PrOH (0.77)	66	70	70:30
10	*t*-BuOH (0.77)	70	80	78:22
11	*t*-BuOH (0.96)	74	85	75:25
12	*t*-BuOH (1.16)	75	87	85:15
13	*t*-BuOH (1.37)	67	87	81:19
14	*t*-BuOH (1.54)	56	85	80:20
15[c]	*t*-BuOH (1.16)	65	-44	50:50
16[d]	*t*-BuOH (1.16)	78	17	60:40
17[e]	*t*-BuOH (1.16)	65	33	64:36

[a] Reaction conditions: $Fe(OTf)_3$ (10 mol %), **L15** (12 mol%), LAGs [η = V (liquid; μL)/m (reagents; mg)], TFA (12.5 mol%) and NaCl (3.0 g) were pre-milled at 25 Hz for 30 min, using two stainless-steel balls (d_{MB} = 1.0 cm) in a 25 mL stainless vial, then, **1a** (0.2 mmol) and **2a** (0.2 mmol) were added and O_2 was filled in and milled for another 30 min. [b] Yields are those of the isolated products, *ee* values were determined by HPLC, *dr* values were determined by ^1H NMR. [c] **L12** was used as ligand. [d] **L14** was used as ligand. [e] **L16** was used as ligand.

Table S4. Screening of the mechanical parameters[a]

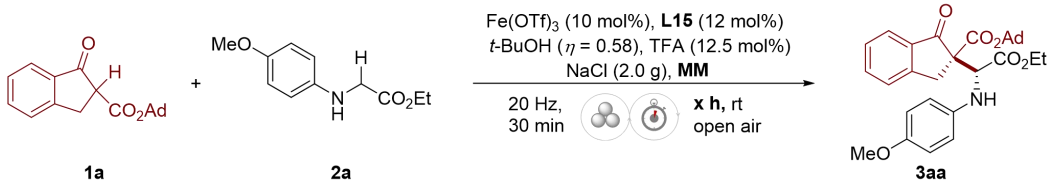


1a **2a** **3aa**

entry	frequency/Hz	balls (n×mm)	time (min+min)	yield (%)[b]	*ee* (%)[b]	*dr*[b]
1	15	2×10	30+30	70	84	75:25
2	20	2×10	30+30	76	87	86:14
3	25	2×10	30+30	75	87	85:15
4	30	2×10	30+30	50	77	60:40
5	20	2×10	30+25	75	90	86:14
6	20	2×10	30+20	67	84	76:24
7	20	2×10	30+15	43	76	55:45
8	20	2×11	30+25	77	91	86:14
9	20	2×14	30+25	87	93	90:10
10[c]	20	2×14	30+25	88	95	90:10
11	20	2×15	30+25	86	82	75:25
12	20	1×15	30+25	75	77	77:23
13	20	1×14	30+25	59	76	74:26

[a] Reaction conditions: $Fe(OTf)_3$ (10 mol %), **L15** (12 mol%), *t*-BuOH (η = 1.16), TFA (12.5 mol%) and NaCl (3.0 g) were pre-milled at a specific frequency for 30 min, using two stainless-steel balls in a 25 mL stainless vial, then, **1a** (0.2 mmol) and **2a** (0.2 mmol) were added and O_2 was filled in and milled for several minutes. [b] Yields are those of the isolated products. *ee* values were determined by HPLC. *dr* values were determined by ^{1}H NMR. [c] NaCl (2.0 g), *t*-BuOH (η = 0.58) were used.

Table S5. Screening of aging conditions[a]

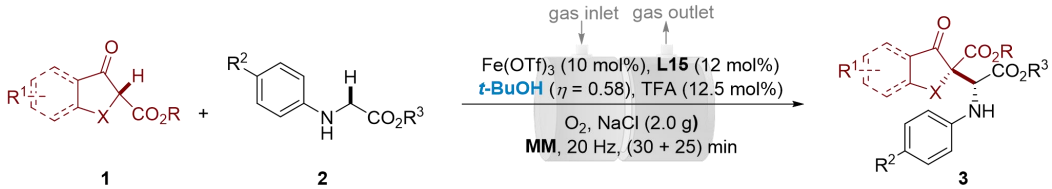


1a **2a** **3aa**

entry	aging time (h)	yield (%)[b]	*ee* (%)[b]	*dr*[b]
1	0	—n.d.	—n.d.	—n.d.
2	2	68	90	88:12
3	4	70	80	80:20
4	6	64	64	72:28
5	12	60	35	60:40
6[c]	12	—n.d.	—n.d.	—n.d.

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.2 mmol), $Fe(OTf)_3$ (10 mol %), **L15** (12 mol%), *t*-BuOH (η = 0.58), TFA (12.5 mol%) and NaCl (2.0 g) were pre-milled at 20 Hz for 30 min, using two stainless-steel balls (d_{MB} = 1.4 cm) in a 25 mL stainless vial, then the contents were scratched off the vessel and aging at in a 50 mL opened flask for several hours. [b] Yields are those of the isolated products. *ee* values were determined by HPLC. *dr* values were determined by ^{1}H NMR. [c] The reaction was initially performed via grinding with a mortar and a pestl.

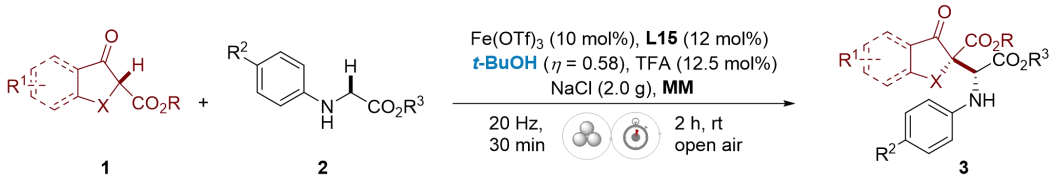
3.2 Typical procedures for LAG induced asymmetric CDC reaction



1 **2** **3**

A mixture of $Fe(OTf)_3$ (10 mol %, 0.1 equiv), **L15** (12 mol%, 0.12 equiv), TFA (12.5 mol%, 0.125 equiv), *t*-BuOH (η = 0.58) and NaCl (2.0 g) was placed in a stainless-steel vessel (25 mL, equipped with gas inlet and outlet valve) with two stainless-steel balls (d_{MB} = 1.4 cm). Then, the ball milling vessel was placed in the mixer mill and pre-milled at 20 Hz for 30 min. After that, **1** (0.2 mmol, 1.0 equiv) and **2** (0.2 mmol, 1.0 equiv) were added and oxygen was filled in through the gas inlet valve. The mixtures were milled at 20 Hz for another 25 min, then the contents were scratched off the vessel and purified directly by column chromatography on silica gel using EtOAc/*n*-hexane as eluent to give the desired products **3**.

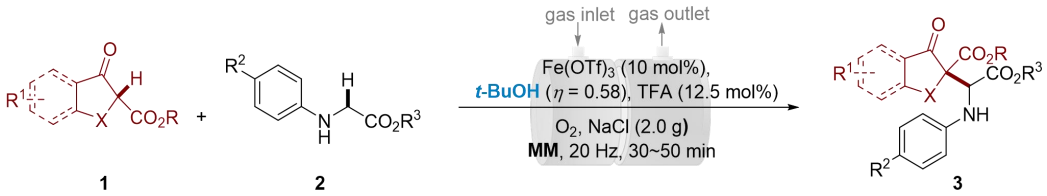
3.3 Typical procedures for asymmetric CDC reaction under accelerating aging conditions



1 **2** **3**

A mixture of **1** (0.2 mmol, 1.0 equiv), **2** (0.2 mmol, 1.0 equiv), $Fe(OTf)_3$ (10 mol %, 0.1 equiv), **L15** (12 mol%, 0.12 equiv), TFA (12.5 mol%, 0.125 equiv), *t*-BuOH (η = 0.58) and NaCl (2.0 g) was placed in a stainless-steel vessel (25 mL) with two stainless-steel balls (d_{MB} = 1.4 cm). Then, the ball milling vessel was placed in the mixer mill and milled at 20 Hz for 30 min. Then the contents were scratched off the vessel and aging in an opened flask (50 mL) for 0.5~2 h. After the reaction was completed, the powders were purified directly by column chromatography on silica gel using EtOAc/*n*-hexane as eluent to give the desired products **3**.

3.4 Typical procedure for the preparation of racemic products

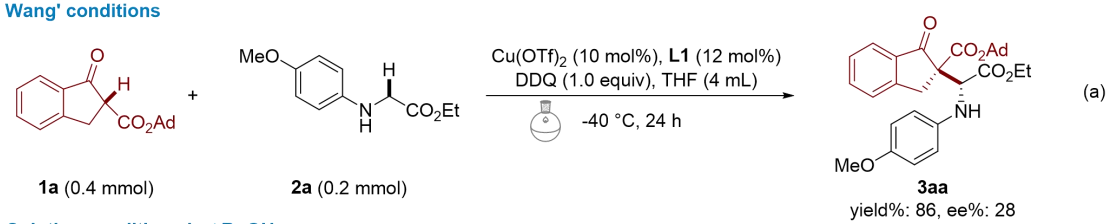


1 **2** **3**

A mixture of **1** (0.2 mmol, 1.0 equiv), **2** (0.2 mmol, 1.0 equiv), $Fe(OTf)_3$ (10 mol %, 0.1 equiv), TFA (12.5 mol%, 0.125 equiv), *t*-BuOH ($\eta = 0.58$) and NaCl (2.0 g) was placed in a stainless-steel vessel (25 mL, equipped with gas inlet and outlet valve) with two stainless-steel balls ($d_{MB} = 1.4$ cm). Then, the ball milling vessel was placed in the mixer mill, oxygen was filled in through the gas inlet valve, and the mixtures were milled at 20 Hz for 30~50 min. After the reaction was completed, the contents were scratched off the vessel and purified directly by column chromatography on silica gel using EtOAc/*n*-hexane as eluent to give the racemic products **3**.

3.5 Comparative experiments under solution-based conditions

Wang' conditions

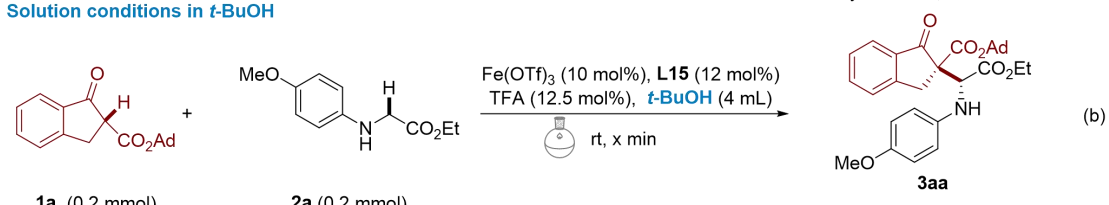


(a)

1a (0.4 mmol) **2a** (0.2 mmol) **3aa**

yield%: 86, ee%: 28

Solution conditions in *t*-BuOH



(b)

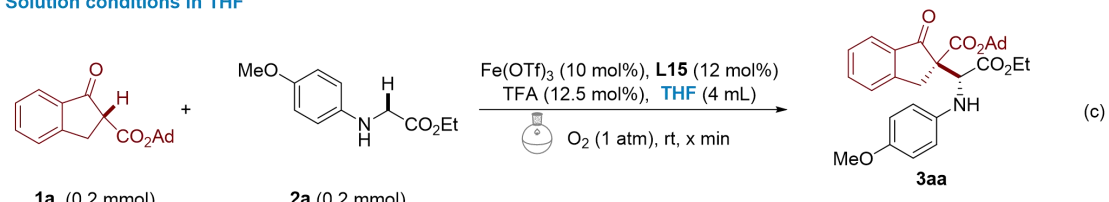
1a (0.2 mmol) **2a** (0.2 mmol) **3aa**

without O_2 (at open air): 720 min, yield%: trace, ee%: n.d.

with O_2 (1 atm):

30 min yield%/ee%	60 min yield%/ee%	240 min yield%/ee%
7, 46	11, 44	30, 11

Solution conditions in THF



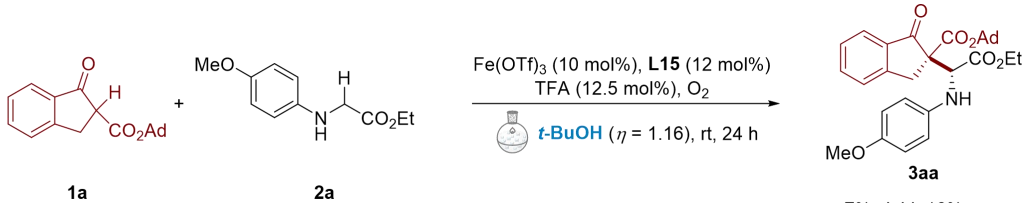
(c)

1a (0.2 mmol) **2a** (0.2 mmol) **3aa**

solvent	30 min yield%/ee%	60 min yield%/ee%	240 min yield%/ee%
THF	n.d., 36	n.d., 33	36, 0
THF/ *t*-BuOH (4 eq.)	n.d., 58	n.d., 57	40, 21

Scheme S1. Reaction of **1a** and **2a** under solution-based conditions. Reaction conditions: (a) the reaction was proceeded under Wang's optimal conditions[6] using THF (4 mL) as solvent and **L1** as ligand. (b) $Fe(OTf)_3$ (10 mol%), **L15** (12 mol%) and TFA (12.5 mol%) were placed in a flask (25 mL) with *t*-BuOH (4 mL) and pre-stirred at rt for 30 min, then **1** (0.2 mmol, 1.0 equiv) and **2** (0.2 mmol, 1.0 equiv) was added, the mixtures were stirring under the air (for 12 h) or oxygen (for 30 min~240 min) atmospheres. To evaluate the yields at different reaction times (30 min, 60 min and 240 min), three individual reactions were carried out respectively. (c) $Fe(OTf)_3$ (10 mol%), **L15** (12 mol%) and TFA (12.5 mol%) were placed in a flask (25 mL) with THF (4 mL) and pre-stirred in the presence/absence of *t*-BuOH (4 equiv. 75 μL) at rt for 30 min, then **1** (0.2 mmol, 1.0 equiv) and **2** (0.2 mmol, 1.0 equiv) was added, the mixtures were stirring under oxygen atmospheres for 30 min~240 min.

3.6 Comparative experiment under neat stirring conditions



1a **2a** **3aa**

7% yield, 16% *ee*

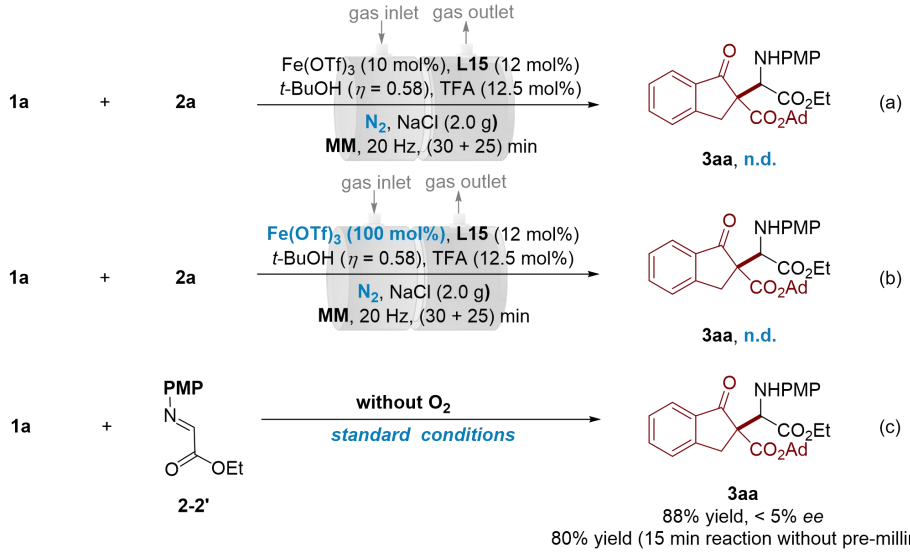
Scheme S2. Reaction of **1a** and **2a** under neat stirring conditions. Reaction conditions: $Fe(OTf)_3$ (10 mol%), **L15** (12 mol%) TFA (12.5 mol%) and *t*-BuOH (η = 1.16, 150 μL) were placed in a flask (25 mL) with and pre-stirred at rt for 30 min, then **1** (0.2 mmol, 1.0 equiv) and **2** (0.2 mmol, 1.0 equiv) was added, and the mixtures were stirring under oxygen atmospheres for 24 h.

To illustrate the advantageous of the mechanochemical LAG conditions, the model reaction was conducted at magnetic stirring with 4 equiv. *t*-BuOH (150 μL) as additive. It has showed that without sufficient mechanical impact, the reactants and the catalyst could not efficiently mix and interact with each other, thus very small amount of the product (7%) was obtained with poor enantioselectivity (16% *ee*).

4. Mechanism study

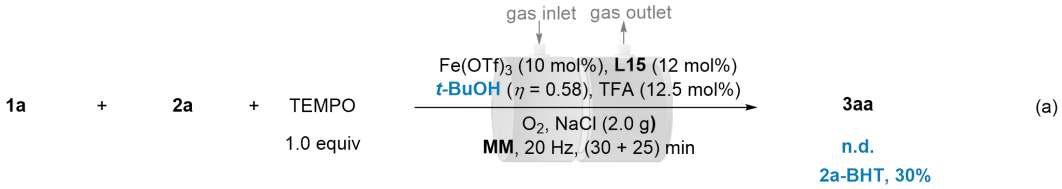
4.1 Control experiments

To demonstrate the actual role of Fe(III) and oxygen, the reactions were carried out under nitrogen atmospheres using either catalytic amount of $Fe(OTf)_3$ (10 mol%) or stoichiometric $Fe(OTf)_3$ (100 mol%). The results clearly showed that oxygen was an indispensable oxidant for this mechanochemical asymmetric CDC reaction, while Fe(III) could not play the role of an oxidant.



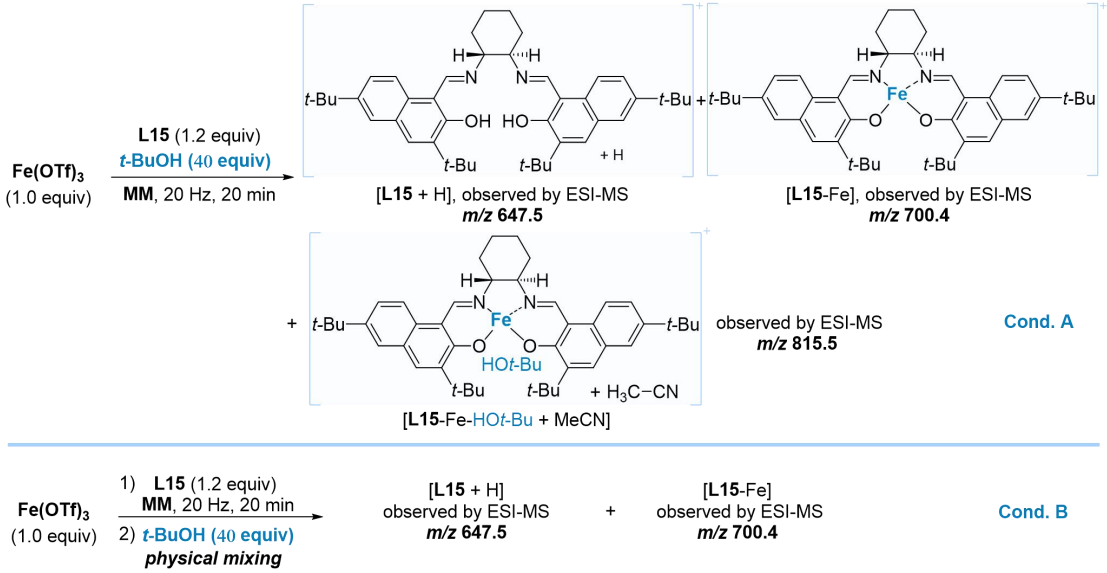
Scheme S3. Reaction of **1a** and **2a** under nitrogen atmospheres. Reaction conditions: (a) $Fe(OTf)_3$ (10 mol%), **L15** (12 mol%), *t*-BuOH (η = 0.58), TFA (12.5 mol%) and NaCl (2.0 g) were placed in a stainless-steel vessel (25 mL, equipped with gas inlet and outlet valve) with two stainless-steel balls (d_{MB} = 1.4 cm) in a mixer mill and pre-milled at 20 Hz for 30 min. Then, **1a** (0.2 mmol) and **2a** (0.2 mmol) were added and the mixtures were milled for another 25 min under nitrogen atmospheres. (b) $Fe(OTf)_3$ (100 mol %) was used. (c) $Fe(OTf)_3$ (10 mol%), **L15** (12 mol%), *t*-BuOH (η = 0.58), TFA (12.5 mol%) and NaCl (2.0 g) were placed in a stainless-steel vessel (25 mL) with two stainless-steel balls (d_{MB} = 1.4 cm) in a mixer mill and pre-milled at 20 Hz for 30 (0) min. Then, **1a** (0.2 mmol) and **2-2'** (0.2 mmol) were added and the mixtures were milled for another 25 (15) min.

4.2 Radical trapping experiments

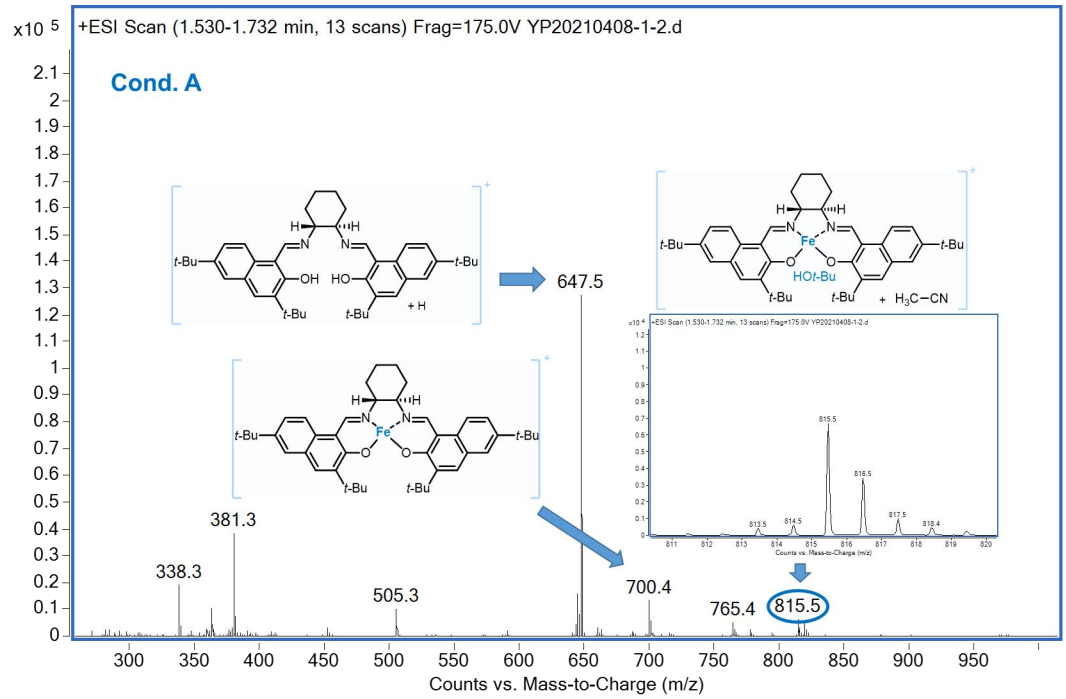


Scheme S4. Radical trapping experiments. Reaction conditions: (a) $Fe(OTf)_3$ (10 mol %), **L15** (12 mol%), *t*-BuOH (η = 0.58), TFA (12.5 mol%) and NaCl (2.0 g) were placed in a stainless-steel vessel (25 mL, equipped with gas inlet and outlet valve) with two stainless-steel balls (d_{MB} = 1.4 cm) in a mixer mill and pre-milled at 20 Hz for 30 min. Then, **1a** (0.2 mmol), **2a** (0.2 mmol) and TEMPO (1.0 equiv.) were added and the mixtures were milled for another 25 min under oxygen atmospheres. (b) **1** (0.2 mmol, 1.0 equiv), **2** (0.2 mmol, 1.0 equiv), $Fe(OTf)_3$ (10 mol %, 0.1 equiv), **L15** (12 mol%, 0.12 equiv), TFA (12.5 mol%, 0.125 equiv), *t*-BuOH (η = 0.58) and NaCl (2.0 g) were milled in the presence of TEMPO (1.0 equiv.) at 20 Hz for 30 min. Then, aging in an opened flask (100 mL) for 2 h. (c) **1** (0.2 mmol, 1.0 equiv), **2** (0.2 mmol, 1.0 equiv), $Fe(OTf)_3$ (10 mol %, 0.1 equiv), **L15** (12 mol%, 0.12 equiv), TFA (12.5 mol%, 0.125 equiv), *t*-BuOH (η = 0.58) and NaCl (2.0 g) were milled in the presence of BHT (2.0 equiv.) at 20 Hz for 30 min. Then, aging in an opened flask (100 mL) for 2 h.

4.3 Iron-complexes capturing experiments



Scheme S5. The reaction of $Fe(OTf)_3$, **L15** and *t*-BuOH. **Condition A**: $Fe(OTf)_3$ (0.02 mmol, 1.0 equiv), **L15** (0.024 mmol, 1.2 equiv), *t*-BuOH (40 equiv, 150 μL) were placed in a stainless-steel vessel (25 mL) with two stainless-steel balls (d_{MB} = 1.4 cm) in a mixer mill and milled at 20 Hz for 30 min. The mixtures were then quickly determined by ESI-MS. **Condition B**: $Fe(OTf)_3$ (0.02 mmol, 1.0 equiv) and **L15** (0.024 mmol, 1.2 equiv) were placed in a stainless-steel vessel (25 mL) with two stainless-steel balls (d_{MB} = 1.4 cm) in a mixer mill and milled at 20 Hz for 30 min. Then, *t*-BuOH (40 equiv, 150 μL) was added and mixed manually. The mixtures were then quickly determined by ESI-MS.



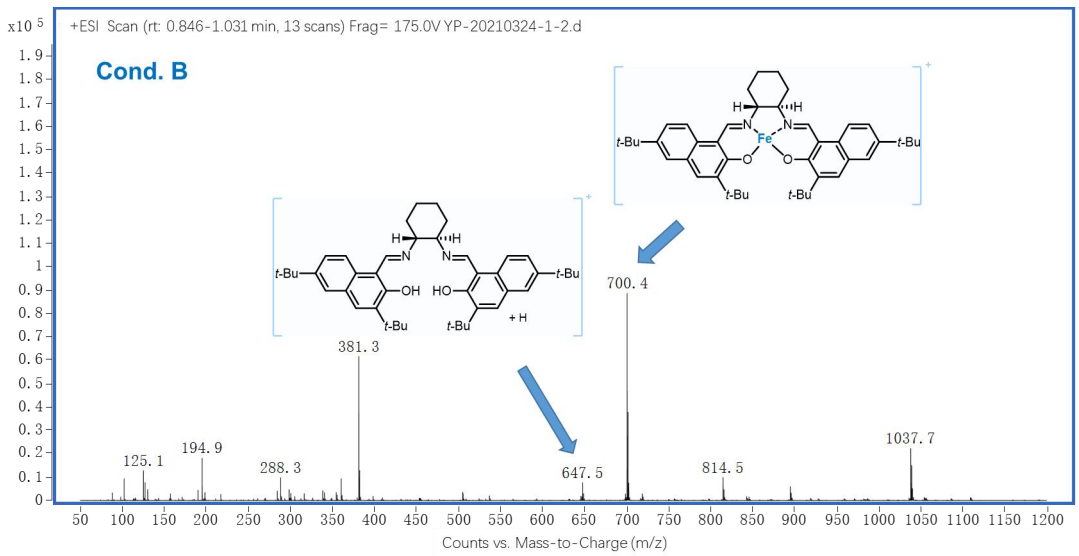
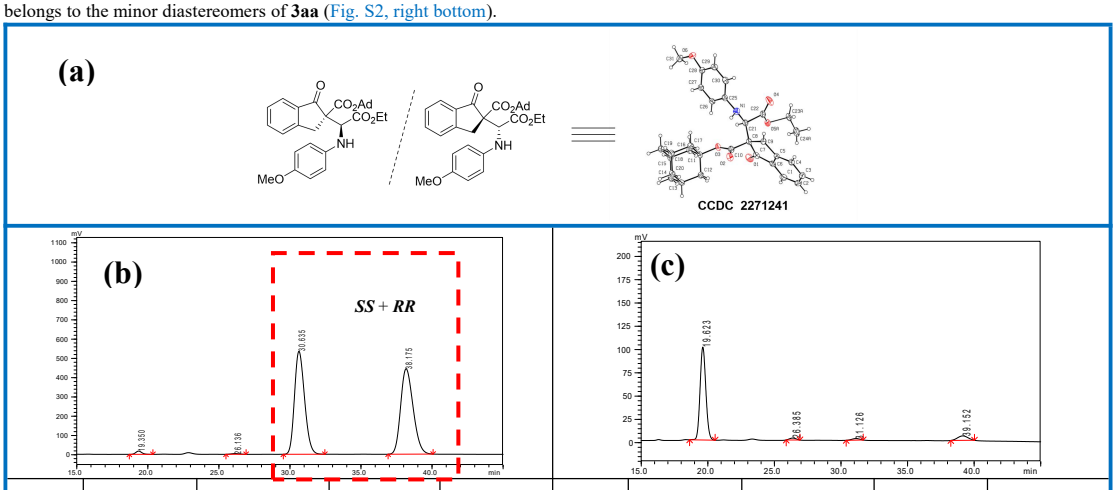


Figure S1. Mass spectra for the reaction of $Fe(OTf)_3$, **L15** and *t*-BuOH under conditions **A** and **B**

To probe the actual catalytic system in the LAG reaction, ESI-MS analysis was employed to detect the mixtures after ball-milling of $Fe(OTf)_3$, **L15** and *t*-BuOH. Two peaks that assigned to Fe-complexes [**L15**-Fe]$^+$ (*m/z* 700.4) and [**L15**-Fe-*t*-BuOH+MeCN]$^+$ (*m/z* 815.5) were found (Figure S1, Cond. A). In stark contrast, neat grinding of $Fe(OTf)_3$ and **L15** followed by physical mixing with *t*-BuOH gave only [**L15**-Fe]$^+$ (*m/z* 700.4) and [**L15**+H]$^+$ (*m/z* 647.5) species, implying that mechanical impact was essential for accessing the **L**-Fe-butanol complex, which is likely an active catalytic species, and the interference caused by ionization during the MS detection could also be excluded.

5. Crystal data for 3aa (minor diastereomers)

We've tried our best to cultivate the single crystal of the chiral products although all of them are oil-like compounds. During the cultivation of **3aa**, trace crystals were appeared. X-ray analysis showed that the space group of its crystal structure is centrally symmetric, where C08 and C21 are in opposite configurations which can be assigned to the racemic mixture of *RR* and *SS* configurations. HPLC analysis of this single crystal showed that the retention times of the main components (> 99% conc.) was at 30.6 minutes and 38.0 minutes, respectively (Fig. S2, left bottom), which belongs to the minor diastereomers of **3aa** (Fig. S2, right bottom).

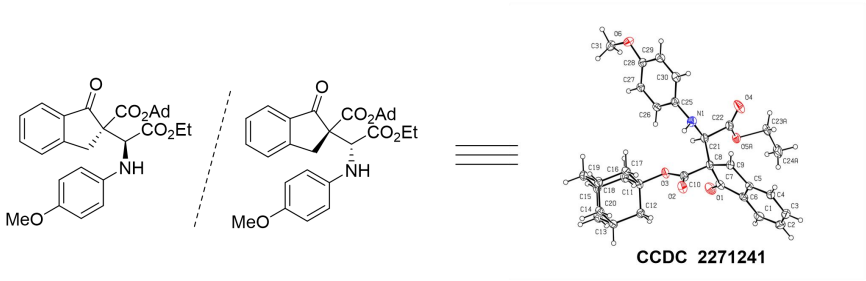


Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	19.350	501255	16826	0.928
2	26.136	23156	1274	0.043
3	30.635	26363969	534315	48.816
4	38.175	27118224	443217	50.213
Total		54006604	995633	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	19.623	3017779	99819	88.456
2	26.385	69577	2053	2.039
3	31.126	65384	1650	1.917
4	39.152	258860	4799	7.588
5		3411601	108321	100.000

Figure S2. X-ray crystal diffraction and HPLC results of **3aa**. (a) X-Ray crystal structure, ellipsoids are drawn at the 30% probability level. (b) HPLC result of the trace crystal from **3aa**. (c) HPLC result of **3aa**.

Single crystal of minor diastereomers of **3aa** suitable for X-ray analysis was obtained by slow evaporation of 0.01 M solution in 7:3 mixture of petroleum ether/ ethyl acetate at room temperature. A suitable crystal was selected on a Bruker APEX-II CCD diffractometer. The crystal was kept at 296.15 K during data collection. Using Olex2,[7] the structure was solved with the SHELXT[8] structure solution program using Intrinsic Phasing and refined with the SHELXL[9] refinement package using Least Squares minimisation.



Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=9.1513(2) b=17.6562(4) c=16.4315(4)
alpha=90 beta=91.946(1) gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	2653.43(11)	2653.42(11)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C31 H34 N O6	C31 H34 N O6
Sum formula	C31 H34 N O6	C31 H34 N O6
Mr	516.59	516.59
Dx, g cm^{-3}	1.293	1.293
Z	4	4
Mu (mm^{-1})	0.089	0.089
F 000	1100.0	1100.0
F000’	1100.55	
h, k, lmax	11, 22, 21	11, 22, 21
Nref	6080	6078
Tmin, Tmax	0.963, 0.974	0.698, 0.746
Tmin’	0.4963	

Correction method= # Reported T Limits: Tmin=0.698 Tmax=0.746
AbsCorr = MULTI-SCAN
Data completeness = 1.000 Theta(max) = 27.497
R(reflections) = 0.0576 (4655) wR2(reflections) = 0.1596 (6078)
S = 1.016 Npar= 374

6. Green chemistry metrics evaluation

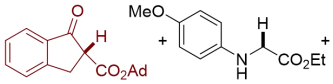
Table S6. Comparison of green chemistry metrics[a]

reaction conditions[a]	LAG method	AA method	stirring in *t*-BuOH	stirring in THF	Wang’s method
yield (%)/ *ee* (%)	87/**95**	68/**90**	30/**11**	40/**21**	86/**28**
oxidant (eq.)/additive (eq.)	O_2/TFA (0.125)	air/TFA (0.125)	O_2	O_2	DDQ (1.0)
time (min)	55	150	240	240	1440
solvent (μL)	*t*-BuOH (75)	*t*-BuOH (75)	*t*-BuOH (4000)	THF (4000)/ *t*-BuOH (4 eq)	THF (4000)
temperature (°C)	rt	rt	rt	rt	-40
atmosphere	O_2	air	O_2	O_2	N_2

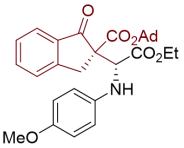
specific operation		–	–	–	–	the solution of DDQ in THF slowly added
***E*-factor**	$\frac{\sum m(\text{Input material}) - m(\text{Product})}{m(\text{Product})}$	23.31 (1.11)[b]	30.11 (1.92)[b]	102.93	89.61	42.02
SI	$\frac{\sum m(\text{Solvents})}{m(\text{Product})}$	0.65	0.83	99.68	85.99	40.00
MI	$\frac{\sum m(\text{Input materials})}{m(\text{Product})}$	24.31 (2.11)[b]	31.11 (2.92)[b]	103.93	90.61	43.02

[a] Details see section 3.5. [b] Grinding auxiliary was excluded (according to our previous work see ref.10, NaCl can be easily recycled and reused).

LAG method



+ $Fe(OTf)_3$ + **L15** + ***t*-BuOH** + TFA —(55 min, NaCl)→



	1a	**2a**	$Fe(OTf)_3$	**L15**	***t*-BuOH**	TFA		**3aa**
MW.	310.39	209.25	503.03	646.96	74.12	98.02		517.62
n/mmol	0.20	0.20	0.02	0.024		0.025		95% *ee*
m/mg	62.1	41.9	10.1	15.5	58.1	2.5	2000	90.1 mg, 87% yield

AA method

1a + **2a** + $Fe(OTf)_3$ + **L15** + ***t*-BuOH** + TFA —(150 min, NaCl)→ **3aa**

MW.	310.39	209.25	503.03	646.96	74.12	98.02		517.62
n/mmol	0.20	0.20	0.02	0.024		0.025		90% *ee*
m/mg	62.1	41.9	10.1	15.5	58.1	2.5	2000	70.4 mg, 68% yield

Stirring in t-BuOH

1a + **2a** + $Fe(OTf)_3$ + **L15** + TFA —(240 min, *t*-BuOH (4 mL))→ **3aa**

MW.	310.39	209.25	503.03	646.96		98.02		517.62
n/mmol	0.20	0.20	0.02	0.024		0.025		11% *ee*
m/mg	62.1	41.9	10.1	15.5		2.5	3100	31.1 mg, 30% yield

Stirring in THF

1a + **2a** + $Fe(OTf)_3$ + **L15** + ***t*-BuOH** + TFA —(240 min, THF (4 mL))→ **3aa**

MW.	310.39	209.25	503.03	646.96	74.12	98.02		517.62
n/mmol	0.20	0.20	0.02	0.024	0.80	0.025		21% *ee*
m/mg	62.1	41.9	10.1	15.5	59.2	2.5	3560	41.4 mg, 40% yield

Wang's method

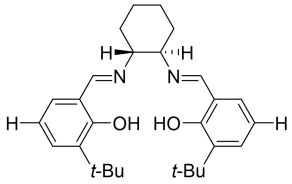
1a + **2a** + $Cu(OTf)_2$ + **L1** + DDQ —(1440 min, THF (4 mL))→ **3aa**

MW.	310.39	209.25	361.67	356.43	227.00			517.62
n/mmol	0.20	0.40	0.02	0.024	0.20			28% *ee*
m/mg	62.1	83.7	7.23	8.55	45.4		3560	89.0 mg, 86% yield

Scheme S6. Green chemistry metrics calculations.

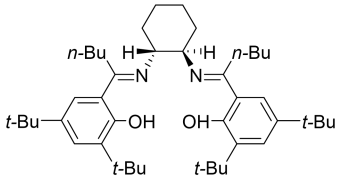
7. Characterization data (HPLC spectra)

7.1 Ligands



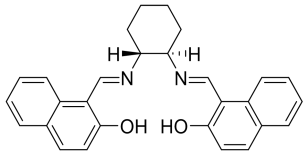
6,6'-((1E,1'E)-(((1R,2R)-cyclohexane-1,2-diyl)bis(azanylylidene))bis(methanylylidene))bis(2-(tert-butyl)phenol) (**L9**)[5a]

Yellow solid; mp 66–67 ˚C (67–69 ˚C[5a]); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 13.84 (s, 2H). 8.30 (s, 2H), [7.53, 7.40] (dd, *J* = 7.6, 1.6 Hz, 1H), 7.24 (d, *J* = 1.6 Hz, 1H), 7.01 (d, *J* = 7.2 Hz, 2H), 6.75–6.69 (m, 2H), 3.43–3.27 (m, 2H), 2.02–1.94 (m, 2H), 1.93–1.85 (m, 2H), 1.81–1.72 (m, 2H), 1.52–1.45 (m, 2H), 1.40 (s, 18H). **Optical Rotation:** $[\alpha]_D^{25}$ = -521.6 (c = 1.0, CH_2Cl_2) {$[\alpha]_D^{20}$ = -523 (c = 1.0, CH_2Cl_2)[5b]}.



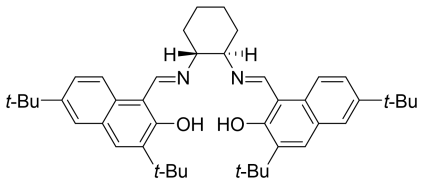
6,6'-((1E,1'E)-(((1R,2R)-cyclohexane-1,2-diyl)bis(azanylylidene))bis(2,2-dimethylpropan-1-yl-1-ylidene))bis(2,4-di-tert-butylphenol) (**L13**)

Yellow solid; mp 120–122 ºC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 2.0 Hz, 2H), 7.27 (d, *J* = 2.4 Hz, 2H), 3.99–3.81 (m, 2H), 2.81–2.57 (m, 4H), 1.94–1.85 (m, 4H), 1.77–1.67 (m, 4H), 1.55–1.47 (m, 8H), 1.41 (s, 18H), 1.27 (s, 18H), 0.99 (t, *J* = 7.0 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 175.0 (2C, Cq), 161.7 (2C, Cq), 137.5 (2C, Cq), 137.3 (2C, Cq), 126.7 (2C, Cq), 122.3 (2C, CH), 116.6 (2C, CH), 62.6 (2C, CH), 35.1 (2C, Cq), 34.1 (2C, Cq), 33.0 (2C, Cq), 31.5 (6C, CH_3), 30.2 (2C, CH_2), 29.6 (6C, CH_3), 27.6 (2C, CH_2), 24.2 (2C, CH_2),23.1 (2C, CH_2), 13.7 (2C, CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{44}H_{71}N_2O_2$ $[M+H]^+$ 659.5516, found 659.5532. **Optical Rotation:** $[\alpha]_D^{25}$ = -273.5 (c = 1.0, CH_2Cl_2).



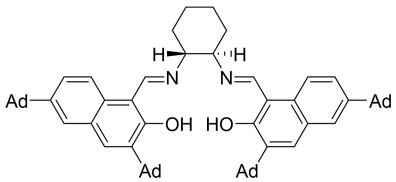
(1R,2R)-cyclohexane-1,2-diyl-bis(azanylylidene)-bis(methanylylidene)-bis(naphthalen-2-ol) (**L14**)

Yellow solid; mp 212–213°C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 14.64 (brs, 2H), 8.77 (s, 2H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 9.2 Hz, 2H), 7.46 (d, *J* = 7.8 Hz, 2H), 7.33–7.27 (m, 2H), 7.16–7.11 (m, 2H), 6.86 (d, *J* = 9.2 Hz, 2H), 3.46–3.40 (m, 2H), 2.23–2.17 (m, 2H), 1.98–21.91 (m, 2H), 1.82–1.74 (m, 2H), 1.55–1.47 (m, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.1 (2C, Cq), 159.2 (2C, CH), 136.4 (2C, CH), 133.2 (2C, Cq), 128.8 (2C, CH), 127.8 (2C, CH), 126.5 (2C, Cq), 122.8 (2C, CH), 122.7 (2C, CH), 118.4 (2C, CH), 107.1 (2C, Cq), 69.1 (2C, CH), 32.7 (2C, CH_2), 24.2 (2C, CH_2). **HRMS (ESI)** *m/z*: calcd for $C_{28}H_{27}N_2O_2$ $[M+H]^+$ 423.2067, found 423.2071. **Optical Rotation:** $[\alpha]_D^{25}$ = -298.6 (c = 1.0, CH_2Cl_2).



3,6-di-tert-butyl-1-(1R,2R)-2-((6-(tert-butyl)-2-hydroxy-3-methylnaphthalen-1-yl)methylene) amino)cyclohexyl) imino) methyl)naphthalen-2-ol (**L15**)

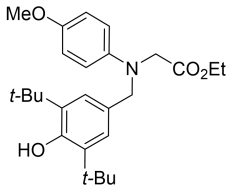
Yellow solid; mp 160–162 ºC; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.66 (s, 2H), 7.45–7.40 (m, 4H, including d, *J* = 9.0 Hz, 2H and s, 2H), 7.27 (s, 2H), 7.16 (dd, *J* = 9.0, 2.4 Hz, 2H), 3.50–3.45 (m, 2H), 2.28–2.23 (m, 2H), 1.99–1.94 (m, 2H), 1.89–1.82 (m, 2H), 1.52–1.50 (m, 2H), 1.47 (s, 18H), 1.30 (s, 18H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.0 (2C, Cq), 159.5 (2C, CH), 144.8 (2C, Cq), 141.1 (2C, Cq), 132.6 (2C, CH), 130.2 (2C, Cq), 125.7 (2C, Cq), 125.3 (2C, CH), 124.0 (2C, CH), 117.0 (2C, CH), 106.9 (2C, Cq), 68.8 (2C, CH), 35.0 (2C Cq), 34.2 (2C Cq), 32.5 (2C, CH_2), 31.3 (6C, CH_3), 29.5 (6C, CH_3), 24.4 (2C, CH_2). **HRMS (ESI)** *m/z*: calcd for $C_{44}H_{59}N_2O_2$ $[M+H]^+$ 647.4571, found 647.4600. **Optical Rotation:** $[\alpha]_D^{25}$ = -359.2 (c = 1.0, CH_2Cl_2).



3,6-di-adamantyl-1-(1R,2R)-2-((6-(adamantyl)-2-hydroxy-3-methylnaphthalen-1-yl)methylene) amino)cyclohexyl) imino) methyl)naphthalen-2-ol (**L16**)

Yellow solid; mp 295–298 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 14.67 (s, 2H), 8.68 (s, 2H), 7.50 (d, *J* = 8.8 Hz, 2H), 7.35 (s, 2H), 7.25 (s, 2H), 7.20 (dd, *J* = 8.8, 2.0 Hz, 2H), 3.45–3.39 (m, 2H), 2.23–2.06 (m, 26H), 1.91–1.87 (m, 12H), 1.85–1.70 (m, 26H), 1.60–1.55 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.6 (2C, Cq), 159.8 (2C, CH), 145.2 (2C, Cq), 141.3 (2C, Cq), 133.0 (2C, Cq), 130.4 (2C, Cq), 126.3 (2C, CH), 124.8 (2C, CH), 124.2 (2C, CH), 117.4 (2C, CH), 107.3 (2C, Cq), 69.4 (2C, CH), 43.2 (4C, CH_2), 40.7 (4C, CH_2), 37.52 (2C, Cq), 37.48 (4C, CH_2), 37.1 (8C, CH_2), 35.9 (2C, CH_2), 32.9 (4C, Cq), 29.3 (4C, CH), 29.0 (8C, CH), 24.7 (2C, CH_2). **HRMS (ESI)** *m/z*: calcd for $C_{68}H_{83}N_2O_2$ $[M+H]^+$ 959.6449, found 959.6485. **Optical Rotation:** $[\alpha]_D^{25}$ = -330.7 (c = 1.0, CH_2Cl_2).

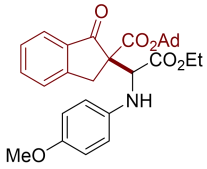
7.2 Radical trapping product



ethyl N-(3,5-di-tert-butyl-4-hydroxybenzyl)-N-(4-methoxyphenyl)glycinate (**2a-BHT**)[10]

Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.07 (s, 2H), 6.81 (d, *J* = 9.2 Hz, 2H), 6.73 (d, *J* = 9.2 Hz, 2H), 4.47 (s, 2H), 4.17 (q, *J* = 7.0 Hz, 2H), 3.94 (s, 2H), 3.75 (s, 3H), 1.41 (s, 18H), 1.24 (t, *J* = 7.0 Hz, 3H).

