Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Stereoselective Control in the Staudinger Reactions Involving Monosubstituted Ketenes with Electron Acceptor Substituents: Experimental Investigation and Theoretical Rationalization

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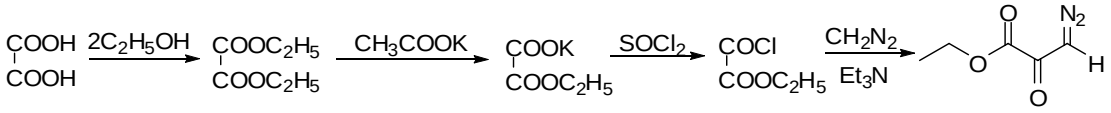
Experimental part

Preparation of 3-diazo-2-oxopropanoic acid derivatives and 2-diazo-3-oxoalkanals

Preparation of ethyl 3-diazo-2-oxopropanoate (2a):



2a

Diethyl oxalate: A mixture of crystallized (hydrated) oxalic acid (63 g, 0.5 mol) and absolute ethanol (97 g, 2 mol) and benzene (100 mL) in a 500 mL flask, equipped with a Dean-Stark trap, was refluxed until the desired amount of water (84 mL) with some alcohol was separated. After removal of the solvent, the residue was distilled under reduced pressure to afford diethyl oxalate as a colorless liquid (75-76 °C/8 mmHg) 61 g in the yield of 83.4%.

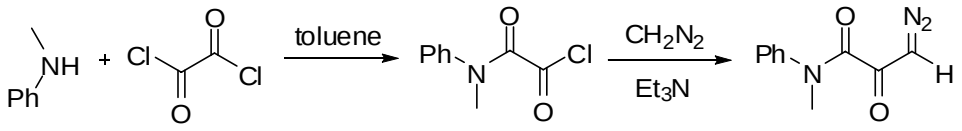
Ethyl potassium oxalate: To a solution of diethyl oxalate (24.3 g, 166 mmol) in water (20 mL) in a round bottom flask was added potassium acetate (17 g, 173 mmol). The resulting mixture was kept in an oil bath at 80°C and became homogeneous in 1.5 h. After removal of the solvent as clean as possible, a mixture of ethanol (34 mL) and diethyl ether (100 mL) was added. A lot of white crystals immediately appeared. These white crystals were filtrated and dried to give ethyl potassium oxalate 16.6 g in 64% yield.

Ethyl chloroglyoxylate: Thionyl chloride (15.4 mL, 25 g, 210 mmol) was added slowly to a suspension of ethyl potassium oxalate (15.6 g, 100 mmol) in appropriate amount of ether (6 mL) in an ice bath. After addition of thionyl chloride, the mixture was heated at 60 °C for about 12 h. After the white solid was filtrated off, the filtrate was distillated fractionally to collect the fraction of 120-130 °C to afford the title product 10.4 g (76.2%).

Ethyl 3-diazo-2-oxopropanoate[1]: To a solution of diazomethane (approximate 105 mmol) and triethylamine (6 mL, 42 mmol) in ether was added a solution of ethyl chloroglyoxylate (4.82 g, 35 mmol) in ether with stirring at 0 °C. After stirring at room temperature for 3 h, the resulting triethylamine hydrochloride precipitate is filtered off. The ethereal part was dried over anhydrous sodium sulfate and evaporated. The residue was separated chromatographically on a silica gel column, eluting with ethyl acetate and petroleum ether (*V*/*V*=1:5) to give ethyl 3-diazo-2-oxopropanoate as yellow crystals 1.01 g (20.2% yield).

Yellow crystals, m.p.79-80 °C, Lit[1]: m.p.72-74 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.38 (t, J = 7.2 Hz, 3H), 4.35 (q, J = 7.2 Hz, 2H), 6.26 (s,1H), ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 13.7, 57.0, 62.7, 160.0, 176.7. IR (KBr) ν (cm^{-1}): 1625, 1735 (C=O), 2158 (CHN_2).

Preparation of 3-diazo-*N*-methyl-2-oxo-*N*-phenylpropanamide (2b):



2b

2-Chloro-*N*-methyl-2-oxo-*N*-phenylacetamide[2]: To a solution of *N*-methylaniline (2.5 g, 23 mmol) in 20 mL toluene was added dropwise oxalyl chloride (14.9 g, 117 mmol) at 0 °C. The

[1] Ohsumi, T.; Neunhoeffer, H. *Tetrahedron* **1992**, 48, 5227-5234.

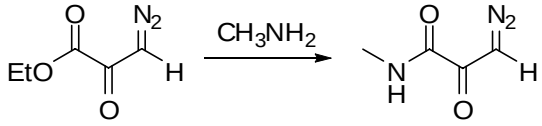
[2] a) Nagasawa, M.; Kawase, N.; Tanaka, N.; Nakamura, H.; Tsuzuike, N.; Murata, M. *PCT Int. Appl*. **2005**, WO2005012248 (*CA* **2005**, *142*, 219153). b) Stolle, R.; Bergdoll, R.; Luther, M.; Auerhahn, A.; Wacker, W. *J. Prak. Chem*. **1930**, *128*, 1-43.

solution was stirred at room temperature for 3 h. After the reaction finished, the solvent and excessive oxalyl chloride were removed under reduced pressure. The crude acyl chloride was acquired as a rufous liquid.

3-Diazo-*N*-methyl-2-oxo-*N*-phenylpropanamide (2b): The diazotization of crude acyl chloride prepared above was followed the same procedure as used for the preparation of ethyl 3-diazo-2-oxopropanoate to afford the title product 1.9 g (40.1% yield).

Yellow crystals, m.p. 54-55 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 3.35 (s, 3H), 5.89 (s, 1H), 7.17-7.41 (m, 5H); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 37.7, 56.5, 125.9, 127.7, 129.3, 142.4, 163.7, 182.3. IR (KBr) ν (cm^{-1}): 1623, 1662 (C=O), 2117 (CHN_2). HRMS calcd for $C_{10}H_9N_3NaO_2$ ([M+Na]$^+$) *m/z*: 226.0586, found: 226.0591.

Preparation of 3-diazo-*N*-methyl-2-oxopropanamide (2c)[3]:

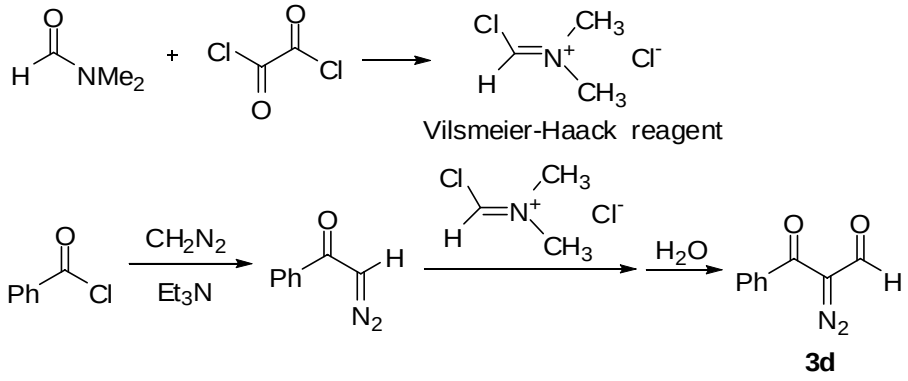


2a **2c**

Ethyl 3-diazo-2-oxopropanoate (1 g, 7 mmol) was dissolved in 5 mL of 33% methylamine in ethanol and the mixture was stirred at room temperature overnight. After removal of the solvent, the residue was purified chromatographically on a silica gel column [elution with ethyl acetate and petroleum ether (V/V=1:5)] to obtain the title compound as yellow crystals 0.64 g (71.6% yield).

Yellow crystals, m.p. 122-123 °C, Lit[3]: m.p.111-125 °C. ^{1}H NMR (200 MHz, $CDCl_3$) δ: 2.91 (d, J = 5.2 Hz, 3H), 6.39 (s, 1H), 7.25(br s, 1H), ^{13}C NMR (50 MHz, $CDCl_3$) δ: 25.9, 54.5, 160.6, 181.5.

Preparation of 2-diazo-3-oxo-3-phenylpropanal (3d)[4]



3d

Diazoacetophenone:[5] To a solution of diazomethane (approximate 342 mmol) and triethylamine (20 mL, 137 mmol) in diethyl ether was added a solution of benzoyl chloride (16 g, 114 mmol) in diethyl ether with stirring at 0 °C. After stirring at room temperature for 3 h, the resulting triethylamine hydrochloride precipitate was filtered off. The ethereal phase was dried over anhydrous sodium sulfate and evaporated. The residue was separated chromatographically on a silica gel column, eluting with ethyl acetate and petroleum ether (1:5, *v/v*) to give

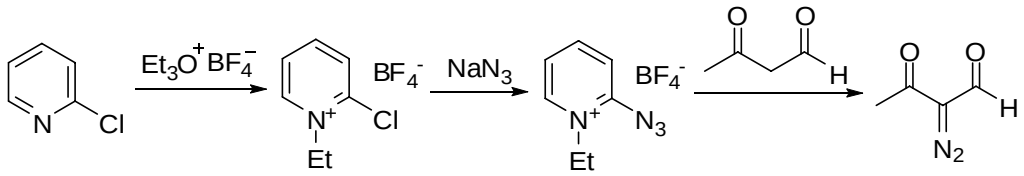
[3] Bycroft, B. W.; Cameron, D.; Croft, L. R.; Hassanali-Walji, A.; Johnson, A. W.; Webb, T. *J. Chem. Soc, Perkin Trans. 1,* **1972,** 827-834.
[4] Stojanovic, F. M.; Arnold, Z. *Collect. Czech. Chem. Commun.* **1967**, *32*, 2155-2160.
[5] Bridson, J. N.; Hooz, J. *Org. Synth.* **1973**, *53*, 35-38.

diazoacetophenone as yellow crystals 7.4 g (44.5% yield). m.p. 50-52 °C, Lit: [5] m.p. 47.5-48.5 °C.

2-Diazo-3-oxo-3-phenylpropanal (3d):[4] To a stirred solution of diazoacetophenone (8.67 g, 60 mmol) prepared from benzoyl chloride and diazomethane in chloroform was added dropwise with a solution of the Vilsmeier-Haack reagent[6] prepared from oxalyl chloride and DMF (3.8 g, 30 mmol) in chloroform at -5 °C over 0.5 h. The reaction mixture was kept at 0 °C for 1 h. After removal of the solvent under reduced pressure, the residue was washed with diethyl ether (50 mL x 3) for three times. Then the precipitate was dissolved in water and the solution was allowed to stand at room temperature for 3 h. The crude product was filtered off and further purified with column chromatography [elution with ethyl acetate and petroleum ether (V/V=1:10)] to afford 2-diazo-3-oxo-3-phenylpropanal as yellow crystals 1.78 g (24% yield).

Yellow crystals, m.p. 66-67 °C, Lit[4]: m.p.60-60.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.50-7.69 (m, 5H), 9.78 (s, 1H).

Preparation of 2-diazo-3-oxobutanal (3e)[7]:



3e

Sodioacetoacetaldehyde:[8] To a stirred suspension of CH_3ONa (54.02 g, 326 mmol) in anhydrous ether (300 mL) cooled in an ice bath was added a mixture of acetone (20.1 g, 346 mmol) and methyl formate (24.4 g, 408 mmol) over 30 min. the reaction mixture was allowed to warm to room temperature and then to stand for 10 h. The suspension was filtered to obtain sodioacetoacetaldehyde as a white solid. 28.5 g (80.8% yield)

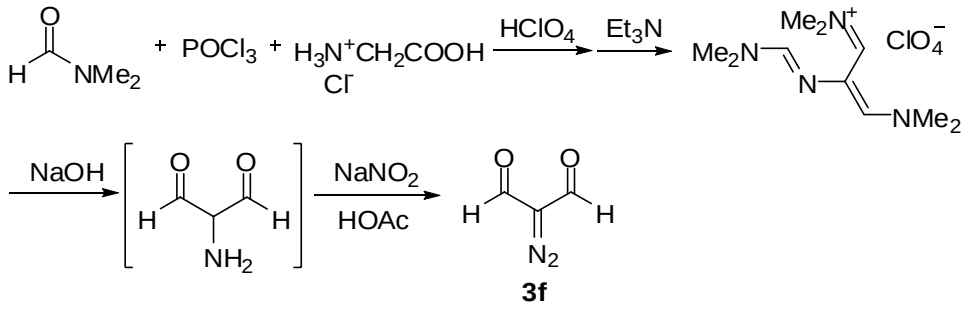
2-Diazo-3-oxobutanal (3e) The solution of 3-oxobutanal was prepared *in situ* by dissolving sodioacetoacetaldehyde (6.16 g, 57 mmol), prepared from condensation of acetone and methyl formate, in a mixture of 35 mL CH_3OH and 10 mL of H_2O and adding AcOH (3.25 mL, 57 mmol).

The solution of 2-azido-1-ethylpyridinium tetrafluoroborate was prepared from 2-chloro-1-ethylpyridinium tetrafluoroborate [9] (16.05 g, 70 mmol) and NaN_3 (4.55 g, 70 mmol) in a mixture 70 mL of CH_3OH and 40 mL of H_2O, then 6 mL of 2M NaOAc was added.

To the solution of 3-oxobutanal was added the above prepared solution of 2-azido-1-ethylpyridinium tetrafluoroborate. The mixture was stirred for 2 h. The product was extracted with CH_2Cl_2 and dried with sodium sulfate. After removal of the solvent, the residue was purified chromatographically on a silica gel column [elution with diethyl ether and petroleum ether (*V/V*=2:1)] to give 2-diazo-3-oxobutanal as a yellow oil 0.766 g (12% yield).

Preparation of 2-diazomalonaldehyde (3f)[10]

6 Fujisawa, T.; Sato, T. *Org. Synth.* **1988**, *66*, 121-123.
7 Sezer, O.; Anac, O.; *Helv. Chim. Acta* **1994**, *77*, 2323-2334.
8 Harris, T. M.; Boatman, S.; Hauser, C. R. *J. Am. Chem. Soc.* **1963**, *85*, 3273-3276.
9 Monteiro, H. J. *Synth. Commun.* **1987**, *17*, 983-992.
10 Arnold, Z.; Sauliova, J. *Collect. Czech. Chem. Commun.* 1973, *38*, 2641-2647.



3f

***N,N*-Dimethyl-*N*-[2-(dimethylaminomethylene)amino-3-dimethylamino]prop-2-enylidenea mmonium diperchlorate**: Phosphorus oxychloride (229 g, 1.5mol) was added dropwise into DMF (300 ml) under stirring and ice-cooling, the mixture was further stirred for 20 min without cooling, and cooled down again with ice. Glycine hydrochloric (56 g, 0.5 mol) was added portionwise. The whole mixture was heated at 80 °C for 4 h and at 125 °C for 2 h, cooled down, and decomposed by pouring into water (300 mL), the temperature being maintained at 15-20 °C by means of efficient external cooling with dry ice/ethanol. Perchloric acid (70%, 100 mL) was then added at -10 °C, the mixture was cooled down to -35 °C under continuous stirring (to deposit a crystalline precipitate), and kept at this temperature for 2 h. The precipitate was rapidly collected with filtration and washed three times with a small amount of precooled ethanol to afford the diperchlorate salt 89.1 g (44.8% yield). m.p. 230-234 °C, Lit[11]: m.p. 226-228 °C.

