

Proline Bulky Substituents Consecutively Act as Steric Hindrances and Directing Groups in a Michael/Conia-Ene Cascade Reaction under Synergistic Catalysis

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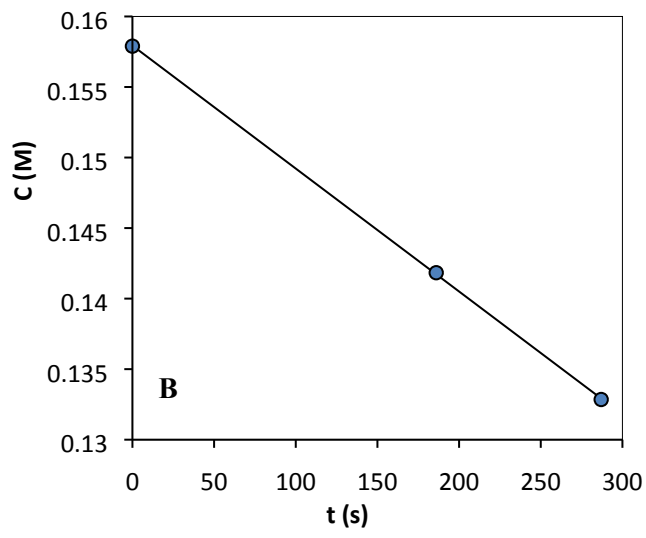
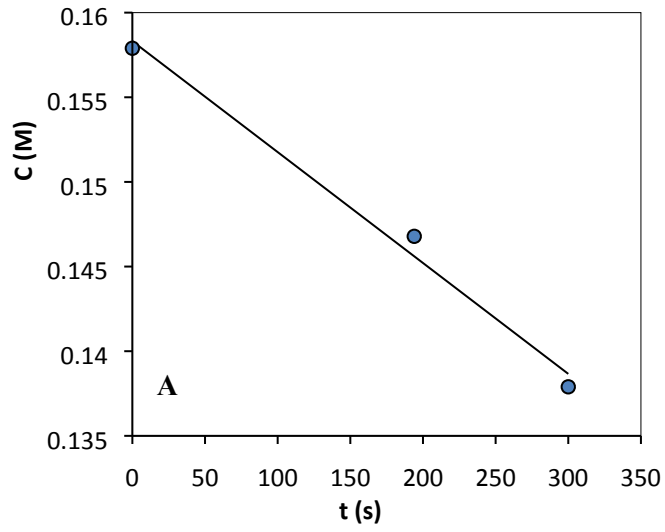
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Initial Experimental Kinetic Studies

General procedure to prepare the Conia-Ene reactions in the kinetic studies: In order to increase the precision of the kinetic studies, we prepared stock solutions of the initial components and added the same amounts of liquid from the stock solutions to all the reactions. The initial reagents were dissolved using AcOEt/CDCl₃ mixtures in order to obtain homogeneous stock solutions (except for the Pd₂(dba)₃ stock solution), which were generated with: (1) 1.05 mmol (223 mg) of pyrazolone **5a** in 700 μL AcOEt and 2.1 mL CDCl₃; (2) 0.7 mmol (89 μL) of cinnamaldehyde (**6a**) in 700 μL AcOEt; (3) 0.21 mmol (58 mg) of Ph₃MeSi in 700 μL AcOEt and 100 μL CDCl₃ (as the internal standard); (4) 0.053 mmol (17.1 mg), 0.070 mmol (22.8 mg) or 0.123 mmol (39.9 mg) of proline derivative **I** (depending on the reaction) in 350 μL AcOEt; and (5) 0.0139 mmol (12.7 mg) or 0.0419 mmol (38.4 mg) of Pd₂(dba)₃ (depending on the reaction) in 700 μL AcOEt and 1.05 mL CDCl₃. In total, we added to the NMR tubes: 400 μL of (1); 100 μL of (2); 100 μL of (3); 100 μL of (4); and 250 μL of (5) in this order. In the resulting solutions, the individual components are dissolved in a total of 487.5 μL AcOEt and 462.5 μL CDCl₃, leading to concentrations of: 0.158 M for pyrazolone **5a**; 0.105 M for cinnamaldehyde; 0.028 M for Ph₃MeSi; 0.0158 M (15 mol%), 0.0211 M (20 mol%) or 0.0368 M (35 mol%) for proline **I**; and 0.0021 M (2 mol%) or 0.0063 M (6 mol%) for Pd₂(dba)₃ (these concentrations are only used for qualitative purposes, since the Pd stock solutions are heterogeneous). All the experiments were carried out on the same day, with the same types of instruments and using the same spinning speed (20 Hz) and temperature (rt, T = 295.9 K) in the NMR measurements. This procedure was followed to measure orders of reaction and equilibrium concentrations.

Orders of reaction: Following the general procedure, we measured the initial rates using varying amounts of catalyst **I** and Pd₂(dba)₃ (Figure S1). These results suggested that the order of reaction of catalyst **I** was 1 (Table S1).



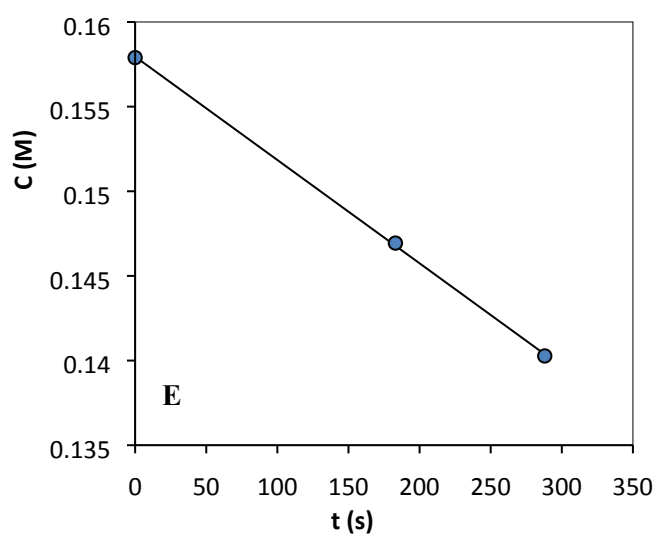
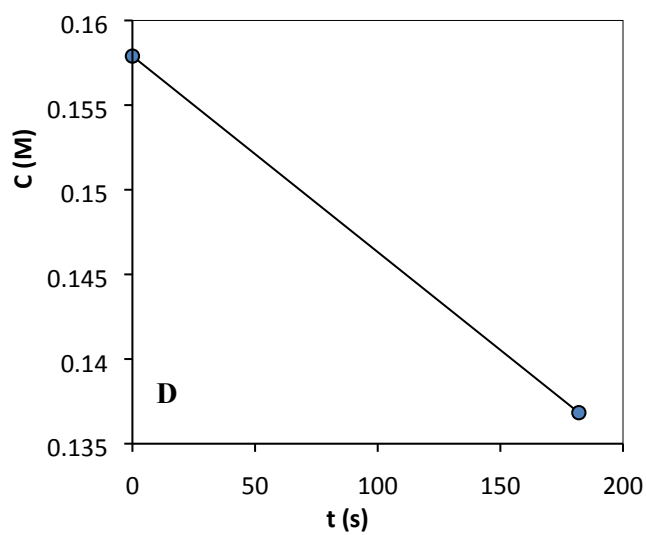
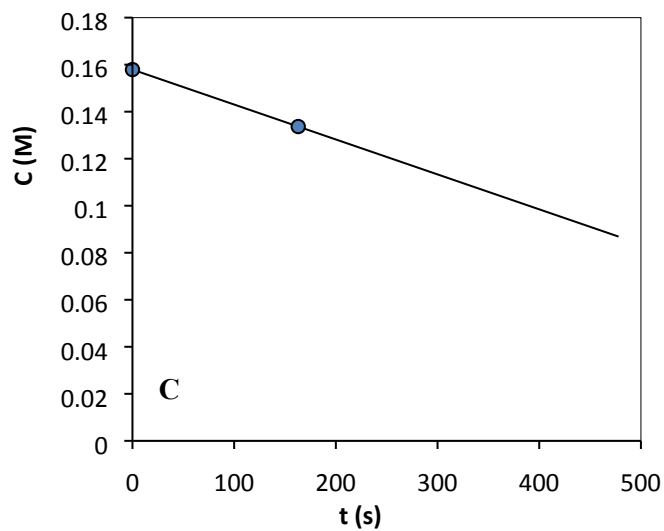


Figure S1. Concentration of cinnamaldehyde (**6a**) vs time plots at the beginning of the reactions when using different amounts of $\text{Pd}_2(\text{dba})_3$ and the proline catalyst **I**. (A) 2 mol% $\text{Pd}_2(\text{dba})_3$ and 15 mol% **I**; (B) 2 mol% $\text{Pd}_2(\text{dba})_3$ and 20 mol% **I**; (C) 2 mol% $\text{Pd}_2(\text{dba})_3$ and 35 mol% **I**; (D) 0 mol% $\text{Pd}_2(\text{dba})_3$ and 15 mol% **I**; (E) 6 mol% $\text{Pd}_2(\text{dba})_3$ and 15 mol% **I**.

Table S1. Initial reaction rates obtained when using 15, 20 and 35 mol% of proline derivative **I** and 2% of Pd₂(dba)₃ (graphs A, B and C in Figure S1, respectively).

Entry ^a	Amount of proline I (mol%)	Initial rate (M s ⁻¹)	Relative initial rate
1	15	-0.0000655	15
2	20	-0.0000872	20
3	35	-0.0001486	34

We also analyzed how the variation of the amount of Pd affected the results but, due to the insolubility of the Pd catalyst, these results were only used qualitatively. The outcomes showed that using 6 mol% of Pd instead of 2 mol% did not have a sharp effect on the results and only a small decrease in the initial rate was observed (Table S2).

Table S2. Initial rates of the reactions when using 15 mol% of proline derivative **I** and different amounts of Pd₂(dba)₃.

Eq. of Pd ₂ (dba) ₃ (mol%)	Relative eq. of I	Initial rate (M s ⁻¹)	Relative initial rate
2	2.0	-0.0000655	2.0
6	6.0	-0.0000610	1.86

Furthermore, we observed that Pd atoms might be forming interactions with proline catalyst **I**, since the ¹H signals of -OSiMe₃ in the proline derivative shift in the NMR spectra when Pd₂(dba)₃ is added (Figure S2).

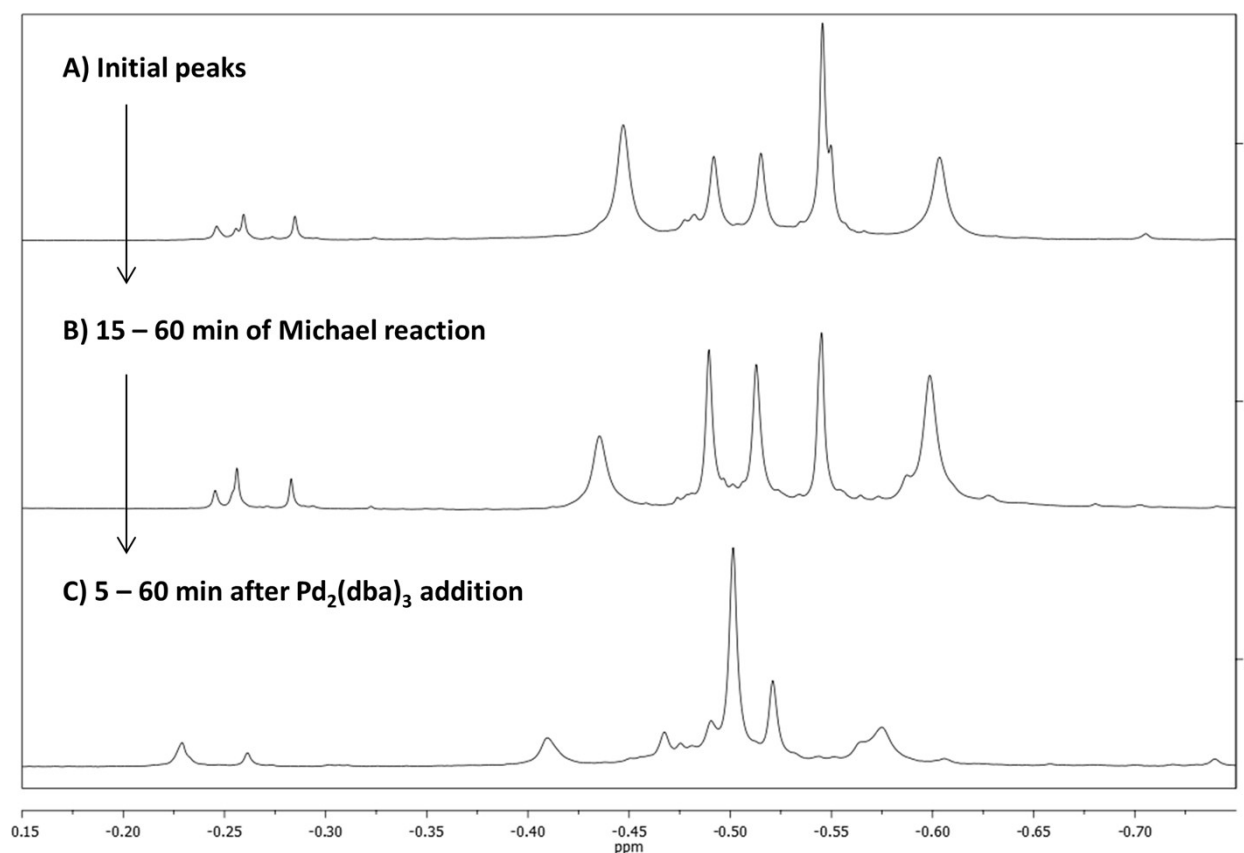
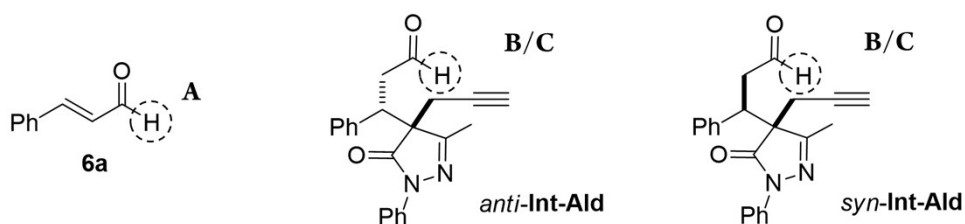
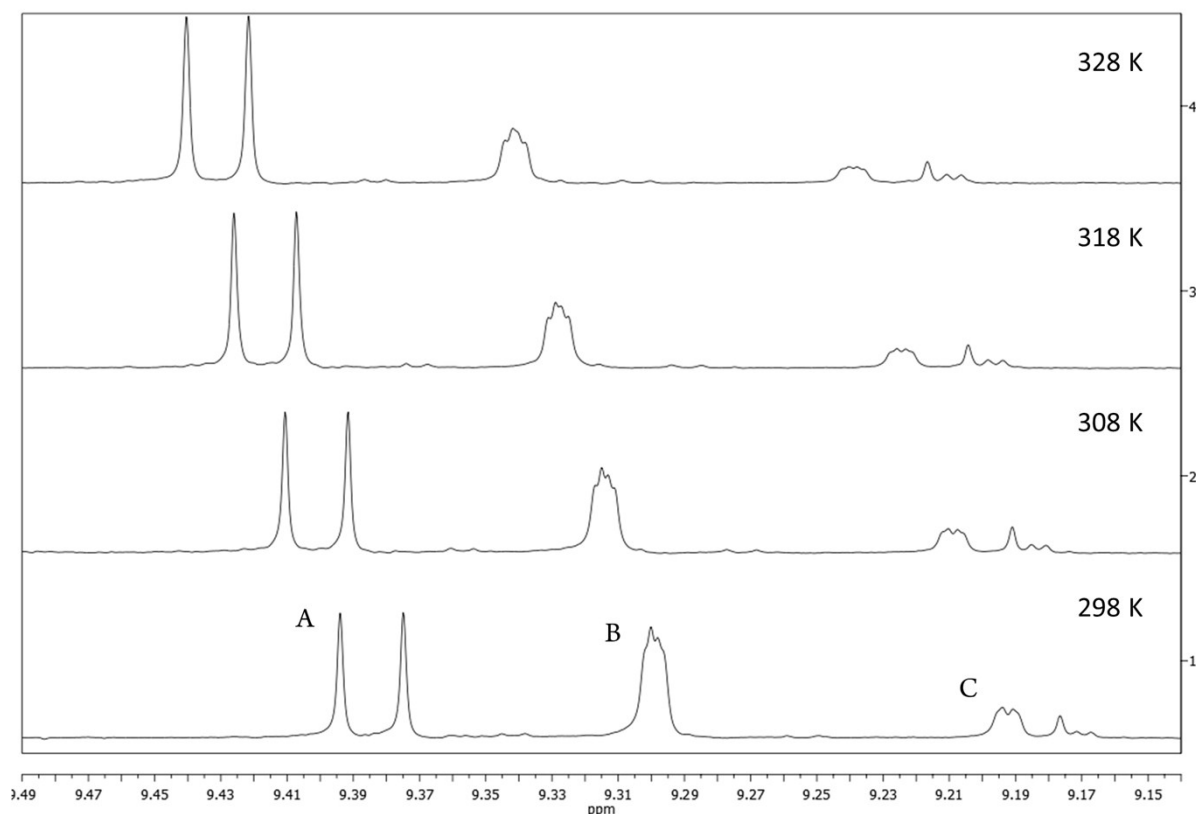


Figure S2. Peaks of the -OSiMe₃ groups of proline derivative **I**: (A) at the beginning of the reaction catalyzed only by 15 mol% **I** (only the Michael addition takes place); (B) after 15 – 60 minutes of this reaction; (C) after 5 – 60 minutes of adding 2 mol% of Pd₂(dba)₃.

Equilibrium concentrations: we carried out variable temperature ^1H NMR experiments in order to study the equilibrium concentrations of the initial Michael reaction, as well as the reversibility of the Michael and cyclization reactions. As seen in Figure S3, when the Michael reaction does not proceed any further, the conversion of the reaction changes when the reaction temperature is modified, showing reversible changes when the reaction is cooled down. For example, the conversion observed at 298 K is 62%, it becomes 40% when the reaction is heated up to 328 K, and conversion is 62% again when the same reaction is cooled down to 298 K (Figure S3, entries 1, 4 and 5, respectively). This indicates that the initial Michael reaction is a reversible process.

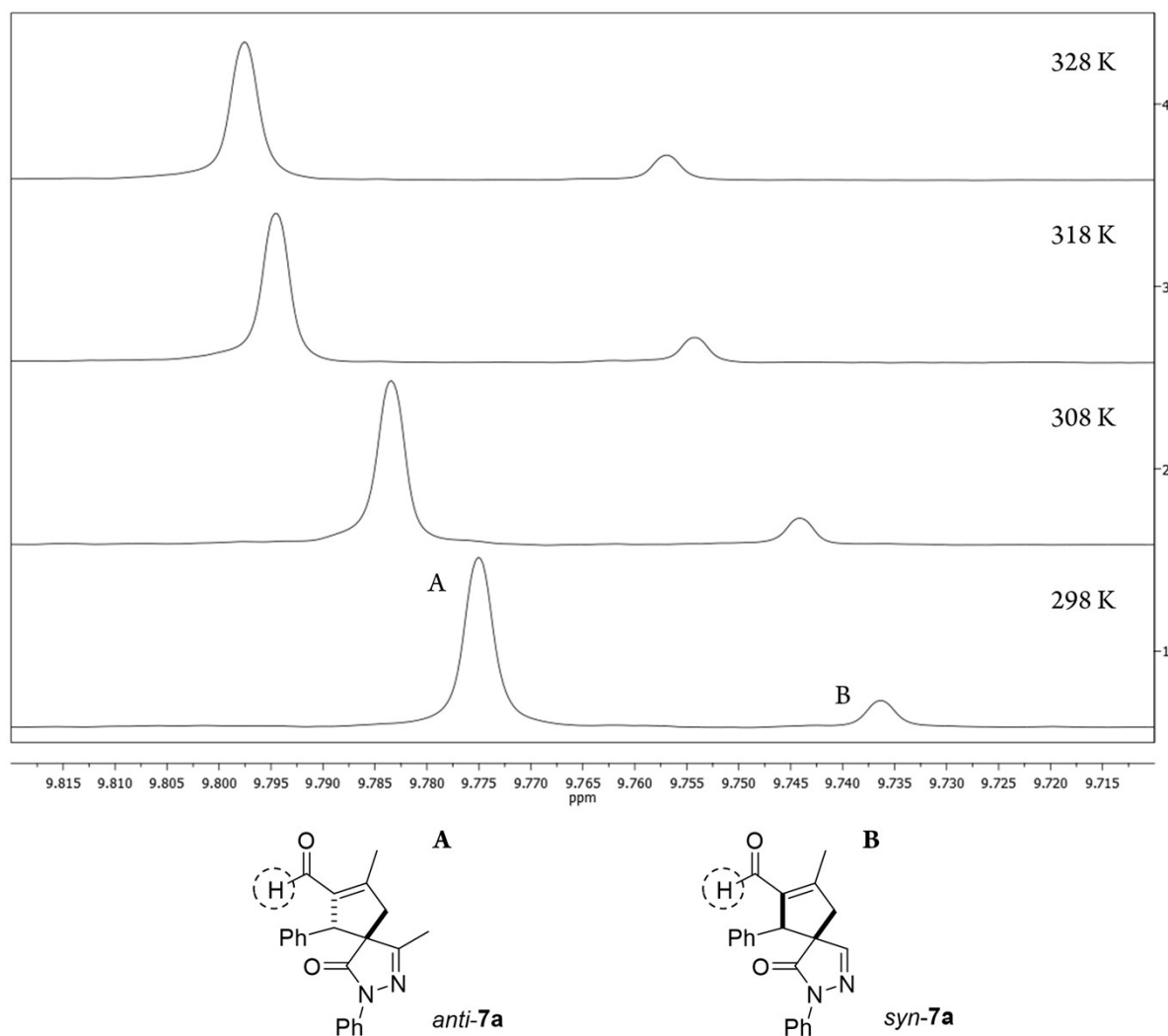


Entry	T (K)	Integral of peak A	Integral of peak B	Integral of peak C	Conversion (%) ^a
1	298	1	1.27	0.37	62
2	308	1	0.92	0.28	55
3	318	1	0.65	0.21	46
4	328	1	0.49	0.17	40
5	298 ^b	1	1.27	0.37	62

^a Conversion was calculated using peaks A, B and C, since **Int-Ald** is the only product observed in part 1. Therefore, for a 62% of reaction conversion, there is 38% of cinnamaldehyde and 62% of *syn-/anti-Int-Ald* compared to the initial amount of cinnamaldehyde (100%). ^b After cooling down the NMR tube at 328 K.

Figure S3. ¹H peaks of the CHO groups of cinnamaldehyde and *anti/syn-Int-Ald* with their corresponding integrals and cinnamaldehyde conversion at different temperatures. Reaction conditions: pyrazolone **5a** (0.158 M), cinnamaldehyde (0.105 M), Ph₃MeSi (0.028 M) and proline **I** (0.0211M) (prepared according to the general procedure).

Contrarily to the previous case, when Pd₂(dba)₃ is added, when the reaction does not proceed any further the conversion of the reaction does not change with temperature (Figure S4). This indicates that the Conia-Ene reaction is an irreversible process.



Entry	T (K)	Integral of peak A	Integral of peak B	Conversion (%) ^a
1	298	6.10	1	100
2	308	6.04	1	100
3	318	6.06	1	100
4	328	6.00	1	100

^a No peaks from initial cinnamaldehyde were observed.

Figure S4. ^1H peaks of the CHO groups of *anti/syn-7a* with their corresponding integrals and cinnamaldehyde conversion at different temperatures. Reaction conditions: pyrazolone **5a** (0.158 M), cinnamaldehyde (0.105 M), Ph_3MeSi (0.028 M), proline **I** (0.0211M) and $\text{Pd}_2(\text{dba})_3$ (0.0021 M) (prepared according to the general procedure).

Additionally, we performed various tests to ensure that condensation intermediates were not formed during part 1 of the reaction (Figures S5-6). We did not detect any condensation products using NMR and MS experiments.

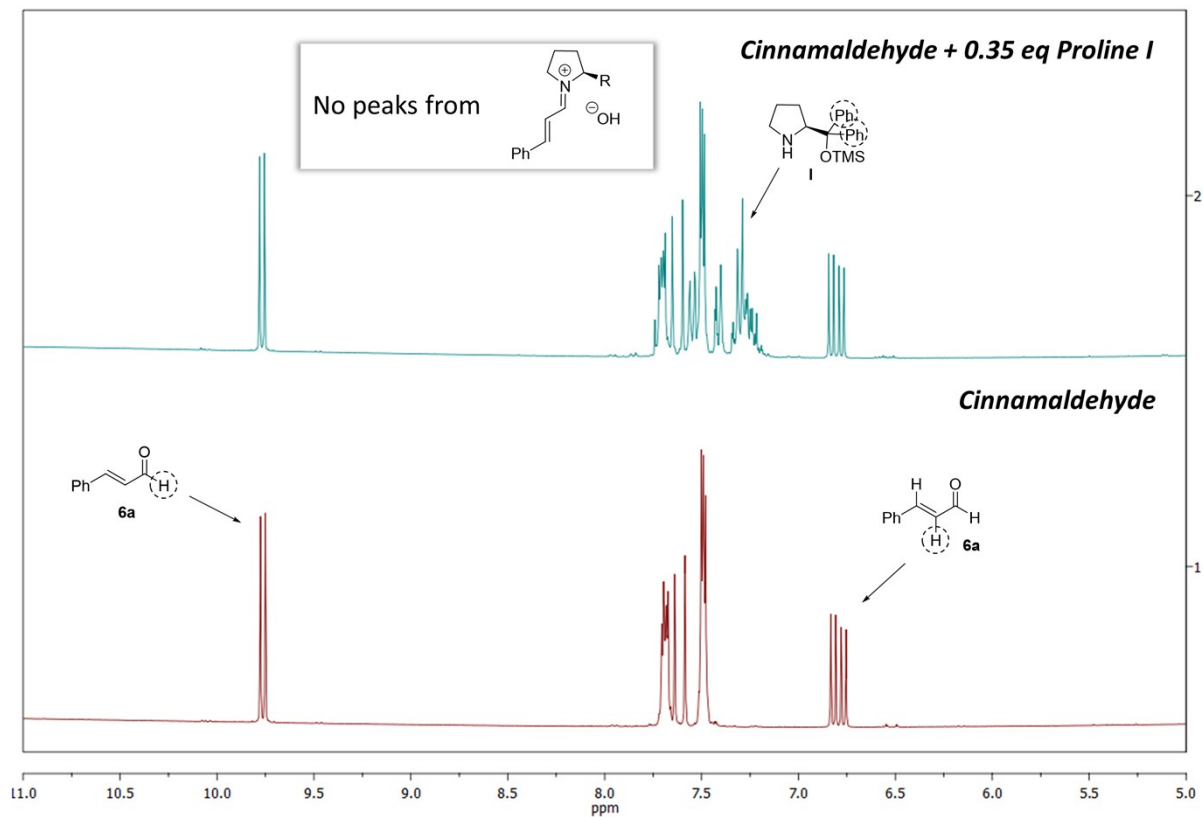


Figure S5. NMR spectra of cinnamaldehyde (0.105 M) and cinnamaldehyde + proline **I** (0.105 M and 0.0368 M, respectively) in the conditions used in the previous NMR kinetic studies (487.5 μL AcOEt and 462.5 μL CDCl_3).

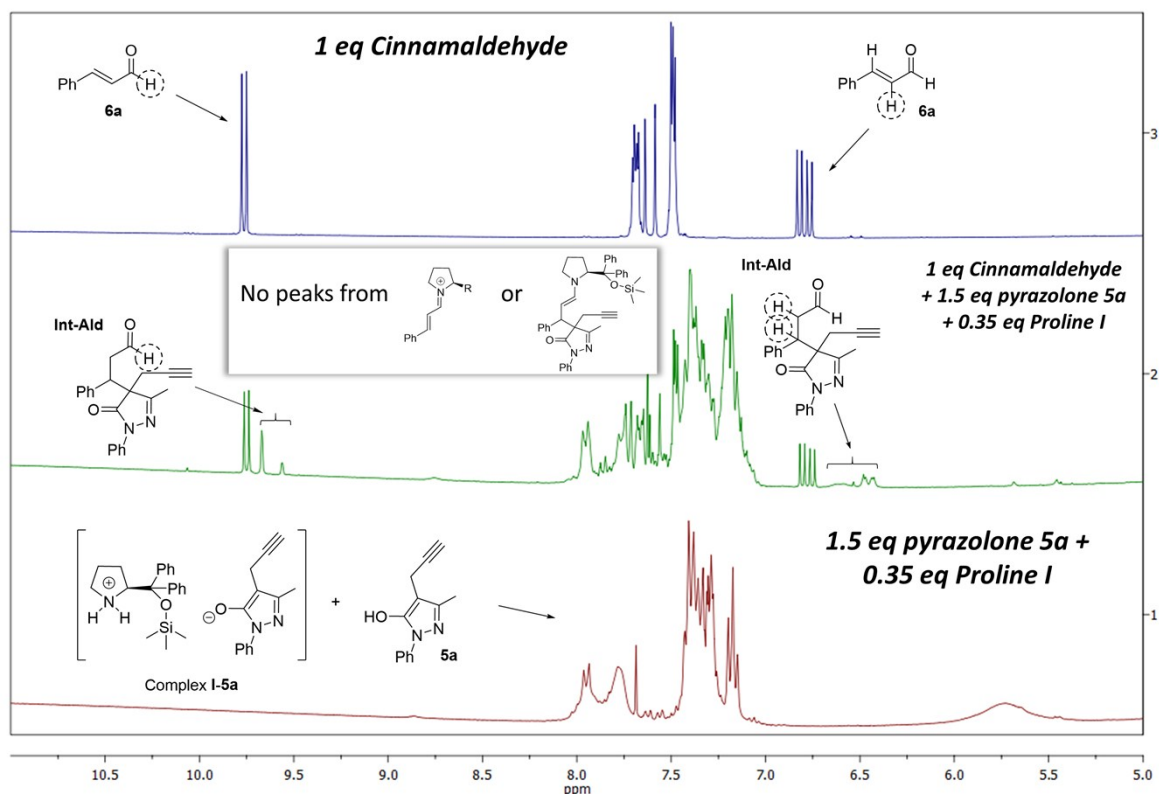
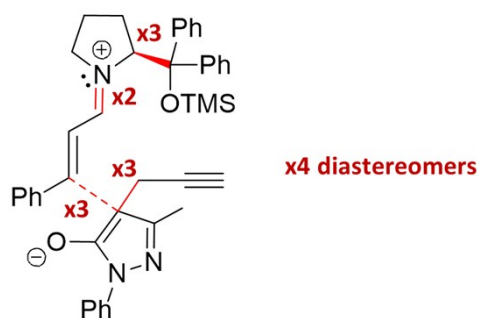


Figure S6. NMR spectra of cinnamaldehyde (0.105 M), pyrazolone **5a** + proline **I** (0.158 M and 0.0368 M, respectively), and the three components together in the conditions used in the previous NMR kinetic studies (487.5 μ L AcOEt and 462.5 μ L CDCl_3).

Previous experimental ^1H NMR shifts of the H atom binding the aldehyde group ($-\text{CHO}$) of cinnamaldehyde in CDCl_3 ⁱ are identical to the $-\text{CHO}$ shift obtained in the mixture used for our NMR experiments (487.5 μ L AcOEt and 462.5 μ L CDCl_3). Based on this finding, the condensation product of proline **I** and cinnamaldehyde should show two characteristic peaks as observed previously in CDCl_3 ,ⁱⁱ one around 8.60 ppm ($-\text{CHN}$, H atom from the iminium group) and one around 5.54 ppm (H atom from the conjugated $\text{C}=\text{C}$). None of these peaks were observed in any experiments, which suggests that the condensation product of proline **I** and cinnamaldehyde reacts very fast when it is produced. We did not observe any peak that suggested the formation of the condensation product of proline **I** with **Int-Ald**.

Computational Details

Methods, protocols and geometry optimization validation: In the **Int-I**, **TS-I**, **Int-II**, **Int-III**, **TS-II**, **Int-IV** reaction steps, a great number of systems were found due to all the possible conformations that the catalyst and the substrates could adopt. In order to find a significant number of conformations, we located and rotated the bonds that led to different conformations through rotations of two (x2) or three groups (x3). Then, the total number of conformations of a diastereomer in a reaction step was determined by the multiplication of all the x2 and x3 bonds (Figure S7).



Number of conformations tested = $3 \times 2 \times 3 \times 3 \times 4 = 216$

Figure S7. Structural analysis used to determine the number of systems calculated in the **TS-I** step.

In order to discard the least energetically favorable systems, for each system we performed relaxed potential energy surface (PES) scans along the coordinate of the bond forming reactions, incrementing this coordinate by 0.1 Å. For each part of the reaction (parts 1 and 2), one scan was needed in order to evaluate the energies of the two transition states (**TS-I** and **TS-II**) and the intermediate steps (**Int-I** to **Int-IV**) (Figure S8). These scans were done at the ω B97X-Dⁱⁱⁱ/6–311G(d)^{iv} level in combination with the UltraFineGrid option and using the SMD solvation model (solvent=ethylethanoate).^v In the calculations including a Pd atom, the calculations were performed using the genecp option with C, H, O, N and Si atoms described using the 6–311G(d) basis set and the Pd atom with the Def2-TZVP^{vi} basis set (including the corresponding effective core potential (ECP) for Pd atoms). After the scans were done, we evaluated the electronic energies obtained at the different reaction steps (Figure S8) and selected the 10 systems with highest energy of each step for each diastereomer, assuming that thermodynamic corrections should not vary in a great extent within similar conformers. For example, for the (*S,R*) diastereomer in the **TS-I** step, we obtained 54 electronic energies that corresponded to all the conformers with the (*S,R*) configuration and, from these 54 structures, we only studied further (optimization without the frozen scan coordinate and G calculation) the 10 structures with the lowest electronic energies.

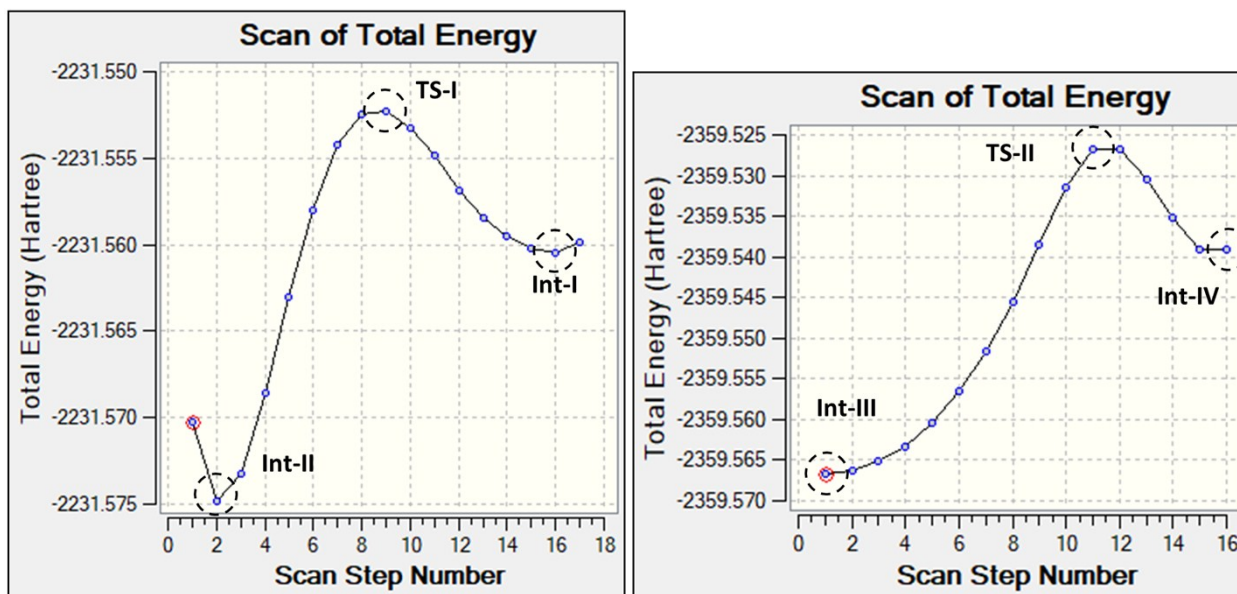


Figure S8. Example of relaxed PES scans along the coordinate of the bond formation of the Michael addition (**TS-I**, left) and the cyclization reaction (**TS-II**, right).

The ω B97X-D/6–311G(d) combination with the UltraFineGrid option was also employed to optimize the geometries of the stationary points (Pd atom with the Def2-TZVP basis set including the corresponding ECP for Pd atoms). This functional has proven to be accurate for systems with non-covalent interactions, such as π -interactions and hydrogen bonds.^{iii,vii} Furthermore, we tested its efficiency for optimizing geometries related to our study by optimizing a molecular geometry obtained from an X-ray structure of proline **I** condensed with cinnamaldehyde (Figure S9).^{viii} Considering that we used solvent (SMD = AcOEt) that creates a medium with

different polarity compared to the original crystal packing (which also contains BF_4^- counterions), the level of agreement between theory and experiment is high: relevant N-C, C-C, O-Si and O-C bond distances differ by less than 2.5% and all angles and dihedrals are also well-reproduced.

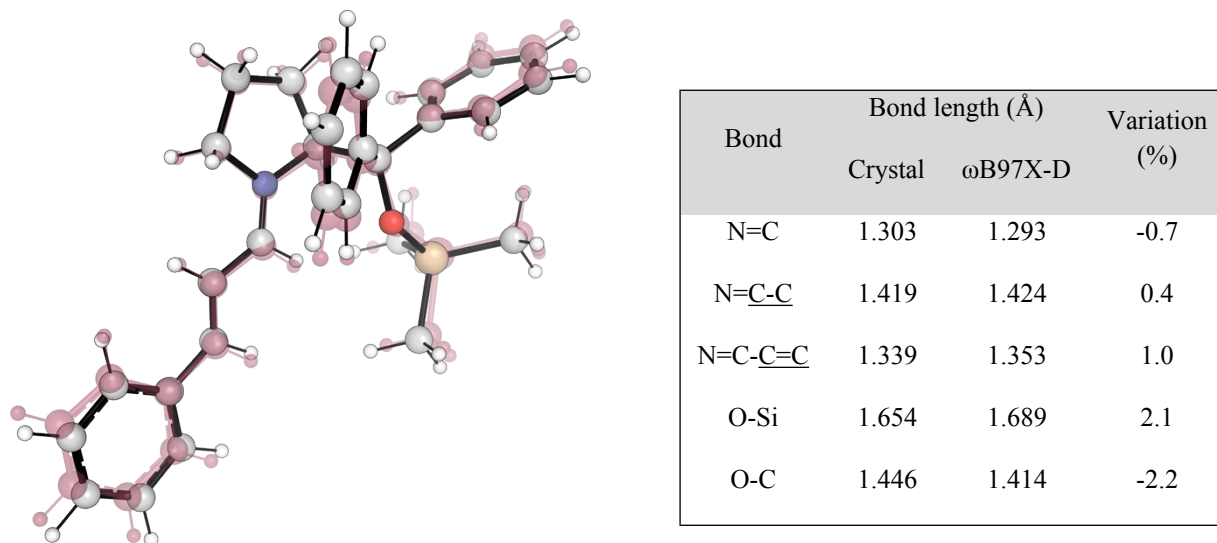


Figure S9. Left: Structure of the condensation product of proline **I** and cinnamaldehyde obtained with ω B97X-D/6-311G(d) (SMD)(UF grid), represented with standard colors, and geometry observed in the original X-ray crystal structure, represented in dark red. Right: Tabulation of relevant bond lengths determined experimentally and computationally.

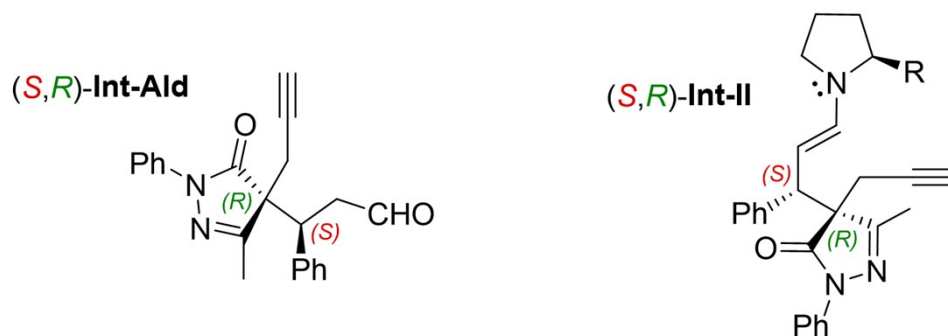
Vibrational frequency calculations were performed in order to (1) verify that the stationary points were either energy minima or transition states and (2) obtain the thermal corrections to Gibbs free energies at 293.15 K (20 °C). Additionally, intrinsic reaction coordinate (IRC) calculations^{ix} were carried out to confirm that **Int-I** and **Int-II** or **Int-III** and **Int-IV** of the different pathways connected to their corresponding transition states. Solvent effects (solvent=ethylethanoate) were also taken into account using the integral equation formalism variant of the polarizable continuum model (IEF-PCM)^x using the SMD solvation model. All the calculations were carried out using *Gaussian 09*.^{xi} Quasi-harmonic (QHA) entropic corrections were calculated from Gaussian frequency calculations with a frequency cut-off value of 100.0 cm^{-1} employing Grimme's model^{xii} with the *GoodVibes* script created by Dr. Robert Paton and Dr. I. Funes-Ardoiz.^{xiii}

In order to reduce basis set superposition errors (BSSEs) and basis set incompleteness errors (BSIEs), after the geometry optimizations, we performed single point energy calculations using ω B97X-D/Def2-QZVPP (using the SMD and ultrafine grids and including the corresponding ECP for Pd atoms). We employed the quadruple zeta basis set Def2-QZVPP because this type of relatively large basis set typically shows less than 2% of ΔE due to BSSEs in combination with different (hybrid)GGA DFT functionals.^{xiv} Then, the G corrections obtained in the frequency calculations obtained at the ω B97X-D/6-311G(d) level (with the quasi-harmonic entropic corrections) were applied to the single point energies obtained at the ω B97X-D/Def2-QZVPP level in order to obtain the final G values.

Graphical representations of the geometries were generated using *PyMol*;^{xv} the display settings were created by Dr. Robert S. Paton from Colorado State University and are openly-accessible.^{xvi}

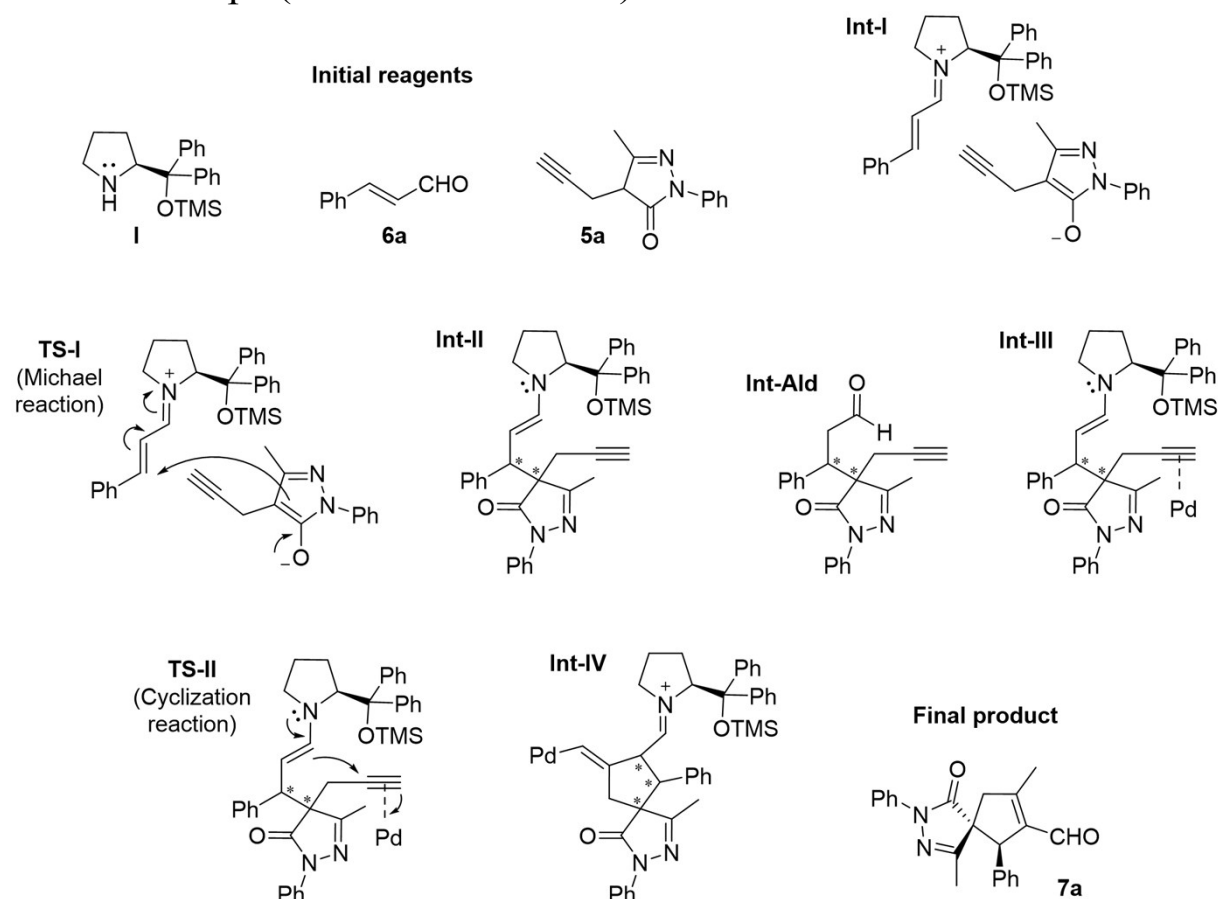
Stereochemistry Nomenclature

At the beginning of the name of each isomer, the absolute configuration of the two stereocenters are specified (*i.e.* (*S,R*)-**Int-Ald**). The first absolute configuration listed is related to the stereocenter created in the original cinnamaldehyde structure (in red) and the second to the stereocenter created in the pyrazolone unit (in green) (see examples below).



For **Int-Ald**, (*R,S*) is equivalent to *anti* and (*R,R*) is equivalent to *syn*.

Reaction Steps (Detailed Structures)



G of the Calculations

The systems were sorted alphabetically using their energies, using suffix “a” for the most stable system of a certain reaction step. For example, **TS-I-a** is the most stable system of the **TS-I** step, **TS-I-b** is the second most stable system, **TS-I-c** is the third most stable system, etc. All the values were obtained at the ω B97X-D/Def2-QZVPP(SMD)(UF grid)// ω B97X-D/6-311G(d)(SMD)(UF grid) level (applying the QHA corrections specified above). These results also include the Boltzmann average energies (G_{av}) calculated as:

$$G_{av} = \sum_i G_i \times p_i \quad (1)$$

In this formula, p_i is the probability of a certain system calculated as:

$$p_i = \frac{e^{\frac{-G_i}{RT}}}{\sum_i \left(e^{\frac{-G_i}{RT}} \right)} \quad (2)$$

where G_i is the relative Gibbs free energy of the corresponding systems.

We used the Boltzmann average G values to represent the reaction coordinates since these values are useful to study reactions with multiple reaction pathways.^{xvii} In order to compare the G of all the reaction coordinates, the corresponding corrections for changing the volume of the species from gas phase at 1 atm to a 1 M solution ($G_{corr}^{1M} = RT \cdot \ln \left(\frac{V_0}{V} \right) = +1.85 \text{ kcal/mol}$) were applied. For V_0 , we considered the volume of a mol of ideal gas at 293.15 K (24.06 l mol⁻¹).

Proline I	G (kcal/mol)	6a	G (kcal/mol)	Pyrazolone 5a	G (kcal/mol)
a	-751553.36	a	-265376.92	a	-431188.10
b	-751552.87	b	-265374.44	b	-431187.73
c	-751551.72	Boltzmann Av. ^a	-265376.89	c	-431186.50
d	-751551.50			d	-431185.02
e	-751549.57	H ₂ O	G (kcal/mol)	e	-431184.87
f	-751547.85	a	-47971.55	f	-431183.51
Boltzmann Average ^a	-751553.10	Boltzmann Av. ^a	-47971.55	Boltzmann Av. ^a	-431187.89

(<i>R,R</i>)- TS-I	G (kcal/mol)	(<i>S,S</i>)- TS-I	G (kcal/mol)	(<i>R,S</i>)- TS-I	G (kcal/mol)
a	-1400128.46	a	-1400131.97	a	-1400129.67
b	-1400127.78	b	-1400129.57	b	-1400129.46
c	-1400127.74	c	-1400129.03	c	-1400129.45
d	-1400126.09	d	-1400128.44	d	-1400126.15
e	-1400125.67	e	-1400128.39	e	-1400125.15
f	-1400125.51	f	-1400125.97	f	-1400124.53
g	-1400125.34	g	-1400125.97	g	-1400124.02
h	-1400124.70	h	-1400125.60	h	-1400123.84
i	-1400124.52	i	-1400124.23	i	-1400122.09

j	-1400124.39
Boltzmann Av. ^a	-1400128.14

j	-1400123.91
Boltzmann Av. ^a	-1400131.90

j	-1400121.74
Boltzmann Av. ^a	-1400129.54

<i>(S,R)</i> -Int-I	G (kcal/mol)
a	-1400141.33
b	-1400138.20
c	-1400137.63
d	-1400136.94
e	-1400136.48
f	-1400136.45
g	-1400135.83
h	-1400135.44
i	-1400134.91
j	-1400130.65
Boltzmann Av. ^a	-1400141.30

<i>(S,R)</i> -TS-I	G (kcal/mol)
a	-1400131.45
b	-1400129.53
c	-1400129.46
d	-1400128.28
e	-1400127.14
f	-1400126.80
g	-1400126.49
h	-1400126.08
i	-1400125.63
j	-1400124.73
Boltzmann Av. ^a	-1400131.31

<i>(S,R)</i> -Int-II	G (kcal/mol)
a	-1400144.98
b	-1400144.11
c	-1400143.69
d	-1400143.34
e	-1400142.44
f	-1400141.99
g	-1400141.89
h	-1400141.19
i	-1400140.77
j	-1400140.38
Boltzmann Av. ^a	-1400144.62

<i>syn</i> -Int-Ald	G (kcal/mol)
a	-696563.77
b	-696563.73
c	-696563.49
d	-696562.95
e	-696562.81
f	-696562.78
g	-696562.34
h	-696561.79
i	-696561.78
j	-696561.46
Boltzmann Av. ^a	-696563.45

<i>anti</i> -Int-Ald	G (kcal/mol)
a	-696562.96
b	-696562.62
c	-696562.42
d	-696562.37
e	-696562.07
f	-696561.64
g	-696561.45
h	-696561.31
i	-696561.30
j	-696561.28
Boltzmann Av. ^a	-696562.50

<i>(S,R)</i> -Int-III	G (kcal/mol)
a	-1480452.48
b	-1480448.96
c	-1480445.81
d	-1480445.79
e	-1480443.65
f	-1480443.30
g	-1480443.15
h	-1480443.00
i	-1480442.92
j	-1480441.51
Boltzmann Av. ^b	-1480452.47

<i>(S,R)</i> -TS-II	G (kcal/mol)
a	-1480424.45
b	-1480421.53
c	-1480421.39
d	-1480421.27
e	-1480421.25
f	-1480418.34
g	-1480417.72
h	-1480417.42
i	-1480417.42

<i>(S,R)</i> -Int-IV	G (kcal/mol)
a	-1480439.78
b	-1480432.65
c	-1480432.60
d	-1480432.26
e	-1480430.38
f	-1480429.50
g	-1480420.82
h	-1480420.81
i	-1480420.38

<i>(S,R)</i> -7a	G (kcal/mol)
a	-696602.13

j	-	j	-1480420.03	b	-696601.13
Boltzmann Av. ^b	-1480424.38	Boltzmann Av. ^b	-1480439.78	Boltzmann Av. ^a	-696601.97

^a For comparison with the other steps, we used Boltzmann averaged G (G_{av}) and the corresponding G_{corr}^{1M} corrections depending on the number of components in the sum of G :

$$G(\text{Initial reagents}) = G_{av}(\mathbf{I}) + G_{av}(\mathbf{5a}) + G_{av}(\mathbf{6a}) + 3G_{corr}^{1M} = -1448112.331 \quad ; \quad G_{rel} = 0$$

$$G((R,R)\text{-TS-I}) = G_{av}((R,R)\text{-TS-I}) + G_{av}(\text{H}_2\text{O}) + 2G_{corr}^{1M} = -1448095.979 \quad ; \quad G_{rel} = 16.4$$

$$G((S,S)\text{-TS-I}) = G_{av}((S,S)\text{-TS-I}) + G_{av}(\text{H}_2\text{O}) + 2G_{corr}^{1M} = -1448099.739 \quad ; \quad G_{rel} = 12.6$$

$$G((R,S)\text{-TS-I}) = G_{av}((R,S)\text{-TS-I}) + G_{av}(\text{H}_2\text{O}) + 2G_{corr}^{1M} = -1448097.379 \quad ; \quad G_{rel} = 15.0$$

$$G((S,R)\text{-Int-I}) = G_{av}((S,R)\text{-Int-I}) + G_{av}(\text{H}_2\text{O}) + 2G_{corr}^{1M} = -1448109.142 \quad ; \quad G_{rel} = 3.2$$

$$G((S,R)\text{-TS-I}) = G_{av}((S,R)\text{-TS-I}) + G_{av}(\text{H}_2\text{O}) + 2G_{corr}^{1M} = -1448099.149 \quad ; \quad G_{rel} = 13.2$$

$$G((S,R)\text{-Int-II}) = G_{av}((S,R)\text{-Int-II}) + G_{av}(\text{H}_2\text{O}) + 2G_{corr}^{1M} = -1448112.459 \quad ; \quad G_{rel} = -0.1$$

$$G(\text{anti-Int-Ald}) = G_{av}(\mathbf{I}) + G_{av}(\text{anti-Int-Ald}) + 2G_{corr}^{1M} = -1448111.896 \quad ; \quad G_{rel} = 0.4$$

$$G(\text{syn-Int-Ald}) = G_{av}(\mathbf{I}) + G_{av}(\text{syn-Int-Ald}) + 2G_{corr}^{1M} = -1448112.849 \quad ; \quad G_{rel} = -0.5$$

$$G_{rel} = -37.2G((S,R)\text{-7a}) = G_{av}(\mathbf{I}) + G_{av}((S,R)\text{-7a}) + 2G_{corr}^{1M} = -1448151.374 \quad ; \quad G_{rel} = -37.2$$

^b **Int-III**, **TS-II** and **Int-IV** contain a Pd atom, while the other steps do not. Also, the only difference between **Int-II** and **Int-III** is the Pd atom introduced. Then, for comparison with the other steps (in kcal/mol):

$$G_{rel}((S,R)\text{-Int-II}) = G_{rel}((S,R)\text{-Int-III}) = -0.1$$

With the new reference system, the $G((S,R)\text{-TS-II})$ and $G((S,R)\text{-Int-IV})$ are compared to $G((S,R)\text{-Int-III})$ (in kcal/mol):

$$G_{rel}((S,R)\text{-TS-II}) = G((S,R)\text{-TS-II}) - G((S,R)\text{-Int-III}) - 0.1 = 28.0$$

$$G_{rel}((S,R)\text{-Int-IV}) = G((S,R)\text{-Int-IV}) - G((S,R)\text{-Int-III}) - 0.1 = 12.6$$

It is worth mentioning that the results of the systems with Pd atoms (**Int-III**, **TS-II** and **Int-IV**) could also have been corrected by subtracting the G of the individual Pd atom to the total G of the systems. This would lead to the same relative activation barrier (G^\ddagger) of **TS-II**, since the difference in G between **Int-III** and **TS-II** remains the same in both approaches. Also, the overall result of the reaction are equal in the two approaches. In this study, we preferred to employ the first approach (normalizing G_{rel} of **Int-III** with respect to **Int-II**) since it allows for a better comparison of the G^\ddagger of **TS-I** and **TS-II**.

Calculation of the dr in the Equilibrium of Part 1

We used the Boltzmann averaged G of the initial reagents and all the isomers from *syn*- and *anti*-**Int-Ald**:

System	G_{av} (kcal/mol)
I	-751553.10
6a	-265376.89
5a	-431187.89
<i>syn/anti-Int-Ald</i>	-696563.28

(using all the *syn* and *anti* isomers)

Then, as seen in section *G of the Calculations*:

$$G(\text{Initial reagents}) = G_{av}(\mathbf{I}) + G_{av}(\mathbf{5a}) + G_{av}(\mathbf{6a}) + 3G_{corr}^{1M} = -1448112.33 \text{ kcal/mol}$$

$$G(\text{syn/anti-Int-Ald}) = G_{av}(\mathbf{I}) + G_{av}(\text{syn/anti-int-Int-Ald}) + 2G_{corr}^{1M} = -1448112.68 \text{ kcal/mol}$$

This leads to a calculated ΔG :

$$\Delta G_{\text{calc}} = G(\text{syn/anti-Int-Ald}) - G(\text{Initial reagents}) = -0.4 \text{ kcal/mol}$$

The experimental value of ΔG (Figure S3) is:

$$\Delta G_{\text{exp}} = -1.7 \text{ kcal/mol}$$

This ΔG_{exp} corresponds to a 62% of reaction conversion at rt (approximately at 298.15 K, but similar results were observed at 293.15 K); since cinnamaldehyde (**6a**) is the limiting reagent, at 62% of reaction conversion the concentration of cinnamaldehyde (**6a**) is 38% of its initial concentration. With this information, we calculated the concentrations of pyrazolone **5a** and **Int-Ald** using the initial concentrations of the two reagents (the initial concentrations were 0.105 M for **6a** and 0.158 M for pyrazolone **5a**). ΔG_{exp} was obtained by using the relationship between the equilibrium constant (K_{eq}) and ΔG , following formulas 3 and 4:

$$K_{\text{eq}} = \frac{[\text{Int - Ald}]_{\text{eq}}}{[\mathbf{6a}]_{\text{eq}}[\mathbf{5a}]_{\text{eq}}} = \frac{0.0651}{0.0399 \cdot 0.0929} = 17.56 \quad (3)$$

$$\Delta G_{\text{exp}} = -RT \ln(K_{\text{eq}}) = -1.7 \text{ kcal/mol} \quad (4)$$

where $R = 0.001985878 \text{ kcal K}^{-1} \text{ mol}^{-1}$, $T = 293.15 \text{ K}$.

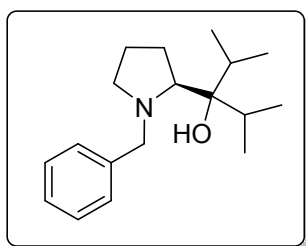
General Information

Chemicals and solvents were either purchased from commercial suppliers in p.a. purity or purified by standard method. Reactions were monitored by thin-layer chromatography (TLC); Merck 60 F 254 silica plates were used for TLC. Column chromatography was performed using silica gel Fluka (40-63 μm). The solvents for column chromatography separation were purified by distillation. ^1H and ^{13}C NMR spectra were recorded with Bruker AVANCE III 600. Chemical shifts are given in ppm and coupling constants J are given in Hz. The NMR spectra were recorded in CDCl_3 and CD_3OD at room temperature unless otherwise stated. High-resolution mass spectra were recorded with a LCQ Fleet spectrometer. Chiral HPLC was carried out using a LC20AD Shimadzu liquid chromatograph with SPD-M20A diode array detector. Chiral column Daicel Chiralpak IA, IB and IC were used for the separation of the enantiomers. Specific optical rotations were measured on AU-Tomatica polarimeter,

Autopol III and CHCl_3 was used as solvent. Specific optical rotations are given in concentration c [g/100 mL]. Infrared spectra were measured on a Nicolet Avatar 370 FT-IR in KBr and IR absorptions are given in wavenumbers as cm^{-1} .

Preparation of Catalysts

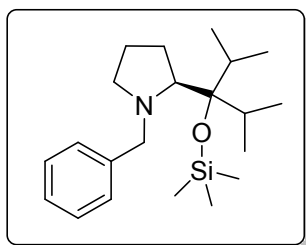
(S)-3-(1-benzylpyrrolidin-2-yl)-2,4-dimethylpentan-3-ol (C1a)



N-Benzyl-L-proline ethyl ester (3.5 g, 15.0 mmol) was taken in 100 mL dry THF and to it, ⁱPrMgBr (15.5 mL, 45.0 mmol, 2.9 M in 2-MeTHF) was added dropwise at 0 °C under argon atmosphere. After the complete addition of ⁱPrMgBr, the reaction mixture was further refluxed for 17 hours under argon atmosphere. Then, the reaction mixture was quenched with dropwise addition of saturated NH₄Cl solution (50 mL). The reaction mixture was extracted with ethyl acetate (3 × 100 mL). The combined organic layer was washed with brine solution (1 × 150 mL). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under reduced pressure. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (10:1) as eluent to give **C1a** as pale yellow oil in 18% yield (750.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 7.33 – 7.30 (m, 4H), 7.25 – 7.22 (m, 1H), 4.05 (d, *J* = 13.8 Hz, 1H), 3.50 (d, *J* = 13.8 Hz, 1H), 3.35 (brs, 1H), 3.14 (dd, *J* = 8.4 Hz, *J'* = 7.0 Hz, 1H), 2.86 – 2.82 (m, 1H), 2.48 – 2.45 (m, 1H), 2.16 – 2.11 (m, 1H), 2.05 – 1.98 (m, 1H), 1.92 – 1.87 (m, 1H), 1.85 – 1.74 (m, 3H), 1.04 (d, *J* = 2.4 Hz, 3H), 1.02 (d, *J* = 2.4 Hz, 3H), 0.97 (d, *J* = 7.1 Hz, 3H), 0.92 (d, *J* = 7.1 Hz, 3H) ppm. ¹³C NMR (151 MHz, CDCl₃) δ = 140.76, 128.48 (2C), 128.18 (2C), 126.90, 77.50, 67.84, 63.42, 53.31, 33.70, 30.95, 29.57, 25.81, 18.76, 18.48, 18.12, 17.68 ppm. FT-IR (KBr): ν = 3449, 3085, 3064, 3028, 2962, 2878, 2803, 1455, 1359, 1317, 1287, 1219, 1099, 1075, 1000, 934, 776, 734, 695 cm⁻¹. HRMS (ESI) *m/z* calcd for C₁₈H₃₀NO [*M* + *H*] = 276.2322, found: 276.2323. [*α*]_D^{rt} = -38.4° (c = 0.625 in CHCl₃).

(S)-1-benzyl-2-(2,4-dimethyl-3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (C1b)

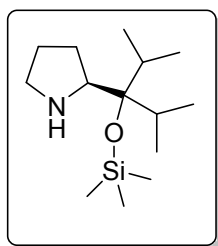


Compound **C1a** (710.0 mg, 2.58 mmol) was taken in 15 mL dry DCM and to it Et₃N (1.08 mL, 7.74 mmol) was added under argon atmosphere. The reaction mixture was then cooled to 0 °C and to it, TMSOTf (0.7 mL, 3.87 mmol) was added dropwise. After complete addition of TMSOTf, the reaction mixture was further stirred at room temperature for 2 hours. The reaction mixture was then quenched with 50 mL saturated NaHCO₃ solution. The reaction mixture was extracted with DCM (2 × 75 mL). The combined organic layer was washed with brine solution (1 × 100 mL). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under reduced pressure. The crude product was

purified by silica gel flash chromatography with n-hexane/ethyl acetate (30:1) as eluent to give **C1b** as pale yellow oil in 93% yield (830.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 7.37 – 7.36 (m, 2H), 7.30 – 7.28 (m, 2H), 7.22 – 7.19 (m, 1H), 4.35 (d, *J* = 13.5 Hz, 1H), 3.24 (d, *J* = 13.5 Hz, 1H), 3.03 (t, *J* = 7.7 Hz, 1H), 2.84 – 2.80 (m, 1H), 2.21 – 2.10 (m, 3H), 1.85 – 1.81 (m, 2H), 1.66 – 1.61 (m, 2H), 1.14 (d, *J* = 6.9 Hz, 3H), 1.09 (d, *J* = 7.0 Hz, 3H), 1.05 (d, *J* = 6.9 Hz, 3H), 1.01 (d, *J* = 7.0 Hz, 3H), 0.14 (s, 9H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 141.92, 128.46 (2C), 128.12 (2C), 126.35, 86.25, 69.33, 62.84, 54.41, 34.30, 32.70, 29.00, 24.32, 19.46, 19.38 (2C), 19.14, 3.23 (3C) ppm. **²⁹Si NMR** (79.46 MHz, CDCl₃) δ = 2.10 ppm. **FT-IR** (KBr): ν = 3088, 3064, 3028, 2965, 2881, 2783, 1383, 1353, 1251, 1144, 1108, 1066, 997, 958, 917, 872, 836, 752, 695 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₁H₃₈NOSi [M + H] = 348.2717, found: 348.2738. [α]_D^{rt} = -46.9° (c = 1.065 in CHCl₃).

(*S*)-2-(2,4-dimethyl-3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (**IV**)

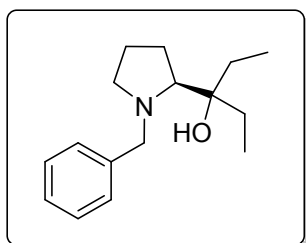


Compound **IV** (810.0 mg, 2.33 mmol) was taken in 10 mL MeOH and to it Pd/C 10 wt. % (250.0 mg, 0.23 mmol) was added. The reaction mixture was stirred for 17 hours at room temperature under H₂ gas atmosphere (H₂ gas filled balloon was used). Then, the reaction mixture was filtered through Celite bed. The Celite bed was washed with MeOH (3 × 10 mL).

The combined organic layer was evaporated under reduced pressure to give **C1c** as white viscous oil in 90% yield (540.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 3.33 – 3.30 (m, 1H), 3.05 – 3.01 (m, 1H), 2.95 – 2.88 (m, 1H), 2.14 – 2.10 (m, 1H), 1.98 – 1.93 (m, 1H), 1.79 – 1.70 (m, 3H), 1.61 – 1.54 (m, 1H), 1.05 (d, *J* = 7.2 Hz, 3H), 1.02 (d, *J* = 7.1 Hz, 3H), 0.99 (d, *J* = 7.1 Hz, 3H), 0.96 (d, *J* = 7.2 Hz, 3H), 0.13 (s, 9H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 84.17, 63.72, 46.63, 35.38, 35.04, 27.04, 25.61, 20.19, 19.82, 19.47 (2C), 2.99 (3C) ppm. **²⁹Si NMR** (79.46 MHz, CDCl₃) δ = 4.60 ppm. **FT-IR** (KBr): ν = 3345, 2965, 2878, 1392, 1245, 1186, 1150, 1102, 1075, 1021, 994, 967, 943, 869, 842, 752 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₄H₃₂NOSi [M + H] = 258.2248, found: 258.2255. [α]_D^{rt} = -26.2° (c = 1.525 in CHCl₃).

(*S*)-3-(1-benzylpyrrolidin-2-yl)pentan-3-ol (**C2a**)

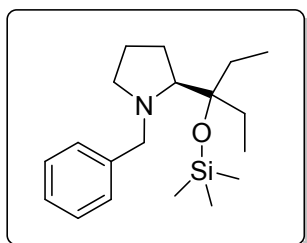


Reaction procedure and work-up same as **C1a**. The crude product was purified by silica gel flash chromatography with n-

hexane/ethyl acetate (10:1) as eluent to give **C2a** as pale yellow oil in 94% yield (3.50 g).

¹H NMR (600 MHz, CDCl₃) δ = 7.37 (d, *J* = 7.2 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 7.0 Hz, 1H), 4.03 (d, *J* = 13.9 Hz, 1H), 3.61 (d, *J* = 13.9 Hz, 1H), 2.90 (t, *J* = 7.4 Hz, 1H), 2.82 (dt, *J* = 10.6 Hz, *J'* = 6.5 Hz, 1H), 2.79 – 2.77 (brs, 1H), 2.47 (dt, *J* = 10.6 Hz, *J'* = 6.2 Hz, 1H), 1.86 (q, *J* = 7.1 Hz, 2H), 1.71 – 1.56 (m, 5H), 1.40 (dq, *J* = 14.8 Hz, *J'* = 7.5 Hz, 1H), 0.90 (dt, *J* = 9.8 Hz, *J'* = 7.5 Hz, 6H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 140.72, 128.43 (2C), 128.18 (2C), 126.95, 76.10, 69.88, 63.27, 55.16, 29.48, 27.40, 26.15, 25.20, 8.22, 7.94 ppm. **FT-IR** (KBr): ν = 3479, 3064, 3025, 2965, 2938, 2881, 2800, 1452, 1374, 1317, 1296, 1213, 1129, 1072, 1027, 961, 917, 872, 734, 698 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₆H₂₆NO [M + H] = 248.2009, found: 248.2005. [α]_D^{rt} = -50.9° (c = 1.650 in CHCl₃).

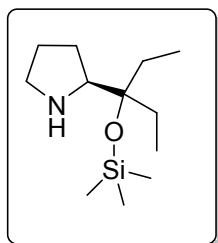
(*S*)-1-benzyl-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (**C2b**)



Reaction procedure and work-up same as **C1b**. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (35:1) as eluent to give **C2b** as pale yellow oil in 95% yield (1.23 g).

¹H NMR (600 MHz, CDCl₃) δ = 7.40 (d, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.24 (t, *J* = 7.3 Hz, 1H), 4.26 (d, *J* = 13.4 Hz, 1H), 3.39 (d, *J* = 13.4 Hz, 1H), 2.87 – 2.83 (m, 2H), 2.26 (dt, *J* = 9.9 Hz, *J'* = 7.5 Hz, 1H), 1.88 – 1.76 (m, 3H), 1.73 – 1.60 (m, 5H), 0.97 (td, *J* = 7.5 Hz, *J'* = 1.1 Hz, 6H), 0.15 (s, 9H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 141.56, 128.61 (2C), 128.16 (2C), 126.51, 82.48, 70.40, 62.47, 55.05, 29.47, 29.07, 27.41, 24.33, 9.18, 8.66, 3.10 (3C) ppm. **²⁹Si NMR** (79.46 MHz, CDCl₃) δ = 5.10 ppm. **FT-IR** (KBr): ν = 3085, 3067, 3028, 2965, 2878, 2789, 1494, 1374, 1353, 1248, 1213, 1135, 1066, 1027, 917, 881, 842, 749, 701 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₉H₃₄NOSi [M + H] = 320.2404, found: 320.2409. [α]_D^{rt} = -42.5° (c = 3.685 in CHCl₃).

(*S*)-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (**III**)



Reaction procedure and work-up same as **IV**. The product **III** was obtained as waxy white solid in 97% yield (750.0 mg).

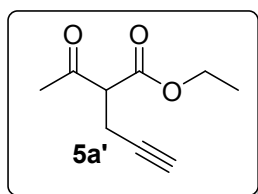
M. P. = 189.5 °C (chloroform).

¹H NMR (600 MHz, CDCl₃) δ = 6.42 (brs, 1H), 3.30 – 3.28 (m, 1H), 3.17 – 3.09 (m, 2H), 1.84 – 1.79 (m, 3H), 1.77 – 1.64 (m, 4H), 1.46 (dq, *J* = 14.7 Hz, *J'* = 7.5 Hz, 1H), 0.90 (t, *J* = 7.5 Hz, 3H), 0.82 (t, *J* = 7.6 Hz, 3H), 0.13 (s, 9H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 79.32, 65.41, 46.69, 30.23, 29.33, 25.96, 25.05, 8.77, 8.56,

3.00 (3C) ppm. **^{29}Si NMR** (79.46 MHz, CDCl_3) $\delta = 9.32$ ppm. **FT-IR** (KBr): $\nu = 2965, 2887, 2768, 2534, 1559, 1455, 1356, 1335, 1299, 1248, 1180, 1138, 1075, 1036, 929, 890, 839, 752, 683$ cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{12}\text{H}_{28}\text{NOSi}$ $[\text{M} + \text{H}] = 230.1935$, found: 230.1934. $[\alpha]_{\text{D}}^{\text{rt}} = -19.3^\circ$ ($c = 2.640$ in CHCl_3).

Preparation of the Starting Materials

Ethyl 2-acetylpent-4-ynoate¹ (**5a'**)



Ethyl acetoacetate (6.3 ml, 50 mmol) was taken in 100 ml dry THF and to this solution, 60% NaH suspension in mineral oil (2.2 g, 55 mmol) was added portionwise at 0 °C under argon atmosphere. Then, the reaction mixture was stirred at room temperature for 3 hours.

Subsequently, the reaction mixture was again cooled to 0 °C and propargyl bromide (4.31 ml, 50 mmol) was added dropwise. After complete addition of propargyl bromide, the reaction mixture was further stirred at room temperature for another 5 hours. After completion of the reaction, the reaction mixture was quenched with dilute HCl solution. The solvent was removed under reduced pressure. Then, the crude was extracted with ethyl acetate (3 × 100 ml). The combined organic layer was washed with water (1 × 100 ml) followed by brine solution (1 × 100 ml). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under vacuo. The crude product thus obtained was fractionally distilled under vacuum (2-3 mbar) at 113-115 °C using Kugelrohr apparatus to get **5a'** as colourless oil in 36% yield (3.0 g).

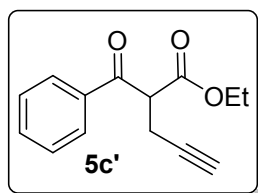
¹H NMR keto form (600 MHz, CDCl₃) δ = 4.25 – 4.16 (m, 2H), 3.67 (t, *J* = 7.5 Hz, 1H), 2.74 – 2.65 (m, 2H), 2.29 (s, 3H), 1.98 (t, *J* = 2.7 Hz, 1H), 1.28 – 1.24 (m, 3H) ppm. ¹³C NMR keto form (151 MHz, CDCl₃) δ = 200.16, 167.16, 79.49, 69.37, 60.95, 57.35, 28.67, 16.50, 13.16 ppm.

¹H NMR enol form (600 MHz, CDCl₃) δ = 4.25 – 4.16 (m, 2H), 2.97 (dd, *J* = 17.4 Hz, *J'* = 2.7 Hz, 1H), 2.90 (dd, *J* = 17.4 Hz, *J'* = 2.7 Hz, 1H), 2.19 (s, 3H), 2.01 (t, *J* = 2.7 Hz, 1H), 1.28 – 1.24 (m, 3H) ppm. ¹³C NMR enol form (151 MHz, CDCl₃) δ = 199.91, 168.25, 77.64, 71.04, 61.38, 61.42, 25.16, 20.87, 13.10 ppm.

FT-IR (KBr): ν = 3542, 3416, 3291, 2986, 2938, 2122, 1742, 1718, 1640, 1619, 1428, 1395, 1359, 1228, 1204, 1180, 1096, 1075, 1018, 929, 857, 791, 665 cm⁻¹. HRMS (ESI) *m/z* calcd for C₉H₁₂NaO₃ [*M* + Na] = 191.0679, found: 191.0676.

¹ Demir, A. S.; Aybey, A.; Kayalar, M. *ARKIVOC* **2005**, xv, 105-116.

Ethyl 2-benzoylpent-4-ynoate² (**5c'**)

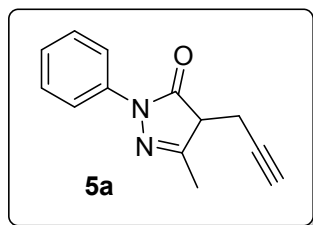


Ethyl 3-oxo-3-phenylpropanoate (4.5 mL, 26 mmol) was taken in 250 mL dry THF and to this solution was, 60% NaH suspension in mineral oil (3.1 g, 78 mmol) was added portionwise at 0 °C under argon atmosphere. Then, the reaction mixture was stirred at room temperature for 10 minutes. Subsequently propargyl bromide (4.2 ml, 39 mmol) was added dropwise. After complete addition of propargyl bromide, the reaction mixture was further stirred at reflux for 48 hours. After completion of the reaction, the reaction mixture was concentrated under reduced pressure. Then, the crude was extracted with H₂O (100 mL) and DCM (3 × 200 ml). The combined organic layer was washed with brine (200 ml). The organic layer was dried over anhyd. MgSO₄ and the solvent was removed under vacuo. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (from 20:1 to 6:1) as eluent to give **5c'** as yellow oil in 48% yield (2.90 g).

¹H NMR keto form (400 MHz, CDCl₃) δ = 8.13 – 7.96 (m, 2H), 7.70 – 7.43 (m, 3), 4.59 (t, *J* = 7.4 Hz, 1H), 4.16 (qd, *J* = 7.1 Hz, *J'* = 1.4 Hz, 2H), 3.01 – 2.82 (m, 2H), 2.01 (t, *J* = 2.7 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H) ppm.

HRMS (ESI) *m/z* calcd for C₁₄H₁₅O₃ [M + H] = 231.1016, found: 231.1018.

5-Methyl-2-phenyl-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one³ (**5a**)



Mono-propargylated ethyl acetoacetate **5a'** (2.0 g, 11.89 mmol) was taken in 12 ml glacial acetic acid and to it, phenyl hydrazine (1.17 ml, 11.89 mmol) was added. The reaction mixture was refluxed for 17 hours under argon atmosphere. Then, the excess glacial AcOH was removed under reduced pressure. The crude mass was extracted with ethyl acetate (3 × 100 ml) and the combined organic layer was washed with satd. NaHCO₃ solution (3 × 200 ml), followed by water (1 × 100 ml) and brine solution (1 × 100 ml). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under vacuo. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (1.5:1) as eluent to give **5a** as pale brown solid in 69% yield (1.75 g).

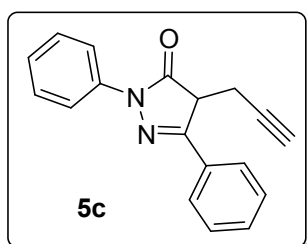
M. P. = 137.6 °C (ethyl acetate).

² Chang, M. Y.; Yu-Chieh Cheng, Y. Ch.; Lu, Y. J. *Org. Lett.*, **2015**, *17*, 1264-1267.

³ Nakagawa, H.; Ohshima, R.; Kimata, A.; Suzuki, T.; Miyata, N. *Bioorg. Med. Chem. Lett.* **2006**, *16*, 5939-5942.

¹H NMR enol form (600 MHz, CD₃OD, 0 °C) δ = 7.64 – 7.62 (m, 2H), 7.49 – 7.46 (m, 2H), 7.32 – 7.29 (m, 1H), 3.26 (d, *J* = 2.7 Hz, 2H), 2.35 (t, *J* = 2.7 Hz, 1H), 2.32 (s, 3H) ppm. **¹³C NMR** enol form (151 MHz, CD₃OD) δ = 162.33, 148.61, 137.84, 130.20 (2C), 127.41, 122.32 (2C), 101.76, 82.20, 69.34, 12.03, 11.16 ppm. **FT-IR** (KBr): ν = 3276, 3076, 2893, 2872, 2797, 2612, 1619, 1571, 1503, 1407, 1371, 1311, 1275, 1240, 1213, 1117, 1033, 905, 827, 806, 755, 743, 686, 662 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₃H₁₃N₂O [M + H] = 213.1022, found: 213.1027.

2,5-Diphenyl-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one³ (**5c**)

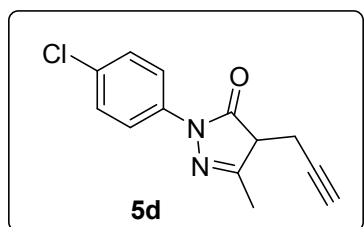


Mono-propargylated ethyl acetoacetate **5c'** (2.3 g, 10 mmol) and phenylhydrazine (1.2 ml, 12 mmol) was heated for 4 hours at 110 °C and then for 6 hours at 180°C. The reaction mixture was extracted with saturated NaHCO₃ (10 mL) and EtOAc (20 mL). The combined organic layers were washed with brine (20 mL). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under vacuo. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (from 10:1 to 5:1) as eluent to give **5c** as pale pink solid in 62% yield (1.7 g).

M. P. = 67.0 °C (n-hexane/ethyl acetate).

¹H NMR keto form (400 MHz, CDCl₃) δ = 8.08 – 7.94 (m, 2H), 7.84 – 7.70 (m, 2H), 7.55 – 7.39 (m, 5H), 7.26 – 7.21 (m, 1H), 3.91 (dd, *J* = 5.4 Hz, *J'* = 4.6 Hz, 1H), 3.08 (ddd, *J* = 16.9 Hz, *J'* = 4.6 Hz, *J''* = 2.7 Hz, 1H), 2.91 (ddd, *J* = 17.0 Hz, *J'* = 5.4 Hz, *J''* = 2.6 Hz, 1H), 1.90 (t, *J* = 2.6 Hz, 1H) ppm. **HRMS** (ESI) *m/z* calcd for C₁₈H₁₅N₂O [M + H] = 275.1179, found: 275.1181.

2-(4-Chlorophenyl)-5-methyl-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one⁴ (**5d**)



4-Chlorophenylhydrazine hydrochloride (426.0 mg, 2.38 mmol) was taken in 5 ml EtOH and to it Et₃N (0.4 ml, 2.90 mmol) was added. To this reaction mixture, the mono-propargylated ethyl acetoacetate **5a'** (400.0 mg, 2.38 mmol) was added and the reaction mixture was refluxed for 17 hours under argon atmosphere. Then, the solvent was removed under reduced pressure and the crude

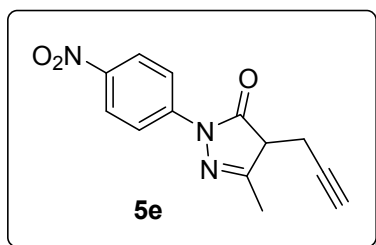
⁴ Sheng, X.; Hua, K.; Yang, C.; Wang, X.; Ji, H.; Xu, J.; Huang, Z.; Zhang, Y. *Bioorg. Med. Chem. Lett.* **2015**, *25*, 3535-3540.

product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (3:1) as eluent to give **5d** as white solid in 53% yield (310.0 mg).

M. P. = 174.0 °C (ethyl acetate/n-hexane).

¹H NMR enol form (600 MHz, CD₃OD, 0 °C) δ = 7.65 (d, *J* = 8.9 Hz, 2H), 7.47 (d, *J* = 8.9 Hz, 2H), 3.25 (d, *J* = 2.7 Hz, 2H), 2.35 (t, *J* = 2.7 Hz, 1H), 2.31 (s, 3H) ppm. **¹³C NMR** enol form (151 MHz, CD₃OD) δ = 162.13, 149.51, 136.82, 132.44, 130.19 (2C), 123.31 (2C), 101.82, 82.12, 69.37, 12.04, 11.31 ppm. **FT-IR** (KBr): ν = 3542, 3461, 3416, 3378, 3282, 3049, 2959, 2887, 2860, 2615, 2340, 2116, 1879, 1619, 1604, 1586, 1497, 1419, 1398, 1374, 1323, 1302, 1263, 1192, 1111, 1096, 1045, 1009, 908, 821, 794, 749, 713, 659, 629, 588 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₃H₁₂ClN₂O [M + H] = 247.0633, found: 247.0634.

5-Methyl-2-(4-nitrophenyl)-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one⁴ (**5e**)



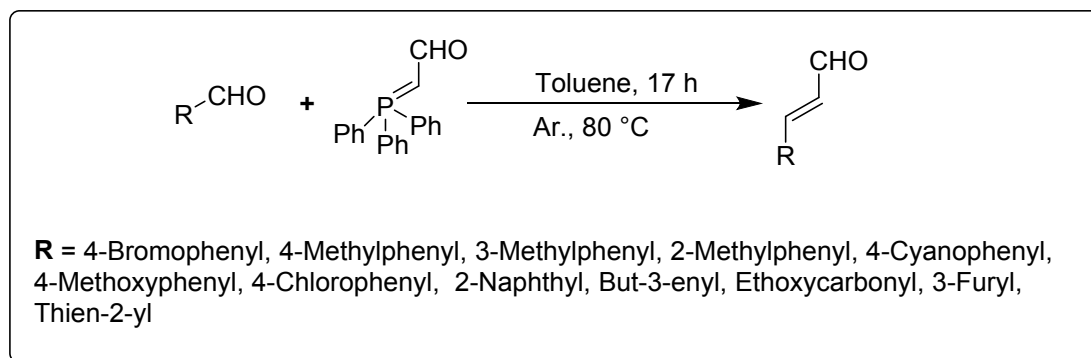
4-Nitrophenylhydrazine hydrochloride (500.0 mg, 2.64 mmol) was taken in 12 ml glacial AcOH and to it anhyd. NaOAc (238.0 mg, 2.90 mmol) was added. To this reaction mixture, the mono-propargylated ethyl acetoacetate **5a'** (444.0 mg, 2.64 mmol) was added and the reaction mixture

was refluxed for 17 hours under argon atmosphere. Then, the excess glacial AcOH was removed under reduced pressure and the crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (3:1) as eluent to give **5e** as pale yellow solid in 44% yield (300.0 mg).

M. P. = 178.7 °C (ethyl acetate/n-hexane).

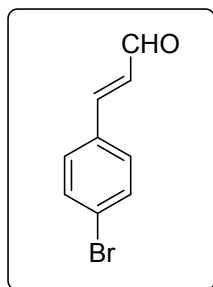
¹H NMR enol form (600 MHz, CD₃OD, 0 °C) δ = 8.34 (d, *J* = 9.3 Hz, 2H), 7.99 (d, *J* = 9.3 Hz, 2H), 3.26 (d, *J* = 2.7 Hz, 2H), 2.36 (t, *J* = 2.7 Hz, 1H), 2.33 (s, 3H) ppm. **¹³C NMR** enol form (151 MHz, CD₃OD) δ = 162.73, 152.04, 145.60, 143.62, 125.83 (2C), 120.16 (2C), 102.52, 81.91, 69.49, 12.03, 11.60 ppm. **FT-IR** (KBr): ν = 3282, 3067, 2980, 2893, 2809, 1634, 1604, 1586, 1521, 1494, 1422, 1419, 1401, 1341, 1326, 1269, 1180, 1108, 857, 845, 812, 794, 749, 689, 665, 576 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₃H₁₂N₃O₃ [M + H] = 258.0873, found: 258.0873.

General procedure for the synthesis of (*E*)- α,β -Unsaturated Aldehydes



Following the reported procedure⁵, to a solution of appropriate aldehyde (1.0 eq.) in toluene, (Formylmethylene)triphenylphosphorane (1.4 eq.) was added and the reaction mixture was heated at 80 °C for 17 hours under argon atmosphere. Then, the reaction mixture was cooled down to room temperature and the solvent was removed. The crude reaction mixture was purified through silica gel flash chromatography (using n-Hex/EtOAc as eluent), affording the desired (*E*)- α,β -unsaturated aldehyde.

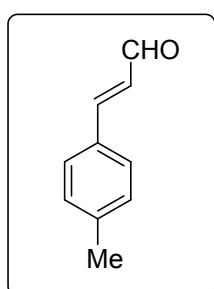
(*E*)-3-(4-Bromophenyl)acrylaldehyde (**6b**)



The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (11:1) as eluent to give **6b** as yellow solid in 48% yield (3.86 g), **M. P.** = 77.6 °C (ethyl acetate/n-hexane).

¹H NMR (600 MHz, CDCl₃) δ = 9.69 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.43 – 7.38 (m, 3H), 6.68 (dd, *J* = 16.0, 7.6 Hz, 1H) ppm. ¹³C NMR (151 MHz, CDCl₃) δ = 193.65, 151.38, 133.20, 132.68 (2C), 130.09

(2C), 129.31, 125.97 ppm. **FT-IR** (KBr): ν = 3082, 3049, 3025, 2824, 2741, 1673, 1628, 1583, 1488, 1410, 1389, 1320, 1302, 1287, 1132, 1075, 1012, 982, 806 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₉H₇BrNaO [M + Na] = 232.9572, found: 232.9573.



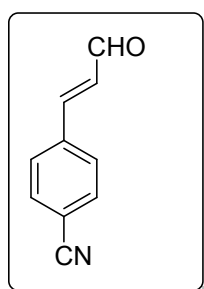
(*E*)-3-(*p*-Tolyl)acrylaldehyde (**6c**)

The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (11:1) as eluent to give **6c** as yellow solid in 37% yield (900.0 mg), **M. P.** = 37.7 °C (ethyl acetate/n-hexane).

⁵ Hirayama, F.; Koshio, H.; Katayama, N.; Kurihara, H.; Taniuchi, Y.; Sato, K.; Hisamichi, N.; Sakai-Moritani, Y.; Kawasaki, T.; Matsumoto, Y.; Yanagisawa, I. *Bioorg. Med. Chem.* **2002**, *10*, 1509-1523.

¹H NMR (600 MHz, CDCl₃) δ = 9.68 (d, *J* = 7.8 Hz, 1H), 7.48 – 7.41 (m, 3H), 7.23 (d, *J* = 8.3 Hz, 2H), 6.68 (dd, *J* = 15.9 Hz, *J'* = 7.7 Hz, 1H), 2.39 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 194.13, 153.28, 142.29, 131.64, 130.16 (2C), 128.85 (2C), 128.02, 21.88 ppm. **FT-IR** (KBr): ν = 3049, 3028, 2983, 2917, 2824, 2735, 1664, 1628, 1607, 1512, 1449, 1413, 1389, 1323, 1293, 1254, 1216, 1183, 1123, 1012, 973, 803 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₀H₁₀NaO [*M* + Na] = 169.0624, found: 169.0624.

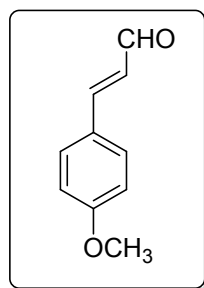
(*E*)-4-(3-Oxoprop-1-en-1-yl)benzonitrile (**6d**)



The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (9:1) as eluent to give **6d** as pale yellow solid in 25% yield (600.0 mg), **M. P.** = 132.7 °C (ethyl acetate/n-hexane).

¹H NMR (600 MHz, CDCl₃) δ = 9.76 (d, *J* = 7.5 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 16.1 Hz, 1H), 6.77 (dd, *J* = 16.0 Hz, *J'* = 7.5 Hz, 1H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 193.02, 149.57, 138.29, 132.96 (2C), 131.33, 128.87 (2C), 118.27, 114.43 ppm. **FT-IR** (KBr): ν = 3554, 3414, 3088, 3058, 2818, 2747, 2720, 2223, 1685, 1622, 1419, 1296, 1129, 976, 818 cm⁻¹. **HRMS** (EI) *m/z* calcd for C₁₀H₇NO [*M*] = 157.0528, found: 157.0529.

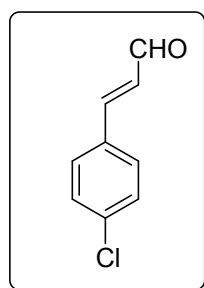
(*E*)-3-(4-Methoxyphenyl)acrylaldehyde (**6f**)



The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (20:1) as eluent to give **6f** as yellow solid in 19% yield (0.5 g), **M. P.** = 57.5 °C (n-hexane/ethyl acetate).

¹H NMR (300 MHz, CDCl₃) δ = 9.66 (d, *J* = 7.7 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 15.9, 1H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.62 (dd, *J* = 15.8 Hz, *J'* = 7.7 Hz, 1H), 3.86 (s, 3H) ppm. **HRMS** (ESI) *m/z* calcd for C₁₀H₁₁O₂ [*M* + H] = 163.0759, found: 163.0755.

(*E*)-3-(4-Chlorophenyl)akrylaldehyde (**6g**)

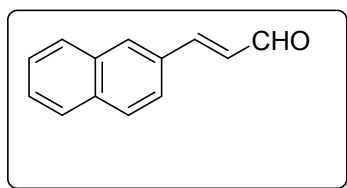


The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (from 20:1 to 10:1) as eluent to give **6g** as yellow solid in 38% yield (0.5 g), **M. P.** = 55.5 °C (n-hexane/ethyl acetate).

¹H NMR (400 MHz, CDCl₃) δ = 9.70 (d, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 8.5 Hz, 2H), 7.41 (m, 3H), 6.68 (dd, *J* = 16.0 Hz, *J'* = 7.6 Hz, 1H) ppm.

HRMS (ESI) m/z calcd for C₉H₈ClO [M + H] = 167.0264, found: 167.0258.

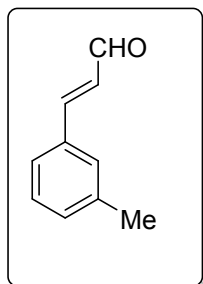
(E)-3-(Naphthalen-2-yl)acrylaldehyde (6h)



The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (11:1) as eluent to give **6h** as pale yellow solid in 32% yield (750.0 mg), **M. P.** = 120.2 °C (ethyl acetate/n-hexane).

¹H NMR (600 MHz, CDCl₃) δ = 9.77 (d, *J* = 7.7 Hz, 1H), 8.00 (s, 1H), 7.91 – 7.84 (m, 3H), 7.69 (dd, *J* = 8.5 Hz, *J'* = 1.8 Hz, 1H), 7.64 (d, *J* = 15.9 Hz, 1H), 7.58 – 7.53 (m, 2H), 6.84 (dd, *J* = 15.9, 7.6 Hz, 1H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 193.83, 152.93, 134.80, 133.35, 131.71, 130.86, 129.14, 128.92, 128.89, 128.03, 127.98, 127.12, 123.68 ppm. **FT-IR** (KBr): ν = 3560, 3470, 3419, 3237, 3055, 2992, 2845, 1682, 1634, 1619, 1353, 1305, 1278, 1248, 1219, 1147, 1129, 1015, 976, 827, 749 cm⁻¹. **HRMS (ESI) m/z** calcd for C₁₃H₁₁O [M + H] = 183.0804, found: 183.0801.

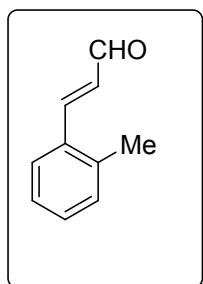
(E)-3-(*m*-Tolyl)acrylaldehyde (6i)



The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (7:1) as eluent to give **6i** as dark yellow oil in 41% yield (1.0 g).

¹H NMR (600 MHz, CDCl₃) δ = 9.69 (d, *J* = 7.7 Hz, 1H), 7.44 (d, *J* = 15.9 Hz, 1H), 7.38 – 7.36 (m, 2H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.26 – 7.24 (m, 1H), 6.71 (dd, *J* = 15.9 Hz, *J'* = 7.7 Hz, 1H), 2.39 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 194.12, 153.41, 139.15, 134.28, 132.46, 129.44, 129.30, 128.75, 126.05, 21.61 ppm. **FT-IR** (KBr): ν = 3031, 2986, 2923, 2818, 2738, 1673, 1622, 1580, 1479, 1425, 1383, 1290, 1266, 1120, 1012, 970, 782 cm⁻¹. **HRMS (ESI) m/z** calcd for C₁₀H₁₁O [M + H] = 147.0804, found: 147.0801.

(E)-3-(*o*-Tolyl)acrylaldehyde (6j)

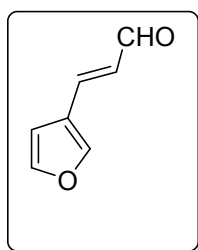


The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (7:1) as eluent to give **6j** as yellow oil in 25% yield (600.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 9.74 (d, *J* = 7.7 Hz, 1H), 7.78 (d, *J* = 15.8 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.34 (td, *J* = 7.3 Hz, *J'* = 1.4 Hz, 1H), 7.27 – 7.25 (m, 2H), 6.67 (dd, *J* = 15.8 Hz, *J'* = 7.7 Hz, 1H), 2.49 (s, 3H)

ppm. ^{13}C NMR (151 MHz, CDCl_3) δ = 193.92, 150.33, 138.01, 132.90, 131.15, 131.11, 129.67, 126.91, 126.68, 19.83 ppm. FT-IR (KBr): ν = 3061, 3022, 2815, 2741, 1673, 1622, 1601, 1482, 1461, 1437, 1296, 1242, 1222, 1189, 1132, 1102, 1033, 973, 755 cm^{-1} . HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{11}\text{O}$ [$\text{M} + \text{H}$] = 147.0804, found: 147.0804.

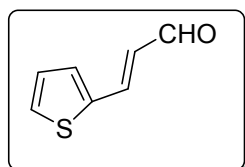
(E)-3-(Furan-3-yl)acrylaldehyde (6n)



The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (20:1) as eluent to give **6n** as dark yellow oil in 12% yield (300.0 mg).

^1H NMR (600 MHz, CDCl_3) δ = 9.59 (d, J = 7.8 Hz, 1H), 7.73 (s, 1H), 7.45 (s, 1H), 7.38 (d, J = 15.8 Hz, 1H), 6.60 (d, J = 2.0 Hz, 1H), 6.41 (dd, J = 15.7 Hz, J' = 7.8 Hz, 1H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ = 193.42, 145.35, 144.91, 142.49, 128.73, 122.84, 107.58 ppm. FT-IR (KBr): ν = 3551, 3470, 3411, 3123, 3043, 3001, 2818, 2732, 1670, 1631, 1568, 1548, 1509, 1404, 1365, 1296, 1284, 1254, 1204, 1156, 1126, 1087, 1021, 967, 869, 794, 743, 597 cm^{-1} . HRMS (ESI) m/z calcd for $\text{C}_7\text{H}_7\text{O}_2$ [$\text{M} + \text{H}$] = 123.0441, found: 123.0435.

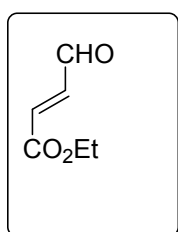
(E)-3-(Thiophen-2-yl)acrylaldehyde (6o)



The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **6o** as dark red oil in 22% yield (550.0 mg).

^1H NMR (600 MHz, CDCl_3) δ = 9.60 (d, J = 7.7 Hz, 1H), 7.56 (d, J = 15.6 Hz, 1H), 7.48 (d, J = 5.0 Hz, 1H), 7.34 (d, J = 3.9 Hz, 1H), 7.09 (dd, J = 5.1 Hz, J' = 3.7 Hz, 1H), 6.48 (dd, J = 15.6 Hz, J' = 7.7 Hz, 1H). ppm. ^{13}C NMR (151 MHz, CDCl_3) δ = 192.92, 144.48, 139.31, 132.17, 130.47, 128.60, 127.37 ppm. FT-IR (KBr): ν = 3533, 3327, 3106, 3082, 3040, 2818, 2756, 2723, 1676, 1655, 1607, 1512, 1419, 1356, 1293, 1248, 1231, 1147, 1129, 1048, 1006, 973, 863, 818, 713 cm^{-1} . HRMS (ESI) m/z calcd for $\text{C}_7\text{H}_7\text{OS}$ [$\text{M} + \text{H}$] = 139.0212, found: 139.0209.

Ethyl (E)-4-oxobut-2-enoate (6p)

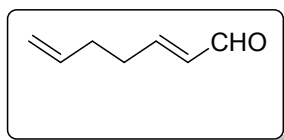


Before setting up the reaction with ethyl glyoxalate in toluene (50%), the commercially available ethyl glyoxalate was distilled to depolymerize it. ^1H NMR of the distilled monomeric ethyl glyoxalate solution provided the exact

amount of ethyl glyoxalate present in the toluene solution. This distilled monomeric ethyl glyoxalate was subsequently used in the reaction. In this reaction, 1.1 eq. of ethyl glyoxalate and 1.0 eq. of (formylmethylene)triphenylphosphorane were used. The reaction temperature was kept at 70 °C. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (7:1) as eluent to give **6p** as pale yellow oil in 48% yield (1.10 g).

¹H NMR (600 MHz, CDCl₃) δ = δ 9.72 (d, *J* = 7.7 Hz, 1H), 6.91 (dd, *J* = 16.0 Hz, *J*' = 7.6 Hz, 1H), 6.69 (d, *J* = 15.9 Hz, 1H), 4.24 (q, *J* = 7.2 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 192.56, 164.85, 140.33, 139.47, 61.73, 14.09 ppm. **FT-IR** (KBr): ν = 3070, 2986, 2941, 2899, 2836, 2741, 1721, 1700, 1640, 1449, 1398, 1368, 1308, 1275, 1248, 1180, 1099, 1033, 979, 866, 695 cm⁻¹. **HRMS** (EI) *m/z* calcd for C₆H₈O₃ [M] = 128.0473, found: 128.0475.

(E)-Hepta-2,6-dienal (6q)

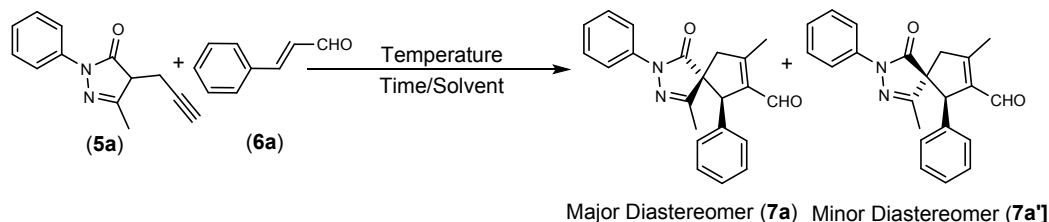


In this reaction, 1.1 eq. of pent-4-enal and 1.0 eq. of (formylmethylene)triphenylphosphorane were used. The reaction temperature was kept at 70 °C. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (7:1) as eluent to give **6q** as pale yellow oil in 28% yield (550.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = δ 9.49 (d, *J* = 7.9 Hz, 1H), 6.83 (dt, *J* = 15.7 Hz, *J*' = 6.7 Hz, 1H), 6.12 (dd, *J* = 15.7 Hz, *J*' = 7.9 Hz, 1H), 5.82 – 5.75 (m, 1H), 5.08 – 5.01 (m, 2H), 2.46 – 2.41 (m, 2H), 2.29 – 2.24 (m, 2H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 194.07, 157.75, 136.72, 133.40, 116.05, 31.94, 31.89 ppm. **FT-IR** (KBr): ν = 3079, 2980, 2923, 2845, 2818, 2738, 1718, 1691, 1640, 1443, 1416, 1302, 1260, 1135, 979, 917 cm⁻¹. **HRMS** (EI) *m/z* calcd for C₇H₁₀O [M] = 110.0732, found: 110.0730.

Optimization of the Reaction Conditions for the Spirocyclization Reaction

Table S3: Solvent Screening



2.0 eq. (**5a**), 1.0 eq. (**6a**), 0.05 eq. Pd₂(dba)₃, 0.20 eq. (*S*)-DPP-TMS and 1 ml Solvent

Entry	Solvent	Temp. °C	Time h	Yield% ^[a] (7a)	ee% ^[b] (7a)	<i>dr</i> ^[c] (7a : 7a')	Yield% ^[a] (7a')	ee% ^[b] (7a')
1	CH ₃ CN	rt	24	57	86	1.4 : 1	37	77
2	MeOH	rt	24	50	92	1.5 : 1	31	83
3	EtOAc	rt	24	70	94	2.0 : 1	26	92
4	DCE	rt	24	64	92	1.8 : 1	30	86
5	Toluene	rt	24	63	92	1.3 : 1	34	90
6	THF	rt	24	55	94	2.3 : 1	26	94
7	CH ₂ Cl ₂	rt	24	48	93	1.4 : 1	33	86
8	CHCl ₃	rt	24	71	94	1.6 : 1	26	89
9	<i>tert</i> -BuOMe	rt	24	62	93	2.0 : 1	19	88

[a] Isolated Yield, [b] Enantioselectivity determined by Chiral HPLC,
[c] Diastereomeric ratio determined through crude NMR spectra.

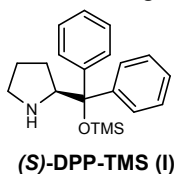
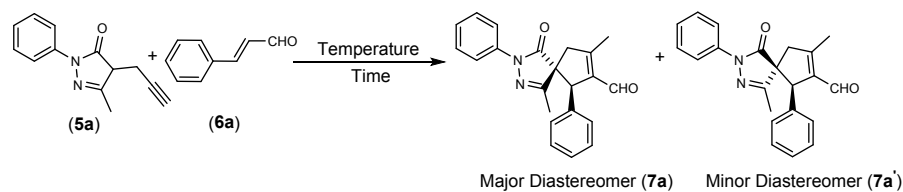
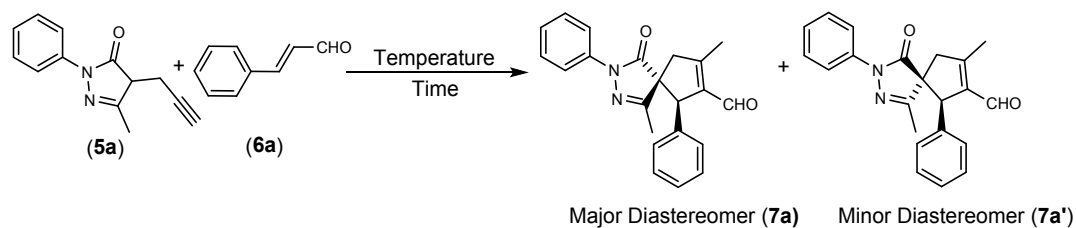


Table S4: Catalyst Screening2.0 eq. (**5a**), 1.0 eq. (**6a**) and 1 ml EtOAc

Entry	Catalyst	Catalyst Amount (eq.)	Temp. °C	Time h	Yield% ^[a] (7a)	ee% ^[b] (7a)	<i>d_r</i> ^[c] (7a : 7a')	Yield% ^[a] (7a')	ee% ^[b] (7a')
1 ^[d]	AgOTf	0.05	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
2 ^[d]	In(OTf) ₃	0.05	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
3 ^[d]	PdCl ₂	0.05	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
4 ^[d]	PdCl ₂ (Ph ₃ P) ₂	0.05	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
5 ^[d]	Pd ₂ (dba) ₃	0.05	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
6 ^[d]	(<i>S</i>)-DPP-TMS	0.20	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
7 ^[d]	No catalyst	No catalyst	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
8	Pd ₂ (dba) ₃ + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	70	94	2:1	26	92
9	Au(PPh ₃)NTf ₂ + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	63	98	2.9:1	21	98
10	Au(PPh ₃) ₃ Cl + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	6.	88	2.8:1	2	92
11 ^[d]	Pd(OAc) ₂ + Ph ₃ P	0.05 + 0.20	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
12 ^[d]	AuCl ₃ + (<i>S</i>)-DPP-TMS	0.02 + 0.05	rt	24	13.	75	1.9:1	7	76
13 ^[d]	FeCl ₃ + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
14 ^[d]	AgOTf + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
15 ^[d]	In(OTf) ₃ + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	n.d.	n.d.	n.d.	n.d.	n.d.
16	Pd(OAc) ₂ + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	62	94	1.7 : 1	10	93
17 ^[e]	Pd(Ph ₃ P) ₄ + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	18	95	1.1 : 1	15	93
18	PdCl ₂ + (<i>S</i>)-DPP-TMS	0.05 + 0.20	rt	24	46	86	4.6 : 1	12	87

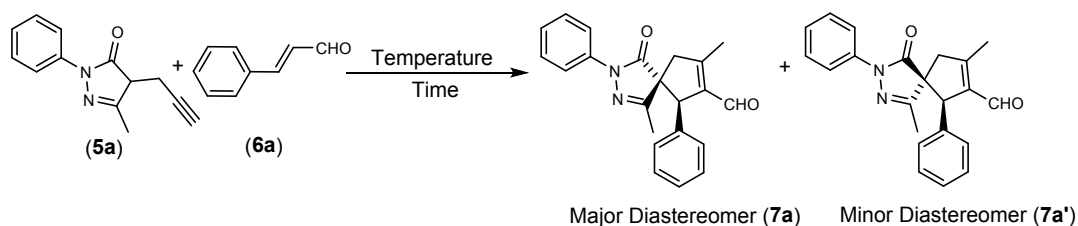
[a] Isolated Yield, [b] Enantioselectivity determined by Chiral HPLC, [c] Diastereomeric ratio determined through crude NMR spectra, [d] No Reaction, n.d.= not detected, [e] Conversion of (**6a**) was less than 40%.

Table S5: Substrate Ratio Screening

0.05 eq. Pd₂(dba)₃, 0.20 eq. (S)-DPP-TMS and 1 ml EtOAc

Entry	Substrate (5a) eq.	Substrate (6a) eq.	Temp. °C	Time h	Yield% ^[a] (7a)	ee% ^[b] (7a)	<i>dr</i> ^[c] (7a : 7a')	Yield% ^[a] (7a')	ee% ^[b] (7a')
1	2.0	1.0	rt	24	70	94	2 : 1	26	92
2	1.5	1.0	rt	24	68	94	2 : 1	30	96
3	1.2	1.0	rt	24	58	92	2.3 : 1	22	96
4	1.0	1.0	rt	24	55	96	2.6 : 1	26	96
5	1.0	1.2	rt	24	53	97	2.2 : 1	31	97

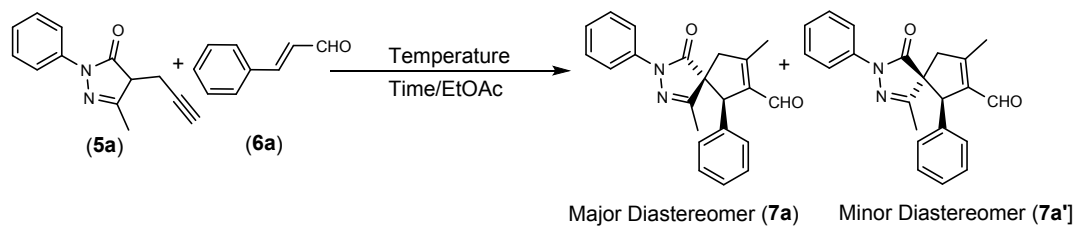
[a] Isolated Yield, [b] Enantioselectivity determined by Chiral HPLC, [c] Diastereomeric ratio determined through crude NMR spectra.

Table S6: Catalyst Loading Screening

1.5 eq. (**5a**), 1.0 eq. (**6a**) and 1 ml EtOAc

Entry	Pd ₂ (dba) ₃ eq.	(S)-DPP-TMS eq.	Temp. °C	Time h	Yield% ^[a] (7a)	ee% ^[b] (7a)	<i>dr</i> ^[c] (7a : 7a')	Yield% ^[a] (7a')	ee% ^[b] (7a')
1	0.05	0.20	rt	24	68	94	2 : 1	30	96
2	0.05	0.10	rt	24	67	93	2.3 : 1	29	96
3	0.05	0.05	rt	24	64	92	2.4 : 1	31	94
4	0.02	0.20	rt	24	70	96	2.1 : 1	28	95
5	0.02	0.10	rt	24	70	93	2 : 1	28	96
6	0.02	0.05	rt	24	69	95	2.2 : 1	26	95
7	0.01	0.05	rt	24	68	93	2.6 : 1	25	95
8	0.01	0.02	rt	24	50	91	2.7 : 1	22	94

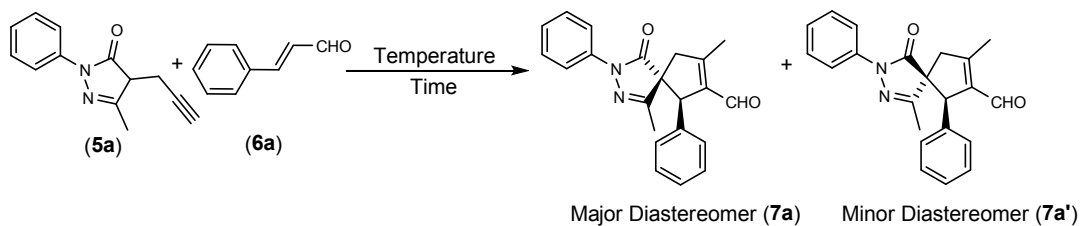
[a] Isolated Yield, [b] Enantioselectivity determined by Chiral HPLC, [c] Diastereomeric ratio determined through crude NMR spectra.

Table S7: Concentration Screening

1.5 eq. **(5a)**, 1.0 eq. **(6a)**, 0.02 eq. Pd₂(dba)₃ and 0.05 eq. (S)-DPP-TMS

Entry	EtOAc ml	Concentration of (5a) in Mol	Temp. °C	Time h	Yield% ^[a] (7a)	ee% ^[b] (7a)	dr ^[c] (7a : 7a')	Yield% ^[a] (7a')	ee% ^[b] (7a')
1	6.0	0.20	rt	24	38	96	1.7 : 1	20	93
2	3.0	0.10	rt	24	53	96	1.7 : 1	22	95
3	1.0	0.05	rt	24	69	95	2.2 : 1	26	95
4	0.6	0.20	rt	24	46	93	1.6 : 1	26	91
5	0.3	0.10	rt	168	43	93	2.2 : 1	12	97

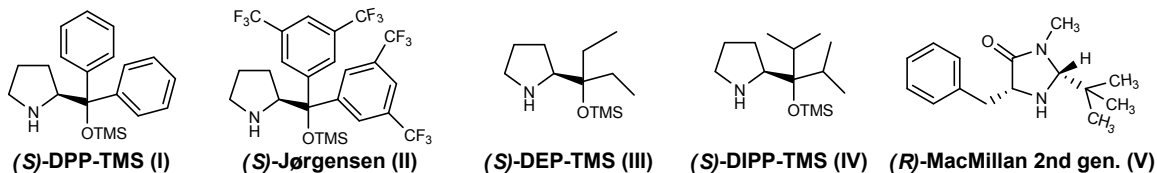
[a] Isolated Yield, [b] Enantioselectivity determined by Chiral HPLC, [c] Diastereomeric ratio determined through crude NMR spectra, [d] Conversion of **(6a)** was less than 65%.

Table S8: Organo-catalyst Screening

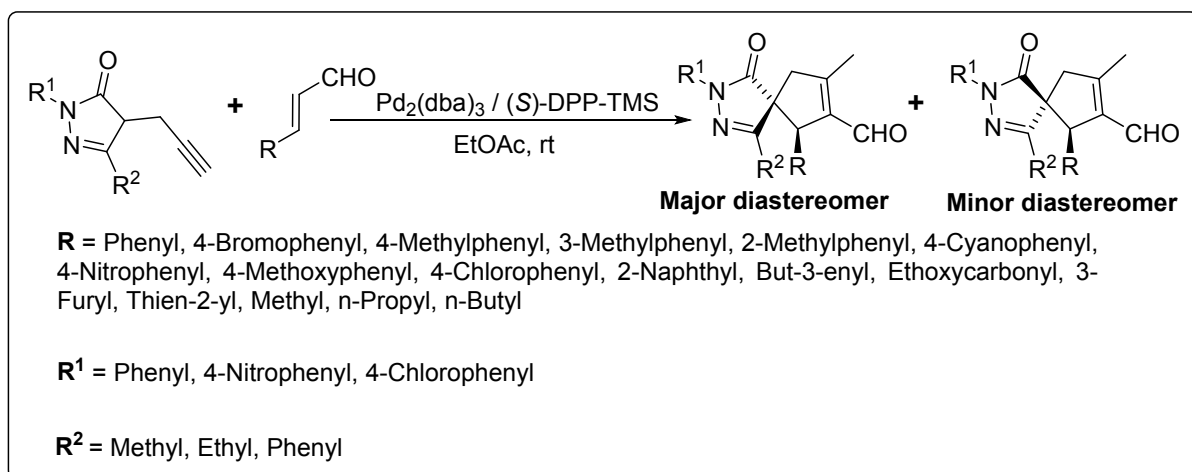
1.5 eq. (**5a**), 1.0 eq. (**6a**), 0.02 eq. Pd₂(dba)₃ in 1 ml EtOAc

Entry	Organo-Catalyst	Catalyst Amount (eq.)	Temp. °C	Time h	Yield% ^[a] (7a)	ee% ^[b] (7a)	dr ^[c] (7a : 7a')	Yield% ^[a] (7a')	ee% ^[b] (7a')
1	(<i>S</i>)-DPP-TMS	0.05	rt	24	69	95	2.2 : 1	26	95
2 ^[d]	(<i>S</i>)-Jørgensen	0.05	rt	36	31	98	2.1 : 1	11	99
3 ^[e]	(<i>S</i>)-Jørgensen	0.05	rt	168	37	98	2.2 : 1	12	97
4 ^[f]	(<i>R</i>)-MacMillan 2nd gen.	0.05	rt	36	48	9	5.6 : 1	26	63
5 ^[g]	(<i>S</i>)-DEP-TMS	0.05	rt	36	29	44	1.8 : 1	17	61
6 ^[h]	(<i>S</i>)-DIPP-TMS	0.05	rt	36	19	80	1.4 : 1	12	91

[a] Isolated Yield, [b] Enantioselectivity determined by Chiral HPLC, [c] Diastereomeric ratio determined through crude NMR spectra, [d] Conversion of (**6a**) was less than 50%, [e] Conversion of (**6a**) was less than 60%, [f] Conversion of (**6a**) was less than 90%, [g] Conversion of (**6a**) was less than 52%, [h] Conversion of (**6a**) was less than 35%.

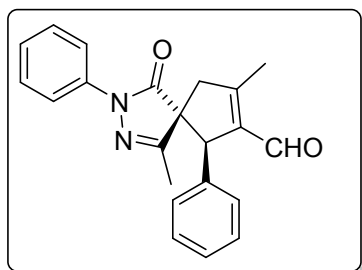


General procedure for the Synthesis of Spirocyclic Compounds



In a screw cap septum vial containing EtOAc (1 ml), pyrazolone (0.18 mmol, 1.5 eq.) was added. The vial was warmed to dissolve the pyrazolone in EtOAc. Then, to this solution, (*E*)- α,β -unsaturated aldehyde (0.12 mmol, 1.0 eq.), Pd₂(dba)₃ (0.0024 mmol, 0.02 eq.) and (*S*)-(-)- α,α -Diphenyl-2-pyrrolidinemethanol trimethylsilyl ether [(*S*)-DPP-TMS] (0.006 mmol, 0.05 eq.) were added. The reaction mixture was stirred at room temperature (rt). ¹H NMR of the crude reaction mixture was measured in order to monitor the progress of the reaction. After the complete consumption of the (*E*)- α,β -unsaturated aldehyde (or after 7 days; whichever is earlier), the solvent of the reaction mixture was removed. The crude reaction mixture was purified through silica gel flash chromatography (using n-Hex/EtOAc as eluent), affording the desired spirocyclic compound.

(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3,6-diphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (**7a**) *major diastereomer*



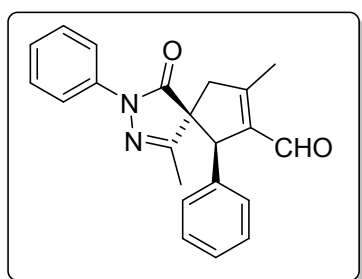
The crude product (1 day reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (3:1) as eluent to give **7a** as brown semisolid in 69% yield (30.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.09 (s, 1H), 7.90 – 7.88 (m, 2H), 7.44 – 7.41 (m, 2H), 7.28 – 7.27 (m, 3H), 7.23 – 7.20 (m, 1H), 7.02 – 7.00 (m, 2H), 4.84 (s, 1H), 2.98 (d, *J* = 18.7

Hz, 1H), 2.93 (d, *J* = 18.7 Hz, 1H), 2.41 (s, 3H), 1.45 (s, 3H) ppm. ¹³C NMR (151 MHz, CDCl₃) δ = 186.93, 176.22, 161.39, 159.44, 138.00, 136.76, 136.69, 129.02 (2C), 128.83 (2C), 128.00, 127.60 (2C), 125.27, 118.97 (2C), 61.81, 59.25, 45.06, 15.17, 14.86 ppm. FT-IR (KBr): ν = 3055, 3034, 2923, 2845, 2757, 2594, 1873, 1811, 1709, 1670, 1598, 1500,

1488, 1365, 1347, 1308, 1260, 1234, 1177, 1117, 1075, 1033, 1000, 973, 911, 761, 711 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{22}\text{H}_{21}\text{N}_2\text{O}_2$ [$\text{M} + \text{H}$] = 345.1598, found: 345.1597. $[\alpha]_{\text{D}}^{25} = -264.8^\circ$ ($c = 0.710$ in CHCl_3). **HPLC analysis** *ee* (major diastereoisomer) = 95%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, $\lambda = 194$ nm, retention time: $t_{\text{major}} = 35.4$ min, $t_{\text{minor}} = 40.9$ min) at 25°C .

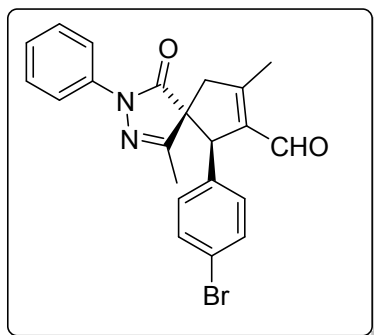
(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3,6-diphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7a') minor diastereomer



The crude product (1 day reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (3:1) as eluent to give **7a'** as dark yellow semisolid in 26% yield (11.0 mg).

^1H NMR (600 MHz, CDCl_3) $\delta = 10.05$ (s, 1H), 7.45 – 7.43 (m, 2H), 7.27 – 7.26 (m, 1H), 7.25 – 7.18 (m, 4H), 7.10 – 7.07 (m, 1H), 7.02 – 7.00 (m, 2H), 4.55 (s, 1H), 3.17 (d, $J = 18.0$ Hz, 1H), 2.77 (d, $J = 18.0$ Hz, 1H), 2.40 (s, 3H), 2.20 (s, 3H) ppm. **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 186.84$, 172.93, 161.77, 160.32, 137.57, 136.84, 135.75, 128.77 (2C), 128.32 (2C), 128.09 (2C), 127.94, 125.07, 119.13 (2C), 61.21, 57.71, 44.86, 14.79, 13.83 ppm. **FT-IR** (KBr): $\nu = 3061$, 3031, 2920, 2851, 2759, 2585, 1841, 1721, 1667, 1598, 1500, 1488, 1368, 1305, 1248, 1213, 1180, 1117, 1078, 1027, 997, 967, 908, 863, 767, 698 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{22}\text{H}_{21}\text{N}_2\text{O}_2$ [$\text{M} + \text{H}$] = 345.1598, found: 345.1596. $[\alpha]_{\text{D}}^{25} = +53.2^\circ$ ($c = 0.235$ in CHCl_3). **HPLC analysis** *ee* (minor diastereoisomer) = 95%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{major}} = 11.3$ min, $t_{\text{minor}} = 23.8$ min) at 25°C .

(5*R*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7b) major diastereomer

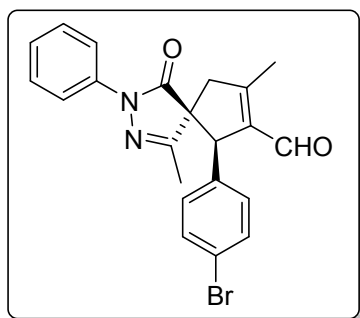


The crude product (3 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (2:1) as eluent to give **7b** as brown semisolid in 63% yield (80.0 mg).

^1H NMR (600 MHz, CDCl_3) $\delta = 10.07$ (s, 1H), 7.86 (d, $J = 7.6$ Hz, 2H), 7.41 (t, $J = 7.9$ Hz, 2H), 7.37 (d, $J = 8.4$ Hz, 2H), 7.20 (t, $J = 7.3$ Hz, 1H), 6.86 (d, $J = 8.4$ Hz, 2H), 4.76 (s, 1H), 3.00 (d, $J = 19.0$ Hz, 1H), 2.89 (d, $J = 19.0$ Hz, 1H), 2.38 (s, 3H), 1.52 (s, 3H) ppm. **^{13}C NMR**

(151 MHz, CDCl₃) δ = 186.66, 175.89, 160.93, 160.19, 137.86, 136.34, 135.78, 131.90 (2C), 129.24 (2C), 129.07(2C), 125.42, 121.87, 118.95 (2C), 61.75, 58.73, 45.09, 15.37, 14.87 ppm. **FT-IR** (KBr): ν = 3064, 3037, 3019, 2914, 2845, 2756, 2591, 1718, 1703, 1667, 1595, 1494, 1395, 1365, 1308, 1257, 1228, 1219, 1177, 1123, 1075, 1009, 973, 908, 869, 764 cm⁻¹. **HRMS** (ESI) m/z calcd for C₂₂H₂₀BrN₂O₂ [M + H] = 423.0703, found: 423.0702. $[\alpha]_D^{25}$ = -254.9° (c = 0.765 in CHCl₃). **HPLC analysis** *ee* (major diastereoisomer) = 90%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 70:30, 1.0 mL/min, λ = 190 nm, retention time: t_{major} = 16.0 min, t_{minor} = 33.1 min) at 25 °C.

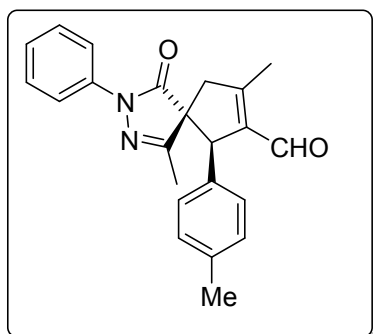
(5*S*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7b') minor diastereomer



The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (3:1) as eluent to give **7b'** as dark yellow semisolid in 24% yield (30.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.04 (s, 1H), 7.46 (d, J = 7.8 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 7.32 – 7.26 (m, 2H), 7.12 (t, J = 7.4 Hz, 1H), 6.88 (d, J = 8.4 Hz, 2H), 4.47 (s, 1H), 3.16 (d, J = 18.9 Hz, 1H), 2.78 (d, J = 19.0 Hz, 1H), 2.40 (s, 3H), 2.18 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 186.58, 172.71, 161.63, 160.82, 137.46, 136.71, 134.92, 131.45 (2C), 129.83 (2C), 128.89 (2C), 125.28, 121.92, 119.10 (2C), 60.88, 56.95, 45.01, 14.79, 13.80 ppm. **FT-IR** (KBr): ν = 3064, 3043, 2917, 2845, 2756, 2726, 1715, 1667, 1595, 1503, 1485, 1434, 1410, 1398, 1371, 1338, 1305, 1216, 1183, 1120, 1072, 1009, 863, 761, 692 cm⁻¹. **HRMS** (ESI) m/z calcd for C₂₂H₂₀BrN₂O₂ [M + H] = 423.0703, found: 423.0707. $[\alpha]_D^{25}$ = -20.7° (c = 0.460 in CHCl₃). **HPLC analysis** *ee* (minor diastereoisomer) = 91%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, λ = 197 nm, retention time: t_{major} = 11.1 min, t_{minor} = 30.6 min) at 25 °C.

(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*p*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*c*) major diastereomer

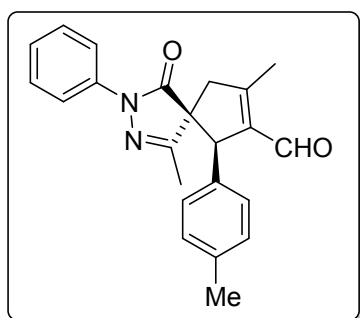


The crude product (2 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7c** as brown semisolid in 55% yield (24.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.05 (s, 1H), 7.87 (d, *J* = 7.5 Hz, 1H), 7.42 – 7.38 (m, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 7.7 Hz, 2H), 4.79 (s, 1H), 2.93 (q, *J* = 18.8 Hz,

2H), 2.38 (s, 3H), 2.29 (s, 3H), 1.46 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 187.05, 176.30, 161.57, 159.13, 138.04, 137.68, 136.79, 133.66, 129.53 (2C), 129.03 (2C), 127.47 (2C), 125.24, 118.98 (2C), 61.92, 59.03, 45.06, 21.26, 15.30, 14.89 ppm. **FT-IR** (KBr): ν = 3025, 2926, 2851, 2762, 2597, 1814, 1718, 1503, 1491, 1401, 1368, 1311, 1260, 1231, 1177, 1123, 1075, 1033, 1000, 970, 908, 761, 689 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₃H₂₃N₂O₂ [M + H] = 359.1754, found: 359.1760. [α]_D^{rt} = -221.3° (c = 0.305 in CHCl₃). **HPLC analysis** *ee* (major diastereoisomer) = 92%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, λ = 194 nm, retention time: *t*_{major} = 32.7 min, *t*_{minor} = 38.1 min) at 25 °C.

(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*p*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*c'*) minor diastereomer



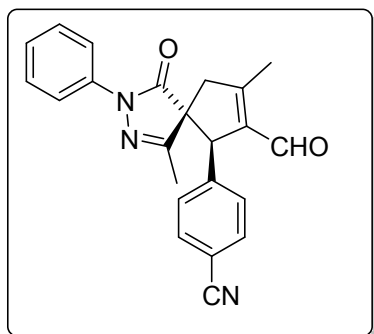
The crude product (2 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7c'** as dark yellow semisolid in 23% yield (10.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.04 (s, 1H), 7.47 (d, *J* = 7.8 Hz, 2H), 7.29 – 7.27 (m, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.03 (d,

J = 7.7 Hz, 2H), 6.89 (d, *J* = 8.1 Hz, 2H), 4.51 (s, 1H), 3.16 (d, *J* = 19.3 Hz, 1H), 2.74 (d, *J* = 18.9 Hz, 1H), 2.39 (s, 3H), 2.26 (s, 3H), 2.18 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 186.99, 173.05, 162.02, 160.12, 137.75, 137.56, 137.12, 132.80, 129.18 (2C), 128.85 (2C), 128.07 (2C), 125.12, 119.26 (2C), 61.28, 57.51, 44.96, 21.41, 14.87, 13.92 ppm. **FT-IR** (KBr): ν = 3022, 2989, 2917, 2848, 2762, 2591, 1718, 1703, 1667, 1595, 1503, 1485, 1431, 1416, 1398, 1365, 1341, 1305, 1248, 1213, 1183, 1120, 1066, 1021, 1000, 973, 911, 866, 758, 692 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₃H₂₃N₂O₂ [M + H] = 359.1754, found: 359.1754. [α]_D^{rt} = +15.5° (c = 0.355 in CHCl₃). **HPLC analysis** *ee* (minor diastereoisomer) = 98%,

(Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{major} = 10.1$ min, $t_{minor} = 27.6$ min) at 25 °C.

4-((5*R*,6*R*)-7-Formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-dien-6-yl)benzotrile (7d) major diastereomer

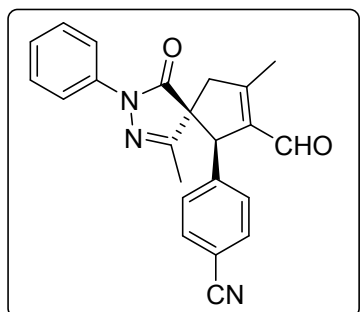


The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (1:1) as eluent to give **7d** as pale red semisolid in 46% yield (20.0 mg).

¹H NMR (600 MHz, CDCl₃) $\delta = 10.10$ (s, 1H), 7.84 (d, $J = 7.7$ Hz, 2H), 7.54 (d, $J = 8.4$ Hz, 2H), 7.43 – 7.39 (m, 2H), 7.22 (t, $J = 7.4$ Hz, 1H), 7.08 (d, $J = 8.2$ Hz, 2H), 4.83 (s, 1H),

3.07 (d, $J = 18.8$ Hz, 1H), 2.89 (d, $J = 19.0$ Hz, 1H), 2.41 (s, 3H), 1.53 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) $\delta = 186.40, 175.47, 161.10, 160.31, 142.16, 137.70, 135.86, 132.46$ (2C), 129.12 (2C), 128.37 (2C), 125.61, 118.92 (2C), 118.52, 111.91, 61.83, 59.15, 45.17, 15.32, 14.89 ppm. **FT-IR** (KBr): $\nu = 3085, 3061, 3052, 3031, 2920, 2896, 2863, 2774, 2597, 2223, 1835, 1712, 1673, 1592, 1503, 1491, 1416, 1401, 1362, 1347, 1332, 1305, 1234, 1198, 1183, 1177, 1117, 1078, 994, 964, 914, 863, 767$ cm⁻¹. **HRMS** (ESI) m/z calcd for C₂₃H₂₀N₃O₂ [M + H] = 370.1550, found: 370.1555. **$[\alpha]_D^{25}$** = -255.3° ($c = 0.235$ in CHCl₃). **HPLC analysis** *ee* (major diastereoisomer) = 86%, (Daicel Chiracel IB column, heptane/*iso*-propanol, 70:30, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{minor} = 15.5$ min, $t_{major} = 19.5$ min) at 25 °C.

4-((5*S*,6*R*)-7-Formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-dien-6-yl)benzotrile (7d') minor diastereomer



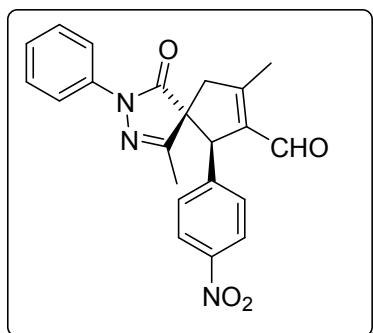
The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (1:1) as eluent to give **7d'** as blackish yellow semisolid in 37% yield (17.0 mg).

¹H NMR (600 MHz, CDCl₃) $\delta = 10.06$ (s, 1H), 7.52 (d, $J = 8.6$ Hz, 1H), 7.44 (d, $J = 7.8$ Hz, 2H), 7.31 – 7.27 (m, 2H), 7.14 –

7.10 (m, 3H), 4.53 (s, 1H), 3.18 (d, $J = 18.9$ Hz, 1H), 2.83 (d, $J = 19.1$ Hz, 1H), 2.42 (s, 3H), 2.20 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) $\delta = 186.32, 172.42, 161.58, 161.38, 141.47, 137.30, 136.32, 132.07$ (2C), 128.98 (2C), 128.95 (2C), 125.44, 118.88 (2C), 118.83, 111.74, 60.84, 57.11, 45.18, 14.80, 13.76 ppm. **FT-IR** (KBr): $\nu = 3070, 3034, 2989, 2917, 2848,$

2762, 2585, 2223, 1721, 1673, 1598, 1500, 1491, 1419, 1398, 1362, 1338, 1308, 1225, 1213, 1183, 1123, 1063, 1018, 997, 967, 908, 872, 758, 695 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_2$ $[\text{M} + \text{H}] = 370.1550$, found: 370.1550. $[\alpha]_{\text{D}}^{25} = -25.9^\circ$ ($c = 0.425$ in CHCl_3). **HPLC analysis** *ee* (minor diastereoisomer) = 82%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{major}} = 9.8$ min, $t_{\text{minor}} = 37.7$ min) at 25°C .

(5*R*,6*R*)-1,8-Dimethyl-6-(4-nitrophenyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7e) major diastereomer

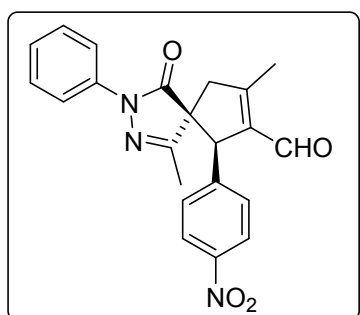


The crude product (4 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (1.5:1) as eluent to give **7e** as yellow semisolid in 48% yield (22.0 mg).

^1H NMR (600 MHz, CDCl_3) $\delta = 10.13$ (s, 1H), 8.11 (d, $J = 8.7$ Hz, 2H), 7.84 (d, $J = 7.7$ Hz, 2H), 7.43 – 7.40 (m, 2H), 7.22 (t, $J = 7.5$ Hz, 1H), 7.14 (d, $J = 8.6$ Hz, 2H), 4.88 (s, 1H),

3.10 (d, $J = 18.9$ Hz, 1H), 2.91 (d, $J = 18.9$ Hz, 1H), 2.43 (s, 3H), 1.58 (s, 3H) ppm. **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 186.37$, 175.38, 161.18, 160.21, 147.54, 144.15, 137.67, 135.94, 129.16 (2C), 128.48 (2C), 125.67, 123.92 (2C), 118.94 (2C), 61.91, 58.97, 45.24, 15.41, 14.93 ppm. **FT-IR** (KBr): $\nu = 3067$, 3040, 2998, 2923, 2851, 2756, 2729, 2594, 2451, 1942, 1867, 1805, 1709, 1670, 1598, 1518, 1500, 1494, 1434, 1422, 1398, 1362, 1347, 1308, 1263, 1228, 1177, 1120, 1015, 1003, 973, 905, 875, 857, 839, 755, 728, 689 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{22}\text{H}_{20}\text{N}_3\text{O}_4$ $[\text{M} + \text{H}] = 390.1448$, found: 390.1452. $[\alpha]_{\text{D}}^{25} = -222.6^\circ$ ($c = 0.420$ in CHCl_3). **HPLC analysis** *ee* (major diastereoisomer) = 86%, (Daicel Chiracel IB column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{minor}} = 24.6$ min, $t_{\text{major}} = 32.5$ min) at 25°C .

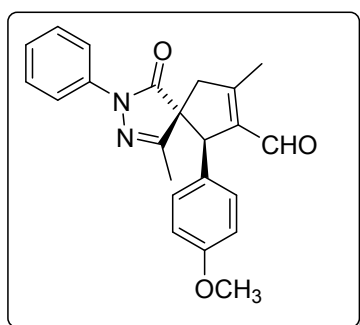
(5*S*,6*R*)-1,8-Dimethyl-6-(4-nitrophenyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7e') minor diastereomer



The crude product (4 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (1.5:1) as eluent to give **7e'** as pale yellow semisolid in 33% yield (15.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.07 (s, 1H), 8.10 (d, *J* = 8.8 Hz, 2H), 7.47 (d, *J* = 7.8 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.17 (d, *J* = 8.7 Hz, 2H), 7.12 (d, *J* = 7.4 Hz, 1H), 4.57 (s, 1H), 3.21 (d, *J* = 19.0 Hz, 1H), 2.85 (d, *J* = 19.2 Hz, 1H), 2.44 (s, 3H), 2.22 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 186.28, 172.34, 161.58, 161.38, 147.52, 143.54, 137.30, 136.50, 129.14 (2C), 128.97 (2C), 125.47, 123.55 (2C), 118.85 (2C), 60.79, 56.76, 45.32, 14.83, 13.79 ppm. **FT-IR** (KBr): ν = 3070, 3061, 3040, 2989, 2914, 2851, 2765, 2579, 2454, 2373, 2349, 1844, 1721, 1673, 1598, 1524, 1506, 1485, 1419, 1401, 1344, 1308, 1263, 1242, 1219, 1180, 1066, 1027, 1018, 997, 967, 914, 875, 758, 695 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₂H₂₀N₃O₄ [M + H] = 390.1448, found: 390.1456. [α]_D^{rt} = -24.2° (c = 0.310 in CHCl₃). **HPLC analysis** *ee* (minor diastereoisomer) = 64%, (Daicel Chiracel IB column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, λ = 190 nm, retention time: *t*_{minor} = 21.2 min, *t*_{major} = 27.3 min) at 25 °C.

(5*R*,6*R*)-6-(4-Methoxyphenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7f) major diastereomer

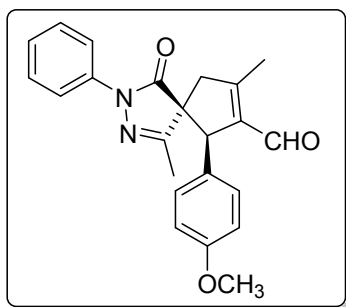


The crude product (4 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (1:1) as eluent to give **7f** as yellow semisolid in 55% yield (24.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.05 (s, 1H), 7.87 (d, *J* = 7.9 Hz, 2H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 6.91 (d, *J* = 8.7, 2H), 6.78 (d, *J* = 8.6 Hz, 2H), 4.78 (s, 1H), 3.76 (s, 3H), 2.92 (q, *J* = 18.8 Hz, 2H), 2.38 (s, 3H), 1.48 (s, 3H) ppm.

¹³C NMR (151 MHz, CDCl₃) δ = 186.91, 176.15, 161.44, 159.11, 159.02, 137.89, 136.70, 128.88 (2C), 128.65, 128.52 (2C), 125.09, 118.80(2C), 114.07(2C), 61.77, 58.56, 55.22, 44.79, 15.17, 14.73 ppm. **FT-IR** (KBr): ν = 2953, 2923, 2860, 1709, 1670, 1613, 1592, 1515, 1398, 1365, 1305, 1248, 1180, 1120, 1084, 1036, 976, 851, 761 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₃H₂₃N₂O₃ [M + H] = 375.1703, found: 375.1700. [α]_D^{rt} = -252.7° (c = 0.440 in CHCl₃). **HPLC analysis** *ee* (major diastereoisomer) = 91%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 60:40, 1.0 mL/min, λ = 252 nm, retention time: *t*_{major} = 22.4 min, *t*_{minor} = 42.4 min) at 25 °C.

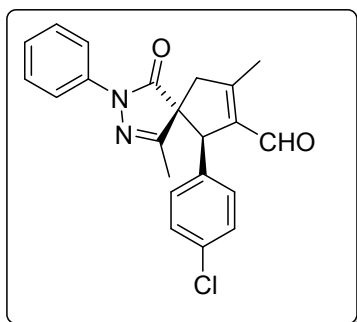
(5*S*,6*R*)-6-(4-Methoxyphenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*f*) minor diastereomer



The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (1:1) as eluent to give **7*f*** as brown semisolid in 20% yield (9.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.03 (s, 1H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.09 (t, *J* = 7.3 Hz, 2H), 6.93 (d, *J* = 8.5 Hz, 2H), 6.76 (d, *J* = 8.5 Hz, 2H), 4.51 (s, 1H), 3.73 (s, 3H), 3.16 (d, *J* = 19.0 Hz, 1H), 2.75 (d, *J* = 18.9 Hz, 1H), 2.39 (s, 3H), 2.18 (s, 3) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 186.79, 172.88, 161.79, 159.82, 159.01, 137.50, 136.91, 129.05 (2C), 128.65 (2C), 127.72, 124.90, 118.97 (2C), 113.61 (2C), 61.09, 57.02, 55.11, 44.63, 14.64, 13.68 ppm. **FT-IR** (KBr): ν = 2953, 2926, 2854, 1715, 1673, 1634, 1613, 1598, 1515, 1500, 1437, 1401, 1365, 1308, 1251, 1213, 1180, 1123, 1084, 1033, 964, 920, 863, 764, 689 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₃H₂₃N₂O₃ [M + H] = 375.1703, found: 375.1701. [α]_D^{rt} = +12.5° (c = 0.20 in CHCl₃). **HPLC analysis** *ee* (minor diastereoisomer) = 92%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, λ = 261 nm, retention time: *t*_{major} = 9.0 min, *t*_{minor} = 24.1 min) at 25 °C

(5*R*,6*R*)-6-(4-Chlorophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*g*) major diastereomer

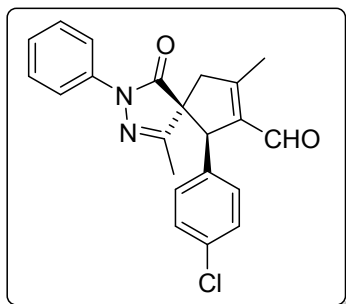


The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7*g*** as yellow semisolid in 44% yield (20.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.08 (s, 1H), 7.85 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.9 Hz, 2H), 7.22 (m, 3H), 6.92 (d, *J* = 8.4 Hz, 2H), 4.78 (s, 1H), 3.00 (d, *J* = 18.9 Hz, 1H), 2.89 (d, *J* = 18.9 Hz, 1H), 2.39 (s, 3H), 1.52 (s, 3) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 186.54, 175.77, 160.81, 159.98, 137.72, 136.27, 135.12, 133.64, 128.93 (2C), 128.83 (2C), 128.75 (2C), 125.27, 118.80 (2C), 61.66, 58.53, 44.92, 15.21, 14.72 ppm. **FT-IR** (KBr): ν = 3061, 2953, 2929, 2854, 1712, 1670, 1595, 1503, 1494, 1398, 1368, 1311, 1278, 1260, 1225, 1183, 1123, 1093, 1012, 973, 869, 851, 836, 764, 689 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₂H₂₀ClN₂O₂ [M + H] = 379.1208, found: 379.1206. [α]_D^{rt} = -272.7° (c = 0.500 in CHCl₃). **HPLC analysis** *ee* (major diastereoisomer) = 89%, (Daicel Chiracel IB

column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 252$ nm, retention time: $t_{minor} = 12.8$ min, $t_{major} = 16.3$ min) at 25 °C.

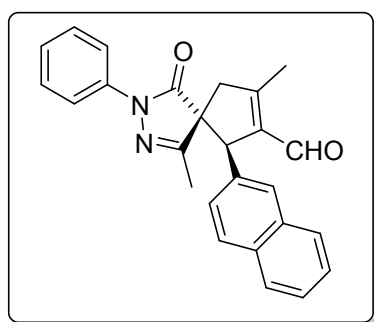
(5*S*,6*R*)-6-(4-Chlorophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7g') *minor diastereomer*



The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7g'** as yellow semisolid in 24% yield (11.0 mg).

¹H NMR (600 MHz, CDCl₃) $\delta = 10.05$ (s, 1H), 7.47 (d, $J = 7.6$ Hz, 2H), 7.31 – 7.27 (m, 2H), 7.20 (d, $J = 8.5$ Hz, 2H), 7.11 (t, $J = 7.4$ Hz, 1H), 6.94 (d, $J = 8.4$ Hz, 2H), 4.49 (s, 1H), 3.17 (d, $J = 18.9$ Hz, 1H), 2.78 (d, $J = 19.0$ Hz, 1H), 2.40 (s, 3H), 2.19 (s, 3) ppm. **¹³C NMR** (151 MHz, CDCl₃) $\delta = 186.46, 172.59, 161.50, 160.62, 137.32, 136.61, 134.25, 133.56, 129.33$ (2C), 128.74 (2C), 128.38 (2C), 125.11, 118.92 (2C), 60.79, 56.74, 44.84, 14.62, 13.64 ppm. **FT-IR** (KBr): $\nu = 2923, 2848, 1709, 1670, 1643, 1595, 1500, 1491, 1413, 1398, 1365, 1305, 1245, 1210, 1180, 1120, 1090, 1015, 872, 758, 689, 585$ cm⁻¹. **HRMS** (ESI) m/z calcd for C₂₂H₂₀ClN₂O₂ [M + H] = 379.1208, found: 379.1207. $[\alpha]_D^{rt} = 0^\circ$ (c = 0.180 in CHCl₃). **HPLC analysis** *ee* (*minor diastereoisomer*) = 91%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 252$ nm, retention time: $t_{major} = 6.9$ min, $t_{minor} = 16.3$ min) at 25 °C.

(5*R*,6*R*)-1,8-Dimethyl-6-(2-naphthyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7h) *major diastereomer*

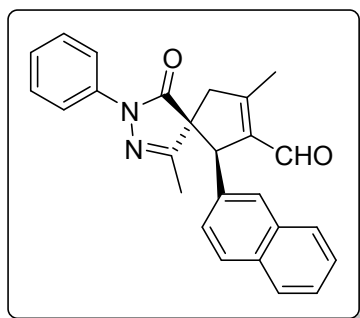


The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7h** as blackish red semisolid in 49% yield (23.0 mg).

¹H NMR (600 MHz, CDCl₃) $\delta = 10.12$ (s, 1H), 7.87 (d, $J = 8.1$ Hz, 2H), 7.80 – 7.68 (m, 4H), 7.45 – 7.40 (m, 6H), 7.21 (t, $J = 7.4$ Hz, 1H), 7.10 (dd, $J = 8.5$ Hz, $J' = 1.9$ Hz, 1H), 4.99 (s, 1H), 2.99 (q, $J = 18.9$ Hz, 2H), 2.44 (s, 3H), 1.41 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) $\delta = 187.02, 176.25, 161.31, 159.56, 137.99, 136.71, 134.32, 133.31, 133.03, 129.05$ (2C), 128.69, 128.01, 127.82, 126.50, 126.37, 126.24, 125.75, 125.34, 119.05 (2C), 61.96, 59.43, 45.20, 15.37, 14.98 ppm. **FT-IR** (KBr): $\nu = 3497, 3455, 3061, 2917, 2842, 2753, 1960, 1712, 1664, 1625, 1592, 1500, 1431,$

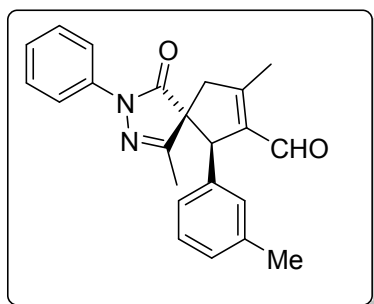
1395, 1365, 1338, 1308, 1272, 1225, 1189, 1120, 908, 863, 827, 800, 755, 695, 656, 588 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_2$ [$\text{M} + \text{H}$] = 395.1754, found: 395.1754. $[\alpha]_{\text{D}}^{25} = -312.5^\circ$ ($c = 0.480$ in CHCl_3). **HPLC analysis** *ee* (major diastereoisomer) = 93%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{minor}} = 29.1$ min, $t_{\text{major}} = 37.3$ min) at 25°C .

(5*S*,6*R*)-1,8-Dimethyl-6-(2-naphthyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7h') minor diastereomer



The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7h'** as brown semisolid in 28% yield (13.0 mg). **^1H NMR** (600 MHz, CDCl_3) $\delta = 10.08$ (s, 1H), 7.79 – 7.70 (m, 4H), 7.48 (m, 1H), 7.43 – 7.35 (m, 5H), 7.18 (t, $J = 7.9$ Hz, 2H), 7.14 (d, $J = 8.7$ Hz, 1H), 7.03 (t, $J = 7.3$ Hz, 1H), 4.71 (s, 1H), 3.26 (d, $J = 19.1$ Hz, 1H), 2.80 (d, $J = 19.4$ Hz, 1H), 2.44 (s, 3H), 2.23 (s, 3H) ppm. **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 186.80, 172.79, 161.98, 160.27, 137.55, 137.06, 133.55, 133.31, 133.13, 128.74$ (2C), 128.11, 127.96, 127.80, 127.14, 126.24, 126.06, 125.92, 125.03, 119.08 (2C), 61.12, 57.76, 45.17, 14.86, 13.86 ppm. **FT-IR** (KBr): $\nu = 3521, 3455, 3058, 2917, 2845, 1712, 1673, 1661, 1628, 1598, 1500, 1431, 1398, 1362, 1335, 1308, 1120, 866, 812, 797, 752, 692$ cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_2$ [$\text{M} + \text{H}$] = 395.1754, found: 395.1758. $[\alpha]_{\text{D}}^{25} = -47.9^\circ$ ($c = 0.240$ in CHCl_3). **HPLC analysis** *ee* (minor diastereoisomer) = 92%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 204$ nm, retention time: $t_{\text{major}} = 8.0$ min, $t_{\text{minor}} = 17.0$ min) at 25°C .

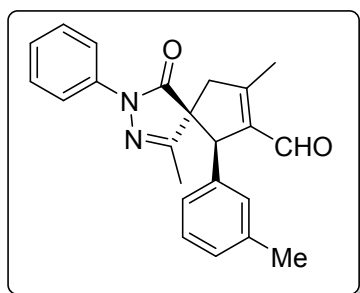
(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*m*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7i) major diastereomer



The crude product (4 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7i** as brown semisolid in 67% yield (29.0 mg). **^1H NMR** (600 MHz, CDCl_3) $\delta = 10.06$ (s, 1H), 7.86 (d, $J = 7.7$ Hz, 2H), 7.42 – 7.38 (m, 2H), 7.22 – 7.12 (m, 2H), 7.04 (d, $J = 7.6$ Hz, 1H), 6.79 – 6.77 (m, 2H), 4.78 (s, 1H), 2.93 (q, $J = 24.0$ Hz, 2H), 2.40 (s, 3H), 2.24 (s, 3H), 1.44 (s, 3H) ppm. **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 187.05, 176.28, 161.49,$

159.26, 138.53, 137.98, 136.77, 136.62, 129.03 (2C), 128.82, 128.67, 128.36, 125.30, 124.60, 119.05 (2C), 61.85, 59.26, 44.99, 21.55, 15.23, 14.91 ppm. **FT-IR** (KBr): ν = 3061, 3046, 3019, 3004, 2929, 2866, 2771, 2732, 1709, 1667, 1628, 1595, 1503, 1488, 1395, 1368, 1347, 1308, 1263, 1189, 1117, 1096, 1057, 1036, 994, 973, 917, 878, 851, 818, 779, 761, 743, 695 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{23}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}] = 359.1754$, found: 359.1753. $[\alpha]_{\text{D}}^{\text{rt}} = -246.3^\circ$ ($c = 0.335$ in CHCl_3). **HRMS** (ESI) m/z calcd for $\text{C}_{23}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}] = 359.1754$, found: 359.1760. $[\alpha]_{\text{D}}^{\text{rt}} = -221.3^\circ$ ($c = 0.305$ in CHCl_3). **HPLC analysis** *ee* (*major diastereoisomer*) = 94%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 70:30, 1.0 mL/min, $\lambda = 238$ nm, retention time: $t_{\text{major}} = 22.0$ min, $t_{\text{minor}} = 40.2$ min) at 25 °C.

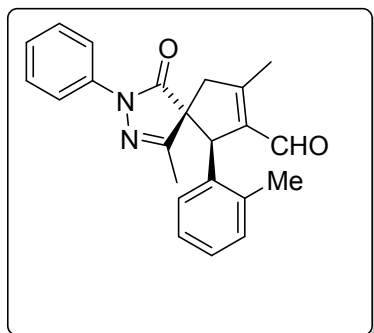
(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*m*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7i'**) *minor diastereomer***



The crude product (4 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (4:1) as eluent to give **7i'** as dark yellow semisolid in 26% yield (11.0 mg).

^1H NMR (600 MHz, CDCl_3) δ = 10.05 (s, 1H), 7.45 (d, $J = 7.9$ Hz, 2H), 7.28 – 7.27 (m, 2H), 7.13 – 7.08 (m, 2H), 7.00 (d, $J = 7.5$ Hz, 1H), 6.80 – 6.79 (m, 2H), 4.51 (s, 1H), 3.16 (d, $J = 18.2$ Hz, 1H), 2.75 (d, $J = 19.0$ Hz, 1H), 2.40 (s, 3H), 2.24 (s, 3H), 2.19 (s, 3H) ppm. **^{13}C NMR** (151 MHz, CDCl_3) δ = 186.92, 172.94, 161.90, 160.20, 137.87, 137.64, 136.88, 135.69, 128.78 (4C), 128.17, 125.15, 125.04, 119.14 (2C), 61.19, 57.70, 44.80, 21.57, 14.82, 13.84 ppm. **FT-IR** (KBr): ν = 3079, 3061, 3046, 3022, 2920, 2845, 2753, 2585, 1850, 1718, 1667, 1628, 1595, 1503, 1491, 1398, 1371, 1302, 1245, 1207, 1183, 1156, 1120, 1096, 1027, 994, 970, 949, 931, 908, 881, 845, 761, 704 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{23}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}] = 359.1754$, found: 359.1754. $[\alpha]_{\text{D}}^{\text{rt}} = +28.1^\circ$ ($c = 0.160$ in CHCl_3). **HPLC analysis** *ee* (*minor diastereoisomer*) = 94%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, $\lambda = 249$ nm, retention time: $t_{\text{major}} = 9.9$ min, $t_{\text{minor}} = 19.5$ min) at 25 °C.

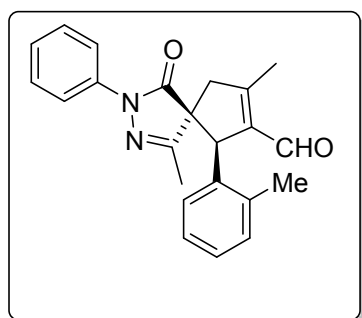
(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*o*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7j) major diastereomer



The crude product (7 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7j** as brown semisolid in 29% yield (12.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.03 (s, 1H), 7.89 – 7.87 (m, 2H), 7.42 – 7.39 (m, 2H), 7.21 – 7.18 (m, 2H), 7.15 – 7.14 (m, 2H), 6.94 (d, *J* = 7.5 Hz, 1H), 4.98 (s, 1H), 3.05 (d, *J* = 18.6 Hz, 1H), 2.85 (d, *J* = 19.0 Hz, 1H), 2.41 (s, 3H), 2.14 (s, 3H), 1.26 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 186.60, 176.84, 161.70, 158.77, 138.03, 137.88, 136.62, 135.74, 131.40, 129.08 (2C), 127.88, 127.17, 126.00, 125.26, 118.88 (2C), 60.26, 54.87, 45.77, 19.70, 15.06, 14.70 ppm. **FT-IR** (KBr): ν = 3058, 3016, 2968, 2956, 2926, 2866, 2774, 1712, 1667, 1649, 1625, 1589, 1488, 1398, 1365, 1341, 1317, 1299, 1257, 1234, 1192, 1114, 1054, 1036, 994, 970, 911, 881, 851, 812, 764, 740, 698 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₃H₂₃N₂O₂ [M + H] = 359.1754, found: 359.1751. [α]_D^{rt} = -217.3° (c = 0.490 in CHCl₃). **HPLC analysis** *ee* (major diastereoisomer) = 91%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 70:30, 1.0 mL/min, λ = 194 nm, retention time: *t*_{minor} = 21.7 min, *t*_{major} = 24.2 min) at 25 °C.

(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*o*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7j') minor diastereomer

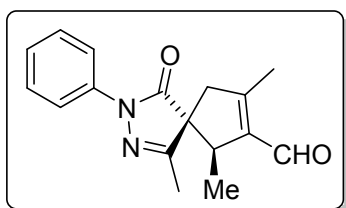


The crude product (7 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7j'** as dark yellow semisolid in 8% yield (4.0 mg).

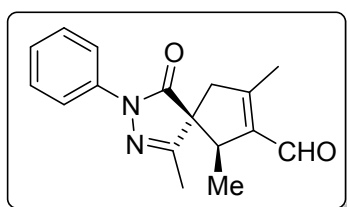
¹H NMR (600 MHz, CDCl₃) δ = 10.03 (s, 1H), 7.60 – 7.58 (m, 2H), 7.32 – 7.29 (m, 2H), 7.14 – 7.11 (m, 3H), 7.09 – 7.08 (m, 1H), 6.97 – 6.95 (m, 1H), 4.75 (s, 1H), 3.27 (d, *J* = 19.3 Hz, 1H), 2.67 (d, *J* = 19.0 Hz, 1H), 2.42 (s, 3H), 2.17 (s, 3H), 2.11 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 186.54, 172.19, 162.74, 159.57, 138.03, 137.82, 135.80, 134.12, 130.71, 128.90 (2C), 127.90, 127.71, 125.75, 125.04, 118.95 (2C), 59.65, 52.68, 45.73, 19.46, 14.65, 13.83 ppm. **FT-IR** (KBr): ν = 3085, 3064, 3046, 2914, 2845, 2777, 2756, 2579, 1832, 1721, 1709, 1667, 1625, 1595, 1503, 1488, 1398, 1365, 1305, 1219, 1120, 1054, 1024, 988, 961, 902, 881, 857, 809, 758, 698 cm⁻¹.

HRMS (ESI) m/z calcd for $C_{23}H_{23}N_2O_2$ $[M + H] = 359.1754$, found: 359.1749. $[\alpha]_D^{25} = -24.0^\circ$ ($c = 0.125$ in $CHCl_3$). **HPLC analysis** *ee* (minor diastereoisomer) = 82%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, $\lambda = 252$ nm, retention time: $t_{major} = 9.5$ min, $t_{minor} = 19.6$ min) at 25 °C.

(5*R*/5*S*,6*R*)-1,6,8-Trimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7k) mixture of diastereomers 1.8:1



The crude product (5 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (3:1) as eluent to give **7k** as a mixture of diastereomers (*dr* 1.8:1) and as brown semisolid in 81% yield (27.0 mg).



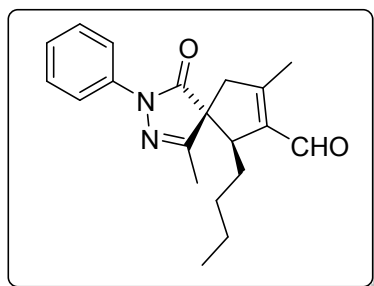
1H NMR major diastereomer ((600 MHz, $CDCl_3$) $\delta = 10.05$ (s, 1H), 7.91 (d, $J = 7.8$ Hz, 2H), 7.41 – 7.37 (m, 2H), 7.20 - 7.16 (m, 1H), 3.64 – 3.60 (m, 1H), 3.04 (d, $J = 18.6$ Hz, 1H), 2.59 (d, $J = 18.6$ Hz, 1H), 2.21 (s, 3H), 2.09 (s, 3H), 1.2 (d, $J = 7.4$ Hz, 3H) ppm. **^{13}C NMR** (151 MHz, $CDCl_3$) $\delta = 187.38, 175.30,$

161.76, 157.98, 138.20, 137.94, 128.88 (2C), 125.09, 118.69 (2C), 61.96, 48.70, 44.62, 14.60, 14.33, 13.49 ppm. **^{13}C NMR** major diastereomer (NMR (151 MHz, $CDCl_3$) $\delta = 187.38, 175.30, 161.76, 157.98, 138.20, 137.94, 128.88$ (2C), 125.09, 118.69 (2C), 61.96, 48.70, 44.62, 14.60, 14.33, 13.49 ppm. **HPLC analysis** *ee* (major diastereoisomer) = 82%, (Daicel Chiracel IB column, heptane/*iso*-propanol, 98:02, 1.0 mL/min, $\lambda = 247$ nm, retention time: $t_{minor} = 46.8$ min, $t_{major} = 59.4$ min) at 25 °C.

1H NMR minor diastereomer (NMR (600 MHz, $CDCl_3$) $\delta = 10.02$ (s, 1H), 7.89 (d, $J = 7.8$ Hz, 2H), 7.41 – 7.37 (m, 2H), 7.20 - 7.16 (m, 1H), 3.39 – 3.34 (m, 1H), 3.10 (d, $J = 18.8$ Hz, 1H), 2.66 (d, $J = 18.9$ Hz, 1H), 2.21 (s, 3H), 2.03 (s, 3H), 1.27 (d, $J = 7.1$, 3H) ppm. **^{13}C NMR** (151 MHz, $CDCl_3$) $\delta = 187.09, 173.81, 162.58, 157.89, 139.53, 137.94, 128.84$ (2C), 124.97, 118.69 (2C), 59.54, 45.70, 45.08, 15.80, 14.21, 13.55 ppm. **^{13}C NMR** minor diastereomer (151 MHz, $CDCl_3$) $\delta = 187.09, 173.81, 162.58, 157.89, 139.53, 137.94, 128.84$ (2C), 124.97, 118.69 (2C), 59.54, 45.70, 45.08, 15.80, 14.21, 13.55 ppm. **HPLC analysis** *ee* (minor diastereoisomer) = 76%, (Daicel Chiracel IB column, heptane/*iso*-propanol, 98:02, 1.0 mL/min, $\lambda = 247$ nm, retention time: $t_{major} = 37.2$ min, $t_{minor} = 42.5$ min) at 25 °C.

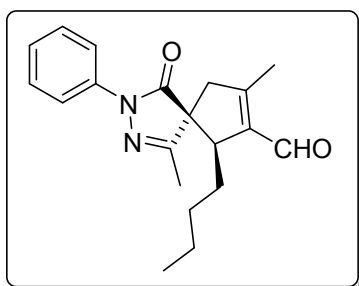
FT-IR (KBr): $\nu = 3056, 2971, 2923, 2917, 2847, 2762, 2724, 1711, 1670, 1597, 1505, 1432, 1397, 1366, 1309, 12883, 1239, 1217, 1188, 1125, 1040, 1002, 960, 907, 869, 831, 764, 694, 637, 580, 514 \text{ cm}^{-1}$. **HRMS** (ESI) m/z calcd for $\text{C}_{17}\text{H}_{19}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}] = 283.1441$, found: 283.1441. $[\alpha]_{\text{D}}^{\text{rt}} = -43.3^\circ$ ($c = 0.90$ in CHCl_3).

(5*R*/5*S*,6*R*)-6-Butyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7I) mixture of diastereomers 2.5:1



The crude product (2 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (5:1) as eluent to give **7I** as a mixture of diastereomers (*dr* 2.5:1) and as pale brown semisolid in 69% yield (27.0 mg).

$^1\text{H NMR}$ major diastereomer (600 MHz, CDCl_3) $\delta = 10.04$ (s, 1H), 7.87 – 7.85 (m, 2H), 7.42 – 7.39 (m, 2H), 7.21 – 7.17 (m, 1H), 3.61 – 3.57 (m, 1H), 3.01 (d, $J = 18.4$ Hz, 1H), 2.55 (d, $J = 18.4$ Hz, 1H), 2.35 – 2.29 (m, 1H), 2.21 (s, 3H), 2.12 (s, 3H), 1.30 – 1.14 (m, 5H), 0.76 (t, $J = 7.1$ Hz, 3H) ppm. **$^{13}\text{C NMR}$** major diastereomer (151 MHz, CDCl_3) $\delta = 187.84, 175.81, 162.24, 157.96, 138.11, 138.06, 129.06$ (2C), 125.34, 119.10 (2C), 61.33, 53.97, 46.41, 29.75, 28.26, 22.58, 16.02, 14.53, 13.92 ppm. **HPLC analysis** *ee* (major diastereoisomer) = 90%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{minor}} = 13.1$ min, $t_{\text{major}} = 17.9$ min) at 25 °C.

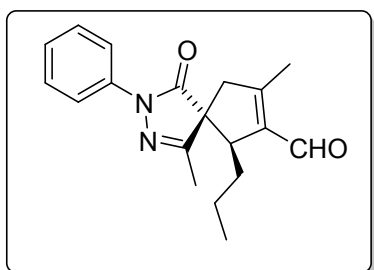


$^1\text{H NMR}$ minor diastereomer (600 MHz, CDCl_3) $\delta = 10.01$ (s, 1H), 7.87 – 7.85 (m, 2H), 7.42 – 7.39 (m, 2H), 7.21 – 7.17 (m, 1H), 3.25 – 3.23 (m, 1H), 3.13 (d, $J = 18.8$ Hz, 1H), 2.62 (d, $J = 18.8$ Hz, 1H), 2.22 (s, 3H), 2.02 (s, 3H), 1.92 – 1.86 (m, 1H), 1.80 – 1.75 (m, 1H), 1.05 – 0.95 (m, 4H), 0.79 (t, $J = 7.3$ Hz, 3H). **$^{13}\text{C NMR}$** minor diastereomer (151 MHz, CDCl_3) $\delta = 187.31, 174.09, 163.31, 158.01, 139.26, 138.11, 129.03$ (2C), 125.13, 118.92 (2C), 58.49, 51.84, 46.27, 30.71, 28.39, 22.71, 14.33, 14.04, 13.64 ppm. **HPLC analysis** *ee* (minor diastereoisomer) = 89%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{major}} = 9.5$ min, $t_{\text{minor}} = 14.3$ min) at 25 °C.

FT-IR (KBr): $\nu = 3569, 3503, 3464, 3422, 3079, 3061, 3043, 3028, 2959, 2929, 2860, 2756, 2726, 2579, 2331, 1867, 1808, 1721, 1706, 1700, 1673, 1658, 1595, 1503, 1488, 1434, 1401,$

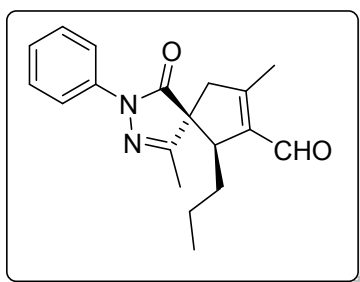
1368, 1302, 1272, 1248, 1234, 1219, 1180, 1123, 1066, 1036, 997, 970, 934, 908, 863, 851, 815, 761, 737, 710, 695, 641 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{20}\text{H}_{25}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}] = 325.1911$, found: 325.1910. $[\alpha]_{\text{D}}^{\text{rt}} = -44.4^\circ$ ($c = 0.540$ in CHCl_3).

(5*R*/5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-propyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7m) mixture of diastereomers 3.4:1



The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (5:1) as eluent to give **7m** as a mixture of diastereomers (*dr* 3.4:1) and as brown semisolid in 84% yield (31.0 mg).

^1H NMR major diastereomer (600 MHz, CDCl_3) $\delta = 10.04$ (s, 1H), 7.89 – 7.87 (m, 2H), 7.42 – 7.39 (m, 2H), 7.21 – 7.17 (m, 1H), 3.62 – 3.59 (m, 1H), 3.01 (d, $J = 18.5$ Hz, 1H), 2.55 (d, $J = 18.5$ Hz, 1H), 2.31 – 2.26 (m, 1H), 2.21 (s, 3H), 2.12 (s, 3H), 1.27 – 1.14 (m, 3H), 0.82 (t, $J = 7.1$ Hz, 3H) ppm. **^{13}C NMR** major diastereomer (151 MHz, CDCl_3) $\delta = 187.84, 175.77, 162.23, 157.97, 138.16, 138.05, 129.07$ (2C), 125.29, 118.99 (2C), 61.37, 53.81, 46.45, 30.88, 20.94, 16.02, 14.53, 14.21 ppm. **HPLC analysis** *ee* (major diastereoisomer) = 86%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 97:3, 1.0 mL/min, $\lambda = 193$ nm, retention time: $t_{\text{minor}} = 18.4$ min, $t_{\text{major}} = 25.1$ min) at 25 $^\circ\text{C}$.