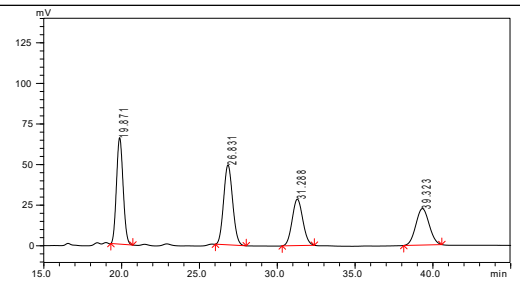
7.3 Products

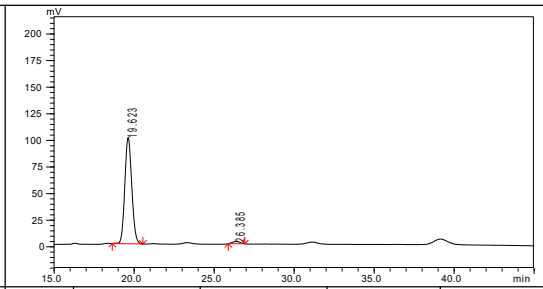


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3aa**)

Colorless oil (90 mg, 87% yield); 90:10 *dr* (88:12 *dr*, **from aging**). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.8 Hz, 1H), 7.61–7.57 (m, 1H), 7.47 (d, *J* = 7.2 Hz, 1H), 7.39–7.35 (m, 1H), 6.87–6.75 (m, 4H), 4.98 (s, 1H), 3.93–3.84 [m, 3H, including 3.90 (q, *J* = 7.2 Hz, 2H); 3.86 (d, *J* = 17.4 Hz, 1H)], 3.75 (s, 3H), 3.36 (d, *J* = 17.4 Hz, 1H), 2.14–2.01 (m, 9H), 1.62–1.56 (m, 6H), 0.89 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.6 (Cq), 171.3 (Cq), 166.9 (Cq), 153.7 (Cq), 152.7 (Cq), 140.8 (Cq), 135.2 (CH), 127.7 (CH), 126.4 (CH), 124.6 (CH), 116.9 (2C, CH), 114.7 (2C, CH), 83.0 (Cq), 65.2 (Cq), 62.2 (CH), 61.6 (CH_2), 55.7 (CH_3), 40.9 (3C, CH_2), 36.0 (3C, CH_2), 33.4 (CH_2), 30.8 (3C, CH), 13.6 (CH_3). **HRMS (ESI)** *m/z*: calcd for $NaC_{31}H_{35}NO_6$ $[M+Na]^+$ 540.2357, found 540.2373.

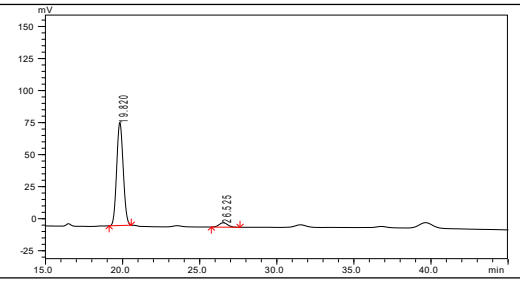
Optical Rotation: $[\alpha]^{25}_D$ = +82.7 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered): 97.7:2.3 *er* (94.7:5.3 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 19.6 min, t_{minor} = 26.4 min; (t_{major} = 19.8 min, t_{minor} = 26.5 min, **from aging**).



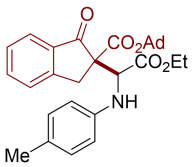


Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)	Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	19.871	1948058	65603	29.388	1	19.623	3017779	99819	97.746
2	26.831	1986413	49213	29.967	2	26.385	69577	2053	2.254
3	31.288	1358795	28592	20.499					
4	39.323	1335476	22457	20.147					
Total		6628743	165865	100.000	Total		3087357	101872	100.000

From aging



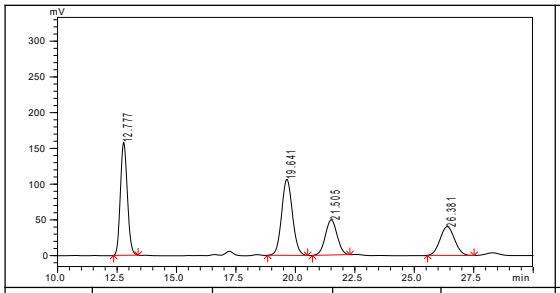
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	19.820	2370344	80422	94.705
2	26.525	132536	3408	5.295
Total		2502880	83829	100.000

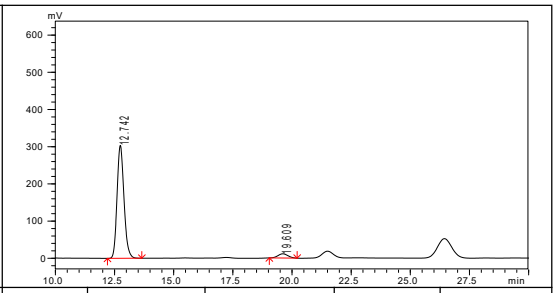


Adamantan-1-yl-2-(2-ethoxy-2-oxo-1-(p-tolylamino)ethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ab**)

Colorless oil (69 mg, 69% yield); 80:20 *dr* (70:30 *dr*, **from aging**). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 1H), 7.61–7.56 (m, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.39–7.34 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.73 (d, *J* = 8.0 Hz, 2H), 5.05 (s, 1H), 3.91 (q, *J* = 7.2 Hz, 2H), 3.85 (d, *J* = 17.2 Hz, 1H), 3.25 (d, *J* = 17.2 Hz, 1H), 2.24 (s, 3H), 2.12-2.02 (m, 9H), 1.61–1.56 (m, 6H), 0.91 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.8 (Cq), 171.5 (Cq), 167.0 (Cq), 152.7 (Cq), 145.1 (Cq), 135.4 (CH), 129.8 (2C, CH), 128.8 (CH), 127.8 (CH), 126.5 (CH), 124.7 (CH), 115.1 (2C, CH), 83.1 (Cq), 65.4(Cq), 61.7 (CH), 61.3 (CH_2), 41.0 (3C, CH_2), 36.2 (3C, CH_2), 33.6 (CH_2), 30.9 (3C, CH), 20.6 (CH_3), 13.8 (CH_3). **HRMS (ESI)** *m/z*: calcd for $NaC_{31}H_{35}NO_5$ $[M+Na]^+$ 524.2407, found 524.2389.

Optical Rotation: $[\alpha]_D^{25}$ = +38.5 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered): 95.5:4.5 *er* (93.0:7.0 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 12.7 min, t_{minor} = 19.6 min; (t_{major} = 12.7 min, t_{minor} = 19.7 min, **from aging**).

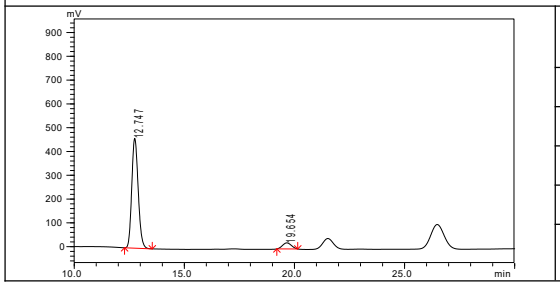




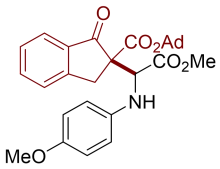
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	12.777	3216615	158150	32.527
2	19.641	3255985	104755	32.925
3	21.505	1701872	49112	20.499
4	26.381	1714725	40243	20.147
Total		9889197	352259	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	12.742	6182467	303506	95.503
2	19.609	291087	10659	4.497
Total		6473554	314166	100.000

From aging



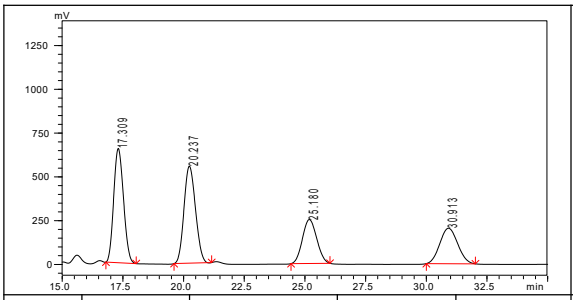
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	12.747	9370228	461446	92.989
2	19.654	706529	25357	7.011
Total		10076757	486802	100.000

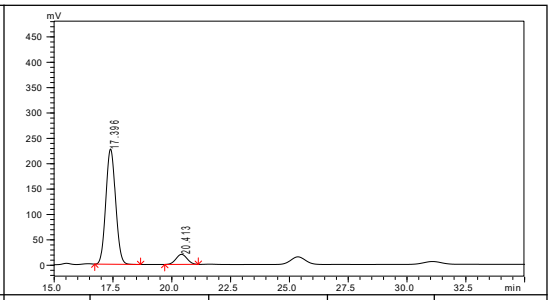


Adamantan-1-yl-2-(2-methoxy-2-oxo-1-(p-tolylamino)ethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ac**)

Colorless oil (89 mg, 88% yield); 92:8 *dr* (85:15 *dr*, **from aging**). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.6 Hz, 1H), 7.62–7.57 (m, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.39–7.33 (m, 1H), 6.81–6.70 (m, 4H), 4.99 (s, 1H), 3.77–3.69 (m, 4H, including 3.73, s, 3H)), 3.62 (s, 3H), 3.35–3.27 (m, 1H), 2.15–2.02 (m, 9H), 1.64–1.57 (m, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 202.9 (Cq), 172.5 (Cq), 167.4 (Cq), 153.5 (Cq), 152.9 (Cq), 140.6 (Cq), 135.7 (Cq), 135.2 (CH), 127.7 (CH), 126.1 (CH), 124.7 (CH), 116.7 (2C, CH), 114.6 (2C, CH), 82.8 (Cq), 63.5(Cq), 62.3 (CH), 55.6 (CH_3), 52.2 (CH_3), 40.9 (3C, CH_2), 36.0 (3C, CH_2), 33.8 (CH_2), 30.8 (3C, CH). **HRMS (ESI)** *m/z*: calcd for $NaC_{30}H_{33}NO_6$ $[M+Na]^+$ 526.2200, found 526.2175.

Optical Rotation: $[\alpha]_D^{25}$ = +69.1 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered): 94.4:5.6 *er* (93.1:6.9 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 85/15, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 17.4 min, t_{minor} = 20.4 min; (t_{major} = 16.6 min, t_{minor} = 19.5 min, **from aging**).

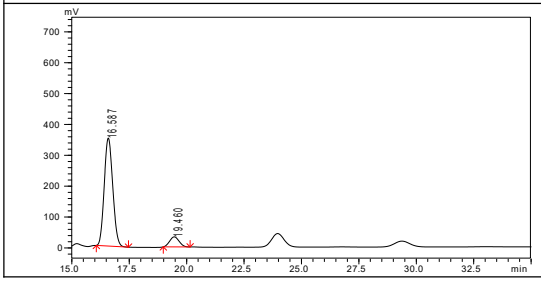




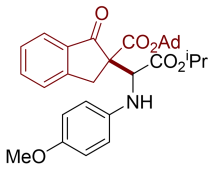
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.309	18348132	652431	32.094
2	20.237	18181916	554130	31.804
3	25.180	10270257	250789	17.965
4	30.913	10368926	202676	18.137
Total		57169231	1660026	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.396	6568169	227057	94.432
2	20.413	387247	15092	5.568
Total		6955415	242148	100.000

From aging



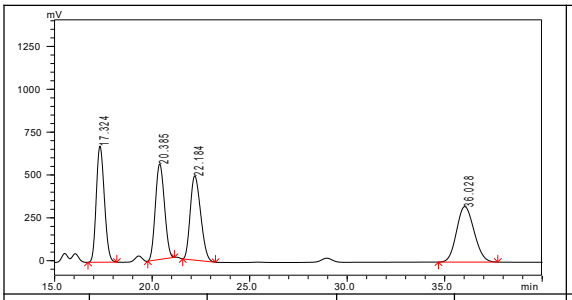
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	16.587	9259479	352372	93.145
2	19.460	681462	27574	6.855
Total		9940942	379946	100.000



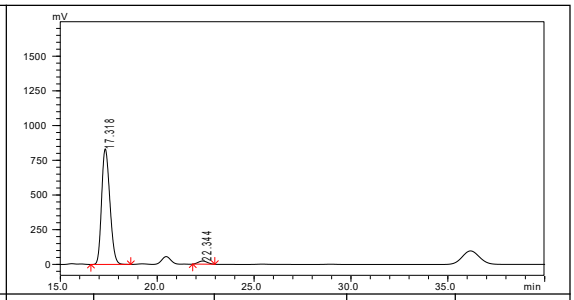
Adamantan-1-yl-2-(2-isopropoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ad**)

Yellow oil (85 mg, 80% yield); 85:15 *dr*. **^{1}H NMR** (500 MHz, $CDCl_3$) [7.76 minor, 7.74 major] (d, J = 8.0 Hz, 1H), 7.61–7.56 (m, 1H), 7.47 (d, J = 7.5 Hz, 1H), 7.39–7.34 (m, 1H), 6.90–6.70 (m, 4H), 5.01–4.71 (m, 2H, including [4.99 minor, 4.93 major] (s, 1H)), [3.75 minor, 3.73 major] (s, 3H), 3.70 (d, J = 17.5 Hz, 1H), 3.30 (d, J = 17.5 Hz, 1H), 2.15–2.03 (m, 9H), 1.64–1.56 (m, 6H), 1.15–0.64 (m, 6H, including [1.11 (d, J = 6.0 Hz), 1.02 (d, J = 6.5 Hz)] major, [1.03 (d, J = 6.5 Hz), 0.67 (d, J = 6.0 Hz)] minor). **^{13}C NMR** (125 MHz, $CDCl_3$) δ [200.2 major, 198.4 minor] (Cq), 171.1 (Cq), [167.6 major, 166.0 minor] (Cq), 153.4 (Cq), 152.7 (Cq), [141.3 minor, 141.0 major] (Cq), 135.9 (Cq), 135.1 (CH), 127.7 (CH), 126.1 (CH), 124.7 (CH), [116.8 major, 116.6 minor] (2C, CH), 114.6 (2C, CH), [82.9 minor, 82.6 major] (Cq), [69.6 minor, 69.3 major] (Cq), [63.0 minor, 62.8 major] (CH), 60.3 (CH), 55.7 (CH_3), 41.0 (3C, CH_2), 36.1 (3C, CH_2), 34.2 (CH_2), 30.8 (3C, CH), 21.6 (CH_3), 21.5 (CH_3), 21.0 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{32}H_{38}NO_6$ $[M+H]^+$ 532.2694, found 532.2701.

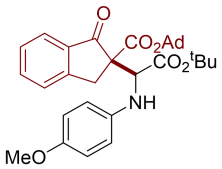
Optical Rotation: $[\alpha]_D^{25}$ = +118.2 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered): 97.1:2.9 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 17.3 min, t_{minor} = 22.3 min.



Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.324	19052006	670875	25.209
2	20.385	18740845	559829	24.798
3	22.184	19090128	498958	25.260
4	36.028	18692504	313278	24.734
Total		75575483	2042939	100.000



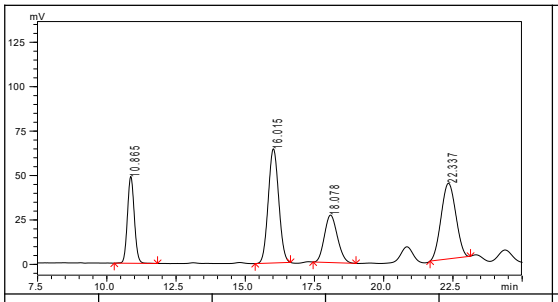
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.318	24626958	832513	97.056
2	22.344	746936	22642	2.944
Total		25373895	855155	100.000

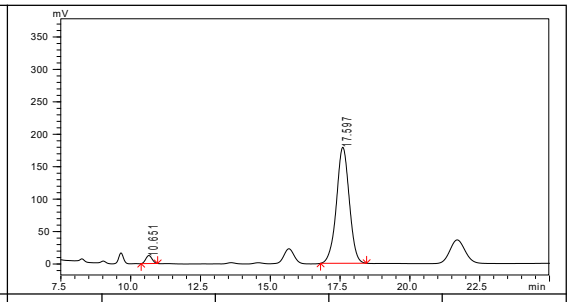


Adamantan-1-yl-2-(2-(tert-butoxy)-1-((4-methoxyphenyl) amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ae**)

Yellow oil (73 mg, 67% yield); 85:15 *dr*. **^{1}H NMR** (400 MHz, $CDCl_3$) δ [7.78 minor, 7.74 major (d, *J* = 7.6 Hz, 1H), 7.62–7.56 (m, 1H), [7.51 minor, 7.47 major (d, *J* = 7.6 Hz, 1H), 7.41–7.34 (m, 1H), 6.90–6.71 (m, 4H), [4.97 minor, 4.83 major] (s, 1H), [3.76 minor, 3.73 major] (s, 3H), 3.69 (d, *J* = 17.6 Hz, 1H), 3.32 (d, *J* = 17.6 Hz, 1H), 2.17–2.00 (m, 9H), 1.63–1.56 (m, 6H), [1.23 major, 1.02 minor] (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.5 (Cq), 170.6 (Cq), 167.8 (Cq), 153.2 (Cq), 152.7 (Cq), 141.1 (Cq), 136.0 (Cq), 135.1 (CH), 127.7 (CH), 126.1 (CH), 124.6 (CH), 116.7 (2C, CH), 114.5 (2C, CH), 82.6 (Cq), 82.4 (Cq), 63.5 (Cq), 62.7 (CH), 55.7 (CH_3), 41.0 (3C, CH_2), 36.0 (3C, CH_2), 34.5 (CH_2), 30.8 (3C, CH), [27.7 major, 27.4 minor] (3C, CH_3). **HRMS (ESI)** *m/z*: calcd for $NaC_{33}H_{39}NO_6$ $[M+Na]^+$ 568.2670, found 568.2653.

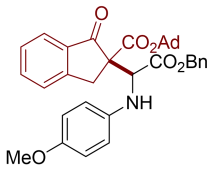
Optical Rotation: $[\alpha]_D^{25}$ = +91.2 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 96.7:3.3 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 17.6 min, t_{minor} =10.7 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	10.865	845305	48856	16.976
2	16.015	1694631	64252	34.032
3	18.078	870838	26701	17.488
4	22.337	1568729	42527	31.504
Total		4979502	182337	100.000

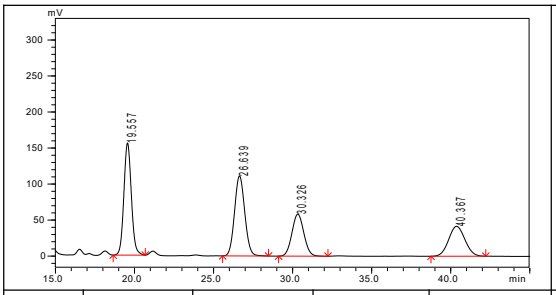
Peak	RetTime (min)	Ara (mV*s)	Height (mV)	Conc. (%)
1	10.651	195606	12378	3.304
2	17.597	5723784	178764	96.696
Total		5919390	191141	100.000

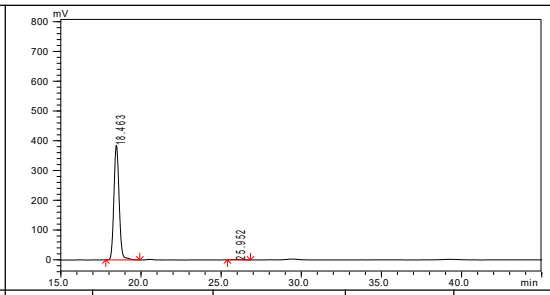


Adamantan-1-yl-2-(2-(benzyloxy)-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3af**)

Colorless oil (105 mg, 90% yield); > 20:1 *dr* (85:15 *dr*, **from aging**). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.6 Hz, 1H), 7.60–7.55 (m, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.39–7.26 (m, 4H), 7.20–7.13 (m, 2H), 6.85–6.63 (m, 4H), 5.16–4.92 (m, 3H, including 3.74, s, 1H), 3.74 (s, 3H), 3.68 (d, *J* = 17.6 Hz, 1H), 3.28 (d, *J* = 17.6 Hz, 1H), 2.09–1.92 (m, 9H), 1.59–1.54 (m, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1 (Cq), 171.8 (Cq), 167.4 (Cq), 153.5 (Cq), 152.8 (Cq), 140.7 (Cq), 135.7 (Cq), 135.2 (CH), 135.1 (Cq), 128.41 (2C, CH), 128.37 (2C, CH), 128.3 (CH), 127.7 (CH), 126.1 (CH), 124.7 (CH), 116.9 (2C, CH), 114.6 (2C, CH), 82.8 (Cq), 67.2 (CH_2), 63.3 (Cq), 62.5 (CH_2), 55.7 (CH_3), 40.8 (3C, CH_2), 36.0 (3C, CH_2), 34.0 (CH_2), 30.8 (3C, CH). **HRMS (ESI)** *m/z*: calcd for $NaC_{36}H_{37}NO_6$ $[M+Na]^+$ 602.2513, found 602.2496.

Optical Rotation: $[\alpha]_D^{25}$ = +192.3 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 99.5:0.5 *er* (96.5:3.5 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 85/15, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 18.5 min, t_{minor} = 26.0 min; (t_{major} = 19.0 min, t_{minor} = 25.9 min, **from aging**).

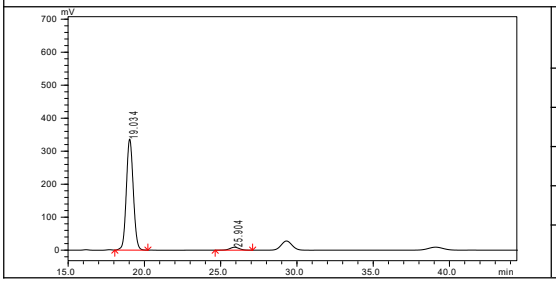




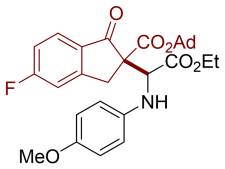
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	19.557	5129380	155646	31.771
2	26.639	4997643	111065	30.955
3	30.326	3049412	58261	18.888
4	40.367	2968614	41464	18.387
Total		16145049	366436	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	18.463	8735464	384652	99.455
2	25.952	47846	1207	0.545
Total		8783310	385859	100.000

From aging



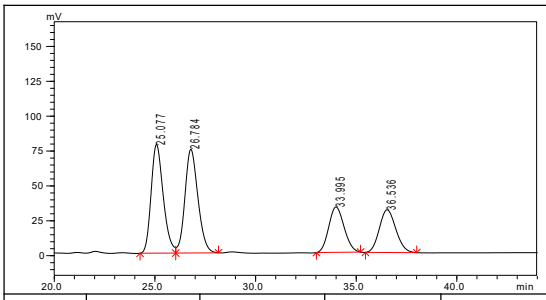
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	19.034	10629697	336616	96.541
2	25.904	380892	8855	3.459
Total		11010589	345471	100.000

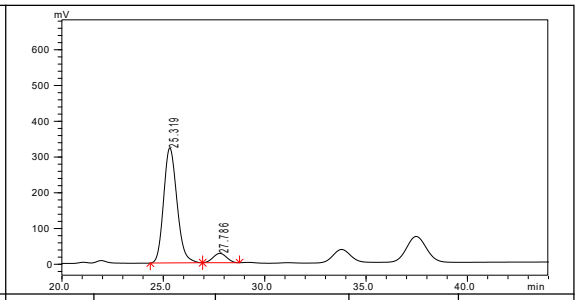


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-5-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ba**)

Yellow oil (76 mg, 71% yield); 80:20 *dr* (72:28 *dr*, **from aging**). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78–7.71 (m, 1H), 7.16–7.11 (m, 1H), 7.09–7.03 (m, 1H), 6.81–6.72 (m, 4H), [4.98 minor, 4.97 major] (s, 1H), [(4.14–4.04) major, (3.95–3.92) minor] (m, 2H), 3.76–3.68 (m, 4H, including [3.75 minor, 3.72 major] (s, 3H)), [3.28 major, 3.23 minor] (d, J = 18.0 Hz, 1H), 2.15–2.02 (m, 9H), 1.63–1.58 (m, 6H), [1.14 major, 0.93 minor] (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ [198.2 major, 196.8 minor] (Cq), [171.8 major, 171.4 minor] (Cq), 167.5 (d, J_1 = 227.5 Hz, Cq), [167.1 major, 166.4 minor] (Cq), 155.9 (Cq), [153.6 major, 153.5 minor] (Cq), 140.7 (Cq), 127.0 (d, J_3 = 10.0 Hz, CH), 123.6 (Cq), 116.9 (2C, CH), 116.0 (d, J_2 = 23.8 Hz, CH), 114.6 (2C, CH), 112.9 (d, J_2 = 22.5 Hz, CH), [83.2 minor, 82.9 major] (Cq), 65.7 (Cq), 63.9 (CH), [61.6 minor, 61.5 major] (CH_2), 55.6 (CH_3), 40.9 (3C, CH_2), 36.0 (3C, CH_2), [33.7 major, 33.3 minor] (CH_2), 30.8 (3C, CH), [14.2 minor, 14.1 major] (CH_3). **^{19}F NMR** (470 MHz, $CDCl_3$) δ -101.8. **HRMS (ESI)** *m/z*: calcd for $C_{31}H_{35}NO_6F$ $[M+H]^+$ 536.2443, found 536.2438.

Optical Rotation: $[\alpha]_D^{25}$ = +26.9 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 95.0:5.0 *er* (92.7:7.3 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 25.3 min, t_{minor} = 27.8 min; (t_{major} = 25.3 min, t_{minor} = 27.9 min, **from aging**).

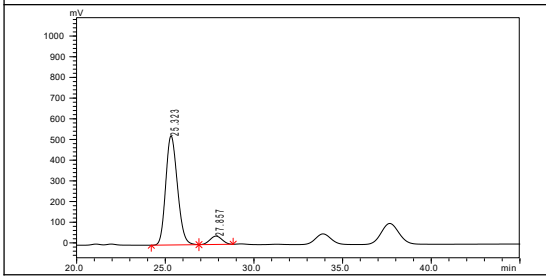




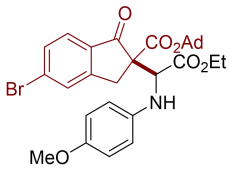
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	25.077	3263565	77863	32.401
2	26.784	3334563	74323	33.106
3	33.995	1727891	32522	17.155
4	36.536	1746374	30606	17.338
Total		10072393	215314	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	25.319	14741828	321629	95.005
2	27.786	775031	20295	4.995
Total		15516860	341924	100.000

From aging



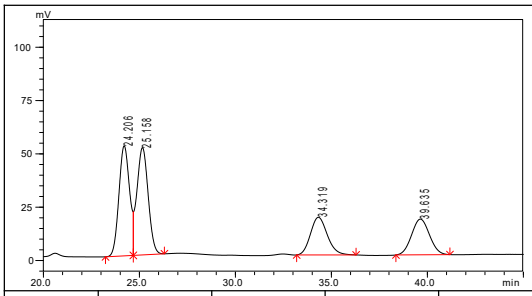
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	25.323	24262899	527926	92.671
2	27.857	1918820	40406	7.329
Total		26181720	568332	100.000

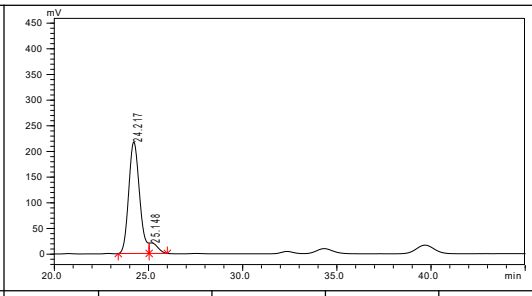


Adamantan-1-yl-5-bromo-2-(2-ethoxy-1-((4-methoxyphenyl) amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ca**)

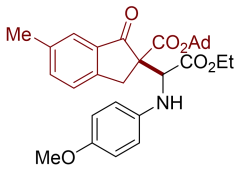
Yellow oil (88.8 mg, 75% yield); 88:12 *dr*. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (brs, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 6.84–6.73 (m, 4H), 5.00 (s, 1H), 4.18–4.07 (m, 1H), 3.83–3.69 (m, 4H, including 3.71, s, 3H), 3.30 (d, *J* = 17.6 Hz, 1H), 2.24–1.99 (m, 9H), 1.65–1.60 (m, 6H), 1.16 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.9 (Cq), 171.8 (Cq), 167.0 (Cq), 154.4 (Cq), 153.5 (Cq), 140.6 (Cq), 131.3 (CH), 129.7 (Cq), 129.4 (CH), 125.8 (CH), 116.8 (2C, CH), 114.5 (2C, CH), 83.0 (Cq), 66.7 (Cq), 63.7 (CH), 61.6 (CH_2), 55.6 (CH_3), 40.9 (3C, CH_2), 36.0 (3C, CH_2), 33.4 (CH_2), 30.8 (3C, CH_2), 14.1 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{31}H_{35}NO_6{}^{79}Br$ $[M+H]^+$ 596.1642, found 596.1666.

Optical Rotation: $[\alpha]_D^{25}$ = +23.6 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 95.1:4.9 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 24.2 min, t_{minor} = 25.2 min.





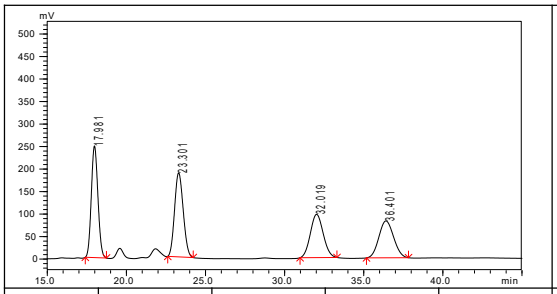
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)	Peak	RetTime (min)	Ara (mV*s)	Height (mV)	Conc. (%)
1	24.206	2000669	51626	32.154	1	24.217	8886927	217369	95.094
2	25.158	2059309	50345	33.097	2	25.171	458455	20460	4.906
3	34.319	1077136	17652	17.311					
4	39.635	1084977	16746	17.438					
Total		6222091	136369	100.000	Total		9345383	237829	100.000

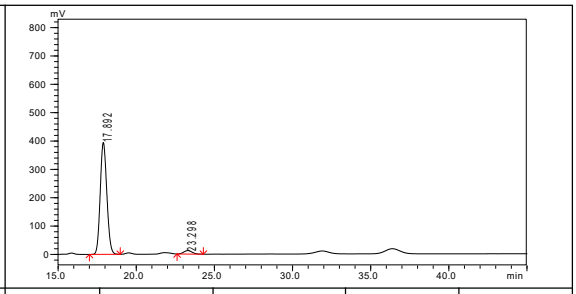


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-6-methyl-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3da**)

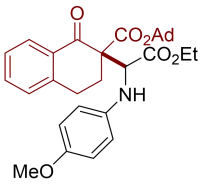
Yellow oil (96 mg, 90% yield); 90:10 *dr*. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 (s, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.37–7.35 (m, 1H), 6.81–6.71 (m, 4H), 4.95 (s, 1H), 3.80–3.64 (m, 4H, including 3.72, s, 3H), 3.25 (d, *J* = 17.5 Hz, 1H), 2.37 (s, 3H), 2.14–2.02 (m, 9H), 1.63–1.57 (m, 6H), 1.11 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 200.2 (Cq), 171.8 (Cq), 167.6 (Cq), 153.4 (Cq), 150.2 (Cq), 141.3 (Cq), 140.9 (Cq), 136.4 (CH), 136.0 (Cq), 125.7 (CH), 124.6 (CH), 116.7 (2C, CH), 114.6 (2C, CH), 82.6 (Cq), 65.6 (Cq), 62.6 (CH), 61.4 (CH_2), 55.6 (CH_3), 40.9 (3C, CH_2), 36.0 (3C, CH_2), 33.6 (CH_2), 30.8 (3C, CH), 21.0 (CH_3), 14.0 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{32}H_{38}NO_6$ $[M+H]^+$ 532.2694, found 532.2681.

Optical Rotation: $[\alpha]_D^{25}$ = +38.5 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 96.2:3.8 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 17.9 min, t_{minor} = 23.3 min.





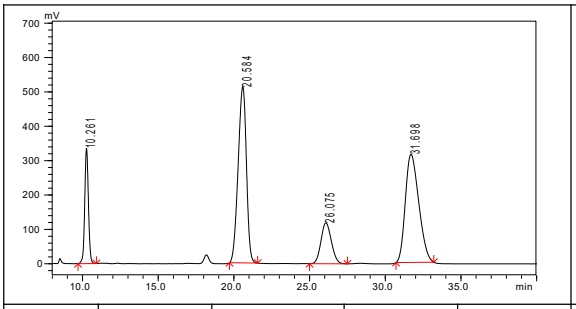
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)	Peak	RetTime (min)	Ara (mV*s)	Height (mV)	Conc. (%)
1	17.981	7200200	248080	28.773	1	17.892	11605629	394695	96.215
2	23.301	7090651	186808	28.335	2	23.298	456539	12237	3.785
3	32.019	5428752	96107	21.694					
4	36.401	5304357	81938	21.197					
Total		6222091	136369	100.000	Total		12062168	406932	100.000

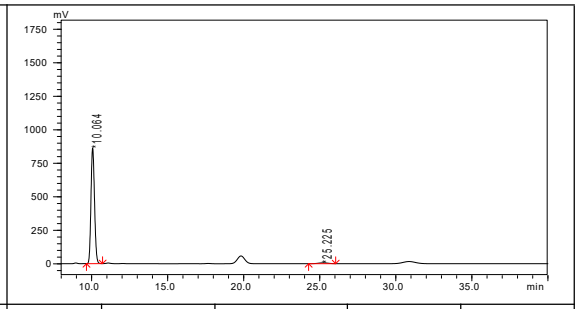


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-1,2,3,4-tetrahydronaphthalene-2-carboxylate (**3ea**)

Yellow oil (101 mg, 95% yield); 88:12 *dr*. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.51–7.42 (m, 1H), 7.33–7.27 (m, 1H), 7.24–7.18 (m, 1H), 6.81–6.62 (m, 4H), 4.38 (s, 1H), 4.25 (q, *J* = 7.2, 7.0 Hz, 2H), 3.74 (s, 3H), 3.18–2.92 (m, 2H), 2.85–2.68 (m, 1H), 2.62–2.46 (m, 1H), 2.16–1.90 (m, 8H), 1.64–1.51 (m, 7H), 1.26 (t, *J* = 7.2, 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.2 (Cq), 172.1 (Cq), 169.7 (Cq), 153.0 (Cq), 142.6 (Cq), 142.5 (Cq), 138.6 (Cq), 133.3 (CH), 128.5 (CH), 127.5 (CH), 126.7 (CH), 115.7 (2C, CH), 114.8 (2C, CH), 82.7 (Cq), 63.7 (Cq), 62.4 (CH), 61.5 (CH_2), 55.7 (CH_3), 41.1 (3C, CH_2), 36.0 (3C, CH_2), 32.4 (CH_2), 30.8 (3C, CH), 26.0 (CH_2), 14.2 (CH_3). **HRMS (ESI)** *m/z*: calcd for $NaC_{32}H_{37}NO_6$ $[M+Na]^+$ 554.2513, found 554.2486.

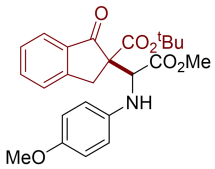
Optical Rotation: $[\alpha]_D^{25}$ = -276.3 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 98.0:2.0 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 85/15, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 10.1 min, t_{minor} = 25.2 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	10.261	5687901	335489	11.315
2	20.584	19516683	513032	38.825
3	26.075	5684746	118813	11.309
4	31.698	19378498	314415	38.550
Total		50267827	1281750	100.000

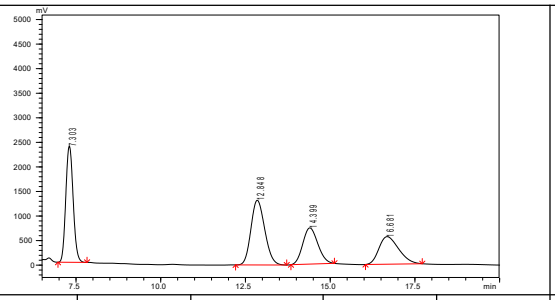
Peak	RetTime (min)	Ara (mV*s)	Height (mV)	Conc. (%)
1	10.064	13982269	864109	98.012
2	25.225	283534	6261	1.988
Total		14265803	870370	100.000

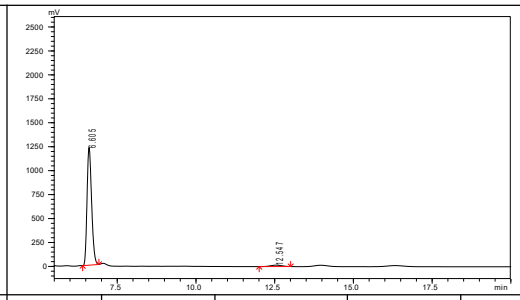


Tert-butyl-2-(2-methoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3fc**)

Pale yellow oil (72.3 mg, 85% yield); 94:6 *dr*. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.6 Hz, 1H), 7.62–7.56 (m, 1H), 7.50–7.46 (m, 1H), 7.37 (d, *J* = 6.8 Hz, 1H), 6.82–6.70 (m, 4H), 5.0 (s, 1H), 3.82–3.76 (m, 1H), 3.72 (s, 1H), [3.61, 3.45] (s, 1H), 3.33 (d, *J* = 17.6, 1H), [1.41, 1.39] (s, 9H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.0 (Cq), 172.4 (Cq), 167.7 (Cq), 153.5 (Cq), 152.8 (Cq), 140.6 (Cq), 135.6 (Cq), 135.2 (CH), 127.7 (CH), 126.1 (CH), 124.7 (CH), 116.7 (2C, CH), 114.6 (2C, CH), 82.7 (Cq), 63.4 (Cq), 62.3 (CH), 55.6 (CH_3), 55.2 (CH_3), 33.7 (CH_2), 27.7 (3C, CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{24}H_{28}NO_6$ $[M+H]^+$ 426.1911, found 426.1920.

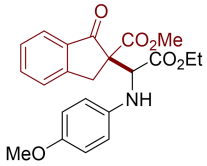
Optical Rotation: $[\alpha]_D^{25}$ = + 25.3 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 97.1:2.9 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 6.6 min, t_{minor} = 12.5 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	7.303	35738285	2365752	30.106
2	12.848	37384493	1316876	31.493
3	14.399	22864996	737071	19.262
4	16.681	22719114	560381	19.139
Total		118706889	4980079	100.000

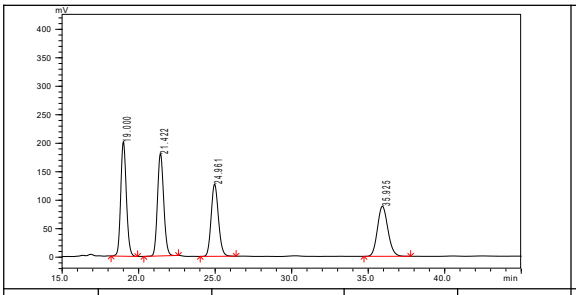
Peak	RetTime (min)	Ara (mV*s)	Height (mV)	Conc. (%)
1	6.605	12480770	1228736	97.078
2	12.547	375714	14716	2.922
Total		12856484	1243452	100.000

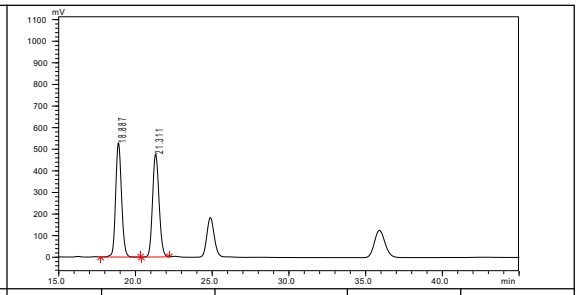


Methyl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3f'a**)

Yellow oil (69.1 mg, 87% yield); 70:30 *dr*. **^{1}H NMR** (500 MHz, $CDCl_3$) δ [7.78 minor, 7.75 major] (d, *J* = 8.0, 7.5 Hz, 1H), 7.63–7.59 (m, 1H), 7.51–7.46 (m, 1H), 7.41–7.35 (m, 1H), 6.87–6.69 (m, 4H), [5.04 major, 5.01 minor] (s, 1H), [4.12–4.04 major, 3.92–3.88 minor] (m, 2H), 3.74 (s, 3H), [3.73 minor, 3.72 major] (s, 3H), [3.33 major, 3.31 minor] (d, *J* = 17.5 Hz, 1H), [1.12 major, 0.89 minor] (t, *J* = 7.5, 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 199.3 (Cq), 171.7 (Cq), 169.3 (Cq), 153.7 (Cq), 152.7 (Cq), 141.0 (Cq), 140.6 (Cq), 135.4 (CH), 127.8 (CH), [126.4 minor, 126.2 major] (CH), [124.9 major, 124.7 minor] (CH), [117.2 major, 116.9 minor] (2C, CH), [114.7 major, 114.6 minor] (2C, CH), [62.9 major, 62.8 minor] (CH), 62.6 (Cq), [61.7 minor, 61.6 major] (CH_2), 55.6 (CH_3), [53.2 minor, 53.1 major] (CH_3), [33.5 minor, 33.4 major] (CH_2), [14.0 major, 13.6 minor] (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{22}H_{24}NO_6$ $[M+H]^+$ 398.1604, found 398.1594.

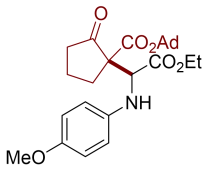
Optical Rotation: n.d. The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 50.2:49.8 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 85/15, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 21.0 min, t_{minor} = 24.7 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	19.000	5161954	201236	27.721
2	21.422	5088019	179656	27.324
3	24.961	4191777	126709	22.511
4	35.925	4179501	87886	22.445
Total		18621251	595486	100.000

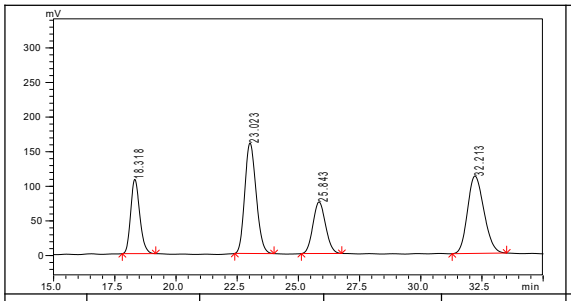
Peak	RetTime (min)	Ara (mV*s)	Height (mV)	Conc. (%)
1	18.887	14166779	528647	50.186
2	21.311	14062023	475438	49.814
Total		28228802	1004085	100.000

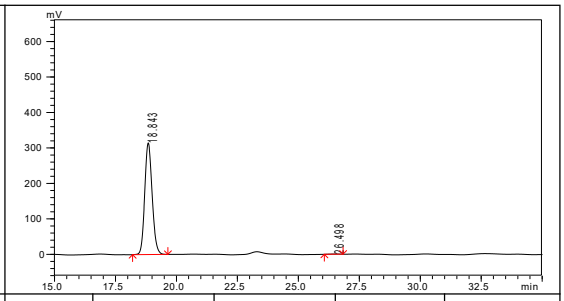


Adamantan-1yl-1-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-2-oxocyclopentane-1-carboxylate (**3ga**)

Yellow oil (73 mg, 78% yield); > 20:1 *dr*. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.81–6.72 (m, 4H), 4.60 (s, 1H), 4.23–4.11 (m, 2H), 3.74 (s, 3H), 2.53–2.40 (m, 2H), 2.30–2.19 (m, 2H), 2.15–2.06 (m, 9H), 2.01–1.95 (m, 2H), 1.66–1.62 (m, 6H), 1.23 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 212.1 (Cq), 171.4 (Cq), 168.4 (Cq), 153.5 (Cq), 141.1 (Cq), 116.7 (CH), 116.3 (CH), 114.7 (2C, CH), 82.9 (Cq), 65.3 (Cq), 61.8 (CH), 61.2 (CH_2), 55.7 (CH_3), 41.1 (3C, CH_2), 37.5 (CH_2), 36.1 (3C, CH_2), 31.4 (CH_2), 30.8 (3C, CH), 19.3 (CH_2), 14.1 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{27}H_{36}NO_6$ $[M+H]^+$ 470.2537, found 470.2553.

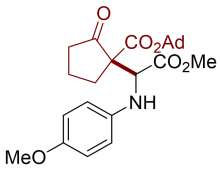
Optical Rotation: $[\alpha]_D^{25}$ = +41.7 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 99.8:0.2 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 18.8 min, t_{minor} = 26.5 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	18.318	2766451	107293	17.490
2	23.023	5163497	159537	32.645
3	25.843	2675785	74433	16.917
4	32.213	5211278	111873	32.947
Total		15817012	453137	100.000

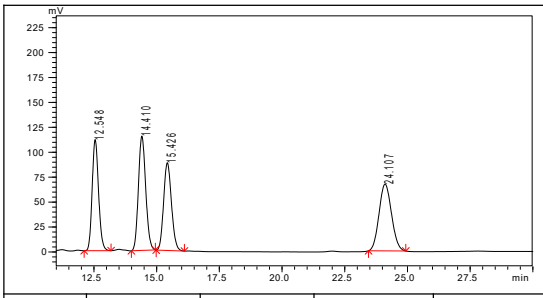
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	18.843	6662447	314743	99.797
2	26.498	13574	471	0.203
Total		6676021	315214	100.000

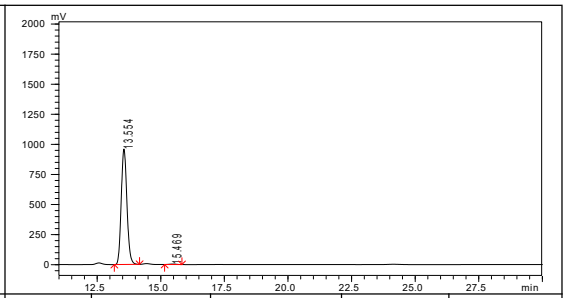


Adamantan-1-yl-1-(2-methoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-2-oxocyclopentane-1-carboxylate (**3gc**)

Yellow oil (76 mg, 83% yield); > 20:1 *dr* (95:5 *dr*, **from aging**). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.76 (brs, 4H), 4.65 (s, 1H), 3.74 (s, 3H), 3.65 (s, 3H), 2.50–2.39 (m, 2H), 2.28–2.23 (m, 2H), 2.20–2.05 (m, 9H), 1.94–1.79 (m, 2H), 1.67–1.60 (m, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 213.0 (Cq), 172.2 (Cq), 168.0 (Cq), 153.5 (Cq), 140.6 (), 116.6 (2C, CH), 114.7 (2C, CH), 82.8 (Cq), 62.9 (Cq), 62.1 (CH), 55.7 (CH_3), 52.2 (CH_3), 41.0 (3C, CH), 38.1 (CH_2), 36.0 (3C, CH), 30.8 (3C, CH), 27.5 (CH_2), 19.8 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{26}H_{34}NO_6$ $[M+H]^+$ 456.2381, found 456.2394.