***N,N*-Dimethyl-*N*-[2-(dimethylaminomethylene)amino-3-dimethylamino]prop-2-enylidenea mmonium perchlorate**: The diperchlorate (89.1g, 0.223 mol) was dissolved in a refluxing mixture of ethanol (600 mL) and Et_3N (45 mL). The solution was filtered with a small amount of active charcoal while hot and the filtrate was allowed to crystallize to give rise to the perchlorate salt 52 g (78.5% yield). m.p. 144-146 °C, Lit[11]: m.p. 139-141 °C.

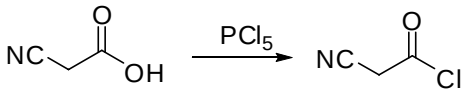
2-Diazomalonaldehyde (3f):[10] A mixture of *N,N*-dimethyl-*N*-[2-(dimethylaminomethylene)amino-3-dimethylamino]prop-2-enylideneammoni um perchlorate (15 g, 0.05 mol) and 125 mL of 2 M NaOH was heated at 40 °C under stirring for 10 h. The solution was filtered with a small amount of charcoal and concentrated on a rotary evaporator to make the volume up to 100 mL and sodium nitrite (4.5 g, 65 mmol) was added. The resulting mixture was cooled at -10°C and acetic acid (15 mL) was added dropwise under stirring (internal temperature not exceeding -5 °C). After the cooling bath was taken off, the mixture was stirred at room temperature for another 2 h during which the dark red turbid solution cleared up. The reaction mixture was extracted with dichloromethane (60 mL x 3). The combined organic phase was washed 2 times with saturated aqueous sodium carbonate and water, dried over sodium sulfate. After removal of the solvent under reduced pressure, the residue was purified chromatographically on a silica gel column (elution with dichloromethane) to give rise to 2-diazomalonaldehyde as a yellow oil 2.4 g (48.6% yield).

Yellow oil, ^{1}H NMR (300 MHz, $CDCl_3$) δ: 9.70 (s, 2H), ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 43.4, 179.3.

Preparation of acyl chloride

Preparation of cyanoacetyl chloride

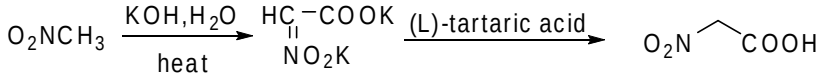
11 Arnold, Z.; Sauliova, J.; Krchnak, V. *Collect. Czech. Chem. Commun.* 1973, *38*, 2633-2640.



Cyanoacetyl chloride was prepared according to literature procedures.[12] To a solution of cyanoacetic acid (17 g, 200 mmol) in anhydrous diethyl ether (100 mL) was added phosphorus pentachloride (42 g, 200 mmol) in portions (5 portions) in an ice-water bath. After the addition was completed, stirring was continued until phosphorus pentachloride dissolved completely. After removal of the solvent, the red residue was distilled under reduced pressure to afford cyanoacetyl chloride as a colorless liquid (30-32 °C/0.01 mmHg) 10.8 g (52% yield).

Preparation of nitroacetyl chloride

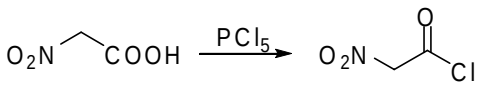
Preparation of nitroacetic acid[13]



In a 250 mL three-necked round bottomed flask equipped with a thermometer and a condenser, potassium hydroxide (120.97 g, 2.156 mol) was added to water (121 mL). When the temperature reached 67 °C, nitromethane (28.2 mL, 0.524 mol) was added dropwise. During the addition the temperature rose to 95 °C. At the end the flask was kept between 95 and 100 °C for 5 h. The mixture was then cooled to room temperature and yellow crystals dipotassium nitroacetate formed. The crystals were filtered and washed with cold methanol. The product obtained (23.58 g, 49.7%) was used without further purification.

In a 100 mL three-necked round bottomed flask, dipotassium nitroacetate (8.00 g, 44.1 mmol) was dissolved in water (20 mL) while stirring. The solution was cooled to -8 °C with an ice-brine bath and a cold solution (-10 °C) of L-tartaric acid (13.24 g, 88.2 mmol) in water (20 mL) was added dropwise, keeping the temperature between -8 and -3 °C. At the end of the addition, the mixture was stirred at -2 °C for 30 min, the solid was filtered and the solution obtained was saturated with sodium chloride. The aqueous solution was extracted twelve times with cold diethyl ether, the organic layer was dried over magnesium sulfate and concentrated under reduced pressure. The oil obtained was taken up in cold chloroform and concentrated in vacuo three times to give 2.87 g (36.1%) of product nitroacetic acid as white crystals. m.p.93-95 °C, Lit[14]:m.p.89-92 °C, ^{1}H NMR (300 MHz, $CDCl_3$) δ: 4.28 (s, 1H), 5.25 (s, 2H).

The preparation of nitroacetyl chloride[15]:



The mixture of nitroacetic acid (1.05 g, 10 mmol) and PCl_5 (2.3 g, 11 mmol) was stirred in $CHCl_3$ (50 mL) at -20 °C for 1h. The distillation of the mixture gave nitroacetyl chloride as a colorless liquid with boiling point 42-44 ^{o}C/2 mmHg. Lit.[16] 53-55 ^{o}C/4 mmHg.

The preparation of *N*-phenylnitroacetamide:

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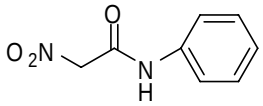
12 Ireland, R. E.; Chaykovsky, M. *Org. Synth.* **1961**, *41*, 5-8.
13 Vanier, S. F.; Larouche, G.; Wurz, R. P.; Charette, A. B. *Org. Lett.* **2010**, *12*, 672-675.
14 Finkbeiner, H. L.; Stiles, M. *J. Am. Chem. Soc.* **1963**, *85*, 616-622.
15 (Hoffmann-La Roche, F., und Co. A.-G., Switz.). Austrian AT 75-2247 (1979), 6 pp. *CA* **1980**, *92*, 6568.
16 Martynov, I. V.; Kruglyak, Yu. L. *Probl. Organ. Sinteza, Akad. Nauk SSSR, Otd. Obshch. Tekhn. Khim*. **1965**, 57-59.

Nitroacetyl chloride was added dropwise to a solution of aniline (93 mg, 1 mmol) in dichloromethane (5 mL) over 0.5 h at room temperature. The reaction mixture was stirred for an additional hour. Evaporation of the solvent and purification of the residue by silica gel column chromatography [elution with ethyl acetate and petroleum ether (*V*/*V*=1:5)] afforded the product 123 mg (yield 68.3%).



Colorless crystals m.p.144-145 °C, Lit[17]:m.p.136-138 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ:5.54 (s, 2H, CH_2), 7.13-7.59 (m, 5H, ArH), 10.57 (s, 1H, NH). ^{13}C NMR (75 MHz, DMSO-d_6) δ: 79.3, 119.4, 124.3, 129.0, 137.9, 159.8.

Preparation of acyl acetic acids

Preparation of ethyl hydrogen malonate[18]

A 250 mL two-neckcd flask equipped with a magnetic stirrer and a dropping funnel were added diethyl malonate (23.14 g, 145 mmol) and commercial absolute ethanol (50 mL). To the solution was added dropwise a solution of potassium hydroxide (8.12 g, 145 mmol) in commercial absolute ethanol (50 mL) under stirring during 1 h. White crystalline precipitates quickly appeared. After stirring for several hours, potassium ethyl malonate (white precipitates) 15.42 g (63% yield) was afforded after filtration, washing with a small amount of diethyl ether and dried *in vacuo*.

To a chilled solution of the potassium salt (15.42 g, 90.6 mmol) in water (30 mL) (immersed in an ice-water bath) was added slowly concentrated hydrochloric acid (8 mL) under stirring. The reaction mixture was extracted with diethyl ether (3 × 50 mL). The ethereal solution was dried over sodium sulfate. After removal of solvent under reduced pressure and dried *in vacuo* at room temperature for 2 h, a colourless liquid residue of ethyl hydrogen malonate was obtained 10.86 g (91% yield).

Preparation of diethoxyphosphorylacetic acid

Triethyl phosphite (12.32 g, 74 mmol)) and ethyl chloroacetate (9.1 g, 74 mmol) were refluxed for 2 h. After vacuum distillation, ethyl diethoxyphosphorylacetate was obtained as a colorless oil 10.46 g (63% yield) at b.p.107-108 °C/2 mmHg.[19]

Ethyl Diethoxyphosphorylacetate (10.46 g, 47 mmol) was added dropwise into a solution of sodium hydroxide (1.87 g, 47 mmol) in water (10 mL). After stirring for 2 h at room temperature and removal of ethanol completely under reduce pressure, the residue was treated with 1mol/L HCl (until pH = 1). The aqueous phase was extracted with CH_2Cl_2 (3 × 30 mL). The combined organic layers were washed with brine and dried over anhydrous Na_2SO_4. After removal of solvent, diethoxyphosphorylacetic acid (7.20 g, 79%) was obtained as a colourless oil.[20]

Preparation of benzenesulfonylacetic acid[21]

To a solution of 11 g (100 mmol) of thiophenol in 60 mL of ethanol was added a solution of

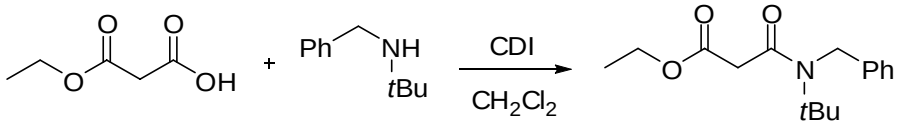
17 Fusco, R.; Rossi, S. *Gazz. Chim. Ital.* **1951**, 81, 511-522.
18 Breslow, D. S.; Baumgarten, E.; Hauser, C. R. *J. Am. Chem. Soc*. **1944**, *66*, 1286–1288.
19 Wu, L.; Ye, H. J.; Xiao, D. J. *Chin. J. Pharm*. **2004**, *35*, 67-68.
20 Teichert, A.; Jantos, K.; Harms, K.; Studer, A. *Org. Lett*. **2004**, *6*, 3477-3480.
21 Kenney, W. J.; Walsh, J. A.; Davenport, D. A. *J. Am. Chem. Soc*. **1961**, *83*, 4019-4022.

sodium hydroxide (9.2 g, 230 mmol) in water (10 mL). To the resulting solution was added a solution of chloroacetic acid (10.4 g, 110 mmol) in ethanol (30 mL). Lots of heat was produced and white precipitate was formed. After filtration, the solid part was dissolved in water. After acidifying with concentrated hydrochloride, the phenylthioacetic acid precipitated. After filtration, dried under infrared light, and recrystallized from benzene, colorless crystals were afforded 13.2 g (78.4% yield), m.p. 65-67 °C. Lit[21] m.p. 63.5 °C.

To a solution of phenylthioacetic acid (6.73 g, 40 mL) dissolved in redistilled acetic acid (30 mL) was added 7.8 mL of hydrogen peroxide (30% by weight) in an ice-water bath at 0 °C. The reaction mixture was stirred overnight and allowed to warm to room temperature. After removal of solvent and recrystallized from benzene, colorless crystalline benzenesulfonylacetic acid was obtained 3.8 g (47.5% yield), m.p. 112-113 °C. Lit.[21] m.p. 111.5-112.5 °C.

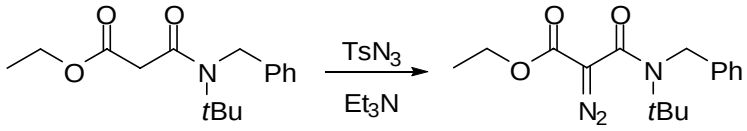
Investigation on the epimerization

Preparation of *N*-benzyl-*N*-*tert*-butyl-3-ethoxy-3-oxopropanamide[22]



A solution of ethyl hydrogen malonate (1.32 g, 10 mmol) and CDI (4.86 g, 30 mmol) in CH_2Cl_2 (50 mL) was stirred at 25 °C for 1 h. To the mixture was added *N*-benzyl-*N*-*tert*-butylamine (1.63 g, 10 mmol) in CH_2Cl_2 (10 mL). The reaction mixture was stirred for another 1 h. After removal of the solvent, the residue was purified chromatographically on a silica gel column [elution with ethyl acetate and petroleum ether (30-60 °C) 1:10), *v/v*] to obtain the title compound as colorless oil. 1.91 g (69% yield). ^{1}H NMR (200 MHz, $CDCl_3$) δ: 1.27 (t, J = 7.2 Hz, 3H, CH_3), 1.46 (s, 9H, CMe_3), 3.38 (s, 2H, CH_2), 4.19 (q, J = 7.2 Hz, 2H, CH_2O), 4.60 (s, 2H, NCH_2), 7.22-7.42 (m, 5H, ArH).

Preparation of *N*-benzyl-*N*-*tert*-butyl-2-diazo-3-ethoxy-3-oxopropanamide[23]

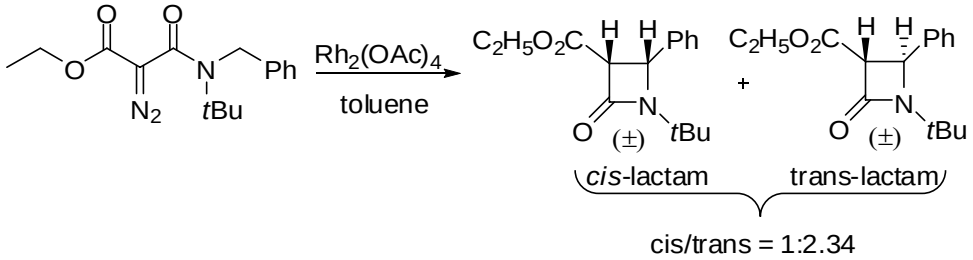


TsN_3 (1.2 g, 6.1 mmol) in 5 mL of acetonitrile was added to a solution of *N*-benzyl-*N*-*tert*-butyl-3-ethoxy-3-oxopropanamide (1.67 g, 6 mmol) and triethylamine (1.68 mL, 13 mmol) in 30 mL of acetonitrile. The mixture was stirred for 36 h at room temperature. After the solvent was evaporated, the residue was purified chromatographically on a silica gel column [elution with ethyl acetate and petroleum ether (30-60 °C) 1:10), *v/v*] to obtain yellow crystals. m.p. 95-96 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.28 (t, J = 7.2 Hz, 3H, CH_3), 1.38 (s, 9H, CMe_3), 4.23 (q, J = 7.2 Hz, 2H, CH_2O), 4.62 (s, 2H, NCH_2), 7.19-7.35 (m, 5H, ArH). ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 14.4, 28.7, 51.5, 58.9, 61.2, 126.7, 127.3, 128.6, 139.5, 162.5, 163.2.

Preparation of ethyl 1-*tert*-butyl-4-phenyl-2-azetidinone-3-carboxylate (11m) via the

[22] Nahmany M.; Melman A. *J. Org. Chem.* **2006**, 71, 5804-5806.
[23] Choi M. K. W.; Yu W. Y.; Che C. M. *Org. lett.* **2005**, *7*, 1081-1084.