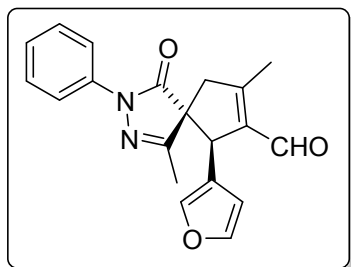


^1H NMR minor diastereomer (600 MHz, CDCl_3) $\delta = 10.01$ (s, 1H), 7.89 – 7.87 (m, 2H), 7.42 – 7.39 (m, 2H), 7.21 – 7.17 (m, 1H), 3.26 – 3.25 (m, 1H), 3.13 (d, $J = 19.0$ Hz, 1H), 2.62 (d, $J = 19.0$ Hz, 1H), 2.22 (s, 3H), 2.02 (s, 3H), 1.91 – 1.85 (m, 1H), 1.76 – 1.70 (m, 1H), 1.12 – 1.05 (m, 2H), 0.84 (t, $J = 7.5$ Hz, 3H). **^{13}C NMR** minor diastereomer (151 MHz, CDCl_3) $\delta = 187.28, 174.08, 163.31, 158.01, 139.28, 138.12, 129.03$ (2C), 125.13, 118.93 (2C), 58.50, 51.61, 46.29, 30.83, 21.82, 14.33, 14.11, 13.64 ppm. **HPLC analysis** *ee* (minor diastereoisomer) = 87%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 97:3, 1.0 mL/min, $\lambda = 204$ nm, retention time: $t_{\text{major}} = 14.0$ min, $t_{\text{minor}} = 19.6$ min) at 25 $^\circ\text{C}$.

FT-IR (KBr): $\nu = 3566, 3536, 3497, 3479, 3461, 3422, 3405, 3396, 3363, 3064, 2962, 2932, 2872, 2765, 1715, 1658, 1634, 1619, 1595, 1500, 1458, 1437, 1395, 1373, 1335, 1311, 1290, 1269, 1240, 1222, 1183, 1123, 1039, 1030, 1006, 994, 967, 931, 908, 851, 767, 737, 713, 689,$

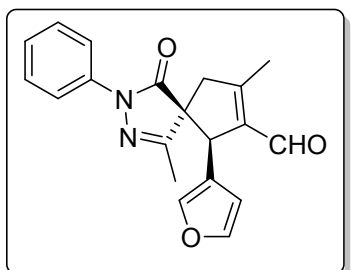
635, 594, 579, 504 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{19}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}] = 311.1754$, found: 311.1753. $[\alpha]_{\text{D}}^{\text{rt}} = -46.2^\circ$ ($c = 0.520$ in CHCl_3).

(5*R*,6*R*)-6-(3-Furyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7n) major diastereomer



The crude product (7 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7n** as brown semisolid in 54% yield (22.0 mg). **^1H NMR** (600 MHz, CDCl_3) $\delta = 10.04$ (s, 1H), 7.89 – 7.87 (m, 2H), 7.42 – 7.39 (m, 2H), 7.32 (t, $J = 1.7$ Hz, 1H), 7.21 – 7.19 (m, 1H), 7.13 (m, 1H), 6.06 – 6.05 (m, 1H), 4.71 (s, 1H), 3.03 (d, $J = 19.0$ Hz, 1H), 2.83 (d, $J = 19.0$ Hz, 1H), 2.34 (s, 3H), 1.77 (s, 3H) ppm. **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 187.01$, 175.62, 161.54, 158.91, 143.48, 140.01, 137.95, 136.23, 129.08 (2C), 125.37, 121.13, 118.95 (2C), 110.10, 61.80, 50.15, 45.02, 15.38, 14.92 ppm. **FT-IR** (KBr): $\nu = 3064$, 2917, 2848, 2753, 1960, 1706, 1667, 1628, 1616, 1598, 1497, 1428, 1398, 1362, 1311, 1266, 1222, 1180, 1159, 1123, 1072, 1027, 878, 857, 791, 758, 695 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}] = 335.1390$, found: 335.1390. $[\alpha]_{\text{D}}^{\text{rt}} = -150.0^\circ$ ($c = 0.400$ in CHCl_3). **HPLC analysis** *ee* (major diastereoisomer) = 88%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{major}} = 22.8$ min, $t_{\text{minor}} = 31.2$ min) at 25 $^\circ\text{C}$.

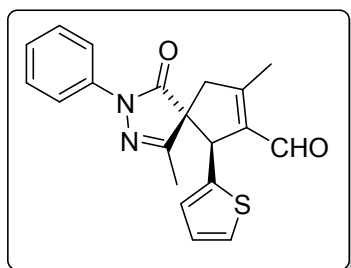
(5*S*,6*R*)-6-(3-Furyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7n') minor diastereomer



The crude product (7 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7n'** as yellow semisolid in 17% yield (7.0 mg). **^1H NMR** (600 MHz, CDCl_3) $\delta = 10.01$ (s, 1H), 7.65 – 7.63 (m, 2H), 7.33 – 7.30 (m, 2H), 7.29 (t, $J = 1.7$ Hz, 1H), 7.20 (m, 1H), 7.14 – 7.11 (m, 1H), 6.17 – 6.16 (m, 1H), 4.45 (s, 1H), 3.13 (d, $J = 18.8$ Hz, 1H), 2.77 (d, $J = 18.8$ Hz, 1H), 2.35 (s, 3H), 2.15 (s, 3H) ppm. **^{13}C NMR** (151 MHz, CDCl_3) $\delta = 186.78$, 173.09, 161.41, 159.55, 143.12, 140.45, 137.74, 136.55, 128.91 (2C), 125.16, 120.49, 119.01 (2C), 110.68, 60.96, 48.10, 44.76, 14.80, 13.85 ppm. **FT-IR**

(KBr): $\nu = 3067, 2920, 2857, 2756, 1721, 1712, 1670, 1619, 1598, 1497, 1491, 1437, 1404, 1365, 1341, 1305, 1204, 1180, 1159, 1123, 1072, 1027, 1000, 970, 875, 758, 695 \text{ cm}^{-1}$. **HRMS** (ESI) m/z calcd for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}] = 335.1390$, found: 335.1388. $[\alpha]_{\text{D}}^{\text{rt}} = +45.8^\circ$ ($c = 0.295$ in CHCl_3). **HPLC analysis** *ee* (minor diastereoisomer) = 94%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 190 \text{ nm}$, retention time: $t_{\text{major}} = 8.3 \text{ min}$, $t_{\text{minor}} = 15.0 \text{ min}$) at 25°C .

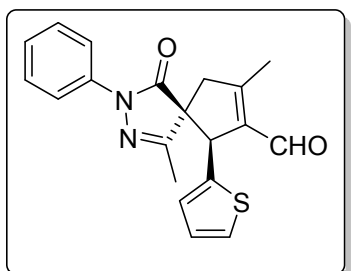
(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(thien-2-yl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7o) major diastereomer



The crude product (5 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7o** as brown semisolid in 64% yield (27.0 mg).

$^1\text{H NMR}$ (600 MHz, CDCl_3) $\delta = 10.03$ (s, 1H), 7.89 – 7.87 (m, 2H), 7.42 – 7.38 (m, 2H), 7.21 – 7.18 (m, 1H), 7.17 (dd, $J = 5.1 \text{ Hz}$, $J' = 1.2 \text{ Hz}$, 1H), 6.93 (dd, $J = 5.1 \text{ Hz}$, $J' = 3.5 \text{ Hz}$, 1H), 6.77 – 6.76 (m, 1H), 5.01 (s, 1H), 3.02 (d, $J = 18.7 \text{ Hz}$, 1H), 2.90 (d, $J = 18.7 \text{ Hz}$, 1H), 2.38 (s, 3H), 1.54 (s, 3H) ppm. **$^{13}\text{C NMR}$** (151 MHz, CDCl_3) $\delta = 186.61, 175.58, 161.09, 159.01, 140.68, 137.97, 137.21, 129.04$ (2C), 127.50, 125.91, 125.30, 124.94, 118.96 (2C), 61.72, 53.66, 44.67, 14.93, 14.90 ppm. **FT-IR** (KBr): $\nu = 3067, 2929, 2851, 2759, 1706, 1670, 1622, 1598, 1503, 1431, 1398, 1362, 1308, 1269, 1234, 1183, 1120, 1048, 1000, 967, 908, 878, 863, 758, 725, 710, 692 \text{ cm}^{-1}$. **HRMS** (ESI) m/z calcd for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}] = 351.1162$, found: 351.1158. $[\alpha]_{\text{D}}^{\text{rt}} = -215.0^\circ$ ($c = 0.200$ in CHCl_3). **HPLC analysis** *ee* (major diastereoisomer) = 87%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, $\lambda = 238 \text{ nm}$, retention time: $t_{\text{major}} = 42.6 \text{ min}$, $t_{\text{minor}} = 47.2 \text{ min}$) at 25°C .

(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(thien-2-yl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7o') minor diastereomer

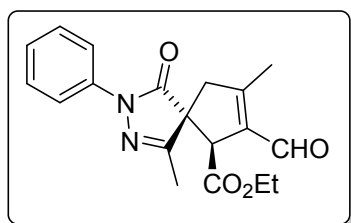


The crude product (7 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7o'** as brown semisolid in 17% yield (7.0 mg).

$^1\text{H NMR}$ (600 MHz, CDCl_3) $\delta = 10.03$ (s, 1H), 7.64 – 7.62 (m, 2H), 7.33 – 7.30 (m, 2H), 7.16 (dd, $J = 5.1 \text{ Hz}$, $J' = 1.2 \text{ Hz}$, 1H), 7.14 – 7.11 (m, 1H), 6.92 (dd, $J = 5.1 \text{ Hz}$, $J' = 3.5 \text{ Hz}$, 1H), 6.77 – 6.76 (m, 1H), 4.78 (s, 1H), 3.26 (d, $J = 18.8 \text{ Hz}$, 1H), 2.70 (d, $J = 18.8 \text{ Hz}$, 1H), 2.38 (s,

3H), 2.13 (s, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ = 186.48, 172.15, 161.58, 159.84, 139.15, 137.78, 137.26, 128.87 (2C), 127.17, 126.34, 125.10, 124.98, 119.03 (2C), 60.96, 52.11, 44.64, 14.80, 13.87 ppm. **FT-IR** (KBr): ν = 3061, 2917, 2851, 2762, 2570, 1844, 1718, 1709, 1673, 1592, 1503, 1491, 1422, 1398, 1365, 1338, 1302, 1216, 1201, 1186, 1123, 1160, 1036, 994, 967, 914, 860, 794, 755, 695 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_2\text{S}$ [$\text{M} + \text{H}$] = 351.1162, found: 351.1161. $[\alpha]_{\text{D}}^{\text{rt}}$ = +14.7° (c = 0.305 in CHCl_3). **HPLC analysis** *ee* (*minor diastereoisomer*) = 90%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, λ = 245 nm, retention time: t_{major} = 13.9 min, t_{minor} = 26.3 min) at 25 °C.

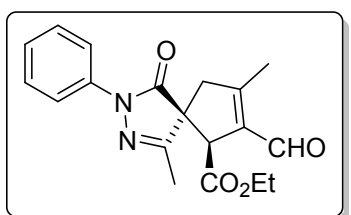
Ethyl (5*R*,6*R*)-7-formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-6-carboxylate (7p) major diastereomer



The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2.5:1) as eluent to give **7p** as brown semisolid in 70% yield (29.0 mg).

^1H NMR (600 MHz, CDCl_3) δ = 9.98 (s, 1H), 7.89 – 7.88 (m, 2H), 7.42 – 7.39 (m, 2H), 7.22 – 7.19 (m, 1H), 4.33 – 4.22 (m, 1H), 4.16 – 4.10 (m, 1H), 4.05 – 4.00 (m, 1H), 3.08 (d, J = 17.9 Hz, 1H), 2.71 (d, J = 17.9 Hz, 1H), 2.27 (s, 3H), 2.05 (s, 3H), 1.08 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ = 186.46, 174.45, 168.91, 160.51, 158.47, 137.74, 134.30, 129.09 (2C), 125.51, 118.93 (2C), 61.62, 59.08, 57.41, 45.76, 14.69, 14.65, 14.08 ppm. **FT-IR** (KBr): ν = 3554, 3524, 3479, 3419, 3058, 2980, 2926, 2848, 2759, 1739, 1712, 1670, 1592, 1500, 1431, 1395, 1365, 1311, 1272, 1231, 1180, 1126, 1102, 1027, 1000, 976, 911, 884, 860, 842, 761, 713, 689 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{19}\text{H}_{21}\text{N}_2\text{O}_4$ [$\text{M} + \text{H}$] = 341.1496, found: 341.1494. $[\alpha]_{\text{D}}^{\text{rt}}$ = -173.3° (c = 0.375 in CHCl_3). **HPLC analysis** *ee* (*major diastereoisomer*) = 92%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, λ = 241 nm, retention time: t_{major} = 43.0 min, t_{minor} = 66.6 min) at 25 °C.

Ethyl (5*S*,6*R*)-7-formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-6-carboxylate (7p') minor diastereomer

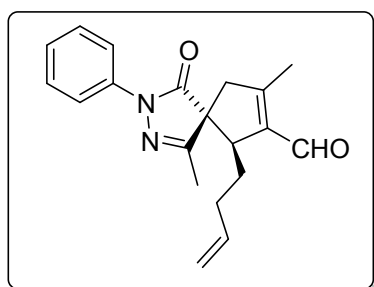


The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2.5:1) as eluent to give **7p'** as yellow semisolid in 18% yield (7.0 mg).

^1H NMR (600 MHz, CDCl_3) δ = 10.04 (s, 1H), 7.91 – 7.89 (m, 2H), 7.43 – 7.40 (m, 2H), 7.22 – 7.19 (m, 1H), 4.13 (qd, J = 7.2

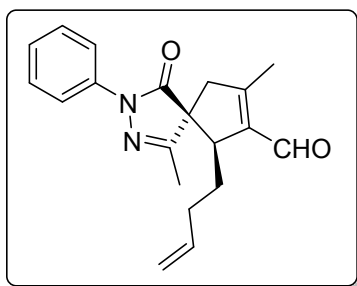
Hz, $J' = 1.7$ Hz, 2H), 3.98 (t, $J = 1.7$ Hz, 1H), 3.28 (d, $J = 17.7$ Hz, 1H), 2.71 (d, $J = 17.7$ Hz, 1H), 2.34 (s, 3H), 2.07 (s, 3H), 1.12 (t, $J = 7.2$ Hz, 2H) ppm. ^{13}C NMR (151 MHz, CDCl_3) $\delta = 186.33, 172.66, 168.38, 161.39, 160.15, 137.98, 134.74, 129.02$ (2C), 125.26, 118.68 (2C), 61.80, 57.74, 54.94, 46.75, 14.59, 14.02, 13.47 ppm. FT-IR (KBr): $\nu = 3560, 3530, 3485, 3449, 3422, 3064, 2983, 2929, 2854, 2759, 2726, 1736, 1715, 1673, 1625, 1595, 1503, 1437, 1398, 1344, 1308, 1284, 1213, 1180, 1123, 1102, 1027, 905, 869, 827, 758, 692, 647, 585$ cm^{-1} . HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{21}\text{N}_2\text{O}_4$ [$\text{M} + \text{H}$] = 341.1496, found: 341.1491. $[\alpha]_{\text{D}}^{25} = -7.9^\circ$ ($c = 0.445$ in CHCl_3). HPLC analysis *ee* (minor diastereoisomer) = 86%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, $\lambda = 239$ nm, retention time: $t_{\text{major}} = 20.6$ min, $t_{\text{minor}} = 71.2$ min) at 25 °C.

(5*R*/5*S*,6*R*)-6-(But-3-en-1-yl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7q) mixture of diastereomers 2.1:1



The crude product (3 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (3:1) as eluent to give **7q** as a mixture of diastereomers (*dr* 2.1:1) and as brown semisolid in 93% yield (36.0 mg).

^1H NMR major diastereomer (600 MHz, CDCl_3) $\delta = 10.04$ (s, 1H), 7.90 – 7.88 (m, 2H), 7.42 – 7.39 (m, 2H), 7.21 – 7.17 (m, 1H), 5.76 – 5.65 (m, 1H), 4.93 – 4.88 (m, 2H), 3.63 – 3.59 (m, 1H), 3.02 (d, $J = 18.5$ Hz, 1H), 2.57 (d, $J = 18.5$ Hz, 1H), 2.46 – 2.40 (m, 1H), 2.22 (s, 3H), 2.12 (s, 3H), 1.96 – 1.88 (m, 3H) ppm. ^{13}C NMR major diastereomer (151 MHz, CDCl_3) $\delta = 187.69, 175.65, 162.07, 158.22, 138.13, 137.93, 137.41, 129.09$ (2C), 125.32, 118.92 (2C), 115.65, 61.23, 53.27, 46.40, 31.80, 27.99, 16.01, 14.52 ppm. HPLC analysis *ee* (major diastereoisomer) = 87%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, $\lambda = 190$ nm, retention time: $t_{\text{minor}} = 15.1$ min, $t_{\text{major}} = 20.1$ min) at 25 °C.

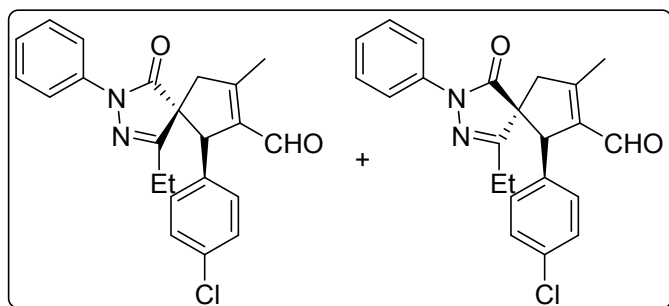


^1H NMR minor diastereomer (600 MHz, CDCl_3) $\delta = 10.01$ (s, 1H), 7.90 – 7.88 (m, 2H), 7.42 – 7.39 (m, 2H), 7.21 – 7.17 (m, 1H), 5.76 – 5.65 (m, 1H), 4.93 – 4.88 (m, 2H), 3.31 – 3.30 (m, 1H), 3.13 (d, $J = 19.0$ Hz, 1H), 2.64 (d, $J = 19.0$ Hz, 1H), 2.23 (s, 3H), 2.02 (s, 3H), 1.87 – 1.82 (m, 2H), 1.36 – 1.29 (m, 2H) ppm. ^{13}C NMR minor diastereomer (151 MHz, CDCl_3) $\delta = 187.22, 174.12, 163.21, 158.22, 139.05, 138.09, 137.72, 129.06$ (2C), 125.19, 118.90 (2C), 115.62, 58.36, 50.56, 46.40, 32.50, 27.60, 14.35, 13.64 ppm. HPLC analysis *ee* (minor

diastereoisomer) = 78%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, λ = 190 nm, retention time: t_{major} = 11.3 min, t_{minor} = 16.4 min) at 25 °C.

FT-IR (KBr): ν = 3554, 3488, 3425, 3363, 3070, 2983, 2923, 2911, 2845, 2756, 2735, 1870, 1706, 1697, 1664, 1592, 1500, 1488, 1425, 1398, 1362, 1344, 1302, 1272, 1254, 1234, 1216, 1189, 1117, 1030, 994, 914, 869, 851, 761, 716, 689, 641, 591 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{20}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M} + \text{H}] = 323.1754$, found: 323.1748. $[\alpha]_D^{rt} = -44.1^\circ$ ($c = 0.340$ in CHCl_3).

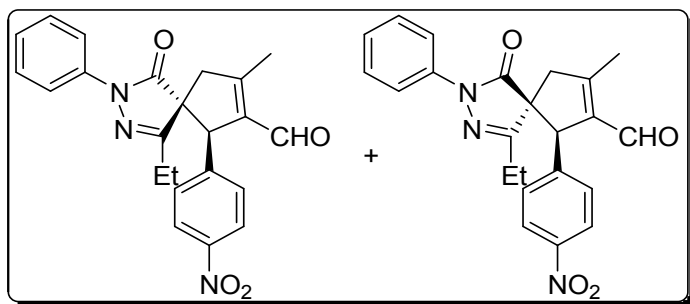
(5*R*/5*S*,6*S*)-6-(4-chlorophenyl)-1-ethyl-8-methyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7r) mixture of major and minor diastereomers



The crude product (3 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (4:1) as eluent to give **7r** as brown semisolid in 88% yield, 1.5:1 dr, as a mixture of diastereomers.

^1H NMR (400 MHz, CDCl_3) δ 10.26 (s, 1H), 10.23 (s, 1H $'$), 8.11 – 8.06 (m, 2H), 7.73 – 7.68 (m, $J = 8.7, 1.1$ Hz, 2H $'$), 7.60 (dd, $J = 8.5, 7.5$ Hz, 3H, H $'$), 7.51 – 7.46 (m, 2H $'$), 7.43 – 7.37 (m, 4H, H $'$), 7.34 – 7.27 (m, 1H $'$), 7.13 (d, $J = 8.4$ Hz, 2H $'$), 7.09 (d, $J = 8.3$ Hz, 2H), 4.98 (d, $J = 1.6$ Hz, 1H), 4.68 (s, 1H $'$), 3.41 – 3.30 (m, 1H $'$), 3.24 – 3.16 (m, 1H), 3.11 – 3.02 (m, 1H), 3.02 – 2.93 (m, 1H $'$), 2.79 – 2.68 (m, 1H $'$), 2.66 – 2.53 (m, 4H $'$ +3H), 2.22 – 2.10 (m, 1H), 1.87 – 1.79 (m, 1H), 1.56 (t, $J = 7.3$ Hz, 3H $'$), 1.10 (t, $J = 7.3$ Hz, 3H). **^{13}C NMR (101 MHz, CDCl_3)** δ 186.6, 186.5, 175.9, 172.8, 165.4, 164.9, 160.8, 160.4, 137.9, 137.6, 136.7, 136.1, 135.1, 134.4, 133.5, 133.5, 129.4, 128.9, 128.7, 128.7, 128.4, 125.2, 125.0, 118.9, 118.8, 61.9, 60.9, 58.8, 57.0, 45.0, 44.9, 22.5, 21.0, 14.7, 14.6, 9.5, 9.5. **HRMS (ESI+)**: Exact mass calculated for $\text{C}_{23}\text{H}_{22}\text{ClN}_2\text{O}_2$ $[\text{M} + \text{H}]^+$: 393.1364, found: 393.1367. The enantiomeric excess was determined by **HPLC** using a Chiralpak OZ-H column (hexane/*i*PrOH = 90:10, flow rate 1.0 mL/min, λ = 210 nm). Major diastereomer: t_r (S) = 26.3, t_r (R) = 33.2, 92% ee. Minor diastereomer: t_r (S) = 13.2, t_r (R) = 15.1, 88% ee.

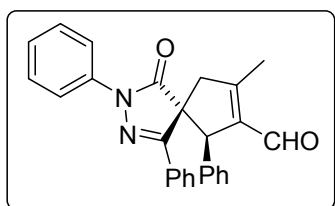
(5*R*/5*S*,6*S*)-6-(4-nitrophenyl)-1-ethyl-8-methyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7s) mixture of major and minor diastereomers



The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (4:1) as eluent to give **7s** as brown semisolid in 65% yield, 1.2:1 dr, as a mixture of diastereomers.

¹H NMR (400 MHz, CDCl₃) δ 10.12 (s, 1H), 10.07 (s, 1H), 8.14 – 8.07 (m, 4H), 7.90 – 7.84 (m, 2H), 7.54 – 7.49 (m, 2H), 7.43 (dd, J = 8.5, 7.6 Hz, 2H), 7.30 (d, J = 7.5 Hz, 2H), 7.26 – 7.20 (m, 1H), 7.19 – 7.15 (m, 2H), 7.15 – 7.09 (m, 3H), 4.89 (d, J = 1.6 Hz, 1H), 4.58 (s, 1H), 3.27 – 3.17 (m, 1H), 3.16 – 3.05 (m, 1H), 2.88 (dd, J = 18.3, 17.5 Hz, 2H), 2.57 (dq, J = 17.7, 7.3 Hz, 1H), 2.50 – 2.35 (m, 7H), 2.10 – 1.97 (m, 1H), 1.67 (dq, J = 17.5, 7.3 Hz, 1H), 1.39 (t, J = 7.3 Hz, 3H), 0.90 (t, J = 7.3 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 186.3, 186.2, 175.4, 172.4, 165.2, 164.2, 161.7, 161.5, 147.3, 147.3, 144.1, 143.6, 137.7, 137.4, 136.4, 135.7, 129.0, 129.0, 128.8, 128.3, 125.4, 125.2, 123.6, 123.4, 118.8, 118.7, 62.0, 60.7, 59.1, 56.8, 45.4, 45.1, 22.6, 21.0, 14.8, 14.7, 9.4, 9.4. **HRMS (ESI+)**: Exact mass calculated for C₂₃H₂₂N₃O₄ [M+H]⁺: 404.1605, found: 404.1603. The enantiomeric excess was determined by **HPLC** using a Chiralpak OZ-H column (hexane/iPrOH = 90:10, flow rate 1.0 mL/min, λ = 230 nm). Diastereomer 1: t_r (S) = 32.2, t_r (R) = 29.7, 55% ee. Diastereomer 2: t_r (S) = 70.9, t_r (R) = 104.8, 90% ee.

(5*R*,6*R*)-8-Methyl-4-oxo-1,3,6-triphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7t**) major diastereomer**

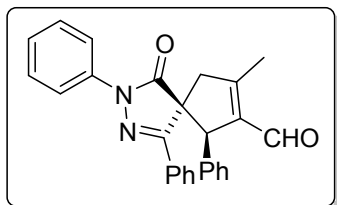


The crude product (7 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (10:1) as eluent to give **7t** as brown semisolid in 26% yield (13.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 10.14 (s, 1H), 7.86 – 7.80 (m, 2H), 7.52 – 7.47 (m, 3H), 7.38 – 7.09 (m, 8H), 7.02 – 6.99 (m, 2H), 5.07 (s, 1H), 3.29 (s, 2H), 2.46 (s, 3H) ppm. **¹³C NMR (151 MHz, CDCl₃)** δ = 187.07, 174.33, 160.85, 159.37, 137.09, 136.17, 135.93, 130.64, 129.62, 129.24 (2C), 128.60 (2C), 128.60 (2C), 127.99 (2C), 127.66, 125.99 (2C), 125.32, 119.53 (2C), 60.24, 59.96, 47.15, 14.86 ppm. **FT-IR (KBr)**: ν = 3064, 3028, 1718, 1670, 1640, 1595, 1497, 1389, 1326, 1311, 1240, 1183, 1129, 1075, 1018, 934, 866, 755, 698 cm⁻¹. **HRMS (ESI)** m/z calcd for for C₂₇H₂₃N₂O₂ [M + H]⁺ = 407.1754, found: 407.1755. [α]_D^{rt} = 0° (c = 0.440 in CHCl₃). **HPLC analysis ee (major diastereoisomer) =**

96%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 318$ nm, retention time: $t_{major} = 7.4$ min, $t_{minor} = 9.4$ min) at 25 °C.

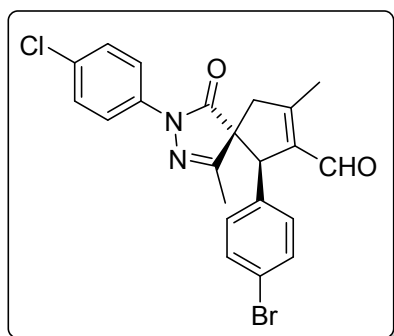
(5*S*,6*R*)-8-Methyl-4-oxo-1,3,6-triphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*t'*) *minor diastereomer*



The crude product (7 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (10:1) as eluent to give **7*t'*** as brown semisolid in 18% yield (9.0 mg).

¹H NMR (600 MHz, CDCl₃) $\delta = 10.09$ (s, 1H), 8.02 – 7.99 (m, 2H), 7.50 – 7.44 (m, 2H), 7.36 – 7.18 (m, 6H), 6.96 – 6.85 (m, 3H), 6.67 – 6.64 (m, 2H), 5.06 (s, 1H), 3.32 (q, $J = 19.0$ Hz, 2H), 2.46 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) $\delta = 187.14, 177.19, 160.14, 159.52, 137.88, 136.76, 135.50, 131.13, 129.95, 128.98$ (2C), 128.06 (2C), 127.70 (2C), 127.59 (2C), 127.22, 126.51 (2C), 125.54, 119.21 (2C), 61.60, 61.50, 47.38, 14.96 ppm. **FT-IR** (KBr): $\nu = 3064, 3028, 2923, 2851, 1709, 1673, 1637, 1598, 1500, 1491, 1428, 1320, 1305, 1290, 1260, 1242, 1180, 1135, 1099, 1078, 1030, 1021, 955, 911, 758, 731, 692$ cm⁻¹. **HRMS** (ESI) m/z calcd for C₂₇H₂₃N₂O₂ [M + H]⁺ = 407.1754, found: 407.1754. $[\alpha]_D^{25} = 0^\circ$ (c = 0.210 in CHCl₃). **HPLC analysis** *ee* (*minor diastereoisomer*) = 99%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, $\lambda = 318$ nm, retention time: $t_{major} = 14.4$ min, $t_{minor} = 17.3$ min) at 25 °C.

(5*R*,6*R*)-6-(4-Bromophenyl)-3-(4-chlorophenyl)-1,8-dimethyl-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*u*) *major diastereomer*

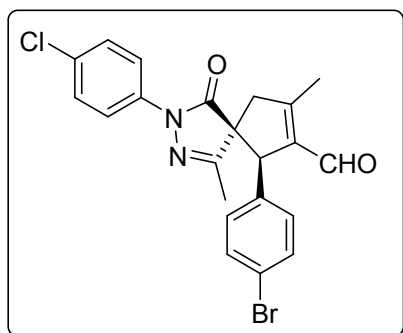


The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7*u*** as dark yellow semisolid in 76% yield (42.0 mg).

¹H NMR (600 MHz, CDCl₃) $\delta = 10.07$ (s, 1H), 7.84 (d, $J = 8.9$ Hz, 2H), 7.38 – 7.36 (m, 4H), 6.84 (d, $J = 8.4$ Hz, 2H), 4.75 (s, 1H), 2.99 (d, $J = 18.8$ Hz, 1H), 2.89 (d, $J = 18.8$ Hz, 1H), 2.39 (s, 3H), 1.52 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) $\delta = 186.59, 175.84, 161.25, 160.02, 136.46, 136.35, 135.67, 131.97$ (2C), 130.49, 129.22 (2C), 129.12 (2C), 121.98, 119.97 (2C), 61.78, 58.78, 45.04, 15.39, 14.87 ppm. **FT-IR** (KBr): $\nu = 3548, 3488, 3461, 3422, 2923, 2848, 2759, 1709, 1670, 1643, 1619, 1494, 1401, 1368, 1338, 1308, 1231, 1177, 1123, 1096, 1072, 1006, 967, 866, 830, 752, 626, 591$ cm⁻¹. **HRMS** (ESI) m/z calcd for

$C_{22}H_{19}BrClN_2O_2$ $[M + H] = 457.0313$, found: 457.0310. $[\alpha]_D^{rt} = -277.8^\circ$ ($c = 0.360$ in $CHCl_3$). **HPLC analysis** *ee* (major diastereoisomer) = 87%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 70:30, 1.0 mL/min, $\lambda = 254$ nm, retention time: $t_{major} = 13.0$ min, $t_{minor} = 31.0$ min) at 25 °C.

(5*S*,6*R*)-6-(4-Bromophenyl)-3-(4-chlorophenyl)-1,8-dimethyl-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7u') minor diastereomer

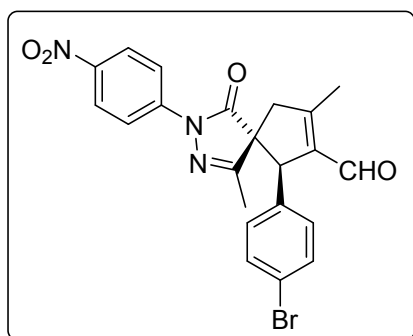


The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2:1) as eluent to give **7u'** as dark brown semisolid in 9% yield (5.0 mg).

¹H NMR (600 MHz, $CDCl_3$) $\delta = 10.03$ (s, 1H), 7.45 (d, $J = 8.8$ Hz, 2H), 7.34 (d, $J = 8.4$ Hz, 2H), 7.25 (d, $J = 8.8$ Hz, 2H), 6.86 (d, $J = 8.4$ Hz, 2H), 4.47 (s, 1H), 3.15 (d, $J = 18.9$

Hz, 1H), 2.78 (d, $J = 18.9$ Hz, 1H), 2.40 (s, 3H), 2.18 (s, 3H) ppm. **¹³C NMR** (151 MHz, $CDCl_3$) $\delta = 186.51$, 172.68, 161.95, 160.65, 136.65, 136.05, 134.80, 131.47 (2C), 130.31, 129.78 (2C), 128.93 (2C), 121.98, 120.07 (2C), 60.96, 57.04, 44.95, 14.77, 13.79 ppm. **FT-IR** (KBr): $\nu = 3551$, 3467, 3408, 2923, 2848, 1715, 1709, 1673, 1643, 1619, 1512, 1494, 1434, 1410, 1365, 1308, 1245, 1222, 1180, 1123, 1096, 1078, 1012, 964, 869, 827 cm^{-1} . **HRMS** (ESI) m/z calcd for $C_{22}H_{19}BrClN_2O_2$ $[M + H] = 457.0313$, found: 457.0311. $[\alpha]_D^{rt} = -14.8^\circ$ ($c = 0.640$ in $CHCl_3$). **HPLC analysis** *ee* (minor diastereoisomer) = 87%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 70:30, 1.0 mL/min, $\lambda = 254$ nm, retention time: $t_{major} = 8.3$ min, $t_{minor} = 14.2$ min) at 25 °C.

(5*R*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-3-(4-nitrophenyl)-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7v) major diastereomer

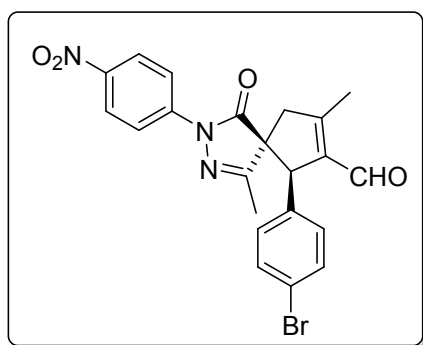


The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (1:1) as eluent to give **7v** as pale brown solid in 62% yield (35.0 mg), **M. P.** = 225.1 °C (ethyl acetate/n-hexane).

¹H NMR (600 MHz, $CDCl_3$) $\delta = 10.08$ (s, 1H), 8.28 (d, $J = 9.2$ Hz, 2H), 8.12 (d, $J = 9.2$ Hz, 2H), 7.39 (d, $J = 8.4$ Hz, 2H), 6.85 (d, $J = 8.4$ Hz, 2H), 4.76 (s, 1H), 2.97 (q, $J = 18.9$ Hz, 2H), 2.41 (s, 3H), 1.53

(s, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ = 186.45, 176.52, 162.24, 159.74, 144.24, 142.86, 136.32, 135.44, 132.10 (2C), 129.22 (2C), 125.06 (2C), 122.19, 118.12 (2C), 61.86, 58.91, 45.06, 15.48, 14.85 ppm. **FT-IR** (KBr): ν = 3482, 3422, 3120, 2920, 2845, 1718, 1661, 1619, 1592, 1521, 1500, 1425, 1401, 1341, 1299, 1260, 1228, 1177, 1123, 1117, 1069, 1009, 967, 857, 809, 749 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{22}\text{H}_{19}\text{BrN}_3\text{O}_4$ [$\text{M} + \text{H}$] = 468.0553, found: 468.0553. $[\alpha]_{\text{D}}^{\text{rt}}$ = -329.1° (c = 0.585 in CHCl_3). **HPLC analysis** *ee* (*major diastereoisomer*) = 92%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 60:40, 1.0 mL/min, λ = 202 nm, retention time: t_{major} = 27.6 min, t_{minor} = 54.6 min) at 25 $^\circ\text{C}$.

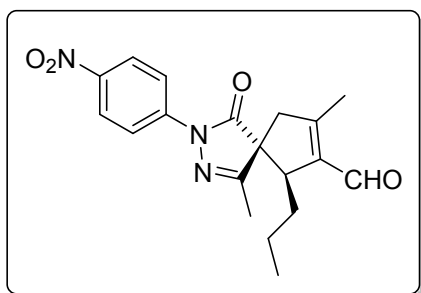
(5*S*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-3-(4-nitrophenyl)-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7v') *minor diastereomer*



The crude product (3 days reaction time) was purified by silica gel flash chromatography with *n*-hexane/ethyl acetate (1:1) as eluent to give **7v'** as dark brown semisolid in 17% yield (10.0 mg).

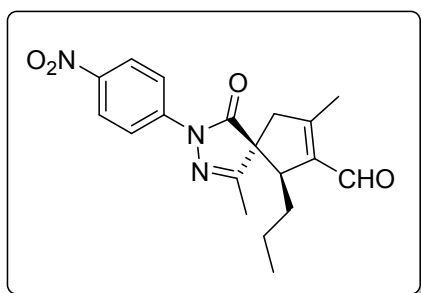
^1H NMR (600 MHz, CDCl_3) δ = 10.04 (s, 1H), 8.16 (d, J = 9.3 Hz, 2H), 7.77 (d, J = 9.3 Hz, 2H), 7.34 (d, J = 8.4 Hz, 2H), 6.86 (d, J = 8.4 Hz, 2H), 4.49 (s, 1H), 3.18 (d, J = 19.0 Hz, 1H), 2.82 (d, J = 19.0 Hz, 1H), 2.41 (s, 3H), 2.22 (s, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ = 186.17, 173.06, 162.82, 160.13, 143.83, 142.32, 136.34, 134.32, 131.36 (2C), 129.51 (2C), 124.68 (2C), 121.95, 117.74 (2C), 60.97, 57.12, 44.75, 14.55, 13.66 ppm. **FT-IR** (KBr): ν = 3551, 3482, 3449, 3428, 3120, 2920, 2848, 1718, 1667, 1634, 1619, 1595, 1515, 1500, 1422, 1401, 1332, 1299, 1219, 1177, 1114, 1072, 1009, 964, 851, 788, 755 cm^{-1} . **HRMS** (ESI) m/z calcd for $\text{C}_{22}\text{H}_{19}\text{BrN}_3\text{O}_4$ [$\text{M} + \text{H}$] = 468.0553, found: 468.0552. $[\alpha]_{\text{D}}^{\text{rt}}$ = $+11.0^\circ$ (c = 0.725 in CHCl_3). **HPLC analysis** *ee* (*minor diastereoisomer*) = 81%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 60:40, 1.0 mL/min, λ = 190 nm, retention time: t_{major} = 22.7 min, t_{minor} = 41.9 min) at 25 $^\circ\text{C}$.

(5*R*/5*S*,6*R*)-1,8-Dimethyl-3-(4-nitrophenyl)-4-oxo-6-propyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7w) *mixture of diastereomers 1.7:1*



The crude product (3 days reaction time) was purified by silica gel flash chromatography with n-hexane/ethyl acetate (1.5:1) as eluent to give **7w** as a mixture of diastereomers (*dr* 1.7:1) and as pale yellow solid in 91% yield (39.0 mg), **M. P.** = 150.6 °C (ethyl acetate/n-hexane).

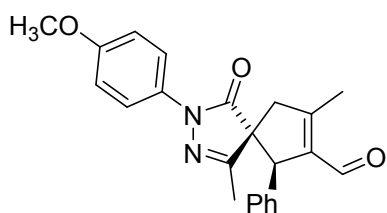
¹H NMR major diastereomer (600 MHz, CDCl₃) δ = 10.05 (s, 1H), 8.29 – 8.26 (m, 2H), 8.16 – 8.13 (m, 2H), 3.63 – 3.60 (m, 1H), 3.02 (d, *J* = 18.4 Hz, 1H), 2.59 (d, *J* = 18.4 Hz, 1H), 2.32 – 2.27 (m, 1H), 2.23 (s, 3H), 2.15 (s, 3H), 1.26 – 1.11 (m, 3H), 0.81 (t, *J* = 7.1 Hz, 3H) ppm. **¹³C NMR** major diastereomer (151 MHz, CDCl₃) δ = 187.64, 176.44, 163.51, 157.50, 144.15, 143.13, 137.87, 125.08 (2C), 118.04 (2C), 61.51, 54.19, 46.44, 30.84, 21.02, 16.08, 14.51, 14.15 ppm. **HPLC analysis** *ee* (major diastereoisomer) = 89%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, λ = 190 nm, retention time: *t*_{major} = 11.5 min, *t*_{minor} = 13.0 min) at 25 °C.



¹H NMR minor diastereomer (600 MHz, CDCl₃) δ = 10.01 (s, 1H), 8.29 – 8.26 (m, 2H), 8.16 – 8.13 (m, 2H), 3.27 – 3.26 (m, 1H), 3.15 (d, *J* = 18.9 Hz, 1H), 2.64 (d, *J* = 18.9 Hz, 1H), 2.24 (s, 3H), 2.05 (s, 3H), 1.86 – 1.80 (m, 1H), 1.76 – 1.70 (m, 1H), 1.05 – 0.97 (m, 2H), 0.83 (t, *J* = 7.4 Hz, 3H) ppm. **¹³C NMR** minor diastereomer (151 MHz, CDCl₃) δ = 187.06, 174.68, 164.59, 157.50, 144.02, 143.13, 139.11, 125.08 (2C), 117.98 (2C), 58.72, 52.00, 46.25, 30.84, 21.87, 14.31, 14.06, 13.70 ppm. **HPLC analysis** *ee* (minor diastereoisomer) = 88%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 90:10, 1.0 mL/min, λ = 190 nm, retention time: *t*_{minor} = 15.2 min, *t*_{major} = 16.3 min) at 25 °C.

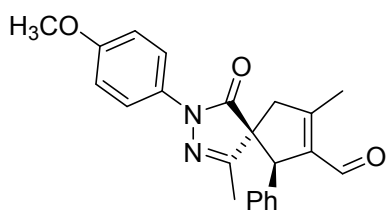
FT-IR (KBr): ν = 3554, 3479, 3422, 3405, 3120, 2953, 2929, 2872, 2848, 2762, 1721, 1670, 1637, 1622, 1592, 1518, 1497, 1425, 1401, 1335, 1299, 1228, 1180, 1129, 1114, 1051, 1000, 967, 854, 752, 689, 621 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₁₉H₂₂N₃O₄ [M + H] = 356.1605, found: 356.1608. [α]_D^{rt} = -20.7° (c = 0.435 in CHCl₃).

(5R,6R)-2-(4-methoxyphenyl)-4,8-dimethyl-6-phenyl-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7x) major diastereomer



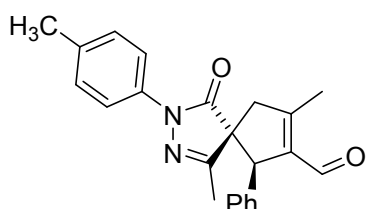
Pale brown solid, yield 56 %, ee 69 %; The ee was determined by HPLC analysis using Chiralpak IA column (90/10 heptane/i-PrOH, flow rate 1.0 ml/min; $\lambda = 190$ nm, 25 °C, $t_{\text{major}} = 18.2$ min; $t_{\text{minor}} = 32.3$ min.); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 10.07 (s, 1H), 7.78 – 7.71 (m, 2H), 7.28 – 7.21 (m, 3H), 7.01 – 6.96 (m, 2H), 6.96 – 6.90 (m, 2H), 4.81 (d, $J = 1.5$ Hz, 1H), 3.82 (s, 3H), 3.01 – 2.82 (m, 2H), 2.39 (d, $J = 1.7$ Hz, 3H), 1.43 (s, 3H) ppm. $^{13}\text{C NMR}$ (101 MHz, CDCl_3) $\delta = 186.8, 175.6, 161.1, 159.4, 157.0, 136.6, 136.5, 131.2, 128.6$ (2C), 127.8 (2C), 127.4 (2C), 120.6 (2C), 114.0, 61.5, 59.1, 55.5, 44.8, 15.0, 14.7 ppm. **IR (KBr):** $\nu = 2944, 2857, 2833, 1700, 1664, 1509, 1296, 1245, 1180, 1168, 1126, 1075, 1033$ cm^{-1} . $[\alpha]_{\text{D}}^{25} = -267,4^\circ$, (0.92, CHCl_3); **HRMS** (ESI) m/z calcd for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}_3$ $[\text{M}+\text{Na}]^+$ 397.1522, found 397.1522.

(5S,6R)-2-(4-methoxyphenyl)-4,8-dimethyl-6-phenyl-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7x') minor diastereomer



Pale brown semi-solid, yield 25 %, ee 94 %; The ee was determined by HPLC analysis using Chiralpak IA column (90/10 heptane/i-PrOH, flow rate 1.0 ml/min; $\lambda = 190$ nm, 25 °C, $t_{\text{major}} = 11.6$ min; $t_{\text{minor}} = 22.9$ min.); $^1\text{H NMR}$ (400 MHz, CDCl_3) $\delta = 10.05$ (s, 1H), 7.29 – 7.27 (m, 2H), 7.25 – 7.19 (m, 3H), 7.04 – 6.98 (m, 2H), 6.81 – 6.76 (m, 2H), 4.54 (s, 1H), 3.75 (s, 3H), 3.19 – 3.10 (m, 1H), 2.81 – 2.72 (m, 1H), 2.39 (d, $J = 1.5$ Hz, 3H), 2.19 (s, $J = 6.8$ Hz, 3H) ppm. $^{13}\text{C NMR}$ (101 MHz, CDCl_3) $\delta = 186.7, 172.5, 161.3, 160.3, 156.9, 136.6, 135.6, 130.8, 128.1$ (2C), 128.0 (2C), 127.7, 121.0 (2C), 113.8 (2C), 61.0, 57.5, 55.4, 44.6, 14.7, 13.7 ppm. **IR (KBr):** $\nu = 2929, 2851, 1703, 1670, 1616, 1515, 1431, 1365, 1308, 1254, 1219, 1183, 1126, 1084$ cm^{-1} . $[\alpha]_{\text{D}}^{25} = +33,9^\circ$, (0.59, CHCl_3); **HRMS** (ESI) m/z calcd for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}_3$ $[\text{M}+\text{Na}]^+$ 397.1522, found 397.1522.

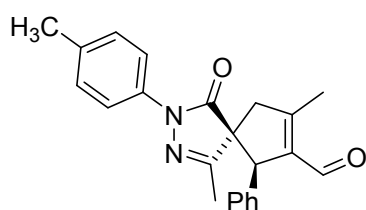
(5R,6R)-4,8-dimethyl-6-phenyl-2-(p-tolyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7y) major diastereomer



Pale brown solid, yield 50 %, ee 91 %; The ee was determined by HPLC analysis using Chiralpak IA column (80/20 heptane/i-

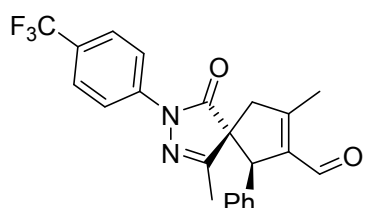
PrOH, flow rate 1.0 ml/min; $\lambda = 190$ nm, 25 °C, $t_{\text{major}} = 14.3$ min; $t_{\text{minor}} = 23.0$ min.); **¹H NMR** (400 MHz, CDCl₃) $\delta = 10.07$ (s, 1H), 7.75 – 7.71 (m, 2H), 7.26 – 7.18 (m, 5H), 7.01 – 6.96 (m, 2H), 4.81 (d, $J = 1.6$ Hz, 1H), 3.01 – 2.86 (m, 2H), 2.39 (d, $J = 1.7$ Hz, 3H), 2.36 (s, 3H), 1.43 (s, 3H) ppm. **¹³C NMR** (101 MHz, CDCl₃) $\delta = 186.8, 175.9, 161.1, 159.3, 136.7, 136.5, 135.42, 134.9, 129.4$ (2C), 128.7 (2C), 127.8, 127.5 (2C), 118.9 (2C), 61.6, 59.1, 44.9, 21.0, 15.0, 14.8 ppm. **IR (KBr):** $\nu = 2998, 2926, 2851, 1712, 1661, 1631, 1616, 1512, 1368, 1344, 1311, 1260, 1231, 1180, 1120$ cm⁻¹. **$[\alpha]^{25}_{\text{D}}$** = -157.1 °, (0.35, CHCl₃); **HRMS** (ESI) m/z calcd for C₂₃H₂₂N₂O₂ [M+Na]⁺ 381.1574, found 381.1574.

(5*S*,6*R*)-4,8-dimethyl-6-phenyl-2-(*p*-tolyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7y') minor diastereomer



Pale brown semi-solid, yield 17 %, ee 97 %; The ee was determined by HPLC analysis using Chiralpak IA column (80/20 heptane/*i*-PrOH, flow rate 1.0 ml/min; $\lambda = 190$ nm, 25 °C, $t_{\text{major}} = 8.9$ min; $t_{\text{minor}} = 15.2$ min.); **¹H NMR** (400 MHz, CDCl₃) $\delta = 10.06$ (d, $J = 6.4$ Hz, 1H), 7.32 – 7.28 (m, 2H), 7.25 – 7.18 (m, 3H), 7.06 (d, $J = 8.3$ Hz, 2H), 7.03 – 6.98 (m, 2H), 4.54 (s, 1H), 3.25 – 3.09 (m, 1H), 2.83 – 2.70 (m, 1H), 2.40 (d, $J = 1.4$ Hz, 3H), 2.28 (s, 3H), 2.20 (s, 3H) ppm. **¹³C NMR** (400 MHz, CDCl₃) $\delta = 186.7, 172.6, 161.4, 160.2, 136.7, 135.6, 135.0, 134.6, 129.1$ (2C), 128.1 (2C), 127.9 (2C), 127.8, 119.0 (2C), 61.0, 57.5, 44.7, 20.9, 14.7, 13.7 ppm. **IR (KBr):** $\nu = 2920, 2854, 1709, 1673, 1637, 1613, 1509, 1434, 1368, 1311, 1251, 1123$ cm⁻¹. **$[\alpha]^{25}_{\text{D}}$** = 17.1 °, (0.35, CHCl₃); **HRMS** (ESI) m/z calcd for C₂₃H₂₂N₂O₂ [M+Na]⁺ 381.1574, found 381.1574.

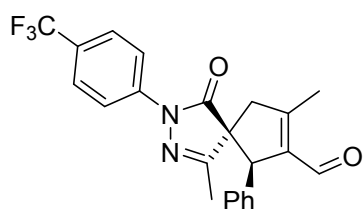
(5*R*,6*R*)-4,8-dimethyl-6-phenyl-2-(4-(trifluoromethyl)phenyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7z) major diastereomer



Pale brown solid, yield 43 %, ee 89 %; The ee was determined by HPLC analysis using Chiralpak IA column (90/10 heptane/*i*-PrOH, flow rate 1.0 ml/min; $\lambda = 190$ nm, 25 °C, $t_{\text{major}} = 13.6$ min; $t_{\text{minor}} = 22.0$ min.); **¹H NMR** (400 MHz, CDCl₃) $\delta = 10.07$ (s, $J = 8.1$ Hz, 1H), 8.05 (d, $J = 8.6$ Hz, 2H), 7.65 (d, $J = 8.7$ Hz, 2H), 7.28 – 7.24 (m, 3H), 7.02 – 6.94 (m, 2H), 4.81 (d, $J = 1.4$ Hz, 1H), 2.95 (d, $J = 1.2$

Hz, 2H), 2.41 (d, $J = 1.5$ Hz, 3H), 1.44 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) $\delta = 186.6$, 176.4, 161.9, 159.1, 140.6, 136.5, 136.4, 128.8 (2C), 128.0, 127.4 (2C), 126.6 (q, $J = 32.7$ Hz), 126.1 (d, $J = 3.6$ Hz, 2C), 124.1 (q, $J = 271.6$ Hz), 118.2 (2C), 61.8, 59.2, 44.8, 15.0, 14.7 ppm. ^{19}F NMR (376 MHz, CDCl_3) $\delta = -62.15$ ppm. IR (KBr): $\nu = 2925, 2857, 1721, 1670, 1616, 1524, 1425, 1365, 1326, 1168, 1123, 1069, 1018$ cm^{-1} . ; $[\alpha]^{25}_{\text{D}} = 209.8$ °, (1.03, CHCl_3); HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{19}\text{F}_3\text{N}_2\text{O}_2$ $[\text{M}+\text{Na}]^+$ 435.1291, found 435.1291.

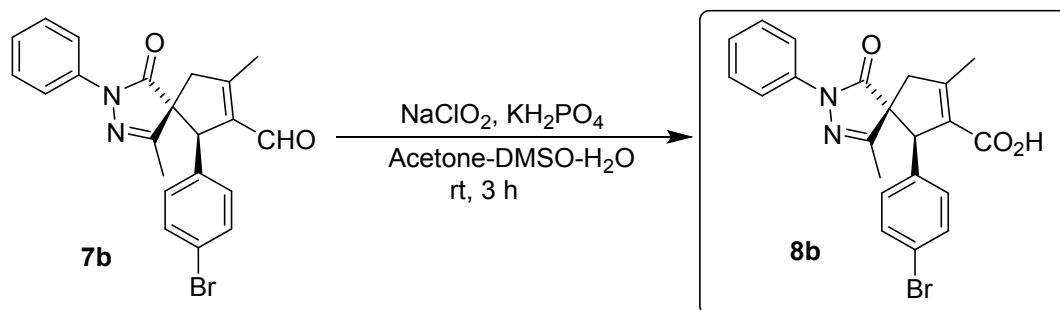
(5*S*,6*R*)-4,8-dimethyl-6-phenyl-2-(4-(trifluoromethyl)phenyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7*z'*) *minor diastereomer*



Pale brown semi-solid, yield 27 %, ee 94 %; The ee was determined by HPLC analysis using Chiralpak IA column (90/10 heptane/*i*-PrOH, flow rate 1.0 ml/min; $\lambda = 190$ nm, 25 °C, $t_{\text{major}} = 10.7$ min; $t_{\text{minor}} = 17.2$ min.); ^1H NMR (400 MHz, CDCl_3) $\delta = 10.06$ (s, 1H), 7.64 (d, $J = 8.6$ Hz, 2H), 7.51 (d, $J = 8.6$ Hz, 2H), 7.25 – 7.16 (m, 3H), 7.02 – 6.96 (m, 2H), 4.55 (s, 1H), 3.23 – 3.11 (m, 1H), 2.86 – 2.74 (m, 1H), 2.41 (d, $J = 1.5$ Hz, 3H), 2.22 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) $\delta = 186.6, 173.1, 162.3, 159.9, 140.2, 136.6, 135.4, 128.2$ (2C), 127.9, 127.9 (2C), 126.4 (q, $J = 32.7$ Hz), 125.9 (d, $J = 2.9$ Hz, 2C), 124.1 (q, $J = 271.6$ Hz), 118.1 (2C), 61.3, 57.8, 44.6, 14.6, 13.7 ppm. ^{19}F NMR (376 MHz, CDCl_3) $\delta = -62.19$ ppm. IR (KBr): $\nu = 2925, 2854, 1721, 1673, 1613, 1518, 1325, 1305, 1260, 1168, 1120, 1063, 1018$ cm^{-1} . $[\alpha]^{25}_{\text{D}} = 26.0$ °, (1.00, CHCl_3); HRMS (ESI) m/z calcd for $\text{C}_{23}\text{H}_{19}\text{F}_3\text{N}_2\text{O}_2$ $[\text{M}+\text{Na}]^+$ 435.1291, found 435.1288.

Derivatization of the Spirocyclic Compounds

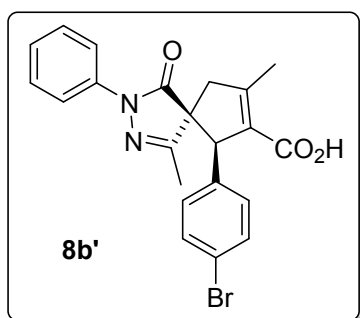
Synthesis of (5*R*,6*S*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carboxylic acid (**8b**)



Compound **7b** (51.5 mg, 0.12 mmol) was taken in 4 ml acetone and to it, 2 ml DMSO was added. To this reaction mixture, NaClO₂ (54.0 mg, 0.6 mmol) and KH₂PO₄ (82.0 mg, 0.6 mmol) dissolved in 4 ml H₂O was added dropwise. The reaction mixture was stirred at room temperature for 3 hours. Then, the solvent was removed under reduced pressure. The crude was extracted with ethyl acetate (4 × 25 ml) and the combined organic layer was washed with H₂O (1 × 50 ml) and brine solution (1 × 50 ml). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under vacuo. The crude product was purified by silica gel flash chromatography with CH₂Cl₂/MeOH (20:1) as eluent to give **8b** as white solid in 54% yield (29.0 mg). **M. P.** = 232.2 °C (diethyl ether/n-heptane).

¹H NMR (600 MHz, CDCl₃) δ = 7.87 – 7.84 (m, 2H), 7.42 – 7.38 (m, 4H), 7.23 – 7.18 (m, 1H), 6.92 (d, *J* = 8.1 Hz, 2H), 4.79 (s, 1H), 2.97 (d, *J* = 18.4 Hz, 1H), 2.83 (d, *J* = 18.4 Hz, 1H), 2.32 (s, 3H), 1.54 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 175.91, 167.89, 161.22, 157.07, 137.90, 136.86, 131.98 (2C), 129.07 (2C), 128.92 (2C), 126.75, 125.39, 121.81, 118.98 (2C), 61.78, 60.17, 45.23, 16.66, 15.35 ppm. **FT-IR** (KBr): ν = 3554, 3476, 3443, 3422, 3408, 3243, 3067, 2965, 2920, 2854, 2603, 2382, 2092, 1862, 1700, 1676, 1619, 1589, 1491, 1422, 1401, 1368, 1308, 1263, 1240, 1222, 1129, 1090, 1072, 1009, 994, 964, 914, 833, 761, 692 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₂H₂₀BrN₂O₃ [M + H] = 439.0652, found: 439.0655. **[α]_D^{rt}** = -345.7° (c = 0.050 in CHCl₃). **HPLC analysis** *ee* (major diastereoisomer) = 90%, (Daicel Chiralcel IC column, heptane/*iso*-propanol, 70:30, 1.0 mL/min, λ = 202 nm, retention time: *t*_{minor} = 5.5 min, *t*_{major} = 10.2 min) at 25 °C.

Synthesis of (5*S*,6*S*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carboxylic acid (**8b'**)

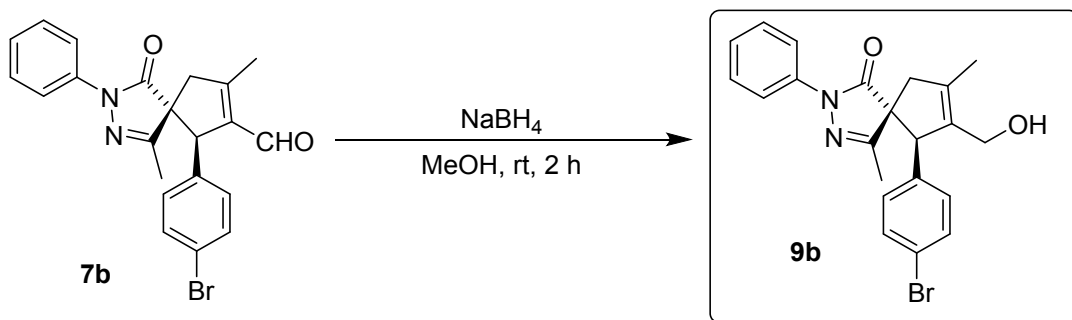


Reaction procedure same as **8b**. The crude product was purified by silica gel flash chromatography with CH₂Cl₂/ MeOH (20:1) as eluent to give **8b'** as white solid in 68% yield (24.0 mg).

M. P. = 235.6 °C (diethyl ether/n-heptane).

¹H NMR (600 MHz, CDCl₃) δ = 7.52 – 7.49 (m, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.31 – 7.28 (m, 2H), 7.13 – 7.09 (m, 1H), 6.91 (d, *J* = 8.1 Hz, 2H), 4.41 (s, 1H), 3.15 (d, *J* = 18.7 Hz, 1H), 2.67 (d, *J* = 18.7 Hz, 1H), 2.34 (s, 3H), 2.18 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 172.57, 169.31, 162.18, 158.40, 137.56, 135.95, 131.50 (2C), 129.73 (2C), 128.88 (2C), 126.95, 125.19, 121.82, 119.03 (2C), 60.49, 58.50, 45.17, 16.71, 13.79 ppm. **FT-IR** (KBr): ν = 3560, 3494, 3479, 3411, 3061, 2920, 2588, 1945, 1894, 1712, 1685, 1619, 1595, 1503, 1488, 1434, 1410, 1365, 1308, 1257, 1228, 1216, 1120, 1069, 1009, 857, 824, 812, 755, 692, 621 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₂H₂₀BrN₂O₃ [M + H] = 439.0652, found: 439.0654. [α]_D^{rt} = -72.7° (c = 0.110 in CHCl₃). **HPLC analysis** *ee* (minor diastereoisomer) = 78%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 40:60, 0.5 mL/min, λ = 198 nm, retention time: *t*_{major} = 11.6 min, *t*_{minor} = 14.1 min) at 39 °C.

Synthesis of (5*R*,6*R*)-6-(4-Bromophenyl)-7-(hydroxymethyl)-4,8-dimethyl-2-phenyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (**9b**)

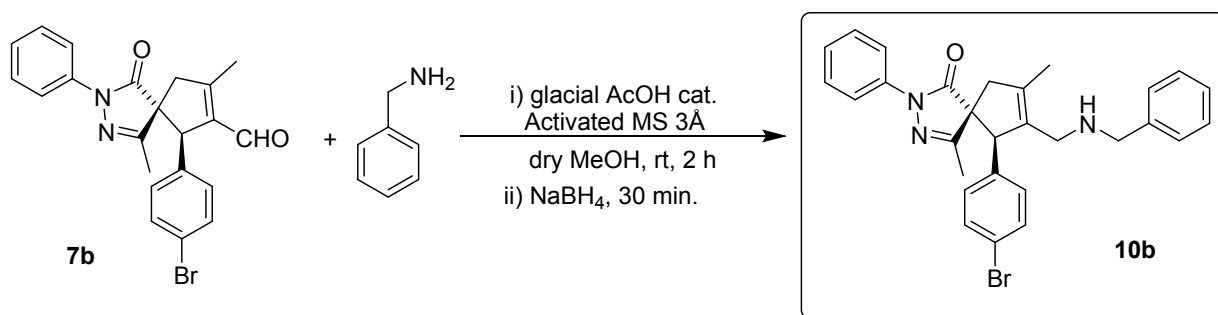


Compound **7b** (40.0 mg, 0.094 mmol) and NaBH₄ (7.1 mg, 0.188 mmol) were taken in 2 ml MeOH and the reaction mixture was stirred at room temperature for 2 hours. Then, the solvent was removed under reduced pressure. The crude was extracted with ethyl acetate (3 × 25 ml) and the combined organic layer was washed with H₂O (1 × 50 ml) and brine solution (1 × 50 ml). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under vacuo. The crude product was purified by silica gel flash chromatography with *n*-

hexane/ethyl acetate (1.5:1) as eluent to give **9b** as pale yellow semisolid in 78% yield (31.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 7.87 – 7.85 (m, 2H), 7.42 – 7.38 (m, 4H), 7.20 – 7.17 (m, 1H), 6.98 (d, *J* = 8.3 Hz, 2H), 4.58 (s, 1H), 4.39 (d, *J* = 12.5 Hz, 1H), 4.02 (d, *J* = 12.5 Hz, 1H), 2.74 (q, *J* = 16.8 Hz, 2H), 1.96 (s, 3H), 1.51 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 176.86, 161.97, 138.08, 137.62, 136.66, 134.09, 132.03 (2C), 130.21 (2C), 129.00 (2C), 125.19, 121.90, 118.97 (2C), 62.41, 60.98, 57.39, 43.78, 15.43, 14.28 ppm. **FT-IR** (KBr): ν = 3482, 3419, 2923, 1706, 1637, 1619, 1589, 1500, 1488, 1395, 1368, 1311, 1126, 1075, 1012, 842, 761, 689 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₂H₂₁BrN₂NaO₂ [*M* + Na] = 447.0679, found: 447.0675. [*α*]_D^{rt} = -286.9° (*c* = 0.420 in CHCl₃). **HPLC analysis** *ee* (*major diastereoisomer*) = 84%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 95:5, 1.0 mL/min, λ = 194 nm, retention time: *t*_{major} = 20.9 min, *t*_{minor} = 24.4 min) at 25 °C.

Synthesis of (5*R*,6*R*)-7-((Benzylamino)methyl)-6-(4-bromophenyl)-4,8-dimethyl-2-phenyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one⁶ (**10b**)



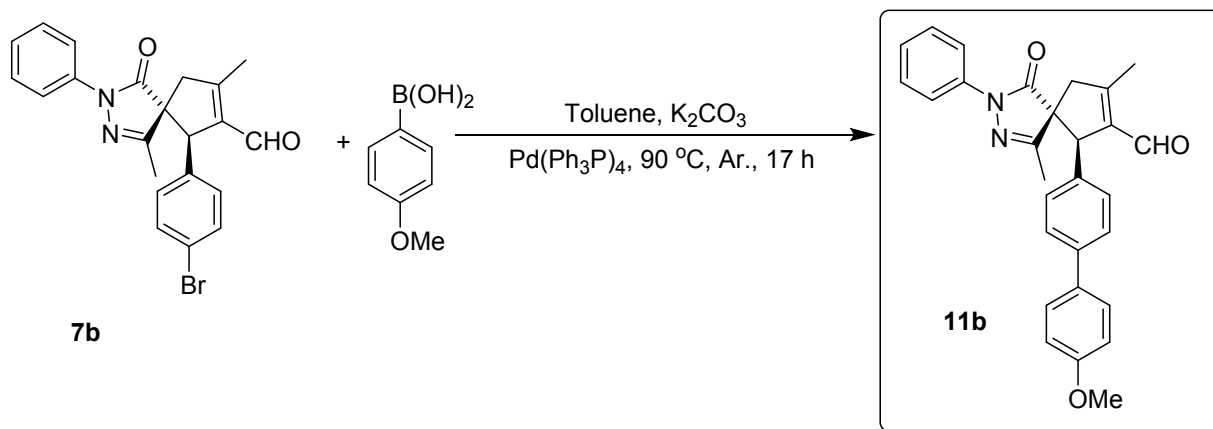
Compound **7b** (100.0 mg, 0.24 mmol) and benzyl amine (38.6 mg, 0.36 mmol) were taken in a flask and to it catalytic amount of glacial AcOH and Molecular sieve 3 Å were added. Then, to the reaction mixture 2 ml dry MeOH was added. The reaction mixture was stirred at room temperature under argon atmosphere for 2 hours. After complete disappearance of the starting aldehyde as indicated by TLC, the reaction mixture was cooled to 0 °C and to it NaBH₄ (18 mg, 0.48 mmol) was added. The reaction mixture was further stirred at room temperature for 30 minutes under argon atmosphere. Then, the solvent was removed under reduced pressure. The crude was extracted with ethyl acetate (3 × 25 ml) and the combined organic layer was washed with H₂O (1 × 50 ml) and brine solution (1 × 50 ml). The organic layer was dried over anhyd. Na₂SO₄ and the solvent was removed under vacuo. The crude product was purified by silica gel flash chromatography with *n*-

⁶ Abdel-Magid, A. F.; Carson, K. G.; Harris, B. D.; Maryanoff, C. A.; Shah, R. D. *J. Org. Chem.*, **1996**, *61*, 3849–3862.

hexane/ethyl acetate (1:1) as eluent to give **10b** as dark yellow semisolid in 74% yield (91.0 mg).

¹H NMR (600 MHz, CDCl₃) δ = 7.89 – 7.87 (m, 2H), 7.41 – 7.38 (m, 4H), 7.25 – 7.17 (m, 6H), 6.97 (d, *J* = 7.1 Hz, 2H), 4.58 (s, 1H), 3.79 (d, *J* = 13.3 Hz, 1H), 3.67 (d, *J* = 13.3 Hz, 1H), 3.48 (d, *J* = 13.2 Hz, 1H), 3.09 (d, *J* = 13.2 Hz, 1H), 2.78 (d, *J* = 16.6 Hz, 1H), 2.67 (d, *J* = 16.6 Hz, 1H), 1.86 (s, 3H), 1.52 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 176.94, 162.08, 140.31, 138.20, 136.90, 136.08, 133.36, 131.91 (2C), 130.30 (2C), 128.98 (2C), 128.41 (2C), 128.21 (2C), 126.95, 125.05, 121.69, 118.91 (2C), 62.45, 61.49, 52.96, 44.28, 43.71, 15.48, 14.25 ppm. **FT-IR** (KBr): ν = 3446, 3061, 3025, 2920, 2905, 2836, 1703, 1646, 1625, 1601, 1503, 1488, 1437, 1395, 1362, 1311, 1299, 1123, 1102, 1072, 1009, 979, 911, 839, 758, 689 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₉H₂₉BrN₃O [M + H] = 514.1489, found: 514.1484. **[α]_D^{rt}** = -217.6° (c = 0.710 in CHCl₃). **HPLC analysis** *ee* = 88%, (Daicel Chiracel IC column, heptane/*iso*-propanol, 98:2, 1.0 mL/min, λ = 190 nm, retention time: *t*_{minor} = 14.2 min, *t*_{major} = 16.0 min) at 25 °C.

Synthesis of (5*R*,6*R*)-6-(4'-Methoxy-[1,1'-biphenyl]-4-yl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde⁷ (**11b**)



Compound **7b** (50.0 mg, 0.12 mmol) and 4-Methoxyphenylboronic acid (36.5 mg, 0.24 mmol) were taken in 2 ml toluene and to this reaction mixture, K₂CO₃ (33.0 mg, 0.24 mmol) was added. The reaction mixture was degassed with argon for 10 minutes and to it Pd(Ph₃P)₄ (7 mg, 0.006 mmol) was added. The reaction mixture was again degassed with argon. Then, the reaction mixture was allowed to stir at 90 °C for 17 hours under argon atmosphere. The crude product was purified by silica gel flash chromatography with n-hexane/ethyl acetate (2.5:1) as eluent to give **11b** as dark yellow semisolid in 81% yield (44.0 mg).

⁷ Shieh, W. C.; Carlson, J. A. *J. Org. Chem.*, **1992**, *57*, 379–381.

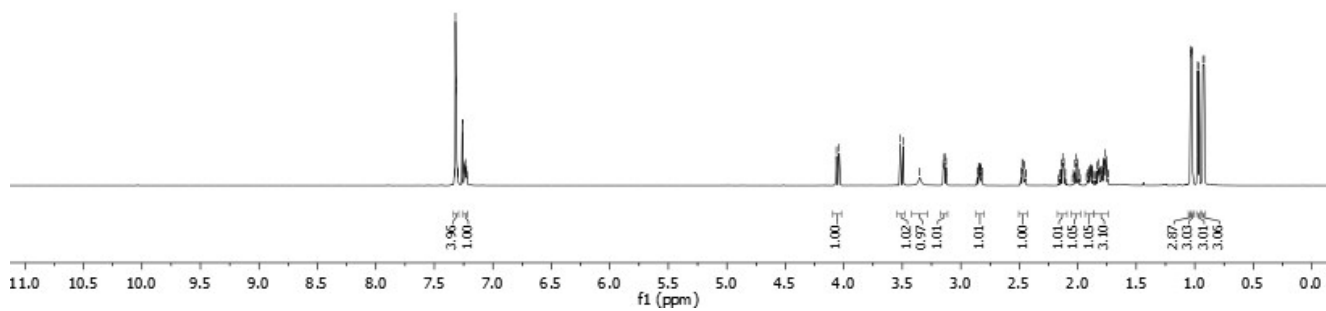
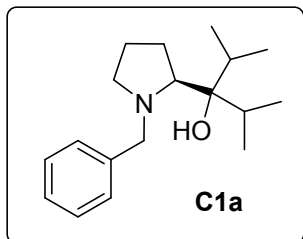
¹H NMR (600 MHz, CDCl₃) δ = 10.10 (s, 1H), 7.89 – 7.88 (m, 2H), 7.48 (d, *J* = 7.5 Hz, 2H), 7.45 – 7.40 (m, 4H), 7.22 – 7.19 (m, 1H), 7.03 (d, *J* = 6.7 Hz, 2H), 6.95 (d, *J* = 7.7 Hz, 2H), 4.86 (s, 1H), 3.84 (s, 3H), 2.96 (q, *J* = 19.0 Hz, 2H), 2.41 (s, 3H), 1.51 (s, 3H) ppm. **¹³C NMR** (151 MHz, CDCl₃) δ = 187.02, 176.23, 161.45, 159.50, 159.38, 140.41, 138.02, 136.73, 135.09, 133.08, 129.06 (2C), 128.15 (2C), 128.01 (2C), 127.00 (2C), 125.31, 119.00 (2C), 114.35 (2C), 61.93, 59.00, 55.50, 45.13, 15.36, 14.92 ppm. **FT-IR** (KBr): ν = 3025, 3007, 2917, 2845, 1709, 1667, 1607, 1598, 1500, 1437, 1428, 1401, 1365, 1308, 1245, 1180, 1120, 1039, 827, 758, 686 cm⁻¹. **HRMS** (ESI) *m/z* calcd for C₂₉H₂₆N₂NaO₃ [M + Na] = 473.1836, found: 473.1832. **[α]_D^{rt}** = -324.5° (c = 0.245 in CHCl₃). **HPLC analysis** *ee* (*major diastereoisomer*) = 78%, (Daicel Chiracel IA column, heptane/*iso*-propanol, 80:20, 1.0 mL/min, λ = 254 nm, retention time: *t*_{minor} = 19.6 min, *t*_{major} = 42.3 min) at 25 °C.

NMR Spectral Data

(S)-3-(1-benzylpyrrolidin-2-yl)-2,4-dimethylpentan-3-ol (C1a)

SP18_281.1.fid

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(S)-3-(1-benzylpyrrolidin-2-yl)-2,4-dimethylpentan-3-ol (C1a)

SP18_281.2.fid

140.76

128.48
128.18
126.90

77.90
77.16 CDCl₃

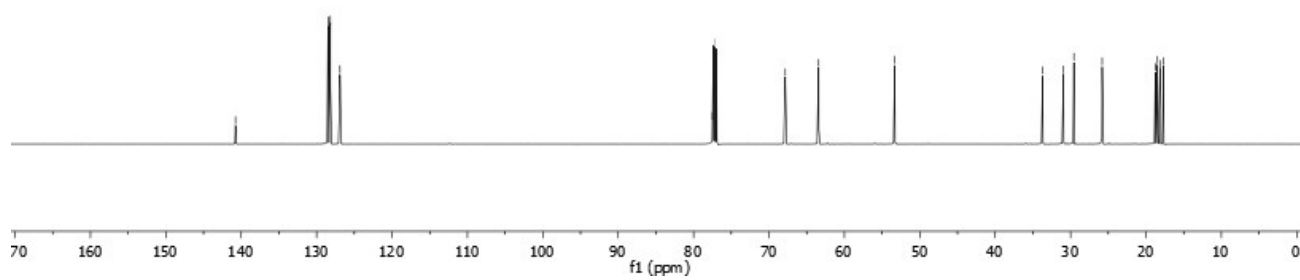
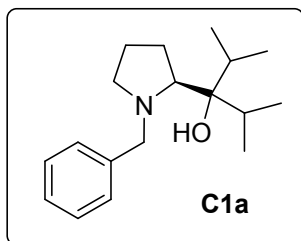
67.84

63.42

53.31

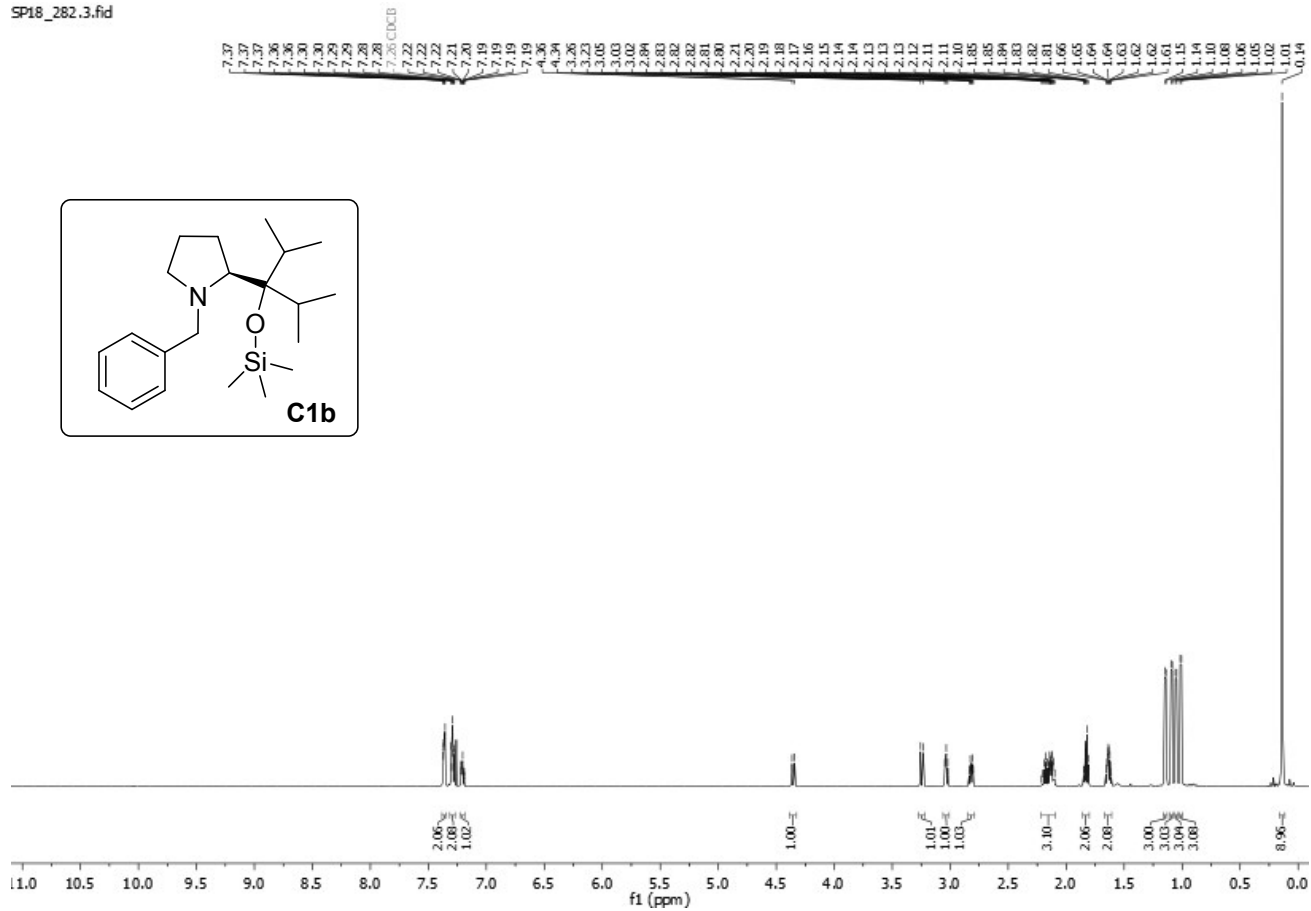
33.70
30.95
29.57
25.81

18.76
18.49
18.12
17.68



(S)-1-benzyl-2-(2,4-dimethyl-3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (C1b)

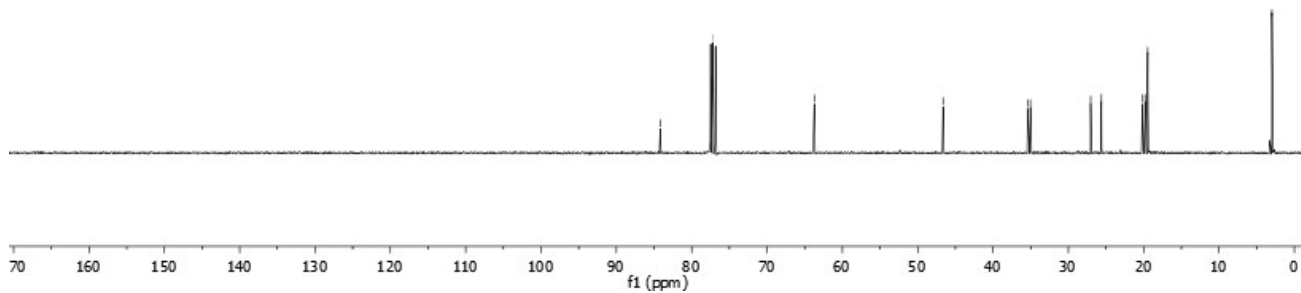
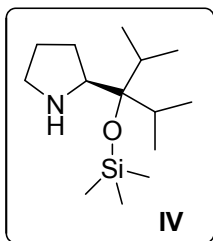
SP18_282.3.fid



(S)-2-(2,4-dimethyl-3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (IV)

SP18-283-FN.2.fid

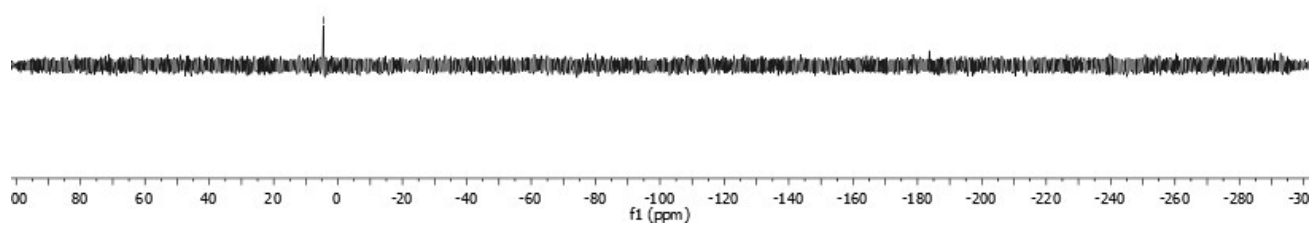
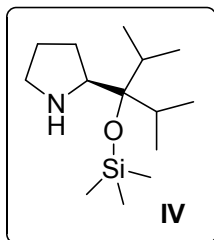
—84.17
—77.16 CDCl₃
—63.72
—46.63
—35.38
—35.04
—27.04
—25.61
—20.19
—19.82
—19.47
—2.99



(S)-2-(2,4-dimethyl-3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (IV)

SP18-283.9.fid

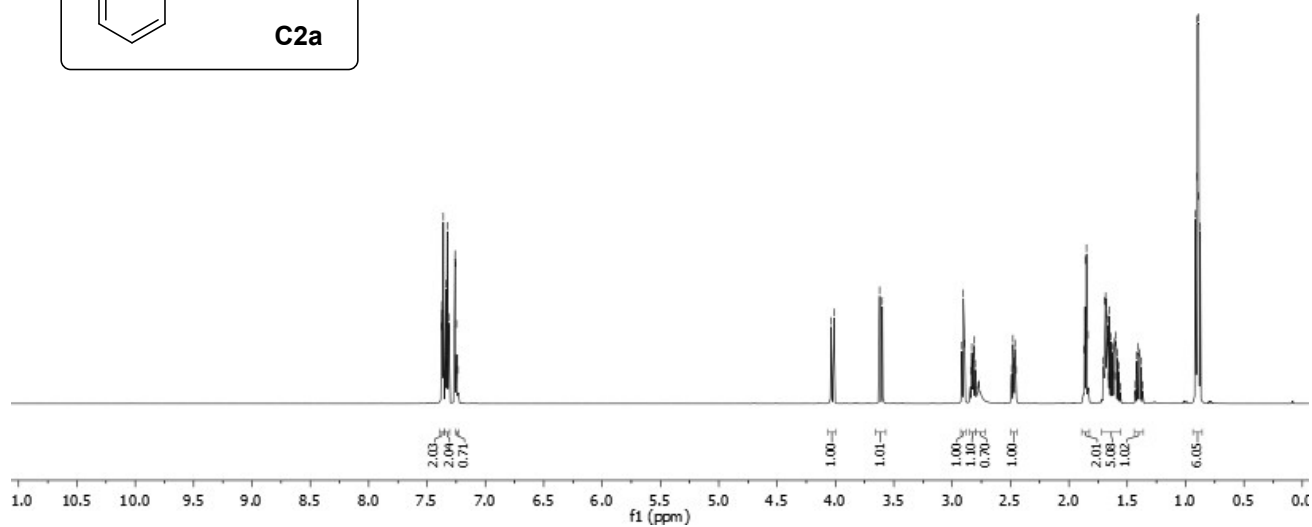
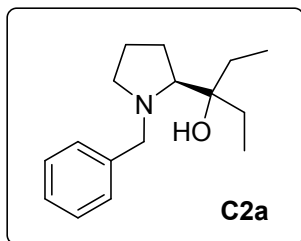
0.00



(S)-3-(1-benzylpyrrolidin-2-yl)pentan-3-ol (C2a)

SP18-285.1.fid
SP18-285

7.37
7.37
7.36
7.34
7.34
7.33
7.31
7.26 CDCl₃
7.25
7.24
4.01
4.01
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3.60
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(S)-3-(1-benzylpyrrolidin-2-yl)pentan-3-ol (C2a)

SP18-285.2.fid
SP18-285

140.72

128.43
128.18
126.95

77.16 CDCl₃
76.10

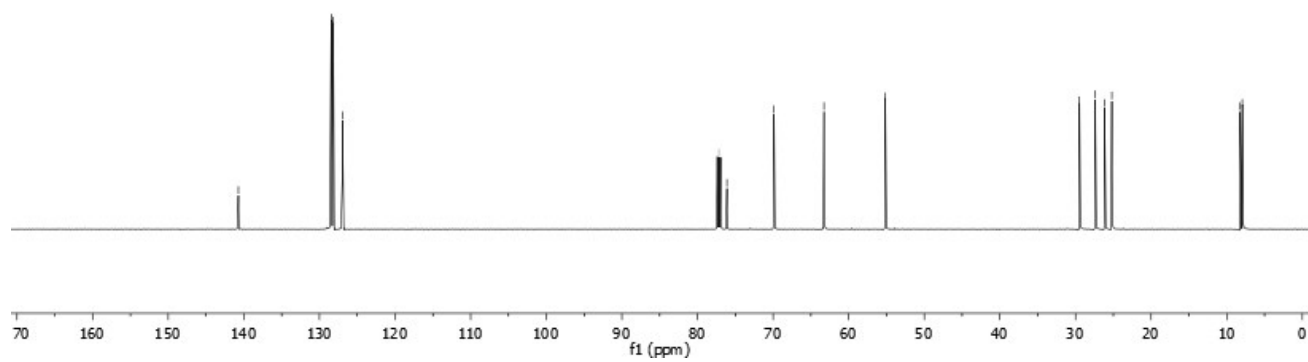
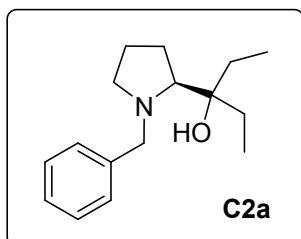
69.88

63.27

55.16

29.48
27.40
26.15
25.20

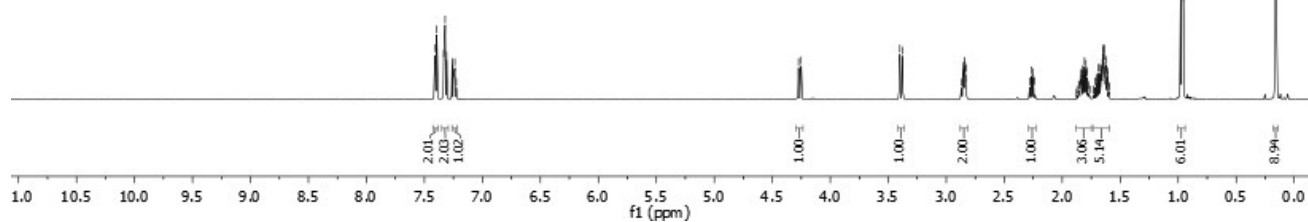
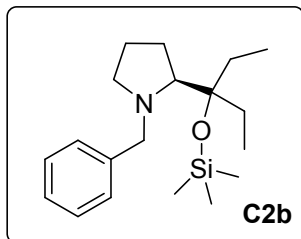
8.22
7.94



(S)-1-benzyl-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (C2b)

SP18-286.1.fid
SP18-286

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1.60
0.98
0.98
0.97
0.95
0.95
0.15



(S)-1-benzyl-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (C2b)

SP18-286.2.fid
SP18-286

141.56

128.61
128.16
126.51

82.48

77.16 CDCl₃

70.40

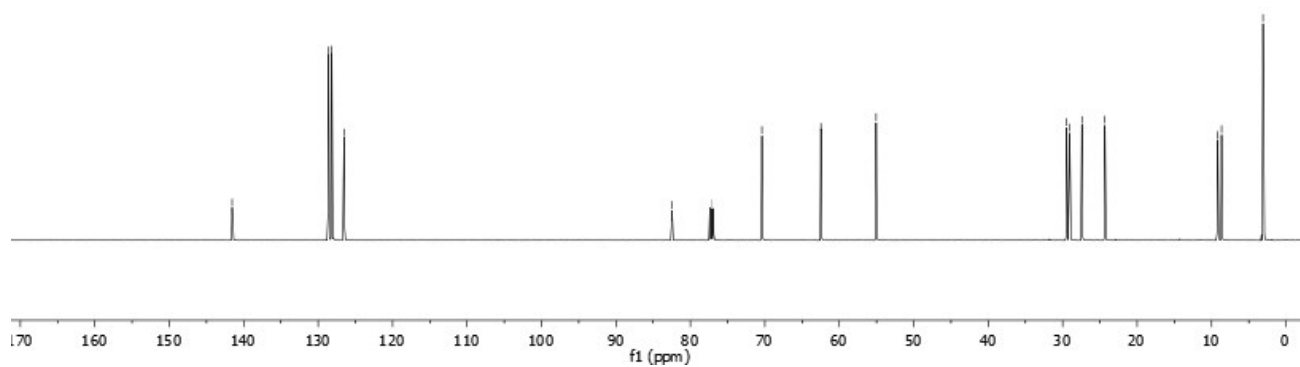
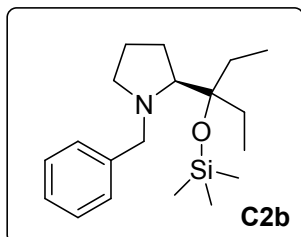
62.47

55.05

29.47
29.07
27.41
24.33

9.18
8.66

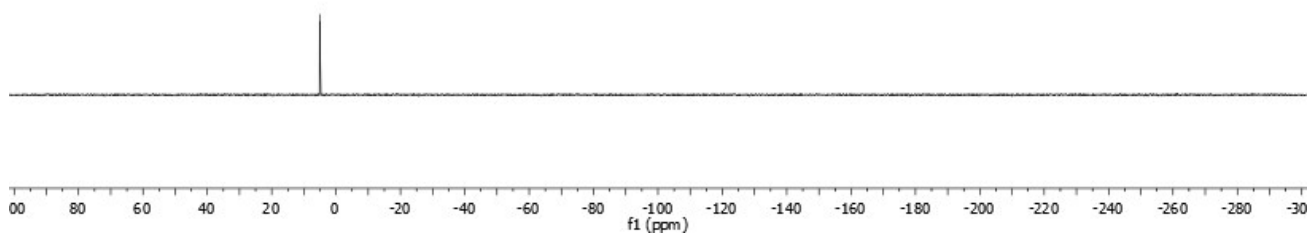
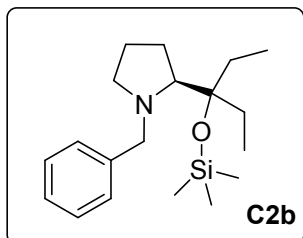
3.10



(S)-1-benzyl-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (C2b)

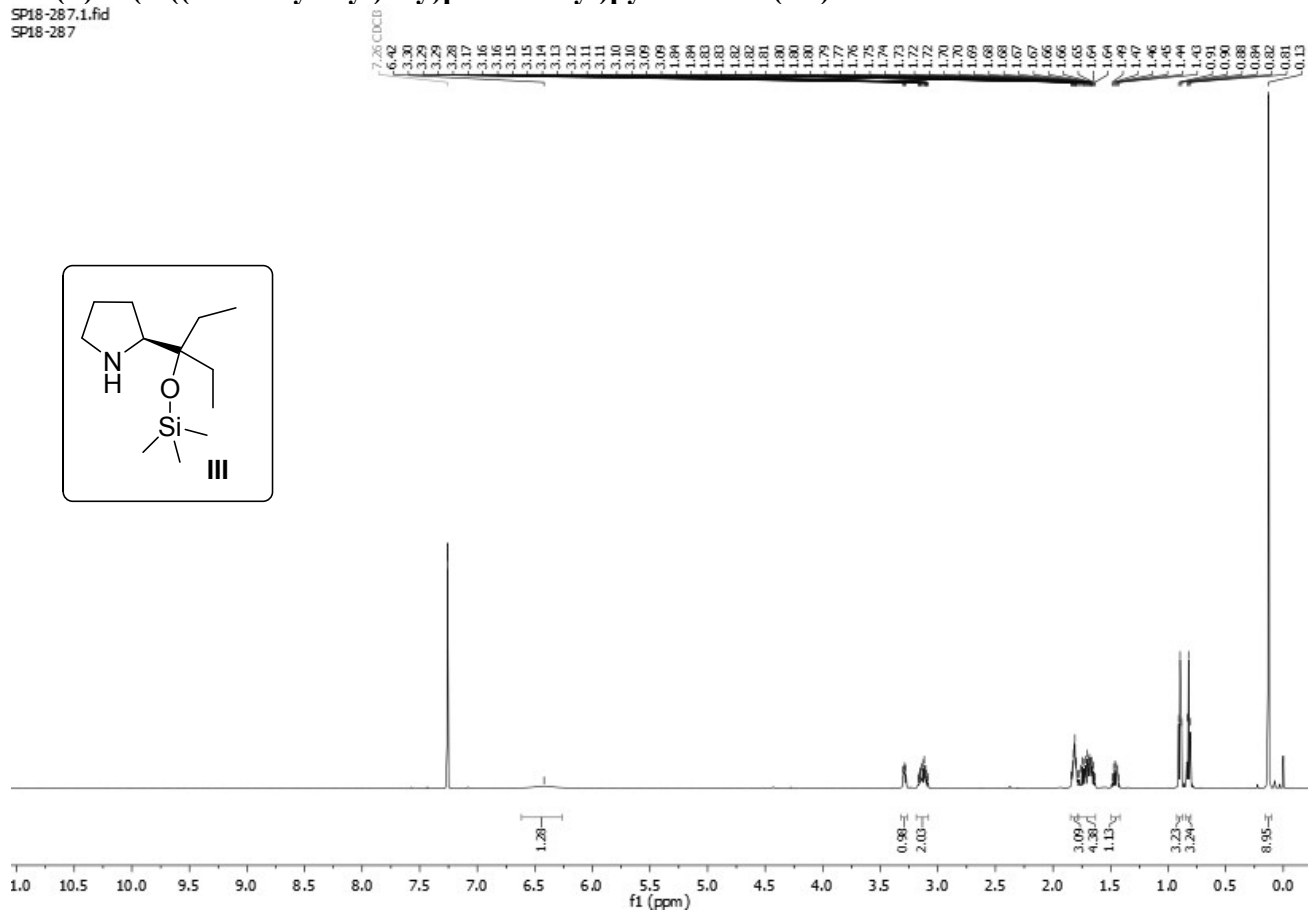
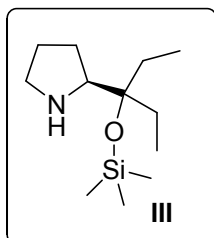
SP18-286.2.fid

5.10



(S)-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (III)

SP18-287.1.fid
SP18-287



(S)-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (III)

SP18-287.4.fid

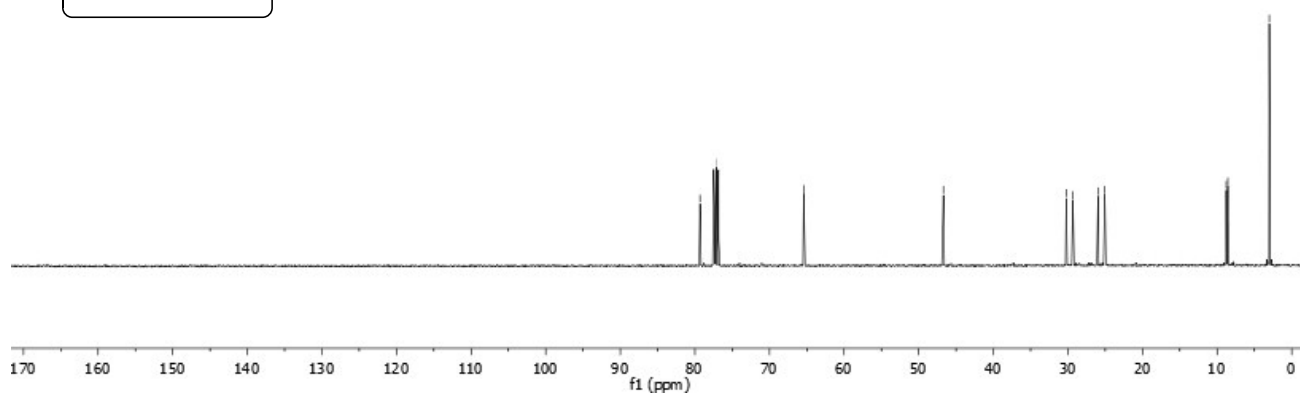
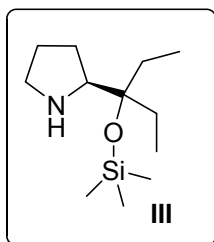
79.32
77.16 CDCl₃

65.41

46.69

30.23
29.33
25.96
25.05

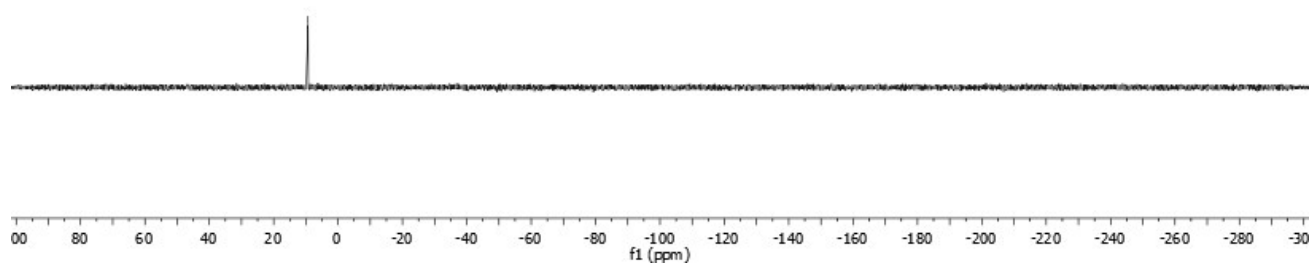
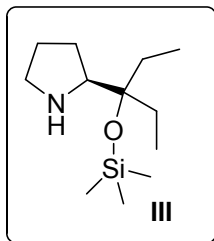
8.77
8.56
3.00



(S)-2-(3-((trimethylsilyl)oxy)pentan-3-yl)pyrrolidine (III)

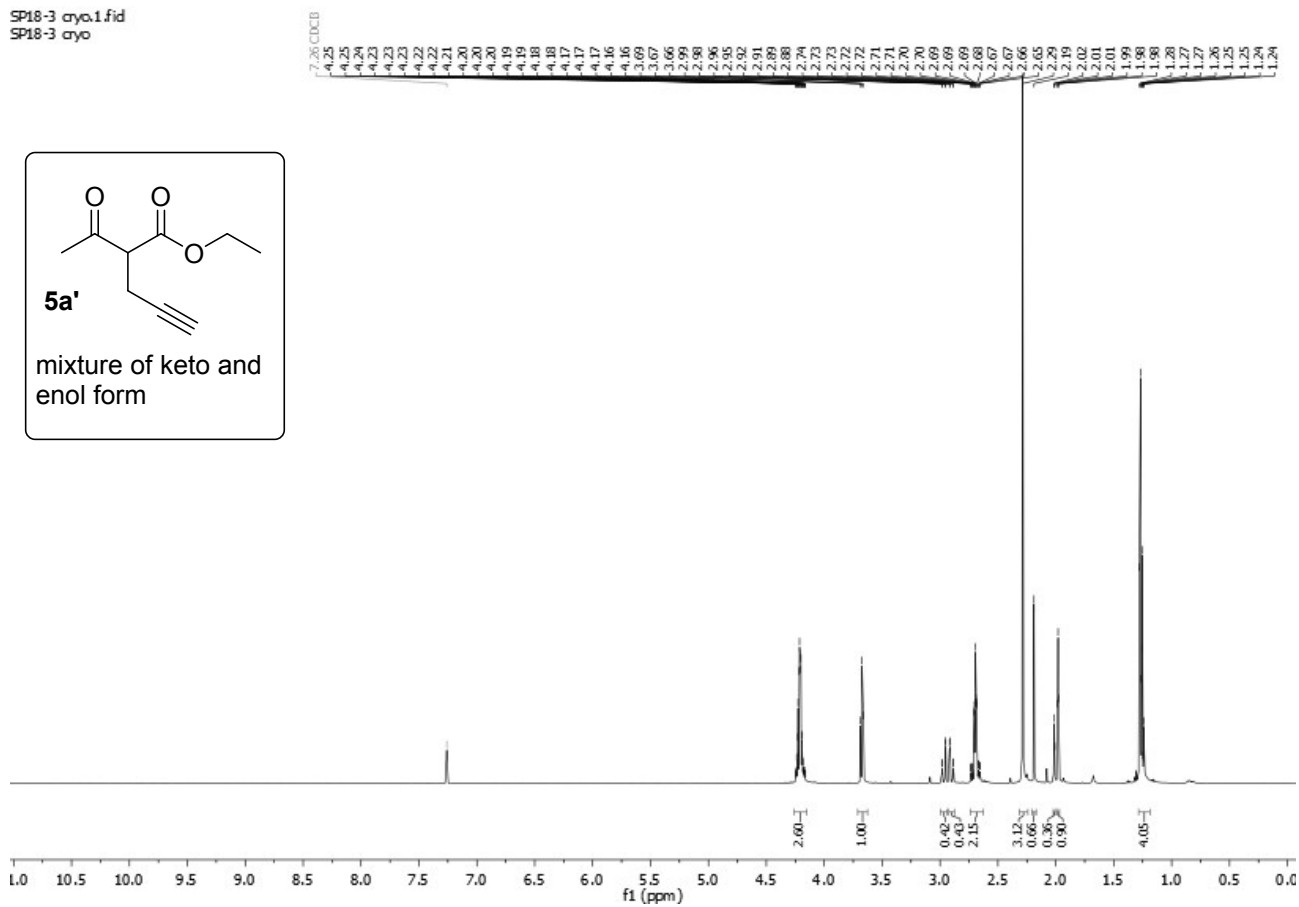
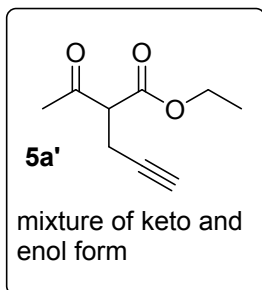
SP18-287.3.fid

9.32



Ethyl 2-acetylpent-4-ynoate (5a')

SP18-3 cryo.1.fid
SP18-3 cryo



Ethyl 2-acetylpent-4-ynoate (5a')

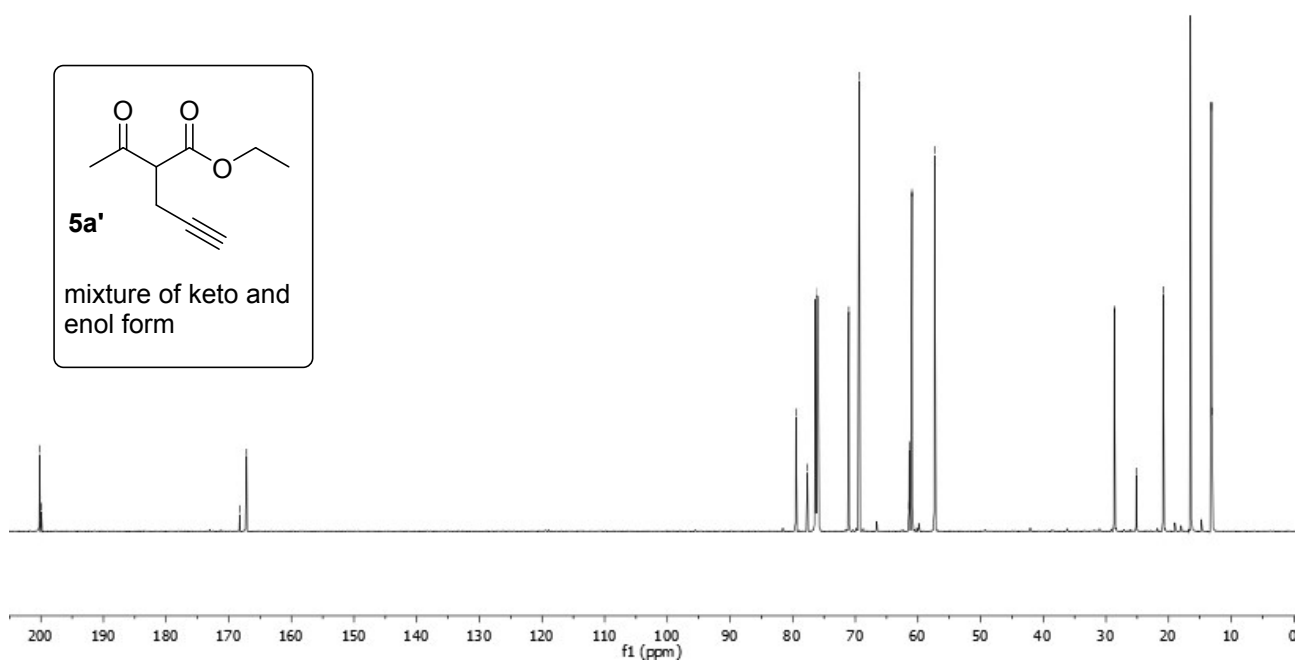
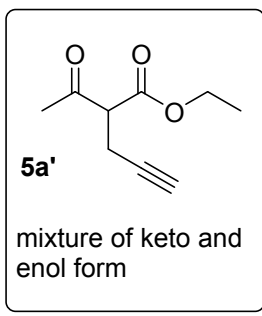
SP18-3 ayv.2.fid
SP18-3 ayv.13C

200.16
199.91

168.25
167.16

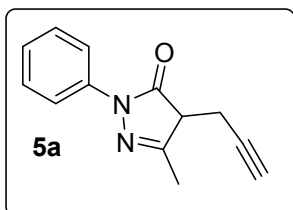
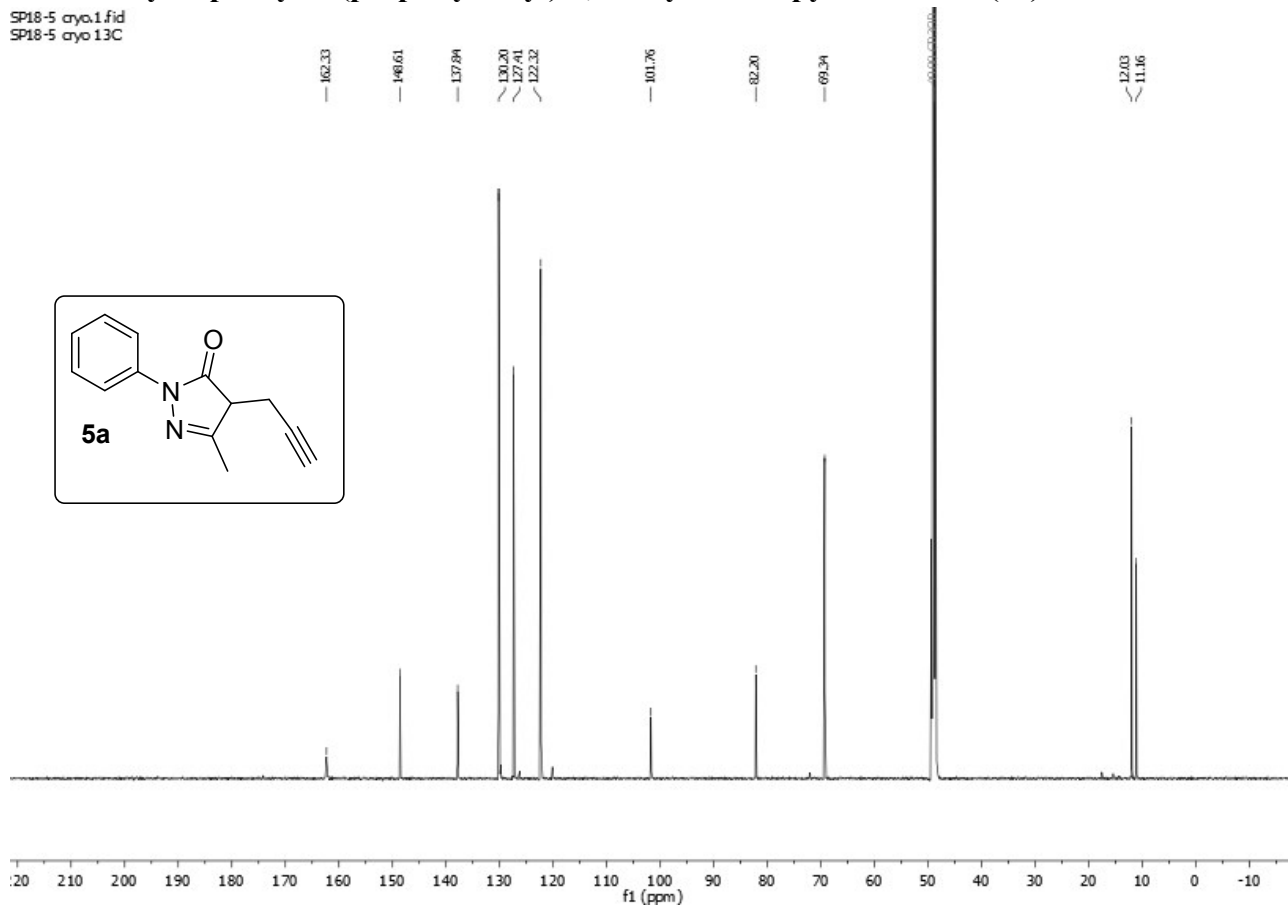
79.49
77.64
76.16 CDCl₃
71.04
69.37
61.42
61.38
60.95
57.35

28.67
25.16
20.87
16.90
13.16
13.10



5-Methyl-2-phenyl-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one (5a)

SP18-5 cryo.1.fid
SP18-5 cryo 13C



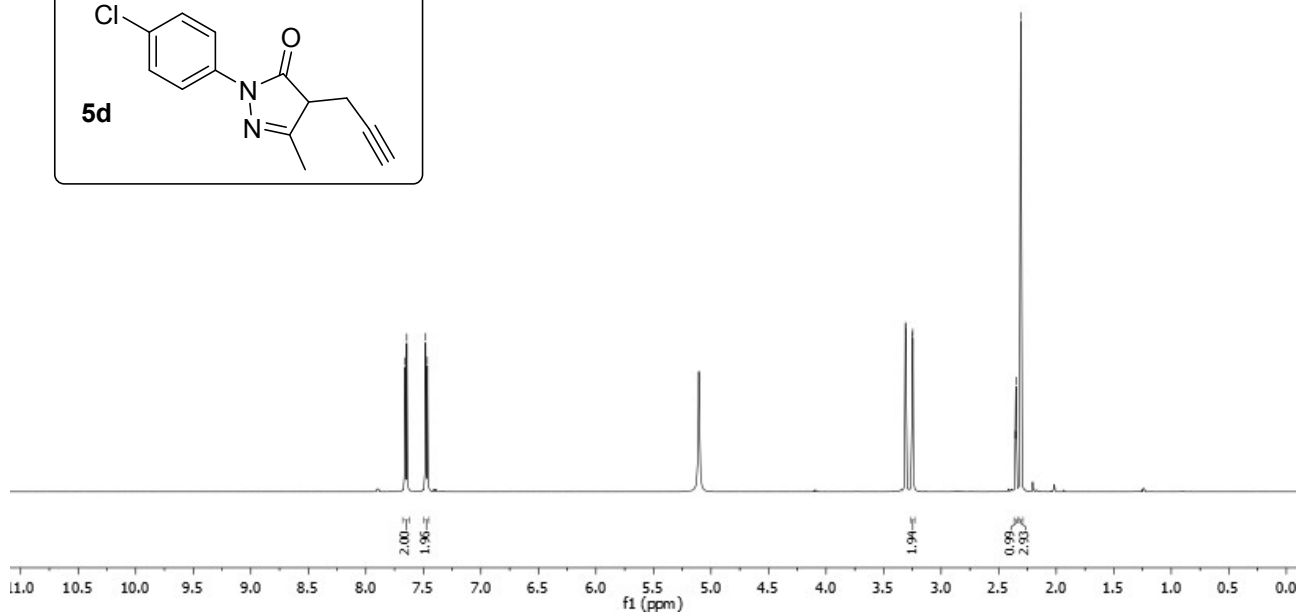
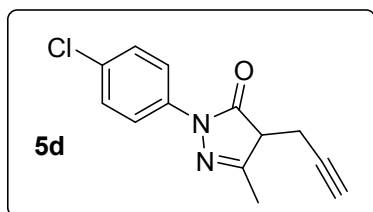
2-(4-Chlorophenyl)-5-methyl-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one (5d)

SP18-94 cryo.7.fid
SP18-94 low temperature 0C cryo

7.66
7.64
7.60
7.57

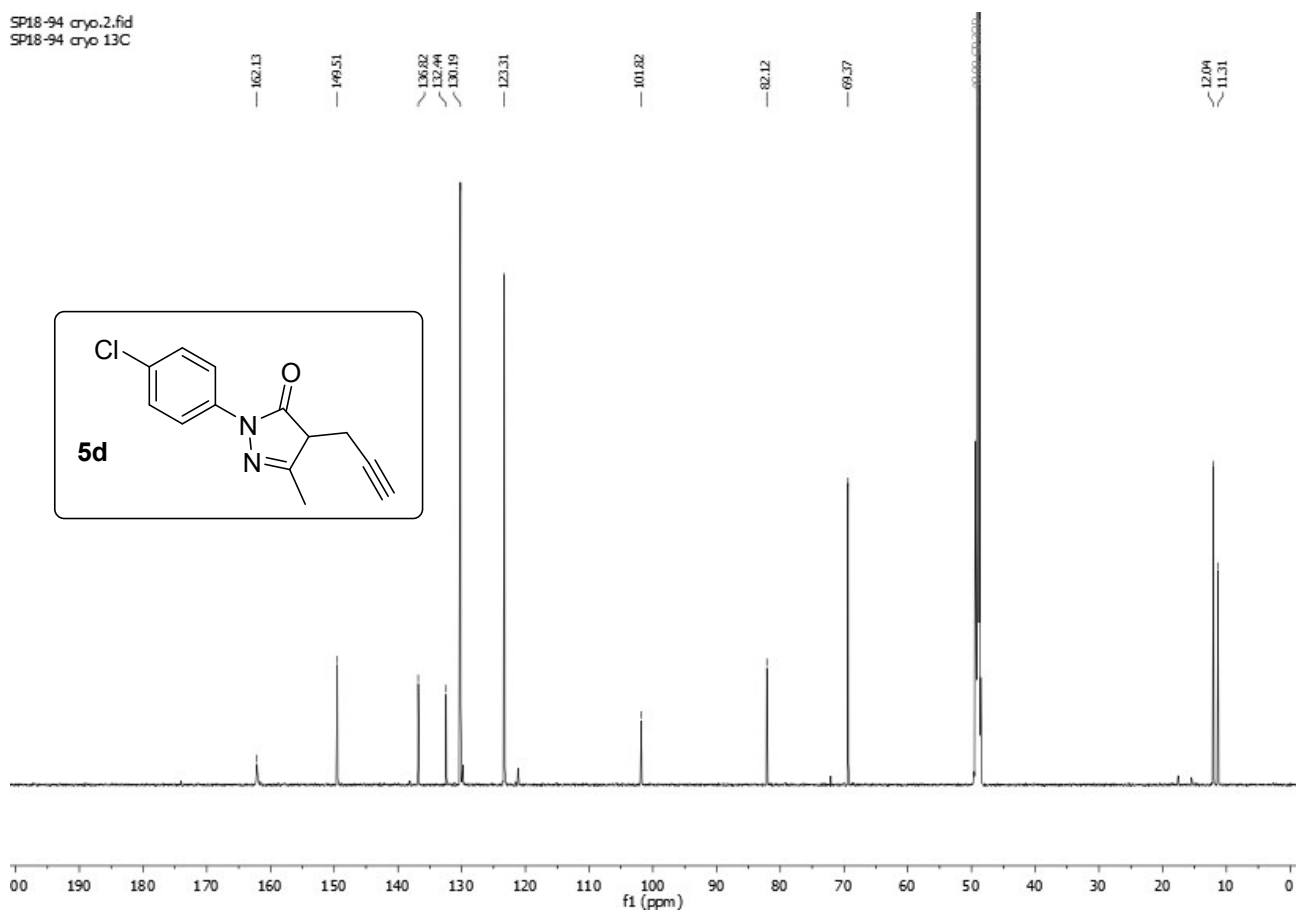
2.31 CDCl₃
2.25
2.25

2.35
2.35
2.35
2.31



2-(4-Chlorophenyl)-5-methyl-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one (5d)

SP18-94 cryo.2.fid
SP18-94 cryo 13C



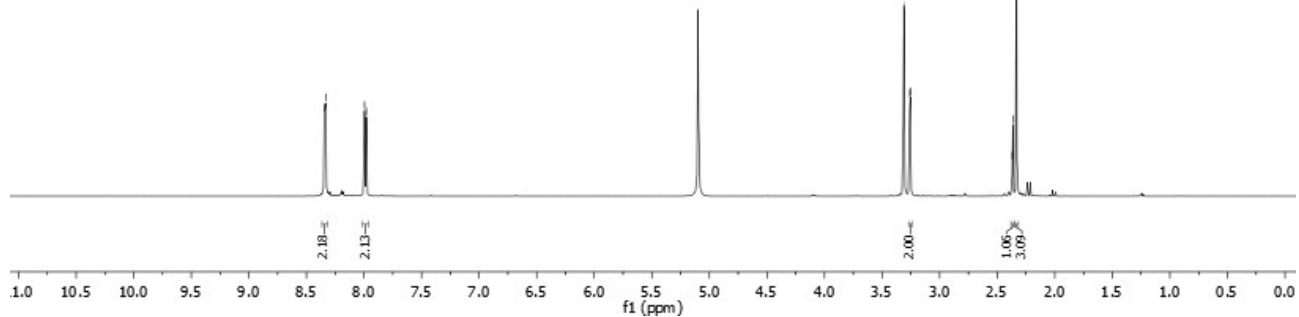
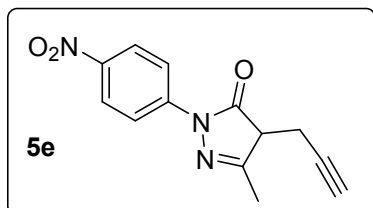
5-Methyl-2-(4-nitrophenyl)-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one (5e)

SP18-104 cryo.11.fid
SP18-104 low temperature 0C cryo

8.35
8.13
8.00
7.98

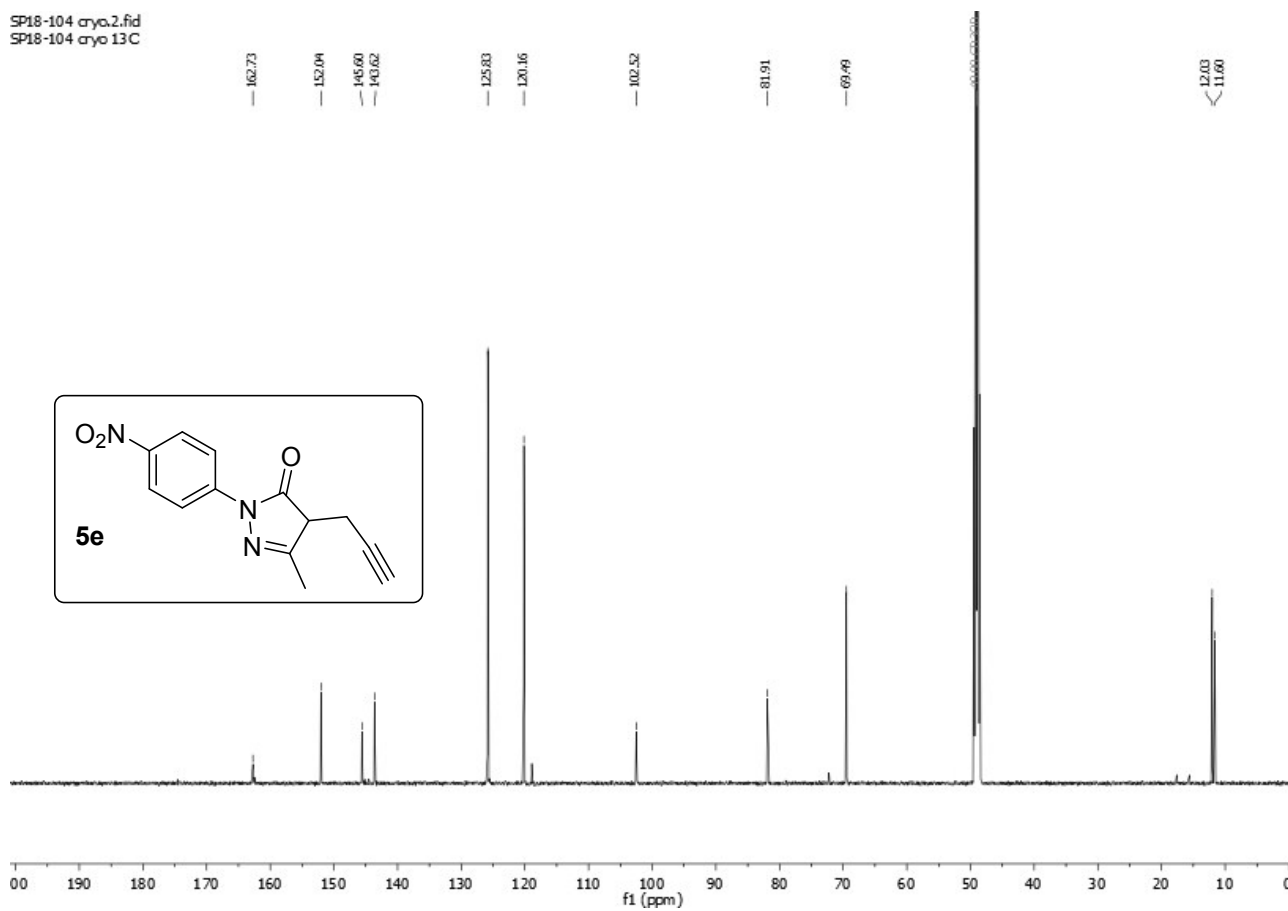
3.31 CD,000
3.26
3.25

2.37
2.36
2.36
2.33



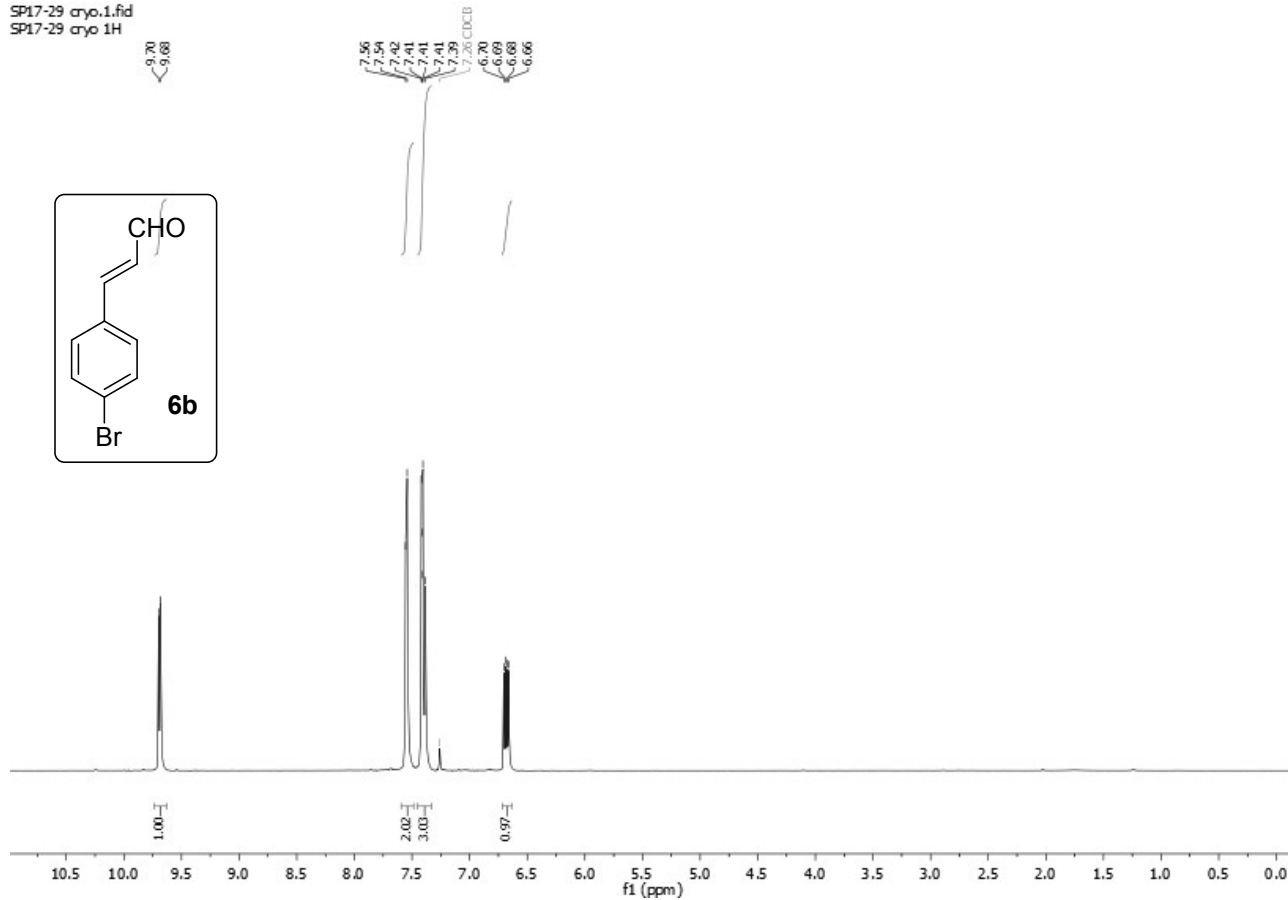
5-Methyl-2-(4-nitrophenyl)-4-(prop-2-yn-1-yl)-2,4-dihydro-3H-pyrazol-3-one (5e)

SP18-104 cryo.2.fid
SP18-104 cryo 13C



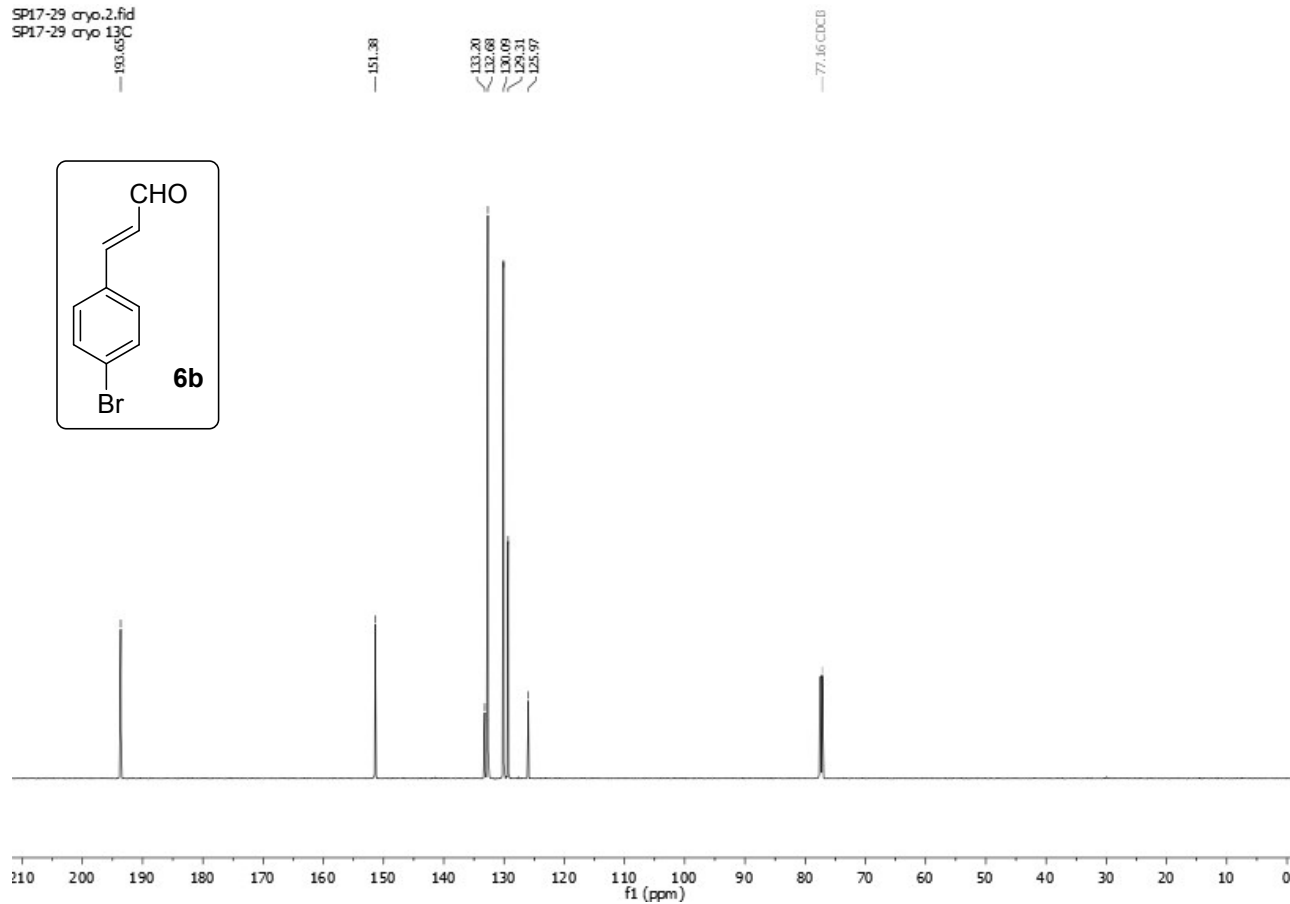
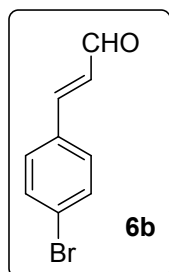
(E)-3-(4-Bromophenyl)acrylaldehyde (6b)

SP17-29 cryo.1.fid
SP17-29 cryo 1H



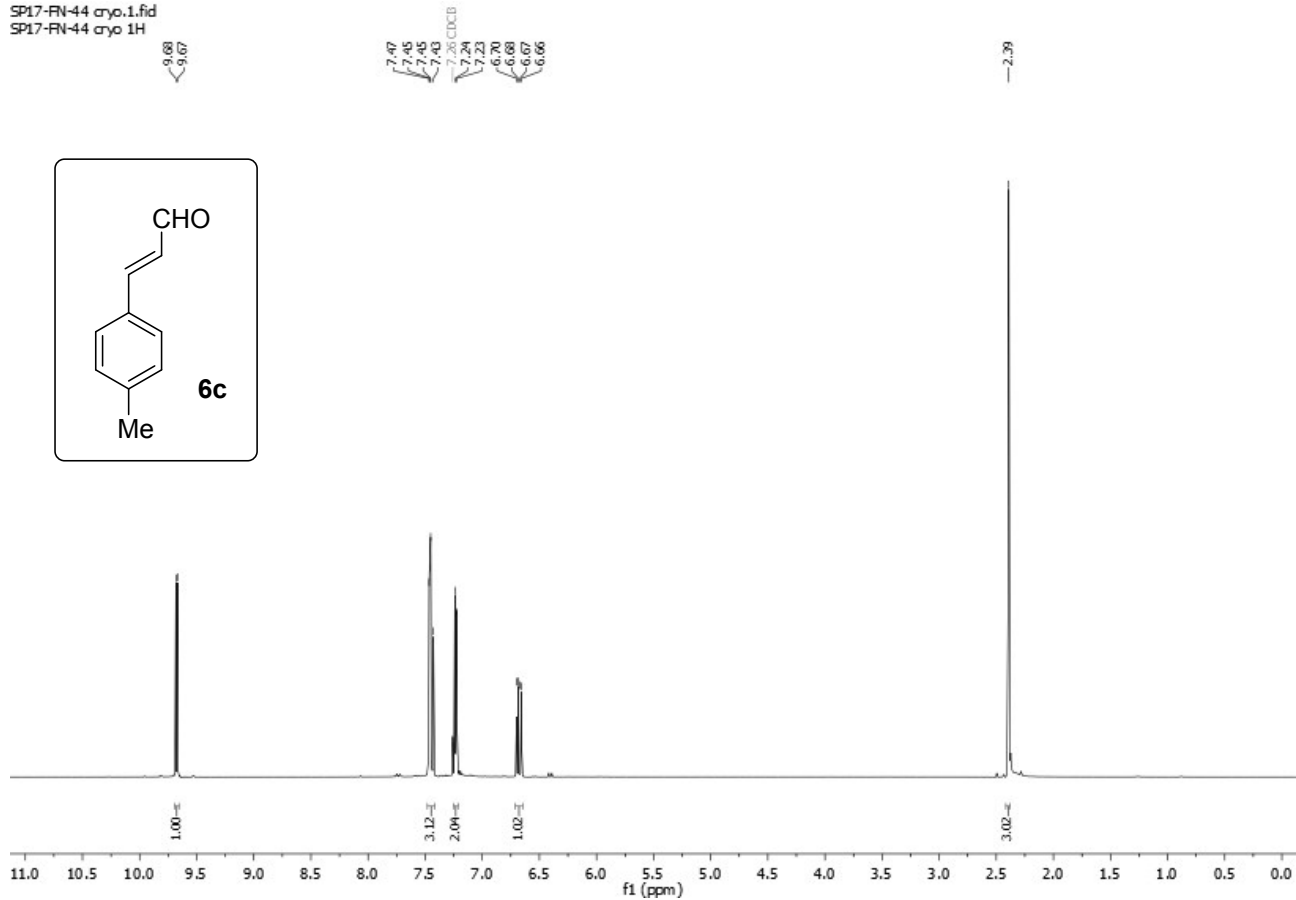
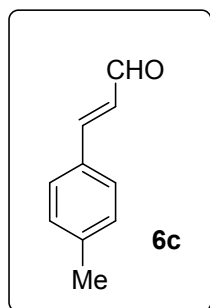
(E)-3-(4-Bromophenyl)acrylaldehyde (6b)

SP17-29 cryo.2.fid
SP17-29 cryo 13C



(E)-3-(p-Tolyl)acrylaldehyde (6c)

SP17-FN-44 cryo.1.fid
SP17-FN-44 cryo 1H



(E)-3-(p-Tolyl)acrylaldehyde (6c)

SP17-FN-44 cryo.2.fid
SP17-FN-44 cryo.13C

194.11

153.28

142.29

131.64

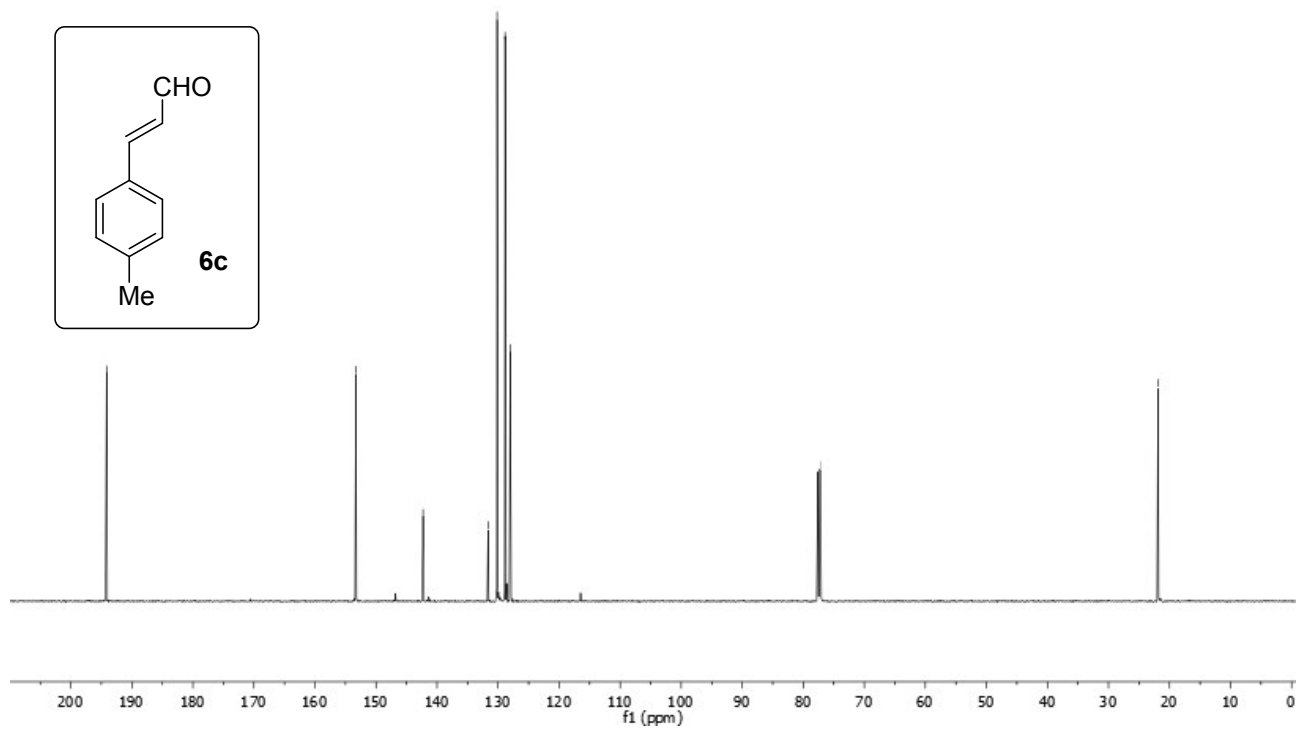
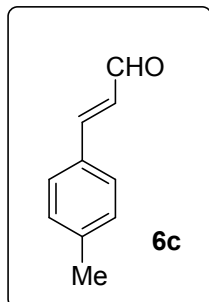
130.16

128.85

128.02

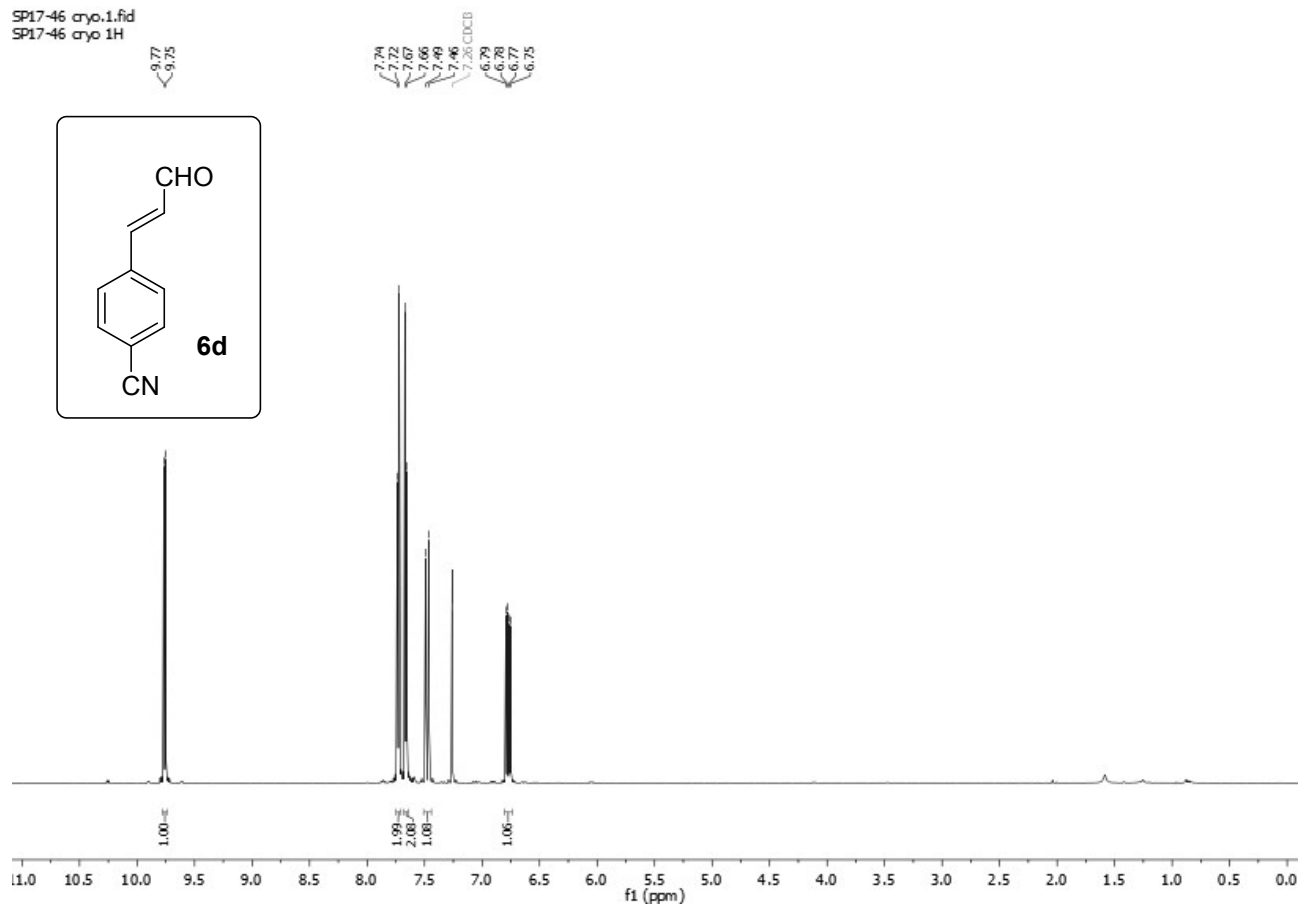
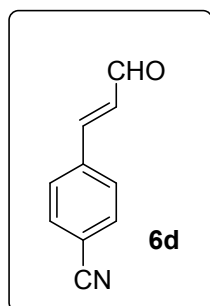
77.16 CDCl₃

21.88



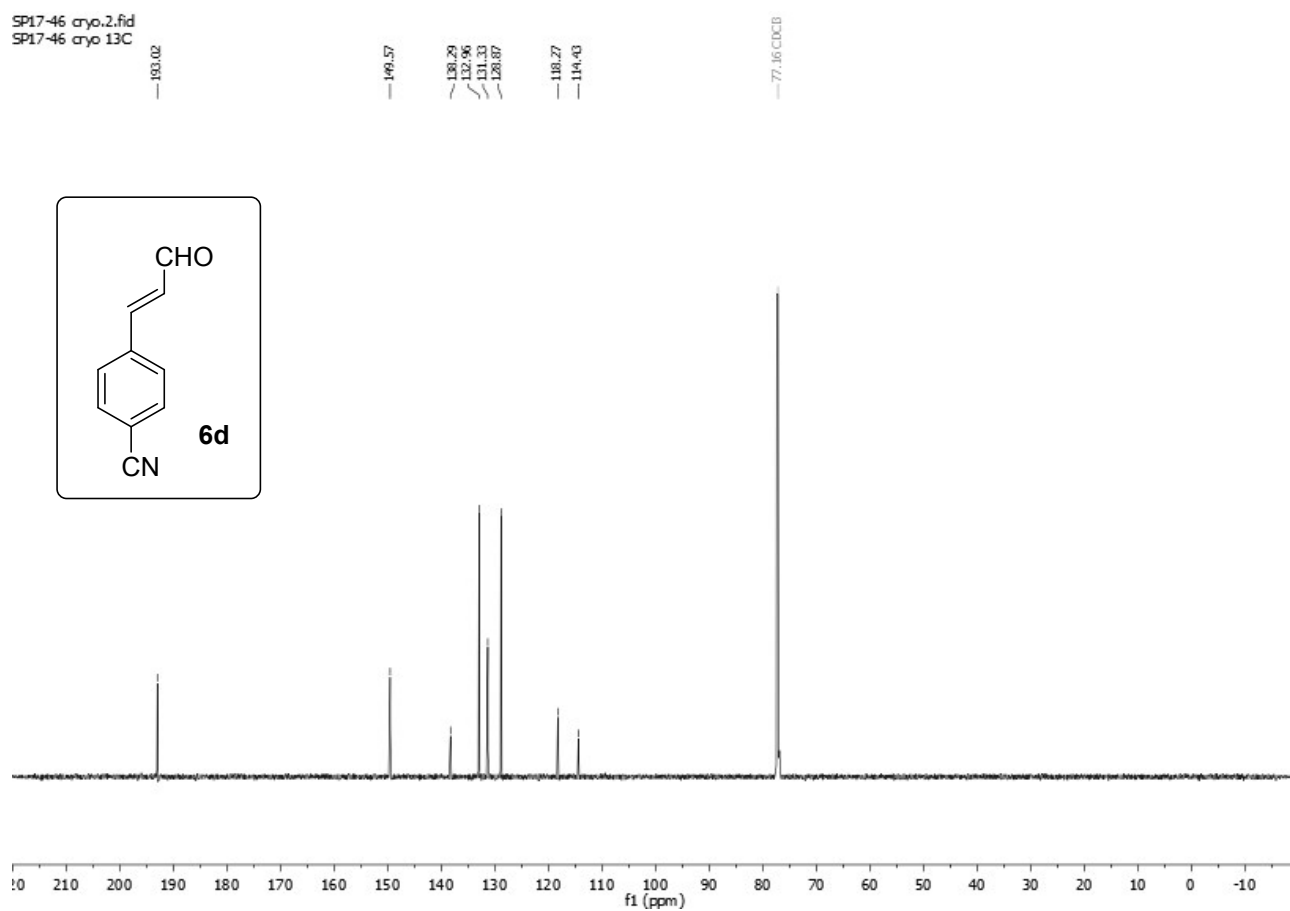
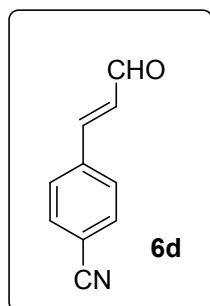
(E)-4-(3-Oxoprop-1-en-1-yl)benzonitrile (6d)

SP17-46 cryo.1.fid
SP17-46 cryo 1H



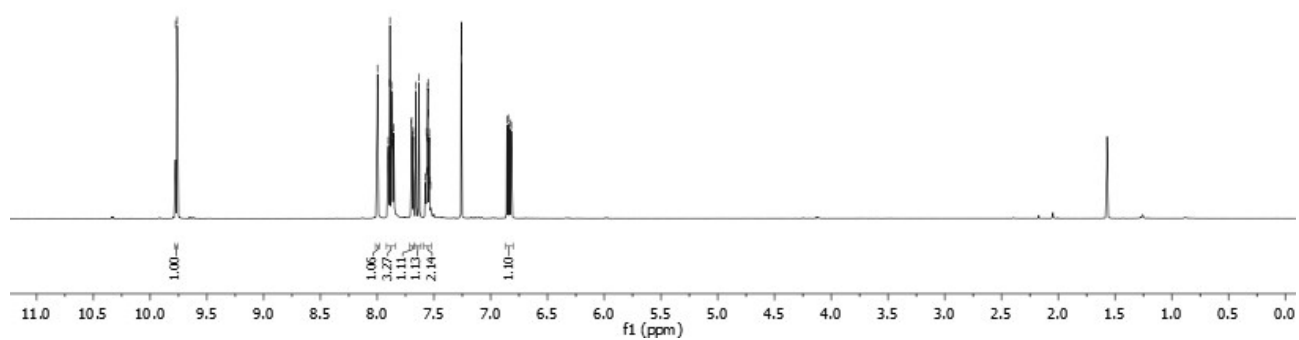
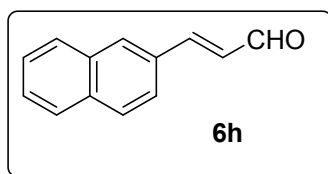
(E)-4-(3-Oxoprop-1-en-1-yl)benzonitrile (6d)

SP17-46 cryo.2.fid
SP17-46 cryo.13C



(E)-3-(Naphthalen-2-yl)acrylaldehyde (6h)

SP17-48 cryo.1.fid
SP17-48 cryo 1H



(E)-3-(Naphthalen-2-yl)acrylaldehyde (6h)

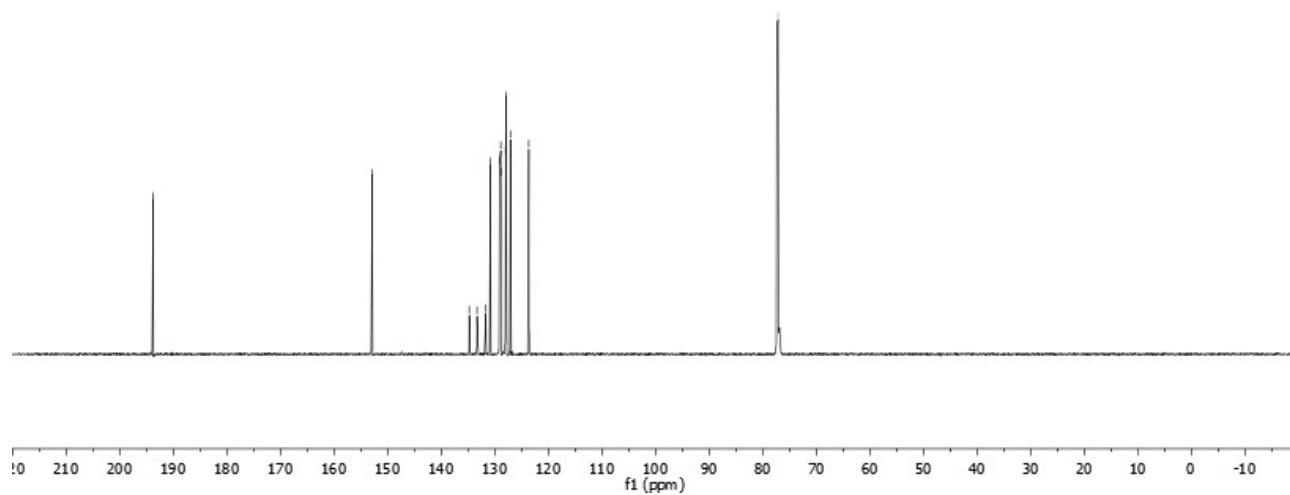
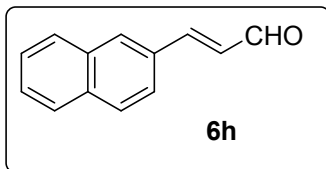
SP17-48 cryo.2.fid
SP17-48 cryo 13C

193.83

152.93

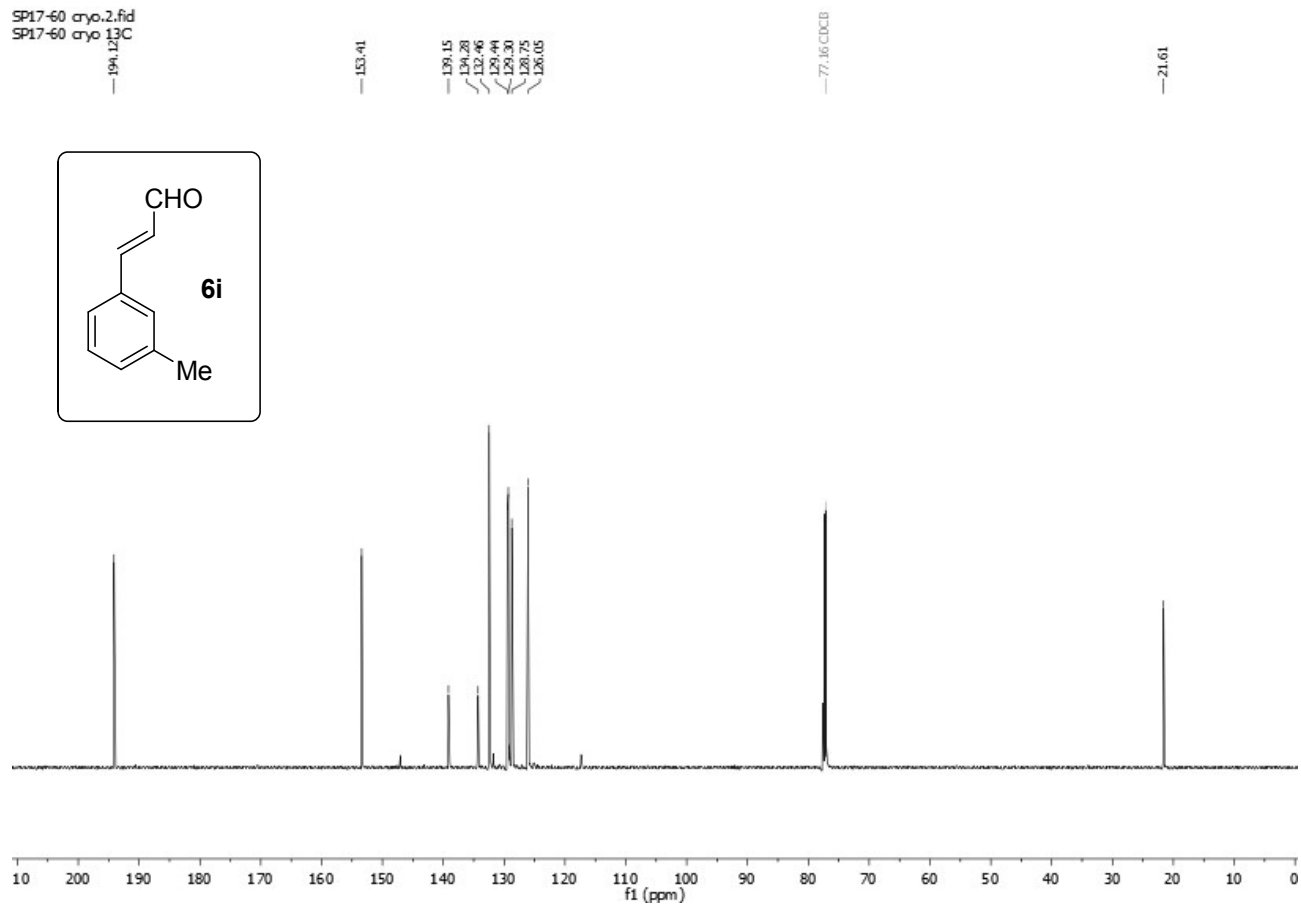
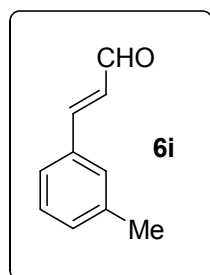
134.80
133.35
131.71
130.86
129.14
128.92
128.03
127.98
127.12
123.68

77.16 CDCl₃



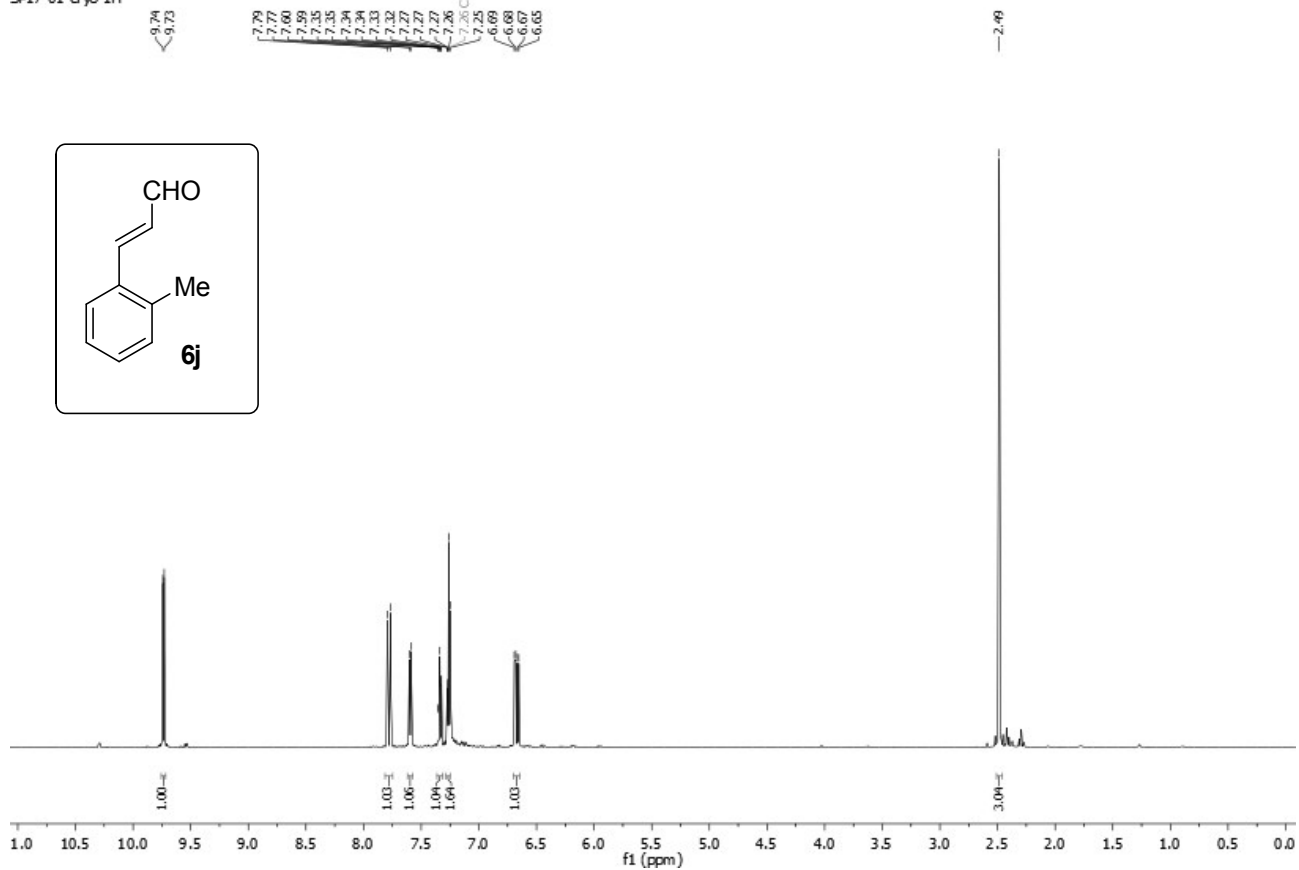
(E)-3-(*m*-Tolyl)acrylaldehyde (6i)

SP17-60 cryo.2.fid
SP17-60 cryo.13C



(E)-3-(o-Tolyl)acrylaldehyde (6j)

SP17-61 cryo.1.fid
SP17-61 cryo 1H



(E)-3-(o-Tolyl)acrylaldehyde (6j)

SP17-61 cryo.2.fid
SP17-61 cryo.13C

193.92

150.33

138.01

132.90

131.15

131.11

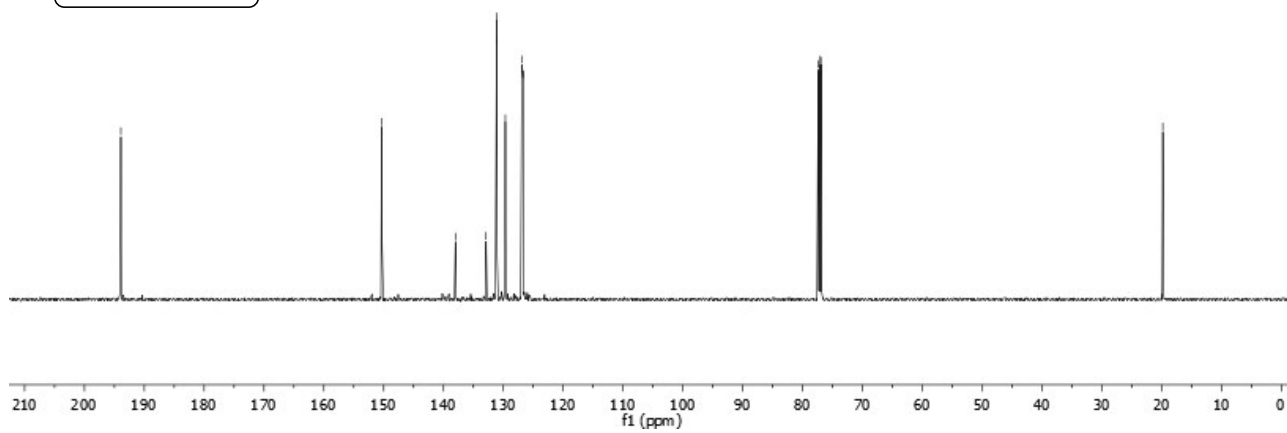
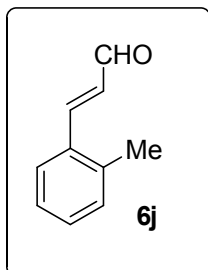
129.67

128.91

126.68

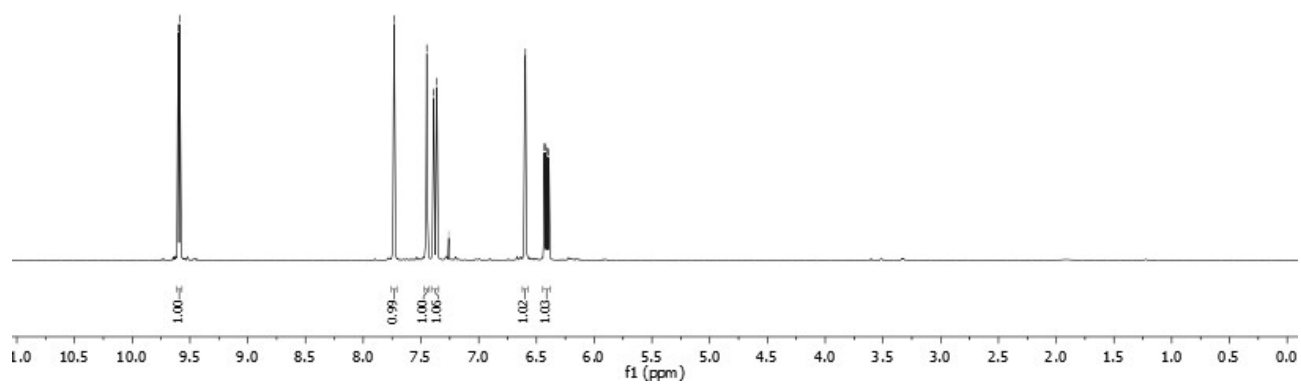
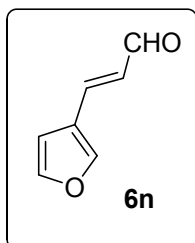
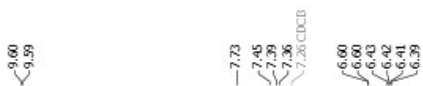
77.37
77.16
76.95

19.83



(E)-3-(Furan-3-yl)acrylaldehyde (6n)

SP17-63 cryo.1.fid
SP17-63 cryo 1H



(E)-3-(Furan-3-yl)acrylaldehyde (6n)

SP17-63 cryo.2.fid
SP17-63 cryo.13C

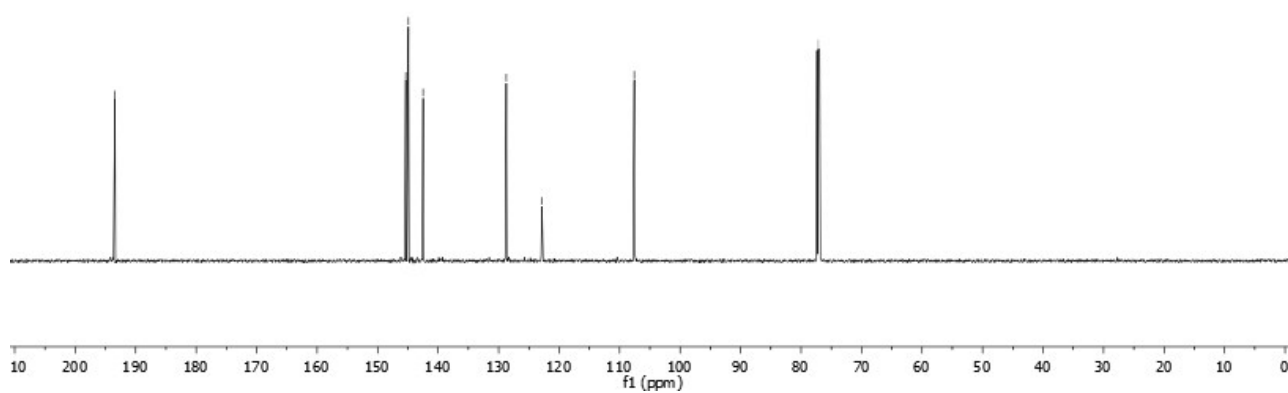
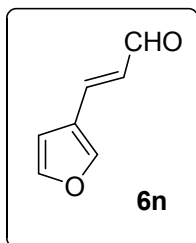
183.62

145.35
144.91
142.49

128.73
122.84

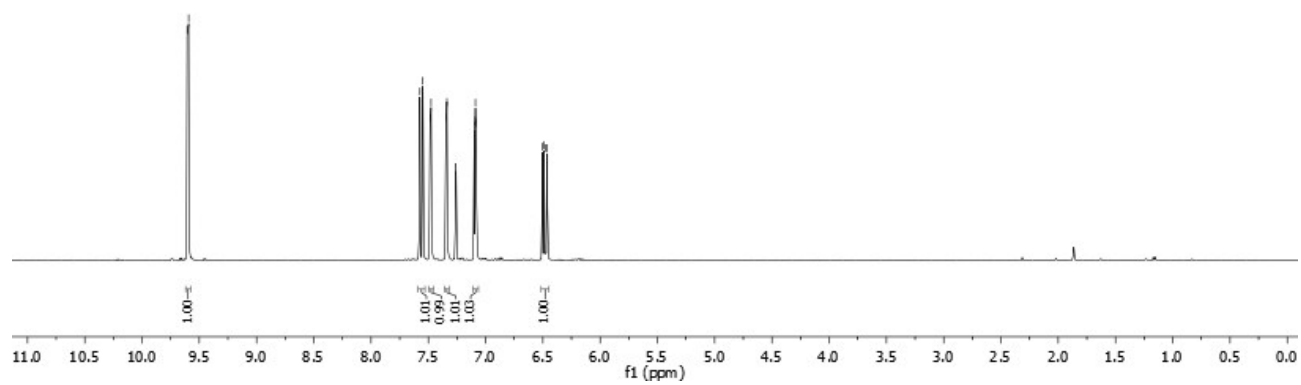
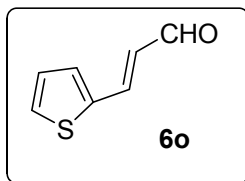
107.59

77.16 CDCl₃



(E)-3-(Thiophen-2-yl)acrylaldehyde (6o)

SP17-80 cryo.1.fid
SP17-80 cryo 1H



(E)-3-(Thiophen-2-yl)acrylaldehyde (6o)

SP17-80 cryo.2.fid
SP17-80 cryo.13C

192.92

144.48

139.31

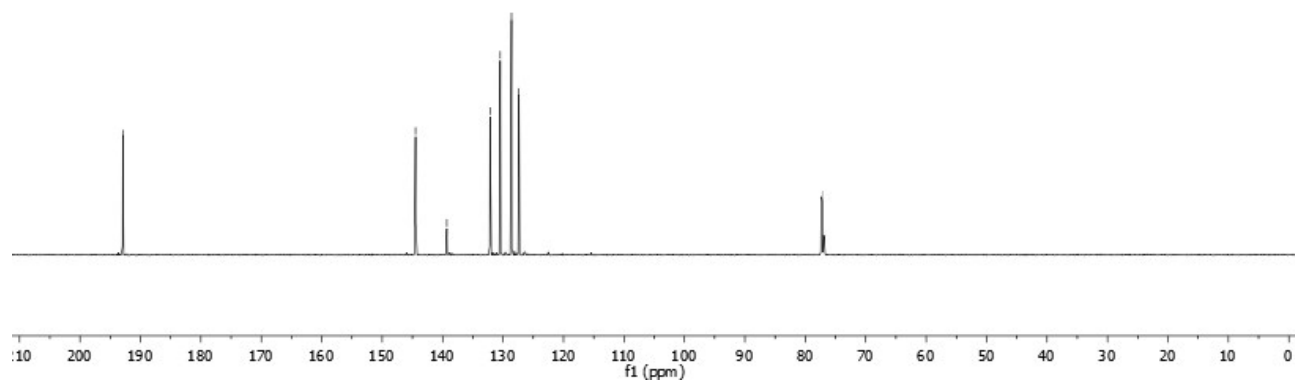
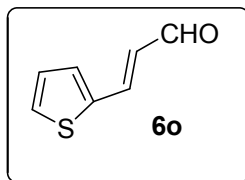
132.17

130.47

128.00

127.37

77.16 CDCl₃



Ethyl (*E*)-4-oxobut-2-enoate (6p)

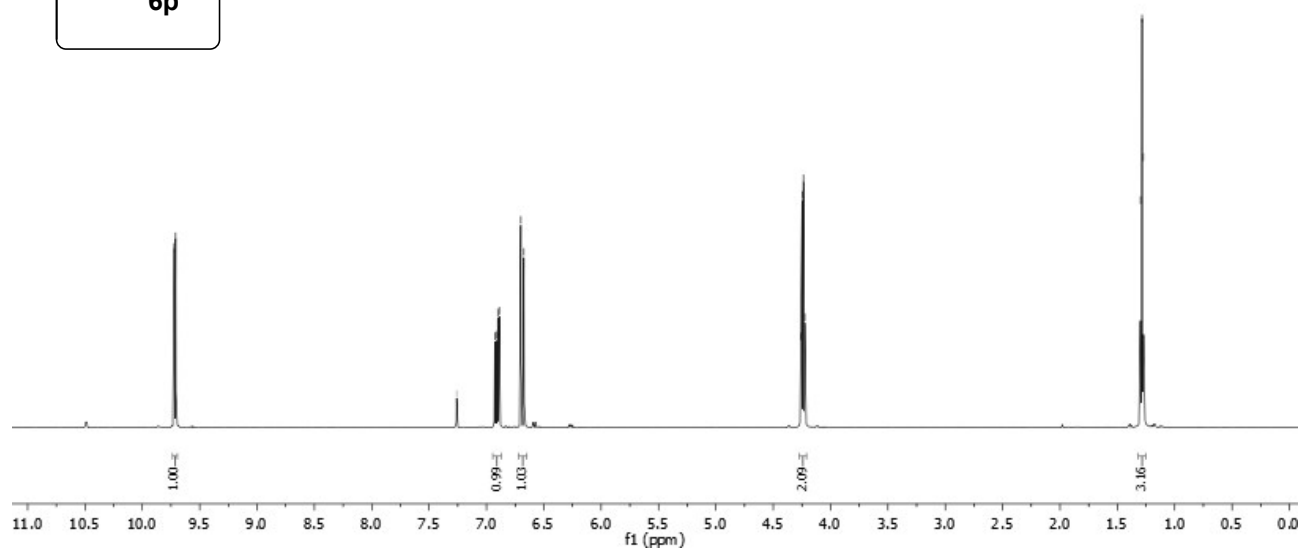
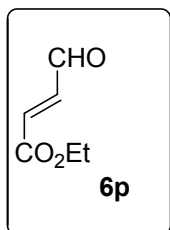
SP17-77 cryo.1.fid
SP17-77 cryo 1H