Optical Rotation: $[\alpha]_D^{25}$ = +25.5 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 99.5:0.5 *er* (95.6:4.4 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 13.6 min, t_{minor} = 15.5 min; (t_{major} = 12.6 min, t_{minor} = 15.5 min, **from aging**).

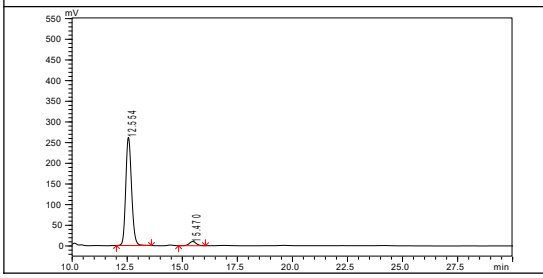




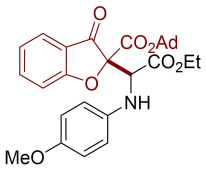
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	12.548	1978393	111406	23.181
2	14.410	2326210	114729	27.257
3	15.426	1914705	88029	22.435
4	24.107	2315087	66938	27.127
Total		8534396	381103	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	13.554	14974891	959339	99.506
2	15.469	74317	3858	0.494
Total		15049208	963198	100.000

From aging



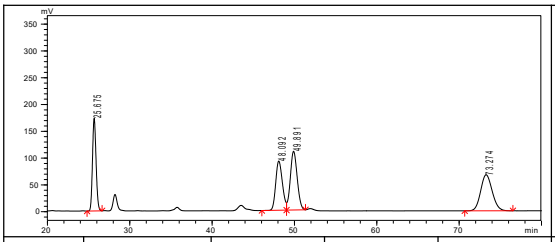
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	12.554	4779517	261480	95.583
2	15.470	220865	10140	4.417
Total		5000383	271619	100.000

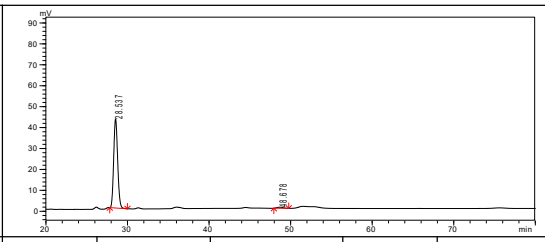


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3ha**)

Pale yellow oil (88.3 mg, 85% yield); >20:1*dr* (93:7 *dr*, **from aging**). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.66–7.59 (m, 1H), 7.25–7.19 (m, 1H), 7.17–7.09 (m, 1H), 6.89–6.74 (m, 4H), 5.06 (s, 1H), 4.32 (brs, 1H), 3.91–3.78 (m, 2H), 3.75 (s, 3H), 2.15–2.00 (m, 9H), 1.63–1.51 (m, 6H), 0.74 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.2 (Cq), 171.6 (Cq), 168.7 (Cq), 161.8 (Cq), 153.6 (Cq), 140.7 (Cq), 138.1 (CH), 124.8 (CH), 122.8 (CH), 120.3 (Cq), 116.7 (2C, CH), 114.6 (2C, CH), 113.4 (CH), 93.0 (Cq), 84.6 (Cq), 62.3 (CH), 61.7 (CH_2), 55.6 (CH_3), 40.8 (3C, CH_2), 35.9 (3C, CH_2), 30.9 (3C, CH), 13.4 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{30}H_{34}NO_7$ $[M+H]^+$ 520.2335, found 520.2332.

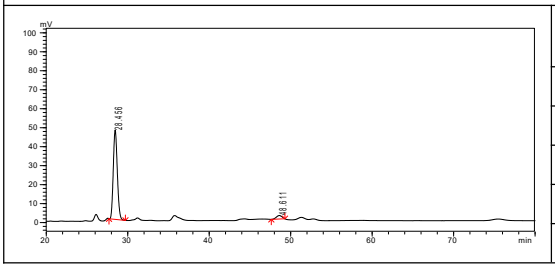
Optical Rotation: $[\alpha]_D^{25}$ = + 63.5 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 98.2: 1.8 *er* (94.8:5.2 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{major} = 28.5 min, t_{minor} = 48.7 min; (t_{major} = 28.5 min, t_{minor} = 48.6 min, **from aging**).



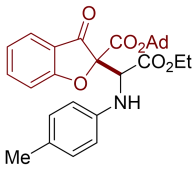


Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)	Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	28.537	1441087	42595	95.074	1	28.537	1441087	42595	98.190
2	48.678	26563	508	1.752	2	48.678	26563	508	1.810
3	51.541	29397	470	1.939					
4	75.593	18713	225	1.235					
Total		1515760	43798	100.000	Total		1467650	43103	100.000

From aging



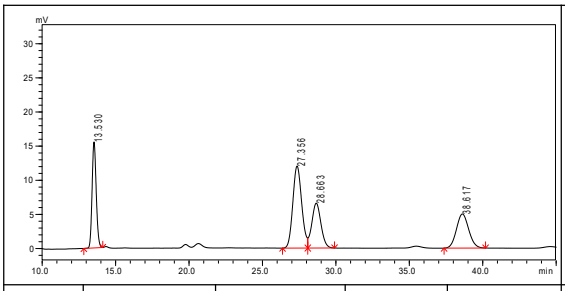
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	28.456	1618769	47032	94.797
2	48.611	88840	1844	5.203
Total		1707609	48876	100.000

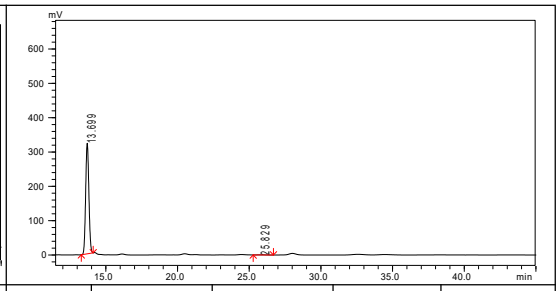


Adamantan-1-yl-2-((S)-2-ethoxy-2-oxo-1-(p-tolylamino)ethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3hb**)

Pale yellow oil (70.5 mg, 70% yield); > 20:1 *dr*. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.8 Hz, 1H), 7.65–7.62 (m, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.16–7.12 (m, 1H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.0 Hz, 2H), 5.14 (s, 1H), 3.89–3.78 (m, 2H), 2.26 (s, 3H), 2.11–1.98 (m, 9H), 1.61–1.54 (m, 6H), 0.76 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.2 (Cq), 171.6 (Cq), 168.6 (Cq), 161.8 (Cq), 144.4 (Cq), 138.1 (CH), 129.7 (2C, CH), 129.1 (Cq), 124.8 (CH), 122.9 (CH), 120.4 (Cq), 115.3 (2C, CH), 113.4 (CH), 93.0 (Cq), 84.7 (Cq), 61.7 (CH), 61.5 (CH_2), 40.8 (3C, CH_2), 35.9 (3C, CH_2), 30.9 (3C, CH), 20.5 (CH_3), 13.4 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{30}H_{34}NO_6$ $[M+H]^+$ 504.2386, found 504.2375.

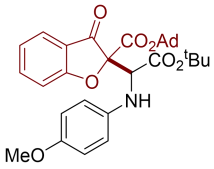
Optical Rotation: $[\alpha]_D^{25}$ = + 40.7 (c = 1.0, CH_2Cl_2). The ee value was determined by **HPLC analysis** (only the major stereoisomers were considered) 99.8:0.2 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{major} = 13.7 min, t_{minor} = 25.8 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	13.530	483798	15522	30.933
2	27.356	505792	12015	32.339
3	28.663	284841	6579	18.212
4	38.617	289591	4996	18.516
Total		1564022	39112	100.000

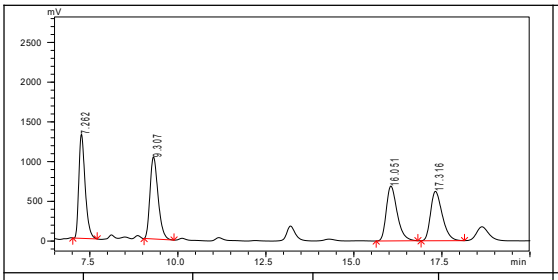
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	13.699	5013378	321757	99.765
2	25.829	11808	341	0.235
Total		5025186	322098	100.000

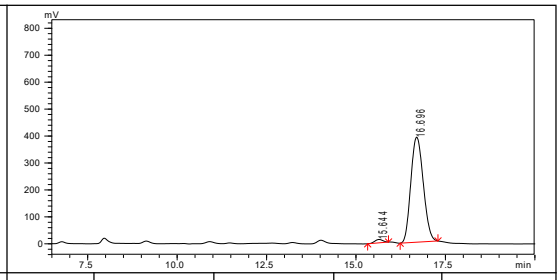


Adamantan-1-yl-2-((S)-2-(tert-butoxy)-1-((4-methoxyphenyl)amino)-2-oxoethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3he**)

Yellow oil (88.7 mg, 81% yield); > 20:1 *dr*. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.6 Hz, 1H), 7.66–7.62 (m, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 7.17–7.12 (m, 1H), 6.90–6.73 (m, 4H), 4.97 (s, 1H), 3.76 (s, 3H), 2.17–2.02 (m, 9H), 1.65–1.56 (m, 6H), 1.0 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.2 (Cq), 171.8 (Cq), 167.4 (Cq), 161.9 (Cq), 153.5 (Cq), 141.0 (Cq), 138.1 (CH), 124.9 (CH), 122.8 (CH), 120.6 (Cq), 116.6 (2C, CH), 114.6 (2C, CH), 113.5 (CH), 93.5 (Cq), 84.6 (Cq), 83.4 (Cq), 62.6 (CH), 55.7 (CH_3), 40.8 (3C, CH_2), 35.9 (3C, CH_2), 30.9 (3C, CH), 27.3 (3C, CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{32}H_{38}NO_7$ $[M+H]^+$ 548.2643, found 548.2635.

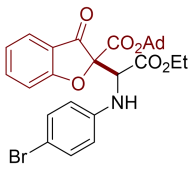
Optical Rotation: $[\alpha]_D^{25}$ = + 101.3 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 98.0:2.0 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{major} = 16.7 min, t_{minor} = 15.6 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	7.262	16373637	1308417	26.382
2	9.307	16491209	1034438	26.572
3	16.051	14857068	690508	23.939
4	17.316	14341238	621131	23.107
Total		62063152	3654494	100.000

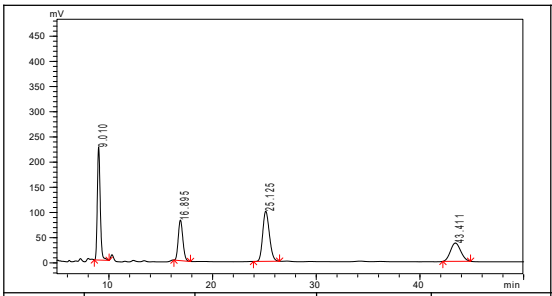
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	15.644	197012	12462	2.044
2	16.696	9440637	389912	97.956
Total		9637649	402373	100.000

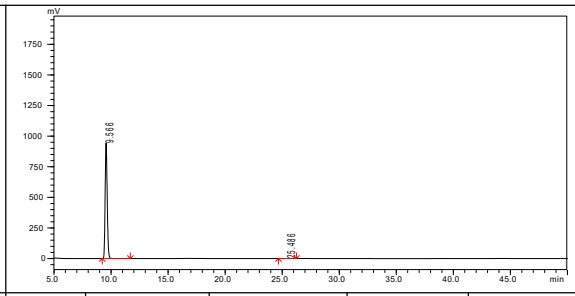


Adamantan-1-yl 2-(1-((4-bromophenyl)amino)-2-ethoxy-2-oxoethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3hg**)

Pale yellow oil (83.0 mg, 73% yield); > 20:1 *dr* (92:8 *dr*, **from aging**). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.8 Hz, 1H), 7.68–7.65 (m, 1H), 7.34 (d, *J* = 9.0 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.20–7.15 (m, 1H), 6.77 (d, *J* = 9.0 Hz, 2H), 5.16 (s, 1H), 3.94–3.84 (m, 2H), 2.17–1.97 (m, 9H), 1.63–1.57 (m, 6H), 0.80 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.0 (Cq), 171.6 (Cq), 168.2 (Cq), 161.7 (Cq), 145.8 (Cq), 138.3 (CH), 132.0 (2C, CH), 124.9 (CH), 123.0 (CH), 120.3 (Cq), 116.5 (2C, CH), 113.4 (CH), 111.6 (Cq), 92.6 (Cq), 85.0 (Cq), 62.0 (CH), 60.8 (CH_2), 40.8 (3C, CH_2), 35.9 (3C, CH_2), 30.9 (3C, CH), 13.4 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{29}H_{31}{}^{79}BrNO_6$ $[M+H]^+$ 568.1335, found 568.1349.

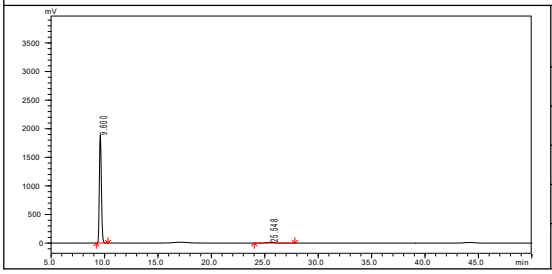
Optical Rotation: $[\alpha]_D^{25}$ = + 32.1 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 99.7:0.3 *er* (97.5:2.5 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{major} = 9.6 min, t_{minor} = 25.5 min (t_{major} = 9.6 min, t_{minor} = 25.5 min, **from aging**).



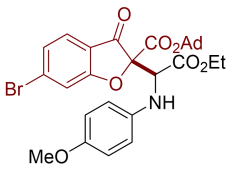


Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)	Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	9.010	4374490	224559	31.717	1	9.566	11970771	942852	99.738
2	16.895	2470747	80578	17.914					
3	25.125	4446080	99432	32.236	2	25.486	31419	734	0.262
4	43.411	2500783	36334	18.132					
Total		13792101	440902	100.000	Total		12002190	943586	100.000

From aging



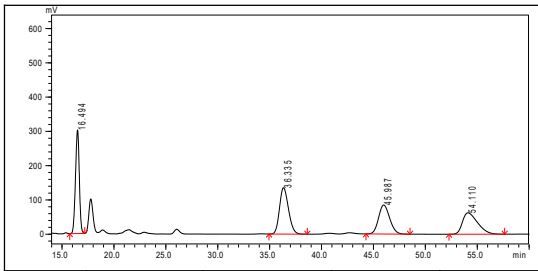
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	9.600	25197027	1889025	97.491
2	25.548	648354	12934	2.509
Total		25845381	1901959	100.000

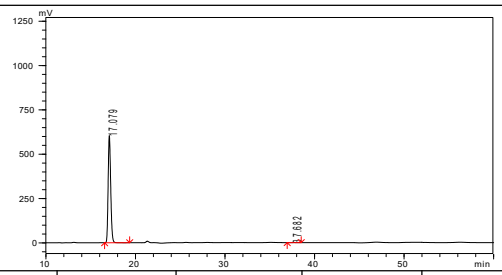


Adamantan-1-yl-6-bromo-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3ia**)

Yellow oil (95.8 mg, 80% yield); >20:1 *dr* (86:14 *dr*, **from aging**). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.14 (d, *J* = 8.8 Hz, 1H), 6.90–6.71 (m, 4H), 5.06 (s, 1H), 3.94–3.82 (m, 2H), 3.76 (s, 3H), 2.14–2.00 (m, 9H), 1.66–1.53 (m, 6H), 0.83 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.8 (Cq), 170.3 (Cq), 168.7 (Cq), 161.3 (Cq), 153.7 (Cq), 141.7 (Cq), 127.3 (CH), 122.2 (Cq), 117.5 (CH), 116.7 (2C, CH), 115.5 (Cq), 115.1 (CH), 114.6 (2C, CH), 93.8 (Cq), 85.1 (Cq), 62.4 (CH), 61.9 (CH_2), 55.7 (CH_3), 40.8 (3C, CH_2), 36.0 (3C, CH_2), 30.9 (3C, CH), 13.6 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{30}H_{33}{}^{79}BrNO_7$ $[M+H]^+$ 598.1435, found 598.1436.

Optical Rotation: $[\alpha]_D^{25}$ = + 31.2 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 99.9:0.1 *er* (96.7:3.3 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 210 nm, retention time: t_{major} = 17.1 min, t_{minor} = 37.7 min (t_{major} = 17.1 min, t_{minor} = 38.7 min, **from aging**).

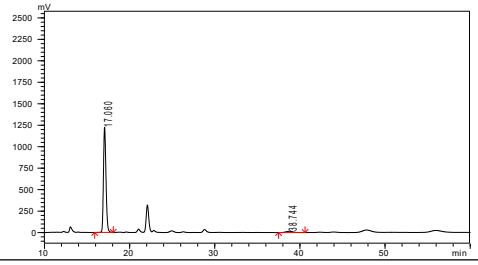




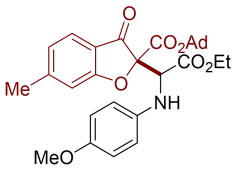
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	16.494	7772692	302504	27.283
2	36.335	8139863	135321	28.572
3	45.987	6288178	84545	22.072
4	54.110	6288021	62343	22.072
Total		21920392	456492	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.079	12031083	604344	99.934
2	37.682	7894	164	0.066
Total		12038977	604508	100.000

From aging



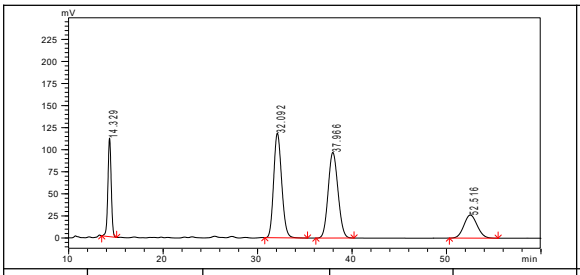
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.060	25310350	1224980	96.669
2	38.744	872095	15169	3.331
Total		26182445	1240149	100.000

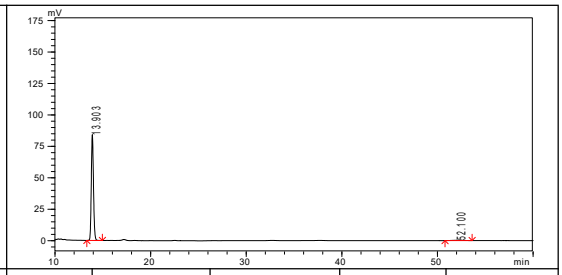


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-6-methyl-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3ja**)

Pale yellow oil (95.0 mg, 89% yield); >20:1 *dr* (92:8 *dr*, **from aging**). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.9 Hz, 1H), 7.02 (s, 1H), 6.94 (d, *J* = 7.9 Hz, 1H), 6.87–6.75 (m, 4H), 5.05 (s, 1H), 3.90–3.79 (m, 2H), 3.76 (s, 3H), 2.44 (s, 3H), 2.17–2.03 (m, 9H), 1.66–1.56 (m, 6H), 0.78 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.5 (Cq), 172.2 (Cq), 168.8 (Cq), 162.0 (Cq), 153.6 (Cq), 140.7 (Cq), 124.4 (2C, CH), 117.4 (Cq), 116.8 (2C, CH), 114.6 (2C, CH), 113.4 (CH), 93.3 (Cq), 84.6 (Cq), 62.2 (CH), 61.7 (CH_2), 55.7 (CH_3), 40.8 (3C, CH_2), 35.9 (3C, CH_2), 30.9 (3C, CH), 22.6 (CH_3), 13.6 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{31}H_{36}NO_7$ $[M+H]^+$ 534.2492, found 534.2482.

Optical Rotation: $[\alpha]_D^{25}$ = + 39.8 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 98.3:1.7 *er* (96.9:3.1 *er*, **from aging**), Chiralcel AD-H colum, hexane/*i*-PrOH = 85/15, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{major} = 13.9 min, t_{minor} = 52.1 min; (t_{major} = 14.0 min, t_{minor} = 52.9 min, **from aging**).

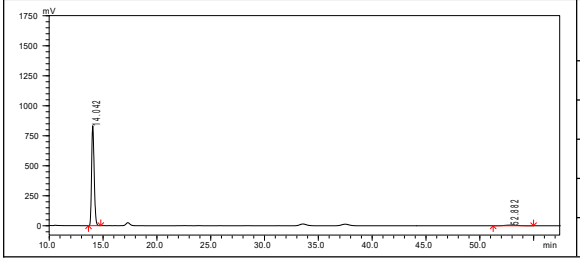




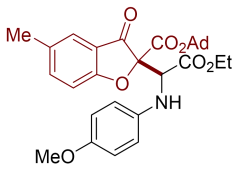
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	14.329	2730537	111687	14.157
2	32.092	6979589	118522	36.186
3	37.966	7016629	97040	36.378
4	52.516	2561311	26210	13.279
Total		19288067	353457	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	13.903	1331872	84150	98.323
2	52.100	22722	275	1.677
Total		1354595	84425	100.000

From aging



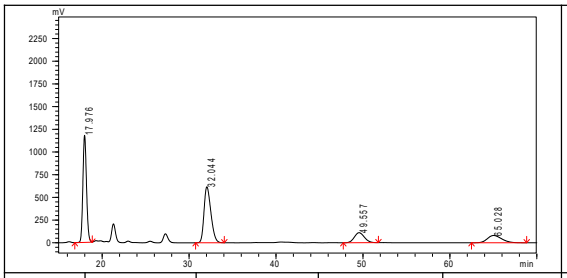
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	14.042	13902359	832880	96.859
2	52.882	450809	5789	3.141
Total		14353167	838669	100.000

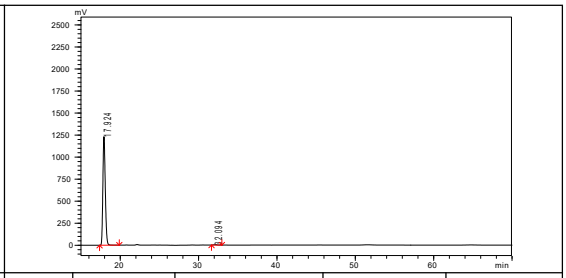


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-5-methyl-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3ka**)

Yellow oil (96.1 mg, 90% yield); >20:1 *dr*. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46–7.40 (m, 2H, including s, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 6.83–6.76 (m, 4H), 5.04 (s, 1H), 3.88–3.76 (m, 2H), 3.74 (s, 3H), 2.34 (s, 3H), 2.13–1.99 (m, 9H), 1.65–1.54 (m, 6H), 0.76 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.2 (Cq), 170.1 (Cq), 168.7 (Cq), 161.9 (Cq), 153.5 (Cq), 140.7 (Cq), 139.4 (CH), 132.6 (Cq), 124.1 (CH), 120.2 (Cq), 116.7 (2C, CH), 114.6 (2C, CH), 112.9 (CH), 93.2 (Cq), 84.5 (Cq), 62.3 (CH), 61.7 (CH_2), 55.6 (CH_3), 40.7 (3C, CH_2), 35.9 (3C, CH_2), 30.8 (3C, CH), 20.6 (CH_3), 13.4 (CH_3). **HRMS (ESI)** *m/z*: calcd for $C_{31}H_{36}NO_7$ $[M+H]^+$ 534.2492, found 534.2508.

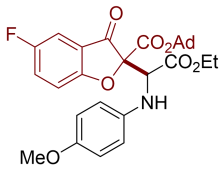
Optical Rotation: $[\alpha]_D^{25}$ = + 41.2 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 99.5:0.5 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{major} = 17.9 min, t_{minor} = 32.1 min.





Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.976	34194662	1180128	39.714
2	32.044	33903344	616602	39.376
3	49.557	8891665	110318	10.327
4	65.028	9112871	80140	10.584
Total		86102541	1987188	100.000

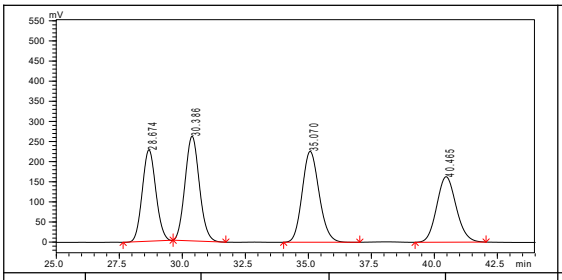
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	17.924	26508925	1231841	99.539
2	32.094	122798	3879	0.461
Total		26631723	1235720	100.000

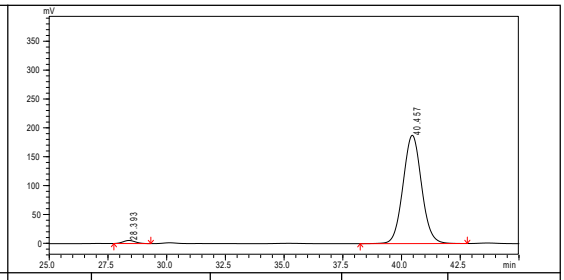


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-5-fluoro-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3la**)

Pale yellow solid (89.2 mg, 83% yield); >20:1 *dr*. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.34 (d, *J* = 1.6 Hz, 1H), 7.26–7.18 (m, 2H), 6.82–6.71 (m, 4H), 5.07 (s, 1H), 4.29–4.19 (m, 2H), 3.72 (s, 3H), 2.18–2.10 (m, 9H), 1.67–1.61 (m, 6H), 1.26 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.1 (Cq), 169.7 (Cq), 168.6 (Cq), 161.7 (Cq), 158.1 (d, J_1 = 243.0 Hz, Cq), 154.1 (Cq), 140.5 (Cq), 125.7 (d, J_2 = 25.5 Hz, CH), 120.7 (d, J_3 = 7.5 Hz, Cq), 117.5 (2C, CH), 114.6 (2C, CH), 114.3 (d, J_3 = 7.5 Hz, CH), 110.1 (d, J_2 = 24.0 Hz, CH), 93.5 (Cq), 84.4 (Cq), 63.2 (CH), 62.3 (CH_2), 55.6 (CH_3), 41.0 (3C, CH_2), 36.0 (3C, CH_2), 30.9 (3C, CH), 14.2 (CH_3). **^{19}F NMR** (564 MHz, $CDCl_3$) δ -120.0. **HRMS (ESI)** *m/z*: calcd for $C_{30}H_{33}{}^{19}FNO_7$ $[M+H]^+$ 538.2241, found 538.2261.

Optical Rotation: $[\alpha]_D^{25}$ = + 25.3 (c = 1.0, CH_2Cl_2). The *ee* value was determined by **HPLC analysis** (only the major stereoisomers were considered) 98.2:1.8 *er*, Chiralcel AD-H colum, hexane/*i*-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_{major} = 40.5 min, t_{minor} = 28.4 min.





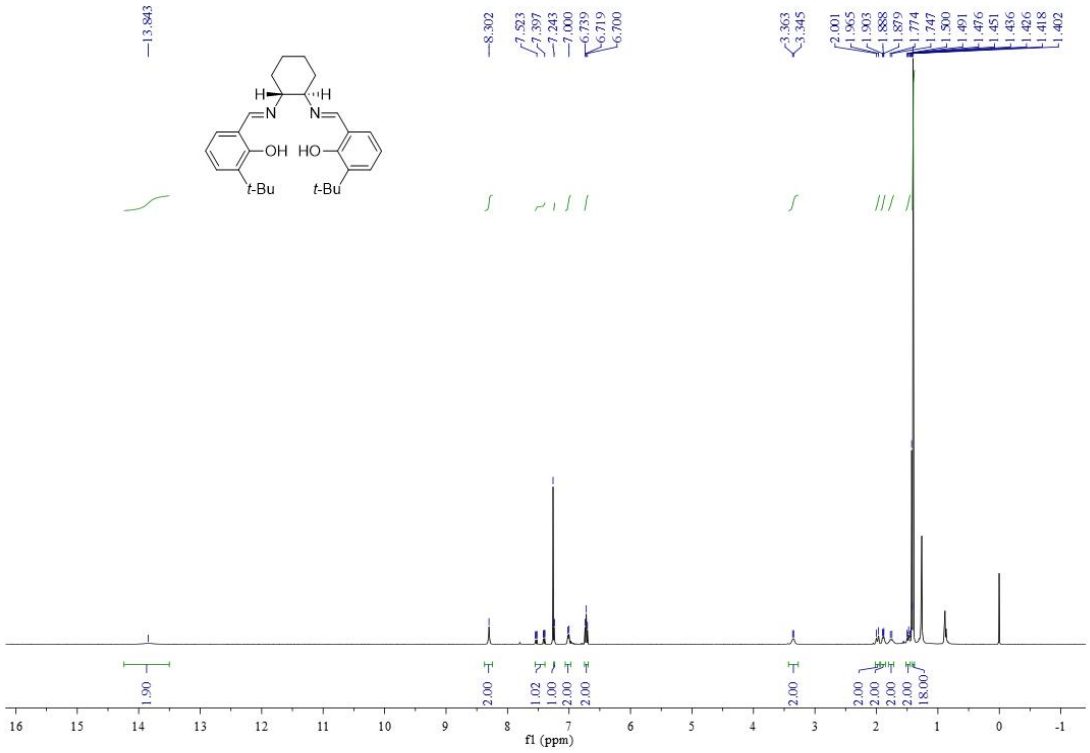
Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	28.674	8486033	227101	22.259
2	30.386	10298564	260044	27.013
3	35.070	10586250	225773	27.768
4	40.465	8753643	162664	22.961
Total		38124490	875582	100.000

Peak	RetTime (min)	Area (mV*s)	Height (mV)	Conc. (%)
1	28.393	193017	5334	1.846
2	40.457	10262870	187395	98.154
Total		23161445	426254	100.000

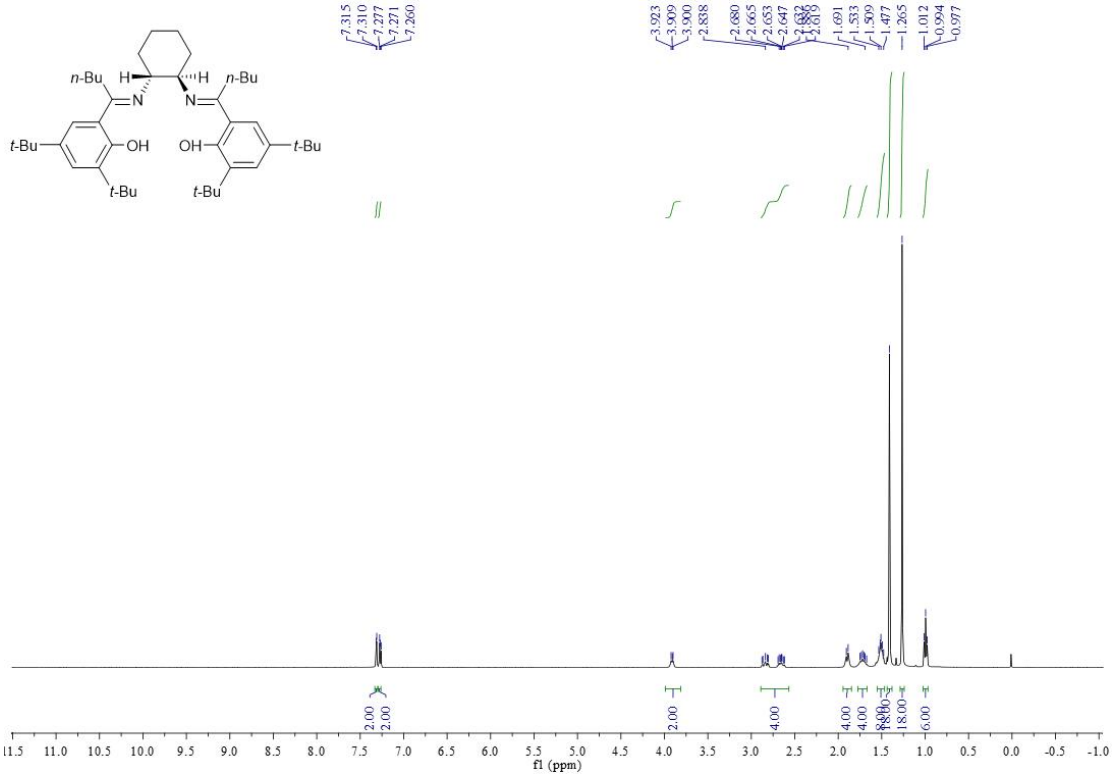
8. NMR spectra

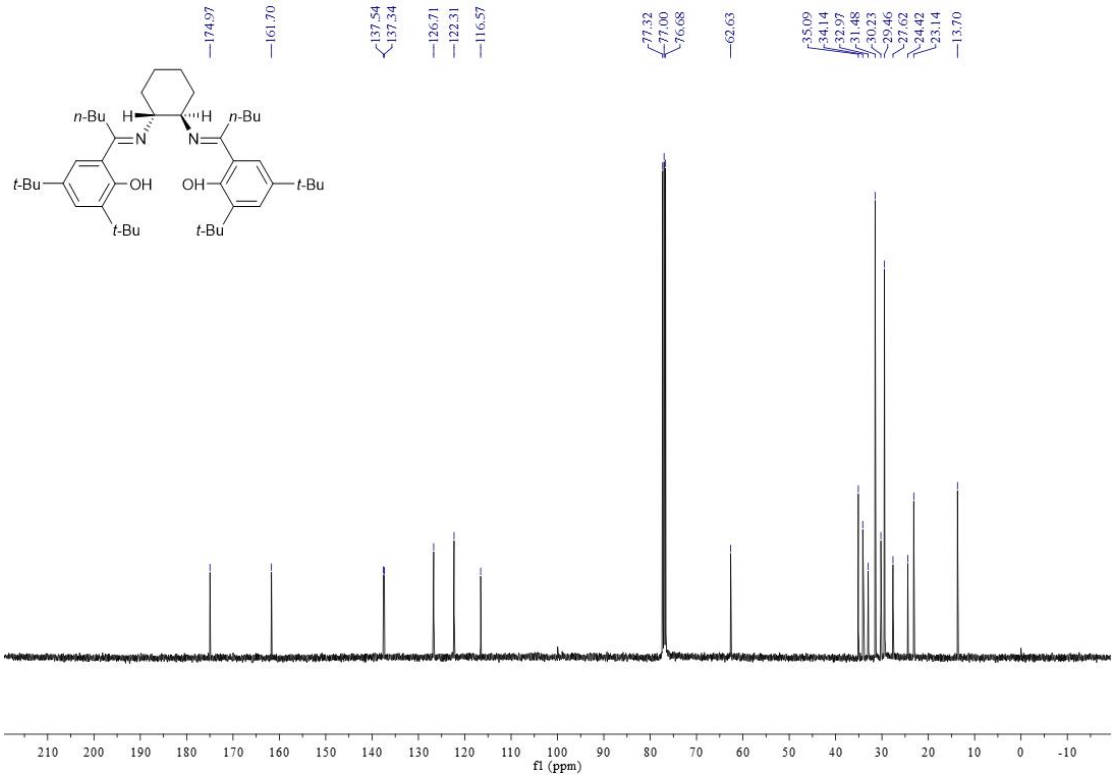
8.1 Ligands

6,6'-((1E,1'E)-(((1R,2R)-cyclohexane-1,2-diyl)bis(azanylylidene))bis(methanylylidene))bis(2-(tert-butyl)phenol) (**L9**)

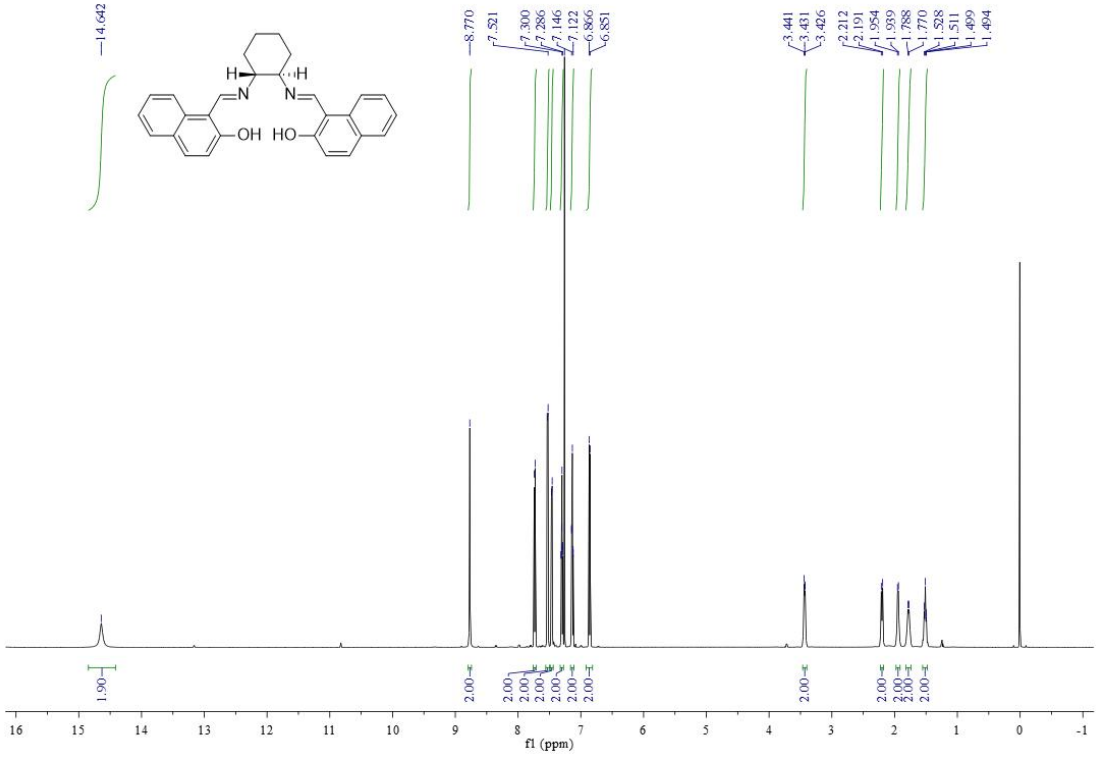


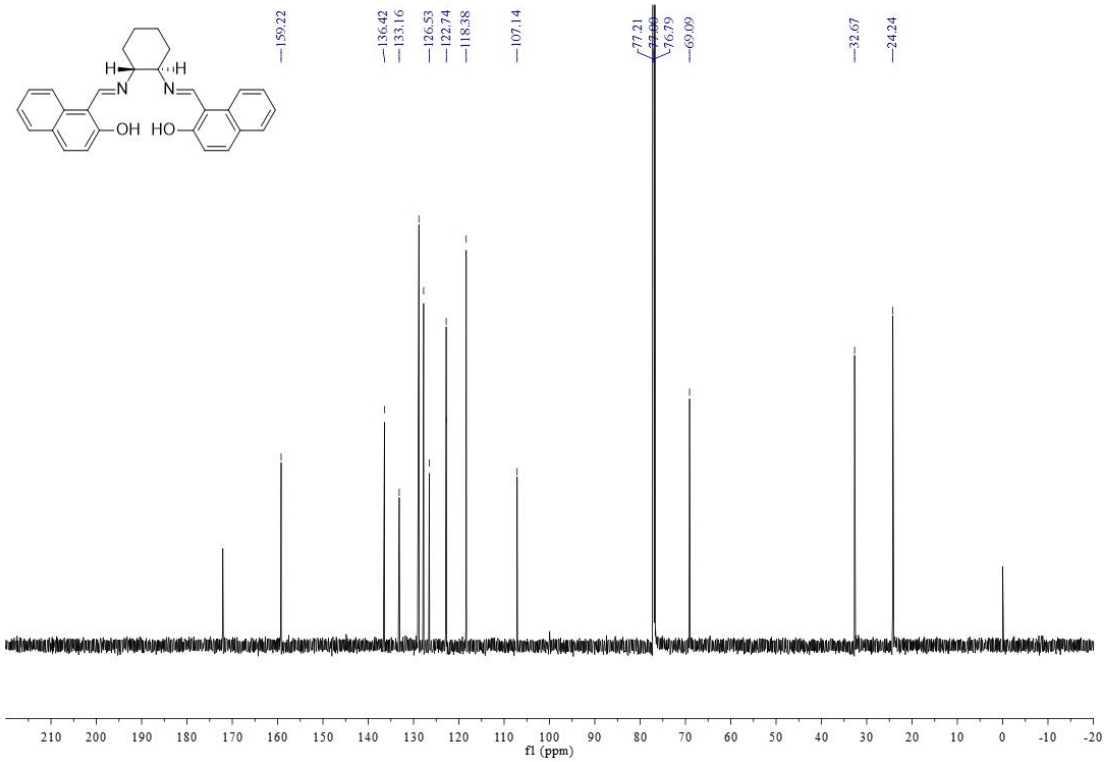
6,6'-((1E,1'E)-(((1R,2R)-cyclohexane-1,2-diyl)bis(azanylylidene))bis(2,2-dimethylpropan-1-yl-1-ylidene))bis(2,4-di-tert-butylphenol) (**L13**)



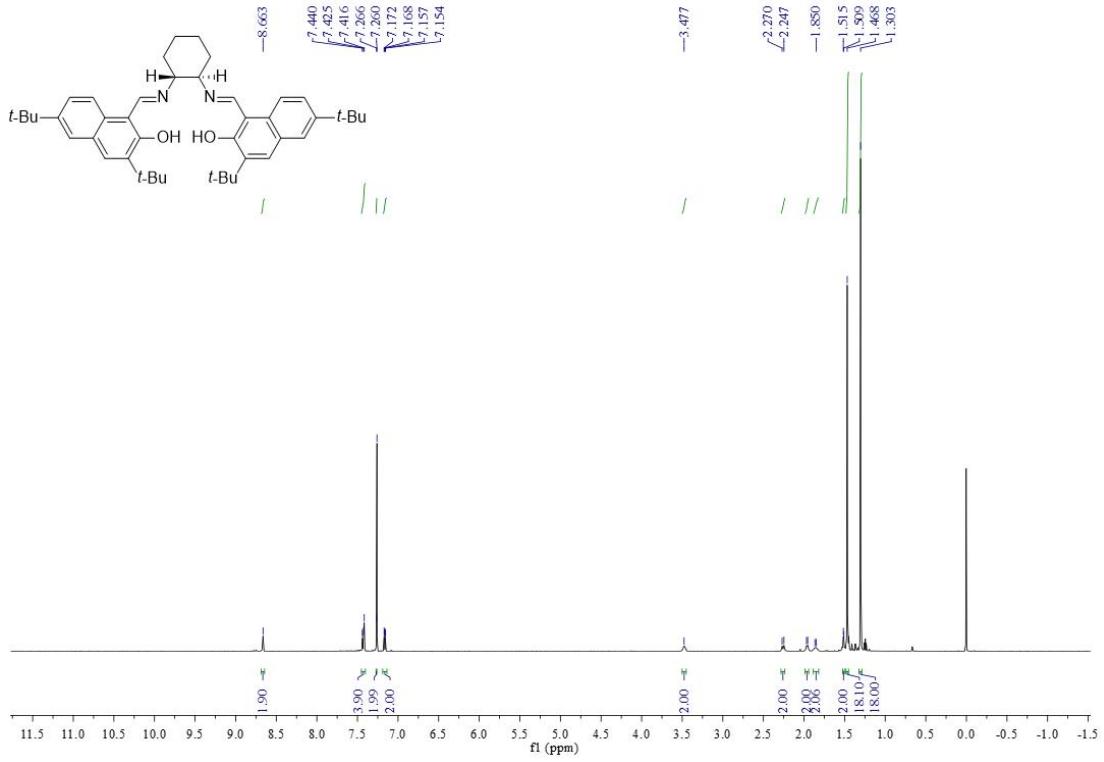


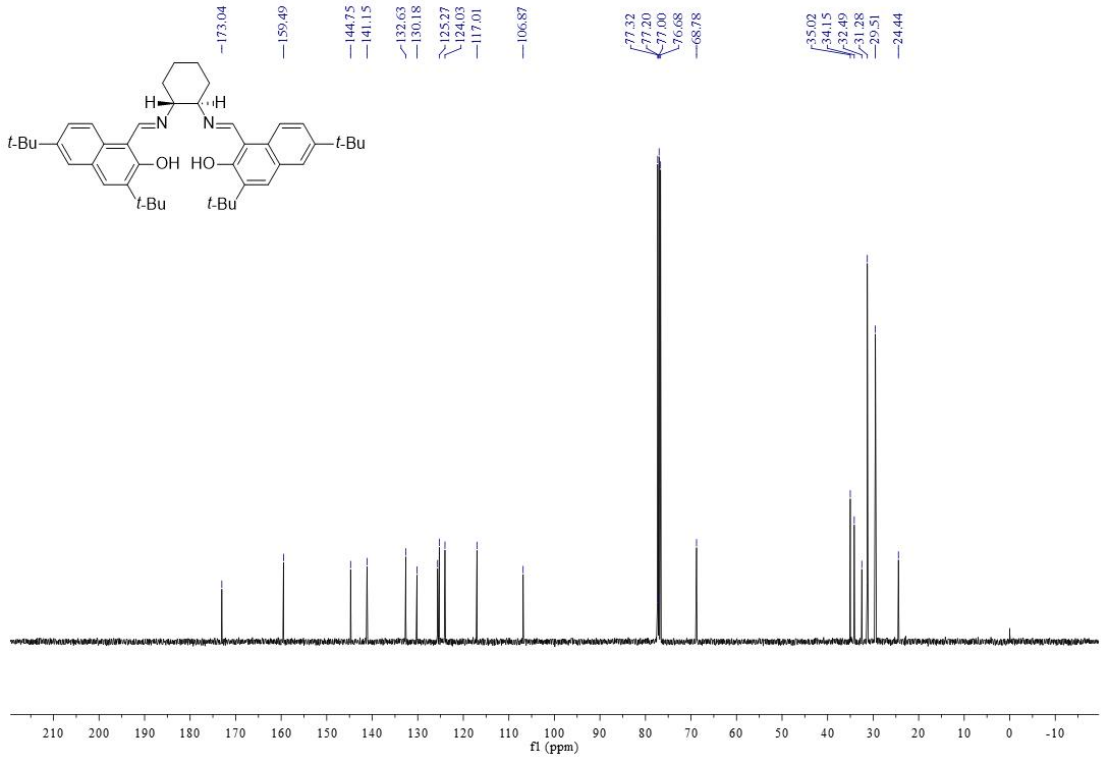
(1R,2R)-cyclohexane-1,2-diyl-bis(azanylylidene)-bis(methanylylidene)-bis(naphthalen-2-ol) (**L14**)