$Rh_2(OAc)_4$ catalyzed intramolecular carbenoid C-H insertion reaction[24]



A solution of *N*-benzyl-*N*-*tert*-butyl-2-diazo-3-ethoxy-3-oxopropanamide (0.512 g, 1.7 mmol) in dry toluene (5 mL) was added to a solution of $Rh_2(OAc)_4$ (2 mol %) in toluene (20 mL). The resulting mixture was stirred at 70 °C for 3 h until the diazo compound had been consumed. After removal of the solvent under reduced pressure, the residue was purified chromatographically on a silica gel column [elution with ethyl acetate and petroleum ether (30-60 °C) 1:10), *v/v*] to give rise to a mixture of *cis*- and *trans*-β-lactam as colorless crystals. 0.28 g (60% yield). *Cis*-**11m**: ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.84 (t, J = 7.2 Hz, 3H, CH_3), 1.31 (s, 9H, CMe_3), 3.76 (q, J = 7.2 Hz, 2H, CH_2), 4.21 (d, J = 6.3 Hz, 1H, CH), 4.91 (d, J = 6.3 Hz, 1H, CH), 7.27-7.40 (m, 5H, ArH). *Trans*-**11m**: ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.27 (s, 9H, CMe_3), 1.29 (t, J = 7.2 Hz, 3H, CH_3), 3.70 (d, J = 2.1 Hz, 1H, CH), 4.24 (dq, J = 2.1, 7.2 Hz, 2H, CH_2), 4.85 (d, J = 2.1 Hz, 1H, CH), 7.27-7.40 (m, 5H, ArH).

Analytic data of known products

***N*-Methyl-*N'*-phenylmalonamide.** Colorless crystals, yield 31%, m.p. 160-162 °C, Lit:[25] m.p.163 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 2.83 (d, J = 4.5 Hz, 3H, CH_3), 3.39 (s, 2H, CH_2), 7.09-7.57 (m, 6H, NH & ArH). 9.68 (s, 1H, NH). ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 26.4, 43.7, 120.2, 124.6, 128.9, 137.6, 165.7, 168.3. IR (KBr) ν (cm^{-1}): 1657, 1652 (C=O). HRMS calcd for $C_{10}H_{12}N_2NaO_2$ ($[M+Na]^+$) *m/z*: 215.0790, found: 215.0783.

2,3-Dihydro-2,3,6-triphenyl-4*H*-1,3-oxazin-4-one (13d). Colorless crystals, yield 74%, m.p. 161-162 °C, Lit.[26] m.p. 146-148 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 6.04 (s, 1H, CH), 6.83 (s, 1H, CH), 7.18-7.71 (m, 15H, ArH). ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 90.0, 98.8, 124.9, 126.2, 126.3, 127.1, 128.6, 128.6, 129.0, 129.4, 131.3, 131.6, 136.4, 139.6, 161.3, 162.9. IR (KBr) ν (cm^{-1}): 1663 (C=O).

(±)-*trans*-3-Methyl-1,4-diphenyl-2-azetidinone (12e).[27] Colorless crystals, yield 19%, m.p. 118-119 °C, ^{1}H NMR (200 MHz, $CDCl_3$) δ: 1.48 (d, J = 7.4 Hz, 3H, CH_3), 3.13 (dq, J = 2.4, 7.4 Hz, 1H, CH), 4.58 (d, J = 2.4 Hz, 1H), 6.98-7.45 (m, 10H, ArH). ^{13}C NMR (50 MHz, $CDCl_3$) δ: 13.1, 55.3, 62.7, 116.9, 123.7, 125.8, 128.4, 129.0, 129.1, 138.0, 168.3. IR (KBr) ν (cm^{-1}): 1742 (C=O).

[24] Grohmann, M.; Maas, G. *Tetrahedron* **2007**, *63*, 12172-12178.
[25] Ziegler, E.; Brus, G. *Monatsh.Chem.* **1967**, *98*, 1100–1103.
[26] Sato, M.; Ogasawara, H.; Kato, T. *Chem. Pharm. Bull*. **1984**, *32*, 2602–2608.
[27] Jian, S. Z.; Ma, C.; Wang, Y. G. *Synthesis* **2005**, *5*, 725–730.

1-Phenyl-1*H*-1,2,3-triazole-4-carboxaldehyde (14). Colorless crystals, yield 68%, m.p. 103-104 °C, Lit.[28] m.p. 98-100 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.50-7.80 (m, 5H, ArH), 8.59 (s, 1H, CH), 10.22 (s, 1H, CHO), ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 120.8, 123.1, 129.8, 130.0, 136.1, 148.1, 185.0. IR (KBr) ν (cm^{-1}): 1689 (C=O).

2-Cyano-*N*-phenylcinnamamide (15). Colorless crystals, yield 17%, m.p. 207-208 °C. Lit.[29] 199 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.04-7.65 (m, 9 H, CH & ArH), 7.96-8.01 (m, 2H, ArH), 8.45 (s, 1H, NH).

Ethyl (±)-*trans*-1,4-diphenyl-azetidin-2-one-3-carboxylate (11a). Colorless crystals, yield 10%, m.p. 92-93 °C, Lit.[30] m.p. 87-89 °C. ^{1}H NMR (200 MHz, $CDCl_3$) δ: 1.33 (t, J = 7.2 Hz, 3H, CH_3), 3.98 (d, J = 2.7 Hz, 1H, CH), 4.30 (q, J = 7.2 Hz, 2H, CH_2O), 5.34 (d, J = 2.7 Hz, 1H, CH), 7.05-7.42 (m, 10H, ArH). ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 14.1, 57.5, 62.1, 63.5, 117.1, 124.3, 126.1, 128.96, 129.03, 129.2, 136.2, 137.1, 159.2, 166.2. IR (KBr) ν (cm^{-1}): 1767 (C=O), 1713 (C=O).

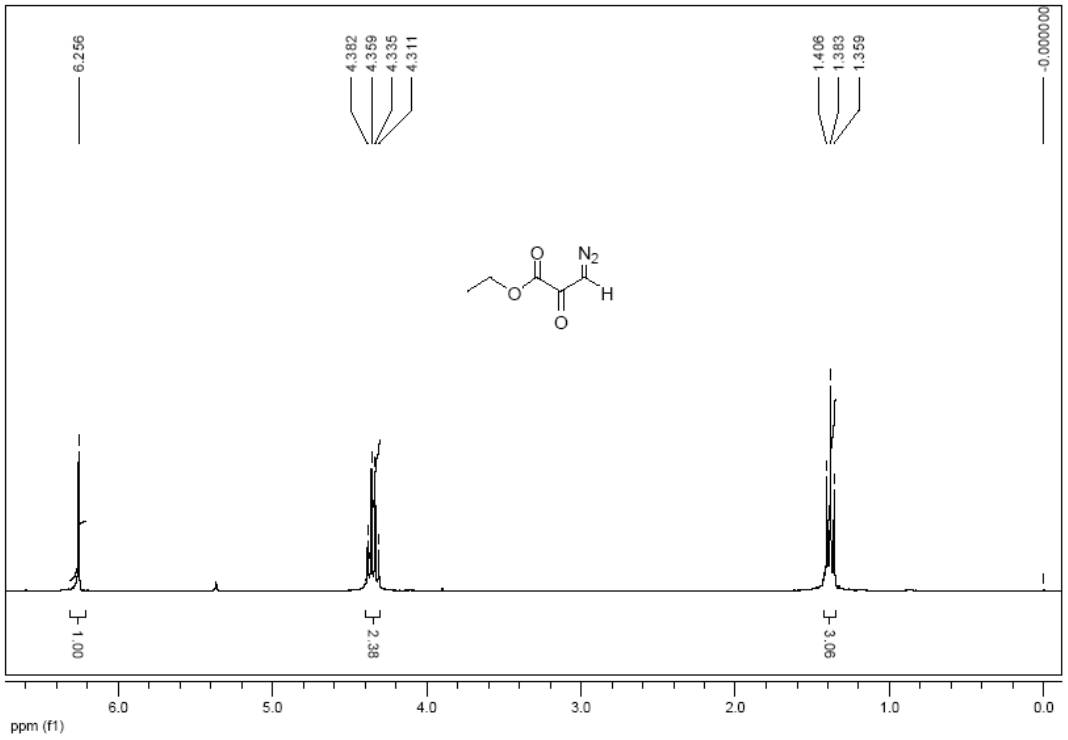
Diethyl (±)-*trans*-1,4-diphenyl-azetidin-2-one-3-phosphonate (11i). Colorless crystals, yield 64%, m.p. 96-97 °C. Lit.[错误！未定义书签。] m.p. 81-83 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.36 (dt, J = 5.7, 6.9 Hz, 6H), 3.55 (dd, J = 2.9, 15.6 Hz, 1H), 4.24 (m, 4H), 5.23 (dd, J = 2.9, 9.2 Hz, 1H), 7.04-7.38 (m, 10H). ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 16.28, 16.36, 55.71, 55.74, 56.2, 58.1, 62.6, 62.7, 63.0, 63.1, 116.9, 124.2, 125.7, 128.8, 129.0, 129.2, 136.42, 136.46, 137.19, 137.23, 158.8, 158.9. IR (KBr) ν (cm^{-1}): 1752 (C=O).

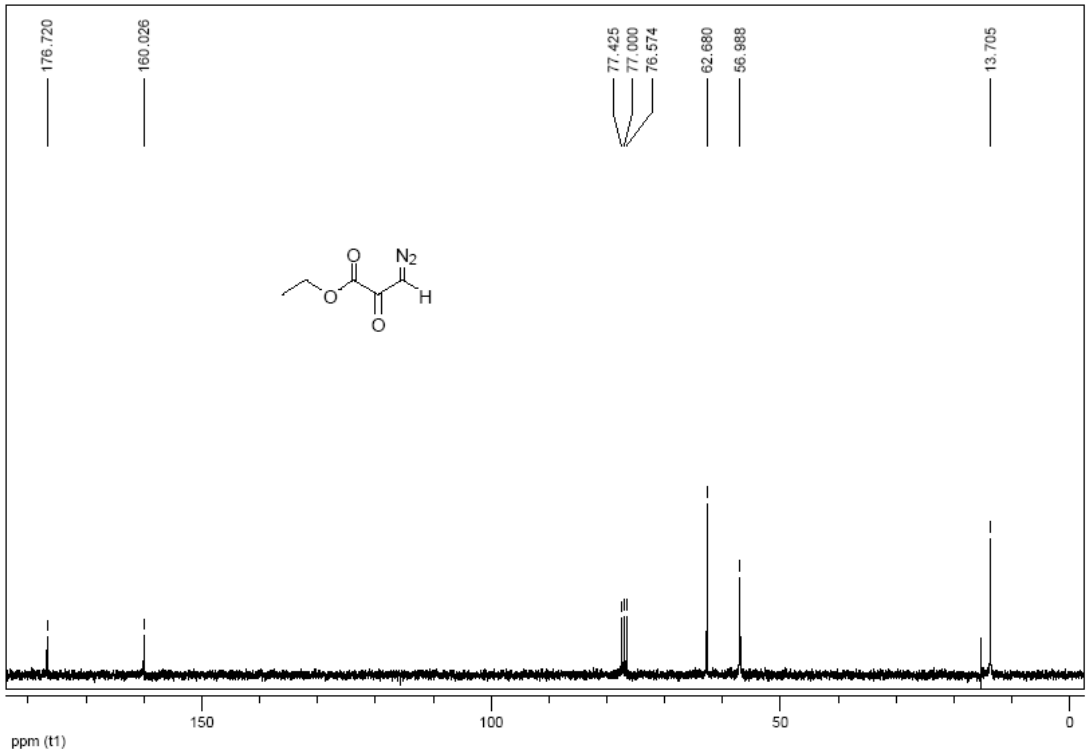
(±)-*trans*-3-Benzenesulfonyl-1,4-diphenyl-azetidin-2-one (11j). Colorless crystals, yield 81%, m.p.179-180 °C. Lit.[错误！未定义书签。] m.p. 156-157 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 4.46 (d, J = 2.6 Hz, 1H)，5.58 (d, J = 2.6 Hz, 1H), 7.10-8.08 (m, 15H). IR (KBr) ν (cm^{-1}): 1748 (C=O).

[28] Cunha, A. C.; Figueiredo, J. M.; Tributino, J. L. M.; Miranda, A. L. P.; Castro, H. C.; Zingali, R. B.; Fraga, C. A. M.; de Souza, M. C. B. V.; Ferreira, V. F.; Barreiro, E. J. *Bioorg. Med. Chem.* **2003**, *11*, 2051–2059.
[29] Ziegler, E.; Wimmer, T. *Monatsh. Chem*. **1965**, *96*, 1252–1260.
[30] Jiao, L.; Zhang, Q. F.; Liang, Y.; Zhang, S. W.; Xu, J. X. *J. Org. Chem.* **2006**, *71*, 815–818.

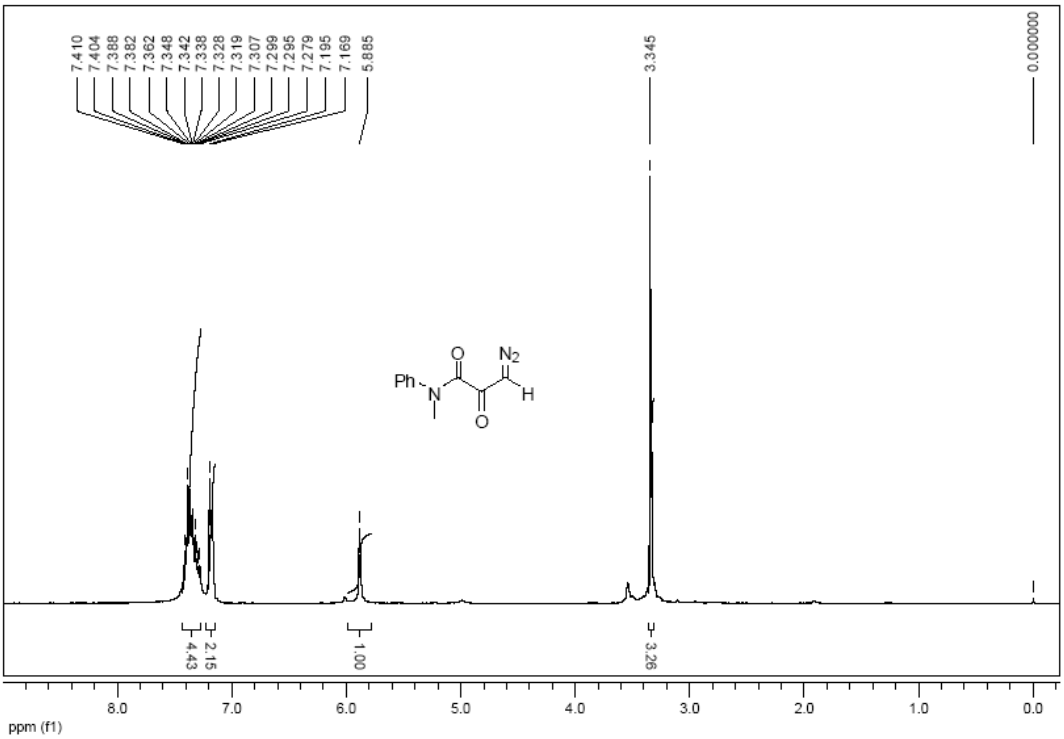
Copies of ^{1}H and ^{13}C NMR Spectra of Diazo Precursors 2 and 3