9.72
9.71

7.26 CDCl₃
6.93
6.92
6.90
6.89
6.70
6.67

4.26
4.25
4.24
4.23

1.30
1.28
1.27



Ethyl (*E*)-4-oxobut-2-enoate (6p)

SP17-77 cryo.2.fid
SP17-77 cryo.13C

192.56

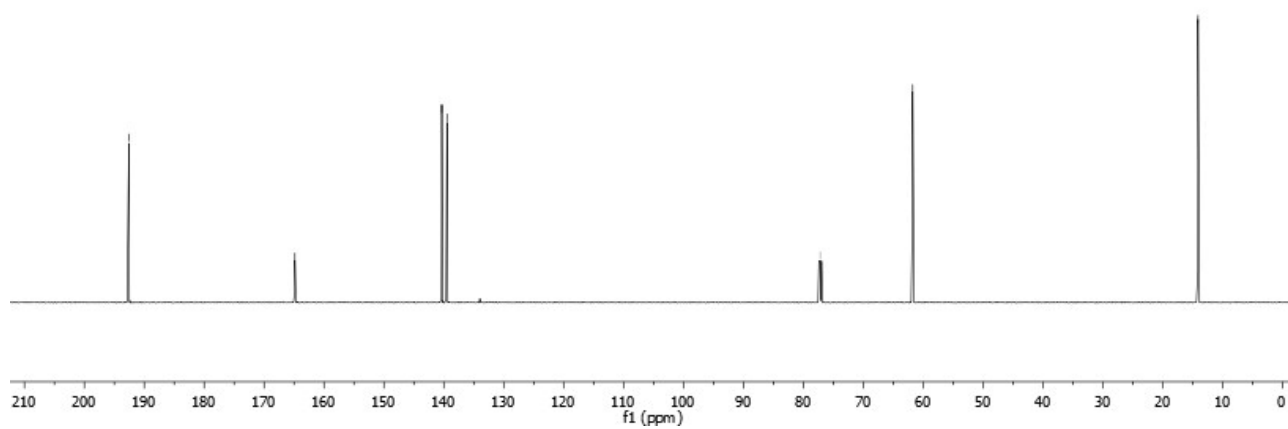
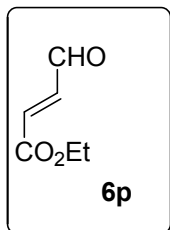
164.85

140.33
138.47

77.16 CDCl₃

61.73

14.09



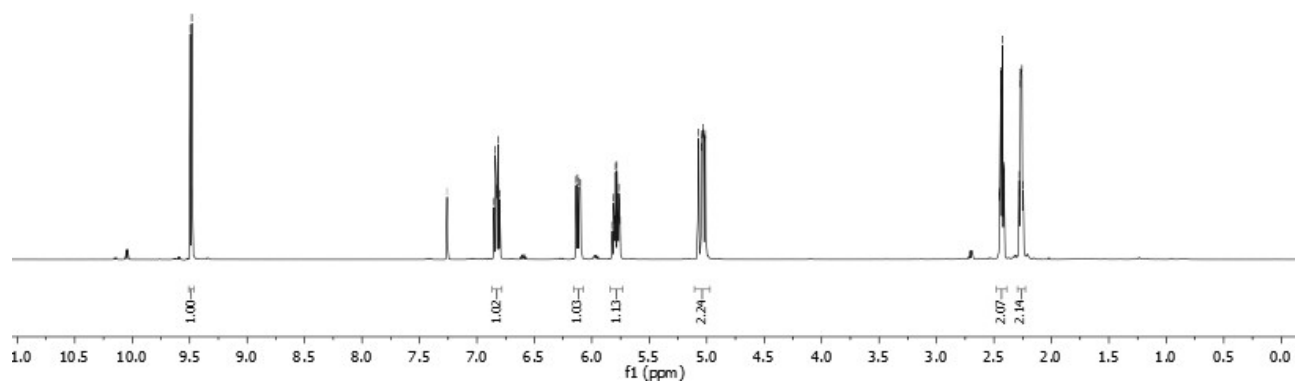
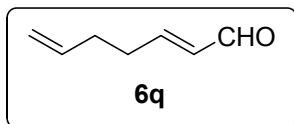
(E)-Hepta-2,6-dienal (6q)

SP17-70.1.fid
SP17-70
1H
CDCl3
HB

9.50
9.48

7.26 CDCl3
6.85
6.84
6.83
6.83
6.81
6.14
6.12
6.10
5.82
5.81
5.80
5.79
5.78
5.77
5.75
5.07
5.04
5.03
5.03
5.02
5.01

2.45
2.44
2.44
2.43
2.42
2.41
2.28
2.28
2.27
2.26
2.25



(E)-Hepta-2,6-dienal (6q)

SP17-70.2.fid
SP17-70
13C
CDCl3
HB

194.07

157.75

136.72

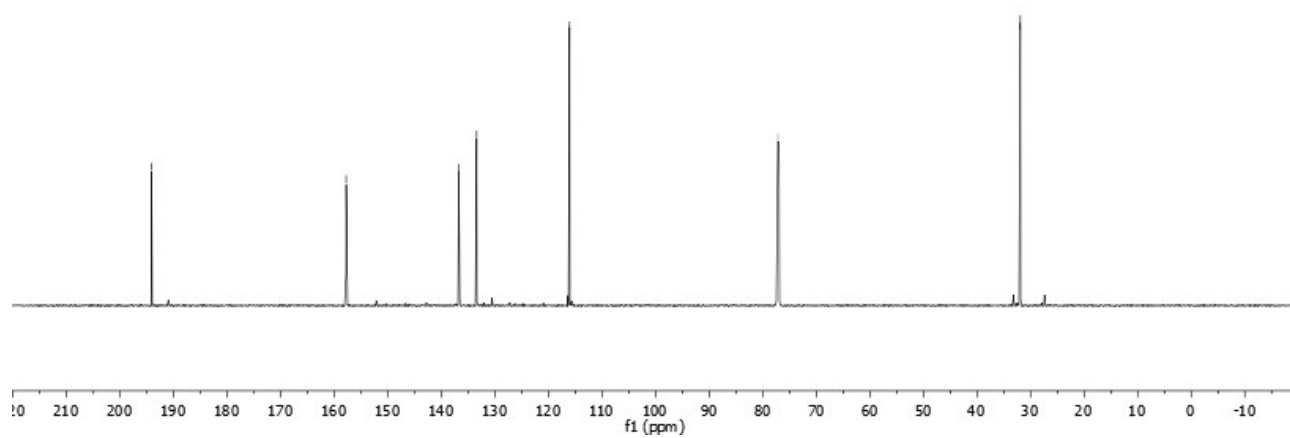
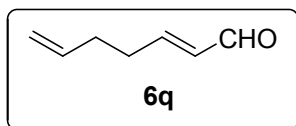
133.40

116.05

77.16 CDCl3

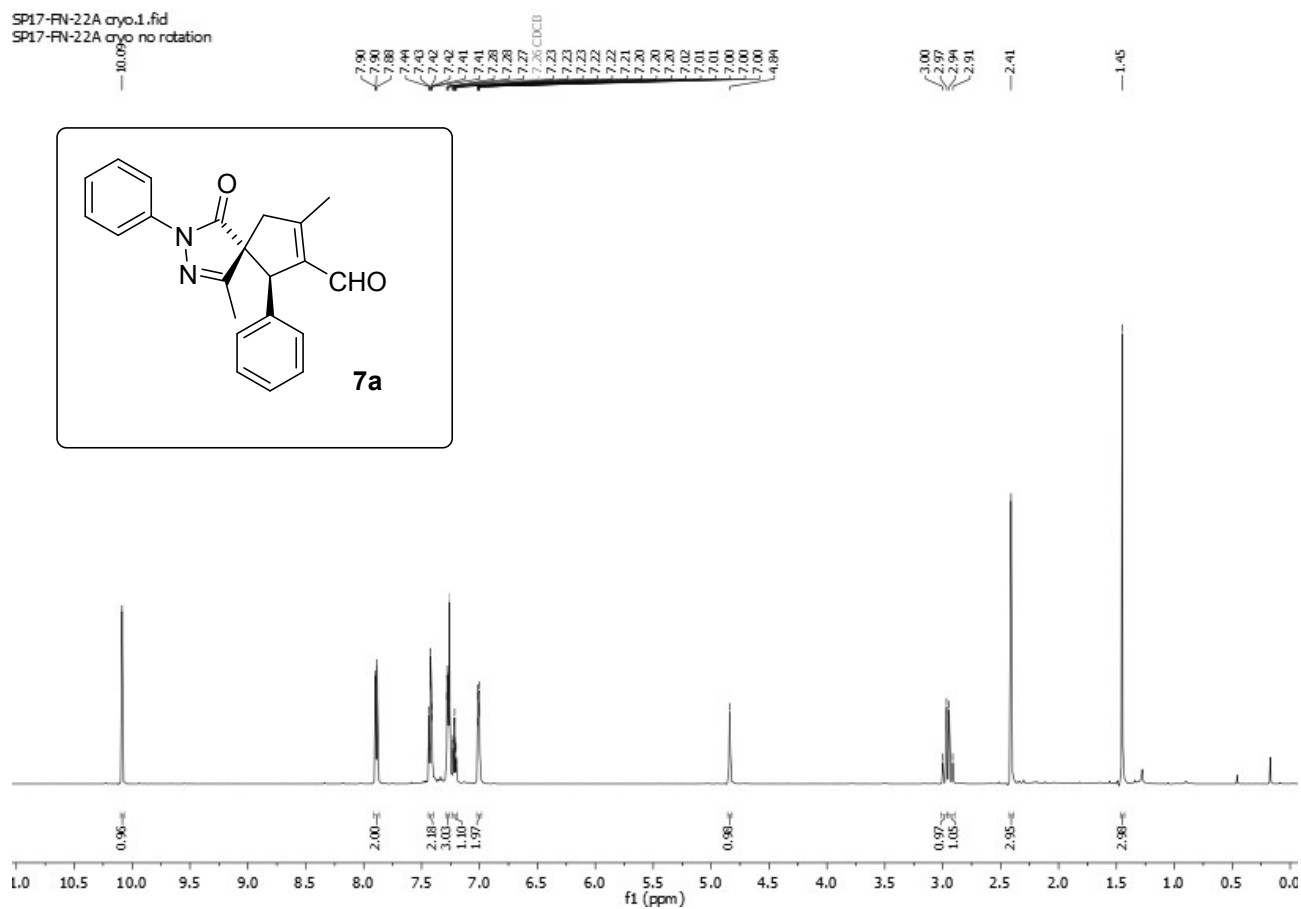
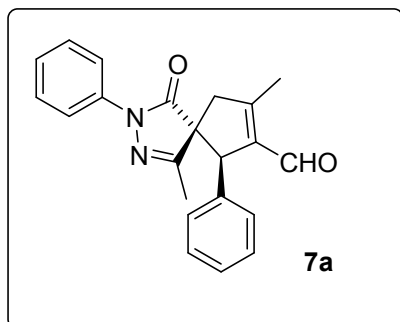
31.94

31.89



(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3,6-diphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7a)

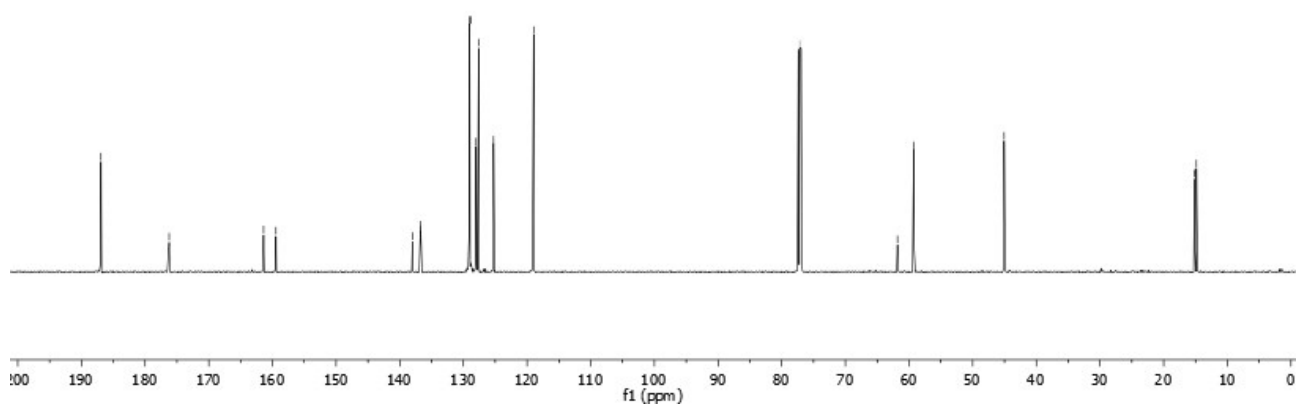
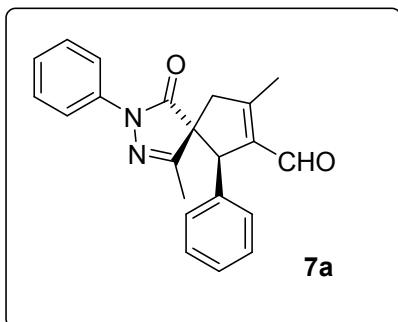
SP17-FN-22A cryo.1.fid
SP17-FN-22A cryo no rotation



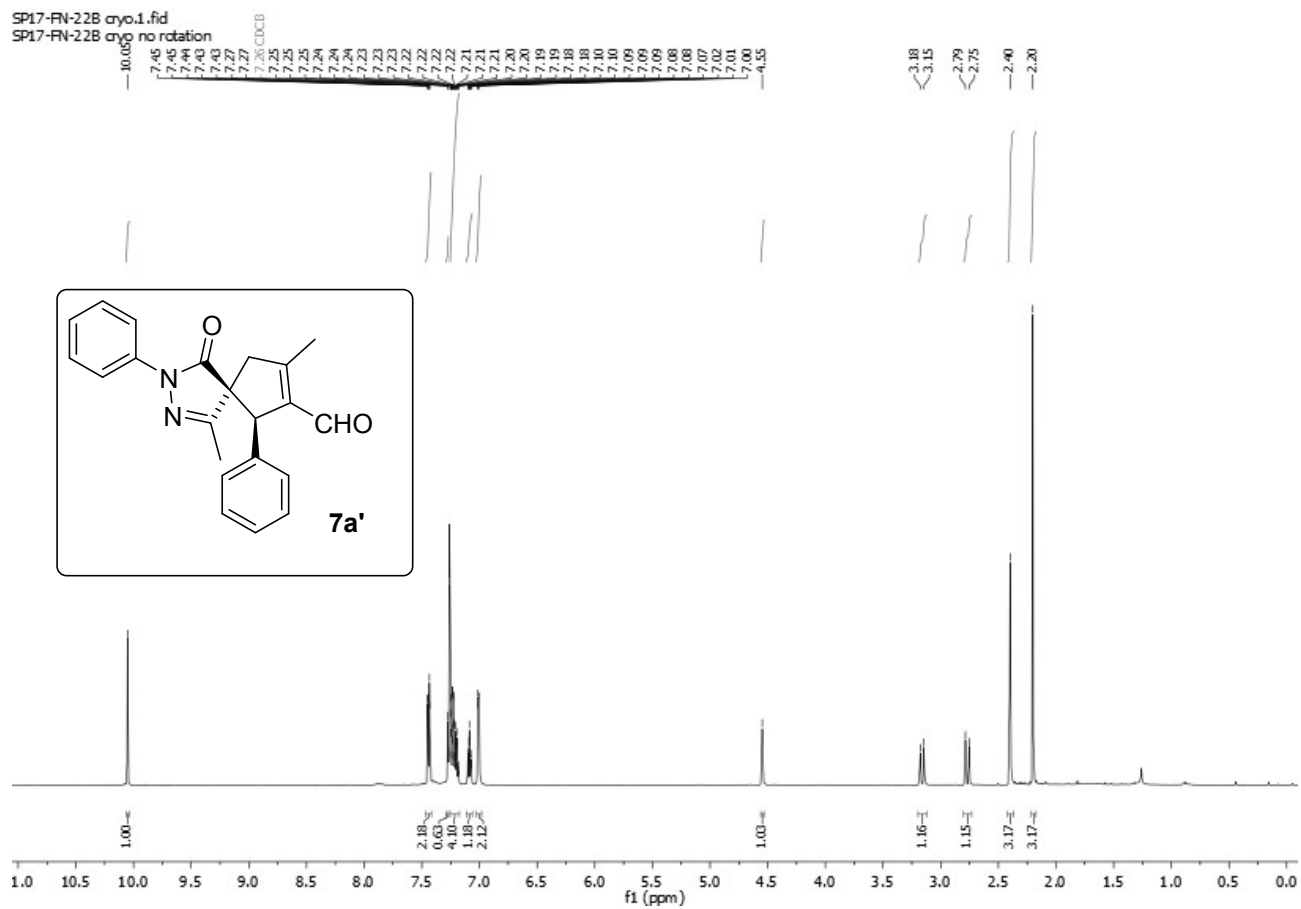
(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3,6-diphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7a)

SP17-FN-22A_cryo.2.fid
SP17-FN-22A_cryo

186.00 176.22 161.39 159.44 138.00 137.06 136.69 129.02 128.83 127.00 125.27 118.97 77.16 CDCl₃ 61.81 59.25 45.06 15.17 14.86



(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3,6-diphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7a')



(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3,6-diphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7a')

SP17-FN-22B cryo.2.fid
SP17-FN-22B cryo

186.84

172.93

161.77

160.32

137.57

136.84

135.75

128.77

128.32

127.68

127.04

125.07

119.13

77.16 CDCl₃

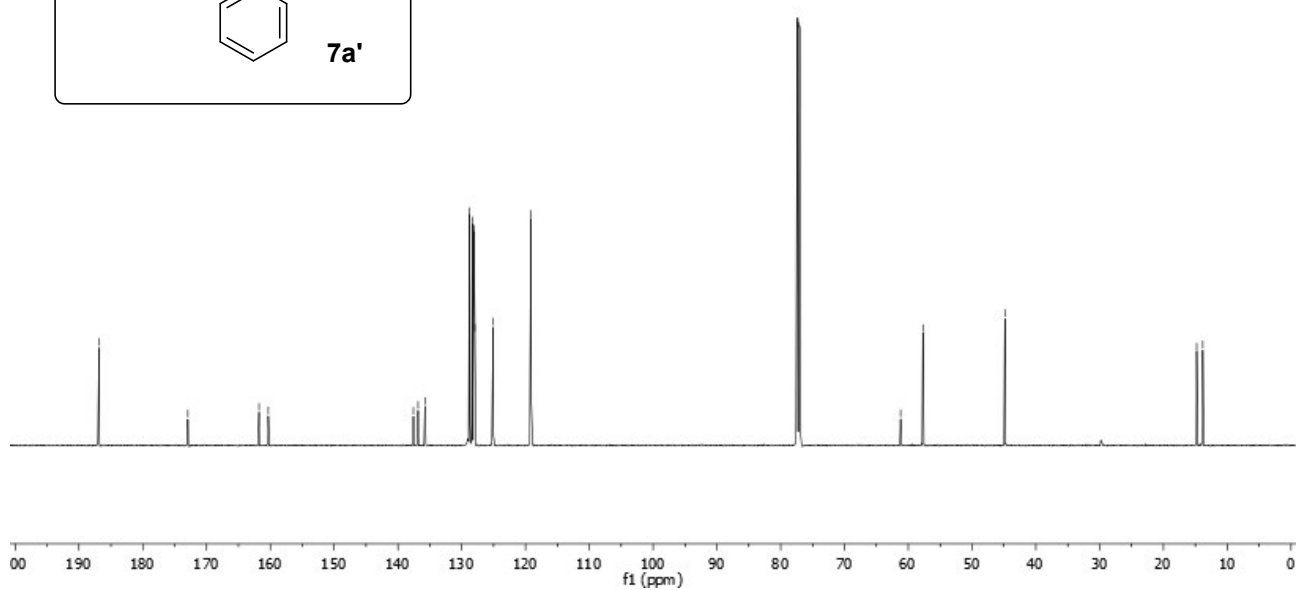
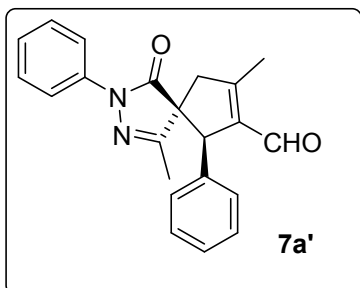
61.21

57.71

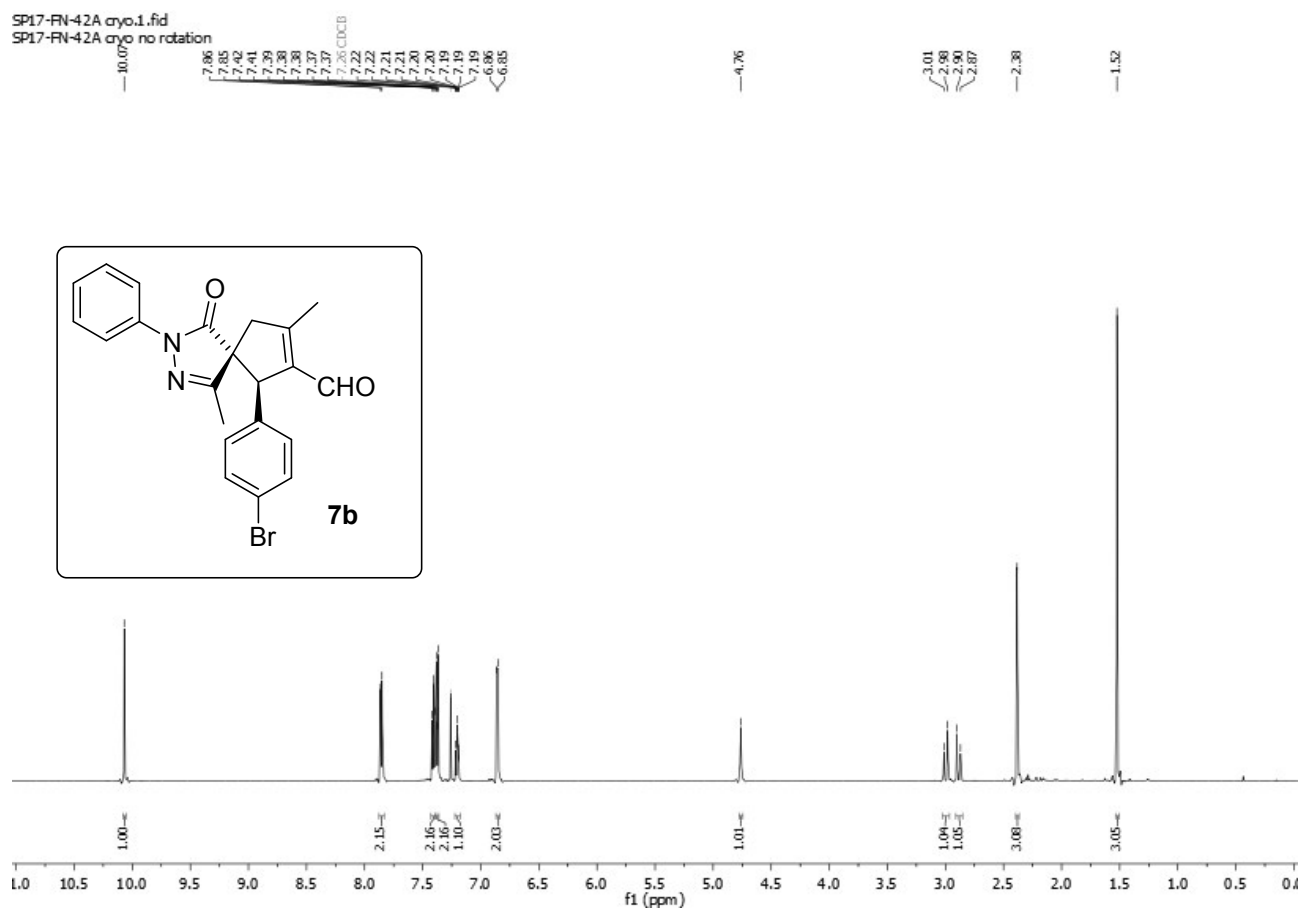
44.86

14.79

13.83



(5*R*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7b)



(5*R*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7b)

SP17-FN-42A cryo.2.fid
SP17-FN-42A cryo.13C

186.67
175.89

160.93
160.19

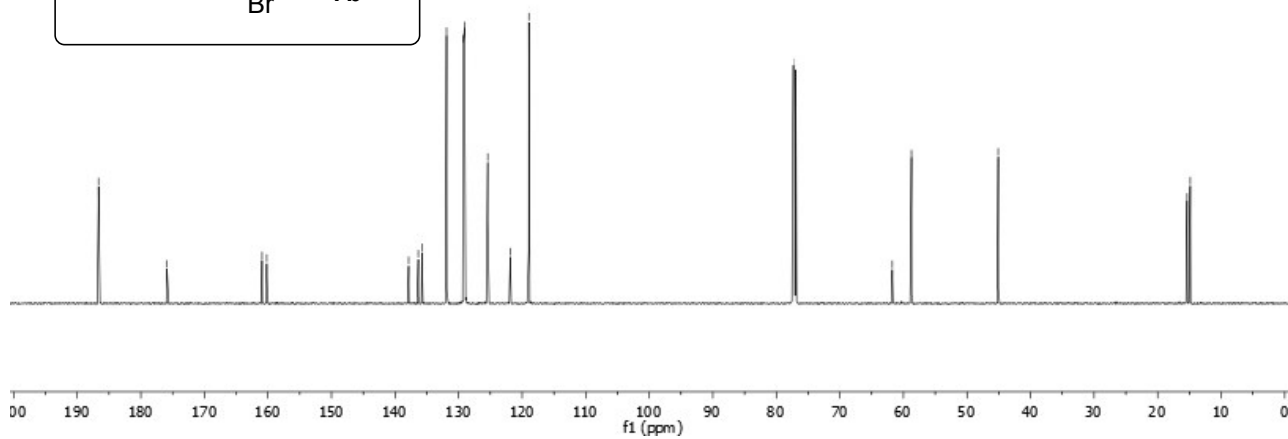
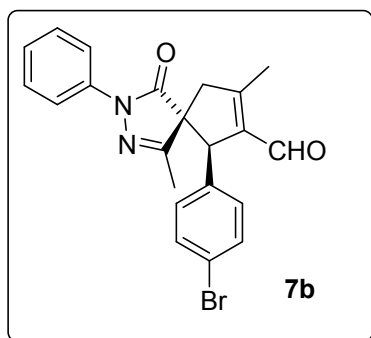
137.86
136.24
135.78
131.90
129.24
125.42
121.87
118.95

77.16 CDCl₃

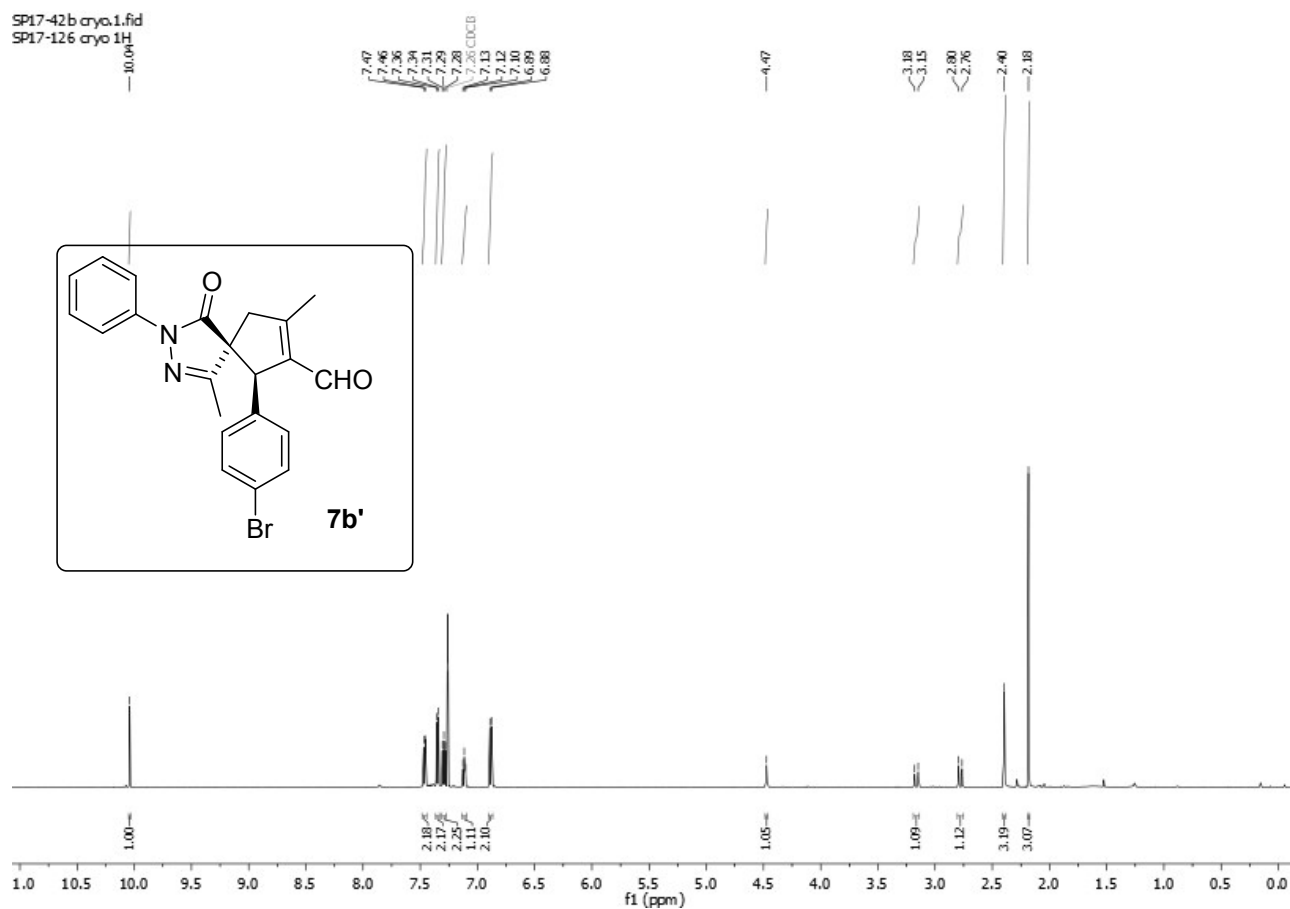
61.75
58.73

45.09

15.37
14.87

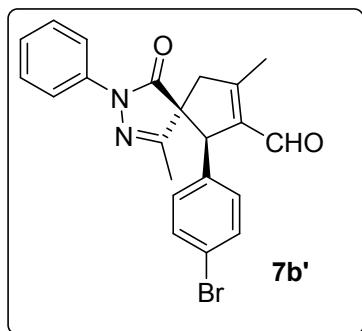
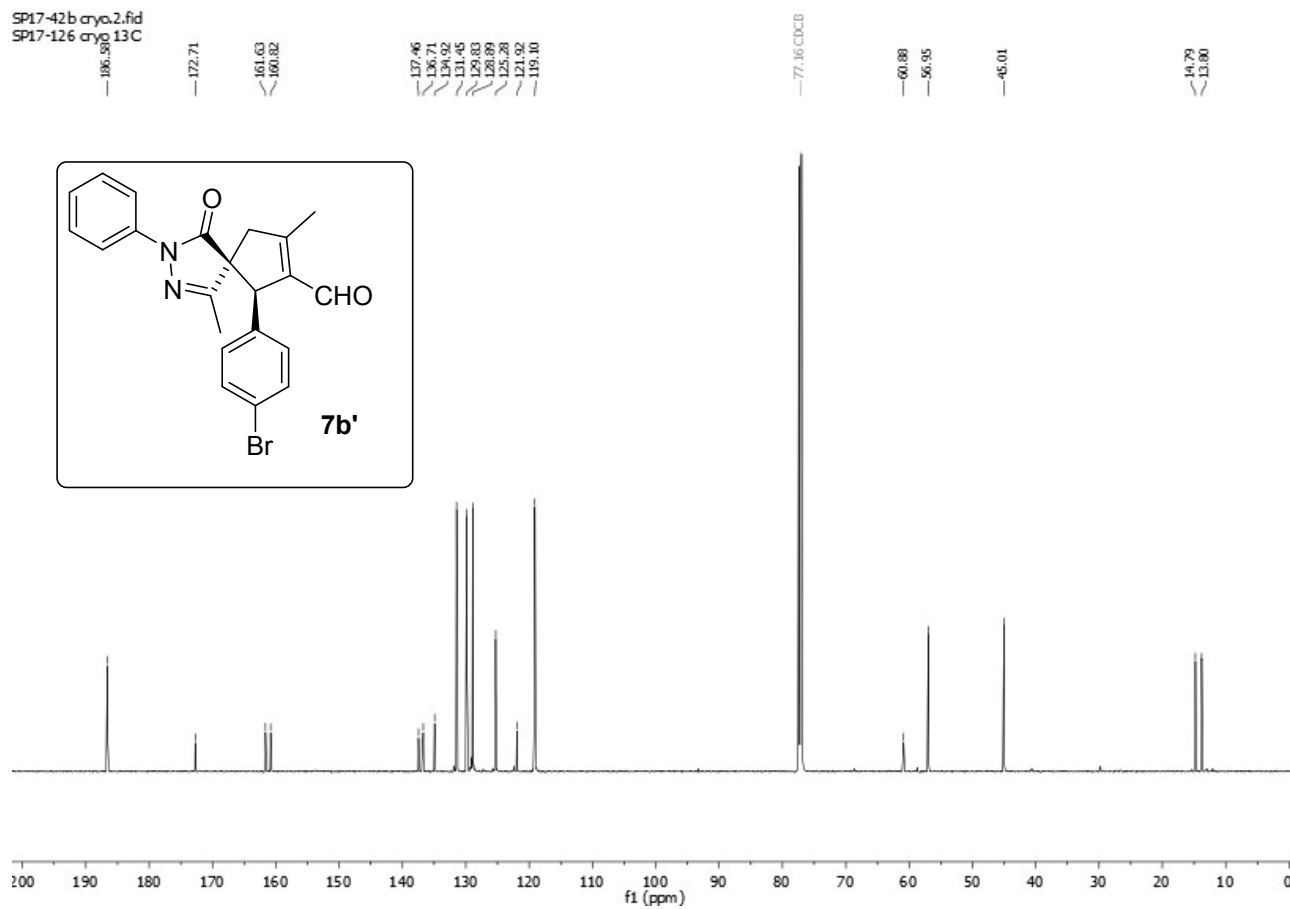


(5*S*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7b')

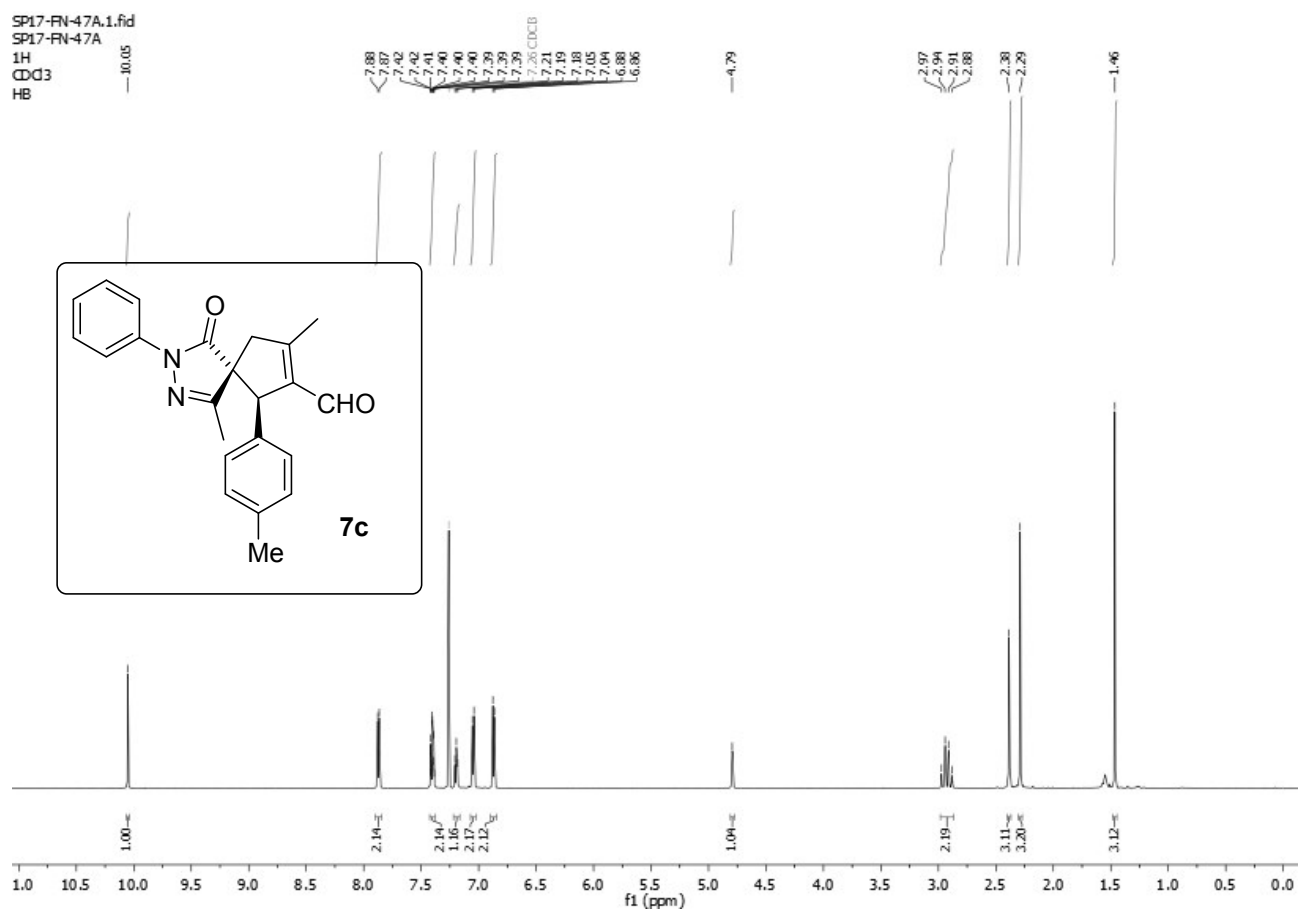


(5*S*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7b')

SP17-42b cryo.2.fid
SP17-126 cryo 13C

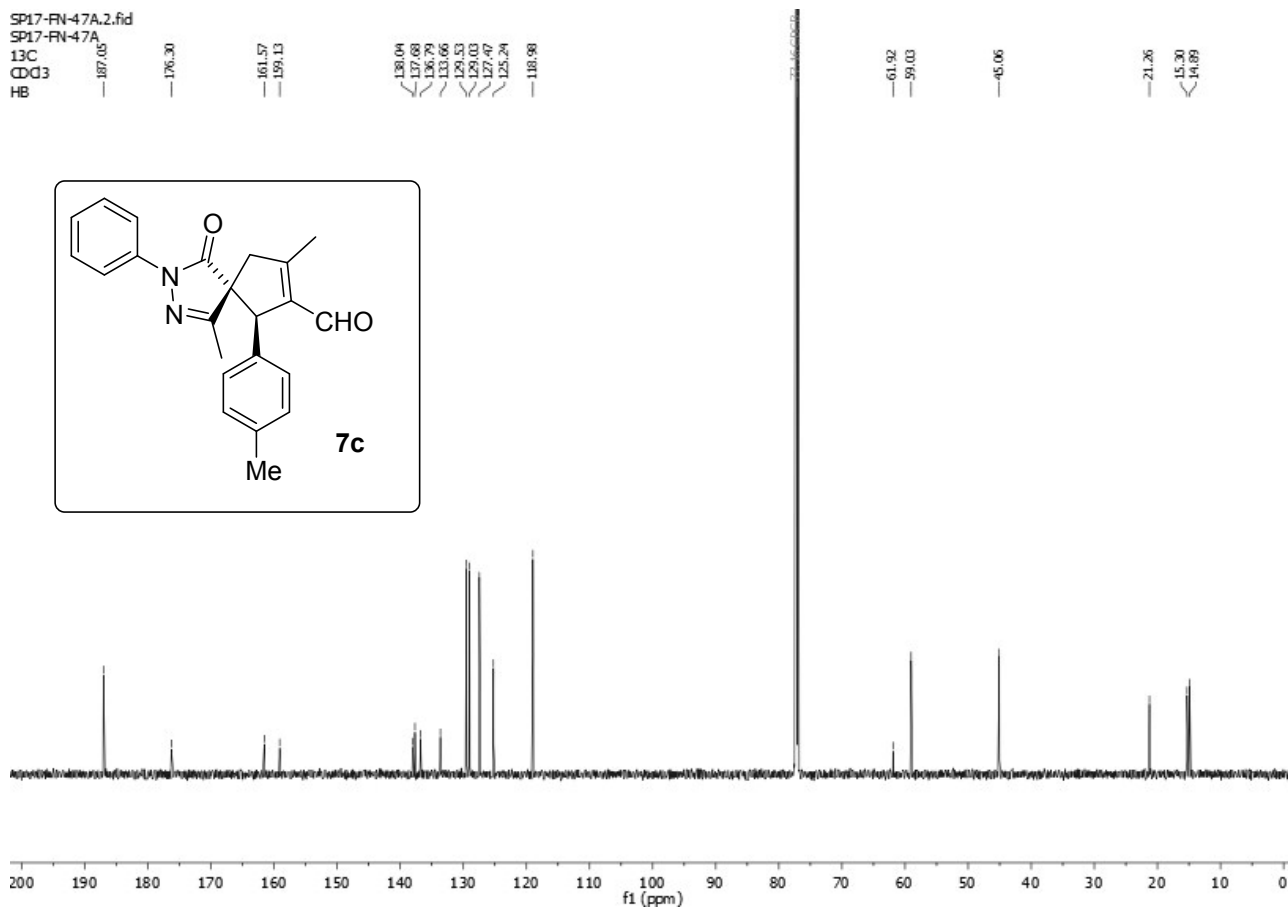
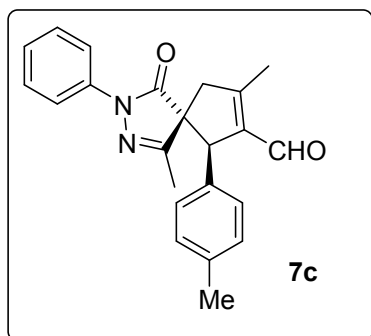


(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*p*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7c)

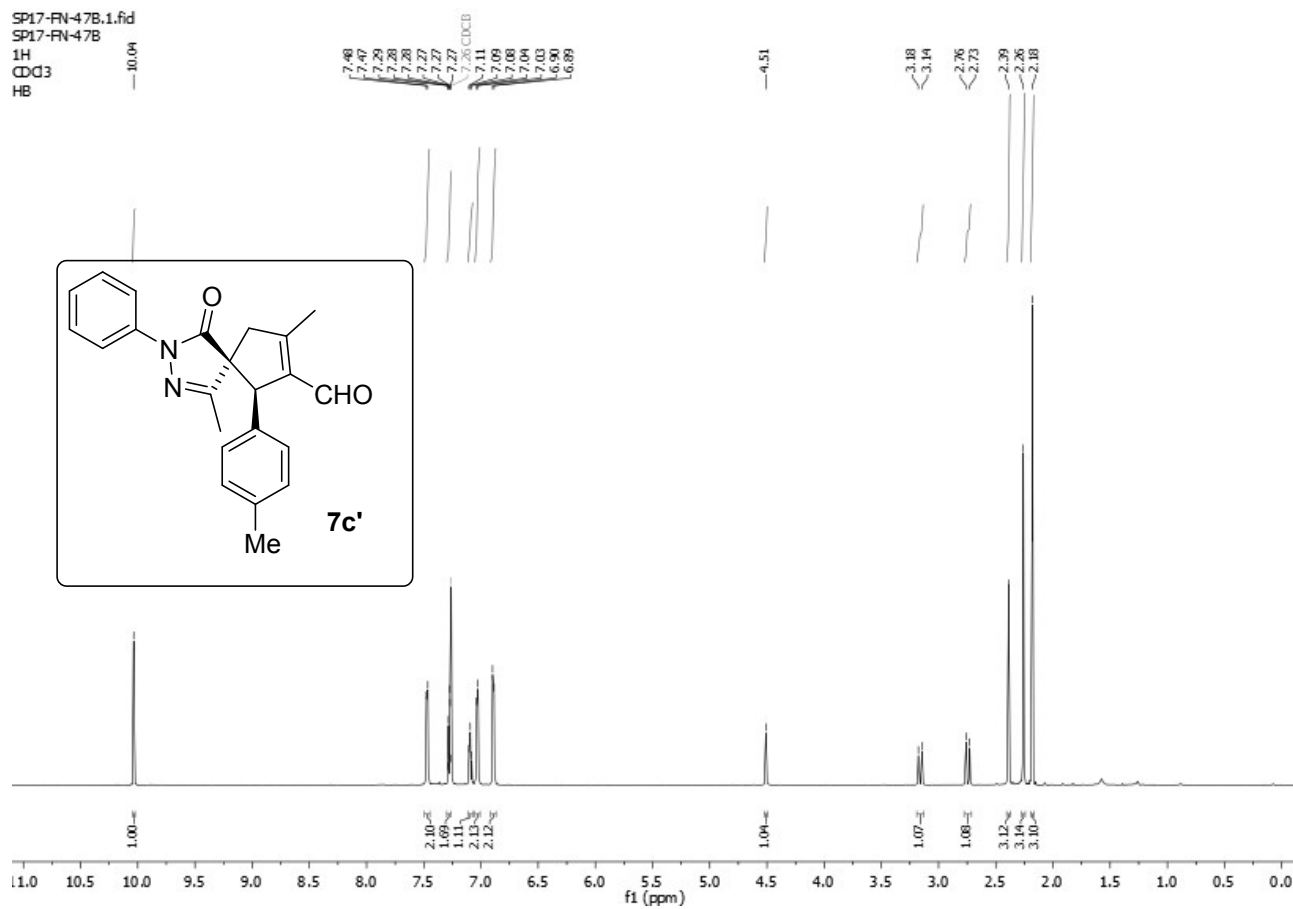


(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*p*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7c)

SP17-FN-47A.2.fid
SP17-FN-47A
13C
CDCl₃
HB



(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*p*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*c'*)



(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*p*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7c')

SP17-FN-47B.2.fid
SP17-FN-47B
13C
CDCl₃
HB

186.99

173.05

162.02

160.12

137.75

137.56

137.12

136.80

128.85

128.07

125.12

119.26

77.26 CDCl₃

61.28

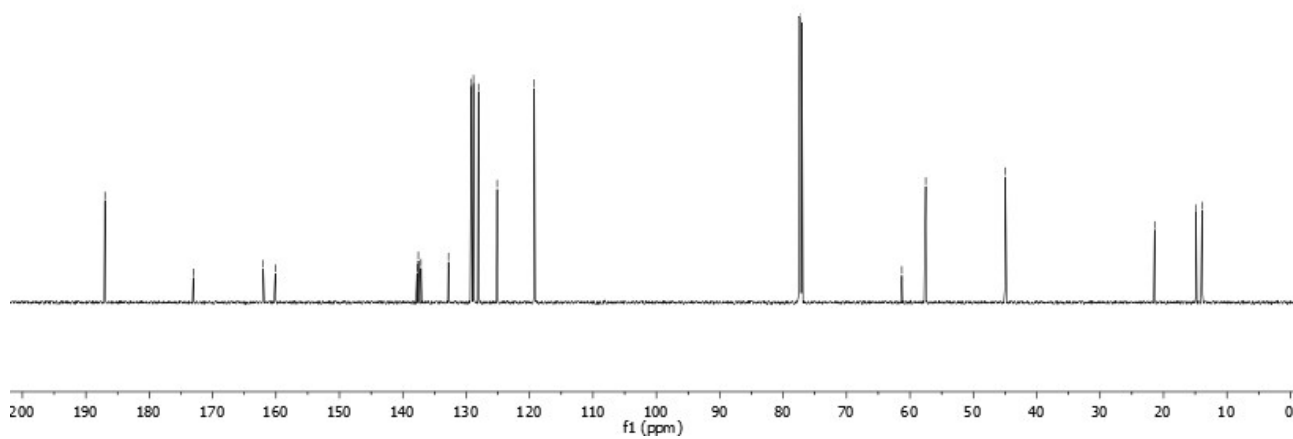
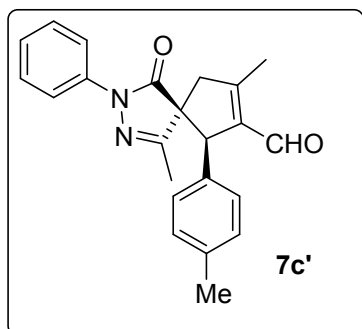
57.51

44.96

21.41

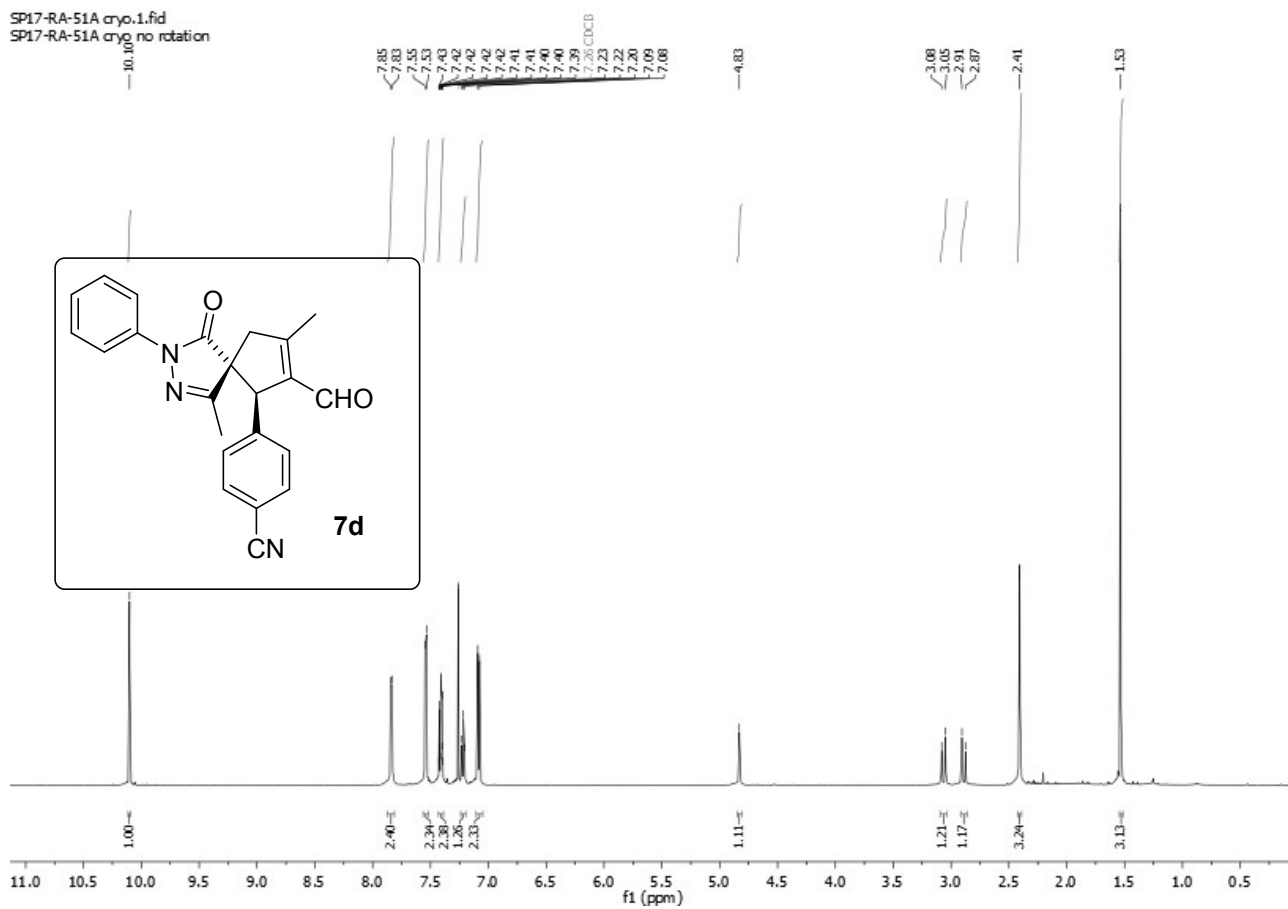
14.87

13.92



4-((5*R*,6*R*)-7-Formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-dien-6-yl)benzonitrile (7d)

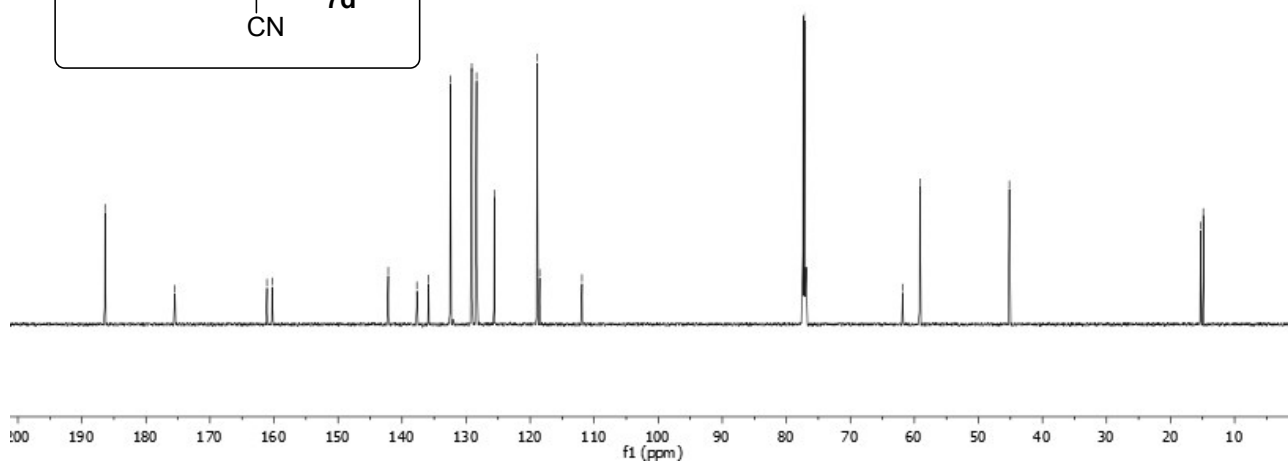
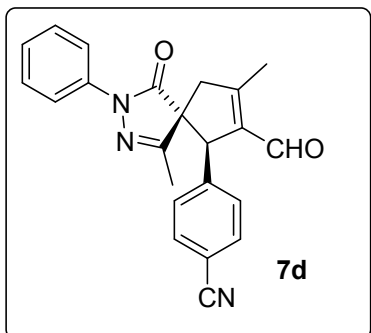
SP17-RA-51A cryo.1.fid
SP17-RA-51A cryo no rotation



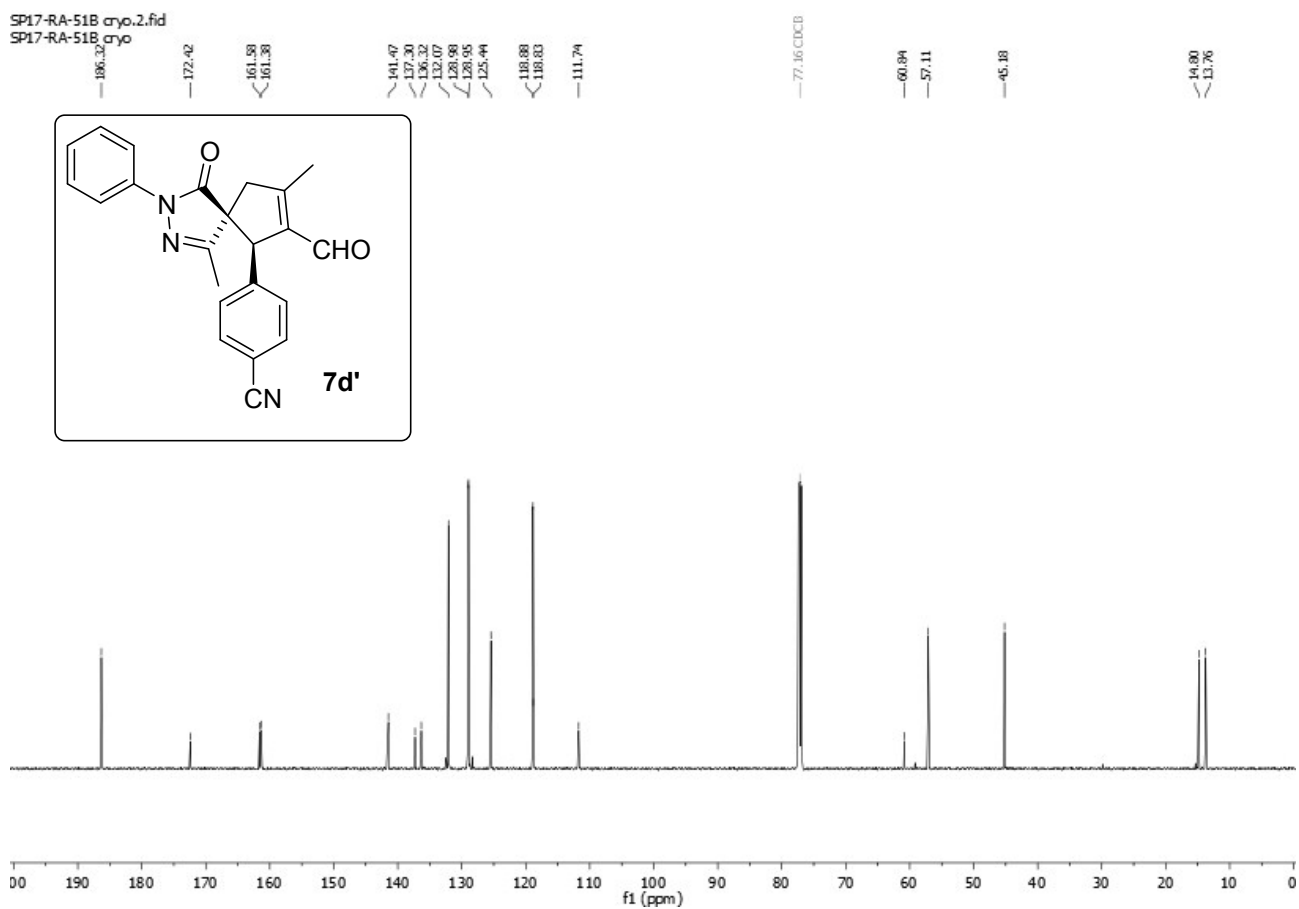
4-((5*R*,6*R*)-7-Formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-dien-6-yl)benzonitrile (7d)

SP17-RA-51A cryo.2.fid
SP17-RA-51A cryo

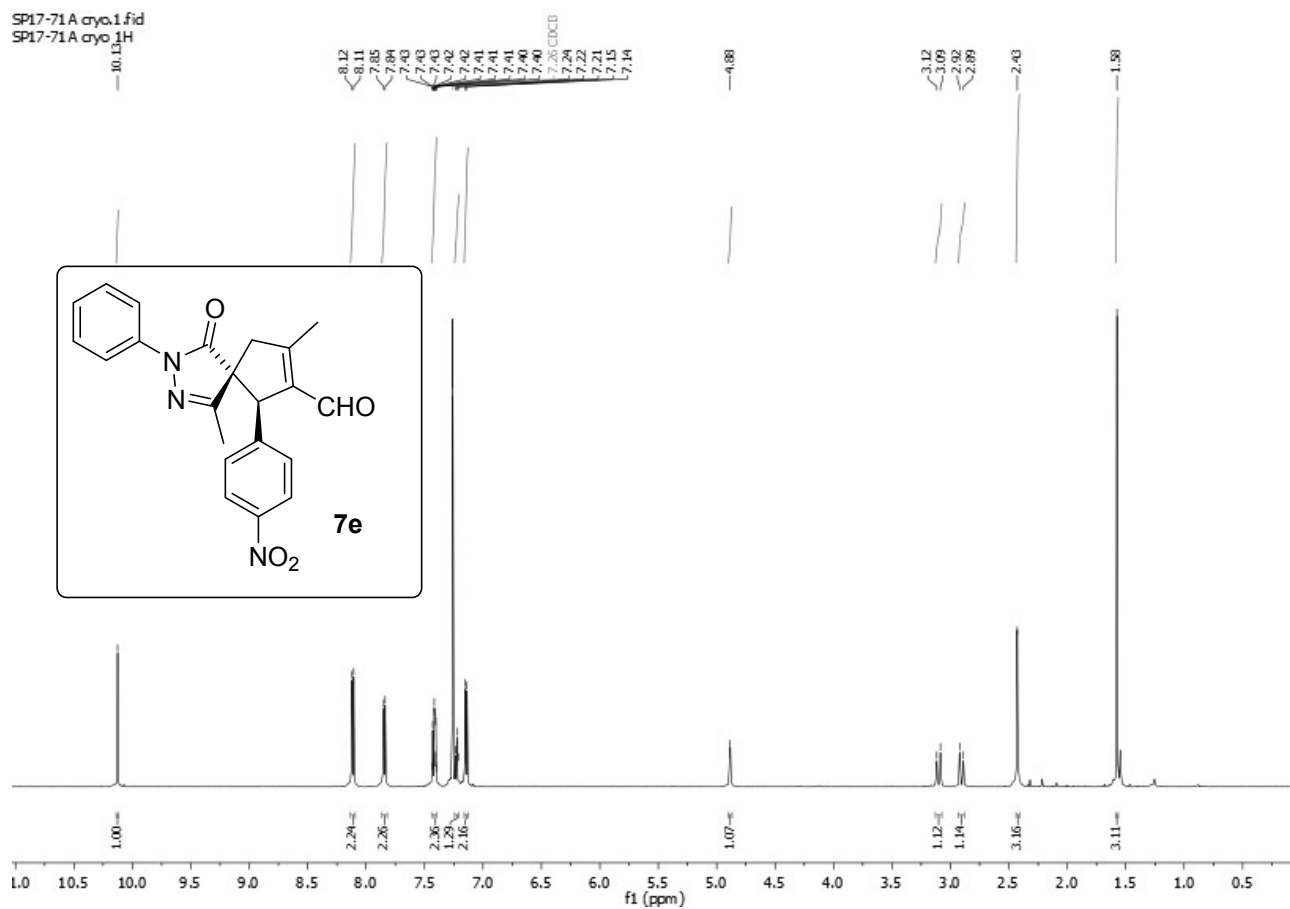
186.90 175.47 161.10 160.31 142.16 137.70 135.86 132.96 129.12 128.37 125.61 118.92 118.52 111.91 77.16 CDCl₃ 61.83 59.15 46.17 15.32 14.89



4-((5*S*,6*R*)-7-Formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-dien-6-yl)benzotrile (7d')

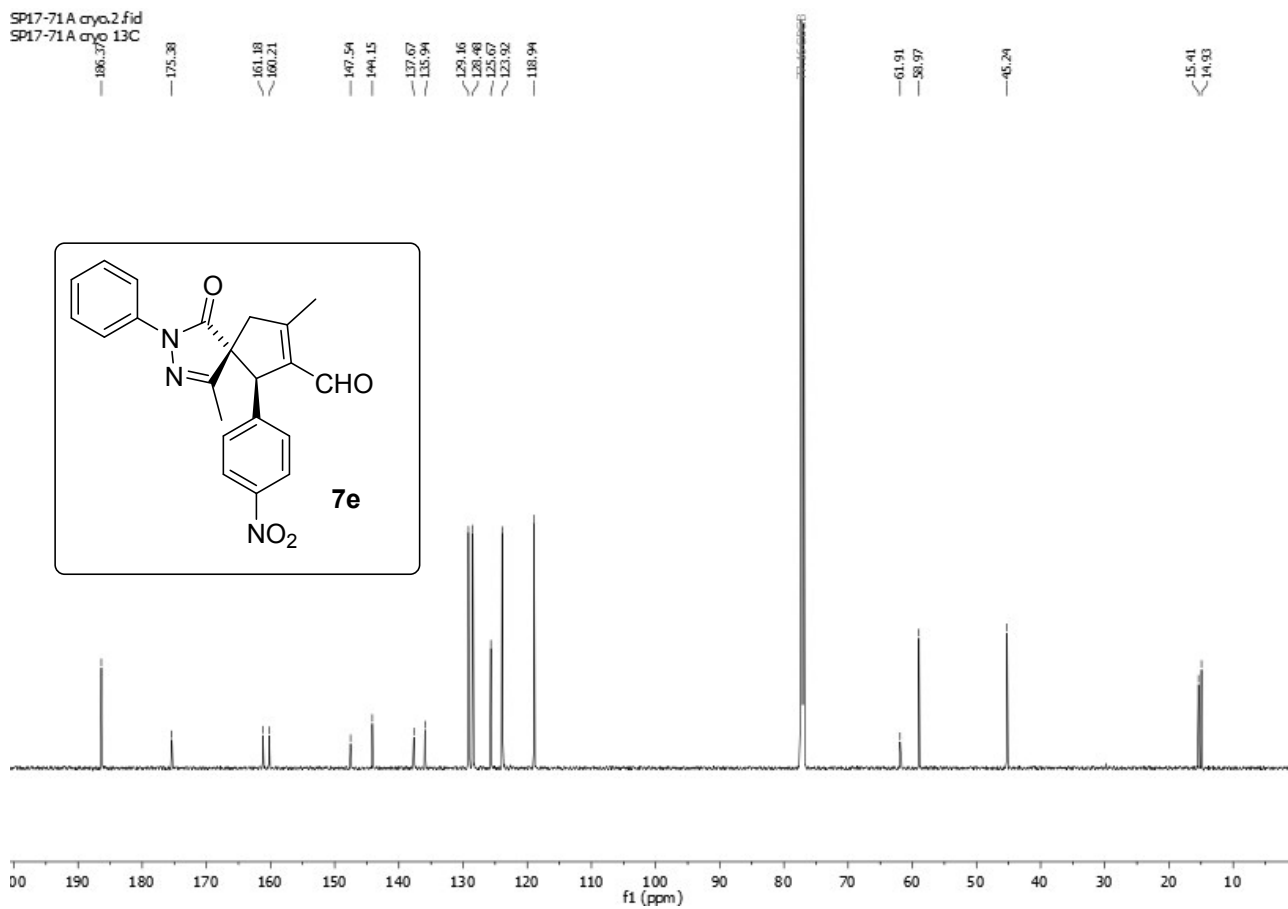


(5*R*,6*R*)-1,8-Dimethyl-6-(4-nitrophenyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7e)



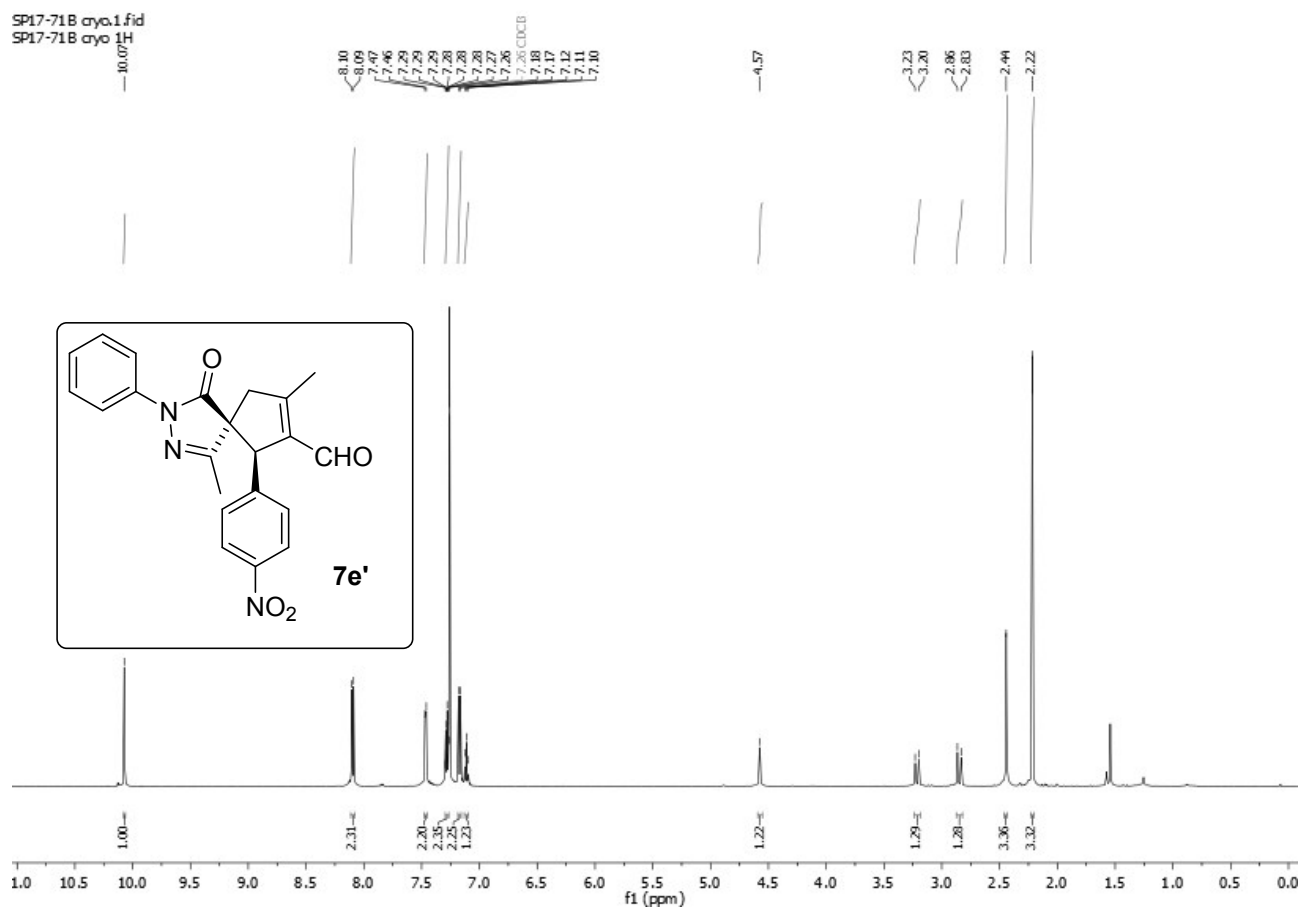
(5*R*,6*R*)-1,8-Dimethyl-6-(4-nitrophenyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7e)

SP17-71A cryo.2.fid
SP17-71A cryo 13C



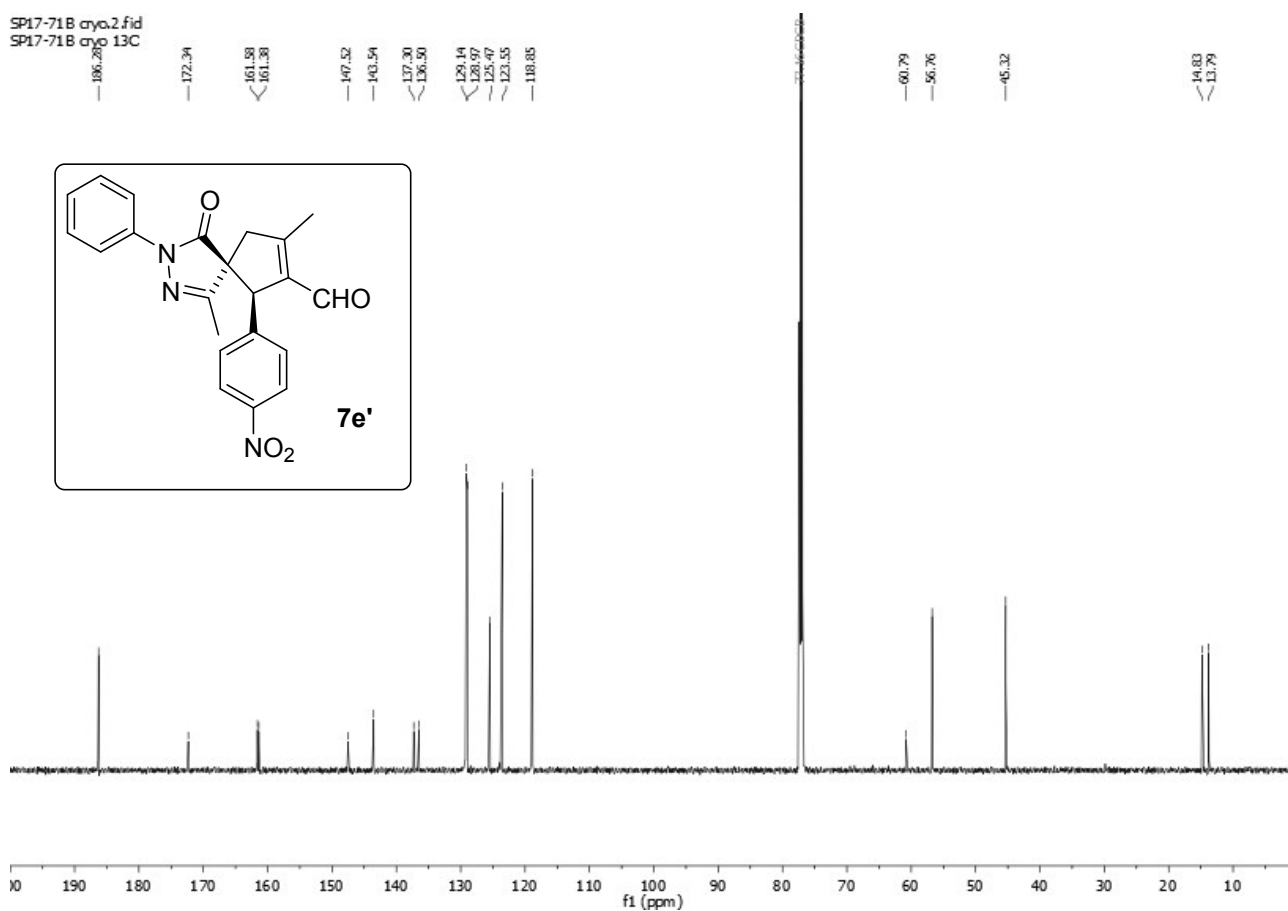
(5*S*,6*R*)-1,8-Dimethyl-6-(4-nitrophenyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7e')

SP17-71B cryo.1.fid
SP17-71B cryo 1H

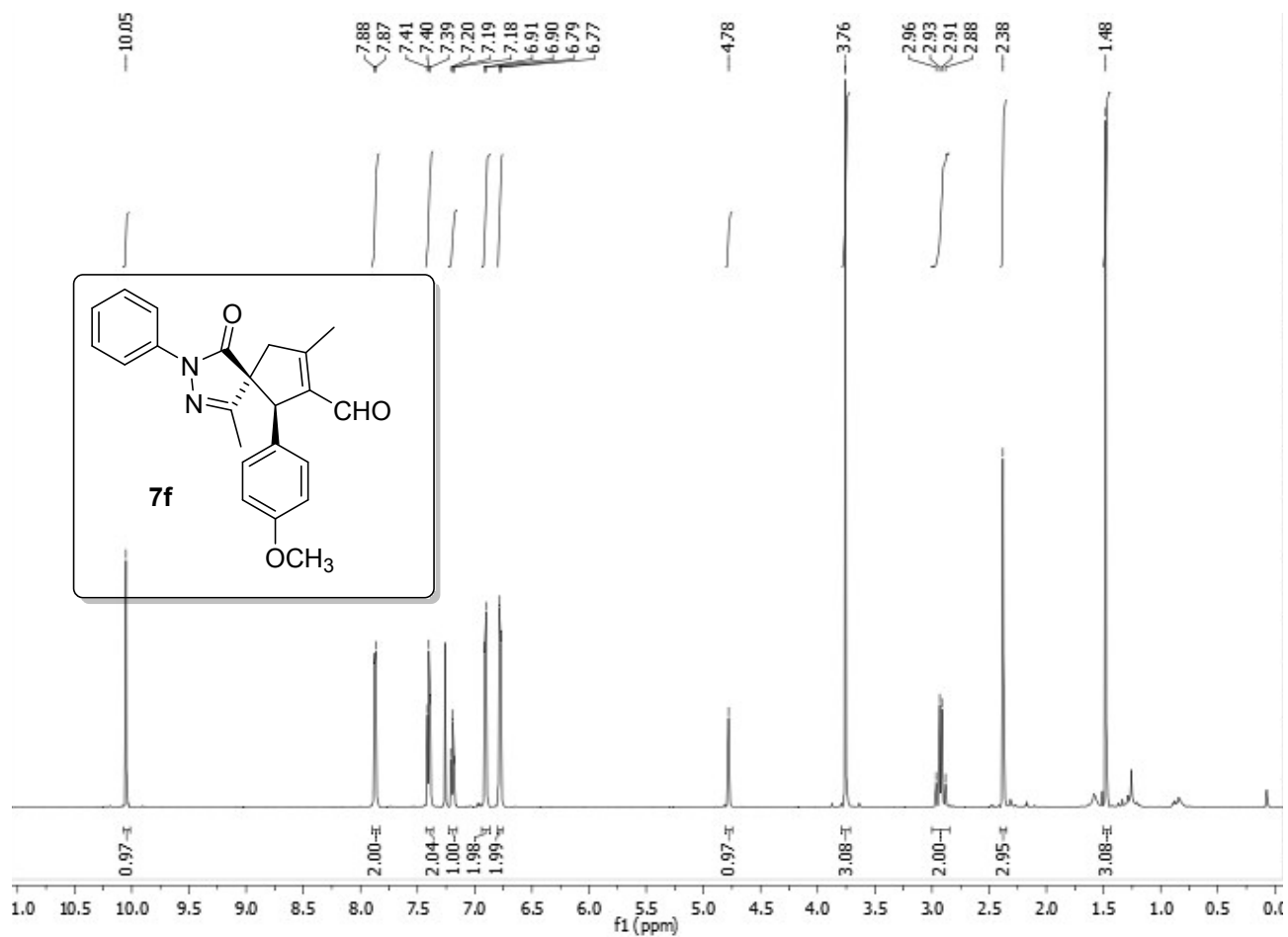


(5*S*,6*R*)-1,8-Dimethyl-6-(4-nitrophenyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7e')

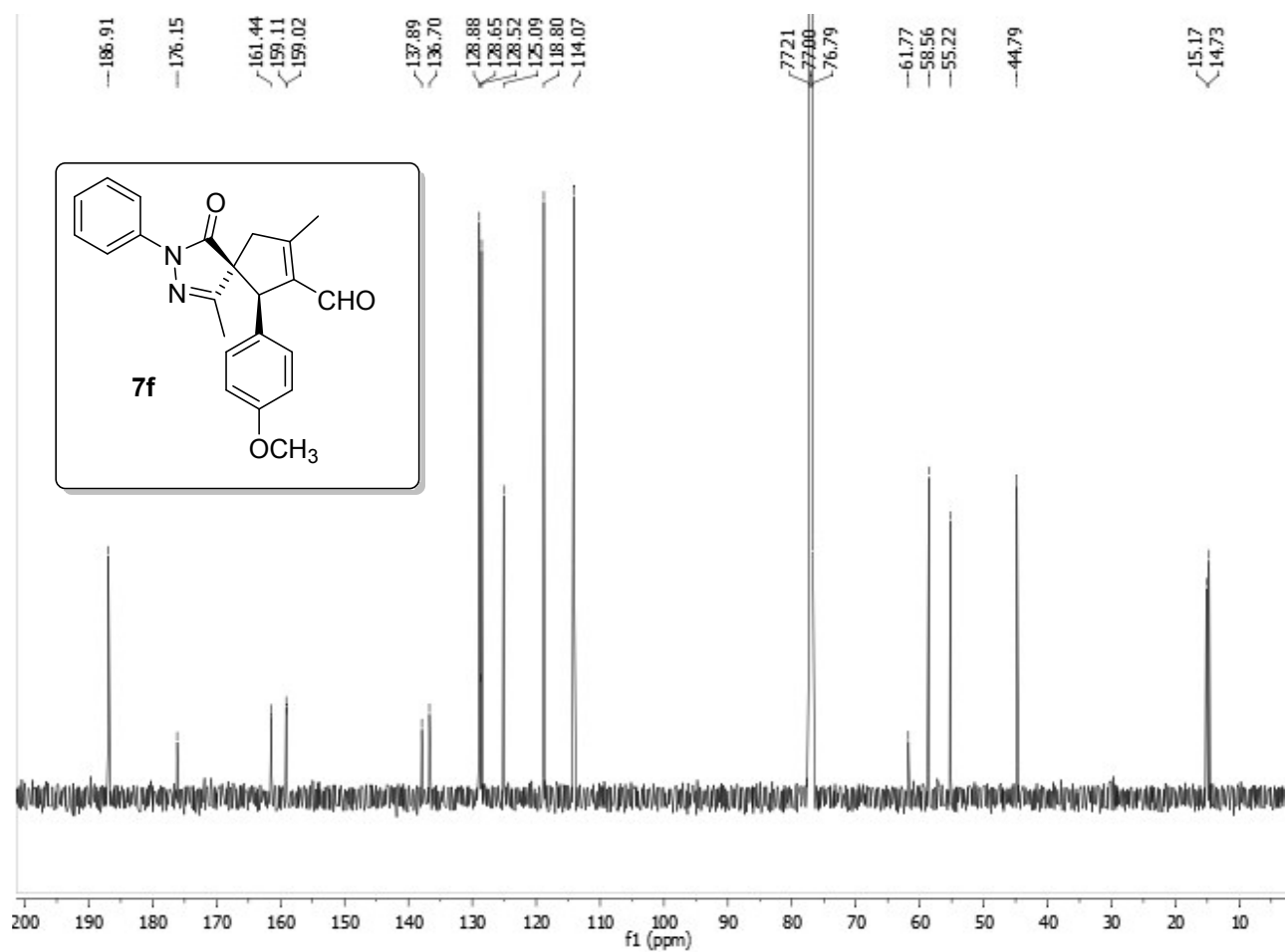
SP17-71B cryo.2.fid
SP17-71B cryo 13C



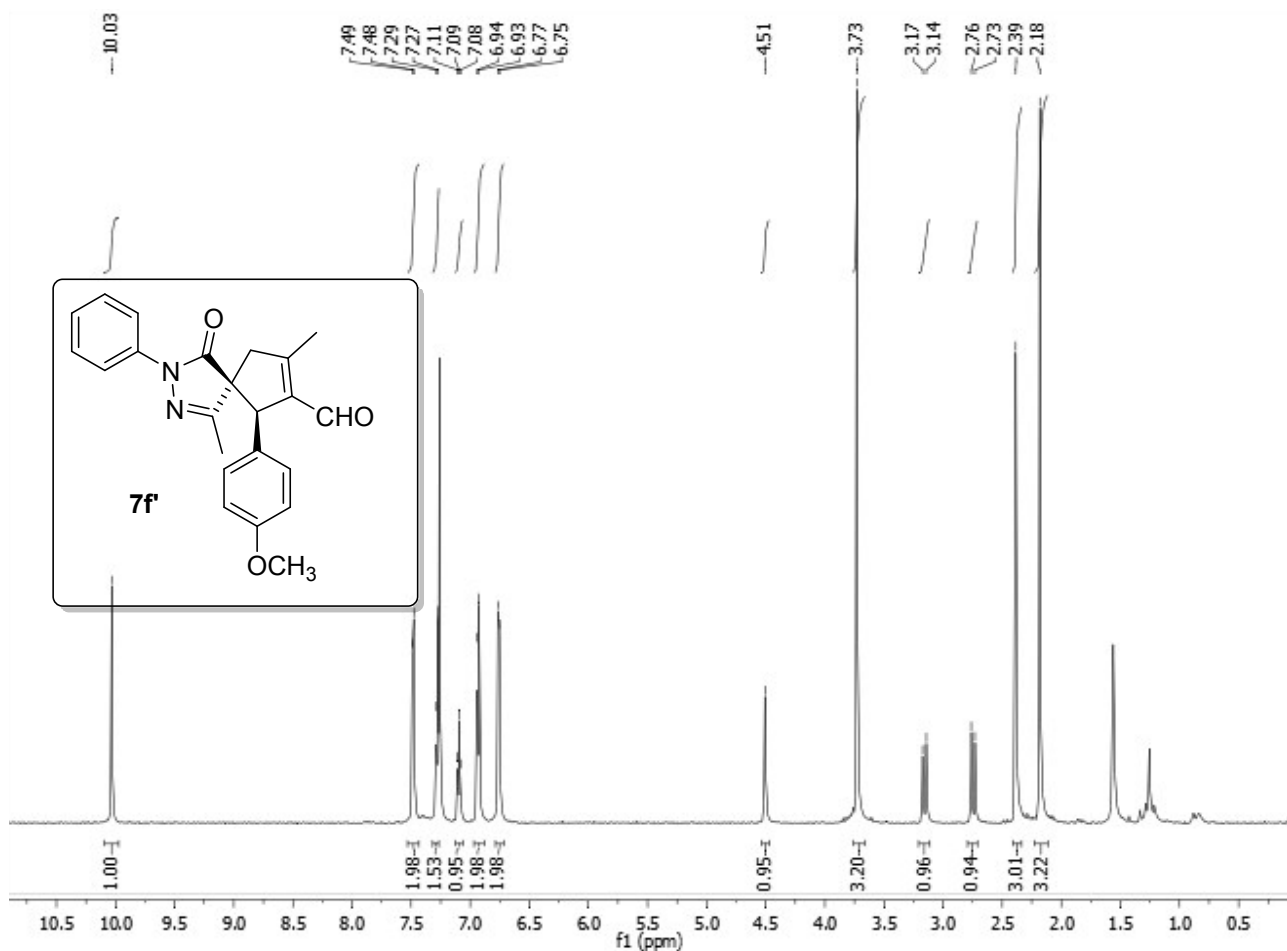
(5*R*,6*R*)-6-(4-Methoxyphenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7f)



(5*R*,6*R*)-6-(4-Methoxyphenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7f)



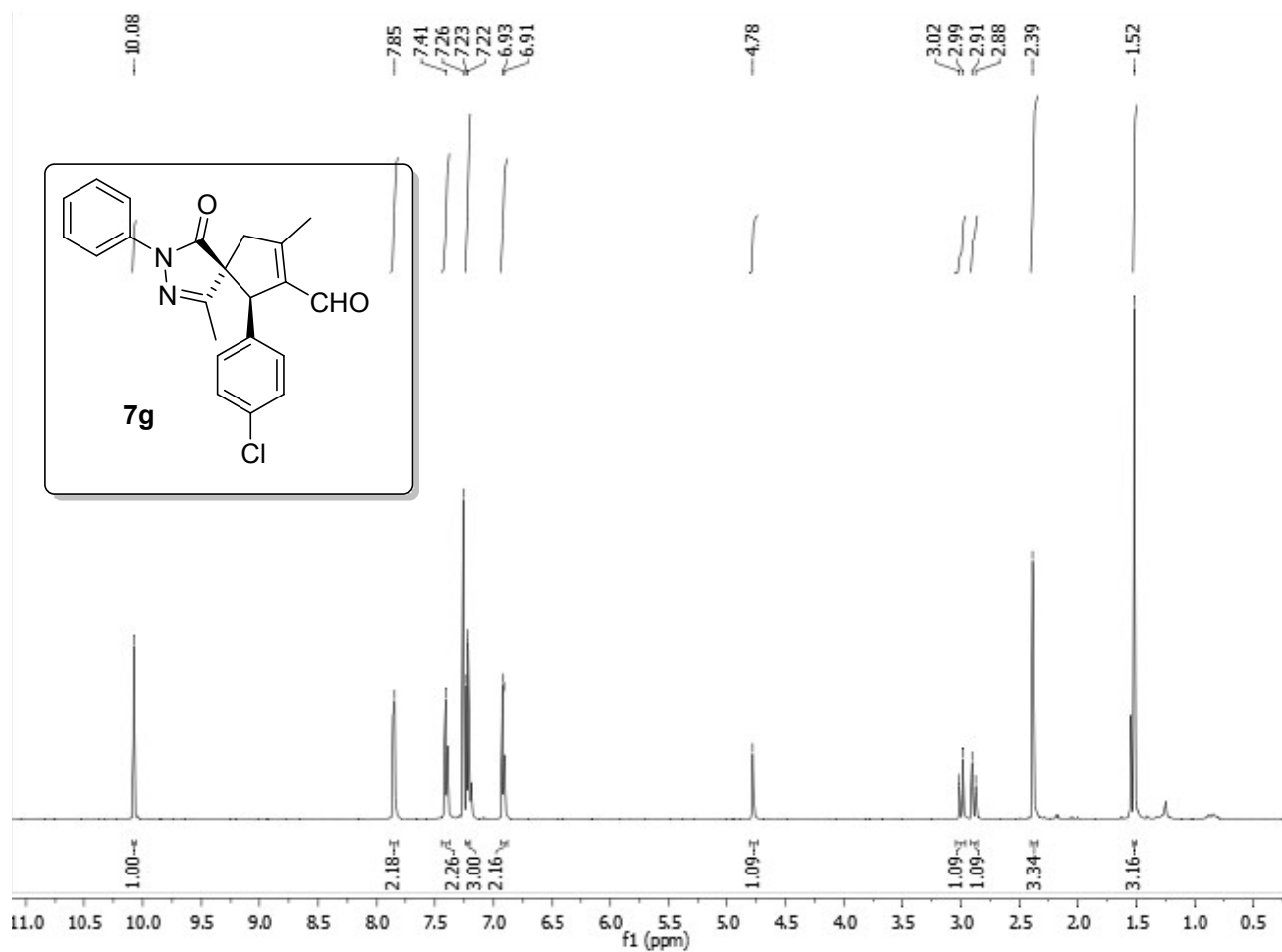
(5*S*,6*R*)-6-(4-Methoxyphenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7f')



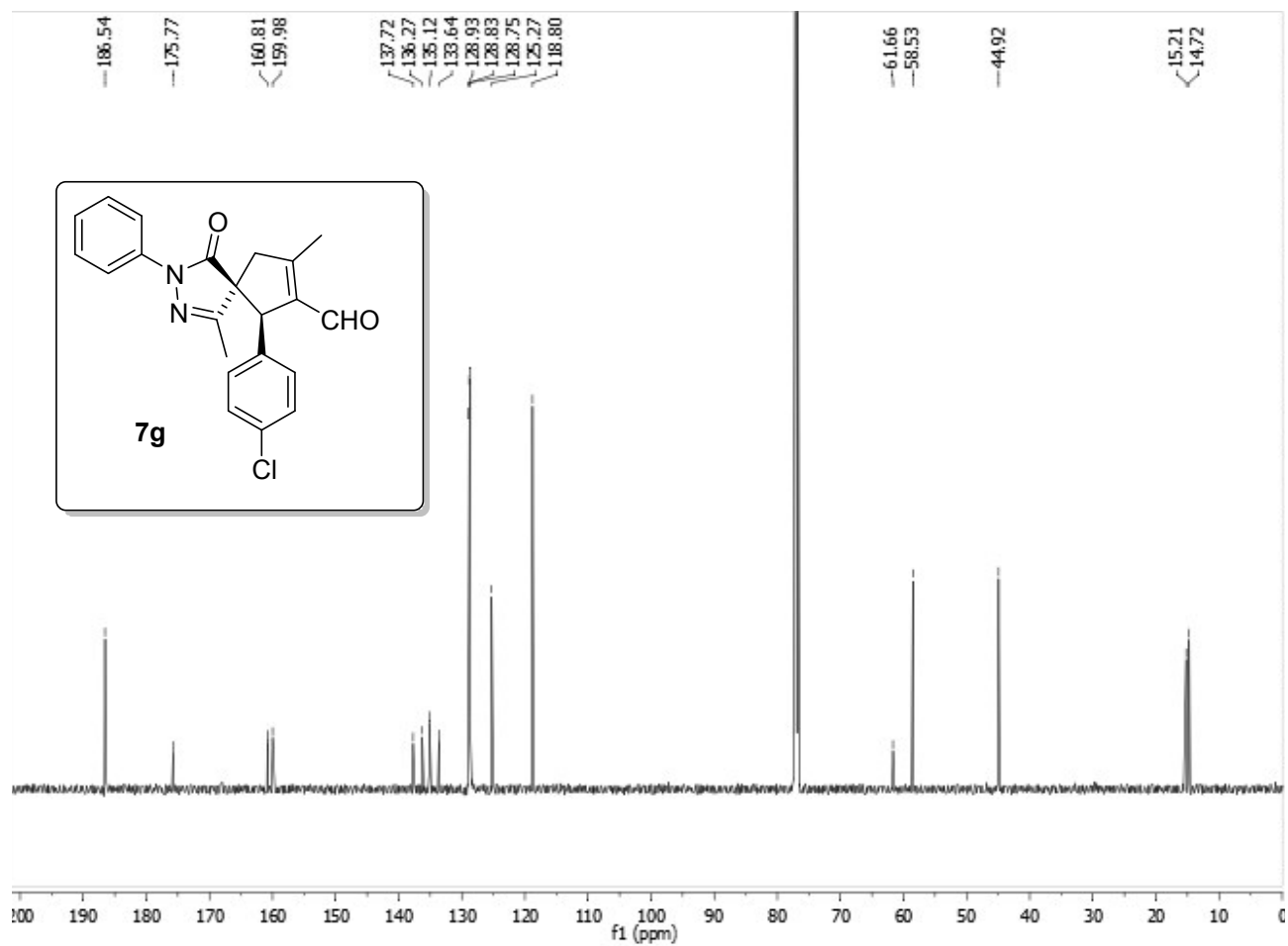
(5*S*,6*R*)-6-(4-Methoxyphenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7f**)**



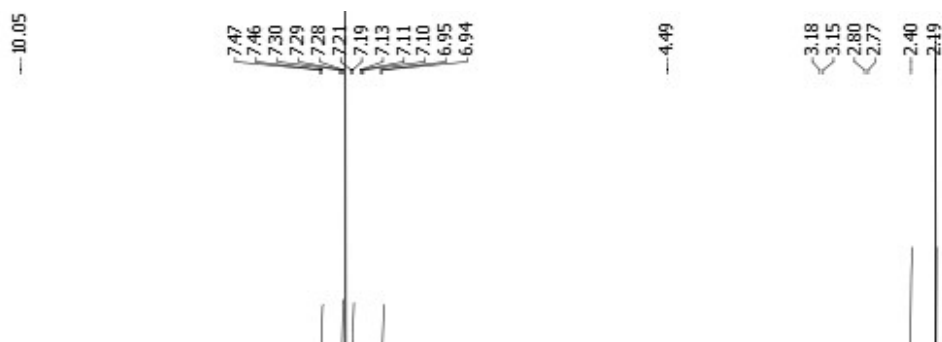
(5*R*,6*R*)-6-(4-Chlorophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7g)

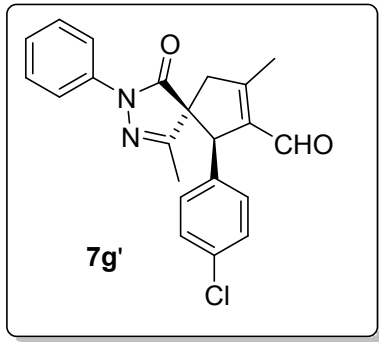


(5*R*,6*R*)-6-(4-Chlorophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7g)

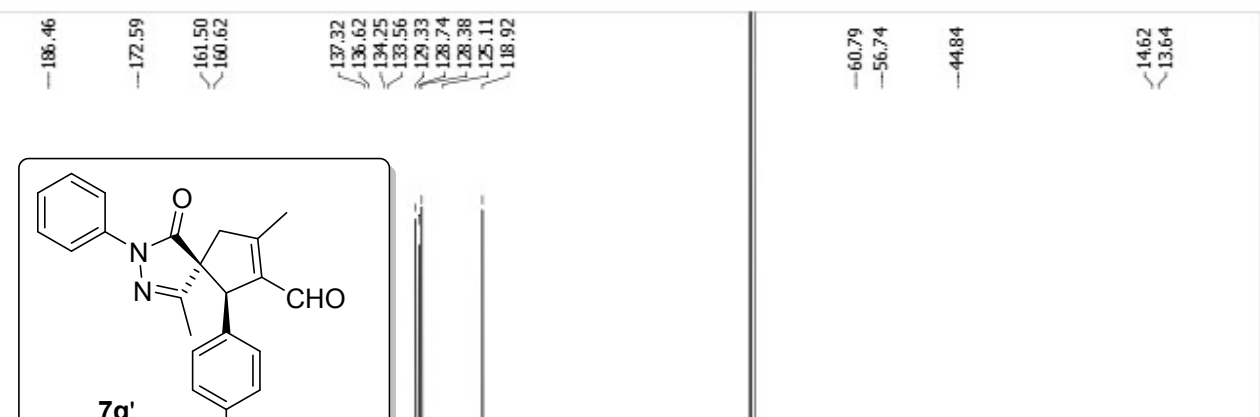


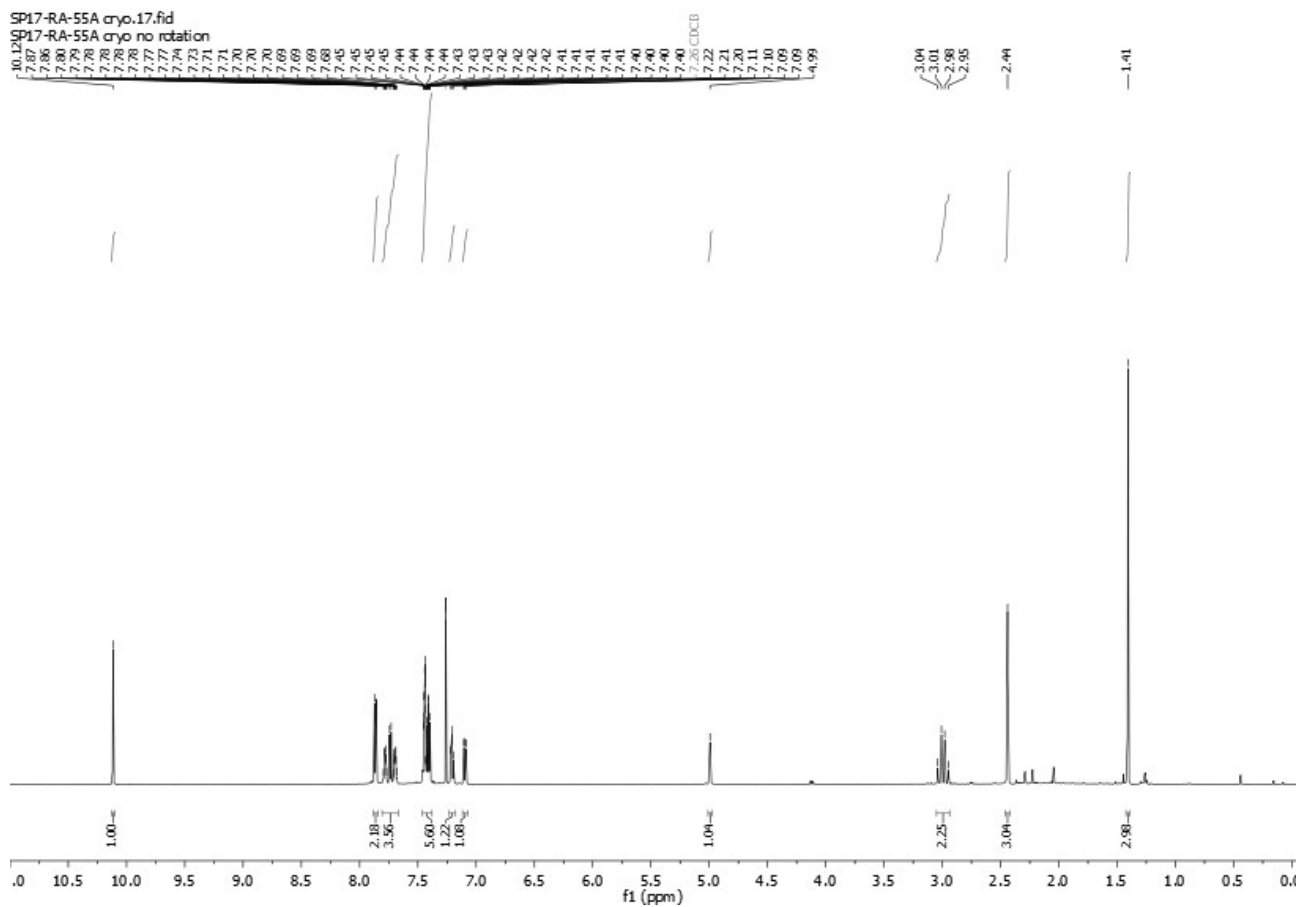
(5*S*,6*R*)-6-(4-Chlorophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7g**)**



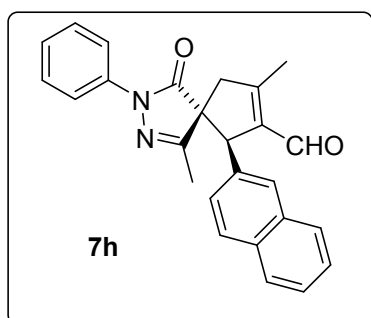


(5*S*,6*R*)-6-(4-Chlorophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7g')

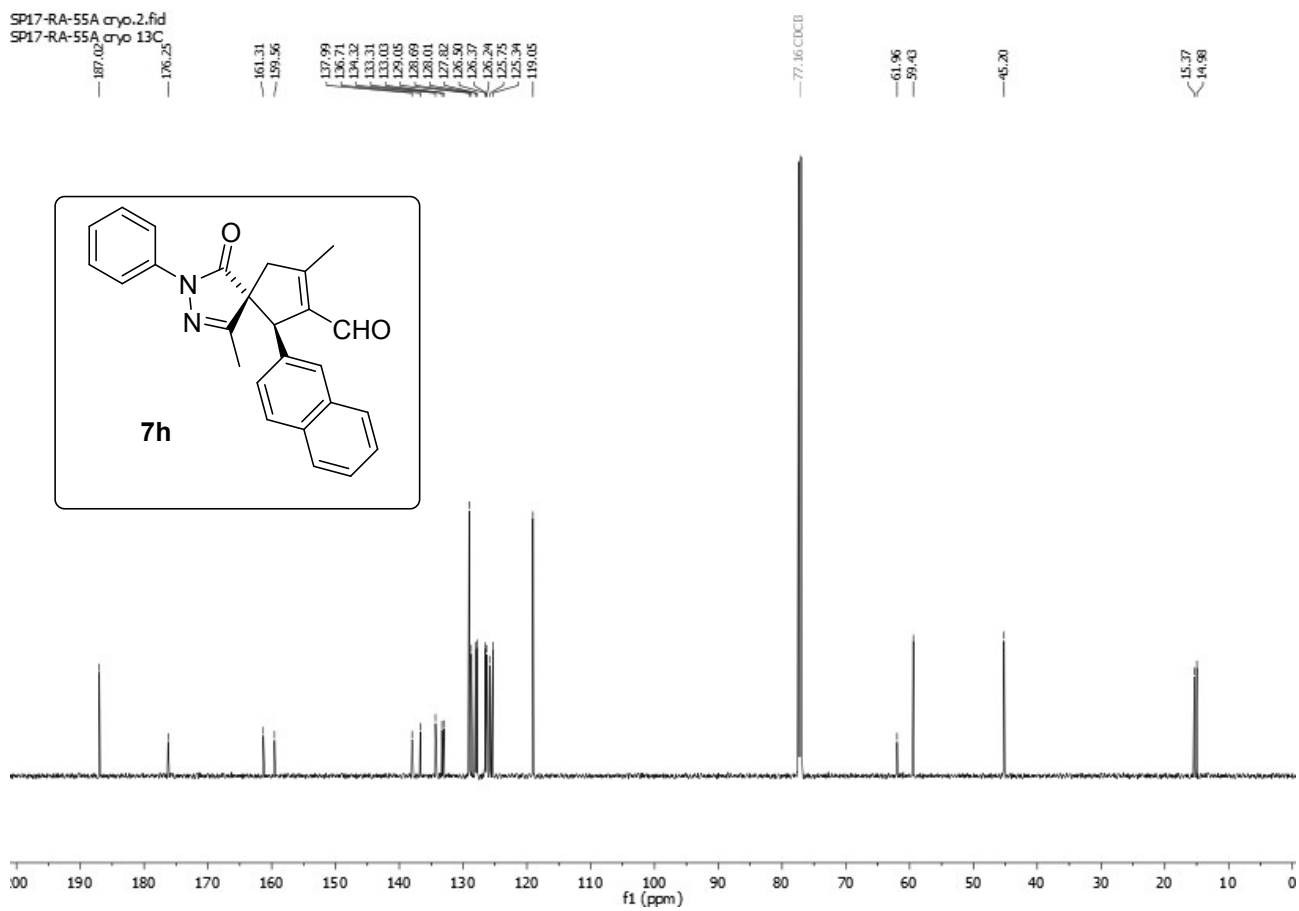




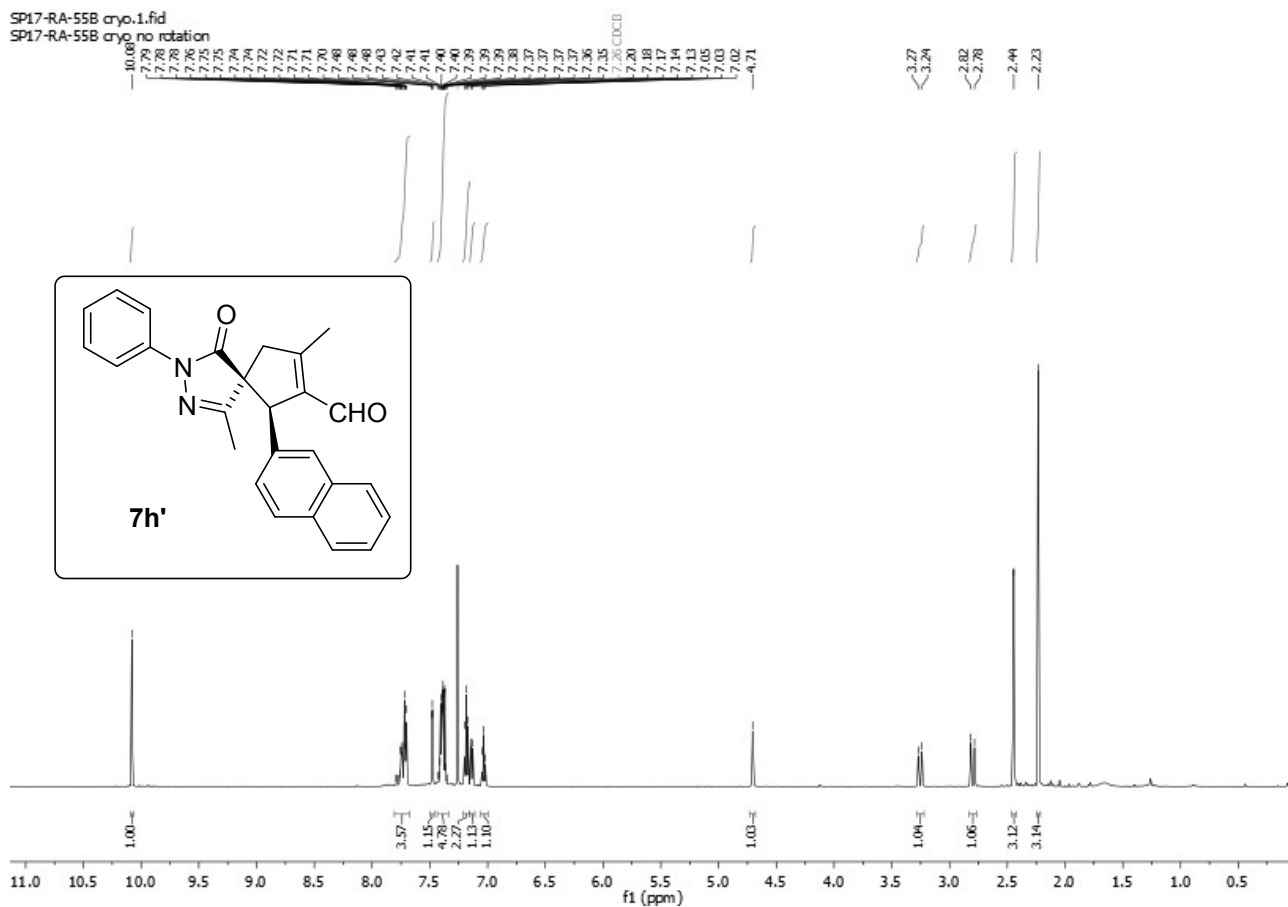
(5*R*,6*R*)-1,8-Dimethyl-6-(2-naphthyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7h)



(5*R*,6*R*)-1,8-Dimethyl-6-(2-naphthyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7h)



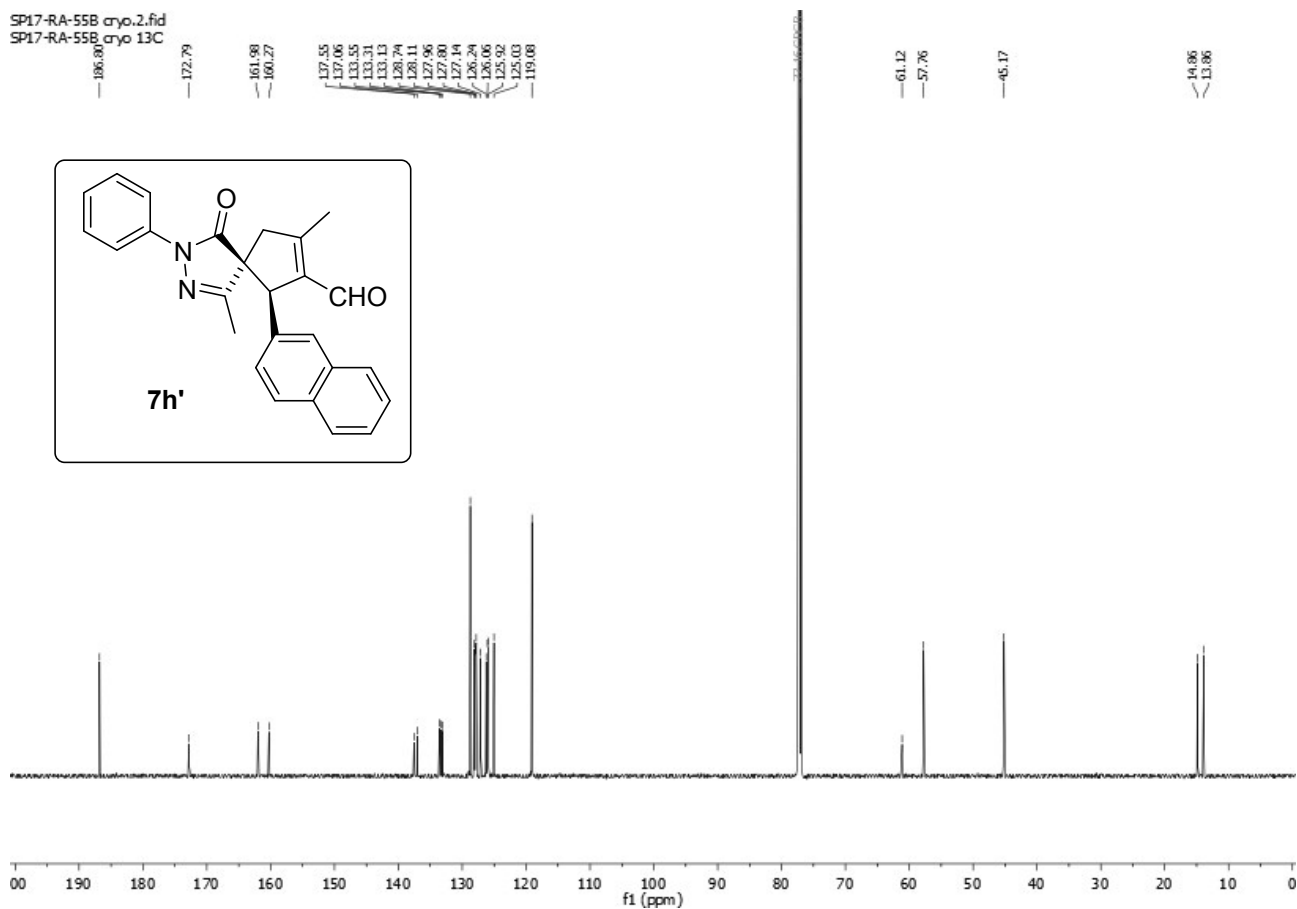
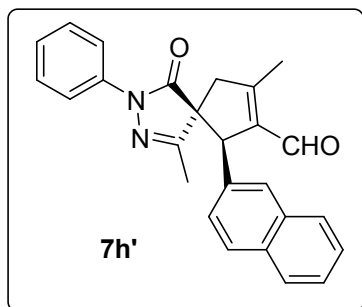
(5*S*,6*R*)-1,8-Dimethyl-6-(2-naphthyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7h')



(5*S*,6*R*)-1,8-Dimethyl-6-(2-naphthyl)-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7h')

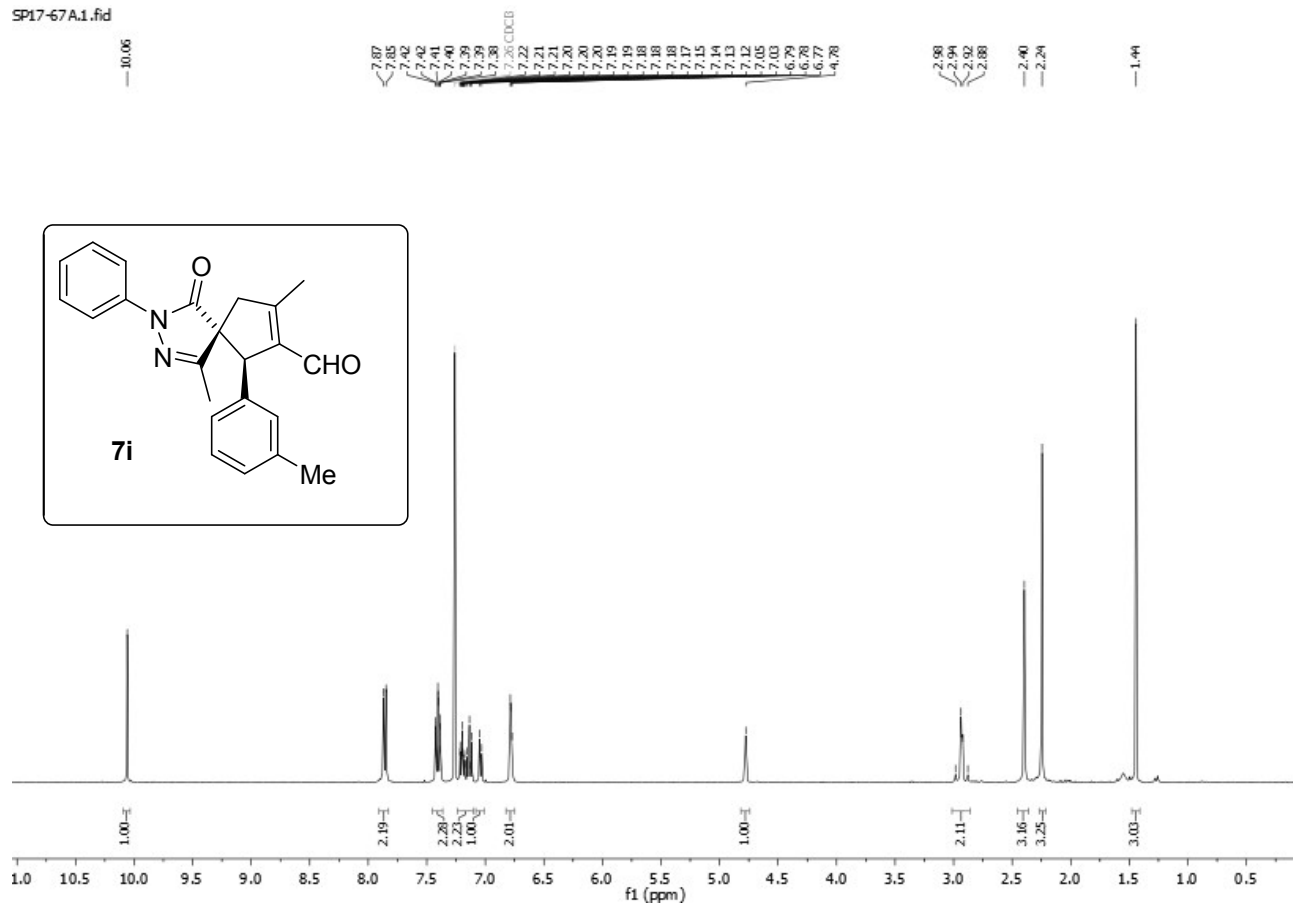
SP17-RA-55B cryo.2.fid
SP17-RA-55B cryo.13C

186.00 172.79 161.98 160.27 137.55 137.06 133.55 133.11 133.11 128.74 128.11 127.96 127.80 127.14 126.24 126.06 125.92 125.03 119.08



(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*m*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7i)

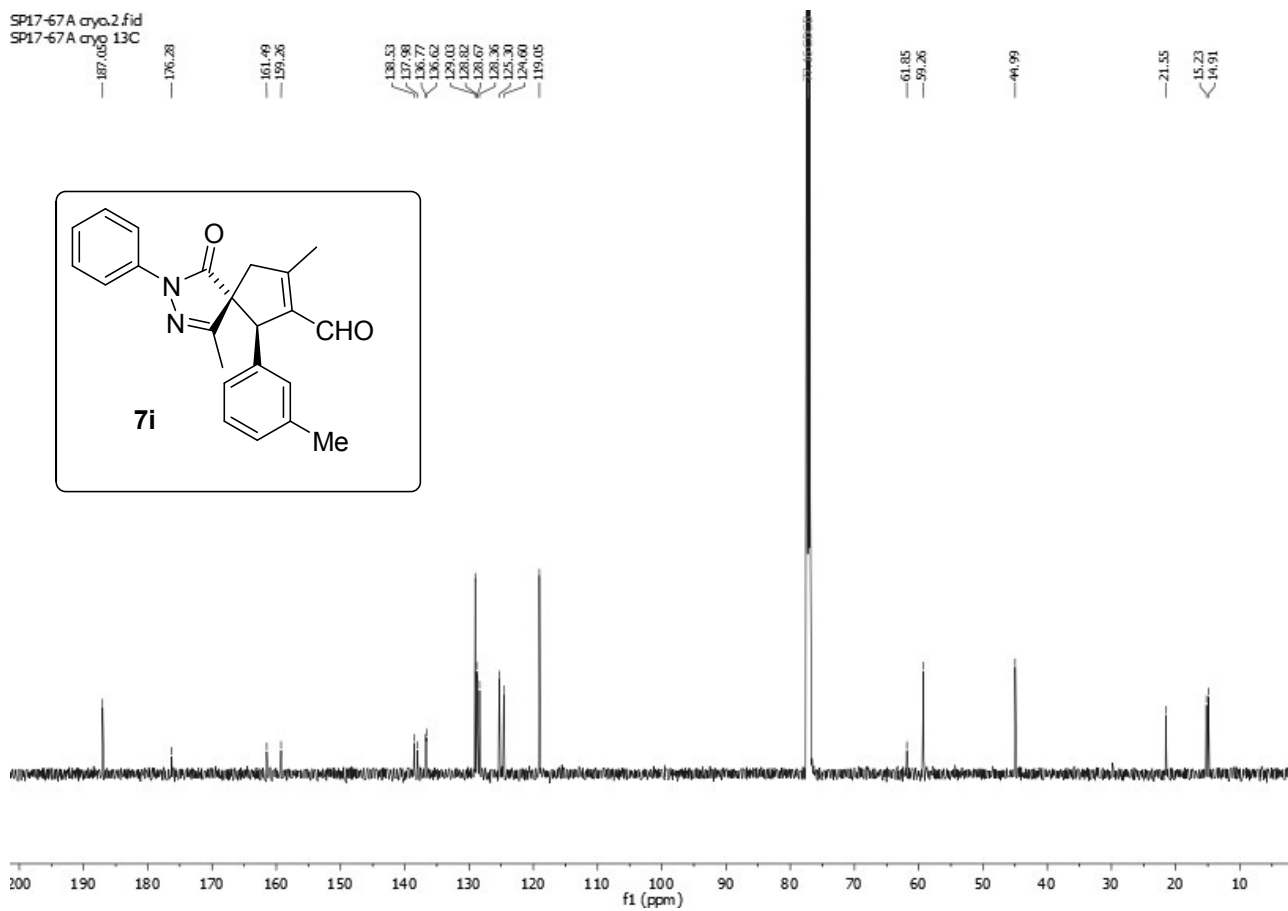
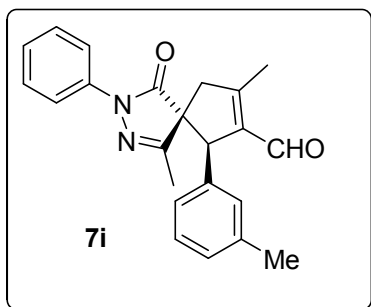
SP17-67A.1.fid



(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*m*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7i)

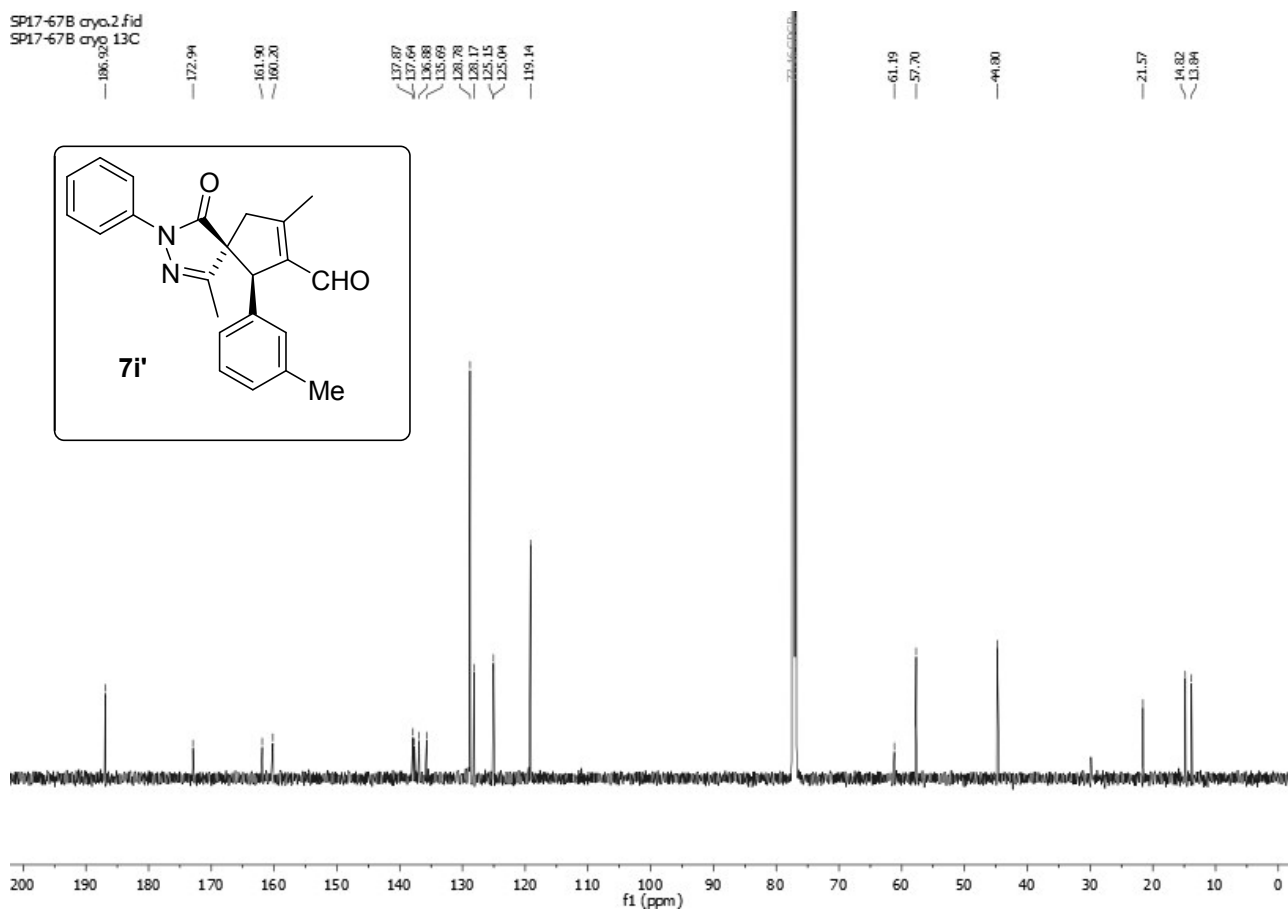
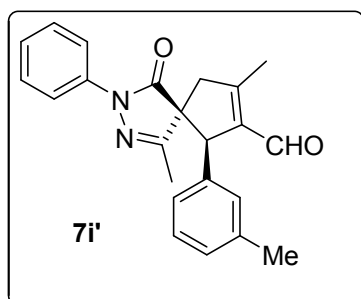
SP17-67A cryo.2.fid
SP17-67A cryo. 13C

187.000 176.28 161.49 159.26 138.53 137.98 136.77 136.62 129.00 128.82 128.97 128.30 128.00 119.05 61.85 59.26 49.99 21.55 15.23 14.91

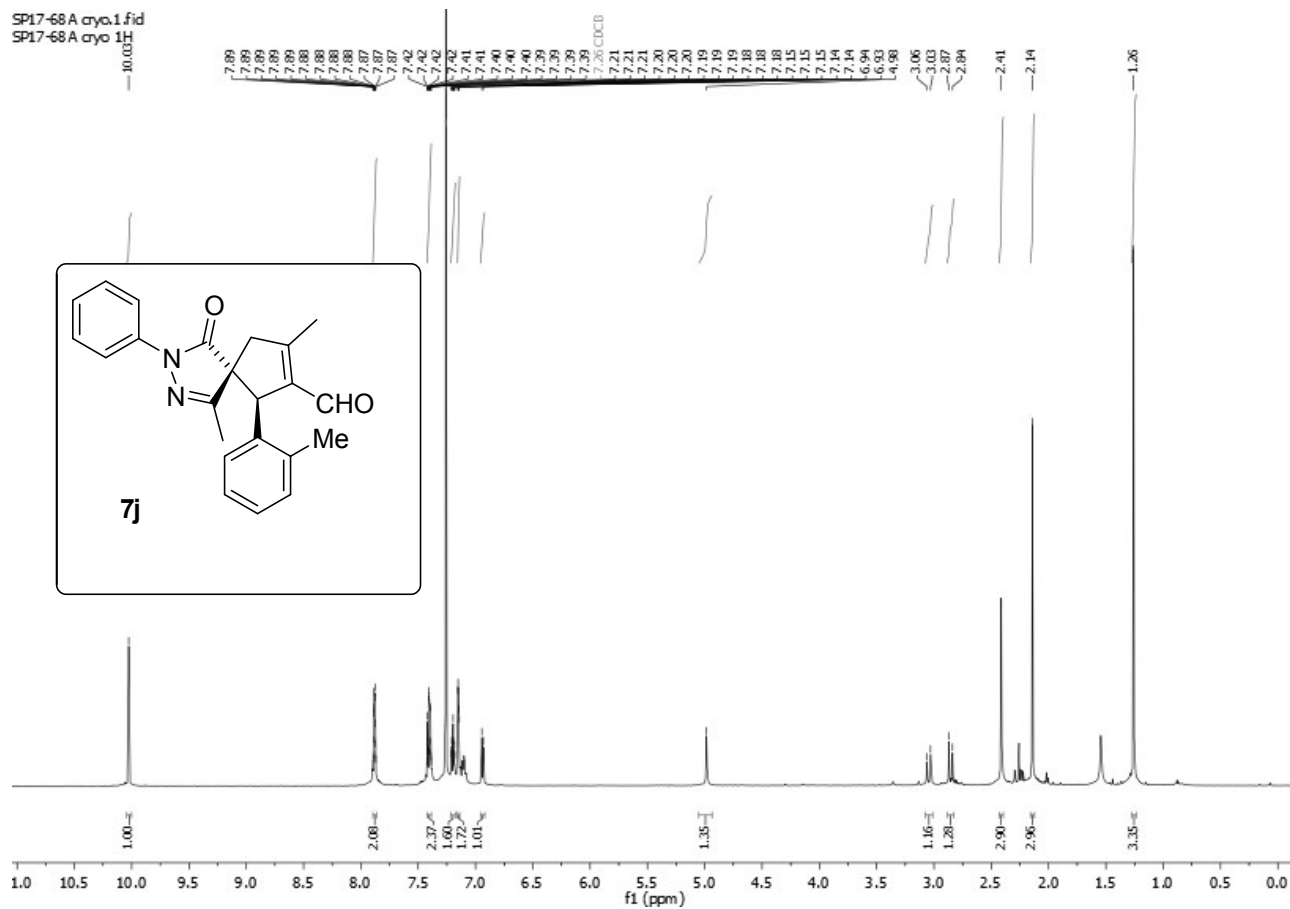


(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(*m*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7i')

SP17-67B cryo.2.fid
SP17-67B cryo.13C

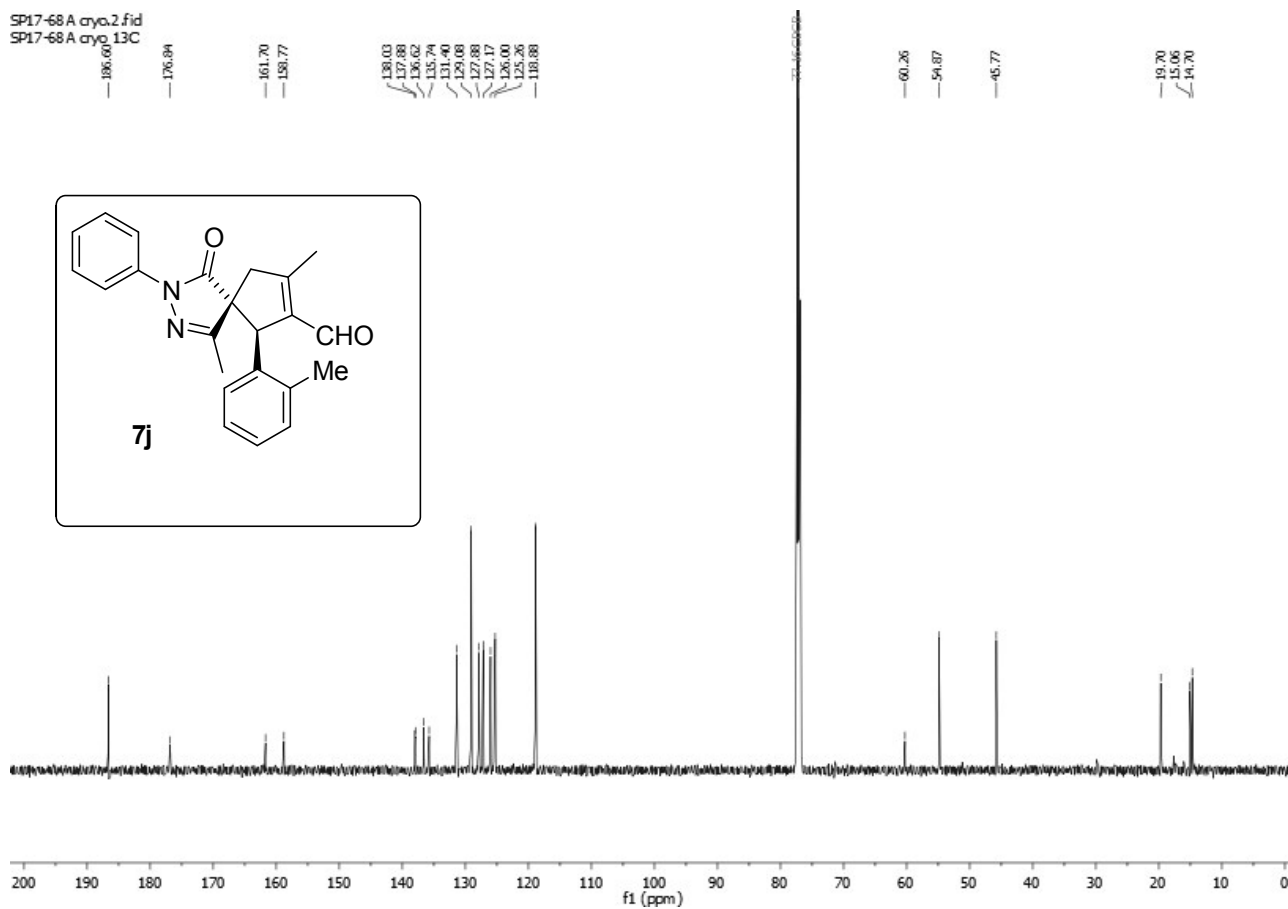
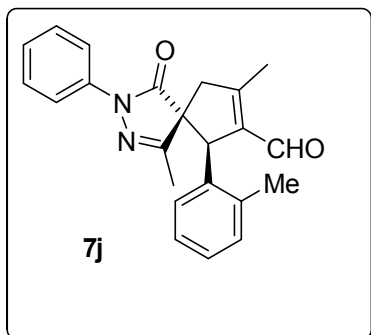


(5*R*,6*R*)-1,8-dimethyl-4-oxo-3-phenyl-6-(*o*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7j)



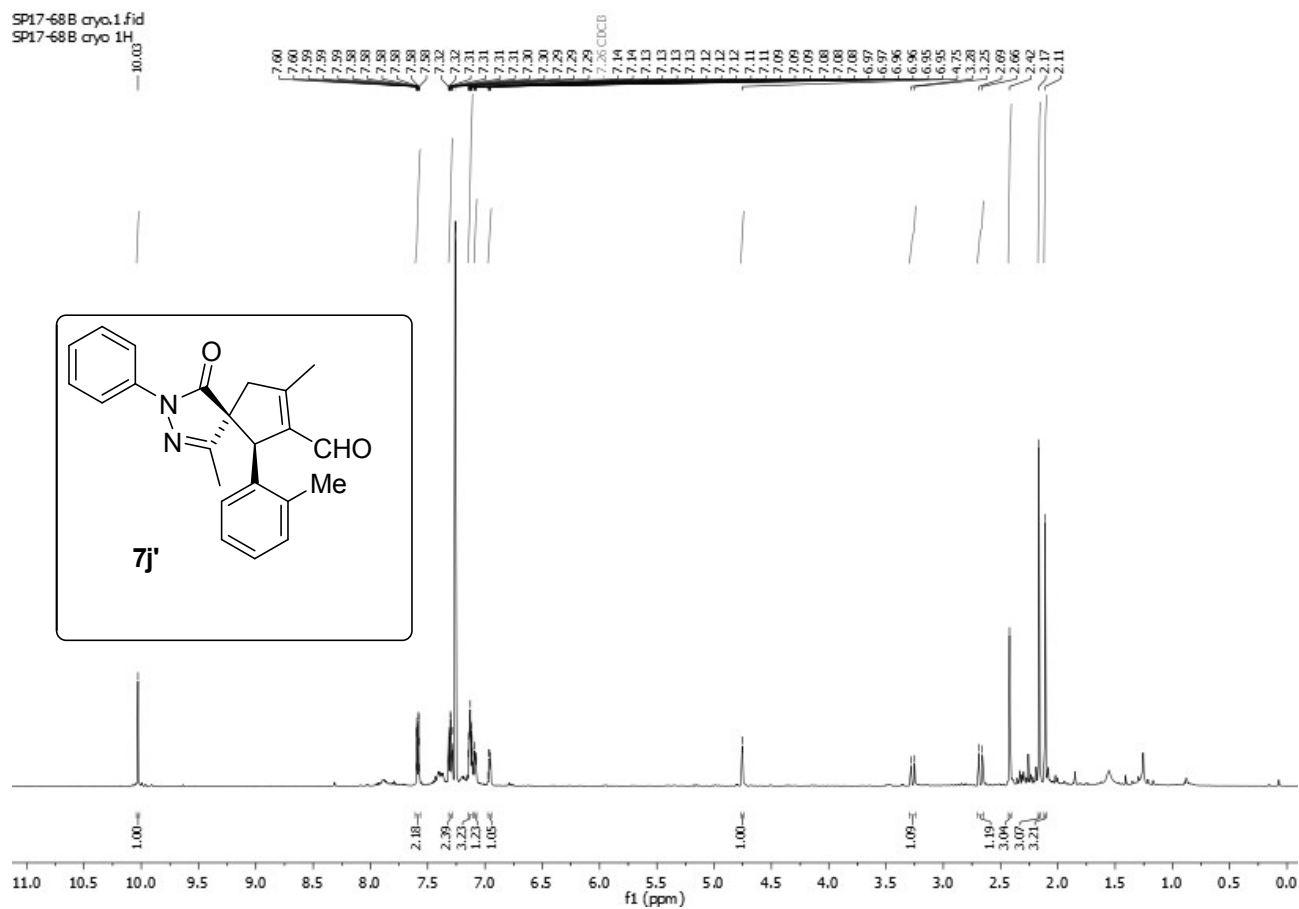
(5*R*,6*R*)-1,8-dimethyl-4-oxo-3-phenyl-6-(*o*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7j)

SP17-68 A cryo.2.fid
SP17-68 A cryo.13C



(5*S*,6*R*)-1,8-dimethyl-4-oxo-3-phenyl-6-(*o*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7j')

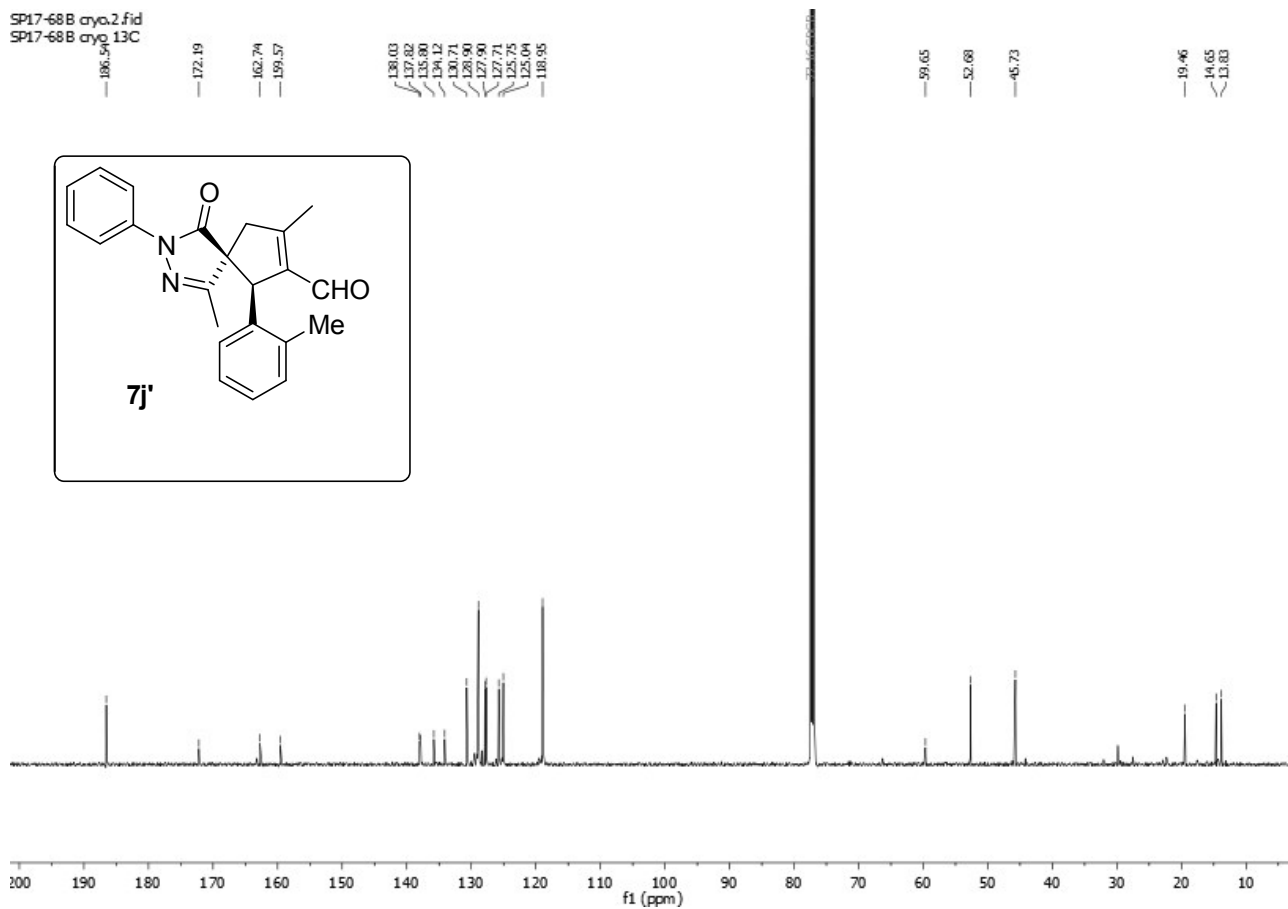
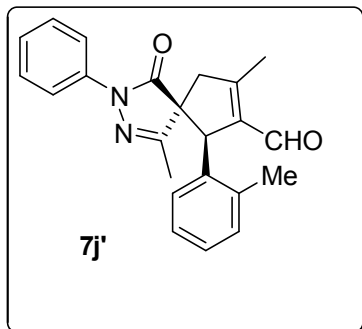
SP17-68B cryo.1.fid
SP17-68B cryo 1H



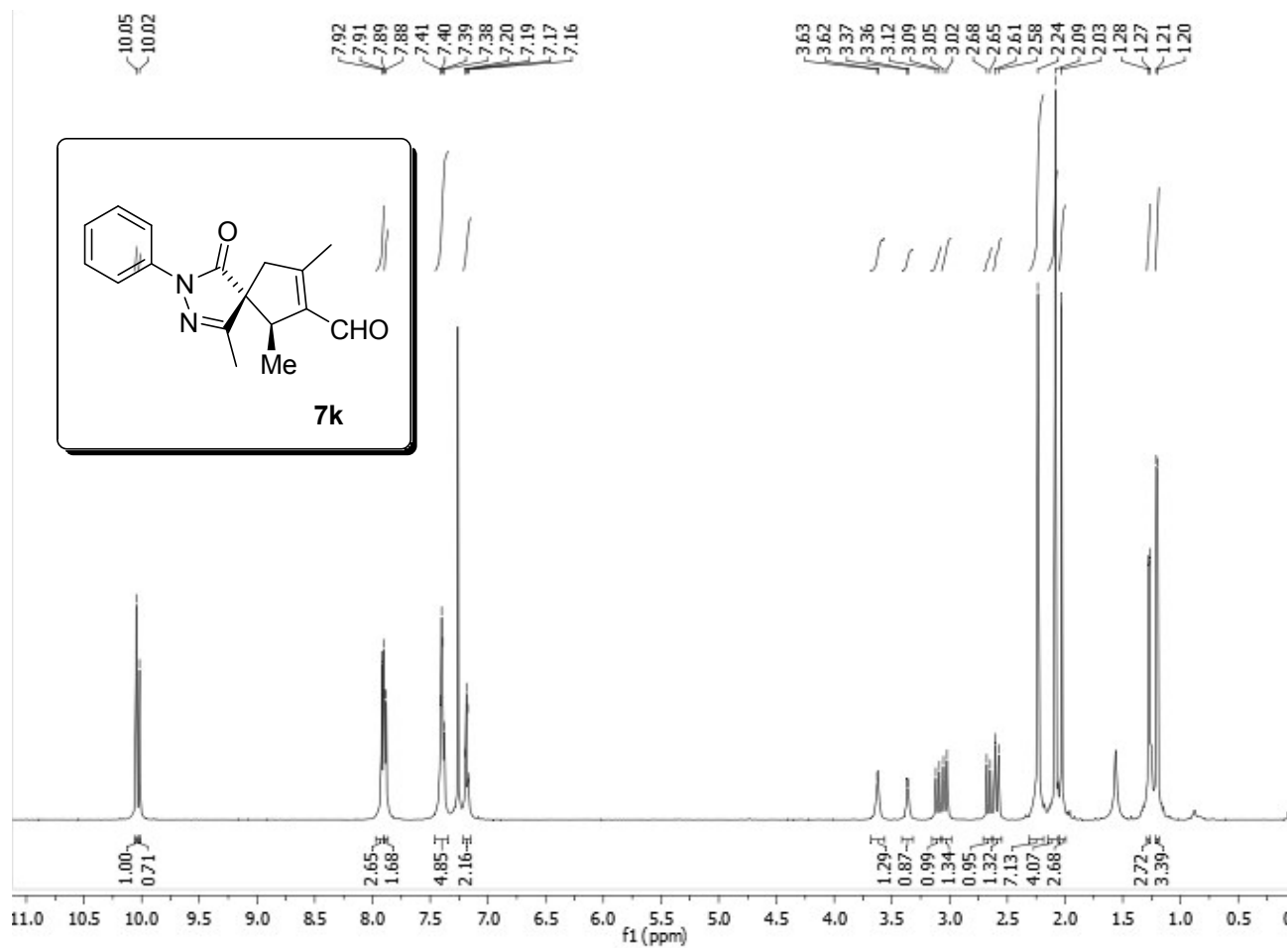
(5*S*,6*R*)-1,8-dimethyl-4-oxo-3-phenyl-6-(*o*-tolyl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7j')

SP17-68 B cryo.2.fid
SP17-68 B cryo.13C

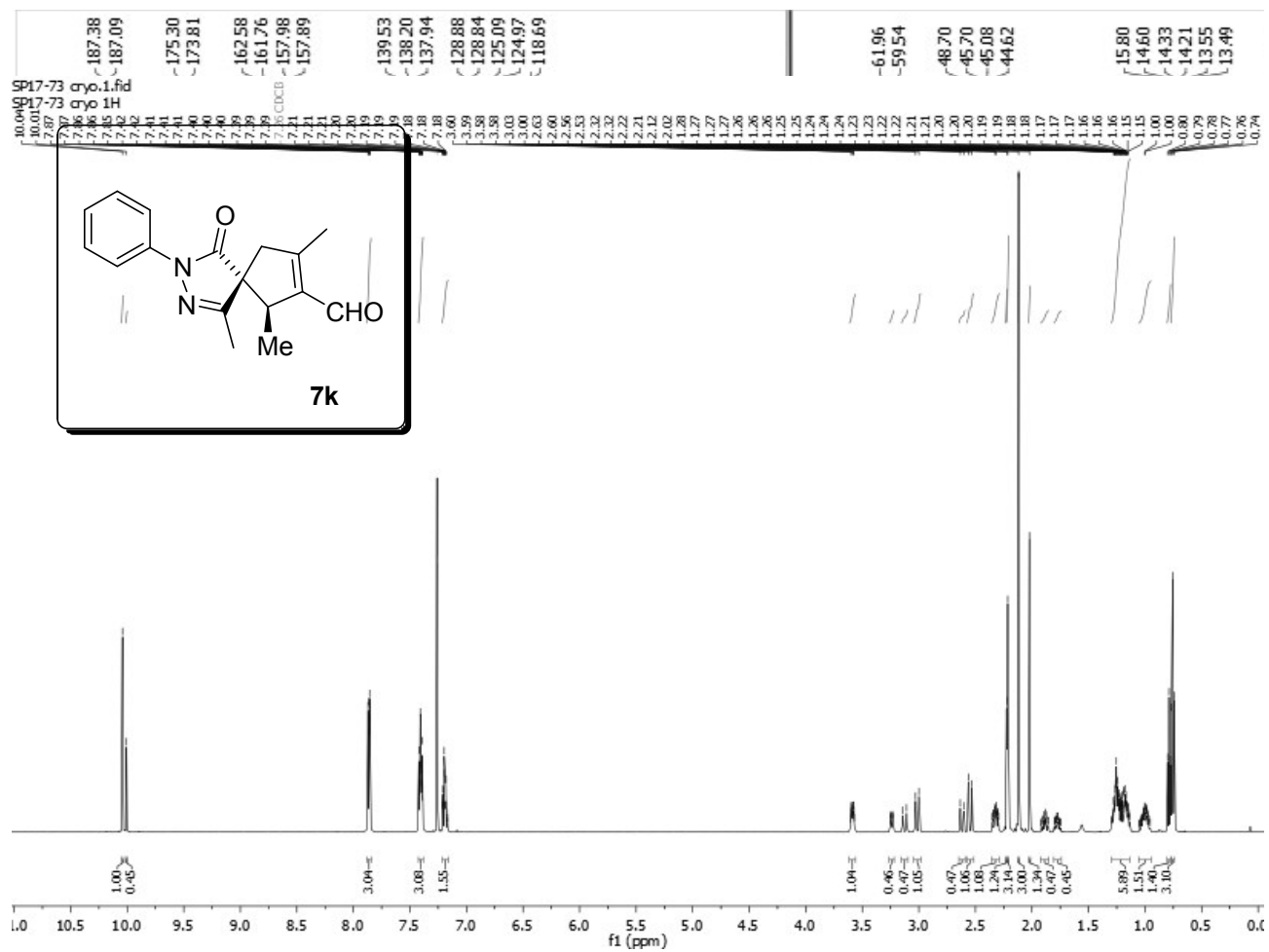
186.540
172.19
162.74
159.57
138.03
137.82
135.80
134.12
130.71
128.90
127.71
125.75
124.64
118.95
59.65
52.68
45.73
19.46
14.65
13.83



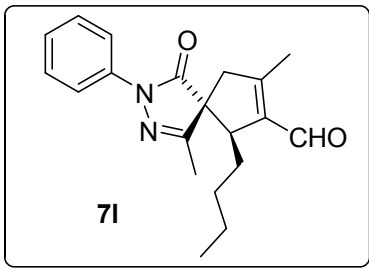
(5*R*/5*S*,6*R*)-1,6,8-Trimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7k) mixture of diastereomers 1.8:1



(5*R*/5*S*,6*R*)-1,6,8-Trimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7k) mixture of diastereomers 1.8:1



(5*R*/5*S*,6*R*)-6-Butyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7l) mixture of diastereomers 2.5:1



(5*R*/5*S*,6*R*)-6-Butyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (71) mixture of diastereomers 2.5:1

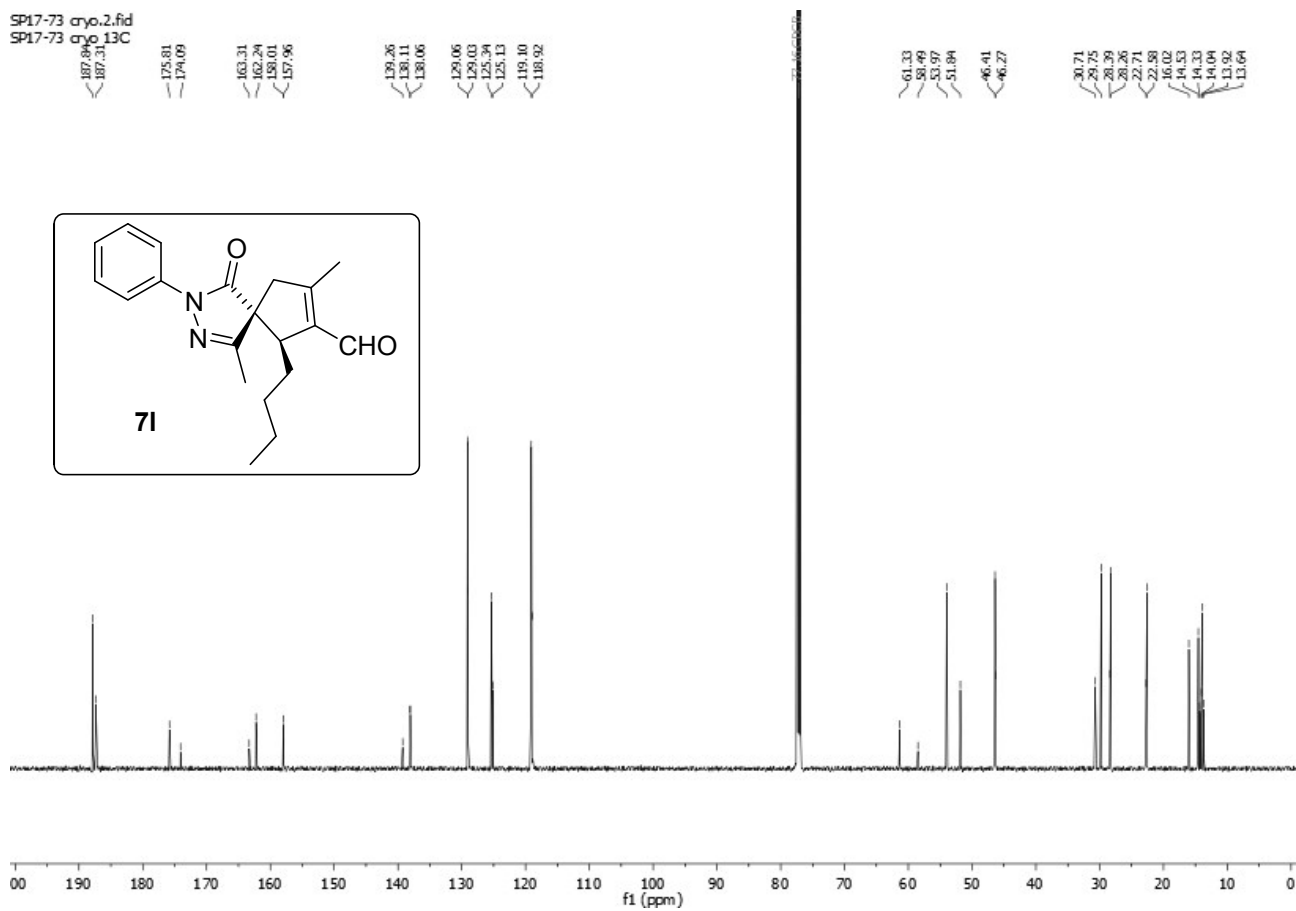
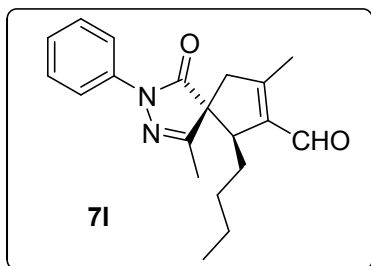
SP17-73 cryo.2.fid
SP17-73 cryo.13C

187.84
187.31
175.81
174.09
163.31
162.24
157.96

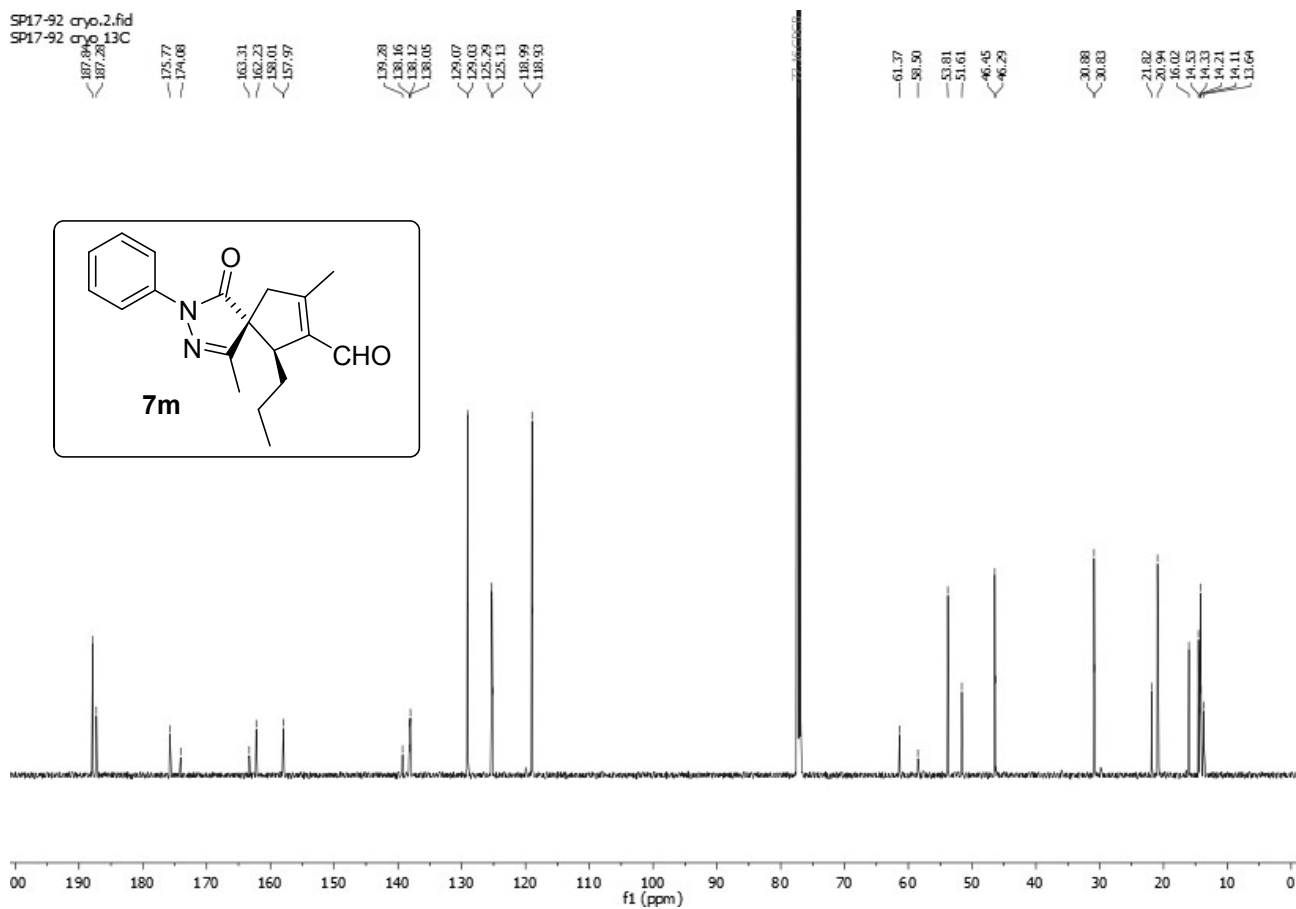
139.26
138.11
138.06
129.06
129.03
125.34
125.13
119.10
118.92

61.33
58.49
53.97
51.84
46.41
46.27

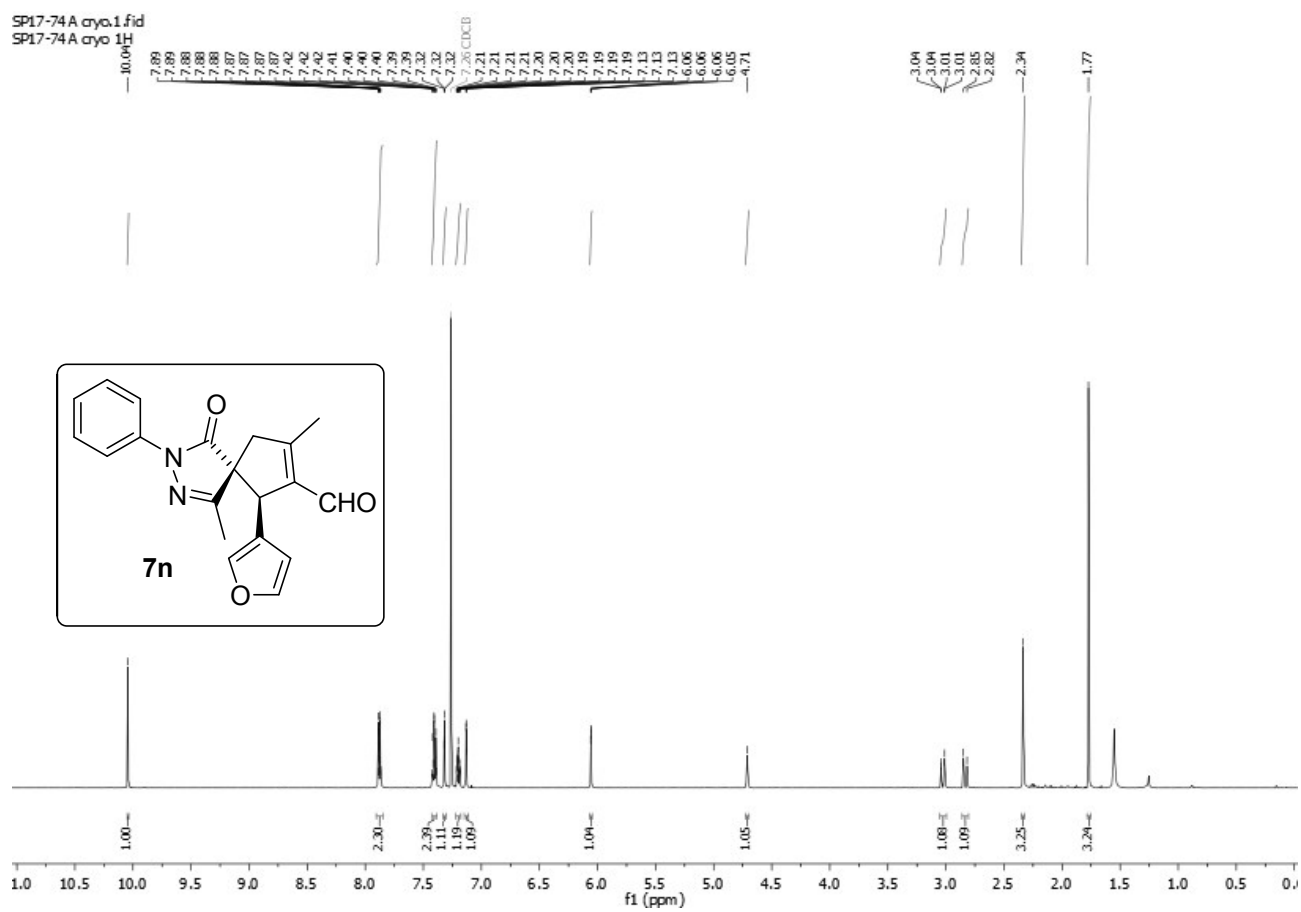
30.71
29.75
28.39
28.26
22.71
22.58
16.02
14.53
14.33
14.04
13.92
13.64



(5*R*/5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-propyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7m) mixture of diastereomers 3.4:1

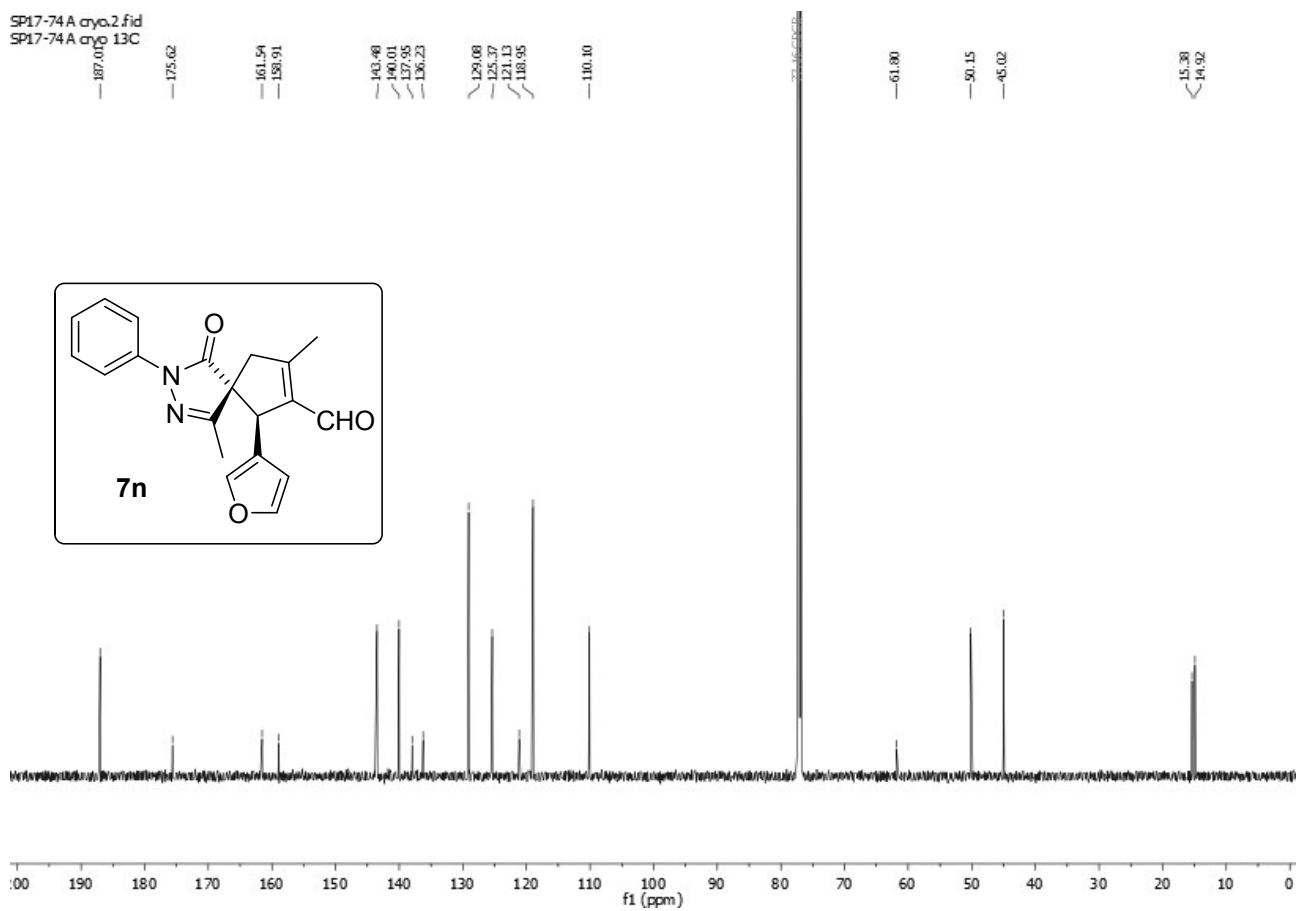


(5*R*,6*R*)-6-(3-Furyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7n)

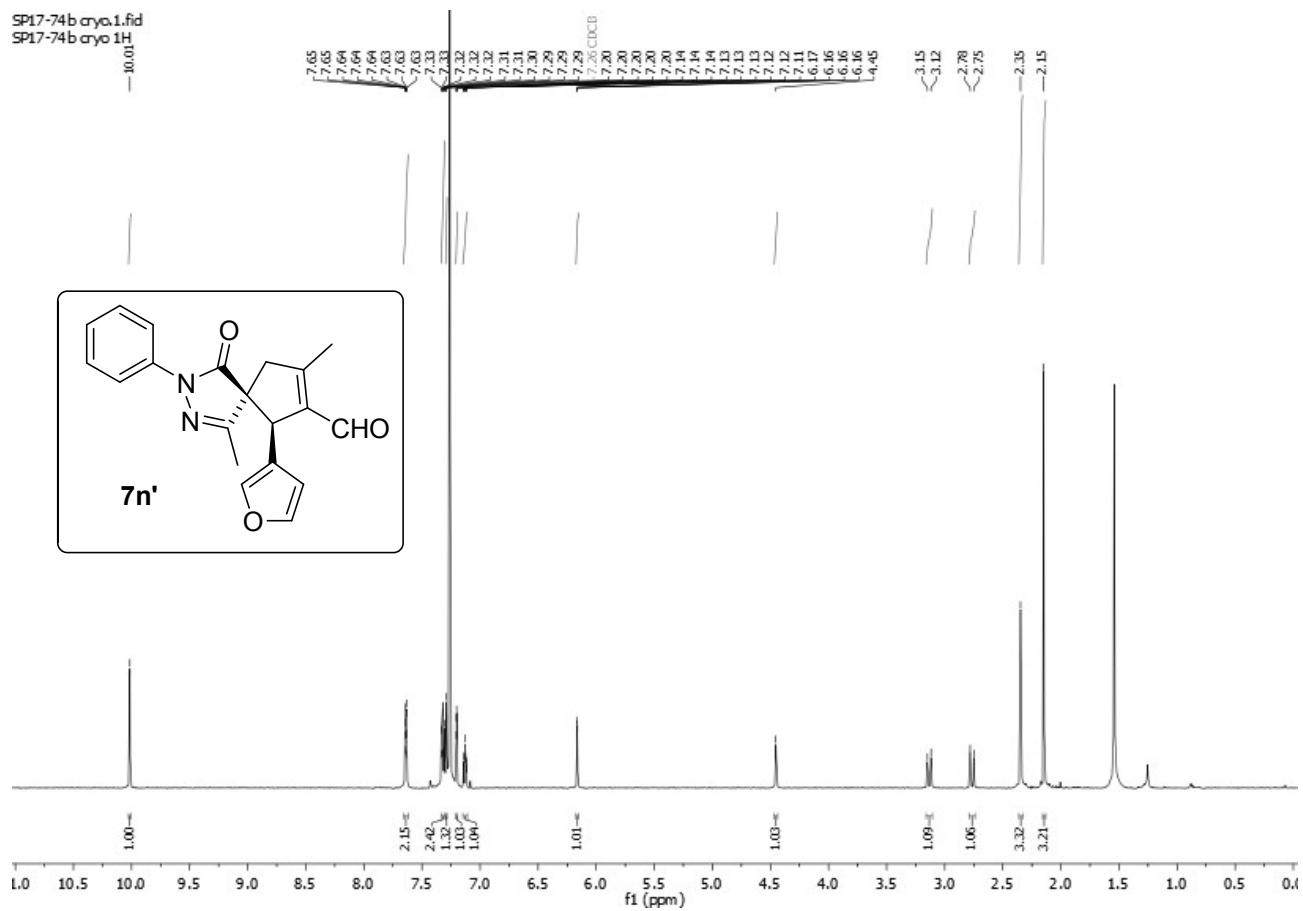


(5*R*,6*R*)-6-(3-Furyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7n)