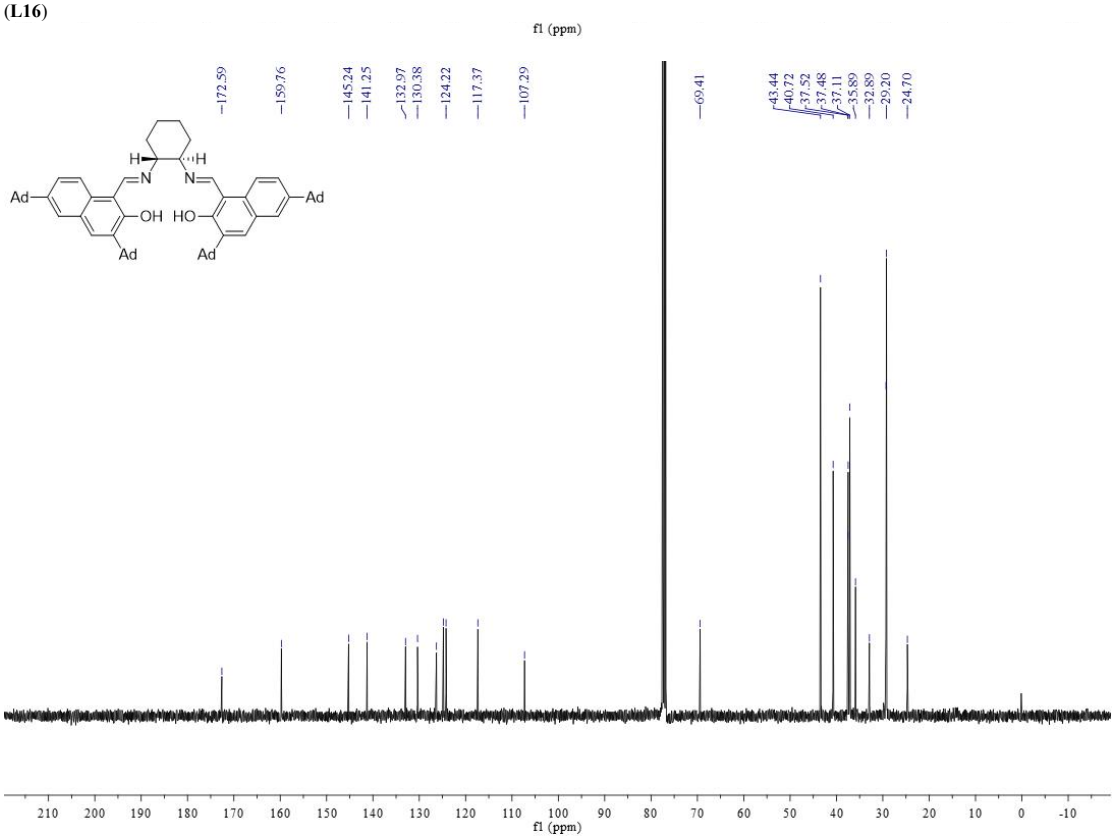


3,6-di-tert-butyl-1-(1R,2R)-2-((6-(tert-butyl)-2-hydroxy-3-methylnaphthalen-1-yl)methylene) amino)cyclohexyl) imino) methyl)naphthalen-2-ol (**L15**)



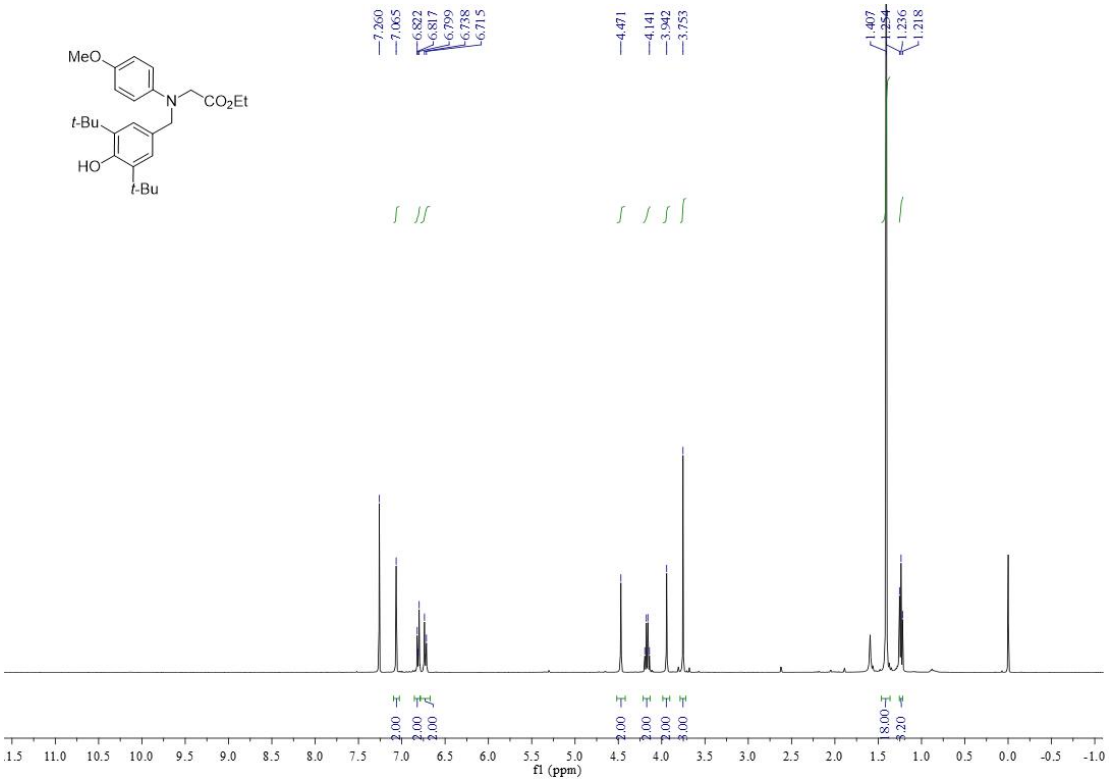


3,6-di-adamantyl-1-(1R,2R)-2-((6-(adamantyl)-2-hydroxy-3-methylnaphthalen-1-yl)methylene) amino)cyclohexyl) imino) methyl)naphthalen-2-ol (**L16**)



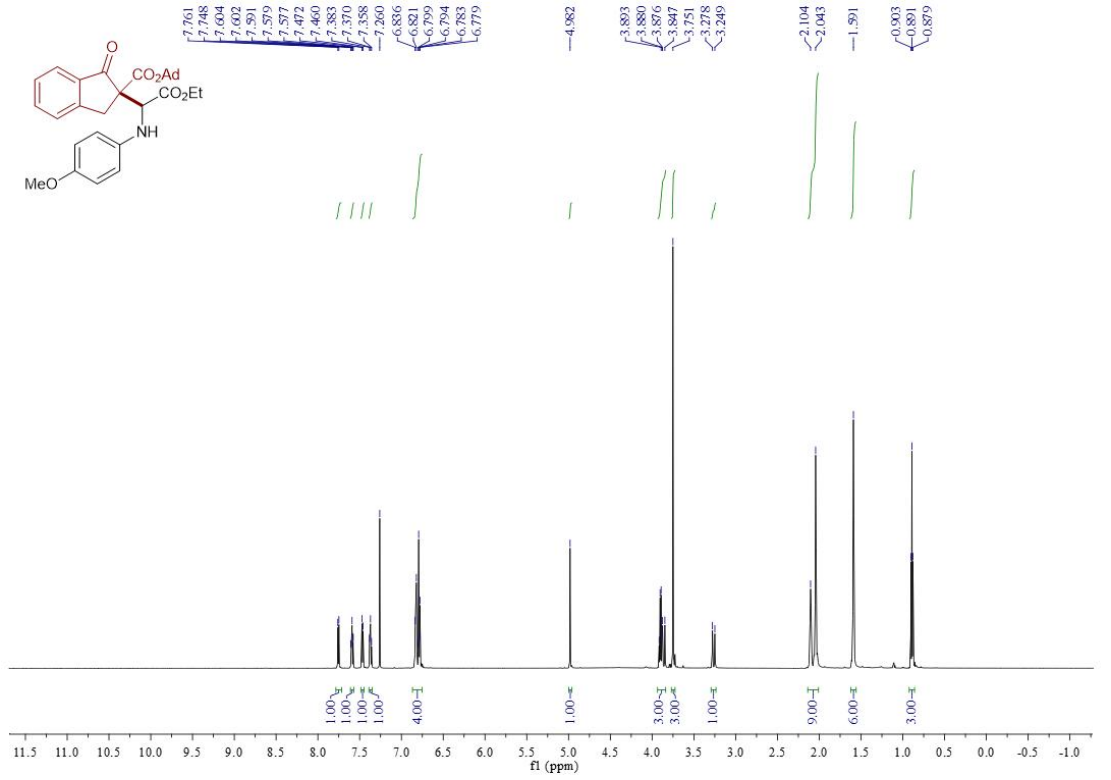
8.2 Radical trapping product

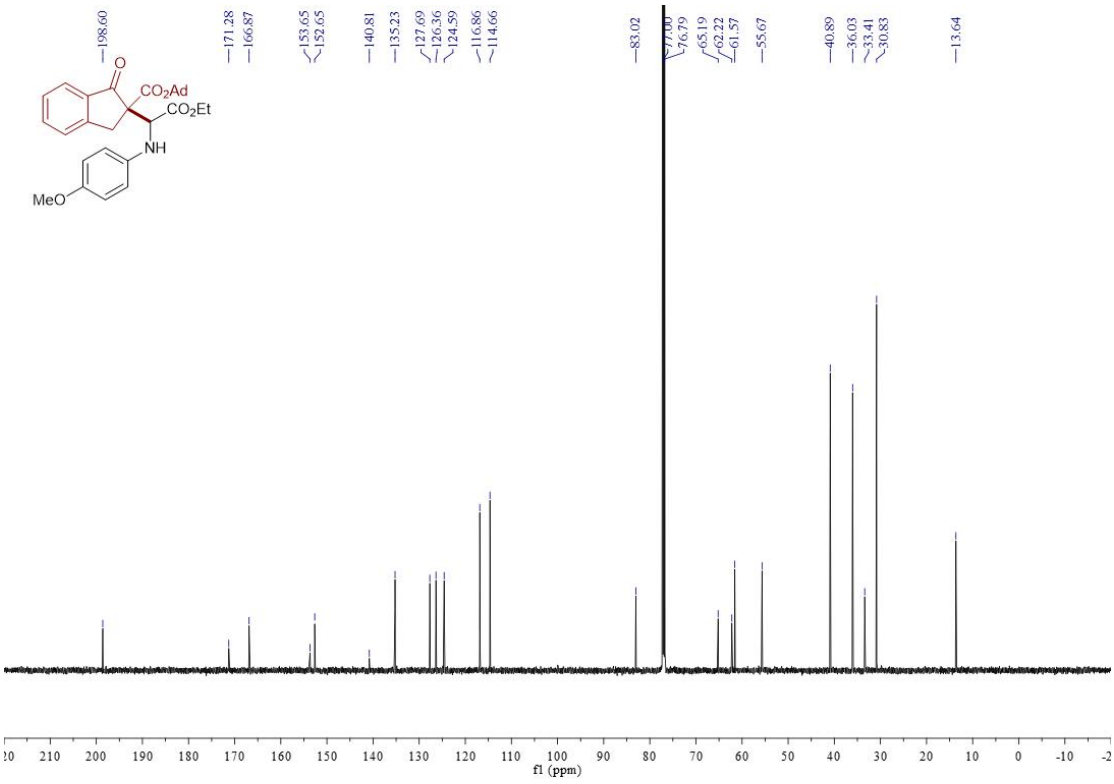
ethyl N-(3,5-di-tert-butyl-4-hydroxybenzyl)-N-(4-methoxyphenyl)glycinate (**2a-BHT**)



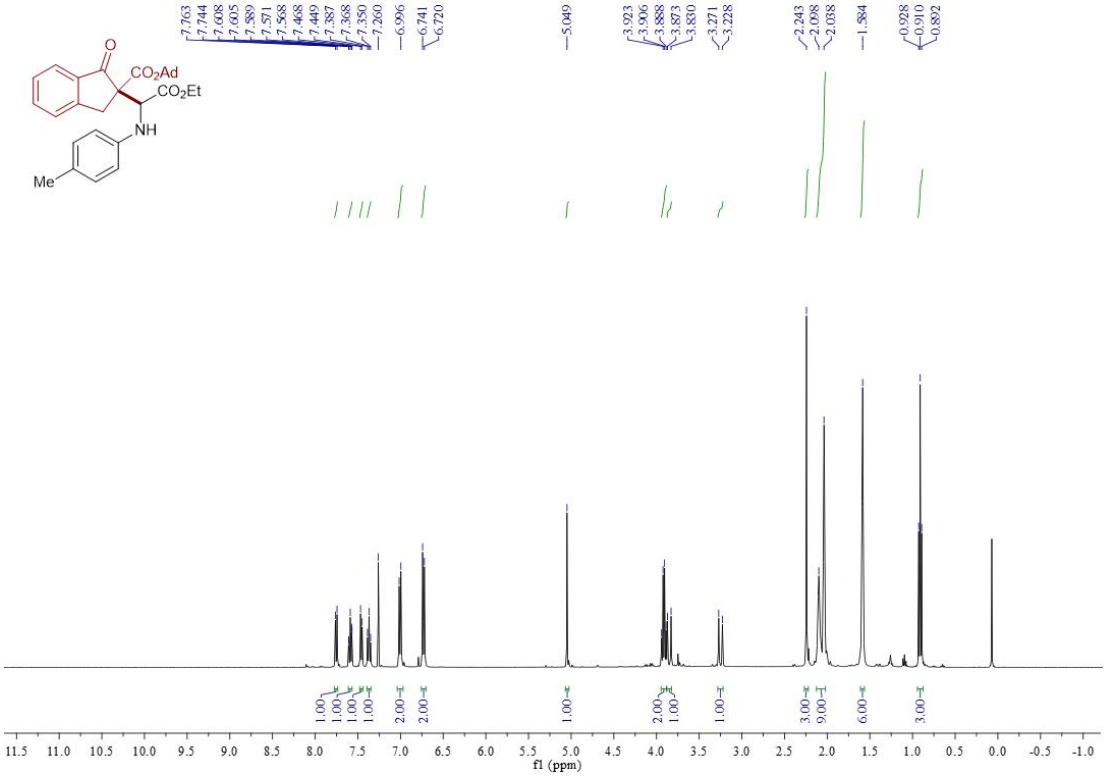
8.3 Products

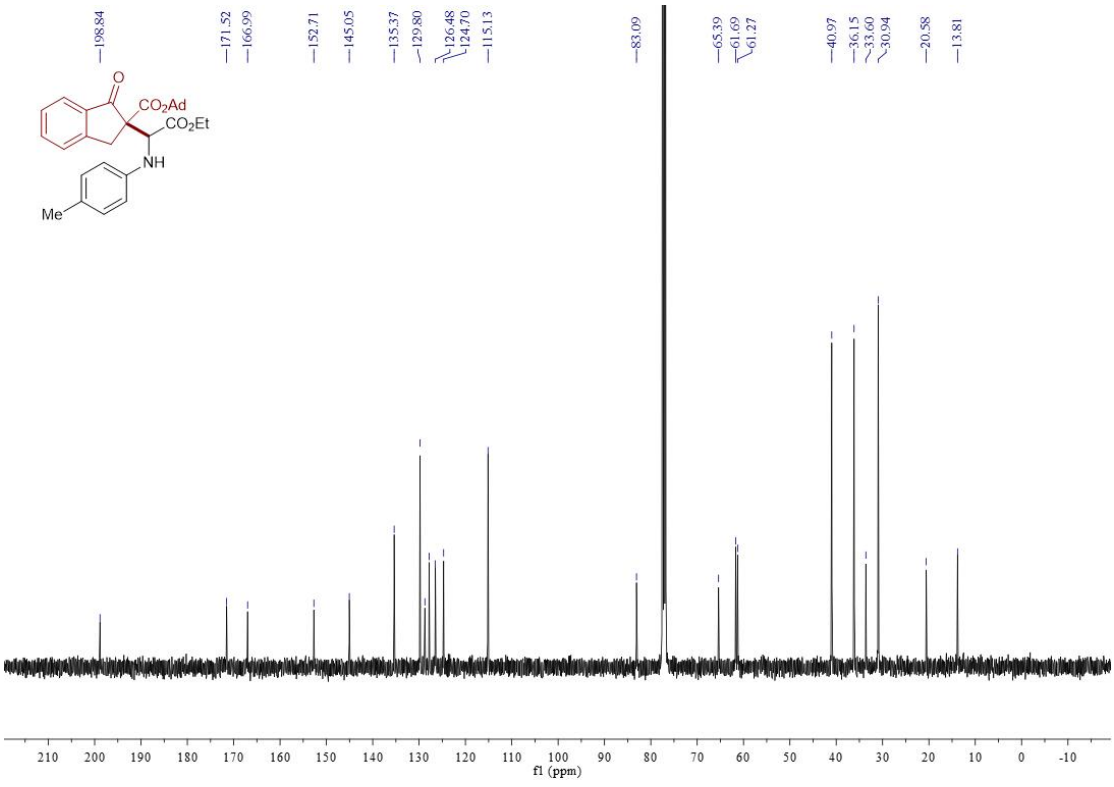
Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3aa**)



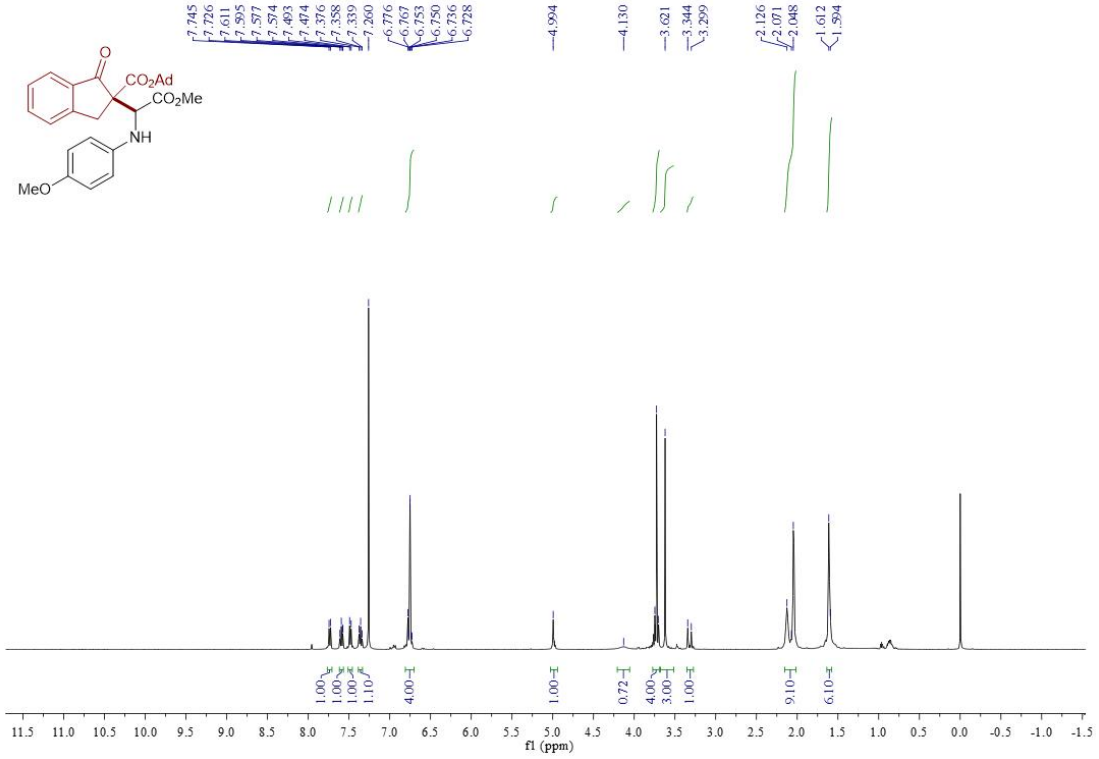


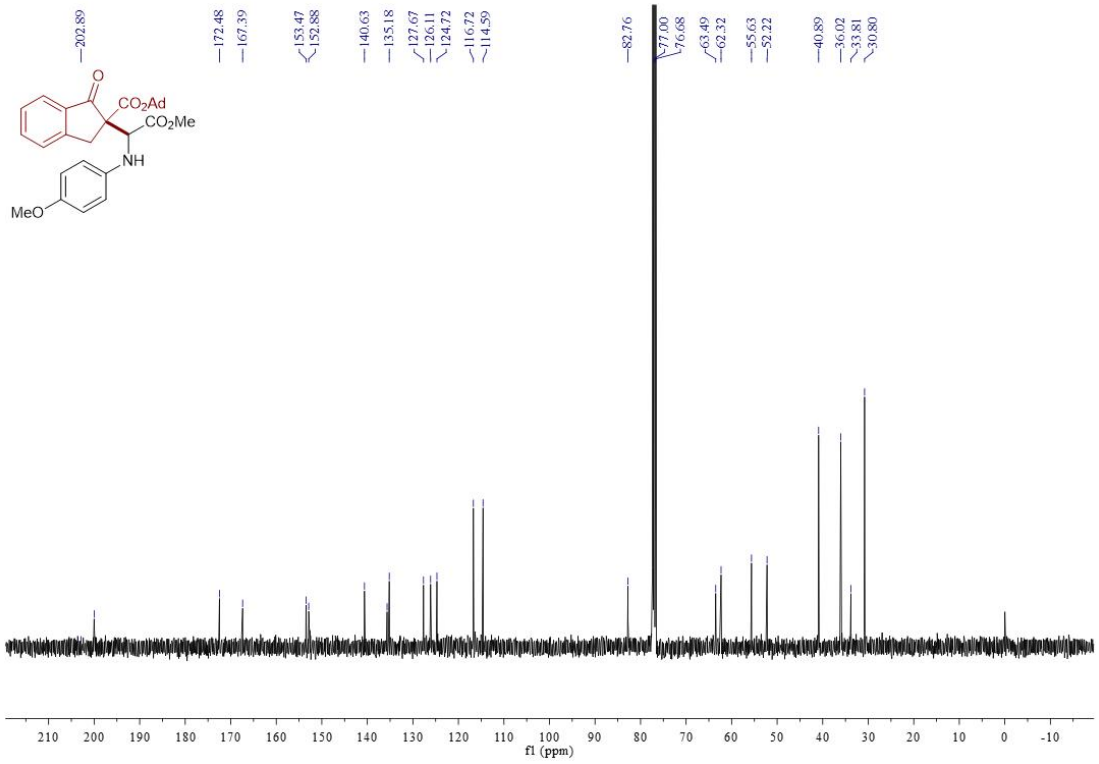
Adamantan-1-yl-2-(2-ethoxy-2-oxo-1-(p-tolylamino)ethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ab**)



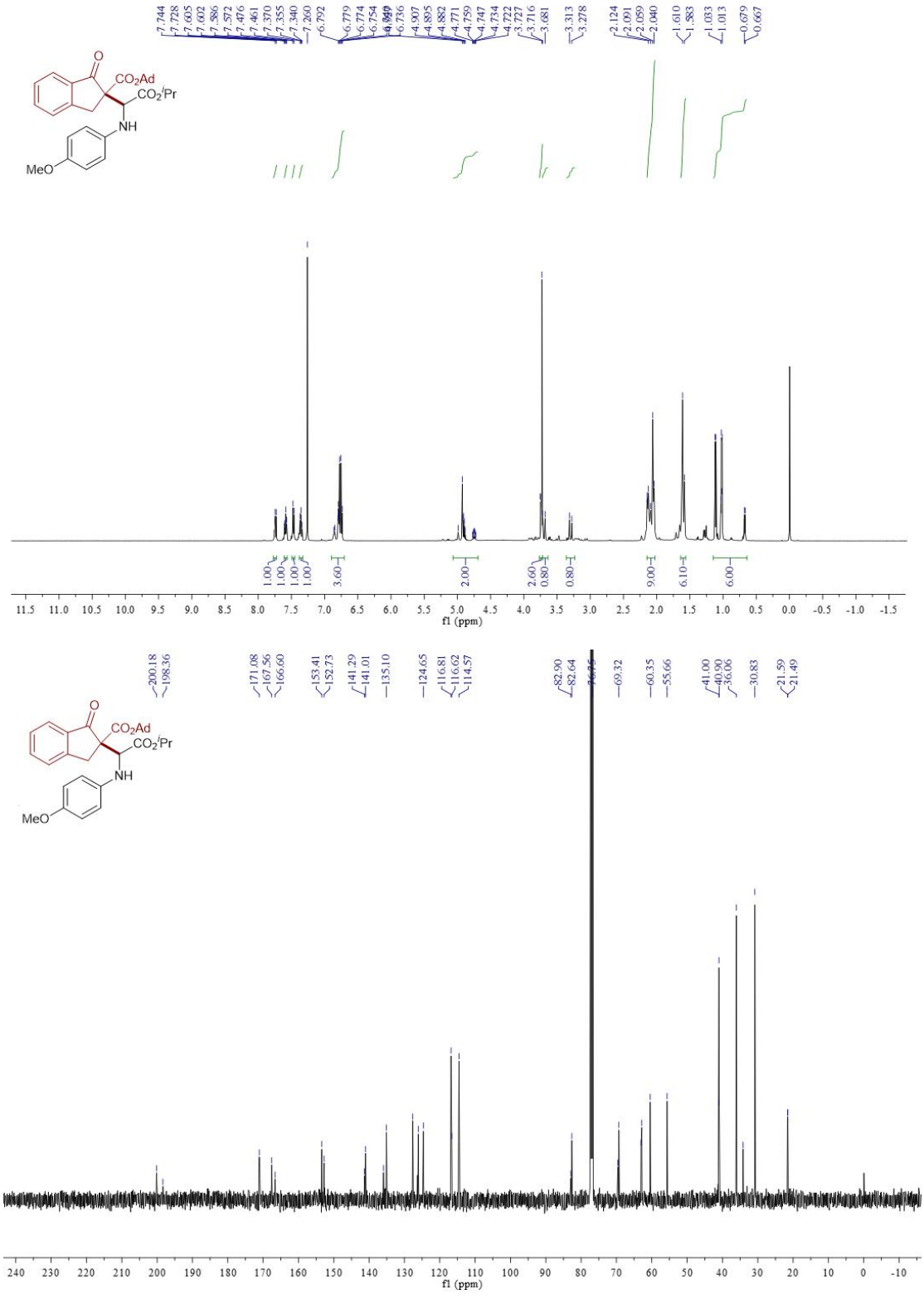


Adamantan-1-yl-2-(2-methoxy-2-oxo-1-(p-tolylamino)ethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ac**)

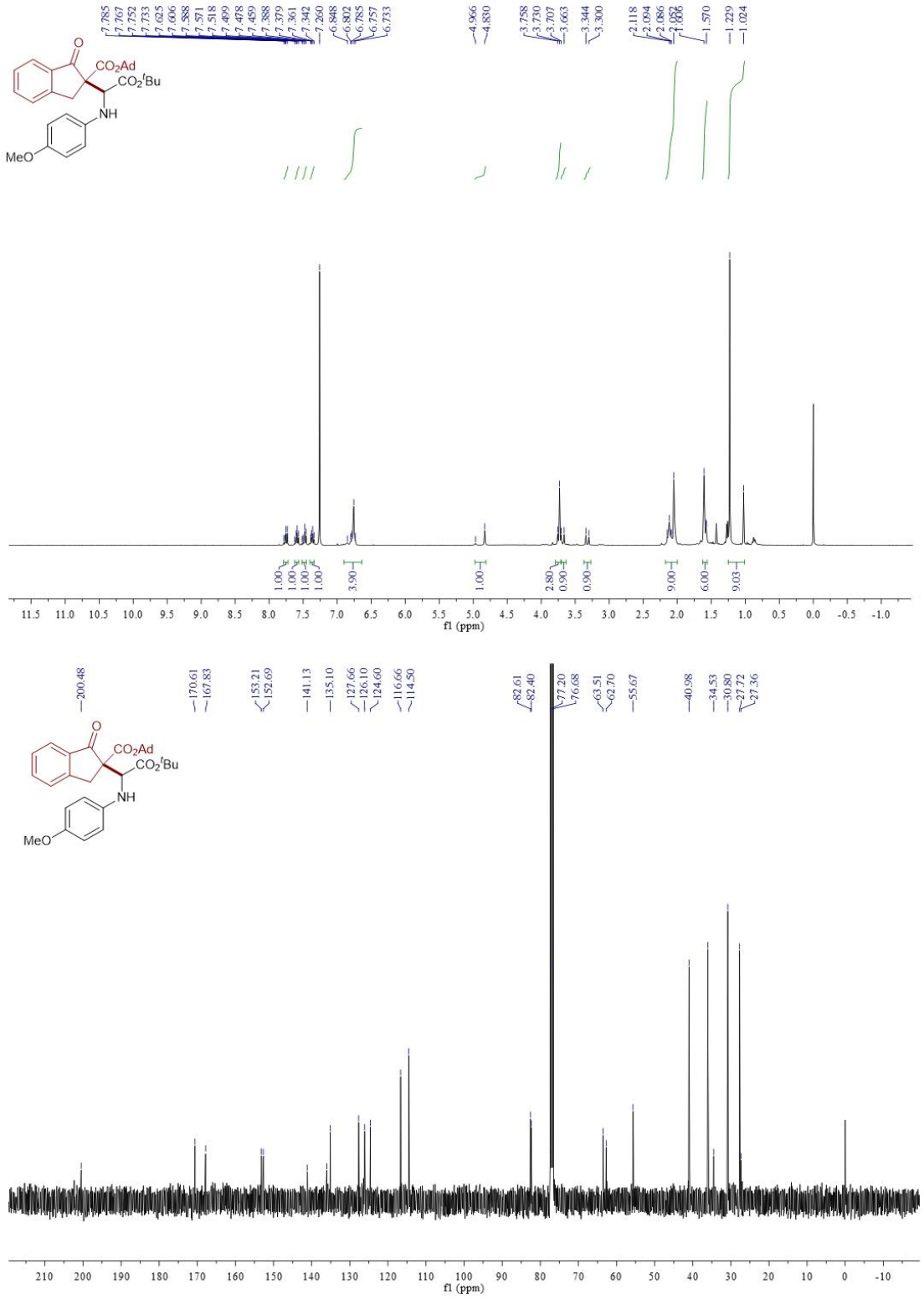




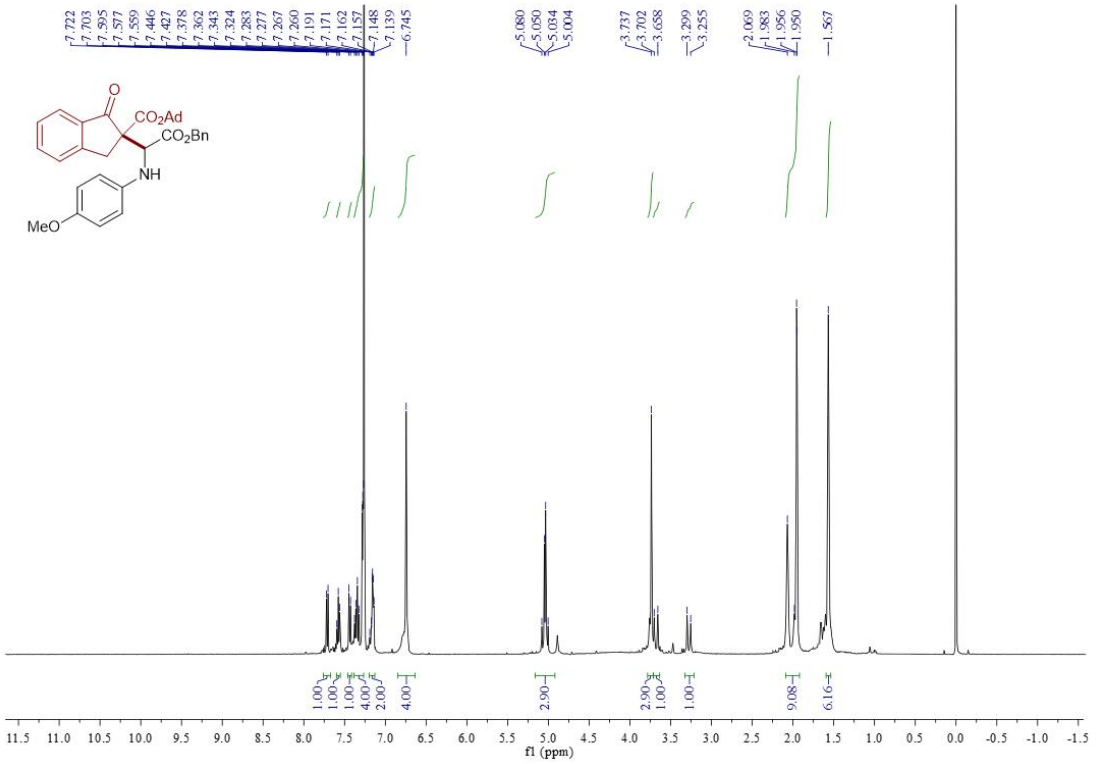
Adamantan-1-yl-2-(2-isopropoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ad**)

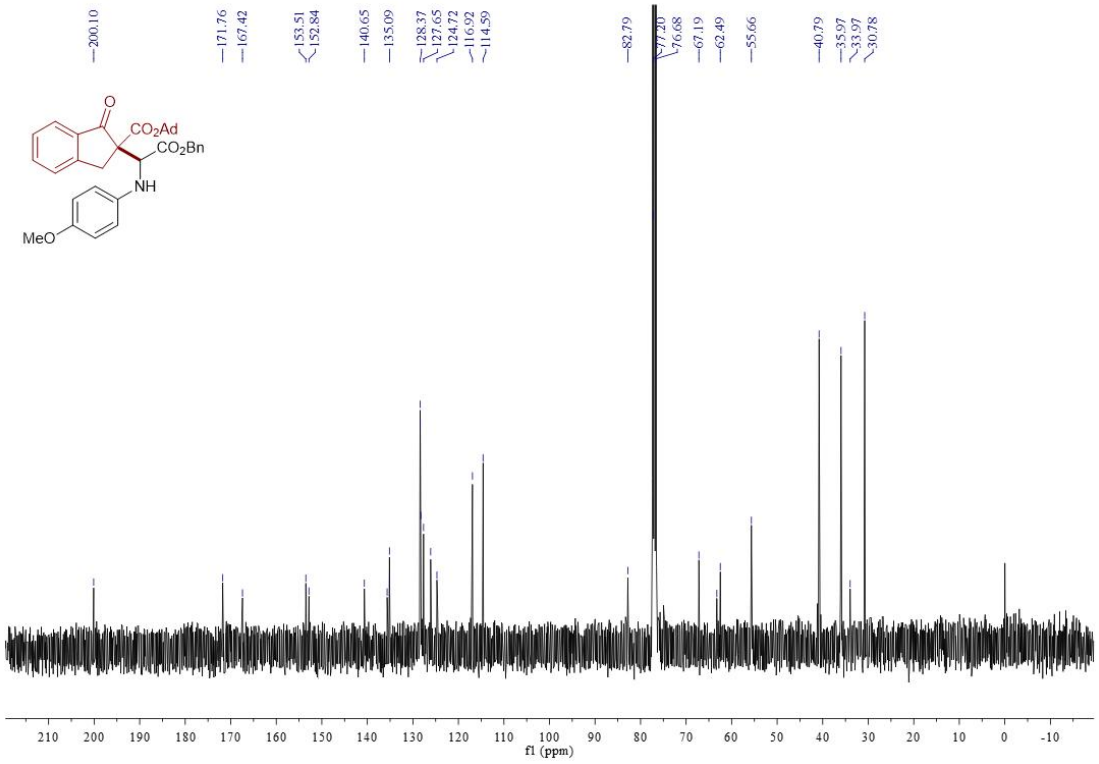


Adamantan-1-yl-2-(2-(tert-butoxy)-1-((4-methoxyphenyl) amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ae**)

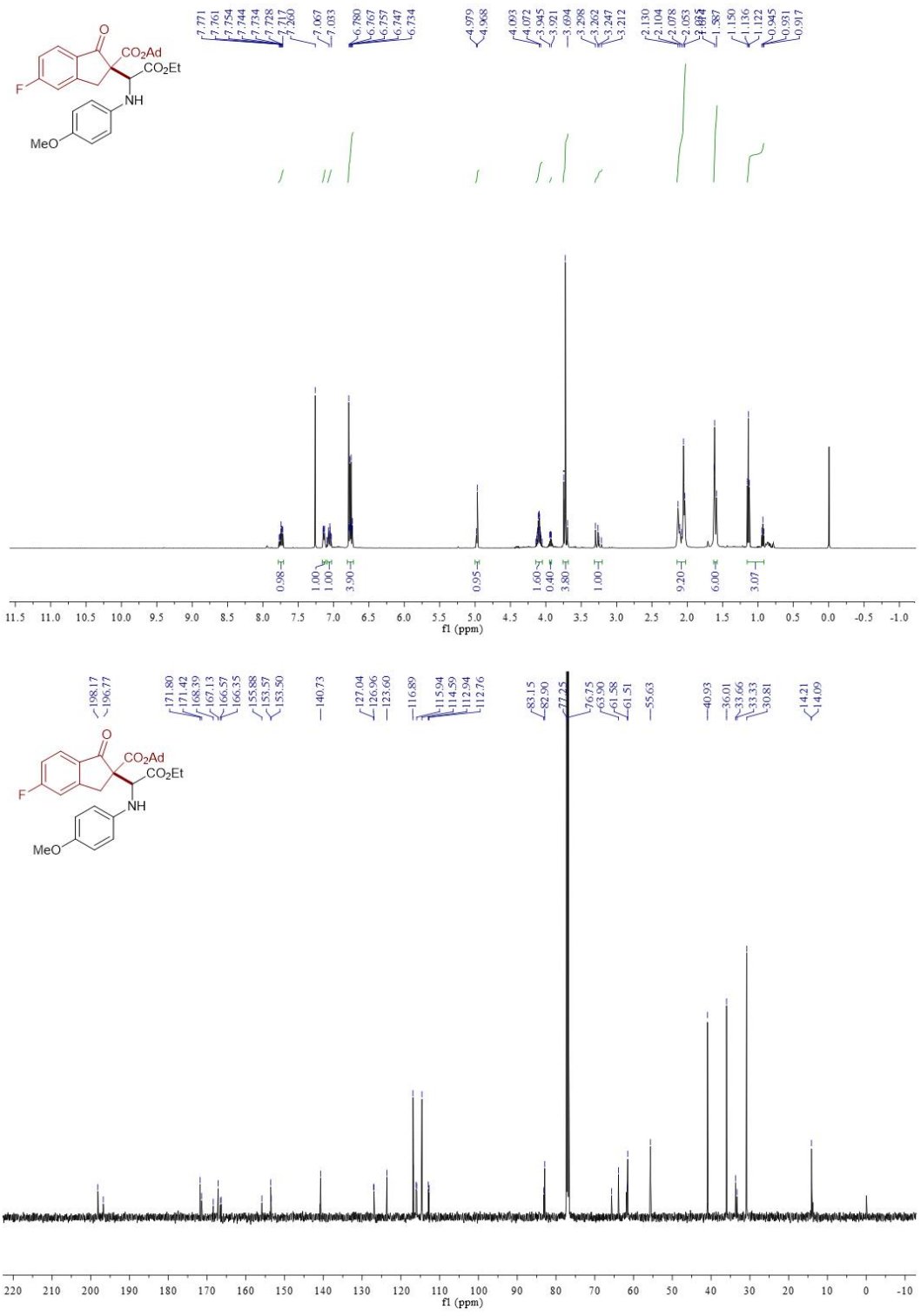


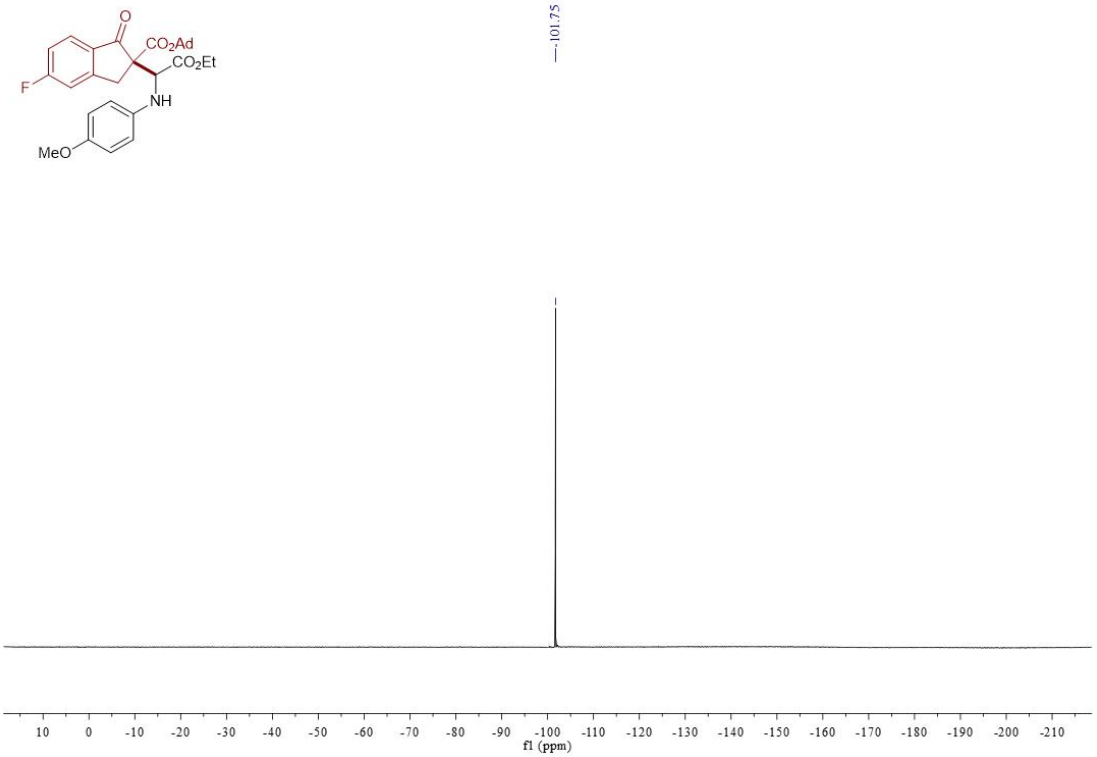
Adamantan-1-yl-2-(2-(benzyloxy)-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3af**)



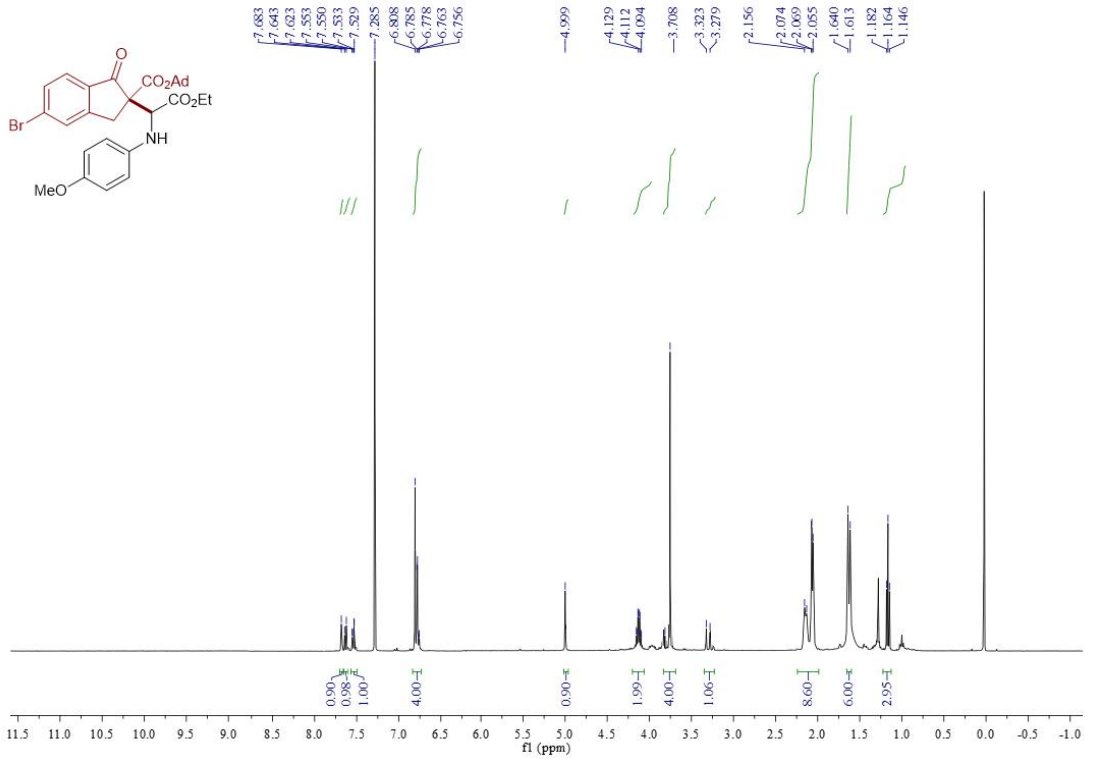


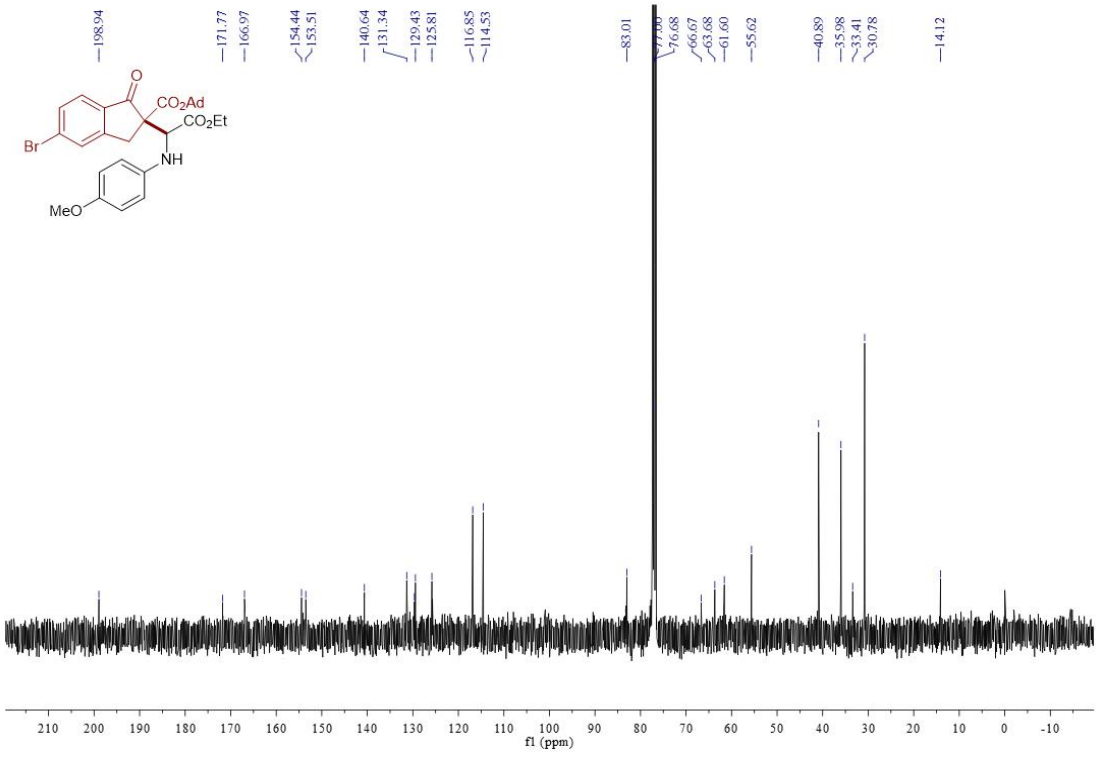
Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-5-fluoro-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ba**)