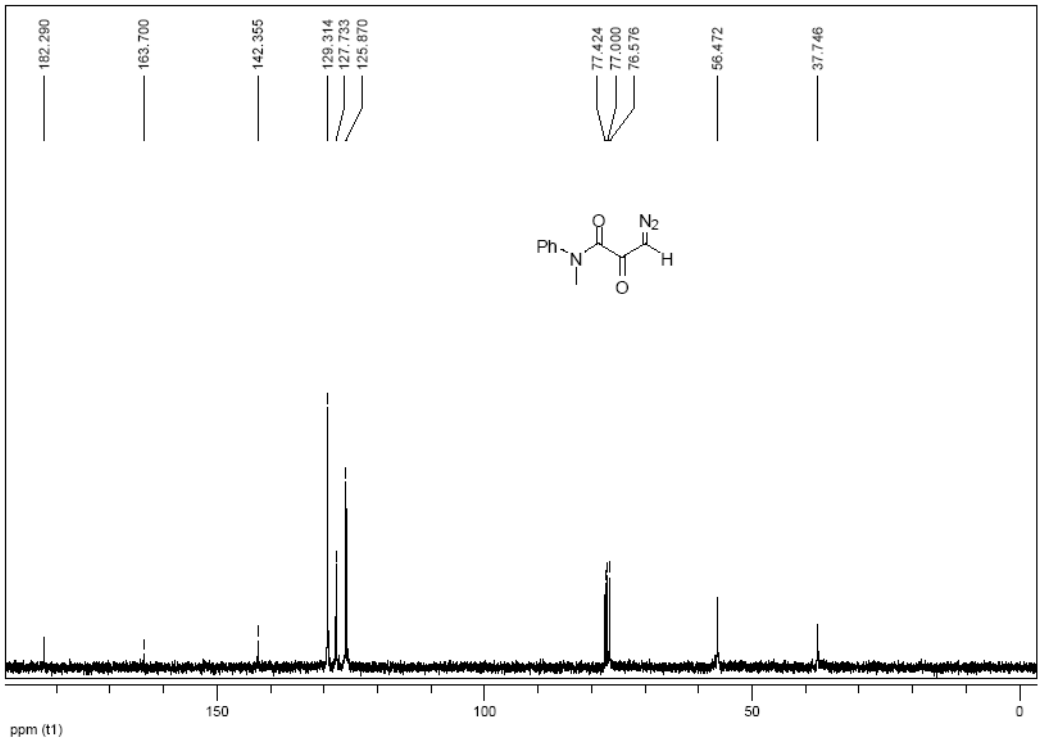
Ethyl 3-diazo-2-oxopropanoate (**2a**)



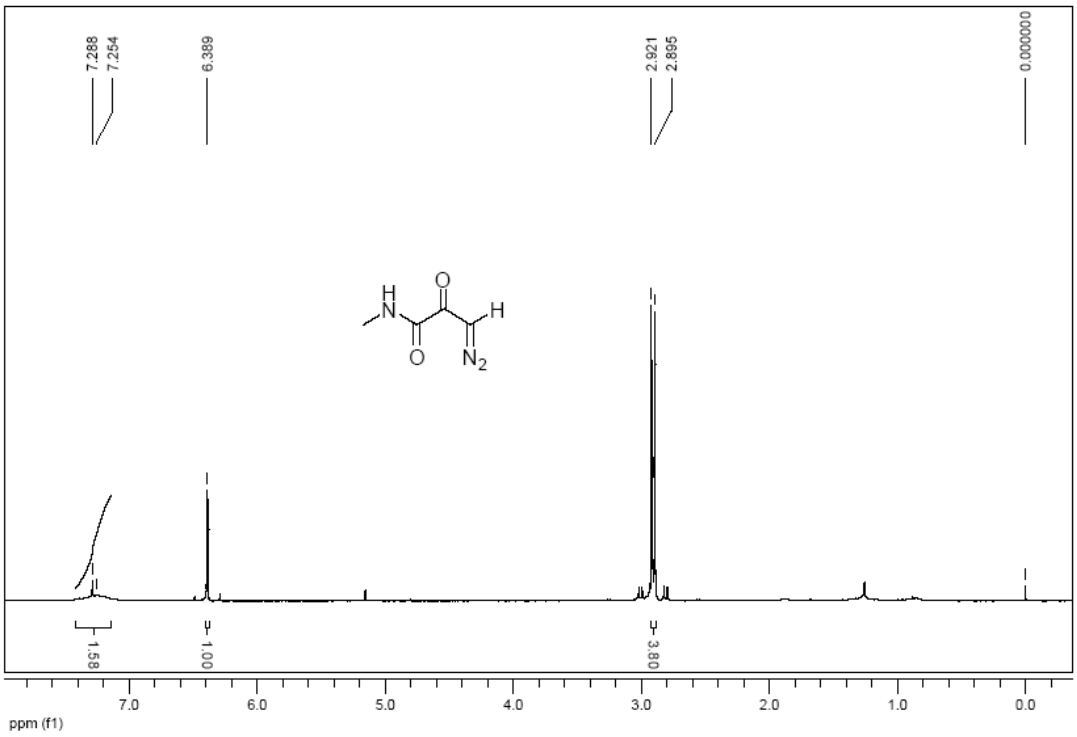


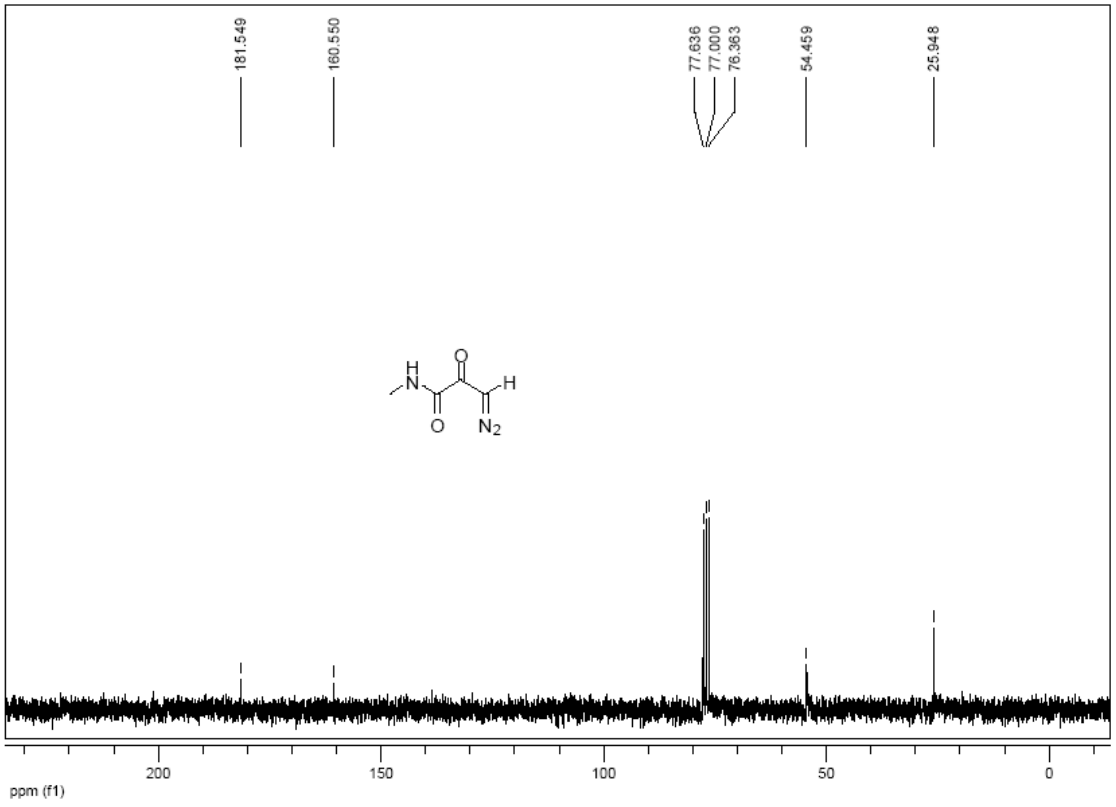
3-Diazo-*N*-methyl-2-oxo-*N*-phenylpropanamide (**2b**)



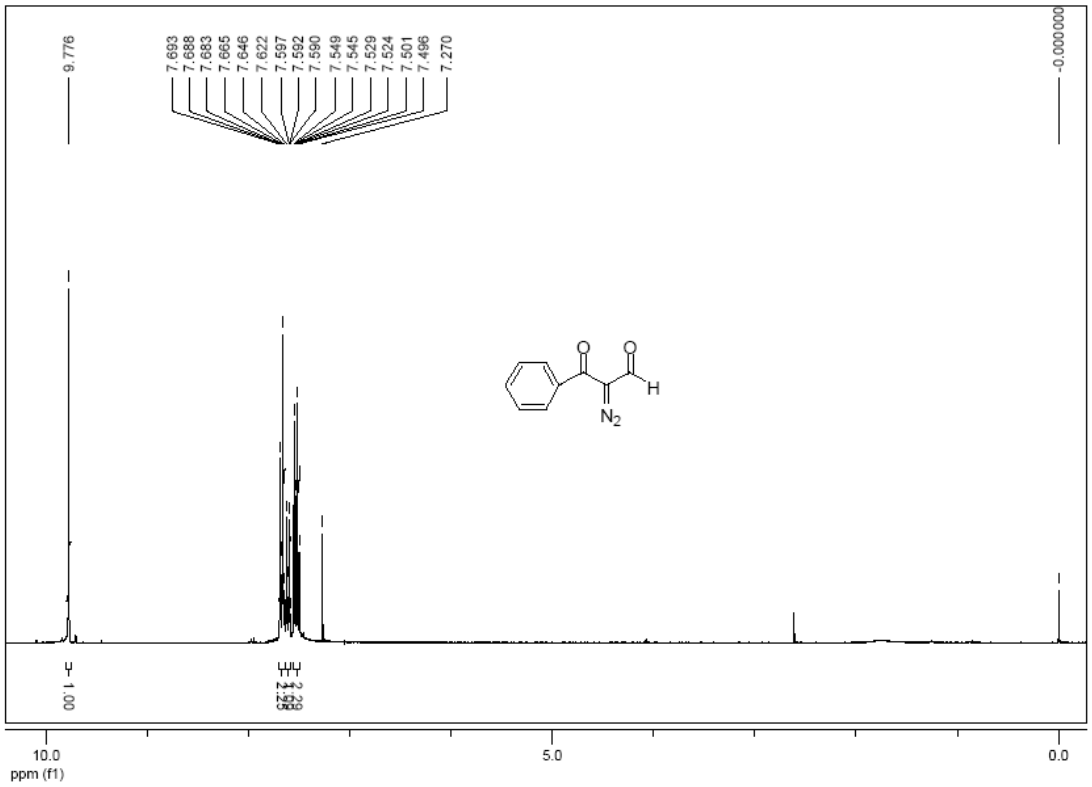


3-Diazo-*N*-methyl-2-oxopropanamide (**2c**)

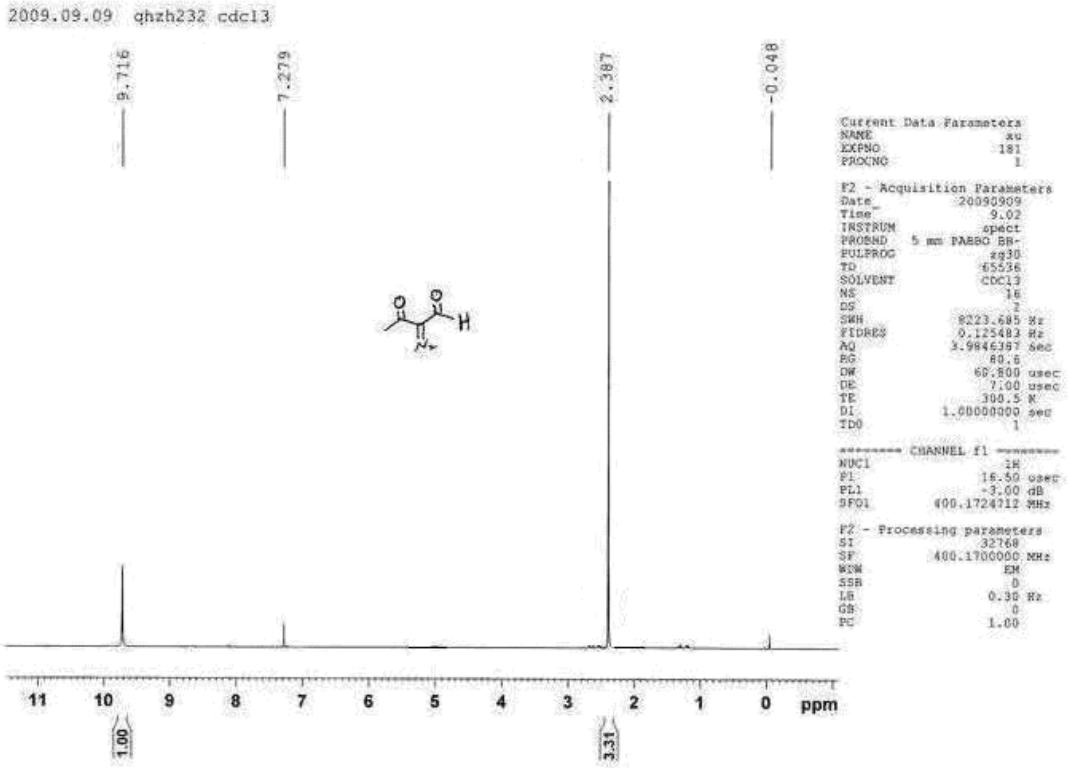


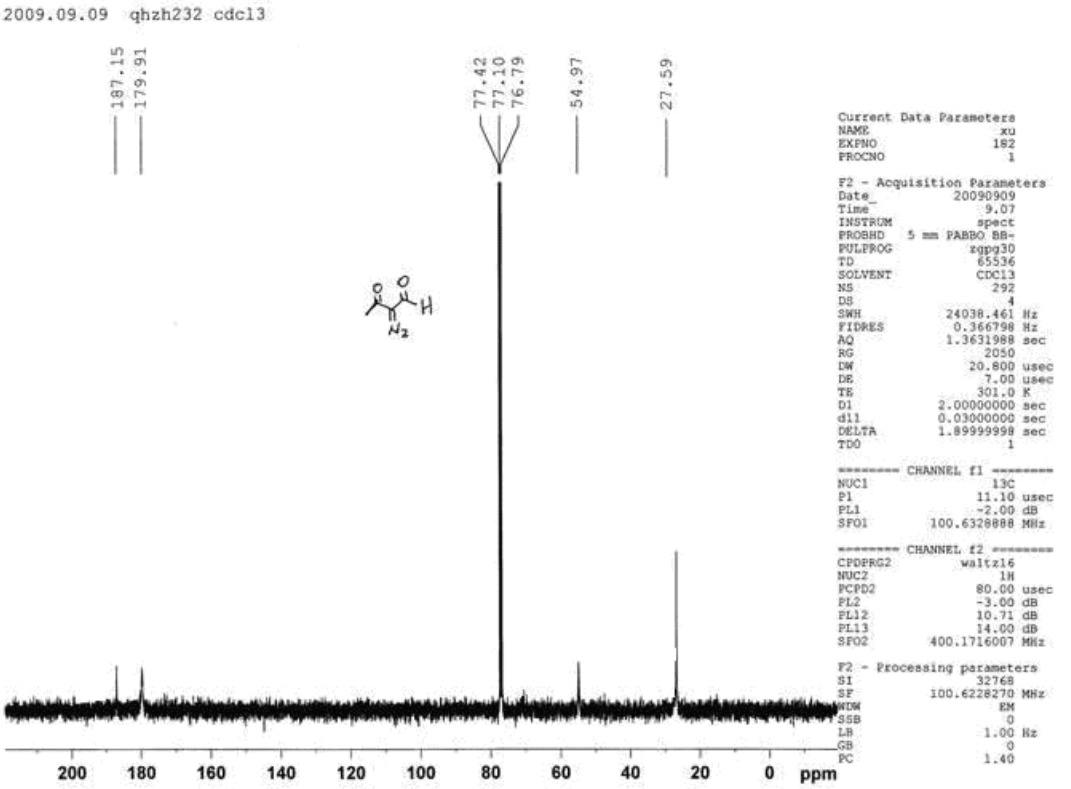


2-Diazo-3-oxo-3-phenylpropanal (**3d**)