SP17-74 A cryo.2.fid
SP17-74 A cryo 13C



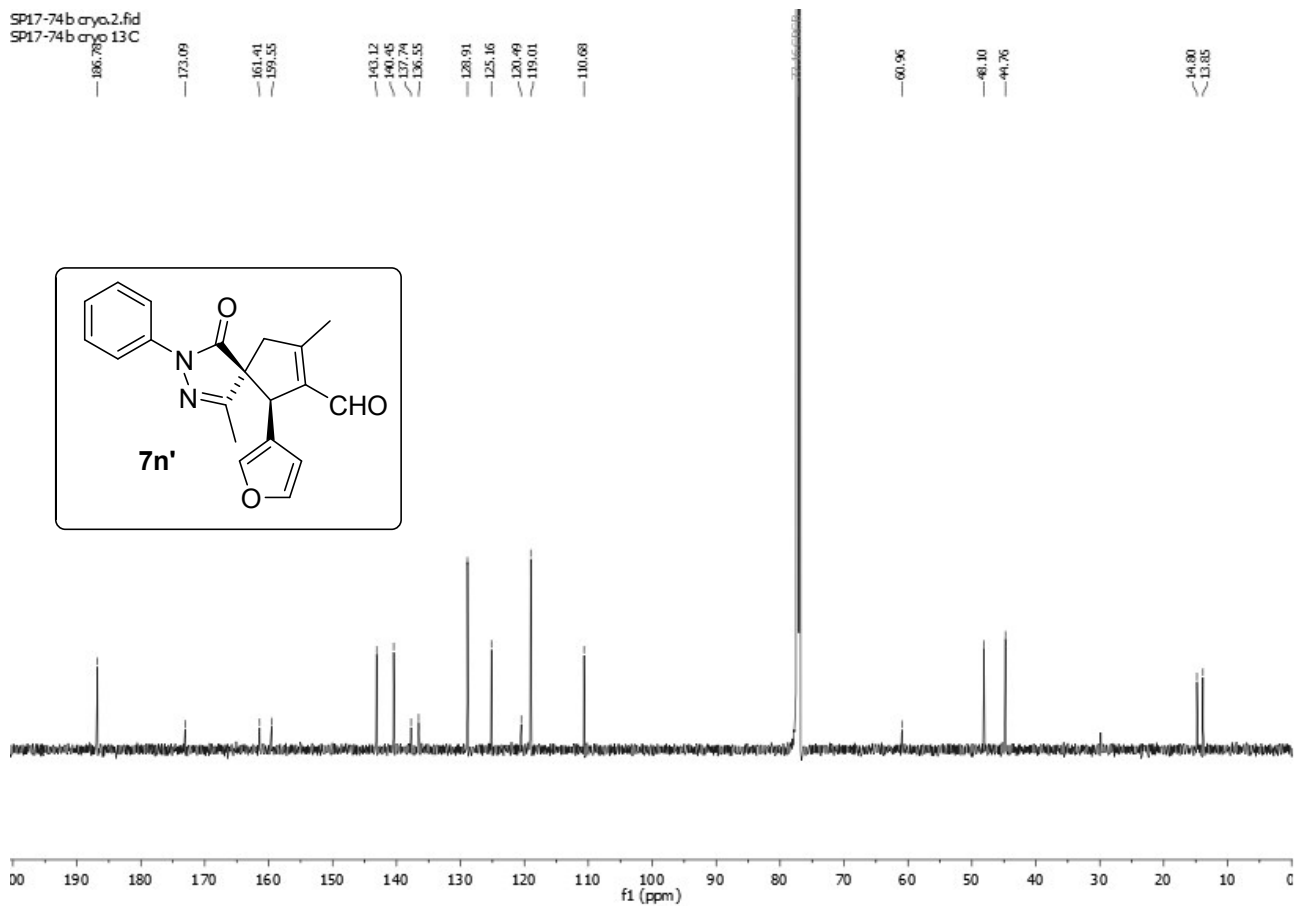
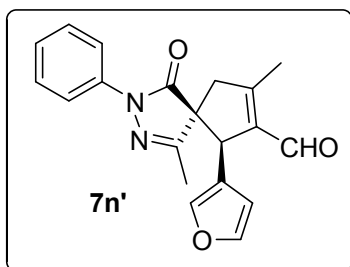
(5*S*,6*R*)-6-(3-Furyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7n')



(5*S*,6*R*)-6-(3-Furyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7n')

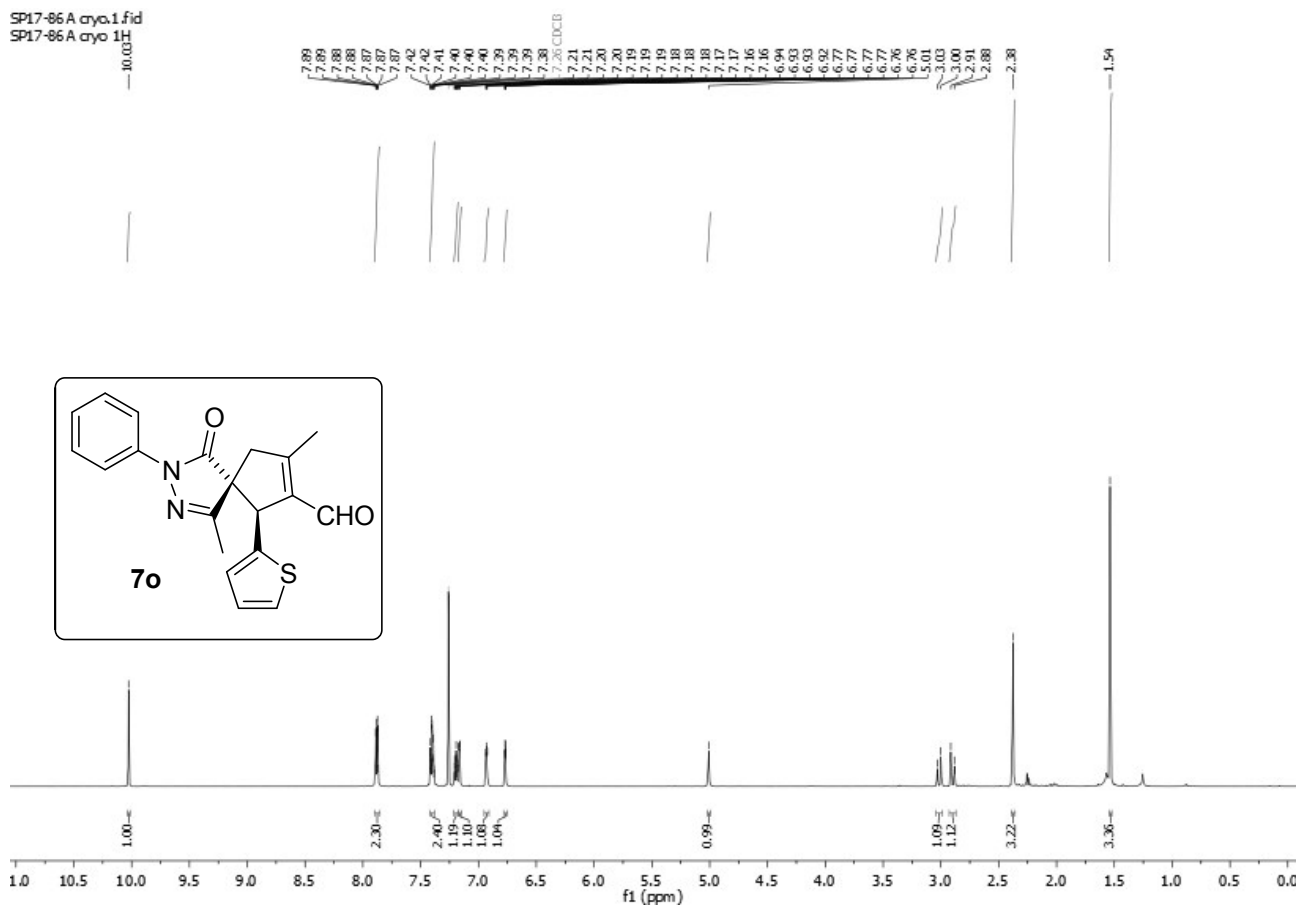
SP17-74b cryo.2.fid
SP17-74b cryo 13C

186.76 173.09 161.41 159.55 143.12 140.45 137.74 136.55 128.91 125.16 120.49 119.01 110.08 60.96 46.10 44.76 14.80 13.85



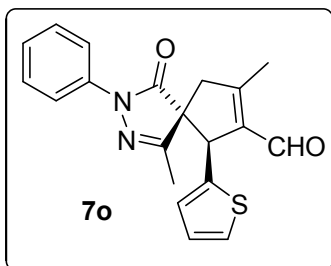
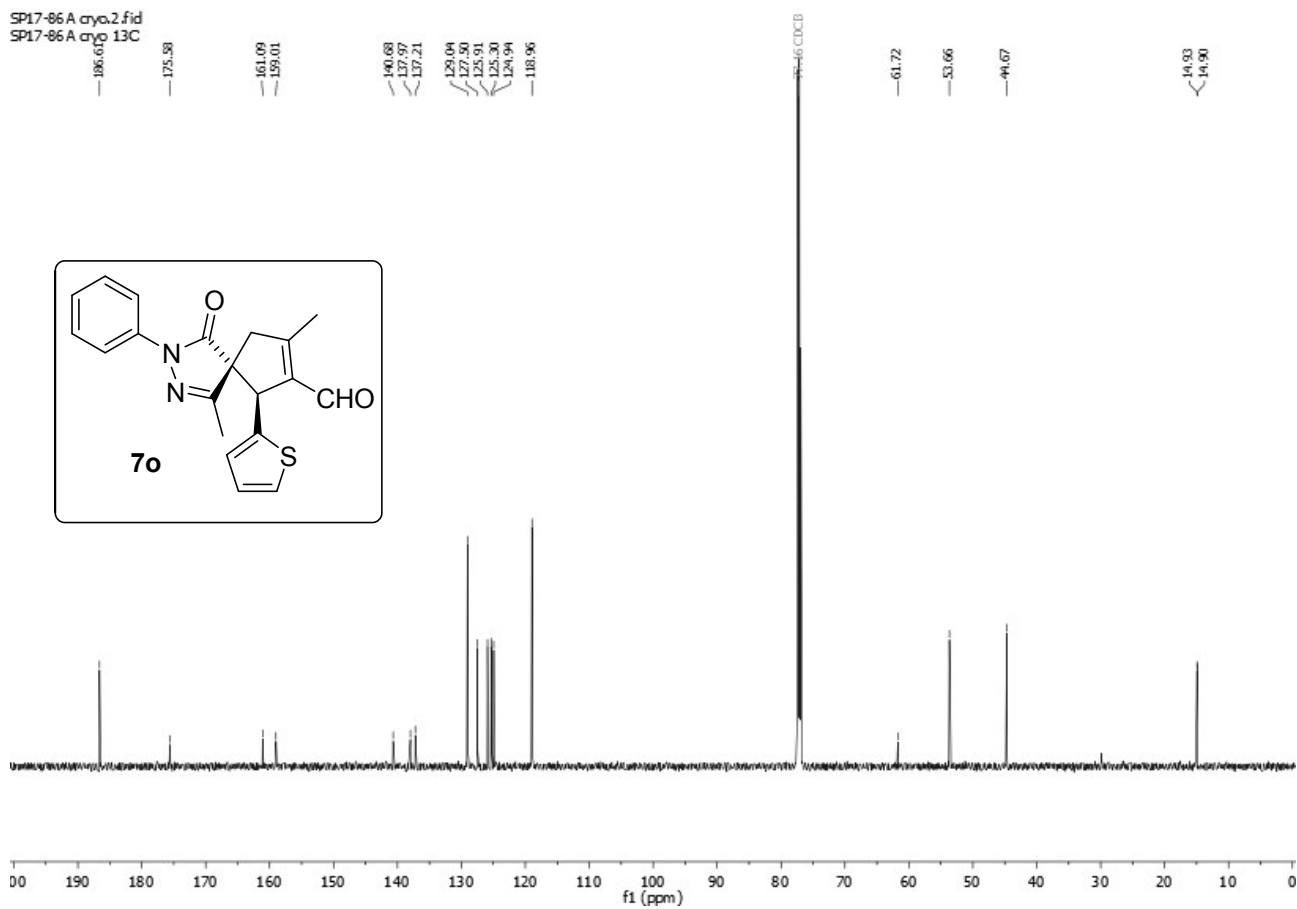
(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(thien-2-yl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7o)

SP17-86 A cryo.1.fid
SP17-86 A cryo 1H



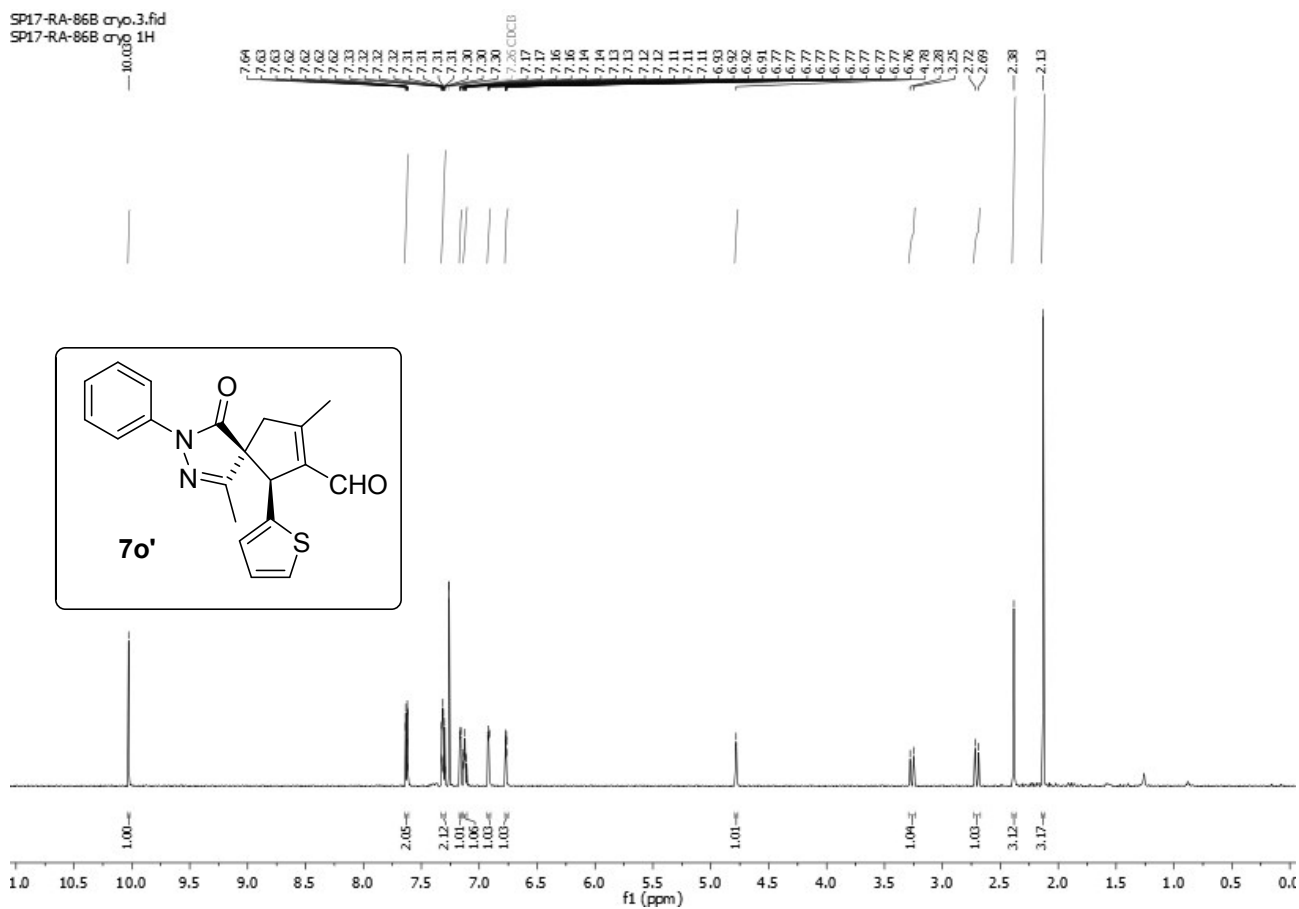
(5*R*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(thien-2-yl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7o)

SP17-86 A cryo.2.fid
SP17-86 A cryo 13C



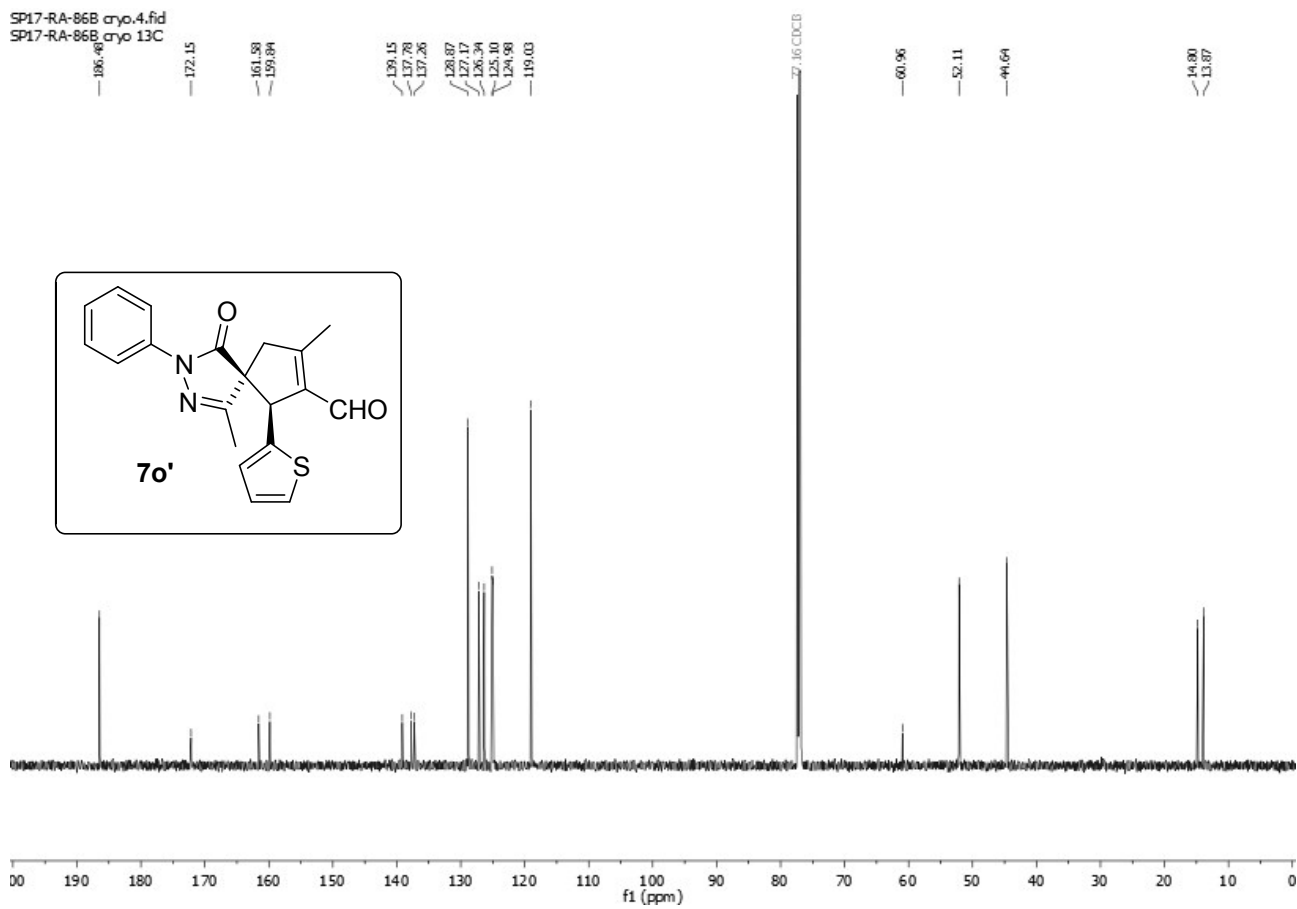
(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(thien-2-yl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7o')

SP17-RA-86B cryo.3.fid
SP17-RA-86B cryo. 1H



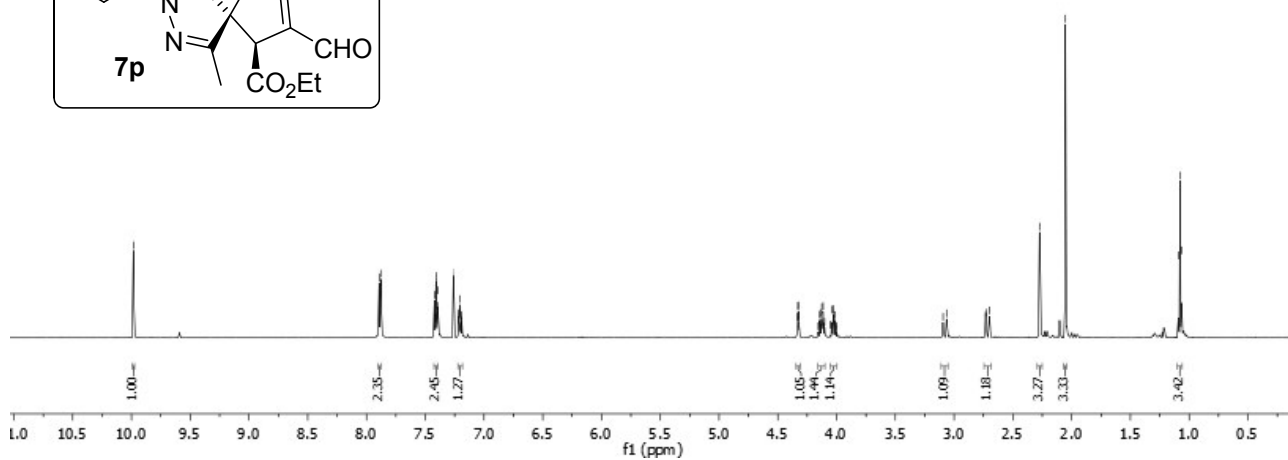
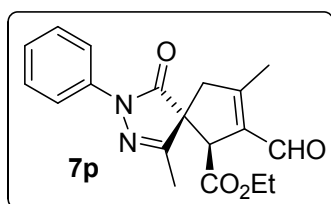
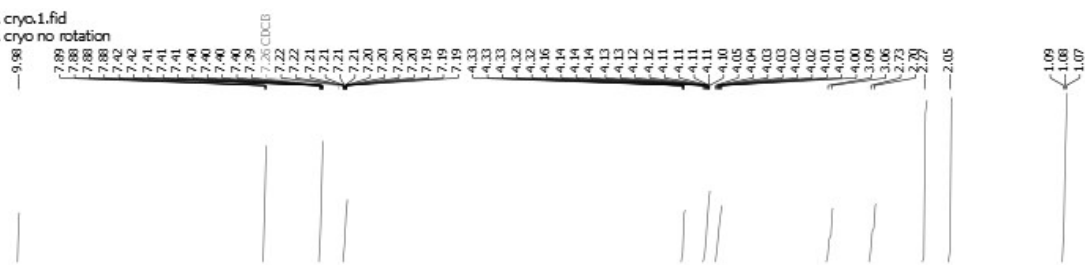
(5*S*,6*R*)-1,8-Dimethyl-4-oxo-3-phenyl-6-(thien-2-yl)-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7o')

SP17-RA-86B_cryo.4.fid
SP17-RA-86B_cryo.13C



Ethyl (5*R*,6*R*)-7-formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-6-carboxylate (7p)

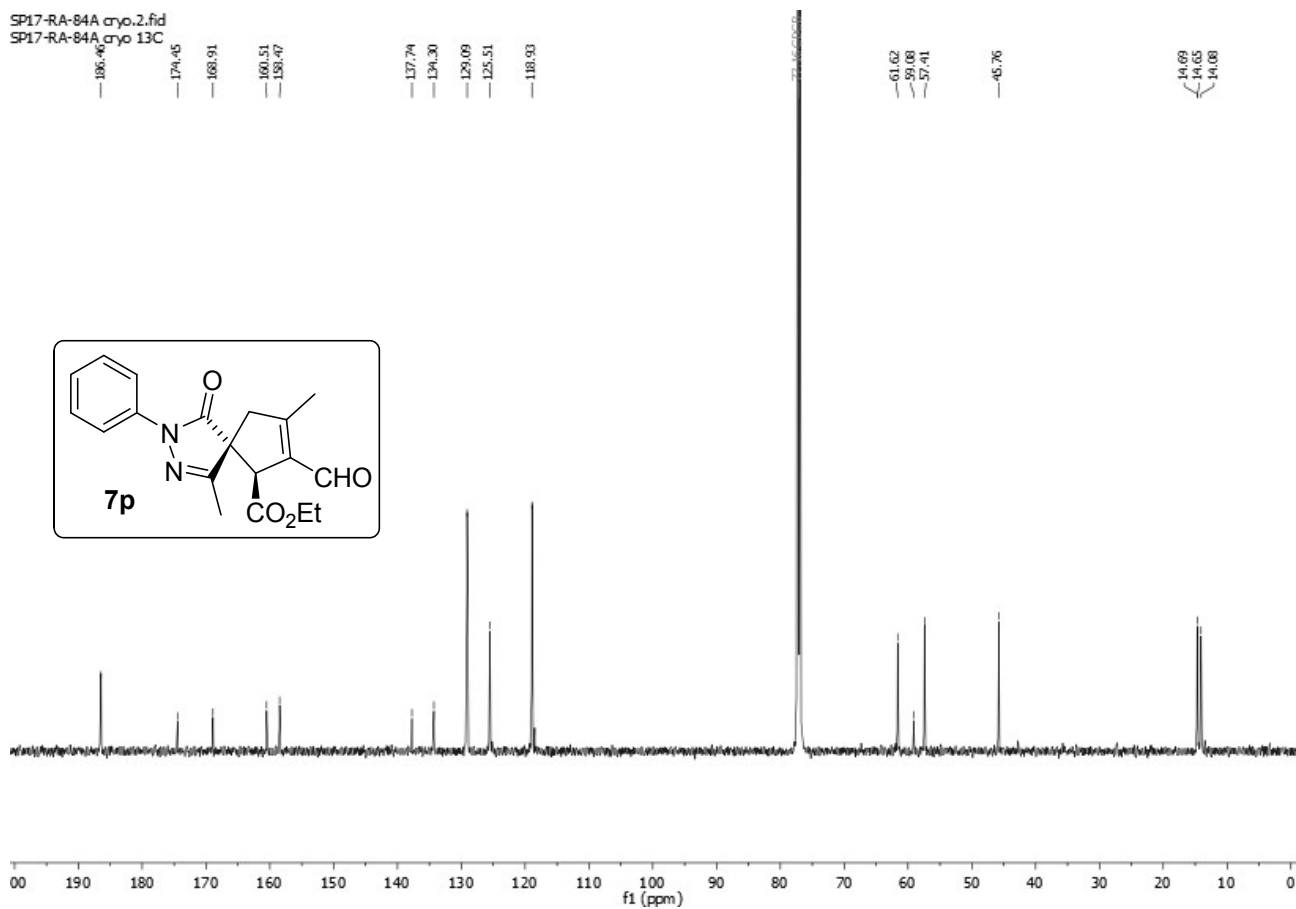
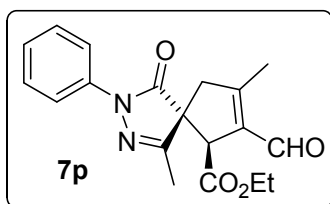
SP17-FRA-894A cryo.1.fid
 SP17-FRA-894A cryo no rotation



Ethyl (5*R*,6*R*)-7-formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-6-carboxylate (7p)

SP17-RA-84A cryo.2.fid
SP17-RA-84A cryo 13C

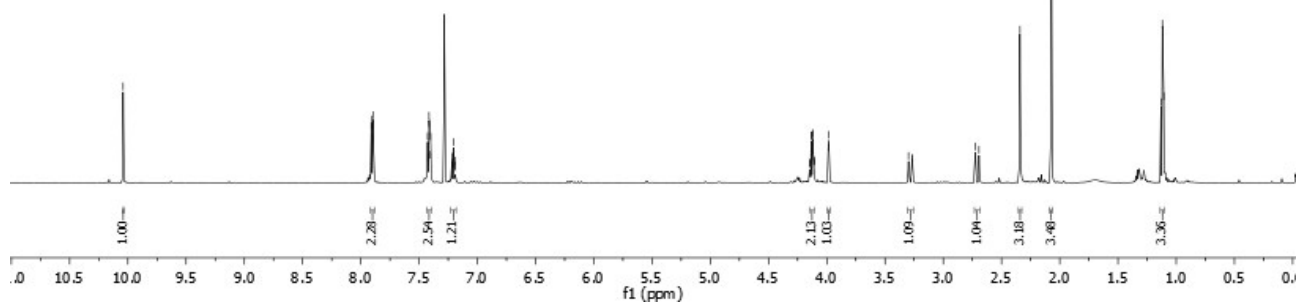
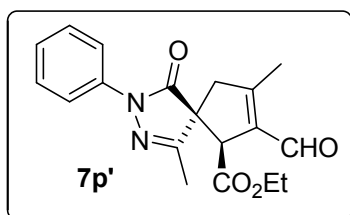
186.46
174.45
168.91
161.51
158.47
137.74
134.30
129.09
125.51
118.93
77.16 (CDCl₃)
61.62
59.08
57.41
45.76
14.69
14.65
14.08



Ethyl (5*S*,6*R*)-7-formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-6-carboxylate (7p')

SP17-FRA-84B cpyo.1.fid
 SP17-FRA-84B cpyo no rotation

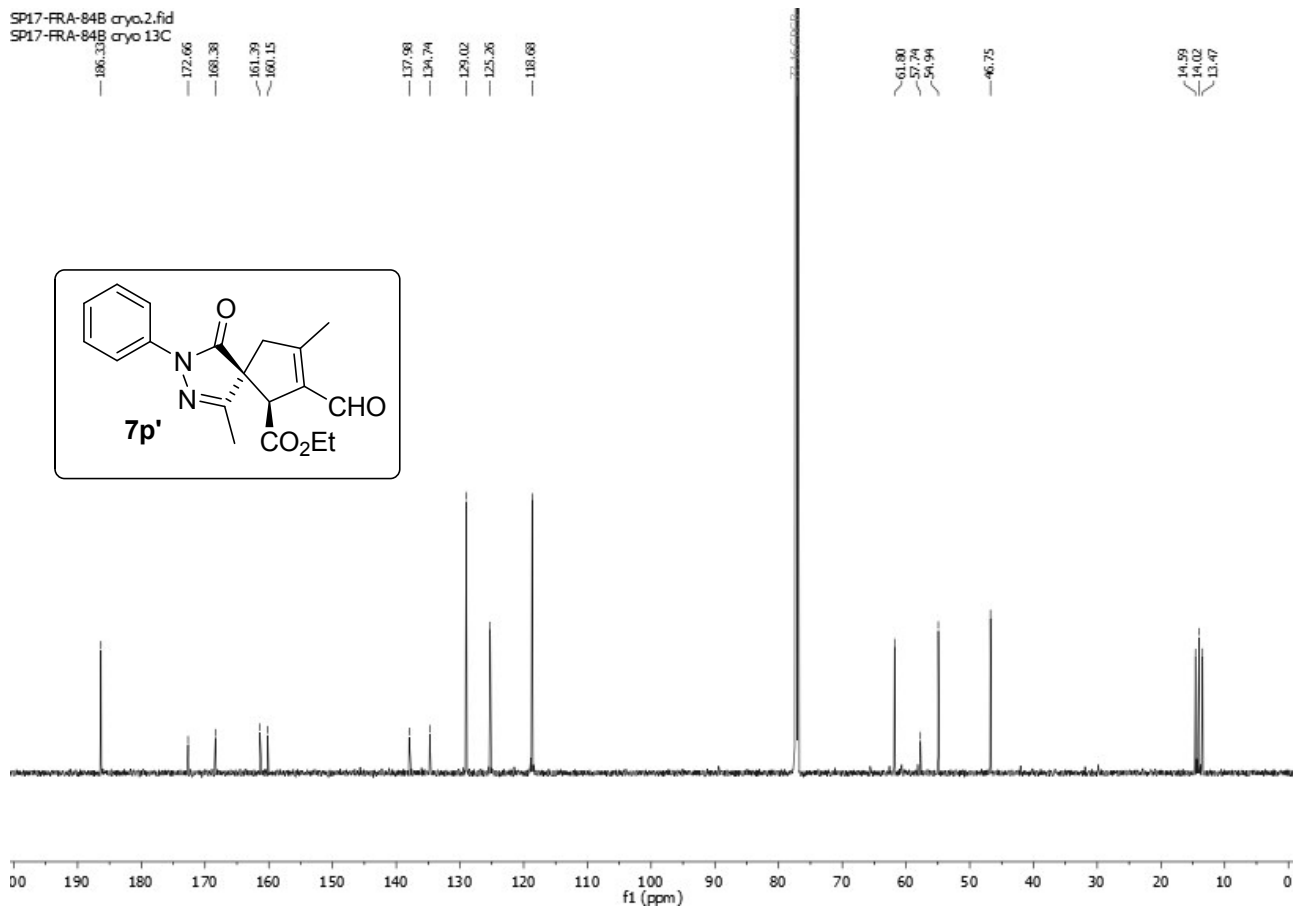
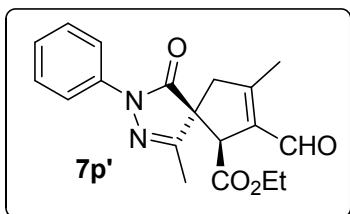
7.91 7.91 7.90 7.89 7.88 7.43 7.42 7.41 7.40 7.39 7.38 7.22 7.21 7.21 7.20 7.19 7.19
 4.15 4.14 4.13 4.12 4.11 3.99 3.98 3.30 3.27 2.72 2.69 2.24 2.07 1.13 1.12 1.11



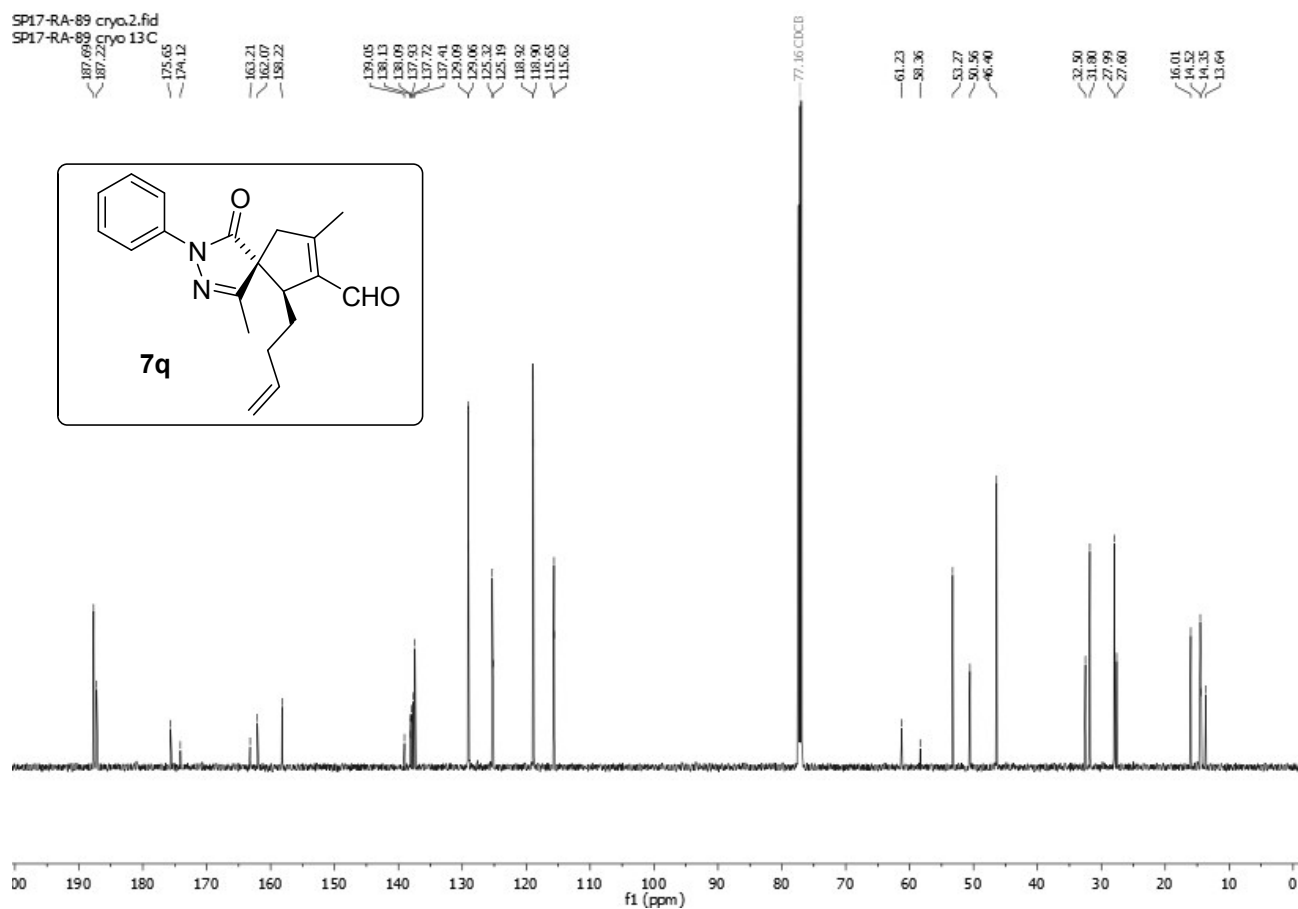
Ethyl (5*S*,6*R*)-7-formyl-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-6-carboxylate (7p')

SP17-FRA-84B cryo.2.fid
SP17-FRA-84B cryo 13C

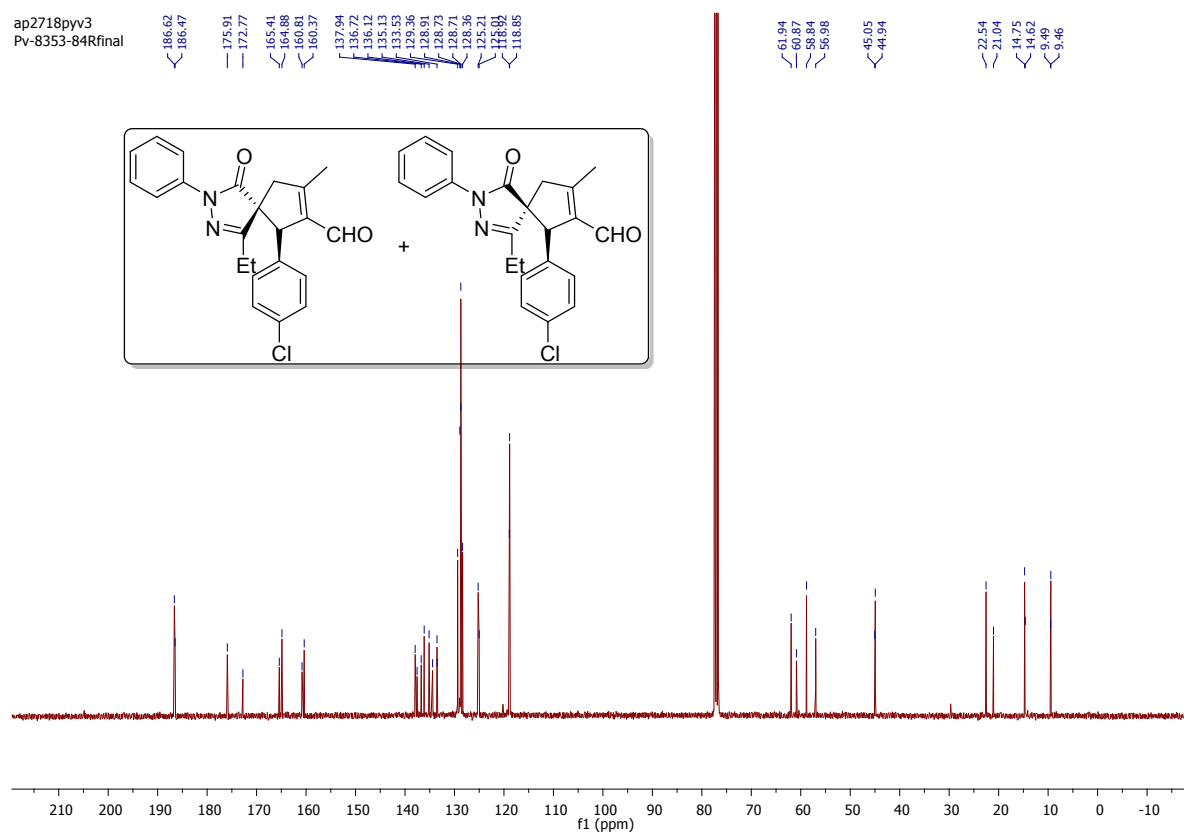
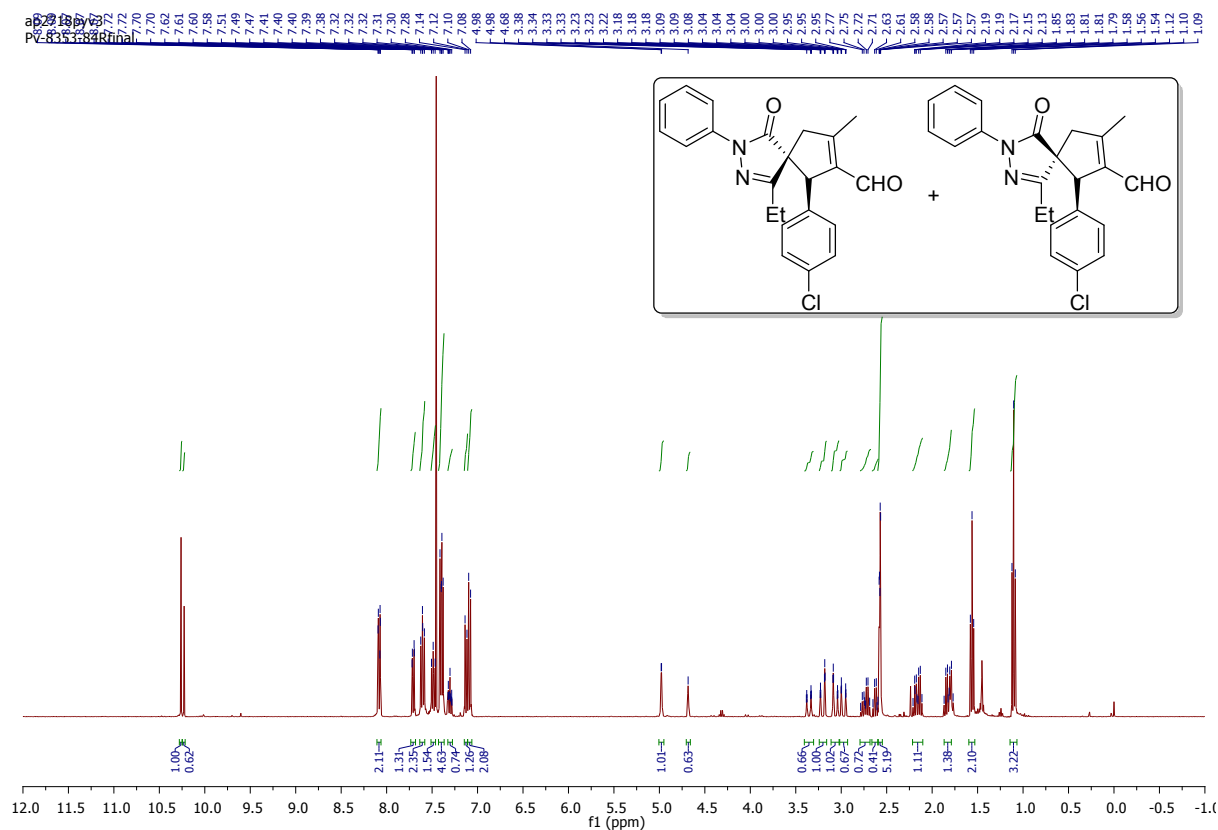
186.33
172.66
168.38
161.39
160.15
137.98
134.74
129.02
125.26
118.68
77.46 (CDCl₃)
61.80
57.74
54.94
46.75
14.59
14.02
13.47



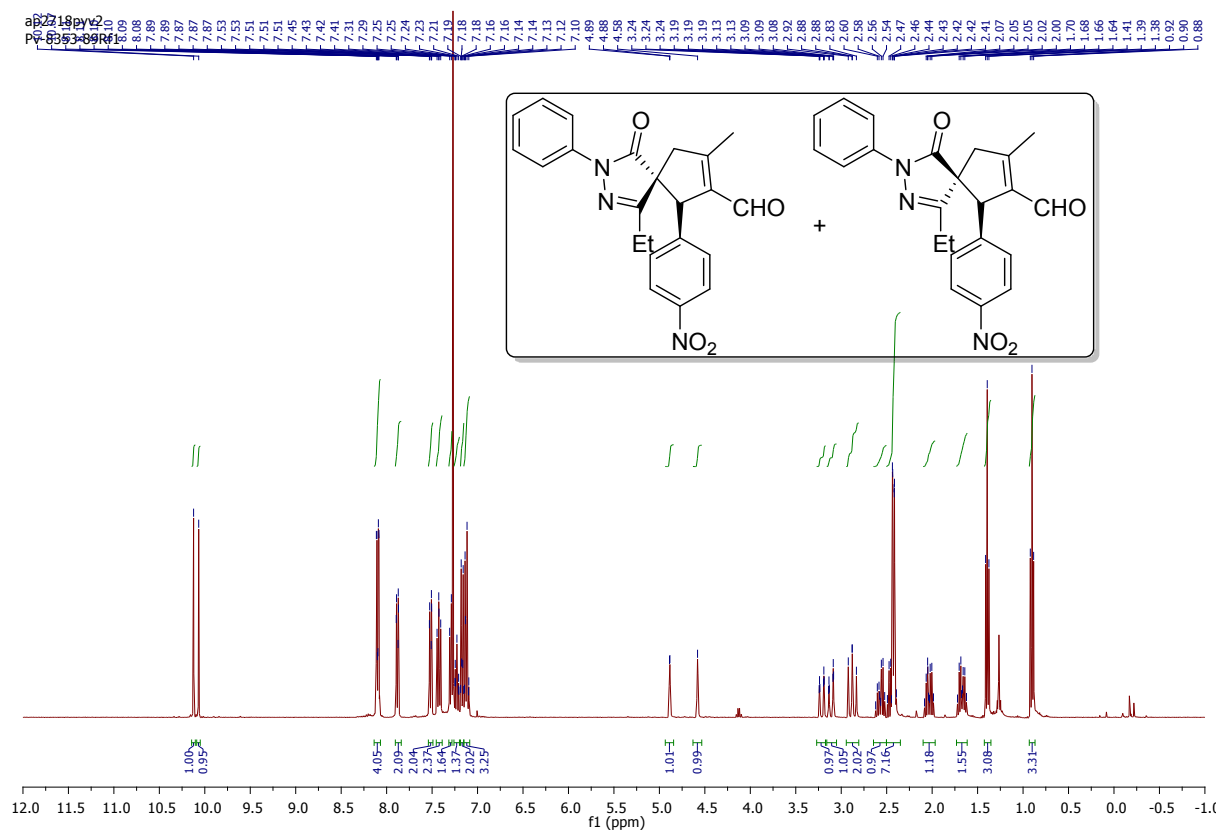
(5*R*/5*S*,6*R*)-6-(But-3-en-1-yl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7q) mixture of diastereomers 2.1:1



(5*R/S*,6*S*)-6-(4-chlorophenyl)-1-ethyl-8-methyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7r) mixture of major and minor diastereomers



(5*R/S*,6*S*)-6-(4-nitrophenyl)-1-ethyl-8-methyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7s) mixture of major and minor diastereomers



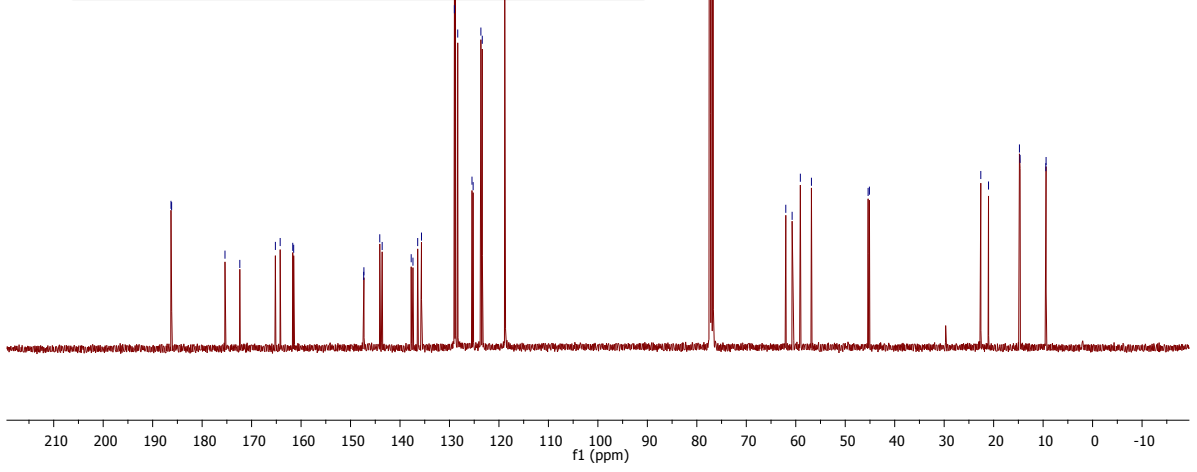
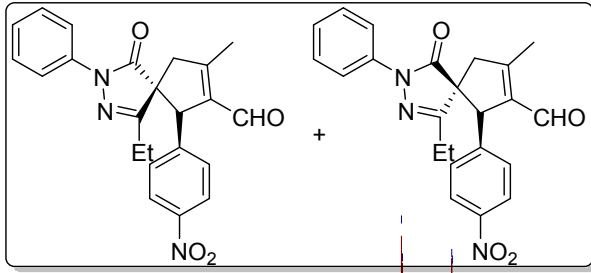
ap2718pyv2
Pv-8353-89Rf1

186.29
186.17
175.38
172.38
165.19
164.22
161.68
161.49
147.34
147.30
144.09
143.61
136.42
135.66
129.01
128.79
128.33
125.45
125.22
123.65
123.37
118.83
118.71

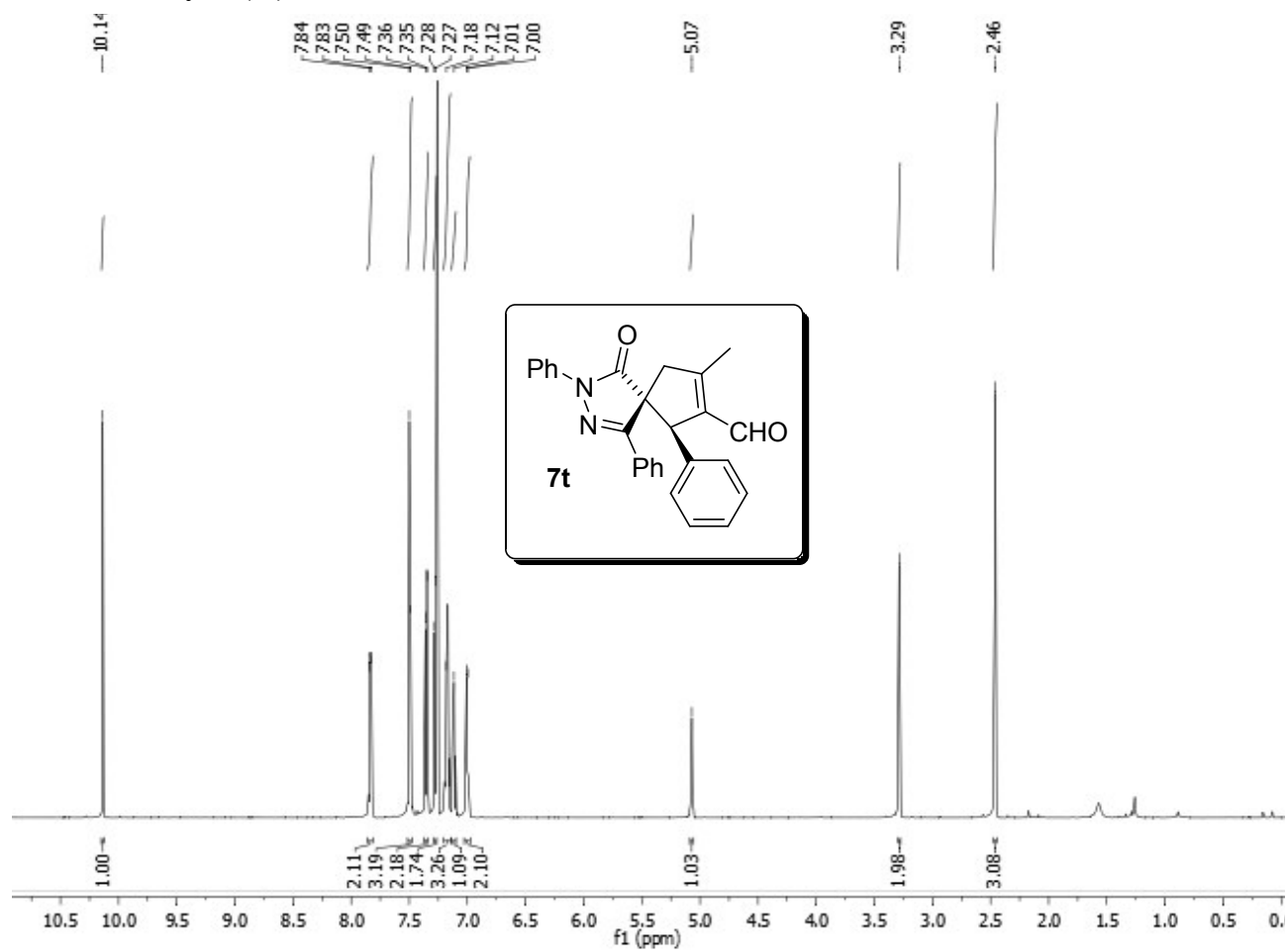
63.02
60.74
59.07
56.83

45.38
45.11

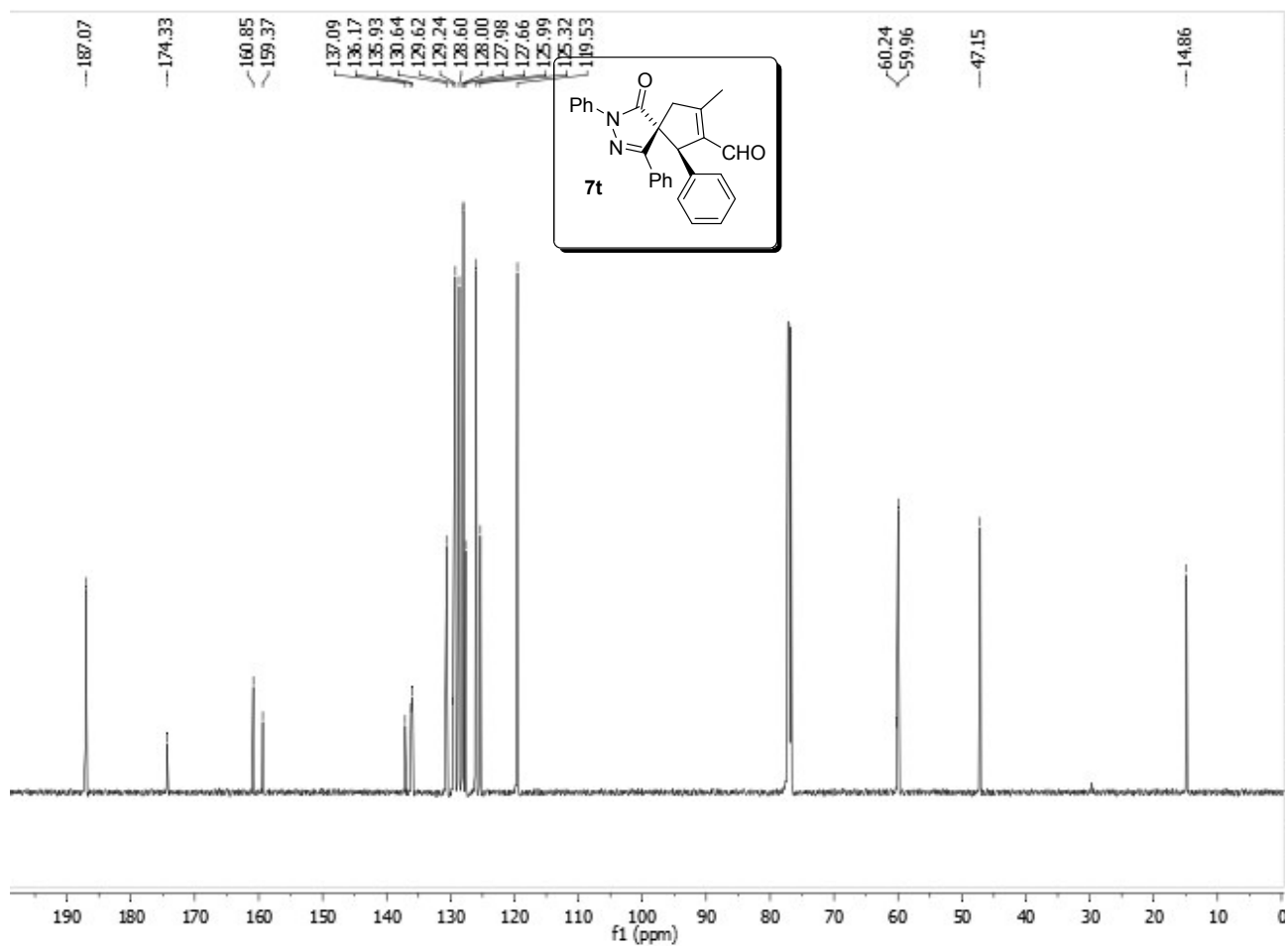
22.60
21.04
14.79
14.66
9.45
9.40



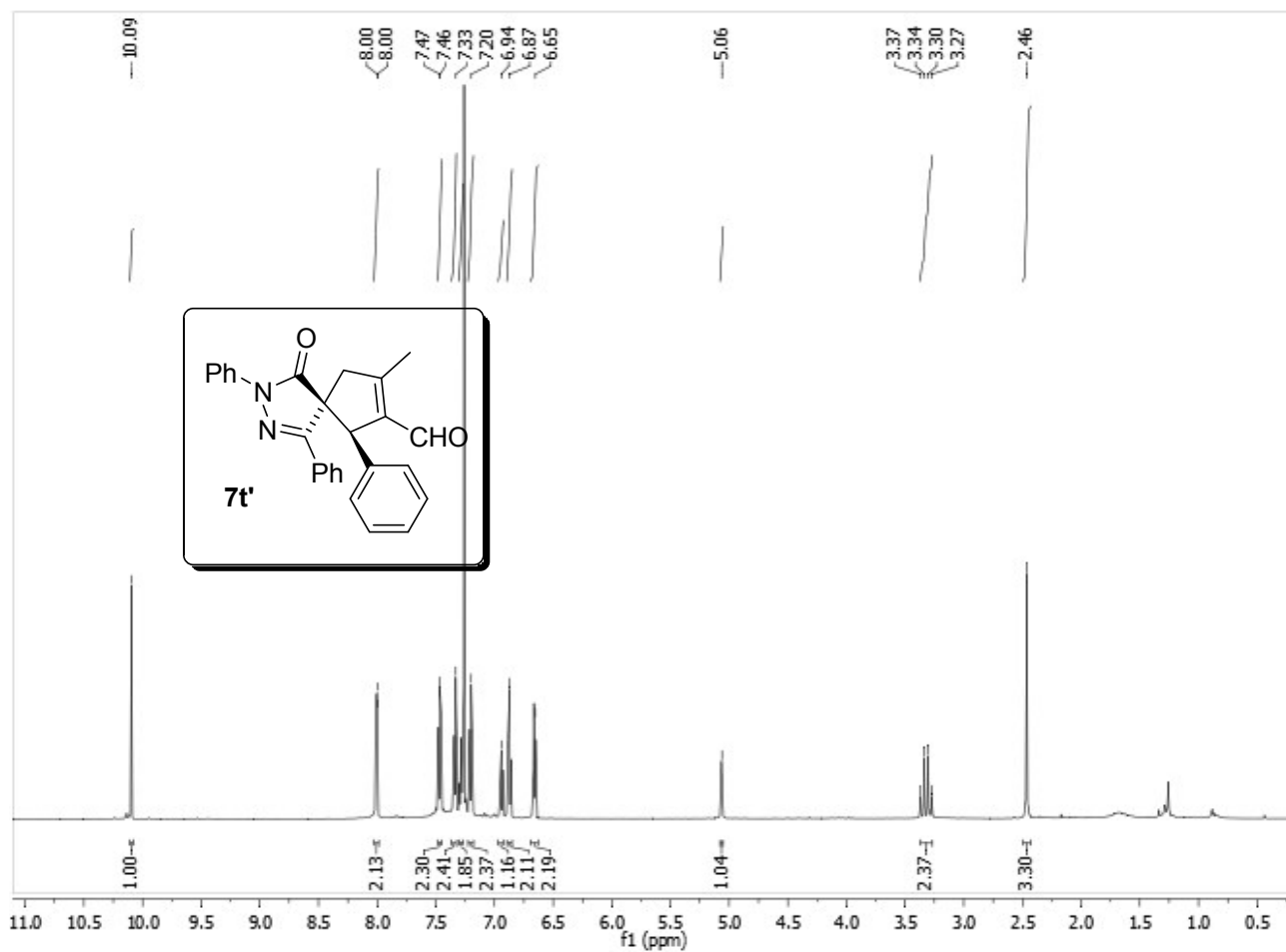
(5*R*,6*R*)-8-Methyl-4-oxo-1,3,6-triphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7t)



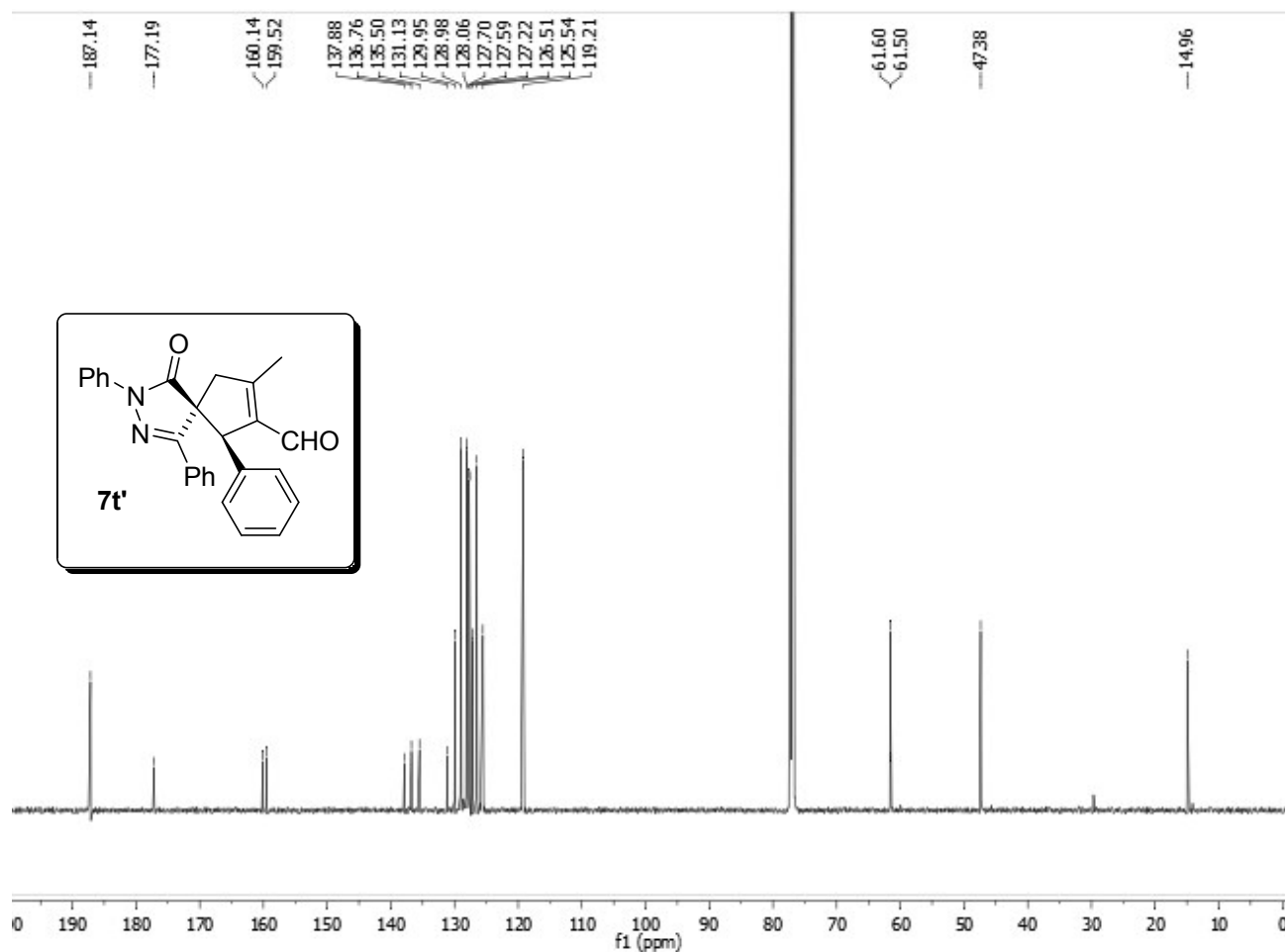
(5*R*,6*R*)-8-Methyl-4-oxo-1,3,6-triphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7t)



(5*S*,6*R*)-8-Methyl-4-oxo-1,3,6-triphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7t')

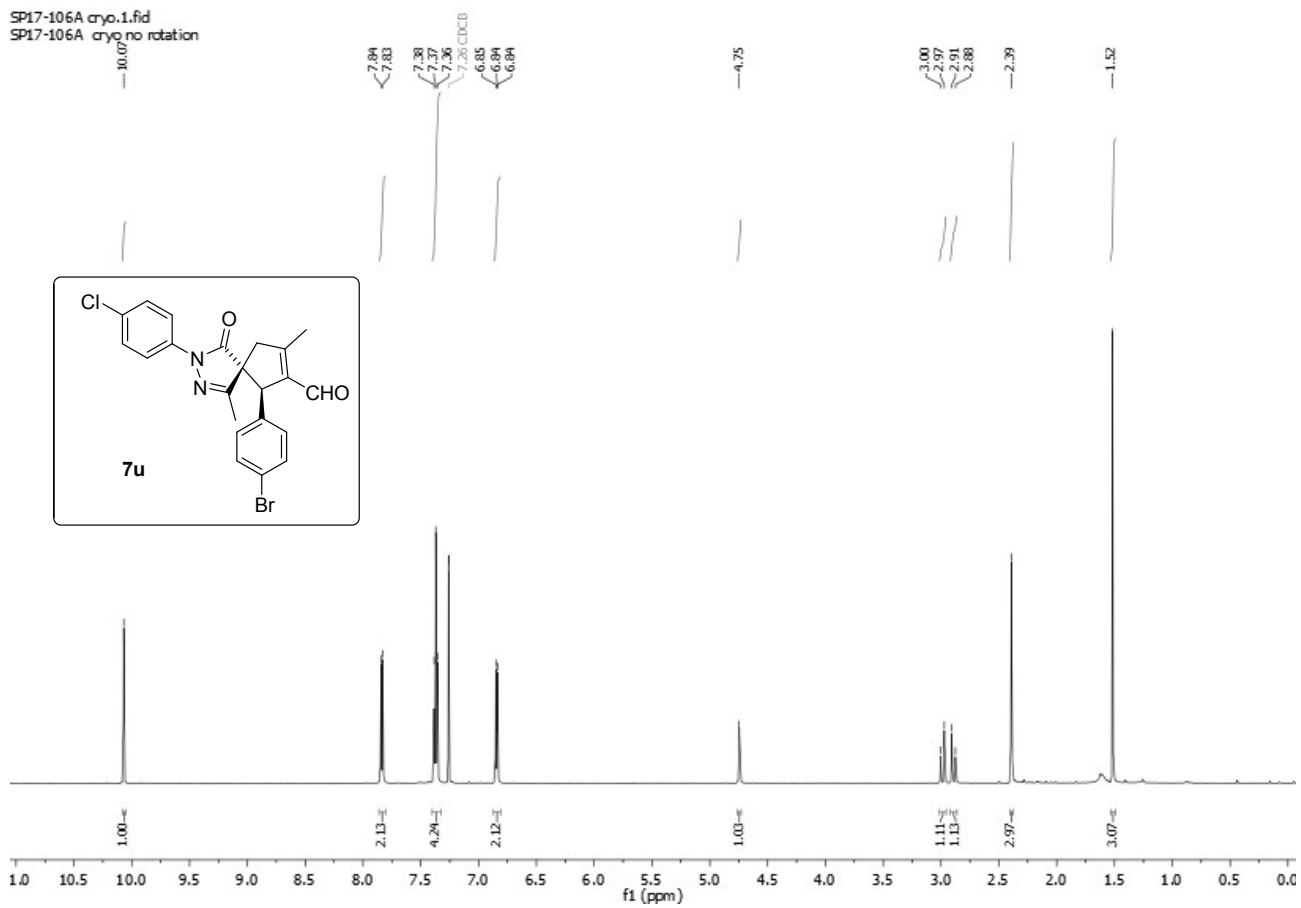


(5*S*,6*R*)-8-Methyl-4-oxo-1,3,6-triphenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7t')

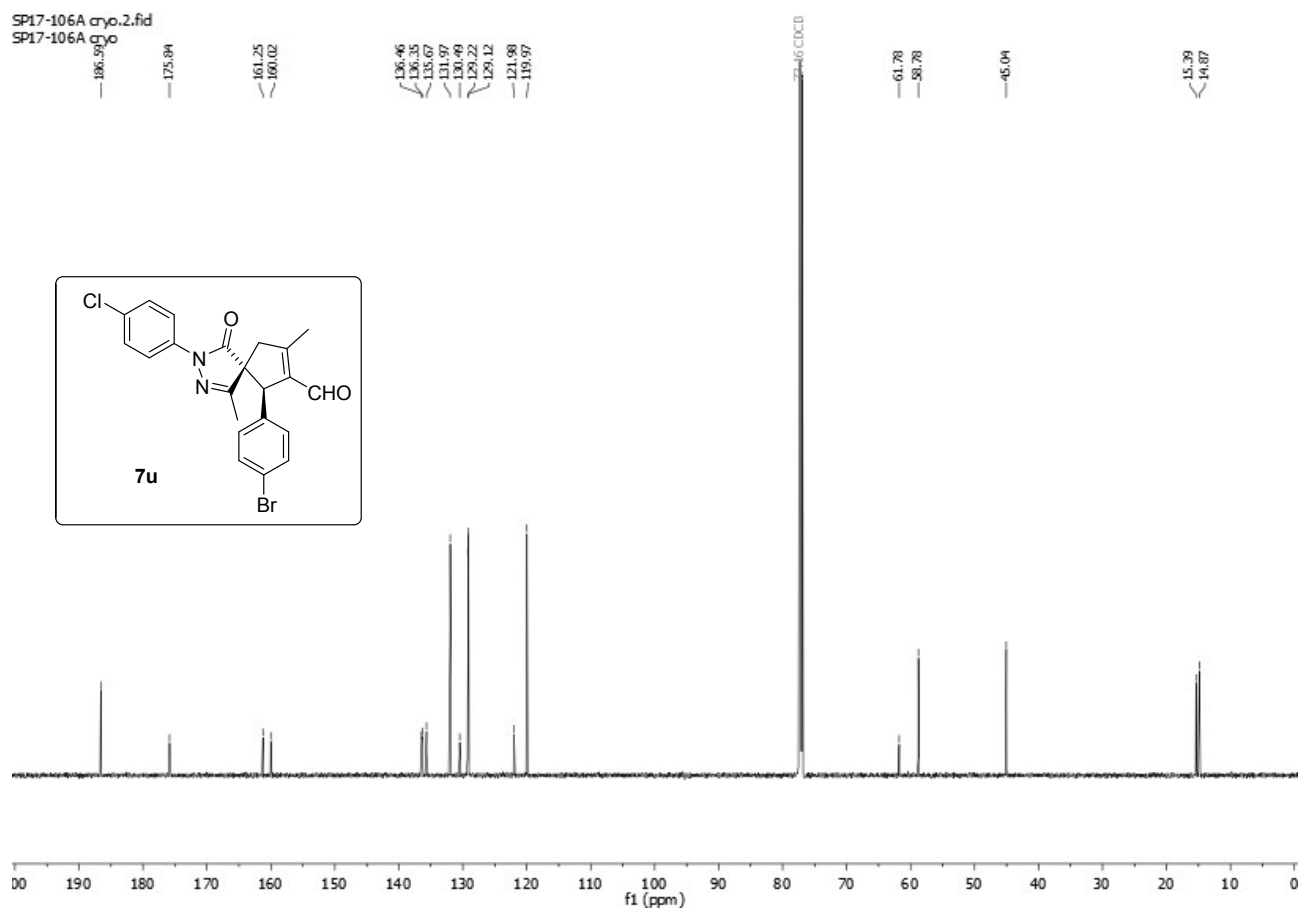


(5*R*,6*R*)-6-(4-Bromophenyl)-3-(4-chlorophenyl)-1,8-dimethyl-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7u)

SP17-106A cryo.1.fid
SP17-106A cryo.no rotation

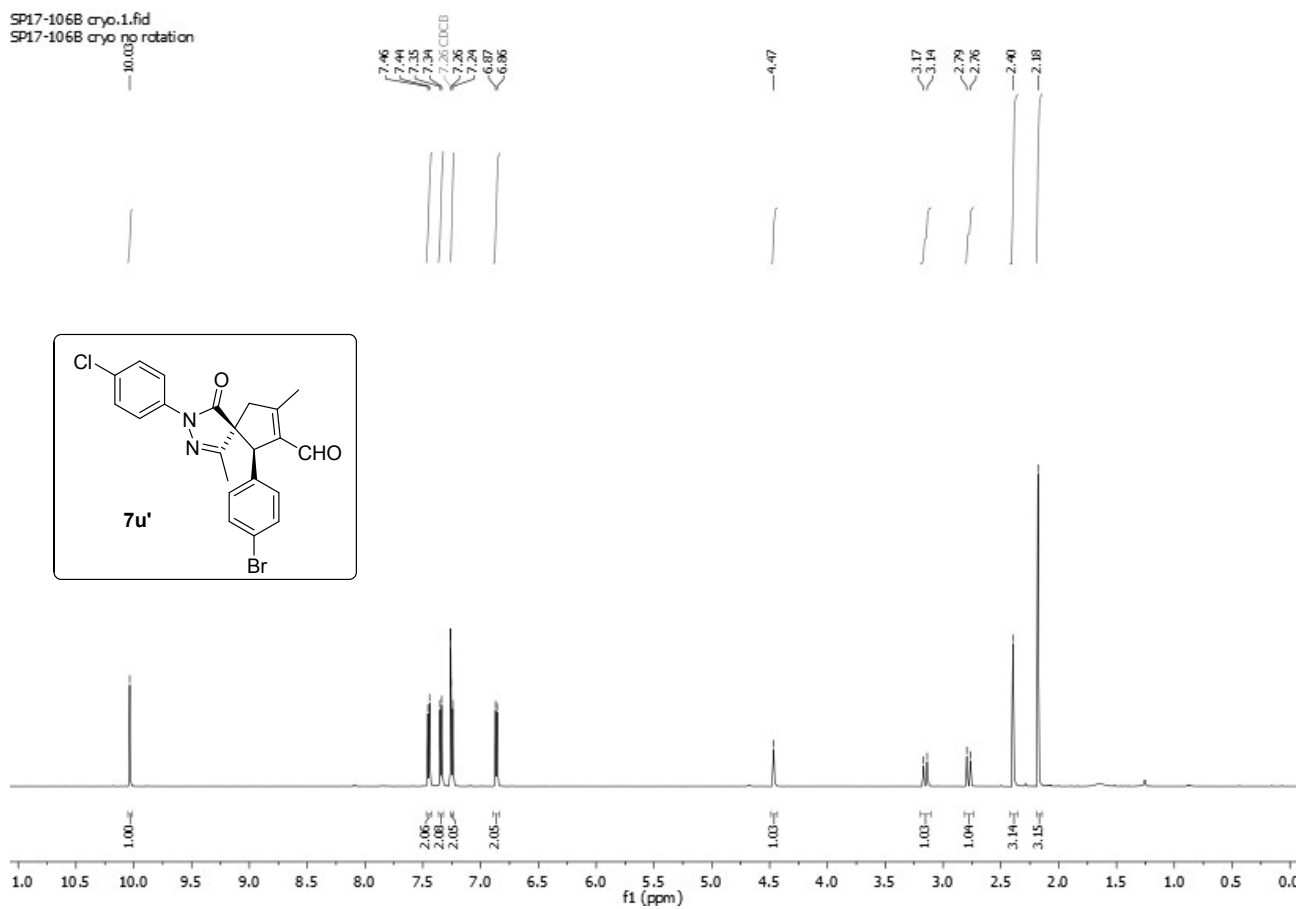


(5*R*,6*R*)-6-(4-Bromophenyl)-3-(4-chlorophenyl)-1,8-dimethyl-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7u)



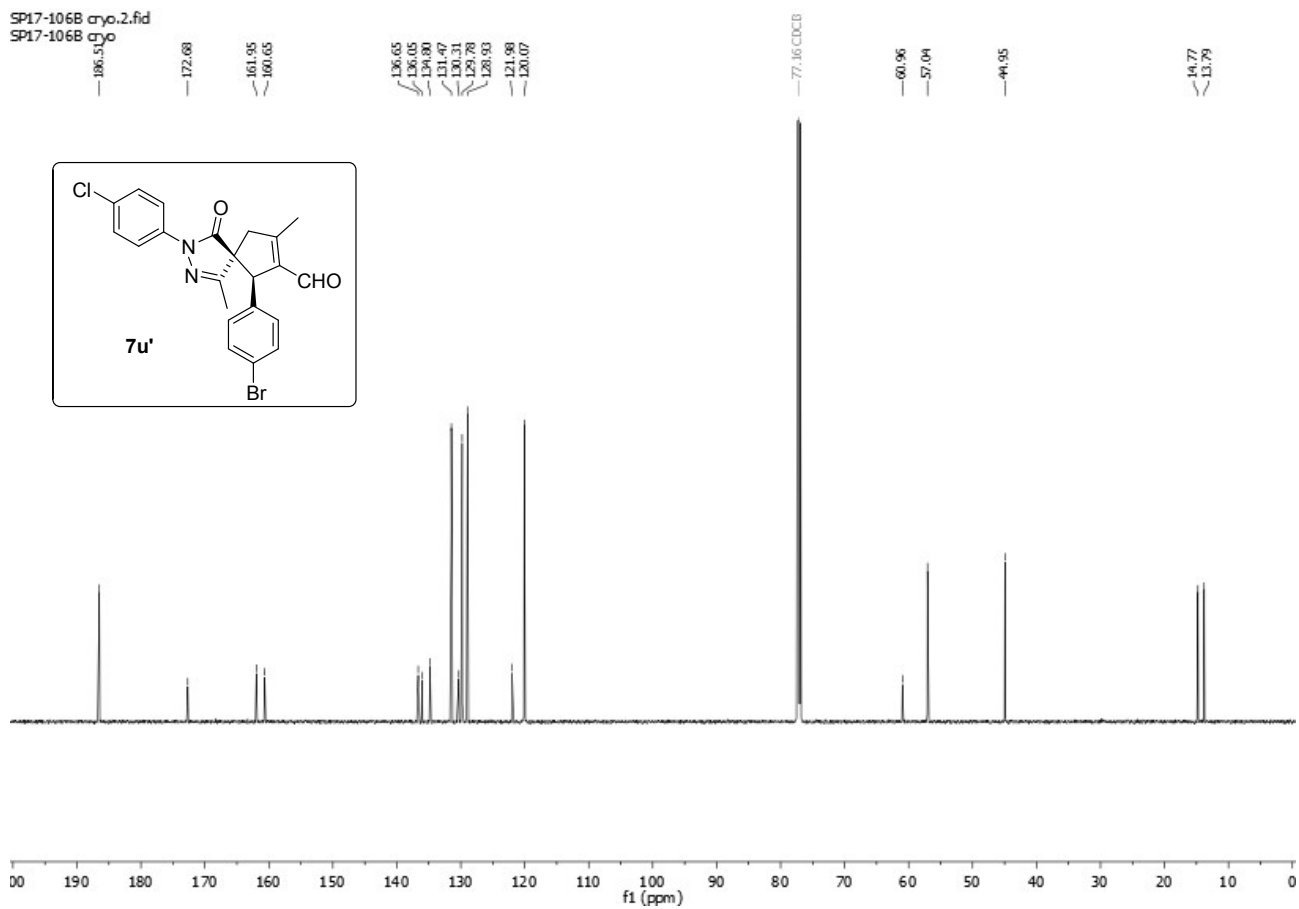
(5*S*,6*R*)-6-(4-Bromophenyl)-3-(4-chlorophenyl)-1,8-dimethyl-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7u')

SP17-106B cryo.1.fid
SP17-106B cryo no rotation



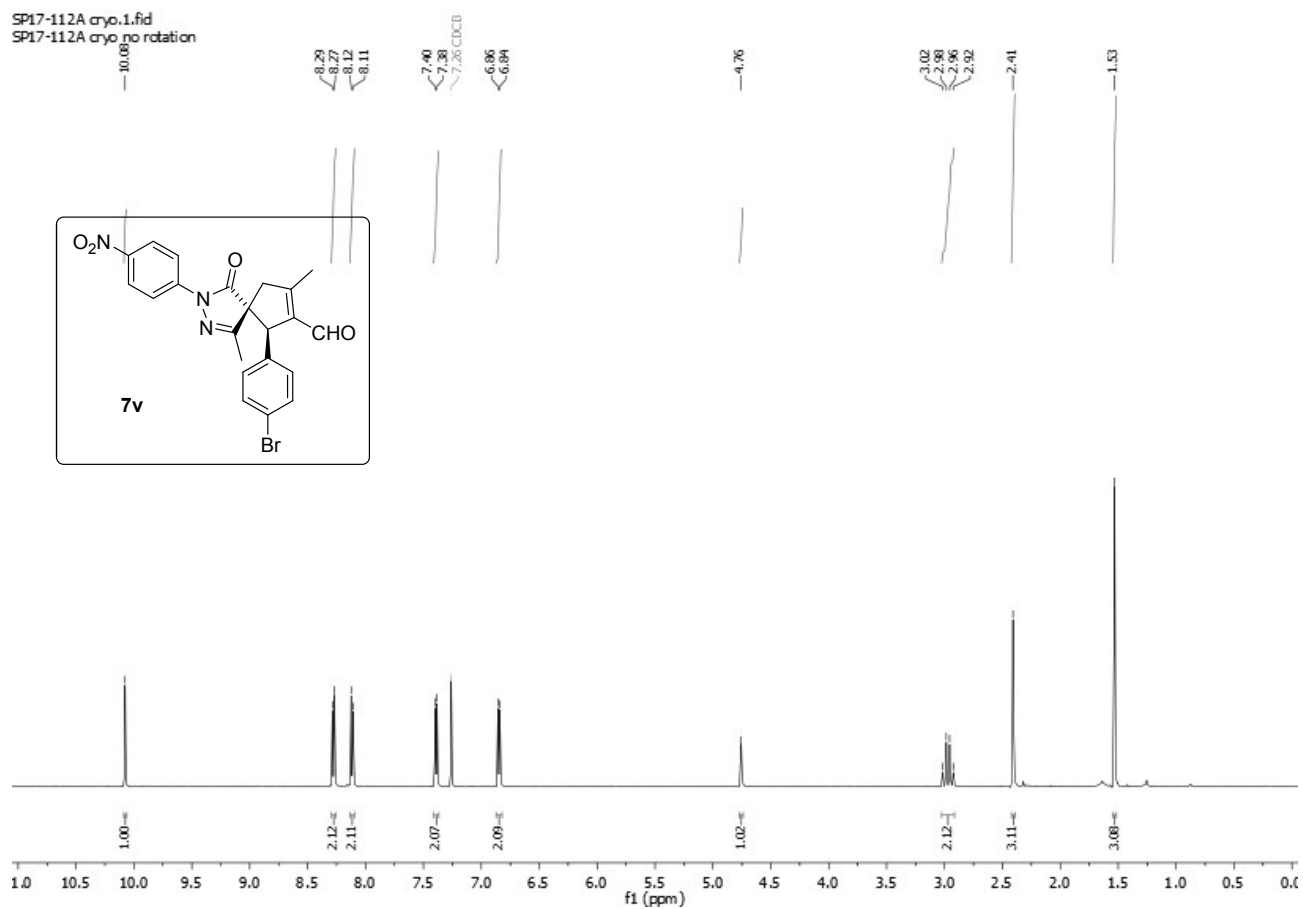
(5*S*,6*R*)-6-(4-Bromophenyl)-3-(4-chlorophenyl)-1,8-dimethyl-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7u')

SP17-106B cryo.2.fid
SP17-106B cryo

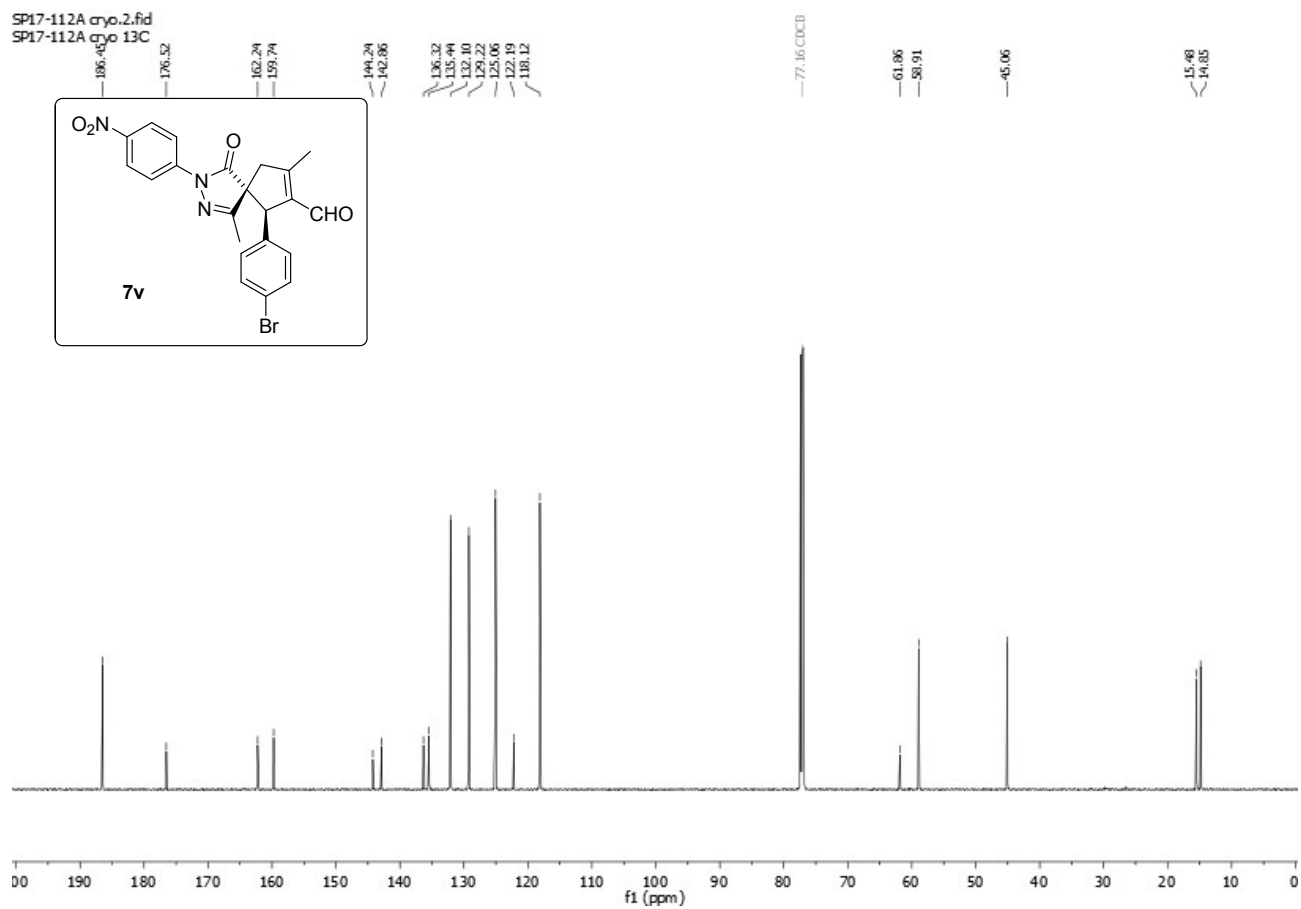


(5*R*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-3-(4-nitrophenyl)-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7v)

SP17-112A cryo.1.fid
SP17-112A cryo no rotation

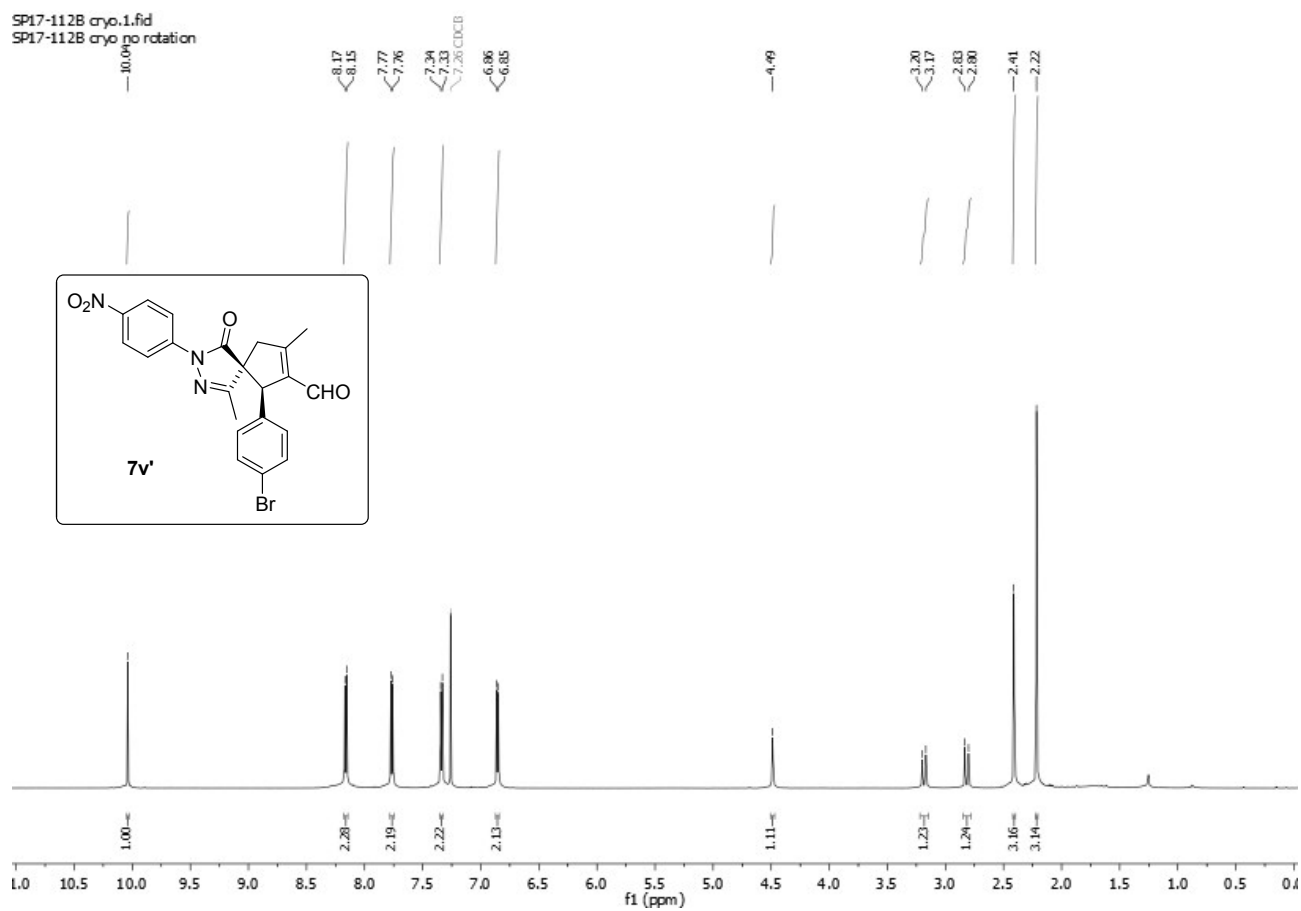


(5*R*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-3-(4-nitrophenyl)-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7v)



(5*S*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-3-(4-nitrophenyl)-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7v')

SP17-112B cryo.1.fid
SP17-112B cryo no rotation



(5*S*,6*R*)-6-(4-Bromophenyl)-1,8-dimethyl-3-(4-nitrophenyl)-4-oxo-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7v')

SP17-112B chp.2.fid
SP17-112B chp.13C

173.06

162.82

160.13

143.83

142.32

136.34

134.32

131.36

129.51

124.68

121.95

117.74

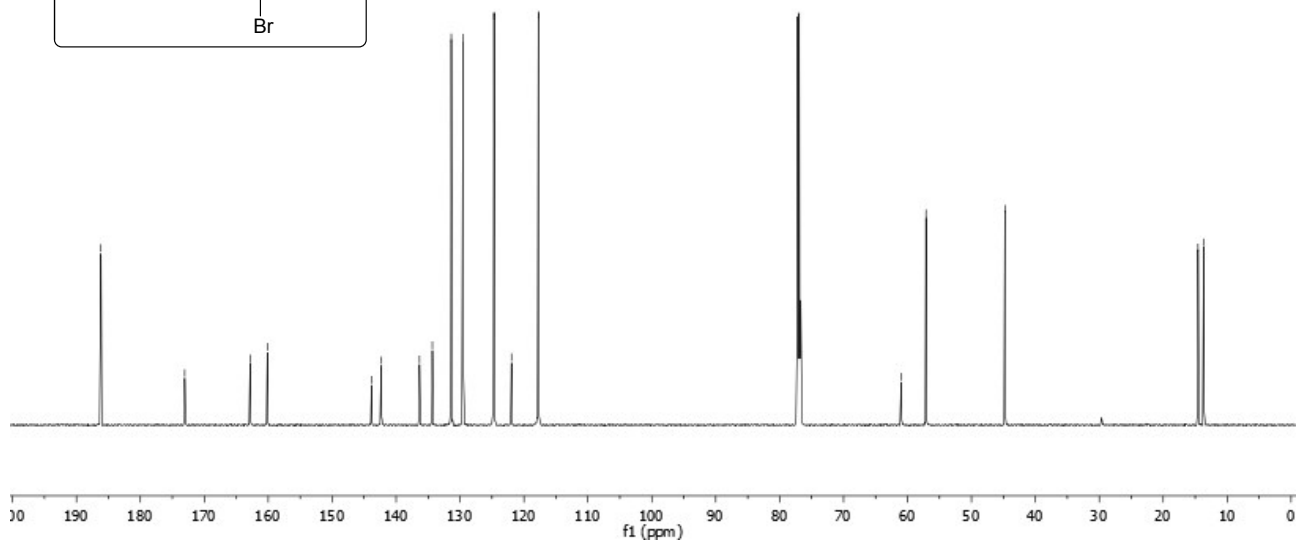
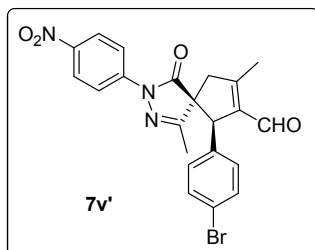
60.97

57.12

41.75

14.55

13.66



(5*R*/5*S*,6*R*)-1,8-Dimethyl-3-(4-nitrophenyl)-4-oxo-6-propyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7w) mixture of diastereomers 1.7:1

SP17-109 cryo.2.fid
SP17-109 13c

187.64
187.06
176.44
174.68
164.59
163.51
157.50

144.15
144.02
143.13
139.11
137.87

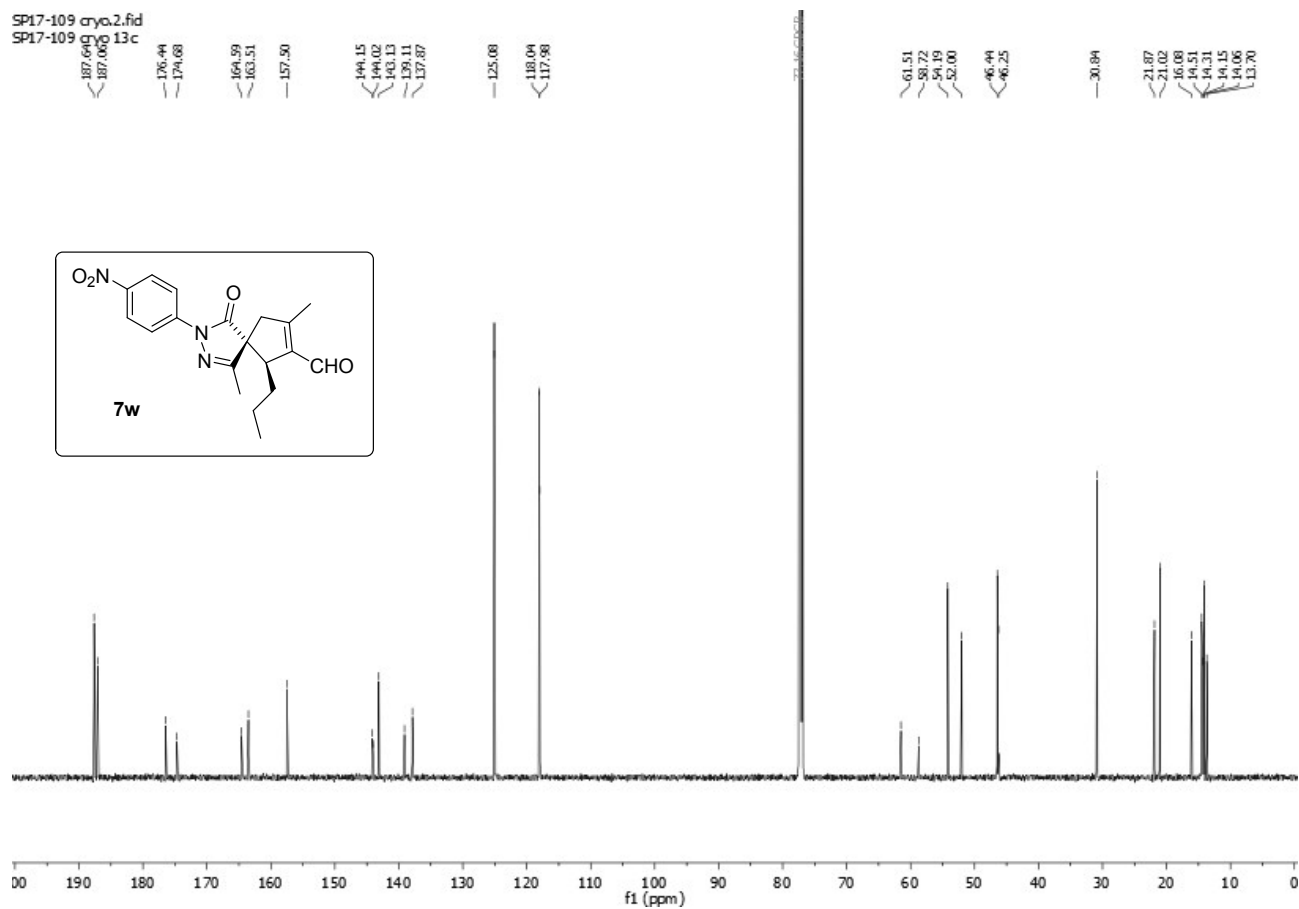
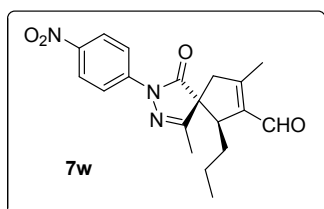
125.08
118.04
117.98

61.51
58.72
54.19
52.00

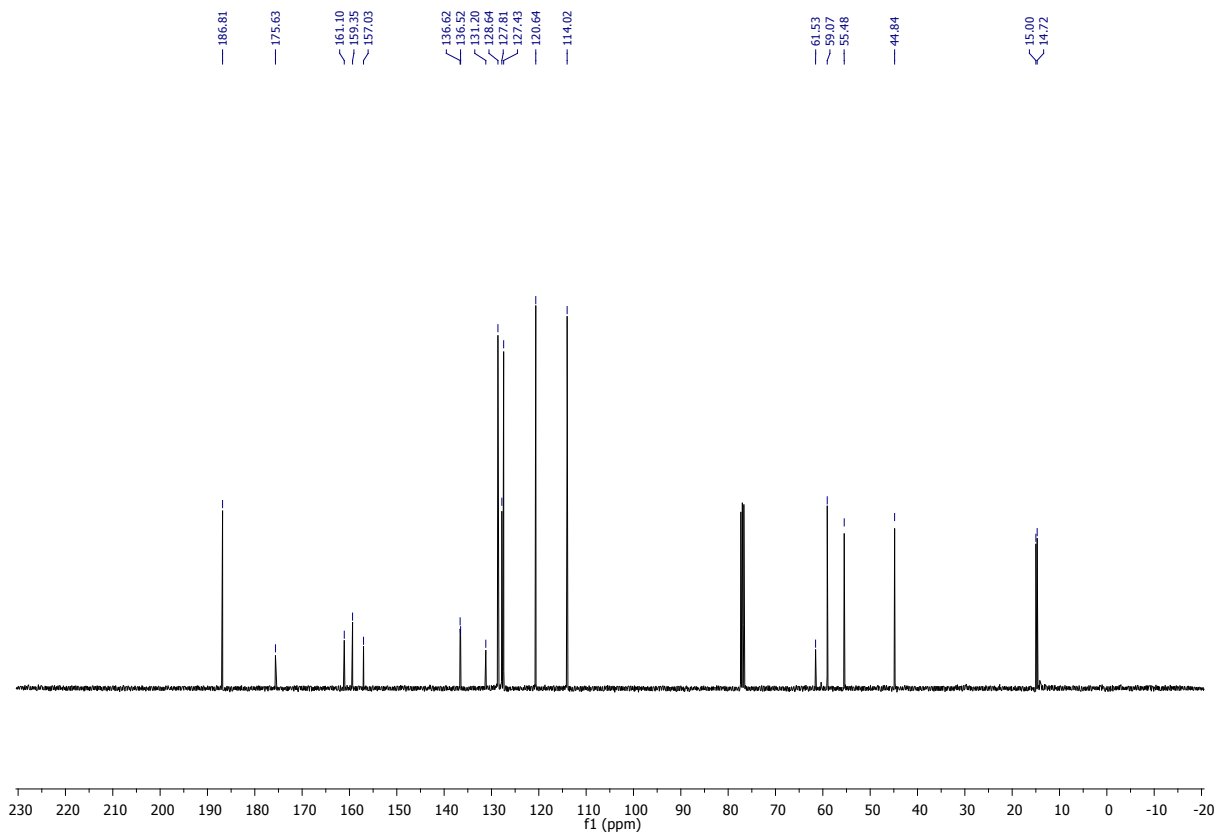
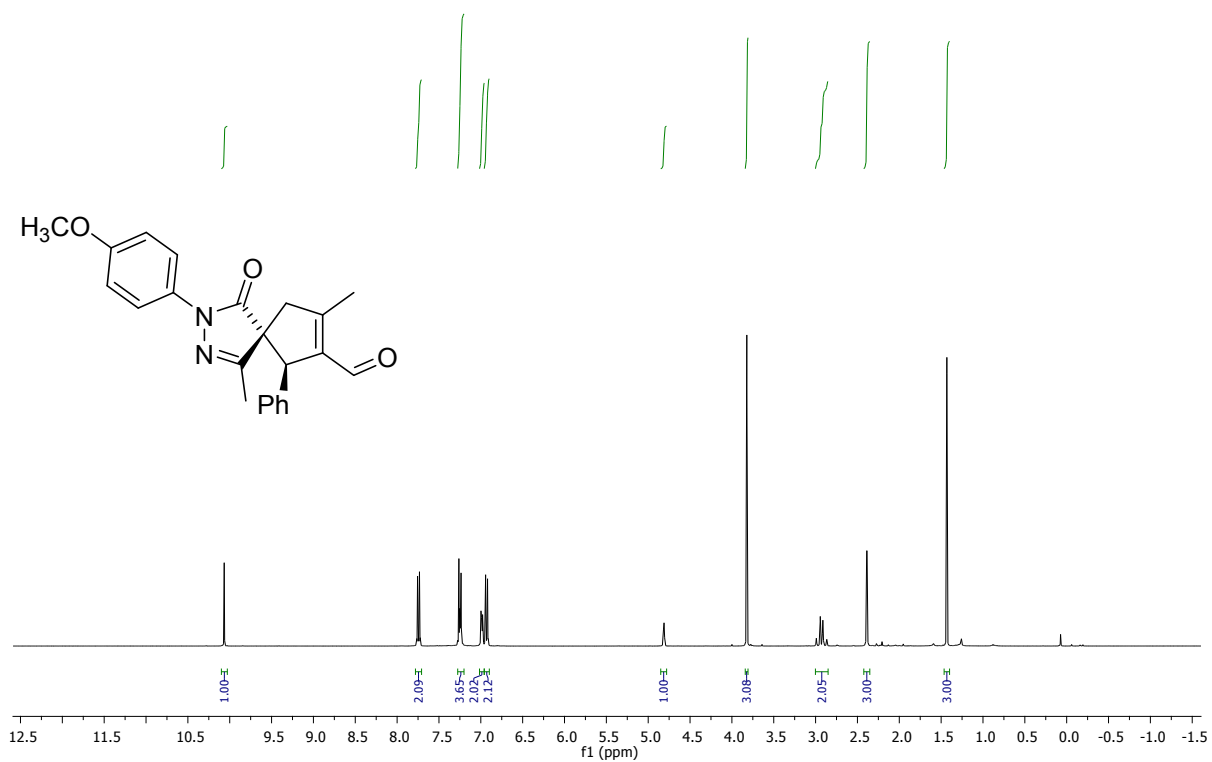
46.44
46.25

30.84

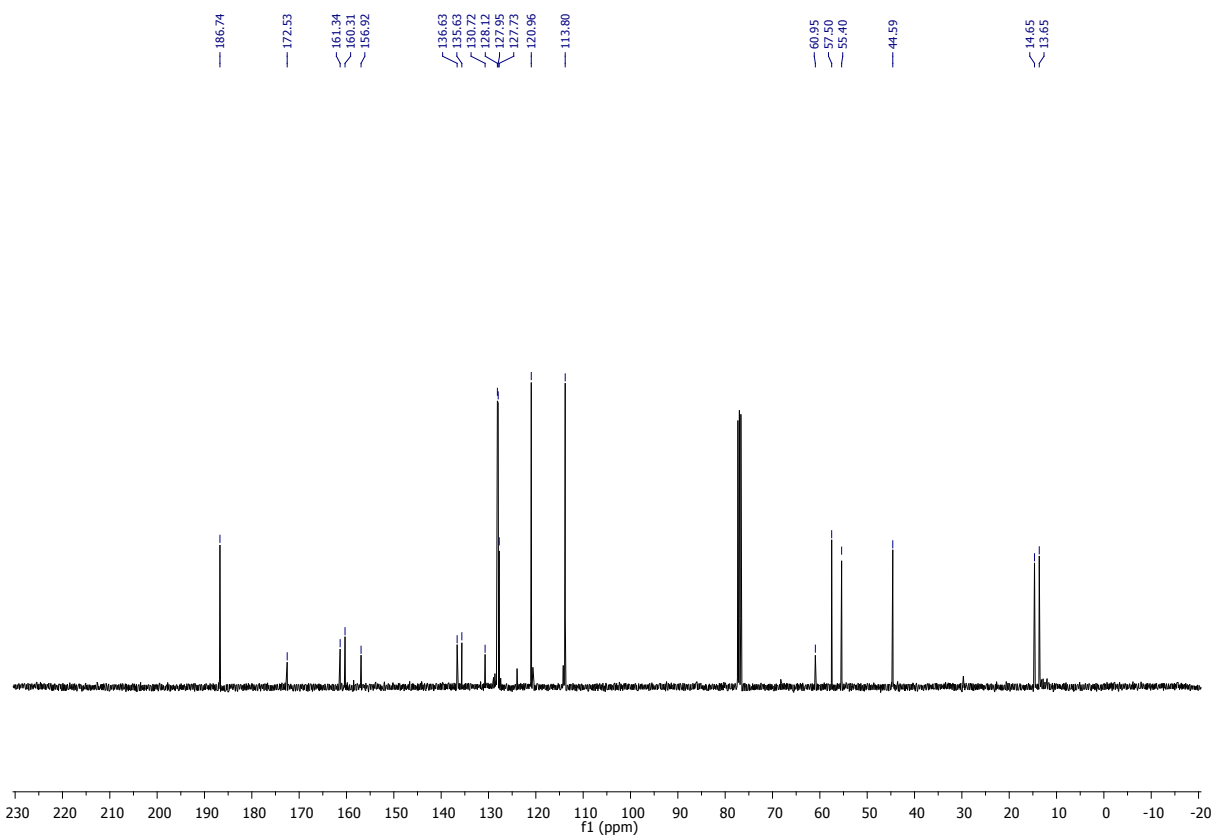
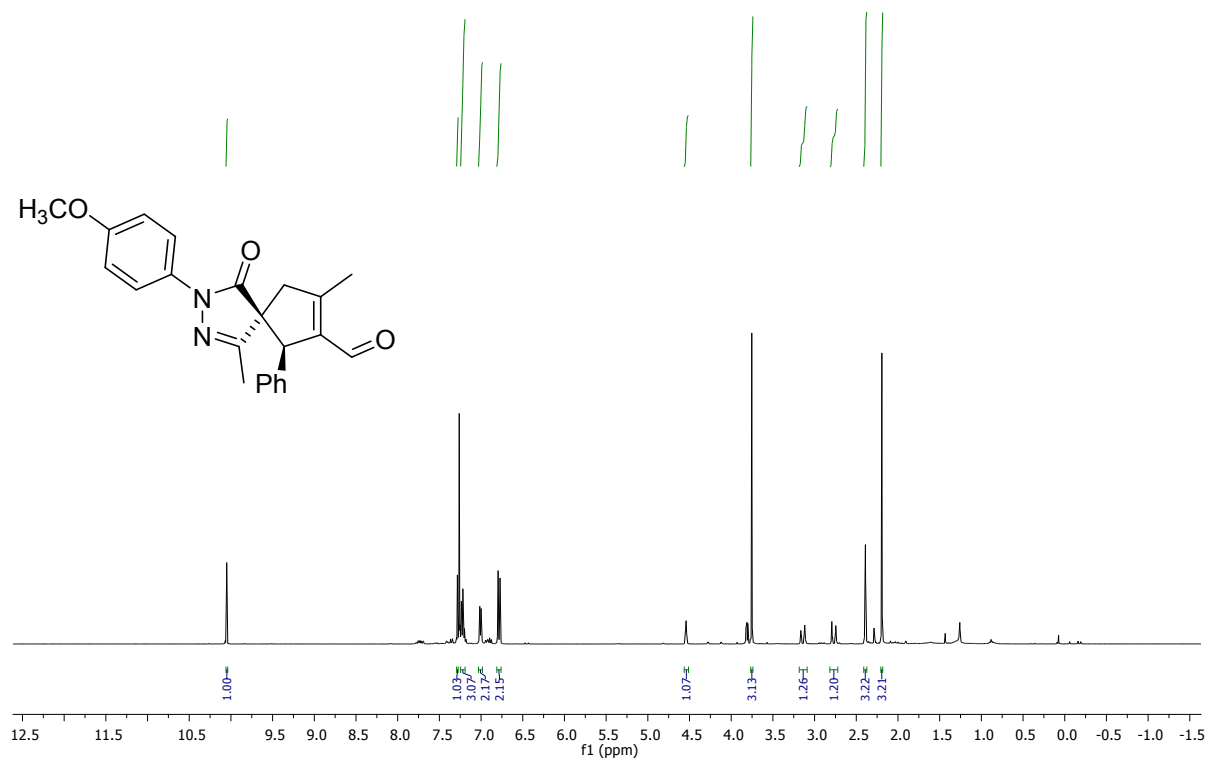
21.87
21.02
18.08
16.51
14.15
14.06
13.70



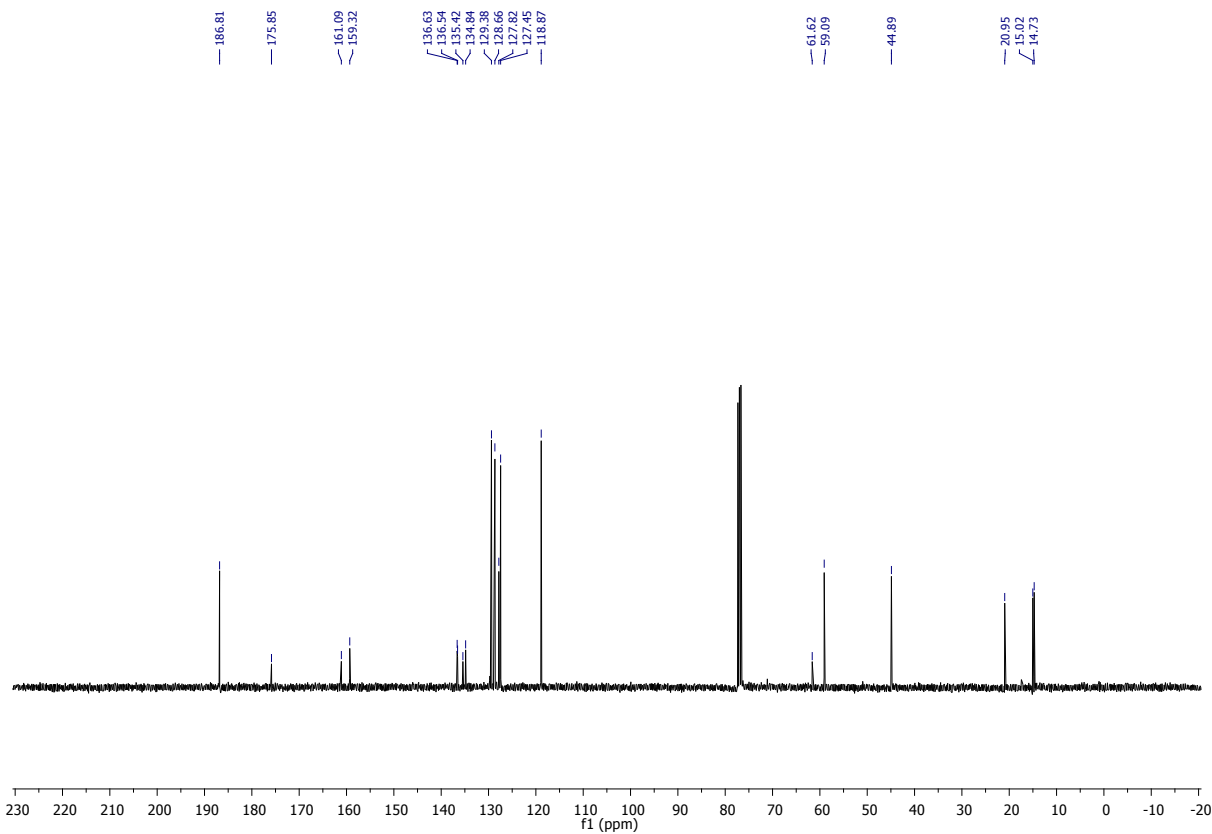
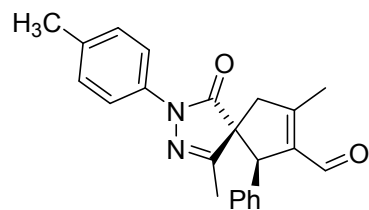
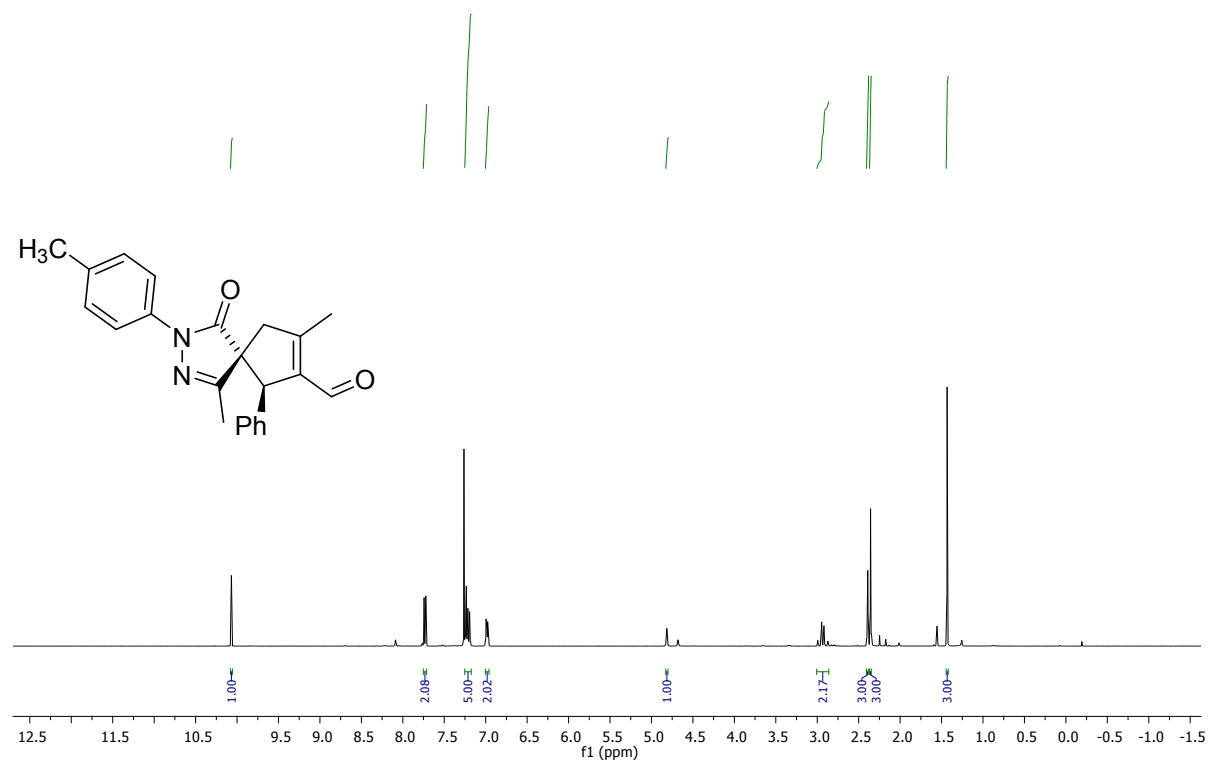
(5*R*,6*R*)-2-(4-methoxyphenyl)-4,8-dimethyl-6-phenyl-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7x)



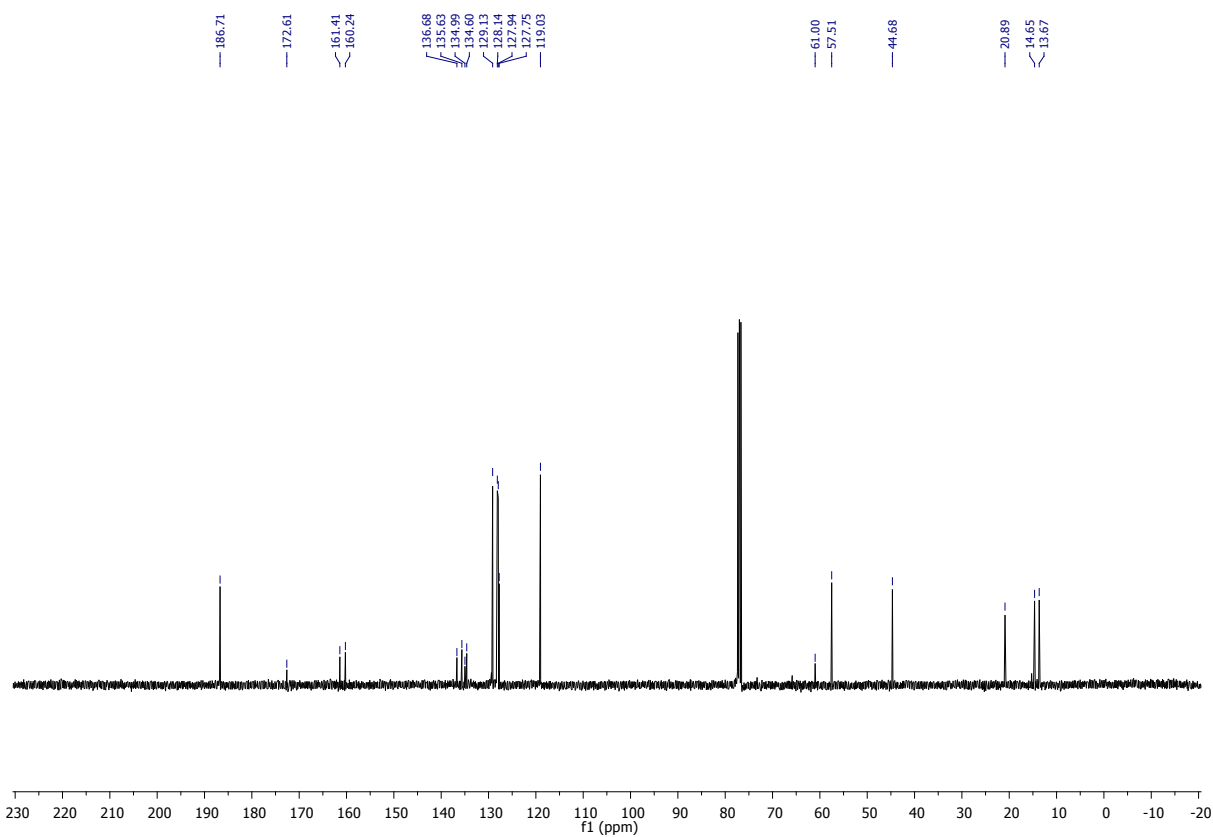
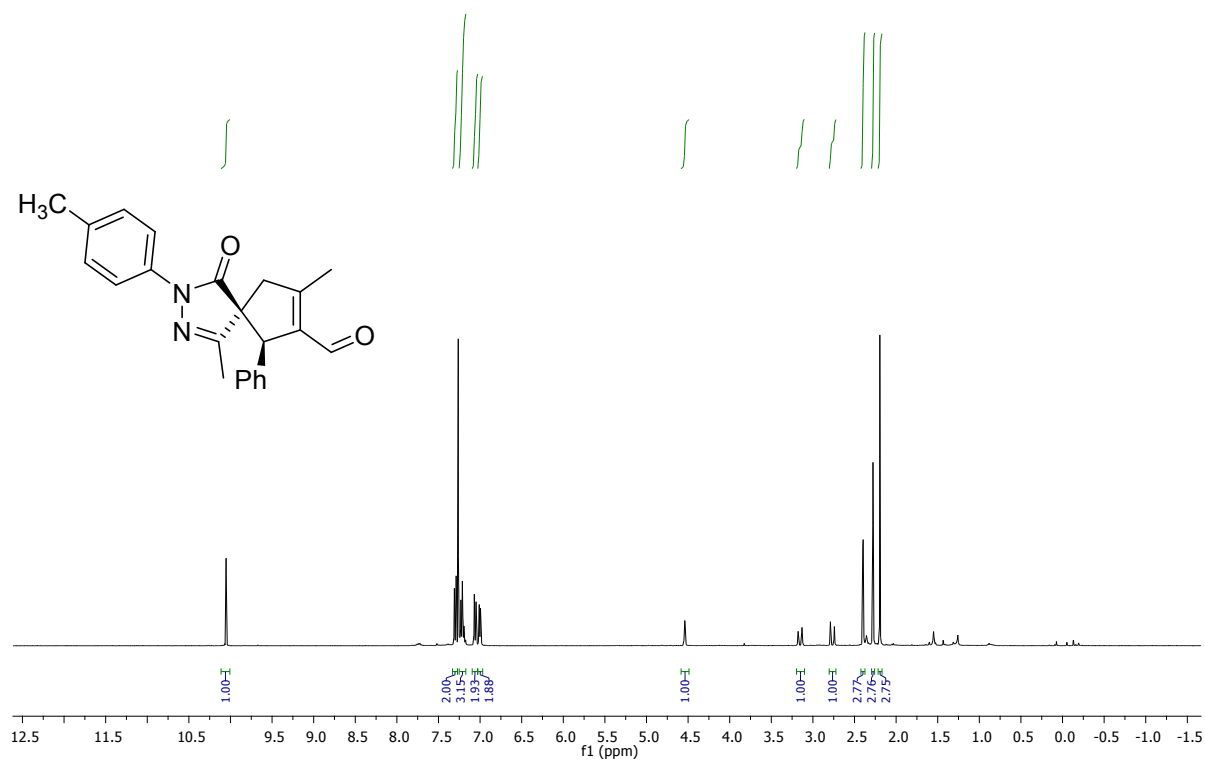
(5*S*,6*R*)-2-(4-methoxyphenyl)-4,8-dimethyl-6-phenyl-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7x')



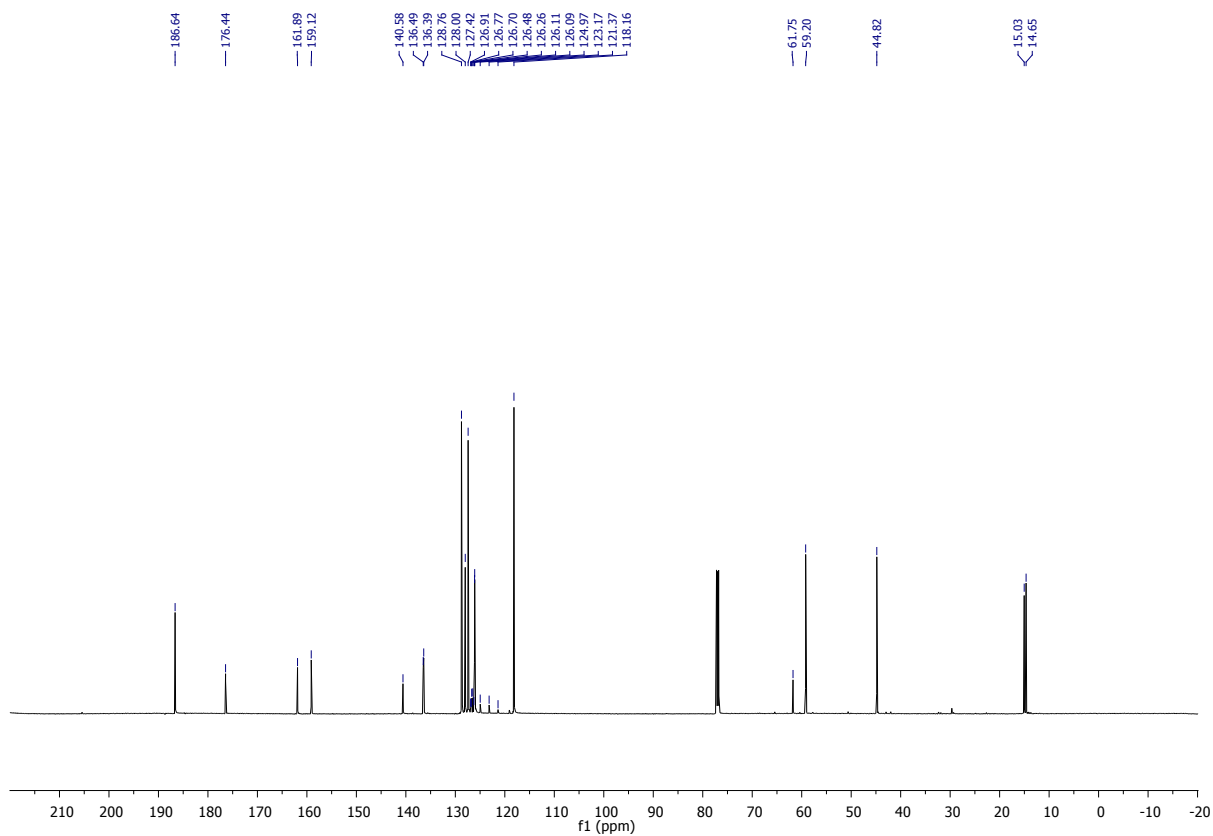
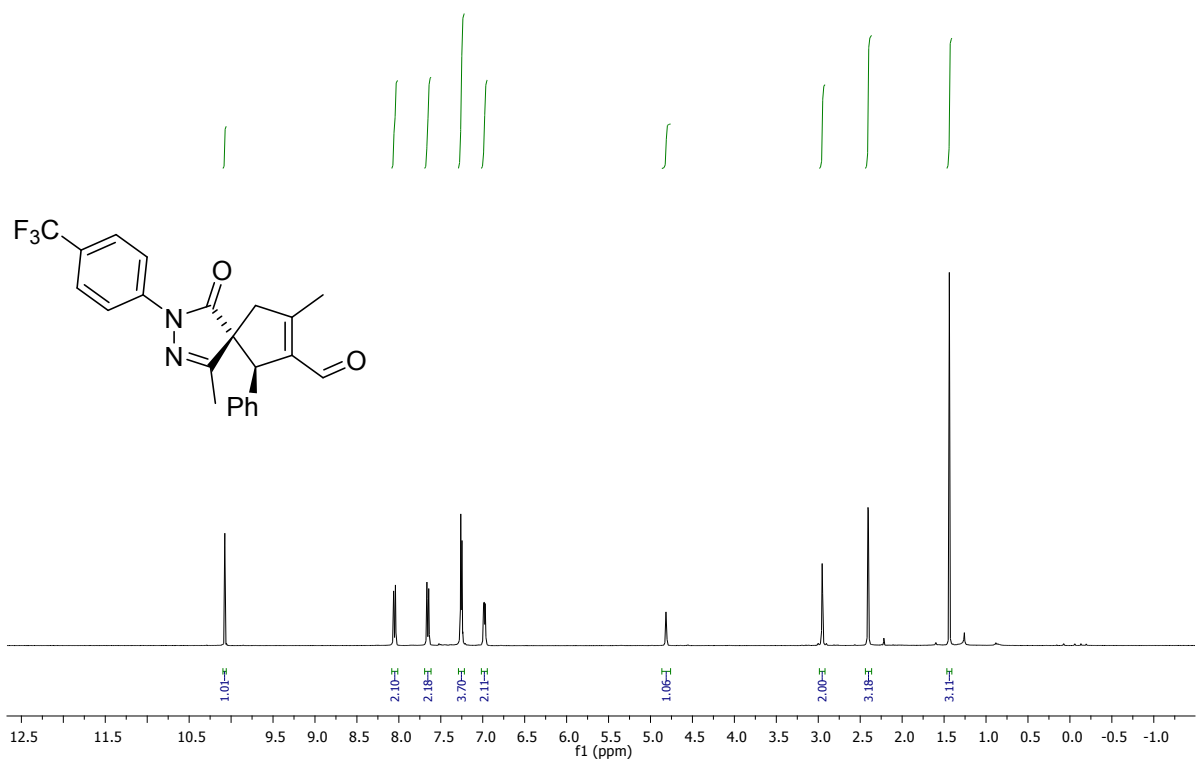
**(5*R*,6*R*)-4,8-dimethyl-6-phenyl-2-(*p*-tolyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one
(7y)**

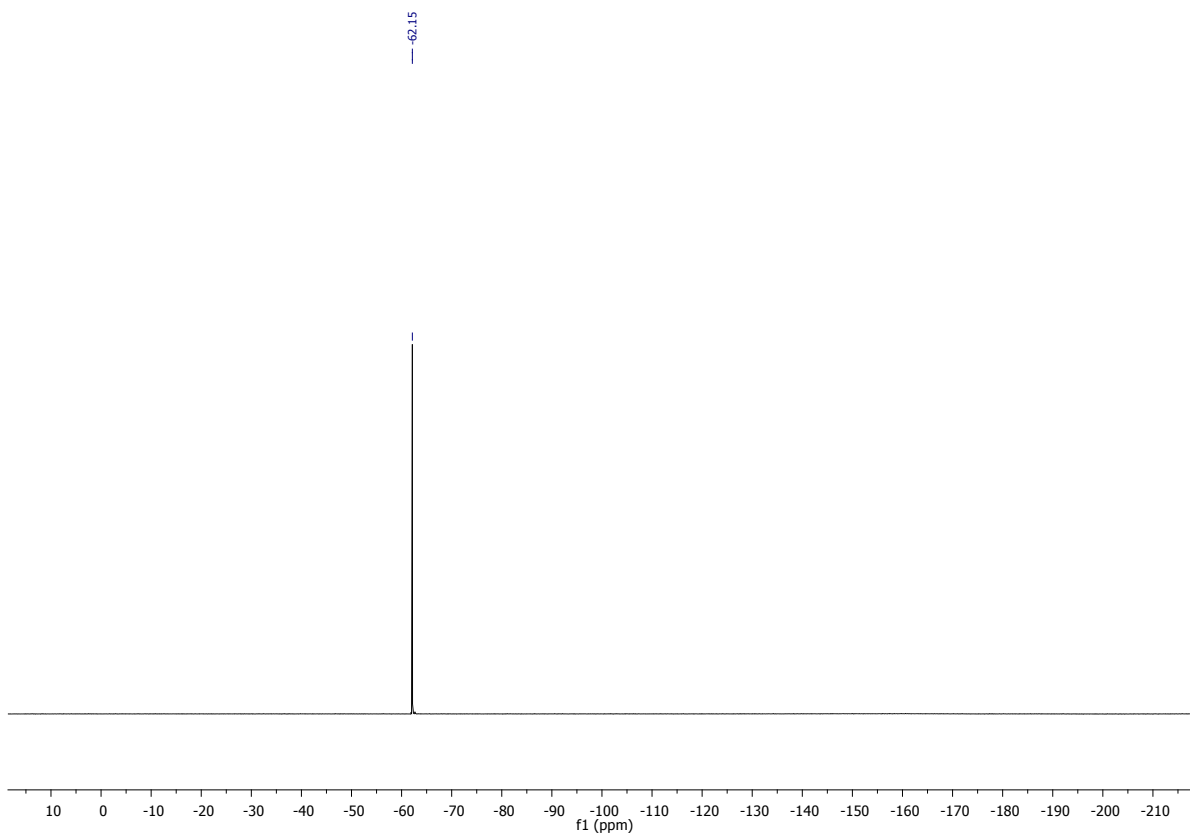


(5*S*,6*R*)-4,8-dimethyl-6-phenyl-2-(*p*-tolyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7y)

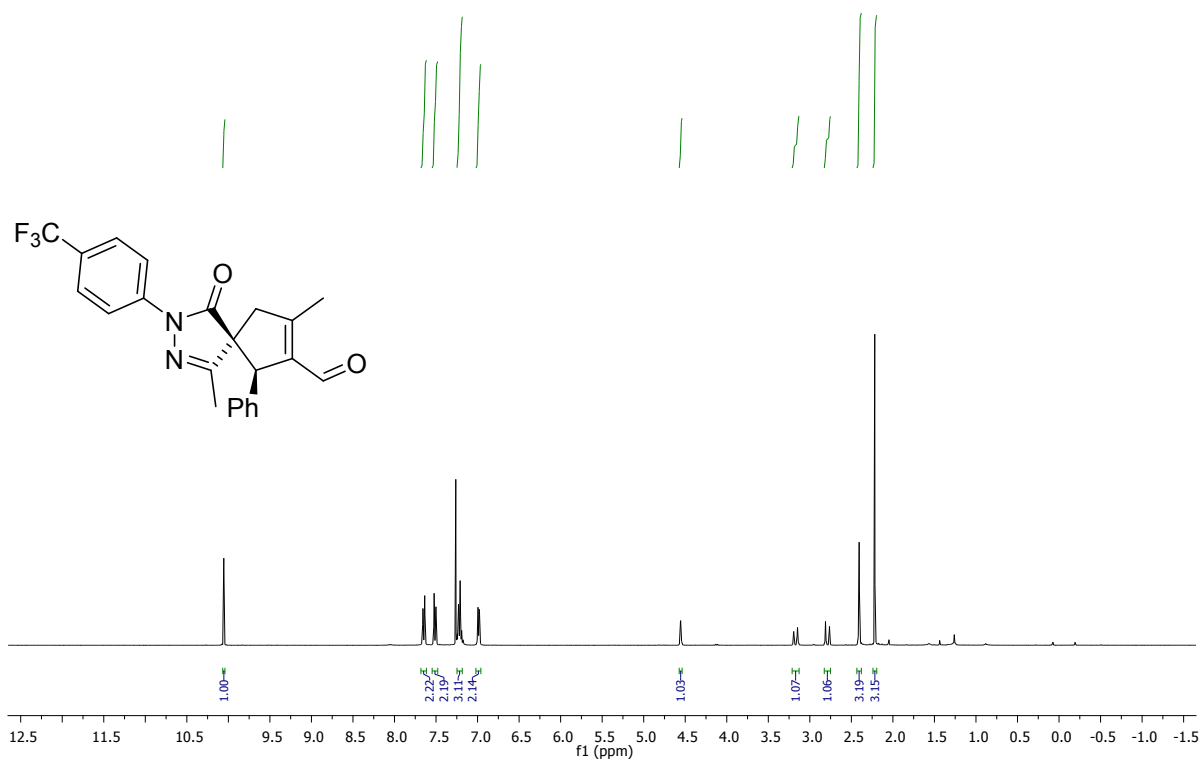


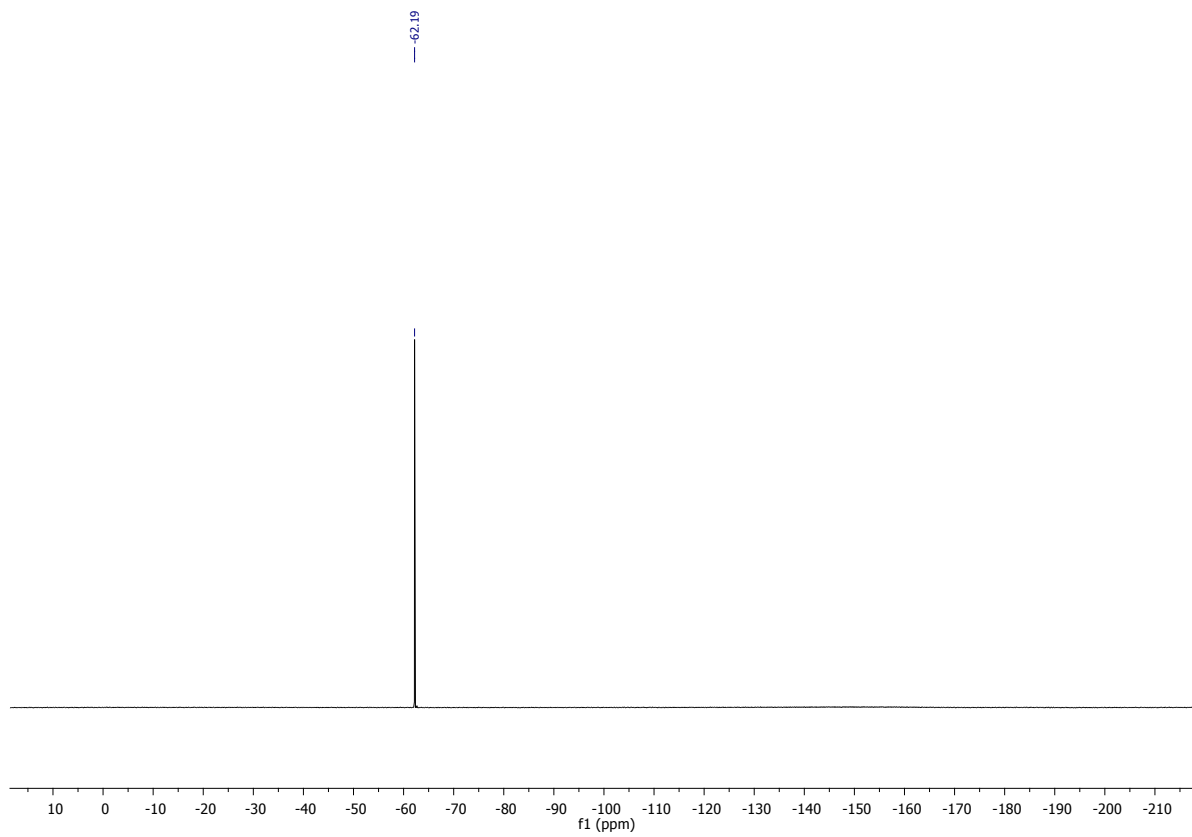
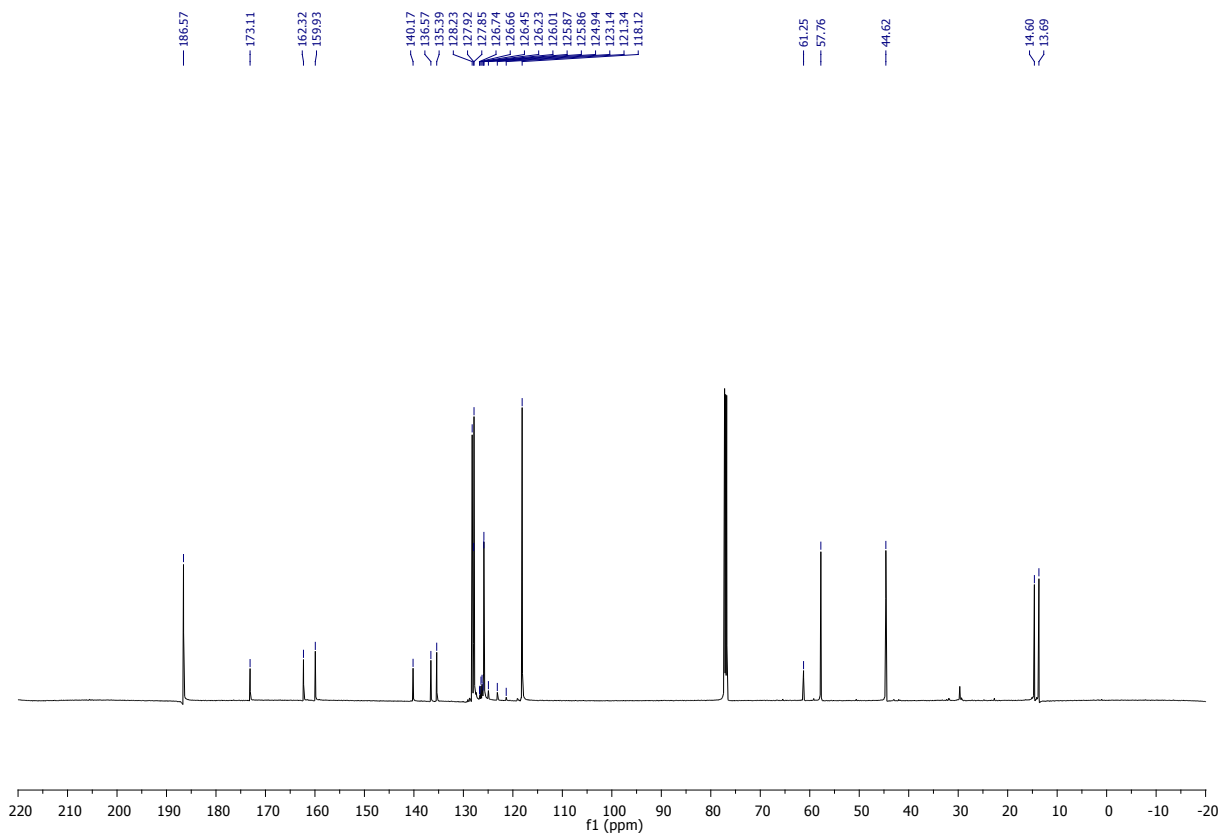
(5*R*,6*R*)-4,8-dimethyl-6-phenyl-2-(4-(trifluoromethyl)phenyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7z)



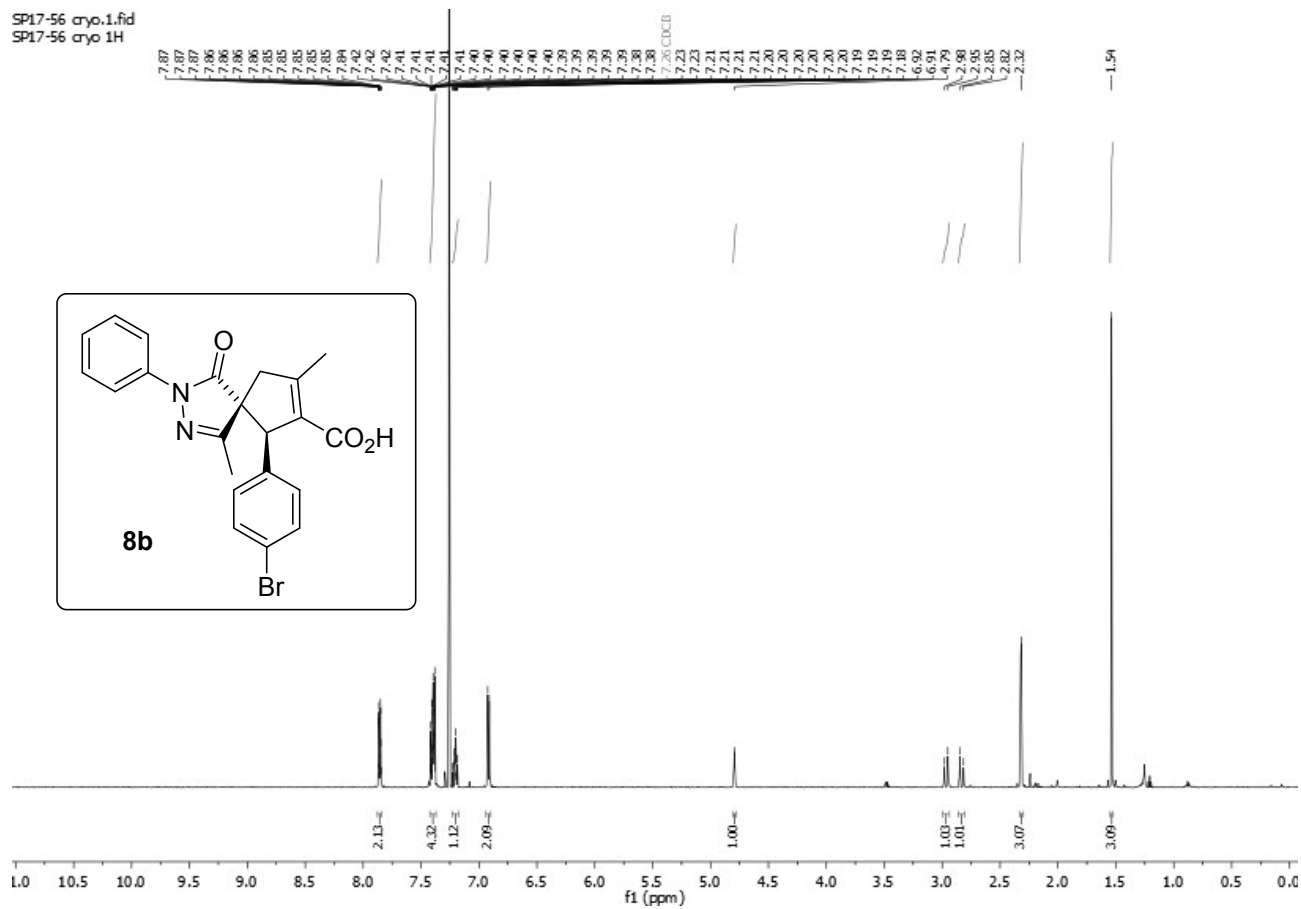


(5*S*,6*R*)-4,8-dimethyl-6-phenyl-2-(4-(trifluoromethyl)phenyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7z')





(5*R*,6*S*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carboxylic acid (8b)



(5*R*,6*S*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carboxylic acid (8b)

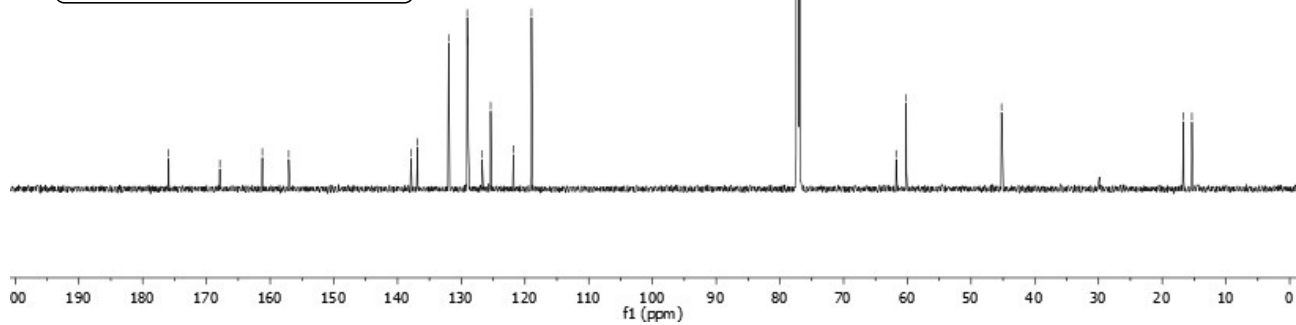
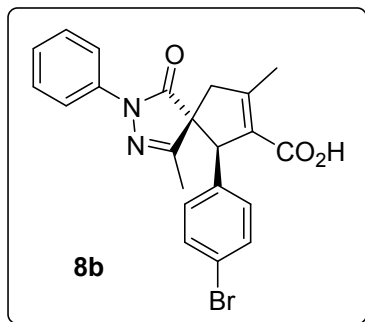
SP17-56 cryo.2.fid
SP17-56 cryo 13C

175.91
167.89
161.22
157.07
137.90
136.86
131.98
129.07
128.92
126.75
125.39
121.81
118.98

61.79
60.17

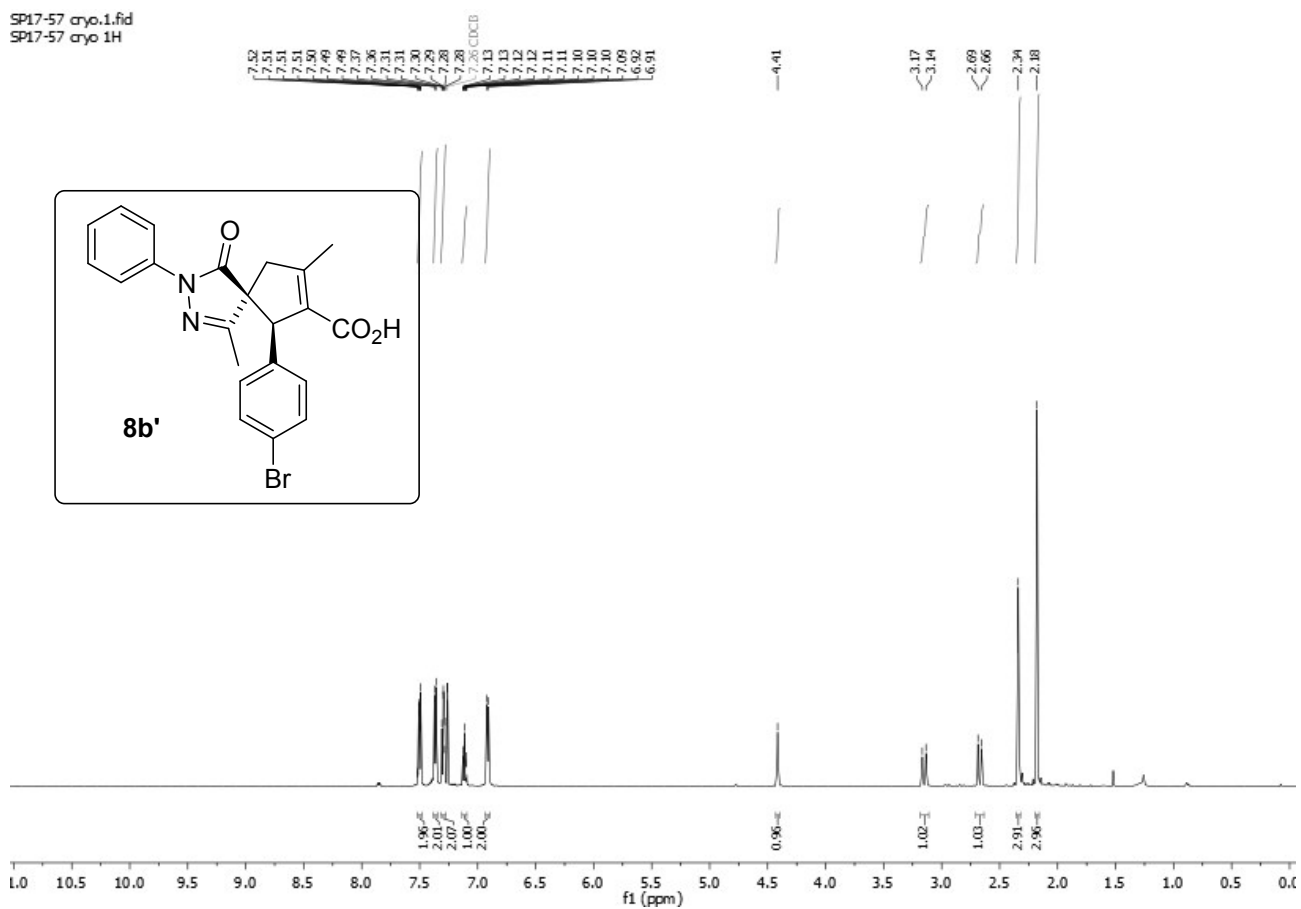
45.23

16.66
15.35



(5*S*,6*S*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carboxylic acid (8b')

SP17-57 cryo.1.fid
SP17-57 cryo.1H



(5*S*,6*S*)-6-(4-Bromophenyl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carboxylic acid (8b')

SP17-57 cryo.2.fid
SP17-567 cryo 13C

172.57
169.31
162.18
158.40

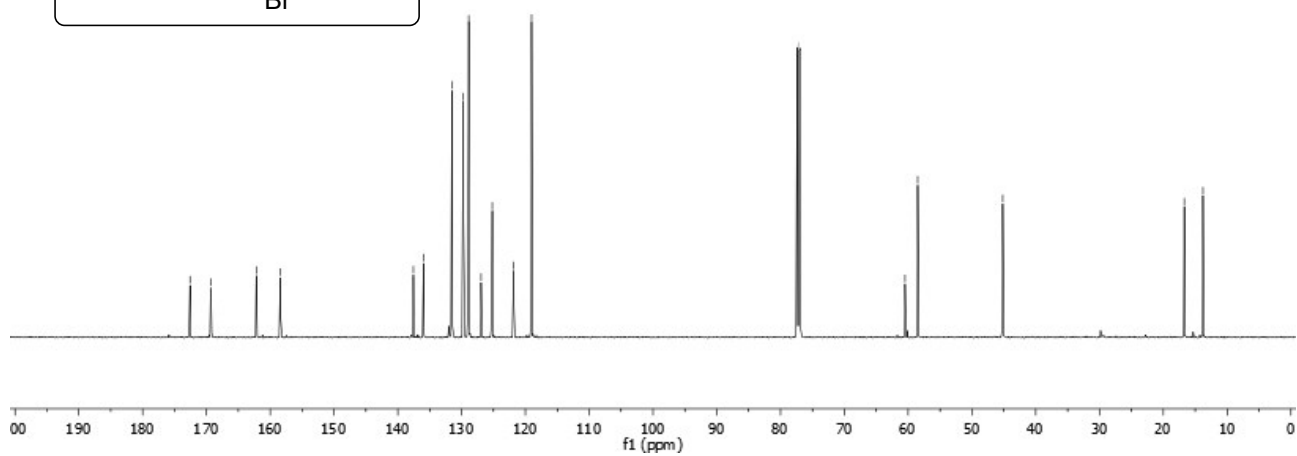
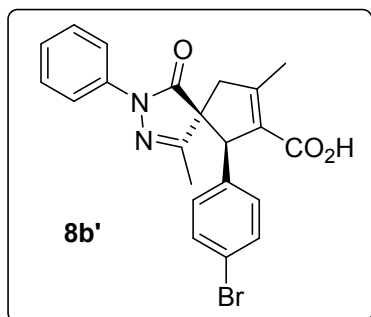
137.56
135.95
131.50
129.73
128.88
126.95
125.19
121.82
119.03

77.16 CDCl₃

60.49
58.50

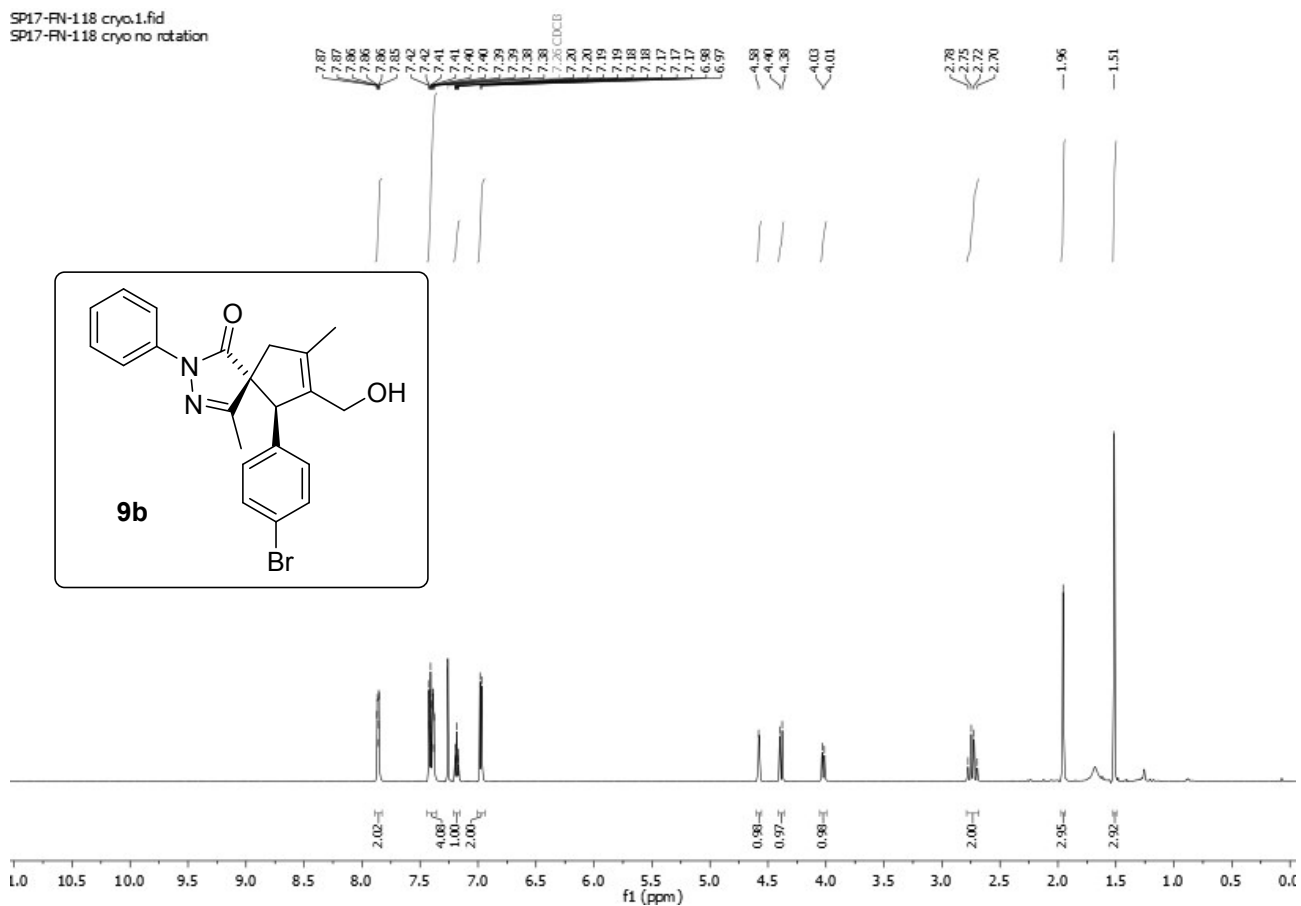
45.17

16.71
13.79



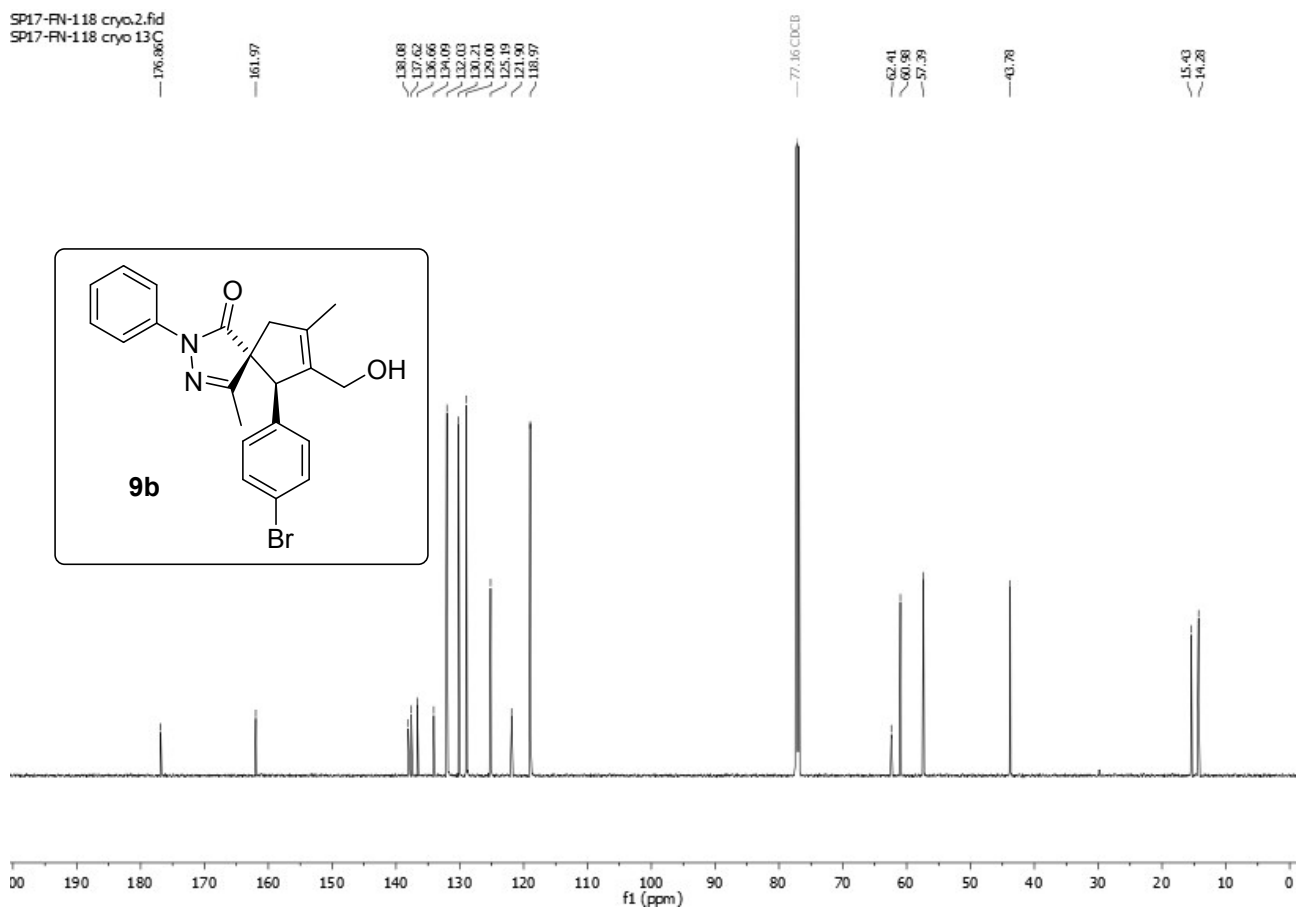
(5*R*,6*R*)-6-(4-Bromophenyl)-7-(hydroxymethyl)-4,8-dimethyl-2-phenyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (9b)

SP17-FN-118 cryo.1.fid
SP17-FN-118 cryo no rotation



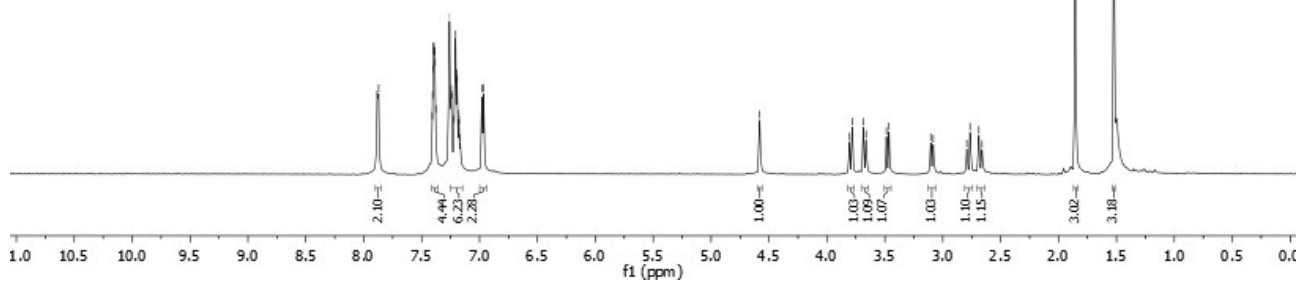
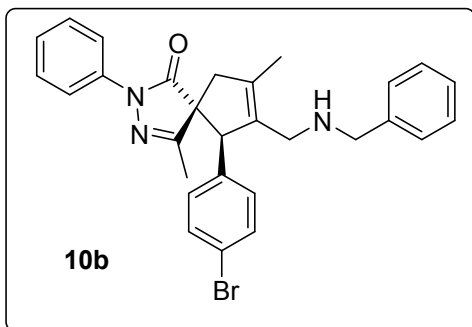
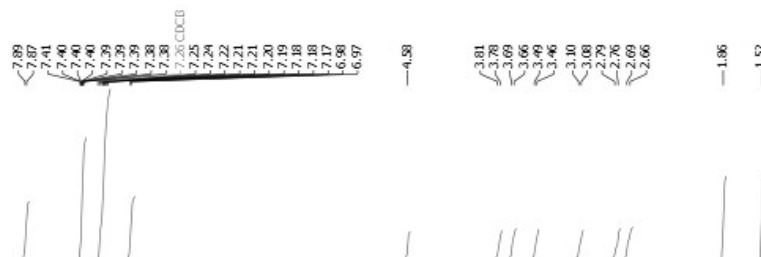
(5*R*,6*R*)-6-(4-Bromophenyl)-7-(hydroxymethyl)-4,8-dimethyl-2-phenyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (9b)

SP17-FN-118 cryo.2.fid
SP17-FN-118 cryo 13C



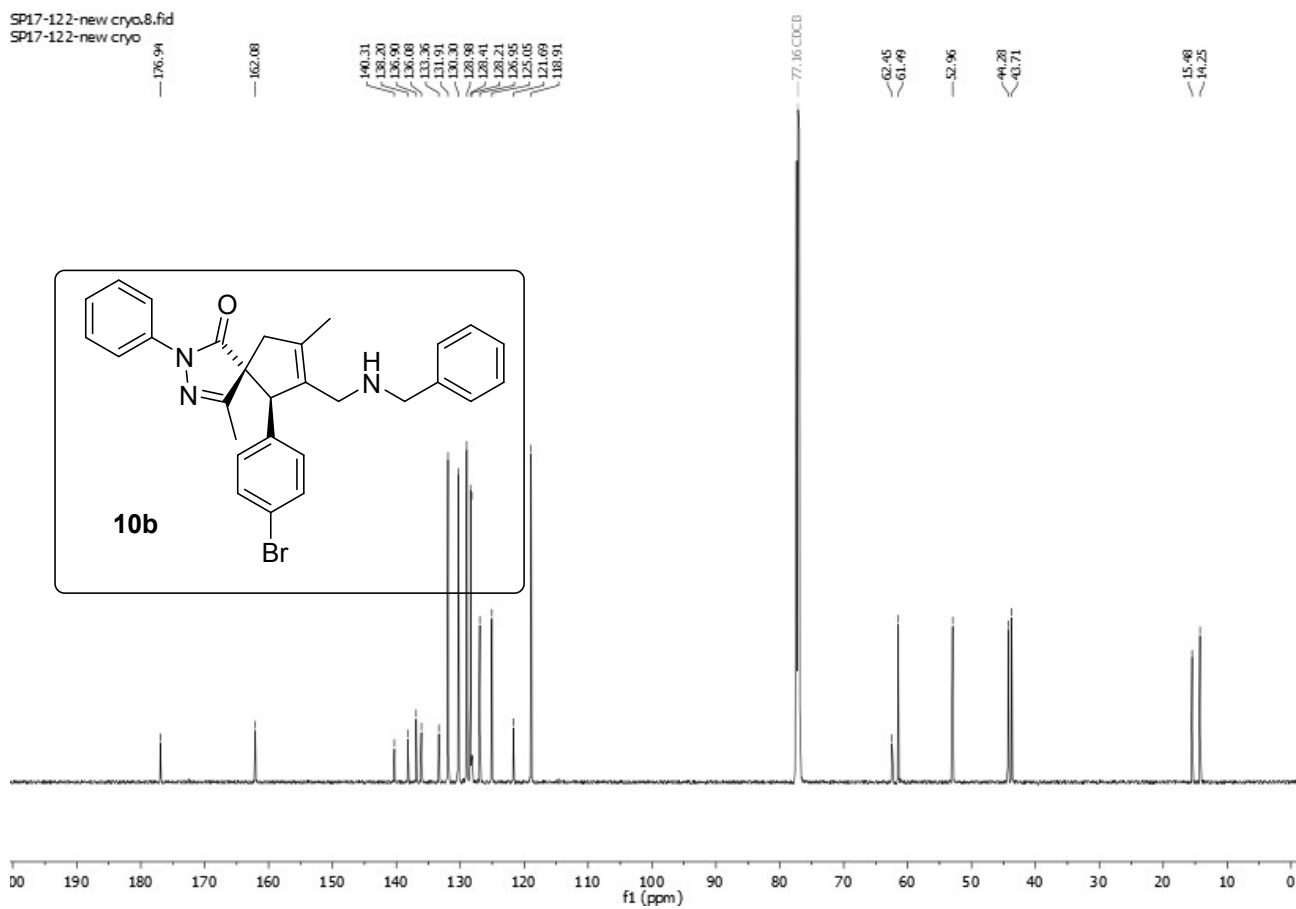
(5*R*,6*R*)-7-((Benzylamino)methyl)-6-(4-bromophenyl)-4,8-dimethyl-2-phenyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (10b)