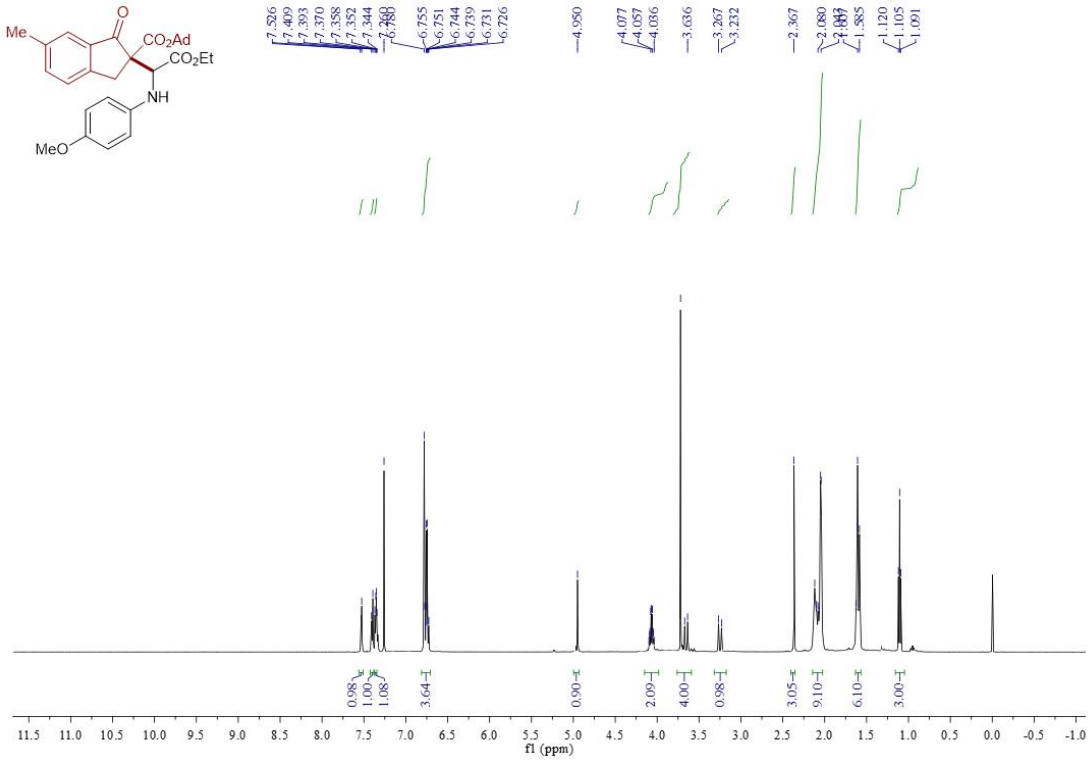

O
CO2Ad
CO2Et
F
NH
MeO
-101.75
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

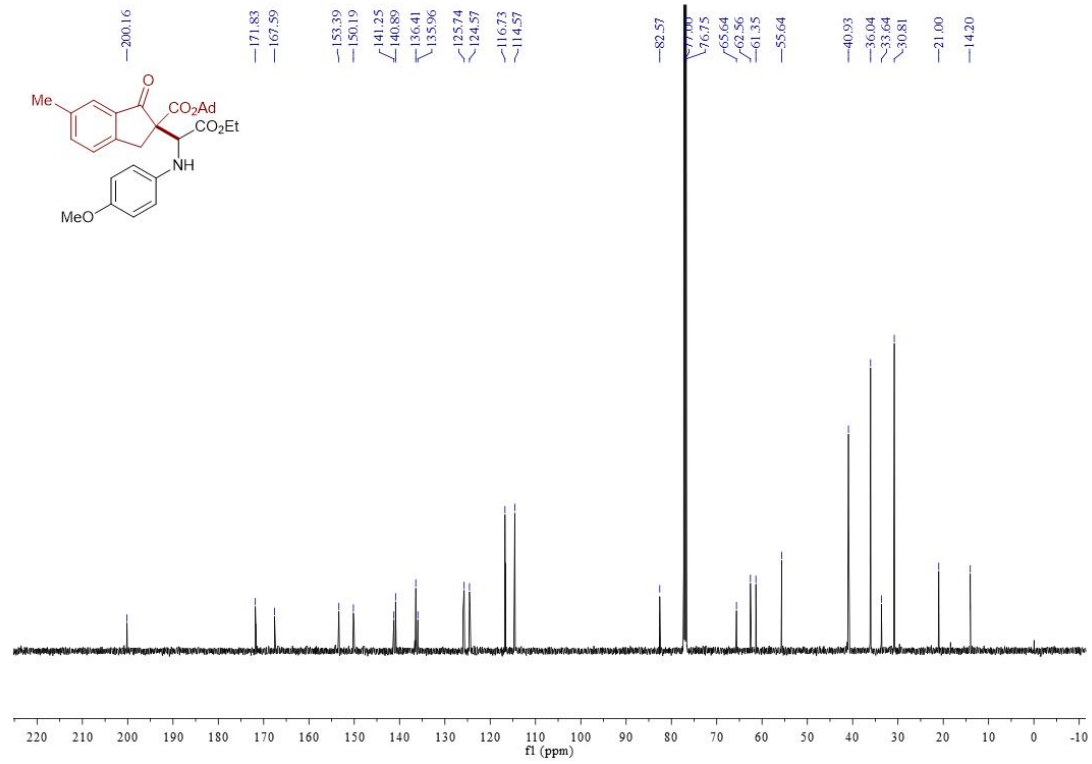
Adamantan-1-yl-5-bromo-2-(2-ethoxy-1-((4-methoxyphenyl) amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3ca**)



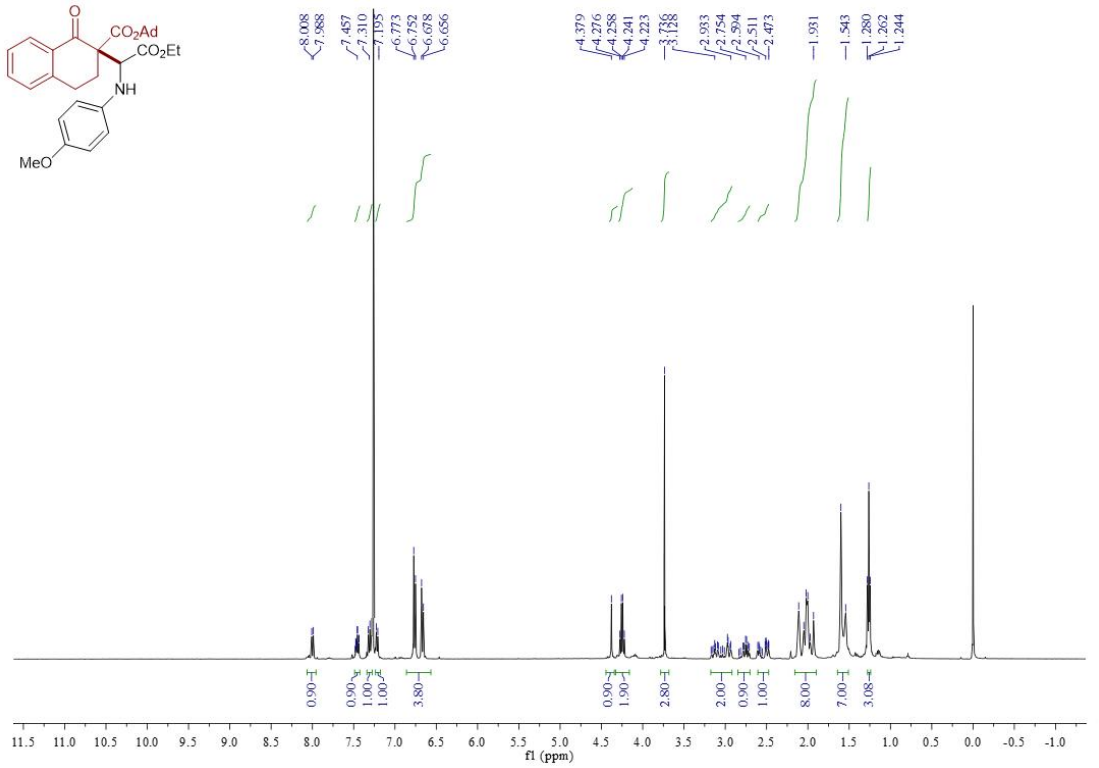


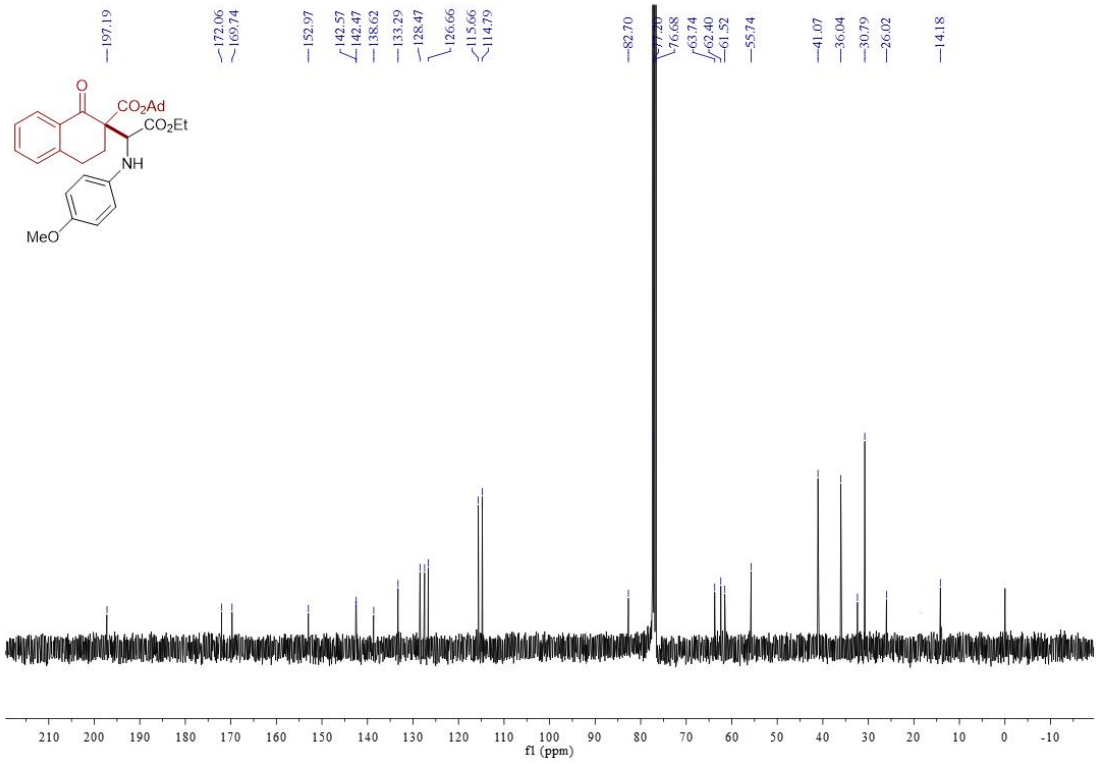
Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-6-methyl-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3da**)



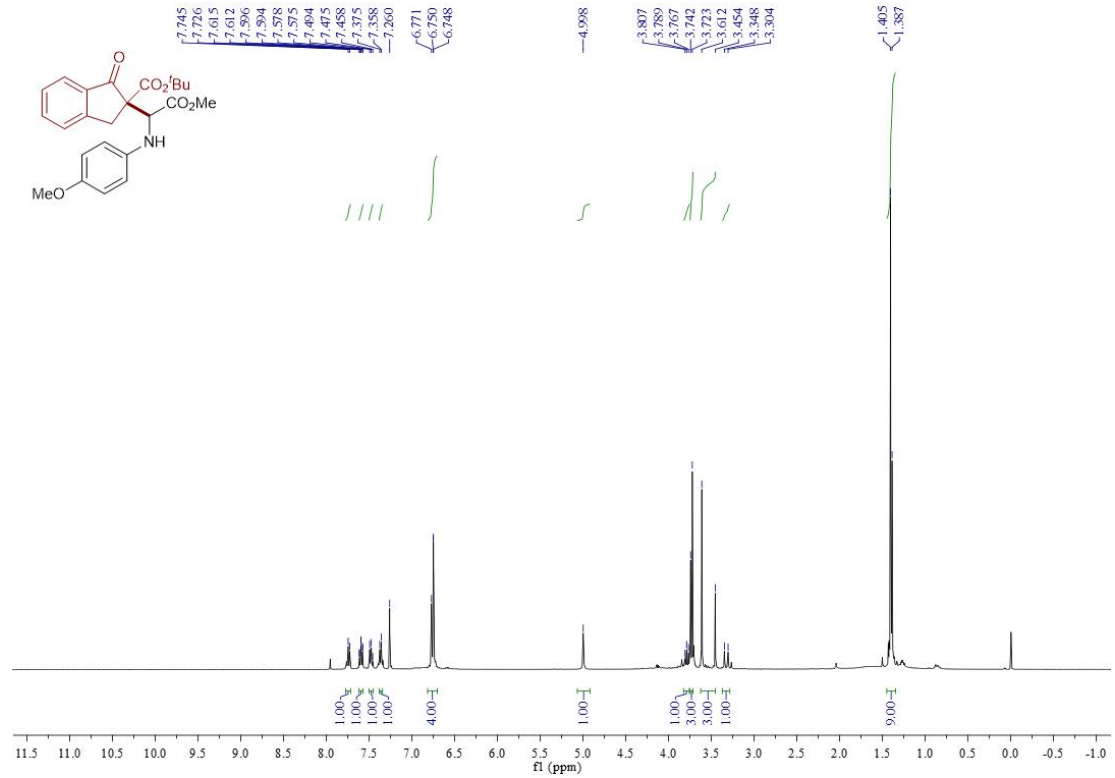


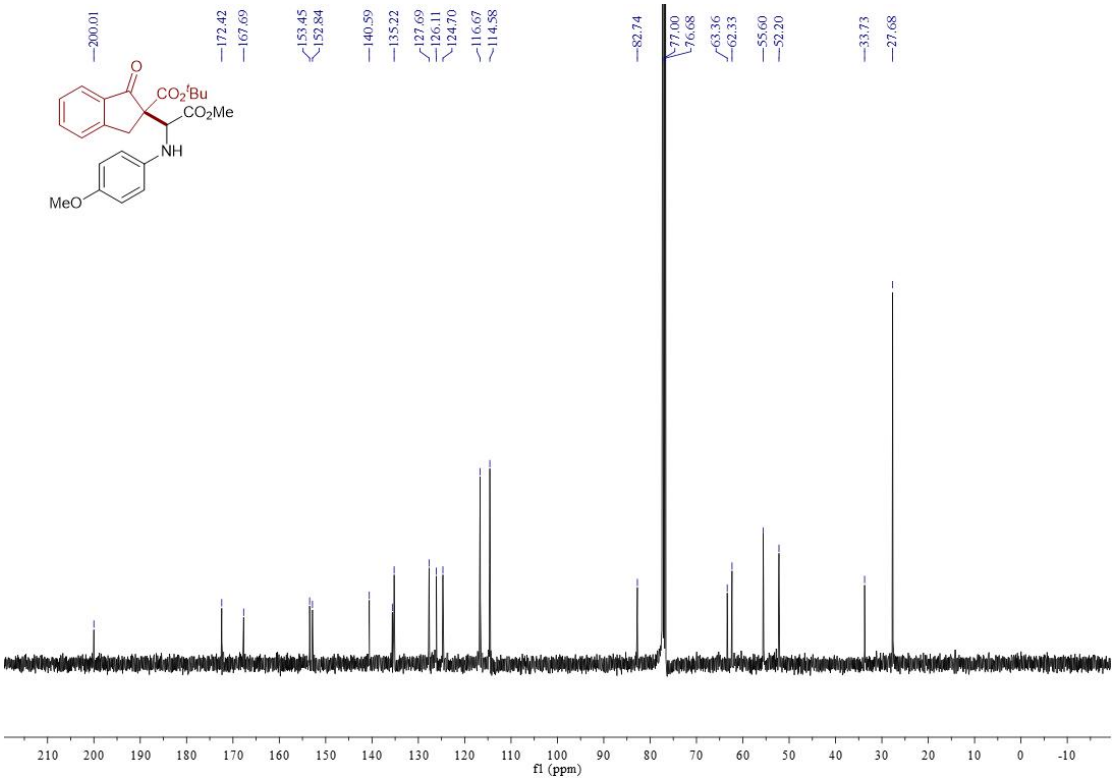
Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-1,2,3,4-tetrahydronaphthalene-2-carboxylate (**3ea**)



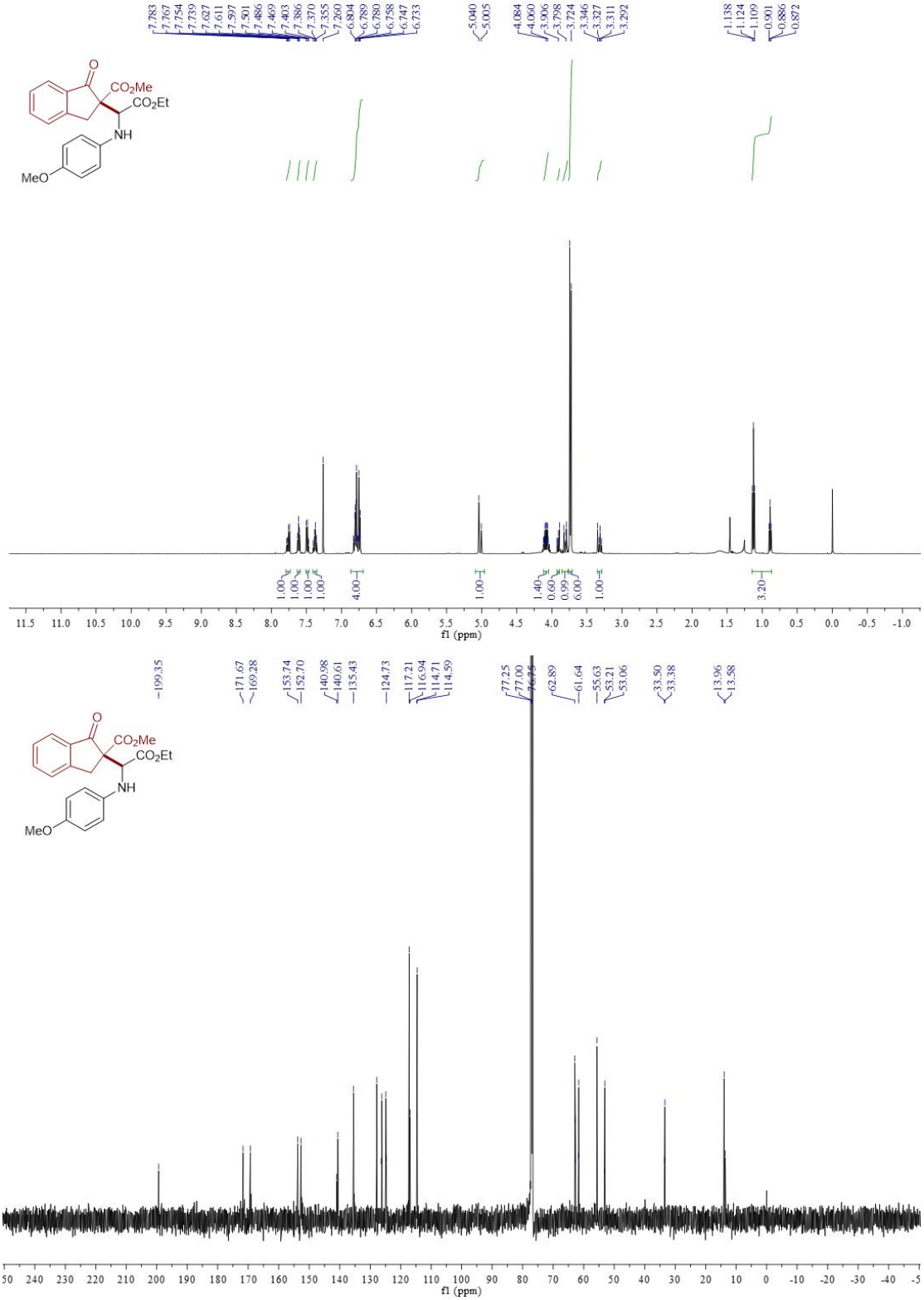


Tert-butyl-2-(2-methoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3fc**)

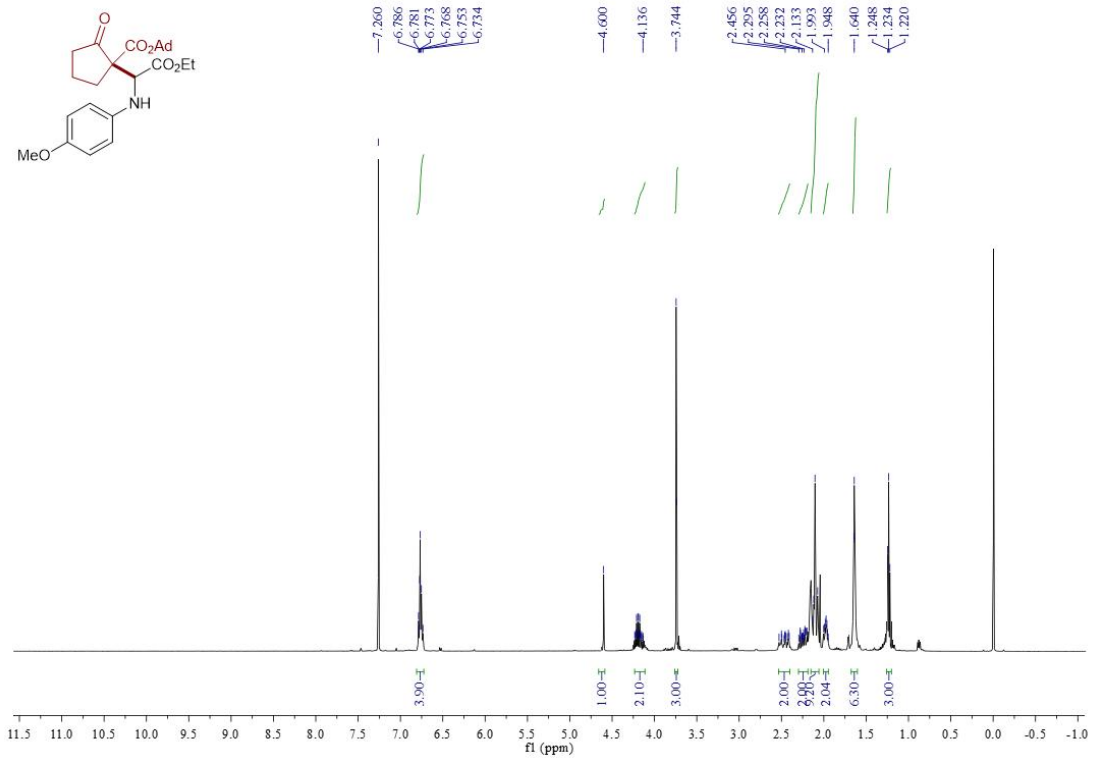


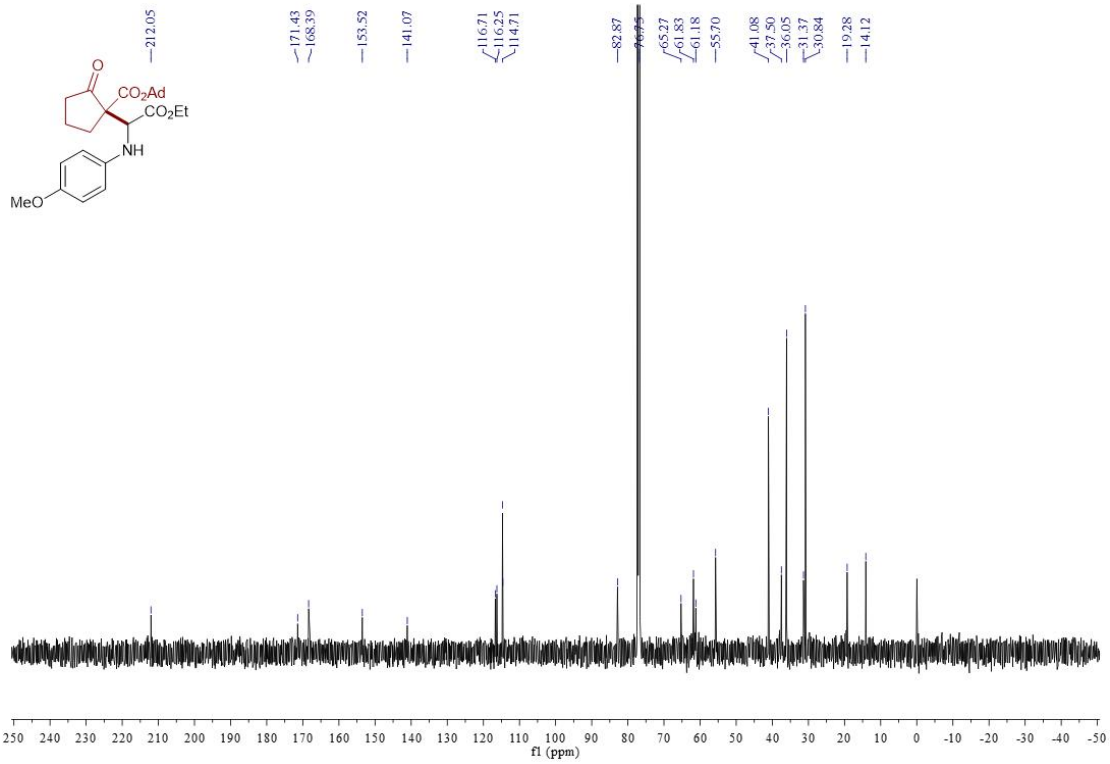


Methyl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-1-oxo-2,3-dihydro-1H-indene-2-carboxylate (**3f'a**)

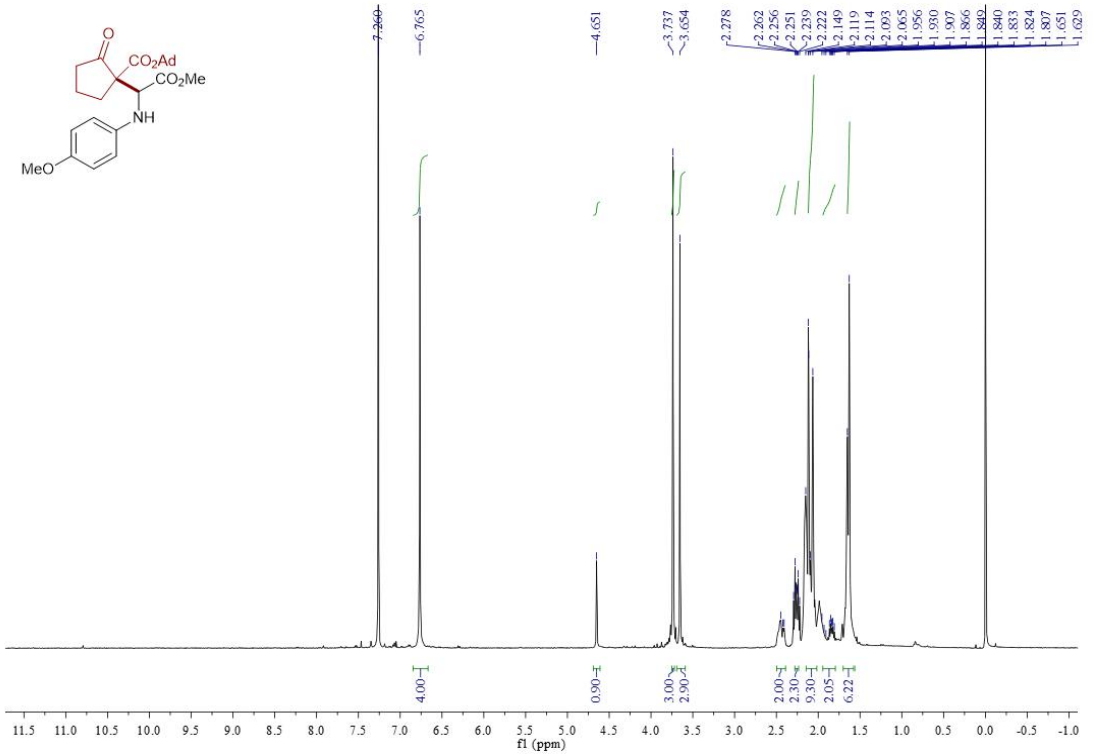


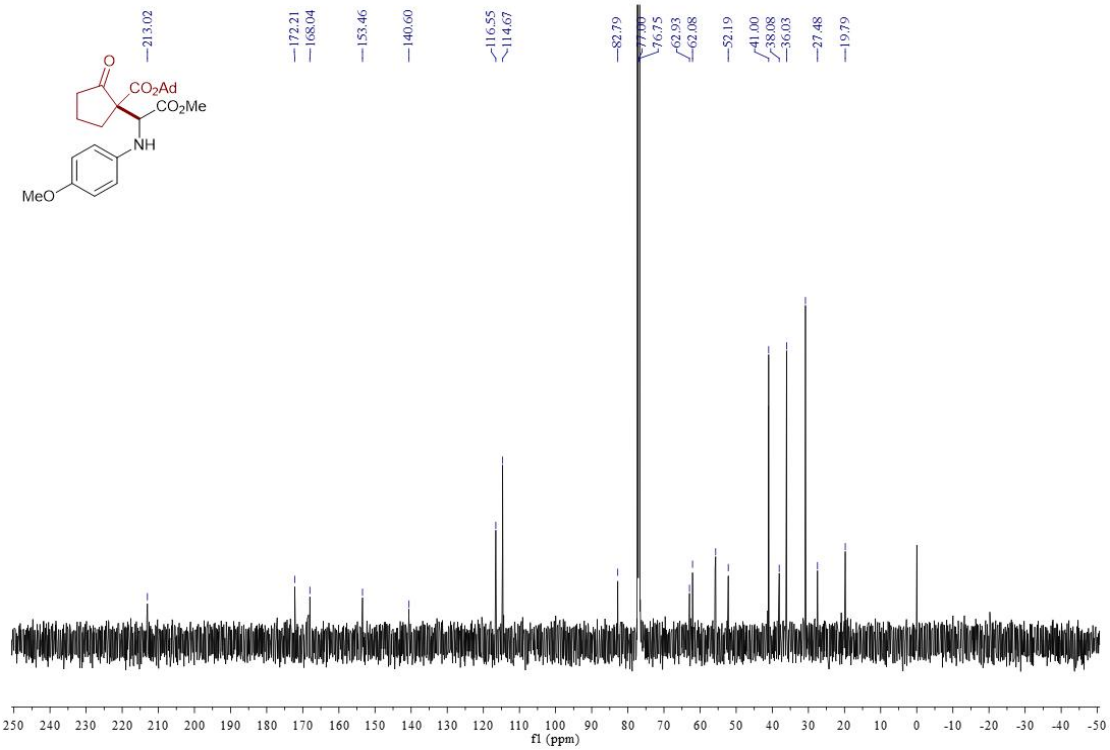
Adamantan-1-yl-1-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-2-oxocyclopentane-1-carboxylate (**3ga**)



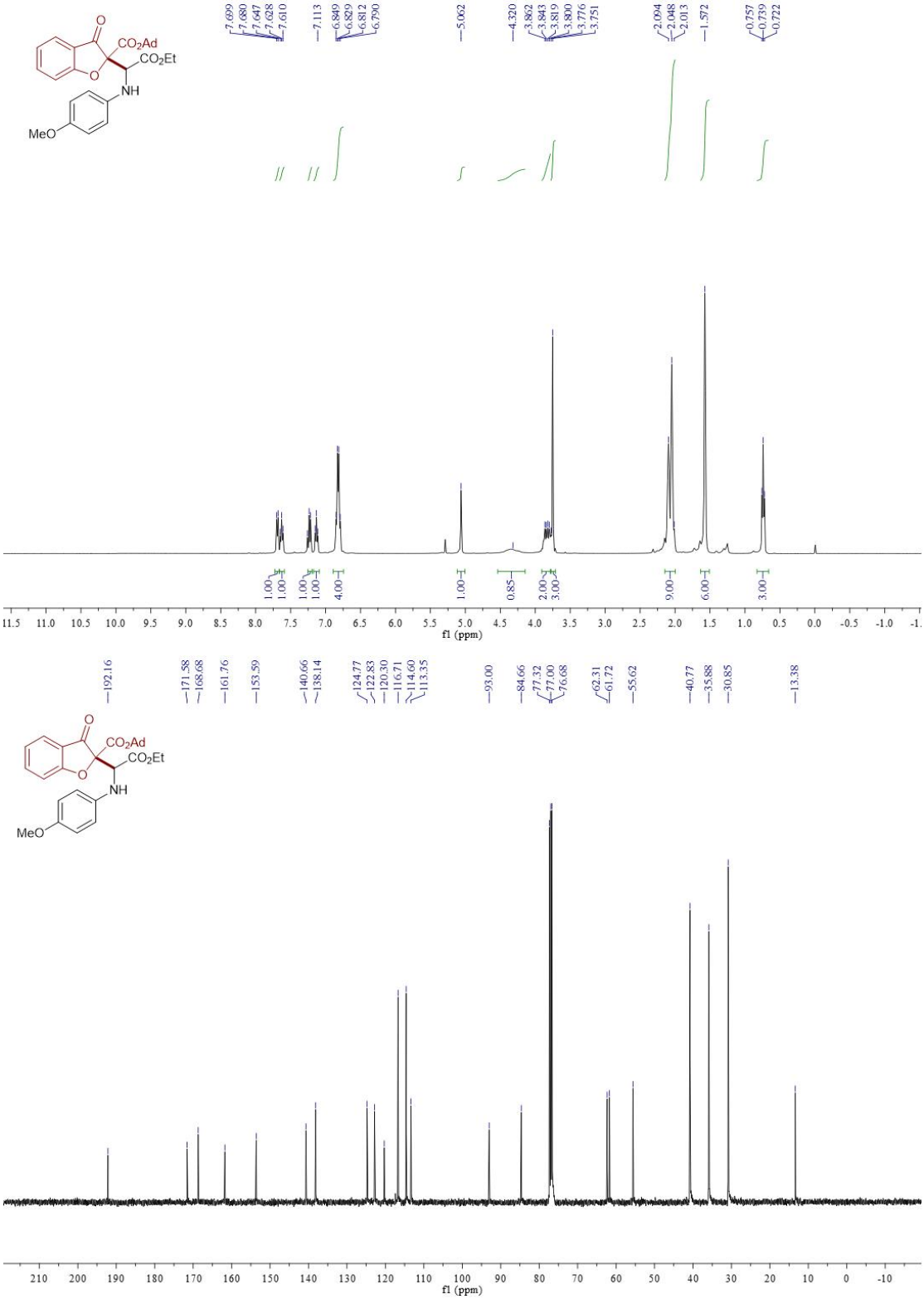


Adamantan-1-yl-1-(2-methoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-2-oxocyclopentane-1-carboxylate (**3gc**)

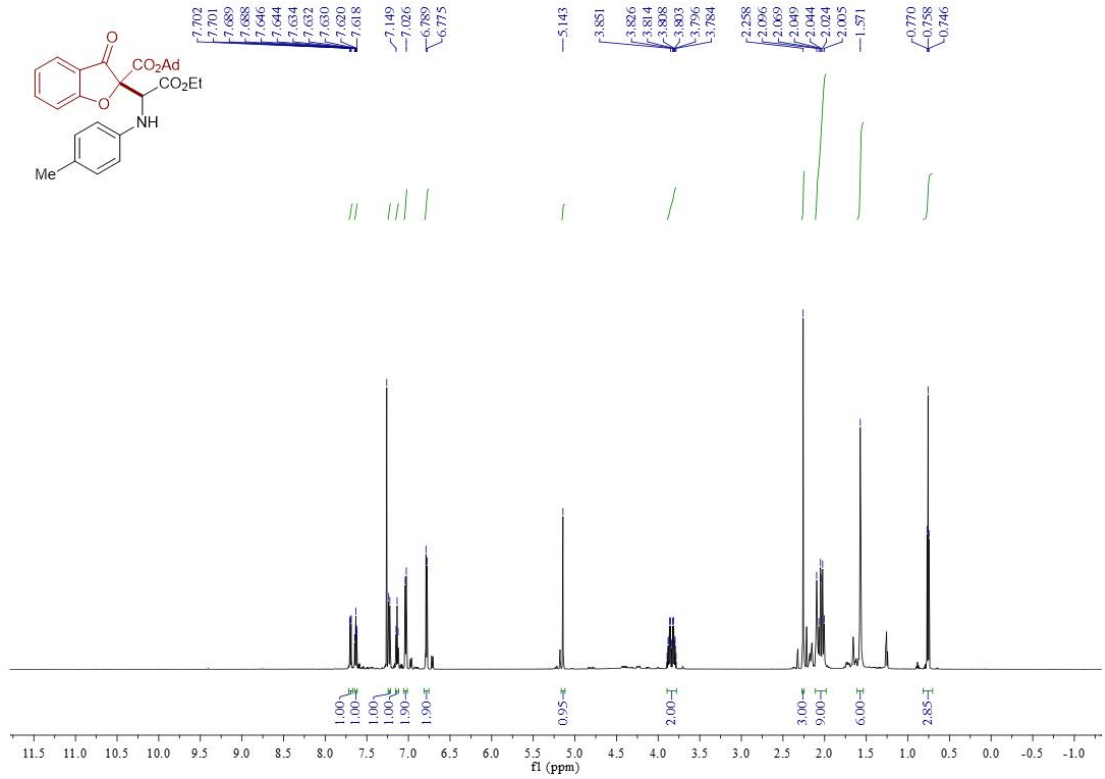


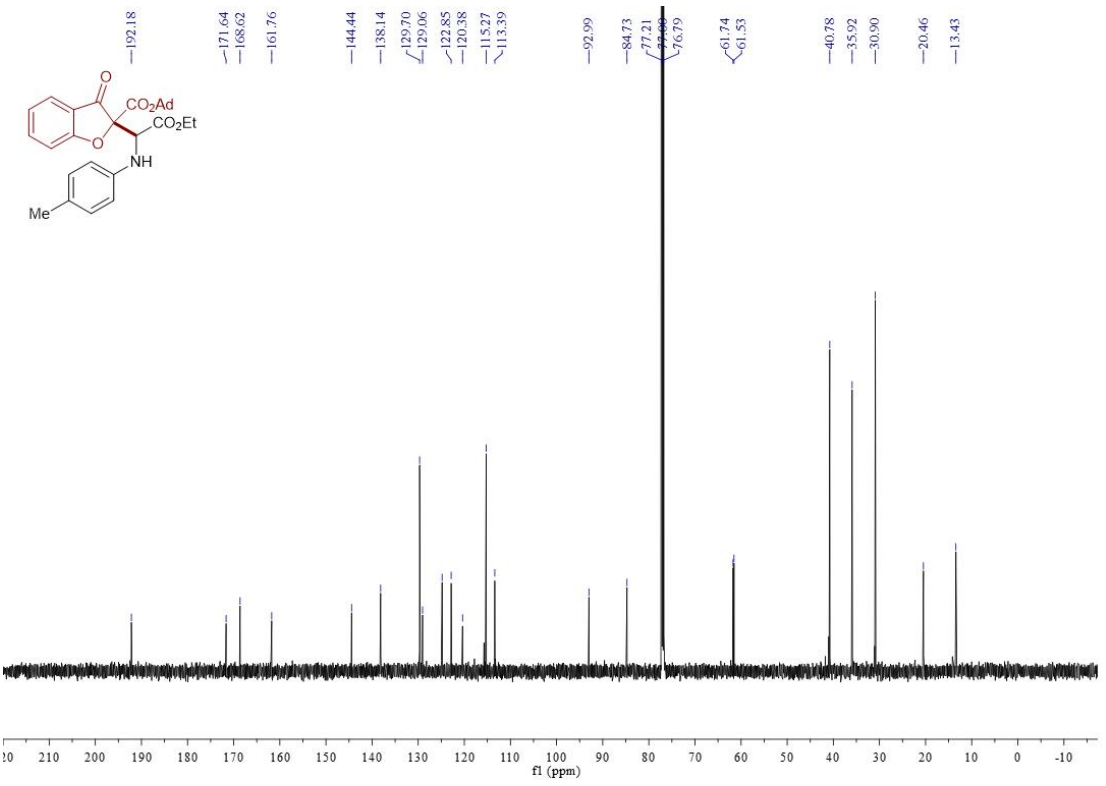


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-3-oxo-2,3 dihydrobenzofuran-2-carboxylate (**3ha**)

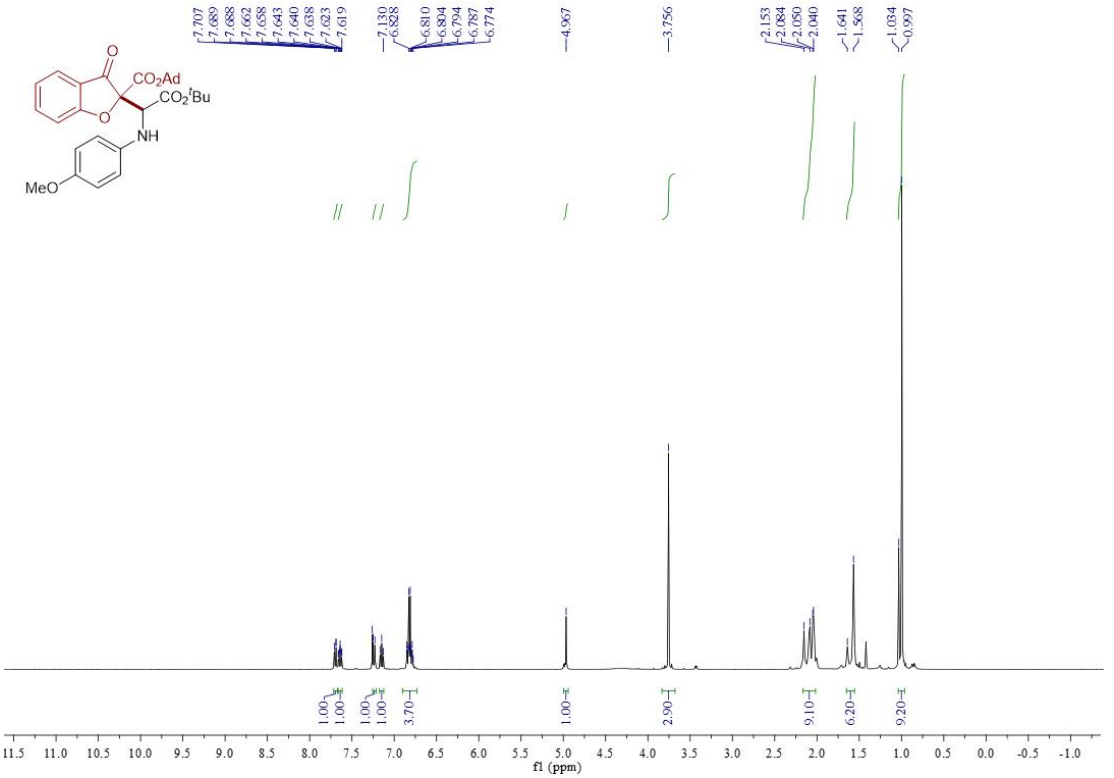


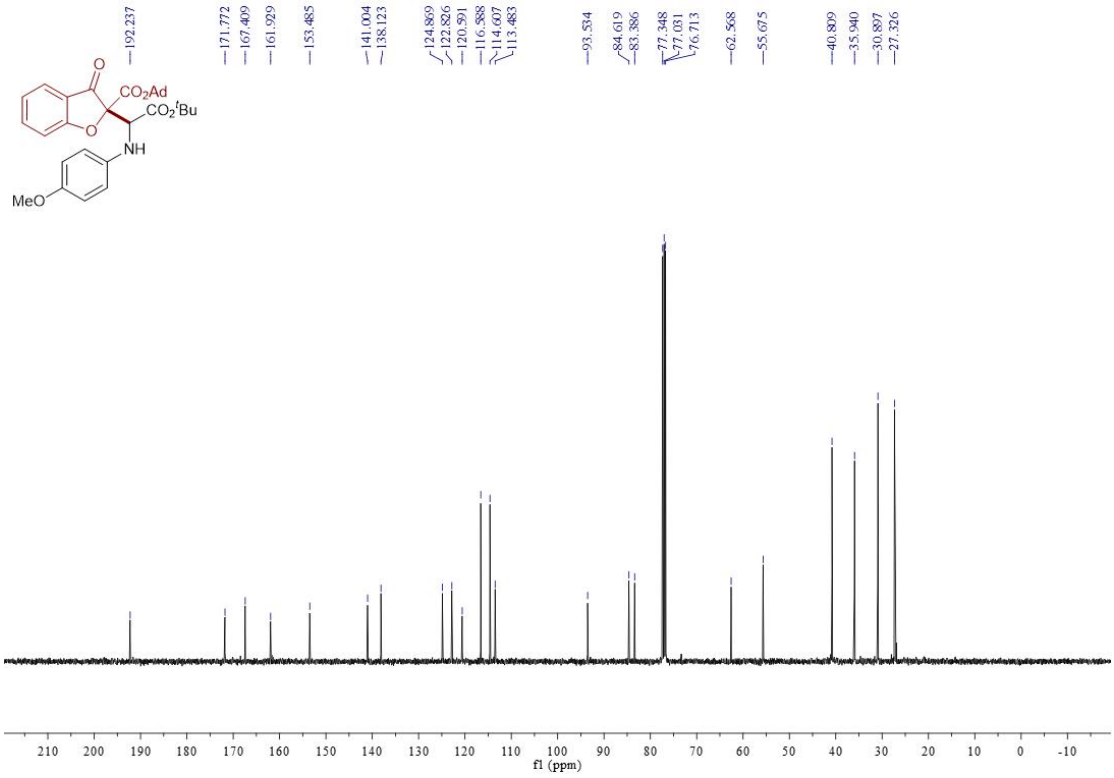
Adamantan-1-yl-2-((S)-2-ethoxy-2-oxo-1-(p-tolylamino)ethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3hb**)