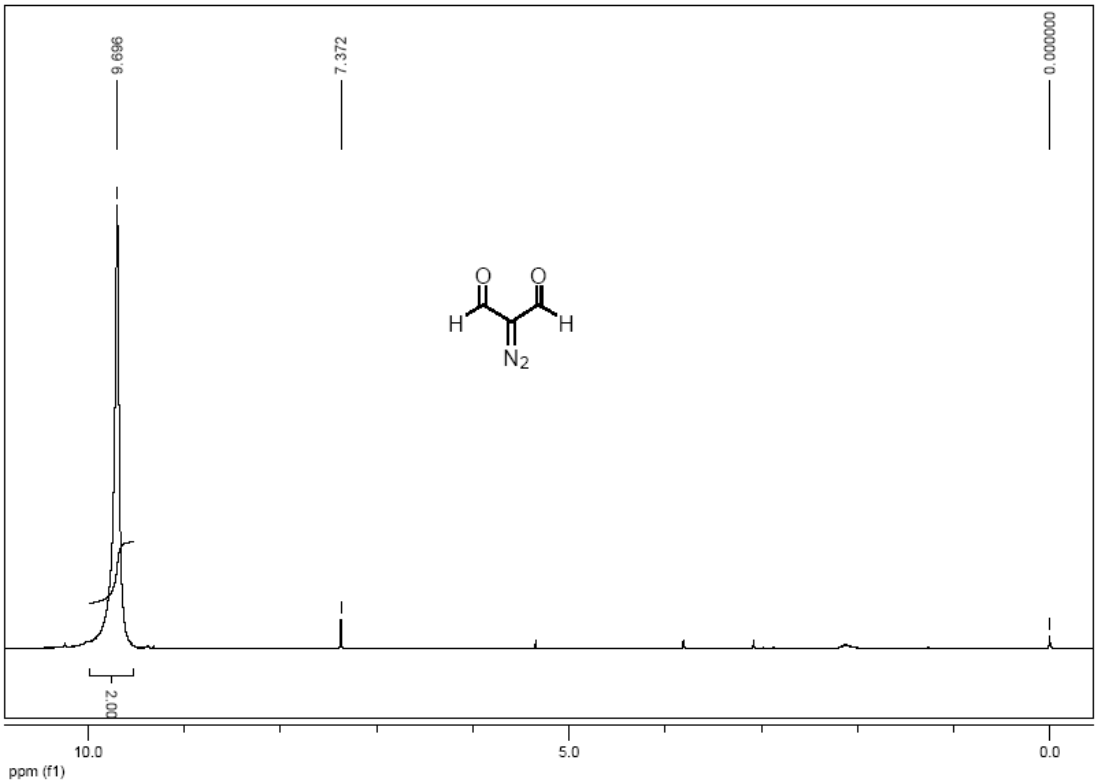


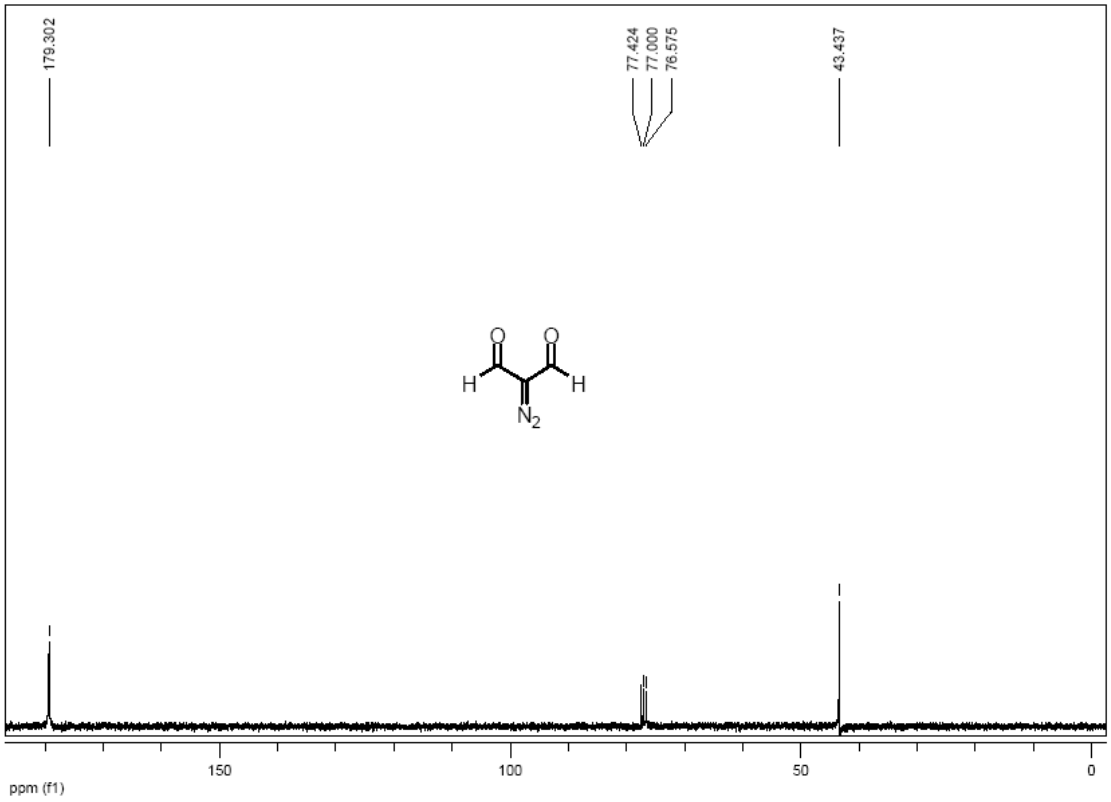
2-Diazo-3-oxobutanal (**3e**)





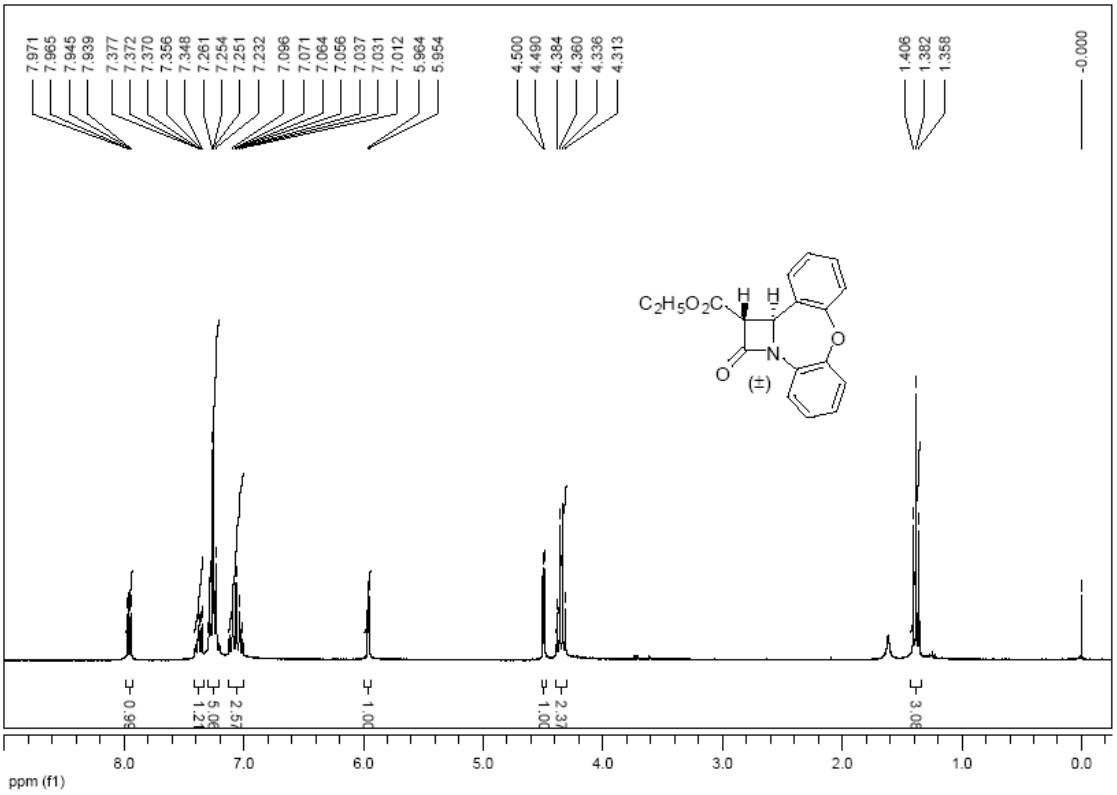
2-Diazomalonaldehyde (**3f**)

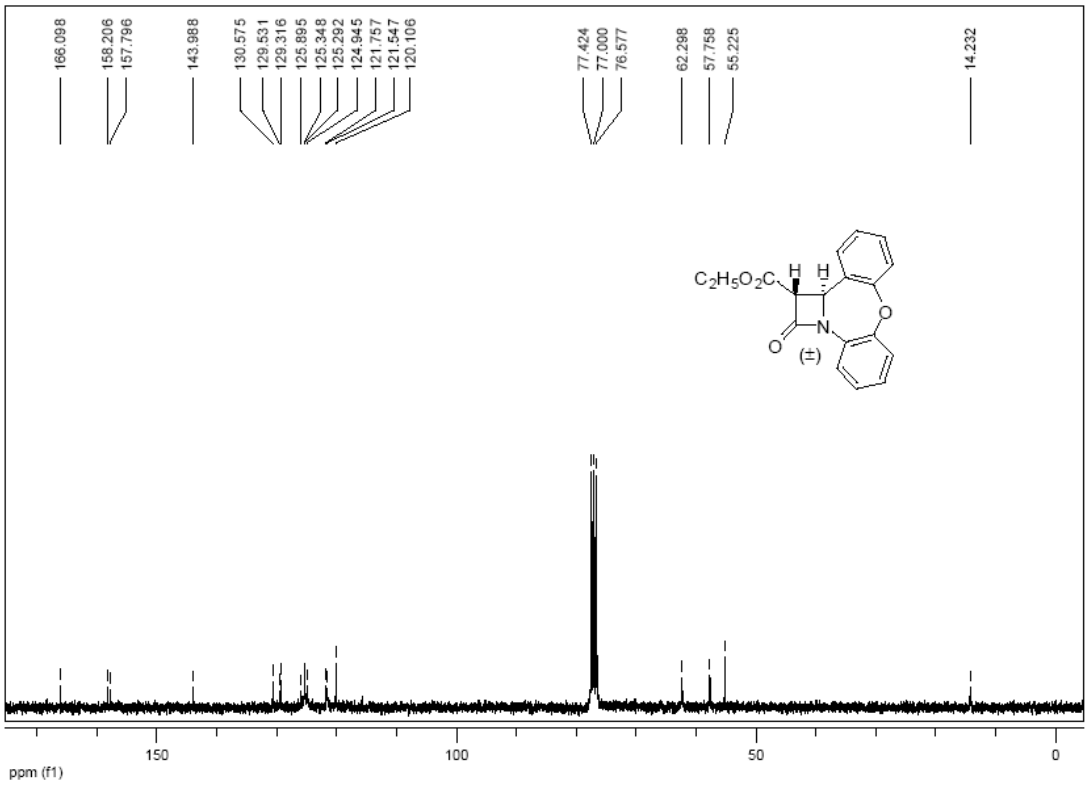




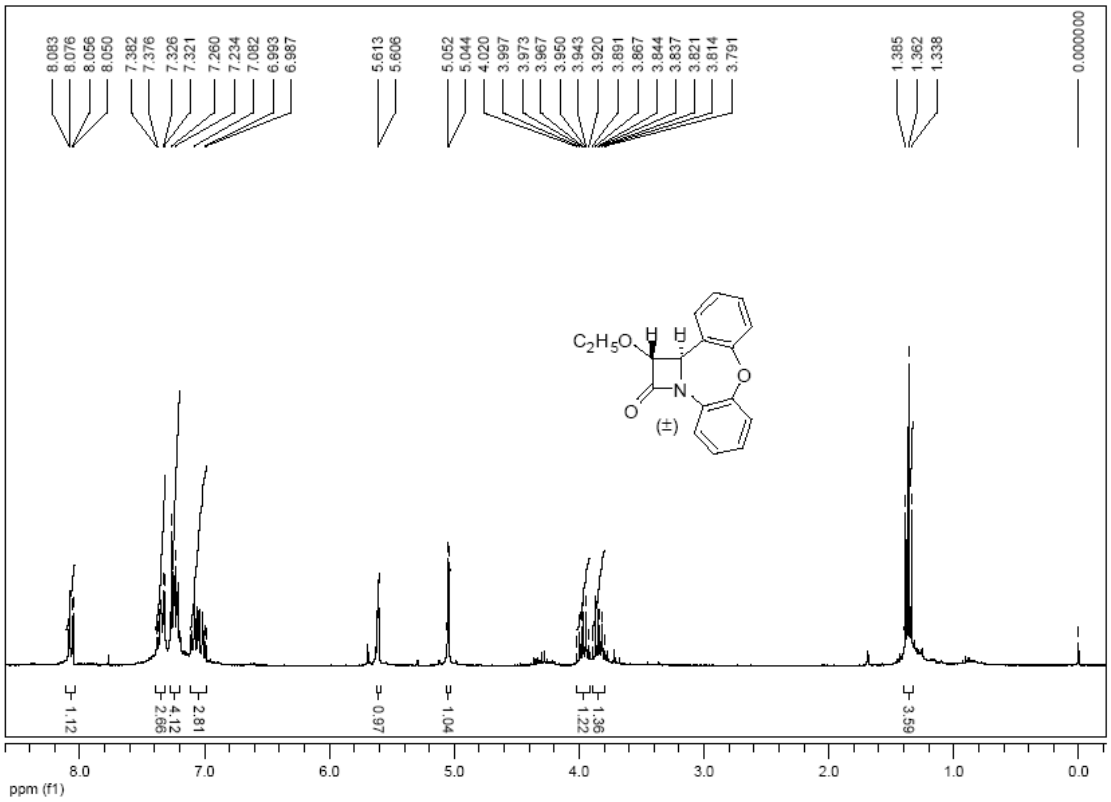
Copies of ^{1}H and ^{13}C NMR Spectra of Products