SP17-122-new cryo.1.fid
 SP17-122-new cryo no rotation

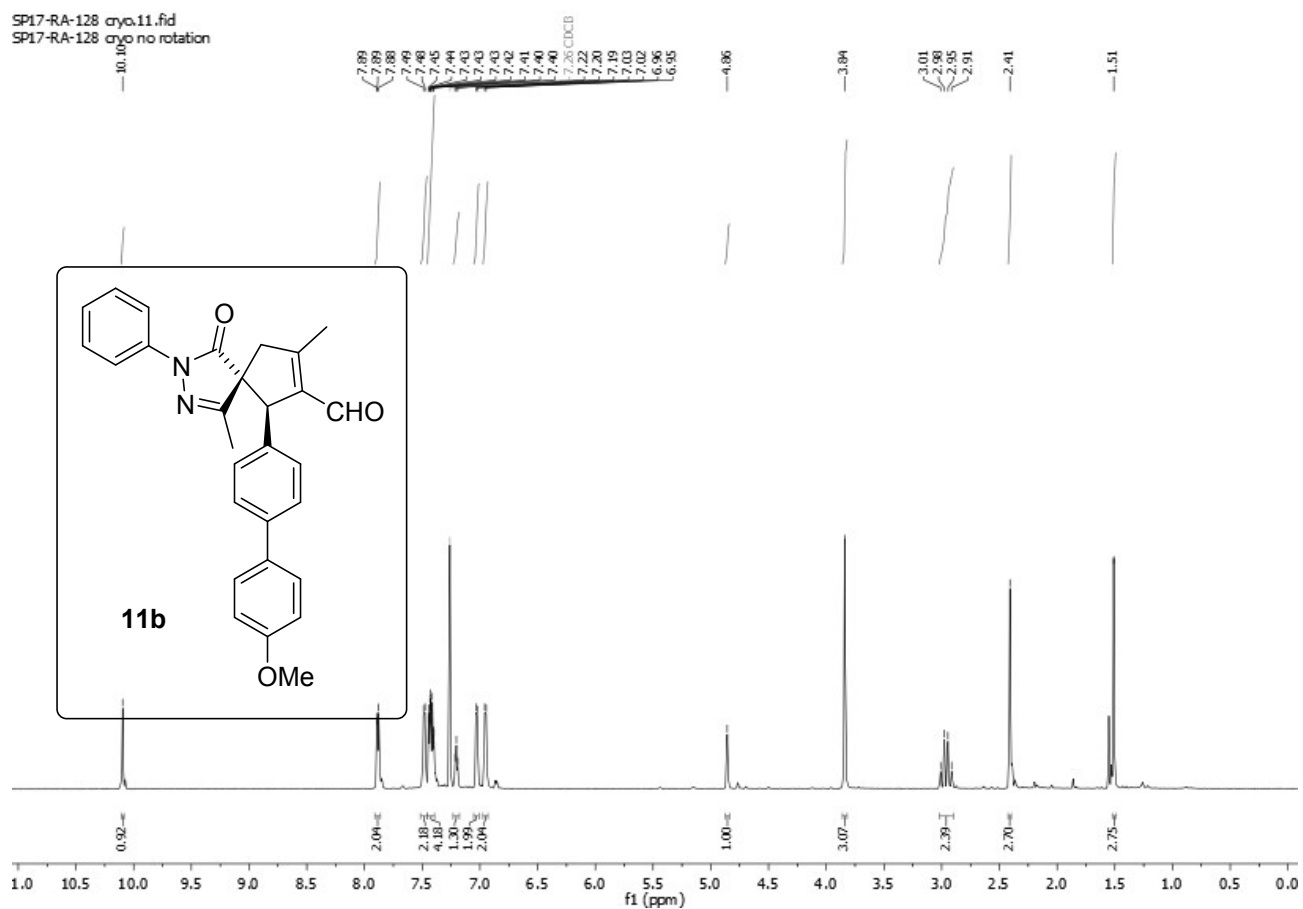


(5*R*,6*R*)-7-((Benzylamino)methyl)-6-(4-bromophenyl)-4,8-dimethyl-2-phenyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (10b)

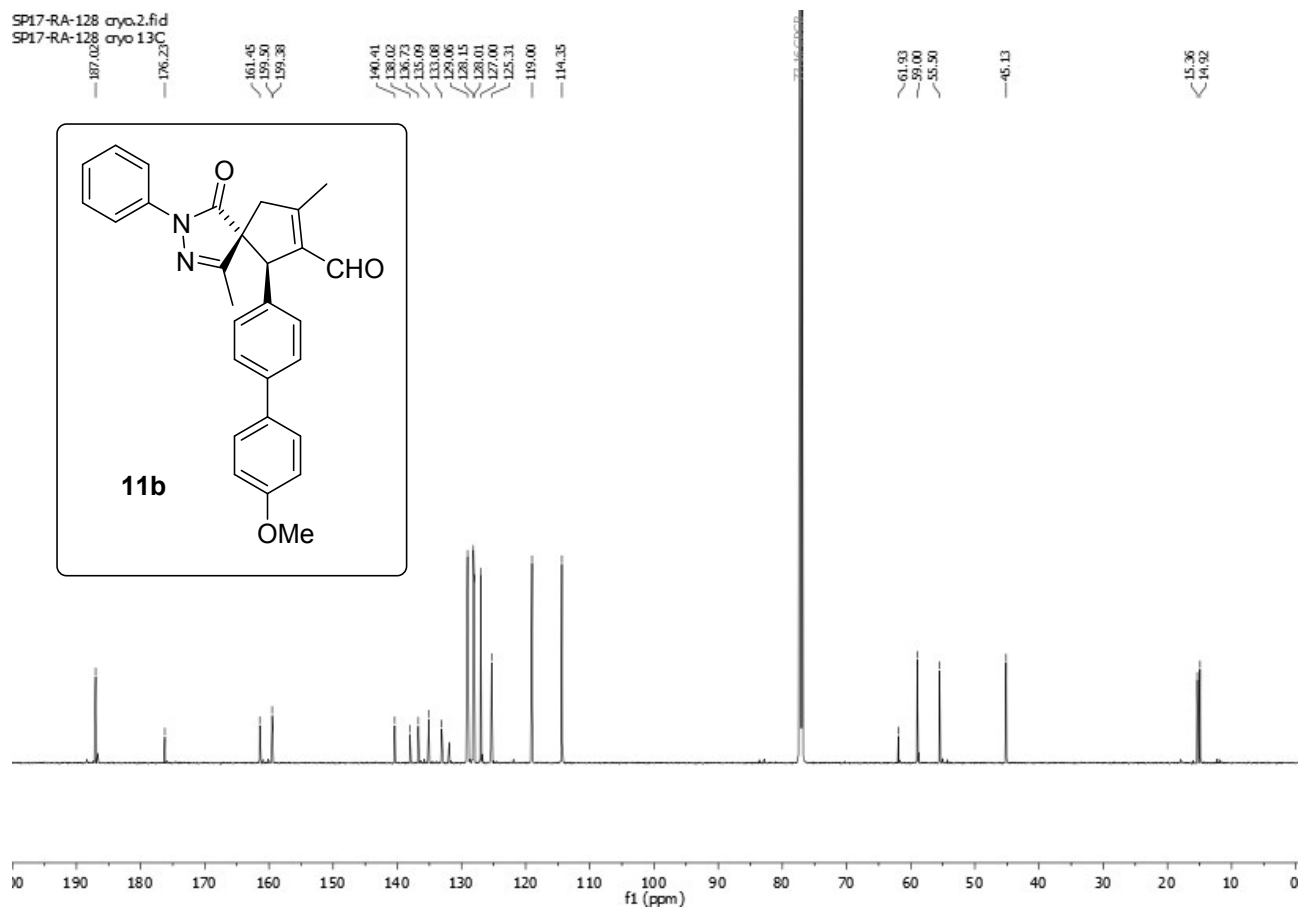
SP17-122-new cryo.8.fid
SP17-122-new cryo



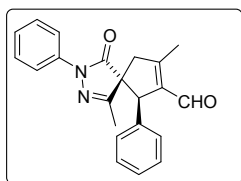
(5*R*,6*R*)-6-(4'-Methoxy-[1,1'-biphenyl]-4-yl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (11b)



(5*R*,6*R*)-6-(4'-Methoxy-[1,1'-biphenyl]-4-yl)-1,8-dimethyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (11b)



HPLC traces



(7a)

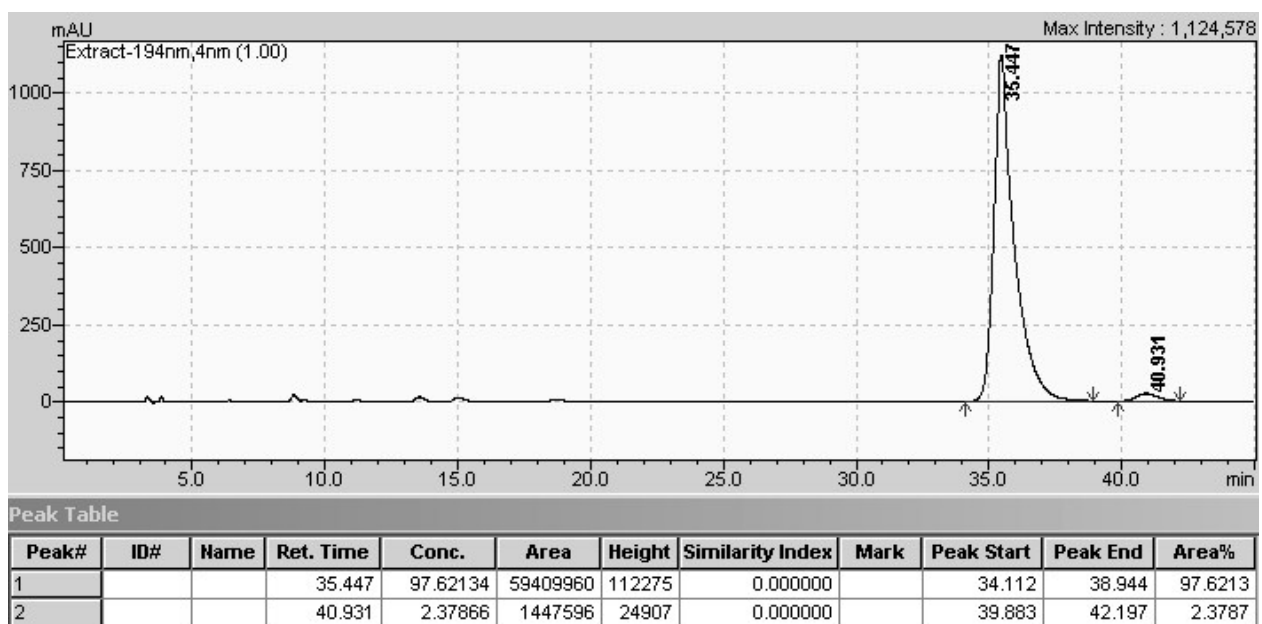
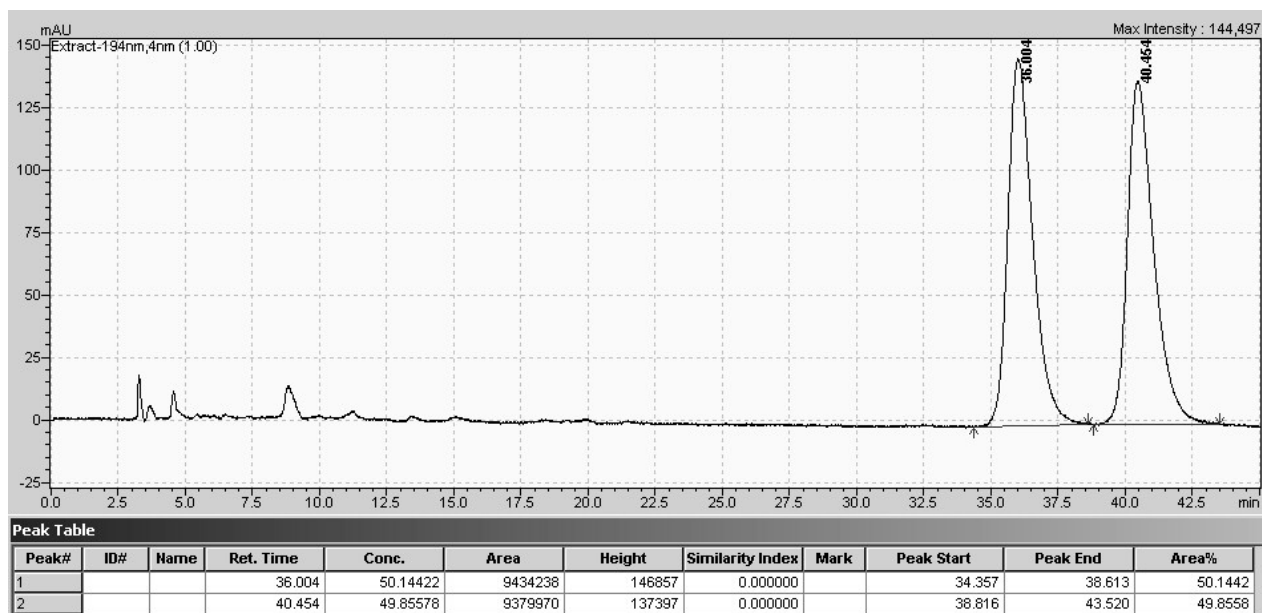
Conditions: IA column

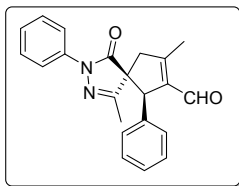
mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 194 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 35.4 \text{ min}$ (major), $t_R = 40.9 \text{ min}$ (minor), ee= 95 %

major diastereoisomer





(7a')

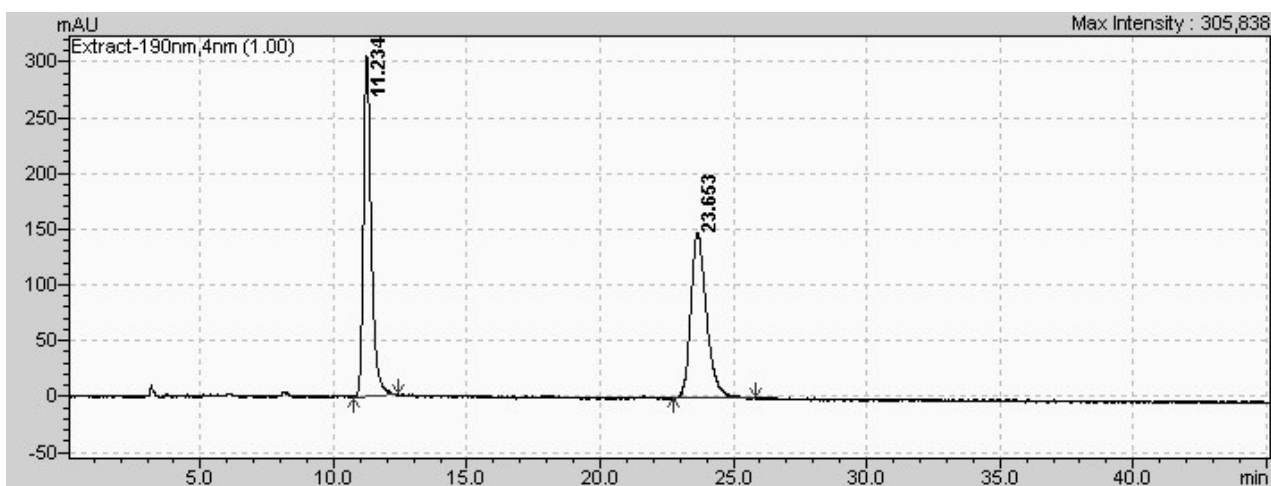
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 90:10

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

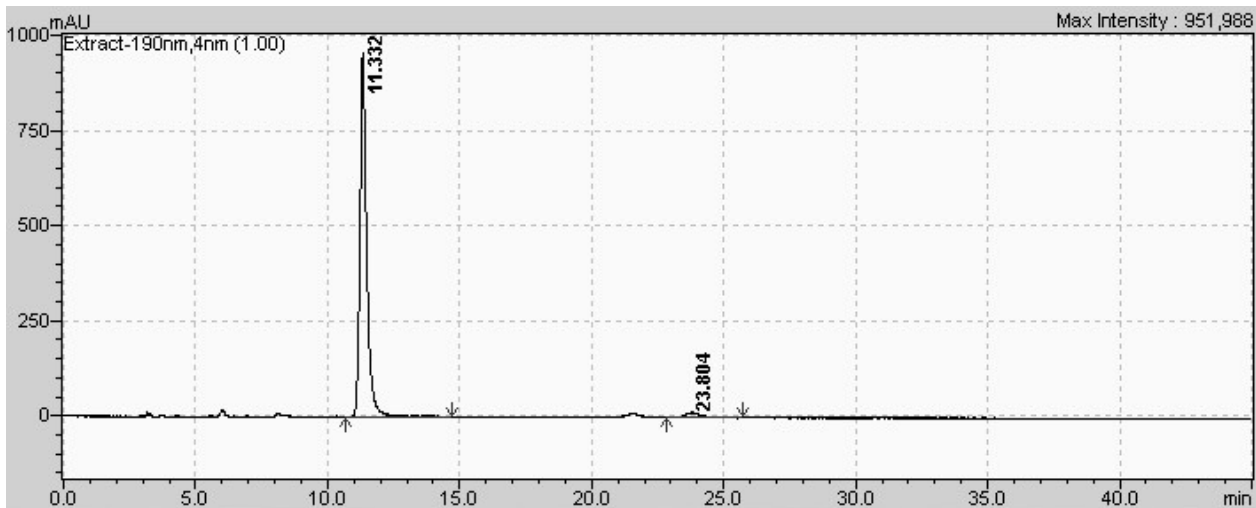
$t_R = 11.3 \text{ min}$ (major), $t_R = 23.8 \text{ min}$ (minor), ee= 95 %

minor diastereoisomer



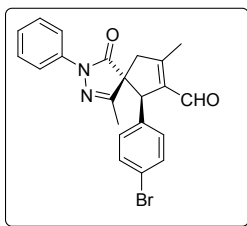
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			11.234	50.85327	6293087	305609	0.000000		10.773	12.427	50.8533
2			23.653	49.14673	6081904	148362	0.000000		22.763	25.867	49.1467



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			11.332	97.38544	16700780	953987	0.000000		10.677	14.720	97.3854
2			23.804	2.61456	448374	12647	0.000000		22.869	25.717	2.6146



(7b)

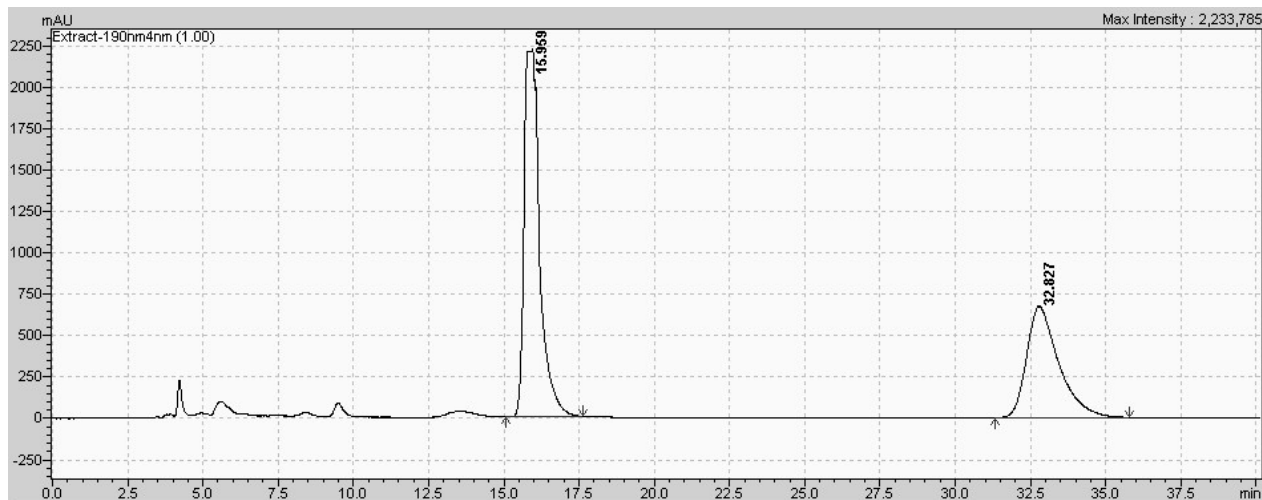
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 70:30

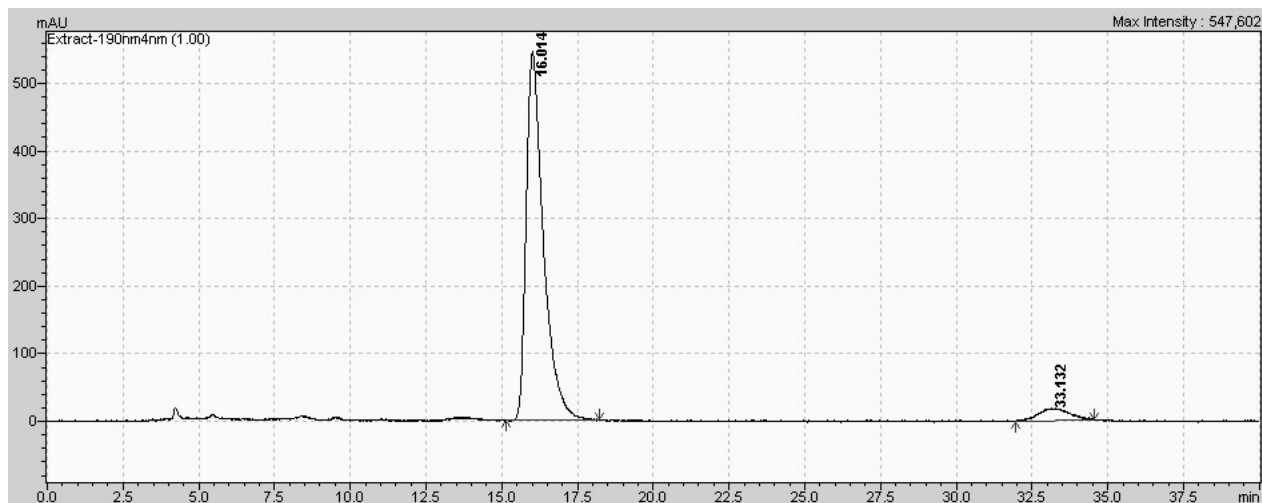
$\lambda = 190$ nm, $V = 1$ ml/min, $t = 25$ °C

$t_R = 16.0$ min (major), $t_R = 33.1$ min (minor), ee= 90 %

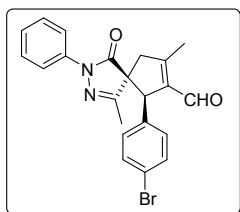
major diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			15.959	61.58879	79786173	2223897	0.000000		15.061	17.632	61.5888
2			32.827	38.41121	49760415	672149	0.000000		31.328	35.787	38.4112



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			16.014	94.78541	21459090	545433	0.000000		15.147	18.219	94.7854
2			33.132	5.21459	1180566	17572	0.000000		31.957	34.549	5.2146



(7b')

Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 90:10

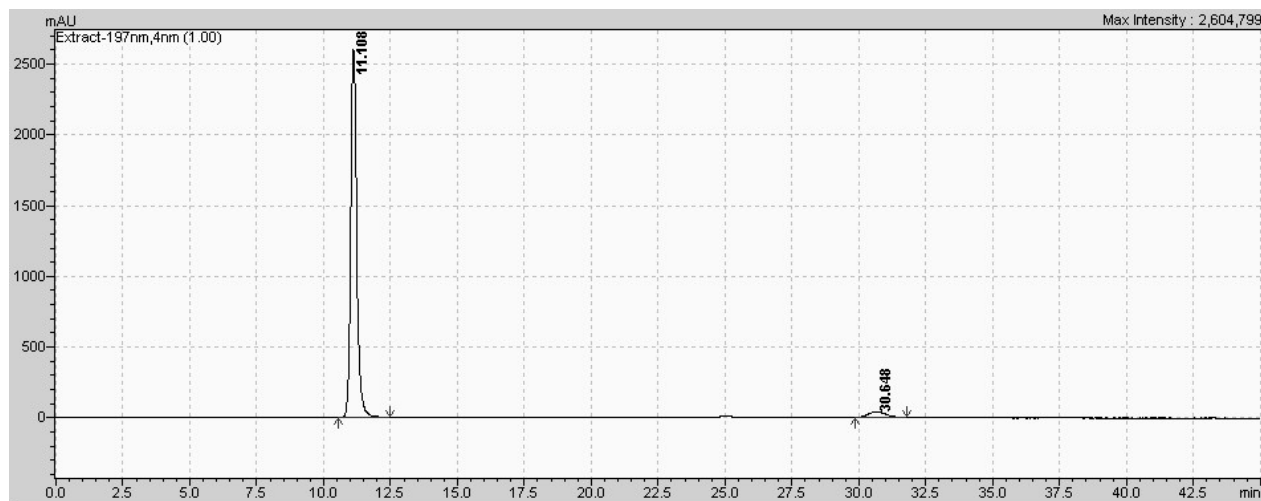
$\lambda = 197 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 11.1 \text{ min}$ (major), $t_R = 30.6 \text{ min}$ (minor), ee= 91 %

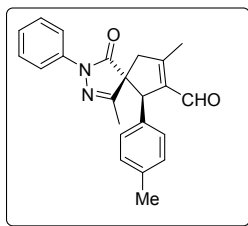
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			10.989	50.40117	4411508	214714	0.000000		10.368	12.811	50.4012
2			30.796	49.59883	4341281	83824	0.000000		29.248	32.928	49.5988



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			11.108	95.60288	41174452	2601533	0.000000		10.528	12.491	95.6029
2			30.648	4.39712	1893760	40134	0.000000		29.856	31.776	4.3971



(7c)

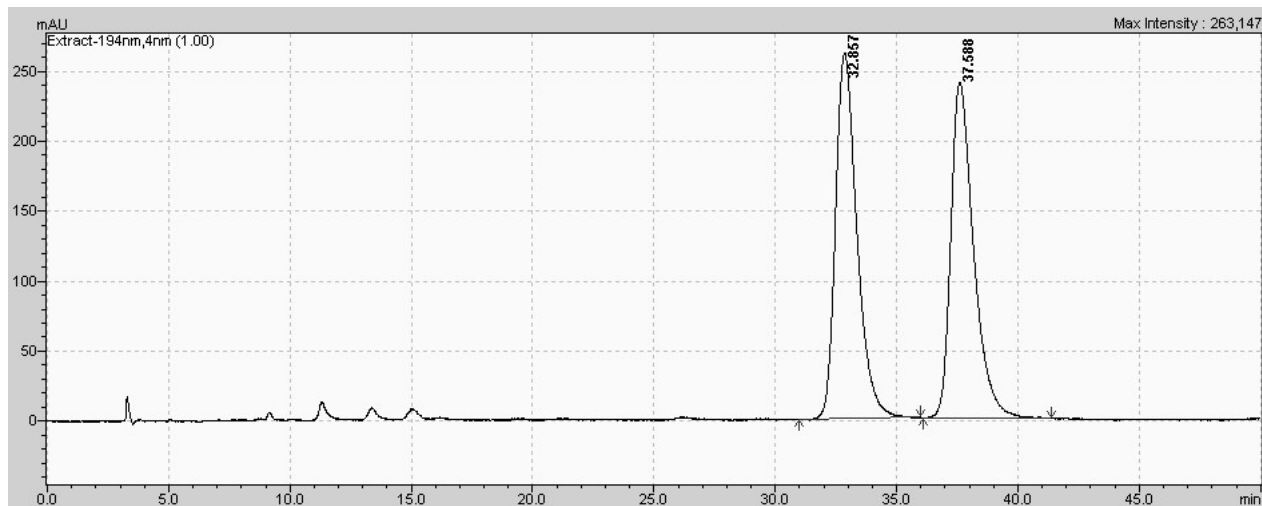
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 194 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

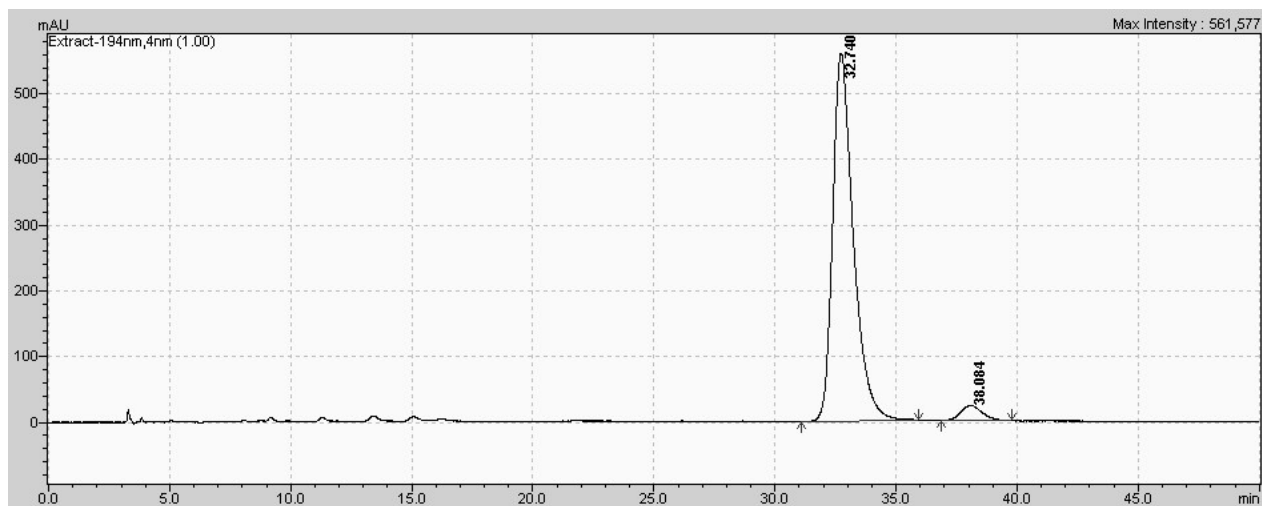
$t_R = 32.7 \text{ min}$ (major), $t_R = 38.1 \text{ min}$ (minor), ee= 92 %

major diastereoisomer



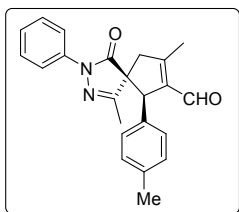
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			32.857	50.60468	16052689	261447	0.000000		30.997	36.011	50.6047
2			37.588	49.39532	15669060	239635	0.000000		36.075	41.376	49.3953



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			32.740	95.90175	33195636	559581	0.000000		31.061	35.957	95.9018
2			38.084	4.09825	1418575	23092	0.000000		36.875	39.755	4.0982



(7c')

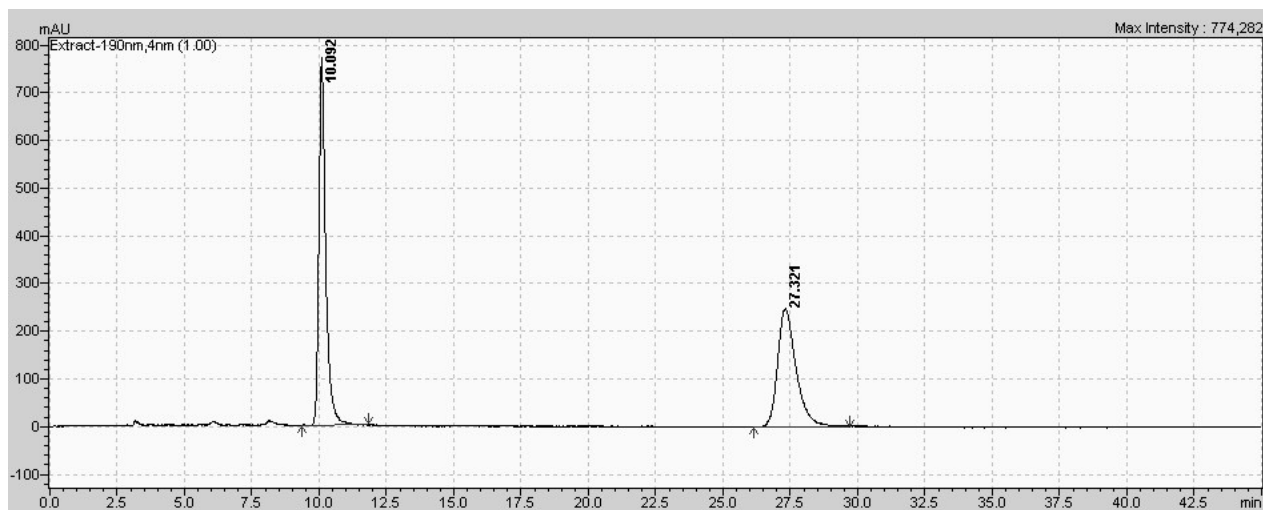
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 90:10

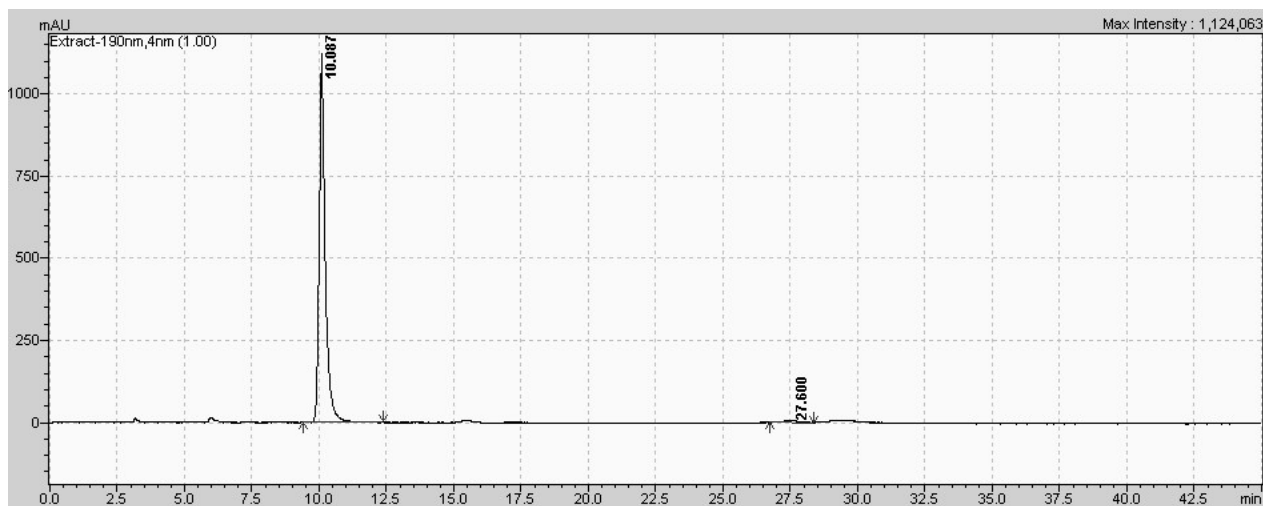
$\lambda = 190$ nm, $V = 1$ ml/min, $t = 25$ °C

$t_R = 10.1$ min (major), $t_R = 27.6$ min (minor), ee= 98 %

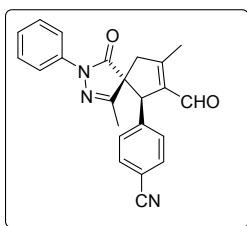
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			10.092	53.78892	13605514	771332	0.000000		9.333	11.819	53.7889
2			27.321	46.21108	11688753	247229	0.000000		26.133	29.707	46.2111



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			10.087	98.82936	17236730	1123064	0.000000		9.387	12.395	98.8294
2			27.600	1.17064	204170	5995	0.000000		26.752	28.363	1.1706



(7d)

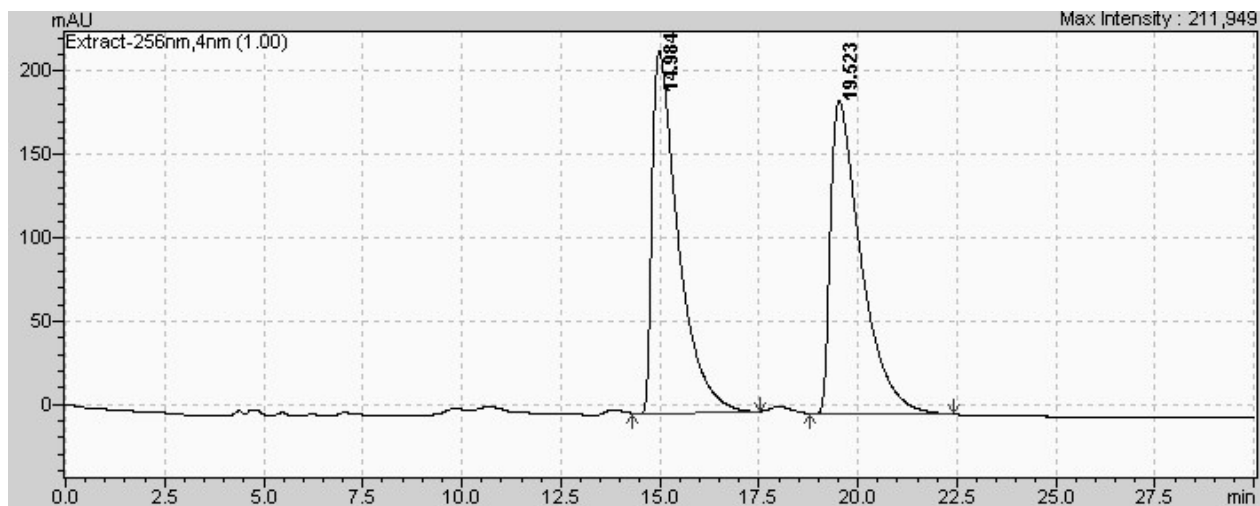
Conditions: IB column

mobile phase: *n*-heptane / propan-2-ol= 70:30

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

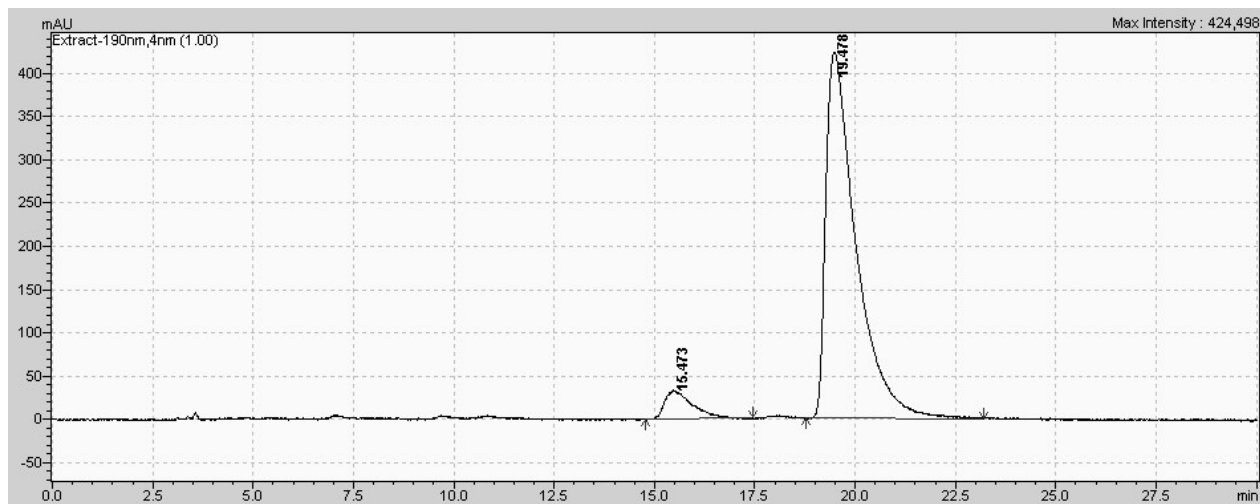
$t_R = 15.5 \text{ min}$ (minor), $t_R = 19.5 \text{ min}$ (major), ee= 86 %

major diastereoisomer



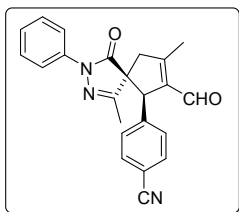
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			14.984	49.40884	9916985	217060	0.000000		14.315	17.525	49.4088
2			19.523	50.59116	10154290	187734	0.000000		18.805	22.400	50.5912



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			15.473	6.77640	1608494	33334	0.000000		14.773	17.461	6.7764
2			19.478	93.22360	22126190	423119	0.000000		18.773	23.189	93.2236



(7d')

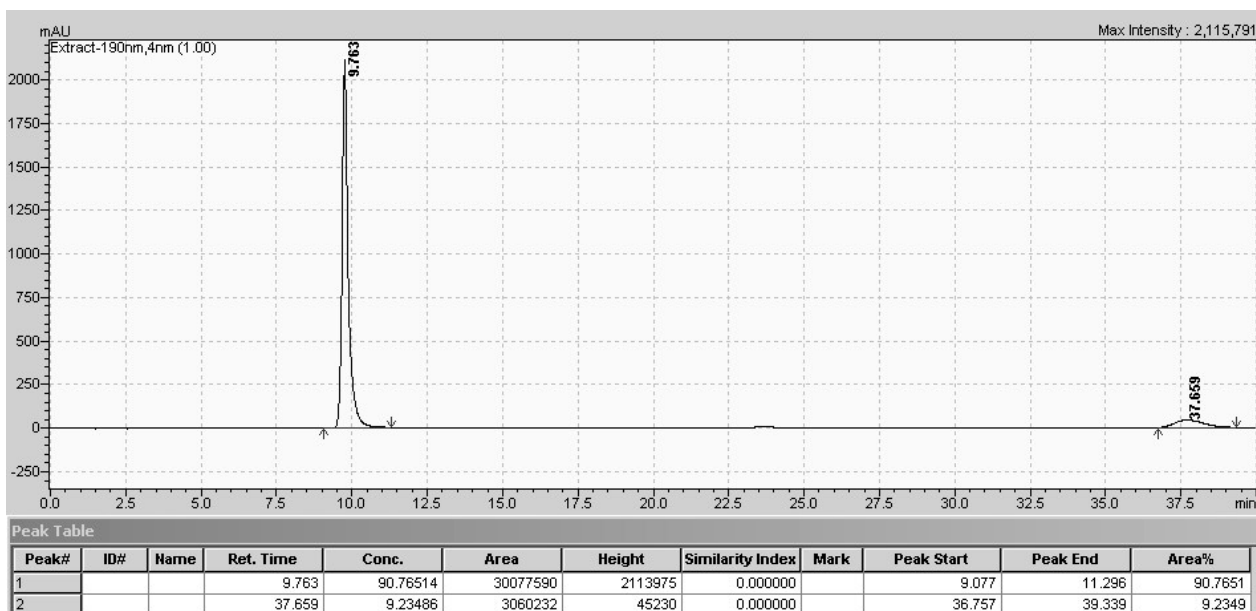
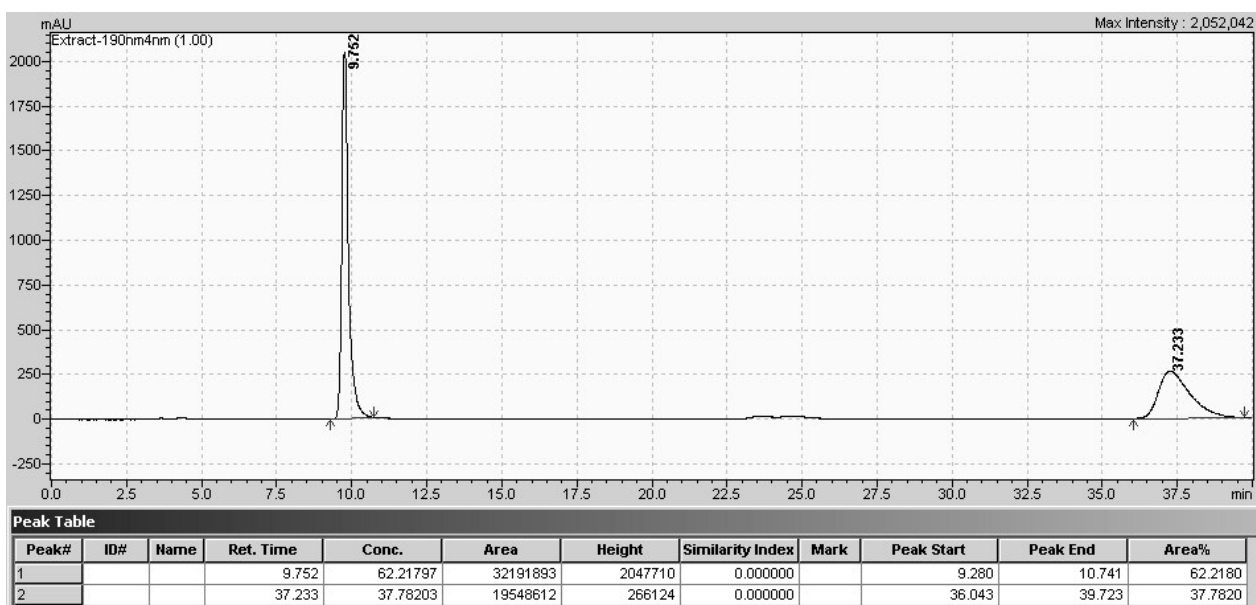
Conditions: IA column

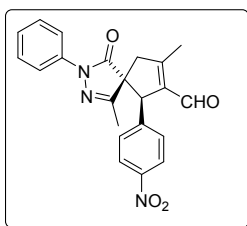
mobile phase: *n*-heptane / propan-2-ol= 80:20

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 9.8 \text{ min}$ (major), $t_R = 37.7 \text{ min}$ (minor), ee= 82 %

minor diastereoisomer





(7e)

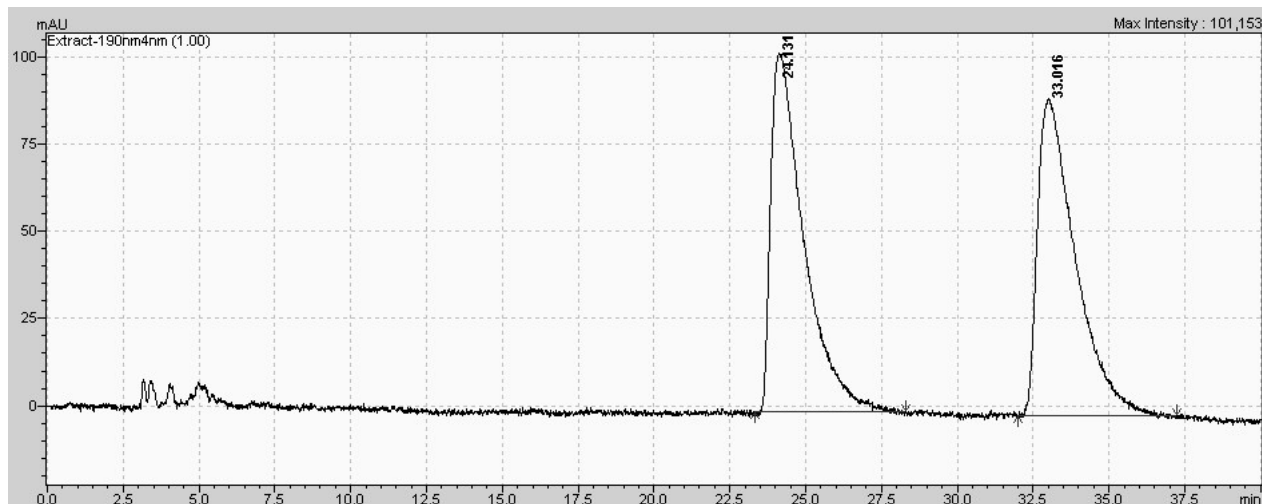
Conditions: IB column

mobile phase: *n*-heptane / propan-2-ol= 80:20

$\lambda = 190$ nm, $V = 1$ ml/min, $t = 25$ °C

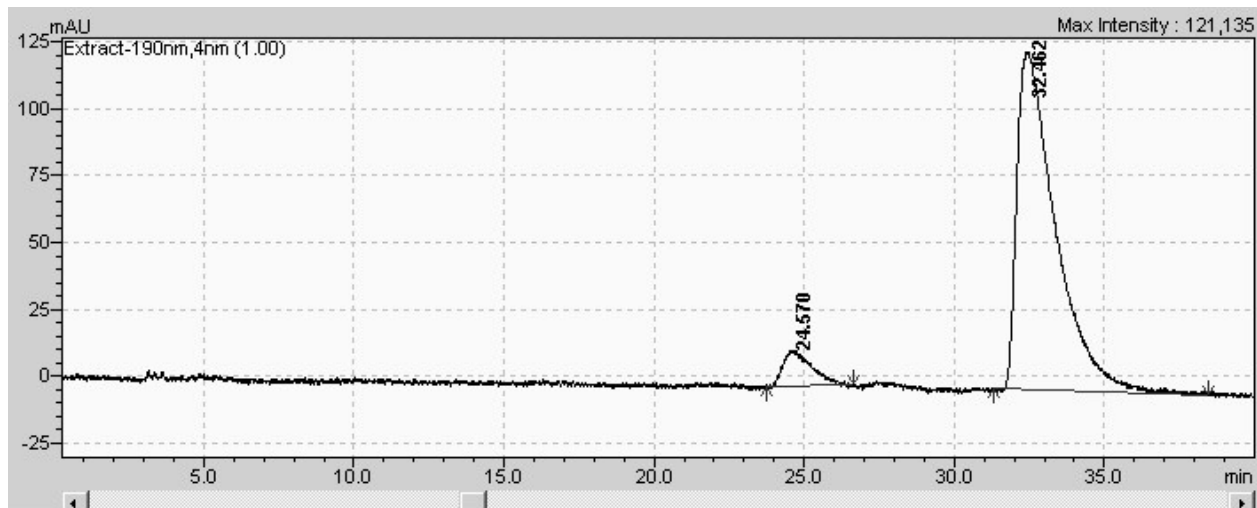
$t_R = 24.6$ min (minor), $t_R = 32.5$ min (major), ee= 86 %

major diastereoisomer



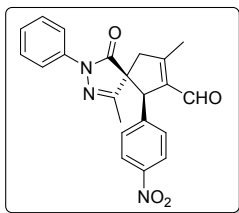
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			24.131	49.67598	7758815	102726	0.000000		23.328	28.299	49.6760
2			33.016	50.32402	7860030	90832	0.000000		32.000	37.237	50.3240



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			24.570	7.00040	846555	13438	0.000000		23.733	26.645	7.0004
2			32.462	92.99960	11246393	126012	0.000000		31.328	38.485	92.9996



(7e')

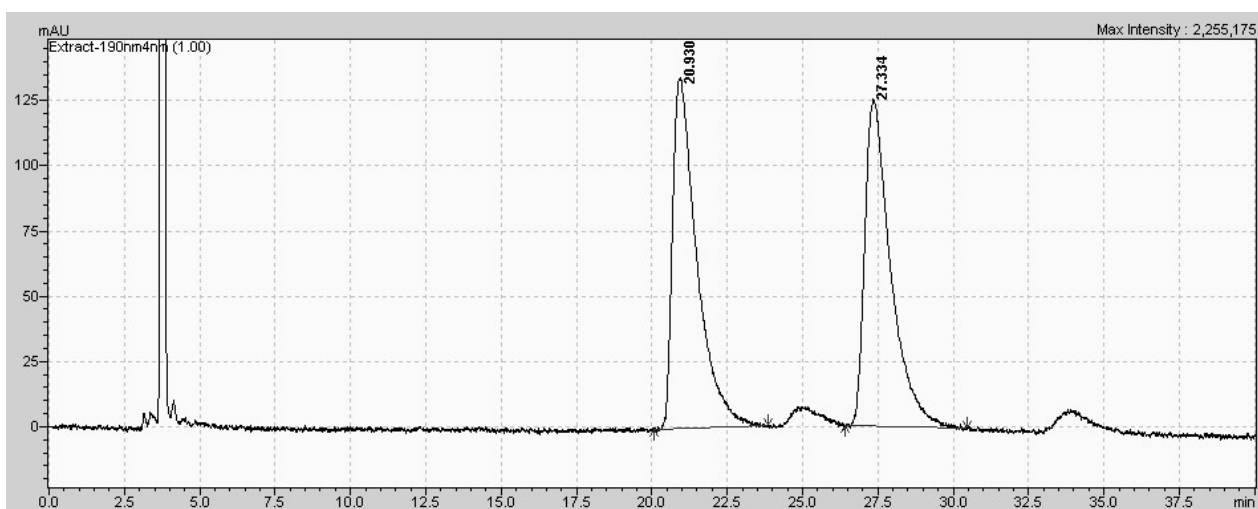
Conditions: IB column

mobile phase: *n*-heptane / propan-2-ol= 80:20

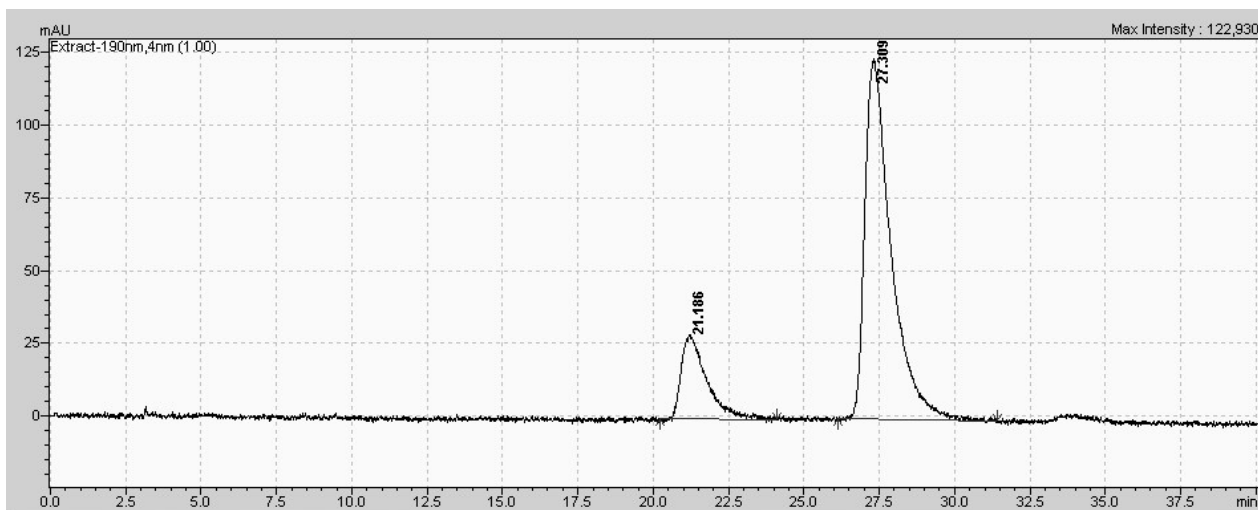
$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 21.2 \text{ min}$ (minor), $t_R = 27.3 \text{ min}$ (major), ee= 64 %

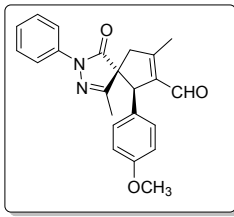
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			20.930	50.23555	7536435	134352	0.000000		20.075	23.861	50.2355
2			27.334	49.76445	7465761	125163	0.000000		26.411	30.464	49.7645



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			21.186	18.19490	1674027	28906	0.000000		20.235	24.096	18.1949
2			27.309	81.80510	7526498	124114	0.000000		26.123	31.413	81.8051



(7f)

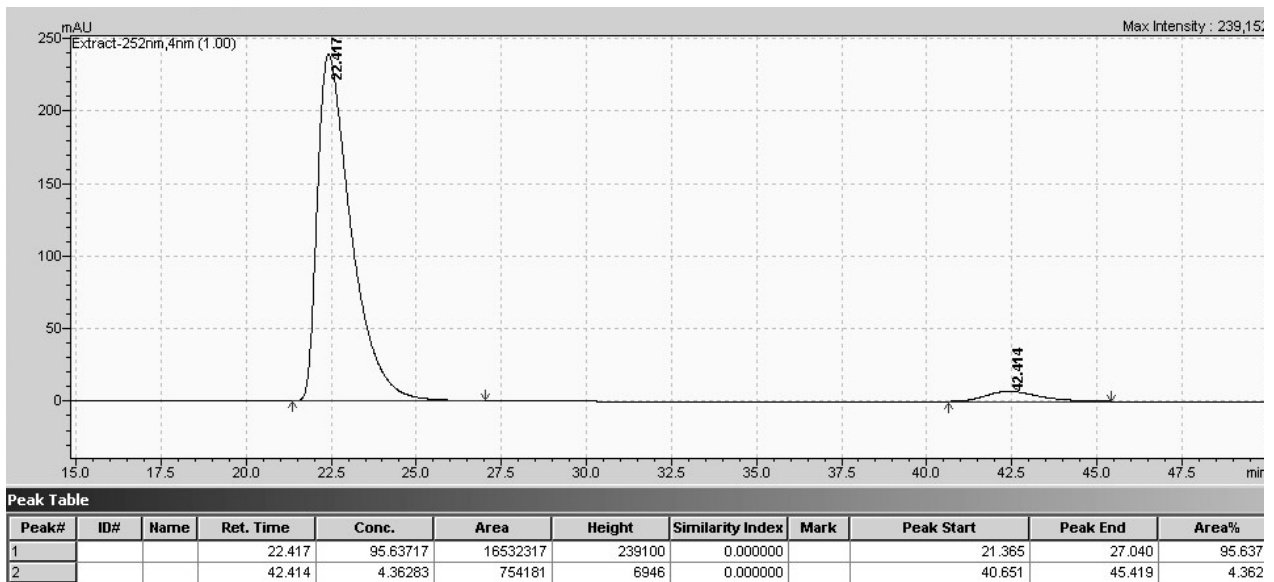
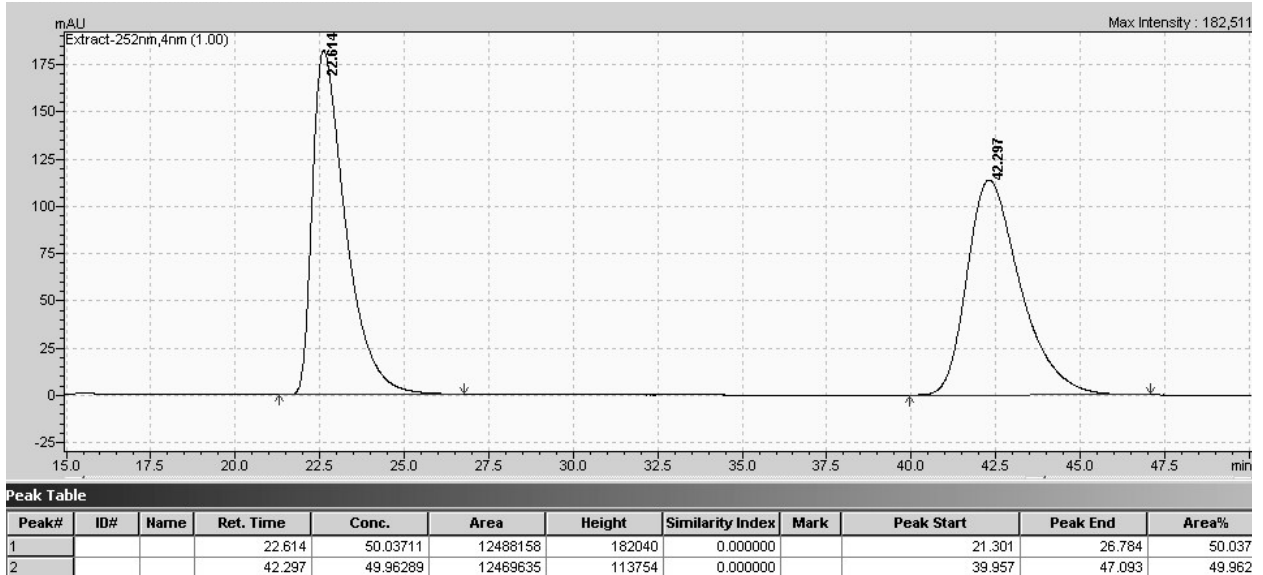
Conditions: IC column

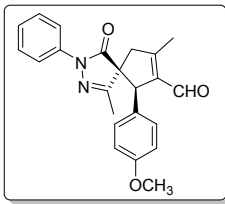
mobile phase: *n*-heptane / propan-2-ol= 60:40

$\lambda = 252\text{nm}$, $V = 1\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

$t_R = 22.4\text{ min}$ (major), $t_R = 42.4\text{ min}$ (minor), ee= 91 %

major diastereoisomer





(7f)

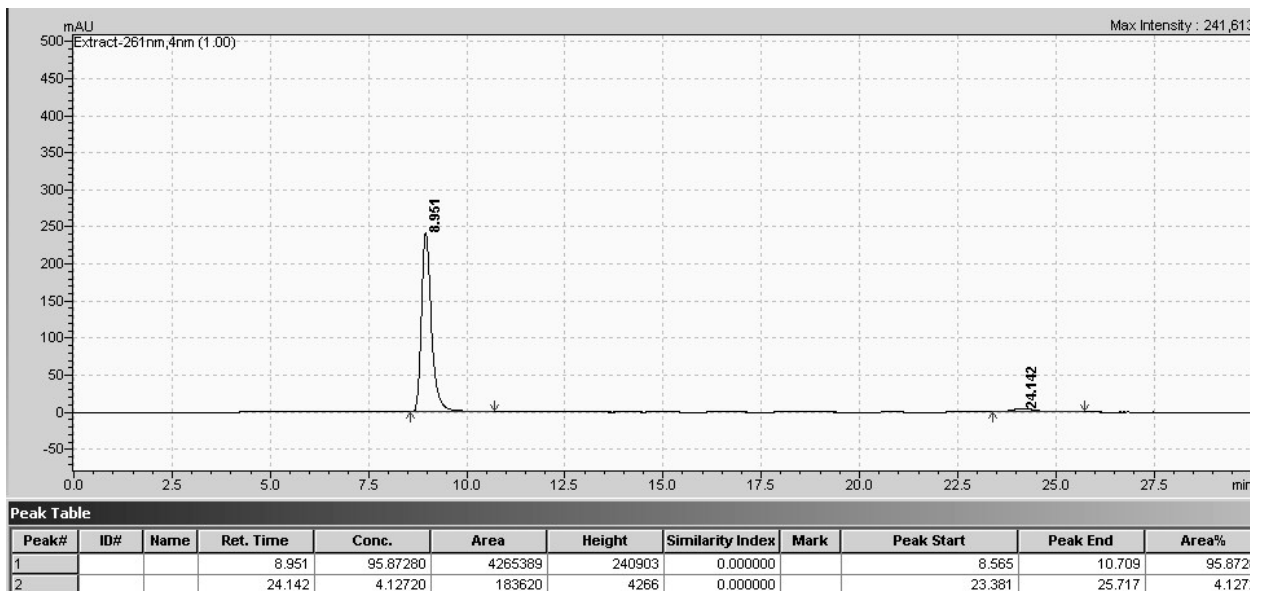
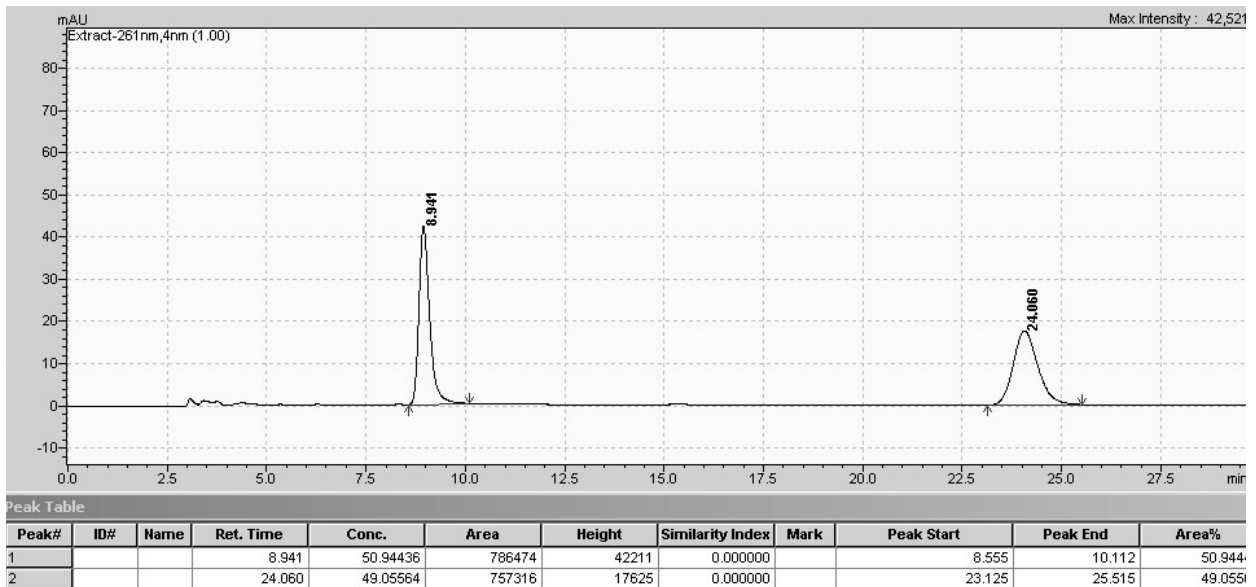
Conditions: IA column

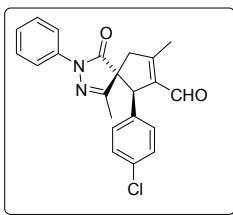
mobile phase: *n*-heptane / propan-2-ol= 80:20

$\lambda = 261\text{nm}$, $V = 1\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

$t_R = 9.0\text{ min}$ (major), $t_R = 24.1\text{ min}$ (minor), $ee = 92\%$

minor diastereoisomer





(7g)

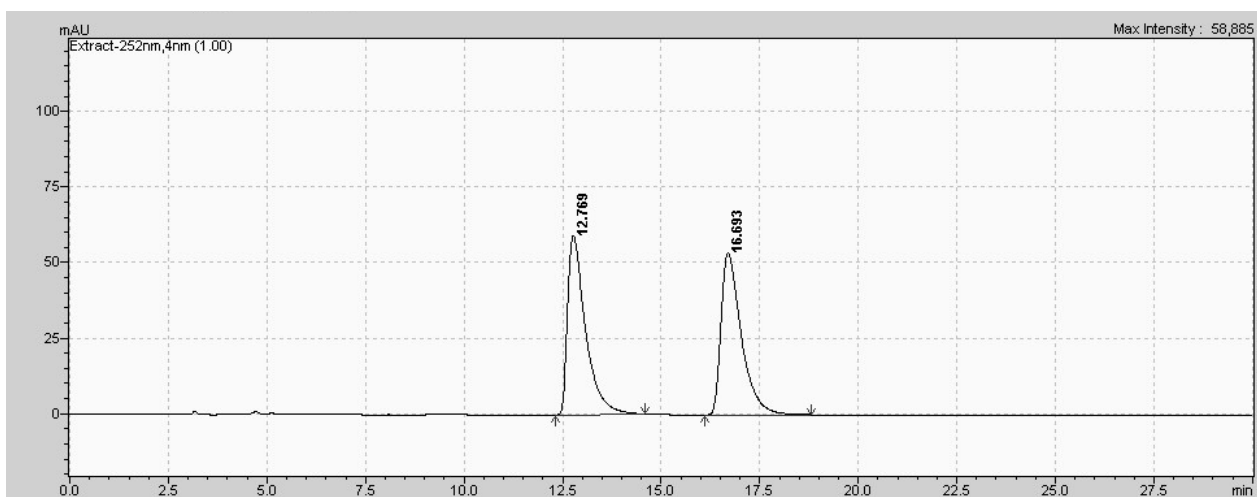
Conditions: IB column

mobile phase: *n*-heptane / propan-2-ol= 80:20

$\lambda = 252\text{nm}$, $V = 1\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

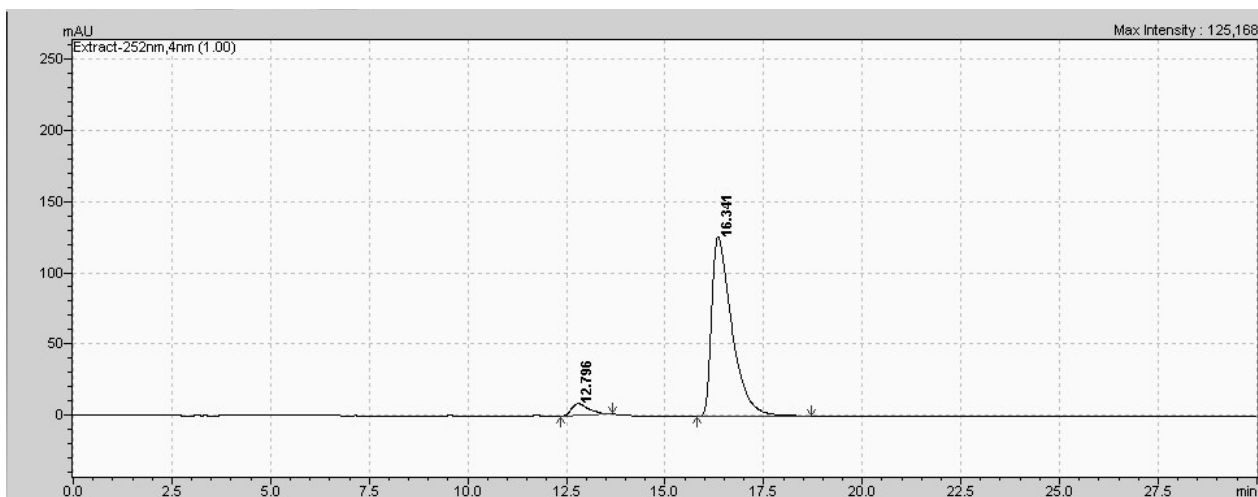
$t_R = 12.8\text{ min}$ (minor), $t_R = 16.3\text{ min}$ (major), ee = 89 %

major diastereoisomer



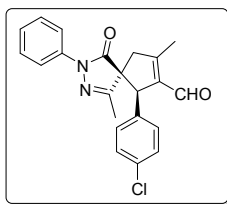
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			12.769	49.41148	1875861	59274	0.000000		12.309	14.603	49.4115
2			16.693	50.58852	1920547	53766	0.000000		16.117	18.795	50.5885



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			12.796	5.39826	256949	8270	0.000000		12.352	13.675	5.3983
2			16.341	94.60174	4502896	125998	0.000000		15.797	18.720	94.6017



(7g)

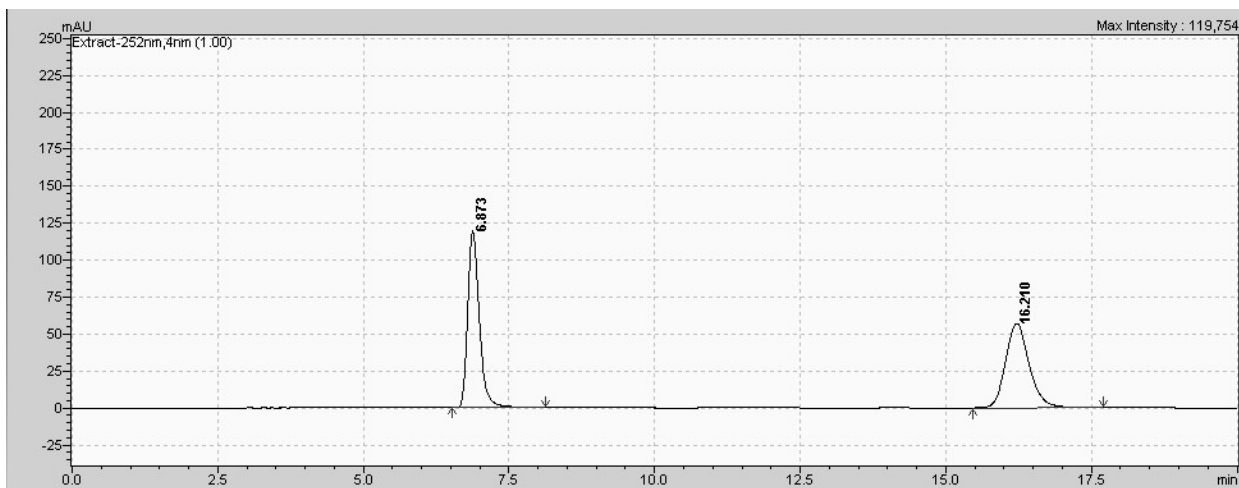
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 80:20

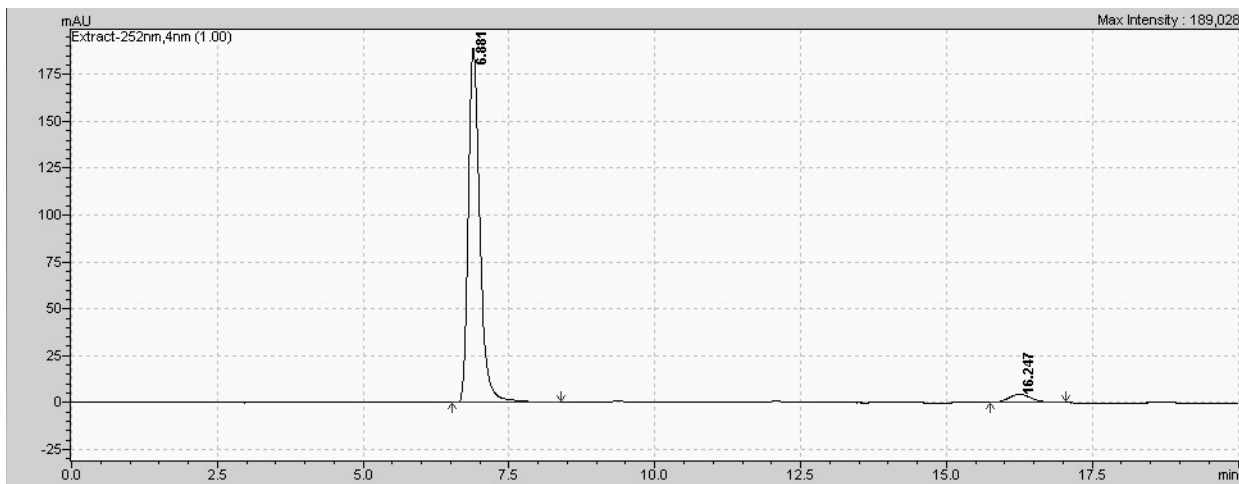
$\lambda = 252\text{nm}$, $V = 1\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

$t_R = 6.9\text{ min}$ (major), $t_R = 16.3\text{ min}$ (minor), ee= 91 %

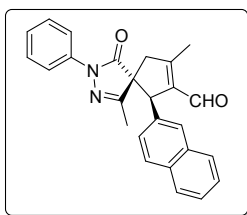
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			6.873	50.34162	1630563	119461	0.000000		6.517	8.117	50.3416
2			16.210	49.65838	1608433	57067	0.000000		15.456	17.707	49.6584



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			6.881	95.60403	2561744	188909	0.000000		6.517	8.395	95.6040
2			16.247	4.39597	117792	4435	0.000000		15.744	17.035	4.3959



(7h)

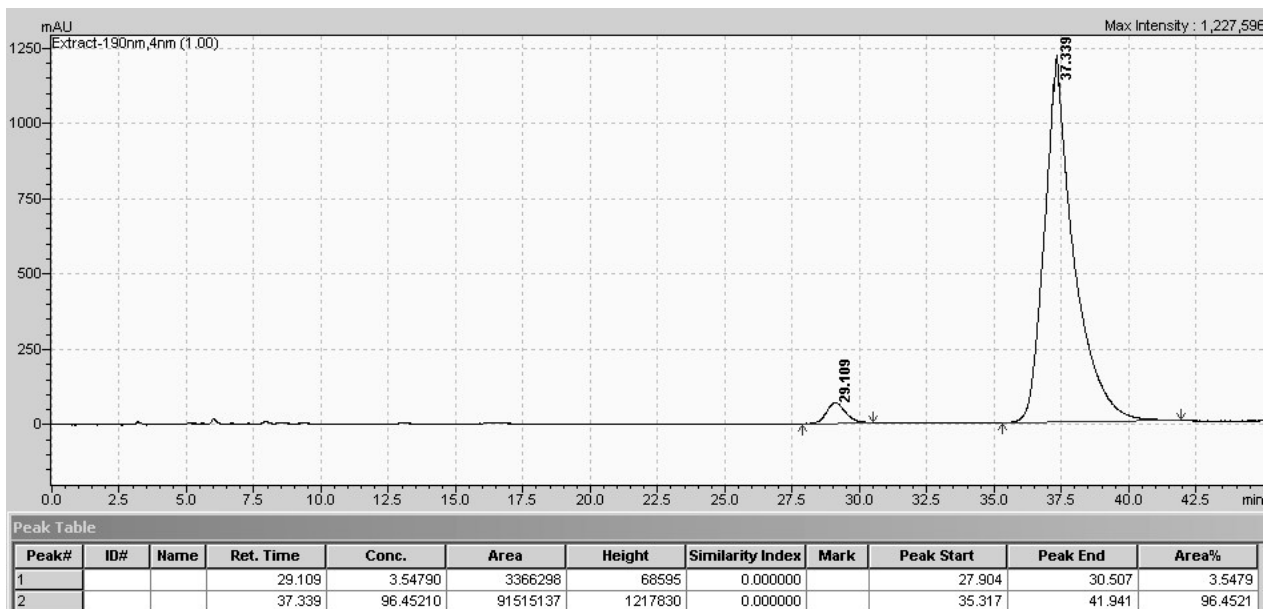
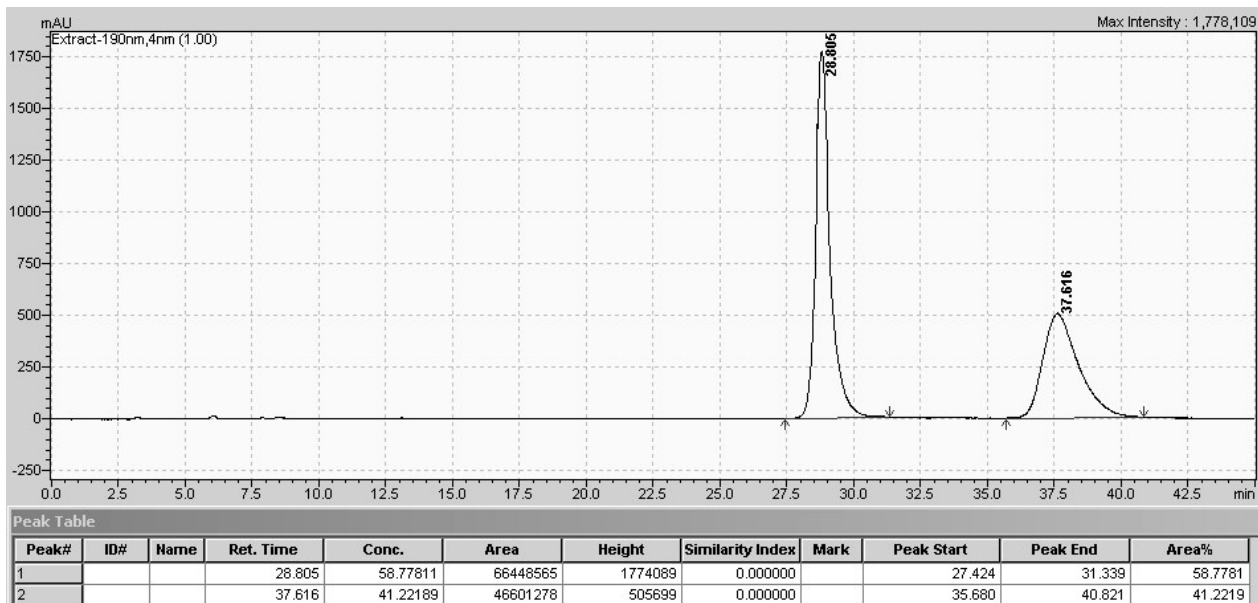
Conditions: IA column

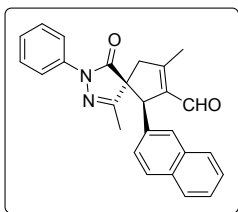
mobile phase: *n*-heptane / propan-2-ol= 90:10

$\lambda = 190$ nm, $V = 1$ ml/min, $t = 25$ °C

$t_R = 29.1$ min (minor), $t_R = 37.3$ min (major), ee= 93 %

major diastereoisomer





(7h')

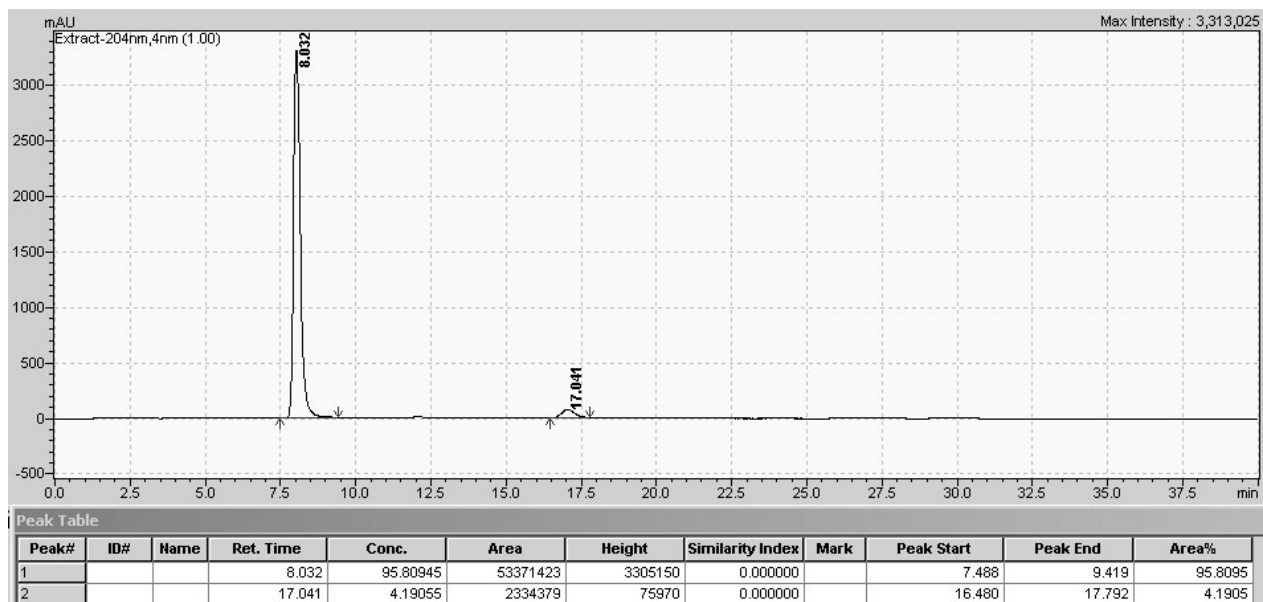
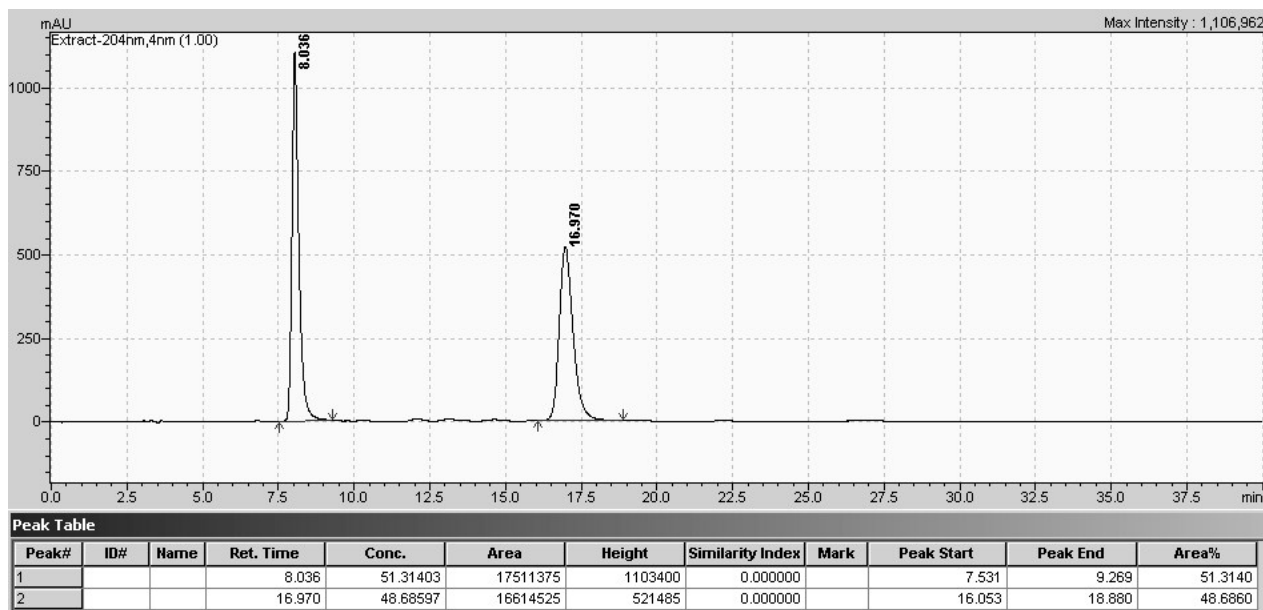
Conditions: IA column

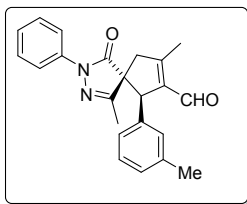
mobile phase: *n*-heptane / propan-2-ol= 80:20

$\lambda = 204 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 8.0 \text{ min}$ (major), $t_R = 17.0 \text{ min}$ (minor), ee= 92 %

minor diastereoisomer





(7i)

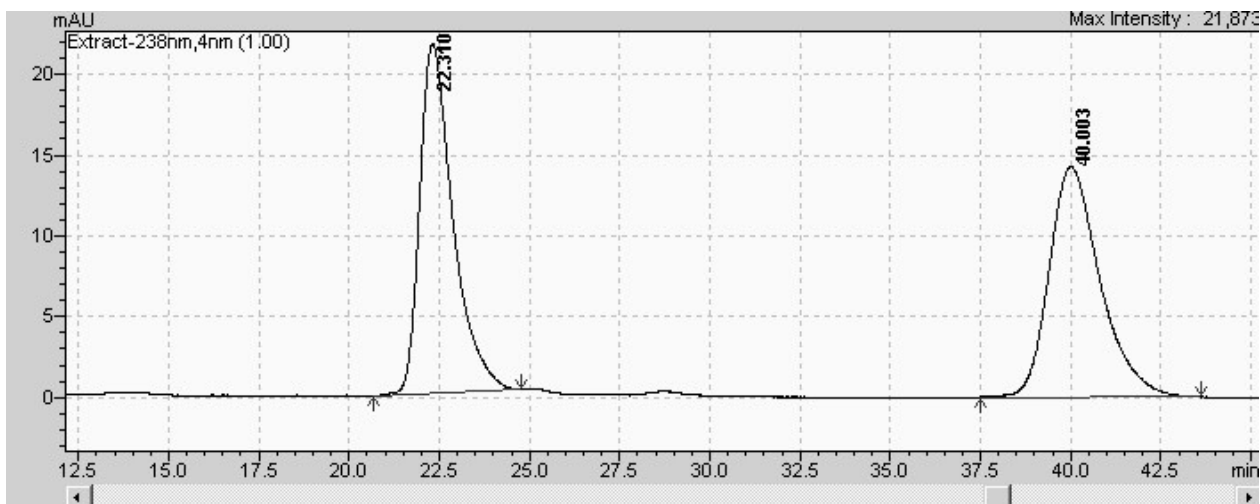
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 70:30

$\lambda = 238 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

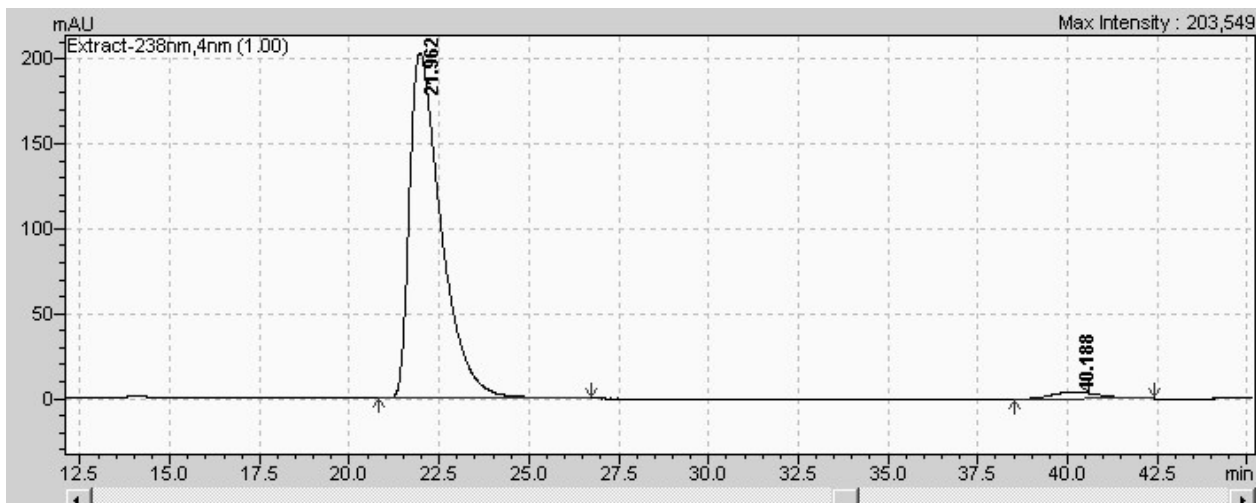
$t_R = 22.0 \text{ min}$ (major), $t_R = 40.2 \text{ min}$ (minor), ee= 94 %

major diastereoisomer



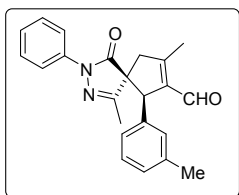
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			22.310	49.77429	1389038	21616	0.000000		20.672	24.757	49.7743
2			40.003	50.22571	1401635	14247	0.000000		37.483	43.595	50.2257



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			21.962	97.02555	12517363	203400	0.000000		20.821	26.720	97.0255
2			40.188	2.97445	383737	4182	0.000000		38.528	42.400	2.9745



(7i')

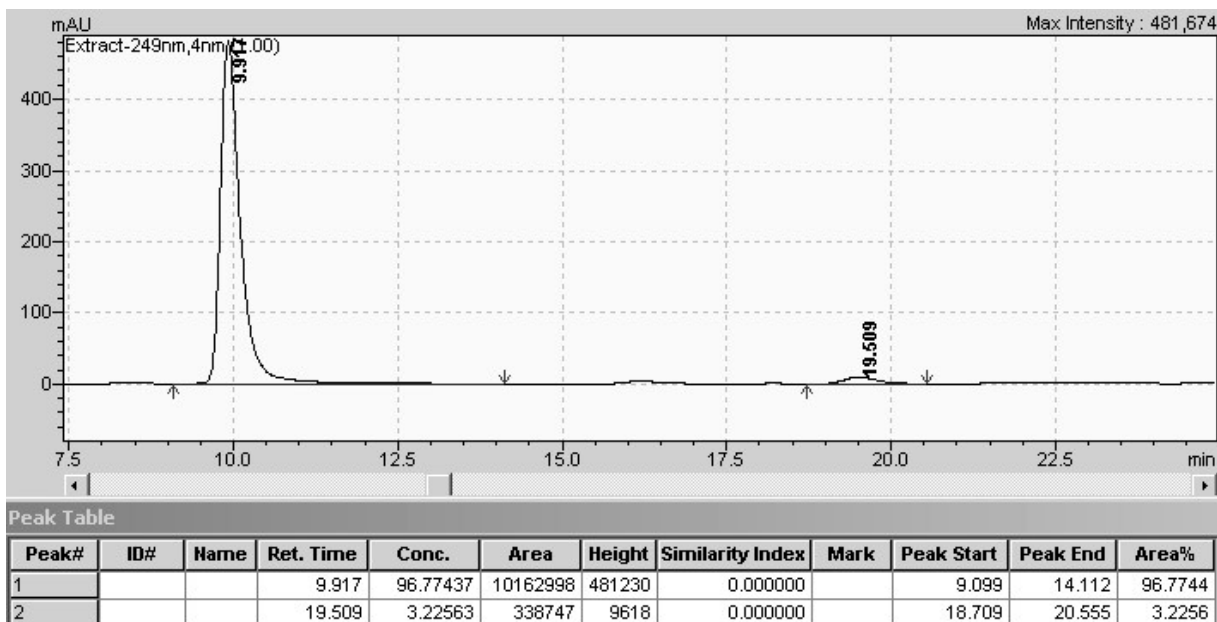
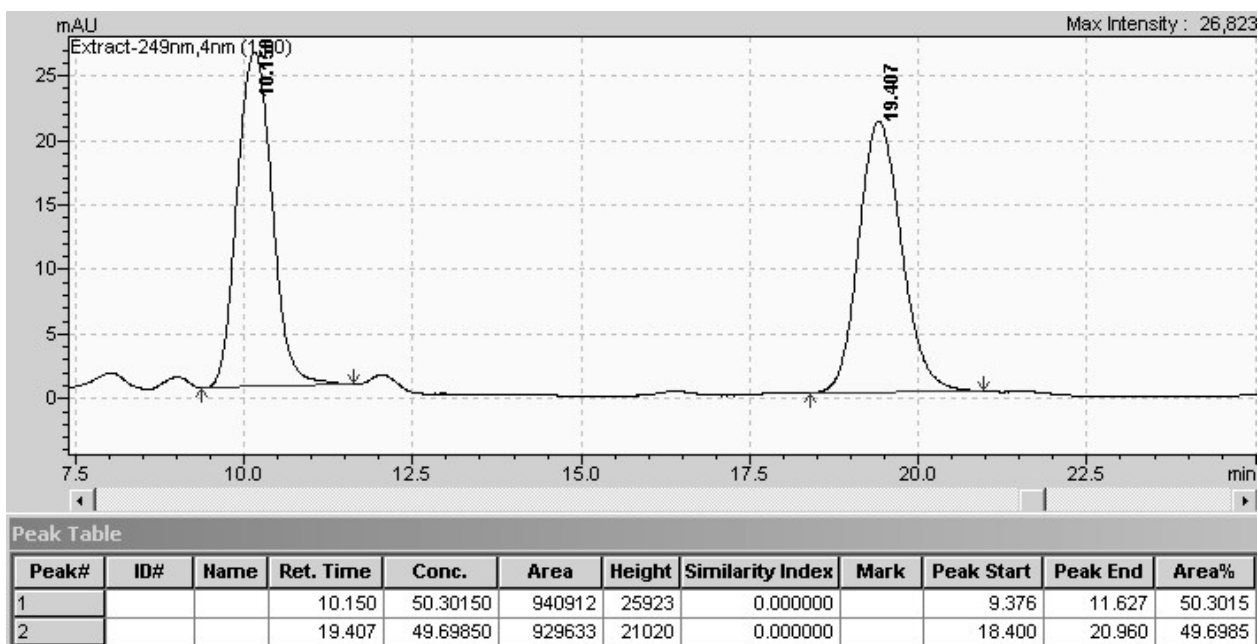
Conditions: IA column

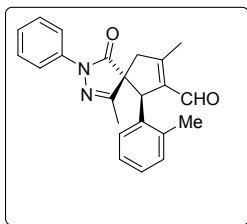
mobile phase: *n*-heptane / propan-2-ol= 90:10

$\lambda = 249 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 9.9 \text{ min}$ (major), $t_R = 19.5 \text{ min}$ (minor), ee= 94 %

minor diastereoisomer





(7j)

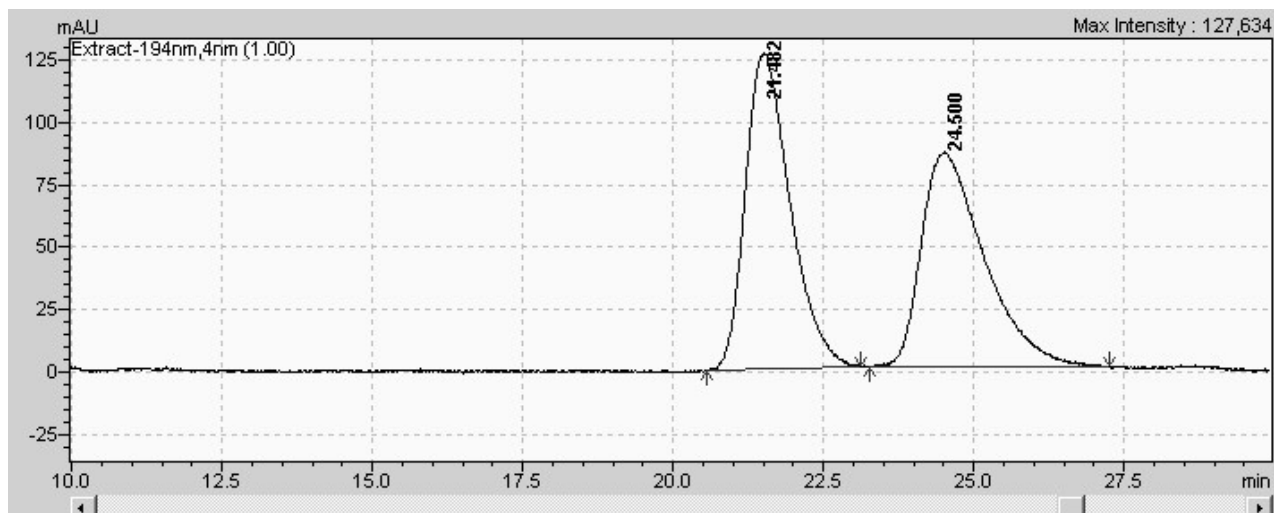
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 70:30

$\lambda = 194 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

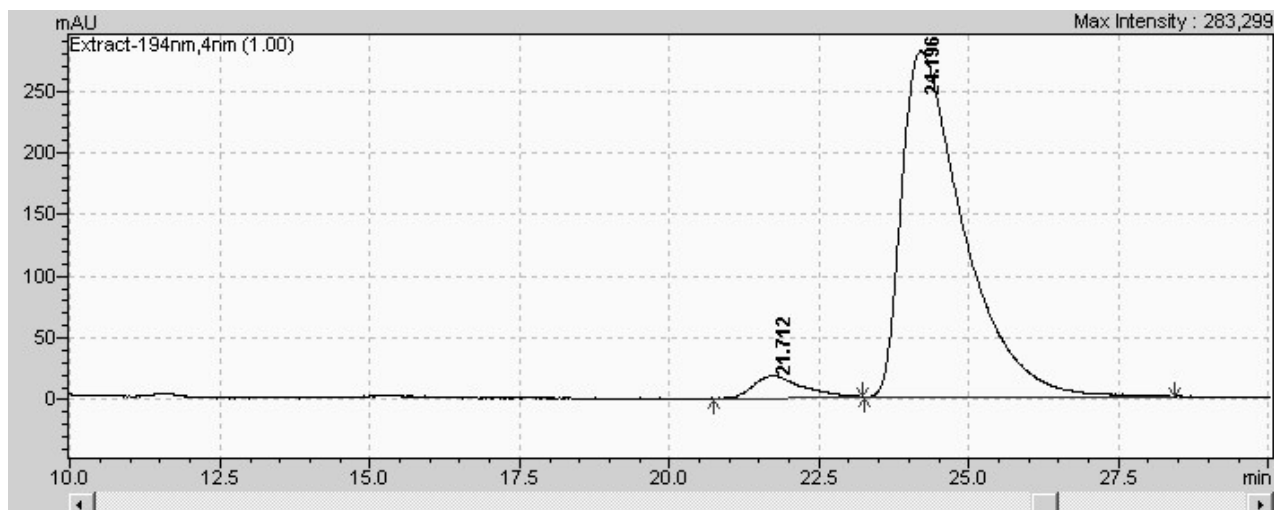
$t_R = 21.7 \text{ min}$ (minor), $t_R = 24.2 \text{ min}$ (major), ee= 91 %

major diastereoisomer



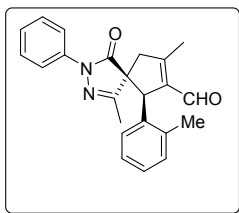
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			21.482	51.57608	6565846	125916	0.000000		20.555	23.115	51.5761
2			24.500	48.42392	6164564	85354	0.000000		23.264	27.253	48.4239



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			21.712	4.69178	988389	18131	0.000000		20.736	23.221	4.6918
2			24.196	95.30822	20078011	280670	0.000000		23.253	28.427	95.3082



(7j)

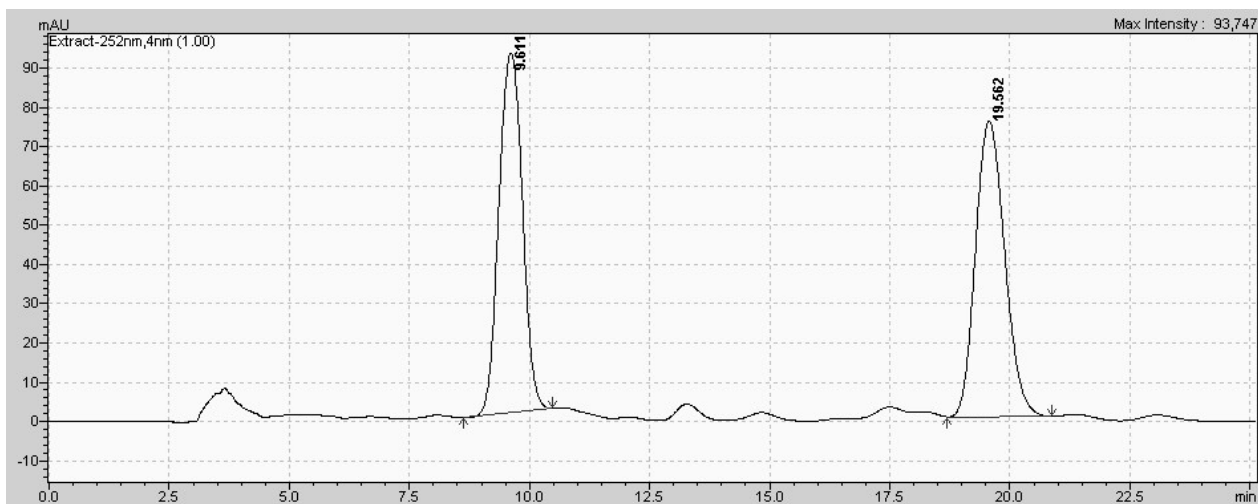
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 90:10

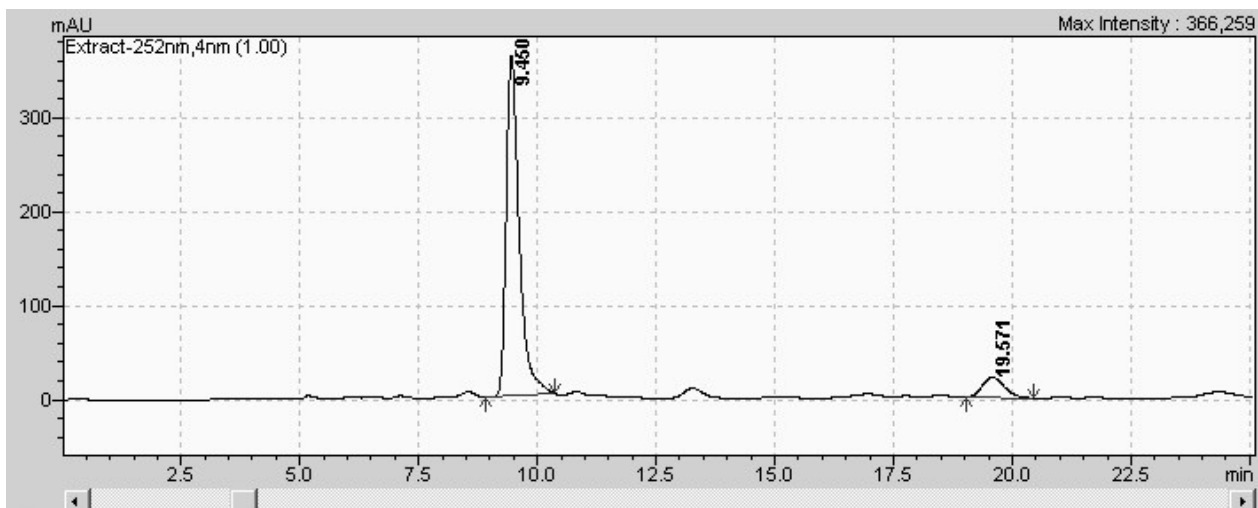
$\lambda = 252 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 9.5 \text{ min}$ (major), $t_R = 19.6 \text{ min}$ (minor), ee= 82 %

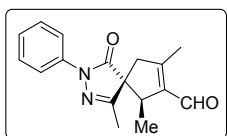
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			9.611	49.57334	3128313	91571	0.000000		8.619	10.485	49.5733
2			19.562	50.42666	3182163	75203	0.000000		18.688	20.865	50.4267



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			9.450	90.85721	6919939	362127	0.000000		8.928	10.379	90.8572
2			19.571	9.14279	696340	21507	0.000000		19.040	20.448	9.1428



(7k)

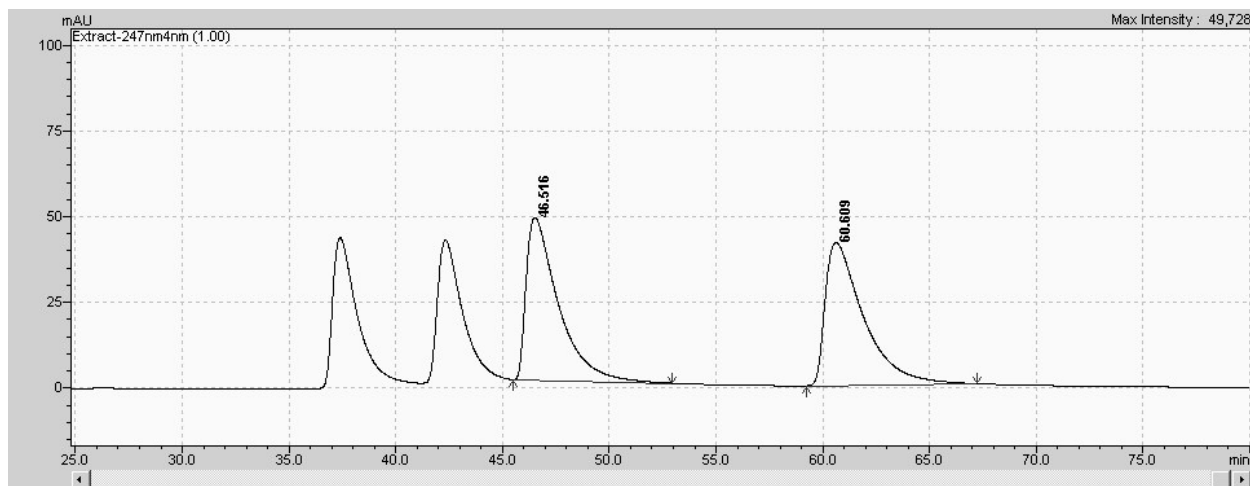
Conditions: IB column

mobile phase: *n*-heptane / propan-2-ol= 98:02

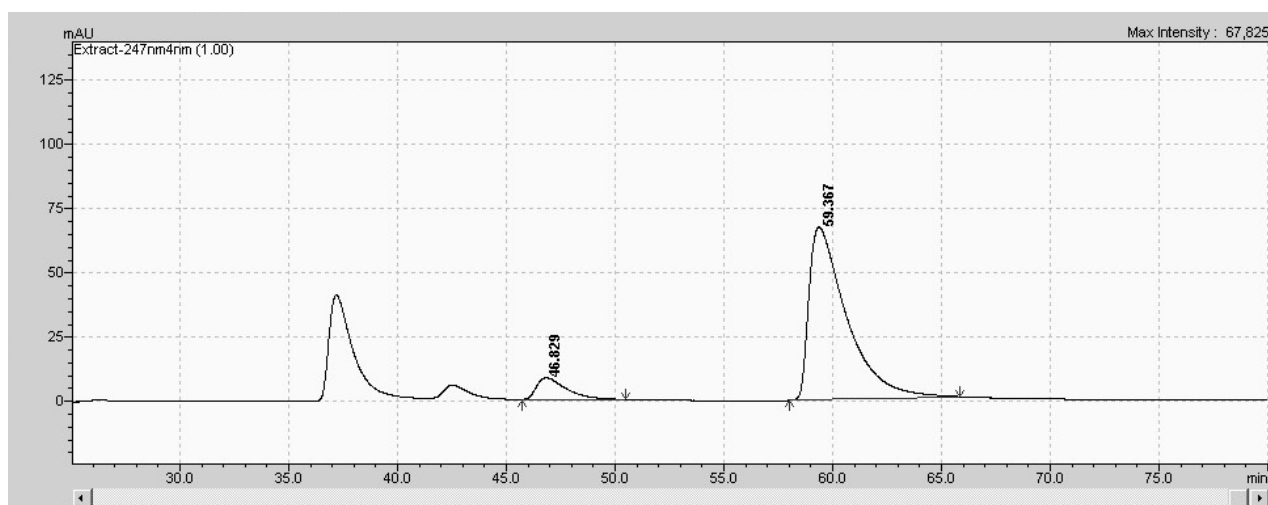
$\lambda = 247\text{nm}$, $V = 0.5\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

$t_{\text{R}} = 46.8\text{ min}$ (minor), $t_{\text{R}} = 59.4\text{ min}$ (major), $ee = 82\%$

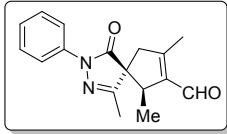
major diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			46.516	48.79855	4974035	47454	0.000000		45.493	52.939	48.798
2			60.609	51.20145	5218963	41733	0.000000		59.232	67.232	51.201



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			46.829	9.06863	809822	8478	0.000000		45.717	50.475	9.068
2			59.367	90.93137	8120100	67173	0.000000		58.005	65.845	90.931



(7k')

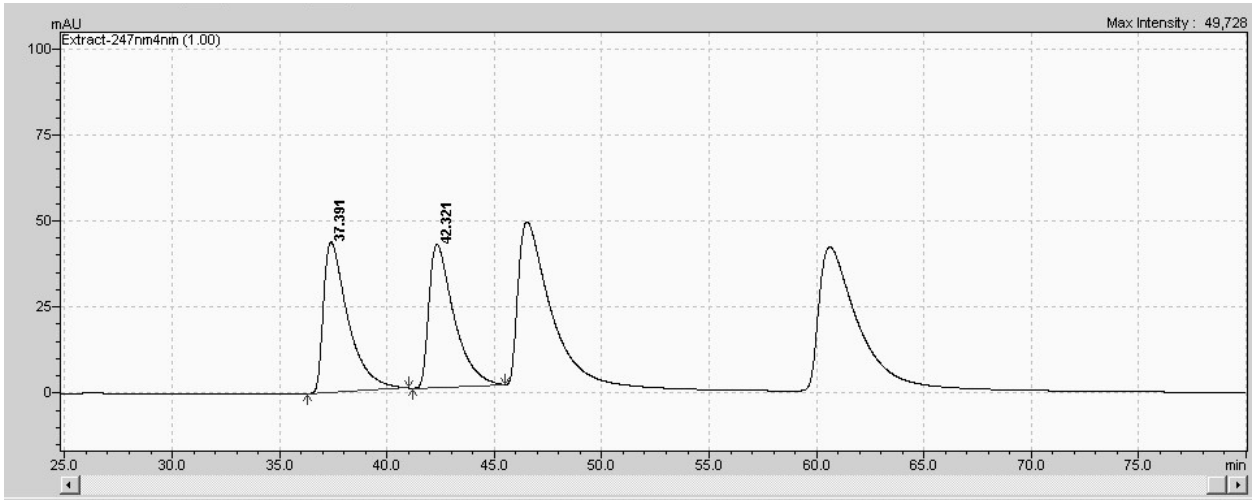
Conditions: IB column

mobile phase: *n*-heptane / propan-2-ol= 98:02

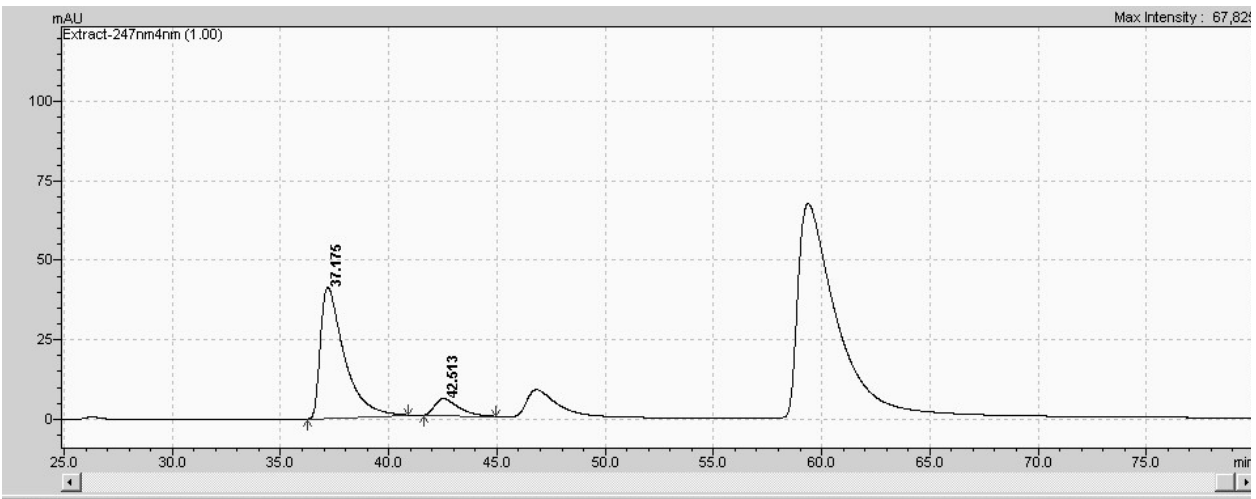
$\lambda = 247\text{nm}$, $V = 0.5\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

$t_R = 37.2\text{ min}$ (major), $t_R = 42.5\text{ min}$ (minor), $ee = 76\%$

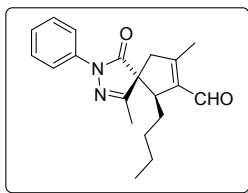
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			37.391	50.91788	3483979	43748	0.000000		36.288	41.013	50.9179
2			42.321	49.08212	3358370	41579	0.000000		41.195	45.493	49.0821



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			37.175	88.79575	3158839	41183	0.000000		36.256	40.896	88.795
2			42.513	11.20425	398582	5271	0.000000		41.621	44.939	11.204



(7I)

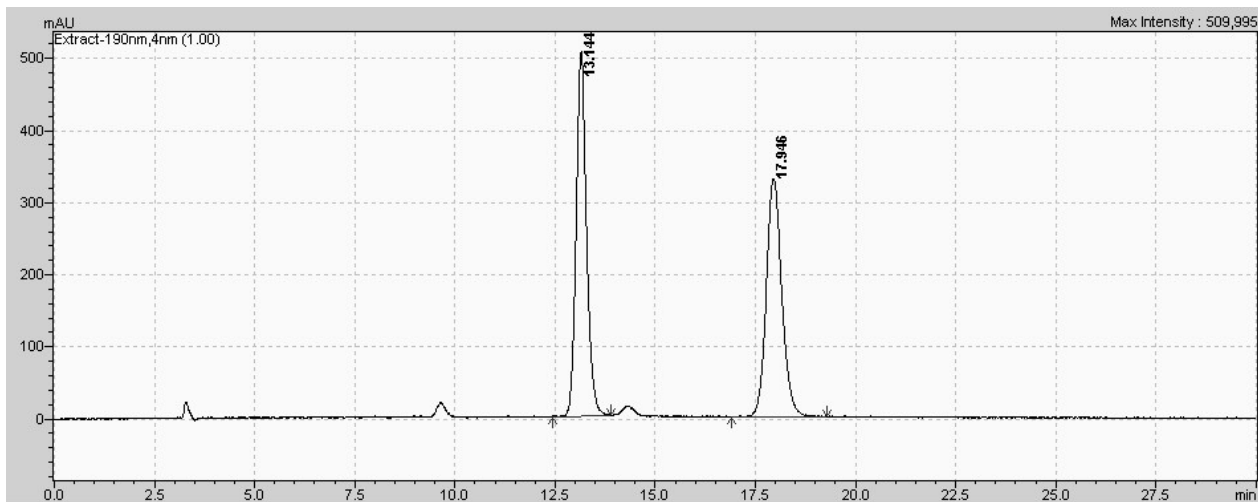
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

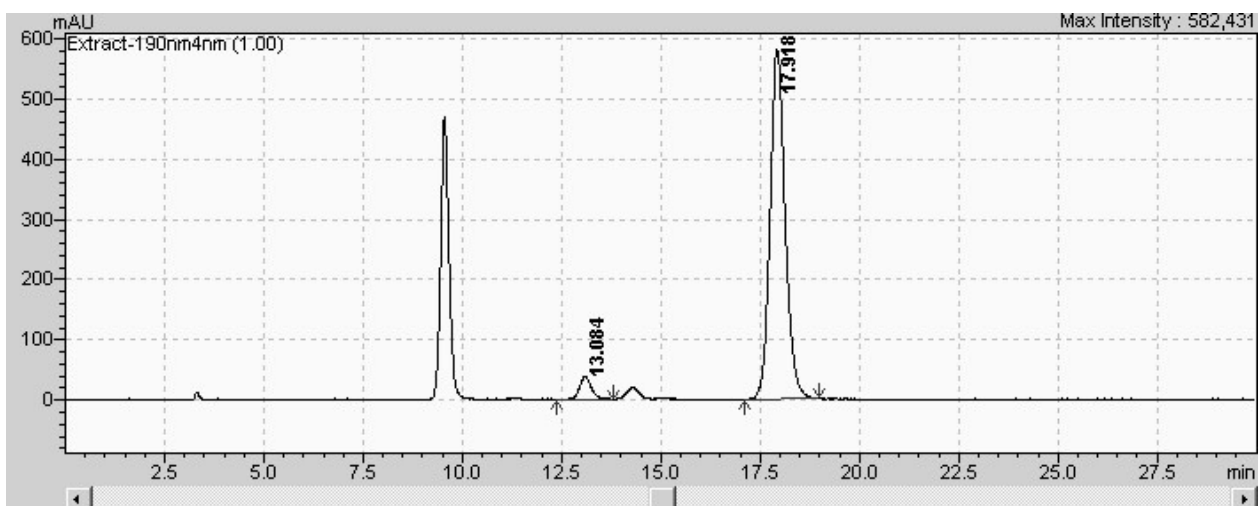
$t_R = 13.1 \text{ min}$ (minor), $t_R = 17.9 \text{ min}$ (major), $ee = 90 \%$

major diastereoisomer



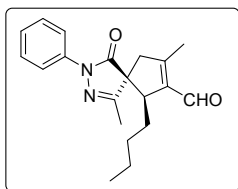
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			13.144	50.64471	9038114	505476	0.000000		12.427	13.909	50.6447
2			17.946	49.35529	8808003	329904	0.000000		16.907	19.275	49.3553



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			13.084	4.91743	791280	39040	0.000000		12.373	13.803	4.9174
2			17.918	95.08257	15300040	580376	0.000000		17.109	18.987	95.0826



(7I')

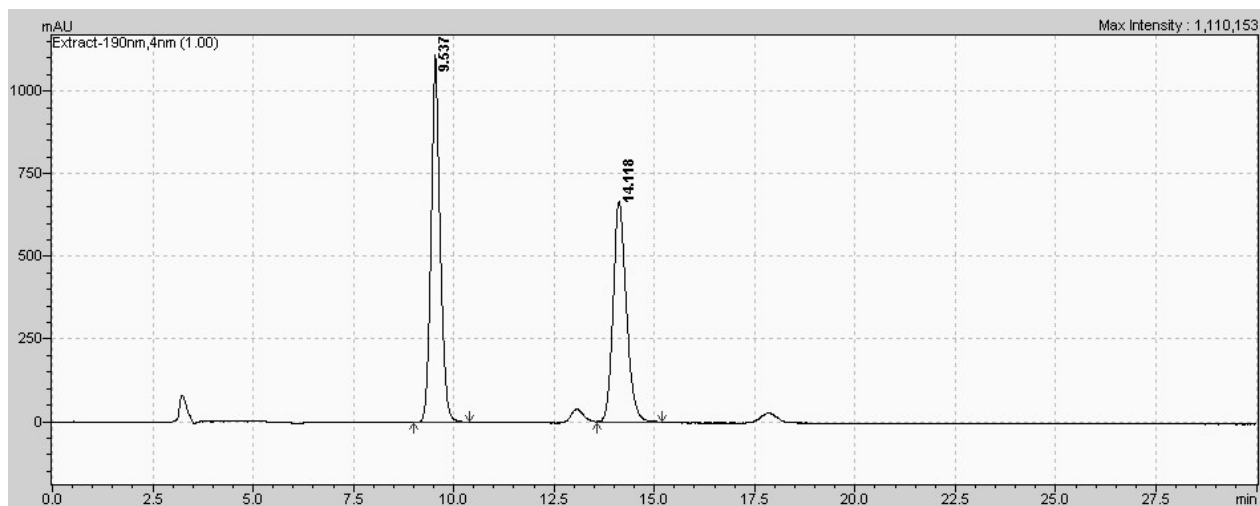
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 95:5

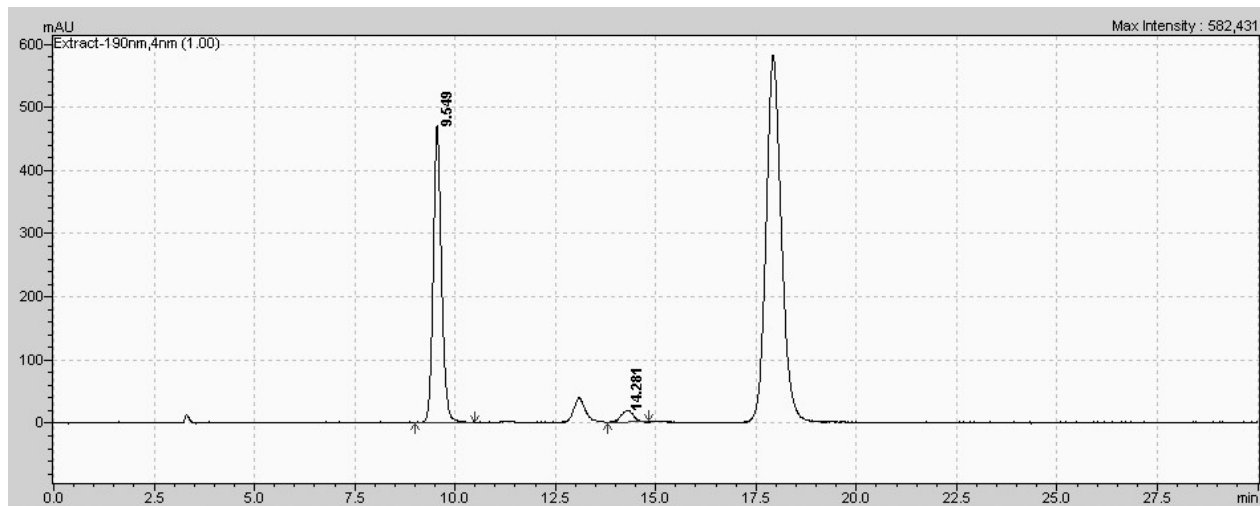
$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 9.5 \text{ min}$ (major), $t_R = 14.3 \text{ min}$ (minor), ee= 89 %

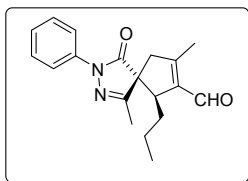
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			9.537	53.35651	17472645	1111484	0.000000		9.003	10.379	53.3565
2			14.118	46.64349	15274507	666483	0.000000		13.557	15.189	46.6435



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			9.549	94.53115	6740678	469173	0.000000		8.992	10.475	94.5312
2			14.281	5.46885	389964	18678	0.000000		13.792	14.816	5.4688



(7m)

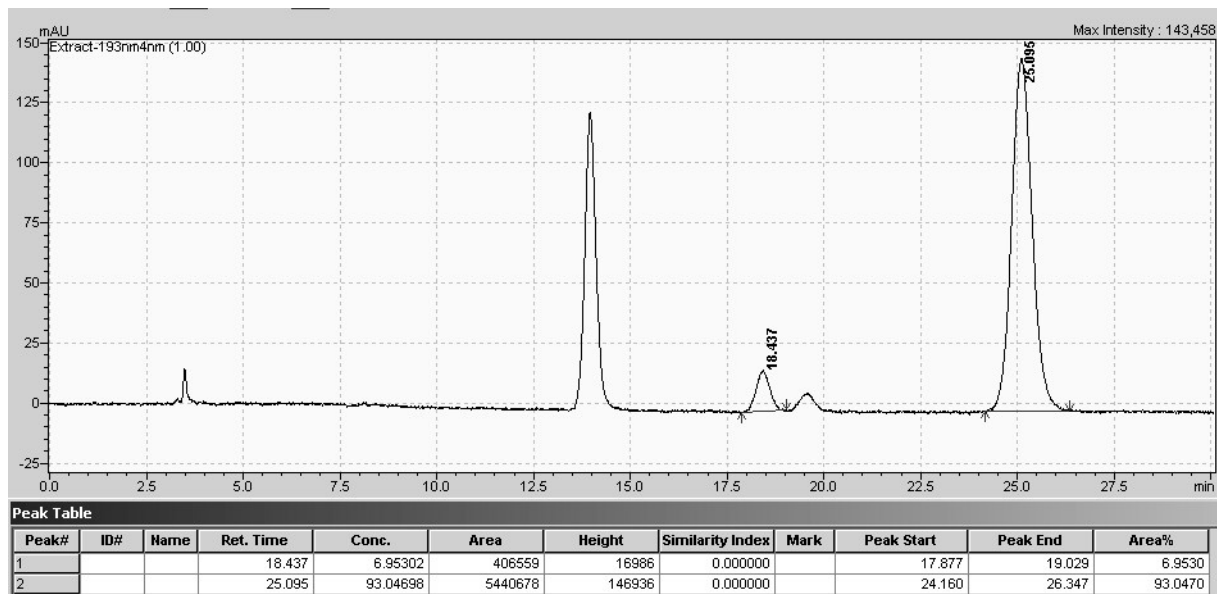
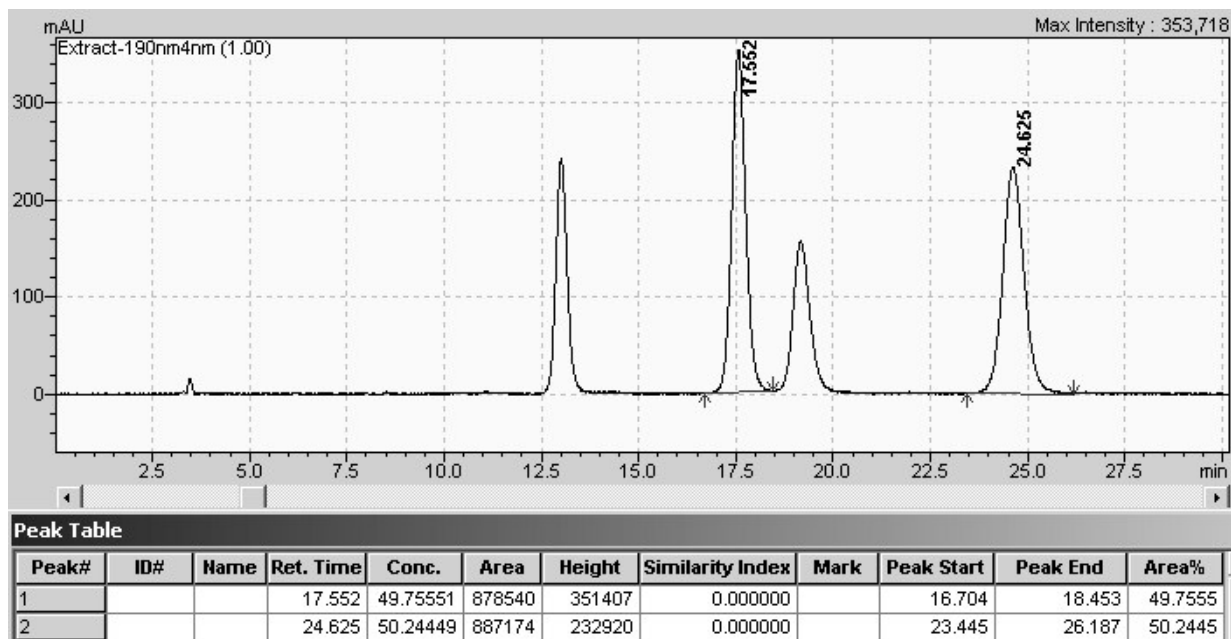
Conditions: IA column

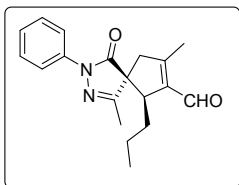
mobile phase: *n*-heptane / propan-2-ol= 97:3

$\lambda = 193 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 18.4 \text{ min}$ (minor), $t_R = 25.1 \text{ min}$ (major), ee= 86 %

major diastereoisomer





(7m')

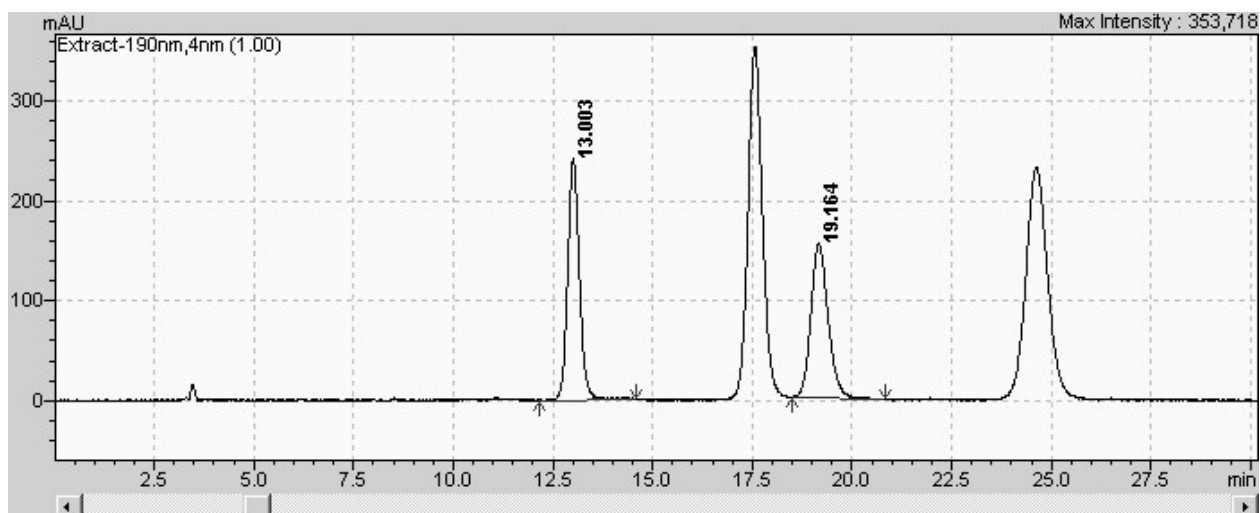
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 97:3

$\lambda = 204 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

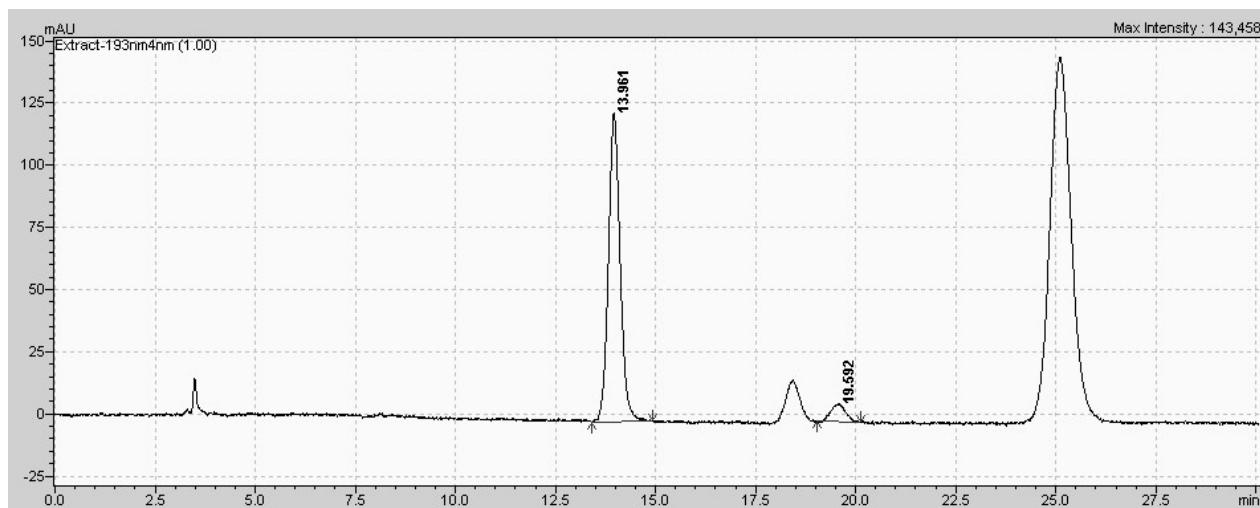
$t_R = 14.0 \text{ min}$ (major), $t_R = 19.6 \text{ min}$ (minor), $ee = 87 \%$

minor diastereoisomer



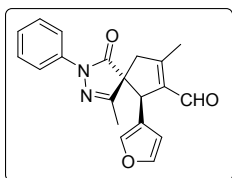
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			13.003	51.32979	490227	242396	0.000000		12.149	14.592	51.3298
2			19.164	48.67021	464826	154648	0.000000		18.496	20.821	48.6702



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			13.961	93.27517	2527968	124160	0.000000		13.408	14.933	93.2752
2			19.592	6.72483	182258	7207	0.000000		19.029	20.128	6.7248



(7n)

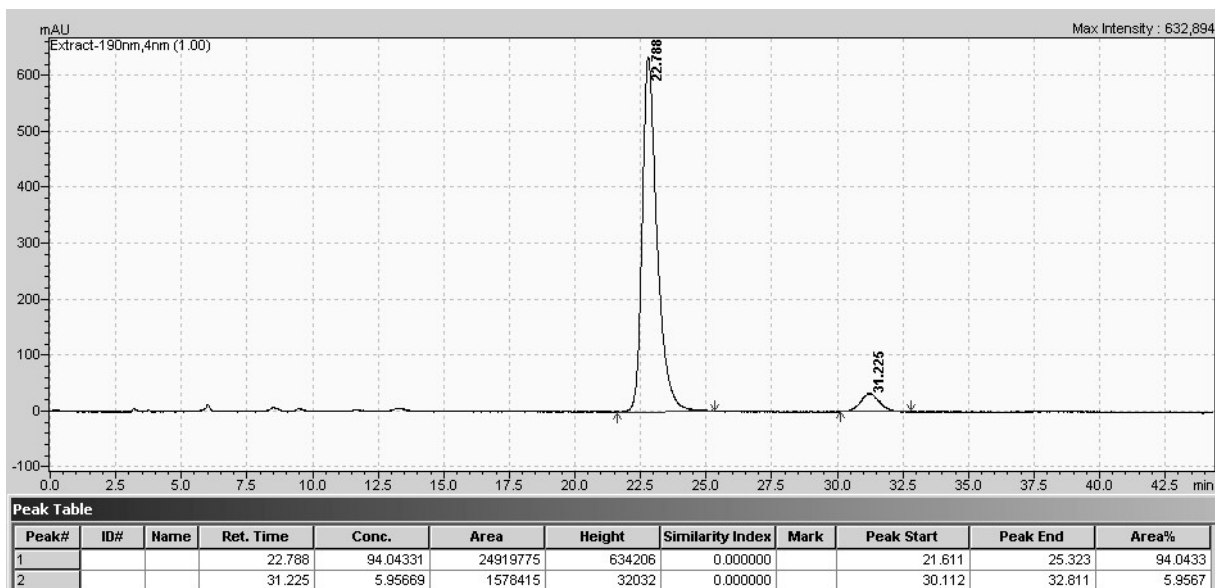
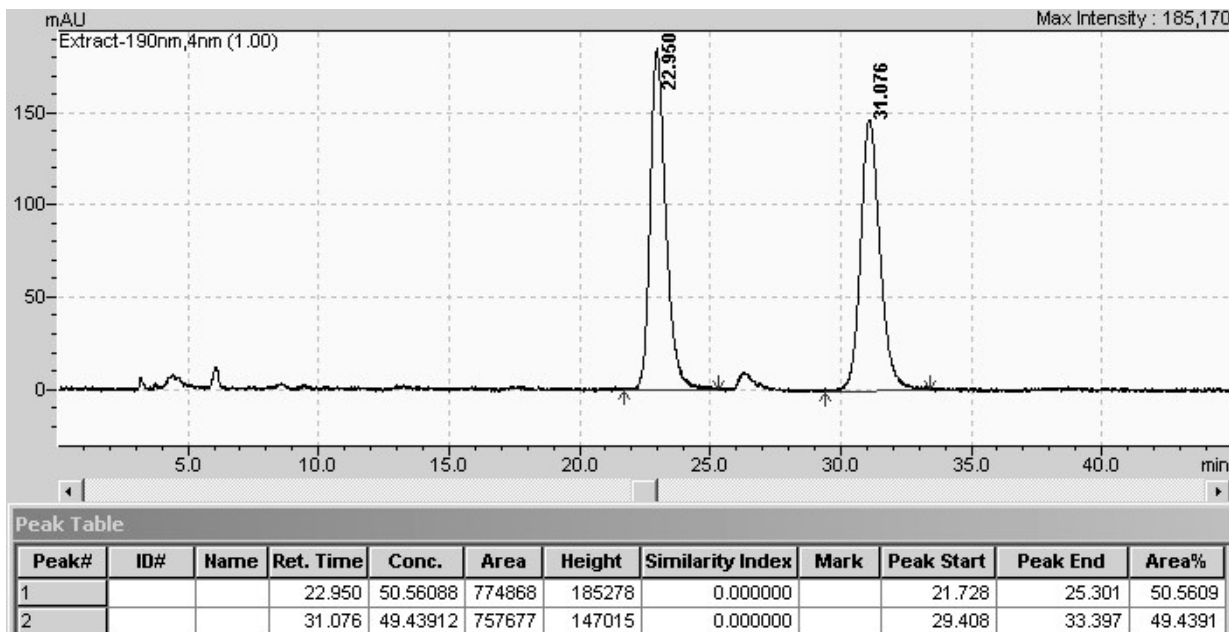
Conditions: IA column

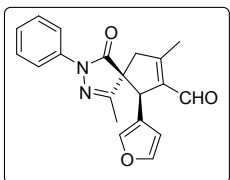
mobile phase: *n*-heptane / propan-2-ol= 90:10

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_{\text{R}} = 22.8 \text{ min}$ (major), $t_{\text{R}} = 31.2 \text{ min}$ (minor), ee= 88 %

major diastereoisomer





(7n')

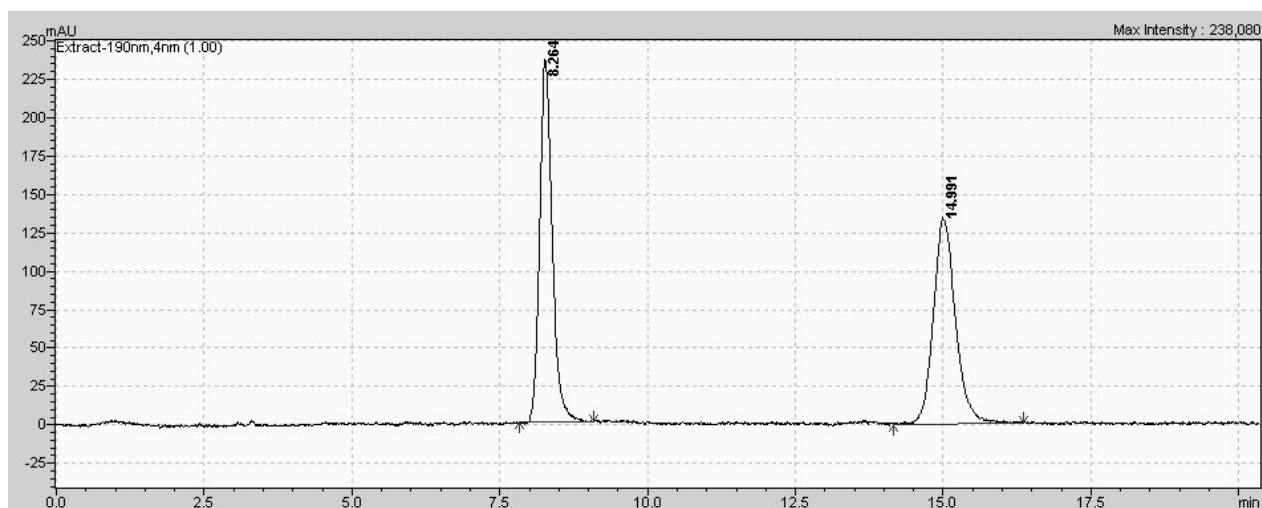
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 80:20

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

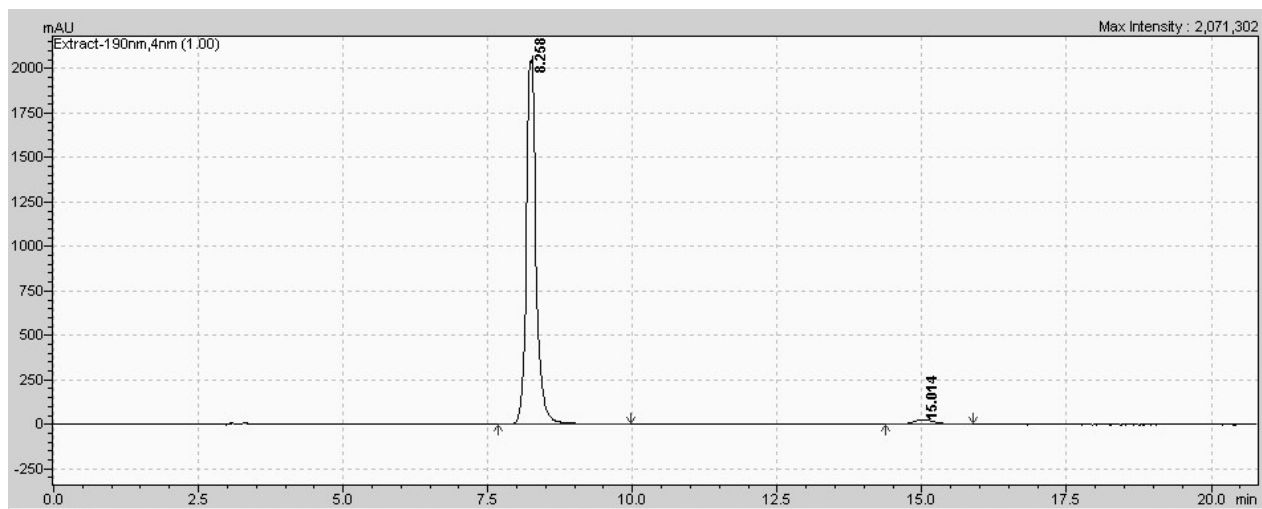
$t_R = 8.3 \text{ min}$ (major), $t_R = 15.0 \text{ min}$ (minor), ee= 94 %

minor diastereoisomer



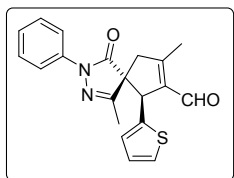
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			8.264	49.93737	3498211	236222	0.000000		7.829	9.088	49.9374
2			14.991	50.06263	3506986	134142	0.000000		14.155	16.352	50.0626



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			8.258	97.15403	24025194	2069556	0.000000		7.680	9.973	97.1540
2			15.014	2.84597	703780	27668	0.000000		14.379	15.883	2.8460



(7o)

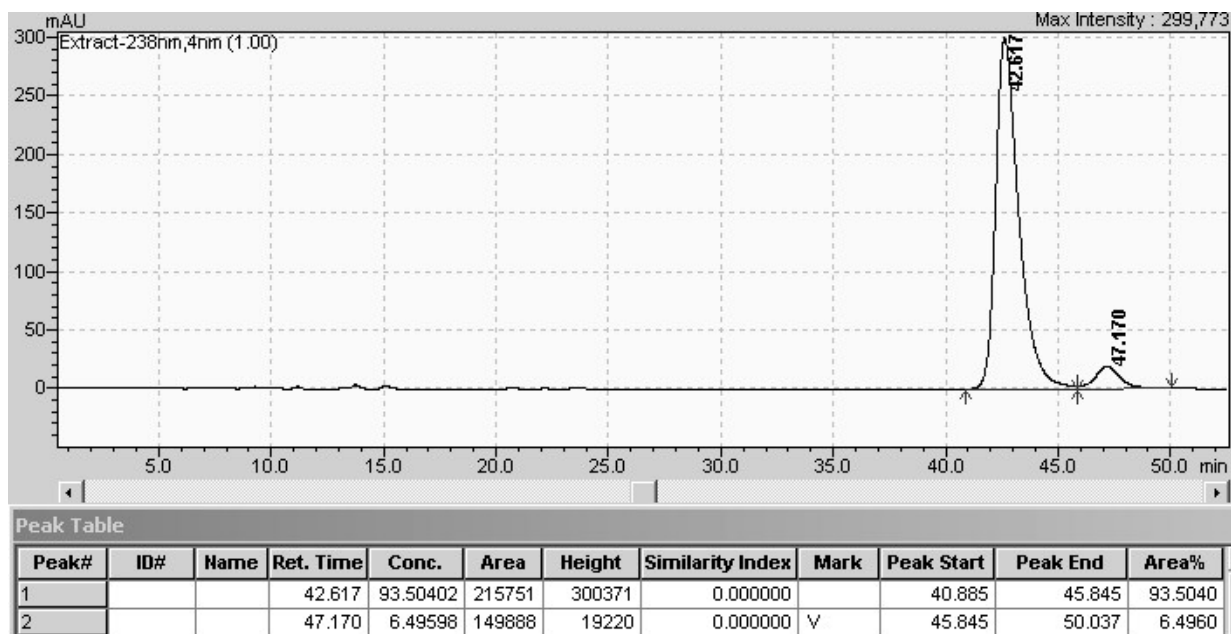
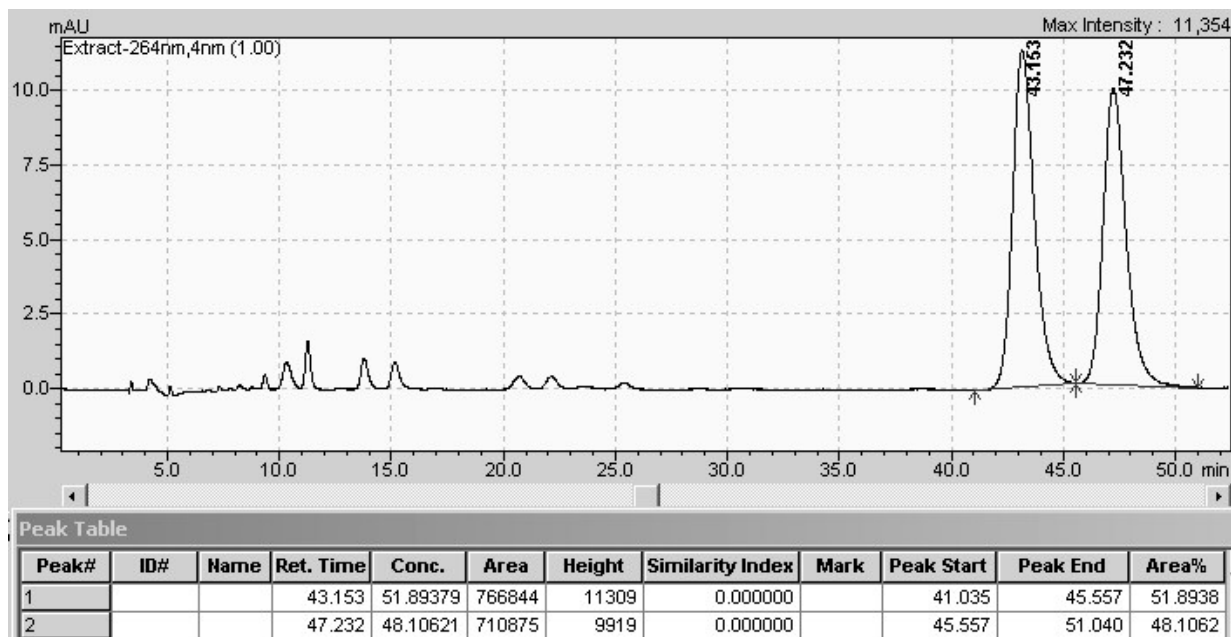
Conditions: IA column

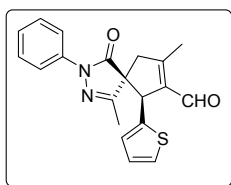
mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 238$ nm, $V = 1$ ml/min, $t = 25$ °C

$t_R = 42.6$ min (major), $t_R = 47.2$ min (minor), ee= 87 %

major diastereoisomer





(7o')

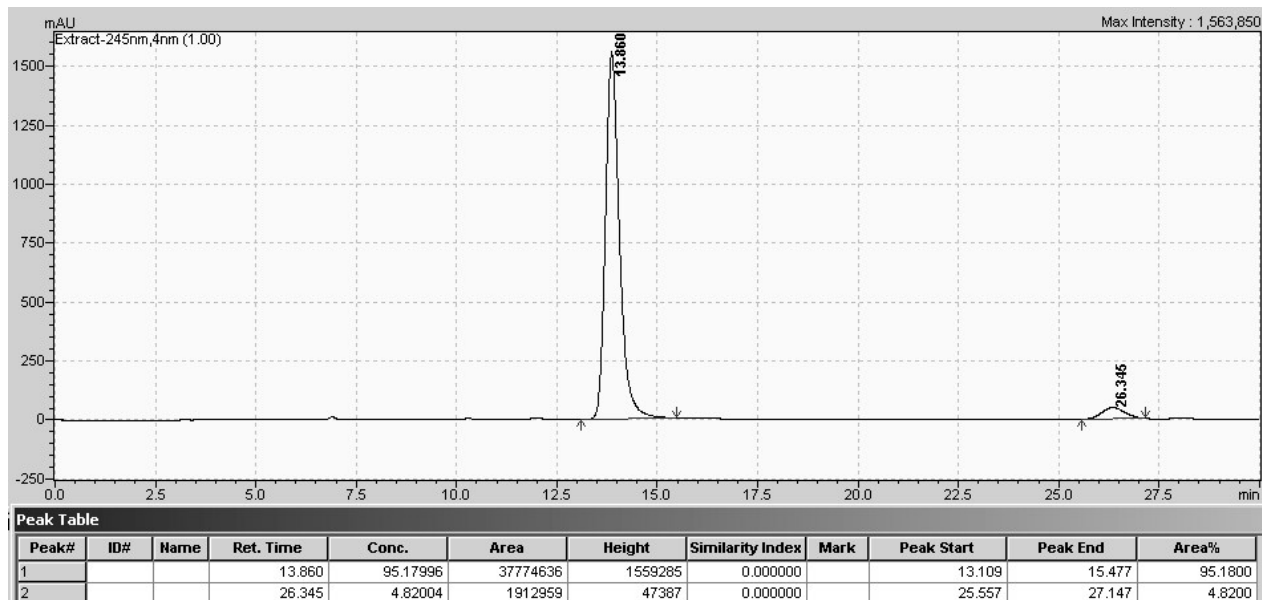
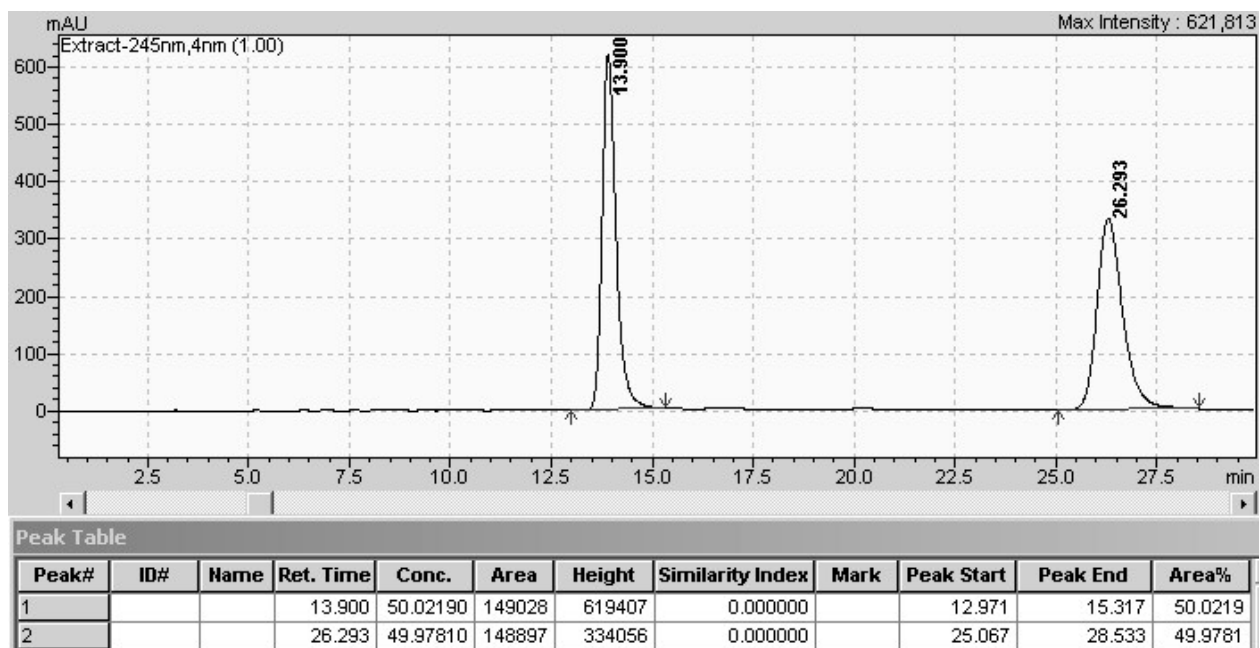
Conditions: IA column

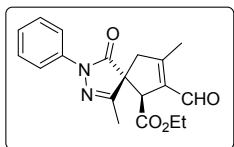
mobile phase: *n*-heptane / propan-2-ol= 90:10

λ = 245 nm, V = 1 ml/min, t = 25 °C

t_R = 13.9 min (major), t_R = 26.3 min (minor), ee= 90 %

minor diastereoisomer





(7p)

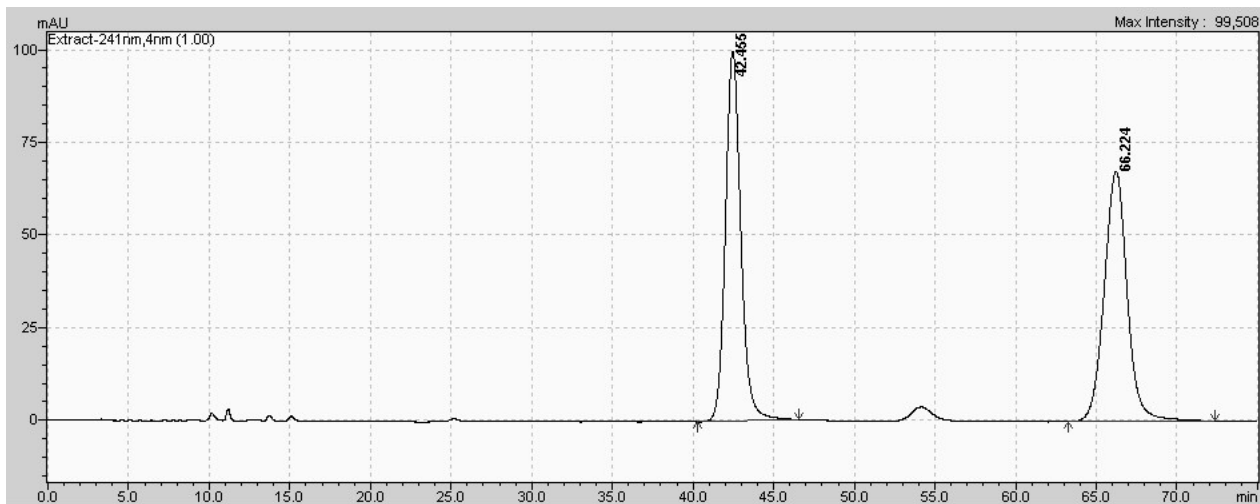
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 241 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

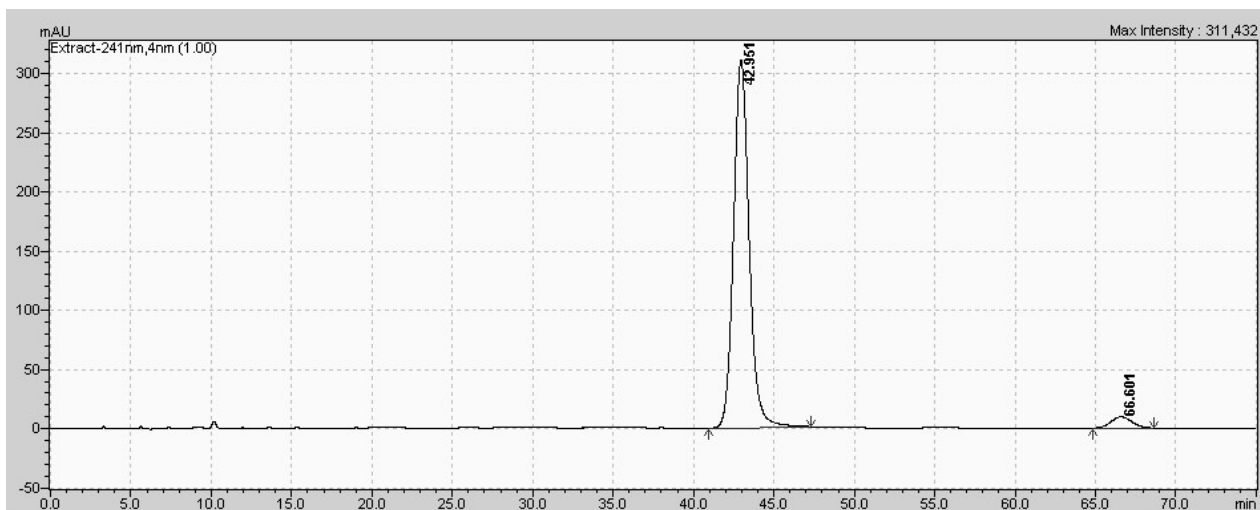
$t_R = 43.0 \text{ min}$ (major), $t_R = 66.6 \text{ min}$ (minor), ee= 92 %

major diastereoisomer



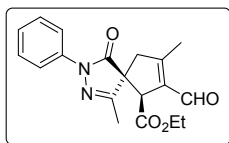
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			42.455	49.78768	6633267	99732	0.000000		40.309	46.539	49.7877
2			66.224	50.21232	6689842	67481	0.000000		63.275	72.352	50.2123



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			42.951	95.95093	20916466	310633	0.000000		40.939	47.264	95.9509
2			66.601	4.04907	882663	9633	0.000000		64.875	68.608	4.0491



(7p')

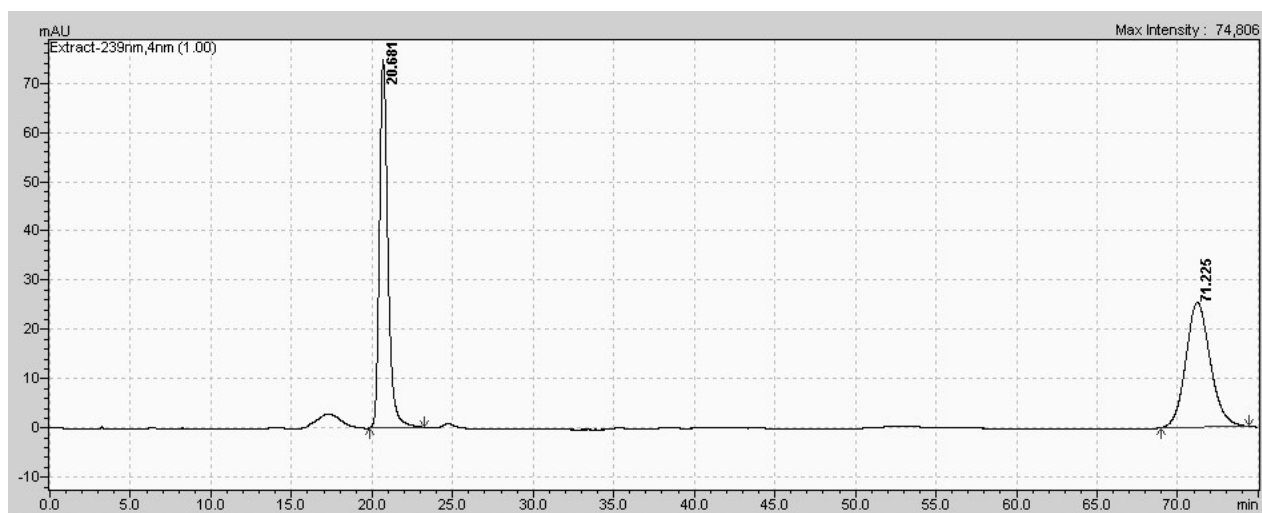
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 90:10

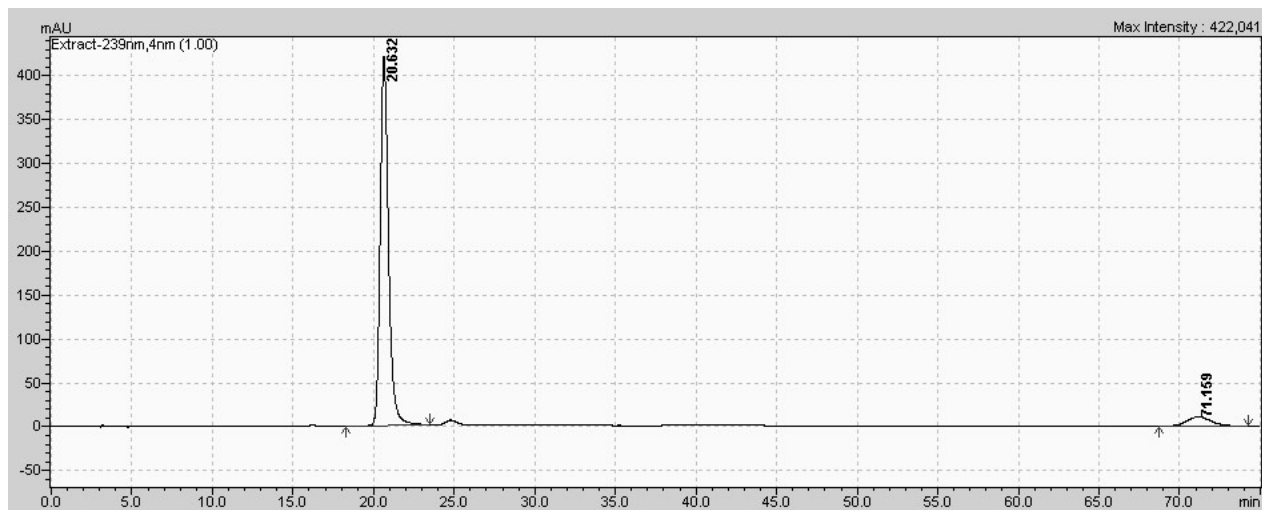
$\lambda = 239 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 20.6 \text{ min}$ (major), $t_R = 71.2 \text{ min}$ (minor), ee= 86 %

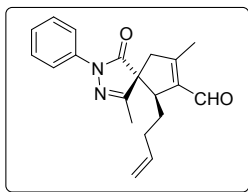
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			20.681	50.54848	2731988	74784	0.000000		19.819	23.221	50.5485
2			71.225	49.45152	2672701	25329	0.000000		68.949	74.389	49.4515



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			20.632	93.05550	15093253	420625	0.000000		18.272	23.477	93.0555
2			71.159	6.94450	1126372	10617	0.000000		68.683	74.293	6.9445



(7q)

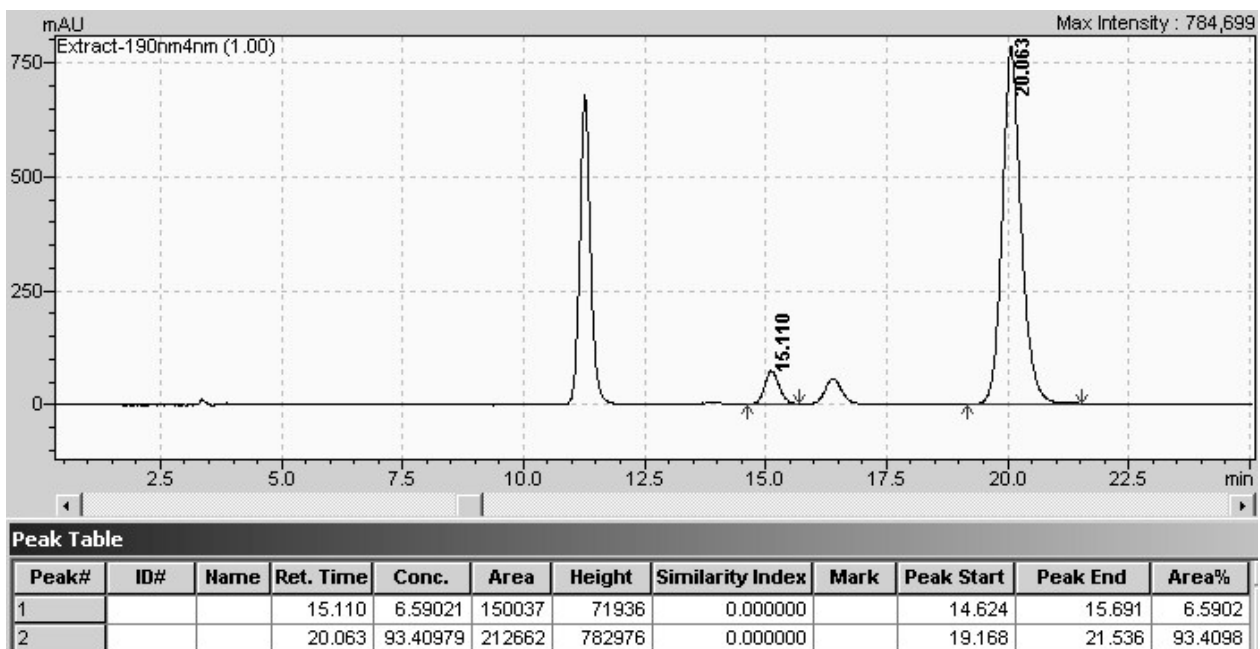
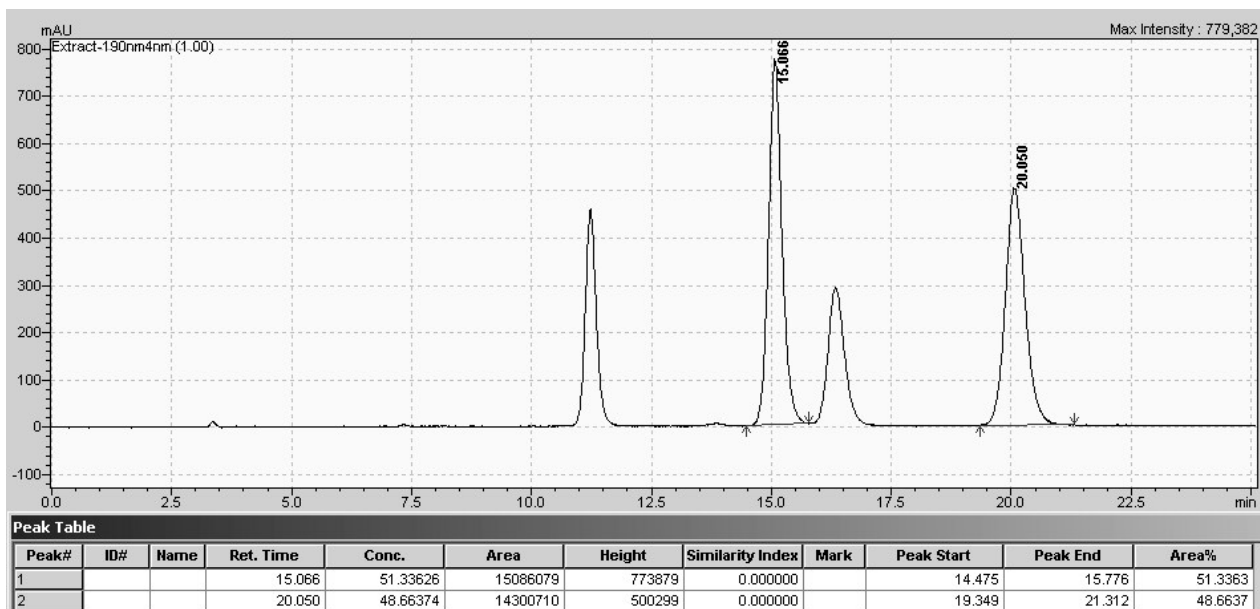
Conditions: IA column