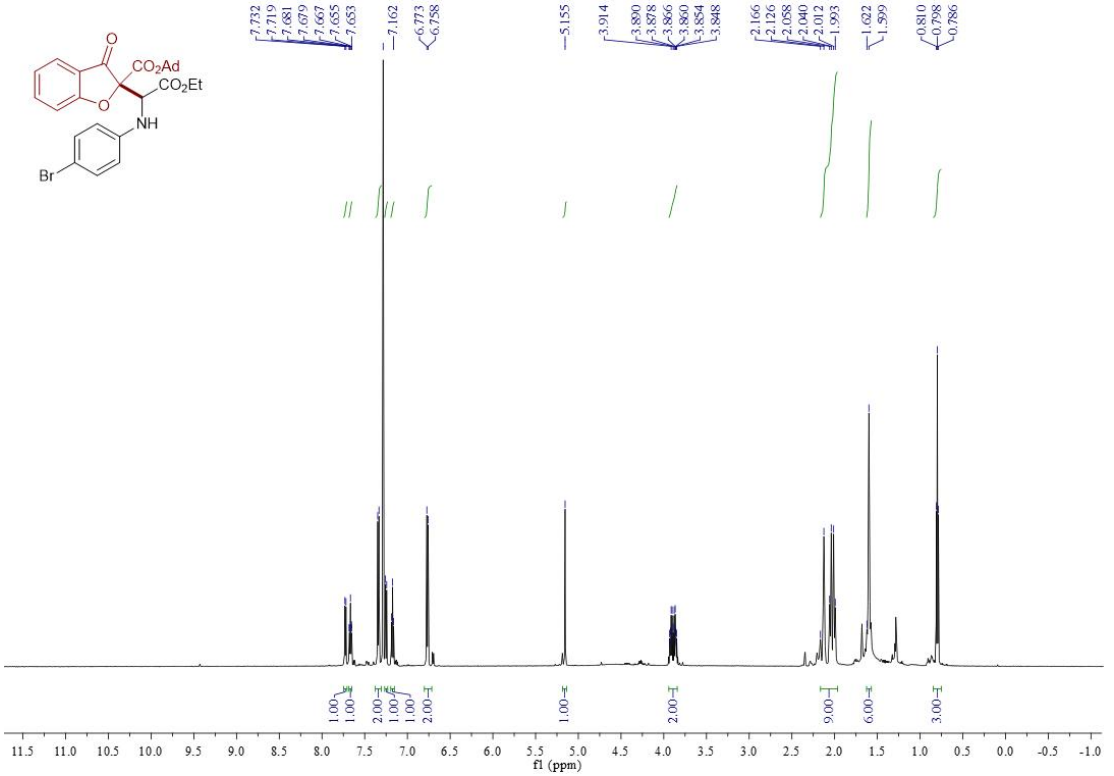


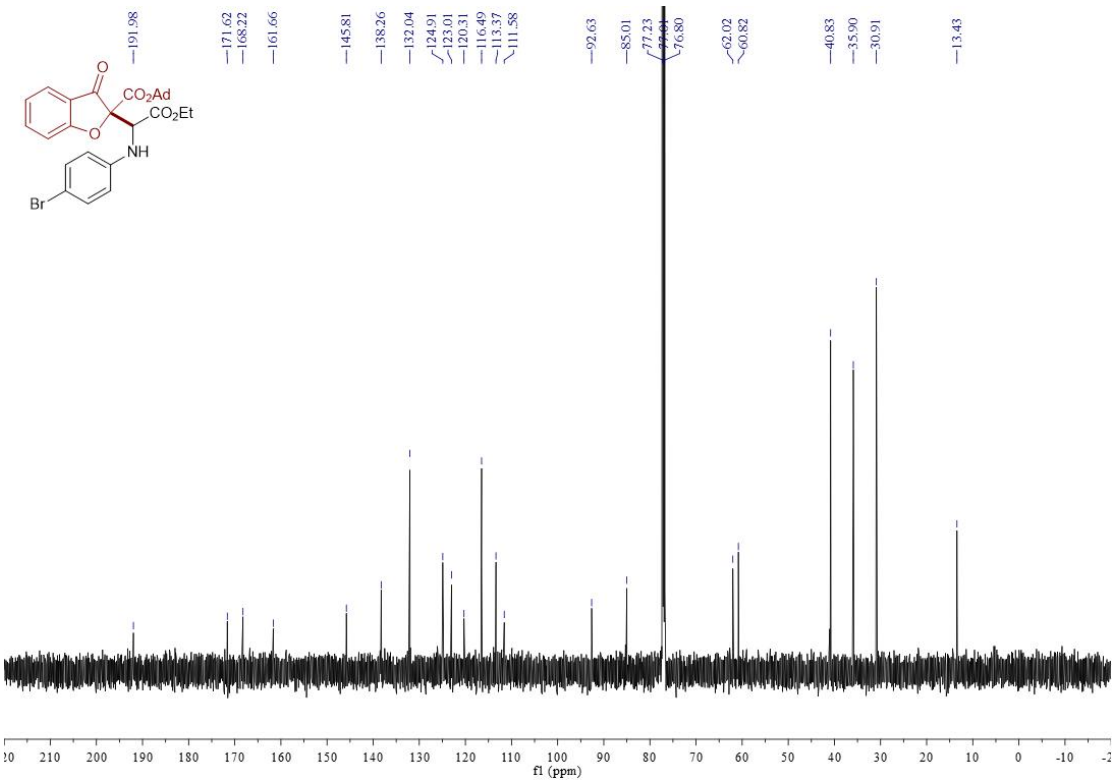
Aadamantan-1-yl-2-(2-(tert-butoxy)-2-oxo-1-(p-tolylamino)ethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3he**)



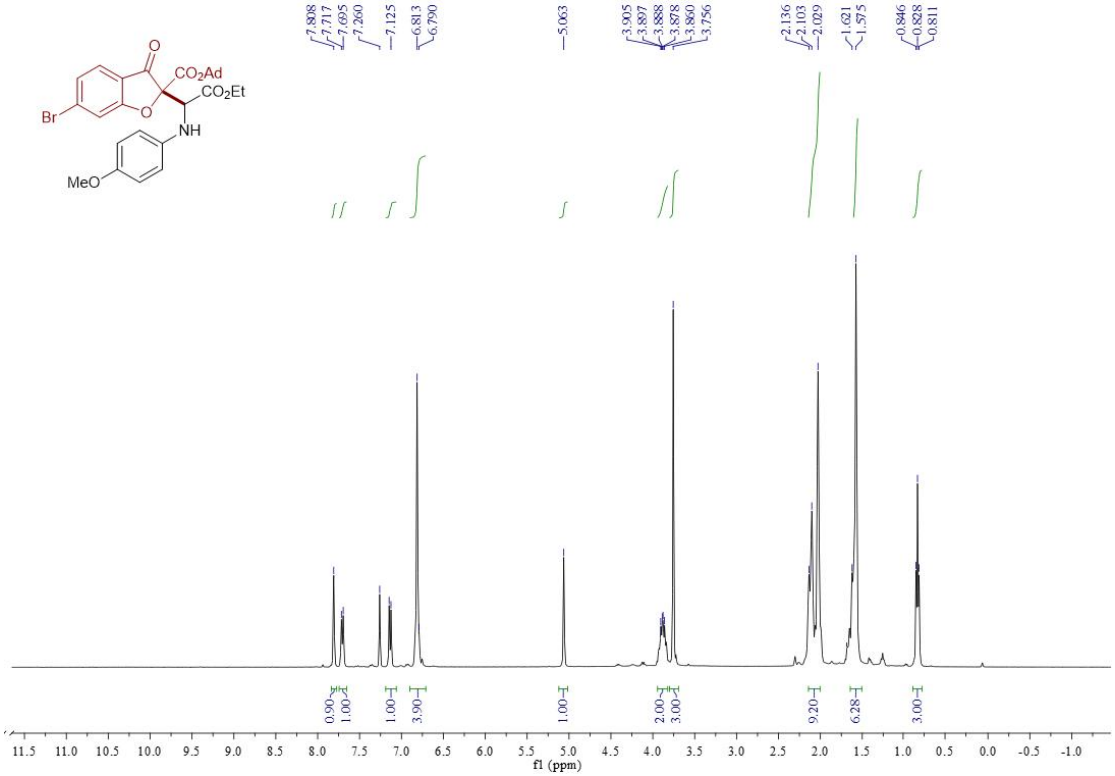


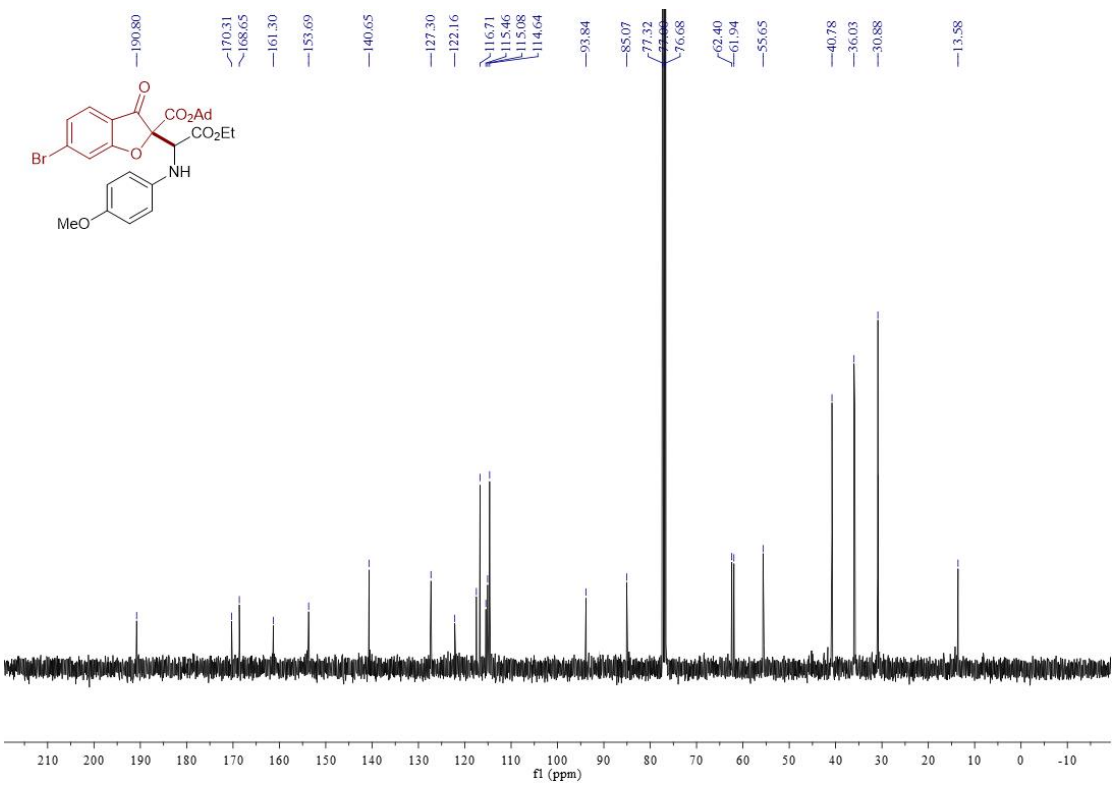
Adamantan-1-yl 2-(1-((4-bromophenyl)amino)-2-ethoxy-2-oxoethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3hg**)



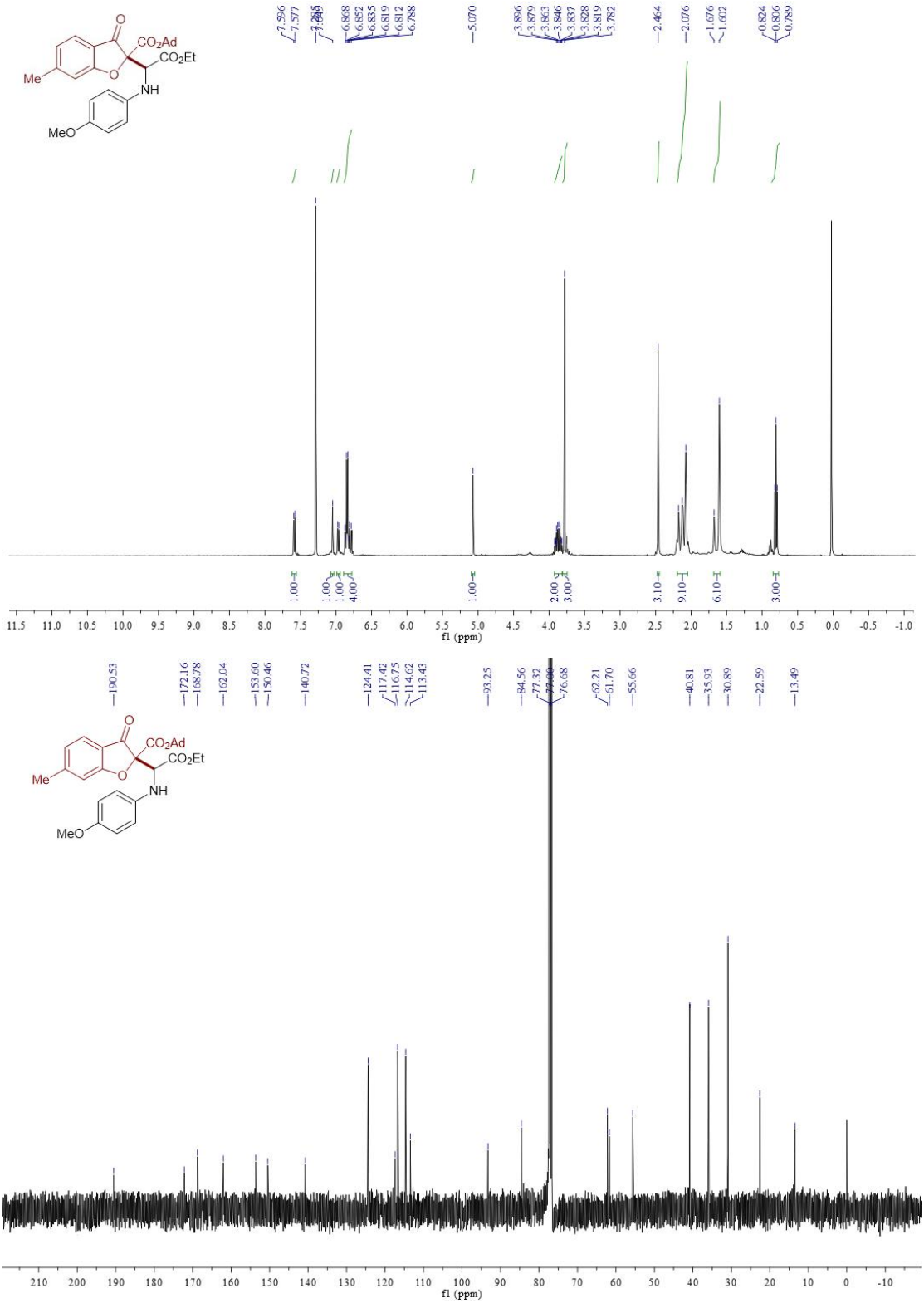


Adamantan-1-yl-6-bromo-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3ia**)

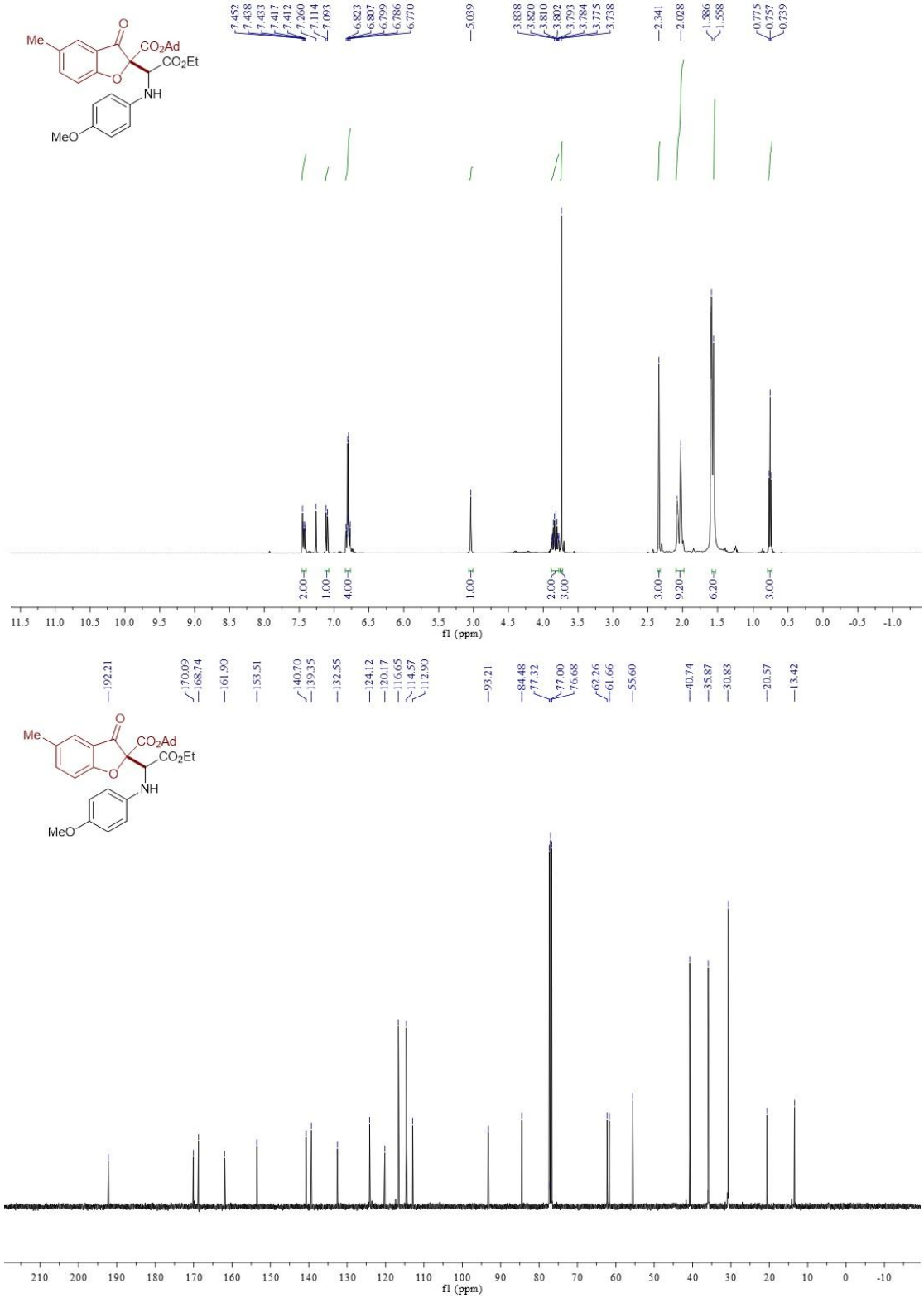




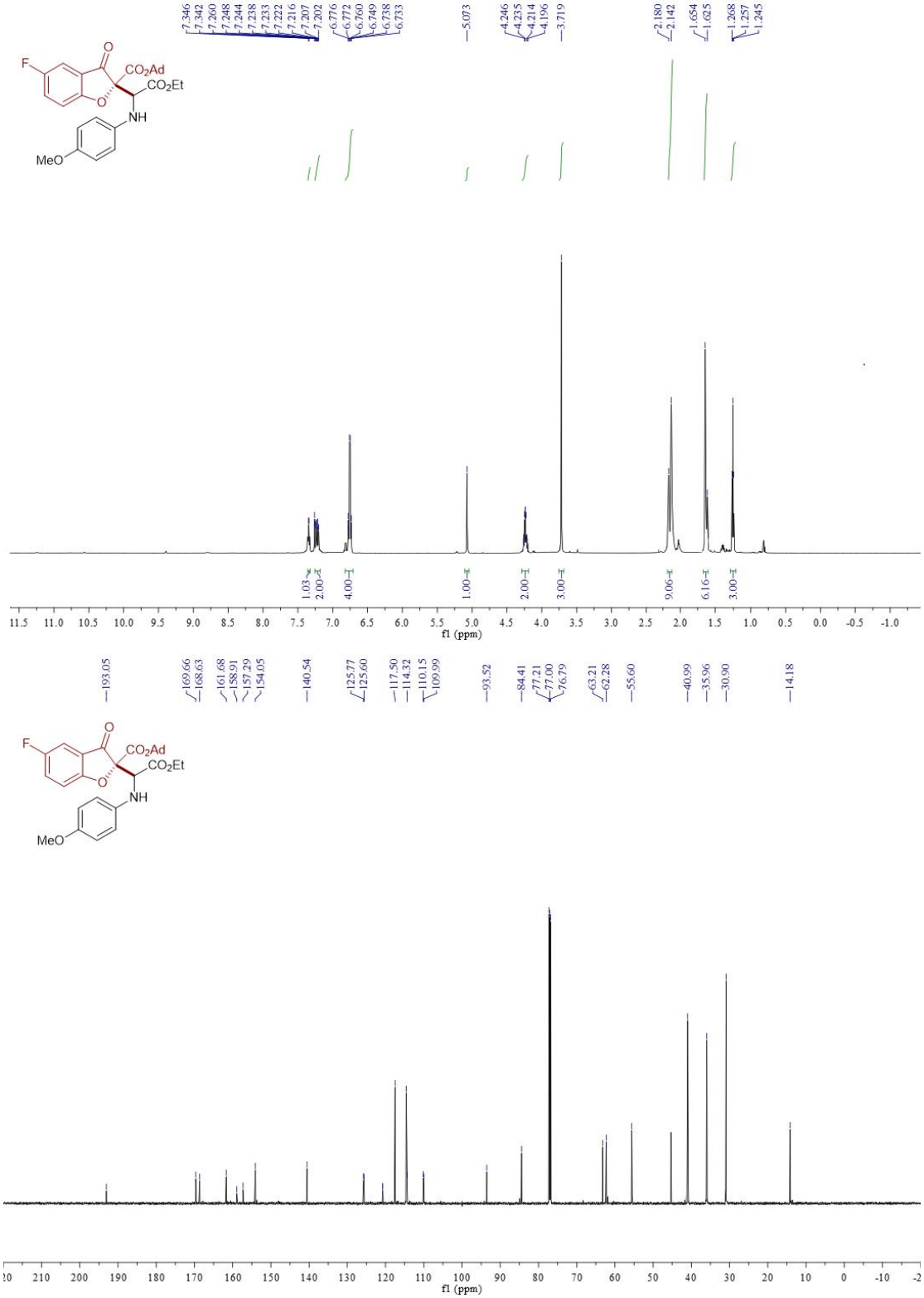
Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-5-methyl-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3ja**)

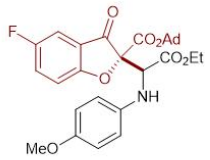


Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-5-fluoro-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3ka**)



Adamantan-1-yl-2-(2-ethoxy-1-((4-methoxyphenyl)amino)-2-oxoethyl)-5-fluoro-3-oxo-2,3-dihydrobenzofuran-2-carboxylate (**3la**)



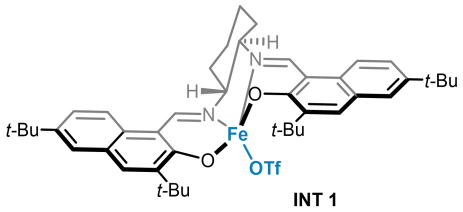

F
O
CO2Ad
CO2Et
O
NH
MeO

-119.965
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

9. DFT Computations

9.1 Computational details

The computations were performed using the Gaussian 16 software package[11]. The PBE0 functional[12] was adopted for all calculations in combination with the D3BJ dispersion correction[13]. During the geometry optimization and frequency calculations, the def2SVP basis set[14] was used to treat Fe, and 6-31G(d)[15,16] was employed for most of the organic and ligand atoms[15,16]. To simplify the calculation, the 3-21G basis set[17] was used to treat the cyclohexyl group of the ligand and the two *tert*-butyl groups of the ligand that distant from the Fe center (noted as the uninterested area). The singlet point energy calculations were performed with a larger basis set combination, in which the def2-TZVP basis set[14] was used for Fe, 6-31G(d) for the uninterested area, and 6-311+G(d,p)[18,19] for others. The free energy was obtained by adding the single point energy to the thermal correction to the Gibbs free energy ($G = E_{PBE0} + G_{corr}$). All calculated structures were illustrated using CYLview[20] software.



G (sextet) = 0 kcal/mol
G (quartet) = 2.1 kcal/mol
G (doublet) = 22.9 kcal/mol

The ground state of the pre-catalyst **INT 1** was determined to be sextet, with a quartet state close in Gibbs free energy (2.1 kcal/mol relative to the sextet). The doublet state lies 22.9 kcal/mol above the sextet state.

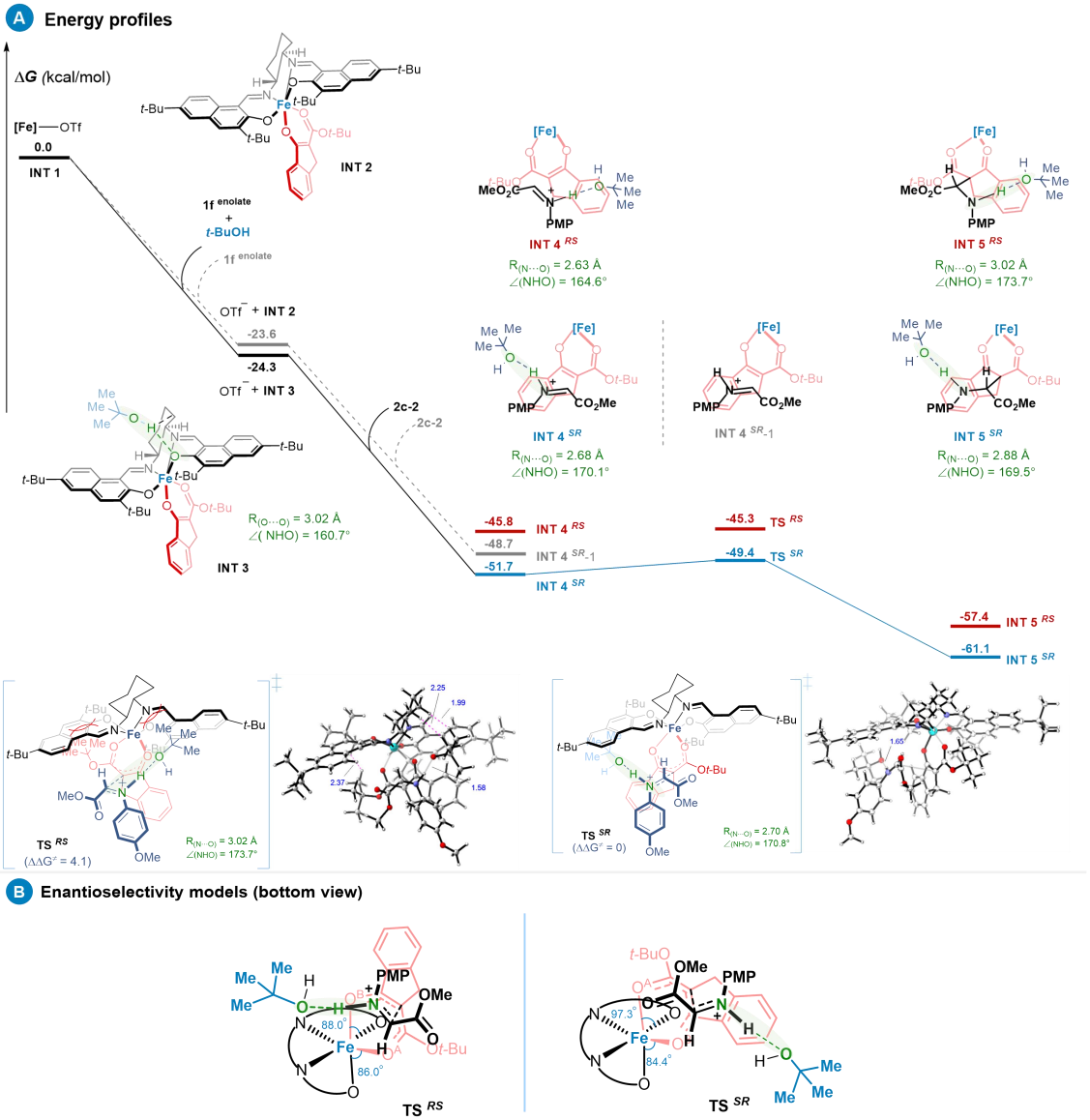
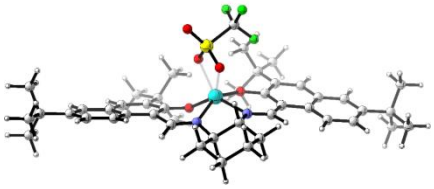
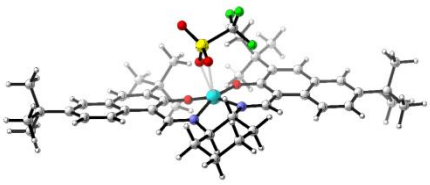


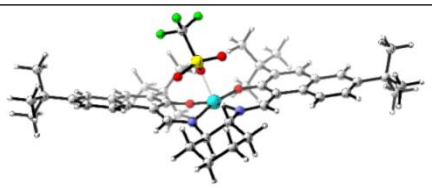
Figure S3. (A) Energy profiles for the asymmetric catalyzed oxidative cross-coupling of **1f** and **2c** after formation of enolate-**1f** and iminium **2c-2**. (B) Enantioselectivity models (bottom view).

9.2 Cartesian Coordinates

Table S7. Coordinates (x,y,z), energy (Hartree) and imaginary frequency (cm^{-1}) of the computed species displayed in Figure 6 and Figure S3 of the manuscript.

INT 1_sextet				INT 1_quartet			
							
E(UPBE1PBE) = -4193.104406 Thermal correction to Gibbs Free Energy = 0.859662				E(UPBE1PBE) = -4193.103565 Thermal correction to Gibbs Free Energy = 0.862200			
C	1.491115	-4.335349	-0.454462	C	-1.448479	4.157827	-0.814163
C	0.643043	-3.125723	-0.091743	C	-0.577432	2.973756	-0.435890
C	-0.646680	-3.085368	-0.917637	C	0.646794	2.872554	-1.339369
C	-1.463187	-4.355953	-0.719459	C	1.498278	4.127778	-1.244687
C	-0.613900	-5.588513	-1.080842	C	0.638197	5.351587	-1.619361
C	0.671680	-5.623879	-0.246180	C	-0.602428	5.444847	-0.720642
H	0.347131	-3.214745	0.962802	H	-0.218078	3.104394	0.593762
H	1.815210	-4.272384	-1.505574	H	-1.835140	4.043999	-1.839825
H	2.389155	-4.380343	0.176793	H	-2.303179	4.245645	-0.129748
H	-1.786041	-4.421129	0.331046	H	1.873402	4.237738	-0.215913
H	-2.361955	-4.349121	-1.349925	H	2.359404	4.076027	-1.924520
H	-1.199498	-6.500947	-0.917018	H	1.240306	6.263298	-1.529401
H	-0.352682	-5.547166	-2.148139	H	0.322255	5.262800	-2.668835
H	0.411509	-5.714800	0.817846	H	-0.285874	5.586045	0.321847
H	1.278815	-6.495920	-0.517078	H	-1.213527	6.309205	-1.006086
H	-0.347966	-3.025775	-1.977747	H	0.291527	2.765824	-2.377784
N	1.259632	-1.809801	-0.225421	N	-1.194921	1.645135	-0.474709
N	-1.318029	-1.830232	-0.597614	N	1.294200	1.611550	-0.972749
C	-2.600096	-1.688917	-0.740570	C	2.587505	1.467695	-0.970604
H	-3.192365	-2.575356	-0.972490	H	3.175311	2.356349	-1.189132
C	2.538977	-1.678896	-0.373450	C	-2.484299	1.488265	-0.581323
H	3.123659	-2.593931	-0.444166	H	-3.064602	2.402746	-0.668490
C	-3.318343	-0.459851	-0.698674	C	3.310387	0.271510	-0.761793
C	-2.629057	0.761136	-0.923161	C	2.629141	-0.970908	-0.820017
C	-4.755365	-0.496410	-0.617118	C	4.746499	0.333277	-0.633288
C	-3.378064	1.976071	-1.176815	C	3.385047	-2.206202	-0.846390
C	-5.470513	0.702363	-0.860540	C	5.466852	-0.885539	-0.662994
C	-5.498262	-1.641663	-0.290240	C	5.481523	1.516006	-0.464680
C	-4.741964	1.894343	-1.141950	C	4.746780	-2.109436	-0.777543
C	-6.871268	0.709627	-0.807530	C	6.865027	-0.882654	-0.562546
C	-6.882023	-1.612480	-0.246911	C	6.863200	1.496536	-0.368057
H	-4.995533	-2.567898	-0.026026	H	4.978202	2.474196	-0.368889
H	-5.332700	2.787772	-1.318808	H	5.342815	-3.016501	-0.787949
C	-7.603234	-0.431895	-0.512645	C	7.590061	0.291705	-0.422503
H	-7.385532	1.649101	-0.999952	H	7.381962	-1.839675	-0.589554
H	-7.414506	-2.518856	0.014054	H	7.388666	2.433677	-0.232152
C	3.288448	-0.465660	-0.426862	C	-3.220603	0.283428	-0.543514
C	2.637752	0.781139	-0.282070	C	-2.549823	-0.945416	-0.315317
C	4.721169	-0.533128	-0.593893	C	-4.661386	0.335965	-0.661473
C	3.395418	2.012935	-0.265840	C	-3.310603	-2.154231	-0.075313
C	5.451363	0.684257	-0.567566	C	-5.385118	-0.864731	-0.453615
C	5.459487	-1.714612	-0.783280	C	-5.403028	1.485392	-0.973930
C	4.751763	1.911944	-0.398792	C	-4.671384	-2.060384	-0.150815
C	6.846678	0.679723	-0.712800	C	-6.784168	-0.874593	-0.540193
C	6.835925	-1.694707	-0.925607	C	-6.785514	1.453638	-1.055888
H	4.967877	-2.681438	-0.831754	H	-4.911054	2.431922	-1.178300
H	5.357930	2.812214	-0.385343	H	-5.273649	-2.946179	0.025237
C	7.566521	-0.490754	-0.890289	C	-7.512318	0.268596	-0.834644
H	7.364478	1.636362	-0.684025	H	-7.299529	-1.817240	-0.367771
H	7.356866	-2.633276	-1.070162	H	-7.312384	2.367551	-1.301756
O	1.347257	0.856415	-0.156265	O	-1.257285	-1.035473	-0.302156
O	-1.331582	0.801688	-0.966657	O	1.334702	-1.042932	-0.903320
Fe	-0.140047	-0.282612	0.098855	Fe	0.095089	0.248229	-0.358938
C	2.690921	3.360769	-0.121886	C	-2.604873	-3.464169	0.266204
C	3.693962	4.518073	-0.103562	C	-3.606925	-4.593822	0.518579

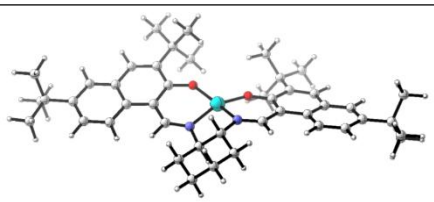
H	4.387136	4.448673	0.743218	H	-4.275235	-4.369566	1.358235
H	4.278026	4.572748	-1.029796	H	-4.216752	-4.812255	-0.366297
H	3.146398	5.461522	-0.004619	H	-3.056486	-5.506248	0.771333
C	1.756259	3.574068	-1.323147	C	-1.705855	-3.893086	-0.904188
H	2.326995	3.578272	-2.259395	H	-2.302507	-4.046938	-1.811359
H	0.996757	2.793545	-1.381026	H	-0.938115	-3.147998	-1.112353
H	1.247287	4.541027	-1.231281	H	-1.208827	-4.839795	-0.661104
C	1.893970	3.420681	1.191888	C	-1.777107	-3.287539	1.550443
H	1.094691	2.680361	1.219385	H	-1.016728	-2.513090	1.448515
H	2.551684	3.252677	2.052342	H	-2.425816	-3.019739	2.392022
H	1.442267	4.414184	1.299390	H	-1.274307	-4.230546	1.796294
C	-2.652323	3.292659	-1.444481	C	2.673075	-3.554784	-0.918623
C	-1.772272	3.162715	-2.698636	C	1.840802	-3.644510	-2.208025
H	-1.036326	2.364572	-2.592439	H	1.095157	-2.850021	-2.260032
H	-2.389946	2.953441	-3.580254	H	2.489915	-3.572539	-3.088949
H	-1.237995	4.104157	-2.874903	H	1.321719	-4.609586	-2.247678
C	-1.799512	3.667432	-0.221369	C	1.779996	-3.724243	0.320760
H	-1.047919	2.909628	-0.002678	H	1.024243	-2.941651	0.383215
H	-1.288085	4.620154	-0.405497	H	1.271483	-4.695114	0.281417
H	-2.431768	3.784940	0.665894	H	2.382775	-3.692028	1.235389
C	-3.634995	4.440410	-1.691493	C	3.667676	-4.719279	-0.933433
H	-4.274566	4.629630	-0.821418	H	4.277456	-4.750995	-0.023044
H	-3.068509	5.357175	-1.887822	H	3.110431	-5.660757	-0.987977
H	-4.274806	4.254782	-2.562441	H	4.336188	-4.681589	-1.801890
O	-0.910870	0.849236	1.744110	O	0.712528	0.060331	1.561116
S	-0.654650	-0.140527	2.849806	S	0.593929	0.968125	2.768087
O	-1.679587	-0.279675	3.860959	O	1.533292	0.614734	3.816732
O	-0.157204	-1.370994	2.165428	O	0.451870	2.380747	2.406161
C	0.835422	0.535999	3.703947	C	-1.065849	0.483456	3.401221
F	1.095324	-0.192552	4.782109	F	-1.368789	1.191511	4.484232
F	0.615051	1.793874	4.061684	F	-1.091047	-0.809701	3.707494
F	1.887083	0.492691	2.888945	F	-2.002651	0.713281	2.471500
C	9.087009	-0.442417	-1.041288	C	-9.037921	0.210448	-0.908507
C	9.444616	0.410384	-2.274050	C	-9.455170	-0.804452	-1.990082
C	9.697986	0.191312	0.223563	C	-9.588596	-0.232441	0.460833
C	9.695318	-1.840114	-1.226048	C	-9.651642	1.573463	-1.259993
H	9.010428	-0.031962	-3.177930	H	-9.062383	-0.499233	-2.966677
H	9.061343	1.431282	-2.168830	H	-9.071846	-1.804271	-1.758529
H	10.534764	0.458580	-2.390012	H	-10.549657	-0.857569	-2.047965
H	9.443083	-0.406397	1.106103	H	-9.293989	0.484484	1.235571
H	10.790218	0.236122	0.127559	H	-10.683939	-0.285116	0.422760
H	9.320413	1.208834	0.372941	H	-9.202526	-1.219871	0.737209
H	10.783014	-1.745331	-1.327301	H	-10.742720	1.473531	-1.300438
H	9.486558	-2.479531	-0.359803	H	-9.405304	2.325204	-0.500435
H	9.308168	-2.322390	-2.131755	H	-9.303923	1.923720	-2.239531
C	-9.130190	-0.372992	-0.468016	C	9.114363	0.242947	-0.315136
C	-9.566177	0.649059	0.599522	C	9.505721	-0.595148	0.917530
C	-9.657088	0.060965	-1.849456	C	9.687501	-0.406937	-1.589432
C	-9.751344	-1.733135	-0.118228	C	9.729452	1.641824	-0.165512
H	-9.188285	0.350877	1.584041	H	9.095851	-0.142435	1.827451
H	-9.179250	1.647363	0.367571	H	9.120392	-1.617457	0.835455
H	-10.661622	0.701606	0.639402	H	10.598598	-0.641732	1.004231
H	-9.352179	-0.662826	-2.613908	H	9.410403	0.181982	-2.471303
H	-10.752794	0.116961	-1.829384	H	10.781800	-0.454230	-1.523220
H	-9.263708	1.045258	-2.126662	H	9.303284	-1.424931	-1.716756
H	-10.843246	-1.633935	-0.105287	H	10.819704	1.546371	-0.098980
H	-9.485241	-2.492216	-0.863759	H	9.492992	2.272347	-1.031263
H	-9.427323	-2.072944	0.872906	H	9.373065	2.134041	0.747323
INT 1_doublet				**[LFe]$^+$**			



E(UPBE1PBE) = -4193.071733

Thermal correction to Gibbs Free Energy = 0.863424

C	1.665163	-3.987607	-1.527765
C	0.802466	-2.870070	-0.967045
C	-0.447684	-2.669628	-1.825940
C	-1.296358	-3.928498	-1.846391
C	-0.450453	-5.095753	-2.393967
C	0.829698	-5.284358	-1.566805
H	0.476338	-3.164297	0.039939
H	2.011099	-3.731253	-2.541144
H	2.546341	-4.162114	-0.896889
H	-1.637185	-4.151886	-0.824661
H	-2.179516	-3.797593	-2.486025
H	-1.044777	-6.016972	-2.383595
H	-0.179942	-4.885235	-3.438812
H	0.557609	-5.559521	-0.538358
H	1.433575	-6.099155	-1.983328
H	-0.108275	-2.456819	-2.853246
N	1.416508	-1.536870	-0.831041
N	-1.086101	-1.448770	-1.326993
C	-2.372952	-1.327043	-1.206809
H	-2.986457	-2.192000	-1.447871
C	2.706677	-1.410401	-0.657895
H	3.282786	-2.328005	-0.718898
C	-3.060946	-0.133744	-0.858633
C	-2.400254	1.118278	-0.952778
C	-4.470160	-0.209589	-0.578421
C	-3.178801	2.341922	-0.937853
C	-5.213108	0.995715	-0.551206
C	-5.152677	-1.405256	-0.305809
C	-4.528791	2.228789	-0.753665
C	-6.593766	0.964761	-0.310396
C	-6.517352	-1.412321	-0.071389
H	-4.606555	-2.340565	-0.220525
H	-5.138703	3.126273	-0.729207
C	-7.273355	-0.223068	-0.080392
H	-7.133255	1.909736	-0.298473
H	-7.004848	-2.355481	0.142764
C	3.440092	-0.228374	-0.404211
C	2.777829	1.028113	-0.295954
C	4.879964	-0.319200	-0.266023
C	3.539603	2.234951	-0.032033
C	5.602181	0.878042	-0.032155
C	5.624530	-1.506583	-0.346917
C	4.893266	2.110530	0.077699
C	6.996853	0.853050	0.103149
C	7.002695	-1.509965	-0.208856
H	5.140611	-2.464056	-0.513891
H	5.495164	2.992461	0.273439
C	7.725367	-0.324319	0.019528
H	7.507941	1.796703	0.283105
H	7.529013	-2.454271	-0.276468
O	1.497378	1.151825	-0.434540
O	-1.110313	1.207984	-1.112110
Fe	0.145557	-0.133431	-0.691640
C	2.830252	3.575240	0.147790
C	3.825300	4.708867	0.410908
H	4.404216	4.545282	1.327357



E(UPBE1PBE) = -3231.892635

Thermal correction to Gibbs Free Energy = 0.840514

C	1.440021	4.150300	-0.371226
C	0.576963	2.895156	-0.520544
C	-0.577047	2.895136	0.520900
C	-1.440103	4.150286	0.371648
C	-0.562738	5.404534	0.520587
C	0.562671	5.404568	-0.520054
H	0.106008	2.899965	-1.517321
H	1.917838	4.149843	0.619275
H	2.224935	4.168129	-1.137805
H	-1.917893	4.149922	-0.618866
H	-2.225034	4.168055	1.138213
H	-1.184808	6.299369	0.406902
H	-0.128994	5.427448	1.530074
H	0.128921	5.427571	-1.529536
H	1.184748	6.299389	-0.406298
H	-0.106067	2.899926	1.517669
N	1.260812	1.603726	-0.356964
N	-1.260872	1.603692	0.357316
C	-2.564104	1.520134	0.314572
H	-3.112753	2.448808	0.446952
C	2.564041	1.520129	-0.314467
H	3.112702	2.448777	-0.446996
C	-3.363629	0.364345	0.095321
C	-2.773663	-0.894106	-0.203345
C	-4.802547	0.495373	0.141213
C	-3.567953	-2.053079	-0.491938
C	-5.579978	-0.657530	-0.152719
C	-5.497585	1.673348	0.460340
C	-4.927915	-1.883192	-0.459386
C	-6.981082	-0.593143	-0.134213
C	-6.880594	1.712756	0.470732
H	-4.973084	2.587468	0.721125
H	-5.572506	-2.729475	-0.673495
C	-7.659669	0.576715	0.169897
H	-7.537860	-1.498009	-0.365230
H	-7.373067	2.643674	0.722753
C	3.363605	0.364345	-0.095284
C	2.773675	-0.894109	0.203485
C	4.802510	0.495383	-0.141336
C	3.568010	-2.053044	0.492068
C	5.579987	-0.657484	0.152641
C	5.497518	1.673333	-0.460652
C	4.927967	-1.883128	0.459446
C	6.981089	-0.593079	0.134016
C	6.880522	1.712755	-0.471162
H	4.972980	2.587413	-0.721499
H	5.572581	-2.729386	0.673590
C	7.659635	0.576752	-0.170275
H	7.537898	-1.497912	0.365088
H	7.372967	2.643653	-0.723317
O	1.471481	-1.019743	0.220425
O	-1.471463	-1.019740	-0.220193
Fe	0.000002	0.066522	0.000263
C	2.917335	-3.399727	0.813504
C	3.973853	-4.473707	1.088142
H	4.620685	-4.647379	0.220546

H	4.523054	4.847086	-0.423748
H	3.271369	5.645456	0.535984
C	2.041940	3.941544	-1.120726
H	2.716820	4.020406	-1.981567
H	1.272475	3.202876	-1.345167
H	1.555463	4.914721	-0.983275
C	1.895301	3.490633	1.366686
H	1.160907	2.690892	1.261189
H	2.475388	3.308363	2.278829
H	1.357897	4.438499	1.489723
C	-2.498066	3.700711	-1.091767
C	-1.744865	3.772048	-2.430095
H	-0.976316	3.000806	-2.497297
H	-2.439289	3.648600	-3.269679
H	-1.262515	4.751889	-2.530610
C	-1.527868	3.916918	0.079368
H	-0.760360	3.143908	0.105225
H	-1.034738	4.891726	-0.020067
H	-2.067003	3.903560	1.033748
C	-3.511905	4.848263	-1.073957
H	-4.060138	4.898614	-0.125989
H	-2.977062	5.796730	-1.194045
H	-4.236981	4.771725	-1.893014
O	-0.481254	-0.294438	1.116276
S	-0.667153	-1.573594	1.950433
O	-1.721446	-2.454046	1.452256
O	0.600876	-2.185800	2.329769
C	-1.350012	-0.750258	3.450692
F	-1.607269	-1.679596	4.365582
F	-2.473525	-0.112986	3.148148
F	-0.471965	0.114343	3.941551
C	9.245474	-0.301061	0.176999
C	9.851826	0.578332	-0.933652
C	9.600255	0.284886	1.557286
C	9.859350	-1.704634	0.075290
H	9.607067	0.164465	-1.918597
H	9.461329	1.600594	-0.880353
H	10.943115	0.616589	-0.825279
H	9.167229	-0.333195	2.351972
H	10.690153	0.312128	1.681766
H	9.214181	1.304706	1.662056
H	10.946024	-1.627474	0.198166
H	9.471425	-2.362656	0.862166
H	9.656750	-2.154884	-0.903990
C	-8.780457	-0.204067	0.176081
C	-9.068195	0.641102	1.432083
C	-9.490324	0.417114	-1.042444
C	-9.347553	-1.613264	0.400608
H	-8.560584	0.208533	2.301723
H	-8.715842	1.670101	1.301290
H	-10.148184	0.664970	1.625538
H	-9.290772	-0.179231	-1.940132
H	-10.573371	0.445807	-0.868102
H	-9.140111	1.439955	-1.220260
H	-10.428953	-1.540163	0.566760
H	-9.177023	-2.251245	-0.474975
H	-8.897657	-2.084450	1.282714