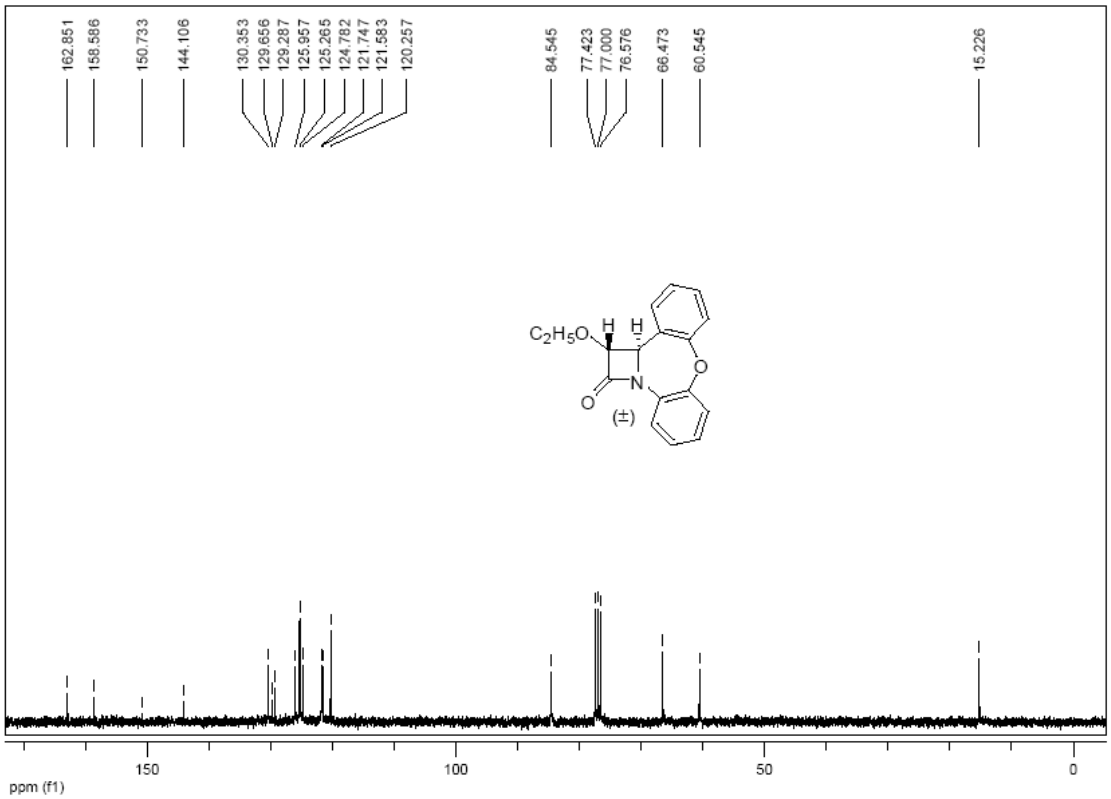
Ethyl (±)-*trans*-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-carboxylate (5a)



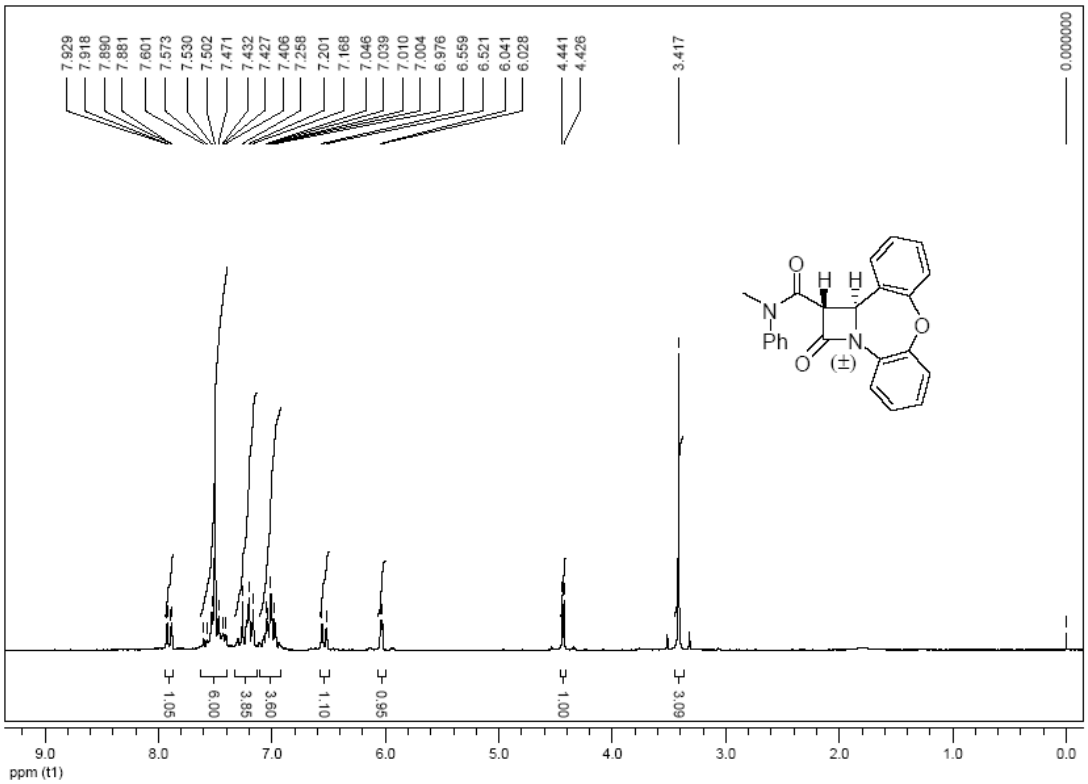


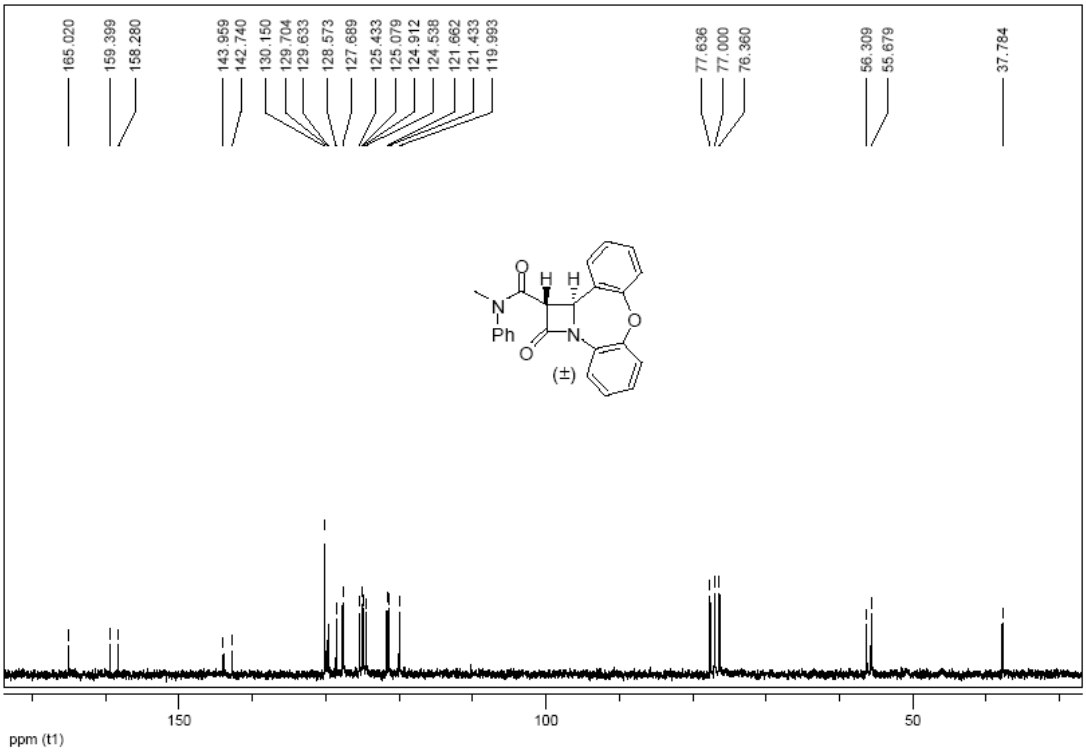
(±)-*trans*-1-Ethoxyl-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one (6a)



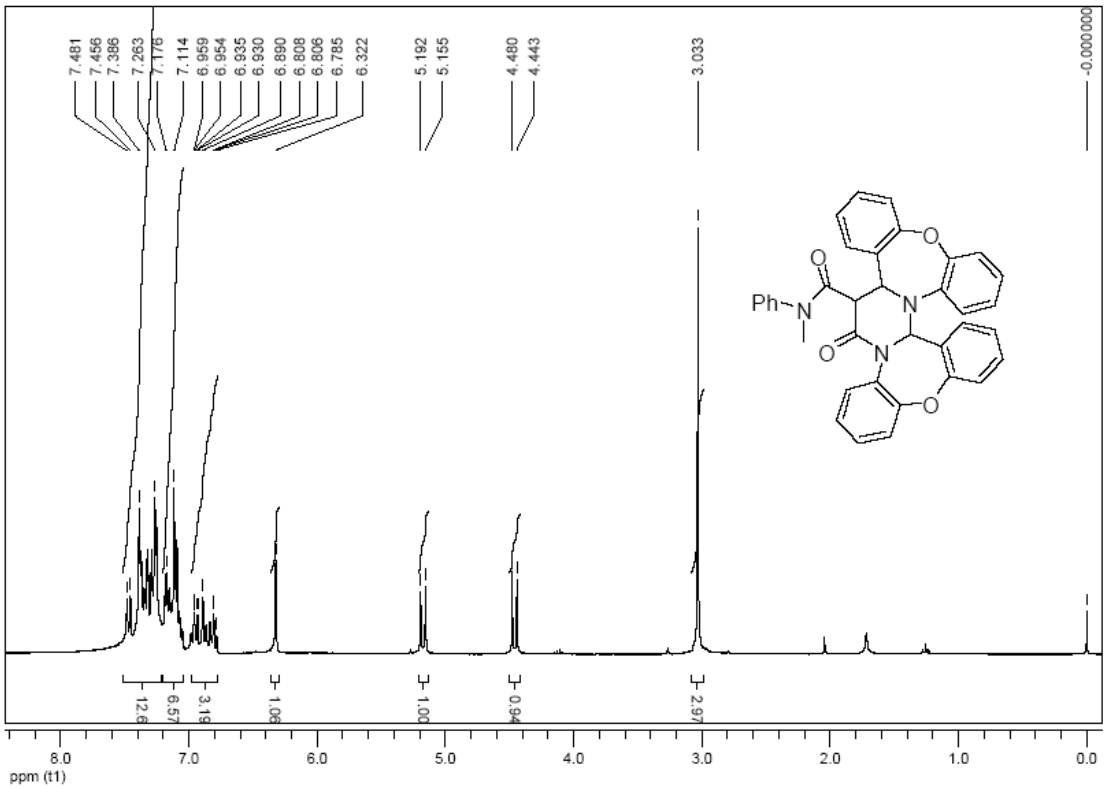


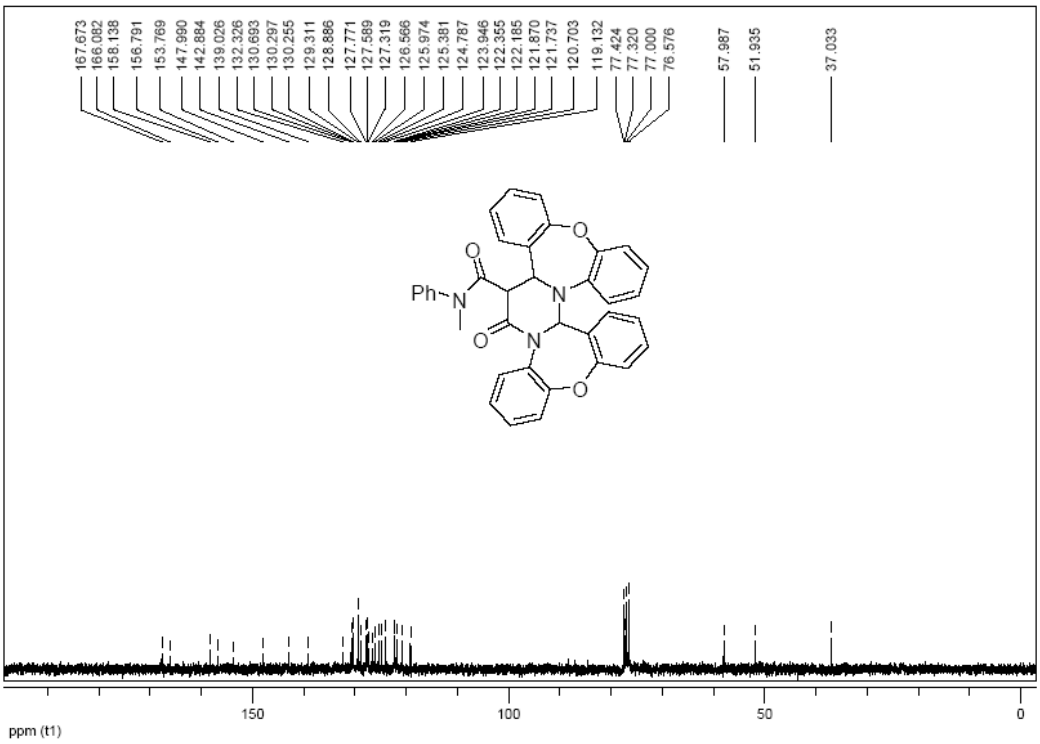
(±)-*trans*-1,12b-Dihydro-*N*-methyl-*N*-phenylazeto[1,2-*d*]dibenzo[*b,f*][1,4] oxazepin-2-one-1-carboxamide (5b)