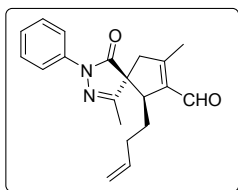
mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 15.1 \text{ min}$ (minor), $t_R = 20.1 \text{ min}$ (major), ee= 87 %

major diastereoisomer





(7q')

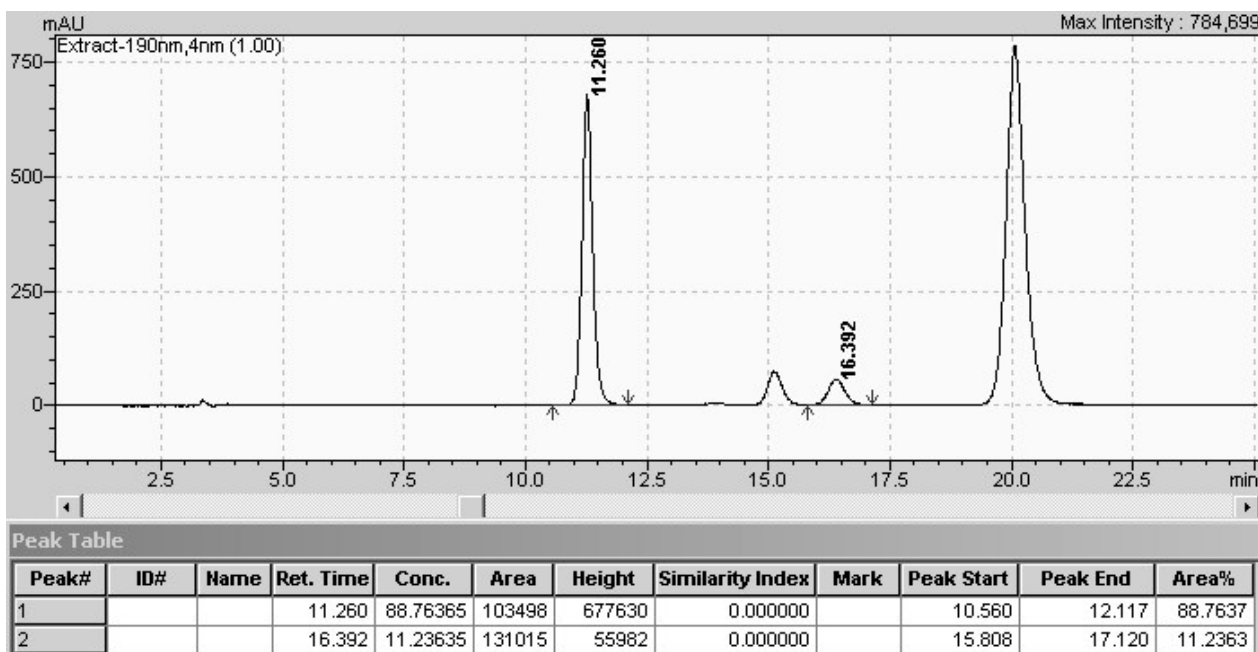
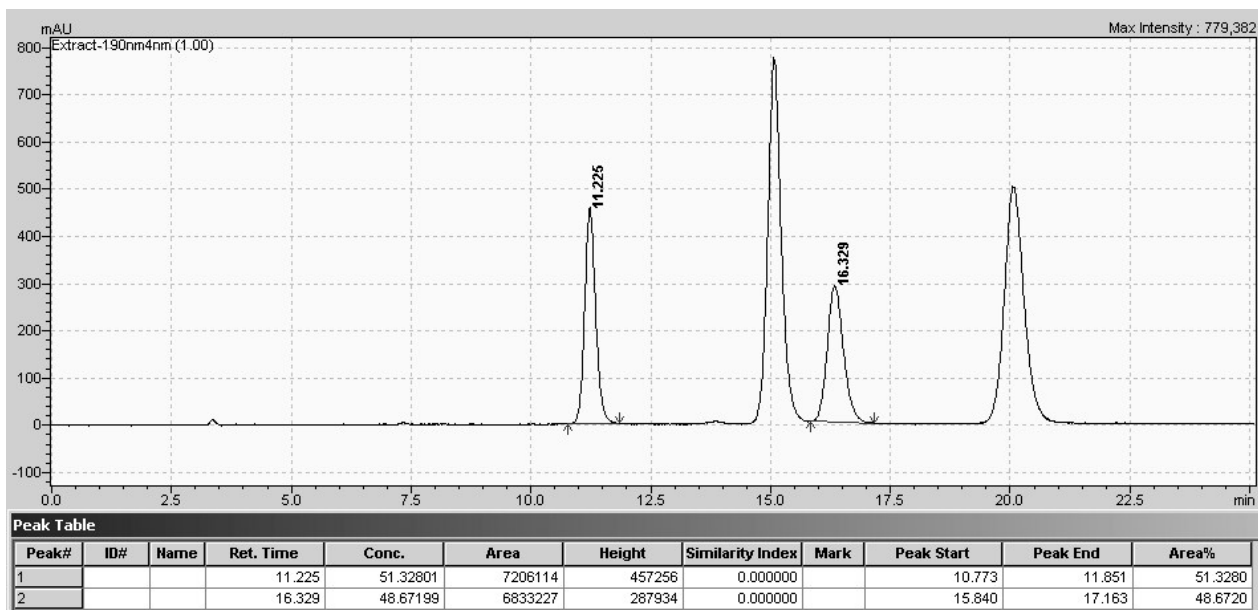
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

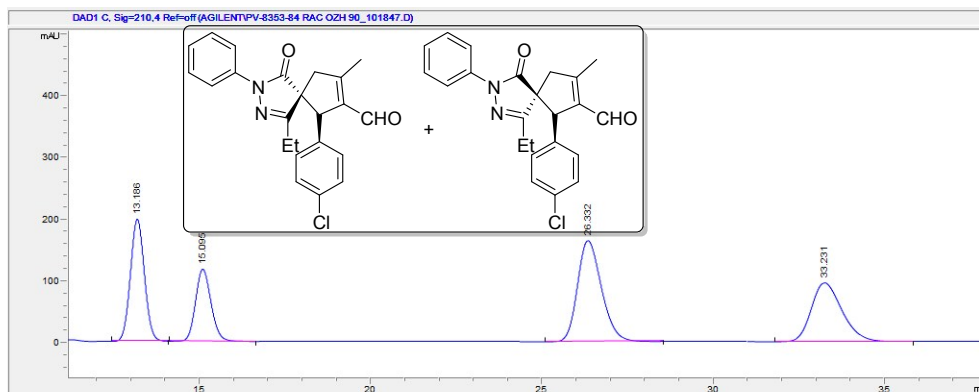
$t_R = 11.3 \text{ min}$ (major), $t_R = 16.4 \text{ min}$ (minor), $ee = 78 \%$

minor diastereoisomer

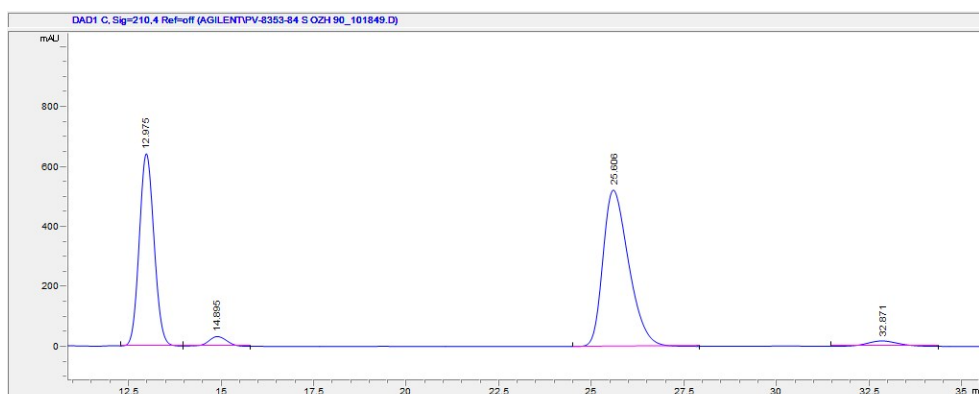


(5*R*/5*S*,6*S*)-6-(4-chlorophenyl)-1-ethyl-8-methyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7*r*) mixture of major and minor diastereomers

Chiralpak OZ-H column (hexane/iPrOH = 90:10, flow rate 1.0 mL/min, $\lambda = 210$ nm). Major diastereomer: t_r (S) = 26.3, t_r (R) = 33.2, 92% ee (S cat). Minor diastereomer: t_r (S) = 13.2, t_r (R) = 15.1, 88% ee



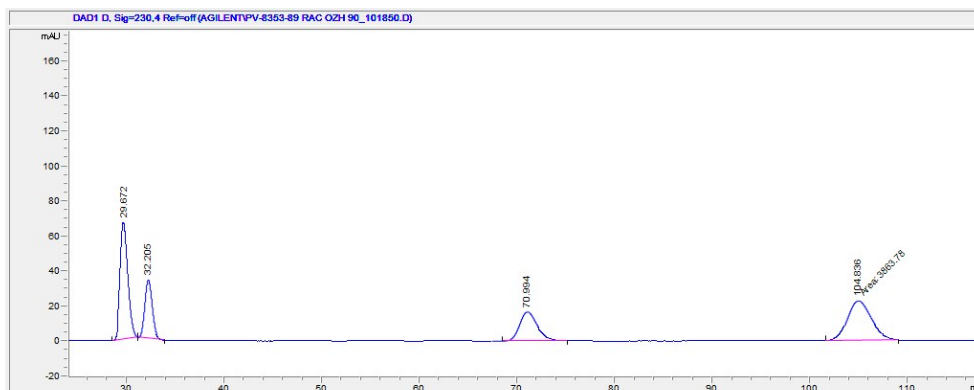
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.186	BB	0.4420	5648.96289	198.52907	24.1968
2	15.095	BB	0.4885	3712.27197	117.51798	15.9012
3	26.332	BB	0.7492	7989.57568	164.34280	34.2226
4	33.231	BB	0.9592	5995.10547	95.92310	25.6795



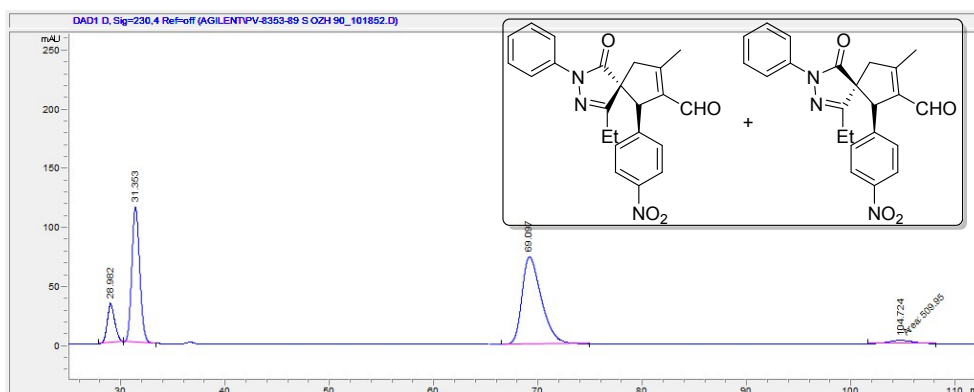
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.975	BB	0.4337	1.78106e4	641.94025	39.3407
2	14.895	BB	0.5421	1093.73975	32.05224	2.4159
3	25.606	BB	0.7453	2.52990e4	522.16455	55.8812
4	32.871	BB	0.8724	1069.42163	18.02011	2.3622

(5*R*/5*S*,6*S*)-6-(4-nitrophenyl)-1-ethyl-8-methyl-4-oxo-3-phenyl-2,3-diazaspiro[4.4]nona-1,7-diene-7-carbaldehyde (7s) mixture of major and minor diastereomers

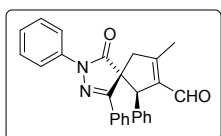
Chiralpak OZ-H column (hexane/iPrOH = 90:10, flow rate 1.0 mL/min, $\lambda = 230$ nm). Diastereomer 1: $t_r(S) = 32.2$, $t_r(R) = 29.7$, 55% ee. Diastereomer 2: $t_r(S) = 70.9$, $t_r(R) = 104.8$, 90% ee.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.672	BB	0.8376	3645.95386	66.92296	31.9114
2	32.205	BB	0.8248	1794.40674	33.61201	15.7056
3	70.994	BB	1.5342	2121.11523	16.62836	18.5651
4	104.836	MM	2.8404	3863.77905	22.67170	33.8179



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.982	BB	0.7907	1737.75159	33.52948	9.7126
2	31.353	BB	0.8224	6067.18457	114.83689	33.9105
3	69.097	BB	1.8412	9576.87695	74.03489	53.5267
4	104.724	MM	2.9117	509.95044	2.91893	2.8502



(7t)

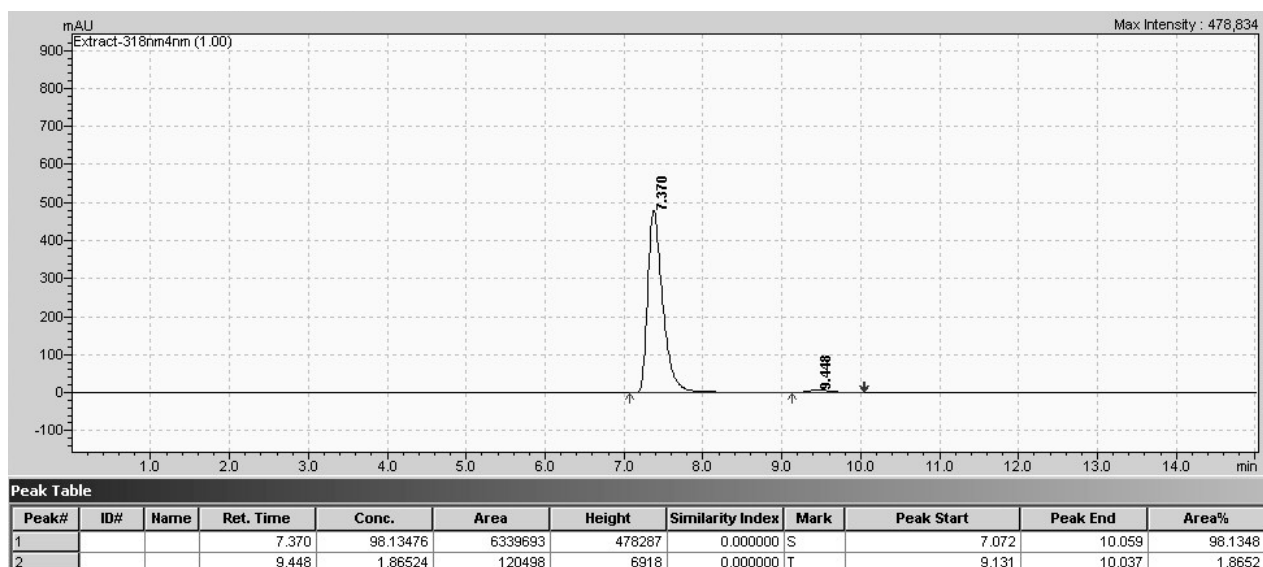
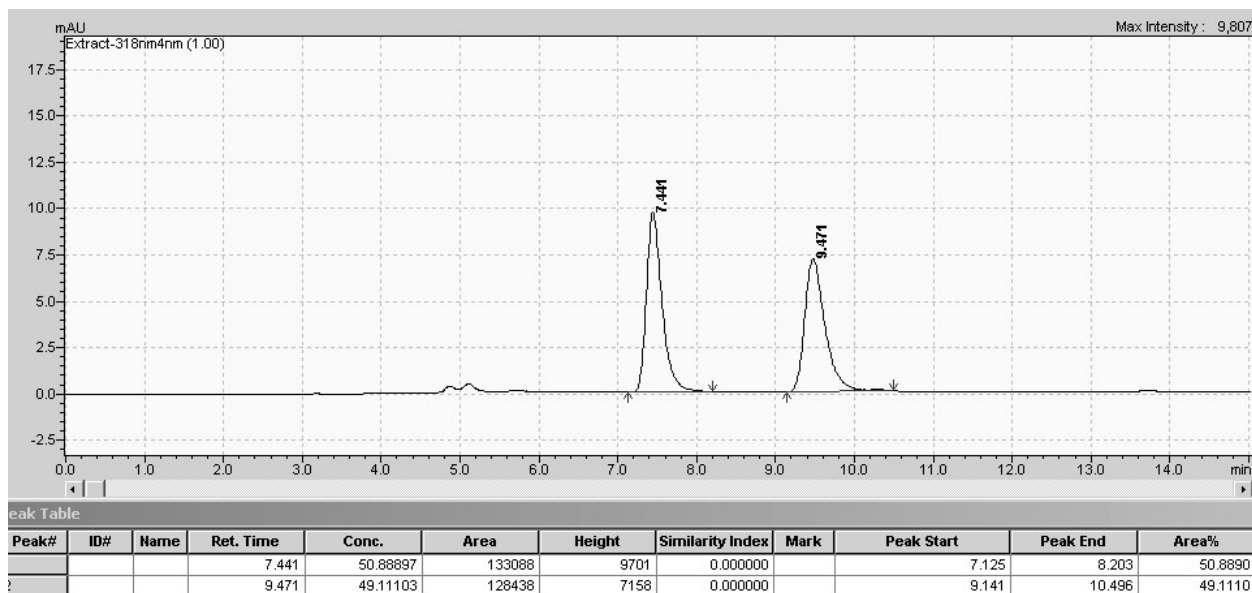
Conditions: IA column

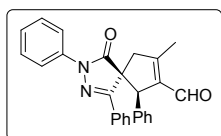
mobile phase: *n*-heptane / propan-2-ol – 80:20

$\lambda = 318\text{nm}$, $V = 1\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

$t_R = 7.4\text{ min}$ (major), $t_R = 9.4\text{ min}$ (minor), ee = 96 %

major diastereoisomer





(7t')

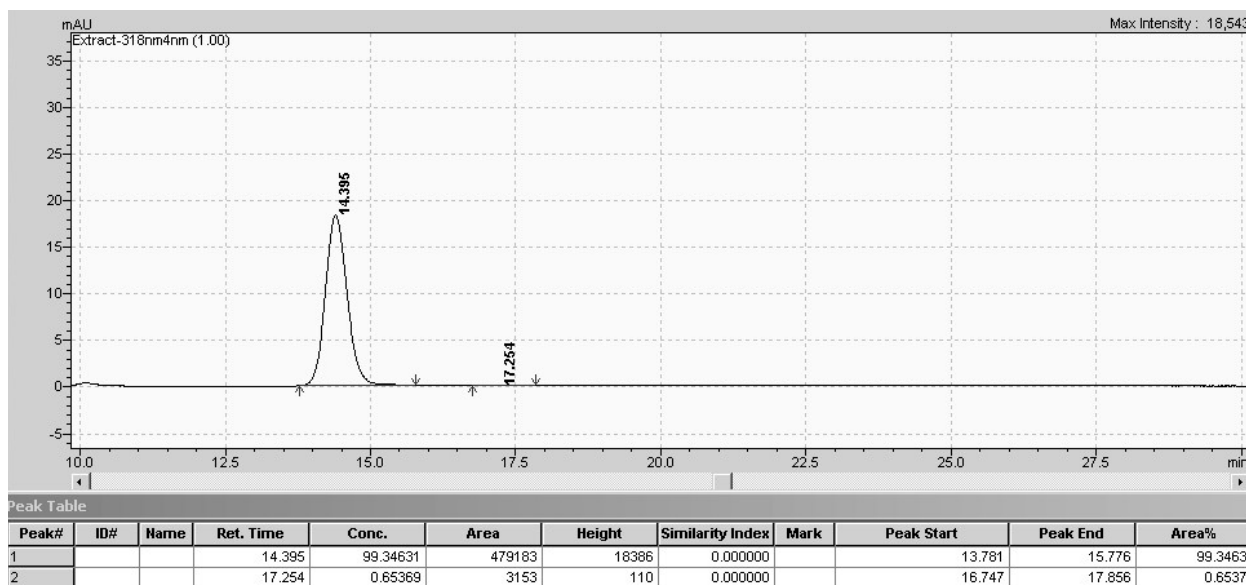
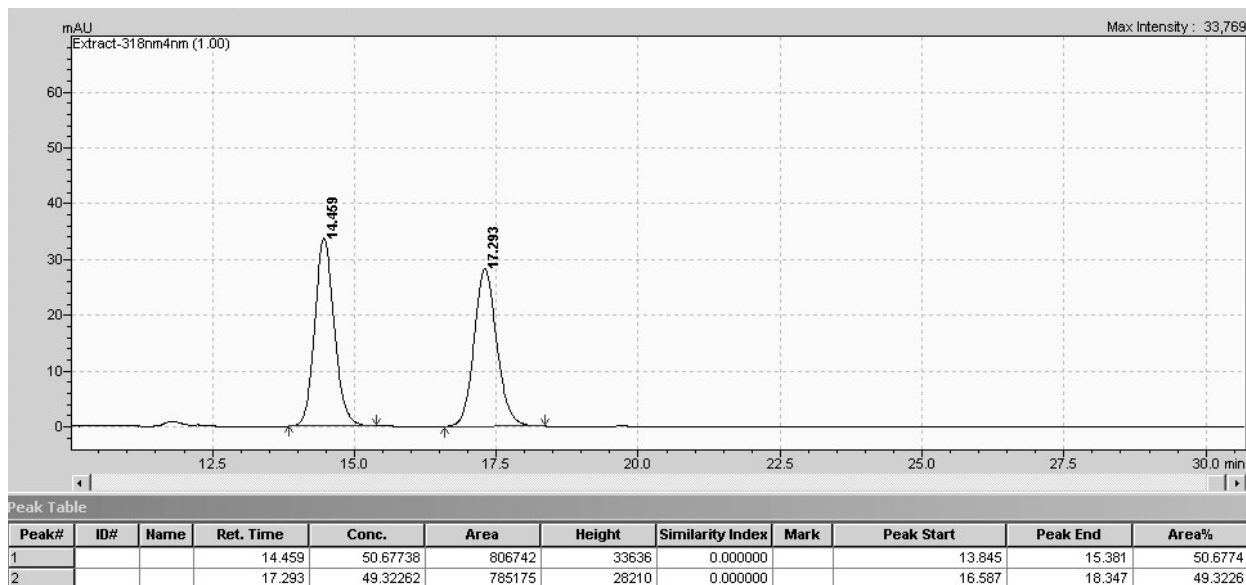
Conditions: IA column

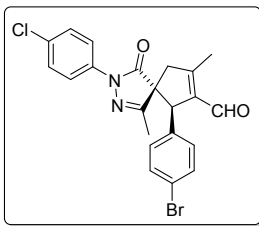
mobile phase: *n*-heptane / propan-2-ol – 80:20

$\lambda = 318\text{nm}$, $V = 1\text{ ml/min}$, $t = 25\text{ }^\circ\text{C}$

$t_R = 14.4\text{min}$ (major), $t_R = 17.3\text{ min}$ (minor), ee = 99%

minor diastereoisomer





(7u)

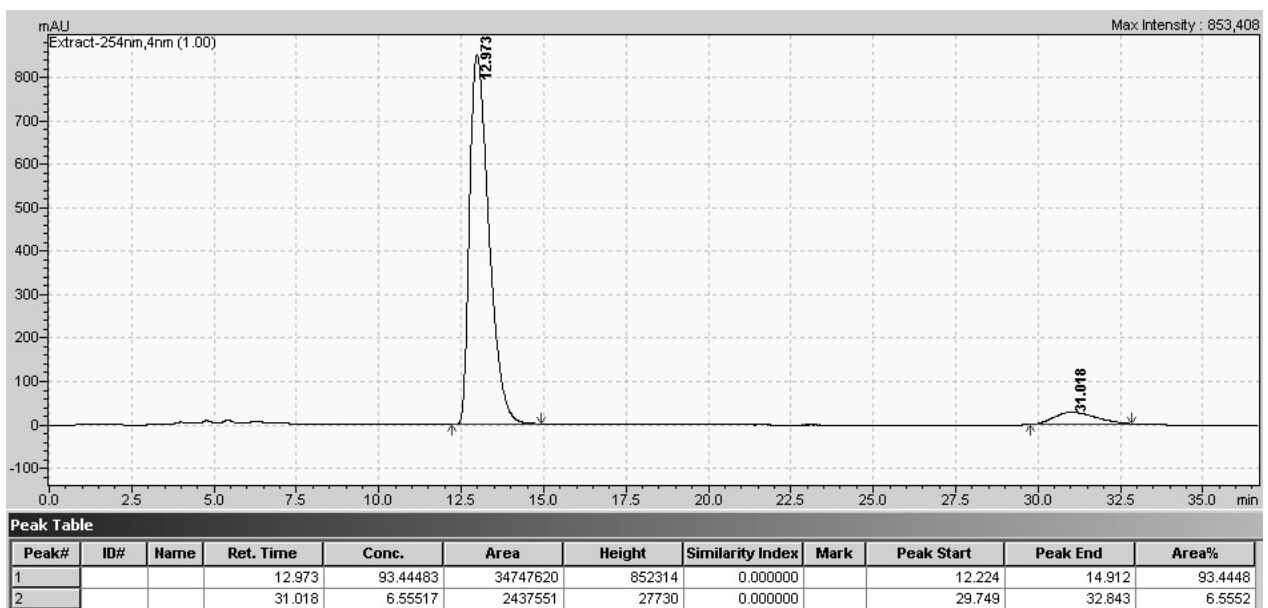
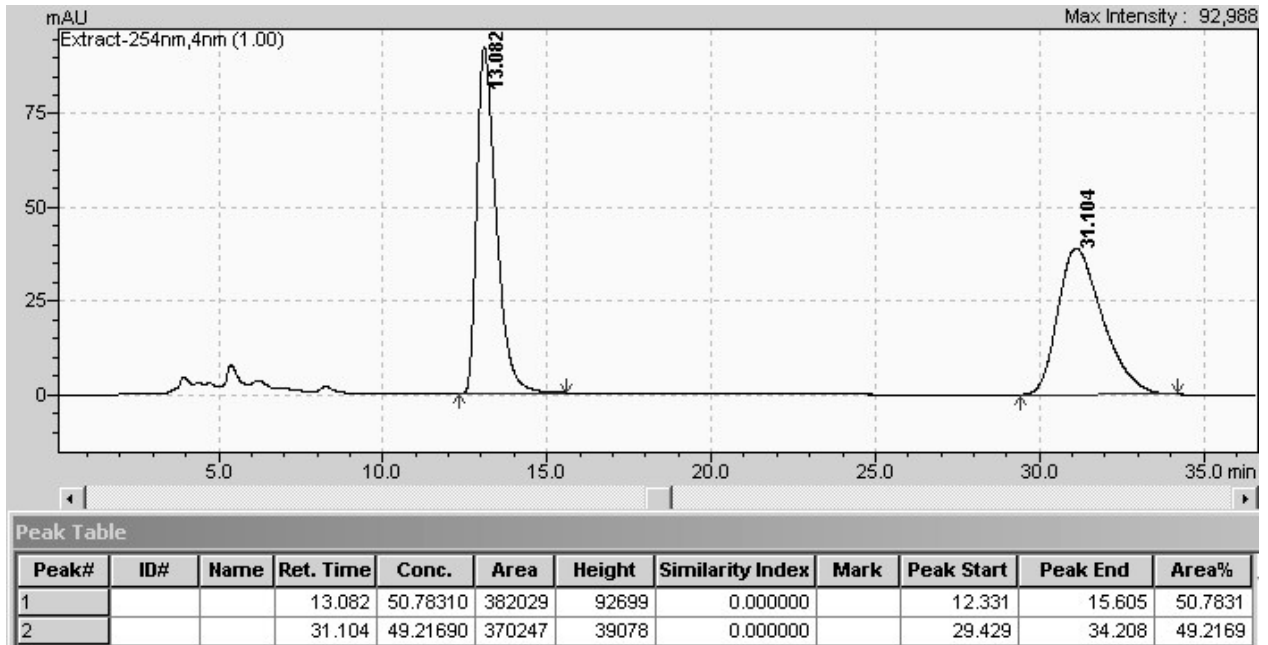
Conditions: IC column

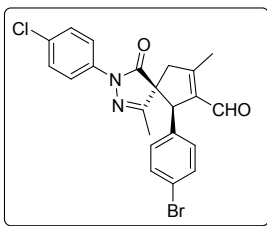
mobile phase: *n*-heptane / propan-2-ol= 70:30

$\lambda = 254 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 13.0 \text{ min}$ (major), $t_R = 31.0 \text{ min}$ (minor), ee= 87 %

major diastereoisomer





(7u')

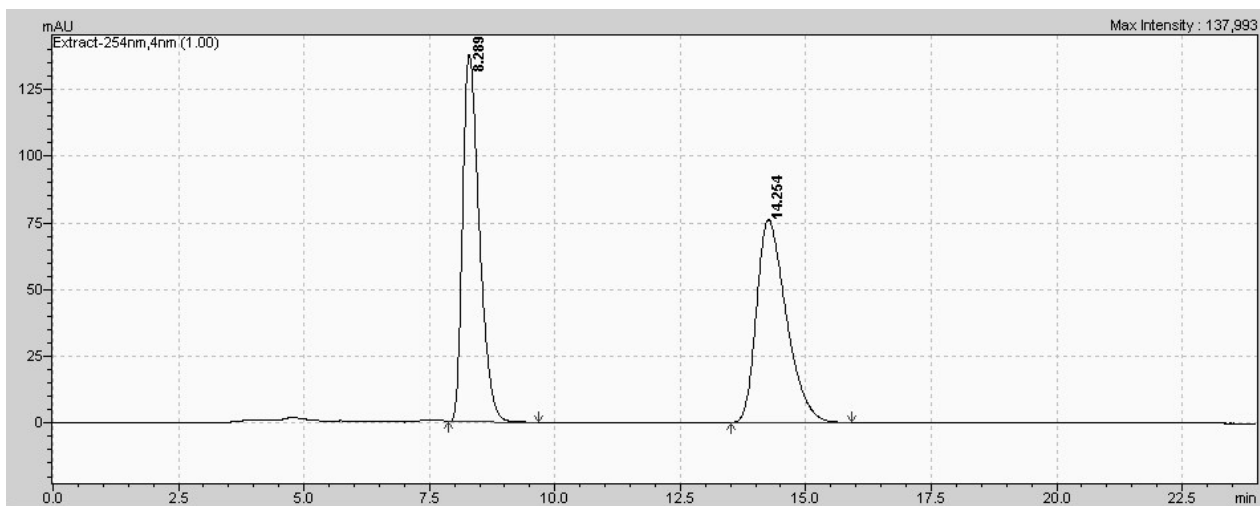
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 70:30

$\lambda = 254 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

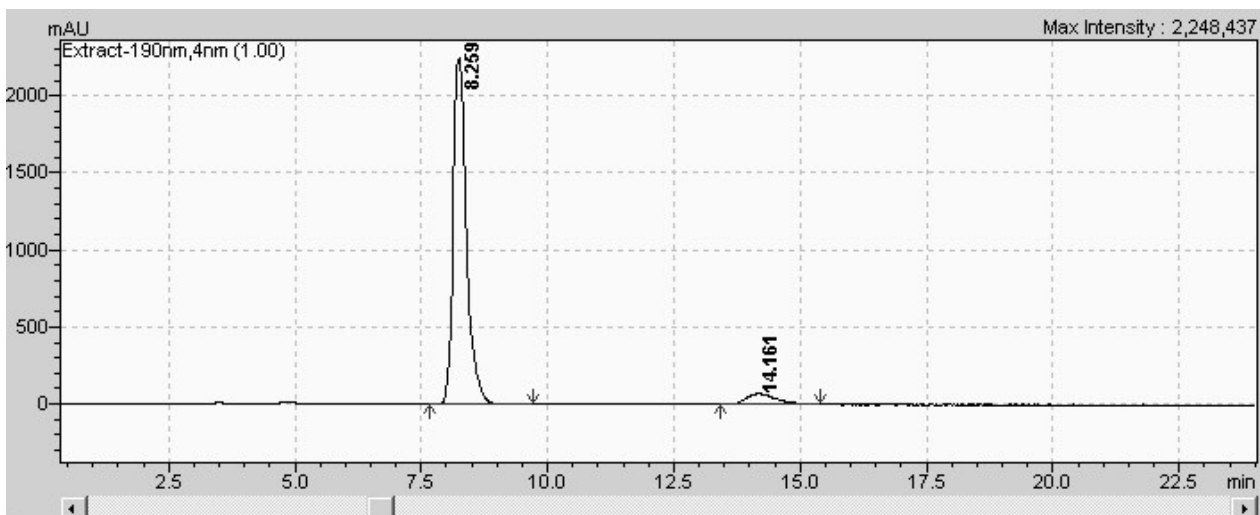
$t_R = 8.3 \text{ min}$ (major), $t_R = 14.2 \text{ min}$ (minor), $ee = 87 \%$

minor diastereoisomer



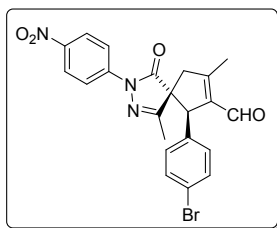
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			8.289	50.29470	3171350	137443	0.000000		7.883	9.664	50.2947
2			14.254	49.70530	3134184	75936	0.000000		13.515	15.904	49.7053



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			8.259	93.49742	414401	2247991	0.000000		7.669	9.717	93.4974
2			14.161	6.50258	288209	69140	0.000000		13.419	15.381	6.5026



(7v)

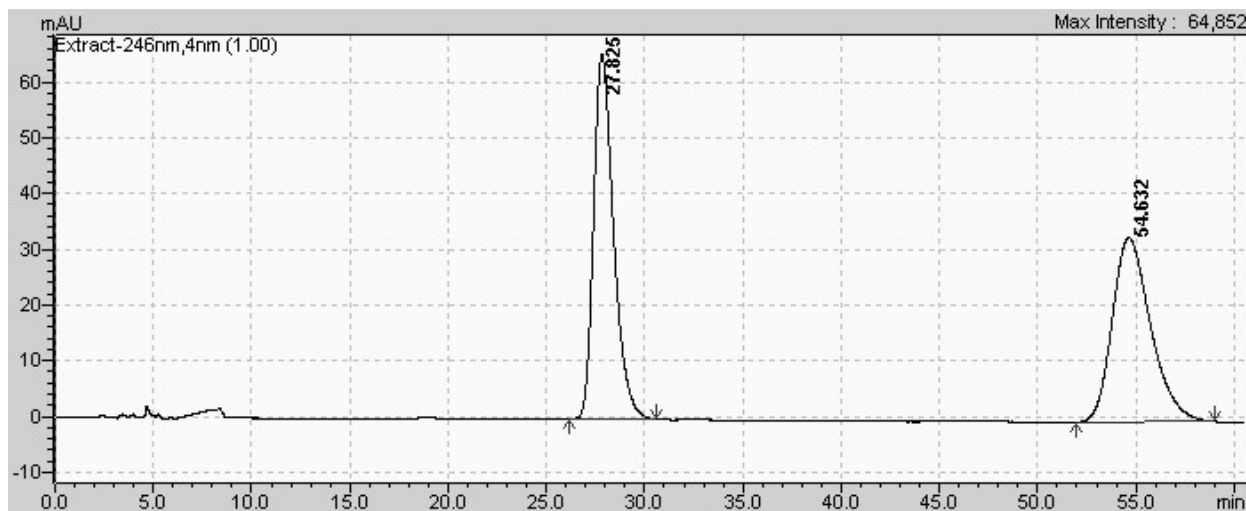
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 60:40

$\lambda = 202 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

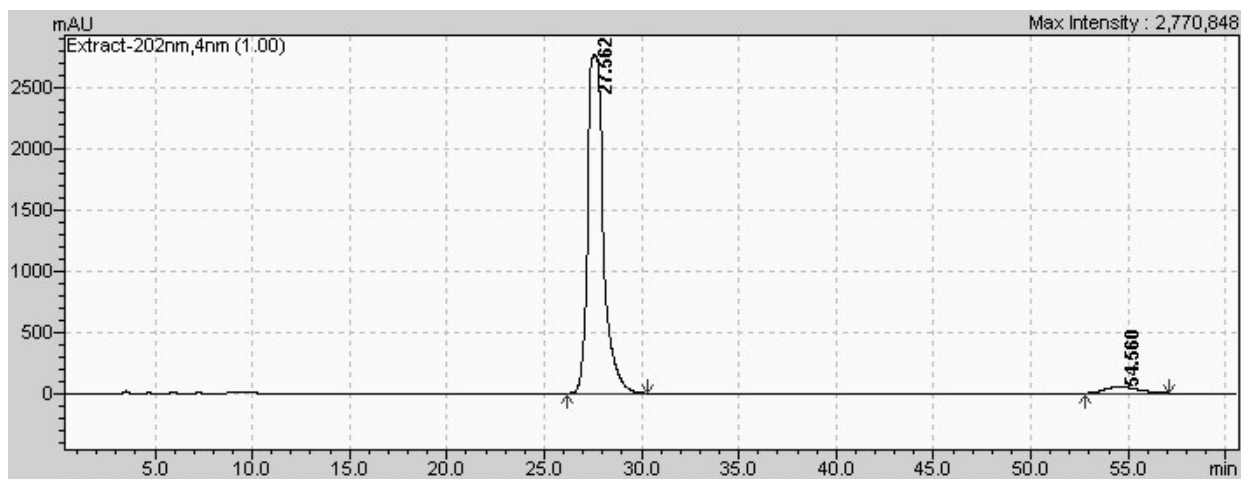
$t_R = 27.6 \text{ min}$ (major), $t_R = 54.6 \text{ min}$ (minor), ee= 92 %

major diastereoisomer



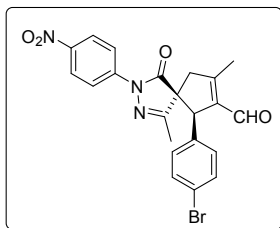
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			27.825	50.76483	461952	65310	0.000000		26.187	30.592	50.7648
2			54.632	49.23517	448032	33037	0.000000		51.936	59.040	49.2352



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			27.562	96.12616	155833	2766661	0.000000		26.176	30.336	96.1262
2			54.560	3.87384	628002	51769	0.000000		52.811	57.088	3.8738



(7v')

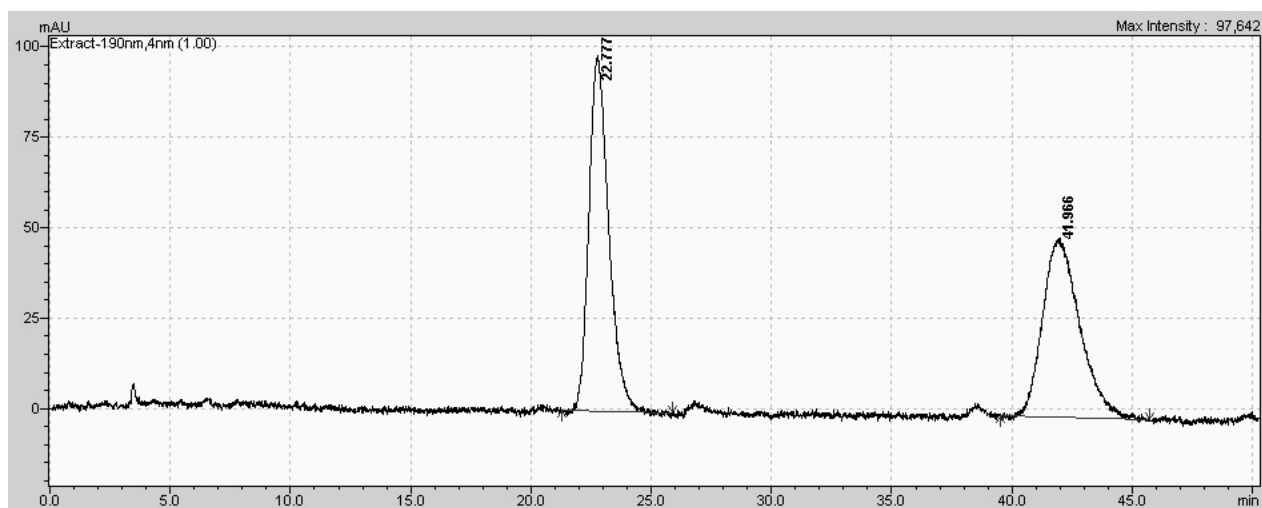
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 60:40

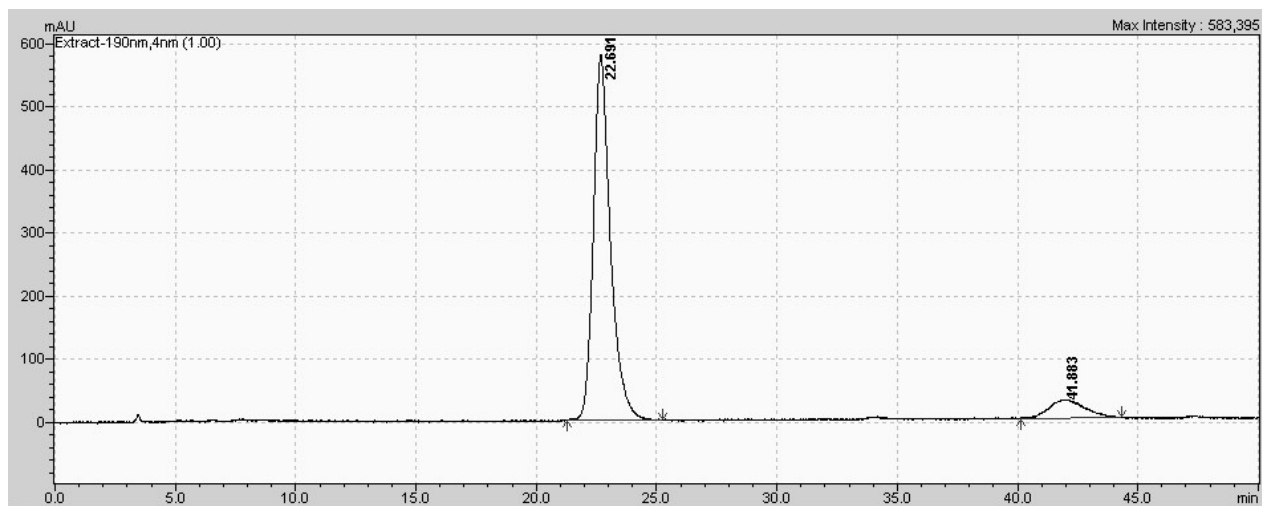
$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_{\text{R}} = 22.7 \text{ min}$ (major), $t_{\text{R}} = 41.9 \text{ min}$ (minor), ee= 81 %

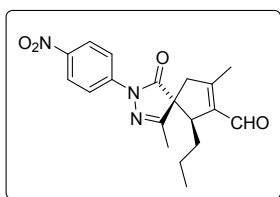
minor diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			22.777	51.37451	5591654	98271	0.000000		21.269	25.867	51.3745
2			41.966	48.62549	5292447	49354	0.000000		39.509	45.728	48.6255



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			22.691	90.37263	28367888	578874	0.000000		21.259	25.259	90.3726
2			41.883	9.62737	3022022	29242	0.000000		40.128	44.341	9.6274



(7w)

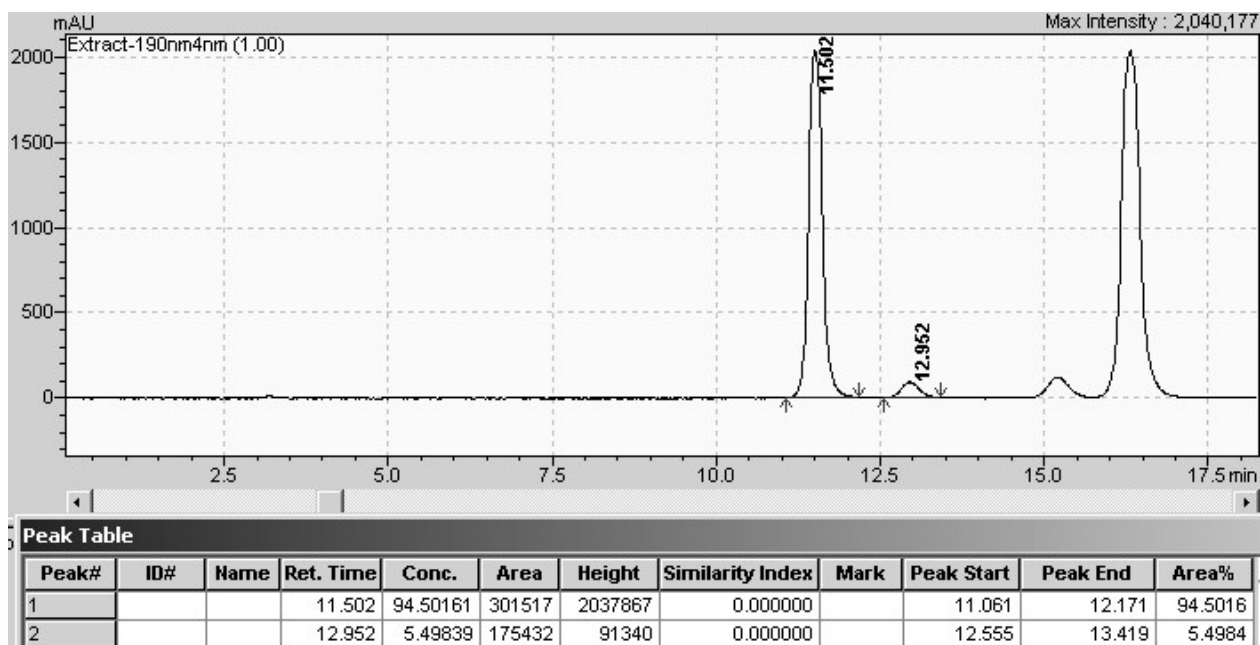
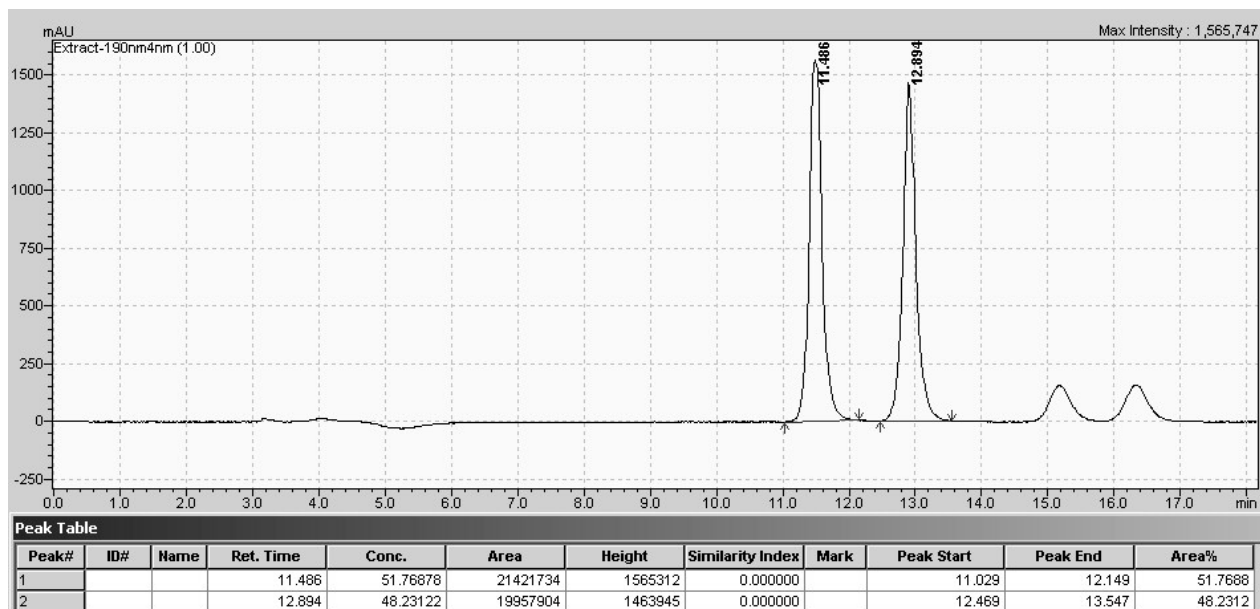
Conditions: IA column

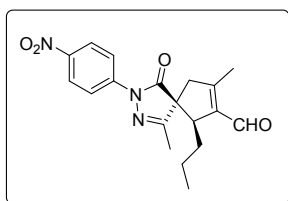
mobile phase: *n*-heptane / propan-2-ol= 90:10

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 11.5 \text{ min}$ (major), $t_R = 13.0 \text{ min}$ (minor), ee= 89 %

major diastereoisomer





(7w')

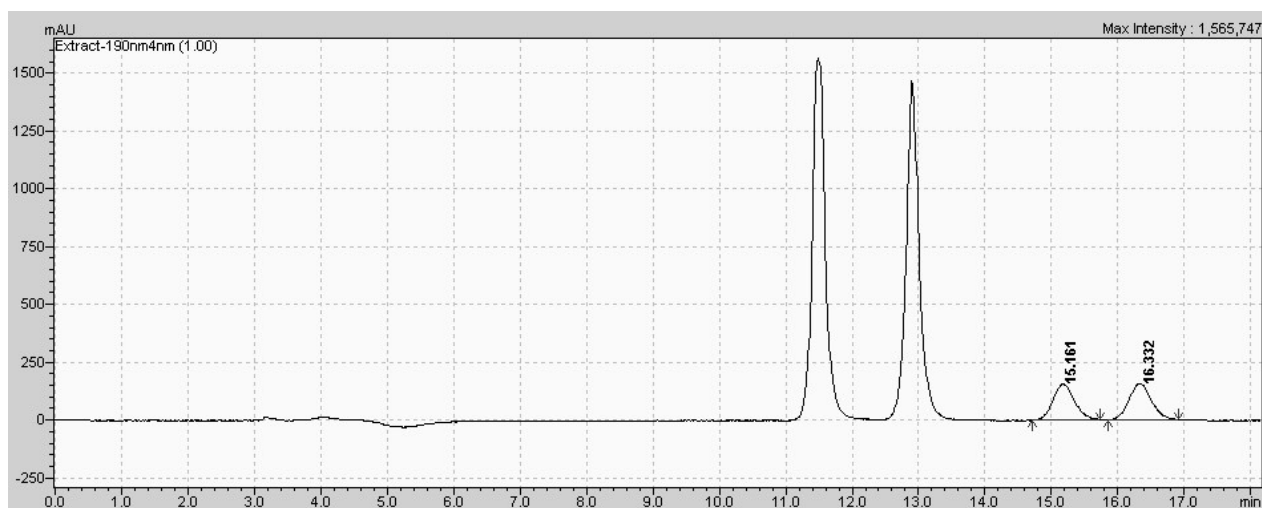
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 90:10

$\lambda = 190 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

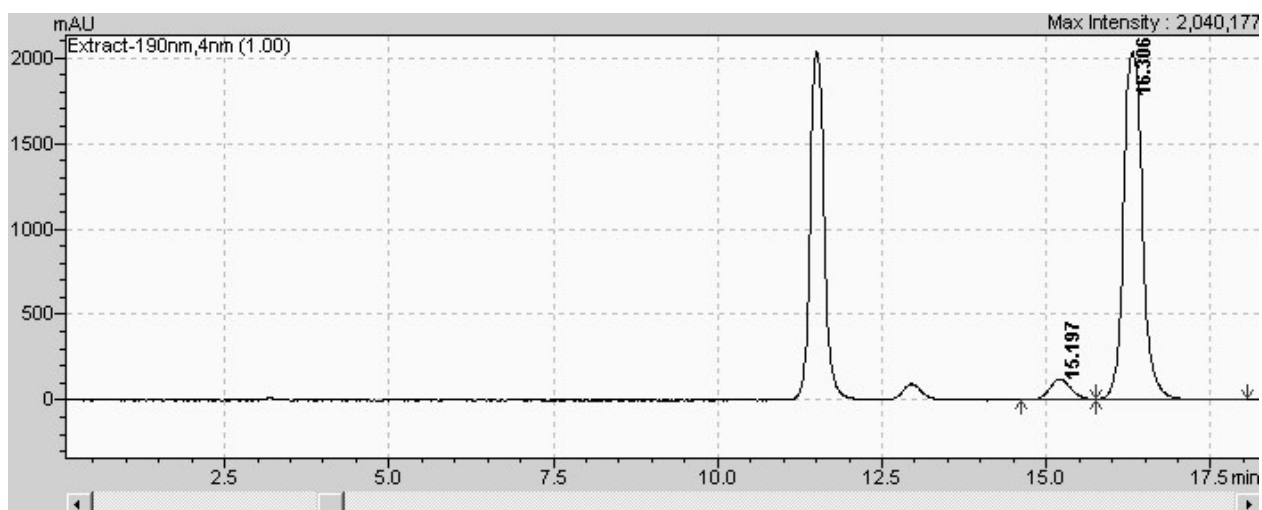
$t_R = 15.2 \text{ min}$ (minor), $t_R = 16.3 \text{ min}$ (major), $ee = 88 \%$

minor diastereoisomer



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			15.161	49.05315	3481585	155478	0.000000		14.709	15.733	49.0531
2			16.332	50.94685	3615993	156404	0.000000		15.851	16.917	50.9469



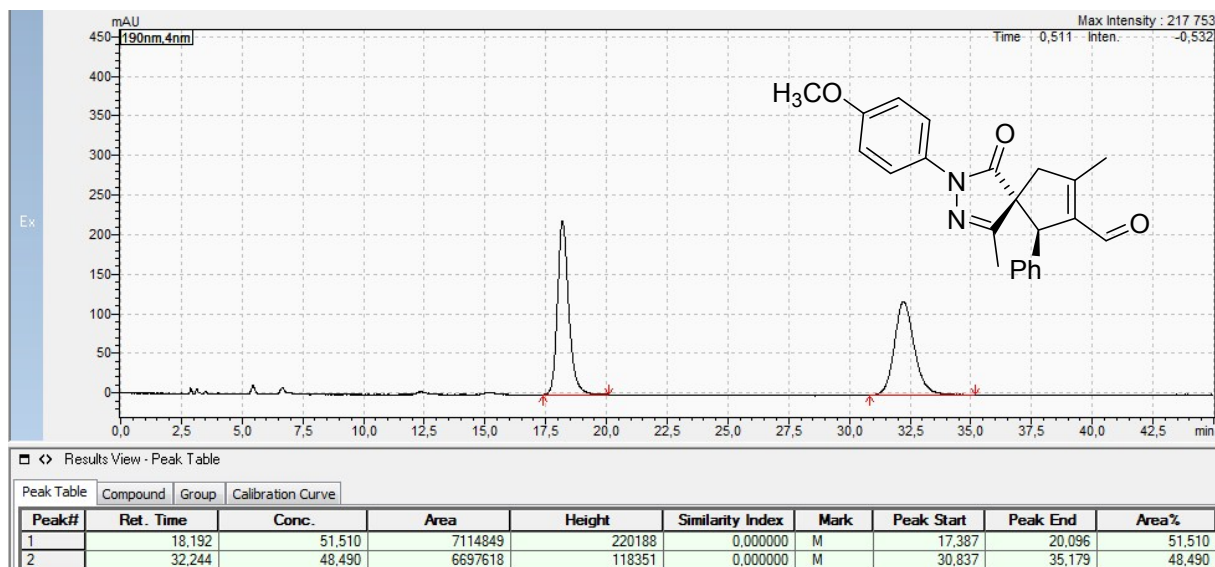
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			15.197	6.14733	264679	120486	0.000000		14.613	15.755	6.1473
2			16.306	93.85267	404091	2030672	0.000000		15.755	18.069	93.8527

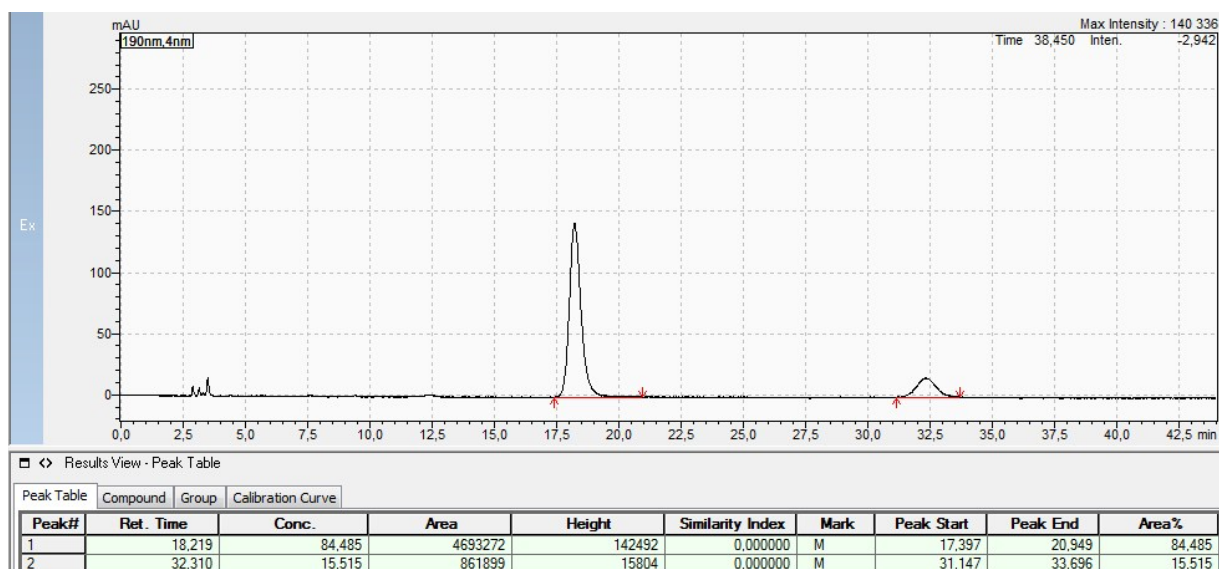
(5*R*,6*R*)-2-(4-methoxyphenyl)-4,8-dimethyl-6-phenyl-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7x)

Column IA (heptane:*i*-PrOH 80:20, 1.0 mL flow, 25 °C)

Racemate



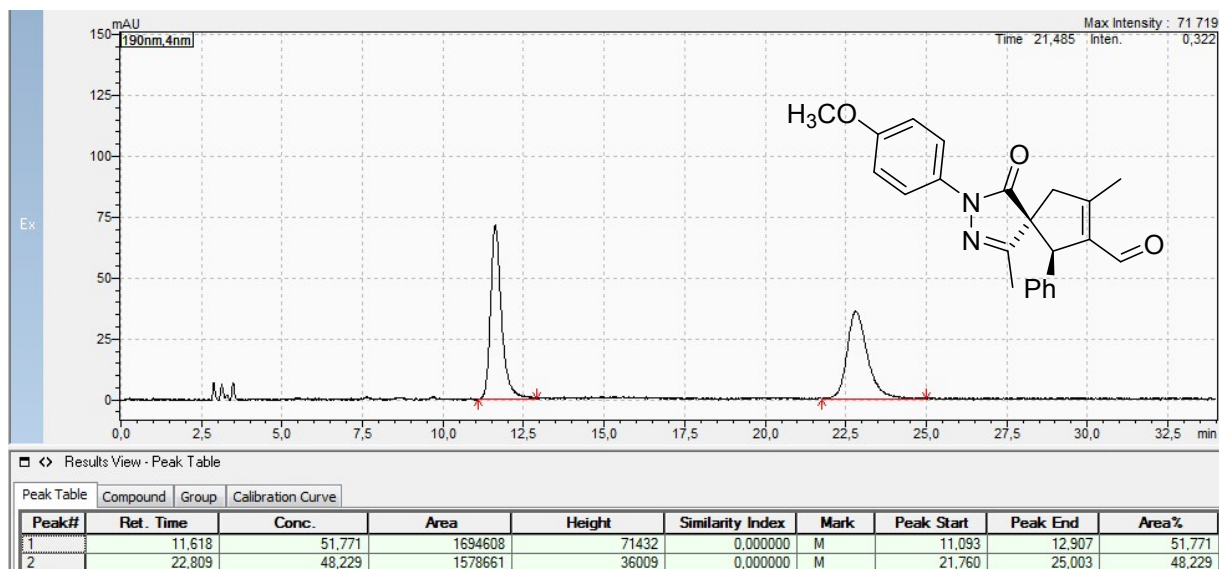
Chiral



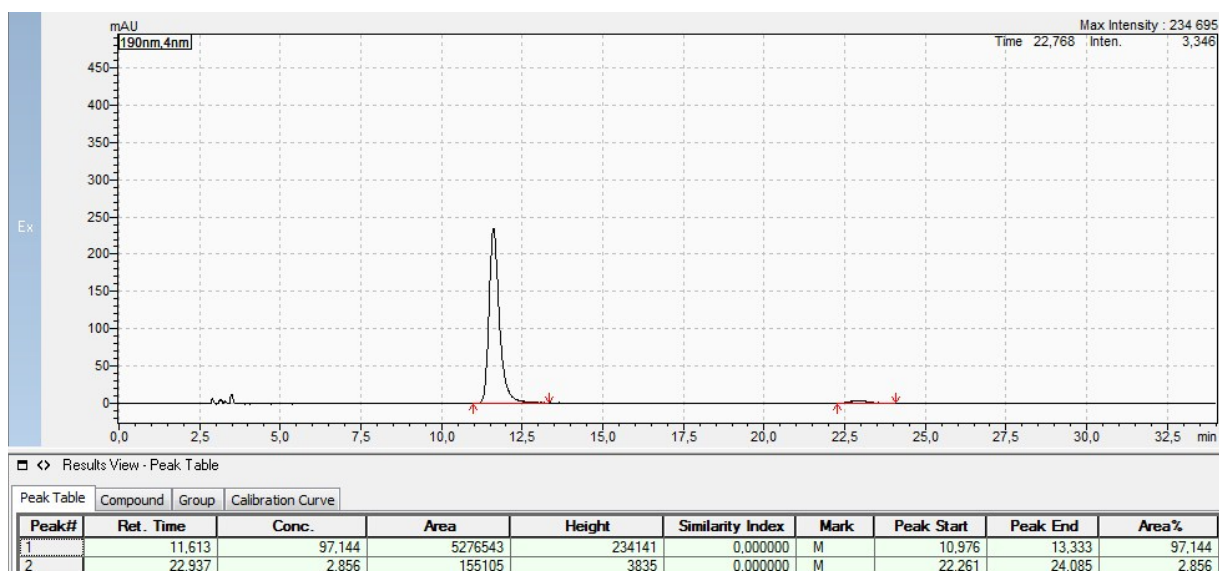
(5*S*,6*R*)-2-(4-methoxyphenyl)-4,8-dimethyl-6-phenyl-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7x')

Column IA (heptane:*i*-PrOH 80:20, 1.0 mL flow, 25 °C)

Racemate



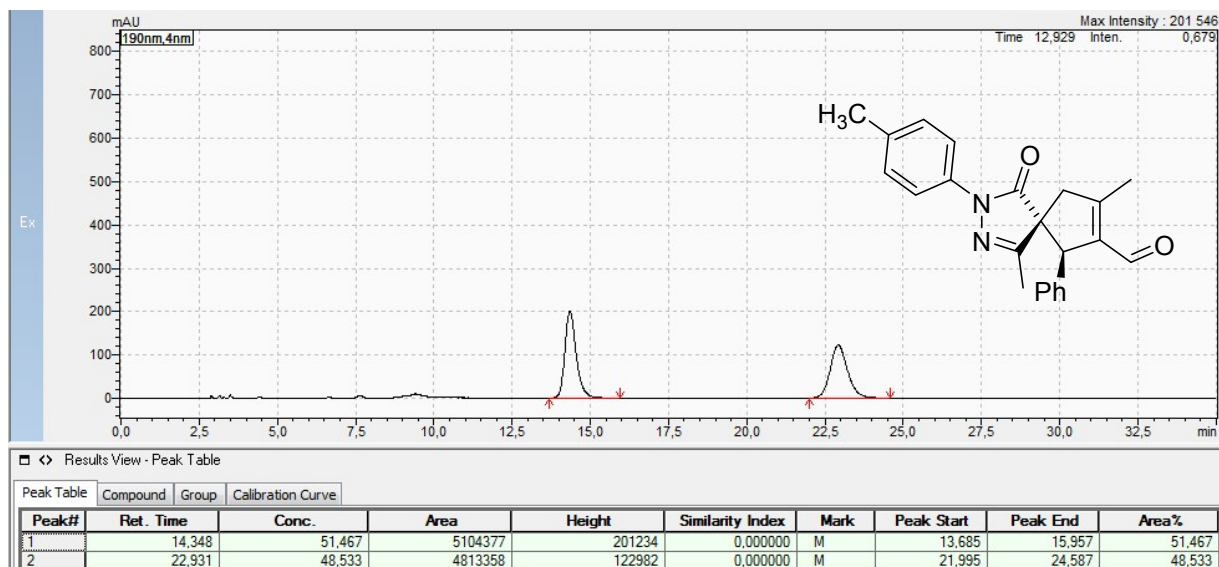
Chiral



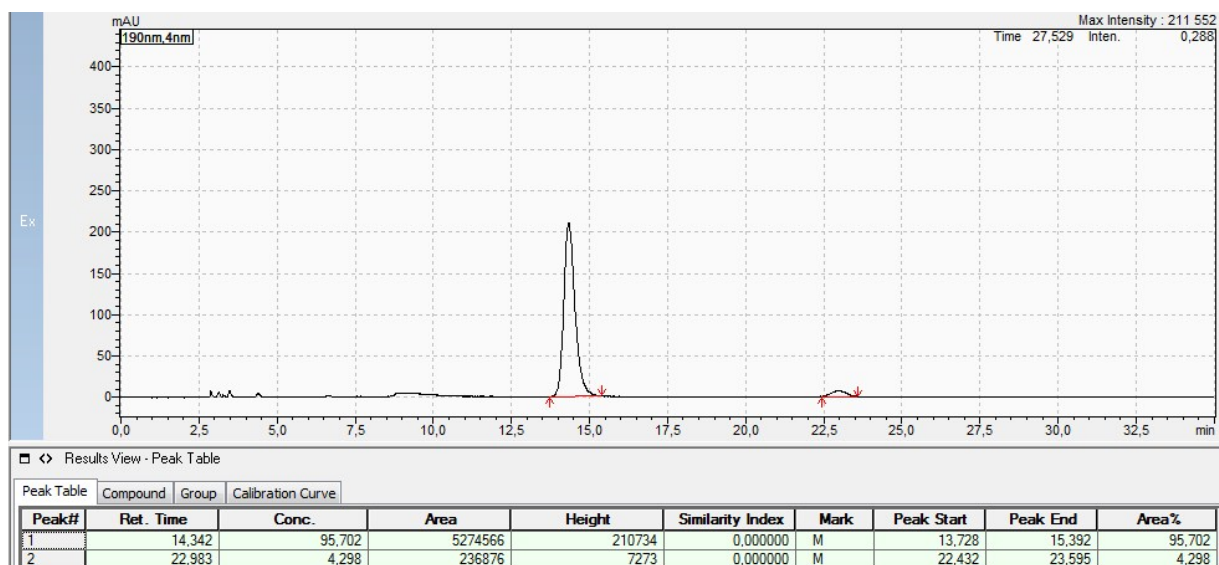
(5*R*,6*R*)-4,8-dimethyl-6-phenyl-2-(*p*-tolyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7y)

Column IA (heptane:*i*-PrOH 80:20, 1.0 mL flow, 25 °C)

Racemate



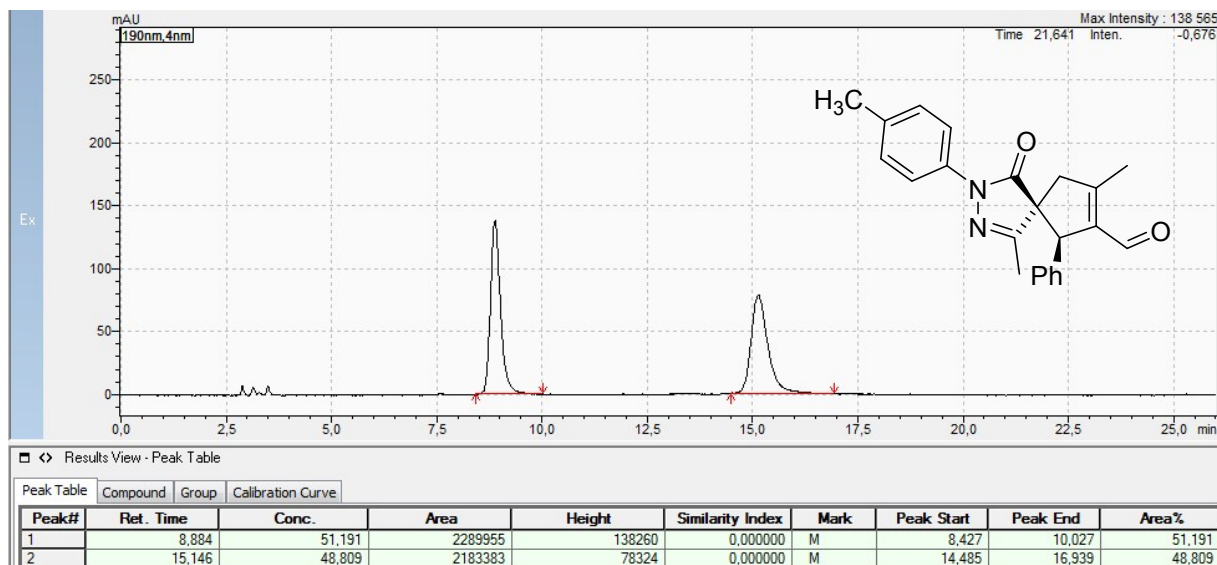
Chiral



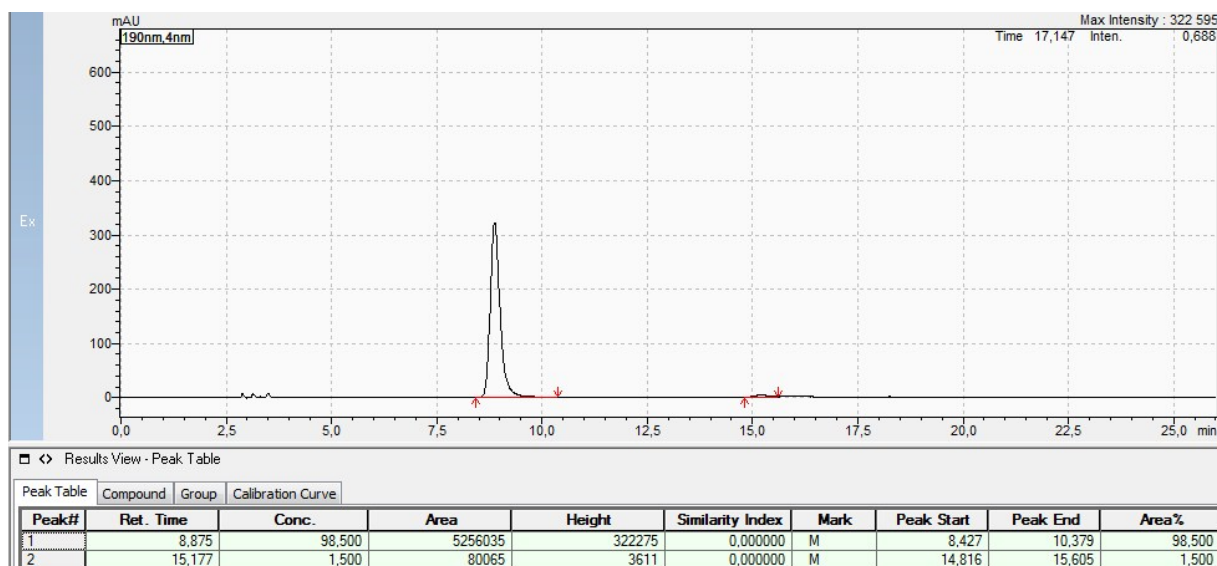
(5*S*,6*R*)-4,8-dimethyl-6-phenyl-2-(*p*-tolyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7y)

Column IA (heptane:*i*-PrOH 80:20, 1.0 mL flow, 25 °C)

Racemate



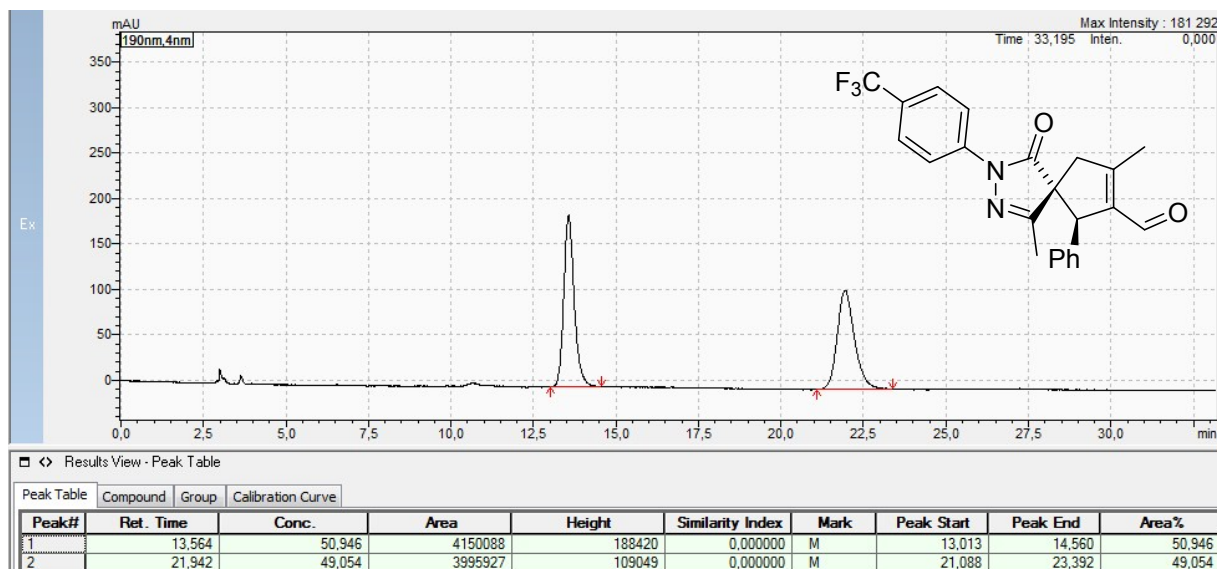
Chiral



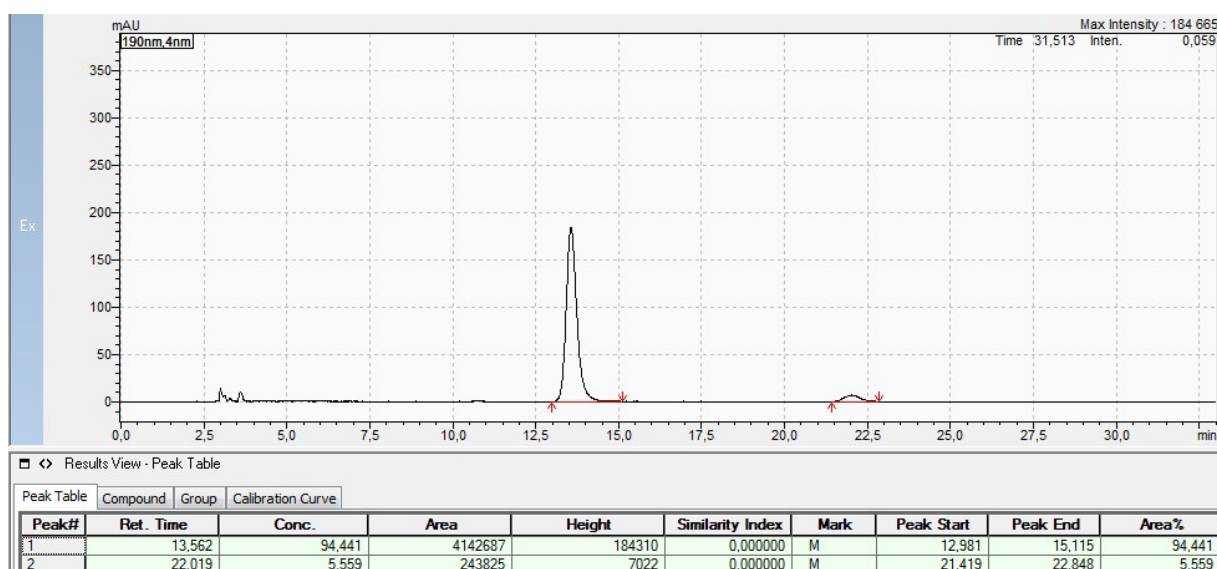
(5*R*,6*R*)-4,8-dimethyl-6-phenyl-2-(4-(trifluoromethyl)phenyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7*z*)

Column IA (heptane:*i*-PrOH 80:20, 1.0 mL flow, 25 °C)

Racemate



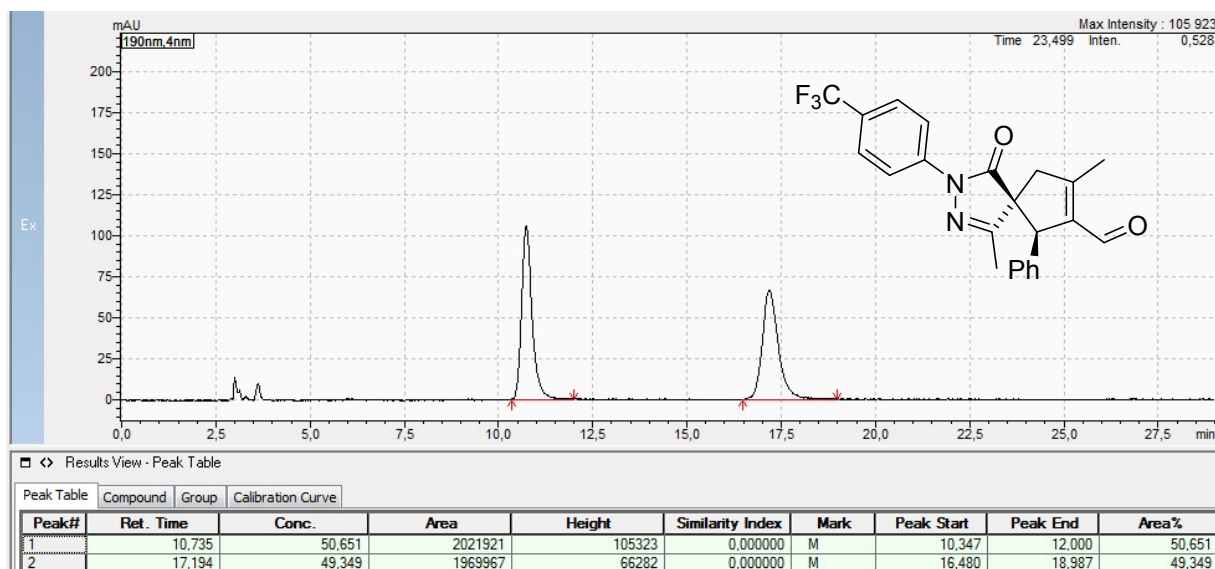
Chiral



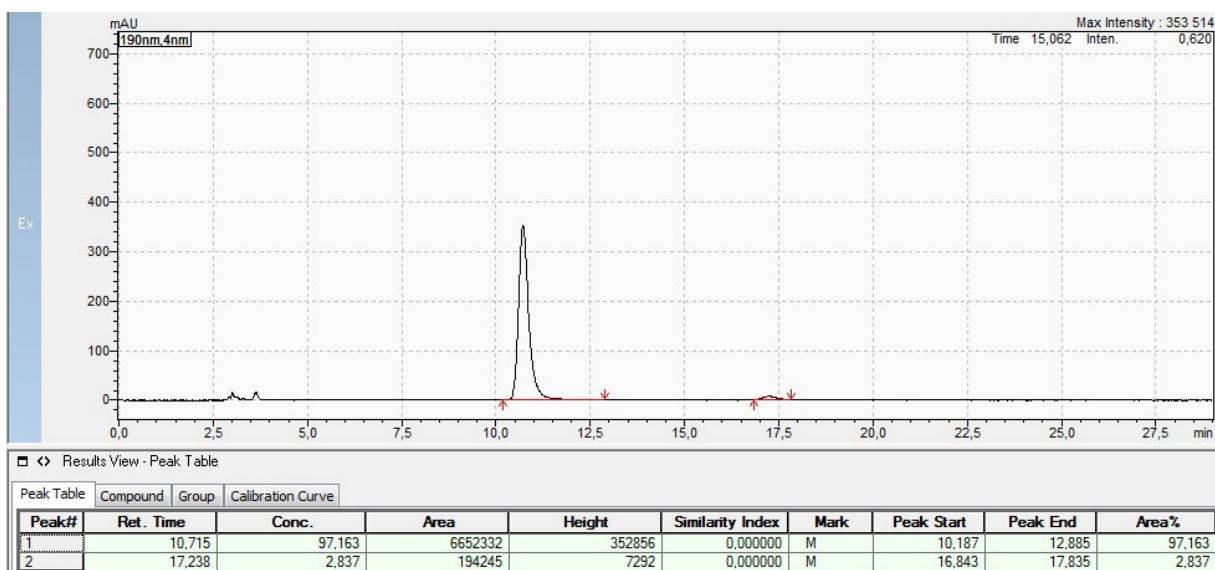
(5*S*,6*R*)-4,8-dimethyl-6-phenyl-2-(4-(trifluoromethyl)phenyl)-7-vinyl-2,3-diazaspiro[4.4]nona-3,7-dien-1-one (7*z'*)

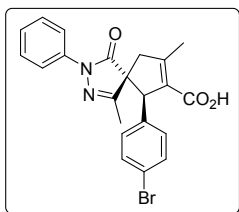
Column IA (heptane:*i*-PrOH 80:20, 1.0 mL flow, 25 °C)

Racemate



Chiral





(8b)

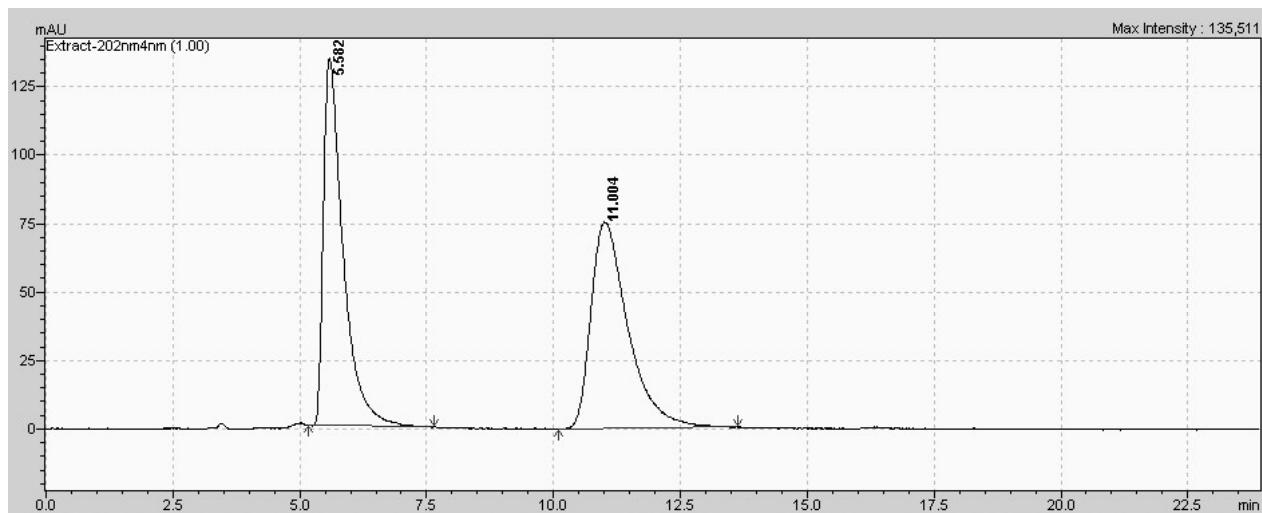
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 70:30

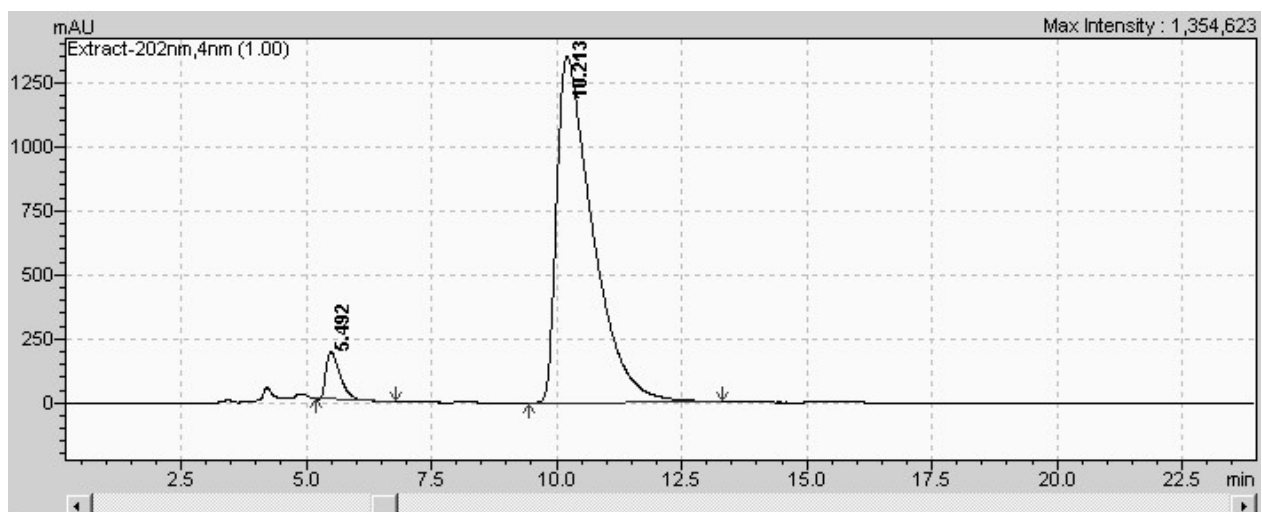
$\lambda = 202 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 5.5 \text{ min}$ (minor), $t_R = 10.2 \text{ min}$ (major), $ee = 90 \%$

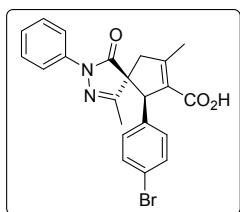
major diastereoisomer



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			5.582	48.80192	3638238	134189	0.000000		5.163	7.648	48.8019
2			11.004	51.19808	3816874	75366	0.000000		10.101	13.632	51.1981



Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			5.492	5.10092	363802	184616	0.000000		5.184	6.784	5.1009
2			10.213	94.89908	676829	1353371	0.000000		9.440	13.323	94.8991



(8b')

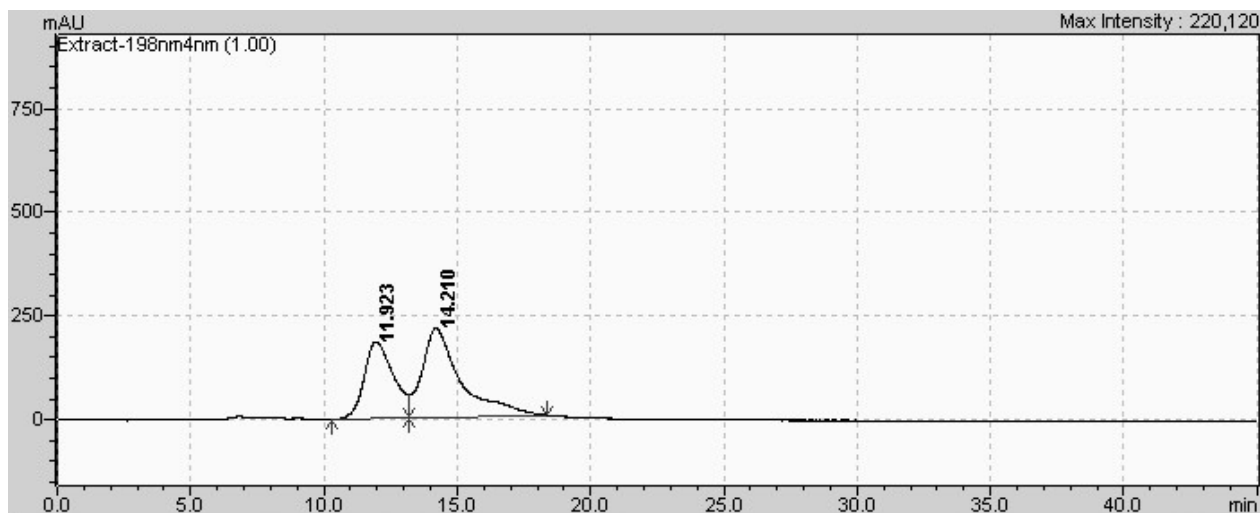
Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 40:60

$\lambda = 198 \text{ nm}$, $V = 0.5 \text{ ml/min}$, $t = 39 \text{ }^\circ\text{C}$

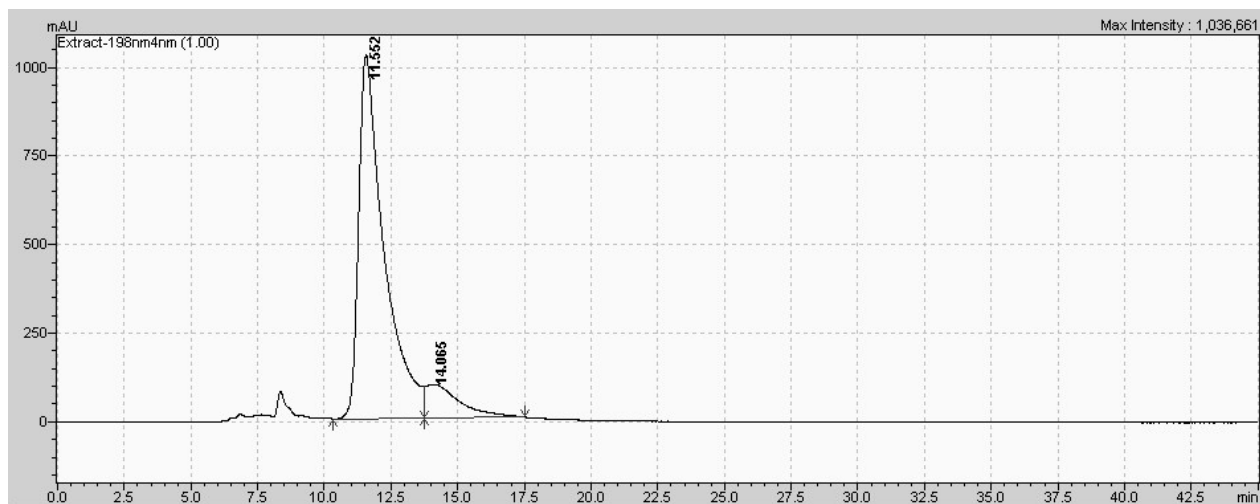
$t_R = 11.6 \text{ min}$ (major), $t_R = 14.1 \text{ min}$ (minor), ee= 78 %

minor diastereoisomer



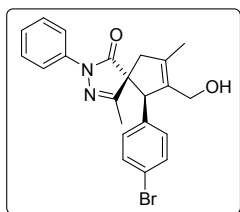
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			11.923	39.49645	142172	185773	0.000000		10.293	13.184	39.4964
2			14.210	60.50355	217790	214496	0.000000	V	13.184	18.368	60.5036



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			11.552	88.86812	68065645	1027606	0.000000		10.325	13.749	88.8681
2			14.065	11.13188	8526097	94531	0.000000	V	13.749	17.515	11.1319



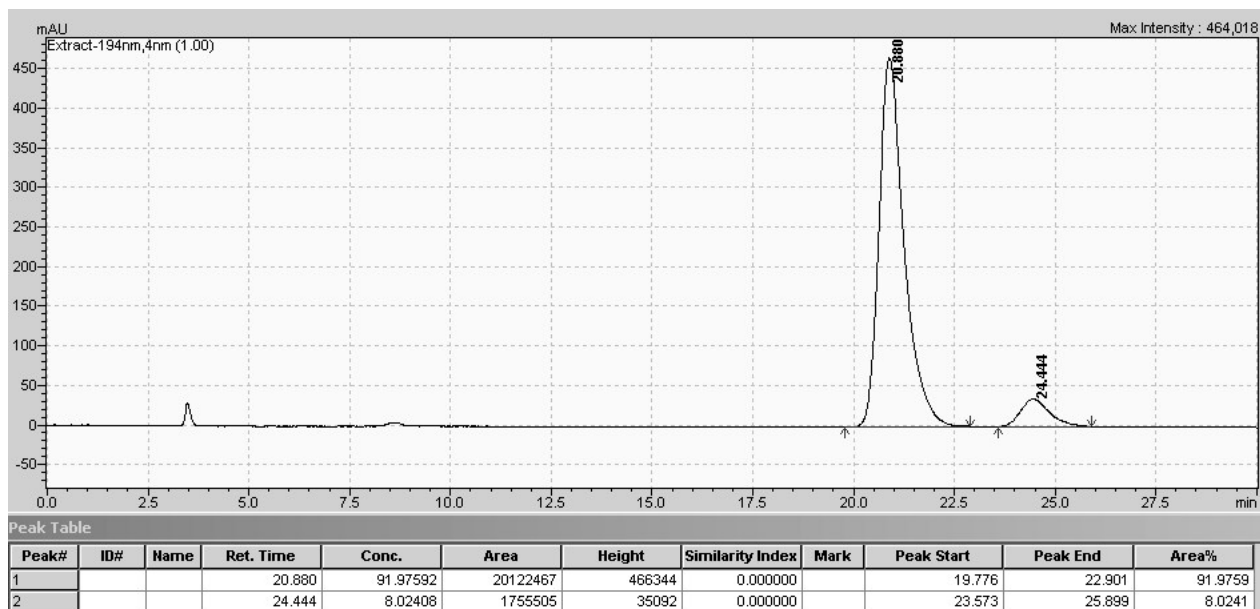
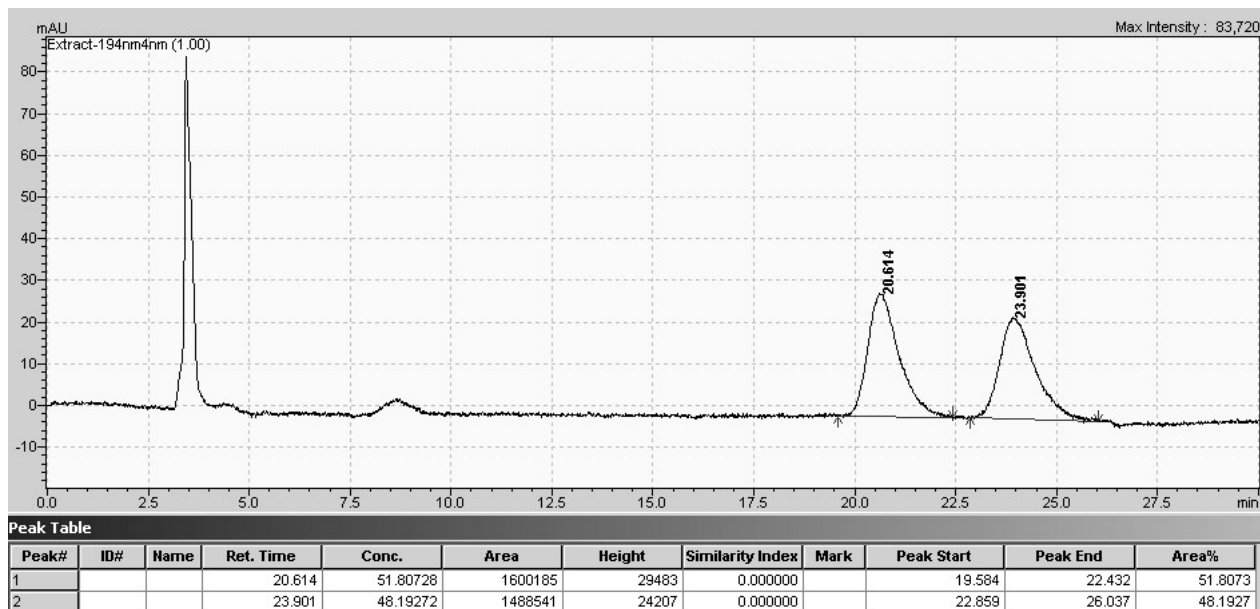
(9b)

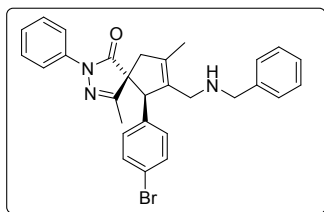
Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 95:5

$\lambda = 194 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 20.9 \text{ min}$ (major), $t_R = 24.4 \text{ min}$ (minor), $ee = 84 \%$





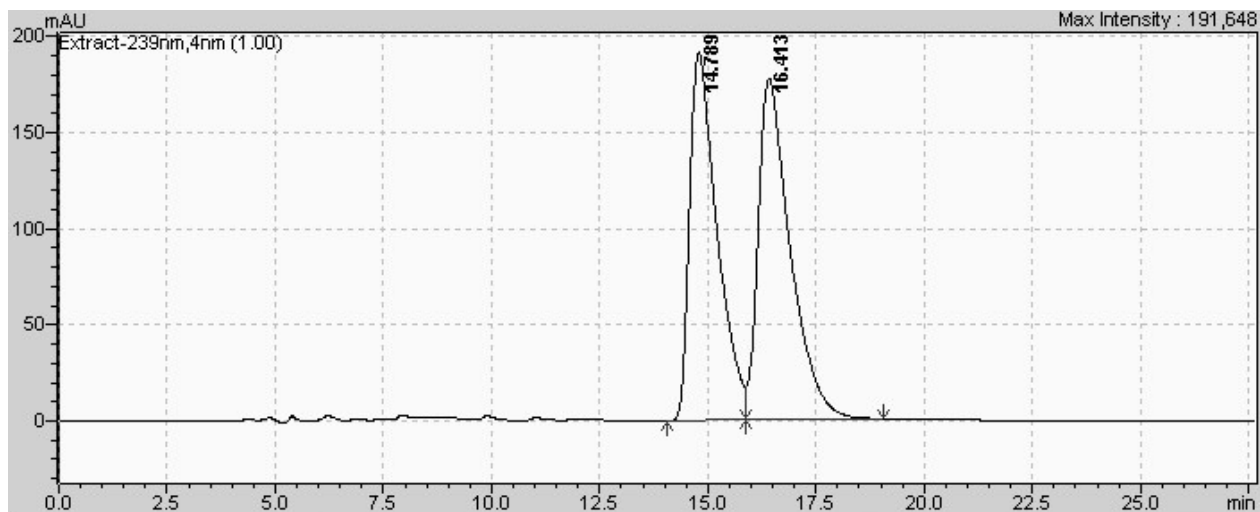
(10b)

Conditions: IC column

mobile phase: *n*-heptane / propan-2-ol= 98:2

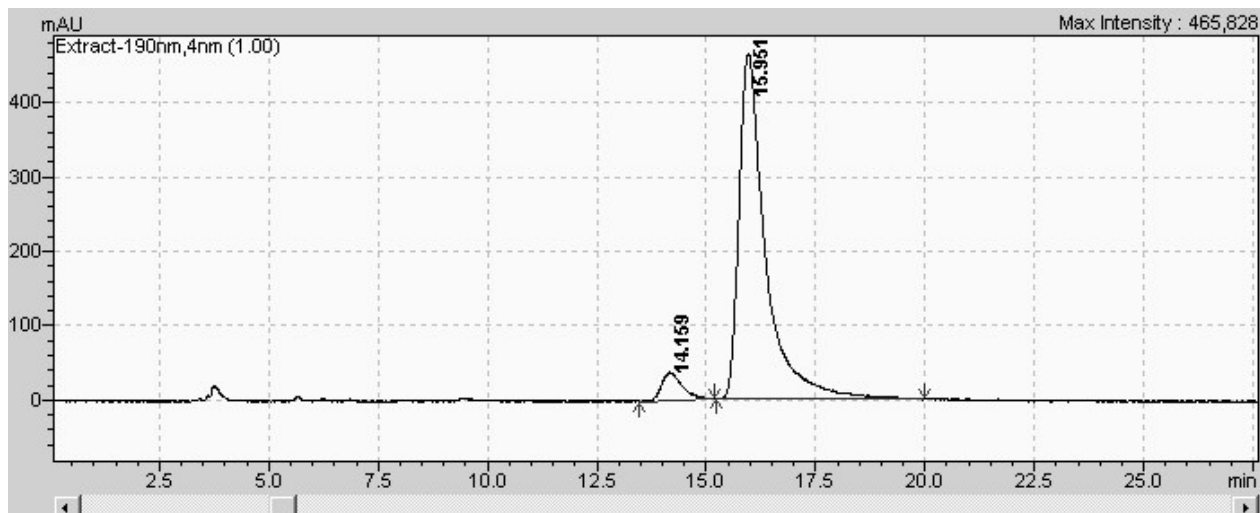
λ = 190 nm, V = 1 ml/min, t = 25 °C

t_R = 14.2 min (minor), t_R = 16.0 min (major), ee= 88 %



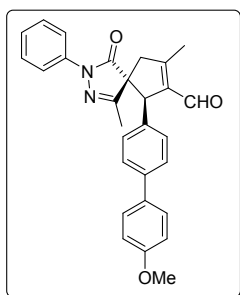
Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			14.789	48.03264	847268	191427	0.000000		14.069	15.872	48.0326
2			16.413	51.96736	916674	177749	0.000000	V	15.872	19.051	51.9674



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			14.159	5.83498	120528	37678	0.000000		13.451	15.179	5.8350
2			15.951	94.16502	194509	463723	0.000000		15.221	20.000	94.1650



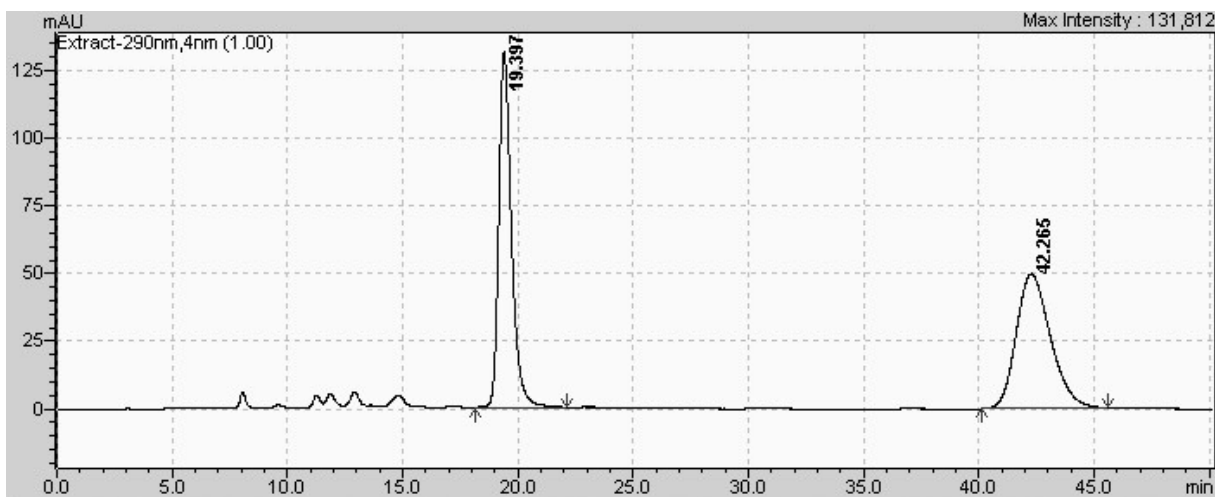
(11b)

Conditions: IA column

mobile phase: *n*-heptane / propan-2-ol= 80:20

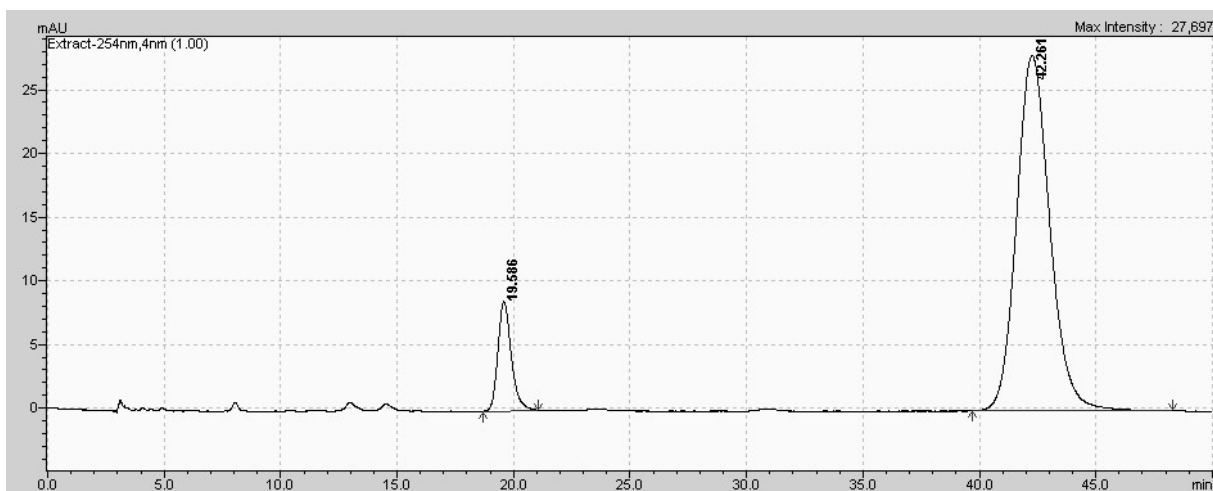
$\lambda = 254 \text{ nm}$, $V = 1 \text{ ml/min}$, $t = 25 \text{ }^\circ\text{C}$

$t_R = 19.6 \text{ min}$ (minor), $t_R = 42.3 \text{ min}$ (major), $ee = 78 \%$



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			19.397	49.39571	499593	131230	0.000000		18.144	22.112	49.3957
2			42.265	50.60429	511817	49702	0.000000		40.139	45.611	50.6043



Peak Table

Peak#	ID#	Name	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1			19.586	10.99424	342915	8596	0.000000		18.688	21.077	10.9942
2			42.261	89.00576	2776125	27915	0.000000		39.712	48.309	89.0058

H	-1.65482700	-3.06865600	1.29590100
H	-2.60771700	-1.63939900	1.73530300
C	-1.97821600	-2.95499500	-2.01697900
H	-1.76471100	-2.53171600	-3.00368300
H	-1.18964000	-3.68034900	-1.79191600
H	-2.92286400	-3.50449200	-2.09145400
C	-3.44119100	-0.41893300	-1.11841200
H	-4.38669200	-0.96606900	-1.21703300
H	-3.58098600	0.33509900	-0.33830800
H	-3.26695400	0.10521100	-2.06278600
C	-0.79574600	1.19137900	0.31640800
C	-1.36780300	1.46918000	1.55574600
C	-2.28087300	2.51226500	1.70304900
C	-2.63380400	3.29428100	0.61275100
C	-2.06391600	3.03021100	-0.63042700
C	-1.15834900	1.99076300	-0.77243200
H	-1.11577900	0.88127800	2.43018700
H	-3.34563700	4.10526300	0.72780900
H	-0.72899000	1.78472500	-1.74737400
C	1.39666500	0.42887100	-0.68847800
C	1.99720600	1.66746800	-0.46107600
C	3.19702500	2.00415500	-1.07927500
C	3.81237400	1.10743400	-1.94450100
C	3.21502000	-0.12522100	-2.18711400
C	2.01967700	-0.46122000	-1.56297700
H	1.52627000	2.38686000	0.20009800
H	4.74622800	1.36935900	-2.43186000
H	1.55906000	-1.42229000	-1.74443100
H	-2.71426900	2.70930500	2.67841700
H	-2.33119500	3.63387800	-1.49182100
H	3.64598000	2.97373900	-0.88799900
H	3.68326800	-0.83177000	-2.86553500
H	0.69369000	-2.78354200	1.01862000

I-d
0 1

C	0.47512800	-0.72467700	1.42309500
N	1.06646000	-2.04892300	1.18038800
C	2.41257000	-2.11144800	1.76547400
C	2.82303400	-0.66757100	2.05685200
C	1.47757400	0.00318400	2.34277300
H	-0.47000300	-0.86184300	1.95168500
H	2.38304100	-2.68795300	2.69865700
H	3.10113600	-2.62297900	1.08797500
H	3.51835500	-0.58740400	2.89597000
H	3.29898600	-0.22099700	1.18058700
H	1.19003000	-0.16964500	3.38473000
H	1.49486500	1.08295900	2.19017700
C	0.11548800	0.00590400	0.08776600
O	-0.54862200	-0.93808400	-0.74566200
Si	-2.06705700	-1.65472500	-0.66018700
C	-2.45313100	-2.32150800	1.04534100
H	-3.32192700	-2.98784000	0.99067100
H	-1.61582000	-2.89809800	1.44949600
H	-2.69925200	-1.52804700	1.75775500
C	-1.92508400	-3.05966600	-1.88124000
H	-1.64743400	-2.69976900	-2.87711000
H	-1.16629400	-3.78366000	-1.56673600
H	-2.87394200	-3.59828200	-1.97766000
C	-3.42904100	-0.48091700	-1.17596900
H	-4.37123500	-1.03561300	-1.26254200
H	-3.58732600	0.31986600	-0.44781300
H	-3.23214500	-0.01698200	-2.14709900
C	-0.80703800	1.21280900	0.29649800
C	-1.34928700	1.57496700	1.52673200
C	-2.23816800	2.64453700	1.62604000
C	-2.59384600	3.36834600	0.49739800
C	-2.05146200	3.01979200	-0.73740200
C	-1.16953100	1.95537200	-0.83188100
H	-1.09291200	1.03521000	2.43024400

H	-3.28677100	4.19976900	0.57599900
H	-0.75878900	1.68510900	-1.79911400
C	1.38891200	0.42199500	-0.65142000
C	2.00672200	1.64733000	-0.39436300
C	3.21936200	1.97320900	-0.98850900
C	3.83382300	1.08093800	-1.86086600
C	3.21440700	-0.13017800	-2.14434700
C	2.00022600	-0.45376200	-1.54774600
H	1.53918800	2.35962900	0.27644900
H	4.78083600	1.33440500	-2.32623100
H	1.51260700	-1.38847400	-1.79578100
H	-2.64940100	2.90848200	2.59506800
H	-2.32019200	3.57811200	-1.62834400
H	3.68312100	2.93022600	-0.77193000
H	3.67348700	-0.82746100	-2.83801800
H	1.07641100	-2.25738400	0.19276200

I-e
0 1

C	-0.58640300	1.28157700	-1.15420100
N	-1.50790100	2.27470900	-0.60234300
C	-1.32395300	3.46878700	-1.42305700
C	0.19704000	3.57077200	-1.52749500
C	0.66197200	2.10063400	-1.55882200
H	-1.00076000	0.83626100	-2.07248700
H	-1.76364300	3.35475400	-2.42816100
H	-1.78430000	4.33993500	-0.95014700
H	0.51578900	4.13512800	-2.40598200
H	0.59515100	4.08153400	-0.64629200
H	0.99401500	1.80219100	-2.55434400
H	1.49939200	1.93599300	-0.88201800
C	-0.33540000	0.05535400	-0.23707100
O	0.52129500	-0.78188000	-0.99377300
Si	2.10463500	-1.31348200	-1.00334900
C	3.33877000	-0.12980600	-0.24166000
H	4.32643900	-0.60681700	-0.24946900
H	3.42969100	0.80378400	-0.80367700
H	3.10752700	0.11818800	0.79772300
C	2.48422400	-1.53601700	-2.81974300
H	1.79770500	-2.24935100	-3.28746900
H	2.39886300	-0.58973100	-3.36371000
H	3.50206300	-1.91293800	-2.96894600
C	2.23550300	-2.97231200	-0.14163300
H	3.13974300	-3.49675200	-0.47163100
H	2.29341200	-2.87867000	0.94630000
H	1.38096400	-3.61532800	-0.37730600
C	0.27277400	0.33093100	1.14212900
C	0.59636900	1.59581200	1.62509600
C	1.21355700	1.74579500	2.86499800
C	1.50807400	0.63594000	3.64506700
C	1.15717600	-0.63116200	3.18732900
C	0.53933800	-0.77555900	1.95418400
H	0.34775800	2.47698200	1.05162500
H	1.99336800	0.75569900	4.60832700
H	0.25717200	-1.76672000	1.61419200
C	-1.67689300	-0.67173600	-0.06492100
C	-2.59261800	-0.25992400	0.90550300
C	-3.83095100	-0.88032200	1.02010900
C	-4.17168200	-1.92722200	0.16946900
C	-3.26456400	-2.34367900	-0.79752900
C	-2.02750600	-1.71742600	-0.91574800
H	-2.33548300	0.54977000	1.58024700
H	-5.13560700	-2.41693500	0.26371500
H	-1.32059600	-2.04483000	-1.66840500
H	1.46241100	2.74129000	3.21882500
H	1.36055300	-1.50777800	3.79410600
H	-4.52869700	-0.54823100	1.78237100
H	-3.51787800	-3.16233800	-1.466398500
H	-2.46395200	1.94310600	-0.64197400

I-f			
0 1			
C	-0.50472700	1.52427800	-1.10113900
N	-1.06241500	2.65505700	-0.35064900
C	-0.73093900	3.82491600	-1.16646100
C	0.68467600	3.57405500	-1.71154700
C	0.73303100	2.04651700	-1.89468400
H	-1.25700100	1.24562600	-1.84680300
H	-1.44841400	3.88964100	-1.99273900
H	-0.82079100	4.73923200	-0.57604600
H	0.88344300	4.11941700	-2.63732100
H	1.42521800	3.90348800	-0.97500200
H	0.63404900	1.76800900	-2.94563800
H	1.67203100	1.61285100	-1.55010900
C	-0.30736100	0.23005400	-0.26430000
O	0.36917200	-0.64176900	-1.15107400
Si	1.53983500	-1.83200900	-1.04154300
C	3.11249300	-1.23699100	-0.22261600
H	3.90586600	-1.97763700	-0.37966800
H	3.46258200	-0.29278900	-0.65153100
H	3.00613900	-1.09646000	0.85622500
C	1.87809700	-2.23219100	-2.83390300
H	0.96989700	-2.56044500	-3.34977900
H	2.26429900	-1.35884900	-3.36938300
H	2.61897800	-3.03347400	-2.92886700
C	0.90352100	-3.35695600	-0.16304900
H	1.64646000	-4.16054200	-0.22965500
H	0.71090700	-3.18268900	0.89893200
H	-0.02171100	-3.72988700	-0.61314800
C	0.50031900	0.38958800	1.03561300
C	1.44999700	1.39532900	1.22466400
C	2.23589700	1.43676700	2.37159900
C	2.09462400	0.46703600	3.35518800
C	1.15041800	-0.53930400	3.18521300
C	0.36099100	-0.56959200	2.04327000
H	1.60660000	2.16051300	0.47746000
H	2.71106600	0.49614900	4.24764300
H	-0.37454400	-1.35827100	1.93511200
C	-1.70651500	-0.33143400	0.03532400
C	-2.51627600	0.24705600	1.01560800
C	-3.79546100	-0.23580500	1.25566400
C	-4.29183200	-1.30711000	0.51814600
C	-3.49671900	-1.88335800	-0.46326200
C	-2.21478500	-1.39528900	-0.70372300
H	-2.14447800	1.07852000	1.60281000
H	-5.29067400	-1.68650600	0.70846000
H	-1.60376000	-1.84425500	-1.47669800
H	2.96603800	2.23089200	2.48930400
H	1.02299600	-1.30308700	3.94544000
H	-4.40716800	0.22614700	2.02415600
H	-3.87114200	-2.71740800	-1.04858200
H	-0.57775600	2.74330200	0.53653300

Pyrazolone 5a

5a-a

0 1			
C	-2.05677900	-0.29681000	-0.90239000
C	-0.68013100	-0.92385000	-0.74782900
C	-1.76081700	1.13895800	-0.59790000
N	-0.52297000	1.34615300	-0.35935400
N	0.15965000	0.12827900	-0.45020900
C	1.54129200	0.10509000	-0.15836400
C	2.14537000	1.24276500	0.38232700
C	2.30819700	-1.03693000	-0.40377300
C	3.50277900	1.23309900	0.67182000
H	1.55126400	2.12657900	0.57116700
C	3.66498600	-1.02870100	-0.10350700
H	1.84743800	-1.92190000	-0.81741000
C	4.27215800	0.09975300	0.43338200
H	3.95885300	2.12384600	1.09149700

H	4.24989900	-1.92200600	-0.29723100
H	5.33219900	0.09681600	0.66348600
O	-0.39321700	-2.09432800	-0.85871000
C	-2.77269700	2.22454200	-0.56510600
H	-2.29531800	3.19033500	-0.39629800
H	-3.33161900	2.25934900	-1.50478600
H	-3.49440700	2.04466200	0.23811200
H	-2.36870600	-0.40174600	-1.94758100
C	-3.11928100	-0.96378300	-0.01529000
H	-3.16451500	-2.02539000	-0.27202000
H	-4.09978300	-0.53717100	-0.24255900
C	-2.83463500	-0.81256500	1.41001200
C	-2.57024400	-0.65933500	2.57081100
H	-2.33751800	-0.53318200	3.60508400

5a-b

0 1			
C	-1.83672000	-0.35874500	-0.38740700
C	-0.45783700	-0.99193400	-0.28579600
C	-1.50295600	1.09409900	-0.23220200
N	-0.24539400	1.29852200	-0.12779900
N	0.41586000	0.06657900	-0.16622300
C	1.82311500	0.05188700	-0.03906800
C	2.50341600	1.25566000	0.16301100
C	2.54141100	-1.14493100	-0.11348200
C	3.88586500	1.25662500	0.28665200
H	1.94942900	2.18250900	0.21966400
C	3.92510200	-1.12312100	0.01375200
H	2.02394000	-2.08027900	-0.26679600
C	4.60725000	0.07037000	0.21404700
H	4.40031900	2.19942800	0.44171100
H	4.47094700	-2.05905000	-0.04653900
H	5.68754600	0.07698800	0.31130100
O	-0.19656300	-2.17399500	-0.30102100
C	-2.48097600	2.21163500	-0.21839700
H	-1.96028200	3.16829000	-0.16021500
H	-3.10042700	2.19209700	-1.11929300
H	-3.15679000	2.12253800	0.63699700
H	-2.21646600	-0.54206100	-1.39932500
C	-2.81738100	-0.96342700	0.63054100
H	-2.52313200	-0.68135600	1.64598800
H	-2.73469300	-2.05212900	0.56739900
C	-4.20324500	-0.57149200	0.39143700
C	-5.33866700	-0.24222400	0.18258500
H	-6.35141000	0.04287100	0.00139200

5a-c

0 1			
C	-1.97299800	0.31456700	-0.39495000
C	-0.73993500	-0.57713500	-0.34302800
C	-1.35651500	1.67205000	-0.23573900
N	-0.08331500	1.62868600	-0.14015500
N	0.32387700	0.29436500	-0.20362100
C	1.69826400	0.00119600	-0.06021800
C	2.57609600	1.01694200	0.32736300
C	2.18992300	-1.28486600	-0.29970700
C	3.92922800	0.74417600	0.47203700
H	2.19541900	2.01302900	0.50870600
C	3.54751400	-1.53916400	-0.14635300
H	1.51789900	-2.07647600	-0.59630400
C	4.42535500	-0.53357600	0.23877900
H	4.59891300	1.54308600	0.77335700
H	3.91693700	-2.54198100	-0.33473500
H	5.48343500	-0.74227400	0.35497700
O	-0.69256100	-1.78352600	-0.40626100
C	-2.10898800	2.95274900	-0.20403500
H	-1.42106400	3.79841300	-0.17782100
H	-2.75382900	3.04160900	-1.08305800
H	-2.75480900	3.00077300	0.67841100
H	-2.42637700	0.22613500	-1.38862000

C	-3.03012500	-0.01521300	0.67492100
H	-3.77354900	0.78710600	0.68416400
H	-2.56256900	-0.02231500	1.66408300
C	-3.72234000	-1.28072300	0.44845300
C	-4.32228300	-2.30407300	0.26708700
H	-4.84302300	-3.22183200	0.10570200

5a-d

O 1			
C	-1.91628400	0.39639900	0.01192600
C	-0.79218800	-0.40005100	0.06422400
C	-1.39847000	1.70328200	-0.16412300
N	-0.08143700	1.70802600	-0.21518000
N	0.29327800	0.40382900	-0.08144100
C	1.66916800	0.06444400	-0.04178400
C	2.56432800	0.96831500	0.52641500
C	2.12608900	-1.13808000	-0.57558100
C	3.91822400	0.66411800	0.55958400
H	2.19261800	1.90215000	0.92942700
C	3.48208700	-1.43750000	-0.52084000
H	1.43171600	-1.83156500	-1.03098000
C	4.38253000	-0.54129000	0.04321900
H	4.61212900	1.37208200	1.00032000
H	3.83477400	-2.37643300	-0.93447500
H	5.44042800	-0.77886400	0.07733800
O	-0.62413000	-1.71402900	0.24509100
C	-3.37086000	0.03160500	0.13148200
H	-3.79758100	0.46017100	1.04529000
H	-3.93305100	0.47108200	-0.69977900
C	-3.61924100	-1.41066900	0.14007200
C	-3.80092600	-2.59879800	0.15011200
H	-3.98542600	-3.65080100	0.15428100
C	-2.18248500	2.96584700	-0.28829900
H	-1.51031300	3.81593400	-0.41543500
H	-2.85941500	2.93142900	-1.14737000
H	-2.79433300	3.14073200	0.60196800
H	-1.49323100	-2.13240200	0.31659800

5a-e

O 1			
C	-1.92297000	0.36597800	-0.14549500
C	-0.78996500	-0.41955300	-0.12599200
C	-1.41892900	1.68941300	-0.14603400
N	-0.10066200	1.71305100	-0.13012100
N	0.28800700	0.40600000	-0.12043000
C	1.66479900	0.07796600	-0.04413000
C	2.51474100	0.91936300	0.67073800
C	2.16806600	-1.05079500	-0.68616200
C	3.86951000	0.62606200	0.74244000
H	2.10844000	1.79724600	1.15741700
C	3.52376500	-1.34190100	-0.59234800
H	1.51070900	-1.69348200	-1.25658700
C	4.37910800	-0.50788700	0.11819400
H	4.52803500	1.28532000	1.29809100
H	3.91247600	-2.22360200	-1.09097000
H	5.43727600	-0.73794000	0.18224800
O	-0.61540300	-1.74502000	-0.09401200
C	-3.36877100	-0.04721700	-0.18759700
H	-3.96391000	0.63679700	0.42598200
H	-3.76829200	0.03211500	-1.20499300
C	-3.59262700	-1.41131700	0.29433100
C	-3.73719900	-2.53893600	0.68457700
H	-3.88759100	-3.53494300	1.03961900
C	-2.21210700	2.95275500	-0.17488300
H	-1.54467500	3.81578700	-0.15225400
H	-2.82609600	3.01665000	-1.07825600
H	-2.88691800	3.01772600	0.68412200
H	-1.47217300	-2.16844600	0.05571000

5a-f

O 1			
C	1.82698000	0.14192500	-0.45179400
C	0.63363500	-0.54322600	-0.49416300
C	1.46948700	1.41331700	0.06004200
N	0.17522200	1.50029100	0.29750000
N	-0.34056600	0.28279800	-0.04095800
C	-1.73729800	0.05345500	0.04780000
C	-2.60830500	1.10239400	-0.23644000
C	-2.23157600	-1.18983300	0.43349800
C	-3.97822400	0.90173600	-0.13454100
H	-2.20624500	2.06506300	-0.52706200
C	-3.60535700	-1.38221800	0.51538600
H	-1.55161900	-1.99716200	0.67240200
C	-4.48261900	-0.34103300	0.23461900
H	-4.65408700	1.72153300	-0.35360300
H	-3.98815700	-2.35217100	0.81471800
H	-5.55381000	-0.49602100	0.30675500
O	0.32092100	-1.77745600	-0.90936500
C	3.19294000	-0.34910800	-0.83838800
H	3.13556400	-1.04609100	-1.68226600
H	3.79215900	0.49176700	-1.20039300
C	3.91180200	-0.99833300	0.26368200
C	4.49149200	-1.52928900	1.17150700
H	5.00264000	-2.00084600	1.98139900
C	2.38589000	2.55871200	0.33121900
H	1.82654300	3.40033100	0.74281300
H	3.16592200	2.27857800	1.04493700
H	2.88409200	2.89242300	-0.58407100
H	1.12395300	-2.25037800	-1.15105700

Cinnamaldehyde (6a)

6a-a			
O 1			
C	-3.34659800	-0.28754200	-0.00005200
C	-1.98302200	0.24248900	0.00011300
H	-3.42227100	-1.39517800	-0.00045000
H	-1.88019400	1.32391100	0.00052200
C	-0.93593300	-0.59468300	-0.00021400
C	0.48667700	-0.24301700	-0.00013000
C	0.93803600	1.08356100	-0.00018700
C	1.43421700	-1.27265900	0.00002700
C	2.29485800	1.36616900	-0.00005500
H	0.22606200	1.90170200	-0.00037200
C	2.79410000	-0.98918900	0.00016600
H	1.09954400	-2.30574000	0.00005900
C	3.22745200	0.33119100	0.00012300
H	2.62898100	2.39832700	-0.00009800
H	3.51523800	-1.79970800	0.00029200
H	4.28880400	0.55646000	0.00023000
H	-1.14758100	-1.66426300	-0.00055300
O	-4.34591400	0.39582100	0.00020200

6a-b

O 1			
C	-3.40933900	-0.38146900	0.00019100
C	-1.97455700	-0.71042800	0.00022700
H	-4.09139400	-1.25385400	0.00060200
H	-1.71863200	-1.76573900	0.00051900
C	-1.04861900	0.25887400	-0.00009100
C	0.40750400	0.10895300	-0.00006800
C	1.04752400	-1.13811200	-0.00017200
C	1.19564400	1.26555200	0.00006300
C	2.43115200	-1.21921800	-0.00010900
H	0.46378700	-2.05245500	-0.00034200
C	2.58220100	1.18395000	0.00012900
H	0.71195200	2.23774700	0.00011400
C	3.20321900	-0.05922100	0.00005300
H	2.91291900	-2.19131000	-0.00019900
H	3.17673200	2.09136700	0.00022700
H	4.28607000	-0.12744400	0.00009900

H	-1.41415700	1.28448100	-0.00035100
O	-3.86695500	0.74049100	-0.00025100

(S,R)-Int-I
(S,R)-Int-I-a

O I			
C	1.48384200	0.64221200	-1.18056800
N	0.17282000	1.14208500	-0.72166500
C	-0.14852900	2.43256000	-1.33665300
C	0.56687400	2.35111500	-2.67849700
C	1.82641300	1.52321000	-2.39013700
H	1.32235700	-0.38995800	-1.47720100
H	-1.22626800	2.54729200	-1.43132200
H	0.24681000	3.23002600	-0.69955000
H	-0.07006400	1.81551300	-3.38159500
H	0.79666300	3.34148300	-3.07351400
H	2.10502900	0.90394000	-3.24210600
H	2.67327400	2.17262400	-2.17254900
C	-0.60203700	0.44825800	0.04982300
C	-1.86467500	0.85335800	0.55902600
H	-0.21846300	-0.52410100	0.33351200
H	-2.25574400	1.83440600	0.32115700
C	-2.57242500	-0.04627200	1.27898200
C	2.51188400	0.63769800	0.00026800
O	1.97802600	-0.30859000	0.90377300
Si	2.58975400	-1.28075300	2.13186200
C	3.70354500	-2.62224000	1.46345800
H	3.91787600	-3.35294200	2.25237000
H	3.22556000	-3.16094800	0.64040200
H	4.66168400	-2.23574400	1.10490400
C	1.02631900	-2.00675500	2.84545100
H	0.36359400	-1.22617300	3.23386500
H	0.47696000	-2.57631300	2.08973100
H	1.24718100	-2.68937100	3.67331700
C	3.49201700	-0.27222400	3.42287600
H	3.82854600	-0.92561900	4.23629000
H	4.37926400	0.22643800	3.02336600
H	2.84946300	0.49557800	3.86405000
C	3.88686300	0.15643500	-0.47948100
C	3.99930900	-0.78141700	-1.50802200
C	5.23207400	-1.32405800	-1.84858300
C	6.37874500	-0.94732400	-1.15960800
C	6.28040000	-0.01995800	-0.12965900
C	5.04639500	0.52519900	0.20442600
H	3.12446800	-1.11717400	-2.05168100
H	7.34082300	-1.37434100	-1.42270500
H	4.99279800	1.24277400	1.01438700
C	2.53140600	2.02517300	0.65554100
C	3.29367700	3.07809300	0.14389300
C	3.20560300	4.35448200	0.68720600
C	2.35275500	4.60446200	1.75575200
C	1.59572000	3.56345800	2.27958000
C	1.68629200	2.28832600	1.73386700
H	3.98141300	2.90721200	-0.67600400
H	2.28440400	5.60054700	2.18054100
H	1.08584000	1.48907100	2.14928500
H	5.29237600	-2.05057500	-2.65222200
H	7.16563300	0.28147800	0.42066100
H	3.81163800	5.15405100	0.27388400
H	0.92994500	3.74086100	3.11803100
C	-3.89785500	0.14920000	1.85385900
C	-4.58162700	1.36978000	1.78629000
C	-4.52581400	-0.94218200	2.46461500
C	-5.85869700	1.48909000	2.31187200
H	-4.12049600	2.22987000	1.31301200
C	-5.80560300	-0.82332700	2.98693300
H	-4.00666400	-1.89432700	2.51131100
C	-6.47569600	0.39315900	2.91009700
H	-6.37993900	2.43845000	2.24960200
H	-6.28268900	-1.68051100	3.44981700

H	-7.47789100	0.48850400	3.31475900
C	-3.14280900	-0.00894200	-2.42953100
C	-1.89225100	-0.67010600	-2.43811600
C	-3.95875900	-0.70544200	-1.53229900
N	-3.33494200	-1.72548700	-0.96004500
N	-2.07026000	-1.71951800	-1.50497200
C	-1.14839700	-2.68644600	-1.09124000
C	-1.47771000	-3.54490200	-0.03340800
C	0.11061700	-2.81054900	-1.69637400
C	-0.56609500	-4.49381200	0.40929000
H	-2.45600300	-3.46314500	0.42105500
C	1.01381900	-3.75830600	-1.23177000
H	0.35668700	-2.16336000	-2.52605400
C	0.69018000	-4.60530300	-0.17727200
H	-0.84344000	-5.14846600	1.22984500
H	1.98451700	-3.38035000	-1.71211400
H	1.40232000	-5.34222900	0.17860900
O	-0.84152400	-0.44731800	-3.07412400
C	-3.47118300	1.19714800	-3.25604200
H	-2.63174300	1.39317900	-3.93172100
H	-4.34432100	1.02558400	-3.89781100
C	-3.72756600	2.40611200	-2.46281300
C	-3.94397300	3.38245800	-1.79409300
H	-4.14084300	4.25379700	-1.21016100
C	-5.37744000	-0.40006300	-1.18257900
H	-5.74413500	-1.09353000	-0.42309800
H	-5.47898300	0.61842200	-0.79650500
H	-6.02554500	-0.47811000	-2.06196200
H	-2.11946500	-1.01601800	1.46746600

(S,R)-Int-I-b

O I			
C	1.74295400	1.04485700	-0.44704700
N	0.51449000	1.08368200	0.36071000
C	0.32999500	2.35511700	1.07715100
C	1.55676300	3.19178200	0.71684600
C	2.15933600	2.51633900	-0.52317600
H	1.45390300	0.65400600	-1.42182000
H	-0.59665700	2.81731600	0.73375500
H	0.25040300	2.15844400	2.14778800
H	1.27480400	4.22520100	0.51420600
H	2.26788900	3.19398300	1.54214600
H	1.73869300	2.94903200	-1.43247900
H	3.24196400	2.63375200	-0.57495700
C	-0.37004800	0.12839500	0.32732900
C	-1.60111300	0.14257100	1.02889300
H	-0.10484200	-0.74306700	-0.25163400
H	-1.89155600	1.02880500	1.58110400
C	-2.41589200	-0.93804800	0.95009700
C	2.78568200	0.04282800	0.15055300
O	2.09511300	-1.18869300	0.15296300
Si	2.47394100	-2.82177000	0.06914300
C	3.23709600	-3.26785500	-1.57575900
H	3.30439500	-4.35811400	-1.66982400
H	2.62711700	-2.90713200	-2.41000500
H	4.24611900	-2.86500600	-1.69909000
C	0.78841200	-3.60803900	0.23786400
H	0.30666700	-3.32622700	1.17989900
H	0.12622800	-3.31406100	-0.58212500
H	0.85917400	-4.70096400	0.22105700
C	3.56988600	-3.34948400	1.48795800
H	3.65341000	-4.44237000	1.50609200
H	4.58482500	-2.95030800	1.41423500
H	3.15656900	-3.03707000	2.45199100
C	4.02765500	-0.06981600	-0.74562700
C	3.98708600	0.20724800	-2.11277200
C	5.09075700	-0.03483000	-2.92355700
C	6.25630800	-0.56410900	-2.38486000
C	6.31146600	-0.84274200	-1.02411800
C	5.20909700	-0.59575500	-0.21677500

C	-4.72437200	-1.62300000	-1.37982200
H	-4.34559900	-2.52400100	-0.88029500
H	-5.52851600	-1.24217900	-0.74099400
C	-5.28891400	-2.02774900	-2.67244100
C	-5.72518200	-2.36497300	-3.74079600
H	-6.11986900	-2.65421800	-4.68917600
C	-1.75541900	-1.82796700	-2.67542600
H	-0.71046700	-1.62108700	-2.91913700
H	-1.79351300	-2.68762700	-1.99755100
H	-2.26706500	-2.12943100	-3.59472000
H	-1.90899200	-1.87231400	0.43203700

(S,R)-Int-I-d

O 1			
C	-1.60010600	-0.31265000	-1.25545300
N	-0.41335300	-1.16168300	-1.08307800
C	-0.44955700	-2.38757600	-1.89100800
C	-1.74507800	-2.27571500	-2.69515300
C	-2.14468500	-0.79712000	-2.60509300
H	-1.23979900	0.71507900	-1.29391200
H	0.43622600	-2.39722600	-2.52954000
H	-0.42414300	-3.26366300	-1.24017800
H	-1.59704100	-2.59506500	-3.72717600
H	-2.51615900	-2.89965800	-2.24849800
H	-1.66501900	-0.22048300	-3.39989200
H	-3.22188900	-0.66863200	-2.69246900
C	0.62676200	-0.74331600	-0.43364100
C	1.80368700	-1.50063100	-0.17438700
H	0.54310700	0.23400300	0.02027000
H	1.89051600	-2.51008400	-0.55842000
C	2.77206800	-0.92038900	0.56757200
C	-2.61263400	-0.43636900	-0.05914800
O	-3.32624400	-1.63658500	-0.25886100
Si	-4.92311700	-2.14020700	-0.13505900
C	-5.50559300	-2.17807900	1.64351100
H	-6.34578300	-2.87439900	1.74570600
H	-4.71585000	-2.52012200	2.32027200
H	-5.85018400	-1.20335300	1.99771600
C	-4.84908800	-3.88148000	-0.80830300
H	-4.61896900	-3.89349700	-1.87834800
H	-4.08980100	-4.48164400	-0.29665500
H	-5.81129600	-4.38874700	-0.67827000
C	-6.07340200	-1.10453600	-1.18379300
H	-7.05237800	-1.59441700	-1.24649900
H	-6.23350400	-0.10228300	-0.77734300
H	-5.70073500	-0.99707200	-2.20760100
C	-1.82465500	-0.53239500	1.25206300
C	-1.58361900	-1.77309100	1.83656000
C	-0.78013000	-1.88051000	2.96715200
C	-0.20445400	-0.74644500	3.52706800
C	-0.44384400	0.49677700	2.95124900
C	-1.24740200	0.60215000	1.82283000
H	-2.02068200	-2.66092400	1.39584200
H	0.42583800	-0.82967300	4.40631600
H	-1.41443500	1.57819100	1.38026400
C	-3.56124400	0.77252700	-0.03313400
C	-3.77302100	1.60282200	-1.13284700
C	-4.70646500	2.63336500	-1.08006100
C	-5.44124000	2.85695600	0.07630300
C	-5.22756900	2.04659000	1.18646800
C	-4.29562000	1.02020600	1.12939400
H	-3.21218100	1.47323100	-2.05012100
H	-6.16808200	3.66154000	0.11669900
H	-4.13072600	0.40769000	2.00853000
H	-0.60171200	-2.85590800	3.40840200
H	-0.00195500	1.39163200	3.37612600
H	-4.85231500	3.26552300	-1.94980000
H	-5.78313500	2.21691400	2.10284200
C	4.02450100	-1.51925900	1.00880200
C	4.97087600	-0.68872200	1.61906900

C	4.32268700	-2.87792300	0.84102800
C	6.19519100	-1.19494200	2.03245000
H	4.74397500	0.36495200	1.74865200
C	5.53988700	-3.38475500	1.26589900
H	3.60265900	-3.54483400	0.37960800
C	6.48163600	-2.54381400	1.85633400
H	6.92439500	-0.53649100	2.49197000
H	5.76064400	-4.43881900	1.13453100
H	7.43607600	-2.94359900	2.18289000
C	3.80083100	1.19096400	-1.77380600
C	2.42163000	1.43552900	-1.63106200
C	4.43923100	1.90539900	-0.74599100
N	3.58644700	2.56047300	0.02544500
N	2.34493100	2.29250200	-0.51827100
C	1.21041200	2.91514800	0.01534800
C	1.23369900	3.38720600	1.33262200
C	0.05246600	3.09589400	-0.75205100
C	0.12404800	4.02883500	1.86561700
H	2.13339400	3.25707100	1.92052900
C	-1.05046700	3.73909800	-0.20320500
H	0.03606700	2.73592000	-1.77153700
C	-1.02832900	4.20777600	1.10593500
H	0.16193000	4.38880000	2.88918200
H	-1.93836800	3.87749000	-0.81123000
H	-1.89666400	4.70282800	1.52747900
O	1.42555800	0.98786500	-2.25158100
C	4.38575800	0.33475000	-2.85645100
H	3.55450400	-0.08563500	-3.43302400
H	4.97878500	0.92372100	-3.56810200
C	5.22714000	-0.76431200	-2.37111600
C	5.93295500	-1.64474800	-1.95681700
H	6.55414300	-2.42527600	-1.57906500
C	5.90586100	1.97635600	-0.47407900
H	6.10095200	2.59526700	0.40486800
H	6.32670300	0.98146300	-0.30316000
H	6.44327900	2.41011800	-1.32398600
H	2.61384700	0.10627600	0.89177300

(S,R)-Int-I-e

O 1			
C	2.01220000	-0.41967200	-1.26373700
N	0.68687800	0.20066700	-1.14425200
C	0.34873300	1.06605600	-2.28209500
C	1.44906300	0.81297600	-3.31896300
C	2.32398900	-0.32425100	-2.75787600
H	1.91034300	-1.45032800	-0.92838400
H	-0.64410900	0.77618000	-2.63117200
H	0.31694400	2.10628400	-1.95304500
H	1.01624200	0.53605200	-4.28048100
H	2.03516400	1.71833600	-3.47036500
H	2.06656900	-1.27347900	-3.22903400
H	3.38462800	-0.15384400	-2.94035600
C	-0.10486400	-0.03033200	-0.14250100
C	-1.31691400	0.65985500	0.11583800
H	0.22369500	-0.79230000	0.55397700
H	-1.62130100	1.47693300	-0.52658800
C	-2.06145800	0.25128700	1.16925200
C	3.01504200	0.26901400	-0.27393100
O	2.45560600	-0.00556000	0.99309600
Si	3.03147400	-0.02446200	2.57603100
C	4.25794000	-1.40602600	2.86158500
H	4.45758600	-1.49344200	3.93626300
H	3.88516800	-2.37795500	2.52566500
H	5.21663900	-1.22885600	2.36670200
C	1.46336300	-0.33289100	3.53859400
H	0.72927500	0.46314500	3.37656600
H	0.99823100	-1.28131200	3.24989600
H	1.66134300	-0.37975000	4.61494100
C	3.80276300	1.60959400	3.05105300
H	4.18115400	1.55348300	4.07843100

H	4.64746000	1.87763700	2.41030300	C	2.70024200	-1.66708800	2.16489100
H	3.08182600	2.43100400	3.01247000	H	1.75545300	0.20188700	1.54958200
C	4.40303200	-0.38014300	-0.36081800	H	0.08145300	-3.09062800	1.51229300
C	4.54591400	-1.73661100	-0.66036800	H	0.96999900	-3.48813800	0.03008500
C	5.78913100	-2.35460300	-0.60435900	H	2.07113700	-3.70775000	2.62610200
C	6.91683400	-1.62886400	-0.24036300	H	3.02301800	-3.56562600	1.15203800
C	6.78847100	-0.27966800	0.06536700	H	2.26602300	-1.39760900	3.13035400
C	5.54387000	0.33577700	0.00587000	H	3.78246100	-1.59152300	2.26145500
H	3.68792600	-2.33994600	-0.93285300	C	-0.01360800	-0.87828900	-0.03366400
H	7.88715900	-2.11183400	-0.19389500	C	-1.14705500	-1.56965800	-0.53644500
H	5.46741900	1.38693700	0.25659600	H	0.02838800	0.19397800	-0.13249700
C	3.02490800	1.77929700	-0.53457500	H	-1.18639300	-2.64972500	-0.47746100
C	3.80280400	2.34248300	-1.54822100	C	-2.19931400	-0.84068200	-0.97488800
C	3.73113600	3.70094900	-1.83020000	C	3.10209800	-0.29590500	-0.06738000
C	2.87602700	4.52287900	-1.10450100	O	2.35322700	0.53037900	-0.93788400
C	2.09570000	3.97300400	-0.09489800	Si	2.04168600	2.19235800	-0.97808300
C	2.16956700	2.61310100	0.18455900	C	1.60414100	2.85320700	0.71167100
H	4.47691200	1.72005800	-2.12604800	H	1.24781600	3.88492600	0.61347100
H	2.82176500	5.58430000	-1.32283900	H	0.80476500	2.27504600	1.18451900
H	1.54741600	2.19618800	0.96663700	H	2.46597400	2.87533900	1.38402500
H	5.87256900	-3.40973000	-0.84297200	C	0.57637100	2.30142000	-2.13022300
H	7.65863700	0.29989500	0.35546200	H	0.78418100	1.80878300	-3.08586300
H	4.34805600	4.11689400	-2.61996500	H	-0.32154200	1.84166900	-1.70674800
H	1.42404800	4.60210900	0.48010100	H	0.32826700	3.34597500	-2.34582900
C	-3.29874700	0.83921600	1.65090800	C	3.48138900	3.14845100	-1.68717200
C	-3.80537000	2.05088900	1.15879000	H	3.14777600	4.15519400	-1.96542800
C	-4.01333200	0.15684300	2.64210300	H	4.30138300	3.26157700	-0.97341400
C	-4.98981500	2.56557200	1.65604400	H	3.88221200	2.67743900	-2.58998200
H	-3.27206600	2.59583200	0.38767400	C	4.33064700	0.46884500	0.44176500
C	-5.20434200	0.67181200	3.13367400	C	4.41660100	1.02228400	1.71774200
H	-3.64462100	-0.79817000	2.99769800	C	5.52137400	1.78254700	2.09196700
C	-5.69167800	1.87724500	2.64390900	C	6.55768800	2.00083600	1.19471100
H	-5.37675200	3.50097900	1.26675400	C	6.48166900	1.45618300	-0.08364400
H	-5.75491200	0.12879500	3.89429400	C	5.37842400	0.70180100	-0.45352800
H	-6.62357100	2.28136800	3.02579200	H	3.62336500	0.88174200	2.44222300
C	-2.07462400	-2.87132500	-0.62631500	H	7.41909400	2.59224800	1.48705700
C	-3.28886100	-2.31331800	-0.15542300	H	5.32577600	0.29356100	-1.45697900
C	-1.73427900	-2.17001100	-1.78734500	C	3.50819600	-1.54210900	-0.86053300
N	-2.60220300	-1.21352200	-2.08441300	C	4.59555800	-2.32727100	-0.47532200
N	-3.56663100	-1.29526200	-1.10224000	C	4.90795400	-3.49440000	-1.16126000
C	-4.65688600	-0.42268500	-1.14963700	C	4.13570500	-3.89597800	-2.24587200
C	-4.66386400	0.62938300	-2.07546200	C	3.05594400	-3.11557400	-2.64213300
C	-5.74870100	-0.56731500	-0.28279500	C	2.74656200	-1.94632200	-1.95568000
C	-5.73764700	1.50819100	-2.13240800	H	5.20870800	-2.02886300	0.36817900
H	-3.82849800	0.73742000	-2.75420900	H	4.37995700	-4.80585900	-2.78441000
C	-6.81224200	0.32159200	-0.35369000	H	1.91323500	-1.33340600	-2.27627900
H	-5.73598600	-1.36897400	0.44098100	H	5.56550700	2.20392100	3.09075500
C	-6.82146700	1.36566000	-1.27309600	H	7.28115100	1.62458000	-0.79747200
H	-5.72264900	2.31323300	-2.86148000	H	5.75966500	-4.08933700	-0.84797100
H	-7.64608700	0.19368000	0.33005900	H	2.45243800	-3.41237100	-3.49395500
H	-7.65808400	2.05537800	-1.31886400	C	-3.49208300	-1.33580000	-1.41615300
O	-3.99642300	-2.59878700	0.82918900	C	-3.81644400	-2.70005900	-1.45583300
C	-1.35838300	-4.00630900	0.04012000	C	-4.46999600	-0.39839800	-1.76862000
H	-1.98172400	-4.35895100	0.86904500	C	-5.08448900	-3.10700000	-1.83341700
H	-1.22845300	-4.86514300	-0.63047100	H	-3.07940300	-3.44646300	-1.18434600
C	-0.03677900	-3.64782600	0.57082200	C	-5.74201300	-0.80761500	-2.14387000
C	1.05103600	-3.33523600	0.98064300	H	-4.22773000	0.65774600	-1.73528100
C	2.01514000	-3.08145300	1.35861000	C	-6.05151000	-2.16162400	-2.17383500
C	-0.57372300	-2.43137700	-2.69078700	H	-5.32716600	-4.16406100	-1.85781400
H	-0.42821300	-1.60070300	-3.38492300	H	-6.49215600	-0.06905800	-2.40438300
H	0.34889300	-2.58895000	-2.12676300	H	-7.04647400	-2.48491100	-2.46190300
H	-0.73923900	-3.33675000	-3.28471500	C	-3.07185200	-0.39269700	2.09301200
H	-1.70765100	-0.61144300	1.72951900	C	-2.32146200	0.72715900	1.68493300
				C	-4.40222100	-0.13752600	1.72069400
				N	-4.54361500	1.03586000	1.13038000
				N	-3.27753200	1.57954800	1.10312700
				C	-3.06426400	2.78065900	0.41743000
				C	-4.03340200	3.25516200	-0.47640700
				C	-1.89212700	3.52233000	0.60302400
				C	-3.81871800	4.43252800	-1.17997700
(S,R)-Int-I-f							
0 1							
C	2.13981200	-0.71369500	1.09973600				
N	0.97841800	-1.45320900	0.57747200				
C	0.98639700	-2.88130700	0.93673400				
C	2.25895200	-3.07859200	1.75586700				

H	-4.95309000	2.69870200	-0.60092700
C	-1.68913400	4.69389700	-0.11518400
H	-1.15540200	3.17224300	1.30940200
C	-2.64263100	5.15771400	-1.01469100
H	-4.58208800	4.78357300	-1.86765900
H	-0.77266300	5.25474800	0.04248000
H	-2.47741200	6.07477200	-1.57057000
O	-1.08551700	0.95318300	1.74366400
C	-2.45149500	-1.57715100	2.76910000
H	-1.36407400	-1.43658600	2.73722600
H	-2.71296000	-1.63034300	3.83417200
C	-2.77324900	-2.87593400	2.16883900
C	-3.05120300	-3.94639100	1.69673000
H	-3.31259900	-4.89298200	1.27952000
C	-5.58014000	-1.04454200	1.86136700
H	-6.49789100	-0.51622400	1.59375100
H	-5.47775900	-1.91108900	1.19958700
H	-5.68152500	-1.42593000	2.88216000
H	-2.09096300	0.24143500	-0.99010100

(S,R)-Int-I-g

0 1

C	2.15521000	1.06106100	0.53454600
N	0.95454900	0.71064300	1.31346900
C	1.05783300	1.08130300	2.73431200
C	2.41965800	1.76341300	2.86782600
C	2.86826900	2.07622400	1.43177800
H	1.81162600	1.50503000	-0.39822600
H	0.22686800	1.75051400	2.96817500
H	0.97026800	0.18749100	3.35356900
H	2.34711100	2.66839000	3.47094600
H	3.12591500	1.09385700	3.35675700
H	2.55354400	3.08101600	1.14082200
H	3.95134600	2.03198300	1.32250600
C	-0.09479900	0.17024900	0.77569600
C	-1.23520600	-0.29523500	1.49197300
H	-0.07148100	0.04969500	-0.30012100
H	-1.31975000	-0.11884000	2.55806500
C	-2.17316100	-0.97323300	0.79599800
C	2.94853000	-0.23132300	0.13909500
O	2.01694900	-1.01356000	-0.57083200
Si	1.87634600	-1.76234500	-2.07268500
C	2.40570100	-0.65566400	-3.48056100
H	2.09188500	-1.10435300	-4.43050100
H	1.92987600	0.32765100	-3.41672600
H	3.48804200	-0.50888500	-3.52689500
C	0.04228100	-2.08769100	-2.16964400
H	-0.31292600	-2.66965600	-1.31306600
H	-0.51224000	-1.14399600	-2.20578300
H	-0.20940700	-2.65077600	-3.07519600
C	2.83687200	-3.36846300	-2.08646400
H	2.46402600	-4.02674400	-2.87922900
H	3.90481200	-3.21735500	-2.26529200
C	2.72729600	-3.90481600	-1.13813900
H	4.14826100	0.10625300	-0.75306300
C	4.30302900	1.33221800	-1.39766600
C	5.35307800	1.54072400	-2.28675600
C	6.26160900	0.52482800	-2.55052500
C	6.11914300	-0.70248600	-1.91082600
C	5.07603500	-0.90423500	-1.01866300
H	3.60825300	2.14672000	-1.23219400
H	7.07640200	0.68699900	-3.24824000
H	4.97865600	-1.86452600	-0.52428700
C	3.36717700	-0.99801800	1.39821500
C	4.55270200	-0.70315900	2.07328500
C	4.87887400	-1.35835900	3.25414300
C	4.02309800	-2.32044400	3.78018700
C	2.84468300	-2.62678200	3.11027600
C	2.52103500	-1.97133100	1.92712400
H	5.23288200	0.04223500	1.67582100

H	4.27830000	-2.83482600	4.70086900
H	1.60675500	-2.22195600	1.40298900
H	5.45223500	2.50253600	-2.77870300
H	6.82285300	-1.50513500	-2.10519500
H	5.80658100	-1.11779600	3.76300100
H	2.17359300	-3.38275800	3.50512100
C	-3.41476700	-1.53460300	1.30597500
C	-3.99003200	-1.11634100	2.51260400
C	-4.07660100	-2.49480100	0.53306400
C	-5.18818900	-1.66401400	2.94061200
H	-3.51710000	-0.33667200	3.09953400
C	-5.26946500	-3.05236800	0.97012500
H	-3.65718700	-2.79066500	-0.42376100
C	-5.82664400	-2.63740300	2.17413500
H	-5.63521500	-1.32437600	3.86876500
H	-5.77385000	-3.79462600	0.36113500
H	-6.76738900	-3.05985400	2.51163700
C	-1.59791500	2.67949700	-0.13476900
C	-1.89471900	1.72404300	-1.13160500
C	-2.73125500	2.75513200	0.69579100
N	-3.69775600	1.94801400	0.30835100
N	-3.20747800	1.31703700	-0.82029300
C	-4.03384000	0.41498700	-1.50132300
C	-5.35468000	0.23123800	-1.07195200
C	-3.56264500	-0.33694200	-2.58601400
C	-6.17660600	-0.68598300	-1.70886900
H	-5.71625400	0.80461100	-0.22946200
C	-4.40031000	-1.25504900	-3.20938800
H	-2.55062500	-0.18115300	-2.93021100
C	-5.70865100	-1.44300400	-2.77889600
H	-7.19505900	-0.81435300	-1.35519000
H	-4.01634600	-1.82831900	-4.04809300
H	-6.35513300	-2.16196700	-3.27159500
O	-1.19264900	1.25117300	-2.05656200
C	-0.31820200	3.45103400	-0.04920100
H	0.21159900	3.26196300	0.89413000
H	0.34227800	3.09999000	-0.84961800
C	-0.47529200	4.90411700	-0.18150800
C	-0.61377000	6.09492500	-0.27015000
H	-0.74522900	7.15016700	-0.36053400
C	-2.91007300	3.62302800	1.89820700
H	-3.83951800	3.37233700	2.41415200
H	-2.08039200	3.50731100	2.60360500
H	-2.94631600	4.68075800	1.61905700
H	-1.98756400	-1.14884900	-0.26110300

(S,R)-Int-I-h

0 1

C	2.22306300	-0.81475700	1.23890800
N	1.03269800	-1.56491200	0.80369800
C	1.08674700	-2.99346900	1.15509200
C	2.38334800	-3.16718900	1.94408100
C	2.85430600	-1.74605100	2.28304100
H	1.87385300	0.11087500	1.69517700
H	0.20113600	-3.23063200	1.74875400
H	1.06724400	-3.59396600	0.24391200
H	2.21654100	-3.75665500	2.84578800
H	3.12351700	-3.68904800	1.34000700
H	2.49409800	-1.45027700	3.27071200
H	3.94069800	-1.67314200	2.29810600
C	0.01772400	-1.01675900	0.20238800
C	-1.09472900	-1.73870000	-0.29955200
H	0.03573600	0.05538000	0.08933200
H	-1.12582300	-2.81662200	-0.19657400
C	-2.10830300	-1.05310000	-0.88264700
C	3.10503700	-0.41737900	0.00132400
O	2.31390600	0.42376100	-0.81475400
Si	1.98053700	2.08335200	-0.77402900
C	1.52786800	2.64223200	0.94811100
H	1.29799700	3.71274400	0.92572400

H	0.64270800	2.12550500	1.33157900	H	-1.99942000	0.02298700	-0.98827900
H	2.35316300	2.51189100	1.65374300				
C	0.53129500	2.22151600	-1.94187300	(S,R)-Int-I			
H	0.80806300	1.89600700	-2.95037900	0 1			
H	-0.31970600	1.61318100	-1.62207500	C	1.96290300	0.85466100	-0.35127700
H	0.17905400	3.25547800	-2.01280300	N	0.66638200	1.04017100	0.32399200
C	3.41396200	3.10034500	-1.40742500	C	0.54244400	2.34579700	0.99366000
H	3.06680800	4.12037400	-1.61162000	C	1.84791600	3.07868000	0.69411600
H	4.22810100	3.17171900	-0.68101200	C	2.52483600	2.28032800	-0.42774600
H	3.82584700	2.70338200	-2.34010500	H	1.75119400	0.46015800	-1.34439200
C	4.38077200	0.32751800	0.41339300	H	-0.32681800	2.86043300	0.58146300
C	4.55871300	0.90610400	1.66837700	H	0.38439800	2.18733400	2.06211000
C	5.69371800	1.66200500	1.94975300	H	1.65264800	4.10645600	0.38810800
C	6.66866900	1.84912300	0.97952500	H	2.47620300	3.10810500	1.58319700
C	6.50096500	1.27722900	-0.27807100	H	2.27005700	2.70046500	-1.40133300
C	5.36736900	0.52846800	-0.55575900	H	3.61015100	2.29800400	-0.33987200
H	3.81680700	0.78524900	2.44904100	C	-0.28552700	0.15335100	0.30615600
H	7.55351400	2.43704200	1.20002900	C	-1.51434800	0.27491000	1.00100000
H	5.24128700	0.10061600	-1.54429800	H	-0.09646600	-0.74894400	-0.25322400
C	3.42658800	-1.67083400	-0.81825000	H	-1.74685700	1.19243900	1.52852800
C	4.50682900	-2.49262300	-0.49520100	C	-2.37531600	-0.77175100	1.00656800
C	4.74582600	-3.66317200	-1.20455300	C	2.84653000	-0.20351800	0.40029900
C	3.90677400	-4.03050500	-2.25108400	O	2.14684300	-1.43474600	0.37717400
C	2.83397500	-3.21276300	-2.58622400	Si	2.02908700	-2.66544000	-0.77407800
C	2.59782500	-2.04066100	-1.87606500	C	1.60346200	-1.98077800	-2.46145100
H	5.17353700	-2.21802900	0.31536000	H	1.33129100	-2.80658600	-3.12854400
H	4.09494700	-4.94288000	-2.80763600	H	0.75797300	-1.28740700	-2.44610400
H	1.76961900	-1.39846800	-2.14881800	H	2.45303100	-1.46832600	-2.92206300
H	5.81046800	2.10398600	2.93368800	C	0.62153000	-3.69141300	-0.10340800
H	7.25230900	1.42051800	-1.04760600	H	0.86248700	-4.09450100	0.88552400
H	5.59370400	-4.28668000	-0.94018900	H	-0.30056100	-3.11015800	-0.00502000
H	2.17914600	-3.48270900	-3.40854300	H	0.40578300	-4.53920700	-0.76211200
C	-3.32829100	-1.61232700	-1.44317100	C	3.58247600	-3.69195200	-0.89757700
C	-3.69433200	-2.95572900	-1.27559400	H	3.36880300	-4.59818900	-1.47680200
C	-4.18651500	-0.76048900	-2.14877100	H	4.39302600	-3.16277800	-1.40586200
C	-4.88383700	-3.42914900	-1.80514400	H	3.94797800	-4.01012800	0.08330400
H	-3.05527700	-3.63409400	-0.72087700	C	4.21078900	-0.39179200	-0.27482100
C	-5.37563900	-1.23773900	-2.68165000	C	4.47416500	0.00325000	-1.58528400
H	-3.91771200	0.28285700	-2.26976900	C	5.69262700	-0.29660800	-2.18834600
C	-5.72683400	-2.57155400	-2.50964500	C	6.66769300	-0.99390200	-1.48837200
H	-5.16070300	-4.46854100	-1.66465600	C	6.41591500	-1.39373600	-0.17954000
H	-6.03314500	-0.56523700	-3.22162300	C	5.19883700	-1.09854000	0.41598500
H	-6.65985300	-2.94494400	-2.91853800	H	3.73736700	0.54822400	-2.16347900
C	-3.46563500	-0.21055000	1.63667400	H	7.61757200	-1.22534800	-1.95876600
C	-2.53383200	0.83042400	1.43436800	H	5.00924900	-1.43103400	1.43066000
C	-4.65105000	0.18145600	0.99189800	C	2.98752100	0.20948900	1.86833500
N	-4.53820900	1.35547200	0.39957600	C	3.98135100	1.09645700	2.28406700
N	-3.24911900	1.76728800	0.66761300	C	4.04868100	1.51978700	3.60575100
C	-2.77001800	2.94572000	0.08085000	C	3.12063400	1.06272500	4.53493500
C	-3.32549000	3.39941300	-1.12034000	C	2.13261300	0.17207300	4.13208100
C	-1.74451600	3.68106800	0.67995800	C	2.06914000	-0.25291500	2.80967500
C	-2.85839200	4.56692500	-1.70843900	H	4.71544000	1.46199600	1.57425400
H	-4.13401800	2.83720000	-1.57075100	H	3.17302300	1.39181400	5.56758300
C	-1.28276400	4.84436100	0.07765100	H	1.30538100	-0.95738500	2.50478400
H	-1.32173900	3.33628400	1.61281200	H	5.87524700	0.02004400	-3.20984600
C	-1.83078700	5.29619200	-1.11785400	H	7.16709100	-1.94446700	0.37685500
H	-3.30206900	4.90732900	-2.63896100	H	4.83144100	2.20728300	3.90920800
H	-0.49031900	5.40924600	0.55897400	H	1.40823700	-0.19961600	4.84963500
H	-1.46694300	6.20809300	-1.57982200	C	-3.64816900	-0.81749000	1.71472300
O	-1.32641700	0.93370900	1.75941300	C	-4.36800400	0.34293400	2.02544700
C	-3.15273300	-1.49676700	2.33157800	C	-4.16969100	-2.06214600	2.08681200
H	-3.34523100	-2.35563000	1.67289100	C	-5.57452200	0.25424000	2.70321800
H	-2.07899100	-1.50909100	2.54932800	H	-4.01291300	1.30733000	1.68579400
C	-3.88708100	-1.71250500	3.58330000	C	-5.37076000	-2.14699200	2.77514000
C	-4.50356200	-1.88764900	4.60040300	H	-3.62523500	-2.96542800	1.83273900
H	-5.04943400	-2.03193500	5.50606200	C	-6.07541100	-0.98751600	3.08411900
C	-5.92178400	-0.59525700	0.90422400	H	-6.13459200	1.15689700	2.92292900
H	-6.64637400	-0.07117700	0.27766500	H	-5.76264500	-3.11703900	3.06160900
H	-5.74446900	-1.58525900	0.47052100	H	-7.02149900	-1.05201300	3.61167200
H	-6.36518400	-0.74905600	1.89316400	C	-3.71263800	-0.54519500	-1.67533600

C	-3.70180900	0.84070100	-1.36079000	H	-5.73513900	0.48026600	-1.75965200
C	-2.47606300	-0.82673500	-2.27106800	C	-3.86628900	1.71336900	-0.35611200
N	-1.68056200	0.23378800	-2.31896600	C	-4.94009200	2.38482500	0.22961800
N	-2.42488300	1.26477800	-1.77145900	C	-5.10141500	3.75385500	0.05674500
C	-1.86550100	2.54025200	-1.69334800	C	-4.18873100	4.47482400	-0.70554300
C	-0.63880800	2.79991500	-2.32029100	C	-3.12065100	3.81290900	-1.29951600
C	-2.48849200	3.57013900	-0.97350900	C	-2.96269200	2.44193200	-1.12790500
C	-0.05464000	4.05473900	-2.22436300	H	-5.66191300	1.83908300	0.82735600
H	-0.15858200	2.00870300	-2.88063600	H	-4.31501700	5.54369800	-0.84310800
C	-1.88553400	4.81940600	-0.88587400	H	-2.13701200	1.92833400	-1.60471100
H	-3.44359600	3.37684400	-0.50664600	H	-6.52141500	-3.13883000	1.50711400
C	-0.66633300	5.07566900	-1.50336400	H	-7.80987600	-0.82841700	-1.86864400
H	0.89175900	4.23626300	-2.72498800	H	-5.94501300	4.25654500	0.51821900
H	-2.38399600	5.60320000	-0.32346700	H	-2.40764200	4.36271800	-1.90535100
H	-0.20413200	6.05461200	-1.43156000	C	2.93745000	1.15901800	-0.91505600
O	-4.57276700	1.56391400	-0.84522400	C	3.48705700	2.24707300	-0.22124400
C	-4.92902000	-1.39545400	-1.45172100	C	3.61201600	0.65085300	-2.03220600
H	-5.48453200	-0.97153800	-0.60640300	C	4.66360900	2.82878600	-0.66151000
H	-5.61752500	-1.35003700	-2.30649300	H	3.00890600	2.61983400	0.67771500
C	-4.65873400	-2.80569700	-1.16696300	C	4.78023900	1.24868700	-2.48014200
C	-4.44014800	-3.96635300	-0.94318400	H	3.21822100	-0.22313600	-2.53866400
H	-4.25020500	-4.99704200	-0.74242300	C	5.30425900	2.34055200	-1.79881900
C	-1.98478100	-2.13232400	-2.81350600	H	5.09387000	3.65858200	-0.11135900
H	-1.16990000	-1.96254400	-3.51872200	H	5.29508200	0.84753400	-3.34570600
H	-1.61720000	-2.79321500	-2.02118000	H	6.22860800	2.79654100	-2.13690900
H	-2.78066200	-2.67005800	-3.33288000	C	2.63989800	-1.59497300	1.42546600
H	-2.07220600	-1.69215100	0.51369800	C	3.62651300	-1.75565600	0.42269400

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C	-2.78080400	0.03587000	1.19680300
N	-1.51610100	0.78457700	1.10791300
C	-1.47077200	1.95992400	1.99252000
C	-2.80796900	1.95393100	2.73056900
C	-3.39456900	0.55347400	2.50342900
H	-2.52126500	-1.02017000	1.27028200
H	-0.61974400	1.83674900	2.66632700
H	-1.31957000	2.86251100	1.39830300
H	-2.67045700	2.16331400	3.79145600
H	-3.46467000	2.72060500	2.32299300
H	-3.10294700	-0.11813700	3.31361300
H	-4.48320200	0.56752100	2.47036100
C	-0.50504600	0.39370600	0.39260800
C	0.70089000	1.10851800	0.21893500
H	-0.61356900	-0.55546000	-0.11360000
H	0.81654900	2.09143400	0.65939500
C	1.67802500	0.54561200	-0.54013800
C	-3.62805800	0.22049500	-0.11074100
O	-2.83933400	-0.25989100	-1.18233800
Si	-2.60276900	-1.78994100	-1.85815900
C	-2.16273900	-3.05906400	-0.55675400
H	-1.91381900	-4.00524400	-1.05131100
H	-1.29357100	-2.78328900	0.04791900
H	-2.99313600	-3.26465600	0.12473600
C	-1.15274700	-1.49181300	-2.99349900
H	-1.39331800	-0.74634200	-3.75811800
H	-0.26881600	-1.13515300	-2.45466800
H	-0.86587100	-2.41321200	-3.51137400
C	-4.07968600	-2.39327000	-2.82538000
H	-3.77895200	-3.24972500	-3.44050900
H	-4.89691300	-2.72485400	-2.17940600
H	-4.47216500	-1.62872000	-3.50233100
C	-4.94441100	-0.56419700	-0.05375900
C	-5.18418500	-1.59346700	0.85503200
C	-6.35643600	-2.34217200	0.78936600
C	-7.30706300	-2.07144500	-0.18513600
C	-7.07816200	-1.04625500	-1.09787000
C	-5.90810300	-0.30532300	-1.03227300
H	-4.46658200	-1.83678100	1.62993100
H	-8.22069600	-2.65440300	-0.23448100

(S,R)-TS-I

(S,R)-TS-I-a

0 1

C	1.80060300	1.08663500	-0.26255900
N	0.57947700	0.91522600	0.52170300
C	0.37513500	1.95188200	1.53080800
C	1.58571300	2.87828600	1.39663600
C	2.21567400	2.53081800	0.03956500
H	1.52914300	0.96047400	-1.31158600
H	-0.56452000	2.47240000	1.32602000
H	0.30549000	1.49927200	2.52426600
H	1.28435500	3.92559600	1.44221000
H	2.29034100	2.69900800	2.20836600
H	1.81253900	3.17832300	-0.74115100
H	3.29878900	2.65857200	0.03959300
C	-0.32586800	-0.01551800	0.24180800