$CF_3SO_3^-$

E(RPBE1PBE) = -961.029680

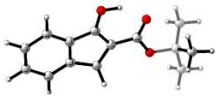
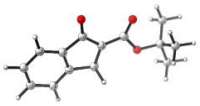
Thermal correction to Gibbs Free Energy= -0.004339

H	4.602502	-4.222198	1.950059
H	3.471120	-5.419078	1.315166
C	2.042186	-3.280985	2.072797
H	2.637652	-2.951756	2.931785
H	1.217450	-2.579361	1.932204
H	1.614523	-4.260337	2.315703
C	2.069238	-3.875545	-0.378592
H	1.251178	-3.186984	-0.599679
H	2.687309	-3.983284	-1.276984
H	1.634407	-4.855331	-0.149972
C	-2.917225	-3.399755	-0.813318
C	-2.069219	-3.875570	0.378842
H	-1.251211	-3.186972	0.600004
H	-2.687365	-3.983348	1.277178
H	-1.634335	-4.855336	0.150245
C	-2.041954	-3.280975	-2.072532
H	-1.217218	-2.579378	-1.931830
H	-1.614291	-4.260329	-2.315436
H	-2.637336	-2.951703	-2.931560
C	-3.973684	-4.473757	-1.088090
H	-4.602266	-4.222226	-1.950047
H	-3.470896	-5.419099	-1.315115
H	-4.620578	-4.647496	-0.220555
C	9.186423	0.600744	-0.178059
C	9.699392	0.222549	1.225441
C	9.698708	-0.420121	-1.213228
C	9.741485	1.985049	-0.542730
H	9.340472	0.942674	1.969446
H	9.359441	-0.778171	1.514660
H	10.795899	0.228140	1.229311
H	9.337320	-0.161481	-2.214955
H	10.795253	-0.415603	-1.221392
H	9.360952	-1.433782	-0.970516
H	10.836372	1.941857	-0.530205
H	9.426932	2.288675	-1.548700
H	9.424520	2.744695	0.182167
C	-9.186464	0.600692	0.177512
C	-9.699226	0.222734	-1.226127
C	-9.698891	-0.420357	1.212423
C	-9.741602	1.984922	0.542352
H	-9.340233	0.943011	-1.969950
H	-9.359171	-0.777916	-1.515467
H	-10.795733	0.228269	-1.230155
H	-9.337656	-0.161892	2.214251
H	-10.795437	-0.415847	1.220421
H	-9.361101	-1.433976	0.969585
H	-10.836488	1.941683	0.529780
H	-9.427093	2.288422	1.548374
H	-9.424655	2.744688	-0.182427

HOTf

E(RPBE1PBE) = -961.515266

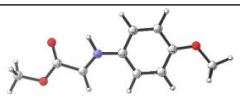
Thermal correction to Gibbs Free Energy= 0.005909

O	1.231635	1.275776	0.662784	O	-1.793755	-0.316390	0.000000
S	0.915153	-0.000035	0.000048	S	-0.254647	-0.819295	0.000000
O	1.232049	-0.063989	-1.436060	O	0.062639	-1.450594	1.261810
O	1.231439	-1.211954	0.773561	O	0.062639	-1.450594	-1.261810
C	-0.931199	0.000036	-0.000002	C	0.453991	0.891847	0.000000
F	-1.430342	-1.105729	-0.576459	F	1.771842	0.766368	0.000000
F	-1.430016	1.052090	-0.669524	F	0.062639	1.538824	1.082810
F	-1.430336	0.053827	1.245645	F	0.062639	1.538824	-1.082810
				H	-2.375859	-1.097892	0.000000
CF_3CO^-				**TFA**			
							
E(RPBE1PBE) = -525.919727				E(RPBE1PBE) = -526.444680			
Thermal correction to Gibbs Free Energy= -0.005146				Thermal correction to Gibbs Free Energy= 0.008361			
C	0.511848	0.013900	0.000001	C	0.599429	-0.000422	0.000000
C	-1.057666	0.009534	-0.000008	C	-0.930413	0.156648	-0.000028
O	-1.582998	1.134970	0.000015	O	-1.492549	1.215673	-0.000025
O	-1.520699	-1.144954	-0.000033	O	-1.511028	-1.042838	0.000012
F	1.025288	-0.625337	1.081966	H	-2.472470	-0.892121	0.000021
F	1.072124	1.244046	-0.000064	F	0.992941	-0.674861	1.083700
F	1.025307	-0.625457	-1.081882	F	1.179304	1.191141	-0.000032
				F	0.992976	-0.674937	-1.083640
1f ^{enol}				**1f** ^{enolate}			
							
E(RPBE1PBE) = -768.186448				E(RPBE1PBE) = - -767.627207			
Thermal correction to Gibbs Free Energy= 0.233515				Thermal correction to Gibbs Free Energy= 0.218350			
C	-2.438644	0.458144	0.000263	C	-2.454254	0.479593	-0.000008
C	-2.253665	-0.934814	0.000078	C	-2.140224	-0.880143	-0.000205
C	-3.356688	-1.774949	-0.000090	C	-3.154979	-1.829235	-0.000204
C	-4.632390	-1.208365	-0.000110	C	-4.485126	-1.400233	0.000047
C	-4.806870	0.178027	0.000004	C	-4.792900	-0.036682	0.000303
C	-3.707036	1.030021	0.000194	C	-3.773610	0.913919	0.000278
C	-0.150670	0.103481	-0.000072	C	-0.130810	0.367793	-0.000354
C	-0.781240	-1.258835	-0.000055	C	-0.644430	-1.050138	-0.000229
H	-3.235518	-2.855280	-0.000161	H	-2.922859	-2.893840	-0.000416
H	-5.504912	-1.856038	-0.000351	H	-5.289197	-2.134139	0.000004
H	-5.811191	0.592016	-0.000108	H	-5.835405	0.277893	0.000537
H	-3.826049	2.109289	0.000270	H	-3.975240	1.982898	0.000436
H	-0.496589	-1.852275	-0.879387	H	-0.315316	-1.633867	-0.875535
H	-0.496309	-1.852148	0.879283	H	-0.315661	-1.633410	0.875568
C	-1.120737	1.074040	0.000156	C	-1.201965	1.314875	-0.000127
O	-0.937022	2.382136	0.000041	O	-1.233817	2.553041	0.000047
C	1.237516	0.472719	-0.000268	C	1.248745	0.682614	-0.000381
O	1.603763	1.655327	-0.000361	O	1.801922	1.778498	-0.000258
O	2.065252	-0.575052	-0.000359	O	2.002375	-0.504426	-0.000578
C	3.513615	-0.405173	0.000060	C	3.426662	-0.451197	0.000140
C	3.956452	0.318082	-1.265428	C	3.953763	0.233051	-1.261528
C	3.955955	0.319187	1.265093	C	3.952513	0.232272	1.262745
C	4.016033	-1.841818	0.000855	C	3.834638	-1.922172	-0.000130
H	3.577214	-0.202800	-2.150894	H	3.545805	-0.264906	-2.148715
H	3.595560	1.347582	-1.276922	H	3.641291	1.278081	-1.271142
H	5.050452	0.325941	-1.316703	H	5.049056	0.171098	-1.301881
H	3.574291	-0.199614	2.150745	H	3.544564	-0.266831	2.149300
H	5.049894	0.324738	1.318029	H	5.047834	0.171229	1.303591
H	3.597185	1.349444	1.274642	H	3.639206	1.277047	1.273069
H	5.110374	-1.857252	0.000269	H	4.926629	-2.023661	0.000747
H	3.660039	-2.372846	0.889232	H	3.432896	-2.425538	0.885912
H	3.659084	-2.374047	-0.886411	H	3.434401	-2.424856	-0.887244
H	0.050748	2.495531	-0.000197				
***t*-BuOH**				**2c-2**			

E(RPBE1PBE) = -233.474250

Thermal correction to Gibbs Free Energy= 0.108271

O	-0.018537	-0.000766	1.444059
H	-0.947913	0.011229	1.711797
C	0.005327	-0.000203	0.017886
C	-0.700156	-1.247682	-0.510073
C	-0.667594	1.265711	-0.508702
C	1.481312	-0.018575	-0.351278
H	-0.234118	-2.147321	-0.095961
H	-1.759305	-1.246234	-0.221360
H	-0.654880	-1.301826	-1.603385
H	-0.177471	2.152476	-0.094601
H	-0.622196	1.319429	-1.602108
H	-1.726032	1.292225	-0.218705
H	1.611645	-0.018408	-1.438076
H	1.983806	0.861077	0.063027
H	1.961425	-0.912024	0.059904

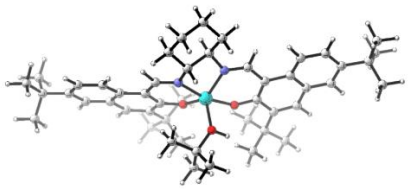


E(UPBE1PBE) = -667.895606

Thermal correction to Gibbs Free Energy = 0.172920

C	-1.939671	-0.533785	0.000194
H	-1.733822	-1.597116	0.000564
N	-0.999274	0.354396	-0.000078
C	0.384155	0.256602	-0.000105
C	1.051433	-0.976907	-0.000283
C	1.111836	1.461519	0.000043
C	2.428903	-1.009714	-0.000200
H	0.502267	-1.913283	-0.000577
C	2.483895	1.431984	0.000142
H	0.589518	2.415302	0.000133
C	3.162758	0.196396	0.000074
H	2.937455	-1.966166	-0.000417
H	3.070058	2.344208	0.000285
O	4.482895	0.268383	0.000227
C	5.258196	-0.927712	-0.000004
H	5.058296	-1.518340	-0.899793
H	6.296176	-0.599258	0.000206
H	5.058125	-1.518791	0.899453
C	-3.315414	0.036109	0.000007
O	-3.481398	1.236958	-0.000355
O	-4.226361	-0.908130	0.000256
C	-5.596704	-0.456579	0.000100
H	-6.196398	-1.363952	0.000444
H	-5.785748	0.141725	0.893388
H	-5.785761	0.141038	-0.893647
H	-1.392652	1.308689	-0.000324

[LFe(*t*-BuOH)]$^+$

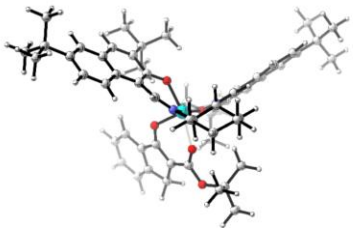


E(UPBE1PBE) = -3465.422068

Thermal correction to Gibbs Free Energy = 0.971785

C	-1.458157	4.240892	0.173311
C	-0.602150	2.995011	0.407050
C	0.585757	2.940605	-0.583949
C	1.443270	4.206055	-0.464326
C	0.575336	5.458026	-0.677856
C	-0.585149	5.496681	0.322155
H	-0.170153	3.046260	1.421154
H	-1.883932	4.211613	-0.840206
H	-2.282967	4.275249	0.896895
H	1.900847	4.234300	0.535314
H	2.244906	4.202722	-1.212603
H	1.198483	6.353416	-0.572939
H	0.174371	5.451345	-1.701173
H	-0.187354	5.546382	1.345469
H	-1.196840	6.391125	0.159249
H	0.155584	2.885686	-1.597479
N	-1.273921	1.699892	0.286051
N	1.272211	1.665833	-0.312918
C	2.563069	1.565105	-0.464259
H	3.087644	2.465832	-0.773512
C	-2.549942	1.608515	0.046376
H	-3.111594	2.539046	0.000048

IINT 2



E(UPBE1PBE) = -3999.744730

Thermal correction to Gibbs Free Energy = 1.087452

C	1.696103	-0.892449	4.474278
C	0.898178	-0.354458	3.286531
C	-0.360151	-1.231718	3.060033
C	-1.258858	-1.129835	4.300944
C	-0.487000	-1.607713	5.542180
C	0.812385	-0.807477	5.731608
H	0.542589	0.655718	3.526129
H	1.983355	-1.938725	4.295256
H	2.610016	-0.300672	4.615324
H	-1.564050	-0.081629	4.419899
H	-2.165694	-1.732963	4.170277
H	-1.120162	-1.514399	6.432931
H	-0.237285	-2.671676	5.420382
H	0.563156	0.246462	5.920641
H	1.362722	-1.182597	6.602843
H	-0.012861	-2.272981	2.941766
N	1.554528	-0.268667	1.996266
N	-0.992019	-0.788859	1.813970
C	-2.091406	-1.361004	1.437432
H	-2.491801	-2.140337	2.090416
C	2.710350	-0.792183	1.754949
H	3.299598	-1.155373	2.600836

C	3.385518	0.414967	-0.302185	C	-2.876662	-1.064923	0.281141
C	2.812509	-0.859698	-0.069966	C	-2.536120	0.027479	-0.556863
C	4.817891	0.556809	-0.440982	C	-4.059281	-1.850183	0.017566
C	3.621979	-2.047299	-0.021458	C	-3.438638	0.451560	-1.610661
C	5.606762	-0.622749	-0.386582	C	-4.908190	-1.446183	-1.046502
C	5.496396	1.774411	-0.611846	C	-4.433441	-3.005830	0.725270
C	4.971705	-1.878577	-0.184746	C	-4.566923	-0.292228	-1.808465
C	7.001689	-0.552017	-0.521132	C	-6.069733	-2.173407	-1.344525
C	6.873618	1.819394	-0.742237	C	-5.584084	-3.709232	0.412660
H	4.962745	2.719996	-0.630802	H	-3.811633	-3.394851	1.525921
H	5.622817	-2.746060	-0.155313	H	-5.261423	-0.014121	-2.595374
C	7.662793	0.651807	-0.704124	C	-6.436320	-3.305616	-0.633394
H	7.567937	-1.479322	-0.476186	H	-6.689501	-1.824684	-2.168652
H	7.352638	2.782005	-0.871905	H	-5.821888	-4.596883	0.986586
C	-3.301746	0.422678	-0.186697	C	3.260588	-1.012057	0.453153
C	-2.651283	-0.820890	-0.395542	C	2.391328	-1.113802	-0.664746
C	-4.739507	0.522822	-0.299888	C	4.661796	-1.309549	0.330728
C	-3.386421	-1.987042	-0.805353	C	2.905962	-1.597956	-1.933012
C	-5.455671	-0.639953	-0.685880	C	5.146418	-1.776206	-0.917713
C	-5.486675	1.682680	-0.040726	C	5.596154	-1.148840	1.368051
C	-4.743722	-1.846386	-0.931233	C	4.234853	-1.908279	-2.004001
C	-6.851420	-0.600255	-0.824199	C	6.504860	-2.084810	-1.075814
C	-6.863284	1.698599	-0.185172	C	6.931997	-1.466910	1.191239
H	-5.008251	2.596155	0.300168	H	5.288130	-0.736548	2.324945
H	-5.339270	-2.700846	-1.235547	H	4.651292	-2.266744	-2.940348
C	-7.581054	0.554454	-0.588293	C	7.418234	-1.948621	-0.040683
H	-7.362219	-1.511647	-1.126020	H	6.837867	-2.435653	-2.050756
H	-7.397999	2.616381	0.025533	H	7.616267	-1.325081	2.019161
O	-1.356527	-0.931753	-0.243753	O	1.124549	-0.850914	-0.574234
O	1.520751	-0.980575	0.093579	O	-1.437506	0.689650	-0.397750
Fe	0.042981	0.152373	0.340008	Fe	0.230398	0.455918	0.554270
C	-2.671161	-3.303207	-1.115655	C	1.982348	-1.712572	-3.144771
C	-3.666399	-4.397655	-1.513350	C	2.716837	-2.274734	-4.365352
H	-4.377739	-4.619826	-0.709349	H	3.546458	-1.631057	-4.680688
H	-4.229370	-4.136126	-2.416451	H	3.108362	-3.282513	-4.181811
H	-3.116372	-5.319442	-1.728693	H	2.015714	-2.340067	-5.204655
C	-1.707685	-3.098454	-2.296565	C	0.803866	-2.654166	-2.845072
H	-2.255296	-2.782225	-3.191375	H	1.168059	-3.654551	-2.582064
H	-0.946204	-2.348206	-2.073356	H	0.189561	-2.280010	-2.025343
H	-1.199455	-4.041827	-2.527425	H	0.174289	-2.748088	-3.738317
C	-1.899018	-3.810249	0.113501	C	1.463596	-0.314387	-3.517019
H	-1.092125	-3.130850	0.393363	H	0.950933	0.159120	-2.679329
H	-2.571139	-3.936827	0.970727	H	2.296335	0.330691	-3.822562
H	-1.454834	-4.787106	-0.109634	H	0.763642	-0.386033	-4.358671
C	2.992450	-3.423150	0.200043	C	-3.130734	1.697064	-2.442494
C	2.014135	-3.744326	-0.941499	C	-1.790024	1.546383	-3.178828
H	1.202327	-3.017248	-0.997901	H	-0.960835	1.433510	-2.481634
H	2.536709	-3.757211	-1.904356	H	-1.808438	0.672210	-3.840288
H	1.574169	-4.736078	-0.783436	H	-1.602394	2.435896	-3.792470
C	2.255717	-3.460318	1.549754	C	-3.084449	2.928120	-1.521945
H	1.408593	-2.771019	1.557491	H	-2.310311	2.823571	-0.760103
H	1.865719	-4.468059	1.732777	H	-2.861776	3.824148	-2.114847
H	2.935943	-3.208972	2.372807	H	-4.052075	3.077455	-1.027302
C	4.053484	-4.526994	0.228008	C	-4.210036	1.949806	-3.498315
H	4.773101	-4.389752	1.043548	H	-5.196859	2.114396	-3.049568
H	3.561377	-5.492592	0.383106	H	-3.950779	2.851303	-4.064105
H	4.604377	-4.590052	-0.717039	H	-4.285270	1.121786	-4.213024
C	-9.099434	0.552349	-0.758684	C	8.890719	-2.290187	-0.269370
C	-9.437932	0.178549	-2.215074	C	9.008431	-3.761800	-0.710734
C	-9.710435	-0.485962	0.202582	C	9.454357	-1.371103	-1.370484
C	-9.717779	1.923785	-0.451261	C	9.733367	-2.097838	0.999843
H	-9.002193	0.908980	-2.906112	H	8.610935	-4.422105	0.068523
H	-9.050706	-0.814870	-2.467155	H	8.448493	-3.940154	-1.635437
H	-10.526169	0.169312	-2.350372	H	10.061514	-4.014384	-0.888364

H	-9.466980	-0.232412	1.240639
H	-10.801032	-0.497589	0.088504
H	-9.331472	-1.491908	-0.009660
H	-10.802888	1.862742	-0.592330
H	-9.527158	2.222712	0.586673
H	-9.330638	2.695124	-1.128144
C	9.183662	0.678148	-0.845868
C	9.815412	0.094909	0.433332
C	9.587829	-0.175742	-2.063836
C	9.721109	2.101678	-1.050366
H	9.529876	0.693946	1.305537
H	9.490667	-0.938616	0.598041
H	10.908196	0.102689	0.341804
H	9.140555	0.230514	-2.978095
H	10.679070	-0.170312	-2.171852
H	9.258877	-1.214188	-1.946072
H	10.811501	2.058051	-1.151674
H	9.313619	2.552604	-1.963350
H	9.486342	2.742994	-0.192096
O	0.305616	-0.083702	2.388782
H	1.110517	-0.621386	2.479158
C	-0.593257	-0.390630	3.517403
C	-0.921995	-1.873343	3.473293
C	0.156610	-0.005032	4.781679
C	-1.828428	0.461970	3.310998
H	-1.400428	-2.137400	2.525688
H	-0.020838	-2.485754	3.593214
H	-1.606584	-2.128258	4.288358
H	0.424628	1.055666	4.765573
H	-0.467149	-0.192420	5.660908
H	1.072538	-0.597230	4.894279
H	-2.504201	0.329950	4.161103
H	-1.565600	1.522269	3.244019
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H	9.366542	-0.321926	-1.066108
H	10.512311	-1.603833	-1.546831
H	8.906802	-1.505999	-2.309677
H	10.774159	-2.365818	0.782000
H	9.712026	-1.053425	1.333816
H	9.375135	-2.742258	1.811774
C	-7.711995	-4.063496	-0.999625
C	-8.921339	-3.124344	-0.827808
C	-7.620778	-4.530175	-2.465229
C	-7.926452	-5.297745	-0.110959
H	-8.993296	-2.789802	0.213426
H	-8.823287	-2.241618	-1.469265
H	-9.845804	-3.650714	-1.097398
H	-6.759469	-5.195106	-2.595995
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H	-7.504511	-3.675914	-3.141172
H	-8.850754	-5.802280	-0.416816
H	-7.097372	-6.008151	-0.215134
H	-8.024679	-5.012582	0.943515
C	0.944490	3.948344	-1.724594
C	0.274900	5.162277	-1.522673
C	0.306376	6.138682	-2.509064
C	1.007345	5.878031	-3.687521
C	1.669021	4.661200	-3.881804
C	1.643380	3.679147	-2.896874
C	-0.077823	3.789481	0.347945
C	-0.414136	5.154663	-0.182989
H	-0.208184	7.087001	-2.373929
H	1.036548	6.631996	-4.469855
H	2.203389	4.483902	-4.811095
H	2.142225	2.723305	-3.026721
H	-1.497832	5.302575	-0.287289
H	-0.050546	5.964234	0.464970
C	0.717421	3.084985	-0.558500
O	1.166623	1.888280	-0.481313
C	-0.552969	3.208382	1.540385
O	-0.279980	2.043075	1.923129
O	-1.348341	4.005743	2.261324
C	-2.142018	3.497863	3.369825
C	-3.032252	2.350035	2.904128
C	-1.239123	3.102975	4.532451
C	-2.989969	4.705375	3.746838
H	-3.607979	2.653015	2.022944
H	-2.451423	1.462934	2.647600
H	-3.739241	2.093378	3.700878
H	-0.580872	3.936236	4.800168
H	-1.851867	2.855692	5.406582
H	-0.623529	2.240004	4.276974
H	-3.644125	4.458532	4.589040
H	-2.352387	5.547674	4.033489
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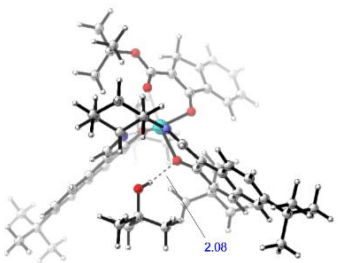
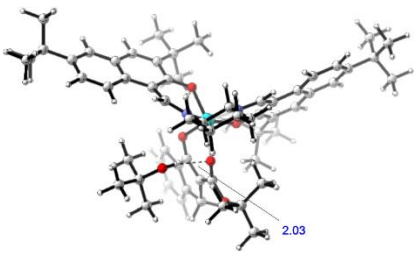
INT 3



E(UPBE1PBE) = -4233.242454

Thermal correction to Gibbs Free Energy = 1.218133

INT 3'



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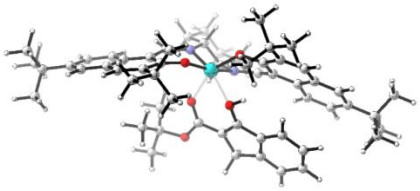
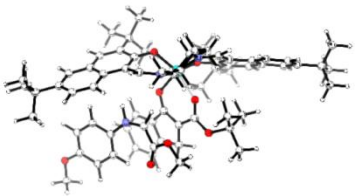
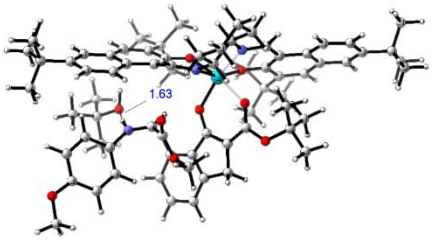
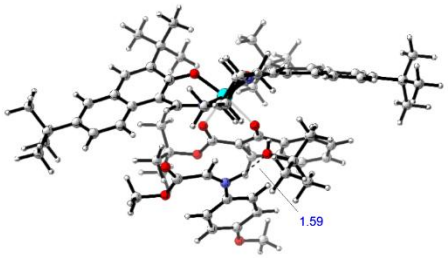
C	0.930978	0.477757	3.297563	C	-0.689394	0.325536	-3.075700
C	-0.246489	-0.517944	3.172472	C	0.631682	-0.466958	-3.194324
C	-1.123001	-0.411343	4.425997	C	1.433041	0.083017	-4.383478
C	-0.277957	-0.752348	5.664769	C	0.597307	-0.022814	-5.670830
C	0.958983	0.157824	5.761470	C	-0.738513	0.723285	-5.527614
H	0.507205	1.470866	3.494929	H	-0.413820	1.381201	-2.971696
H	2.164524	-0.962765	4.350056	H	-1.790239	-0.877554	-4.507404
H	2.681336	0.733678	4.555001	H	-2.464023	0.755675	-4.202188
H	-1.512614	0.611834	4.499602	H	1.677509	1.133669	-4.177053
H	-1.977491	-1.095795	4.348628	H	2.374566	-0.465843	-4.506785
H	-0.886452	-0.655835	6.572331	H	1.168620	0.381093	-6.515647
H	0.052811	-1.798496	5.592960	H	0.395325	-1.083147	-5.881281
H	0.632124	1.198375	5.900519	H	-0.542801	1.792627	-5.364444
H	1.564669	-0.121317	6.632187	H	-1.325663	0.627706	-6.448854
H	0.185071	-1.528187	3.096282	H	0.368999	-1.522322	-3.380214
N	1.528429	0.539586	1.972247	N	-1.272509	-0.092855	-1.815146
N	-0.945567	-0.227902	1.919126	N	1.305860	-0.362105	-1.891638
C	-1.843304	-1.074448	1.529668	C	2.505577	-0.835320	-1.773395
H	-2.045088	-1.915835	2.194161	H	2.954152	-1.269738	-2.668665
C	2.654637	-0.027584	1.703645	C	-2.396291	-0.721248	-1.733800
H	3.250892	-0.399582	2.538887	H	-3.016118	-0.786981	-2.629641
C	-2.624241	-1.018463	0.334048	C	3.336664	-0.836141	-0.611241
C	-2.525811	0.096096	-0.535001	C	2.907374	-0.197453	0.579005
C	-3.548680	-2.088001	0.051743	C	4.639000	-1.456525	-0.684258
C	-3.450307	0.245238	-1.641281	C	3.806828	-0.073519	1.710103
C	-4.403957	-1.956494	-1.074111	C	5.490085	-1.359817	0.448427
C	-3.656897	-3.274934	0.799884	C	5.135326	-2.168204	-1.791037
C	-4.332672	-0.774015	-1.864523	C	5.037568	-0.655234	1.599615
C	-5.310676	-2.976257	-1.399904	C	6.763594	-1.947285	0.434978
C	-4.557102	-4.269001	0.457248	C	6.396840	-2.737886	-1.783243
H	-3.016125	-3.452084	1.658353	H	4.531448	-2.306504	-2.682671
H	-5.029217	-0.707584	-2.694798	H	5.734398	-0.595255	2.429885
C	-5.411787	-4.141243	-0.655514	C	7.246758	-2.639607	-0.664027
H	-5.944672	-2.833636	-2.273123	H	7.377296	-1.848926	1.328430
H	-4.594234	-5.166551	1.062727	H	6.728054	-3.277506	-2.662516
C	3.179160	-0.269498	0.390629	C	-2.867609	-1.411535	-0.574036
C	2.303811	-0.332287	-0.718538	C	-1.938727	-1.849326	0.405304
C	4.566917	-0.620552	0.256148	C	-4.247089	-1.809231	-0.518371
C	2.813574	-0.701654	-2.024881	C	-2.366049	-2.783585	1.430801
C	5.030874	-1.063690	-1.009442	C	-4.648985	-2.711583	0.498757
C	5.507533	-0.553032	1.299308	C	-5.237460	-1.342532	-1.400535
C	4.128628	-1.069414	-2.109172	C	-3.676631	-3.172089	1.431930
C	6.367972	-1.454152	-1.175158	C	-5.985588	-3.126577	0.583752
C	6.820671	-0.947880	1.113572	C	-6.550830	-1.768359	-1.298743
H	5.223901	-0.163208	2.272554	H	-4.991584	-0.610338	-2.165100
H	4.540123	-1.371119	-3.067246	H	-4.028539	-3.862909	2.191944
C	7.281394	-1.418201	-0.132997	C	-6.955303	-2.677987	-0.301156
H	6.682243	-1.789456	-2.161671	H	-6.255741	-3.819007	1.378671
H	7.507736	-0.880341	1.948329	H	-7.280938	-1.379538	-1.998033
O	1.017661	-0.147291	-0.583783	O	-0.691344	-1.488280	0.375138
O	-1.633597	1.018862	-0.358875	O	1.720028	0.306886	0.687664
Fe	0.051438	1.109605	0.584996	Fe	0.036111	0.200646	-0.244418
C	1.925812	-0.606569	-3.266820	C	-1.378137	-3.268891	2.490575
C	2.667548	-1.055308	-4.529083	C	-2.016998	-4.286374	3.440071
H	3.552933	-0.440867	-4.728903	H	-2.861156	-3.860298	3.994766
H	2.976998	-2.105841	-4.471977	H	-2.364568	-5.180835	2.909413
H	1.997741	-0.954141	-5.389987	H	-1.270347	-4.606108	4.175278
C	0.664997	-1.477646	-3.151231	C	-0.165069	-3.950586	1.835364
H	0.935329	-2.533529	-3.031258	H	-0.484313	-4.810931	1.235062
H	0.037887	-1.175155	-2.312356	H	0.381898	-3.260144	1.192338
H	0.075730	-1.388646	-4.072092	H	0.514640	-4.315591	2.614927
C	1.532852	0.866999	-3.452476	C	-0.921314	-2.066700	3.331836
H	1.030953	1.262610	-2.567953	H	-0.493477	-1.281756	2.707509
H	2.428264	1.472529	-3.639325	H	-1.771805	-1.646146	3.881994

H	0.861509	0.976162	-4.312943	H	-0.166695	-2.382357	4.062841
C	-3.425778	1.506588	-2.504346	C	3.386380	0.699292	2.960616
C	-2.064367	1.656986	-3.201133	C	2.121424	0.086999	3.581601
H	-1.255144	1.754212	-2.478585	H	1.278878	0.128759	2.893162
H	-1.858060	0.787249	-3.836117	H	2.293426	-0.960657	3.855247
H	-2.067474	2.551735	-3.835763	H	1.850156	0.638447	4.490018
C	-3.702171	2.738630	-1.625318	C	3.129272	2.168181	2.586457
H	-2.950732	2.843294	-0.840839	H	2.350293	2.251420	1.826988
H	-3.681466	3.645015	-2.243406	H	2.803308	2.724731	3.474201
H	-4.692628	2.665962	-1.159691	H	4.045816	2.635313	2.206197
C	-4.502013	1.465432	-3.592438	C	4.480025	0.679989	4.032170
H	-5.511274	1.388025	-3.170958	H	5.409798	1.144964	3.683444
H	-4.456710	2.392733	-4.173942	H	4.134061	1.248259	4.902521
H	-4.350960	0.632211	-4.288981	H	4.705147	-0.338304	4.370805
C	8.725307	-1.864495	-0.364450	C	-8.400483	-3.156482	-0.158745
C	8.728299	-3.337954	-0.815567	C	-8.440269	-4.692357	-0.277536
C	9.357910	-0.984196	-1.459468	C	-8.938079	-2.728661	1.220672
C	9.579677	-1.745100	0.905943	C	-9.316317	-2.564538	-1.239882
H	8.277452	-3.969538	-0.041545	H	-8.056373	-5.005092	-1.255232
H	8.156426	-3.463506	-1.741516	H	-7.829170	-5.161593	0.501282
H	9.758212	-3.672912	-0.993182	H	-9.473049	-5.047562	-0.169911
H	9.351690	0.066670	-1.148377	H	-8.908893	-1.637053	1.313789
H	10.394748	-1.296740	-1.637475	H	-9.974621	-3.069008	1.340421
H	8.803128	-1.070598	-2.400118	H	-8.334715	-3.161173	2.026430
H	10.599462	-2.080737	0.682355	H	-10.333893	-2.945969	-1.093316
H	9.628941	-0.705815	1.252513	H	-9.348516	-1.470252	-1.174909
H	9.180648	-2.374302	1.710733	H	-8.981620	-2.855657	-2.242902
C	-6.406984	-5.228271	-1.061903	C	8.636330	-3.275050	-0.621857
C	-7.828421	-4.634147	-1.085598	C	9.686508	-2.188112	-0.323023
C	-6.036993	-5.745406	-2.465537	C	8.662507	-4.341829	0.490146
C	-6.395822	-6.415719	-0.088633	C	9.004958	-3.948888	-1.951276
H	-8.096850	-4.258295	-0.091693	H	9.668732	-1.421697	-1.106171
H	-7.895891	-3.805852	-1.799360	H	9.489665	-1.705317	0.640275
H	-8.550350	-5.406005	-1.381339	H	10.687063	-2.637437	-0.286988
H	-5.026646	-6.170104	-2.455880	H	7.916040	-5.117794	0.285413
H	-6.747154	-6.521462	-2.778570	H	9.655314	-4.807123	0.540791
H	-6.063056	-4.932085	-3.199105	H	8.437300	-3.893526	1.464234
H	-7.131672	-7.157491	-0.421270	H	10.011414	-4.376051	-1.867924
H	-5.411092	-6.897815	-0.065320	H	8.307655	-4.760943	-2.189910
H	-6.663917	-6.096123	0.925572	H	9.006102	-3.222626	-2.773105
C	0.188510	4.607036	-1.801741	C	-0.851821	2.532724	3.205228
C	-0.711595	5.670874	-1.650629	C	-0.336423	3.816623	3.426915
C	-0.834232	6.621344	-2.654609	C	-0.392127	4.370718	4.698607
C	-0.047319	6.492185	-3.799753	C	-0.965478	3.624950	5.729476
C	0.850990	5.430110	-3.941697	C	-1.476433	2.343414	5.498758
C	0.977665	4.472978	-2.940062	C	-1.423050	1.781614	4.227496
C	-0.847802	4.299537	0.246274	C	-0.001902	3.255078	1.174835
C	-1.433150	5.554952	-0.334381	C	0.234476	4.374094	2.149063
H	-1.529871	7.451218	-2.556107	H	0.004362	5.364149	4.893734
H	-0.134050	7.228263	-4.594728	H	-1.013540	4.045963	6.730335
H	1.452292	5.352960	-4.843414	H	-1.914103	1.784470	6.321200
H	1.666793	3.639934	-3.032408	H	-1.804210	0.785559	4.023758
H	-2.519799	5.475423	-0.477638	H	1.301556	4.612414	2.255750
H	-1.265851	6.436251	0.299921	H	-0.266548	5.306070	1.852791
C	0.088630	3.736322	-0.621757	C	-0.633123	2.172387	1.798678
O	0.748573	2.643660	-0.495701	O	-0.962653	1.039957	1.306795
C	-1.193204	3.698001	1.472619	C	0.375309	3.217953	-0.177620
O	-0.686225	2.634105	1.910051	O	0.142621	2.241604	-0.946204
O	0.636933	-2.621421	1.096903	O	-2.513371	2.638748	-2.192915
H	0.648860	-1.941542	0.400509	H	-1.769233	2.437104	-1.601010
C	0.867306	-3.901363	0.516746	C	-3.550222	3.224739	-1.409232
C	-0.236011	-4.219674	-0.489984	C	-3.987065	2.261422	-0.307460
C	2.241193	-3.928925	-0.149530	C	-3.054610	4.539220	-0.806884
C	0.819843	-4.874008	1.687149	C	-4.689450	3.477421	-2.386066

H	-1.218566	-4.205392	-0.007775	H	-4.395611	1.340364	-0.735273
H	-0.249618	-3.476242	-1.294029	H	-3.140148	1.985459	0.330621
H	-0.086022	-5.205700	-0.944852	H	-4.758516	2.712305	0.327389
H	3.017172	-3.641279	0.567763	H	-2.691229	5.202471	-1.599462
H	2.474471	-4.927443	-0.536665	H	-3.852599	5.053638	-0.259504
H	2.284067	-3.224427	-0.987308	H	-2.232538	4.354838	-0.104459
H	0.985808	-5.902213	1.349878	H	-5.550218	3.923737	-1.877709
H	1.590138	-4.618406	2.422795	H	-4.363276	4.152158	-3.184678
H	-0.157754	-4.823039	2.179512	H	-5.006318	2.533123	-2.842389
O	-2.123821	4.360745	2.165312	O	0.992372	4.313011	-0.615960
C	-2.788328	3.771133	3.318242	C	1.575849	4.398449	-1.949479
C	-3.445946	2.452417	2.926349	C	2.585338	3.275779	-2.160153
C	-1.807675	3.620218	4.475151	C	0.475162	4.416418	-3.002643
C	-3.845906	4.813026	3.656571	C	2.286609	5.744575	-1.907827
H	-4.100190	2.601426	2.060586	H	3.314564	3.266023	-1.342838
H	-2.707338	1.690669	2.672495	H	2.103483	2.298702	-2.201106
H	-4.058315	2.089195	3.759203	H	3.126356	3.447717	-3.097316
H	-1.326359	4.580319	4.689387	H	-0.231204	5.226953	-2.796181
H	-2.346059	3.299028	5.373847	H	0.918547	4.591570	-3.989242
H	-1.035256	2.886082	4.244339	H	-0.086087	3.482443	-3.030374
H	-4.425965	4.492421	4.527719	H	2.763315	5.947214	-2.871991
H	-3.377378	5.775963	3.883541	H	1.574197	6.547576	-1.694450
H	-4.529447	4.951269	2.813114	H	3.056165	5.747773	-1.129583
INT 2'				**INT 4 ^{SR}-1**			
							
E(RPBE1PBE) = -4000.146916 Thermal correction to Gibbs Free Energy = 1.102925				E(RPBE1PBE) = -4667.708848 Thermal correction to Gibbs Free Energy = 1.289005			
C	0.849053	3.387943	2.770164	C	-0.10193	-3.49267	3.3087
C	0.101956	2.323759	1.964338	C	-0.71034	-2.57386	2.24928
C	-0.970089	1.618990	2.847310	C	-1.88391	-3.2746	1.50659
C	-1.951431	2.648277	3.414166	C	-2.94497	-3.73795	2.51272
C	-1.189990	3.710977	4.220930	C	-2.3158	-4.64807	3.57984
C	-0.147785	4.410380	3.339015	C	-1.18355	-3.91933	4.31214
H	-0.435755	2.802928	1.131494	H	-1.12803	-1.67604	2.73006
H	1.388524	2.903671	3.597050	H	0.30994	-4.39063	2.82541
H	1.581453	3.901195	2.133589	H	0.71435	-2.976	3.83143
H	-2.485940	3.136956	2.585978	H	-3.38518	-2.85482	2.9994
H	-2.688319	2.154019	4.060143	H	-3.74513	-4.28345	1.99653
H	-1.899269	4.442808	4.624009	H	-3.08819	-4.96576	4.28971
H	-0.686973	3.231878	5.072414	H	-1.915	-5.55123	3.09847
H	-0.656043	4.924256	2.510541	H	-1.58646	-3.03094	4.81904
H	0.393746	5.167547	3.917318	H	-0.74319	-4.56973	5.07658
H	-0.431590	1.132465	3.675989	H	-1.45579	-4.15088	0.99339
N	0.910865	1.242004	1.409798	N	0.18728	-2.12419	1.19368
N	-1.547077	0.565970	2.008622	N	-2.32777	-2.32382	0.48406
C	-2.827808	0.464771	1.822007	C	-3.5854	-2.06764	0.31437
H	-3.468819	1.139917	2.385369	H	-4.29566	-2.63084	0.91599
C	2.200170	1.217980	1.490026	C	1.41561	-2.51532	1.10505
H	2.721918	2.105975	1.851798	H	1.85702	-3.06779	1.93811
C	-3.504401	-0.433177	0.944074	C	-4.16619	-1.10812	-0.57238
C	-2.828077	-1.533416	0.360009	C	-3.38857	-0.47642	-1.57289
C	-4.904392	-0.207384	0.674553	C	-5.56346	-0.78504	-0.41765
C	-3.545507	-2.516705	-0.411546	C	-3.99096	0.44696	-2.50206
C	-5.588324	-1.158656	-0.126569	C	-6.13509	0.14925	-1.31793
C	-5.632518	0.915450	1.103604	C	-6.39789	-1.28548	0.60219
C	-4.879695	-2.290221	-0.618972	C	-5.32264	0.71874	-2.33545
C	-6.942953	-0.975392	-0.442800	C	-7.48443	0.53173	-1.19399

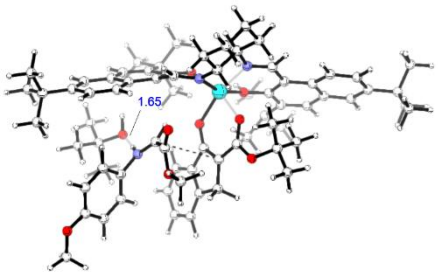
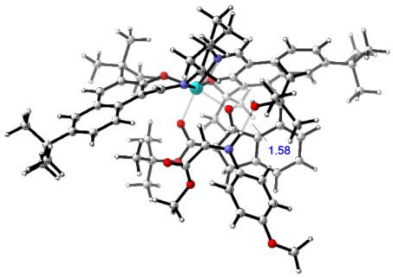
C	-6.968778	1.074223	0.779473	C	-7.71775	-0.89664	0.70333
H	-5.160927	1.700943	1.686990	H	-6.02033	-1.98026	1.34634
H	-5.453188	-2.997456	-1.209512	H	-5.80987	1.42379	-3.00148
C	-7.660136	0.125848	-0.001524	C	-8.29786	0.02525	-0.19904
H	-7.430749	-1.727926	-1.058151	H	-7.8759	1.24918	-1.9091
H	-7.490341	1.954514	1.134688	H	-8.32583	-1.30987	1.50148
C	3.018952	0.077726	1.194109	C	2.24764	-2.30981	-0.04617
C	2.476117	-1.225217	1.310891	C	1.65058	-2.25581	-1.33753
C	4.412001	0.273251	0.906155	C	3.67636	-2.33813	0.10965
C	3.339381	-2.381533	1.232348	C	2.49095	-2.27588	-2.51895
C	5.249731	-0.869015	0.828229	C	4.48133	-2.31998	-1.05674
C	4.984797	1.524790	0.628119	C	4.3325	-2.31569	1.35822
C	4.676089	-2.156438	1.016908	C	3.84617	-2.29872	-2.33171
C	6.609533	-0.723656	0.510276	C	5.88462	-2.28023	-0.94617
C	6.325585	1.642351	0.311538	C	5.71072	-2.2993	1.44003
H	4.371936	2.421764	0.615436	H	3.75989	-2.29939	2.28235
H	5.352779	-3.002499	0.950688	H	4.50284	-2.29151	-3.19578
C	7.173103	0.515529	0.246994	C	6.52422	-2.27294	0.28357
H	7.223272	-1.620643	0.460534	H	6.46549	-2.25808	-1.86346
H	6.726681	2.624398	0.094468	H	6.17809	-2.29146	2.41858
O	1.191950	-1.413567	1.493717	O	0.36349	-2.23663	-1.48126
O	-1.542960	-1.690677	0.533007	O	-2.1137	-0.72507	-1.6854
Fe	-0.223117	-0.375264	0.759143	Fe	-0.80834	-1.14982	-0.38991
C	2.760616	-3.792600	1.346833	C	1.86571	-2.24103	-3.91244
C	3.856255	-4.858062	1.255951	C	2.93183	-2.29509	-5.01017
H	4.378957	-4.836303	0.292247	H	3.60966	-1.4338	-4.97343
H	4.596788	-4.753799	2.056934	H	3.52919	-3.21303	-4.96136
H	3.401043	-5.848391	1.357390	H	2.43725	-2.27755	-5.9868
C	2.042980	-3.972274	2.694450	C	0.93959	-3.45395	-4.10397
H	2.741199	-3.818395	3.524674	H	1.49863	-4.38969	-3.98814
H	1.210781	-3.274997	2.804250	H	0.11581	-3.44691	-3.38862
H	1.651205	-4.993195	2.768864	H	0.52008	-3.4356	-5.11646
C	1.776809	-4.040368	0.189725	C	1.07258	-0.93714	-4.09901
H	0.907359	-3.381568	0.244849	H	0.28416	-0.82837	-3.35448
H	2.276654	-3.914157	-0.781500	H	1.7347	-0.066	-4.03101
H	1.405504	-5.070750	0.226438	H	0.61095	-0.92881	-5.0933
C	-2.825687	-3.737214	-0.984368	C	-3.16136	1.08998	-3.61311
C	-2.189449	-4.554666	0.151977	C	-2.63303	-0.00493	-4.55411
H	-1.467112	-3.967518	0.721639	H	-2.03054	-0.73929	-4.01662
H	-2.959589	-4.918485	0.841341	H	-3.46498	-0.52584	-5.04132
H	-1.673642	-5.426932	-0.266879	H	-2.01103	0.44632	-5.33667
C	-1.751902	-3.287572	-1.989717	C	-1.9874	1.88863	-3.01965
H	-0.997923	-2.651734	-1.523035	H	-1.26816	1.23678	-2.52385
H	-1.249756	-4.166406	-2.411369	H	-1.46538	2.42656	-3.81987
H	-2.207575	-2.730688	-2.816983	H	-2.34743	2.63024	-2.29557
C	-3.793528	-4.661053	-1.729245	C	-3.99937	2.06057	-4.44956
H	-4.254899	-4.167694	-2.592523	H	-4.38502	2.89366	-3.84992
H	-3.241548	-5.528594	-2.105562	H	-3.37049	2.48584	-5.23861
H	-4.588432	-5.036501	-1.074750	H	-4.84398	1.56141	-4.93784
C	8.652837	0.624167	-0.120297	C	8.04296	-2.2535	0.43373
C	9.501986	0.044474	1.027456	C	8.48693	-3.60925	1.01924
C	8.909491	-0.175635	-1.412739	C	8.74936	-2.04142	-0.91232
C	9.085099	2.078091	-0.358860	C	8.46275	-1.11844	1.38802
H	9.321502	0.603664	1.952289	H	8.01494	-3.78671	1.99234
H	9.260826	-1.009305	1.204696	H	8.20655	-4.42439	0.34277
H	10.566370	0.116541	0.773272	H	9.57554	-3.61841	1.15366
H	8.318411	0.240317	-2.237613	H	8.44748	-1.09105	-1.37086
H	9.971383	-0.119067	-1.680442	H	9.83226	-2.01348	-0.74748
H	8.642277	-1.230759	-1.284444	H	8.53508	-2.8602	-1.60916
H	10.150755	2.094507	-0.613844	H	9.55587	-1.09738	1.47053
H	8.529522	2.527097	-1.191448	H	8.11879	-0.1495	1.01018
H	8.941503	2.687000	0.541709	H	8.05048	-1.26563	2.39193
C	-9.133165	0.284778	-0.375132	C	-9.76433	0.4122	-0.03512
C	-9.251273	0.382018	-1.908803	C	-10.21165	1.43105	-1.09224