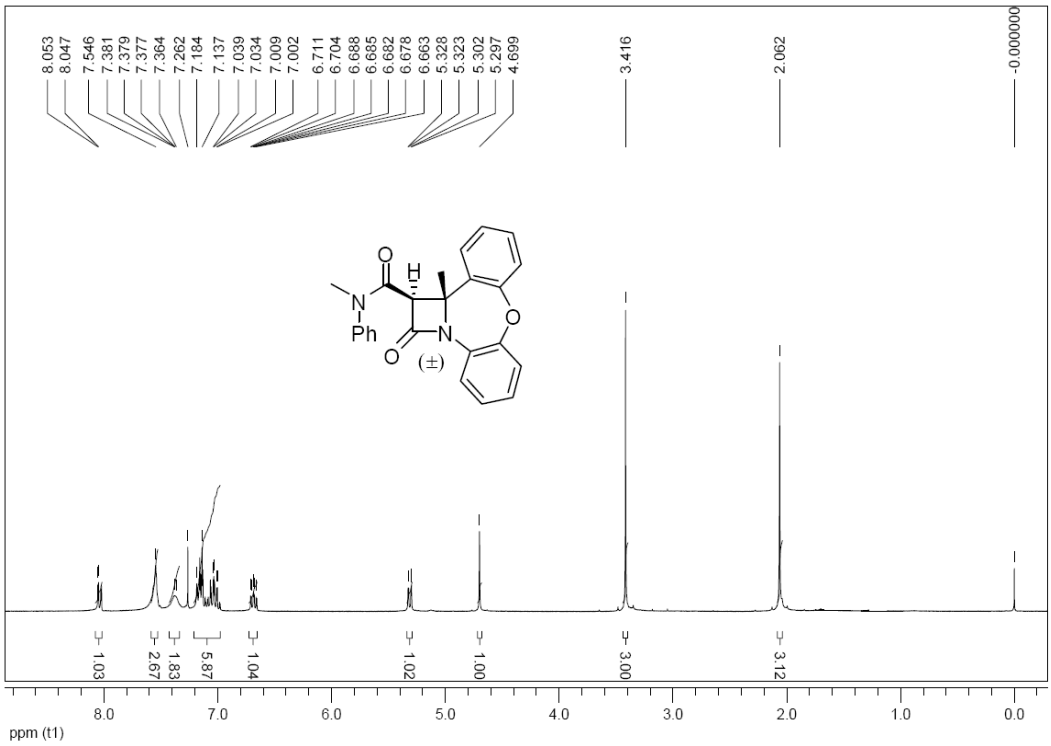


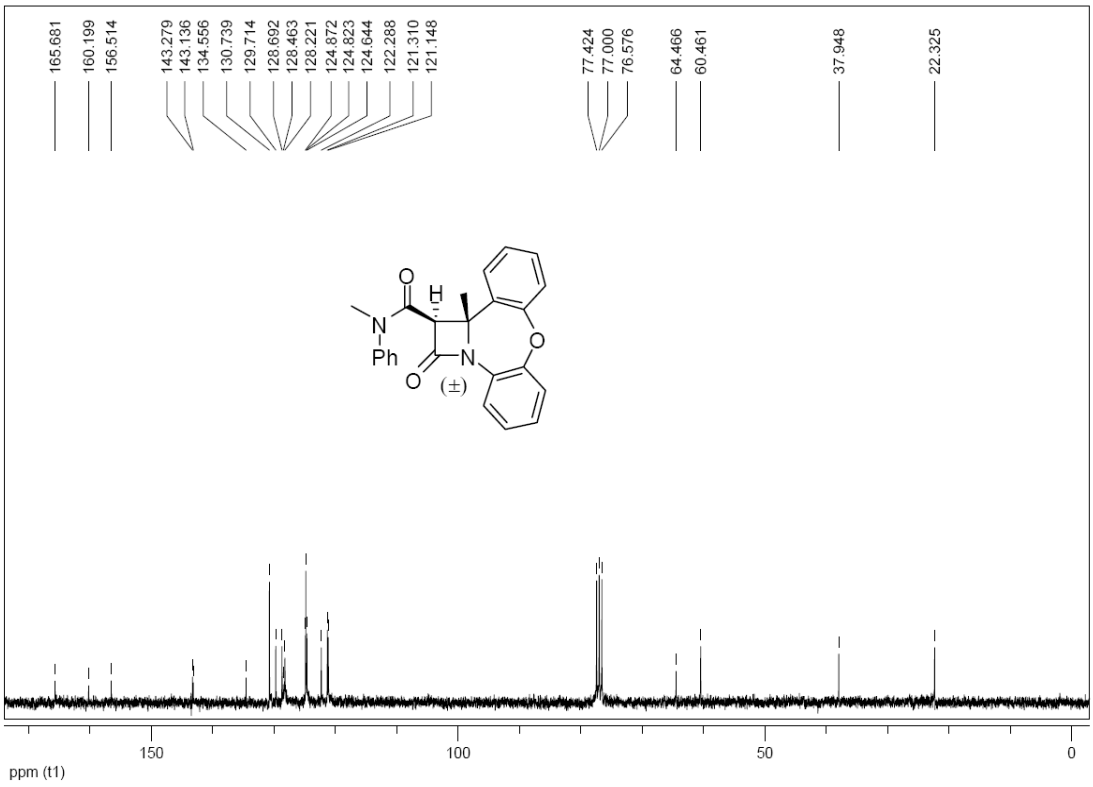
22,23-Dihydro-*N*-methyl-*N*-phenyl-10a*H*,21*H*-tetrabenzo[*b*,*b*',*f*,*f*']pyrimido [1,2-*d*:3,4-*d*']bis[1,4]oxazepin-21-one-22-carboxamide (7b)



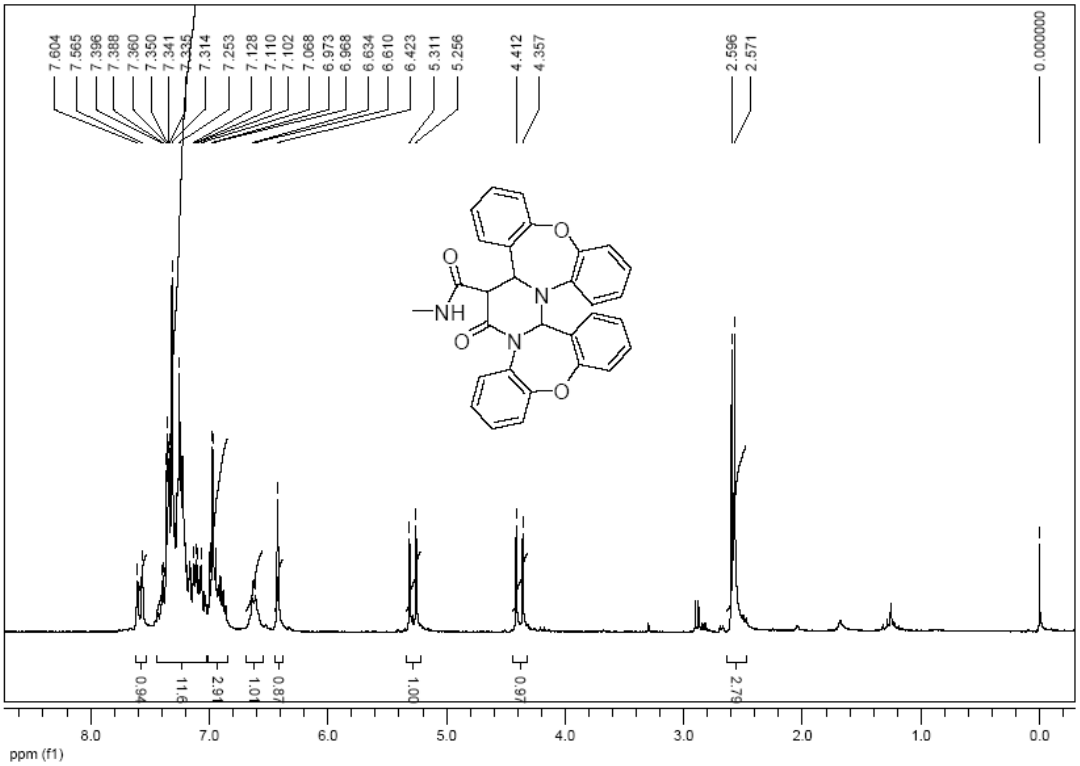


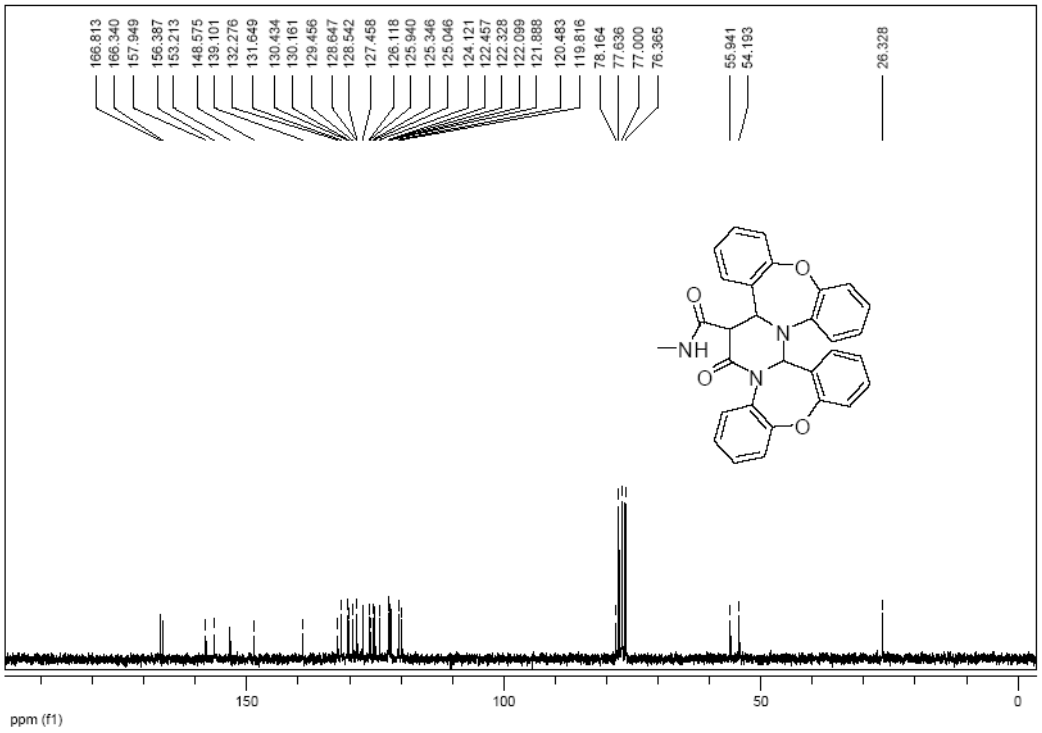
(±)-*trans*-1,12b-Dihydro-12b,*N*-dimethyl-*N*-phenyl-azeto[1,2-*d*]dibenzo[*b,f*] [1,4] oxazepin-2-one-1-carboxamide (5bb)



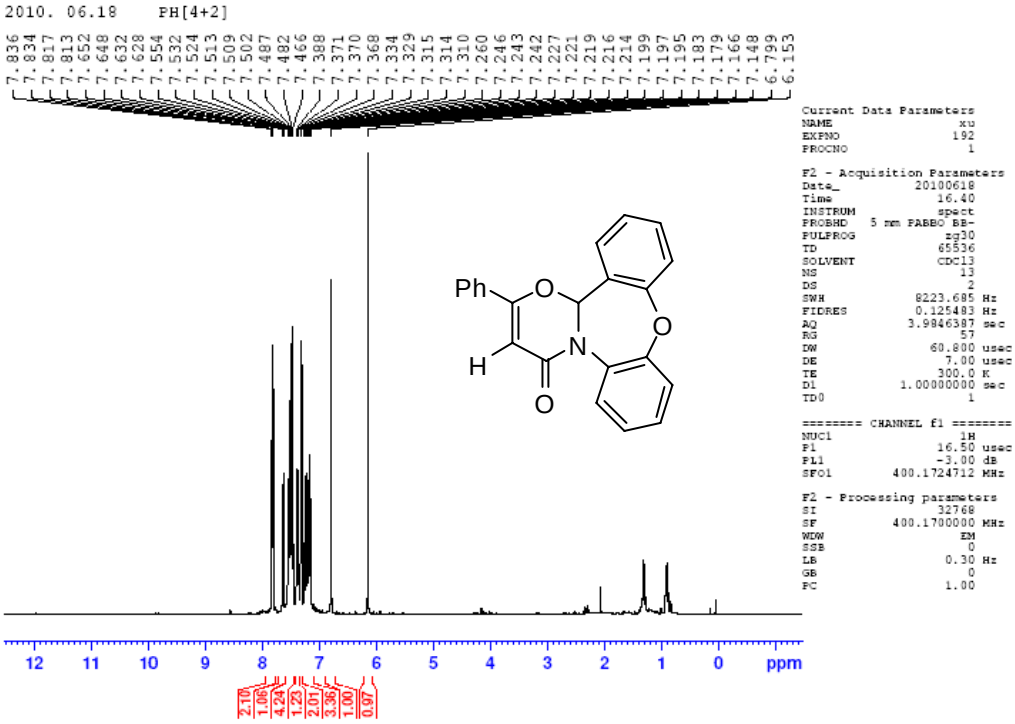


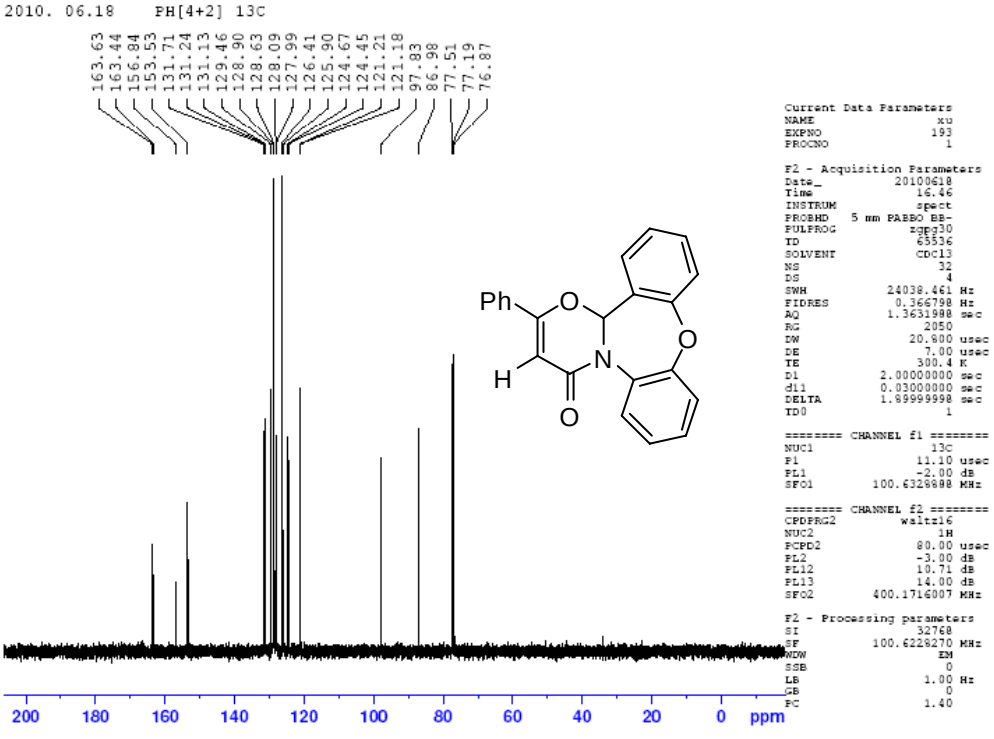
22,23-Dihydro-*N*-methyl-10a*H*,21*H*-tetrabenzo[*b*,*b*',*f*,*f*']pyrimido[1,2-*d*:3,4-*d*']bis[1,4]oxazepin-21-one-22-carboxamide (7c)