C	-1.51800200	-0.21160600	0.91088200	H	-4.28048600	-2.47610400	-1.45601900
H	-0.04929700	-0.68840400	-0.55809500	H	-5.38838200	-1.36542700	-0.67268000
H	-1.79990100	0.45041000	1.72175500	C	-5.37836100	-1.27050100	-2.76578000
C	-2.41150200	-1.20640700	0.47893500	C	-5.93842500	-1.11267100	-3.81697000
C	2.85888800	-0.02358200	0.05408600	H	-6.44392500	-0.96622100	-4.74553900
O	2.19804900	-1.21860700	-0.31856600	C	-1.80555000	-1.34775900	-2.98135300
Si	2.64811400	-2.77548200	-0.74693300	H	-0.85256400	-1.00263600	-3.38696700
C	3.52490100	-2.80869700	-2.39719600	H	-1.63397900	-2.26809900	-2.41309100
H	3.62057400	-3.84292300	-2.74822900	H	-2.46518600	-1.60545800	-3.81578000
H	2.96336200	-2.25806400	-3.15865200	H	-1.99804800	-1.97587700	-0.16685800
H	4.53135200	-2.38397200	-2.35128300				
C	0.99368700	-3.63314500	-0.88340300	(S,R)-TS-I-b			
H	0.43218700	-3.56884300	0.05434600	0 1			
H	0.38269200	-3.19340100	-1.67798000	C	2.29106400	-0.71768100	1.36962300
H	1.11863300	-4.69574900	-1.11862600	N	1.07125800	-1.49506000	1.12971800
C	3.68475500	-3.59455700	0.57528500	C	1.13122900	-2.86123700	1.64858500
H	3.88703500	-4.63570200	0.29776900	C	2.51957100	-2.99144200	2.27171600
H	4.65181300	-3.10695800	0.72370100	C	3.02198400	-1.55106800	2.43436700
H	3.16776700	-3.60831500	1.53947100	H	1.99412800	0.25135700	1.77169900
C	4.12348400	0.13345800	-0.80361900	H	0.32989800	-2.99280900	2.38318500
C	4.08399000	0.72956100	-2.06578700	H	0.97130100	-3.57835800	0.83892700
C	5.20603500	0.74488600	-2.88664500	H	2.47903000	-3.51391600	3.22818000
C	6.39317700	0.15924500	-2.46524500	H	3.17547400	-3.55884400	1.61258500
C	6.44768300	-0.43911600	-1.21221700	H	2.75221200	-1.16443500	3.41995600
C	5.32502500	-0.44975400	-0.39404400	H	4.10579700	-1.48434300	2.34483400
H	3.17646500	1.18874800	-2.43829200	C	-0.01208200	-1.00895300	0.54448500
H	7.26768400	0.16924900	-3.10735300	C	-1.14656500	-1.73873800	0.23228300
H	5.39171900	-0.92419900	0.57744100	H	0.02751500	0.03626500	0.28109600
C	3.14420400	-0.03030600	1.55840400	H	-1.19433300	-2.79380700	0.47298700
C	4.10650700	0.80492800	2.12905500	C	-2.23254400	-1.11965800	-0.39969700
C	4.28584500	0.85007600	3.50621000	C	3.07301100	-0.43644200	0.03786100
C	3.49894500	0.06409900	4.34068500	O	2.22133000	0.33404500	-0.79417600
C	2.53413200	-0.76690900	3.78394500	Si	1.86789600	1.98481100	-0.84773900
C	2.35965100	-0.81188100	2.40536300	C	1.50826500	2.67326500	0.85212700
H	4.72554000	1.43214500	1.49722700	H	1.26879100	3.73774200	0.75691700
H	3.63855900	0.09811400	5.41624500	H	0.65009700	2.19109400	1.32895000
H	1.59910400	-1.45668400	1.98290000	H	2.37142300	2.60313500	1.51982200
H	5.14691400	1.21598900	-3.86230000	C	0.34432300	2.04281700	-1.92436600
H	7.36613800	-0.90248800	-0.86702100	H	0.54685500	1.63788900	-2.92143300
H	5.04263500	1.50443800	3.92663000	H	-0.48263400	1.46778800	-1.49723600
H	1.91061800	-1.38376300	4.42308100	H	-0.00777500	3.07200400	-2.04920800
C	-3.52390400	-1.67303800	1.32399800	C	3.24666100	2.97819200	-1.62549700
C	-3.89913400	-3.01980400	1.27059500	H	2.87925900	3.98632000	-1.85216800
C	-4.21823700	-0.81590900	2.18474500	H	4.10937700	3.08561900	-0.96210500
C	-4.93371100	-3.50297100	2.06057600	H	3.59570900	2.53870000	-2.56476700
H	-3.36797400	-3.69519500	0.60640500	C	4.37325100	0.34316100	0.27293800
C	-5.25708400	-1.29812000	2.96832200	C	4.64709600	1.03537000	1.45108600
H	-3.96756300	0.23651100	2.22039800	C	5.79304100	1.81747700	1.56997300
C	-5.61770600	-2.64115400	2.91108800	C	6.68549100	1.91754300	0.51164200
H	-5.20713100	-4.55178100	2.01052900	C	6.42299100	1.23158000	-0.67050300
H	-5.79281500	-0.61974100	3.62421800	C	5.27789700	0.45813800	-0.78646200
H	-6.43036200	-3.01328900	3.52636300	H	3.97174100	0.98408300	2.29676700
C	-3.57104700	-0.45229800	-1.29416700	H	7.57944200	2.52531600	0.60534000
C	-3.82044200	0.87014100	-0.75230100	H	5.07797300	-0.05811500	-1.71909900
C	-2.42287000	-0.29869100	-2.12503800	C	3.33122300	-1.76219400	-0.68151400
N	-1.86528300	0.87067800	-1.98257900	C	4.45594300	-2.53725900	-0.39678000
N	-2.70096700	1.60302700	-1.14638500	C	4.63770800	-3.77619900	-0.99951900
C	-2.29292300	2.88039700	-0.73788700	C	3.69360500	-4.26171500	-1.89751800
C	-1.13501100	3.44126000	-1.28837200	C	2.57305800	-3.49348800	-2.19235400
C	-2.99538700	3.58783800	0.24458000	C	2.39541000	-2.25256700	-1.59081400
C	-0.68569100	4.67929900	-0.85203400	H	5.20171200	-2.17465300	0.30248500
H	-0.59047500	2.89427800	-2.04602600	H	3.83474100	-5.22822300	-2.37052500
C	-2.52751700	4.82484300	0.67143100	H	1.52566700	-1.65428400	-1.83151300
H	-3.89735000	3.16467300	0.66212600	H	5.98383300	2.34815900	2.49704000
C	-1.37185900	5.37995100	0.13442700	H	7.10921700	1.30518100	-1.50783200
H	0.21525300	5.09842300	-1.28938800	H	5.52143000	-4.36150300	-0.76661400
H	-3.08078100	5.35815700	1.43818000	H	1.83257400	-3.85811200	-2.89716600
H	-1.01401000	6.34594300	0.47458400	C	-3.26798800	-1.89299200	-1.10597900
O	-4.75456100	1.27565300	-0.06608800	C	-3.61651200	-3.19726800	-0.73798600
C	-4.67214400	-1.45380200	-1.49444200	C	-3.93086600	-1.30174500	-2.18666600

H	-1.60487600	0.36421500	-1.72200200	C	-0.98956800	3.83604200	-0.95245500
H	0.63275300	-2.76172400	-2.30143800	H	0.02940000	2.22097600	-1.94359800
H	-0.77496800	-3.41908600	-1.43570200	C	-0.90402400	4.87032000	-0.02810900
H	-0.72040100	-1.73064400	-3.97976000	H	0.39282100	5.88870600	1.35334000
H	-1.66025800	-3.20721100	-3.71107300	H	-1.92211000	3.65390300	-1.47799100
H	-2.82522200	-0.73257400	-3.40438700	H	-1.76426500	5.49788900	0.17861700
H	-3.25289500	-2.06021100	-2.34300000	O	1.70785100	0.92377000	-2.43127400
C	0.48691300	-0.75854300	-0.61674800	C	4.59077600	-0.27573800	-2.02698600
C	1.70507100	-1.32013000	-0.29340000	H	5.12222700	0.31242700	-2.78542700
H	0.26062300	0.23893000	-0.25998400	H	5.37198100	-0.72612800	-1.40413700
H	1.93349100	-2.34202200	-0.56885300	C	3.89458000	-1.36130000	-2.71991300
C	2.68174900	-0.52444000	0.33488900	C	3.41728900	-2.28676900	-3.31858500
C	-2.64658400	-0.67032300	-0.15453700	H	2.96946500	-3.09482300	-3.85247100
O	-1.90615700	0.18113600	0.69777300	C	5.76245000	1.56842600	0.23892000
Si	-2.23275600	1.09087400	2.06980100	H	5.87562800	2.26562500	1.07110200
C	-3.41052600	2.49706800	1.71152200	H	6.03401600	0.56666900	0.57814600
H	-3.38076200	3.22340100	2.53231700	H	6.47588900	1.85093600	-0.54322100
H	-3.13183600	3.02933800	0.79841600	H	2.31893100	0.39042900	0.79774300
H	-4.44615000	2.16204600	1.60512000				
C	-0.54424200	1.74484700	2.51303200				
H	0.16892500	0.93059100	2.67979300	(S,R)-TS-I-e			
H	-0.14775000	2.38557500	1.71990500	O I			
H	-0.57764600	2.34407800	3.42954500	C	1.87302600	1.09539300	-0.19676200
C	-2.91161600	0.02704800	3.45093400	N	0.59435200	0.90664500	0.48302400
H	-3.09122900	0.64203900	4.34054000	C	0.35171800	1.86267500	1.56033500
H	-3.86232100	-0.44432900	3.18588100	C	1.57946600	2.77764300	1.56367000
H	-2.21468900	-0.76678600	3.73548100	C	2.29839300	2.50337600	0.23365500
C	-4.03878600	-0.06639600	-0.37600000	H	1.67971800	1.04768600	-1.26924700
C	-4.24183400	0.93806300	-1.32477800	H	-0.57014400	2.41189600	1.35122200
C	-5.46891300	1.58020200	-1.43740400	H	0.22546900	1.33438200	2.51002500
C	-6.52055900	1.23511900	-0.59691700	H	1.28673600	3.82464400	1.65154100
C	-6.33108000	0.24311600	0.35731900	H	2.22456100	2.54037000	2.40931800
C	-5.10253700	-0.39776000	0.46534300	H	1.96846400	3.21250600	-0.52771800
H	-3.43932700	1.24718300	-1.98392900	H	3.38130600	2.60065300	0.31922500
H	-7.47832700	1.73755700	-0.68331900	C	-0.30843800	0.01829900	0.08105300
H	-4.97453900	-1.16068300	1.22411100	C	-1.53387700	-0.21415300	0.67234100
C	-2.67212100	-2.09198600	0.42060400	H	-0.00130800	-0.58976700	-0.75844400
C	-3.59519000	-3.05107700	-0.00286000	H	-1.84473500	0.37391600	1.52849100
C	-3.52114100	-4.36420400	0.44843200	C	-2.41734100	-1.15450000	0.11337300
C	-2.51973200	-4.74556400	1.33323100	C	2.87614700	-0.06602400	0.11845300
C	-1.59832600	-3.79899000	1.76612700	O	2.21918700	-1.20937600	-0.39575400
C	-1.67601700	-2.48758500	1.31327000	Si	2.66039000	-2.74309600	-0.90640200
H	-4.39526700	-2.77853100	-0.68154100	C	3.66939100	-2.68019700	-2.47817100
H	-2.46075700	-5.77032200	1.68533800	H	3.79102100	-3.69075300	-2.88577500
H	-0.94246800	-1.76495400	1.64678700	H	3.17240700	-2.07797300	-3.24544900
H	-5.59939500	2.35698100	-2.18375700	H	4.66948400	-2.26522900	-2.32557900
H	-7.14019600	-0.03376300	1.02525100	C	0.99922900	-3.52796800	-1.24826100
H	-4.25294600	-5.08894200	0.10649600	H	0.36469600	-3.53046900	-0.35584200
H	-0.81004300	-4.08024100	2.45704600	H	0.46566100	-2.99940400	-2.04493200
C	3.80725100	-1.13867700	1.07119000	H	1.11338000	-4.56875100	-1.57086800
C	4.45724600	-2.29431100	0.62696500	C	3.56294100	-3.69467600	0.42541900
C	4.22776200	-0.55017900	2.26778500	H	3.76310200	-4.71628200	0.08194900
C	5.50511000	-2.83881300	1.35823300	H	4.52577300	-3.24733800	0.68627500
H	4.15247700	-2.76600300	-0.30160300	H	2.97097200	-3.76738200	1.34269600
C	5.26684700	-1.10219100	3.00541200	C	4.20988200	0.11437700	-0.62080500
H	3.73690700	0.35367500	2.61615500	C	4.28545100	0.79513700	-1.83756700
C	5.91266100	-2.24665700	2.55000900	C	5.47011800	0.83504500	-2.56399600
H	6.00504900	-3.73123200	0.99593300	C	6.60624600	0.19017200	-2.09132900
H	5.57662700	-0.63384300	3.93386100	C	6.54605300	-0.49287600	-0.88267200
H	6.72904000	-2.67682100	3.12081600	C	5.36072200	-0.52867400	-0.15900900
C	3.76209100	0.64712800	-1.17116100	H	3.42014700	1.30169700	-2.24747700
C	2.53713500	1.28365900	-1.60149400	H	7.53008200	0.22006500	-2.65950100
C	4.37263400	1.61187700	-0.29515900	H	5.33771400	-1.07150900	0.77817900
N	3.56356400	2.58680500	0.00535800	C	3.03791600	-0.19262700	1.63551200
N	2.41641700	2.38881600	-0.74612900	C	3.96126200	0.57985300	2.34263900
C	1.31118300	3.23114600	-0.54572200	C	4.03013100	0.51788300	3.72898400
C	1.40370800	4.27910800	0.37694900	C	3.16987400	-0.31497400	4.43591400
C	0.10215800	3.01957100	-1.22012100	C	2.24337100	-1.08458600	3.74262700
C	0.30290800	5.08600600	0.62827400	C	2.17901200	-1.02191400	2.35520000
H	2.33554200	4.44063700	0.90188600	H	4.63644600	1.24157000	1.81140500
				H	3.22246500	-0.36400600	5.51867200

H	1.44581300	-1.61777800	1.82589200	H	2.48791400	2.55384300	1.60760000
H	5.50051300	1.37208100	-3.50637000	C	0.31164000	2.14584400	-1.76005800
H	7.42331200	-1.00342600	-0.49893500	H	0.44864000	1.73715000	-2.76674700
H	4.75839500	1.12507600	4.25680500	H	-0.51269800	1.59954700	-1.29275800
H	1.56318800	-1.73639600	4.28140900	H	-0.00882200	3.18764200	-1.86432500
C	-3.55398600	-1.70031800	0.87402000	C	3.24805400	3.00673700	-1.56485400
C	-4.27574400	-0.93300500	1.79407100	H	2.89340300	4.02641000	-1.75743500
C	-3.91360000	-3.03874500	0.68497700	H	4.13772600	3.08345000	-0.93350800
C	-5.33041000	-1.49244200	2.49935500	H	3.55158200	2.57927200	-2.52528200
H	-4.03686000	0.11405600	1.93153600	C	4.38692700	0.28032600	0.21725100
C	-4.96628100	-3.59950700	1.39490700	C	4.71089300	0.92193600	1.41155500
H	-3.35617900	-3.64539800	-0.02295600	C	5.87658200	1.67509300	1.52437900
C	-5.68044900	-2.82536200	2.30237200	C	6.73962300	1.79636100	0.44401600
H	-5.89010800	-0.88234800	3.20071500	C	6.42731900	1.16103600	-0.75411100
H	-5.23178300	-4.63961100	1.23648400	C	5.26220500	0.41691700	-0.86392700
H	-6.50799600	-3.25862500	2.85483000	H	4.06085100	0.85254600	2.27568800
C	-3.50902800	-0.23500700	-1.62107700	H	7.64912100	2.38134200	0.53311900
C	-3.73654400	1.04924400	-0.97561000	H	5.02368700	-0.05951400	-1.80853100
C	-2.31996200	-0.04722500	-2.39025700	C	3.26177800	-1.75556000	-0.79655700
N	-1.73369300	1.08727000	-2.13594000	C	4.37413100	-2.57140100	-0.58811900
N	-2.57884000	1.77465900	-1.27583800	C	4.50238000	-3.78390700	-1.25501200
C	-2.15293900	3.00816700	-0.76297200	C	3.51557500	-4.20187400	-2.14104100
C	-0.97067400	3.57894900	-1.24854800	C	2.40653200	-3.39247300	-2.35980700
C	-2.85828200	3.66132700	0.25459300	C	2.28263300	-2.17786800	-1.69437400
C	-0.50159000	4.77125500	-0.71697000	H	5.15278900	-2.26149400	0.10048700
H	-0.42366900	3.07362100	-2.03269900	H	3.61469000	-5.14808500	-2.66316200
C	-2.37083300	4.85373400	0.77669800	H	1.42160300	-1.54622100	-1.87418200
H	-3.77699800	3.23130400	0.62524100	H	6.10600200	2.16673500	2.46413000
C	-1.19219700	5.41765300	0.30294400	H	7.08973900	1.25181000	-1.60874000
H	0.41790500	5.19718800	-1.10656900	H	5.37751300	-4.40164700	-1.08074800
H	-2.92752500	5.34467200	1.56886200	H	1.63254400	-3.70433800	-3.05384800
H	-0.81952200	6.34852300	0.71706300	C	-3.32581200	-1.57896400	-1.05294600
O	-4.66286000	1.44569400	-0.27718800	C	-3.67952900	-2.92411600	-0.90737000
C	-4.56622200	-1.22165900	-2.05137200	C	-3.99846700	-0.81043000	-2.00951100
H	-4.79274300	-1.05534200	-3.11189500	C	-4.68858800	-3.47668900	-1.68286400
H	-4.15708500	-2.23870100	-1.99886600	H	-3.18152900	-3.54246600	-0.17039600
C	-5.83484000	-1.21124200	-1.32425300	C	-5.00830700	-1.36320900	-2.78587400
C	-6.90511600	-1.26846400	-0.78433400	H	-3.72970800	0.23279800	-2.13720700
H	-7.84243700	-1.29461300	-0.27603400	C	-5.36006400	-2.69801200	-2.62167200
C	-1.70122900	-1.04119600	-3.31041400	H	-4.95535800	-4.52045900	-1.55228500
H	-0.73080800	-0.68624900	-3.66228100	H	-5.52103200	-0.74955900	-3.51912400
H	-1.56329500	-2.00788100	-2.81454100	H	-6.15083400	-3.13251200	-3.22448300
H	-2.33947100	-1.22049600	-4.18160300	C	-3.37245900	-0.10794600	1.51940800
H	-1.97948600	-1.86443900	-0.58222100	C	-2.50906400	1.05290600	1.51962500
				C	-4.58294300	0.34374300	0.89410100
(S,R)-TS-I-f				N	-4.44431000	1.53026400	0.36894600
0 1				N	-3.18007900	1.97595900	0.72106300
C	2.32425100	-0.79077900	1.33987400	C	-2.69770200	3.18429300	0.19083500
N	1.07949700	-1.52792600	1.11117500	C	-3.23100300	3.67298700	-1.00516600
C	1.12688100	-2.92145900	1.54793100	C	-1.68131500	3.89401000	0.83352600
C	2.52925800	-3.11105400	2.12558000	C	-2.74591000	4.85375700	-1.54985600
C	3.07712200	-1.69183500	2.33163500	H	-4.02685800	3.12554100	-1.49409800
H	2.06597400	0.16410300	1.79924000	C	-1.20067800	5.07010800	0.27122000
H	0.34074900	-3.08257400	2.29343500	H	-1.27049400	3.52085100	1.76044700
H	0.93304200	-3.58843600	0.70312800	C	-1.72417900	5.55810100	-0.92033000
H	2.50167600	-3.67013500	3.06157700	H	-3.16879000	5.22205800	-2.47911900
H	3.15119200	-3.66898600	1.42666700	H	-0.41041000	5.61283100	0.78036500
H	2.86289800	-1.34552800	3.34544400	H	-1.34466500	6.47860500	-1.35120700
H	4.15738600	-1.64815700	2.19546600	O	-1.39827400	1.19439700	2.03606700
C	-0.01454900	-0.98202200	0.59885900	C	-3.17903900	-1.12261200	2.60880200
C	-1.18060500	-1.65290300	0.28261600	H	-2.11145100	-1.37566300	2.63798300
H	0.04368900	0.07839900	0.40727500	H	-3.39670900	-0.66895800	3.58349700
H	-1.26126900	-2.72036200	0.45034500	C	-3.94922400	-2.35875600	2.49132400
C	-2.26260000	-0.93739900	-0.25863500	C	-4.57410100	-3.38205900	2.42458100
C	3.06211600	-0.46068100	-0.00591700	H	-5.13342200	-4.28780800	2.34953200
O	2.19733700	0.36523400	-0.76772800	C	-5.87501900	-0.38618400	0.76115100
Si	1.88013500	2.02281000	-0.75595800	H	-6.56342500	0.19287100	0.14289200
C	1.60171500	2.66555700	0.97684700	H	-5.73313000	-1.36962700	0.30773600
H	1.38082200	3.73741100	0.92678300	H	-6.33560900	-0.54508000	1.74105900
H	0.75257600	2.18322600	1.46927400	H	-2.04050300	0.06758900	-0.60026400

(S,R)-TS-I-g

O 1			
C	-2.83784300	0.44587500	1.36337000
N	-1.58166000	1.12602600	1.04493500
C	-1.53646300	2.51945500	1.48831600
C	-2.89813200	2.76267400	2.14076600
C	-3.45769500	1.36075600	2.42675700
H	-2.58071100	-0.53425100	1.76867200
H	-0.70843100	2.63127300	2.19645100
H	-1.35178900	3.18454500	0.64142500
H	-2.80255700	3.35358000	3.05224600
H	-3.54966200	3.30819100	1.45861300
H	-3.13550500	1.01720200	3.41307500
H	-4.54759000	1.33978000	2.41369200
C	-0.53679600	0.48981000	0.54605500
C	0.67835400	1.05615100	0.19827300
H	-0.67714100	-0.57416100	0.39909900
H	0.82479800	2.12743600	0.27374800
C	1.70539900	0.22824700	-0.25870600
C	-3.69323300	0.18190500	0.07723200
O	-2.82042500	-0.49176800	-0.80446800
Si	-2.73974800	-1.94379000	-1.64002800
C	-3.13216500	-3.39679700	-0.53013500
H	-2.78996000	-4.32824500	-0.99608000
H	-2.63088400	-3.31177100	0.43925800
H	-4.20485700	-3.49995200	-0.34248300
C	-0.95600000	-1.99139700	-2.19282600
H	-0.67333700	-1.06978600	-2.71204500
H	-0.26760500	-2.12469000	-1.35358800
H	-0.78444700	-2.82340300	-2.88470900
C	-3.84645100	-1.94122100	-3.14904700
H	-3.50630500	-2.70345100	-3.85948600
H	-4.89171500	-2.15818700	-2.91603300
H	-3.80858600	-0.97678600	-3.66654100
C	-4.91794800	-0.68928300	0.38323800
C	-5.09529000	-1.37752700	1.58248000
C	-6.17777000	-2.23481500	1.75936900
C	-7.10031600	-2.42098300	0.73920400
C	-6.94021500	-1.73247100	-0.45922400
C	-5.86449700	-0.87312700	-0.62862400
H	-4.39589600	-1.26959500	2.40227100
H	-7.94064500	-3.09331000	0.87678400
H	-5.75799500	-0.33610500	-1.56456500
C	-4.08458600	1.51408600	-0.56806400
C	-5.26098300	2.18161900	-0.22474800
C	-5.54784600	3.43322700	-0.75621900
C	-4.66069300	4.03806100	-1.64007600
C	-3.49066900	3.37620900	-1.99456300
C	-3.20681800	2.12280100	-1.46412700
H	-5.96374000	1.72646100	0.46441000
H	-4.88444900	5.01495600	-2.05609300
H	-2.29719800	1.60672200	-1.74634600
H	-6.29311900	-2.76071900	2.70138000
H	-7.65687700	-1.86145300	-1.26371400
H	-6.46875500	3.93596400	-0.47924400
H	-2.79487100	3.83413900	-2.69025600
C	2.87550100	0.71060900	-0.98624900
C	3.41557800	1.98685700	-0.78692400
C	3.46912400	-0.13526100	-1.93318600
C	4.51147500	2.40721600	-1.52747800
H	2.98892000	2.64956400	-0.04243200
C	4.55884500	0.29073200	-2.67591200
H	3.07176700	-1.13440000	-2.07402400
C	5.08325300	1.56376800	-2.47410300
H	4.92977000	3.39351600	-1.35629000
H	5.01100900	-0.37611400	-3.40201200
H	5.94622800	1.89193400	-3.04379600
C	2.72303100	-0.66408400	1.73647500
C	3.79353800	-1.32882700	1.03681200

C	3.29379200	0.53938000	2.23981500
N	4.52062600	0.72240400	1.83314800
N	4.84688200	-0.40161200	1.09285400
C	6.08235300	-0.43690800	0.43096400
C	6.93414800	0.67140500	0.50733500
C	6.47594000	-1.54666800	-0.32618800
C	8.14417500	0.67108100	-0.17093600
H	6.62962100	1.53012200	1.08975500
C	7.69069400	-1.52827300	-1.00058100
H	5.82148000	-2.40345000	-0.38606600
C	8.53294100	-0.42456200	-0.93536500
H	8.78747100	1.54305500	-0.10236100
H	7.97674500	-2.39617400	-1.58709000
H	9.47899700	-0.41905200	-1.46672900
O	3.82605300	-2.41909900	0.46380300
C	1.51750800	-1.30876300	2.35424200
H	1.75414900	-1.67129800	3.36266200
H	0.74555500	-0.53946500	2.50100200
C	0.90543100	-2.41238600	1.61146300
C	0.34050500	-3.30442800	1.03802000
H	-0.11905400	-4.11654700	0.52058800
C	2.60981900	1.55158500	3.09157700
H	3.26527700	2.40663500	3.26775800
H	1.69116600	1.90640800	2.61144300
H	2.32290100	1.13050300	4.06069800
H	1.45437600	-0.81173100	-0.44478500

(S,R)-TS-I-h

O 1			
C	-2.87757000	0.21201000	1.18783500
N	-1.60851000	0.92816300	1.03073200
C	-1.55100000	2.19497200	1.75911700
C	-2.93783200	2.35496900	2.37629800
C	-3.53776800	0.94283500	2.36695400
H	-2.63975500	-0.82011300	1.45003900
H	-0.76335800	2.12179800	2.51737000
H	-1.29658000	3.01246400	1.08014700
H	-2.88019000	2.76475100	3.38529100
H	-3.54069700	3.03547700	1.77578700
H	-3.28345800	0.41537100	3.28982000
H	-4.62481800	0.95904300	2.29195500
C	-0.54507700	0.40530500	0.44705200
C	0.68256400	1.01868700	0.28614100
H	-0.66932200	-0.59884500	0.06534300
H	0.83317800	2.04112100	0.61135400
C	1.73295600	0.30268200	-0.29933400
C	-3.69298800	0.17031500	-0.14985900
O	-2.87539800	-0.46849200	-1.11635100
Si	-2.58812000	-2.08323700	-1.50064100
C	-2.19665800	-3.11088800	0.01691700
H	-1.90426800	-4.11867700	-0.30071900
H	-1.37260900	-2.71611600	0.61903900
H	-3.06556800	-3.22250600	0.67212300
C	-1.09713600	-1.97113100	-2.61800500
H	-1.31816300	-1.38564000	-3.51614600
H	-0.24369600	-1.49690300	-2.12298400
H	-0.77526900	-2.96602900	-2.94376300
C	-4.01644400	-2.87885700	-2.40361400
H	-3.67596200	-3.81571600	-2.86044800
H	-4.84723400	-3.12292700	-1.73612100
H	-4.40333500	-2.24530400	-3.20717000
C	-5.00330000	-0.61309500	-0.00636600
C	-5.27384600	-1.46309800	1.06442900
C	-6.43653700	-2.22935900	1.09066800
C	-7.34797200	-2.15492100	0.04657700
C	-7.08850800	-1.31025900	-1.02878400
C	-5.92753100	-0.55277000	-1.05342800
H	-4.58549100	-1.54937700	1.89670500
H	-8.25476900	-2.75030600	0.06826500
H	-5.72931900	0.08949200	-1.90456400

C	-3.88171300	-2.83280000	-2.12148700
C	-3.37511500	-3.89792000	-2.34923600
H	-2.93006000	-4.84561900	-2.55616800
C	-1.45255100	-0.92938100	-3.01460900
H	-0.57257100	-0.36616900	-3.33167200
H	-1.12272600	-1.81684200	-2.46770200
H	-1.98033300	-1.28327400	-3.90462200
H	-2.07923300	-1.92805900	-0.17011000

(S,R)-TS-I-j

0 1

C	2.76918500	1.11464000	-0.53007200
N	1.54068800	1.13162200	0.26096600
C	1.67243000	1.87592300	1.50815200
C	2.94746600	2.71062200	1.33457800
C	3.46505300	2.40886500	-0.08180600
H	2.49553400	1.14466000	-1.58666300
H	0.78047700	2.49439400	1.63988800
H	1.74206400	1.18599500	2.35403000
H	2.74033700	3.77429800	1.46017100
H	3.68761200	2.43513600	2.08373600
H	3.18557200	3.20808600	-0.77229400
H	4.54997000	2.32566100	-0.09949400
C	0.41578300	0.55895700	-0.12946100
C	-0.73455700	0.41795700	0.62261200
H	0.43116900	0.15329200	-1.13608400
H	-0.75111100	0.72351000	1.66215100
C	-1.86328200	-0.16050800	0.03647400
C	3.58599100	-0.19493500	-0.27062200
O	3.93884600	-0.17681700	1.09358300
Si	5.30663900	-0.21117400	2.06005000
C	6.09838600	-1.90701000	2.14097200
H	6.65284600	-2.00012700	3.08214800
H	5.34764700	-2.70393700	2.12995300
H	6.80477200	-2.09599300	1.32933400
C	4.62437900	0.18071600	3.75493200
H	4.14681800	1.16306300	3.80702000
H	3.88128500	-0.56469100	4.05725400
H	5.42240000	0.16580900	4.50542600
C	6.56816500	1.05894500	1.52194700
H	7.44370300	1.01226000	2.18001900
H	6.92043200	0.88070100	0.50130500
H	6.17958200	2.08072200	1.57273800
C	2.65248300	-1.38452000	-0.52396600
C	2.05593300	-2.06031800	0.53522000
C	1.10981000	-3.05311100	0.29871200
C	0.74752500	-3.37946500	-1.00171200
C	1.35107900	-2.71762600	-2.06776200
C	2.29870900	-1.73093000	-1.82922900
H	2.31724900	-1.78912900	1.55052300
H	0.00256300	-4.14655300	-1.18593200
H	2.75966000	-1.21993900	-2.66924400
C	4.81305200	-0.31590800	-1.18450500
C	5.22222800	0.66479900	-2.08618600
C	6.36781400	0.48822600	-2.85916300
C	7.11966600	-0.67264100	-2.74681900
C	6.70342100	-1.67247500	-1.87268100
C	5.55751400	-1.49646400	-1.11206400
H	4.66113400	1.58205600	-2.21285400
H	8.01437700	-0.80642500	-3.34579100
H	5.22692200	-2.29681900	-0.45938600
H	0.64465900	-3.56176100	1.13683200
H	1.08259800	-2.97076500	-3.08827500
H	6.66826000	1.26743300	-3.55193500
H	7.26595800	-2.59679200	-1.79094900
C	-2.93977800	-0.77660200	0.81196500
C	-3.32727800	-0.30461000	2.07071300
C	-3.59291600	-1.89588800	0.27965100
C	-4.32801300	-0.95008000	2.78449300
H	-2.85409200	0.57625900	2.49093500

C	-4.58699600	-2.54249500	0.99698700
H	-3.31947700	-2.24971500	-0.70865500
C	-4.95613600	-2.07097200	2.25303200
H	-4.62715500	-0.56925500	3.75543700
H	-5.08615800	-3.40548600	0.56965600
H	-5.74344500	-2.56832200	2.80977500
C	-2.96078400	1.60298300	-1.07670600
C	-4.00781400	0.74017500	-1.56277200
C	-3.52605300	2.28162600	0.04388200
N	-4.72212900	1.83946600	0.33223100
N	-5.03918400	0.90186700	-0.63492300
C	-6.22493700	0.16458800	-0.50120400
C	-7.03231200	0.35975000	0.62438500
C	-6.60569900	-0.78152900	-1.45940600
C	-8.19084900	-0.38499500	0.78970100
H	-6.73396700	1.08685300	1.36699300
C	-7.76738700	-1.52190200	-1.27503200
H	-5.98280000	-0.93452100	-2.32860400
C	-8.56753600	-1.33557100	-0.15385800
H	-8.80147300	-0.22120400	1.67240300
H	-8.04637900	-2.25515900	-2.02567300
H	-9.47280600	-1.91831500	-0.01837000
O	-4.00589600	-0.01223300	-2.54182200
C	-1.87008800	2.02777900	-2.02275500
H	-1.32334100	1.14451400	-2.37765700
H	-2.32462800	2.45284700	-2.92615400
C	-0.89812400	2.99812300	-1.51948400
C	-0.08644800	3.80409800	-1.15164300
H	0.61830700	4.52883400	-0.81013600
C	-2.89454800	3.30393100	0.92738200
H	-3.55171300	3.51034900	1.77476600
H	-1.92936300	2.95190300	1.30416800
H	-2.70698400	4.24069600	0.39666700
H	-1.73840800	-0.56915200	-0.96318000

(S,R)-Int-II

(S,R)-Int-II-a

0 1

C	3.20540500	1.58188400	-0.88924800
N	1.90351400	2.03863800	-0.43621400
C	1.97968500	3.04737500	0.60245100
C	3.41001500	3.60112700	0.51277000
C	4.11229200	2.78413000	-0.59056000
H	3.14039700	1.38901700	-1.96231800
H	1.21836800	3.81393500	0.41791900
H	1.77492800	2.61721500	1.59227200
H	3.40645200	4.66430400	0.26643600
H	3.91965400	3.49312500	1.47021700
H	4.20918300	3.38006300	-1.50068200
H	5.11960700	2.48126100	-0.30347700
C	0.75130600	1.35619500	-0.69302300
C	-0.41131900	1.47346700	-0.02821100
H	0.83471100	0.64855900	-1.51128800
H	-0.48087600	2.12723600	0.83425500
C	-1.58365800	0.60090300	-0.37112700
C	3.63355900	0.20995600	-0.24989600
O	2.71312900	-0.70959700	-0.80921400
Si	2.65775900	-2.36838100	-1.03745300
C	3.88547300	-2.92245400	-2.33534600
H	3.69379200	-3.96790700	-2.60456300
H	3.80063700	-2.32941900	-3.25140200
H	4.92119200	-2.85775100	-1.98962600
C	0.90779000	-2.62607200	-1.63368100
H	0.18734500	-2.28965100	-0.88147800
H	0.70654900	-2.07907200	-2.56030400
H	0.70590700	-3.68519100	-1.82864500
C	2.93188700	-3.32179200	0.54871900
H	2.91159900	-4.39797500	0.33971200
H	3.89592000	-3.10217200	1.01527600
H	2.14995500	-3.11688400	1.28573000

C	5.05168400	-0.20618300	-0.66603200	H	-0.41042900	2.21662500	1.73311900
C	5.55947400	0.13337000	-1.92261600	H	0.01409600	0.90334900	2.84326100
C	6.78662700	-0.35245800	-2.35620800	H	1.60313400	3.17171900	2.58232900
C	7.53322300	-1.19813200	-1.54402800	H	2.26026800	1.59258100	3.01691900
C	7.04032800	-1.54771700	-0.29320200	H	2.22018100	2.92835200	0.29148700
C	5.81385300	-1.05519000	0.13851400	H	3.53460400	2.02011700	1.02704300
H	4.99858200	0.77677900	-2.58985700	C	-0.42791900	-0.07275900	0.26989800
H	8.48994300	-1.58090200	-1.88399600	C	-1.67776500	-0.19271000	0.75206800
H	5.44832600	-1.34657800	1.11612000	H	-0.18082000	-0.54838600	-0.66975500
C	3.44490100	0.28324500	1.26798600	H	-1.96232300	0.28024600	1.68653300
C	4.39257400	0.89558900	2.09052100	C	-2.78097100	-0.85655800	-0.03623600
C	4.16635000	1.04212100	3.45379300	C	2.80521900	-0.47378100	0.29399700
C	2.98531000	0.57632500	4.02186500	O	2.10818100	-1.54765400	-0.32533000
C	2.03615500	-0.03661000	3.21267800	Si	1.89439800	-2.00137100	-1.92694100
C	2.26515700	-0.17825100	1.84898000	C	1.45680700	-0.55354600	-3.03652400
H	5.32239300	1.26228800	1.66894800	H	1.20710000	-0.93002200	-4.03531000
H	2.80927600	0.68756800	5.08699200	H	0.60210400	0.03048400	-2.68567200
H	1.50600900	-0.63420900	1.22749700	H	2.30270400	0.13025800	-3.15711100
H	7.15658200	-0.07140300	-3.33698700	C	0.47257500	-3.20989900	-1.82636800
H	7.60893600	-2.20913900	0.35248800	H	0.75605300	-4.10047300	-1.25595100
H	4.91843800	1.52003100	4.07349400	H	-0.39984400	-2.77459000	-1.32911300
H	1.10842400	-0.40618800	3.63827700	H	0.16262100	-3.54332400	-2.82257300
C	-1.88969800	-0.44040900	0.70203600	C	3.39791300	-2.84554000	-2.64799700
C	-1.79879900	-0.14559200	2.06336500	H	3.12358500	-3.33175800	-3.59195100
C	-2.29157100	-1.72489700	0.33082300	H	4.20567800	-2.14118800	-2.86537700
C	-2.10898200	-1.10151800	3.02352700	H	3.79618600	-3.61966600	-1.98522100
H	-1.47333900	0.83677400	2.38697300	C	4.15003300	-0.29683000	-0.42153600
C	-2.60388300	-2.68413800	1.28791200	C	4.41956000	0.74853600	-1.30315800
H	-2.36745000	-1.97829600	-0.72167100	C	5.62269200	0.80031600	-2.00342000
C	-2.51544000	-2.37499200	2.63972200	C	6.57764900	-0.19186200	-1.83075900
H	-2.03316300	-0.84839400	4.07640100	C	6.32086500	-1.24137600	-0.95298500
H	-2.91605900	-3.67455800	0.97298600	C	5.11952100	-1.29175000	-0.26272700
H	-2.75826700	-3.12118600	3.38920000	H	3.69950300	1.54190600	-1.46371000
C	-2.88597000	1.39744200	-0.76635300	H	7.51563900	-0.14973700	-2.37465100
C	-3.88851700	0.37590200	-1.29696200	H	4.92391700	-2.12280600	0.40622500
C	-3.64915600	1.93967800	0.41166600	C	2.98095600	-0.84016300	1.76639400
N	-4.75117500	1.32317300	0.61324000	C	4.04552900	-0.35204200	2.52412600
N	-4.90843400	0.35273700	-0.37816800	C	4.12540600	-0.60874400	3.88848400
C	-5.97935600	-0.55929900	-0.27608900	C	3.13751600	-1.35741300	4.51742600
C	-6.61437500	-0.72926300	0.95570800	C	2.07523400	-1.85299000	3.76868700
C	-6.39376500	-1.30274500	-1.38283200	C	1.99903100	-1.59779200	2.40476700
C	-7.66063400	-1.63331500	1.07283700	H	4.82278300	0.23931000	2.05240100
H	-6.28495800	-0.15453100	1.81135700	H	3.19694500	-1.55765500	5.58248300
C	-7.43716300	-2.21021400	-1.24474100	H	1.16923200	-1.98470100	1.82690100
H	-5.90380900	-1.17341400	-2.33695400	H	5.80952700	1.62456000	-2.68411900
C	-8.07714800	-2.38140700	-0.02327200	H	7.05616100	-2.02682400	-0.81194000
H	-8.14816100	-1.75672600	2.03437800	H	4.96299900	-0.22068200	4.45933600
H	-7.75255900	-2.78433400	-2.10985700	H	1.29864500	-2.44087000	4.24777100
H	-8.89250400	-3.09022600	0.07422700	C	-3.74135700	-1.59387600	0.88082900
O	-3.77491000	-0.29802400	-2.29788700	C	-4.53065700	-0.93055300	1.82310400
C	-2.55943100	2.45460300	-1.83248400	C	-3.80598900	-2.98584700	0.82306000
H	-1.81636700	3.14851400	-1.43163400	C	-5.36530600	-1.64294000	2.67651200
H	-2.09281200	1.95111000	-2.68467100	H	-4.50401400	0.15188900	1.87832700
C	-3.73959900	3.19063800	-2.27796700	C	-4.63402100	-3.70173200	1.68027700
C	-4.73184300	3.77887900	-2.61129400	H	-3.20081600	-3.51829800	0.09487200
H	-5.61066500	4.30232400	-2.91658500	C	-5.41976300	-3.03121300	2.61015700
C	-3.25189300	3.09654200	1.25595500	H	-5.97514600	-1.10871700	3.39829600
H	-4.03077900	3.30527200	1.99032200	H	-4.66665000	-4.78486700	1.61783500
H	-2.31376500	2.90837200	1.78232100	H	-6.07017400	-3.58600900	3.27875100
H	-3.10500000	3.98630800	0.63632100	C	-3.47125300	0.18367700	-1.02823500
H	-1.32935600	0.05216800	-1.28491800	C	-3.44071500	1.56903100	-0.38183600
				C	-2.51915700	0.41362400	-2.17603600
				N	-1.93275700	1.54825500	-2.11898600
				N	-2.44459200	2.26116500	-1.03504300
				C	-1.73615100	3.39275100	-0.57992700
				C	-0.45142200	3.63432800	-1.07195700
				C	-2.28180200	4.24440100	0.38352900
				C	0.27619900	4.71828500	-0.60121100
				H	-0.02909200	2.97190000	-1.81561900
				C	-1.53201700	5.31580700	0.85408800
(S,R)-Int-II-b							
0 1							
C	1.89488500	0.80075800	0.20282100				
N	0.60029100	0.61227400	0.84115400				
C	0.36739600	1.48021600	1.98142000				
C	1.71716000	2.14006700	2.24498800				
C	2.45186700	2.05353800	0.90263800				
H	1.73765900	0.99582800	-0.86100700				

H	-3.27557200	4.06391600	0.76572300
C	-0.25328400	5.56178600	0.36919900
H	1.27094500	4.89839700	-0.99560700
H	-1.96319300	5.96770200	1.60673000
H	0.32252100	6.40327200	0.73900600
O	-4.13418100	1.97948000	0.52275000
C	-4.90551700	-0.17790200	-1.45254100
H	-5.55104400	-0.10828100	-0.57313100
H	-5.26925100	0.56987400	-2.16439600
C	-5.04539600	-1.50637100	-2.04315200
C	-5.16412800	-2.59525700	-2.53426600
H	-5.27280800	-3.56795900	-2.96003200
C	-2.21880100	-0.54386800	-3.27380300
H	-1.45191200	-0.13006300	-3.92861500
H	-1.87473900	-1.50604800	-2.88446800
H	-3.11549600	-0.74340300	-3.86601800
H	-2.33935900	-1.61407400	-0.68884300

(S,R)-Int-II-c

O 1			
C	-2.21268900	-1.25167800	-1.56761300
N	-0.79112200	-1.14718200	-1.31073800
C	-0.19219300	-2.38597300	-0.85332900
C	-1.20558600	-3.47723700	-1.23337600
C	-2.39559300	-2.74316000	-1.88394800
H	-2.44788400	-0.62864800	-2.43351500
H	0.77775300	-2.51646700	-1.34714100
H	-0.00477300	-2.36998400	0.22822700
H	-0.76673000	-4.19759600	-1.92591800
H	-1.51858200	-4.02994200	-0.34770200
H	-2.37427200	-2.87203700	-2.96836500
H	-3.35693800	-3.12559500	-1.53923300
C	-0.11591800	0.03730100	-1.27780300
C	1.09143700	0.23564300	-0.72362300
H	-0.64087200	0.85942300	-1.75627100
H	1.56416400	-0.56806200	-0.16617700
C	1.78503900	1.57500200	-0.75901400
C	-3.09168200	-0.68055200	-0.39509000
O	-2.82094100	0.71038900	-0.42954100
Si	-3.57588300	2.06463400	0.21272100
C	-5.14417600	2.47261700	-0.72284600
H	-5.51422800	3.45901600	-0.41893200
H	-4.97005600	2.50831000	-1.80305600
H	-5.94560800	1.75130600	-0.53867600
C	-2.28643400	3.39023100	-0.02483000
H	-1.36508400	3.11249100	0.49453000
H	-2.04077100	3.54642900	-1.08006500
H	-2.61687600	4.35129800	0.38373500
C	-3.95131500	1.89667600	2.03806200
H	-4.45083900	2.80827200	2.38765300
H	-4.61396300	1.05829300	2.26719600
H	-3.04045900	1.77519800	2.63106300
C	-4.59211500	-0.88892300	-0.64756600
C	-5.10884000	-0.83088900	-1.94493300
C	-6.47716900	-0.88609400	-2.17679400
C	-7.36541900	-0.99315300	-1.11267700
C	-6.86813900	-1.04765300	0.18300800
C	-5.49705000	-0.99675700	0.40974400
H	-4.44825100	-0.72892000	-2.79750000
H	-8.43469200	-1.03197900	-1.29294300
H	-5.13552100	-1.03555800	1.43012200
C	-2.59896400	-1.27783200	0.92547400
C	-2.99650900	-2.54551300	1.35328500
C	-2.45622100	-3.11373900	2.50117400
C	-1.50315100	-2.42417500	3.24222100
C	-1.09720200	-1.16252700	2.82300600
C	-1.63958400	-0.59868800	1.67497300
H	-3.73526700	-3.10324900	0.78793800
H	-1.08010700	-2.86733800	4.13795500
H	-1.29390900	0.37125700	1.34167700

H	-6.84975100	-0.83938200	-3.19495100
H	-7.54734300	-1.12733100	1.02561800
H	-2.78221600	-4.10025700	2.81506500
H	-0.34813200	-0.61521400	3.38675600
C	1.42490000	2.47719900	0.41508300
C	1.31727900	3.85498100	0.22501300
C	1.13574700	1.95834700	1.67723200
C	0.93826300	4.69691700	1.26526600
H	1.51279100	4.27632400	-0.75708800
C	0.75178900	2.79371400	2.71864000
H	1.20080000	0.88936200	1.84441300
C	0.65192400	4.16740300	2.51732400
H	0.85182500	5.76458900	1.09058500
H	0.52767900	2.37028200	3.69271300
H	0.34529400	4.81799200	3.32997800
C	3.33101500	1.38023000	-0.94572200
C	3.93391400	0.54423700	0.18297100
C	3.56941700	0.46382400	-2.11619600
N	4.09317300	-0.65190900	-1.78283300
N	4.30896600	-0.64575000	-0.40216400
C	4.81084900	-1.81479900	0.20802800
C	4.84734800	-3.00421000	-0.52467800
C	5.25998900	-1.80178300	1.53118900
C	5.33066700	-4.16437000	0.06404700
H	4.50254500	-3.01211200	-1.54990500
C	5.73578000	-2.97471300	2.10476600
H	5.23548100	-0.88587500	2.10251900
C	5.77576300	-4.16025800	1.38145700
H	5.35430700	-5.08070800	-0.51679400
H	6.08226300	-2.95225100	3.13288100
H	6.15117800	-5.07009600	1.83746200
O	4.05924400	0.86279500	1.34423000
C	4.07055500	2.72485300	-1.07188000
H	3.58863500	3.32812200	-1.84730400
H	3.96700600	3.26962100	-0.13026500
C	5.48794300	2.56315000	-1.38599400
C	6.64714700	2.38975000	-1.64539300
H	7.68015000	2.24171500	-1.87018900
C	3.22894900	0.78546000	-3.52429600
H	3.49234800	-0.04661900	-4.17796600
H	2.15790700	0.98616100	-3.62302100
H	3.76680800	1.67926200	-3.85525200
H	1.46440400	2.10690600	-1.66149600

(S,R)-Int-II-d

O 1			
C	3.20590200	-0.61730900	1.67267000
N	1.87627600	-1.19310300	1.82524900
C	1.87933300	-2.64330200	1.77779900
C	3.32318700	-3.05066200	2.09796200
C	4.12502700	-1.73662200	2.18681600
H	3.26638200	0.26716700	2.31057200
H	1.16031200	-3.03203700	2.50742300
H	1.56604900	-3.00545200	0.78828400
H	3.37785700	-3.60150200	3.03855700
H	3.71616200	-3.70409300	1.31841100
H	4.38869700	-1.52172500	3.22438400
H	5.06077600	-1.78873900	1.63019200
C	0.74072600	-0.48873700	1.53964700
C	-0.46068900	-1.00738100	1.23223900
H	0.87850700	0.58642100	1.54023700
H	-0.58715800	-2.08119500	1.15046800
C	-1.57282000	-0.12999500	0.72957600
C	3.50183500	-0.08880200	0.21818900
O	2.67571700	1.05776700	0.10936900
Si	2.64180100	2.43058000	-0.84991800
C	4.07171400	3.57777100	-0.47900300
H	3.90430300	4.54535600	-0.96741700
H	4.16987300	3.76787300	0.59433600
H	5.02925600	3.19188200	-0.83999300

C	1.03280400	3.22486100	-0.33460800
H	0.18862400	2.54111500	-0.46789700
H	1.05440900	3.52092000	0.71876300
H	0.82286200	4.12387800	-0.92440100
C	2.61895300	2.02688600	-2.67652000
H	2.64969700	2.95561400	-3.25854300
H	3.48035100	1.42591200	-2.98163100
H	1.71491400	1.48519700	-2.96956500
C	4.96141400	0.35431300	0.04933900
C	5.65585900	0.93810700	1.11218500
C	6.93019700	1.46074900	0.93491900
C	7.53724600	1.42044600	-0.31543200
C	6.85672300	0.84914700	-1.38303000
C	5.58274500	0.32200700	-1.19974700
H	5.20457300	1.00293800	2.09521300
H	8.53127500	1.83249000	-0.45531100
H	5.06877500	-0.11315300	-2.04884200
C	3.06851100	-1.14957500	-0.79759500
C	3.85678200	-2.27349800	-1.05415600
C	3.40331600	-3.28557300	-1.89129800
C	2.15074900	-3.19205300	-2.49055300
C	1.36164700	-2.07431000	-2.24883900
C	1.82091500	-1.06518000	-1.41063700
H	4.83790900	-2.36385700	-0.60042300
H	1.79614700	-3.98368000	-3.14286900
H	1.18404500	-0.21506800	-1.21138200
H	7.44742800	1.90814300	1.77755400
H	7.31450800	0.81348800	-2.36629800
H	4.03268000	-4.15028700	-2.07661300
H	0.37914900	-1.98287800	-2.70220700
C	-1.97066600	-0.52456100	-0.68603500
C	-2.36553100	-1.82524300	-1.00651500
C	-1.91467300	0.42056300	-1.71052200
C	-2.70094100	-2.16802300	-2.31050300
H	-2.40235000	-2.58968900	-0.23731400
C	-2.23999000	0.07982800	-3.01916000
H	-1.61995400	1.43929400	-1.47924500
C	-2.63717200	-1.21677200	-3.32356600
H	-3.00774400	-3.18422600	-2.53682100
H	-2.18727500	0.83224800	-3.79954500
H	-2.89598600	-1.48512500	-4.34266500
C	-2.81368100	0.00284800	1.68481300
C	-3.81357000	0.93228600	0.99774200
C	-3.64803800	-1.24370300	1.81496300
N	-4.79979000	-1.13053600	1.27083700
N	-4.92296800	0.15446900	0.74658600
C	-6.07091400	0.47109800	-0.01030500
C	-6.88685900	-0.56310500	-0.47468500
C	-6.39786000	1.79769600	-0.30067900
C	-8.01993600	-0.26785200	-1.21946400
H	-6.62940400	-1.58947100	-0.24994800
C	-7.53257000	2.07378200	-1.05408100
H	-5.76907300	2.60133600	0.05345900
C	-8.35055500	1.05001600	-1.51601700
H	-8.64571700	-1.08036600	-1.57416600
H	-7.77702600	3.10764400	-1.27527000
H	-9.23579200	1.27572900	-2.10098500
O	-3.65168800	2.09305500	0.69576500
C	-2.38451400	0.51870100	3.07548400
H	-3.27011500	0.65015400	3.70505900
H	-1.77051200	-0.25523400	3.54507400
C	-1.61562100	1.76049800	3.05868900
C	-0.95702100	2.76410100	3.07100700
H	-0.39110500	3.66865800	3.08125400
C	-3.26531900	-2.48901900	2.53227800
H	-4.07445000	-3.21783400	2.46891000
H	-2.35628400	-2.92931700	2.11795300
H	-3.06555100	-2.27994300	3.58763900
H	-1.19197000	0.89434600	0.67449800

(S,R)-Int-II-e

0 1			
C	-2.53359300	1.30764600	-0.80567800
N	-1.91734700	0.64018600	-1.95417600
C	-2.63331300	1.03189300	-3.16848600
C	-3.02159000	2.48157300	-2.89767800
C	-3.40165400	2.44246600	-1.41518700
H	-1.73674900	1.73896200	-0.19868000
H	-2.00128400	0.89423800	-4.04677600
H	-3.52493100	0.40840500	-3.28473200
H	-2.15344100	3.12795800	-3.06171700
H	-3.83669300	2.83410800	-3.53357400
H	-3.22353000	3.39043300	-0.90587500
H	-4.45929400	2.19969100	-1.30857300
C	-0.54651900	0.51298700	-2.01520300
C	0.32951000	0.52817600	-0.99907500
H	-0.17401100	0.35804000	-3.02598800
H	-0.01786000	0.63808100	0.02129500
C	1.80989800	0.40785700	-1.22771400
C	-3.38896900	0.37334300	0.11213000
O	-4.45093300	-0.08944300	-0.69549100
Si	-5.43977200	-1.44152400	-0.76333100
C	-4.85003900	-2.60652100	-2.10513100
H	-5.66518500	-3.27348100	-2.40863400
H	-4.53274900	-2.05599300	-2.99710500
H	-4.01543200	-3.23617700	-1.78674800
C	-7.10518600	-0.76264100	-1.27671600
H	-7.55974200	-0.12925300	-0.50871500
H	-7.01844800	-0.16373000	-2.18945800
H	-7.80850700	-1.57609800	-1.48616200
C	-5.56879100	-2.33146200	0.87612400
H	-6.39353400	-3.05298500	0.83893200
H	-4.65921100	-2.88629400	1.12215100
H	-5.77397600	-1.64267000	1.70172800
C	-2.61442800	-0.84031300	0.66402700
C	-2.13943700	-1.80178000	-0.23408500
C	-1.56383400	-2.98282500	0.21330700
C	-1.44381800	-3.23401400	1.57645300
C	-1.90405500	-2.28667900	2.48014100
C	-2.48486400	-1.10500000	2.02772300
H	-2.23792200	-1.62319000	-1.29620000
H	-0.99485000	-4.15753700	1.92677900
H	-2.86523200	-0.40633200	2.76160500
C	-3.92317500	1.27270500	1.23567400
C	-3.03797400	1.96509600	2.06926000
C	-3.50571200	2.81122700	3.06495600
C	-4.87413000	2.98649400	3.24900800
C	-5.76155600	2.30934400	2.42442700
C	-5.28742500	1.46357100	1.42488400
H	-1.96648900	1.83446900	1.95499900
H	-5.24185000	3.64835100	4.02622300
H	-5.99341000	0.96399000	0.77511200
H	-1.21105900	-3.71428100	-0.50692700
H	-1.82531200	-2.46708000	3.54736500
H	-2.79827800	3.33498600	3.69979900
H	-6.83147600	2.44119000	2.55038800
C	2.58598300	1.66977900	-0.87075600
C	2.35446300	2.36736300	0.31586300
C	3.58573900	2.13362200	-1.72696800
C	3.10737900	3.48880000	0.64202200
H	1.57660000	2.04000500	0.99741500
C	4.34190200	3.25476600	-1.40404700
H	3.78220700	1.60381200	-2.65360400
C	4.10690200	3.93526800	-0.21547000
H	2.91316800	4.01457400	1.57146000
H	5.11678700	3.59481700	-2.08355400
H	4.69709500	4.80906900	0.04072600
C	2.44242800	-0.85266400	-0.52549400
C	3.92008200	-0.89639800	-0.90666100
C	2.55124800	-0.74060900	0.97146700

H	-6.98613800	-0.12512700	-3.49789200
H	-7.95784800	0.93890300	0.54026200
H	-4.85699400	-3.01537500	3.45115900
H	-1.38019600	-0.52761900	3.83904800
C	3.19557000	-0.52644100	-1.78002300
C	3.92110600	0.44873700	-2.47458900
C	3.81762600	-1.75168400	-1.49484900
C	5.22696500	0.20747400	-2.88168700
H	3.45234500	1.40034000	-2.70161000
C	5.12267100	-1.98495600	-1.89415200
H	3.28941700	-2.51877300	-0.94200600
C	5.83168300	-1.00794700	-2.59021900
H	5.77542900	0.97625300	-3.41550700
H	5.59735000	-2.93029800	-1.65401700
H	6.85699100	-1.19333500	-2.89238700
C	2.19311400	0.93675200	0.65412900
C	3.23985300	0.05979300	1.11451900
C	2.85907600	2.09362700	0.15963200
N	4.15718800	1.95637200	0.16758100
N	4.41509200	0.72258100	0.74521800
C	5.73868800	0.26354500	0.79891500
C	6.76173000	1.04866300	0.25567500
C	6.05621900	-0.97703400	1.36333600
C	8.07161800	0.59209300	0.26535700
H	6.51466000	2.00621400	-0.18200100
C	7.37356900	-1.41917600	1.36182900
H	5.26827000	-1.58384100	1.78455300
C	8.39021800	-0.64696600	0.81225800
H	8.85042800	1.21404500	-0.16525800
H	7.60213800	-2.38631800	1.79931700
H	9.41576500	-1.00135500	0.81492100
O	3.15770200	-1.04067900	1.66362700
C	0.79916200	0.83748800	1.17861500
H	0.06278700	1.02472400	0.38856500
H	0.63350800	-0.19452000	1.50347700
C	0.49820800	1.74062400	2.29151400
C	0.21517700	2.49423000	3.18419300
H	-0.01662500	3.15841600	3.98675600
C	2.22106700	3.32394700	-0.38698200
H	2.98212000	4.02567300	-0.73338700
H	1.56003200	3.08564400	-1.22695100
H	1.60925400	3.82084400	0.37204200

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O 1			
C	-1.41699800	0.54413500	0.32026100
N	-0.63662200	0.85310300	-0.87810900
C	-1.26236200	1.92350700	-1.65546500
C	-2.01568600	2.75727100	-0.61556800
C	-2.02974400	1.91463000	0.67384700
H	-0.72578300	0.19924800	1.09121800
H	-0.49126700	2.48914000	-2.17868900
H	-1.94102300	1.48533500	-2.38974500
H	-1.50346300	3.70402200	-0.44597300
H	-3.02627500	2.98462800	-0.95569600
H	-1.41236800	2.38597800	1.44039000
H	-3.03459900	1.81594400	1.07889700
C	0.58661800	0.41664800	-1.13645100
C	1.28356800	-0.59293000	-0.50444600
H	1.06658000	0.92463900	-1.96938500
H	0.81476500	-1.17565300	0.27456500
C	2.59789800	-0.87350900	-0.89603100
C	-2.48494200	-0.56814100	0.06578400
O	-3.36113000	-0.05877500	-0.91806200
Si	-4.97526400	0.32541600	-1.13399100
C	-4.96361900	1.34733400	-2.69803700
H	-5.98557100	1.62000000	-2.98426500
H	-4.39822500	2.27704100	-2.58912000
H	-4.53113500	0.78859700	-3.53442300
C	-5.67274800	1.31005000	0.29387100

H	-5.59630900	0.77604500	1.24568000
H	-5.18158500	2.28097600	0.40851400
H	-6.73679000	1.50543900	0.11550200
C	-6.03288300	-1.19106700	-1.43965900
H	-6.92411000	-0.90473900	-2.01015900
H	-5.49919200	-1.94201500	-2.03162800
H	-6.37811600	-1.66922000	-0.51983300
C	-1.78525700	-1.80628600	-0.50477200
C	-1.64275400	-1.95712200	-1.88118500
C	-0.91370600	-3.01951600	-2.40452400
C	-0.32815800	-3.95305200	-1.55787200
C	-0.48510600	-3.82153700	-0.18275400
C	-1.20510700	-2.75431500	0.33879600
H	-2.09616300	-1.22934400	-2.54325800
H	0.24684000	-4.77809300	-1.96523100
H	-1.30787500	-2.65902400	1.41501900
C	-3.23665500	-0.95023400	1.34836100
C	-4.19787700	-1.96031400	1.25497600
C	-4.95427300	-2.33814600	2.35367300
C	-4.74680600	-1.72439200	3.58576500
C	-3.76710400	-0.74882000	3.70292900
C	-3.01570800	-0.36615100	2.59374500
H	-4.34450900	-2.46939400	0.30901900
H	-5.33528000	-2.01629000	4.44933100
H	-2.25837800	0.39558700	2.73007700
H	2.96271700	-0.37035100	-1.78773800
H	-0.80130300	-3.11531900	-3.47980600
H	-0.03898700	-4.54863800	0.48767300
H	-5.69983000	-3.11987600	2.25074400
H	-3.58044600	-0.27545000	4.66131400
C	3.21622300	-2.18762700	-0.65270300
C	4.18813900	-2.65184000	-1.54459300
C	2.84375400	-3.01064300	0.41606600
C	4.77492400	-3.89954000	-1.37497500
H	4.48011900	-2.02789400	-2.38376300
C	3.43520300	-4.25307900	0.59127100
H	2.08770800	-2.68072700	1.11913700
C	4.40339200	-4.70256000	-0.30301900
H	5.52426300	-4.24336200	-2.08020100
H	3.13785000	-4.87615600	1.42851600
H	4.86329300	-5.67553600	-0.16481400
C	4.01115800	0.45447700	0.31117800
C	3.55896000	1.62319600	-0.41068600
C	3.29578100	0.48092200	1.54620300
N	2.37187600	1.40021000	1.56155400
N	2.51507600	2.11358100	0.37343500
C	1.77158600	3.29076800	0.19845500
C	1.06562600	3.83110100	1.27881700
C	1.73240400	3.94389200	-1.03876100
C	0.35126400	5.01108500	1.12505500
H	1.09499000	3.32605900	2.23487000
C	1.01350800	5.12538100	-1.17445600
H	2.28617700	3.53576500	-1.87171000
C	0.32129700	5.67094100	-0.09926500
H	-0.18475500	5.41841600	1.97658700
H	0.99985500	5.62366700	-2.13880200
H	-0.23490800	6.59530900	-0.21357100
O	3.91891800	2.06417300	-1.50302600
C	5.37585400	-0.13489200	0.10059400
H	5.41028600	-1.16647600	0.46437300
H	5.59221900	-0.17738900	-0.97137500
C	6.43234900	0.63281700	0.76755800
C	7.28460700	1.26646600	1.32969000
H	8.04139200	1.83500900	1.82274700
C	3.50644700	-0.42186500	2.71142400
H	2.67294800	-0.34968600	3.41297600
H	3.62290700	-1.46196500	2.39916200
H	4.42401700	-0.14375900	3.24072200

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O 1				N	2.35357400	1.15409400	1.56234800
C	-1.37192200	0.98769600	0.50097500	N	2.83600000	1.88757000	0.48169700
N	-0.61252700	1.39111800	-0.68188700	C	2.36246500	3.19215500	0.28100500
C	-0.95839700	2.74376900	-1.14680000	C	1.53677100	3.77963500	1.24490600
C	-1.89389400	3.31032700	-0.07308000	C	2.67451000	3.90666500	-0.88154900
C	-1.80173700	2.32976700	1.10584200	C	1.02573200	5.05348100	1.04165200
H	-0.66665200	0.47377100	1.15329300	H	1.30248000	3.22906000	2.14557500
H	-0.04326400	3.33009600	-1.24392000	C	2.15388700	5.18174000	-1.06749800
H	-1.44324000	2.69058800	-2.12366600	H	3.32395900	3.46090100	-1.62081500
H	-1.58794200	4.31502100	0.21981500	C	1.32413400	5.76435300	-0.11617300
H	-2.91334500	3.37089900	-0.45195500	H	0.38523000	5.49190900	1.80057100
H	-1.02799600	2.65217200	1.80496400	H	2.40310700	5.72282400	-1.97497500
H	-2.73588200	2.25566100	1.66380800	H	0.92061500	6.75935100	-0.27115700
C	0.51391700	0.80201800	-1.07232600	O	4.43137900	1.60057200	-1.21181200
C	1.00714200	-0.42118900	-0.66996600	C	5.00567800	-1.03477100	0.27896200
H	1.08443500	1.37873300	-1.79732700	H	4.71747800	-2.06657700	0.50301900
H	0.40635500	-1.04423800	-0.02468900	H	5.37132500	-1.03130800	-0.75215300
C	2.27283300	-0.85891900	-1.08963400	C	6.10224800	-0.64780500	1.17216100
C	-2.53101300	-0.01696500	0.19225600	C	6.98560500	-0.32182300	1.91857100
O	-1.90164500	-1.09812500	-0.46304500	H	7.77328300	-0.02716500	2.57565000
Si	-2.23444300	-2.72534800	-0.70530400	C	2.75796100	-1.00907800	2.59668700
C	-3.99282600	-3.05507000	-1.26328400	H	1.96464600	-0.69017300	3.27572700
H	-4.02094700	-4.00095800	-1.81710900	H	2.48629000	-1.97378000	2.16121300
H	-4.69997700	-3.14486900	-0.43558100	H	3.66974800	-1.16829500	3.18124700
H	-4.35911700	-2.27593500	-1.93915000				
C	-1.85291700	-3.68719300	0.85348300	(R,R)-TS-I-d			
H	-0.86680800	-3.42906500	1.25322300	O 1			
H	-2.58808900	-3.49813700	1.64191100	C	-1.56326300	0.53825700	-1.14035800
H	-1.85357900	-4.76482300	0.65352300	N	-0.86064300	-0.29139300	-2.11981400
C	-1.07766100	-3.18804900	-2.09477100	C	-1.36822800	-0.11193400	-3.48840500
H	-1.08672200	-4.26962000	-2.27016000	C	-2.54064600	0.85880600	-3.35337500
H	-1.37889200	-2.70241700	-3.02915500	C	-2.30073700	1.56247600	-2.01144800
H	-0.04494700	-2.89632700	-1.89108100	H	-0.79603500	1.02573100	-0.53867800
C	-3.17399400	-0.52775000	1.49470800	H	-0.57034500	0.30886600	-4.10703500
C	-2.46521200	-0.58808100	2.69702100	H	-1.66864100	-1.07215100	-3.91387100
C	-3.01716500	-1.18254500	3.82646700	H	-2.56774500	1.56596800	-4.18374000
C	-4.28900800	-1.73863500	3.77836900	H	-3.48633100	0.31727400	-3.34861400
C	-5.00693400	-1.68675200	2.58966200	H	-1.64744800	2.42580300	-2.15302000
C	-4.45438800	-1.08596700	1.46576200	H	-3.22167300	1.92189400	-1.55034700
H	-1.46657300	-0.17826300	2.78118500	C	0.39258900	-0.72254200	-1.94309700
H	-4.71773300	-2.20531800	4.65906600	C	1.09818200	-0.77976400	-0.76610700
H	-5.03431500	-1.05732500	0.55162300	H	0.86839100	-1.07990800	-2.85186400
C	-3.53792100	0.63370500	-0.76330700	H	0.61782600	-0.48467300	0.15481900
C	-4.60981000	1.40488900	-0.31068500	C	2.45755200	-1.15135000	-0.74156800
C	-5.45948400	2.04097500	-1.20765400	C	-2.46261800	-0.28496300	-0.15797500
C	-5.24802400	1.92261900	-2.57681700	O	-1.60208000	-1.26322000	0.38807500
C	-4.18153200	1.16023600	-3.03853300	Si	-1.47619000	-2.10517900	1.83277800
C	-3.33596700	0.52187200	-2.13836400	C	-0.92879400	-0.96163600	3.20863300
H	-4.78983600	1.51701200	0.75263000	H	-0.59319700	-1.54028500	4.07702300
H	-5.91173500	2.41799200	-3.27796400	H	-0.09016000	-0.33194900	2.89459800
H	-2.50362000	-0.06716900	-2.50352600	H	-1.73322100	-0.29984100	3.54339400
H	2.75956500	-0.28158600	-1.87141200	C	-0.16056400	-3.37882300	1.47403800
H	-2.44350000	-1.21208700	4.74706900	H	-0.45571800	-4.03520200	0.64857800
H	-6.00265500	-2.11438500	2.53296200	H	0.79481700	-2.92063100	1.20769100
H	-6.28884600	2.63197400	-0.83282700	H	0.01300900	-4.01079100	2.35222700
H	-4.00433500	1.05961600	-4.10455800	C	-3.05998700	-2.99472600	2.29701300
C	2.62689200	-2.28977000	-1.09604700	H	-2.82208100	-3.85349700	2.93563400
C	3.55897900	-2.75322900	-2.02943300	H	-3.76188700	-2.36669400	2.85040000
C	2.04149900	-3.21513900	-0.22410100	H	-3.57792000	-3.38321500	1.41408100
C	3.89998100	-4.09868900	-2.08951500	C	-2.99973300	0.60564400	0.97586000
H	4.01703500	-2.04930000	-2.71749800	C	-2.34180800	1.76654900	1.38708300
C	2.38548900	-4.55756400	-0.27851100	C	-2.77044600	2.47483100	2.50435600
H	1.30371000	-2.88908800	0.49962200	C	-3.86253300	2.03589300	3.24098000
C	3.31763400	-5.00494800	-1.21111100	C	-4.52957800	0.88302200	2.84311800
H	4.62253100	-4.43882200	-2.82385600	C	-4.10231700	0.18178800	1.72318000
H	1.92027100	-5.25909000	0.40624800	H	-1.47804500	2.14524900	0.85498200
C	3.58426900	-6.05573000	-1.25437300	H	-4.19215500	2.58735600	4.11540200
H	3.82254100	-0.11614800	0.39200300	H	-4.63768400	-0.71413400	1.43283800
C	3.80924800	1.19063100	-0.23314100	C	-3.57244900	-0.98435800	-0.94915800
C	2.98619700	0.01622900	1.54230300	C	-4.80446800	-0.38046600	-1.20585700

C	-4.37544700	-0.09421100	4.03748900
H	-4.10291400	-0.31897800	5.04459700
C	-5.39052800	0.22677500	-1.59366200
H	-5.22544800	0.28180300	-2.67084200
H	-5.51887900	-0.81971400	-1.30873400
H	-6.32951100	0.74298700	-1.36452100

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0 1

C	-1.44708200	0.97208800	-0.07299000
N	-0.63661600	1.10408000	-1.28260600
C	-1.07726400	2.20385700	-2.15414400
C	-2.21631100	2.88648300	-1.39212700
C	-2.13647400	2.33506900	0.03885500
H	-0.75076900	0.81488400	0.75082700
H	-0.23188500	2.87645200	-2.31664700
H	-1.40181500	1.81333300	-3.12085900
H	-2.10324900	3.97156900	-1.40457500
H	-3.17537000	2.64774100	-1.85138600
H	-1.52015600	2.98326600	0.65940200
H	-3.11626900	2.26740400	0.51268100
C	0.56837800	0.56746500	-1.44043800
C	1.20294700	-0.33161300	-0.60769400
H	1.09795100	0.91841300	-2.32111500
H	0.67409200	-0.73495200	0.24180400
C	2.52508300	-0.72102000	-0.86556100
C	-2.41188800	-0.25906700	-0.10448900
O	-1.57961700	-1.36672600	-0.37277200
Si	-1.61015400	-3.01626400	-0.06967900
C	-1.25543000	-3.33944900	1.73803300
H	-1.04891800	-4.40266600	1.90651700
H	-0.37683500	-2.77964600	2.07502300
H	-2.09466100	-3.05977900	2.38231800
C	-0.23838900	-3.67279400	-1.15002800
H	-0.45988400	-3.50566200	-2.20956600
H	0.72131600	-3.19777300	-0.93537400
H	-0.11175400	-4.75156700	-1.00579200
C	-3.21479500	-3.83449600	-0.59027700
H	-3.02502500	-4.89344500	-0.80150400
H	-3.99233700	-3.79444200	0.17596400
H	-3.61803100	-3.39134100	-1.50642800
C	-3.09245300	-0.45293300	1.26234100
C	-2.53703600	0.02390500	2.45148500
C	-3.10426100	-0.28805500	3.68269600
C	-4.23679800	-1.08851900	3.75338700
C	-4.80531500	-1.56507900	2.57778000
C	-4.23992600	-1.24530400	1.35065200
H	-1.65154200	0.64737600	2.44895900
H	-4.67557500	-1.33489700	4.71466100
H	-4.70228900	-1.62271100	0.44681600
C	-3.41409300	-0.09342300	-1.25244500
C	-4.63087800	0.57183200	-1.09371800
C	-5.47757300	0.77693300	-2.17637700
C	-5.11909300	0.32401900	-3.44115500
C	-3.90961600	-0.33984300	-3.61050600
C	-3.06654000	-0.54668800	-2.52451100
H	-4.92835300	0.93732500	-0.11724200
H	-5.77972000	0.48385700	-4.28707700
H	-2.12389500	-1.06235100	-2.66137000
H	2.92140700	-0.47439600	-1.84540600
H	-2.65149900	0.09787200	4.59015200
H	-5.69371700	-2.18730300	2.61260500
H	-6.42024600	1.29391000	-2.02876300
H	-3.61823300	-0.69979300	-4.59210900
C	3.06938100	-1.95406800	-0.26525000
C	4.07549600	-2.65894800	-0.93152900
C	2.57961500	-2.46991600	0.94142100
C	4.57576200	-3.84762000	-0.41227800
H	4.46093600	-2.27707200	-1.87184900
C	3.07570700	-3.65666300	1.45781300

H	1.81854900	-1.93181000	1.49527900
C	4.07639800	-4.35137900	0.78290900
H	5.35380200	-4.38254200	-0.94699200
H	2.68338400	-4.03961300	2.39422800
H	4.46360500	-5.28065300	1.18766800
C	3.99375100	0.79539800	-0.07844800
C	3.14194200	1.91983500	-0.39513500
C	3.82387900	0.60059300	1.33305900
N	2.86320900	1.32924300	1.82336800
N	2.43006800	2.14637200	0.78240800
C	1.46240300	3.12463300	1.05189700
C	0.83159200	3.14035100	2.30261600
C	1.12882400	4.10557600	0.10924100
C	-0.08782500	4.13401100	2.60914900
H	1.08530300	2.38343600	3.03232100
C	0.20705600	5.09355100	0.43539700
H	1.60877900	4.09497400	-0.85789300
C	-0.40499400	5.12292600	1.68294700
H	-0.55990300	4.13181200	3.58660600
H	-0.02894600	5.85284900	-0.30359600
H	-1.12198700	5.89901100	1.92850400
O	2.95931800	2.50448000	-1.46356100
C	5.28836300	0.48775200	-0.78815000
H	6.04509500	1.23681900	-0.52418800
H	5.67693500	-0.46803300	-0.41874600
C	5.22557000	0.40744400	-2.24887600
C	5.22269100	0.29929300	-3.44520300
H	5.20854700	0.22667400	-4.50983900
C	4.63379800	-0.29190000	2.20953500
H	5.59570500	0.18187500	2.43509500
H	4.11810900	-0.47673300	3.15369400
H	4.84966700	-1.24928500	1.73186800

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C	-1.99000100	-0.69077300	-0.97010200
N	-1.57365100	-2.02091800	-0.50001800
C	-2.34474200	-3.06722800	-1.17392400
C	-2.53943400	-2.49090800	-2.57110700
C	-2.66416200	-0.97781600	-2.33460800
H	-1.07591900	-0.10933800	-1.10617100
H	-1.79330400	-4.00742100	-1.15676500
H	-3.29802500	-3.21589500	-0.66092200
H	-1.65933300	-2.71046000	-3.18124700
H	-3.41367400	-2.90812400	-3.07332400
H	-2.17270200	-0.40800000	-3.12340900
H	-3.70884700	-0.67056600	-2.33061400
C	-0.38470500	-2.28465500	0.03441200
C	0.53012700	-1.38889600	0.54125600
H	-0.12765400	-3.34158300	0.04475500
H	0.26369200	-0.34902500	0.63124300
C	1.85397600	-1.79726900	0.76146500
C	-2.89446700	0.06117800	0.07006300
O	-2.07409500	0.38997400	1.17470600
Si	-1.30484600	1.78125400	1.72172500
C	-0.10208000	2.46213900	0.45426500
H	0.72311200	2.98201300	0.95374400
H	0.33643900	1.69625600	-0.19137100
H	-0.58802100	3.19259400	-0.19883900
C	-0.42962300	1.15350500	3.24712600
H	-1.15695300	0.89614700	4.02488500
H	0.16619300	0.25908900	3.04691500
H	0.24112600	1.91200100	3.66488500
C	-2.49397800	3.13559700	2.22150400
H	-1.95868400	3.87073300	2.83492000
H	-2.91629100	3.66856100	1.36603100
H	-3.32253600	2.75167900	2.82470400
C	-3.48908400	1.34513000	-0.52412500
C	-2.82484300	2.06413900	-1.51942300
C	-3.31658800	3.28453500	-1.96950100

C	-4.48360700	3.81106500	-1.43040500	H	4.19448200	2.75726400	-1.94449200
C	-5.15005900	3.11018200	-0.43161400	H	2.24244700	0.88928100	-3.07278800
C	-4.65343600	1.89398200	0.01796200	H	3.78160300	0.47868900	-2.33996100
H	-1.90462000	1.69121900	-1.95263400	C	0.36356900	1.91825800	0.14877300
H	-4.86867600	4.76222800	-1.78316200	C	-0.61298900	0.96600700	0.34948500
H	-5.17576300	1.37330400	0.81225600	H	0.14198400	2.94637200	0.42251800
C	-3.96677600	-0.91122900	0.57610100	H	-0.41179100	-0.07186200	0.13234500
C	-5.14478600	-1.15892000	-0.13193000	C	-1.87878200	1.34682600	0.81208600
C	-6.04279000	-2.13076600	0.29445400	C	2.98329400	-0.29865400	0.04389000
C	-5.77913400	-2.87365000	1.43925100	O	4.08299300	0.53122800	0.35330500
C	-4.61527000	-2.62592900	2.15827100	Si	5.75223600	0.55893000	0.24078400
C	-3.71963600	-1.65271900	1.73070700	C	6.56912500	-0.44507300	1.59596000
H	-5.38313300	-0.58394700	-1.01920800	H	7.56160600	-0.02987600	1.80674100
H	-6.47909900	-3.63270600	1.77330900	H	5.99768800	-0.40540000	2.52912700
H	-2.81185000	-1.46503500	2.28984100	H	6.70882500	-1.49581700	1.32947200
H	2.03518400	-2.86833200	0.76206000	C	6.16149600	2.36096600	0.51617400
H	-2.78118400	3.82284500	-2.74476700	H	5.72448100	3.00780300	-0.25011700
H	-6.05609700	3.51492300	0.00744000	H	5.80377100	2.70826100	1.49105900
H	-6.95356500	-2.30280900	-0.27015100	H	7.24569200	2.51762400	0.49496900
H	-4.40062400	-3.19282900	3.05873400	C	6.37449900	-0.00030800	-1.43130100
C	2.79549600	-1.03307000	1.59365800	H	7.47100300	-0.00183600	-1.42667400
C	3.81415700	-1.71645600	2.26593500	H	6.05078500	-1.01418900	-1.68399000
C	2.70963400	0.35326900	1.74738600	H	6.05875600	0.66899000	-2.23744000
C	4.71178900	-1.03837300	3.07861400	C	2.18316800	-0.54906900	1.32667600
H	3.89626000	-2.79325100	2.15326400	C	2.27744000	0.33510900	2.39740500
C	3.60596200	1.03325600	2.55905000	C	1.47542100	0.17125800	3.52192800
H	1.94987200	0.91498600	1.21940000	C	0.57420900	-0.88417300	3.59270700
C	4.60943700	0.34078000	3.22847400	C	0.48699700	-1.78132000	2.53401500
H	5.49274100	-1.58659600	3.59524300	C	1.28405800	-1.61262800	1.40926400
H	3.52442100	2.11039900	2.65961300	H	2.97735800	1.16024600	2.34257700
H	5.31140100	0.87408000	3.86119300	H	-0.05681300	-1.00903500	4.46649600
C	2.80468200	-1.70785100	-1.29405400	H	1.19608400	-2.31531900	0.58661900
C	2.33269200	-0.37217500	-1.57988300	C	3.43859500	-1.63947300	-0.54628300
C	4.19864500	-1.54567600	-1.00257200	C	3.11889000	-2.08286700	-1.82742600
N	4.53816000	-0.28934600	-0.92599000	C	3.59987500	-3.30260500	-2.29877300
N	3.41435300	0.44567300	-1.26250900	C	4.40393500	-4.09885100	-1.49587800
C	3.46977600	1.84806600	-1.22106400	C	4.70630800	-3.67903200	-0.20347900
C	4.49176000	2.47171400	-0.49917300	C	4.21813700	-2.46884800	0.26447700
C	2.51301700	2.62973000	-1.87532200	H	2.48916800	-1.49540900	-2.48396800
C	4.54793700	3.85663600	-0.43040500	H	4.78091800	-5.04636600	-1.86640500
H	5.22925300	1.86114000	0.00469300	H	4.43411000	-2.16790100	1.28365100
C	2.57861100	4.01501600	-1.78847200	H	-1.99506900	2.38085900	1.12350200
H	1.72050200	2.14970000	-2.43065000	H	1.55427800	0.87491900	4.34470300
C	3.59028800	4.63934100	-1.06823200	H	-0.21051000	-2.61088600	2.58024900
H	5.34714100	4.32612300	0.13458900	H	3.33914000	-3.62585500	-3.30124900
H	1.82582300	4.60980200	-2.29640800	H	5.31489200	-4.30077600	0.44504400
H	3.63467900	5.72166400	-1.00663500	C	-2.79242300	0.40481100	1.46948000
O	1.21828700	-0.00392200	-1.96304100	C	-3.80183000	0.90194800	2.29831400
C	2.13373300	-2.86784600	-1.97566900	C	-2.68516400	-0.98272000	1.30780000
H	1.05601000	-2.66649700	-1.99166500	C	-4.66359100	0.04251500	2.96929400
H	2.43273900	-2.91199600	-3.03009500	H	-3.90608200	1.97528900	2.42384600
C	2.36222300	-4.18069400	-1.37250200	C	-3.55134100	-1.83987700	1.96575000
C	2.53896800	-5.25941900	-0.87369700	H	-1.93802800	-1.39838800	0.64245600
C	2.70149500	-6.22043100	-0.43826500	C	-4.53989600	-1.33085900	2.80496600
H	5.20210400	-2.61861900	-0.75479000	H	-5.43784100	0.44870100	3.61172600
H	6.15737800	-2.17742300	-0.46461300	H	-3.46628100	-2.91049500	1.81180900
H	4.87283800	-3.29606000	0.03685600	H	-5.21802800	-2.00549400	3.31733500
H	5.35564600	-3.22692200	-1.65180200	C	-3.03942700	1.91792300	-1.11313100
(R,R)-TS-I-h				C	-3.05432500	0.55686000	-1.59387000
0.1				C	-4.35809100	2.14903300	-0.61326600
C	2.09080100	0.51228200	-0.94980700	N	-5.08018100	1.06258900	-0.61766500
N	1.58407200	1.74319100	-0.34288200	N	-4.30587600	0.07415300	-1.19934000
C	2.49471500	2.86108100	-0.58875500	C	-4.79354600	-1.24026500	-1.23205400
C	3.12720900	2.53308600	-1.94485600	C	-6.00426700	-1.53923300	-0.59800600
C	2.85856400	1.03257900	-2.18329800	C	-4.07761700	-2.26655800	-1.85776900
H	1.23835600	-0.10462600	-1.23629900	C	-6.48404800	-2.84064400	-0.58976400
H	1.93312500	3.79567500	-0.59142200	C	-6.54829300	-0.74688500	-0.10227600
H	3.24360100	2.90083000	0.20375400	H	-4.57168100	-3.56581400	-1.83558500
H	2.66713000	3.13274100	-2.73218400	H	-3.14216100	-2.03875100	-2.34776000
				C	-5.77279000	-3.86657900	-1.20448300

H	-7.42321100	-3.05314500	-0.08826200
H	-4.00326200	-4.35133400	-2.32418400
H	-6.15019500	-4.88374400	-1.19229000
O	-2.17241200	-0.07474000	-2.17979400
C	-2.09257100	2.90259000	-1.73267100
H	-1.12288500	2.40456100	-1.85391300
H	-2.41671800	3.15499500	-2.74991000
C	-1.89496500	4.14537400	-0.98667500
C	-1.72072900	5.16291200	-0.37162100
H	-1.57830900	6.07332900	0.16716300
C	-4.92131900	3.41581700	-0.06418300
H	-5.93954500	3.24432300	0.29028800
H	-4.31809000	3.79112700	0.76736700
H	-4.94370900	4.20434000	-0.82216000

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C	2.61047500	0.95136700	-1.40183500
N	1.13139600	0.88342700	-1.33476000
C	0.53249500	1.85149800	-2.26519900
C	1.71786900	2.59895700	-2.87067000
C	2.82108200	2.40198000	-1.83742300
H	2.89831500	0.30141600	-2.23420100
H	-0.05959200	1.33189800	-3.02289400
H	-0.13769300	2.50484300	-1.69969600
H	2.00562400	2.14827300	-3.82460700
H	1.48759000	3.64935700	-3.05000400
H	3.82020300	2.58550600	-2.23008600
H	2.65272900	3.07210000	-0.99287800
C	0.37757500	-0.02006800	-0.72238200
C	-0.97982500	-0.19305400	-0.93380200
H	0.89577900	-0.67778500	-0.03756300
H	-1.50202500	0.43007500	-1.64660600
C	-1.68673500	-1.16335000	-0.21790800
C	3.40435200	0.44818300	-0.16224200
O	3.01656400	-0.88799000	0.11178100
Si	3.32892500	-2.37599400	-0.60999100
C	3.00912000	-2.32267600	-2.45334700
H	3.03597600	-3.34112800	-2.85775200
H	2.02209300	-1.90971100	-2.68646700
C	3.76213500	-1.74383500	-2.99658100
H	2.08107000	-3.48191400	0.22729100
H	2.21770700	-3.47961500	1.31291600
H	1.05458600	-3.16316900	0.01846000
H	2.17758100	-4.51723200	-0.11720500
C	5.06827100	-2.96811700	-0.27949400
H	5.17553800	-4.00380600	-0.62330800
H	5.82141300	-2.37111100	-0.80128800
H	5.30699200	-2.95095200	0.78815500
C	4.92166200	0.44227500	-0.43338600
C	5.48121600	0.45140400	-1.71017800
C	6.85455300	0.30470600	-1.88938400
C	7.69110600	0.13811800	-0.79495100
C	7.14378600	0.11995000	0.48435700
C	5.77645100	0.26985900	0.65930900
H	4.86538500	0.56483100	-2.59379200
H	8.76059400	0.02189500	-0.93558700
H	5.36439500	0.24182900	1.66197300
C	3.08704300	1.28176100	1.08364600
C	3.63304000	2.55760100	1.24937200
C	3.33964800	3.31569100	2.37457500
C	2.50535300	2.80568900	3.36505200
C	1.98178400	1.52859600	3.22128900
C	2.27353800	0.77280900	2.08941000
H	4.31824000	2.95655400	0.50943200
H	2.27817400	3.39620400	4.24659100
H	1.88320600	-0.23230800	2.00291700
H	-1.10435300	-1.79847700	0.44355000
H	7.26553600	0.31893900	-2.89342600
H	7.78374400	-0.01537600	1.35000500

H	3.77455600	4.30399900	2.48321700
H	1.34495900	1.10686400	3.99251400
C	-2.93059000	-1.77364500	-0.70168300
C	-3.27096500	-3.05469700	-0.25389800
C	-3.79271300	-1.12782700	-1.59339900
C	-4.43419800	-3.67572500	-0.68570900
H	-2.61087200	-3.56655600	0.43993100
C	-4.95956000	-1.74468300	-2.02068100
H	-3.56884900	-0.12638100	-1.94310100
C	-5.28468900	-3.01985600	-1.56928900
H	-4.68029000	-4.67021200	-0.32832400
H	-5.62305300	-1.22133800	-2.70089000
H	-6.19946400	-3.49873000	-1.90280100
C	-2.45068100	-0.05748400	1.70012200
C	-2.96971100	1.04329800	0.92859600
C	-3.59865300	-0.81646200	2.08248200
N	-4.68582700	-0.38447100	1.50301700
N	-4.32786800	0.73779400	0.77835100
C	-5.29587100	1.38153100	-0.00405700
C	-6.56651400	0.80838700	-0.13330300
C	-5.01108100	2.57258800	-0.68232700
C	-7.52984300	1.41967200	-0.92277100
H	-6.78109000	-0.11633500	0.38465500
C	-5.98775200	3.16752300	-1.47263800
H	-4.03167800	3.01765200	-0.58323200
C	-7.25077300	2.60191600	-1.60156000
H	-8.50931100	0.95954400	-1.00995200
H	-5.75095900	4.09117200	-1.99200500
H	-8.00681200	3.07459000	-2.21979000
O	-2.37793700	2.01623000	0.45655900
C	-1.14395300	0.09626000	2.41890300
H	-0.46063800	0.64462100	1.75941600
H	-1.26052200	0.73489200	3.30361300
C	-0.50360700	-1.15353500	2.82709800
C	0.03748900	-2.17725800	3.14938700
H	0.51197200	-3.08407500	3.45150400
C	-3.65551500	-1.99562400	2.99327100
H	-4.67281400	-2.39070500	3.02377700
H	-2.98085900	-2.78935500	2.66431400
H	-3.35650900	-1.72199400	4.01012700

(R,R)-TS-I-j

0 1			
C	-2.04154800	-2.23184200	-0.33062500
N	-0.63975800	-2.30422400	0.13154400
C	-0.40478500	-3.39765200	1.07374400
C	-1.79716400	-3.78781100	1.54061600
C	-2.68004300	-3.46687900	0.33332600
H	-2.03572100	-2.32962400	-1.41900700
H	0.09642400	-4.22680300	0.55928500
H	0.24304200	-3.05254900	1.88287500
H	-1.85153200	-4.83890500	1.82666400
H	-2.08713400	-3.18560200	2.40323400
H	-2.66495200	-4.29855800	-0.37624100
H	-3.71803500	-3.29827300	0.61631900
C	0.36540300	-1.63761100	-0.42288200
C	1.70762600	-1.93394700	-0.28000300
H	0.07322000	-0.82192100	-1.06703400
H	2.01216300	-2.79947600	0.29594100
C	2.66657200	-1.13217000	-0.91215100
C	-2.72668400	-0.86335000	-0.01823900
O	-1.92462200	0.12764200	-0.63386700
Si	-1.98915100	1.08958800	-2.01342200
C	-3.04842900	0.38861100	-3.38761200
H	-2.84999600	0.96415800	-4.30030600
H	-2.80815400	-0.65588500	-3.60958700
H	-4.12052100	0.45354800	-3.18665100
C	-0.22300700	1.13916900	-2.63321600
H	0.49907900	1.28439200	-1.82679700
H	0.03915800	0.21911400	-3.16726400

H	-0.09150400	1.96653900	-3.33865200	C	1.36330100	0.63692300	0.38525200
C	-2.58514700	2.78880000	-1.53201800	N	0.59891300	0.39606700	1.61415800
H	-2.35543300	3.52224000	-2.31191300	C	1.15908600	1.17330700	2.71758100
H	-3.66687900	2.80722300	-1.36814200	C	1.57412300	2.46804800	2.03008500
H	-2.10016200	3.12091300	-0.61058300	C	2.01341200	2.02232300	0.62734900
C	-4.15071400	-0.78861700	-0.58362900	H	0.66666400	0.66948500	-0.45357000
C	-4.71635900	-1.75173200	-1.41517700	H	0.40894200	1.31089300	3.49611400
C	-5.98293600	-1.56465800	-1.96279000	H	2.01709000	0.64453400	3.13734100
C	-6.70087400	-0.40850100	-1.69184100	H	0.70625200	3.12884500	1.95896200
C	-6.14705900	0.56042300	-0.85949300	H	2.36356000	2.99451600	2.56990000
C	-4.88873200	0.36688100	-0.31009100	H	1.68515800	2.73510000	-0.12756400
H	-4.18130900	-2.65929600	-1.66688600	H	3.09731900	1.95214100	0.55870900
H	-7.68564000	-0.26192700	-2.12323000	C	-0.64675900	-0.07158300	1.65546600
H	-4.46722700	1.12671200	0.33964400	C	-1.35502300	-0.66255000	0.63165900
C	-2.71816600	-0.62258600	1.49225200	H	-1.11144000	-0.00760600	2.63462700
C	-3.77227300	-1.03823900	2.30702700	H	-0.90592600	-0.77309400	-0.34446400
C	-3.69909900	-0.89719700	3.68831200	C	-2.67869600	-1.07229400	0.82855300
C	-2.57045400	-0.33519800	4.27530500	C	2.40298900	-0.50265600	0.12703100
C	-1.52101400	0.08880500	3.46758800	O	3.29236900	-0.48300900	1.22326200
C	-1.59506000	-0.05355100	2.08691600	Si	4.91955800	-0.27385200	1.55128800
H	-4.66256400	-1.47539400	1.86787000	C	5.84689800	-1.89053700	1.37684400
H	-2.51411600	-0.22198200	5.35330500	H	6.77085500	-1.86042500	1.96570600
H	-0.76596800	0.28339600	1.47897900	H	5.25423700	-2.73471300	1.74426900
H	2.27721900	-0.31592100	-1.51274300	H	6.13064600	-2.10575800	0.34320100
H	-6.40231100	-2.32733000	-2.61084200	C	4.91938800	0.26132400	3.34168600
H	-6.69774600	1.46843700	-0.63640400	H	4.41245200	1.22293200	3.47225100
H	-4.52993200	-1.22392400	4.30561700	H	4.41905000	-0.47104400	3.98328100
H	-0.63520300	0.53717700	3.90725200	H	5.94280100	0.37784100	3.71506400
C	3.97956400	-1.61934300	-1.34686600	C	5.74880700	1.03928900	0.50675200
C	4.67584400	-0.89068800	-2.31882100	H	6.80692100	1.09210700	0.79102300
C	4.56562000	-2.78230800	-0.83268300	H	5.71307600	0.82237600	-0.56410400
C	5.91925700	-1.31358100	-2.76767500	H	5.32736500	2.03659700	0.66419300
H	4.24325300	0.02719200	-2.70269700	C	1.66587600	-1.84651300	0.11900800
C	5.81005400	-3.20222000	-1.28039100	C	1.55291900	-2.59350500	1.28750600
H	4.05508500	-3.36419700	-0.07282200	C	0.79936400	-3.76234300	1.30953300
C	6.49070900	-2.47092900	-2.24951200	C	0.15422300	-4.20297600	0.16003800
H	6.44490300	-0.73577900	-3.52052500	C	0.27617800	-3.47086600	-1.01575000
H	6.25221900	-4.10422300	-0.87023600	C	1.02626200	-2.30188800	-1.03442100
H	7.46329700	-2.80236500	-2.59797600	H	2.05075200	-2.24763000	2.18512600
C	3.51162100	0.39850800	0.67739500	H	-0.43946500	-5.11102300	0.17820400
C	3.02021300	1.54292000	-0.06082200	H	1.10407000	-1.73545500	-1.95725200
C	2.54036100	0.17180500	1.69462000	C	3.15235300	-0.32440800	-1.19894900
N	1.48969600	0.92821200	1.55833100	C	2.98688100	0.76475400	-2.04955000
N	1.73794200	1.76636700	0.47668500	C	3.73684300	0.87630400	-3.21848000
C	0.96515300	2.93772000	0.35394800	C	4.66139800	-0.10137500	-3.55606900
C	0.07338600	3.29363600	1.37072100	C	4.81614300	-1.20922900	-2.72647300
C	1.08430400	3.76307900	-0.76942000	C	4.06192600	-1.31985000	-1.56860900
C	-0.66579400	4.46485800	1.27144300	H	2.27062800	1.54520100	-1.82932500
H	-0.02438400	2.65611300	2.23886800	H	5.24767400	-0.01141100	-4.46461200
C	0.34298300	4.93520400	-0.84907900	H	4.17310500	-2.19993300	-0.94411100
H	1.77051400	3.49253000	-1.55823400	H	-3.02053200	-1.13085500	1.85797000
C	-0.53280700	5.29911200	0.16702100	H	0.71421000	-4.32885600	2.23156200
H	-1.35035100	4.72495900	2.07265600	H	-0.22034100	-3.80674500	-1.92006600
H	0.45392700	5.56787500	-1.72418300	H	3.59048700	1.73661000	-3.86373800
H	-1.11029800	6.21470100	0.09543300	H	5.51957000	-1.99322300	-2.98738500
O	3.53929300	2.17683200	-0.97512400	C	-3.34193800	-2.02565100	-0.07514200
C	4.98153600	0.11754100	0.81475800	C	-4.28227600	-2.91700100	0.45280000
H	5.16297500	-0.94422000	1.01185700	C	-3.04927600	-2.09202200	-1.44178100
H	5.48398800	0.34357300	-0.12970000	C	-4.90909100	-3.85490100	-0.35666000
C	5.60759500	0.90583200	1.88104000	H	-4.51491300	-2.87934900	1.51292900
C	6.10359100	1.55090100	2.76537400	C	-3.68123100	-3.02459100	-2.25189800
H	6.54428400	2.13230200	3.54431800	H	-2.34133800	-1.40102300	-1.88034200
C	2.61549400	-0.85825300	2.76559800	C	-4.61098000	-3.90948300	-1.71387100
H	1.69858900	-0.86691300	3.35768100	H	-5.63067000	-4.54259300	0.07200000
H	2.76678400	-1.85508500	2.34006600	H	-3.44950500	-3.05828200	-3.31141900
H	3.46011500	-0.65910200	3.43289800	H	-5.10163100	-4.63811400	-2.35096900
				C	-4.02457900	0.72981700	0.54942200
				C	-3.37554700	1.18625700	-0.66516400
				C	-3.42561200	1.48722500	1.59662700
				N	-2.39605700	2.17535100	1.18062000

(R,S)-TS-I
(R,S)-TS-I-a
0 1

N	-2.34276800	1.99591800	-0.19445400
C	-1.39048200	2.70351800	-0.94229100
C	-0.88089100	3.90918800	-0.45470200
C	-0.93098600	2.20354100	-2.16375200
C	0.07777000	4.60238200	-1.18124400
H	-1.24197600	4.29251900	0.49118500
C	0.02587800	2.90990600	-2.88219400
H	-1.33666800	1.27768500	-2.54814600
C	0.53878600	4.10899000	-2.39776200
H	0.46606500	5.53753500	-0.79052400
H	0.37694100	2.51147900	-3.82890700
H	1.28819900	4.65341600	-2.96254500
O	-3.60938800	0.92486700	-1.84163600
C	-5.41388100	0.16047900	0.54965500
H	-5.56077700	-0.41462200	-0.36910400
H	-5.54728500	-0.54256400	1.37928500
C	-6.45066900	1.19310100	0.63805300
C	-7.28529900	2.05341200	0.72187600
H	-8.02703100	2.81842200	0.78388200
C	-3.78876300	1.44438500	3.04001000
H	-3.11929900	2.07991300	3.62277000
H	-4.81578400	1.78907200	3.19376900
H	-3.73073200	0.42336900	3.43335800

(R,S)-TS-I-b

0 1			
C	1.34909600	0.44072000	0.75231000
N	0.53822800	-0.20691000	1.79042600
C	1.11618200	0.04418000	3.10902400
C	1.63253000	1.47137900	2.98105100
C	2.08828900	1.56857400	1.51775600
H	0.67358500	0.84973600	-0.00195800
H	0.35700400	-0.08155200	3.88133600
H	1.92699500	-0.66399200	3.29080600
H	0.81139600	2.16834200	3.16731400
H	2.43635000	1.69182400	3.68621800
H	1.84204200	2.54198100	1.09589300
H	3.16606300	1.44173000	1.43396300
C	-0.75298100	-0.51510100	1.65473900
C	-1.47744900	-0.65336400	0.49512100
H	-1.25422000	-0.72058000	2.59674000
H	-0.99832200	-0.51595600	-0.46312200
C	-2.85905300	-0.91061900	0.54909500
C	2.31548200	-0.57456800	0.06119200
O	3.16506900	-1.06522400	1.07704900
Si	4.78958900	-1.13780200	1.46859200
C	4.76944200	-1.34996000	3.32500000
H	5.78766100	-1.46439900	3.71352300
H	4.32713300	-0.48130800	3.82359500
H	4.20304800	-2.23593200	3.62925700
C	5.75157300	0.40862800	1.03428600
H	5.74561000	0.63023500	-0.03609100
H	5.38958700	1.29435900	1.56471000
H	6.79785800	0.26454800	1.33018500
C	5.59898800	-2.62815800	0.67304100
H	6.46626700	-2.94758200	1.26212600
H	4.91069300	-3.47782500	0.61810800
H	5.95572300	-2.42098100	-0.33965100
C	1.48853000	-1.73911500	-0.49279600
C	1.27163000	-2.87746300	0.27710300
C	0.43942600	-3.89281500	-0.18196100
C	-0.17950800	-3.78624700	-1.42180200
C	0.04706400	-2.65962100	-2.20462000
C	0.87272800	-1.64321900	-1.74141100
H	1.74949500	-2.95823600	1.24572200
H	-0.83476500	-4.57471000	-1.77720900
H	1.02938200	-0.76310900	-2.35728700
C	3.11920500	0.05874800	-1.07974100
C	3.03191500	1.39787800	-1.44553200
C	3.81864400	1.90645800	-2.47692200

C	4.70154600	1.08220400	-3.15914600
C	4.77518400	-0.26720400	-2.82140700
C	3.98402100	-0.77022400	-1.80081000
H	2.34511800	2.07037300	-0.94893200
H	5.31727700	1.48060700	-3.95886400
H	4.02635000	-1.82872000	-1.56733800
H	-3.25369600	-1.23076600	1.50967300
H	0.27136700	-4.77014300	0.43479300
H	-0.42826200	-2.56694400	-3.17556100
H	3.73192300	2.95480900	-2.74342600
H	5.44331600	-0.93001700	-3.36173100
C	-3.57984600	-1.46477400	-0.60991300
C	-4.68720200	-2.29300000	-0.39544800
C	-3.17647700	-1.21929400	-1.92738700
C	-5.36547300	-2.86880200	-1.46142900
H	-5.01428400	-2.49069800	0.62018900
C	-3.85418500	-1.79402100	-2.99274000
H	-2.32739000	-0.57828300	-2.12642900
C	-4.95035000	-2.62002500	-2.76525200
H	-6.21845500	-3.51248500	-1.27276100
H	-3.52814600	-1.59122200	-4.00776600
H	-5.47852000	-3.06737100	-3.60110200
C	-3.92977800	1.04335800	0.83749300
C	-3.35166800	1.65045500	-0.34813400
C	-3.11428900	1.50289200	1.91581500
N	-2.03484600	2.10264400	1.48857400
N	-2.14711200	2.18293000	0.11134600
C	-1.16025100	2.84954400	-0.62957800
C	-0.33783800	3.79167400	-0.00803400
C	-0.97581500	2.56166100	-1.98575600
C	0.64647200	4.44447600	-0.73930600
H	-0.47740000	4.00657400	1.04380300
C	0.00819100	3.22740900	-2.70529400
H	-1.61825500	1.83957000	-2.47052400
C	0.82275900	4.17325700	-2.09176400
H	1.27648600	5.17624500	-0.24352500
H	0.14045500	2.99649300	-3.75739500
H	1.58889500	4.68968300	-2.66020300
O	-3.77176600	1.69312600	-1.49934800
C	-5.40081700	0.72796600	0.86208900
H	-5.97973400	1.65759200	0.92477200
H	-5.67498300	0.27346200	-0.09548000
C	-5.82730700	-0.15520300	1.94668100
C	-6.17832200	-0.88121400	2.83702400
H	-6.49663000	-1.52275900	3.62837600
C	-3.29186800	1.24503600	3.37280800
H	-2.47078900	1.69799500	3.93259100
H	-4.23521700	1.65830000	3.73985500
H	-3.31308700	0.17154800	3.58581400

(R,S)-TS-I-c

0 1			
C	1.47215200	-0.99772300	-0.63420800
N	0.71855100	-0.77611200	-1.86939000
C	1.10049300	-1.70567100	-2.94642300
C	2.23112100	-2.54763600	-2.36074500
C	2.07040500	-2.39576200	-0.84365100
H	0.74642800	-0.99959900	0.18003400
H	0.23346200	-2.32356000	-3.19781500
H	1.40536500	-1.15187200	-3.83688300
H	2.15359300	-3.58951800	-2.67461900
H	3.19890900	-2.17193600	-2.69198000
H	1.35953000	-3.13206000	-0.46447300
H	3.00758200	-2.53876700	-0.30513000
C	-0.48649200	-0.20940800	-1.91024700
C	-1.13181100	0.52569100	-0.93971500
H	-0.99542800	-0.34390600	-2.86155200
H	-0.64597200	0.72086900	0.00499400
C	-2.44500900	0.96587900	-1.16057100
C	2.50766200	0.13277300	-0.32053500

O	1.78050900	1.34436600	-0.36969900	H	-7.92252400	-2.74436900	-0.88984900
Si	1.56806900	2.69094400	0.60731600	C	-3.41354100	-1.96421500	-2.92311700
C	0.90047200	2.18114700	2.28064000	H	-2.70716400	-2.70934600	-3.29362200
H	0.39431200	3.02154700	2.76891800	H	-4.42921100	-2.33032700	-3.10084300
H	0.17795800	1.36298500	2.20267900	H	-3.29494400	-1.04714000	-3.51117100
H	1.69961700	1.84419500	2.94812200				
C	0.35231000	3.72646700	-0.35914900	(R,S)-TS-I-d			
H	0.82959600	4.12499100	-1.26143900	O 1			
H	-0.52853300	3.16505900	-0.67413900	C	1.90819300	0.26421000	-1.71891000
H	0.00823500	4.58141300	0.23329900	N	0.50165600	0.60829500	-1.41375500
C	3.12011400	3.72426900	0.80300700	C	0.09564500	1.84844700	-2.07745400
H	2.83388600	4.75794200	1.03133700	C	1.40131700	2.59799000	-2.25194400
H	3.78141000	3.38612900	1.60329400	C	2.39907900	1.47706800	-2.53763100
H	3.69852500	3.75212000	-0.12678800	H	1.89044700	-0.62776400	-2.34776500
C	3.12117500	-0.06537600	1.07506000	H	-0.36793200	1.61751600	-3.04603200
C	2.56629600	-0.90600300	2.04030400	H	-0.62962700	2.38251400	-1.46492500
C	3.09922800	-0.97041800	3.32363200	H	1.35003200	3.33301800	-3.05642900
C	4.19670200	-0.19419500	3.66999300	H	1.65129900	3.11932000	-1.32536500
C	4.76661300	0.64114900	2.71515300	H	2.37037800	1.21607100	-3.59876000
C	4.23612500	0.69697300	1.43390500	H	3.42772200	1.75057500	-2.30886100
H	1.70663000	-1.52724700	1.82386000	C	-0.39934700	-0.27417700	-0.97947600
H	4.60869400	-0.24247200	4.67264300	C	-1.76458600	-0.15617500	-1.15627700
H	4.69932400	1.34687700	0.70052600	H	0.01732800	-1.16271900	-0.51749800
C	3.57463200	0.17716600	-1.41949000	H	-2.15890100	0.70362100	-1.68436400
C	4.75627400	-0.56137200	-1.34332300	C	-2.64972000	-1.14671800	-0.71267200
C	5.65872300	-0.57127400	-2.40036900	C	2.76845300	-0.13794200	-0.48041600
C	5.39228500	0.15627100	-3.55488200	O	2.22281600	-1.38655800	-0.07405500
C	4.22061000	0.90018200	-3.63787400	Si	2.84301400	-2.77007500	0.65847300
C	3.32207800	0.91262700	-2.57712300	C	4.14730200	-3.62234000	-0.37475200
H	4.97946100	-1.14199300	-0.45525900	H	4.33645400	-4.61799900	0.04422100
H	6.09650900	0.14917300	-4.38059600	H	3.82112900	-3.76254800	-1.40975200
H	2.41122800	1.49463900	-2.64195000	H	5.10009300	-3.08732100	-0.39092500
H	-2.80753900	0.90861200	-2.18360600	C	1.33665600	-3.86533900	0.77423700
H	2.64467500	-1.63273500	4.05283800	H	0.56964400	-3.42959400	1.41988200
H	5.62922600	1.25008500	2.96575300	H	0.88924000	-4.04120000	-0.20938300
H	6.57307800	-1.15021900	-2.31937300	H	1.59907800	-4.84267000	1.19365700
H	4.00458500	1.47762900	-4.53124800	C	3.51845200	-2.42000800	2.36691200
C	-3.05332300	2.04582300	-0.37027400	H	3.90838500	-3.34683500	2.80380400
C	-3.99219000	2.88753000	-0.97750700	H	4.33868600	-1.69746300	2.35577400
C	-2.69583400	2.29261000	0.95991400	H	2.74929800	-2.03877800	3.04487100
C	-4.54951000	3.95226700	-0.28273500	C	4.23847800	-0.35008800	-0.88827700
H	-4.27669700	2.71077000	-2.01041600	C	4.58237300	-0.81047100	-2.16176100
C	-3.25341100	3.35555100	1.65473200	C	5.89996800	-1.10764500	-2.48518200
H	-1.98256200	1.65077100	1.45988000	C	6.90498100	-0.96336500	-1.53592300
C	-4.18048500	4.18931000	1.03722800	C	6.57766900	-0.51411300	-0.26296400
H	-5.27020600	4.59878300	-0.77254200	C	5.25900100	-0.20803300	0.05346300
H	-2.96598000	3.53095600	2.68620700	H	3.82534800	-0.95255300	-2.92349700
H	-4.61486500	5.02029100	1.58330800	H	7.93383500	-1.19931400	-1.78694700
C	-3.87257100	-0.73843700	-0.68088600	H	5.02817500	0.14391100	1.05168000
C	-3.36670300	-0.92982100	0.66237500	C	2.64032400	0.88700900	0.65054900
C	-3.19083200	-1.70000300	-1.47516000	C	3.28082000	2.12773700	0.57711500
N	-2.21783700	-2.27767600	-0.82109400	C	3.17915400	3.04476600	1.61385900
N	-2.29327400	-1.80741800	0.48158700	C	2.44412200	2.73417400	2.75462200
C	-1.43133700	-2.32840000	1.45681400	C	1.79943200	1.50814200	2.83347600
C	-0.72587100	-3.50821600	1.20387100	C	1.88832700	0.59978700	1.78302900
C	-1.25606200	-1.67373800	2.68155300	H	3.89190800	2.37741000	-0.28288900
C	0.13287300	-4.02566100	2.16477400	H	2.36989800	3.44702400	3.56930800
H	-0.86166500	-4.01298700	0.25628000	H	1.35895000	-0.34013900	1.84304300
C	-0.40307400	-2.21174800	3.63674600	H	-2.20689200	-2.03847400	-0.27776200
H	-1.80774100	-0.76741700	2.88568600	H	6.13947100	-1.45947000	-3.48333100
C	0.29613100	-3.38804400	3.38987400	H	7.34943700	-0.39782500	0.49087600
H	0.67346600	-4.94244200	1.95138400	H	3.68778900	4.00028200	1.53567400
H	-0.28104300	-1.69409400	4.58286000	H	1.20059900	1.26071100	3.70367100
H	0.96301200	-3.80055400	4.13948300	C	-3.96116900	-1.36160700	-1.33935800
O	-3.73340000	-0.43825900	1.72482600	C	-4.49783500	-2.65463100	-1.35777500
C	-5.22982600	-0.15764000	-0.95037700	C	-4.68587400	-0.32833200	-1.94629800
H	-5.44429100	0.60338600	-0.19485100	C	-5.71953000	-2.91194500	-1.96375200
H	-5.24940700	0.35206100	-1.92033900	H	-3.94841000	-3.46423500	-0.88962400
C	-6.29512700	-1.16399200	-0.92728500	C	-5.90948900	-0.58594300	-2.54770300
C	-7.15720400	-2.00065500	-0.91294000	H	-4.30572800	0.68464900	-1.93581900

C	-6.43134300	-1.87575100	-2.55901600
H	-6.11625300	-3.92180600	-1.96913000
H	-6.46164000	0.22737400	-3.00701200
H	-7.38872200	-2.07180300	-3.03091600
C	-3.40277800	-0.54590700	1.42647900
C	-3.68710800	0.80992600	1.01009300
C	-2.09374300	-0.49270900	1.98368400
N	-1.51716700	0.66021200	1.77044400
N	-2.46814400	1.46968400	1.17115700
C	-2.09281200	2.74983000	0.74004500
C	-0.80165300	3.21281300	1.01627100
C	-2.96351900	3.55446200	-0.00395200
C	-0.39150900	4.45411300	0.55358000
H	-0.12069700	2.58228100	1.56933200
C	-2.53176400	4.79285900	-0.46607200
H	-3.96574000	3.20653800	-0.20907700
C	-1.24828900	5.25381400	-0.19658700
H	0.61635300	4.78986200	0.77773300
H	-3.21760000	5.40346300	-1.04535900
H	-0.92200800	6.22204400	-0.56169200
O	-4.73466100	1.29966700	0.58871700
C	-4.53643300	-1.47123400	1.76918600
H	-5.01080100	-1.14647200	2.70412300
H	-5.31046500	-1.37521400	1.00044400
C	-4.17785800	-2.88259400	1.90514400
C	-3.89278300	-4.04325700	2.02681300
H	-3.64181300	-5.07485000	2.13600900
C	-1.34702400	-1.59070400	2.66071900
H	-0.35535600	-1.24589200	2.95754900
H	-1.87358800	-1.93471500	3.55516400
H	-1.24214700	-2.45840400	2.00471300

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C	1.60171200	-0.84842800	-0.65582400
N	0.86758900	-0.62635500	-1.90261300
C	1.40052200	-1.41186200	-3.02847100
C	2.60108700	-2.16171700	-2.45716500
C	2.37408800	-2.14479100	-0.94112700
H	0.85603700	-0.99834400	0.12651300
H	0.62417900	-2.10294400	-3.36928100
H	1.67099900	-0.75406300	-3.85725700
H	2.65469400	-3.17929900	-2.84664200
H	3.52936100	-1.65575300	-2.72118800
H	1.74719200	-2.98719500	-0.64481200
H	3.30426200	-2.21470900	-0.37667200
C	-0.39612100	-0.20729800	-1.95896800
C	-1.16146700	0.37394500	-0.97119900
H	-0.84608500	-0.32721700	-2.94126700
H	-0.74427700	0.55314200	0.00890100
C	-2.50169900	0.69094600	-1.23208000
C	2.48495700	0.36728000	-0.21771200
O	1.63074200	1.49368000	-0.21113700
Si	1.16320900	2.67977800	0.87858500
C	0.45309500	1.90651000	2.42975500
H	-0.18927100	2.62159300	2.95587200
H	-0.15080500	1.01928700	2.21687500
H	1.24411900	1.60334500	3.12258100
C	-0.10544600	3.65635300	-0.08150600
H	0.37926300	4.20956100	-0.89381200
H	-0.87698100	3.02687300	-0.52700000
H	-0.60419100	4.39000600	0.56113400
C	2.53904500	3.87405600	1.32494000
H	2.09463900	4.83740000	1.60274600
H	3.15396900	3.54520300	2.16527200
H	3.20057500	4.06185600	0.47261500
C	3.07156600	0.12987900	1.18317300
C	2.61567800	-0.86824900	2.04422400
C	3.11488200	-0.98003500	3.33784300
C	4.08012900	-0.09475300	3.79792400

C	4.55138500	0.89963000	2.94702100
C	4.05467000	1.00346600	1.65526000
H	1.86165700	-1.58066000	1.73594200
H	4.46672400	-0.18033200	4.80819100
H	4.43894700	1.77966800	1.00340600
C	3.57836400	0.61660900	-1.26176100
C	4.83503800	0.01561500	-1.18202600
C	5.77180500	0.18789500	-2.19425000
C	5.46517800	0.96364700	-3.30662700
C	4.21826900	1.57312700	-3.39143600
C	3.28453400	1.40247000	-2.37569200
H	5.09046200	-0.59832600	-0.32576600
H	6.19570700	1.09821900	-4.09774700
H	2.31498900	1.88035700	-2.44069900
H	-2.80461800	0.66593700	-2.27525900
H	2.73918900	-1.76618000	3.98475500
H	5.31005500	1.59670500	3.28781100
H	6.74391200	-0.28739800	-2.11174400
H	3.97022500	2.18714600	-4.25148400
C	-3.25428900	1.66095100	-0.42387300
C	-3.05578000	1.80566800	0.95316100
C	-4.16414800	2.50785800	-1.06503600
C	-3.75951800	2.76322900	1.66650600
H	-2.36644500	1.15401300	1.47325300
C	-4.85892200	3.47508200	-0.35279000
H	-4.32159000	2.40953400	-2.13510700
C	-4.66256200	3.60089000	1.01780500
H	-3.60423200	2.85563100	2.73648300
H	-5.55856800	4.12626400	-0.86638300
H	-5.20910200	4.35133900	1.57986200
C	-3.77686600	-1.16951400	-0.92107600
C	-3.23975800	-1.45850400	0.39706000
C	-3.00287800	-1.96666700	-1.81212500
N	-1.97597500	-2.52184100	-1.22517300
N	-2.08991500	-2.20937900	0.11895600
C	-1.18456400	-2.76199900	1.03622000
C	-0.39017900	-3.84853400	0.65848000
C	-1.05231600	-2.23357000	2.32608300
C	0.51485500	-4.39678100	1.55785200
H	-0.48951500	-4.25460200	-0.33977800
C	-0.15168000	-2.80232000	3.21754100
H	-1.67021700	-1.40063900	2.62757500
C	0.63878100	-3.88383700	2.84452400
H	1.12472700	-5.23891100	1.24632500
H	-0.06403800	-2.38177800	4.21425900
H	1.34349900	-4.31924700	3.54498400
O	-3.61430700	-1.13217800	1.51709500
C	-5.18384900	-0.73301100	-1.24509700
H	-5.16366600	-0.03848900	-2.09556000
H	-5.75726600	-1.60094400	-1.59310500
C	-5.94805300	-0.10068500	-0.16968800
C	-6.63825800	0.43106800	0.65548300
H	-7.21848700	0.90355400	1.41567000
C	-3.20503900	-2.09178400	-3.28217800
H	-2.45839000	-2.75965400	-3.71573800
H	-4.19830400	-2.48968400	-3.51178800
H	-3.12910000	-1.11715300	-3.77783800

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C	-2.04748100	-2.20560100	-0.20923200
N	-0.65975200	-2.25065000	0.30643900
C	-0.44997200	-3.32541000	1.27656300
C	-1.85497100	-3.68350300	1.72951100
C	-2.70479500	-3.41342300	0.48708200
H	-1.99629200	-2.35607800	-1.29031700
H	0.04542800	-4.17337700	0.78794200
H	0.19153100	-2.96654400	2.08382500
H	-1.92493700	-4.71908100	2.06429800
H	-2.15972400	-3.03696400	2.55456600

H	-2.67286400	-4.27403500	-0.18644000	H	-1.47556800	4.22468300	2.03638400
H	-3.74924500	-3.23174900	0.73597800	H	-1.46103000	5.91859200	0.21768300
C	0.35328200	-1.59023500	-0.23035400	O	1.30783800	0.45996500	1.79310600
C	1.69887700	-1.90581000	-0.10239400	C	4.18528000	-0.59103800	1.75699900
H	0.07090400	-0.77531400	-0.87954500	H	3.45753500	-1.34530700	2.07636700
H	2.00270500	-2.78406200	0.45528500	H	4.99500500	-1.12441300	1.24937600
C	2.63793100	-1.13183400	-0.78087100	C	4.73905800	0.06473700	2.94610100
C	-2.76340000	-0.83556700	0.00906100	C	5.19720000	0.62144400	3.90750100
O	-1.94694900	0.14779500	-0.60242900	H	5.59672200	1.11858600	4.76321500
Si	-1.94938700	1.02645000	-2.03809100	C	5.59609900	1.35808100	-0.40007100
C	-2.87752900	0.19733700	-3.43696300	H	5.75418200	2.01376700	-1.25888600
H	-2.61847900	0.70989900	-4.37172400	H	6.20616800	1.73043100	0.42993900
H	-2.59591000	-0.85319100	-3.56071900	H	5.96073600	0.35901100	-0.64662000
H	-3.96353300	0.24539800	-3.32695600				
C	-0.14828900	1.12133000	-2.53833700				
H	0.51152200	1.35911100	-1.70148700	(R,S)-TS-I-g			
H	0.19307100	0.18298700	-2.98928100	O 1			
H	-0.00928300	1.90537500	-3.29070400	C	-1.33838300	-0.64804900	0.63430800
C	-2.64416200	2.72717000	-1.72188400	N	-0.53031000	-0.39662400	1.83616300
H	-2.36267400	3.41762500	-2.52438300	C	-0.87463000	-1.34017600	2.90725000
H	-3.73684300	2.71607200	-1.66607600	C	-1.33768900	-2.58484000	2.15040700
H	-2.26241100	3.13842000	-0.78439500	C	-1.93780900	-2.05694200	0.83786700
C	-4.15448900	-0.81157600	-0.63835800	H	-0.65667600	-0.68270600	-0.21603800
C	-4.66591100	-1.82731900	-1.44205500	H	0.00287100	-1.52943700	3.52467400
C	-5.90258300	-1.68688900	-2.06678700	H	-1.65035300	-0.91977300	3.55018200
C	-6.64450300	-0.52598200	-1.90151400	H	-0.46780400	-3.20891700	1.93543500
C	-6.14566900	0.49477000	-1.09681400	H	-2.04694100	-3.17894400	2.73007500
C	-4.91730400	0.34796100	-0.47053100	H	-1.67029100	-2.69302400	-0.00401000
H	-4.11174800	-2.74257400	-1.61105900	H	-3.02542500	-2.02565700	0.86914800
H	-7.60558400	-0.41560000	-2.39288300	C	0.71714700	0.08994300	1.79136900
H	-4.53920900	1.14812800	0.15723300	C	1.35713000	0.71108600	0.74173600
C	-2.84277900	-0.53884100	1.50746800	H	1.25139000	0.01051200	2.73249300
C	-3.95005000	-0.90860300	2.27251600	H	0.85841200	0.84637500	-0.20746800
C	-3.95299500	-0.72336100	3.65065400	C	2.68799400	1.11598900	0.88384000
C	-2.84715900	-0.16603900	4.28354400	C	-2.37958200	0.44761700	0.21062000
C	-1.74284700	0.20696500	3.52537100	O	-2.87968000	-0.10127400	-0.99348700
C	-1.74168000	0.02483300	2.14735300	Si	-4.35417000	-0.39949300	-1.72632900
H	-4.82250600	-1.34477800	1.79830900	C	-5.59112700	-1.21683500	-0.58638000
H	-2.84835800	-0.02171700	5.35937100	H	-6.46599500	-1.52954600	-1.16912800
H	-0.86511400	0.30790600	1.58056400	H	-5.18522700	-2.11452300	-0.10972200
H	2.25066000	-0.29869300	-1.36163900	H	-5.94813200	-0.54829700	0.20181100
H	-6.27936100	-2.49046500	-2.69112900	C	-3.89053200	-1.56780500	-3.10683000
H	-6.71577500	1.40704900	-0.95468500	H	-3.17999200	-1.10698500	-3.80030300
H	-4.82445600	-1.01365000	4.22901500	H	-3.43062800	-2.48035800	-2.71523300
H	-0.86788100	0.63632300	4.00293500	H	-4.77209700	-1.86180600	-3.68723900
C	3.92293800	-1.65306800	-1.26816800	C	-5.08913600	1.16708900	-2.44504900
C	4.50607500	-1.04660100	-2.38669100	H	-5.78588400	0.91793300	-3.25371400
C	4.56453900	-2.75780400	-0.69559100	H	-5.64501900	1.74936900	-1.70544500
C	5.69503100	-1.52656300	-2.91807600	H	-4.31658600	1.81571300	-2.87095400
H	4.02262800	-0.18427000	-2.83559400	C	-3.54145200	0.78090300	1.16073100
C	5.76101000	-3.22832900	-1.21864200	C	-3.92945800	0.02302300	2.26253000
H	4.13502600	-3.25349600	0.16799300	C	-5.05499500	0.36056700	3.01014400
C	6.33001100	-2.61618700	-2.33158300	C	-5.82617000	1.46002000	2.66365900
H	6.13044500	-1.04418500	-3.78684800	C	-5.45308900	2.22973600	1.56623500
H	6.24971400	-4.08031700	-0.75761400	C	-4.32350500	1.89587700	0.83473400
H	7.26283700	-2.98978200	-2.74074600	H	-3.38243400	-0.85786700	2.55775300
C	3.51656300	0.36955200	0.82133900	H	-6.70667600	1.71835600	3.24264700
C	2.21180600	0.90560400	1.08152100	H	-4.04387700	2.51580200	-0.00976000
C	4.15851700	1.33914700	-0.00591200	C	-1.60662000	1.73069300	-0.11329300
N	3.34243500	2.28960100	-0.37807600	C	-1.24826400	2.61980900	0.89913900
N	2.13653100	2.03879900	0.26146200	C	-0.46517700	3.73197500	0.61956700
C	1.14927800	3.04141000	0.24882800	C	-0.03442000	3.97604800	-0.68021000
C	1.14494700	3.98194500	-0.78617500	C	-0.40175500	3.10319900	-1.69697700
C	0.18833400	3.13143900	1.25966800	C	-1.18105600	1.98581900	-1.41429700
C	0.21381000	5.01044900	-0.78922200	H	-1.57275300	2.43666200	1.91811000
H	1.88798200	3.90886600	-1.56981000	H	0.58692400	4.83837700	-0.89823600
C	-0.73937100	4.16622700	1.24076500	H	-1.45325200	1.29764100	-2.20555700
H	0.18151500	2.40387700	2.05813900	H	3.08486100	1.14462600	1.89445700
C	-0.73219500	5.11494000	0.22545200	H	-5.32847600	-0.25110900	3.86376900
H	0.22959900	5.73635200	-1.59622200	H	-6.03973600	3.09712600	1.28151600
				H	-0.18436700	4.40710300	1.42147100

H	-0.07213200	3.28528800	-2.71494500
C	3.33222800	2.05340400	-0.04474800
C	4.30725900	2.93028800	0.44442200
C	2.99243800	2.11604600	-1.40060800
C	4.92013400	3.85270700	-0.39259300
H	4.57724000	2.89355700	1.49568500
C	3.61085900	3.03267600	-2.23824700
H	2.25600100	1.43636500	-1.80783800
C	4.57401500	3.90434000	-1.73880700
H	5.66858200	4.53009200	0.00520000
H	3.34247500	3.06415000	-3.28911200
H	5.05437200	4.62032100	-2.39776900
C	4.02490900	-0.73592700	0.53105900
C	3.32455600	-1.14564300	-0.67026200
C	3.44055500	-1.49336200	1.58169900
N	2.38090100	-2.15122900	1.18487100
N	2.28850200	-1.93966400	-0.18186100
C	1.30970100	-2.62162500	-0.92165900
C	0.88438500	-3.88626600	-0.51244200
C	0.74278300	-2.03248700	-2.05333000
C	-0.10211100	-4.55137500	-1.22846700
H	1.33278000	-4.33771000	0.36417100
C	-0.24165900	-2.70840800	-2.76266400
H	1.07709300	-1.05362000	-2.37084700
C	-0.67080500	-3.96789200	-2.35617200
H	-0.42652300	-5.53396600	-0.90095900
H	-0.68310900	-2.24021300	-3.63619400
H	-1.44231400	-4.48915600	-2.91303000
O	3.52692200	-0.86963700	-1.84943500
C	5.41293500	-0.16677100	0.50253200
H	5.53961200	0.40820300	-0.41940100
H	5.56458800	0.53656700	1.32897700
C	6.45258000	-1.19806800	0.57003600
C	7.29037300	-2.05649100	0.64046000
H	8.03466400	-2.81997200	0.68948900
C	3.84968700	-1.48725700	3.01377900
H	3.18984500	-2.12576800	3.60436300
H	4.87572700	-1.84964700	3.12829800
H	3.81858800	-0.47413300	3.43044300

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C	-1.51507300	1.06354300	0.83389800
N	-0.45569200	1.58602700	-0.02831500
C	-0.37537000	3.05491700	-0.00893400
C	-1.44708700	3.50088700	0.98728800
C	-1.78861400	2.23618300	1.78678900
H	-1.08898100	0.21573700	1.37041500
H	0.62665900	3.34461700	0.31672400
H	-0.54404700	3.45927400	-1.00921000
H	-1.08000300	4.29929200	1.63381400
H	-2.32405200	3.87785200	0.46147300
H	-1.12044800	2.14002300	2.64595300
H	-2.81161700	2.24581800	2.16474300
C	0.62747700	0.88037500	-0.35182300
C	0.80740600	-0.48351200	-0.27441300
H	1.44088500	1.48347700	-0.74716000
H	-0.00137800	-1.11916700	0.05147800
C	2.06764800	-1.04000800	-0.54517700
C	-2.75144500	0.52317600	0.04364500
O	-2.22674300	-0.38983200	-0.89932600
Si	-2.51311700	-1.96547200	-1.39239700
C	-2.38519500	-3.14417600	0.05816100
H	-2.19802600	-4.16550100	-0.29235200
H	-1.56594800	-2.87468500	0.73261400
H	-3.30492000	-3.16241100	0.65106400
C	-1.17308200	-2.26921400	-2.65593400
H	-1.34225200	-1.65497100	-3.54720500
H	-0.17633200	-2.03322900	-2.27961900
H	-1.16926400	-3.31691500	-2.97633700

C	-4.16011000	-2.17174200	-2.26626000
H	-4.09100100	-3.00330700	-2.97747300
H	-4.99180200	-2.38757700	-1.59189600
H	-4.41661100	-1.27831700	-2.84546100
C	-3.73237200	-0.19298300	0.98544200
C	-3.39944600	-0.58257000	2.28283900
C	-4.28479600	-1.32600500	3.05739500
C	-5.52215600	-1.69627300	2.54838600
C	-5.87403400	-1.30201400	1.26173000
C	-4.99023000	-0.55447200	0.49605800
H	-2.44549300	-0.31442600	2.71819600
H	-6.21063300	-2.27964500	3.15080300
H	-5.28497700	-0.24774600	-0.50101200
C	-3.42449800	1.66577800	-0.72316300
C	-4.44171100	2.43935500	-0.16242400
C	-4.97289300	3.52332400	-0.85116000
C	-4.49279800	3.85329400	-2.11372200
C	-3.48331100	3.08513000	-2.68280500
C	-2.95587100	1.99922300	-1.99318700
H	-4.82640800	2.20097200	0.82301200
H	-4.90729100	4.69930200	-2.65233400
H	-2.16949800	1.40144900	-2.43712900
H	2.77631200	-0.39538500	-1.05968300
H	-4.00027000	-1.61523900	4.06395900
H	-6.84137500	-1.57440200	0.85221800
H	-5.76481200	4.11077300	-0.39780300
H	-3.10417400	3.33005600	-3.66990700
C	2.20731100	-2.46656500	-0.90418000
C	3.14410600	-2.82682900	-1.87739600
C	1.39974200	-3.46562800	-0.35124700
C	3.26512700	-4.14591000	-2.29558400
H	3.78125400	-2.06215700	-2.31115400
C	1.52739500	-4.78555100	-0.76112400
H	0.66796900	-3.21463600	0.40770200
C	2.45785000	-5.13079500	-1.73692100
H	3.99245500	-4.40438800	-3.05813200
H	0.89364700	-5.54731600	-0.31879900
H	2.55151100	-6.16221400	-2.06061700
C	3.28975600	-0.95368600	1.30410700
C	3.10338200	0.47516300	1.38805700
C	4.58881200	-1.11015800	0.70856700
N	5.06334200	0.01589400	0.25616000
N	4.15845300	0.99592000	0.62433800
C	4.35593000	2.31452600	0.18391500
C	5.34504900	2.57973200	-0.77026000
C	3.57081000	3.36899000	0.66598700
C	5.54048200	3.87445600	-1.22984100
H	5.95451000	1.76672000	-1.14171000
C	3.77656000	4.65796100	0.18771300
H	2.81213000	3.17131700	1.40859800
C	4.75720100	-4.92386200	-0.76024000
H	6.31372700	4.06002100	-1.96868700
H	3.15895100	5.46379000	0.57228300
H	4.91191300	5.93348900	-1.12568000
O	2.18962200	1.12905500	1.88582500
C	2.74892500	-1.95584400	2.29039600
H	2.90344900	-2.96311100	1.88660700
H	3.34350500	-1.91440100	3.21146300
C	1.33943600	-1.85117900	2.67253900
C	0.19520300	-1.87198200	3.03850000
H	-0.81890500	-1.88113200	3.36986100
C	5.36670900	-2.37583400	0.59759500
H	6.20934900	-2.24754200	-0.08434500
H	5.76068200	-2.66726500	1.57736700
H	4.74613800	-3.20064100	0.24037200

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C	-2.84966400	-0.73332400	-1.57938800
N	-1.65004600	-1.48047500	-1.15952000

C	-1.89802500	-2.92033500	-1.19705400	C	6.65237100	1.19443000	0.36137900
C	-2.88683000	-3.05967400	-2.34703500	C	5.00640300	2.96185500	0.32272100
C	-3.74967900	-1.79788700	-2.23686100	C	7.62342700	2.09801900	-0.04615900
H	-2.52253200	0.00554900	-2.31138200	H	6.90149600	0.15585700	0.53108300
H	-0.97515500	-3.47345800	-1.35852400	C	5.99211200	3.85088800	-0.08993100
H	-2.33016300	-3.23684000	-0.24249900	H	3.98847000	3.29292400	0.46708100
H	-2.33995800	-3.07062300	-3.29384500	C	7.30375700	3.43215700	-0.27793600
H	-3.47386300	-3.97698300	-2.28229300	H	8.64187500	1.74952900	-0.18744100
H	-4.10799400	-1.45594200	-3.20785800	H	5.72250200	4.88813800	-0.26354100
H	-4.62946900	-1.99696600	-1.62691400	H	8.06628000	4.13379000	-0.59956700
C	-0.45168100	-0.91252600	-1.06725200	O	2.35051100	1.89989000	0.87061900
C	0.77275000	-1.54665500	-0.97149400	C	1.12746900	-0.65470300	1.92019900
H	-0.47469000	0.17187200	-1.11929500	H	1.10957900	-0.18575500	2.91210900
H	0.83102800	-2.62652400	-0.93909500	H	0.38884400	-0.10368800	1.32446700
C	1.95112300	-0.78634000	-0.94725200	C	0.66790300	-2.03635900	2.05572100
C	-3.49288300	0.07318500	-0.40393900	C	0.26454500	-3.15954800	2.19022300
O	-2.51710500	1.05781800	-0.10782900	H	-0.09788700	-4.15648300	2.30528500
Si	-2.56499100	2.57856600	0.61685400	C	3.75931000	-2.70867200	1.89719700
C	-3.58750300	3.80738900	-0.35628100	H	4.79853600	-3.03431100	1.82275100
H	-3.40030800	4.81384000	0.03720400	H	3.42010600	-2.85440800	2.92693600
H	-3.30440600	3.81679200	-1.41339500	H	3.14221400	-3.34872200	1.26379000
H	-4.66373900	3.62889400	-0.29805400				
C	-0.78546500	3.12151900	0.56872400	(R,S)-TS-I-j			
H	-0.09213300	2.42644000	1.04936200	0 1			
H	-0.44049600	3.24963700	-0.46289800	C	2.08466500	-0.05326800	-1.51610400
H	-0.66862700	4.09115000	1.06657800	N	0.66189700	0.33400800	-1.36549600
C	-3.19474200	2.47124900	2.37450400	C	0.29097900	1.38655300	-2.31263900
H	-3.22526100	3.47321900	2.81800100	C	1.59995200	2.10972800	-2.55827300
H	-4.20654200	2.06028900	2.43406200	C	2.62166700	0.97551500	-2.53707400
H	-2.54836100	1.85380500	3.00524700	H	2.09759400	-1.04620400	-1.96909400
C	-4.79126300	0.76286900	-0.85244700	H	-0.10076900	0.93725700	-3.23502400
C	-4.95400100	1.20942500	-2.16564600	H	-0.48070600	2.02297300	-1.88153700
C	-6.07648200	1.93646300	-2.54276100	H	1.59801200	2.65828100	-3.50099500
C	-7.06004700	2.24207600	-1.61008700	H	1.78336900	2.81802000	-1.74767500
C	-6.90721700	1.81462800	-0.29702700	H	2.66605000	0.49906000	-3.51993200
C	-5.78467000	1.08474200	0.07482700	H	3.62979200	1.31327700	-2.30593100
H	-4.19859700	1.01152100	-2.91653900	C	-0.26000500	-0.42735500	-0.77862800
H	-7.93553100	2.81209300	-1.90299300	C	-1.61844200	-0.39104100	-1.04155000
H	-5.68475600	0.77301200	1.10739500	H	0.12666600	-1.16485600	-0.08691200
C	-3.69680700	-0.85382900	0.80089700	H	-2.01027400	0.30372900	-1.77515700
C	-4.81364300	-1.68837500	0.91306800	C	-2.48800300	-1.27022900	-0.39002200
C	-4.94363400	-2.57145700	1.97712800	C	2.86866500	-0.20168000	-0.17579800
C	-3.96127500	-2.63320300	2.95944400	O	2.28766100	-1.29348100	0.52501800
C	-2.85043900	-1.80611800	2.86124400	Si	2.47329900	-2.96289100	0.44314100
C	-2.71728800	-0.93320700	1.78676800	C	2.19397700	-3.60523400	-1.29343100
H	-5.61109300	-1.63684000	0.18103500	H	2.19404100	-4.70154200	-1.27956900
H	-4.06515900	-3.31580800	3.79664800	H	1.22561900	-3.28995300	-1.69615400
H	-1.83986100	-0.30434300	1.71346200	H	2.97236400	-3.29519400	-1.99617400
H	1.81752600	0.28940800	-1.03072100	C	1.09677600	-3.57408100	1.54574800
H	-6.17692400	2.26992600	-3.57045700	H	1.17739300	-3.17141300	2.55973000
H	-7.66134000	2.05193500	0.44610000	H	0.11487600	-3.29538900	1.15039300
H	-5.82275500	-3.20447300	2.04232500	H	1.11811000	-4.66670000	1.62210800
H	-2.07420100	-1.84275200	3.61752600	C	4.13047900	-3.53640500	1.08434700
C	3.23724900	-1.28360600	-1.45413700	H	4.11474800	-4.62485400	1.21512400
C	4.17957800	-0.36112000	-1.91600500	H	4.95286800	-3.29872900	0.40428800
C	3.56130200	-2.64538400	-1.48974000	H	4.36227900	-3.09417800	2.05800400
C	5.41272400	-0.78172300	-2.39844000	C	4.35455600	-0.52346700	-0.41955200
H	3.94565500	0.69846600	-1.89441100	C	4.82500000	-1.08450400	-1.60720600
C	4.79398800	-3.06521300	-1.96350400	C	6.15457600	-1.47478200	-1.73608300
H	2.85300800	-3.38422000	-1.13121900	C	7.03786000	-1.31472800	-0.67672200
C	5.72547400	-2.13468200	-2.41852600	C	6.58062800	-0.75953600	0.51370900
H	6.13098400	-0.04771500	-2.74760400	C	5.25477500	-0.36963500	0.63779200
H	5.03333800	-4.12358800	-1.97527400	H	4.16669700	-1.23067700	-2.45487000
H	6.69116200	-2.46646100	-2.78569200	H	8.07445900	-1.61908900	-0.77701200
C	2.47958800	-0.48409700	1.29130600	H	4.91304400	0.05119100	1.57680800
C	2.97595200	0.84911900	1.03349900	C	2.73349500	1.03515900	0.71812900
C	3.65781700	-1.27649900	1.49327300	C	3.36657700	2.23698600	0.39047300
N	4.74682500	-0.60825000	1.23622100	C	3.27534500	3.33981800	1.22845500
N	4.35852800	0.68794000	0.94165500	C	2.56236000	3.25761100	2.42131100
C	5.33250700	1.61997400	0.55116100	C	1.94025000	2.06409500	2.75918200

C	2.02358800	0.96459500	1.91031200
H	3.96676200	2.31381900	-0.50867800
H	2.49410800	4.11807400	3.07889200
H	1.53714100	0.03714000	2.17467700
H	-2.02803400	-2.01611700	0.25336600
H	6.49670700	-1.90501600	-2.67163800
H	7.25825800	-0.63115300	1.35131500
H	3.77667500	4.26285300	0.95526400
H	1.37020400	1.98590200	3.67913300
C	-3.78984600	-1.66804000	-0.93570600
C	-4.56431700	-0.82157500	-1.73785000
C	-4.26369000	-2.95735000	-0.66482700
C	-5.78011000	-1.25528900	-2.24350200
H	-4.23239200	0.18819000	-1.94099800
C	-5.47482500	-3.39359200	-1.18206100
H	-3.66889000	-3.62476500	-0.04793800
C	-6.23942000	-2.54044400	-1.96973200
H	-6.37742000	-0.58394500	-2.85163500
H	-5.82512800	-4.39707600	-0.96385200
H	-7.19143200	-2.87501300	-2.36905100
C	-3.28467500	-0.21938100	1.56594100
C	-3.52353800	1.02564000	0.86793100
C	-1.97387700	-0.09875300	2.10191100
N	-1.35436600	0.96900100	1.67731500
N	-2.27887700	1.66770400	0.91821700
C	-1.86161300	2.82323900	0.24212800
C	-0.57378100	3.32159500	0.47054300
C	-2.68355100	3.46254000	-0.69425800
C	-0.11972000	4.43100400	-0.22668200
H	0.07050100	2.81928400	1.17720600
C	-2.20767200	4.56865500	-1.38955700
H	-3.68323100	3.09131500	-0.86478800
C	-0.92711100	5.06184000	-1.16808200
H	0.88408900	4.79593500	-0.03227400
H	-2.85674800	5.04882800	-2.11554400
H	-0.56596400	5.92583200	-1.71614800
O	-4.52547500	1.46025200	0.30431000
C	-4.30746800	-1.15553300	2.15168900
H	-3.97446000	-2.19328800	2.01664000
H	-4.34740100	-1.00512500	3.23806400
C	-5.67572700	-1.06054100	1.64518200
C	-6.82358200	-1.05819700	1.29505300
H	-7.83327700	-1.02673900	0.95274200
C	-1.30337000	-1.08814600	2.99089300
H	-0.27003000	-0.79945200	3.18522200
H	-1.82328300	-1.16552300	3.95158700
H	-1.30820000	-2.08838900	2.54685100

(S,S)-TS-I

(S,S)-TS-I-a

0 1

C	1.795771	-0.244495	-1.143803
N	0.507620	0.408092	-1.391204
C	0.375805	0.961484	-2.736933
C	1.742053	0.741346	-3.382245
C	2.392618	-0.372506	-2.551054
H	1.592075	-1.221343	-0.704049
H	-0.427207	0.424600	-3.254026
H	0.103722	2.019032	-2.688578
H	1.648343	0.463679	-4.432877
H	2.331861	1.657000	-3.331465
H	2.124319	-1.351869	-2.951869
H	3.480721	-0.304431	-2.549219
C	-0.491884	0.395347	-0.524838
C	-1.712070	1.026172	-0.674735
H	-0.293933	-0.150199	0.388299
H	-1.928168	1.593971	-1.571449
C	-2.673526	0.909432	0.341916
C	2.653748	0.542723	-0.096759
O	1.826113	0.649720	1.042799

Si	1.855941	0.272586	2.675650
C	2.502704	-1.448763	3.009646
H	2.275885	-1.729316	4.044985
H	2.024189	-2.187964	2.360459
H	3.584586	-1.531634	2.874633
C	0.051342	0.381061	3.146555
H	-0.379445	1.342790	2.848466
H	-0.543802	-0.415218	2.687508
H	-0.072633	0.289405	4.231331
C	2.837857	1.545336	3.634938
H	2.555639	1.520795	4.693737
H	3.916482	1.374963	3.583317
H	2.639774	2.557741	3.267637
C	3.939234	-0.211005	0.261455
C	4.159615	-1.545868	-0.071870
C	5.294242	-2.214805	0.377629
C	6.227171	-1.560420	1.170456
C	6.022881	-0.224644	1.503242
C	4.893387	0.440259	1.048073
H	3.448633	-2.096101	-0.675035
H	7.109018	-2.084039	1.524612
H	4.748719	1.482523	1.311280
C	2.937154	1.952466	-0.620920
C	4.068674	2.238728	-1.385533
C	4.255239	3.501935	-1.934395
C	3.308801	4.499932	-1.730123
C	2.181277	4.225920	-0.964078
C	1.999105	2.963072	-0.412002
H	4.815335	1.471668	-1.558834
H	3.452735	5.486373	-2.158905
H	1.121498	2.755821	0.188180
H	5.441220	-3.255674	0.108009
H	6.745741	0.301840	2.117901
H	5.143872	3.705405	-2.523193
H	1.438824	4.998694	-0.791912
C	-3.785602	1.866508	0.477657
C	-4.287749	2.136212	1.754841
C	-4.350236	2.531898	-0.616468
C	-5.327668	3.038994	1.936613
H	-3.853802	1.632537	2.613195
C	-5.395396	3.426585	-0.436519
H	-3.975994	2.349944	-1.617863
C	-5.889543	3.682215	0.840012
H	-5.700912	3.236813	2.935941
H	-5.826538	3.928975	-1.296206
H	-6.706007	4.383363	0.977413
C	-3.839089	-1.014525	0.058520
C	-2.712151	-1.785600	0.537667
C	-3.779945	-1.121520	-1.364631
N	-2.681425	-1.690566	-1.770776
N	-2.012202	-2.108819	-0.622308
C	-0.802933	-2.806241	-0.759305
C	-0.300302	-3.062580	-2.039797
C	-0.073922	-3.230597	0.359167
C	0.901985	-3.738042	-2.194830
H	-0.861476	-2.732937	-2.903328
C	1.129547	-3.903026	0.183122
H	-0.459597	-3.039097	1.349805
C	1.629281	-4.162553	-1.087875
H	1.271611	-3.932275	-3.196821
H	1.682295	-4.226246	1.059546
H	2.568916	-4.690090	-1.213913
O	-2.368324	-2.037683	1.694057
C	-5.092614	-0.857376	0.871050
H	-4.828551	-0.631567	1.908559
H	-5.683465	-0.010372	0.508982
C	-5.930822	-2.060247	0.847682
C	-6.611112	-3.049883	0.808906
H	-7.207671	-3.934394	0.779677
C	-4.796601	-0.628112	-2.332953

H	-4.412394	-0.679933	-3.353403
H	-5.703479	-1.238947	-2.274834
H	-5.092098	0.400499	-2.113339
H	-2.330249	0.502879	1.288846

(S,S)-TS-I-b

0 1

C	-1.854988	0.493848	-1.121812
N	-0.497330	0.066353	-1.477083
C	-0.345436	-0.154658	-2.908596
C	-1.386705	0.784065	-3.508893
C	-2.516649	0.813209	-2.471971
H	-1.763155	1.385929	-0.502667
H	0.672232	0.092593	-3.214758
H	-0.542630	-1.205227	-3.151937
H	-0.951332	1.779079	-3.623936
H	-1.727896	0.447312	-4.488943
H	-3.014916	1.782170	-2.437606
H	-3.275461	0.071264	-2.719044
C	0.477745	-0.050111	-0.588465
C	1.742770	-0.557779	-0.797243
H	0.203273	0.264645	0.410624
H	2.030105	-0.937589	-1.769867
C	2.656223	-0.579085	0.274286
C	-2.576469	-0.581169	-0.239407
O	-1.800511	-0.612947	0.939866
Si	-2.008605	-0.953097	2.566081
C	-3.091320	0.327426	3.389964
H	-3.082115	0.188098	4.477225
H	-2.732361	1.341258	3.186877
H	-4.132521	0.267321	3.059500
C	-0.253800	-0.862573	3.198765
H	0.369725	-1.629271	2.725838
H	0.206009	0.111263	3.000488
H	-0.213369	-1.031470	4.280580
C	-2.701767	-2.669341	2.840366
H	-2.586601	-2.953075	3.893069
H	-3.766914	-2.737025	2.603476
H	-2.175921	-3.419315	2.241144
C	-4.006344	-0.156043	0.112141
C	-4.370907	1.189420	0.181043
C	-5.628268	1.566228	0.638644
C	-6.544178	0.604203	1.046132
C	-6.192548	-0.739465	0.986798
C	-4.937398	-1.112548	0.522496
H	-3.674226	1.968315	-0.104262
H	-7.523961	0.898941	1.407389
H	-4.680209	-2.164880	0.486387
C	-2.497860	-1.943452	-0.938458
C	-3.422822	-2.334337	-1.909109
C	-3.267825	-3.528473	-2.604184
C	-2.183347	-4.356978	-2.340396
C	-1.261959	-3.983551	-1.368999
C	-1.420587	-2.789404	-0.675718
H	-4.288367	-1.715748	-2.118192
H	-2.061696	-5.289360	-2.882125
H	-0.692909	-2.506708	0.074220
H	-5.887297	2.619166	0.682681
H	-6.895852	-1.502637	1.303791
H	-4.002346	-3.812435	-3.350880
H	-0.412493	-4.621582	-1.147159
C	3.817926	-1.487755	0.266368
C	4.442040	-1.899016	-0.916542
C	4.294611	-1.989121	1.481521
C	5.526436	-2.761684	-0.880283
H	4.086605	-1.535905	-1.874340
C	5.377182	-2.858224	1.518192
H	3.805406	-1.697457	2.405941
C	6.002485	-3.240331	0.337932
H	6.005003	-3.062816	-1.806499

H	5.734564	-3.233583	2.471327
H	6.852417	-3.914418	0.363883
C	3.654459	1.413361	0.477945
C	2.437417	2.000500	1.006658
C	3.672839	1.805144	-0.901727
N	2.553818	2.367083	-1.262966
N	1.787941	2.508635	-0.109890
C	0.520490	3.104590	-0.202482
C	0.038802	3.497900	-1.455466
C	-0.285207	3.284443	0.928431
C	-1.223732	4.061598	-1.571367
H	0.659624	3.351691	-2.328584
C	-1.547241	3.851167	0.792649
H	0.082358	2.982060	1.897906
C	-2.028945	4.242539	-0.451309
H	-1.579988	4.359835	-2.552457
H	-2.159836	3.984426	1.678671
H	-3.015340	4.684154	-0.546842
O	2.016809	1.998304	2.165341
C	4.807930	1.248283	1.436228
H	5.035903	2.222186	1.887131
H	4.487263	0.616735	2.271728
C	6.048729	0.704336	0.889122
C	7.088939	0.271439	0.474090
H	8.005083	-0.123576	0.096203
C	4.737668	1.571976	-1.918393
H	4.369963	1.852657	-2.907501
H	5.627250	2.168764	-1.698282
H	5.054852	0.527838	-1.935819
H	2.240824	-0.411070	1.264684

(S,S)-TS-I-c

0 1

C	-1.846249	0.538079	-0.619620
N	-0.531622	0.149607	-1.126245
C	-0.402504	0.246223	-2.578060
C	-1.729150	0.837863	-3.058734
C	-2.451919	1.320394	-1.791655
H	-1.684529	1.186773	0.241976
H	0.454200	0.890834	-2.799820
H	-0.207826	-0.739615	-3.008525
H	-1.562124	1.660798	-3.755303
H	-2.313726	0.078724	-3.577658
H	-2.260214	2.380909	-1.628892
H	-3.531586	1.190478	-1.861901
C	0.484281	-0.171502	-0.345785
C	1.716621	-0.627528	-0.771578
H	0.315518	-0.040311	0.715677
H	1.891253	-0.808532	-1.824369
C	2.740181	-0.828320	0.165755
C	-2.659676	-0.702604	-0.116937
O	-1.905935	-1.306831	0.919164
Si	-1.755681	-1.012527	2.570892
C	-1.370707	0.779252	2.944613
H	-1.326382	0.906989	4.033162
H	-0.400133	1.096800	2.551830
H	-2.139680	1.465309	2.577389
C	-0.301492	-2.086588	3.035342
H	-0.500995	-3.143779	2.833235
H	0.598215	-1.807462	2.477043
H	-0.067552	-1.990641	4.101128
C	-3.279727	-1.521976	3.525331
H	-3.046562	-1.537242	4.596715
H	-4.111269	-0.826291	3.382383
H	-3.626251	-2.522655	3.250634
C	-4.035804	-0.304077	0.430315
C	-4.354959	0.999770	0.807826
C	-5.578343	1.289776	1.406025
C	-6.504135	0.280622	1.633407
C	-6.197313	-1.024539	1.260853

C -4.975293 -1.310443 0.670649
 H -3.659664 1.815141 0.645771
 H -7.457740 0.507632 2.098724
 H -4.742393 -2.334865 0.401361
 C -2.764187 -1.724687 -1.251324
 C -3.783042 -1.661118 -2.202556
 C -3.811377 -2.544916 -3.274716
 C -2.817933 -3.507825 -3.413546
 C -1.803294 -3.584062 -2.466150
 C -1.778534 -2.700544 -1.392961
 H -4.566276 -0.916391 -2.110799
 H -2.839657 -4.199291 -4.249731
 H -0.989687 -2.766000 -0.653979
 H -5.804192 2.312013 1.691389
 H -6.909032 -1.824252 1.437864
 H -4.613995 -2.479863 -4.002317
 H -1.026319 -4.336218 -2.559135
 C 3.899485 -1.684467 -0.149374
 C 4.380077 -1.838498 -1.455765
 C 4.516171 -2.407862 0.876118
 C 5.446487 -2.683918 -1.723282
 H 3.932828 -1.279440 -2.270343
 C 5.583728 -3.256210 0.608251
 H 4.150317 -2.307029 1.892052
 C 6.054182 -3.395403 -0.691942
 H 5.808373 -2.785531 -2.741159
 H 6.046849 -3.809288 1.418670
 H 6.889017 -4.055415 -0.903547
 C 3.752145 1.161051 0.615011
 C 2.500500 1.809681 0.942494
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 C 0.724138 3.616975 -1.828627
 C 0.017742 3.455808 0.473644
 C -0.380518 4.409380 -2.107113
 H 1.439234 3.379337 -2.604207
 C -1.084821 4.247988 0.175240
 H 0.180725 3.097720 1.478833
 C -1.293536 4.735951 -1.109518
 H -0.524574 4.775561 -3.118749
 H -1.784326 4.489770 0.969743
 H -2.155217 5.356335 -1.331934
 O 1.851888 1.809174 1.991130
 C 4.830411 0.846615 1.619603
 H 5.556248 0.160499 1.168147
 H 5.392445 1.758495 1.857773
 C 4.378032 0.256239 2.880886
 C 4.064998 -0.247347 3.925117
 H 3.763067 -0.679367 4.852925
 C 5.299998 1.359856 -1.479691
 H 5.145180 1.525801 -2.547595
 H 6.063251 2.065840 -1.134392
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 H 2.452257 -0.818582 1.213371

(S,S)-TS-I-d
01

C 2.757224 -0.312176 -1.543629
 N 1.428156 0.300106 -1.475345
 C 1.189754 1.306371 -2.510531
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 C 3.247286 0.077982 -2.941988
 H 2.624172 -1.390245 -1.451661
 H 0.338673 0.985506 -3.119693
 H 0.936241 2.265738 -2.052162
 H 2.303376 1.433082 -4.377946
 H 3.069479 2.245793 -3.017067
 H 2.987145 -0.722887 -3.638103

H 4.329704 0.203505 -2.980518
 C 0.505475 -0.071526 -0.604834
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 H -1.032851 1.352671 -1.050743
 C -1.602482 -0.000733 0.533628
 C 3.650520 0.123169 -0.330921
 O 2.917583 -0.338698 0.786434
 Si 3.225004 -0.704047 2.394481
 C 4.326054 -2.204893 2.558528
 H 4.337570 -2.545178 3.600644
 H 3.958427 -3.036948 1.949629
 H 5.361170 -2.008747 2.267144
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 H 0.834655 -0.241973 2.900323
 H 1.078162 -1.957888 2.524896
 H 1.535340 -1.323912 4.105011
 C 3.940440 0.757729 3.312126
 H 4.122434 0.489459 4.359330
 H 4.892934 1.095933 2.895422
 H 3.255239 1.610637 3.307244
 C 5.019344 -0.572816 -0.352549
 C 5.205599 -1.812612 -0.965718
 C 6.416598 -2.488403 -0.862095
 C 7.466884 -1.940084 -0.137339
 C 7.295385 -0.707129 0.480961
 C 6.085086 -0.034675 0.373202
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 H 8.410794 -2.468599 -0.054789
 H 5.972885 0.922858 0.867652
 C 3.754587 1.650381 -0.299881
 C 4.733607 2.333509 -1.024017
 C 4.757493 3.722197 -1.055841
 C 3.796329 4.454622 -0.367748
 C 2.815239 3.784922 0.353359
 C 2.796265 2.395006 0.386122
 H 5.487424 1.781163 -1.574003
 H 3.814264 5.539320 -0.391491
 H 2.023199 1.884581 0.947263
 H 6.534765 -3.450071 -1.350609
 H 8.104482 -0.265041 1.053037
 H 5.530243 4.231888 -1.621997
 H 2.058357 4.343533 0.894426
 C -2.721642 0.754283 1.096502
 C -3.270559 1.877258 0.459179
 C -3.256113 0.354715 2.325949
 C -4.312754 2.577215 1.042790
 H -2.900889 2.191240 -0.509762
 C -4.293868 1.065873 2.915691
 H -2.845160 -0.515155 2.827933
 C -4.824728 2.177614 2.275769
 H -4.739337 3.432810 0.530329
 H -4.694180 0.741321 3.870377
 H -5.644780 2.726444 2.726754
 C -2.723023 -1.795534 -0.549243
 C -3.638280 -0.919692 -1.232706
 C -3.459592 -2.342315 0.537688
 N -4.648434 -1.814988 0.645419
 N -4.781207 -0.939133 -0.420790
 C -5.914897 -0.116914 -0.483908
 C -6.849807 -0.153116 0.556274
 C -6.116573 0.763838 -1.552757
 C -7.953319 0.686915 0.532111
 H -6.689720 -0.830591 1.383760
 C -7.225890 1.601085 -1.558224
 H -5.397019 0.792287 -2.357846
 C -8.149460 1.576274 -0.519862
 H -8.664331 0.647659 1.351778
 H -7.364437 2.282469 -2.392215
 H -9.011642 2.235050 -0.531781

O -3.475067 -0.252904 -2.256498
C -1.540341 -2.415292 -1.222730
H -1.116420 -1.688840 -1.923591
H -0.752613 -2.645649 -0.494714
C -1.865893 -3.641981 -1.956523
C -2.142853 -4.652854 -2.544305
H -2.398244 -5.543842 -3.073602
C -2.969314 -3.351758 1.517348
H -3.722674 -3.538052 2.284949
H -2.735173 -4.299779 1.022858
H -2.051738 -3.008865 2.008574
H -1.197943 -0.769634 1.185348

(S,S)-TS-I-e

0 1

C 2.627185 0.455594 -1.544484
N 1.284618 0.917404 -1.192680
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C 2.248855 2.720970 -2.391900
C 3.055595 1.436561 -2.640688
H 2.531622 -0.561159 -1.926822
H 0.111133 2.210632 -2.335065
H 0.721532 2.914942 -0.829736
H 2.012796 3.235878 -3.323856
H 2.808235 3.413799 -1.764118
H 2.796323 1.008124 -3.611653
H 4.131583 1.614628 -2.640739
C 0.398308 0.146642 -0.580583
C -0.861418 0.526193 -0.162453
H 0.733921 -0.864424 -0.389900
H -1.204829 1.540133 -0.320733
C -1.695115 -0.423859 0.444664
C 3.545289 0.360394 -0.277716
O 2.848009 -0.542862 0.554146
Si 3.180111 -1.632947 1.780642
C 4.216799 -3.059263 1.158945
H 4.257444 -3.851571 1.915404
H 3.789354 -3.496957 0.251020
H 5.246593 -2.768344 0.933597
C 1.471826 -2.229274 2.246216
H 0.842065 -1.405327 2.597093
H 0.966138 -2.702048 1.398010
H 1.519412 -2.970925 3.051328
C 3.991286 -0.806187 3.247641
H 4.068463 -1.513844 4.081164
H 5.002583 -0.453367 3.029274
H 3.407676 0.050669 3.598204
C 4.926136 -0.221332 -0.610994
C 5.145465 -1.028200 -1.727755
C 6.373007 -1.650316 -1.931229
C 7.405813 -1.481969 -1.018316
C 7.202888 -0.677611 0.097477
C 5.977714 -0.054977 0.294421
H 4.364294 -1.193436 -2.459623
H 8.361521 -1.970958 -1.175636
H 5.841294 0.569205 1.169695
C 3.628210 1.731116 0.398454
C 4.578045 2.679686 0.014763
C 4.582352 3.950465 0.576065
C 3.631248 4.297289 1.529567
C 2.680810 3.360714 1.917909
C 2.680623 2.088479 1.356203
H 5.324333 2.429684 -0.731277
H 3.633755 5.289481 1.968885
H 1.932331 1.367352 1.661681
H 6.517467 -2.271773 -2.808896
H 7.999699 -0.533743 0.819851
H 5.331384 4.671344 0.264891
H 1.933345 3.618243 2.661362
C -2.822261 -0.059260 1.309092

C -3.394485 1.220836 1.301511
C -3.344644 -1.016876 2.183749
C -4.448577 1.527450 2.145332
H -3.031762 1.978309 0.616533
C -4.395277 -0.705943 3.038445
H -2.915987 -2.014026 2.197859
C -4.950674 0.566249 3.020384
H -4.892562 2.516745 2.112283
H -4.785352 -1.463244 3.710312
H -5.779876 0.809821 3.676477
C -2.735191 -1.511238 -1.335690
C -3.540713 -0.353945 -1.644934
C -3.617411 -2.409652 -0.662452
N -4.780250 -1.867127 -0.424870
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C -5.840304 0.255893 -0.790172
C -6.899434 -0.153096 0.027255
C -5.868173 1.535937 -1.354456
C -7.960841 0.705023 0.274835
H -6.871763 -1.136889 0.475179
C -6.937746 2.383886 -1.091824
H -5.050952 1.854466 -1.984924
C -7.990078 1.981503 -0.278118
H -8.771241 0.369983 0.914939
H -6.942171 3.374683 -1.535858
H -8.821027 2.650088 -0.078591
O -3.245429 0.654102 -2.289068
C -1.554155 -1.840716 -2.198892
H -1.888558 -2.202191 -3.179253
H -1.015150 -0.907705 -2.404198
C -0.613308 -2.814167 -1.643515
C 0.172856 -3.603659 -1.192792
H 0.862490 -4.318975 -0.802960
C -3.326783 -3.789318 -0.177105
H -4.202865 -4.192421 0.334567
H -3.065296 -4.458474 -1.001906
H -2.482054 -3.795640 0.518093
H -1.246451 -1.386155 0.672684

(S,S)-TS-I-f

0 1

C 1.751207 -0.358097 -0.778984
N 0.486636 0.222786 -1.264412
C 0.383663 0.227530 -2.724242
C 1.429610 -0.796581 -3.159933
C 2.495314 -0.761594 -2.060988
H 1.507337 -1.252359 -0.201653
H -0.627764 -0.068145 -3.009095
H 0.570308 1.225934 -3.132811
H 0.967063 -1.783869 -3.206973
H 1.839824 -0.568818 -4.144927
H 2.982427 -1.728397 -1.933768
H 3.269676 -0.035615 -2.306012
C -0.572333 0.394624 -0.480750
C -1.775322 0.972125 -0.830825
H -0.448461 0.054220 0.540953
H -1.918458 1.382563 -1.823524
C -2.804807 1.017108 0.121029
C 2.601968 0.503301 0.224575
O 3.602372 -0.397806 0.650417
Si 5.185476 -0.829330 0.321794
C 5.866162 -0.192421 -1.302194
H 6.947995 -0.373179 -1.312687
H 5.447782 -0.708961 -2.169828
H 5.718974 0.882176 -1.439423
C 5.172666 -2.697207 0.304646
H 4.790093 -3.104438 1.245790
H 4.544147 -3.081696 -0.504786
H 6.182417 -3.096819 0.158184
C 6.267397 -0.213387 1.719459

C	-1.392491	5.121708	0.334218
H	-0.979698	3.506111	1.689380
C	-3.261844	4.811340	-1.130594
H	-4.332947	2.957704	-0.919726
C	-2.206083	5.599829	-0.687470
H	-0.565200	5.722765	0.698435
H	-3.910298	5.167454	-1.924980
H	-2.021868	6.573229	-1.129585
O	-4.974781	1.139437	0.197088
C	-4.507936	-1.342316	1.859585
H	-5.132292	-0.972509	2.682639
H	-5.190737	-1.494153	1.017038
C	-3.947333	-2.634763	2.253926
C	-3.494619	-3.695984	2.588399
H	-3.097248	-4.640657	2.886190
C	-1.559863	-0.700319	3.196227
H	-0.673200	-0.147393	3.513955
H	-2.168038	-0.922720	4.078335
H	-1.253008	-1.659114	2.771542
H	-2.170876	-0.010237	-0.620292

(S,S)-TS-I-h

0 1

C	-1.784496	0.648280	-0.753984
N	-0.501243	0.115135	-1.215849
C	-0.472727	-0.045568	-2.665032
C	-1.391877	1.075938	-3.138552
C	-2.455039	1.177947	-2.039982
H	-1.571871	1.456068	-0.054342
H	0.547456	0.062379	-3.033238
H	-0.849617	-1.034964	-2.942237
H	-0.817373	2.002422	-3.207039
H	-1.822678	0.869494	-4.119688
H	-2.811259	2.198068	-1.899021
H	-3.312369	0.553541	-2.289509
C	0.554682	-0.004629	-0.423894
C	1.782626	-0.546188	-0.743225
H	0.390618	0.332574	0.595140
H	1.961044	-0.939515	-1.736243
C	2.786326	-0.619396	0.238700
C	-2.707809	-0.400127	-0.028326
O	-3.010015	-1.383322	-0.993828
Si	-3.606383	-2.958061	-0.949058
C	-2.251178	-4.159630	-1.421683
H	-2.694791	-5.108061	-1.745186
H	-1.655977	-3.780878	-2.259375
H	-1.568434	-4.385496	-0.598913
C	-4.907094	-3.035345	-2.291681
H	-5.812136	-2.465536	-2.061998
H	-4.511252	-2.656571	-3.239968
H	-5.214857	-4.073299	-2.460633
C	-4.326064	-3.396446	0.718940
H	-4.880276	-4.339244	0.642001
H	-3.551882	-3.532436	1.479048
H	-5.023401	-2.637249	1.085352
C	-2.008943	-1.064548	1.173090
C	-1.018594	-2.019638	0.919068
C	-0.352538	-2.666842	1.949405
C	-0.671336	-2.382716	3.272776
C	-1.666244	-1.453471	3.542749
C	-2.328746	-0.803614	2.504706
H	-0.757968	-2.263531	-0.101611
H	-0.154908	-2.886153	4.083367
H	-3.115655	-0.106217	2.758758
C	-3.960358	0.397626	0.370371
C	-3.850132	1.544784	1.164474
C	-4.965360	2.304990	1.488067
C	-6.223316	1.938405	1.021025
C	-6.344741	0.811081	0.220936
C	-5.221925	0.055317	-0.104782

H	-2.884407	1.859000	1.542464
H	-7.096663	2.531307	1.272014
H	-5.340286	-0.796801	-0.758290
H	0.418302	-3.393473	1.713571
H	-1.940847	-1.231436	4.568815
H	-4.846896	3.189696	2.105506
H	-7.315863	0.516462	-0.163671
C	3.902735	-1.574902	0.122239
C	4.394188	-2.014910	-1.112152
C	4.474580	-2.090777	1.289794
C	5.440913	-2.921481	-1.173567
H	3.966366	-1.639258	-2.034848
C	5.522734	-2.999603	1.229075
H	4.089639	-1.775460	2.254685
C	6.013419	-3.413556	-0.003181
H	5.814915	-3.245978	-2.139117
H	5.956306	-3.384202	2.146234
H	6.834578	-4.121036	-0.053986
C	3.914898	1.336451	0.343119
C	2.795066	1.960762	1.020534
C	3.779338	1.736737	-1.025438
N	2.645677	2.342166	-1.245873
N	2.030471	2.497404	-0.007970
C	0.798278	3.165308	0.063529
C	0.218252	3.662388	-1.107929
C	0.123392	3.318935	1.280842
C	-1.015495	4.295806	-1.060240
H	0.740967	3.542983	-2.046890
C	-1.108573	3.961736	1.308697
H	0.569934	2.939122	2.188040
C	-1.691794	4.449672	0.145211
H	-1.451593	4.670630	-1.980916
H	-1.618566	4.075289	2.260409
H	-2.658700	4.940264	0.176296
O	2.522136	1.968437	2.221788
C	5.166231	1.106072	1.152007
H	5.492614	2.062479	1.579392
H	4.919509	0.478089	2.014915
C	6.304960	0.513469	0.454293
C	7.267155	0.041294	-0.086889
H	8.111846	-0.390214	-0.575262
C	4.704032	1.471613	-2.163824
H	4.232897	1.778660	-3.099861
H	5.637944	2.028374	-2.046786
H	4.971776	0.415087	-2.225286
H	2.475298	-0.433311	1.263169

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0 1

C	1.804794	-0.335523	-0.761759
N	0.474343	0.094366	-1.230690
C	0.333030	0.033474	-2.686756
C	1.484580	-0.866929	-3.124011
C	2.562389	-0.665671	-2.056744
H	1.673555	-1.243812	-0.169025
H	-0.642388	-0.391919	-2.930680
H	0.385135	1.032049	-3.133075
H	1.148621	-1.905061	-3.131614
H	1.840055	-0.619388	-4.125286
H	3.178052	-1.555714	-1.929845
H	3.222632	0.155573	-2.336321
C	-0.578671	0.213385	-0.428588
C	-1.830868	0.666694	-0.785041
H	-0.406960	-0.061608	0.605645
H	-2.018453	1.005356	-1.796720
C	-2.849112	0.703031	0.181016
C	2.580606	0.630346	0.211446
O	3.667534	-0.148919	0.659635
Si	5.242055	-0.564128	0.278482
C	5.872823	0.099204	-1.355082