C	-9.917526	-0.941791	0.130344
C	-9.754171	1.546071	0.242058
H	-8.698838	1.254134	-2.277375
H	-8.849530	-0.515768	-2.391587
H	-10.305327	0.485369	-2.193771
H	-9.832660	-1.024792	1.219649
H	-10.976556	-0.837688	-0.135200
H	-9.539987	-1.866309	-0.320354
H	-10.809324	1.601196	-0.048771
H	-9.704347	1.517700	1.337285
H	-9.255653	2.453636	-0.119925
C	2.920278	0.297192	-2.344692
C	3.014187	1.549615	-2.977728
C	4.226121	1.956450	-3.514264
C	5.324094	1.101529	-3.407813
C	5.218424	-0.146171	-2.786258
C	4.009455	-0.565844	-2.247430
C	0.841501	1.302748	-2.114442
C	1.682848	2.252302	-2.922775
H	4.325570	2.920994	-4.004245
H	6.282612	1.411311	-3.814303
H	6.092199	-0.783368	-2.705626
H	3.939439	-1.527157	-1.743933
H	1.265068	2.410086	-3.926021
H	1.756890	3.242961	-2.455998
C	1.574146	0.187855	-1.827223
O	1.077676	-0.873648	-1.165456
C	-0.521258	1.465427	-1.692747
O	-1.038795	0.769302	-0.793971
O	-1.180323	2.406537	-2.328422
C	-2.616103	2.673937	-2.088509
C	-3.433082	1.431413	-2.412374
C	-2.818495	3.147471	-0.656888
C	-2.903080	3.791858	-3.076866
H	-3.225869	1.094999	-3.433333
H	-3.230991	0.616298	-1.716119
H	-4.497515	1.677571	-2.343178
H	-2.166444	4.000082	-0.436483
H	-3.857214	3.470323	-0.533513
H	-2.622964	2.344150	0.053503
H	-3.953192	4.088913	-3.002217
H	-2.279008	4.666448	-2.868404
H	-2.709256	3.461138	-4.101503
H	1.765124	-1.538846	-0.987953
C	-10.6331	-0.8531	-0.17669
C	-9.96971	1.03364	1.36009
H	-9.63301	2.35963	-1.01609
H	-10.10649	1.02172	-2.10412
H	-11.26842	1.67301	-0.93078
H	-10.36982	-1.60057	0.58
H	-11.69104	-0.59188	-0.05125
H	-10.49385	-1.29808	-1.16839
H	-11.02397	1.3057	1.49207
H	-9.69464	0.32885	2.15268
H	-9.35591	1.93576	1.46535
C	1.48017	2.53395	-1.03034
C	1.21291	3.77911	-0.44684
C	1.9817	4.87962	-0.79981
C	3.00767	4.70474	-1.73019
C	3.26958	3.45553	-2.30443
C	2.49969	2.35093	-1.9604
C	-0.19971	2.18045	0.53439
C	0.08178	3.65854	0.54197
H	1.79619	5.85733	-0.36303
H	3.61752	5.55775	-2.01552
H	4.07983	3.35318	-3.0201
H	2.68487	1.36709	-2.38222
H	-0.79702	4.23531	0.22172
H	0.36452	4.04328	1.53025
C	0.57575	1.53746	-0.45253
O	0.59313	0.31201	-0.78413
C	-1.28446	1.52159	1.17954
O	-1.56372	0.31509	1.01191
C	1.87174	0.8995	1.90099
H	1.20453	0.04888	1.81802
N	2.9626	0.80368	1.18804
C	4.0974	1.59194	0.93114
C	4.23198	2.93901	1.27869
C	5.11705	0.94823	0.2083
C	5.37351	3.63123	0.91056
H	3.44254	3.4454	1.81519
C	6.24679	1.64012	-0.15951
H	5.03591	-0.10156	-0.05122
C	6.38917	2.99391	0.18482
H	5.45367	4.67829	1.17735
H	7.03848	1.1543	-0.71957
O	7.51644	3.585	-0.2268
C	7.72089	4.9499	0.09095
H	7.74568	5.10398	1.17596
H	8.68886	5.21175	-0.33569
H	6.94235	5.58029	-0.35476
C	1.50063	1.89665	2.93031
O	1.94545	3.01186	3.08917
O	0.55866	1.34486	3.69851
C	0.0396	2.2027	4.72033
H	-0.67302	1.59389	5.27445
H	0.84568	2.54714	5.37162
H	-0.45947	3.05919	4.26291
H	2.96873	-0.05584	0.62895
O	-1.9757	2.3009	2.00354
C	-3.32939	1.95876	2.4659
C	-4.25412	1.98283	1.25915
C	-3.36519	0.62301	3.19977
C	-3.64998	3.09795	3.4212
H	-4.2519	2.9745	0.79567
H	-3.94976	1.24279	0.51701
H	-5.27811	1.74445	1.56364
H	-2.55091	0.56286	3.93011

				H	-4.31399	0.54667	3.74153
				H	-3.28273	-0.21828	2.51199
				H	-4.68556	3.01282	3.76345
				H	-2.99621	3.07406	4.29927
				H	-3.52869	4.06353	2.92143
INT 4 *SR*				**INT 4 *RS***			
							
E(UPBE1PBE) = -4901.206977 Thermal correction to Gibbs Free Energy= 1.416355				E(UPBE1PBE) = -4901.202737 Thermal correction to Gibbs Free Energy= 1.421506			
C	-0.255144	-0.003113	4.491613	C	1.365996	-1.033712	4.441732
C	-0.961439	-0.096588	3.139013	C	0.534890	-0.973786	3.158559
C	-2.112896	-1.144104	3.175969	C	-0.424676	-2.193612	3.056534
C	-3.099594	-0.815760	4.304510	C	-1.319214	-2.285363	4.296190
C	-2.369775	-0.695289	5.650938	C	-0.469922	-2.323680	5.575355
C	-1.272993	0.373867	5.578445	C	0.431886	-1.085777	5.659693
H	-1.417795	0.872945	2.892241	H	-0.110587	-0.081615	3.175993
H	0.185940	-0.976896	4.749983	H	1.989676	-1.939476	4.431810
H	0.550591	0.740683	4.435120	H	2.033742	-0.163609	4.502578
H	-3.598263	0.136734	4.074220	H	-1.972394	-1.403216	4.326588
H	-3.866099	-1.597425	4.379477	H	-1.952404	-3.180247	4.244357
H	-3.093851	-0.448859	6.436349	H	-1.128028	-2.379492	6.450361
H	-1.915649	-1.662464	5.909032	H	0.155704	-3.227117	5.571975
H	-1.724866	1.347225	5.339484	H	-0.192568	-0.180237	5.683563
H	-0.766147	0.467603	6.545813	H	1.024329	-1.105924	6.581620
H	-1.640962	-2.120753	3.372852	H	0.211395	-3.091376	2.994838
N	-0.142904	-0.499590	2.000244	N	1.275025	-0.985005	1.899540
N	-2.670988	-1.167707	1.820518	N	-1.108938	-2.041509	1.772602
C	-3.949898	-1.202417	1.628652	C	-2.390079	-2.182395	1.652219
H	-4.585186	-1.289800	2.507577	H	-2.958975	-2.438428	2.546164
C	1.060994	-0.938560	2.155450	C	2.564865	-1.131505	1.863528
H	1.541782	-0.807362	3.125294	H	3.128832	-0.981551	2.785903
C	-4.648984	-1.113388	0.383462	C	-3.153160	-2.057448	0.450327
C	-3.958793	-1.198290	-0.849353	C	-2.523265	-2.129625	-0.818216
C	-6.076587	-0.906139	0.408961	C	-4.581644	-1.892183	0.551150
C	-4.672395	-1.142325	-2.101229	C	-3.324776	-2.243980	-2.019122
C	-6.762082	-0.828522	-0.829843	C	-5.336727	-1.850427	-0.649845
C	-6.843366	-0.717070	1.577121	C	-5.280322	-1.689033	1.755244
C	-6.028037	-0.963266	-2.039560	C	-4.674790	-2.075658	-1.889741
C	-8.149451	-0.591907	-0.868748	C	-6.712916	-1.583853	-0.612507
C	-8.201592	-0.483508	1.513990	C	-6.640599	-1.428031	1.767701
H	-6.383119	-0.735501	2.560377	H	-4.763331	-1.713298	2.710153
H	-6.599976	-0.898623	-2.959818	H	-5.303756	-2.102725	-2.773694
C	-8.892902	-0.416838	0.282256	C	-7.389806	-1.356018	0.576709
H	-8.628281	-0.542926	-1.842172	H	-7.251449	-1.551950	-1.557447
H	-8.752615	-0.344333	2.438399	H	-7.132892	-1.273473	2.720151
C	1.813612	-1.683507	1.184590	C	3.321429	-1.558226	0.728691
C	1.126494	-2.390412	0.161274	C	2.698799	-2.377090	-0.251291
C	3.214479	-1.904941	1.421485	C	4.738373	-1.315784	0.687089
C	1.834337	-3.397281	-0.617839	C	3.508189	-3.107892	-1.207322
C	3.876678	-2.922114	0.690404	C	5.497125	-1.933936	-0.339675
C	3.982547	-1.151561	2.331837	C	5.417981	-0.470290	1.580163
C	3.144840	-3.643162	-0.302290	C	4.848703	-2.840103	-1.228957
C	5.240664	-3.185065	0.913851	C	6.867734	-1.663734	-0.460361
C	5.322494	-1.427083	2.533126	C	6.777401	-0.230743	1.449108
H	3.534440	-0.318232	2.866996	H	4.885386	0.024502	2.387190
H	3.683773	-4.420867	-0.836619	H	5.480975	-3.335672	-1.959138

C	5.986726	-2.456151	1.825720	C	7.532877	-0.811911	0.410757
H	5.704132	-3.989447	0.348496	H	7.415696	-2.149650	-1.265019
H	5.877832	-0.830996	3.251196	H	7.265796	0.415151	2.169770
O	-0.129175	-2.221028	-0.062761	O	1.414292	-2.540052	-0.281057
O	-2.664946	-1.342823	-0.885657	O	-1.228962	-2.130295	-0.931775
Fe	-1.305731	-0.701903	0.260266	Fe	0.057248	-1.266472	0.219203
C	1.116111	-4.122120	-1.753682	C	2.861000	-4.122870	-2.150370
C	2.027545	-5.145176	-2.436214	C	3.908921	-4.836493	-3.008703
H	2.912248	-4.680690	-2.886288	H	4.444574	-4.142965	-3.667634
H	2.357569	-5.928947	-1.744360	H	4.642326	-5.375361	-2.397711
H	1.472534	-5.634333	-3.243108	H	3.407071	-5.570558	-3.647823
C	-0.114582	-4.881490	-1.228447	C	2.124948	-5.193960	-1.327091
H	0.181573	-5.622734	-0.477025	H	2.817879	-5.703296	-0.647247
H	-0.847464	-4.206770	-0.785537	H	1.313559	-4.758607	-0.741052
H	-0.590347	-5.416057	-2.058791	H	1.699979	-5.946232	-2.001956
C	0.692250	-3.084625	-2.809648	C	1.874457	-3.428941	-3.103484
H	0.013573	-2.338068	-2.393359	H	1.103877	-2.880997	-2.559099
H	1.569513	-2.565119	-3.215320	H	2.400805	-2.735426	-3.768715
H	0.182574	-3.588618	-3.638891	H	1.379881	-4.181468	-3.729051
C	-3.922432	-1.256511	-3.428395	C	-2.670812	-2.549154	-3.365814
C	-3.214414	-2.619117	-3.511220	C	-1.907501	-3.880125	-3.261555
H	-2.507489	-2.754096	-2.690807	H	-1.141915	-3.843713	-2.484465
H	-3.945786	-3.434808	-3.479191	H	-2.597638	-4.700706	-3.034388
H	-2.665823	-2.694017	-4.458151	H	-1.419164	-4.103736	-4.217633
C	-2.894636	-0.118313	-3.559099	C	-1.716512	-1.418442	-3.780108
H	-2.111721	-0.193186	-2.803764	H	-0.902958	-1.294524	-3.064935
H	-2.422576	-0.160966	-4.548125	H	-1.284973	-1.642690	-4.763240
H	-3.383119	0.858669	-3.460654	H	-2.264173	-0.471714	-3.855229
C	-4.876657	-1.154999	-4.621485	C	-3.713869	-2.695752	-4.476873
H	-5.393499	-0.188640	-4.654623	H	-4.266025	-1.764174	-4.648866
H	-4.302133	-1.252878	-5.548713	H	-3.205858	-2.953972	-5.412059
H	-5.628437	-1.952448	-4.615318	H	-4.433309	-3.493898	-4.261484
C	7.467038	-2.719136	2.088795	C	9.026338	-0.543212	0.228210
C	7.646948	-3.119108	3.566125	C	9.795848	-1.872066	0.359339
C	8.015596	-3.847634	1.204778	C	9.261876	0.058760	-1.170780
C	8.274996	-1.438922	1.796542	C	9.570558	0.438022	1.276110
H	7.297839	-2.324663	4.235007	H	9.631838	-2.308445	1.351032
H	7.078680	-4.030687	3.782018	H	9.465359	-2.593065	-0.396325
H	8.707519	-3.306012	3.773720	H	10.869982	-1.695888	0.223256
H	7.926167	-3.596693	0.140365	H	8.716889	1.004697	-1.272711
H	9.077552	-3.995762	1.431177	H	10.331869	0.249570	-1.318128
H	7.491599	-4.791054	1.398452	H	8.922282	-0.625419	-1.956124
H	9.338618	-1.620279	1.991972	H	10.639857	0.596045	1.094764
H	8.157861	-1.146239	0.745578	H	9.066027	1.409988	1.208686
H	7.947637	-0.610724	2.436582	H	9.453284	0.039464	2.291001
C	-10.394600	-0.147917	0.278465	C	-8.883556	-1.033660	0.559907
C	-10.970894	-0.124044	-1.143998	C	-9.104418	0.259003	-0.250553
C	-11.107699	-1.257369	1.075691	C	-9.646228	-2.198259	-0.100256
C	-10.659567	1.220326	0.936669	C	-9.446136	-0.821720	1.972658
H	-10.511366	0.671178	-1.743515	H	-8.563199	1.092359	0.214711
H	-10.820799	-1.086939	-1.647114	H	-8.749219	0.141224	-1.280485
H	-12.048533	0.068693	-1.090207	H	-10.172942	0.505689	-0.277802
H	-10.755875	-1.288736	2.112767	H	-9.490423	-3.121773	0.468504
H	-12.188657	-1.070974	1.083521	H	-10.719743	-1.974197	-0.125045
H	-10.920073	-2.233694	0.614793	H	-9.303138	-2.361484	-1.127867
H	-11.737614	1.421880	0.952717	H	-10.515646	-0.592963	1.900212
H	-10.289495	1.240391	1.967960	H	-9.331495	-1.725253	2.583256
H	-10.159687	2.014483	0.370016	H	-8.951382	0.018645	2.474979
C	0.739445	2.167904	-2.359611	C	-2.791105	1.499605	-1.264472
C	0.404753	3.522169	-2.509747	C	-2.641027	2.169838	-2.489713
C	1.157878	4.335864	-3.343155	C	-3.751645	2.723834	-3.111804
C	2.241109	3.776887	-4.023824	C	-5.001927	2.590544	-2.501315
C	2.560047	2.422893	-3.883415	C	-5.146841	1.901861	-1.293892
C	1.807611	1.598286	-3.050352	C	-4.036632	1.348780	-0.661915

C	-1.069536	2.548455	-0.967535	C	-0.557268	1.327009	-1.829319
C	-0.798384	3.848524	-1.668583	C	-1.203144	2.107750	-2.934967
H	0.910535	5.386490	-3.472331	H	-3.661202	3.232835	-4.068759
H	2.837648	4.399825	-4.684667	H	-5.879445	3.011324	-2.984341
H	3.394643	2.011919	-4.442588	H	-6.133204	1.771417	-0.858491
H	2.043139	0.542236	-2.941491	H	-4.144337	0.769165	0.248824
H	-1.644406	4.171689	-2.290694	H	-0.757172	3.104593	-3.053755
H	-0.601253	4.674280	-0.971581	H	-1.109142	1.607994	-3.908437
C	-0.179933	1.563890	-1.381472	C	-1.478366	0.990547	-0.848707
O	-0.069853	0.340858	-0.993704	O	-1.264389	0.373061	0.269030
C	-2.105281	2.294701	-0.037525	C	0.815596	0.982941	-1.712461
O	-2.293774	1.185822	0.514573	O	1.246075	0.142385	-0.888800
C	2.588733	1.197767	0.017684	C	1.516101	2.393227	2.389808
H	1.797471	0.522966	-0.323065	H	1.091613	1.723657	3.129817
N	3.795532	0.974009	-0.341958	N	0.624464	2.954560	1.634355
C	4.912101	1.816342	-0.074173	C	0.549435	3.846487	0.568374
C	4.898001	3.137908	-0.507473	C	-0.744876	3.997107	0.041238
C	6.030370	1.272586	0.562478	C	1.612618	4.577959	0.007600
C	6.010699	3.942763	-0.286859	C	-0.992071	4.840132	-1.022417
H	4.037389	3.524386	-1.045556	H	-1.567372	3.434663	0.467991
C	7.130822	2.075296	0.784657	C	1.371795	5.408386	-1.061490
H	6.002869	0.246913	0.916926	H	2.608182	4.494658	0.415340
C	7.132925	3.415382	0.362604	C	0.075444	5.543635	-1.598176
H	5.998865	4.967667	-0.638340	H	-2.000232	4.915143	-1.411910
H	8.010811	1.690358	1.289082	H	2.174329	5.981281	-1.513749
O	8.255732	4.101319	0.622008	O	-0.035365	6.357794	-2.645535
C	8.327260	5.454723	0.216520	C	-1.313586	6.534495	-3.238411
H	7.553477	6.057734	0.706952	H	-2.016757	6.980403	-2.526466
H	9.311088	5.806317	0.526783	H	-1.158363	7.214493	-4.075117
H	8.233694	5.548577	-0.872178	H	-1.710529	5.581167	-3.605771
C	2.207975	2.249253	1.016742	C	2.996211	2.417615	2.470653
O	2.183861	1.967634	2.190474	O	3.526195	1.713522	3.304045
O	1.859768	3.392923	0.464677	O	3.633019	3.204153	1.620936
C	1.317446	4.377333	1.359801	C	5.071056	3.140579	1.669171
H	1.266387	5.295764	0.778194	H	5.413813	3.928878	1.001104
H	0.317933	4.064317	1.671588	H	5.416235	3.313839	2.690058
H	1.964239	4.497889	2.230254	H	5.404622	2.160807	1.319236
H	3.953933	0.124050	-0.956967	H	-0.335411	2.585839	1.921282
O	3.972161	-1.089677	-2.041110	O	1.611106	1.650545	-2.536960
C	5.157620	-1.323095	-2.844267	C	3.047935	1.387288	-2.661914
C	5.201483	-0.174322	-3.836965	C	3.755149	1.636071	-1.338042
C	6.390378	-1.321573	-1.947940	C	3.260963	-0.027913	-3.168974
C	4.999263	-2.658369	-3.556763	C	3.474924	2.413821	-3.699637
H	4.321014	-0.196705	-4.486918	H	3.551778	2.653371	-0.989930
H	5.227787	0.787291	-3.311905	H	3.438339	0.920363	-0.578670
H	6.097283	-0.243999	-4.461330	H	4.835710	1.526056	-1.480309
H	6.278243	-2.042443	-1.131891	H	2.702402	-0.188934	-4.096880
H	7.284378	-1.583901	-2.523238	H	4.324784	-0.188014	-3.372636
H	6.552585	-0.331749	-1.508293	H	2.945550	-0.764019	-2.430308
H	5.832750	-2.828426	-4.245201	H	4.549326	2.329192	-3.888505
H	4.989645	-3.486266	-2.838096	H	2.942527	2.254475	-4.642229
H	4.066705	-2.681595	-4.129623	H	3.260053	3.428093	-3.347069
H	3.727800	-1.915576	-1.583644	O	-1.529238	1.716528	2.498967
O	-2.868635	3.350924	0.225801	C	-2.677081	2.157977	3.255003
C	-4.179856	3.239321	0.874710	C	-2.118286	2.590950	4.602185
C	-5.104413	2.457019	-0.046125	C	-3.351127	3.324173	2.540406
C	-4.072191	2.613749	2.260114	C	-3.641675	0.993128	3.412991
C	-4.615613	4.692621	0.982261	H	-1.618716	1.750071	5.095240
H	-5.198296	2.965010	-1.011326	H	-1.391359	3.401996	4.478500
H	-4.732321	1.444483	-0.212031	H	-2.917365	2.951818	5.256475
H	-6.100456	2.375628	0.400719	H	-3.700490	3.025164	1.545310
H	-3.283094	3.103793	2.841969	H	-4.219456	3.672627	3.108911
H	-5.021122	2.758234	2.787759	H	-2.660664	4.168729	2.435443
H	-3.859516	1.546945	2.199904	H	-4.502166	1.286998	4.022405

H	-5.623472	4.748122	1.404325	H	-4.024020	0.651012	2.446069
H	-3.936107	5.256233	1.629939	H	-3.145754	0.151386	3.904245
H	-4.626028	5.163492	-0.005288	H	-1.748591	1.133577	1.725560
TS ***SR***				**TS** ***RS***			
							
E(UPBE1PBE) = -4901.206377				E(UPBE1PBE) = -4901.200180			
Thermal correction to Gibbs Free Energy= 1.419386				Thermal correction to Gibbs Free Energy= 1.419693			
C	0.680905	-2.079880	-4.382407	C	1.245979	-0.353742	4.542231
C	1.265309	-1.563320	-3.067962	C	0.503576	-0.612151	3.229583
C	2.484999	-2.418002	-2.617340	C	-0.256423	-1.974189	3.287624
C	3.548618	-2.458906	-3.721211	C	-1.210959	-2.016417	4.482615
C	2.940015	-2.969312	-5.036570	C	-0.442525	-1.750469	5.785556
C	1.768086	-2.079266	-5.467086	C	0.261598	-0.389561	5.720868
H	1.623743	-0.534863	-3.203180	H	-0.255033	0.168711	3.069459
H	0.310262	-3.106352	-4.244775	H	2.010428	-1.131095	4.686853
H	-0.160150	-1.444527	-4.689863	H	1.751947	0.620243	4.505208
H	3.945250	-1.444627	-3.875924	H	-1.978203	-1.241128	4.356833
H	4.378844	-3.112557	-3.424610	H	-1.711765	-2.992022	4.533569
H	3.712727	-2.987202	-5.813959	H	-1.135345	-1.782058	6.634567
H	2.582619	-3.999431	-4.898320	H	0.305257	-2.541313	5.937350
H	2.127530	-1.052054	-5.623997	H	-0.490389	0.401727	5.591571
H	1.346649	-2.434737	-6.414494	H	0.796716	-0.190810	6.656615
H	2.106628	-3.437598	-2.438135	H	0.512105	-2.754750	3.406542
N	0.372492	-1.564832	-1.917945	N	1.336627	-0.715539	2.032807
N	2.906372	-1.861177	-1.328838	N	-0.856461	-2.146970	1.966345
C	4.152955	-1.604517	-1.091356	C	-2.113402	-2.398602	1.795733
H	4.875566	-1.875364	-1.858603	H	-2.726824	-2.536842	2.685761
C	-0.849160	-1.960665	-1.995443	C	2.633985	-0.615794	2.069383
H	-1.285357	-2.148637	-2.977398	H	3.104467	-0.149410	2.939114
C	4.709315	-1.003234	0.080562	C	-2.798266	-2.497097	0.540545
C	3.924870	-0.829183	1.245273	C	-2.080009	-2.653694	-0.671242
C	6.095667	-0.606452	0.066888	C	-4.237487	-2.398003	0.528869
C	4.515976	-0.343901	2.468461	C	-2.782061	-2.844862	-1.920548
C	6.657335	-0.102318	1.266860	C	-4.899532	-2.438502	-0.727154
C	6.931771	-0.645794	-1.067051	C	-5.041067	-2.190093	1.665707
C	5.841636	-0.005687	2.428041	C	-4.140982	-2.697475	-1.902341
C	8.002465	0.310559	1.308932	C	-6.282455	-2.217549	-0.808953
C	8.247206	-0.234767	-1.001620	C	-6.405355	-1.976818	1.560746
H	6.556481	-0.985783	-2.027867	H	-4.609697	-2.183352	2.662116
H	6.321818	0.376667	3.323398	H	-4.700419	-2.774930	-2.829145
C	8.819776	0.251503	0.196253	C	-7.058647	-1.965766	0.312007
H	8.388132	0.685479	2.252262	H	-6.743313	-2.242619	-1.794186
H	8.856949	-0.283623	-1.897866	H	-6.977390	-1.816270	2.466488
C	-1.681187	-2.258817	-0.861784	C	3.526329	-1.170835	1.104533
C	-1.076307	-2.655591	0.359514	C	3.135766	-2.347789	0.407638
C	-3.101331	-2.329124	-1.049856	C	4.876960	-0.688190	1.026685
C	-1.900172	-3.269737	1.389036	C	4.147097	-3.201830	-0.182863
C	-3.891223	-2.929863	-0.039924	C	5.832496	-1.470880	0.331812
C	-3.763753	-1.795067	-2.175088	C	5.285097	0.550967	1.541036
C	-3.241376	-3.410341	1.137018	C	5.429297	-2.725509	-0.214078
C	-5.289712	-3.009716	-0.190622	C	7.146824	-1.005366	0.192269
C	-5.138062	-1.873403	-2.292524	C	6.591536	0.988313	1.393757
H	-3.197331	-1.292176	-2.954515	H	4.562313	1.212297	2.011771
H	-3.868915	-3.900186	1.875841	H	6.206993	-3.322027	-0.680755
C	-5.937475	-2.482923	-1.296023	C	7.554416	0.215967	0.713840

H	-5.862154	-3.497881	0.593946	H	7.858313	-1.627663	-0.346425
H	-5.615068	-1.463417	-3.177703	H	6.867622	1.955148	1.795882
O	0.195796	-2.539367	0.560274	O	1.894510	-2.718698	0.345726
O	2.657273	-1.123919	1.247163	O	-0.777380	-2.642215	-0.691710
F	1.345569	-1.115942	-0.113478	Fe	0.365815	-1.548142	0.382247
C	-1.275318	-3.693385	2.716330	C	3.778538	-4.596924	-0.693473
C	-2.294242	-4.380178	3.629339	C	5.011947	-5.350261	-1.198500
H	-3.127126	-3.719482	3.896336	H	5.479503	-4.848718	-2.054247
H	-2.702869	-5.291405	3.177056	H	5.766945	-5.478069	-0.414235
H	-1.798755	-4.669294	4.561695	H	4.709339	-6.348876	-1.530455
C	-0.119825	-4.683092	2.491562	C	3.181623	-5.406714	0.471216
H	-0.477782	-5.582724	1.977487	H	3.894843	-5.475243	1.300782
H	0.683198	-4.239670	1.902556	H	2.257498	-4.954368	0.837487
H	0.287135	-4.990155	3.461798	H	2.955938	-6.425225	0.134413
C	-0.769291	-2.430606	3.437151	C	2.767440	-4.537589	-1.849234
H	-0.039827	-1.884355	2.836293	H	1.853207	-4.015811	-1.561871
H	-1.608625	-1.758802	3.658226	H	3.201081	-4.038844	-2.722739
H	-0.297967	-2.708957	4.387000	H	2.499190	-5.557630	-2.149245
C	3.675712	-0.213013	3.738813	C	-2.021014	-3.184482	-3.202107
C	3.130104	-1.592387	4.145576	C	-1.241831	-4.494390	-2.998421
H	2.512245	-2.027168	3.357600	H	-0.526671	-4.411690	-2.177718
H	3.952331	-2.282775	4.365944	H	-1.927692	-5.321223	-2.781916
H	2.518498	-1.494897	5.050946	H	-0.690472	-4.743467	-3.912973
C	2.509766	0.764773	3.511168	C	-1.051706	-2.054432	-3.584295
H	1.816188	0.393228	2.756540	H	-0.264296	-1.935711	-2.839652
H	1.955665	0.902100	4.447752	H	-0.583667	-2.284807	-4.549337
H	2.882009	1.746744	3.194783	H	-1.587954	-1.103443	-3.684368
C	4.506791	0.322541	4.907376	C	-2.975184	-3.386566	-4.382155
H	4.900282	1.325909	4.706265	H	-3.524585	-2.470234	-4.629027
H	3.871650	0.390394	5.796954	H	-2.395416	-3.669709	-5.266924
H	5.346166	-0.338355	5.152242	H	-3.698742	-4.187371	-4.192277
C	-7.451752	-2.529851	-1.480011	C	8.996009	0.685716	0.518301
C	-7.776324	-3.357633	-2.739022	C	9.952777	-0.343924	1.150124
C	-8.159027	-3.171243	-0.278078	C	9.281939	0.804832	-0.991564
C	-7.985632	-1.093081	-1.652364	C	9.254040	2.051631	1.169920
H	-7.311769	-2.920232	-3.629810	H	9.750525	-0.439904	2.222837
H	-7.407802	-4.382914	-2.622911	H	9.835438	-1.328757	0.684794
H	-8.861828	-3.386853	-2.893566	H	10.991338	-0.018586	1.013093
H	-7.969265	-2.606357	0.642796	H	8.603526	1.535163	-1.447962
H	-9.239849	-3.173992	-0.459240	H	10.315902	1.135289	-1.149758
H	-7.836512	-4.209820	-0.137830	H	9.146745	-0.158986	-1.494976
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H	-7.744481	-0.485133	-0.772728	H	8.615188	2.827623	0.730885
H	-7.552269	-0.614830	-2.538330	H	9.082651	2.012488	2.252390
C	10.282259	0.686685	0.204693	C	-8.552270	-1.678093	0.164958
C	10.726751	1.182264	1.587554	C	-8.725354	-0.395960	-0.673565
C	11.164575	-0.512991	-0.192161	C	-9.235234	-2.861529	-0.546739
C	10.472093	1.832042	-0.809109	C	-9.237651	-1.466464	1.522373
H	10.141569	2.055222	1.901375	H	-8.244537	0.450871	-0.167807
H	10.627224	0.391089	2.340337	H	-8.274555	-0.514179	-1.665474
H	11.781330	1.477559	1.540244	H	-9.791382	-0.170359	-0.800138
H	10.905102	-0.882035	-1.190726	H	-9.109931	-3.778171	0.040266
H	12.219221	-0.211350	-0.198434	H	-10.306968	-2.657948	-0.661039
H	11.034373	-1.330872	0.525495	H	-8.807498	-3.024894	-1.541818
H	11.522906	2.146505	-0.820283	H	-10.302358	-1.265570	1.356952
H	10.196943	1.514257	-1.821052	H	-9.152898	-2.360914	2.150971
H	9.848916	2.689559	-0.530335	H	-8.808245	-0.608930	2.054890
C	-0.761025	2.188366	1.854563	C	-2.556083	1.099883	-1.400752
C	-0.656388	3.546629	1.522450	C	-2.377282	1.797388	-2.605353
C	-1.315462	4.499875	2.286389	C	-3.475529	2.353343	-3.247727
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C	-1.498943	1.755452	2.952272	C	-3.820511	0.893686	-0.853941
C	0.594964	2.297882	-0.019807	C	-0.301462	0.954526	-1.904928

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H	-1.244933	5.557318	2.044718	H	-3.360222	2.899208	-4.180626
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H	-2.708122	2.419955	4.601650	H	-5.919158	1.262167	-1.125920
H	-1.561593	0.699093	3.193147	H	-3.949941	0.283176	0.034385
H	1.118612	4.320870	0.559121	H	-0.492900	2.769589	-3.077860
H	-0.285384	4.232473	-0.496443	H	-0.796060	1.296136	-3.993586
C	0.012701	1.402983	0.879150	C	-1.249508	0.615195	-0.939339
O	0.061400	0.122121	0.892981	O	-1.075786	0.021714	0.187332
C	1.589919	1.890299	-0.946748	C	1.014867	0.435432	-1.888011
O	1.975160	0.710703	-1.093607	O	1.446064	-0.337936	-0.993695
C	-2.371577	0.886320	-0.618797	C	0.829476	2.393416	0.619575
H	-1.707721	0.087971	-0.292265	H	0.920230	1.375711	0.999767
N	-3.375276	1.169966	0.123016	N	-0.260974	3.030522	0.842752
C	-4.419812	2.081803	-0.208095	C	-0.561510	4.359253	0.441829
C	-4.649786	3.184480	0.603884	C	-1.752303	4.582853	-0.242524
C	-5.239024	1.795454	-1.300934	C	0.311177	5.413424	0.726080
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H	-3.991524	3.390338	1.443826	H	-2.410734	3.751540	-0.476377
C	-6.294485	2.639098	-1.589046	C	-0.008580	6.689578	0.306393
H	-5.076801	0.884307	-1.870442	H	1.218684	5.237723	1.297435
C	-6.533332	3.770173	-0.793486	C	-1.197674	6.927056	-0.402356
H	-5.872220	4.908823	0.929004	H	-2.988580	6.020122	-1.225689
H	-6.965877	2.437404	-2.416956	H	0.638253	7.532059	0.527002
O	-7.581247	4.524446	-1.159105	O	-1.410093	8.198581	-0.766930
C	-7.892345	5.666666	-0.384880	C	-2.600856	8.510272	-1.466195
H	-7.067547	6.389560	-0.392978	H	-3.486829	8.268686	-0.867061
H	-8.769067	6.113470	-0.853487	H	-2.566449	9.584522	-1.646086
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C	-2.045753	1.545021	-1.922990	C	2.032708	3.025693	-0.007331
O	-1.719624	0.883282	-2.880103	O	3.060311	3.084705	0.622691
O	-2.111581	2.862008	-1.858671	O	1.791893	3.467916	-1.224321
C	-1.646823	3.554939	-3.026615	C	2.841298	4.194313	-1.880231
H	-1.867908	4.605046	-2.844369	H	2.762265	3.942744	-2.936656
H	-0.569798	3.399027	-3.133510	H	2.661788	5.260962	-1.723826
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H	-3.508472	0.608082	1.014831	H	-1.018069	2.492851	1.369972
O	-3.872471	-0.418103	2.252627	O	1.771043	0.826503	-2.904747
C	-5.189040	-0.376617	2.864811	C	3.090366	0.242919	-3.190253
C	-5.170010	0.823197	3.795278	C	4.080129	0.641497	-2.108176
C	-6.251549	-0.219789	1.783004	C	2.970671	-1.265765	-3.332179
C	-5.395960	-1.664125	3.650358	C	3.446876	0.881129	-4.523518
H	-4.429294	0.682490	4.588370	H	4.188192	1.728962	-2.058248
H	-4.920174	1.735728	3.244705	H	3.772883	0.267087	-1.132550
H	-6.153266	0.959274	4.255818	H	5.065277	0.220387	-2.332767
H	-6.135635	-0.992710	1.016863	H	2.184708	-1.523943	-4.049723
H	-7.254203	-0.308919	2.214904	H	3.919595	-1.666876	-3.702973
H	-6.181676	0.759309	1.298648	H	2.748854	-1.740431	-2.377500
H	-6.332332	-1.621404	4.215073	H	4.434998	0.539726	-4.846162
H	-5.453767	-2.529561	2.980546	H	2.716418	0.609869	-5.291833
H	-4.574407	-1.819754	4.356992	H	3.472087	1.972583	-4.438699
H	-3.714917	-1.318669	1.914407	O	-1.945115	1.534300	2.226397
O	2.107439	2.893300	-1.653243	C	-3.131141	1.953315	2.942885
C	3.391007	2.779718	-2.354798	C	-2.610650	2.561506	4.236565
C	4.481853	2.469740	-1.339761	C	-3.890768	2.991225	2.125591
C	3.327127	1.737447	-3.463721	C	-3.998924	0.736641	3.218145
C	3.564249	4.172739	-2.940200	H	-2.051822	1.817283	4.812714
H	4.513648	3.241704	-0.564062	H	-1.944184	3.405083	4.024912
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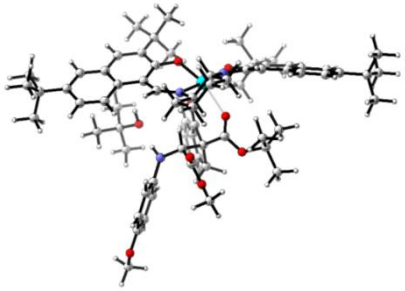
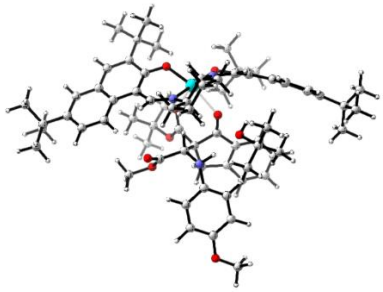
H	2.414461	1.861229	-4.057275	H	-4.788965	3.314545	2.661834
H	4.185871	1.870324	-4.130481	H	-3.270538	3.876498	1.948711
H	3.353395	0.726944	-3.056001	H	-4.879372	1.019845	3.803538
H	4.524722	4.242854	-3.459192	H	-4.355082	0.269667	2.293718

H	2.766305	4.395606	-3.656352	H	-3.438640	-0.010478	3.787976
H	3.541810	4.927123	-2.148089	H	-2.096299	0.811134	1.579967
INT 5 *SR*				**INT 5 *RS***			
							
E(UPBE1PBE) = -4901.224388				E(UPBE1PBE) = -4901.220753			
Thermal correction to Gibbs Free Energy= 1.418839				Thermal correction to Gibbs Free Energy= 1.421043			
C	0.357370	0.086156	4.482577	C	1.006204	0.473939	4.287889
C	-0.412107	-0.189154	3.192896	C	0.377725	-0.200663	3.070328
C	-1.628807	-1.122549	3.439578	C	-0.332213	-1.532438	3.450667
C	-2.552746	-0.512842	4.499532	C	-1.378538	-1.281328	4.536274
C	-1.769586	-0.223784	5.791086	C	-0.727050	-0.611855	5.757349
C	-0.590540	0.716741	5.512214	C	-0.075215	0.717159	5.351447
H	-0.800502	0.765188	2.811512	H	-0.402104	0.459147	2.658468
H	0.764781	-0.851498	4.887878	H	1.789889	-0.173143	4.708161
H	1.183925	0.775350	4.269167	H	1.459632	1.426202	3.982557
H	-2.970483	0.427329	4.109124	H	-2.146310	-0.608599	4.134682
H	-3.382378	-1.195610	4.723425	H	-1.853806	-2.224998	4.835209
H	-2.444264	0.217930	6.533647	H	-1.487833	-0.444277	6.528917
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C	-4.214191	-1.339030	0.694814	C	-2.732692	-2.669737	0.771817
C	-3.567815	-1.759207	-0.492149	C	-1.985741	-2.986745	-0.385988
C	-5.605598	-0.960718	0.671687	C	-4.163867	-2.507592	0.697982
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C	-6.307479	-1.074785	-0.555375	C	-4.785968	-2.647340	-0.571771
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C	-7.653409	-0.671657	-0.650888	C	-6.143016	-2.326405	-0.736434
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C	2.286981	-2.036344	1.336989	C	3.540232	-0.996072	1.209425
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C	4.390537	-3.165672	0.773959	C	5.877554	-1.190837	0.496662
C	4.501320	-1.221886	2.207969	C	5.155991	0.897097	1.484888
C	3.637211	-4.035526	-0.065142	C	5.580435	-2.515549	0.066174
C	5.787201	-3.303352	0.885577	C	7.157656	-0.642529	0.326137
C	5.867636	-1.383406	2.310308	C	6.429459	1.413468	1.308022
H	4.043520	-0.362576	2.690142	H	4.386665	1.545952	1.893886
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C	6.545411	-2.437612	1.654275	C	7.462350	0.652200	0.721741
H	6.265104	-4.113543	0.343034	H	7.924638	-1.261823	-0.134117

H	6.438156	-0.669148	2.893849	H	6.627674	2.429700	1.626860
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C	1.541288	-4.836276	-1.249507	C	4.066311	-4.512314	-0.349063
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C	-3.606872	-2.417542	-2.986546	C	-1.859917	-3.721165	-2.861223
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H	-2.303049	-3.823555	-1.928187	H	-0.321768	-4.788838	-1.725631
H	-3.829828	-4.529845	-2.498090	H	-1.682449	-5.803395	-2.245415
H	-2.530524	-4.178849	-3.651668	H	-0.466088	-5.283030	-3.424190
C	-2.481981	-1.450131	-3.394867	C	-0.938440	-2.578088	-3.316612
H	-1.692013	-1.416141	-2.643795	H	-0.205342	-2.331127	-2.547654
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H	-2.875526	-0.436598	-3.542307	H	-1.523273	-1.679984	-3.552287
C	-4.583190	-2.511648	-4.162019	C	-2.782665	-4.067227	-4.033243
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H	7.952278	-3.688465	3.647967	H	9.846978	-0.706868	0.926763
H	9.497454	-2.834889	3.396527	H	10.893183	0.716300	1.130661
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H	9.710708	-3.767615	1.121547	H	10.209895	1.569266	-1.163748
H	8.204370	-4.682443	1.329781	H	9.155192	0.156681	-1.391460
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C	-9.789747	0.311843	0.360960	C	-8.370022	-1.440014	0.064268
C	-10.389536	0.116794	-1.038129	C	-8.356799	-0.257052	-0.925775
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H	-9.842820	0.700866	-1.788500	H	-7.781635	0.578486	-0.507398
H	-10.380925	-0.940968	-1.327276	H	-7.905386	-0.552942	-1.880207
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H	-10.247991	-0.372816	2.390301	H	-9.172048	-3.461184	0.159631
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C	1.531009	0.376449	-5.194434	C	-4.449717	1.310004	-2.499511
C	1.166871	-0.124128	-3.956323	C	-3.551831	0.644020	-1.683776
C	0.027882	1.839437	-0.931346	C	0.148479	1.358891	-1.271796
C	0.223810	2.919715	-2.005577	C	-0.291550	2.357140	-2.358478

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C	0.352321	0.520587	-1.625882	C	-1.111508	0.558051	-0.937406
O	0.264227	-0.593997	-1.103773	O	-1.144869	-0.316627	-0.073696
C	-1.353250	1.709450	-0.335298	C	1.208164	0.359834	-1.699238
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C	1.034508	1.976430	0.316910	C	0.533597	1.979548	0.135577
H	0.913930	1.036712	0.861827	H	0.635908	1.112128	0.790849
N	2.399279	2.157078	-0.035219	N	-0.472740	2.808913	0.732557
C	3.069319	3.399588	-0.075987	C	-0.820086	4.070291	0.200506
C	3.501689	3.959857	-1.277917	C	-2.108672	4.320587	-0.272224
C	3.366421	4.078850	1.114736	C	0.109334	5.120854	0.172873
C	4.208315	5.161671	-1.306966	C	-2.469903	5.567765	-0.779124
H	3.277047	3.450965	-2.211601	H	-2.840341	3.517629	-0.269052
C	4.032142	5.291708	1.096743	C	-0.229230	6.351475	-0.362875
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C	4.465961	5.842951	-0.115993	C	-1.522097	6.589674	-0.845199
H	4.537018	5.559675	-2.260599	H	-3.483861	5.718826	-1.132548
H	4.262873	5.821703	2.015718	H	0.487584	7.166251	-0.388292
O	5.122828	7.020392	-0.026272	O	-1.750903	7.827601	-1.340421
C	5.605924	7.596659	-1.218450	C	-3.049542	8.118239	-1.801389
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C	0.545380	3.060305	1.271010	C	1.910079	2.625857	0.212928
O	0.382029	2.881218	2.457370	O	2.460362	2.839498	1.267952
O	0.309184	4.210963	0.650067	O	2.438996	2.894024	-0.978600
C	-0.043982	5.310945	1.489766	C	3.748994	3.473400	-0.951076
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O	3.440806	-0.177893	-1.351490	O	1.838560	0.694057	-2.785730
C	4.690590	-0.285143	-2.060375	C	2.970181	-0.072560	-3.368496
C	4.704552	0.867569	-3.050885	C	4.091676	-0.178747	-2.351860
C	5.846525	-0.157402	-1.076600	C	2.465949	-1.426096	-3.834013
C	4.720759	-1.626622	-2.784845	C	3.368389	0.805209	-4.542759
H	3.805327	0.853351	-3.673608	H	4.361350	0.805618	-1.959185
H	4.755192	1.824801	-2.523407	H	3.825229	-0.831039	-1.521510
H	5.579759	0.794659	-3.704112	H	4.975450	-0.598326	-2.842388
H	5.850085	-0.973931	-0.348736	H	1.611567	-1.309345	-4.507835
H	6.806257	-0.176793	-1.604986	H	3.266015	-1.931230	-4.384875
H	5.774866	0.789316	-0.530336	H	2.177127	-2.059213	-2.994284
H	5.652437	-1.748913	-3.347413	H	4.210600	0.349401	-5.071144
H	4.645420	-2.452256	-2.068825	H	2.538163	0.917098	-5.246903
H	3.880420	-1.698560	-3.483423	H	3.672033	1.798400	-4.197734
H	3.447266	-0.840076	-0.641701	O	-2.684864	1.183497	1.983973
O	-2.104352	2.765722	-0.488557	C	-3.846996	1.815484	2.558466
C	-3.492334	2.854166	0.036871	C	-3.386583	3.206671	2.964416
C	-4.367467	1.945037	-0.807185	C	-4.962465	1.864664	1.519447
C	-3.533812	2.513015	1.519766	C	-4.301932	1.038010	3.789557
C	-3.821525	4.319641	-0.190418	H	-2.516320	3.133420	3.625688
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H	-3.709438	4.582812	-1.246476	H	-2.956198	0.364214	1.542735

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