H	6.959507	-0.046493	-1.385544
H	5.455836	-0.424569	-2.218620
H	5.688290	1.169223	-1.482682
C	5.278822	-2.432035	0.257272
H	4.915066	-2.848352	1.201886
H	4.656277	-2.836453	-0.546420
H	6.298592	-2.802819	0.103890
C	6.333878	0.070089	1.658703
H	7.323379	-0.398392	1.611176
H	6.485122	1.152474	1.604803
H	5.908410	-0.158152	2.641222
C	3.076630	1.959606	-0.364460
C	2.582166	2.548735	-1.523099
C	3.066091	3.778606	-1.963500
C	4.046962	4.444738	-1.243300
C	4.528364	3.879711	-0.065436
C	4.041639	2.656066	0.368545
H	1.803665	2.068796	-2.097794
H	4.425674	5.401419	-1.587678
H	4.407117	2.238471	1.300015
C	1.702077	0.913573	0.937724
C	0.925422	2.067220	1.534613
C	0.031956	2.233785	2.587534
C	-0.089739	1.252112	3.563405
C	0.700347	0.109425	3.486919
C	1.589730	-0.056750	2.433019
H	0.992738	2.835813	0.772767
H	-0.793084	1.375984	4.380296
H	2.193532	-0.953252	2.368042
H	2.666933	4.213429	-2.874160
H	5.280955	4.397400	0.520464
H	-0.574639	3.132183	2.637771
H	0.615260	-0.661808	4.245639
C	-4.017213	1.588687	0.409757
C	-4.642718	2.054049	1.211201
C	-4.501346	2.023518	-1.189564
C	-5.732240	2.912030	1.139114
H	-4.263945	1.743317	2.180047
C	-5.589663	2.878604	-1.261844
H	-4.031805	1.688169	-2.107427
C	-6.213567	3.321690	-0.098062
H	-6.205718	3.259648	2.051259
H	-5.956079	3.201515	-2.230816
H	-7.066539	3.989684	-0.157778
C	-3.882096	-1.343763	0.245218
C	-2.744424	-1.906317	0.944745
C	-3.684125	-1.706441	-1.124096
N	-2.508424	-2.236682	-1.323061
N	-1.918101	-2.373500	-0.071235
C	-0.650866	-2.969167	0.022861
C	-0.039274	-3.469282	-1.131312
C	0.027341	-3.044977	1.244628
C	1.229159	-4.028535	-1.061895
H	-0.565339	-3.410549	-2.074360
C	1.294933	-3.612336	1.295418
H	-0.442646	-2.659494	2.137249
C	1.908159	-4.105338	0.149662
H	1.688343	-4.409448	-1.968892
H	1.809244	-3.662175	2.250106
H	2.898737	-4.543858	0.200362
O	-2.509743	-1.929172	2.153863
C	-5.164731	-1.187527	1.020208
H	-5.455000	-2.164530	1.426852
H	-4.974204	-0.559521	1.897353
C	-6.311609	-0.641437	0.298038
C	-7.279549	-0.203766	-0.261666
H	-8.130441	0.195606	-0.766338
C	-4.590961	-1.474873	-2.284115
H	-4.078492	-1.739659	-3.211347
H	-5.495510	-2.083902	-2.202289

H	-4.915647	-0.433804	-2.337273
H	-2.544411	0.525578	1.208997

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0	1		
C	-1.766533	0.845955	-0.335360
N	-0.526062	0.435361	-0.995487
C	-0.542837	0.753706	-2.419541
C	-1.398380	2.014999	-2.456811
C	-2.436793	1.792669	-1.353289
H	-1.486448	1.372570	0.576020
H	0.472909	0.918752	-2.778536
H	-0.991795	-0.070437	-2.982069
H	-0.771039	2.876995	-2.222746
H	-1.853999	2.177554	-3.435025
H	-2.740665	2.725646	-0.878852
H	-3.327320	1.316196	-1.762528
C	0.536433	0.027451	-0.322631
C	1.734047	-0.420435	-0.848848
H	0.422298	0.042639	0.757270
H	1.868660	-0.482881	-1.920761
C	2.744077	-0.856223	0.020166
C	-2.728856	-0.331902	0.065960
O	-3.128516	-0.941687	-1.141665
Si	-3.838072	-2.416056	-1.548141
C	-2.589535	-3.495238	-2.431028
H	-3.108919	-4.284851	-2.985846
H	-2.005112	-2.922892	-3.159069
H	-1.890063	-3.986106	-1.749954
C	-5.189918	-1.998890	-2.773798
H	-6.063262	-1.524722	-2.316269
H	-4.818726	-1.325155	-3.553195
H	-5.543466	-2.908498	-3.271704
C	-4.538021	-3.302228	-0.058610
H	-5.153546	-4.146325	-0.391165
H	-3.755087	-3.702460	0.591296
H	-5.176257	-2.653655	0.548985
C	-2.032966	-1.378245	0.956411
C	-1.109670	-2.244430	0.360797
C	-0.449091	-3.217674	1.095864
C	-0.705924	-3.359021	2.455188
C	-1.636553	-2.523595	3.057048
C	-2.294403	-1.546095	2.315320
H	-0.900557	-2.160248	-0.696804
H	-0.192463	-4.118509	3.035538
H	-3.032754	-0.934366	2.816208
C	-3.909989	0.367308	0.760265
C	-3.702814	1.180565	1.881316
C	-4.756027	1.856677	2.482058
C	-6.044784	1.744513	1.970530
C	-6.260075	0.958815	0.847389
C	-5.200174	0.284893	0.247217
H	-2.710391	1.291632	2.304619
H	-6.868741	2.272613	2.438860
H	-5.388774	-0.288908	-0.648701
H	0.269038	-3.864407	0.602120
H	-1.864404	-2.631716	4.112477
H	-4.565478	2.475509	3.352842
H	-7.255499	0.872726	0.423691
C	3.825550	-1.733405	-0.466706
C	4.292474	-1.678521	-1.785992
C	4.378612	-2.684004	0.396952
C	5.280405	-2.547807	-2.223857
H	3.901487	-0.933928	-2.471024
C	5.367785	-3.555894	-0.042198
H	4.025374	-2.741149	1.420850
C	5.822478	-3.490385	-1.353741
H	5.634077	-2.486410	-3.247800
H	5.781904	-4.287732	0.643546
H	6.595598	-4.169138	-1.698520

C	3.940328	0.908560	0.841719
C	2.739750	1.635273	1.189720
C	4.375045	1.492374	-0.391210
N	3.502742	2.327059	-0.881850
N	2.493530	2.429792	0.070471
C	1.452688	3.344925	-0.145488
C	1.512358	4.210981	-1.243774
C	0.350666	3.413057	0.715756
C	0.493063	5.126531	-1.466747
H	2.361919	4.159530	-1.911078
C	-0.662115	4.333060	0.474487
H	0.308397	2.756284	1.571896
C	-0.603216	5.196577	-0.612907
H	0.559580	5.791045	-2.322481
H	-1.509739	4.368581	1.152225
H	-1.398439	5.911956	-0.793524
O	2.006665	1.542653	2.176545
C	4.888290	0.304387	1.844857
H	5.596101	-0.350586	1.323820
H	5.497055	1.093589	2.303931
C	4.271679	-0.471157	2.922841
C	3.815978	-1.138272	3.811245
H	3.388139	-1.710638	4.603669
C	5.670617	1.243573	-1.084391
H	5.625199	1.586529	-2.119929
H	6.476195	1.789377	-0.580819
H	5.942027	0.186432	-1.072930
H	2.461457	-1.009425	1.057400

(R,R)-Int-Ald (or syn-Int-Ald)

(R,R)-Int-Ald-a

0 1			
C	-3.41196500	0.91218300	-2.11106700
C	-2.30853100	-0.05271900	-1.77588000
H	-3.66362100	0.96461700	-3.18960400
H	-2.72978900	-1.04319100	-1.99097400
C	-1.82873800	0.05971500	-0.32876600
H	-2.72003500	0.06865800	0.30380500
C	-1.08160900	1.36072700	-0.06826800
C	-1.47858100	2.19090300	0.97968500
C	0.02412600	1.74057700	-0.83176000
C	-0.78017700	3.35532900	1.27526900
H	-2.35166700	1.92589700	1.56766000
C	0.72991300	2.90100700	-0.53573000
H	0.35201300	1.13106000	-1.66734900
C	0.33299500	3.71075200	0.52205100
H	-1.10797100	3.98633000	2.09513200
H	1.59301500	3.16997800	-1.13583400
H	0.88381400	4.61674600	0.75305800
C	-1.00006600	-1.18110100	0.14555900
C	0.31949100	-1.28087100	-0.61797400
C	-0.48431500	-0.94443800	1.54386900
N	0.78635100	-0.81575300	1.58941900
N	1.29609100	-0.99564000	0.30161600
C	2.66354700	-0.73342800	0.06591400
C	3.33964000	0.14672600	0.91151700
C	3.32902200	-1.32896700	-1.00537600
C	4.68120400	0.42108800	0.68609600
H	2.81149300	0.60854000	1.73597200
C	4.66994200	-1.03505100	-1.22326700
H	2.80416400	-2.00911900	-1.66140300
C	5.35280100	-0.16471600	-0.38213600
H	5.20119200	1.10516400	1.34857900
H	5.18336500	-1.50118600	-2.05771000
H	6.40045700	0.05573400	-0.55675200
O	0.46753500	-1.54443800	-1.79245900
C	-1.75888900	-2.52048300	-0.00082300
H	-1.76539100	-2.80268800	-1.05723300
H	-1.19818500	-3.30396100	0.51801600
C	-3.12835300	-2.49048300	0.50281000

C	-4.25664000	-2.44843400	0.91075400
H	-5.26093400	-2.41894000	1.27166400
C	-1.32208800	-0.87653200	2.76874800
H	-0.72458400	-0.53787700	3.61581800
H	-2.16744500	-0.19956600	2.62973400
H	-1.73640800	-1.86253300	3.00058700
H	-1.50143000	0.07175000	-2.50289500
O	-4.02947800	1.56989100	-1.31314900

(R,R)-Int-Ald-b

0 1			
C	-3.98256300	0.03791200	-1.79785700
C	-2.54310200	0.46108700	-1.71435200
H	-4.36133800	-0.08364100	-2.83196000
H	-1.95080700	-0.20125200	-2.35401800
C	-1.97663700	0.57514400	-0.29297600
H	-2.82444400	0.72112800	0.38274600
C	-1.04911800	1.76861700	-0.13049300
C	-1.22920000	2.64977100	0.93504200
C	0.01302600	1.99595500	-1.00901700
C	-0.36273800	3.71899600	1.13373400
H	-2.05707800	2.49832000	1.62083200
C	0.88541500	3.05885800	-0.80963700
H	0.17146200	1.33608700	-1.85596400
C	0.70270700	3.92260500	0.26510500
H	-0.52114800	4.39205200	1.97010700
H	1.71058800	3.21044500	-1.49758300
H	1.38463900	4.75209100	0.42080100
C	-1.28321500	-0.74486200	0.19715200
C	-0.00719900	-1.01693800	-0.59868200
C	-0.70296200	-0.53287900	1.57198500
N	0.57432800	-0.54624700	1.58146900
N	1.02097900	-0.81931000	0.28617300
C	2.40132400	-0.72781900	0.00388900
C	3.19056600	0.13879200	0.76003300
C	2.96718300	-1.47704700	-1.02675300
C	4.54655400	0.24807700	0.48527200
H	2.73742100	0.71796000	1.55497800
C	4.32432700	-1.34719400	-1.29709600
H	2.35421300	-2.15111000	-1.60887200
C	5.11945300	-0.48990600	-0.54559500
H	5.15618500	0.92199700	1.07801500
H	4.76182200	-1.93172400	-2.09972300
H	6.17888500	-0.39847300	-0.76027500
O	0.07949300	-1.32158200	-1.77003500
C	-2.23646500	-1.95347500	0.13034600
H	-3.15943100	-1.71575500	0.66479400
H	-2.50849400	-2.13880300	-0.91242100
C	-1.63661800	-3.16404000	0.68634200
C	-1.10678600	-4.13327700	1.15608600
H	-0.64188200	-5.00103200	1.56896100
C	-1.50338400	-0.35265100	2.80923200
H	-0.85820100	-0.07222000	3.64235400
H	-2.27148100	0.41322400	2.67659600
H	-2.01568400	-1.28673500	3.06252400
H	-2.50546000	1.43566200	-2.21773100
O	-4.72078400	-0.13762800	-0.86099100

(R,R)-Int-Ald-c

0 1			
C	3.81179200	-0.36667600	-1.99126300
C	2.51070500	0.34509700	-1.73932800
H	4.08340900	-0.46448100	-3.06147000
H	2.69906100	1.38612200	-2.03093400
C	2.03445100	0.22831800	-0.29035600
H	2.89231900	0.45498100	0.34957300
C	1.58505900	-1.18853000	0.04278300
C	2.16688500	-1.86857900	1.11207200
C	0.57232600	-1.82694800	-0.67671200
C	1.73727100	-3.14019900	1.47165800

H	2.97134000	-1.39796000	1.66795200
C	0.13443600	-3.09589100	-0.31602400
H	0.10701000	-1.33856000	-1.52681000
C	0.71250000	-3.75576500	0.76239200
H	2.20527900	-3.64989200	2.30764900
H	-0.66211200	-3.56789100	-0.88175700
H	0.37085200	-4.74640600	1.04420500
C	0.94575000	1.28159500	0.10172300
C	-0.33708100	1.08630100	-0.70373700
C	0.43937400	0.99204200	1.49230800
N	-0.78158900	0.61869300	1.50976300
N	-1.27226600	0.65201700	0.20205600
C	-2.55359700	0.12100800	-0.06019100
C	-3.09009100	-0.82247600	0.81688300
C	-3.26947400	0.51493500	-1.19093500
C	-4.34215800	-1.36383200	0.56128700
H	-2.52496200	-1.12338400	1.68973800
C	-4.51754900	-0.04491900	-1.43724900
H	-2.85314900	1.24598000	-1.86947500
C	-5.06105000	-0.98226100	-0.56690200
H	-4.75340100	-2.09575600	1.24859200
H	-5.06999400	0.26431800	-2.31843900
H	-6.03733300	-1.41174800	-0.76470500
O	-0.48785200	1.25785700	-1.89455800
C	1.47359000	2.72253600	-0.05029900
H	2.44386700	2.80383200	0.44927300
H	1.63539500	2.93604800	-1.10933100
C	0.55361200	3.71968900	0.49109500
C	-0.22696400	4.50992300	0.94587600
H	-0.91966700	5.21756100	1.34491500
C	1.24215200	1.13945400	2.73267200
H	0.70997600	0.71199300	3.58299100
H	2.21315500	0.64791400	2.63382000
H	1.42970700	2.19933200	2.93356500
H	1.77016900	-0.01536600	-2.45763900
O	4.55465600	-0.78042500	-1.13806500

(R,R)-Int-Ald-d

0 1			
C	-3.23644000	1.59967000	-1.67092500
C	-2.44535200	0.32434100	-1.55481200
H	-3.88176900	1.83797100	-0.79879000
H	-3.15226900	-0.48761300	-1.76607200
C	-1.87560500	0.15349100	-0.14018300
H	-2.72514700	0.09246600	0.54788200
C	-1.03181300	1.34455200	0.29132000
C	-1.25192200	1.93631200	1.53525400
C	-0.01418800	1.85499100	-0.51766300
C	-0.46533900	2.99552300	1.97268600
H	-2.04870600	1.56271200	2.17147500
C	0.77892200	2.90885400	-0.08064400
H	0.17412000	1.42811800	-1.49698600
C	0.55848500	3.48049800	1.16744000
H	-0.65261700	3.44095500	2.94432100
H	1.57086900	3.28339200	-0.72055800
H	1.17798000	4.30384000	1.50746000
C	-1.10365700	-1.19737200	0.04087700
C	0.18676300	-1.18861000	-0.78041700
C	-0.53277700	-1.26807900	1.43564300
N	0.74185700	-1.17992000	1.45410000
N	1.20254300	-1.10997400	0.13837100
C	2.56694800	-0.82615600	-0.09207700
C	3.29814100	-0.17215800	0.90037900
C	3.17414900	-1.16951400	-1.29998900
C	4.63474600	0.13026100	0.68228600
H	2.81602200	0.09515500	1.83188600
C	4.51103900	-0.84957000	-1.50589400
H	2.60782300	-1.67484100	-2.06936500
C	5.24784700	-0.20254900	-0.52122300
H	5.19670300	0.63830600	1.45897900

H	4.97839400	-1.11751300	-2.44768400
H	6.29152600	0.04050400	-0.68945600
O	0.28664900	-1.23011200	-1.98787100
C	-1.94036000	-2.43366700	-0.35258600
H	-2.02850900	-2.45777900	-1.44244400
H	-1.39264600	-3.33807400	-0.07027500
C	-3.27279900	-2.46871900	0.24261400
C	-4.37030400	-2.48132700	0.72929500
H	-5.34781000	-2.50621800	1.15779400
C	-1.31970700	-1.42718400	2.68584600
H	-0.68211200	-1.25594700	3.55396600
H	-2.16276800	-0.73363900	2.71484000
H	-1.73483200	-2.43791400	2.74716600
H	-1.67859000	0.29890300	-2.32935500
O	-3.22629000	2.32447900	-2.63156000

(R,R)-Int-Ald-e

0 1			
C	-1.87529900	2.99172300	-0.53287200
C	-0.98508400	1.88166600	-0.03919400
H	-2.16161500	2.92664600	-1.60352100
H	0.02436400	2.12819800	-0.39442200
C	-1.40055300	0.51286800	-0.59787400
H	-1.31984300	0.57022700	-1.68931300
C	-2.84566800	0.15744900	-0.28632500
C	-3.58766300	-0.56441800	-1.22508300
C	-3.48002300	0.55068400	0.89259600
C	-4.90957800	-0.91360500	-0.98161100
H	-3.12171600	-0.85395900	-2.16220100
C	-4.80432600	0.20499700	1.14025000
H	-2.95225500	1.14700800	1.62798900
C	-5.52190500	-0.53401800	0.20802500
H	-5.46408800	-1.47520900	-1.72625200
H	-5.27687800	0.52362000	2.06349800
H	-6.55559200	-0.80125200	0.40085300
C	-0.35932900	-0.58204000	-0.20809400
C	0.97244400	-0.22040500	-0.87414100
C	0.06428800	-0.61814200	1.23827100
N	1.30764000	-0.36813000	1.39401800
N	1.88176400	-0.11156800	0.14701600
C	3.26354200	0.17943900	0.08602400
C	4.00765700	0.20240700	1.26806300
C	3.89044200	0.44600700	-1.13406900
C	5.36441700	0.49117000	1.22474200
H	3.52174300	-0.00513300	2.21141600
C	5.25017600	0.73234300	-1.15651500
H	3.32282600	0.42692300	-2.05255400
C	5.99595200	0.75818100	0.01527100
H	5.92981100	0.50592100	2.15077700
H	5.72679900	0.93683600	-2.10970300
H	7.05660000	0.98349500	-0.01293600
O	1.15529400	-0.05852200	-2.06068000
C	-0.78702100	-1.98466800	-0.70164500
H	-1.72913700	-2.26656100	-0.22627200
H	-0.97287100	-1.92825700	-1.77823500
C	0.22185600	-3.00525700	-0.43165900
C	1.08003400	-3.80727700	-0.18537700
H	1.83967600	-4.52684800	0.02581600
C	-0.79642100	-0.96862300	2.39818500
H	-0.17765200	-1.16133800	3.27527100
H	-1.48846400	-0.15693900	2.63268200
H	-1.39801900	-1.85528700	2.18225900
H	-0.95103200	1.90789400	1.05213900
O	-2.24605800	3.91714700	0.14113900

(R,R)-Int-Ald-f

0 1			
C	3.95452100	-0.62188700	-1.33061500
C	2.82730100	0.37707900	-1.31620300
H	4.54563600	-0.68628000	-0.39235500

H	3.29340900	1.35340200	-1.49790200
C	2.10205200	0.39237000	0.03809000
H	2.80719200	0.77687500	0.78340400
C	1.68432900	-1.00312000	0.48151000
C	1.91450800	-1.41658800	1.79346800
C	1.04731200	-1.88626800	-0.39324900
C	1.50676800	-2.67204600	2.22875000
H	2.41835400	-0.74812500	2.48527000
C	0.63370500	-3.13981500	0.04009600
H	0.86540500	-1.59918500	-1.42347700
C	0.85981700	-3.53609300	1.35328400
H	1.69489000	-2.97373700	3.25398800
H	0.13460300	-3.80844700	-0.65334000
H	0.53706700	-4.51541200	1.69092100
C	0.88966600	1.38350900	0.06031600
C	-0.25403300	0.86176900	-0.81032900
C	0.22810500	1.36208400	1.41450100
N	-0.94392400	0.85658400	1.38694200
N	-1.24717600	0.50912700	0.06875500
C	-2.49552000	-0.09012900	-0.20656800
C	-3.52443400	0.00878000	0.73094400
C	-2.69989400	-0.79193400	-1.39576900
C	-4.74843400	-0.59411200	0.47603300
H	-3.35822600	0.54768200	1.65445100
C	-3.93354500	-1.38349000	-1.63750300
H	-1.90724800	-0.86945900	-2.12580300
C	-4.96282900	-1.29035900	-0.70842700
H	-5.54111600	-0.51371200	1.21264300
H	-4.08398200	-1.92692400	-2.56459700
H	-5.92178200	-1.75829600	-0.90377700
O	-0.27131800	0.77609000	-2.01935800
C	1.30836000	2.79901300	-0.38096600
H	2.19329600	3.10549700	0.18536200
H	1.59080800	2.77097900	-1.43587800
C	0.24277100	3.78254100	-0.20617200
C	-0.65695700	4.56172900	-0.05186600
H	-1.45496400	5.25894700	0.07789000
C	0.83473600	1.88581400	2.66478500
H	0.22218200	1.61736400	3.52600500
H	1.84481000	1.49497700	2.80959900
H	0.90932600	2.97707700	2.61569500
H	2.15551200	0.17905900	-2.15203300
O	4.25165500	-1.29801100	-2.28071800

(R,R)-Int-Ald-g

O 1			
C	-1.71283200	3.14016200	0.28650500
C	-0.99637700	1.85224100	0.58643100
H	-1.52175900	3.95374800	1.01486600
H	0.07121200	2.08553900	0.46808900
C	-1.41151700	0.68445300	-0.30899500
H	-1.33823500	1.03043100	-1.34438700
C	-2.85495000	0.25383800	-0.10049900
C	-3.60827700	-0.14805400	-1.20607700
C	-3.47442000	0.25588900	1.14895900
C	-4.92563900	-0.56487600	-1.06694400
H	-3.15676200	-0.12464800	-2.19337500
C	-4.79442900	-0.15854500	1.29438700
H	-2.94017300	0.59724400	2.02814900
C	-5.52373100	-0.57700100	0.18858800
H	-5.48891600	-0.87020300	-1.94277000
H	-5.25436300	-0.14648700	2.27726200
H	-6.55410700	-0.89776400	0.30152700
C	-0.36998300	-0.47524100	-0.22792700
C	0.94704700	0.03441100	-0.82280100
C	0.09500900	-0.87778300	1.14827800
N	1.34765400	-0.69106900	1.32064500
N	1.89032500	-0.13484100	0.16040900
C	3.27494300	0.14638900	0.12808800
C	4.05517100	-0.13626300	1.25195100

C	3.87024300	0.70375400	-1.00681400
C	5.41552800	0.13834600	1.23569800
H	3.59509700	-0.56972200	2.12919800
C	5.23392200	0.97116300	-1.00346900
H	3.27534900	0.92269300	-1.88098000
C	6.01537400	0.69346500	0.11104000
H	6.00900900	-0.08718900	2.11572000
H	5.68466800	1.40342200	-1.89085800
H	7.07899400	0.90612600	0.10371900
O	1.09854600	0.49574100	-1.93211500
C	-0.82478000	-1.70995400	-1.04295300
H	-1.75278100	-2.10344000	-0.62229200
H	-1.04756400	-1.38320600	-2.06254700
C	0.18401300	-2.76507800	-1.07705300
C	1.04202600	-3.60424700	-1.07603400
H	1.80090200	-4.55209000	-1.08427200
C	-0.73550000	-1.50196900	2.21112600
H	-0.09286500	-1.95629800	2.96608400
H	-1.36975400	-0.75922900	2.69982700
H	-1.39456200	-2.26685000	1.79338100
H	-1.11220400	1.63526000	1.65355600
O	-2.41880600	3.33383000	-0.66865600

(R,R)-Int-Ald-h

O 1			
C	-3.78163700	-0.13076500	-1.72407500
C	-2.31927800	0.23006800	-1.73336400
H	-4.43127000	0.56209400	-1.15002600
H	-1.75128100	-0.55387300	-2.23575700
C	-1.74074000	0.58796000	-0.35027500
H	-2.55218500	0.99439400	0.26308500
C	-0.66327200	1.65848700	-0.43358600
C	-0.68443400	2.74216400	0.44351900
C	0.38591200	1.56433200	-1.35068500
C	0.32443400	3.69892700	0.42118200
H	-1.49772000	2.83910400	1.15661400
C	1.39937800	2.51428200	-1.37105000
H	0.42374300	0.73825900	-2.05355200
C	1.37404100	3.58375100	-0.48231500
H	0.28986300	4.53377700	1.11371500
H	2.21129700	2.41570900	-2.08393600
H	2.16594500	4.32544800	-0.49770400
C	-1.21485800	-0.67033800	0.43159800
C	0.02200500	-1.24508200	-0.26297500
C	-0.60489000	-0.23470300	1.74201500
N	0.66519300	-0.37467800	1.76900500
N	1.07317100	-0.96163400	0.57098900
C	2.45326100	-1.02922700	0.27763400
C	3.31276000	-0.09522200	0.85643900
C	2.94959200	-1.99546300	-0.59640500
C	4.66859800	-0.13657700	0.56359300
H	2.91377100	0.65553300	1.52683000
C	4.30854900	-2.01589600	-0.88813200
H	2.28194200	-2.71748800	-1.04553200
C	5.17320400	-1.09330000	-0.31138600
H	5.33235700	0.59183000	1.01750200
H	4.69102100	-2.76866500	-1.56946300
H	6.23295500	-1.11893000	-0.54155200
O	0.06712200	-1.81907100	-1.32992200
C	-2.27067400	-1.78679100	0.57363600
H	-2.45487100	-2.21821600	-0.41481900
H	-1.85488200	-2.59358500	1.18483400
C	-3.53477600	-1.34460500	1.15351900
C	-4.57606300	-0.96814600	1.61720300
H	-5.50627600	-0.64440800	2.02900700
C	-1.34858800	0.30906800	2.90806600
H	-0.65090000	0.73580600	3.62964900
H	-2.06220700	1.07535900	2.59823800
H	-1.92225300	-0.48328100	3.39809400
H	-2.26250700	1.12836000	-2.36123500

O -4.26215000 -1.05600400 -2.32618800

(R,R)-Int-Ald-i

O 1

C -4.17755500 0.03926100 -1.20591200
C -2.80569800 0.65552200 -1.28928000
H -4.73383400 0.25264900 -0.26736800
H -2.24893000 0.20370400 -2.11155400
C -2.02787900 0.64997000 0.03755100
H -2.75894500 0.73463800 0.85034000
C -1.08084300 1.83410800 0.15757800
C -0.98255900 2.53206400 1.36041900
C -0.26748200 2.22546700 -0.90838700
C -0.08791500 3.58680300 1.50317200
H -1.61277500 2.24961500 2.19836700
C 0.63108100 3.27554800 -0.76755000
H -0.32669400 1.70440400 -1.85795800
C 0.72581000 3.95864300 0.43995600
H -0.02688200 4.11668100 2.44812200
H 1.25998200 3.55860900 -1.60513600
H 1.42904500 4.77746100 0.55011000
C -1.26906000 -0.69939500 0.29498000
C -0.05936500 -0.82373200 -0.63201700
C -0.57891400 -0.66376700 1.63287000
N 0.69376200 -0.65083700 1.53622000
N 1.03902300 -0.70670900 0.18386900
C 2.40647800 -0.67759300 -0.16716800
C 3.37236600 -0.80911400 0.83276600
C 2.80081800 -0.50276800 -1.49574900
C 4.71924100 -0.76642000 0.50086100
H 3.06533700 -0.93675000 1.86193300
C 4.15402700 -0.46570500 -1.80910600
H 2.05945200 -0.40629500 -2.27507500
C 5.12045400 -0.59663700 -0.81956000
H 5.45998200 -0.86874400 1.28720600
H 4.44931800 -0.33066000 -2.84452700
H 6.17461400 -0.56591300 -1.07342100
O -0.07772900 -0.98586700 -1.83337800
C -2.20061800 -1.91656000 0.13720100
H -3.10544600 -1.76172900 0.73415400
H -2.50815200 -1.99618400 -0.90838600
C -1.56133100 -3.16897500 0.53190100
C -1.00004200 -4.17602800 0.86508000
H -0.50453100 -5.07667300 1.15330400
C -1.27203500 -0.67550700 2.94569700
H -0.56448000 -0.48058300 3.75198500
H -2.06918300 0.07081200 2.98226300
H -1.73304000 -1.65404000 3.11546300
H -2.99254700 1.70195600 -1.56410400
O -4.69672600 -0.59929000 -2.08389100

(R,R)-Int-Ald-j

O 1

C -0.12733500 -2.75807300 -0.44549200
C 0.98695700 -2.02946500 0.26489200
H 0.03924100 -2.93162100 -1.52771300
H 0.66253700 -1.79018200 1.28083600
C 1.54653000 -0.81099900 -0.49201100
H 1.50600200 -1.04000300 -1.56349100
C 3.00299100 -0.53755200 -0.15747300
C 3.53062800 -0.78207800 1.11083900
C 3.85994800 -0.04946200 -1.14641700
C 4.86611200 -0.51752000 1.39205400
H 2.90117900 -1.19585600 1.89104400
C 5.19570900 0.21689600 -0.87030100
H 3.47811200 0.11795600 -2.14924600
C 5.70251200 -0.01077900 0.40412200
H 5.25411100 -0.71421600 2.38617600
H 5.84245900 0.59491200 -1.65534900
H 6.74521700 0.19426200 0.62288900

C 0.61714500 0.43825700 -0.34008500
C -0.76819500 0.06118600 -0.87400300
C 0.26089400 0.84803800 1.06798100
N -0.98932600 0.73634900 1.31058200
N -1.62740600 0.22754200 0.17911100
C -3.03200800 0.07171000 0.20111700
C -3.78180400 0.76757700 1.14952600
C -3.66553100 -0.77191400 -0.71150600
C -5.16143200 0.61750100 1.17999700
H -3.28198000 1.41515600 1.85808400
C -5.04793400 -0.90399000 -0.67237800
H -3.08572500 -1.31940900 -1.44006400
C -5.80296400 -0.21419900 0.26873700
H -5.73694700 1.16077100 1.92226800
H -5.53419300 -1.56302100 -1.38404500
H -6.88156300 -0.32664000 0.29467400
O -1.02655600 -0.31929300 -1.99553000
C 1.14495300 1.64372400 -1.15204600
H 2.12445300 1.94172800 -0.77121700
H 1.28321300 1.32703300 -2.18970400
C 0.23648500 2.78628600 -1.10628900
C -0.54056300 3.69824900 -1.03663000
H -1.22851700 4.51301600 -0.98531300
C 1.18548200 1.41186500 2.08811600
H 0.61395700 1.94732000 2.84731600
H 1.75856400 0.62503100 2.58282800
H 1.90342900 2.09706000 1.63153300
H 1.78778900 -2.77503000 0.34974800
O -1.10915700 -3.19033800 0.09983100

(R,S)-Int-Ald (or anti-Int-Ald)

(R,S)-Int-Ald-a

O 1

C 4.36704400 -0.30503800 -0.79272800
C 3.34837500 0.69234200 -0.30453900
H 4.17495000 -0.72614300 -1.80147000
H 3.49198100 0.84278000 0.76625600
C 1.92230800 0.27632900 -0.68799700
H 1.86316300 0.31021100 -1.78181200
C 1.58365600 -1.14569700 -0.26169100
C 1.99139600 -1.66126500 0.96918200
C 0.81632500 -1.95651100 -1.10055100
C 1.62876400 -2.94557900 1.35810300
H 2.60468500 -1.06553900 1.63654300
C 0.44765600 -3.23858000 -0.71248500
H 0.49749600 -1.57719800 -2.06624300
C 0.85099400 -3.73657700 0.52114000
H 1.95669700 -3.32711900 2.31947500
H -0.15380000 -3.84937400 -1.37765200
H 0.56502500 -4.73782100 0.82606700
C 0.82231800 1.28070300 -0.21373400
C -0.48492700 0.85801500 -0.89232600
C 0.42363200 1.15515900 1.23596200
N -0.76425700 0.70863700 1.38323400
N -1.32208100 0.48005300 0.12522000
C -2.63637600 -0.03047700 0.04727500
C -3.42875400 -0.05930600 1.19620600
C -3.14203300 -0.51722000 -1.16002900
C -4.71691600 -0.57202000 1.13253600
H -3.03151800 0.31370400 2.13055200
C -4.43531700 -1.02307600 -1.20546600
H -2.53450300 -0.49193400 -2.05281200
C -5.22997800 -1.05538000 -0.06604000
H -5.32294800 -0.59015100 2.03239100
H -4.81952600 -1.39839200 -2.14830200
H -6.23799000 -1.45347800 -0.11063100
O -0.70344100 0.84771200 -2.08354200
C 1.16473700 2.73352100 -0.60307300
H 2.06581600 3.05571500 -0.07614500
H 1.38466000 2.76443800 -1.67440000

C	0.07770400	3.65952800	-0.29548500
C	-0.83909300	4.38161200	-0.01545600
H	-1.65248200	5.03043900	0.22350400
C	1.23846200	1.56304900	2.41013000
H	0.66868200	1.41333900	3.32768600
H	2.16542700	0.98980700	2.47626200
H	1.51105800	2.62023400	2.33440800
H	3.60081300	1.63644400	-0.80204400
O	5.35179300	-0.62296000	-0.17825800

(R,S)-Int-Ald-b

O 1			
C	4.51396900	-0.63297500	-0.19404000
C	3.38200400	0.13938800	0.43166000
H	5.45254200	-0.63018400	0.39572200
H	3.32396200	-0.16961900	1.47946200
C	2.05487500	-0.03433900	-0.30942100
H	2.28466200	-0.06485900	-1.37801800
C	1.38034900	-1.35378100	0.03688900
C	1.10204000	-1.71119400	1.35738300
C	0.97532800	-2.21439000	-0.98377100
C	0.42303700	-2.88852900	1.64812300
H	1.40510300	-1.06733400	2.17684800
C	0.29901900	-3.39398500	-0.69668200
H	1.18590900	-1.95249600	-2.01521000
C	0.01632800	-3.73280700	0.62149000
H	0.20784900	-3.14347100	2.68070300
H	-0.00836900	-4.04815700	-1.50611900
H	-0.51721500	-4.65015400	0.84791100
C	1.06381500	1.16903600	-0.16504000
C	-0.22357400	0.76877500	-0.89221700
C	0.53059800	1.38539500	1.22681500
N	-0.70791200	1.08774900	1.33309100
N	-1.17540300	0.66146300	0.09094600
C	-2.51491500	0.23296300	-0.02726900
C	-3.44865500	0.62385900	0.93235600
C	-2.90200900	-0.58842300	-1.08696500
C	-4.76415300	0.19284300	0.82762100
H	-3.13908400	1.25482200	1.75544800
C	-4.22402000	-1.00445800	-1.18095900
H	-2.17793900	-0.89590900	-1.82830500
C	-5.16111600	-0.61898600	-0.22933000
H	-5.48378700	0.50082500	1.57901900
H	-4.51781000	-1.64333600	-2.00735700
H	-6.19101300	-0.95030100	-0.30870700
O	-0.35529100	0.57780000	-2.07952300
C	1.64181100	2.44748300	-0.80402000
H	2.58082500	2.72449900	-0.31947900
H	1.87147800	2.22868400	-1.85092200
C	0.71889400	3.57751900	-0.73242500
C	-0.06378300	4.48383900	-0.65116600
H	-0.75907200	5.29165400	-0.58960000
C	1.29626200	1.92052100	2.38287500
H	0.62840300	2.07786800	3.23050200
H	2.09309200	1.23796400	2.68805600
H	1.76482100	2.87437200	2.12277000
H	3.72192200	1.18192800	0.46413500
O	4.46532900	-1.20377700	-1.25254600

(R,S)-Int-Ald-c

O 1			
C	1.93866300	-0.49522300	3.09159800
C	0.99542100	-0.41898800	1.92230500
H	1.62510900	-1.19194300	3.89410400
H	0.68869700	-1.43733700	1.66298700
C	1.55788000	0.35014400	0.72520100
H	2.02394100	1.25844700	1.11682600
C	2.66435800	-0.40810200	0.01070200
C	2.52659100	-1.73672700	-0.39338100
C	3.86962100	0.24389700	-0.25284200

C	3.56343800	-2.38886100	-1.05083400
H	1.59880600	-2.26661700	-0.21815200
C	4.90828100	-0.40434700	-0.91049700
H	3.99948300	1.27306100	0.06889000
C	4.75715600	-1.72591400	-1.31361200
H	3.43543500	-3.42121400	-1.36028300
H	5.83740200	0.12279200	-1.10204900
H	5.56553300	-2.23757100	-1.82577100
C	0.41664400	0.86020000	-0.21387900
C	-0.62668800	-0.21066600	-0.54180300
C	-0.44519300	1.85846900	0.51598600
N	-1.65941400	1.48170400	0.63288600
N	-1.80177000	0.23537900	0.01899100
C	-3.07314500	-0.38194000	0.03710500
C	-4.10801200	0.21421500	0.76250600
C	-3.30824000	-1.57398200	-0.65331700
C	-5.36163300	-0.38034600	0.79461600
H	-3.92734700	1.13938100	1.29252600
C	-4.57001000	-2.15481400	-0.60712300
H	-2.51578900	-2.03851100	-1.22051700
C	-5.60281800	-1.56787400	0.11291800
H	-6.15592600	0.09484500	1.36097200
H	-4.74052200	-3.07981000	-1.14833600
H	-6.58435500	-2.02861400	0.14168600
O	-0.45726100	-1.23016000	-1.17355000
C	0.99448400	1.44476000	-1.52081800
H	1.78779100	2.15686000	-1.27428800
H	1.45968000	0.63353300	-2.08630100
C	-0.02050900	2.09684300	-2.34345000
C	-0.88631800	2.62380500	-2.98634200
H	-1.65157300	3.08970000	-3.56681000
C	0.02934100	3.15545400	1.06209800
H	-0.81230000	3.73309600	1.44489600
H	0.74482100	2.99942400	1.87537000
H	0.53586500	3.73684000	0.28632000
H	0.08631900	0.05767500	2.31730800
O	2.94618000	0.15345400	3.21038300

(R,S)-Int-Ald-d

O 1			
C	2.05938800	-1.94779500	2.28322900
C	0.99174800	-1.17342700	1.55660200
H	2.80533400	-1.32837000	2.82507700
H	0.48971400	-1.84084800	0.85251400
C	1.56111000	0.08555200	0.88772500
H	2.01682400	0.69483900	1.67594900
C	2.67557500	-0.23426500	-0.09422100
C	2.57962800	-1.27249100	-1.02191900
C	3.84871400	0.52198000	-0.05985800
C	3.62374800	-1.53355500	-1.90107500
H	1.68247800	-1.87644400	-1.07410000
C	4.89428600	0.26400900	-0.93840900
H	3.94634800	1.32308400	0.66777400
C	4.78259300	-0.76576900	-1.86516100
H	3.53017700	-2.34318800	-2.61738800
H	5.79753200	0.86375200	-0.89417400
H	5.59670800	-0.97368400	-2.55172200
C	0.42239200	0.98208000	0.30032500
C	-0.57131100	0.19026100	-0.55307600
C	-0.48904500	1.45380900	1.40449600
N	-1.68372800	1.01992200	1.28583300
N	-1.76574900	0.24381500	0.12821000
C	-3.00741300	-0.34653000	-0.19973700
C	-4.06548300	-0.25264700	0.70800600
C	-3.18926700	-1.02284700	-1.40889000
C	-5.28950800	-0.83229600	0.40543100
H	-3.92585300	0.27486500	1.64162300
C	-4.42208000	-1.59841300	-1.69250700
H	-2.37824300	-1.09648500	-2.11783000
C	-5.47775600	-1.50984800	-0.79395200

H	-6.10188700	-0.75157100	1.12032100
H	-4.55139100	-2.12097400	-2.63468000
H	-6.43595700	-1.96265300	-1.02509400
O	-0.35127100	-0.35926700	-1.60919700
C	1.00211400	2.15306900	-0.52009400
H	1.75397600	2.67493400	0.07969200
H	1.51789000	1.74333600	-1.39192000
C	-0.02365200	3.09613100	-0.95672000
C	-0.89661000	3.84718700	-1.29499800
H	-1.66760100	4.51734800	-1.60490300
C	-0.08221400	2.33217300	2.53107000
H	-0.93803200	2.54099400	3.17343200
H	0.70267500	1.86303200	3.13187500
H	0.31445500	3.27958200	2.15408800
H	0.24862700	-0.88621800	2.31272900
O	2.12387400	-3.14819500	2.32430000

(R,S)-Int-Ald-e

0 1

C	-4.29265800	-0.07029500	-1.12968700
C	-3.32338300	0.74600200	-0.31520400
H	-4.04547900	-0.15790100	-2.20866500
H	-3.57723900	1.78696900	-0.55539300
C	-1.84717700	0.52842300	-0.68114800
H	-1.80370100	0.31993700	-1.75691700
C	-0.98594800	1.75743500	-0.42241400
C	-1.22461700	2.60465000	0.66057800
C	0.10462400	2.03024200	-1.25013000
C	-0.38792300	3.68385600	0.91950600
H	-2.07323400	2.43031300	1.31353800
C	0.94690900	3.10506500	-0.99079800
H	0.30530700	1.39007900	-2.10331400
C	0.70522000	3.93437200	0.09814100
H	-0.59153700	4.32854100	1.76835600
H	1.79219100	3.29387500	-1.64421800
H	1.36123300	4.77406200	0.30267000
C	-1.20557700	-0.73677500	-0.01287100
C	0.13399500	-0.98196800	-0.71370800
C	-0.73164700	-0.50918700	1.40171600
N	0.54233300	-0.52259100	1.50328200
N	1.09014900	-0.78355600	0.24694100
C	2.48913300	-0.69556900	0.07810500
C	3.22625200	0.11800700	0.93858600
C	3.12678300	-1.39608500	-0.94529000
C	4.60040200	0.22280400	0.77521300
H	2.71993000	0.66123300	1.72632100
C	4.50202300	-1.27139400	-1.10217600
H	2.55437700	-2.02737500	-1.61052400
C	5.24515300	-0.46706500	-0.24628700
H	5.16815500	0.85612900	1.44888100
H	4.99410800	-1.81792800	-1.89989000
H	6.31886100	-0.37872100	-0.37324700
O	0.29836900	-1.25743400	-1.88160700
C	-2.10163300	-1.98397800	-0.14759100
H	-3.03848600	-1.83131200	0.39327000
H	-2.35216500	-2.12390500	-1.20407600
C	-1.45394000	-3.18923900	0.36366800
C	-0.88521000	-4.14908300	0.80573100
H	-0.38588900	-5.01007300	1.19185200
C	-1.59855700	-0.35122900	2.59840800
H	-0.98402100	-0.25382300	3.49384600
H	-2.24014700	0.52845500	2.51584800
H	-2.25052900	-1.22265500	2.71334600
H	-3.54205100	0.60228600	0.74415500
O	-5.29966600	-0.56495200	-0.69357900

(R,S)-Int-Ald-f

0 1

C	-4.47050000	-0.08391200	-0.78958400
C	-3.42693900	0.51292500	0.11669600

H	-5.49531700	-0.07530100	-0.36817000
H	-3.74344900	1.55414100	0.25781200
C	-1.99128700	0.45965900	-0.41967000
H	-2.06344700	0.35951300	-1.50681100
C	-1.19495100	1.72249000	-0.13071200
C	-1.25249100	2.36259500	1.10830900
C	-0.34420700	2.24285400	-1.10721800
C	-0.47202600	3.48235600	1.36954000
H	-1.91687400	1.99176100	1.88205900
C	0.44124900	3.36013700	-0.84848500
H	-0.29093700	1.76310600	-2.07915700
C	0.38231300	3.98199300	0.39313000
H	-0.53030300	3.96346400	2.34050700
H	1.09920100	3.74482800	-1.62081100
H	0.99548800	4.85335600	0.59832000
C	-1.19294700	-0.81278600	0.02744200
C	0.11572100	-0.81881400	-0.76886100
C	-0.64902700	-0.75994600	1.43394400
N	0.62502800	-0.67004200	1.46678900
N	1.11225900	-0.65526900	0.16023300
C	2.50312300	-0.52783200	-0.04540900
C	3.37103200	-0.66332600	1.03973300
C	3.01483400	-0.25370000	-1.31567100
C	4.73906100	-0.52569700	0.85023200
H	2.97003900	-0.86946700	2.02301100
C	4.38742600	-0.12277300	-1.48684800
H	2.34823700	-0.15116200	-2.15928700
C	5.25740800	-0.25686300	-0.41172400
H	5.40361100	-0.63294900	1.70124800
H	4.77475400	0.09008200	-2.47787100
H	6.32750900	-0.15196700	-0.55483300
O	0.22627700	-0.92557600	-1.96966400
C	-1.98080600	-2.10823800	-0.25544100
H	-2.92095400	-2.10059800	0.30346200
H	-2.23828800	-2.13081500	-1.31697000
C	-1.22710800	-3.30878300	0.09672200
C	-0.57719300	-4.27051100	0.40222400
H	-0.00210500	-5.13139400	0.66272400
C	-1.43516000	-0.87408600	2.69096700
H	-0.76052700	-0.89140400	3.54756900
H	-2.12950700	-0.03974800	2.81364100
H	-2.02397300	-1.79647100	2.68979900
H	-3.54978800	0.05356600	1.10282800
O	-4.27621900	-0.51840000	-1.89585100

(R,S)-Int-Ald-g

0 1

C	1.56628600	0.03869000	3.11394200
C	0.67129900	-0.04073000	1.90735500
H	1.15042600	-0.42736800	4.02930700
H	0.24597300	-1.04857200	1.86298400
C	1.35940500	0.36624200	0.60119200
H	1.92042400	1.28106500	0.80596300
C	2.38659800	-0.66469000	0.15566400
C	2.08208000	-2.02052600	0.02001400
C	3.69551600	-0.25314800	-0.09922000
C	3.05340800	-2.93119500	-0.37930800
H	1.07686700	-2.37626700	0.20529900
C	4.66974800	-1.16078700	-0.49754800
H	3.95751600	0.79226600	0.02252700
C	4.35037900	-2.50551200	-0.64274700
H	2.79271800	-3.97961100	-0.48385300
H	5.68088000	-0.81573700	-0.68853700
H	5.10782800	-3.21789300	-0.95345400
C	0.31477600	0.76897900	-0.49460600
C	-0.79745400	-0.27115300	-0.66923800
C	-0.50224100	1.94794600	-0.01675800
N	-1.74060000	1.66860200	0.13214700
N	-1.95032300	0.33880200	-0.23295200
C	-3.26191500	-0.18414800	-0.15139200

C	-4.29355000	0.63761900	0.31027300
C	-3.53885400	-1.50435500	-0.51696300
C	-5.58560700	0.13955800	0.40288400
H	-4.07952500	1.65913000	0.59262600
C	-4.83924900	-1.98443700	-0.41634700
H	-2.74941600	-2.14517800	-0.87965200
C	-5.86926300	-1.17256500	0.04123400
H	-6.37647900	0.78969100	0.76237600
H	-5.04179300	-3.01092200	-0.70396600
H	-6.88095300	-1.55660400	0.11477900
O	-0.69152700	-1.38784300	-1.12676500
C	0.95665700	0.99474800	-1.88306400
H	1.35620000	0.03576800	-2.22488700
H	0.17512100	1.28055400	-2.59389000
C	2.01568400	1.99850000	-1.91386600
C	2.88388200	2.82653900	-1.95214500
H	3.65946100	3.55944800	-1.98540600
C	0.01414300	3.30408900	0.30825300
H	0.40777500	3.79453600	-0.58543500
H	-0.78859700	3.91423200	0.72388900
H	0.83185500	3.25233900	1.03239300
H	-0.18007000	0.61502200	2.14109000
O	2.63901200	0.58463000	3.14499300

(R,S)-Int-Ald-h

0 1			
C	2.14042300	2.99198400	1.21979300
C	1.64963800	1.61790600	1.58011400
H	2.49885200	3.59033800	2.08166200
H	2.38768800	1.16545100	2.25031300
C	1.33860500	0.74516300	0.36250300
H	0.78130700	1.37190400	-0.33997500
C	2.59939600	0.31503200	-0.36459000
C	2.70390000	0.54191400	-1.73711300
C	3.66153800	-0.31252100	0.28733200
C	3.82487500	0.13118200	-2.44722600
H	1.89195800	1.04100400	-2.25703100
C	4.78344900	-0.73068000	-0.42036300
H	3.62720100	-0.47958400	1.35898900
C	4.86728500	-0.51465300	-1.79091500
H	3.88464800	0.31822800	-3.51442400
H	5.59642900	-1.22287200	0.10355400
H	5.74399000	-0.83803800	-2.34239700
C	0.36826800	-0.44261800	0.71879600
C	-1.01525900	0.18035700	0.93989700
C	0.07237400	-1.31854700	-0.47778500
N	-1.11041100	-1.14965200	-0.93122100
N	-1.77164600	-0.21106800	-0.13765600
C	-3.11239600	0.11183200	-0.44852500
C	-3.75041900	-0.55927800	-1.49447200
C	-3.79976100	1.09808100	0.26388300
C	-5.06273000	-0.24488400	-1.81889400
H	-3.21711500	-1.32055600	-2.04692400
C	-5.11365200	1.39763900	-0.07508300
H	-3.31563700	1.61947600	1.07627100
C	-5.75435500	0.73326800	-1.11347100
H	-5.54577200	-0.77430800	-2.63366100
H	-5.63729800	2.16525900	0.48531800
H	-6.77994000	0.97501900	-1.37099800
O	-1.35536400	0.89486900	1.85830300
C	0.80665100	-1.25807400	1.94988700
H	1.79637600	-1.68628800	1.77289500
H	0.88979500	-0.59248700	2.81215400
C	-0.13319900	-2.33219800	2.26347400
C	-0.92845400	-3.20491900	2.47912900
H	-1.63347900	-3.98022600	2.68250800
C	0.95917900	-2.36900200	-1.04878900
H	0.43466600	-2.89611500	-1.84670400
H	1.88810200	-1.95694400	-1.44441800
H	1.22690800	-3.09243600	-0.27239100

H	0.75417000	1.77257800	2.19447600
O	2.13904000	3.46559900	0.11262700

(R,S)-Int-Ald-i

0 1			
C	-3.95917100	1.13044900	-0.79366500
C	-3.24815500	0.15123000	0.10235800
H	-3.78274700	0.98754100	-1.88026300
H	-3.33162500	0.49415000	1.13370900
C	-1.80552100	-0.07566900	-0.36766800
H	-1.86375300	-0.50090800	-1.37533000
C	-0.99850500	1.21209200	-0.46674000
C	-1.07947600	2.20984800	0.50580700
C	-0.11045100	1.39146600	-1.52931100
C	-0.28356700	3.34679100	0.42711800
H	-1.76854600	2.11208900	1.33750900
C	0.69174800	2.52326800	-1.60716600
H	-0.03321500	0.62678800	-2.29543700
C	0.60939300	3.50465700	-0.62616200
H	-0.36219300	4.11027500	1.19426300
H	1.38212900	2.63637200	-2.43642200
H	1.23447800	4.38968300	-0.68433300
C	-1.03687000	-1.15781200	0.46419000
C	0.29113000	-1.39501900	-0.26453600
C	-0.52475000	-0.64828800	1.79212900
N	0.74546600	-0.50492100	1.80972900
N	1.26142300	-0.91947400	0.58492600
C	2.60817900	-0.62831300	0.27436000
C	3.21312200	0.48198900	0.86308800
C	3.31637800	-1.42033200	-0.62783900
C	4.52988200	0.79091300	0.55275900
H	2.64789000	1.09517700	1.55409400
C	4.63044800	-1.09012100	-0.93824500
H	2.84473700	-2.28017400	-1.08319700
C	5.24373500	0.01013000	-0.35087900
H	4.99595700	1.65515700	1.01432400
H	5.17871200	-1.70768300	-1.64204000
H	6.27101900	0.25853500	-0.59537500
O	0.45138300	-1.85748900	-1.37023100
C	-1.82842200	-2.47203200	0.64260200
H	-1.17738100	-3.21467900	1.11402600
H	-2.65107300	-2.29792600	1.34215100
C	-2.37795600	-3.02303500	-0.59292100
C	-2.86968100	-3.46980100	-1.59244400
H	-3.28866600	-3.87548200	-2.48648900
C	-1.33632300	-0.36855700	3.00648800
H	-0.68058900	-0.07331800	3.82632700
H	-2.05941500	0.43163800	2.83485900
H	-1.89936000	-1.25549600	3.31184400
H	-3.80830000	-0.78844900	0.02212900
O	-4.69479500	2.00053300	-0.40587800

(R,S)-Int-Ald-j

0 1			
C	-0.43495000	1.61653700	-2.74165700
C	-0.87711400	0.36763500	-2.02637000
H	0.29837500	1.44622500	-3.55360300
H	-1.55841900	-0.11804700	-2.73781800
C	-1.60028000	0.58429600	-0.68720100
H	-2.08078100	1.56515100	-0.73961100
C	-2.70873000	-0.42778400	-0.45989500
C	-2.53426400	-1.79065600	-0.70646800
C	-3.95099900	0.01113800	-0.00024800
C	-3.57086200	-2.68918800	-0.48556800
H	-1.57988800	-2.15974400	-1.06196100
C	-4.99049700	-0.88518800	0.22232800
H	-4.10926300	1.07001700	0.18341500
C	-4.80164100	-2.24093000	-0.01740000
H	-3.41500100	-3.74544000	-0.67981700
H	-5.94888500	-0.52173500	0.57876700

H	-5.60988700	-2.94432400	0.15404600	C	-4.16746300	3.30966600	-2.30466800
C	-0.59597800	0.68383000	0.52103500	C	-4.07829600	2.01205200	-1.82562400
C	0.42015300	-0.45961200	0.50514300	H	-2.26441600	2.58697000	0.97213000
C	0.32591300	1.86352900	0.34419200	H	-3.64795300	5.37304400	-1.96519000
N	1.53931700	1.52050400	0.13838600	H	-4.52710200	1.20576300	-2.39482000
N	1.62693400	0.12618600	0.19717000	C	-2.72580500	-0.66489400	-1.15752100
C	2.88583100	-0.47923100	-0.01323700	C	-1.93377000	-0.22725800	-2.19990900
C	3.96697100	0.31618700	-0.40243100	C	-1.31257900	-1.14007400	-3.07236500
C	3.06225600	-1.85601900	0.15081000	C	-1.49227200	-2.49636500	-2.91781200
C	5.20808900	-0.26407300	-0.62362500	C	-2.32147000	-2.98133900	-1.87773700
H	3.83114300	1.38181600	-0.52603800	C	-2.91823400	-2.06348800	-0.99481500
C	4.31255300	-2.41820300	-0.07730800	H	-1.76635800	0.83249100	-2.35223200
H	2.23380700	-2.47693500	0.45692400	H	-1.03270700	-3.19729100	-3.60633900
C	5.39127500	-1.63310000	-0.46429300	H	-3.67919000	-2.40784500	-0.30143300
H	6.03865700	0.36632600	-0.92392000	H	-2.42503400	4.88086400	0.13624200
H	4.43751500	-3.48789700	0.05538800	H	-4.69295700	3.50521600	-3.23389800
H	6.36339800	-2.08182900	-0.63784000	H	-0.69067900	-0.76307500	-3.87752900
O	0.20418700	-1.63347300	0.70952900	H	-2.62765600	-4.02272200	-1.87478800
C	-1.34370500	0.72043900	1.86777000	C	2.92875500	1.75503100	0.44335100
H	-2.10331700	1.50746500	1.83710700	C	3.49218400	2.05535600	1.68536000
H	-1.86990400	-0.22768500	2.00080800	C	3.27716700	2.54826700	-0.65054300
C	-0.44910200	0.94125200	3.00102900	C	4.39027900	3.10634300	1.82517500
C	0.31755800	1.12455500	3.90623800	H	3.23622300	1.46295500	2.55802700
H	0.99351700	1.28239000	4.71724800	C	4.17255700	3.60312200	-0.51417100
C	-0.07896500	3.28789700	0.45396800	H	2.85084700	2.32896200	-1.62428900
H	0.74861100	3.93763400	0.16779300	C	4.73706200	3.88248700	0.72463300
H	-0.93704200	3.50825400	-0.18228700	H	4.82371900	3.31679600	2.79768100
H	-0.35622900	3.51304700	1.48904900	H	4.43141900	4.20443100	-1.37985500
H	-0.02419700	-0.31463900	-1.95997500	H	5.44231200	4.70006700	0.83292700
O	-0.85881800	2.72512900	-2.53296000	C	2.81028400	-0.78727000	0.20087600

(S,R)-Int-III

(S,R)-Int-III-a

0 1

C	-2.87291300	0.00454200	1.28941900
N	-1.52880400	0.47934100	1.62904200
C	-1.38785000	0.69723500	3.06059300
C	-2.78674700	0.45805300	3.63264600
C	-3.71151100	0.59561900	2.42485900
H	-2.90684100	-1.08906300	1.39274300
H	-0.65023300	0.00676800	3.48908600
H	-1.02444900	1.71668200	3.24560400
H	-2.85622200	-0.55545800	4.03757600
H	-3.03121000	1.15433100	4.43630800
H	-4.64956000	0.05911400	2.55886600
H	-3.94159300	1.64534600	2.23026300
C	-0.41880900	0.41287100	0.84131800
C	0.85252400	0.59852400	1.23871600
H	-0.61275700	0.21451500	-0.20433900
H	1.08530100	0.80079800	2.27773600
C	1.98957000	0.57086700	0.25932000
C	-3.42846400	0.26779300	-0.15064100
O	-4.76444700	-0.21590200	-0.08536700
Si	-6.33392200	0.35619200	0.02614100
C	-6.49865400	2.05359800	0.79634800
H	-7.55677800	2.34187100	0.77567900
H	-6.17959300	2.07575000	1.84134900
H	-5.94334100	2.82437000	0.25499800
C	-7.19827800	-0.91114000	1.09453800
H	-7.11220300	-1.91656800	0.66963200
H	-6.78099100	-0.94364000	2.10620400
H	-8.26610000	-0.68448500	1.18796900
C	-7.13295800	0.36752900	-1.66799600
H	-8.22380800	0.33359500	-1.56604900
H	-6.89124000	1.26427400	-2.24527400
H	-6.83468100	-0.50386800	-2.25985500
C	-3.41487700	1.72202400	-0.62845900
C	-2.81279900	2.77302400	0.05917900
C	-2.89897100	4.07860800	-0.41994300
C	-3.58073900	4.35479500	-1.59626700

C	-4.16746300	3.30966600	-2.30466800
C	-4.07829600	2.01205200	-1.82562400
H	-2.26441600	2.58697000	0.97213000
H	-3.64795300	5.37304400	-1.96519000
H	-4.52710200	1.20576300	-2.39482000
C	-2.72580500	-0.66489400	-1.15752100
C	-1.93377000	-0.22725800	-2.19990900
C	-1.31257900	-1.14007400	-3.07236500
C	-1.49227200	-2.49636500	-2.91781200
C	-2.32147000	-2.98133900	-1.87773700
C	-2.91823400	-2.06348800	-0.99481500
H	-1.76635800	0.83249100	-2.35223200
H	-1.03270700	-3.19729100	-3.60633900
H	-3.67919000	-2.40784500	-0.30143300
H	-2.42503400	4.88086400	0.13624200
H	-4.69295700	3.50521600	-3.23389800
H	-0.69067900	-0.76307500	-3.87752900
H	-2.62765600	-4.02272200	-1.87478800
C	2.92875500	1.75503100	0.44335100
C	3.49218400	2.05535600	1.68536000
C	3.27716700	2.54826700	-0.65054300
C	4.39027900	3.10634300	1.82517500
H	3.23622300	1.46295500	2.55802700
C	4.17255700	3.60312200	-0.51417100
H	2.85084700	2.32896200	-1.62428900
C	4.73706200	3.88248700	0.72463300
H	4.82371900	3.31679600	2.79768100
H	4.43141900	4.20443100	-1.37985500
H	5.44231200	4.70006700	0.83292700
C	2.81028400	-0.78727000	0.20087600
C	3.93352600	-0.54193200	-0.80770800
C	3.61972600	-1.06760500	1.43740300
N	4.87528400	-0.89144100	1.25782500
N	5.09236300	-0.53378900	-0.07165800
C	6.40397400	-0.22978400	-0.49207900
C	7.48569300	-0.62088400	0.29865700
C	6.62565200	0.47166900	-1.67882000
C	8.77871200	-0.31087800	-0.09986000
H	7.30739500	-1.15639000	1.22187200
C	7.92660100	0.76877000	-2.06494200
H	5.79009100	0.77709100	-2.29196600
C	9.00891700	0.38225100	-1.28316900
H	9.61233600	-0.61799500	0.52329500
H	8.08952900	1.31531600	-2.98816100
H	10.02137400	0.62093300	-1.59091800
O	3.81275200	-0.37761900	-2.00244800
C	1.97436800	-1.96912600	-0.33650000
H	1.52167200	-1.63700100	-1.27308300
H	2.66142200	-2.77938800	-0.60534100
C	0.94438000	-2.56839000	0.53743800
C	0.40114900	-3.21081700	1.45552600
H	0.34775300	-3.72474900	2.39695000
C	3.10752500	-1.50082700	2.76512800
H	3.88571700	-1.38053300	3.52055700
H	2.22096800	-0.93673500	3.05716400
H	2.81592000	-2.55430500	2.73210700
H	1.57216000	0.64304700	-0.75043400
Pd	-1.04971300	-2.87577600	-0.00458000

(S,R)-Int-III-b

0 1

C	2.82033900	0.13083800	-1.08968900
N	1.52583000	0.78948700	-1.26280600
C	1.34481200	1.32976200	-2.59926800
C	2.75626400	1.42851900	-3.15643400
C	3.48160900	0.26657000	-2.47407100
H	2.64246300	-0.92515300	-0.86023900
H	0.72203200	0.64987000	-3.20224800
H	0.83470700	2.29739400	-2.55625400
H	2.77569300	1.35135000	-4.24497800

H	6.55211300	-0.60882800	3.90599500	H	1.29984100	-4.00118700	-1.15041000
H	2.82689600	-2.72125200	4.15424600	H	0.22722900	-2.60420700	-1.22939000
C	-2.78830800	-1.31256500	0.99349600	H	0.64410600	-3.48043700	-2.70614100
C	-3.30145000	-0.89082000	2.22185500	C	3.86646900	-2.94616900	-2.90329500
C	-3.19045400	-2.55504200	0.50109300	H	3.44291900	-3.43318500	-3.78985100
C	-4.20328800	-1.67838000	2.92716800	H	4.67404400	-2.29201700	-3.24289200
H	-3.00369200	0.06607600	2.63806100	H	4.30808800	-3.73022500	-2.28073600
C	-4.09114900	-3.34687400	1.20437200	C	5.01108000	-0.41105300	-0.78188800
H	-2.80758200	-2.89901700	-0.45442400	C	5.20084100	0.68331600	-1.62373000
C	-4.60528900	-2.90842500	2.41867100	C	6.29410600	0.74070300	-2.48531900
H	-4.59473200	-1.32714800	3.87666400	C	7.21719300	-0.29524600	-2.51630200
H	-4.39494600	-4.30634100	0.79828400	C	7.04088000	-1.39259600	-1.67806100
H	-5.31402000	-3.52122300	2.96616100	C	5.94855500	-1.44753900	-0.82605600
C	-2.65262800	0.69639400	-0.59591700	H	4.50136900	1.51080200	-1.62684400
C	-3.79252200	-0.04519600	-1.29833900	H	8.06900900	-0.24961900	-3.18703700
C	-3.44814200	1.58999700	0.31968200	H	5.81378900	-2.31405600	-0.18754100
N	-4.70375900	1.33897100	0.28793300	C	4.16266800	-1.03476500	1.52365700
N	-4.94159700	0.34137000	-0.65409100	C	5.34625900	-0.61546100	2.13127000
C	-6.21966300	-0.25425000	-0.71163100	C	5.62431400	-0.94586300	3.45293200
C	-7.09630200	-0.08960100	0.36228700	C	4.71893800	-1.70109300	4.18930000
C	-6.60280100	-1.02101600	-1.81353000	C	3.53931900	-2.12937300	3.58945800
C	-8.34817200	-0.68721600	0.32771900	C	3.26465900	-1.80013300	2.26735700
H	-6.79070800	0.49972200	1.21667600	H	6.06224900	-0.02094700	1.57441900
C	-7.85719500	-1.61918700	-1.82715100	H	4.93389700	-1.95964600	5.22125200
H	-5.92479200	-1.15313500	-2.64407200	H	2.34558200	-2.13415100	1.80311300
C	-8.73660900	-1.45695400	-0.76369600	H	6.42029500	1.60295000	-3.13206700
H	-9.02159900	-0.55362400	1.16798200	H	7.75299900	-2.21130900	-1.69381600
H	-8.14589000	-2.21517600	-2.68681400	H	6.55175900	-0.61054000	3.90617600
H	-9.71465600	-1.92569900	-0.78403600	H	2.82693800	-2.72385700	4.15286300
O	-3.68725400	-0.83222500	-2.21389900	C	-2.78849000	-1.31299500	0.99217900
C	-1.83566700	1.38870100	-1.70861000	C	-3.30130300	-0.89230000	2.22103700
H	-1.52948300	0.59787500	-2.40205800	C	-3.19091000	-2.55497500	0.49873500
H	-2.52803900	2.02641200	-2.26988600	C	-4.20309300	-1.68039500	2.92582800
C	-0.64596200	2.21641500	-1.39867900	H	-3.00328300	0.06415000	2.63808400
C	0.46473600	2.71046900	-1.72543700	C	-4.09157200	-3.34731600	1.20146700
H	1.31409300	2.80278700	-2.37964300	H	-2.80825500	-2.89813700	-0.45715800
C	-2.94121300	2.65994800	1.22065500	C	-4.60539200	-2.90990700	2.41627900
H	-3.74372000	3.00059600	1.87694600	H	-4.59427500	-1.32998900	3.87573600
H	-2.10256400	2.30994400	1.82598000	H	-4.39558000	-4.30637500	0.79457500
H	-2.58940900	3.51656000	0.63115200	H	-5.31409800	-3.52311300	2.96334500
H	-1.46314100	-1.05642100	-0.63994700	C	-2.65286900	0.69709200	-0.59582600
Pd	-0.10874600	3.58004800	0.02634900	C	-3.79292700	-0.04397900	-1.29855000
(S,R)-Int-III-d				C	-3.44818100	1.59015400	0.32048200
0 1				N	-4.70381900	1.33919300	0.28878500
C	2.91411700	0.71589900	0.21744300	N	-4.94186500	0.34224300	-0.65386900
N	1.70434400	0.51250000	1.00715200	C	-6.21985100	-0.25357800	-0.71131400
C	1.64569300	1.33027600	2.20360100	C	-7.09574500	-0.09052600	0.36345200
C	3.04961000	1.90633300	2.34536300	C	-6.60353000	-1.01905200	-1.81390400
C	3.58801800	1.91270500	0.91014600	C	-8.34747300	-0.68843400	0.32901600
H	2.62269700	0.97693100	-0.80270700	H	-6.78963800	0.49776500	1.21837300
H	0.89450500	2.12717000	2.06208100	C	-7.85776700	-1.61756500	-1.82739400
H	1.34089800	0.73592400	3.07138400	H	-5.92606300	-1.14992300	-2.64508900
H	3.03745300	2.90500700	2.78575700	C	-8.73645300	-1.45691000	-0.76310200
H	3.65938500	1.26718200	2.98553900	H	-9.02035300	-0.55611600	1.16991900
H	3.27731200	2.82823300	0.39783600	H	-8.14692100	-2.21255200	-2.68759500
H	4.67711900	1.86835300	0.87420300	H	-9.71438100	-1.92591100	-0.78333100
C	0.55848400	0.03409700	0.44979700	O	-3.68787600	-0.83036000	-2.21469100
C	-0.67698400	0.05591300	0.97527500	C	-1.83604300	1.39000400	-1.70823800
H	0.69036300	-0.37864600	-0.54079400	H	-1.53030400	0.59960300	-2.40236400
H	-0.85438200	0.45613200	1.96715400	H	-2.52841200	2.02831000	-2.26884200
C	-1.84727000	-0.43751900	0.17743500	C	-0.64601300	2.21714000	-1.39808100
C	3.77953000	-0.58587700	0.11496900	C	0.46491900	2.71086200	-1.72445700
O	2.95173900	-1.59915800	-0.43918600	H	1.31435600	2.80362800	-2.37848000
Si	2.51700600	-2.01246500	-2.00662400	C	-2.94109900	2.65950000	1.22208300
C	2.03611200	-0.53190400	-3.05318800	H	-3.74366400	3.00010800	1.87832200
H	1.74012200	-0.88653300	-4.04788300	H	-2.10274700	2.30891800	1.82748000
H	1.19007200	0.03238200	-2.65043700	H	-2.58882100	3.51629300	0.63312000
H	2.86955700	0.16186200	-3.19809500	H	-1.46333700	-1.05568500	-0.64110300
C	1.03911700	-3.12252300	-1.74912900	Pd	-0.10849100	3.57991500	0.02771300

(S,R)-Int-III-e

0 1			
C	3.17618500	1.14789500	-0.49313800
N	1.84933500	1.43129900	0.01960800
C	1.86068600	2.24698600	1.21686500
C	3.24200300	2.91875700	1.22327200
C	4.00132200	2.34028600	0.01116200
H	3.12017000	1.13519400	-1.58378100
H	1.03700500	2.97204800	1.15590700
H	1.70044400	1.64193700	2.11944000
H	3.15106000	4.00353300	1.14087900
H	3.76515100	2.70738000	2.15630700
H	4.06152000	3.08241700	-0.78754100
H	5.02554800	2.05998400	0.25942800
C	0.74077600	0.74492000	-0.37910500
C	-0.43194300	0.68262800	0.26976600
H	0.86017300	0.23535700	-1.32957400
H	-0.54489600	1.14463000	1.24389700
C	-1.59647800	-0.05644600	-0.31309400
C	3.69666800	-0.28043700	-0.09058000
O	2.83141000	-1.15035000	-0.79609400
Si	2.85959800	-2.75635800	-1.26819600
C	4.05898700	-3.01674300	-2.67949900
H	3.93434600	-4.02024700	-3.10304900
H	3.89361100	-2.29821300	-3.48847200
H	5.10096300	-2.92466700	-2.35829300
C	1.09568500	-3.03111000	-1.81729000
H	0.40483400	-2.82490300	-0.99336000
H	0.82248600	-2.38279400	-2.65584400
H	0.92901900	-4.06645300	-2.13412500
C	3.27241100	-3.92444200	0.13407500
H	3.27225900	-4.95568500	-0.23860600
H	4.25876900	-3.73792400	0.56672600
H	2.53698600	-3.86919100	0.94179500
C	5.13327500	-0.52982100	-0.57001000
C	5.60111800	0.04019000	-1.75691900
C	6.85264400	-0.28565600	-2.26444600
C	7.66358000	-1.19863000	-1.59991600
C	7.21052600	-1.77690500	-0.42088200
C	5.95992400	-1.44292800	0.08657800
H	4.98892300	0.74208000	-2.31058000
H	8.63932600	-1.45709100	-1.99810400
H	5.62685200	-1.90790100	1.00672900
C	3.51226500	-0.47008600	1.41743800
C	4.42478300	0.04873700	2.33778600
C	4.18692400	-0.03691700	3.70451400
C	3.02808700	-0.64333100	4.17733000
C	2.11300700	-1.16381400	3.26968300
C	2.35488200	-1.07556800	1.90396700
H	5.33461700	0.52656800	1.99080200
H	2.84177300	-0.71044600	5.24443500
H	1.61974800	-1.45692600	1.20777300
H	7.19189100	0.17272200	-3.18775900
H	7.82963000	-2.49333800	0.10940000
H	4.91186100	0.37197800	4.40114500
H	1.20030700	-1.63526800	3.62044800
C	-2.08365900	-1.17889100	0.59618400
C	-2.32384200	-0.97014200	1.95589500
C	-2.32061000	-2.45031000	0.07115300
C	-2.79649400	-1.99775700	2.76327300
H	-2.14103200	0.00409800	2.39751800
C	-2.79177300	-3.48200000	0.87580200
H	-2.14605300	-2.63153300	-0.98448100
C	-3.03470400	-3.25823700	2.22543000
H	-2.98154500	-1.81144800	3.81644600
H	-2.97234000	-4.46069100	0.44315600
C	-3.40661000	-4.06005700	2.85498800
H	-2.80251500	0.85769600	-0.78700600
C	-3.82202100	-0.11692900	-1.38086000
C	-3.61225300	1.41784400	0.35584700

N	-4.74020200	0.82791500	0.49735400
N	-4.88553000	-0.11887500	-0.51319400
C	-5.95885100	-1.03207200	-0.44678500
C	-6.62157800	-1.21798800	0.76775300
C	-6.34568700	-1.76226900	-1.57195000
C	-7.66867700	-2.12494800	0.84922100
H	-6.31143500	-0.65448500	1.63800400
C	-7.39038800	-2.67295800	-1.46964600
H	-5.83132300	-1.62218900	-2.51167500
C	-8.05829000	-2.85990300	-0.26559300
H	-8.17762700	-2.26194000	1.79771800
H	-7.68386900	-3.23770900	-2.34855900
H	-8.87425600	-3.57130700	-0.19571700
O	-3.69156200	-0.77323100	-2.39132700
C	-2.41718000	1.84204800	-1.91067300
H	-2.07919200	1.23153100	-2.75467900
H	-3.33493200	2.33899600	-2.24465400
C	-1.40640400	2.89618200	-1.66563100
C	-0.49194400	3.67196200	-2.04340500
H	0.22194700	4.03327600	-2.76257100
C	-3.24947900	5.22259500	1.28528200
H	-3.98138200	2.57986900	2.09255800
H	-2.25459000	2.38087000	1.71342900
H	-3.25110400	3.48266700	0.75149400
H	-1.26034700	-0.52395400	-1.24516700
Pd	-0.98984500	4.16946900	-0.12298200

(S,R)-Int-III-f

0 1			
C	2.95633800	0.76075900	-0.72566400
N	1.71147700	0.95553900	-0.00980700
C	1.87603900	1.70555700	1.21537900
C	3.18350900	2.48635100	1.01463700
C	3.74723900	2.02435200	-0.34228300
H	2.73973100	0.72504600	-1.79734300
H	1.01091400	2.37011400	1.34138200
H	1.92458300	1.04379800	2.08980400
H	2.99840400	3.56248400	1.01167700
H	3.88691400	2.28193900	1.82151500
H	3.57444900	2.78619100	-1.10634700
H	4.82081100	1.84995100	-0.29217600
C	0.52944900	0.39269800	-0.37736800
C	-0.60605300	0.35838400	0.33714900
H	0.53729800	-0.02687400	-1.38007500
H	-0.62791900	0.72837100	1.35594700
C	-1.86110000	-0.20179700	-0.25555200
C	3.67454700	-0.57762000	-0.34311800
O	4.00512400	-0.47991400	1.02611100
Si	5.33823100	-0.52546600	2.02941000
C	6.01875600	-2.25710700	2.25959600
H	6.55418400	-2.31369800	3.21463000
H	5.22050700	-3.00583900	2.29224800
H	6.72301900	-2.54899900	1.47680100
C	4.65347600	0.04690900	3.67214000
H	4.26898600	1.07004100	3.63298900
H	3.83597100	-0.60093800	4.00536100
H	5.42878600	0.01823900	4.44584500
C	6.70297200	0.61080600	1.44114200
H	7.56196800	0.53629100	2.11824900
H	7.05548700	0.34528800	0.43974800
H	6.39262800	1.66000700	1.42439400
C	2.66934300	-1.72010100	-0.52350400
C	2.02095500	-2.28215900	0.57082400
C	1.02662200	-3.23844700	0.39213000
C	0.66799200	-3.64493100	-0.88655000
C	1.31938000	-3.09549600	-1.98728900
C	2.31449300	-2.14377600	-1.80514700
H	2.27877200	-1.94536700	1.56711200
H	-0.11488400	-4.38330300	-1.02550700
H	2.81237500	-1.72067300	-2.67272600

H	-3.33790400	2.37231300	-2.05153500	C	-3.09804000	-2.78082900	2.38216500
C	-1.35532700	2.70876500	-1.48631600	H	-2.26255200	-0.82333100	2.57664400
C	-0.36813700	3.38878200	-1.86781400	C	-3.42763700	-3.58130500	0.14241700
H	0.37642700	3.67321600	-2.59045100	H	-2.85135800	-2.23759400	-1.42690100
C	-3.16316300	2.42620900	1.48805100	C	-3.51956700	-3.78280900	1.51444800
H	-3.86391100	2.52972300	2.31813000	H	-3.16452500	-2.92721700	3.45563100
H	-2.18073700	2.15317800	1.87814600	H	-3.75358700	-4.35454100	-0.54593100
H	-3.06943600	3.40294500	0.99483400	H	-3.91722600	-4.71362900	1.90576500
H	-1.57748600	-0.72006700	-1.19028500	C	-3.06046600	1.04942900	-0.12962100
Pd	-0.80274300	3.93520000	0.05085400	C	-4.18343500	0.45630700	-0.98017600
(S,R)-Int-III-h				C	-3.78929500	1.24666900	1.17246400
O 1				N	-4.97801100	0.77193800	1.15088700
C	2.89051500	0.82760300	-0.48627800	N	-5.24045200	0.27153100	-0.12381100
N	1.66004500	0.96166800	0.26725200	C	-6.44809500	-0.42249300	-0.34853900
C	1.87833700	1.45294300	1.61103100	C	-7.20410600	-0.84829000	0.74571400
C	3.20540300	2.22188500	1.51928300	C	-6.88759400	-0.69485500	-1.64596700
C	3.74582800	1.96693100	0.09827700	C	-8.39073900	-1.53713100	0.53828100
H	2.66933200	0.98496100	-1.54633900	H	-6.85785700	-0.63933400	1.74902800
H	1.04133300	2.09875100	1.89366600	C	-8.07481900	-1.39228100	-1.83410400
H	1.93319200	0.63022500	2.33541200	H	-6.30457500	-0.36881200	-2.49486200
H	3.04756800	3.28902200	1.68900700	C	-8.83417200	-1.81544600	-0.75016900
H	3.91042300	1.87534100	2.27492900	H	-8.96945700	-1.86255900	1.39663000
H	3.61588700	2.85509900	-0.52605500	H	-8.40694900	-1.60002300	-2.84613000
H	4.80919300	1.73294300	0.10895800	H	-9.76109900	-2.35678000	-0.90682700
C	0.45065800	0.50424200	-0.16355200	O	-4.12793000	0.18019600	-2.15971400
C	-0.66209000	0.35611500	0.57077200	C	-2.55826700	2.32938700	-0.83565100
H	0.42364700	0.27267000	-1.22556900	H	-2.10484900	2.00967800	-1.77670200
H	-0.64314500	0.53666400	1.63965600	H	-3.42920000	2.93531500	-1.10922700
C	-1.94524200	-0.07333400	-0.06952700	C	-1.62773400	3.21363700	-0.09539600
C	3.54533400	-0.58967000	-0.34839400	C	-1.26721300	4.00910100	0.80822600
O	3.89384600	-0.74221700	1.01123500	H	-1.40671300	4.53591200	1.73582000
Si	5.23242800	-1.02862300	1.96664300	C	-3.27720200	1.90367400	2.40642000
C	5.82338700	-2.80606500	1.88814500	H	-3.87867700	1.59915500	3.26447500
H	6.36947800	-3.04623400	2.80805600	H	-2.22949900	1.66474300	2.58848100
H	4.98749500	-3.50995600	1.81872500	H	-3.34363700	2.99051100	2.30755400
H	6.49931100	-2.99884000	1.05165400	H	-1.73401500	-0.26086500	-1.12783700
C	4.59637500	-0.70852600	3.69484300	Pd	0.22654500	3.96602600	-0.56606700
H	4.25673500	0.32188000	3.83339200	(S,R)-Int-III-i			
H	3.75478500	-1.36805000	3.93140700	O 1			
H	5.37866400	-0.89934900	4.43782500	C	2.89138800	0.81507200	-0.48644000
C	6.64738200	0.12088300	1.55123900	N	1.65830900	0.96422800	0.26012800
H	7.50264900	-0.09439100	2.20245200	C	1.87752400	1.44382500	1.60802700
H	6.98795500	-0.00003400	0.51830200	C	3.21273900	2.19954800	1.52482600
H	6.38383000	1.17233100	1.70068800	C	3.75875200	1.94084800	0.10644000
C	2.48301000	-1.63598900	-0.70101900	H	2.67844900	0.97768800	-1.54737100
C	1.80398600	-2.32733400	0.29673000	H	1.04641600	2.09610400	1.89294700
C	0.75601400	-3.18467700	-0.02153000	H	1.92217100	0.61560300	2.32677700
C	0.37692700	-3.36425000	-1.34568500	H	3.06414500	3.26806300	1.69448300
C	1.05967500	-2.68687900	-2.35167000	H	3.90994900	1.84560300	2.28436500
C	2.10596500	-1.83143900	-2.03024900	H	3.64545600	2.83244300	-0.51623700
H	2.07935100	-2.16508700	1.33133700	H	4.81854700	1.69157600	0.12302900
H	-0.44768300	-4.02466300	-1.59245000	C	0.44545000	0.52200500	-0.17737600
H	2.62812700	-1.30613200	-2.82457700	C	-0.66999800	0.38010800	0.55393700
C	4.76020000	-0.77793000	-1.26821800	H	0.41866900	0.29889200	-1.24123800
C	5.30689200	0.22937900	-2.06145100	H	-0.64951000	0.55337100	1.62394600
C	6.43395800	-0.01120200	-2.84430000	C	-1.95829000	-0.02609200	-0.08990700
C	7.03182400	-1.26360800	-2.84959900	C	3.52685800	-0.61111500	-0.34800800
C	6.47916800	-2.28564100	-2.08325000	O	3.86771400	-0.77026100	1.01284400
C	5.35123100	-2.04353000	-1.31360400	Si	5.19715000	-1.07991700	1.97370400
H	4.86746200	1.21840700	-2.09041700	C	5.76337600	-2.86519400	1.88830200
H	7.91260500	-1.44840400	-3.45581900	H	6.29233100	-3.12272300	2.81347100
H	4.91109100	-2.85573100	-0.74553600	H	4.91814300	-3.55559300	1.79944900
H	0.22048200	-3.69819900	0.77058700	H	6.44828600	-3.05980600	1.05952900
H	0.77610500	-2.82391500	-3.39045500	C	4.55705100	-0.75811900	3.70002600
H	6.84232200	0.78998100	-3.45183600	H	4.23164400	0.27661100	3.84072900
H	6.92108800	-3.27677000	-2.09331900	H	3.70510000	-1.40642500	3.93035800
C	-2.49408400	-1.37243400	0.50497900	H	5.33304100	-0.96277900	4.44591500
C	-2.59090300	-1.58813900	1.88057300	C	6.62935400	0.05224600	1.57046900
C	-2.91752600	-2.38699800	-0.35400900	H	7.47957100	-0.17814700	2.22310300

H	6.97159700	-0.06703100	0.53788200	C	-1.07871800	-2.75943100	-1.10533500
H	6.37949100	1.10624700	1.72539000	C	-2.43351600	-3.24612000	-1.61297500
C	2.45159000	-1.64177800	-0.70648900	C	-3.16137800	-1.96638400	-2.04251700
C	1.75750000	-2.32264200	0.28790800	H	-2.44524500	0.06715900	-1.73773900
C	0.69618400	-3.16155200	-0.03524900	H	-0.29380500	-2.83502300	-1.87474200
C	0.31852800	-3.33289100	-1.36083900	H	-0.73568400	-3.32593100	-0.23168400
C	1.01678500	-2.66654200	-2.36359600	H	-2.33089800	-3.95485200	-2.43665200
C	2.07664900	-1.82978200	-2.03739500	H	-2.97631200	-3.74668500	-0.81055600
H	2.03109300	-2.16584300	1.32379400	H	-2.93142400	-1.73298900	-3.08563400
H	-0.51680400	-3.97829000	-1.61121200	H	-4.24451000	-2.06269400	-1.96336700
H	2.61052300	-1.31226100	-2.82905700	C	-0.27658800	-0.60045500	-0.29091100
C	4.74310400	-0.81382100	-1.26274200	C	0.96291600	-1.02002400	0.02191300
C	5.30662500	0.18802000	-2.05107900	H	-0.52671500	0.44350300	-0.16668400
C	6.43421400	-0.06555000	-2.82904100	H	1.25232100	-2.05565500	-0.12284400
C	7.01573600	-1.32566300	-2.83427500	C	1.99718200	-0.06534100	0.53381200
C	6.44613700	-2.34207000	-2.07288800	C	-3.48056300	-0.43777200	0.07862100
C	5.31781100	-2.08690800	-1.30803400	O	-2.78532200	0.57959700	0.78994600
H	4.88006700	1.18272000	-2.07955600	Si	-2.63480400	2.23907000	0.56488600
H	7.89695500	-1.52059700	-3.43667600	C	-2.23622400	2.69166000	-1.20821500
H	4.86501300	-2.89441600	-0.74323900	H	-2.09153000	3.77664700	-1.27351100
H	0.14909500	-3.66688800	0.75421500	H	-1.32306500	2.21763300	-1.57833600
H	0.73463700	-2.79748100	-3.40354900	H	-3.05486500	2.44240400	-1.88986200
H	6.85607600	0.73154100	-3.43270900	C	-1.20703000	2.69573300	1.67944200
H	6.87519400	-3.33883800	-2.08291400	H	-1.41153100	2.42190000	2.71954600
C	-2.52863300	-1.32042800	0.47513200	H	-0.27808000	2.19707900	1.38651500
C	-2.98816300	-2.31370000	-0.39029200	H	-1.02070200	3.77484700	1.65402300
C	-2.61755400	-1.54880800	1.84910400	C	-4.17082200	3.17195700	1.08033600
C	-3.52657800	-3.49867300	0.09852100	H	-3.94421300	4.24366700	1.13251200
H	-2.93037100	-2.15408400	-1.46219200	H	-4.99066300	3.04636900	0.36748900
C	-3.15241600	-2.73255200	2.34321000	H	-4.53172600	2.86528700	2.06663400
H	-2.26336600	-0.80001600	2.54988000	C	-4.85355400	0.11239600	-0.32666300
C	-3.61063100	-3.71266800	1.46916200	C	-5.15716100	0.53528600	-1.61974600
H	-3.88163900	-4.25436700	-0.59481500	C	-6.38349100	1.12970800	-1.90774900
H	-3.21217700	-2.88874400	3.41571000	C	-7.32853600	1.30747300	-0.90676000
H	-4.03064300	-4.63614200	1.85452400	C	-7.03767300	0.88987400	0.38876300
C	-3.05755400	1.11619000	-0.13821900	C	-5.81292500	0.30480800	0.67212200
C	-4.18785000	0.53765500	-0.98848600	H	-4.44402200	0.41529200	-2.42650800
C	-3.77713600	1.30158400	1.17117100	H	-8.28442700	1.76907200	-1.13205900
N	-4.96248400	0.81730200	1.15623100	H	-5.59185100	0.00019700	1.68937400
N	-5.23312600	0.33256400	-0.12231500	C	-3.59861200	-1.64130600	1.01249500
C	-6.40228200	-0.42819400	-0.33183100	C	-4.62549000	-2.57616600	0.87902400
C	-7.02253500	-1.03672000	0.76055500	C	-4.65717900	-3.71744800	1.67268200
C	-6.92781400	-0.59126100	-1.61424800	C	-3.65759800	-3.94335200	2.61210300
C	-8.16638400	-1.79797400	0.56640800	C	-2.63218700	-3.01473100	2.75507200
H	-6.60342200	-0.91180800	1.75056200	C	-2.60467400	-1.87321900	1.96268900
C	-8.06837300	-1.36531100	-1.79205300	H	-5.41039100	-2.42037500	0.14677700
H	-6.44703800	-0.12297100	-2.46122700	H	-3.68060800	-4.83398100	3.23193800
C	-8.69501600	-1.96960100	-0.70881600	H	-1.80460800	-1.15305100	2.07803700
H	-8.64181100	-2.26703400	1.42161700	H	-6.59612500	1.45110400	-2.92221700
H	-8.47114500	-1.48796800	-2.79220300	H	-7.76448600	1.02790600	1.18268300
H	-9.58749100	-2.56842000	-0.85625000	H	-5.46626200	-4.43114700	1.55444700
O	-4.14737500	0.27747700	-2.17178900	H	-1.84712400	-3.17727100	3.48678600
C	-2.53910300	2.39430700	-0.83294500	C	2.77872800	-0.57958500	1.73305600
H	-2.09526600	2.07781400	-1.77967400	C	3.17098600	-1.90963900	1.87613300
H	-3.40217300	3.01600100	-1.09591500	C	3.12844700	0.32390800	2.73931400
C	-1.59150600	3.25656600	-0.08828700	C	3.91733100	-2.31786400	2.97612600
C	-1.21493900	4.03893000	0.82012000	H	2.91421600	-2.63813900	1.11577900
H	-1.34306100	4.56024300	1.75245500	C	3.87530600	-0.07842400	3.83981600
C	-3.25851000	1.95184400	2.40578900	H	2.82279700	1.36284700	2.65230800
H	-3.86410900	1.65255300	3.26282300	C	4.27902300	-1.40367300	3.95942500
H	-2.21361500	1.70030100	2.58843500	H	4.21818300	-3.35735400	3.06209700
H	-3.31180300	3.03958900	2.30881300	H	4.13854800	0.64414100	4.60564000
H	-1.75058400	-0.20768500	-1.14996500	H	4.86328800	-1.72284500	4.81651800
Pd	0.27391600	3.98319600	-0.55891800	C	2.93593700	0.52268900	-0.64346300
				C	2.17206800	1.76335100	-1.09843400
				C	4.17155500	1.17277300	-0.08174100
				N	4.05421400	2.44347400	0.03030700
				N	2.81585300	2.82175000	-0.49719000
				C	2.42701400	4.17535300	-0.43389700
				C	3.34875200	5.13814400	-0.01712100
(S,R)-Int-III-j							
O 1							
C	-2.59489000	-0.84388700	-1.15338400				
N	-1.29466000	-1.36854100	-0.76046100				

C	1.12080900	4.55767300	-0.75197900
C	2.96243300	6.46840400	0.07783400
H	4.35698800	4.83965900	0.23709700
C	0.75348100	5.89361400	-0.65396000
H	0.40316400	3.81996700	-1.07949700
C	1.66593100	6.85699300	-0.23997800
H	3.68806200	7.20607800	0.40467600
H	-0.26327300	6.17857200	-0.90485800
H	1.37039000	7.89794400	-0.16477100
O	1.18424000	1.80669300	-1.79861900
C	3.15205200	-0.40593900	-1.84532000
H	2.17449600	-0.54907000	-2.30859600
H	3.77187800	0.12014500	-2.58034200
C	3.77467700	-1.71784900	-1.56556000
C	4.69879500	-2.52447800	-1.29876500
H	5.71466900	-2.77143700	-1.04462300
C	5.44408100	0.49356600	0.28171900
H	6.10678700	1.19344200	0.79278200
H	5.27259000	-0.37566900	0.91730500
H	5.94270600	0.13791900	-0.62589400
H	1.46728800	0.81424200	0.91123300
Pd	2.99960100	-3.61562200	-1.59276100

(S,R)-TS-II

(S,R)-TS-II-a

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C	-2.989887	0.067698	1.220692
N	-1.601630	0.231188	1.689827
C	-1.575351	0.363115	3.153647
C	-3.047162	0.516020	3.554512
C	-3.771617	0.876580	2.255114
H	-3.240701	-0.984273	1.398543
H	-1.112463	-0.508099	3.617569
H	-0.976680	1.243432	3.407297
H	-3.429734	-0.432897	3.938086
H	-3.178066	1.267603	4.333554
H	-4.820489	0.588209	2.284599
H	-3.714917	1.948121	2.054432
C	-0.500859	0.198487	0.961122
C	0.784243	-0.023495	1.444748
H	-0.630162	0.284378	-0.110041
H	0.929145	-0.040129	2.518176
C	1.953150	0.399471	0.590847
C	-3.322469	0.281429	-0.289011
O	-4.708963	-0.020598	-0.361534
Si	-6.181631	0.784634	-0.400978
C	-6.133075	2.540619	0.244727
H	-7.137006	2.970679	0.142344
H	-5.865161	2.600471	1.302326
H	-5.449177	3.183143	-0.316067
C	-7.300017	-0.260038	0.671700
H	-7.333780	-1.295475	0.317531
H	-6.966035	-0.278854	1.714087
H	-8.325848	0.124388	0.661960
C	-6.843485	0.794106	-2.151433
H	-7.922568	0.986183	-2.142823
H	-6.382959	1.567534	-2.772064
H	-6.688902	-0.170512	-2.645637
C	-3.057275	1.682118	-0.843993
C	-2.378885	2.684138	-0.154943
C	-2.223364	3.952322	-0.710508
C	-2.739434	4.237645	-1.966035
C	-3.402079	3.238512	-2.673899
C	-3.552789	1.977760	-2.118289
H	-1.959164	2.500185	0.824457
H	-2.620881	5.226755	-2.395816
H	-4.058035	1.204422	-2.685777
C	-2.628914	-0.814745	-1.130619
C	-1.767632	-0.559562	-2.178538
C	-1.170454	-1.611695	-2.901249

C	-1.439436	-2.924282	-2.586428
C	-2.340130	-3.231517	-1.533762
C	-2.913503	-2.171505	-0.800228
H	-1.519505	0.458863	-2.452829
H	-0.995367	-3.730611	-3.160797
H	-3.743473	-2.383164	-0.134157
H	-1.695213	4.717395	-0.151047
H	-3.799879	3.441217	-3.662858
H	-0.489552	-1.375508	-3.712327
H	-2.730140	-4.240084	-1.435220
C	2.790712	1.556660	1.105653
C	2.989676	1.803482	2.464239
C	3.448305	2.373355	0.182319
C	3.828464	2.828800	2.887208
H	2.492304	1.196008	3.212116
C	4.292495	3.394353	0.600979
H	3.304529	2.203175	-0.880471
C	4.487186	3.625186	1.957962
H	3.969543	3.001824	3.949328
H	4.796949	4.010022	-0.136470
H	5.145305	4.421867	2.288923
C	2.818599	-0.876269	0.276507
C	3.707922	-0.559266	-0.915794
C	3.851225	-1.191157	1.321495
N	5.045224	-0.989251	0.906904
N	4.990975	-0.587575	-0.430234
C	6.174622	-0.147518	-1.058932
C	7.233539	0.307113	-0.271391
C	6.286878	-0.147722	-2.449925
C	8.399397	0.753836	-0.877401
H	7.136356	0.307501	0.806669
C	7.457484	0.313203	-3.040561
H	5.467712	-0.499761	-3.060786
C	8.518129	0.762975	-2.263297
H	9.218139	1.103908	-0.257304
H	7.537897	0.311017	-4.122672
H	9.429680	1.117353	-2.732597
O	3.348315	-0.286612	-2.041689
C	1.787318	-1.960367	-0.022759
H	1.336099	-1.710081	-0.986710
H	2.237928	-2.950213	-0.111763
C	0.744800	-1.993316	1.067522
C	0.242917	-2.833146	1.931451
H	-0.225545	-2.591246	2.879693
C	3.596954	-1.712423	2.690377
H	4.531666	-1.758097	3.250955
H	2.884735	-1.086475	3.231425
H	3.162136	-2.714521	2.637790
H	1.562145	0.687160	-0.390872
Pd	-1.120044	-2.915137	0.293398

(S,R)-TS-II-b

0 1

C	-2.375608	1.245030	-1.216842
N	-0.945110	0.936297	-0.929327
C	-0.194555	0.700787	-2.171264
C	-1.147399	1.119473	-3.282086
C	-2.529255	0.869187	-2.694112
H	-2.485577	2.330789	-1.135263
H	0.713364	1.301275	-2.178638
H	0.081217	-0.357495	-2.235825
H	-1.016055	2.183326	-3.498105
H	-0.967683	0.563635	-4.202934
H	-3.299500	1.473491	-3.168677
H	-2.813973	-0.177899	-2.806726
C	-0.394188	1.038807	0.269329
C	0.892269	0.776698	0.753914
H	-1.103097	1.308312	1.040741
H	1.018796	1.206017	1.741120
C	2.171258	0.649299	-0.037090

C	-3.513365	0.667814	-0.296055
O	-4.682524	1.089976	-0.982332
Si	-5.988741	0.391298	-1.768735
C	-5.557338	-1.133131	-2.764771
H	-6.475053	-1.525203	-3.219998
H	-4.861866	-0.917862	-3.580971
H	-5.131582	-1.933958	-2.154098
C	-6.552732	1.754807	-2.915502
H	-6.844297	2.652201	-2.360211
H	-5.763326	2.041992	-3.617628
H	-7.419367	1.439481	-3.506844
C	-7.369099	-0.011731	-0.568776
H	-8.330820	-0.001061	-1.094631
H	-7.260867	-0.999058	-0.112271
H	-7.430275	0.727092	0.236797
C	-3.524114	-0.844650	-0.070001
C	-2.556182	-1.737853	-0.609722
C	-2.645474	-3.126886	-0.329120
C	-3.705472	-3.612177	0.474464
C	-4.640698	-2.738442	0.980703
C	-4.536564	-1.363047	0.713720
H	-1.894666	-1.417450	-1.402782
H	-3.784047	-4.677682	0.663786
H	-5.264844	-0.691584	1.154291
C	-3.518724	1.423005	1.051095
C	-3.080150	0.853006	2.245788
C	-3.058177	1.593918	3.423644
C	-3.479111	2.917500	3.427247
C	-3.924988	3.493898	2.242120
C	-3.944009	2.752764	1.067523
H	-2.734124	-0.174982	2.262686
H	-3.465354	3.494776	4.346007
H	-4.307997	3.206870	0.153136
H	-2.051081	-3.832508	-0.901779
H	-5.458503	-3.103543	1.592987
H	-2.712283	1.127371	4.340427
H	-4.263643	4.524982	2.231539
C	3.041684	1.893363	-0.106758
C	3.060196	2.862623	0.896645
C	3.905407	2.051003	-1.194083
C	3.928879	3.946019	0.824203
H	2.390349	2.786820	1.745931
C	4.777676	3.130152	-1.267421
H	3.901235	1.316005	-1.993389
C	4.795706	4.081179	-0.253814
H	3.927268	4.687334	1.616945
H	5.443116	3.225826	-2.119165
H	5.476199	4.924722	-0.306462
C	2.947784	-0.601260	0.506077
C	3.991141	-1.003788	-0.526927
C	3.823541	-0.340269	1.699910
N	5.068839	-0.451948	1.426889
N	5.203168	-0.831076	0.088557
C	6.495665	-0.889344	-0.475079
C	7.548133	-0.237063	0.169928
C	6.727271	-1.578667	-1.666900
C	8.822884	-0.278938	-0.376966
H	7.360785	0.295208	1.093281
C	8.008876	-1.603431	-2.203966
H	5.914931	-2.084827	-2.168082
C	9.062025	-0.958824	-1.566529
H	9.634108	0.230462	0.132731
H	8.180604	-2.141824	-3.130359
H	10.059832	-0.986390	-1.991132
O	3.780526	-1.359853	-1.668182
C	1.865161	-1.666888	0.668102
H	1.559791	-1.961046	-0.340275
H	2.234485	-2.558235	1.177805
C	0.701735	-1.108097	1.446275
C	0.058789	-1.358565	2.554038

H	-0.458929	-0.640105	3.181687
C	3.378733	-0.018525	3.081218
H	4.247890	0.136181	3.721930
H	2.759450	0.880595	3.102835
H	2.773350	-0.834243	3.485757
H	1.945594	0.348234	-1.057730
Pd	-1.147808	-2.172623	0.993743

(S,R)-TS-II-c

0 1

C	2.375617	1.244563	1.217207
N	0.945148	0.935912	0.929499
C	0.194571	0.699526	2.171245
C	1.147340	1.117458	3.282422
C	2.529303	0.868041	2.694307
H	2.485599	2.330347	1.136060
H	-0.713331	1.300031	2.179022
H	-0.081245	-0.358793	2.235025
H	1.015718	2.181079	3.499397
H	0.967752	0.560763	4.202776
H	3.299248	1.472462	3.169221
H	2.814508	-0.178969	2.806406
C	0.394266	1.039058	-0.269122
C	-0.892149	0.777076	-0.753901
H	1.103179	1.309060	-1.040354
H	-1.018594	1.206706	-1.740975
C	-2.171194	0.649450	0.036977
C	3.513360	0.667699	0.296215
O	4.682542	1.090121	0.982290
Si	5.988615	0.391835	1.769276
C	5.557264	-1.132481	2.765521
H	6.475300	-1.525600	3.219188
H	4.863213	-0.916808	3.582823
H	5.129829	-1.932720	2.155254
C	6.552087	1.755639	2.915930
H	6.843905	2.652909	2.360570
H	5.762360	2.042974	3.617632
H	7.418451	1.440479	3.507761
C	7.369239	-0.011211	0.569618
H	8.330972	0.000158	1.095431
H	7.261427	-0.998777	0.113538
H	7.430138	0.727362	-0.236215
C	3.524347	-0.844754	0.070077
C	2.556148	-1.738052	0.609171
C	2.645446	-3.127002	0.328177
C	3.705753	-3.612134	-0.475098
C	4.641268	-2.738326	-0.980658
C	4.537107	-1.362993	-0.713337
H	1.894400	-1.417870	1.402124
H	3.784329	-4.677588	-0.664706
H	5.265578	-0.691446	-1.153468
C	3.518374	1.422909	-1.050924
C	3.080321	0.852633	-2.245675
C	3.058022	1.593528	-3.423536
C	3.478104	2.917379	-3.427084
C	3.923458	3.494064	-2.241897
C	3.942808	2.752946	-1.067295
H	2.734907	-0.175558	-2.262620
H	3.464093	3.494648	-4.345845
H	4.306395	3.207308	-0.152873
H	2.050814	-3.832756	0.900427
H	5.459319	-3.103306	-1.592687
H	2.712540	1.126750	-4.340358
H	4.261447	4.525365	-2.231271
C	-3.041799	1.893369	0.106733
C	-3.905599	2.050695	1.194041
C	-3.060543	2.862669	-0.896623
C	-4.778118	3.129635	1.267459
H	-3.901368	1.315490	1.993168
C	-3.929468	3.945865	-0.824092

H	-2.390707	2.787088	-1.745942
C	-4.796336	4.080741	0.253927
H	-5.443624	3.225069	2.119176
H	-3.928040	4.687233	-1.616785
H	-5.477022	4.924126	0.306629
C	-2.947612	-0.601111	-0.506364
C	-3.990767	-1.003953	0.526732
C	-3.823619	-0.339752	-1.699941
N	-5.068859	-0.451468	-1.426659
N	-5.202915	-0.831070	-0.088447
C	-6.495297	-0.889575	0.475431
C	-7.547929	-0.237164	-0.169176
C	-6.726610	-1.579225	1.667118
C	-8.822557	-0.279229	0.377989
H	-7.360792	0.295366	-1.092423
C	-8.008100	-1.604190	2.204451
H	-5.914136	-2.085480	2.167988
C	-9.061411	-0.959447	1.567420
H	-9.633911	0.230285	-0.131388
H	-8.179606	-2.142840	3.130736
H	-10.059122	-0.987158	1.992238
O	-3.779916	-1.360326	1.667850
C	-1.864819	-1.666535	-0.668580
H	-1.559301	-1.960606	0.339781
H	-2.234002	-2.557972	-1.178224
C	-0.701542	-1.107490	-1.446787
C	-0.058668	-1.357644	-2.554664
H	0.459116	-0.639023	-3.182075
C	-3.379312	-0.017332	-3.081258
H	-4.248740	0.139625	-3.721058
H	-2.758401	0.880658	-3.102463
H	-2.775876	-0.833743	-3.487293
H	-1.945586	0.348288	1.057593
Pd	1.148025	-2.172268	-0.994687

(S,R)-TS-II-d

0 1			
C	2.328203	0.913019	1.386986
N	0.955355	0.531334	0.963696
C	0.125619	0.115641	2.100282
C	1.113079	-0.202764	3.205517
C	2.286016	0.731164	2.918327
H	2.443654	1.972193	1.153570
H	-0.532991	0.940224	2.391292
H	-0.481437	-0.744687	1.822034
H	0.678493	-0.031767	4.191040
H	1.412810	-1.248734	3.147090
H	2.104782	1.705866	3.378518
H	3.226543	0.361543	3.322370
C	0.483002	0.792624	-0.248285
C	-0.795548	0.652351	-0.805698
H	1.262795	1.082430	-0.940766
H	-0.838302	1.122417	-1.781154
C	-2.108495	0.652838	-0.053733
C	3.497858	0.203823	0.616266
O	3.460824	0.681622	-0.717762
Si	4.064216	2.010747	-1.546212
C	3.415778	3.607171	-0.812688
H	3.699283	4.452711	-1.450027
H	2.322835	3.609667	-0.743012
H	3.820180	3.807363	0.183675
C	3.352351	1.759801	-3.253099
H	3.702501	0.823686	-3.699406
H	2.258054	1.723515	-3.231488
H	3.639644	2.574587	-3.926628
C	5.929836	2.036759	-1.614048
H	6.258640	2.800033	-2.329216
H	6.387102	2.271642	-0.649253
H	6.333659	1.077905	-1.952849
C	4.862614	0.575253	1.226064

C	5.076566	1.772199	1.912764
C	6.350208	2.136681	2.335651
C	7.438143	1.313865	2.072652
C	7.239434	0.121464	1.386388
C	5.965454	-0.241260	0.969499
H	4.255684	2.444966	2.129921
H	8.432399	1.598956	2.400426
H	5.831959	-1.172103	0.430011
C	3.321909	-1.317032	0.547078
C	3.322899	-2.104031	1.678993
C	3.107879	-3.492839	1.602078
C	2.942492	-4.108727	0.382918
C	3.033025	-3.348121	-0.808548
C	3.217996	-1.947554	-0.721723
H	3.512209	-1.663067	2.650445
H	2.801944	-5.183094	0.322316
H	3.508244	-1.377149	-1.595526
H	6.488933	3.070194	2.871179
H	8.079628	-0.530491	1.170908
H	3.091004	-4.078219	2.515841
H	3.189408	-3.861904	-1.753485
C	-2.923336	1.935321	-0.114541
C	-2.875978	2.828202	-1.184841
C	-3.814523	2.202928	0.928634
C	-3.706228	3.943664	-1.219760
H	-2.188469	2.665896	-2.006714
C	-4.650862	3.311473	0.893936
H	-3.860783	1.529371	1.779400
C	-4.601981	4.186442	-0.185373
H	-3.653025	4.623872	-2.063780
H	-5.339402	3.490689	1.713159
H	-5.253103	5.053813	-0.217420
C	-2.939085	-0.604220	-0.510197
C	-3.977424	-0.902048	0.561309
C	-3.826971	-0.354546	-1.698397
N	-5.070218	-0.378510	-1.394413
N	-5.192459	-0.695444	-0.039232
C	-6.463124	-0.613865	0.568539
C	-7.439985	0.200018	-0.006620
C	-6.739856	-1.320261	1.739369
C	-8.689757	0.299522	0.588683
H	-7.213266	0.745758	-0.913665
C	-7.993119	-1.201191	2.328268
H	-5.983460	-1.951146	2.184565
C	-8.972951	-0.396063	1.759647
H	-9.444467	0.933107	0.134422
H	-8.202746	-1.753190	3.238692
H	-9.949794	-0.311986	2.223855
O	-3.766813	-1.206694	1.717204
C	-1.898659	-1.715068	-0.649406
H	-1.569967	-1.984091	0.357815
H	-2.313427	-2.611301	-1.114046
C	-0.756832	-1.212112	-1.493981
C	-0.254061	-1.473198	-2.673612
H	0.220320	-0.764924	-3.346788
C	-3.396859	-0.112362	-3.100678
H	-4.259939	0.162297	-3.709011
H	-2.649572	0.680986	-3.158133
H	-2.936537	-1.012485	-3.516933
H	-1.929224	0.450742	0.997865
Pd	1.148456	-2.291248	-1.326039

(S,R)-TS-II-e

0 1			
C	-2.271243	0.539536	1.523714
N	-0.932217	0.242221	0.980532
C	-0.402829	1.473332	0.384397
C	-0.852753	2.559569	1.359267
C	-2.096473	1.977957	2.063202
H	-2.476936	-0.174406	2.320633

H	0.667342	1.444660	0.232519
H	-0.874518	1.594630	-0.590432
H	-0.061008	2.759859	2.084653
H	-1.069394	3.494499	0.841019
H	-1.946547	1.943615	3.143934
H	-2.982981	2.580807	1.879937
C	-0.296941	-0.881171	1.303692
C	1.017840	-1.332496	1.134081
H	-0.974789	-1.616766	1.726827
H	1.164776	-2.271096	1.651616
C	2.244018	-0.450943	1.027187
C	-3.423167	0.425332	0.474687
O	-3.199828	1.421763	-0.495115
Si	-3.935762	2.762056	-1.177784
C	-5.203659	2.272941	-2.466775
H	-5.306261	3.077881	-3.203742
H	-4.898995	1.373962	-3.012498
H	-6.195737	2.092077	-2.045137
C	-2.513742	3.622456	-2.028944
H	-1.729098	3.914955	-1.325134
H	-2.055722	2.981002	-2.788919
H	-2.857161	4.532144	-2.533806
C	-4.717074	3.888743	0.093696
H	-5.210515	4.722260	-0.420270
H	-5.479753	3.382982	0.692950
H	-3.980940	4.324128	0.776548
C	-3.390137	-0.948198	-0.201969
C	-2.992194	-1.071665	-1.540967
C	-3.065964	-2.318995	-2.208737
C	-3.418312	-3.463327	-1.456534
C	-3.772659	-3.333957	-0.115934
C	-3.790305	-2.082452	0.497815
H	-2.772016	-0.174561	-2.104675
H	-3.491378	-4.427797	-1.946967
H	-4.129407	-1.997489	1.525501
C	-4.804799	0.599241	1.131995
C	-5.009399	0.907189	2.474939
C	-6.296392	1.101485	2.972876
C	-7.398194	0.988625	2.137550
C	-7.207769	0.652638	0.799979
C	-5.926618	0.450580	0.311332
H	-4.178700	1.004287	3.162732
H	-8.398961	1.145815	2.525934
H	-5.794587	0.161347	-0.725577
H	-3.013866	-2.365844	-3.292208
H	-4.068983	-4.213520	0.446184
H	-6.430236	1.344541	4.021917
H	-8.059990	0.537975	0.138170
C	3.299927	-0.620617	2.109347
C	3.524932	-1.809848	2.801604
C	4.133534	0.468194	2.382236
C	4.561014	-1.912822	3.724138
H	2.895801	-2.675933	2.631609
C	5.173427	0.367551	3.297222
H	3.967501	1.412667	1.871707
C	5.393470	-0.828315	3.971555
H	4.717054	-2.849469	4.249685
H	5.808154	1.227255	3.485544
H	6.203284	-0.912232	4.688842
C	2.864481	-0.585572	-0.423173
C	3.504560	0.744373	-0.792407
C	4.055781	-1.502152	-0.521631
N	5.136946	-0.875145	-0.797691
N	4.838516	0.480810	-0.956664
C	5.898237	1.399244	-1.117198
C	7.173637	1.051255	-0.669806
C	5.677950	2.645940	-1.704071
C	8.221948	1.949349	-0.814738
H	7.334841	0.082508	-0.214601
C	6.736759	3.536896	-1.832542

H	4.690454	2.916636	-2.050345
C	8.010556	3.196681	-1.392875
H	9.210898	1.669815	-0.466597
H	6.559112	4.504477	-2.290420
H	8.832151	3.896724	-1.501049
O	2.951094	1.823114	-0.871762
C	1.690499	-0.949804	-1.338951
H	1.061870	-0.063258	-1.452314
H	2.025366	-1.247480	-2.334417
C	0.928323	-2.085455	-0.715212
C	0.761665	-3.373352	-0.880941
H	0.632611	-4.117417	-0.100530
C	4.060001	-2.981741	-0.374908
H	5.087604	-3.345685	-0.330934
H	3.526846	-3.294833	0.523428
H	3.548846	-3.447445	-1.221664
H	1.938889	0.589938	1.094656
Pd	-1.046494	-2.495621	-1.504190

(S,R)-TS-II-f

O 1

C	3.169425	1.093418	-0.770620
N	1.849990	1.448378	-0.233768
C	1.954458	2.498947	0.780355
C	3.140202	3.319121	0.287450
C	4.051801	2.309287	-0.433400
H	3.055060	0.959588	-1.846052
H	1.032232	3.076622	0.821687
H	2.142805	2.048052	1.761077
H	2.785785	4.081151	-0.410796
H	3.650703	3.826106	1.107368
H	4.478301	2.733038	-1.343021
H	4.890836	2.021057	0.197486
C	0.757424	0.760369	-0.512650
C	-0.502891	1.014264	0.009101
H	0.874494	0.016756	-1.291639
H	-0.545198	1.551575	0.948232
C	-1.558839	-0.033777	-0.221604
C	3.658729	-0.290474	-0.205641
O	2.758107	-1.216870	-0.779564
Si	2.740377	-2.876221	-1.043698
C	3.948968	-3.353315	-2.387133
H	3.785631	-4.395962	-2.683840
H	3.819998	-2.735830	-3.281466
H	4.990342	-3.263197	-2.064853
C	0.979371	-3.162183	-1.592756
H	0.270454	-2.872867	-0.809508
H	0.733649	-2.595058	-2.496186
H	0.801642	-4.220343	-1.814224
C	3.086427	-3.850822	0.514099
H	3.084526	-4.922685	0.283303
H	4.059818	-3.617557	0.953620
H	2.324713	-3.680628	1.280382
C	5.079123	-0.620431	-0.683541
C	5.534571	-0.193830	-1.933180
C	6.765510	-0.609421	-2.425874
C	7.565876	-1.467883	-1.681534
C	7.123836	-1.903468	-0.438599
C	5.893725	-1.482567	0.052643
H	4.930964	0.459993	-2.551633
H	8.525392	-1.795564	-2.067785
H	5.567292	-1.841509	1.021281
C	3.506576	-0.291030	1.321140
C	4.463746	0.284126	2.161004
C	4.248478	0.379760	3.530890
C	3.071488	-0.102969	4.091095
C	2.116835	-0.687430	3.267699
C	2.333727	-0.778046	1.898107
H	5.399829	0.650270	1.755730
H	2.903769	-0.030906	5.160736

H	1.569901	-1.220221	1.271465
H	7.096093	-0.263424	-3.399740
H	7.734963	-2.576572	0.153749
H	5.008882	0.829051	4.161371
H	1.195004	-1.077407	3.686927
C	-1.768917	-1.038141	0.898006
C	-1.499023	-0.747347	2.235193
C	-2.268082	-2.305436	0.584740
C	-1.731519	-1.690569	3.230841
H	-1.093833	0.218434	2.515285
C	-2.502949	-3.249542	1.576793
H	-2.471939	-2.559477	-0.451017
C	-2.236228	-2.944300	2.906736
H	-1.516081	-1.441678	4.265166
H	-2.890969	-4.226203	1.306778
H	-2.415698	-3.679670	3.684125
C	-2.872072	0.702358	-0.658284
C	-3.798250	-0.310481	-1.317764
C	-3.732310	1.157296	0.488139
N	-4.837947	0.515922	0.558856
N	-4.899976	-0.387982	-0.504026
C	-5.975909	-1.299051	-0.560980
C	-6.721331	-1.544447	0.593742
C	-6.289674	-1.964345	-1.747819
C	-7.776764	-2.444639	0.554835
H	-6.471460	-1.027391	1.510771
C	-7.344824	-2.868601	-1.766347
H	-5.713735	-1.778839	-2.642922
C	-8.093733	-3.114778	-0.621995
H	-8.350242	-2.626660	1.457877
H	-7.581672	-3.381292	-2.692950
H	-8.917064	-3.820713	-0.646519
O	-3.579772	-0.942854	-2.329971
C	-2.400135	1.767956	-1.646509
H	-2.187344	1.250662	-2.588709
H	-3.178968	2.504074	-1.851759
C	-1.137557	2.464539	-1.175767
C	-0.314742	3.347156	-1.723009
H	0.773998	3.294585	-1.684890
C	-3.421670	2.231157	1.466257
H	-4.250178	2.351299	2.165632
H	-2.512686	2.007099	2.028562
H	-3.248516	3.179762	0.942862
H	-1.269508	-0.599422	-1.114771
Pd	-1.314471	4.387391	-0.252820

(S,R)-TS-II-g
01

C	2.972203	0.684674	-1.046976
N	1.724646	1.027006	-0.359646
C	1.960475	1.945500	0.757100
C	3.224930	2.707742	0.351342
C	3.809490	1.962285	-0.865843
H	2.738077	0.489638	-2.094577
H	1.102701	2.605370	0.877525
H	2.103426	1.366107	1.673432
H	2.977859	3.737575	0.088440
H	3.937823	2.744204	1.175535
H	3.722805	2.572756	-1.766770
H	4.865078	1.738199	-0.728439
C	0.566347	0.445171	-0.613690
C	-0.635484	0.773275	-0.000452
H	0.560337	-0.233385	-1.460892
H	-0.574888	1.249065	0.969643
C	-1.807952	-0.143311	-0.225535
C	3.630295	-0.600687	-0.441240
O	3.927630	-0.301063	0.903358
Si	5.237702	-0.201215	1.940817
C	5.837148	-1.885693	2.499700
H	6.341518	-1.787205	3.468053

H	5.006915	-2.585837	2.638670
H	6.551130	-2.339180	1.807918
C	4.526471	0.685676	3.423189
H	4.160336	1.685996	3.175173
H	3.692447	0.123612	3.856220
H	5.282761	0.799789	4.207651
C	6.657237	0.762141	1.199951
H	7.495609	0.776033	1.906231
H	7.023109	0.313222	0.271603
H	6.393862	1.803919	0.993352
C	2.597914	-1.733185	-0.476375
C	1.882102	-2.082676	0.664862
C	0.867336	-3.033115	0.600951
C	0.555136	-3.642296	-0.607372
C	1.272065	-3.303968	-1.751715
C	2.287923	-2.359380	-1.684693
H	2.108715	-1.590534	1.602852
H	-0.242990	-4.375453	-0.658493
H	2.839231	-2.104054	-2.584597
C	4.879008	-1.037049	-1.220389
C	5.411862	-0.341026	-2.303391
C	6.569055	-0.788091	-2.937126
C	7.209234	-1.939249	-2.500729
C	6.669700	-2.658829	-1.438386
C	5.512301	-2.215489	-0.816693
H	4.940218	0.558699	-2.678280
H	8.113120	-2.283422	-2.992336
H	5.083799	-2.801919	-0.011400
H	0.306990	-3.283841	1.495929
H	1.040352	-3.778280	-2.699896
H	6.967109	-0.227884	-3.776774
H	7.145223	-3.573583	-1.099920
C	-2.082416	-1.164890	0.864398
C	-2.732639	-2.354153	0.526537
C	-1.716274	-0.969434	2.195465
C	-3.016880	-3.315570	1.488190
H	-3.010473	-2.537779	-0.506872
C	-1.994732	-1.930970	3.161043
H	-1.193967	-0.067980	2.495116
C	-2.647288	-3.107528	2.812599
H	-3.523232	-4.230825	1.199382
H	-1.697164	-1.758235	4.190464
H	-2.863313	-3.857878	3.566054
C	-3.051055	0.749720	-0.570679
C	-4.100065	-0.124636	-1.243956
C	-3.819334	1.225554	0.632029
N	-4.982536	0.696858	0.713890
N	-5.175864	-0.131503	-0.393298
C	-6.340083	-0.925942	-0.457908
C	-7.036522	-1.210369	0.717907
C	-6.791607	-1.433452	-1.677405
C	-8.179823	-1.995542	0.668462
H	-6.679151	-0.814875	1.659751
C	-7.933231	-2.225427	-1.707404
H	-6.253324	-1.214914	-2.588730
C	-8.634066	-2.509830	-0.541461
H	-8.715225	-2.209824	1.587646
H	-8.278464	-2.615795	-2.659158
H	-9.526697	-3.125357	-0.574748
O	-3.984825	-0.721580	-2.293884
C	-2.504742	1.813206	-1.521598
H	-2.371420	1.325878	-2.494097
H	-3.211592	2.631990	-1.664944
C	-1.166207	2.355445	-1.059674
C	-0.283630	3.197291	-1.578953
H	0.796651	3.042649	-1.582745
C	-3.366927	2.204647	1.653676
H	-4.140664	2.338354	2.410989
H	-2.446259	1.876547	2.140081
H	-3.152352	3.171740	1.181459

H -1.621240 -0.698728 -1.151808
Pd -1.129836 4.219866 -0.004437

(S,R)-TS-II-h

0 1

C 3.172174 0.807065 -0.707285
N 1.866110 1.205926 -0.177816
C 1.961454 2.323709 0.769411
C 3.302589 2.992118 0.450329
C 3.998747 2.097263 -0.595316
H 3.029376 0.524417 -1.750373
H 1.116774 2.995142 0.621736
H 1.927542 1.935918 1.792190
H 3.145789 3.995436 0.051883
H 3.903170 3.087727 1.354790
H 4.005000 2.588746 -1.569767
H 5.037489 1.897827 -0.336526
C 0.760924 0.516288 -0.388003
C -0.498299 0.879544 0.072210
H 0.846546 -0.303402 -1.089265
H -0.536719 1.541448 0.927772
C -1.596528 -0.145569 -0.032518
C 3.727777 -0.461478 0.033333
O 2.838557 -1.525968 -0.242876
Si 2.643609 -2.618130 -1.505565
C 2.492770 -1.747460 -3.156437
H 2.265289 -2.484354 -3.935492
H 1.687396 -1.006241 -3.174682
H 3.420044 -1.247772 -3.451959
C 1.028007 -3.437507 -1.058458
H 1.095838 -3.955890 -0.096818
H 0.216664 -2.706266 -0.978400
H 0.732345 -4.174669 -1.812469
C 4.030389 -3.866007 -1.586608
H 3.762716 -4.667251 -2.285577
H 4.968605 -3.425978 -1.935982
H 4.217331 -4.330142 -0.613619
C 5.129571 -0.849418 -0.449806
C 5.637414 -0.447114 -1.684784
C 6.859664 -0.929140 -2.144066
C 7.593562 -1.822634 -1.375176
C 7.096845 -2.231219 -0.141507
C 5.877258 -1.749954 0.312513
H 5.090986 0.245614 -2.314149
H 8.546241 -2.198367 -1.733621
H 5.494950 -2.088963 1.269190
C 3.677380 -0.227660 1.545134
C 4.659265 0.518147 2.197327
C 4.547848 0.807528 3.552074
C 3.453952 0.349023 4.278129
C 2.480460 -0.411300 3.639911
C 2.592729 -0.698319 2.284268
H 5.526667 0.872633 1.651014
H 3.367669 0.574137 5.336216
H 1.830724 -1.287114 1.789199
H 7.235175 -0.601228 -3.107850
H 7.658058 -2.932606 0.467147
H 5.322423 1.389065 4.041518
H 1.627173 -0.785697 4.196522
C -1.913758 -0.921061 1.234936
C -1.639322 -0.429670 2.511358
C -2.532739 -2.169463 1.126113
C -1.986782 -1.156839 3.645226
H -1.139621 0.524461 2.636308
C -2.886005 -2.895692 2.256460
H -2.737389 -2.583551 0.143481
C -2.616530 -2.389524 3.523131
H -1.762664 -0.754864 4.628216
H -3.368631 -3.861037 2.144581
H -2.888310 -2.955375 4.408160

C -2.848872 0.560784 -0.658597
C -3.787361 -0.499218 -1.219216
C -3.750511 1.224081 0.345784
N -4.896438 0.659452 0.427800
N -4.946353 -0.387558 -0.494803
C -6.075970 -1.233417 -0.505105
C -6.904394 -1.277440 0.617787
C -6.366871 -2.023801 -1.618476
C -8.015766 -2.108752 0.621642
H -6.673673 -0.661494 1.477188
C -7.479158 -2.856554 -1.594018
H -5.728273 -1.991489 -2.489463
C -8.309576 -2.904358 -0.480758
H -8.653590 -2.135151 1.499069
H -7.698116 -3.467914 -2.463353
H -9.177762 -3.554670 -0.471654
O -3.538979 -1.296387 -2.099844
C -2.272443 1.439825 -1.768257
H -2.019757 0.771397 -2.599236
H -3.004081 2.157308 -2.142753
C -1.016236 2.161405 -1.321150
C -0.145193 2.950459 -1.937410
H 0.938368 2.882863 -1.822935
C -3.432625 2.407381 1.184922
H -4.279018 2.646845 1.830090
H -2.551413 2.227379 1.804074
H -3.206471 3.272086 0.547399
H -1.300939 -0.872785 -0.797737
Pd -1.193377 4.194075 -0.669238

(S,R)-TS-II-i

0 1

C 3.172183 0.807168 -0.707154
N 1.866126 1.205979 -0.177594
C 1.961484 2.323711 0.769728
C 3.302839 2.991872 0.451046
C 3.998757 2.097340 -0.595019
H 3.029381 0.524670 -1.750280
H 1.116971 2.995310 0.621877
H 1.927233 1.935838 1.792461
H 3.146392 3.995456 0.053137
H 3.903411 3.086800 1.355580
H 4.004746 2.589097 -1.569333
H 5.037566 1.897843 -0.336535
C 0.760941 0.516480 -0.387896
C -0.498364 0.879885 0.072242
H 0.846506 -0.303239 -1.089125
H -0.536794 1.541761 0.927826
C -1.596500 -0.145397 -0.032330
C 3.727757 -0.461486 0.033285
O 2.838431 -1.525882 -0.242966
Si 2.643353 -2.617843 -1.505826
C 2.492518 -1.746909 -3.156563
H 2.264699 -2.483652 -3.935662
H 1.687344 -1.005467 -3.174592
H 3.419878 -1.247440 -3.452178
C 1.027644 -3.437092 -1.058857
H 1.095205 -3.955119 -0.097008
H 0.216267 -2.705831 -0.979320
H 0.732215 -4.174531 -1.812688
C 4.029993 -3.865858 -1.587139
H 3.762211 -4.666921 -2.286274
H 4.968247 -3.425857 -1.936448
H 4.216915 -4.330221 -0.614255
C 5.129486 -0.849456 -0.450021
C 5.637344 -0.446919 -1.684915
C 6.859546 -0.928952 -2.144322
C 7.593383 -1.822672 -1.375638
C 7.096654 -2.231483 -0.142049
C 5.877113 -1.750220 0.312092

H	5.090975	0.245999	-2.314122
H	8.546025	-2.198407	-1.734181
H	5.494792	-2.089403	1.268702
C	3.677518	-0.227826	1.545114
C	4.659594	0.517727	2.197305
C	4.548359	0.806949	3.552101
C	3.454453	0.348539	4.278201
C	2.480752	-0.411508	3.639976
C	2.592839	-0.698366	2.284283
H	5.526974	0.872172	1.650927
H	3.368317	0.573523	5.336328
H	1.830673	-1.286949	1.789213
H	7.235068	-0.600863	-3.108040
H	7.657818	-2.933048	0.466445
H	5.323080	1.388289	4.041547
H	1.627446	-0.785816	4.196618
C	-1.913548	-0.920777	1.235236
C	-1.639010	-0.429271	2.511592
C	-2.532466	-2.169227	1.126580
C	-1.986303	-1.156375	3.645554
H	-1.139359	0.524900	2.636430
C	-2.885574	-2.895386	2.257018
H	-2.737202	-2.583401	0.144001
C	-2.615993	-2.389105	3.523623
H	-1.762104	-0.754311	4.628488
H	-3.368158	-3.860767	2.145265
H	-2.887642	-2.954906	4.408724
C	-2.848909	0.560725	-0.658510
C	-3.787266	-0.499424	-1.219054
C	-3.750641	1.224078	0.345745
N	-4.896543	0.659390	0.427740
N	-4.946330	-0.387712	-0.494770
C	-6.075885	-1.233657	-0.505093
C	-6.904059	-1.278094	0.617959
C	-6.366956	-2.023685	-1.618667
C	-8.015380	-2.109476	0.621773
H	-6.673193	-0.662406	1.477507
C	-7.479177	-2.856528	-1.594251
H	-5.728529	-1.991033	-2.489772
C	-8.309360	-2.904739	-0.480831
H	-8.653021	-2.136212	1.499322
H	-7.698278	-3.467621	-2.463737
H	-9.177502	-3.555110	-0.471760
O	-3.538770	-1.296717	-2.099538
C	-2.272388	1.439623	-1.768254
H	-2.019495	0.771067	-2.599065
H	-3.004001	2.156993	-2.143019
C	-1.016291	2.161310	-1.320929
C	-0.145456	2.950511	-1.937527
H	0.938114	2.882921	-1.822957
C	-3.432864	2.407457	1.184815
H	-4.279191	2.646748	1.830133
H	-2.551494	2.227646	1.803798
H	-3.207015	3.272204	0.547240
H	-1.300854	-0.872685	-0.797459
Pd	-1.193701	4.194088	-0.669376

(S,R)-Int-IV

(S,R)-Int-IV-a

0 1

C	3.19093400	1.17979900	0.31540900
N	1.83536100	1.24293100	0.90063700
C	1.85438200	1.50544300	2.35625900
C	3.32346000	1.75283700	2.70362600
C	4.06091000	1.88042300	1.36106600
H	3.15318500	1.73603800	-0.61889400
H	1.22711100	2.37427600	2.55140800
H	1.43780000	0.64130600	2.87486100
H	3.43210400	2.65821100	3.30036400

H	3.71435100	0.92236300	3.28841000
H	4.15930200	2.93050000	1.08006100
H	5.06526300	1.45963800	1.40194100
C	0.76816200	1.09808600	0.19797200
C	-0.60675700	1.18668000	0.70361700
H	0.91004800	0.93926100	-0.86412400
H	-0.63704500	1.24831400	1.79039100
C	-1.47083800	0.02892000	0.16810400
C	3.54818400	-0.30043300	-0.05749800
O	2.60289700	-0.62059800	-1.05807300
Si	2.53078300	-1.74720800	-2.31269900
C	3.77055400	-1.35458000	-3.65224400
H	3.56029200	-1.96808200	-4.53613900
H	3.70936100	-0.30690400	-3.96231700
H	4.80235200	-1.55650200	-3.35241800
C	0.79132400	-1.51228600	-2.94228500
H	0.05236700	-1.75409900	-2.17282800
H	0.60604500	-0.48682600	-3.27672800
H	0.59323800	-2.17183600	-3.79420100
C	2.75117500	-3.49634500	-1.69287100
H	2.64593800	-4.19559000	-2.53509300
H	3.73328100	-3.67333200	-1.24720300
H	1.99387300	-3.76120900	-0.94898700
C	4.96324300	-0.38687100	-0.64655200
C	5.51328700	0.67232000	-1.37128100
C	6.73665400	0.53763500	-2.01617400
C	7.43313700	-0.66326100	-1.95562700
C	6.89634000	-1.72607500	-1.23976600
C	5.67491400	-1.58657100	-0.59217100
H	4.99531200	1.62037600	-1.45555500
H	8.38635400	-0.76951600	-2.46265200
H	5.27439400	-2.42982800	-0.04280100
C	3.34156400	-1.20234500	1.16391300
C	4.31446100	-1.32283800	2.15821800
C	4.07629300	-2.08131500	3.29730900
C	2.85822300	-2.73238500	3.46381200
C	1.88309100	-2.61886900	2.48089800
C	2.12533100	-1.85879400	1.34236100
H	5.27050700	-0.82340300	2.04526000
H	2.67294400	-3.32666300	4.35254300
H	1.35353900	-1.77674300	0.58776800
H	7.14245600	1.37606400	-2.57236300
H	7.42656800	-2.67100400	-1.18391700
H	4.84749000	-2.16411200	4.05619500
H	0.92748600	-3.11989500	2.59234800
C	-1.57216500	-1.22252800	1.01011800
C	-1.65389300	-1.19718900	2.40290800
C	-1.64380500	-2.45929600	0.36518700
C	-1.81280000	-2.37212700	3.12837600
H	-1.59621900	-0.25741500	2.94047400
C	-1.79993700	-3.63658200	1.08699700
H	-1.59199900	-2.49982000	-0.71827900
C	-1.88862300	-3.59612900	2.47370500
H	-1.87683100	-2.32877200	4.21070500
H	-1.85721000	-4.58472900	0.56278800
H	-2.01409500	-4.51273700	3.04048900
C	-2.83254200	0.70758600	-0.19717700
C	-3.59381800	-0.22769100	-1.11972100
C	-3.80579500	0.84352200	0.93695300
N	-4.83929500	0.10372700	0.78836000
N	-4.72486200	-0.58270800	-0.42526700
C	-5.70061400	-1.54661000	-0.75535700
C	-6.56862900	-2.00580200	0.23806600
C	-5.80217900	-2.05106000	-2.05411800
C	-7.52812400	-2.95982500	-0.07036500
H	-6.48791800	-1.61286000	1.24271700
C	-6.76517200	-3.01056100	-2.34263700
H	-5.13353700	-1.69941800	-2.82601900
C	-7.63279100	-3.47056200	-1.35966100
H	-8.19688600	-3.30778900	0.71012600

H	-6.83560900	-3.39552300	-3.35477900
H	-8.38322900	-4.21763400	-1.59513300
O	-3.24149800	-0.61639400	-2.21342200
C	-2.36758700	2.03499900	-0.80974100
H	-2.06847600	1.84144600	-1.84705000
H	-3.14727400	2.79810300	-0.83048200
C	-1.19258900	2.45905000	0.04715700
C	-0.72833300	3.70296700	0.26093300
H	0.15437700	3.71374400	0.92023500
C	-3.68751900	1.78321300	2.08295500
H	-4.54786600	1.67814500	2.74501600
H	-2.77449000	1.61150400	2.65657400
H	-3.63910600	2.81357000	1.71794400
H	-1.07005800	-0.26238000	-0.80902500
Pd	-1.36819000	5.42681900	-0.41709900

(S,R)-Int-IV-b

O 1			
C	3.13046500	-0.24702800	-1.00104100
N	1.77271000	-0.24177700	-1.57122800
C	1.76987300	0.07587300	-2.99807400
C	3.09814300	0.78044800	-3.21824200
C	4.02715200	0.12343200	-2.19781700
H	3.36145600	-1.25957800	-0.66642400
H	1.69548600	-0.84786800	-3.58775700
H	0.92109500	0.71231200	-3.24985600
H	3.45558700	0.66557600	-4.24250300
H	2.99179500	1.84722000	-3.01310700
H	4.45295200	-0.79358900	-2.61389500
H	4.86023300	0.76705400	-1.91712300
C	0.73028900	-0.86195300	-0.95607000
C	-0.67676200	-0.77493300	-1.49365400
H	0.78557500	-0.80149000	0.12721100
H	-0.72255400	-0.33320900	-2.48638000
C	-1.66407800	-0.12801800	-0.51073600
C	3.25265800	0.67562600	0.25841800
O	2.38778500	0.15706000	1.26348700
Si	2.51625400	-1.11626800	2.35433800
C	3.02438500	-2.71668200	1.51317600
H	2.99611300	-3.53573200	2.24020000
H	2.32624600	-3.01206900	0.70851200
H	4.03146400	-2.69072100	1.09032800
C	0.77022500	-1.28574200	2.98604600
H	0.36455400	-0.32339700	3.31319100
H	0.09584900	-1.68553400	2.22162200
H	0.72498500	-1.96881500	3.84089200
C	3.70992700	-0.76262600	3.74272700
H	3.60264600	-1.52786900	4.52042500
H	4.75180100	-0.77517700	3.41133400
H	3.51777800	0.20778000	4.20957900
C	4.67513600	0.70162100	0.83080700
C	5.63381700	-0.26606700	0.53364200
C	6.86700500	-0.27115600	1.18029100
C	7.16069300	0.69170800	2.13607800
C	6.21107700	1.66166900	2.44288100
C	4.98283000	1.66165200	1.79875000
H	5.44052900	-1.03582500	-0.20405100
H	8.12166000	0.68765500	2.63977500
H	4.24537100	2.41305100	2.05923800
C	2.74500100	2.07089600	-0.10115600
C	3.58610000	3.02566900	-0.67300900
C	3.08694100	4.25435600	-1.08995900
C	1.73583100	4.54723300	-0.94109100
C	0.89197300	3.60558700	-0.36334300
C	1.39449800	2.37909900	0.05365900
H	4.64298600	2.81493400	-0.79580700
H	1.34435200	5.50534400	-1.26758000
H	0.73185900	1.65462300	0.50954300
H	7.59772900	-1.03369900	0.93147000
H	6.42495800	2.41705200	3.19185700

H	3.75876200	4.98402500	-1.53052400
H	-0.16392600	3.82106500	-0.23667800
C	-2.05320700	1.32003100	-0.71995200
C	-2.02231800	1.95229000	-1.96272700
C	-2.51119700	2.05089600	0.38028800
C	-2.45049900	3.26817200	-2.10471000
H	-1.66200000	1.42873800	-2.84095600
C	-2.94636700	3.36254400	0.24150900
H	-2.52972800	1.58485000	1.36103000
C	-2.92013200	3.97688500	-1.00601800
H	-2.41501900	3.73932100	-3.08159800
H	-3.30242200	3.90519700	1.11101600
H	-3.25658600	5.00226300	-1.11862500
C	-2.87573500	-1.12577800	-0.47767900
C	-3.67215200	-0.90734100	0.79577500
C	-3.92538200	-0.86204500	-1.51612600
N	-5.04119200	-0.49655500	-1.00844300
N	-4.91382400	-0.48834500	0.38539500
C	-5.99766700	-0.02664900	1.16205600
C	-7.06973800	0.60638700	0.52829600
C	-6.00886100	-0.18687300	2.55022700
C	-8.14045400	1.07005100	1.27962000
H	-7.05806900	0.72940900	-0.54613100
C	-7.08766500	0.28854300	3.28598600
H	-5.18331300	-0.67555200	3.04614400
C	-8.15800300	0.91694600	2.66165100
H	-8.96702800	1.55909600	0.77454700
H	-7.08583500	0.15774300	4.36325800
H	-8.99679300	1.28234400	3.24444500
O	-3.27089800	-1.03815500	1.93396900
C	-2.18909400	-2.49927600	-0.57518200
H	-1.83878300	-2.76082700	0.42807800
H	-2.85966400	-3.29193000	-0.91075200
C	-1.04754000	-2.26893000	-1.56061000
C	-0.57253100	-3.15528000	-2.51691100
H	0.03622900	-2.58642500	-3.25032500
C	-3.75959700	-1.03734400	-2.98189000
H	-4.67905800	-0.76639800	-3.50212100
H	-2.94180200	-0.42190100	-3.36298600
H	-3.50962200	-2.07730500	-3.21264900
H	-1.24087500	-0.20952500	0.49705500
Pd	0.90948500	-2.96331100	-0.90779800

(S,R)-Int-IV-c

O 1			
C	-3.00040100	0.00500900	1.18092000
N	-1.59479900	0.05581300	1.65490500
C	-1.55782600	0.27582100	3.11781600
C	-3.02017800	0.46991000	3.51537100
C	-3.72667000	0.85876300	2.21634000
H	-3.29909700	-1.03365600	1.35738200
H	-1.09593800	-0.57878400	3.61018000
H	-0.95202500	1.16365400	3.30944300
H	-3.43122200	-0.46885900	3.89358700
H	-3.12581200	1.22294500	4.29617200
H	-4.78765000	0.62194000	2.25087800
H	-3.61772300	1.92432800	2.00575900
C	-0.55129600	-0.21363900	0.94021400
C	0.79703100	-0.48948500	1.45761900
H	-0.66709200	-0.22349700	-0.13428000
H	0.88714900	-0.32030200	2.52772300
C	1.88746600	0.20914800	0.63077500
C	-3.31299700	0.25407500	-0.32853300
O	-4.70302200	-0.00915300	-0.41393200
Si	-6.17063100	0.80996700	-0.39679900
C	-6.09107200	2.54693600	0.29709700
H	-7.07114900	3.01746300	0.15155300
H	-5.88191800	2.57074400	1.36927300
H	-5.35354300	3.17646900	-0.20731700
C	-7.27555900	-0.25430900	0.66908800

H	-7.35183700	-1.27135000	0.27104000	(S,R)-Int-IV-d			
H	-6.90168900	-0.32958300	1.69540300	0 1			
H	-8.29000100	0.15635300	0.71823700	C	-3.11944800	-0.24288500	1.00492000
C	-6.85968700	0.87412000	-2.13464000	N	-1.75774300	-0.26503400	1.56540800
H	-7.94030100	1.05443800	-2.10210600	C	-1.74151300	0.01925200	2.99903200
H	-6.41814300	1.67452900	-2.73471200	C	-3.06001900	0.73372700	3.24472400
H	-6.70341000	-0.07072000	-2.66484800	C	-4.00362200	0.11143300	2.21599700
C	-2.98813500	1.65872800	-0.83974700	H	-3.36360400	-1.24560900	0.65036700
C	-2.17807300	2.57051500	-0.16720300	H	-1.67384100	-0.91857000	3.56700700
C	-1.93722100	3.83670800	-0.69607000	H	-0.88391200	0.64027700	3.25945100
C	-2.49879700	4.21014300	-1.90828600	H	-3.41180900	0.59937300	4.26857000
C	-3.29406200	3.30065600	-2.59986900	H	-2.94261700	1.80362900	3.06343800
C	-3.52804200	2.04073500	-2.07154200	H	-4.43795800	-0.80951100	2.61408100
H	-1.71688500	2.32049400	0.77890300	H	-4.83067600	0.77110100	1.95554900
H	-2.31331000	5.19768000	-2.31728100	C	-0.72820500	-0.88542200	0.92851900
H	-4.12813100	1.33282800	-2.63169500	C	0.68188100	-0.83665600	1.46247400
C	-2.63755000	-0.83467000	-1.19270100	H	-0.78830200	-0.79471300	-0.15288700
C	-1.81911100	-0.55856100	-2.26849500	H	0.73997300	-0.41788700	2.46448800
C	-1.19998100	-1.59685300	-2.99410400	C	1.67864400	-0.18767600	0.49096700
C	-1.41074400	-2.91357300	-2.65697500	C	-3.23973500	0.70696700	-0.23470100
C	-2.27156800	-3.24312200	-1.57677400	O	-2.39745000	0.19195800	-1.26070900
C	-2.85645300	-2.19635400	-0.83384800	Si	-2.56376900	-1.05681400	-2.37483200
H	-1.61236200	0.46402500	-2.55862800	C	-3.07527300	-2.66766400	-1.55564900
H	-0.95099500	-3.70979800	-3.23301900	H	-3.10739300	-3.46391000	-2.30758300
H	-3.65708100	-2.43322400	-0.14145300	H	-2.34385300	-3.01183800	-0.80074300
H	-1.30512600	4.52957200	-0.15046400	H	-4.05838600	-2.62931100	-1.08095900
H	-3.72854200	3.57124500	-3.55653600	C	-0.83228100	-1.23425000	-3.04236900
H	-0.54948200	-1.34567400	-3.82528100	H	-0.43329000	-0.27517900	-3.38695600
H	-2.63222000	-4.26168400	-1.46655300	H	-0.14207800	-1.62689800	-2.28842000
C	2.46542300	1.50006700	1.16849000	H	-0.80592800	-1.92570100	-3.89127400
C	2.57387000	1.78053600	2.53090600	C	-3.77803100	-0.66069800	-3.73367600
C	2.95758800	2.43971700	0.25815400	H	-3.69920400	-1.41605600	-4.52428700
C	3.15867000	2.96334300	2.97071100	H	-4.81366700	-0.65920500	-3.38301900
H	2.20270800	1.07906700	3.26960900	H	-3.57635100	0.31294900	-4.18959900
C	3.54817500	3.61889400	0.69414300	C	-4.66807400	0.77160900	-0.78919200
H	2.88026500	2.24247700	-0.80678100	C	-5.63765000	-0.19056500	-0.50967700
C	3.65037100	3.88557100	2.05495900	C	-6.87819000	-0.15811500	-1.14113400
H	3.23183600	3.16127500	4.03523300	C	-7.16850300	0.83708200	-2.06433700
H	3.92692800	4.33059100	-0.03197500	C	-6.20791400	1.80144900	-2.35379800
H	4.10917500	4.80648200	2.39939900	C	-4.97242000	1.76411000	-1.72480300
C	2.92930400	-0.91847900	0.33232700	H	-5.44706600	-0.98581500	0.20125100
C	3.78227900	-0.50669700	-0.85445700	H	-8.13526600	0.86229100	-2.55616600
C	3.98077200	-1.11343100	1.38425900	H	-4.22704000	2.51220100	-1.97170200
N	5.15454500	-0.82301700	0.96600400	C	-2.70101100	2.08460900	0.14688500
N	5.06668300	-0.43200700	-0.37427500	C	-3.51640200	3.04069100	0.75280700
C	6.23254000	0.02326600	-1.02555200	C	-2.98950800	4.25046300	1.19036400
C	7.36452200	0.32596900	-0.26510700	C	-1.63561900	4.52270900	1.02842500
C	6.26582100	0.18080900	-2.41343700	C	-0.81734200	3.58004300	0.41661100
C	8.51614000	0.78094500	-0.89176600	C	-1.34766400	2.37270700	-0.02139600
C	7.33597600	0.20124700	0.80902700	H	-4.57497500	2.84541600	0.88627400
H	7.42626800	0.64301700	-3.02251600	H	-1.22207500	5.46570900	1.37129500
H	5.39351400	-0.05146600	-3.00662600	H	-0.70405300	1.64777400	-0.50327800
C	8.55602400	0.94493100	-2.27214500	H	-7.61729800	-0.91706600	-0.90656500
H	9.38891600	1.01177800	-0.28963700	H	-6.41901000	2.58205400	-3.07726600
H	7.44111700	0.76195200	-4.10105600	H	-3.64172200	4.98139100	1.65756000
H	9.45799700	1.30318900	-2.75672800	H	0.24038300	3.77979700	0.27987300
O	3.39253800	-0.25777300	-1.97647500	C	2.08991600	1.25056800	0.72362400
C	2.01639600	-2.12837100	0.07660100	C	2.07517700	1.85940800	1.97824000
H	1.62901800	-2.02638800	-0.94156000	C	2.55547900	1.99427000	-0.36477200
H	2.53344600	-3.08583100	0.14580400	C	2.52592600	3.16494500	2.14340100
C	0.92167000	-2.01592300	1.13900000	H	1.70959900	1.32454700	2.84742700
C	0.35542800	-3.03624200	1.85360200	C	3.01462400	3.29511100	-0.20277700
H	-0.24906200	-2.62554400	2.68409000	C	2.56342100	1.54623200	-1.35396400
C	3.76118600	-1.64352400	2.75508700	H	3.00379900	3.88601300	1.05627400
H	4.70523300	-1.67602700	3.30056800	H	2.50252800	3.61788900	3.12921800
H	3.05063000	-1.02787100	3.31117200	H	3.37728300	3.84763300	-1.06326900
H	3.33848700	-2.65119600	2.70670800	H	3.35873000	4.90300700	1.18680300
H	1.46757900	0.42621100	-0.35775500	C	2.87574300	-1.20447200	0.44380100
Pd	-0.99021000	-2.95982100	0.18897600	C	3.68090000	-0.96069700	-0.81938500
				C	3.91874400	-0.96513900	1.49548200

N	5.03381200	-0.57500800	1.00400700	C	-4.57859400	-0.47653000	1.34018100
N	4.91457000	-0.53802600	-0.38949000	C	-5.31823100	0.61099500	1.79644600
C	5.97694000	-0.00416400	-1.14858400	C	-6.43720300	0.42327400	2.60518600
C	6.92792500	0.80002200	-0.51709900	C	-6.83170700	-0.85505700	2.97267800
C	6.07846300	-0.25904500	-2.51773200	C	-6.08565700	-1.94942500	2.54296000
C	7.97322900	1.33936000	-1.25363000	C	-4.96938100	-1.75735000	1.74385400
H	6.84289300	0.99631500	0.54368400	H	-5.04155800	1.62342900	1.53299400
C	7.12723000	0.29625000	-3.24098100	H	-7.70601100	-1.00011300	3.59857100
H	5.34415600	-0.87982300	-3.01029100	H	-4.38564400	-2.61684000	1.43127100
C	8.07929700	1.09448200	-2.61863700	H	0.09494100	-3.50698900	0.12313600
H	8.70734900	1.96179200	-0.75253500	H	-0.41811000	-1.44925600	3.85034100
H	7.19800100	0.09260200	-4.30449100	H	-7.00044800	1.28626800	2.94521600
H	8.89639700	1.52109200	-3.19052100	H	-6.37076600	-2.95432100	2.83685000
O	3.29301400	-1.06969000	-1.96411800	C	2.01181500	-1.09029000	-0.79884800
C	2.16683400	-2.56708700	0.50892900	C	1.40654300	-1.45122400	-2.00079300
H	1.81716300	-2.80237300	-0.50101200	C	2.77311200	-2.05574700	-0.13139500
H	2.82263200	-3.37748500	0.83109700	C	1.56694400	-2.73037100	-2.52708400
C	1.02547200	-2.33842800	1.49527300	H	0.78340000	-0.74775200	-2.54080400
C	0.53236200	-3.23776300	2.43016000	C	2.94723300	-3.32721700	-0.65846300
H	-0.06727300	-2.67550900	3.17609800	H	3.21799700	-1.82028200	0.83000000
C	3.74638500	-1.18293200	2.95494400	C	2.34328800	-3.67128800	-1.86399100
H	4.66392000	-0.92786700	3.48659600	H	1.07906900	-2.98782700	-3.46176800
H	2.92755200	-0.57799000	3.35095400	H	3.54664300	-4.05393000	-0.11984100
H	3.49469700	-2.22875400	3.15515600	H	2.47115600	-4.66633700	-2.27737200
H	1.25523800	-0.24751300	-0.51824500	C	3.22195300	1.11199600	-0.17946500
Pd	-0.94345100	-2.98040200	0.82631400	C	4.21772400	0.54842100	0.81746000

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C	-2.88299500	1.09981500	0.17735700
N	-1.64325200	1.10114200	-0.61706300
C	-1.95182400	1.44970300	-2.00134300
C	-3.07730000	2.46781500	-1.86133500
C	-3.86096900	1.98842500	-0.63150400
H	-2.67297200	1.53076800	1.15846500
H	-1.07899200	1.85694500	-2.50655000
H	-2.28223700	0.55424200	-2.53268400
H	-2.64173700	3.45454200	-1.67637600
H	-3.69778000	2.53482200	-2.75706700
H	-4.21160800	2.83113300	-0.03427800
H	-4.73834200	1.41620400	-0.92987900
C	-0.44048900	1.35652400	-0.01974300
C	0.86134600	1.26462200	-0.78339600
H	-0.39020200	0.95273100	0.99643800
H	0.70591400	1.08380300	-1.84556800
C	1.88696600	0.28970100	-0.18201300
C	-3.37730400	-0.36556100	0.39147800
O	-3.69176500	-0.86574600	-0.88703800
Si	-4.97401400	-1.56767800	-1.70015800
C	-4.97723000	-3.41990100	-1.43661400
H	-5.61301100	-3.90898000	-2.18354700
H	-3.97195700	-3.84211500	-1.53659300
H	-5.36085000	-3.70132100	-0.45192800
C	-4.59549900	-1.17469700	-3.48682900
H	-4.59854300	-0.09449800	-3.66591600
H	-3.61632600	-1.56026500	-3.78807300
H	-5.34136100	-1.61931500	-4.15492900
C	-6.64316800	-0.85655100	-1.24149700
H	-7.39855900	-1.26164200	-1.92575500
H	-6.95278000	-1.11401600	-0.22538400
H	-6.67753400	0.23287500	-1.33741400
C	-2.21371400	-1.17230800	0.97648400
C	-1.52017000	-2.09725900	0.20607800
C	-0.44194600	-2.79498500	0.74109500
C	-0.03618800	-2.56450900	2.04885700
C	-0.72345900	-1.63603800	2.82571700
C	-1.80731800	-0.95021300	2.29326800
H	-1.82074000	-2.26323900	-0.82079500
H	0.81245000	-3.10099700	2.46038100
H	-2.34515500	-0.23891100	2.91349700

C	-4.57859400	-0.47653000	1.34018100
C	-5.31823100	0.61099500	1.79644600
C	-6.43720300	0.42327400	2.60518600
C	-6.83170700	-0.85505700	2.97267800
C	-6.08565700	-1.94942500	2.54296000
C	-4.96938100	-1.75735000	1.74385400
H	-5.04155800	1.62342900	1.53299400
H	-7.70601100	-1.00011300	3.59857100
H	-4.38564400	-2.61684000	1.43127100
H	0.09494100	-3.50698900	0.12313600
H	-0.41811000	-1.44925600	3.85034100
H	-7.00044800	1.28626800	2.94521600
H	-6.37076600	-2.95432100	2.83685000
C	2.01181500	-1.09029000	-0.79884800
C	1.40654300	-1.45122400	-2.00079300
C	2.77311200	-2.05574700	-0.13139500
C	1.56694400	-2.73037100	-2.52708400
H	0.78340000	-0.74775200	-2.54080400
C	2.94723300	-3.32721700	-0.65846300
H	3.21799700	-1.82028200	0.83000000
C	2.34328800	-3.67128800	-1.86399100
H	1.07906900	-2.98782700	-3.46176800
H	3.54664300	-4.05393000	-0.11984100
H	2.47115600	-4.66633700	-2.27737200
C	3.22195300	1.11199600	-0.17946500
C	4.21772400	0.54842100	0.81746000
C	4.00745500	1.00686800	-1.45400300
N	5.15814800	0.47448800	-1.28370800
N	5.31217400	0.17899400	0.07497700
C	6.46251300	-0.52447300	0.48967100
C	7.22752300	-1.20122700	-0.46267800
C	6.83627200	-0.55773200	1.83486900
C	8.35803100	-1.90246500	-0.06747600
H	6.93343200	-1.17159500	-1.50352800
C	7.96743600	-1.27097700	2.21322900
H	6.24698200	-0.03563200	2.57462900
C	8.73461400	-1.94484300	1.27074200
H	8.94544300	-2.42378400	-0.81624100
H	8.25032400	-1.29087800	3.26066900
H	9.61766700	-2.49665600	1.57467800
O	4.06161800	0.43068500	2.01551600
C	2.75263900	2.53347600	0.18021500
H	2.64073300	2.57257900	1.26781200
H	3.46703100	3.30579200	-0.11059100
C	1.42803100	2.68089600	-0.55793400
C	0.93275800	3.83864800	-1.14662300
H	0.12917300	3.56166500	-1.85842500
C	3.55707200	1.46878500	-2.79200300
H	4.34964700	1.32546700	-3.52743400
H	2.67396000	0.91039300	-3.11414600
H	3.28011300	2.52645900	-2.76151000
H	1.65324800	0.15567600	0.88119000
Pd	-0.26225500	3.33275900	0.62361800

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0 1

C	2.89148200	1.13208100	-0.17932900
N	1.65871800	1.13922400	0.62563800
C	1.97555500	1.46534400	2.01325800
C	3.12678800	2.45546700	1.88271000
C	3.89731200	1.96942700	0.64806000
H	2.68599100	1.59991300	-1.14442500
H	1.11269600	1.89361900	2.51915100
H	2.28121700	0.55756300	2.53876800
H	2.71638000	3.45487100	1.70789000
H	3.74927000	2.49864400	2.77844300
H	4.28152200	2.80929000	0.06786700
H	4.75203200	1.35987900	0.93791100
C	0.44915600	1.40146500	0.04706400
C	-0.84664000	1.26333800	0.81123200

C	-1.45385900	-1.92185400	3.06501100
H	-0.75702100	-0.04342900	2.33553000
C	-2.69737000	-3.27754000	1.52423500
H	-2.95582700	-2.47170000	-0.44037800
C	-2.15018400	-3.09161500	2.78983300
H	-1.01563400	-1.76708400	4.04575400
H	-3.23807100	-4.18886200	1.29082900
H	-2.26217400	-3.85485900	3.55287300
C	-3.08810100	0.71685900	-0.53344000
C	-4.11621700	-0.19130600	-1.18818100
C	-3.82235500	1.11667100	0.71538200
N	-4.96934900	0.55728900	0.81426400
N	-5.17225200	-0.24344900	-0.31352900
C	-6.32098600	-1.06035300	-0.37181500
C	-7.01114500	-1.35137500	0.80642600
C	-6.76647900	-1.58220900	-1.58794700
C	-8.13893500	-2.15904700	0.76332700
H	-6.66085800	-0.94272300	1.74514900
C	-7.89307900	-2.39557200	-1.61134200
H	-6.23482000	-1.35829000	-2.50168300
C	-8.58608000	-2.68811200	-0.44277200
H	-8.66873100	-2.37773700	1.68475200
H	-8.23296100	-2.79629000	-2.56073800
H	-9.46684900	-3.32073700	-0.47115400
O	-4.00544200	-0.77223000	-2.24778200
C	-2.62549600	1.85457100	-1.44981000
H	-2.58323300	1.44926100	-2.46757100
H	-3.32042500	2.69448200	-1.46344200
C	-1.21495000	2.26356500	-0.99971300
C	-0.44985700	3.23275900	-1.61550100
H	0.62798000	3.11194900	-1.41448200
C	-3.33920600	2.05932600	1.75592400
H	-4.10948700	2.21741200	2.51177200
H	-2.43982700	1.67320600	2.24290800
H	-3.06546600	3.02006100	1.29932000
H	-1.58179700	-0.59884200	-1.22443000
Pd	-1.28972700	4.26296100	-0.01929800

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0 1			
C	3.00194100	0.79266600	-1.00314500
N	1.72523900	1.08799300	-0.31544800
C	1.94441200	1.99762600	0.82281000
C	3.10980400	2.86271500	0.35952300
C	3.86079000	2.03609200	-0.70288200
H	2.78201800	0.68293900	-2.06473200
H	1.04653600	2.57925400	1.01604300
H	2.19616300	1.38581200	1.68972100
H	2.72370300	3.78529600	-0.07685600
H	3.75177900	3.13225900	1.19878500
H	4.00068300	2.61829500	-1.61405800
H	4.84777900	1.74356000	-0.35280400
C	0.58681200	0.63117500	-0.70461100
C	-0.69615800	1.01607700	-0.13409300
H	0.59427700	0.00697300	-1.59317100
H	-0.59340600	1.33571800	0.89795800
C	-1.76340700	-0.07134900	-0.28037700
C	3.60075800	-0.54759100	-0.46489800
O	3.83868300	-0.34575600	0.90661400
Si	5.11473700	-0.34387700	1.99907500
C	5.50526700	-2.07809700	2.58326400
H	5.99234300	-2.03585600	3.56413300
H	4.59879100	-2.68128000	2.69701400
H	6.18177200	-2.60997700	1.90939900
C	4.42588400	0.65640700	3.41688600
H	4.20115800	1.68411900	3.11389400
H	3.50762000	0.21530200	3.81760900
H	5.14669500	0.71129800	4.23999300
C	6.66101300	0.46817100	1.33269600
H	7.44654800	0.40757500	2.09557200

H	7.04510400	-0.02119800	0.43342800
H	6.51740200	1.52936500	1.10873200
C	2.55576500	-1.65508700	-0.63728800
C	1.84860700	-2.15054900	0.45248200
C	0.85597700	-3.11005800	0.27285300
C	0.55374800	-3.57457700	-0.99959700
C	1.25833800	-3.08286600	-2.09557900
C	2.25528900	-2.13430700	-1.91421900
H	2.07072100	-1.77772000	1.44474400
H	-0.22820100	-4.31357900	-1.13872200
H	2.80224900	-1.76312200	-2.77574800
C	4.87737800	-0.95335300	-1.21169500
C	5.48993000	-0.18434800	-2.19714200
C	6.67716700	-0.60713400	-2.79083100
C	7.26523800	-1.80461000	-2.40973200
C	6.64472600	-2.59502700	-1.44604100
C	5.45866000	-2.17580500	-0.86408500
H	5.06025100	0.75462200	-2.52329200
H	8.19267900	-2.12961900	-2.86928900
H	4.96940100	-2.81190000	-0.13403000
H	0.30571000	-3.47935500	1.13186700
H	1.03212600	-3.44112500	-3.09449300
H	7.14017200	0.00891700	-3.55449400
H	7.08077200	-3.54479600	-1.15444400
C	-1.85963800	-1.11223400	0.81734800
C	-2.54609900	-2.30036600	0.54954600
C	-1.31270000	-0.94114600	2.08755400
C	-2.69756700	-3.27755300	1.52350900
H	-2.95579900	-2.47133200	-0.44098000
C	-1.45383200	-1.92233000	3.06450600
H	-0.75669100	-0.04388100	2.33537300
C	-2.15036300	-3.09193100	2.78913600
H	-3.23840100	-4.18875100	1.28992800
H	-1.01557300	-1.76781600	4.04527400
H	-2.26248200	-3.85526700	3.55206600
C	-3.08800500	0.71704500	-0.53345500
C	-4.11597100	-0.19123900	-1.18827300
C	-3.82227300	1.11660500	0.71540200
N	-4.96911100	0.55688700	0.81434100
N	-5.17184600	-0.24387600	-0.31345100
C	-6.32037900	-1.06107000	-0.37170700
C	-7.01046300	-1.35218000	0.80655200
C	-6.76572300	-1.58314200	-1.58780000
C	-8.13802500	-2.16017700	0.76352000
H	-6.66029100	-0.94334300	1.74523800
C	-7.89209100	-2.39682900	-1.61113100
H	-6.23412200	-1.35915600	-2.50155300
C	-8.58501300	-2.68946700	-0.44253800
H	-8.66776700	-2.37893600	1.68495800
H	-8.23185500	-2.79772600	-2.56049400
H	-9.46559800	-3.32235400	-0.47086800
O	-4.00515600	-0.77197300	-2.24797500
C	-2.62545400	1.85486300	-1.44960600
H	-2.58308500	1.44971400	-2.46742600
H	-3.32046500	2.69470500	-1.46310200
C	-1.21500600	2.26390800	-0.99936900
C	-0.44992000	3.23334300	-1.61467500
H	0.62796100	3.11257100	-1.41395600
C	-3.33936000	2.05941900	1.75590300
H	-4.10978800	2.21761400	2.51157700
H	-2.44004200	1.67343900	2.24311000
H	-3.06552100	3.02008600	1.29920400
H	-1.58152100	-0.59833200	-1.22465000
Pd	-1.29036200	4.26360700	-0.01919600

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0 1			
C	3.18486600	0.93657700	-0.65770100
N	1.85141300	1.32300500	-0.16056700
C	1.92526900	2.37723700	0.87417900

C	2.43551400	-0.75614900	2.20621600
H	5.42802900	0.76846000	1.75851700
H	3.18195400	0.24452500	5.36486000
H	1.66830900	-1.28539200	1.65483100
H	7.30653600	-0.43456600	-2.95740700
H	7.45407500	-3.04188400	0.44477700
H	5.18496500	1.10505800	4.17633900
H	1.43086100	-0.96975800	4.08660600
C	-1.55798100	-0.96609100	1.00622800
C	-1.26735400	-0.54298500	2.30308200
C	-1.92006000	-2.30204400	0.81096900
C	-1.34765600	-1.42646400	3.37465000
H	-0.96912200	0.48141600	2.49657300
C	-1.99928600	-3.18680600	1.87839100
H	-2.13897200	-2.65458100	-0.19217700
C	-1.71410200	-2.75048100	3.16756900
H	-1.12309900	-1.07478600	4.37640800
H	-2.28231600	-4.21905900	1.70067300
H	-1.77476600	-3.43870100	4.00416700
C	-2.90838700	0.57165500	-0.59168300
C	-3.81402700	-0.52357200	-1.13225100
C	-3.74447600	1.09135500	0.54200500
N	-4.84720200	0.45563300	0.67287100
N	-4.91201500	-0.53813700	-0.30842900
C	-6.02934500	-1.40019700	-0.32511500
C	-7.00120300	-1.27756200	0.67144900
C	-6.17638600	-2.37136100	-1.31982800
C	-8.10358600	-2.12067100	0.66971900
H	-6.88627000	-0.52512800	1.43959000
C	-7.28648200	-3.20710600	-1.30338700
H	-5.43108600	-2.46924100	-2.09509000
C	-8.25584600	-3.09058800	-0.31495200
H	-8.84996600	-2.01387400	1.45017200
H	-7.38896900	-3.95717700	-2.08093000
H	-9.11937800	-3.74709500	-0.31112100
O	-3.58574200	-1.24683800	-2.07983400
C	-2.50022400	1.60188200	-1.65331600
H	-2.38250800	1.06088400	-2.59922700
H	-3.25943400	2.36822100	-1.81026000
C	-1.14462500	2.19123800	-1.22184900
C	-0.41710600	3.09778500	-1.97268500
H	0.65248600	3.10020800	-1.69693700
C	-3.41674900	2.23786700	1.42712100
H	-4.24741200	2.44287800	2.10356200
H	-2.52065800	2.03442400	2.01794500
H	-3.20224300	3.13059900	0.82438400
H	-1.26738300	-0.64738100	-1.06737300
Pd	-1.41219400	4.28529200	-0.57807400

(S,R)-7a
(S,R)-7a-a
O 1

O	0.83790000	-1.82881200	-1.62203300
O	-4.12600500	1.00644500	-1.69216500
N	1.58563400	-0.79060500	0.31702800
N	1.02543500	-0.37592700	1.52889300
C	5.68281900	-0.09508100	-0.30811500
H	6.73977100	0.09031500	-0.46648100
C	4.99372200	-0.98055000	-1.12758200
H	5.51114800	-1.49400800	-1.93135100
C	3.64021000	-1.22870600	-0.93259900
H	3.11403000	-1.91899600	-1.57563200
C	2.96309200	-0.57336700	0.09822700
C	3.64804400	0.32174200	0.92287900
H	3.11817600	0.82900800	1.71804300
C	5.00111500	0.55140700	0.71736400
H	5.52309800	1.24811300	1.36510600
C	0.65058800	-1.33255700	-0.53248600
C	-0.68865800	-1.12204700	0.15761100
C	-0.23770200	-0.56331900	1.47931700

C	-1.10428600	-0.32556500	2.66301200
H	-0.53092100	0.14704900	3.46120900
H	-1.49977500	-1.27694400	3.03389400
H	-1.95883200	0.30489900	2.41494100
C	-1.57145100	-2.37037300	0.28966900
H	-1.35303600	-3.07541200	-0.52183700
H	-1.41966000	-2.90744100	1.22959600
C	-2.97564400	-1.85516200	0.11889800
C	-4.11652500	-2.75001200	0.45877400
H	-5.09526800	-2.31875900	0.25256000
H	-4.07243100	-3.01225200	1.52112400
H	-4.03001300	-3.68882800	-0.09816800
C	-2.97077400	-0.62321600	-0.42226600
C	-4.15870200	0.05934400	-0.93732900
C	-1.56332500	-0.12878700	-0.69625400
H	-1.33274100	-0.33920800	-1.74803000
C	-1.22337400	1.32372800	-0.43592000
C	-0.07411800	1.85406800	-1.02516700
H	0.50645100	1.24666400	-1.71406500
C	0.33851200	3.15077700	-0.74531000
H	1.23871300	3.54079000	-1.20896400
C	-0.40356500	3.94544000	0.12142800
C	-1.56131300	3.43453800	0.69699600
H	-2.15519900	4.05111700	1.36406600
C	-1.96567600	2.13372300	0.42097000
H	-2.87467500	1.75461000	0.87590700
H	-5.13278700	-0.35206800	-0.61304200
H	-0.08662800	4.95986400	0.34055700

(S,R)-7a-b

O 1	0.87761300	-1.83678300	-1.62974800
O	-5.22836300	0.15190100	-0.67106700
N	1.59702700	-0.81307600	0.32784100
N	1.01321800	-0.37677600	1.52137900
C	5.72177700	-0.20057800	-0.19628200
H	6.78580600	-0.03649200	-0.32864600
C	5.03546600	-1.07311900	-1.03176900
H	5.56214800	-1.59778700	-1.82217200
C	3.67289500	-1.29425500	-0.86985000
H	3.14936000	-1.97497300	-1.52516300
C	2.98388100	-0.62450300	0.14374000
C	3.66626600	0.25753000	0.98451700
H	3.12743700	0.77584700	1.76642800
C	5.02819200	0.46025400	0.81191400
H	5.54790200	1.14689800	1.47208600
C	0.67292400	-1.33467400	-0.54591100
C	-0.67889400	-1.08671700	0.10551400
C	-0.25225200	-0.53403000	1.43733700
C	-1.14756700	-0.26407600	2.59214700
H	-0.58920800	0.21096300	3.39952500
H	-1.56905100	-1.20340200	2.96516700
H	-1.98591500	0.37423700	2.31065100
C	-1.61056500	-2.30219000	0.20781600
H	-1.40858100	-3.00250900	-0.61220400
H	-1.49175000	-2.85851300	1.14120900
C	-2.99210500	-1.72649900	0.03483600
C	-4.18146800	-2.55481000	0.36557200
H	-5.11089700	-2.09946200	0.03167000
H	-4.23763400	-2.69441300	1.45143700
H	-4.07881700	-3.55333200	-0.07194400
C	-2.93106800	-0.49146100	-0.49350000
C	-4.06464000	0.31415700	-0.96917700
C	-1.49792000	-0.06988100	-0.76967700
H	-1.26433600	-0.31328700	-1.81443100
C	-1.10783100	1.37550700	-0.53971300
C	0.05417700	1.86110100	-1.14403000
H	0.62063200	1.21940800	-1.81308100
C	0.49642000	3.15515500	-0.90251300
H	1.40619700	3.50977700	-1.37556500

C	-0.22859600	3.99389500	-0.06237200	H	-2.74339800	1.88377300	0.76967100
C	-1.39724600	3.52865600	0.52810300	H	-3.78799400	1.13025600	-1.66585600
H	-1.97545000	4.17766300	1.17771500	H	0.11195600	5.00685000	0.12533000
C	-1.83086600	2.22829100	0.29332200				

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