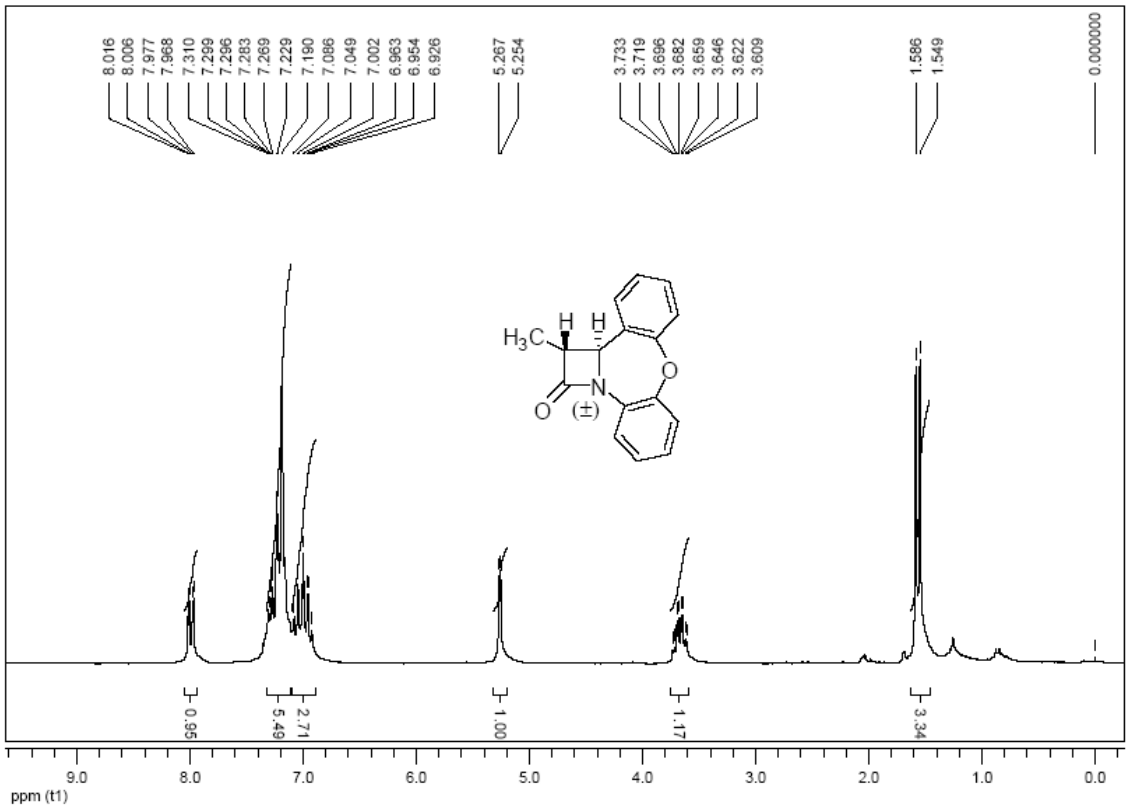


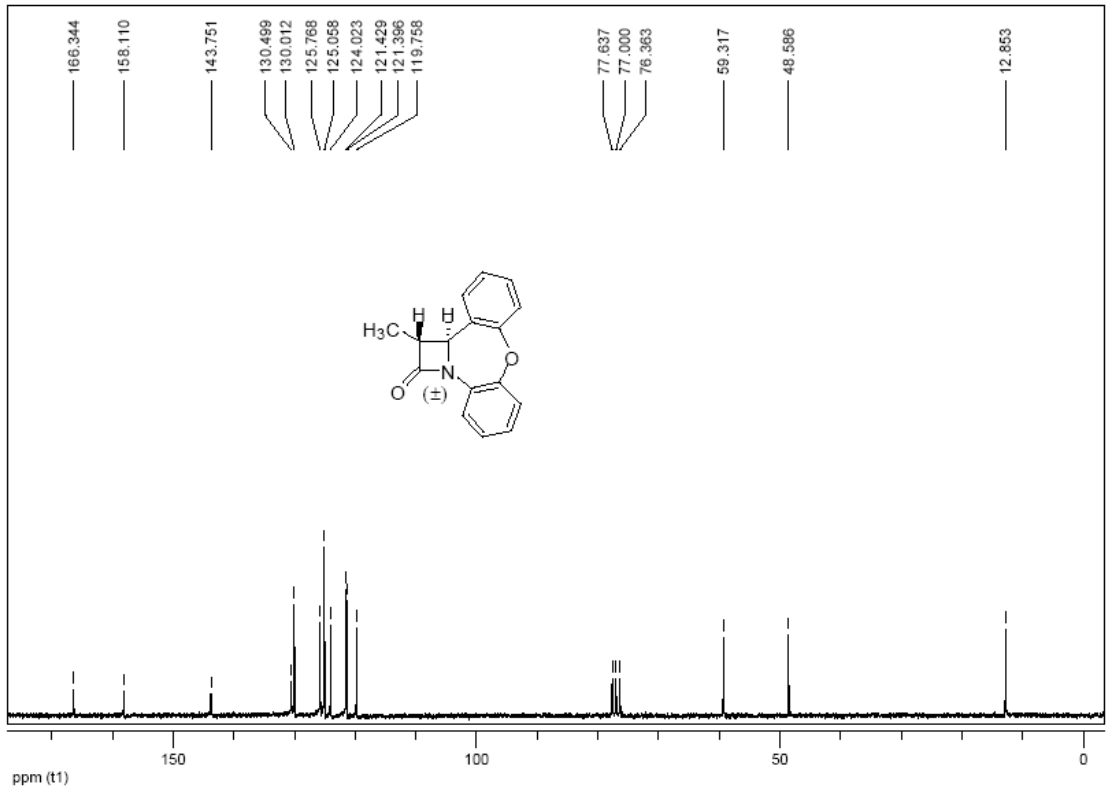
2-Phenyldibenzo[*b,f*][1,3]oxazino[3,2-*d*][1,4]oxazepin-4(14b*H*)-one (8d).



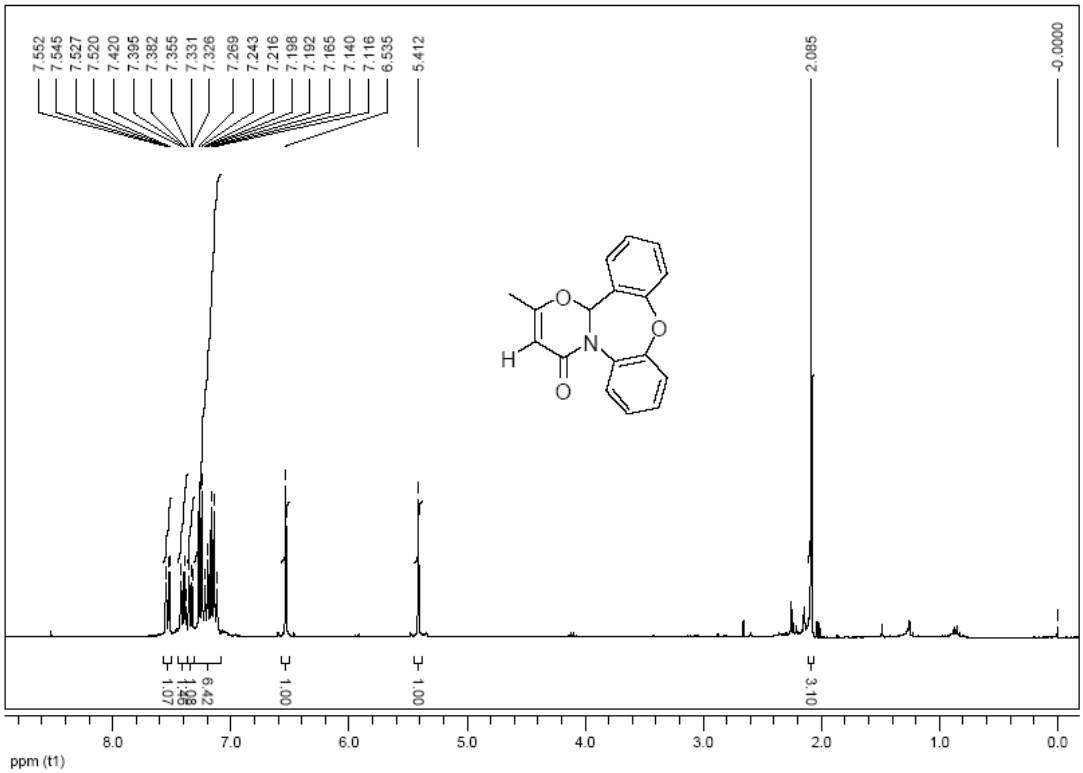


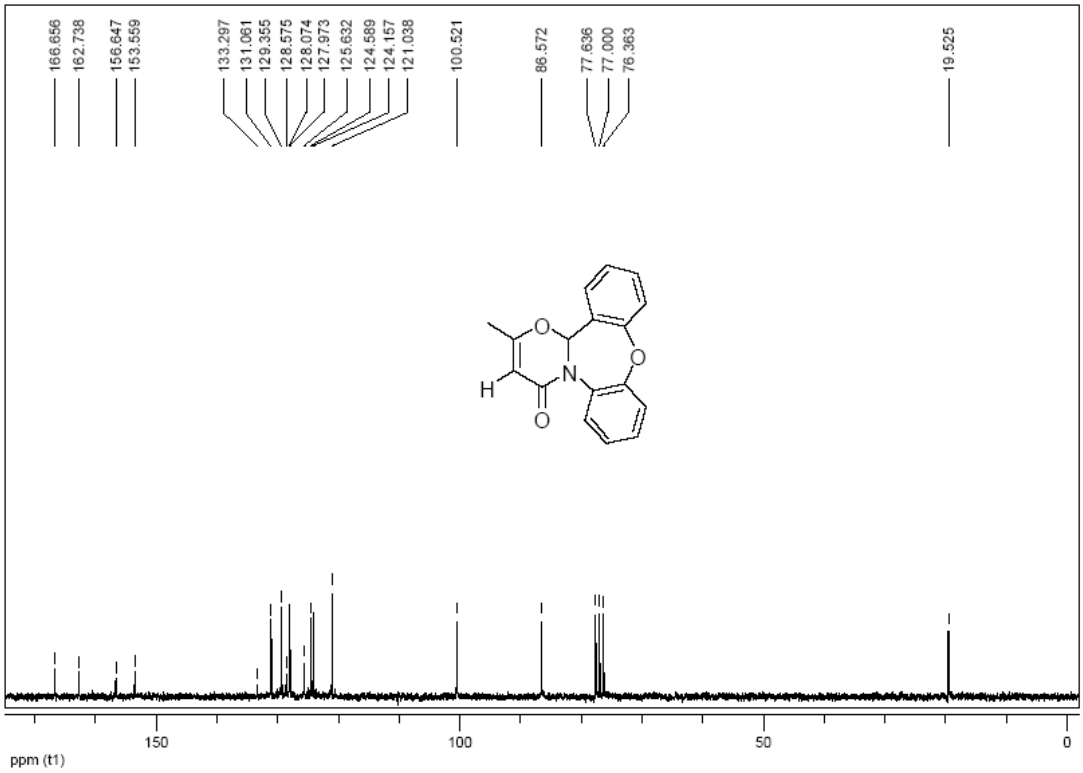
(±)-*trans*-1,12b-Dihydro-1-methyl-azeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepin-2-one (6e)



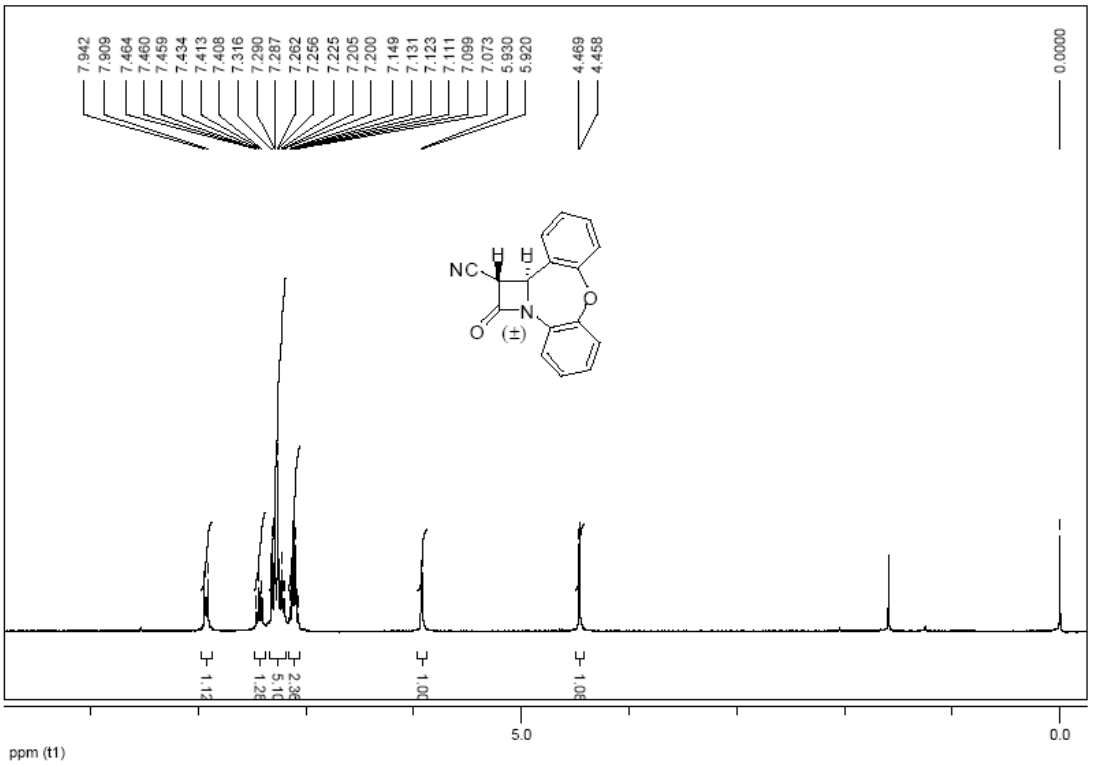


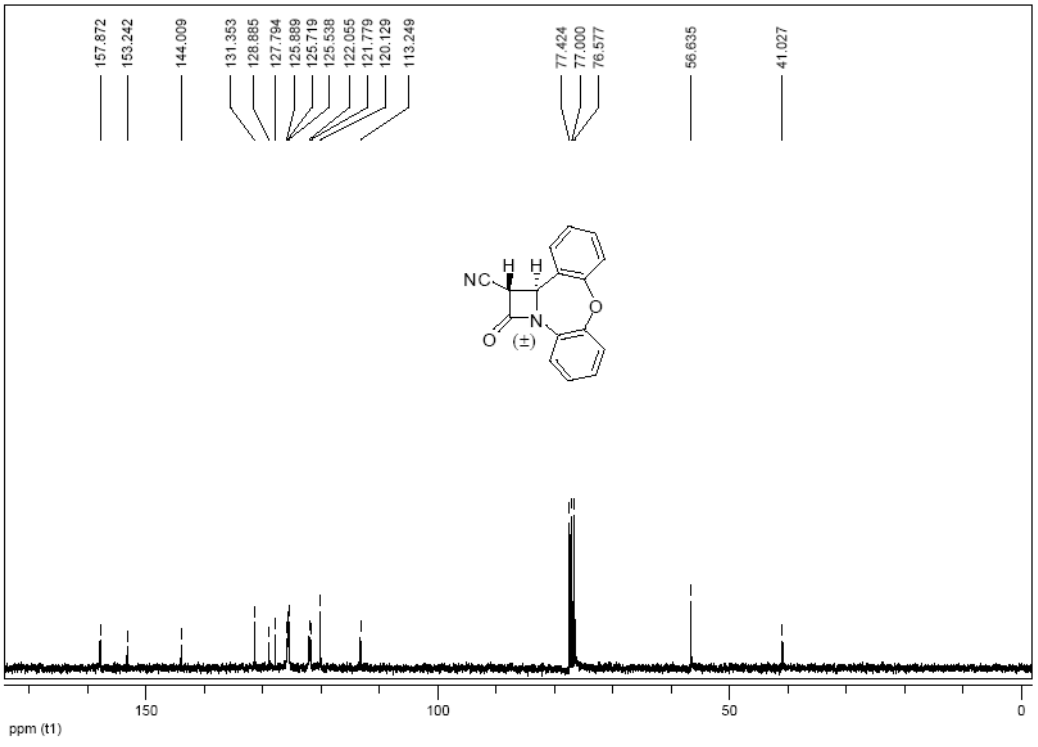
2-Methyldibenzo[*b*,*f*][1,3]oxazino[3,2-*d*][1,4]oxazepin-4(14b*H*)-one (8e)



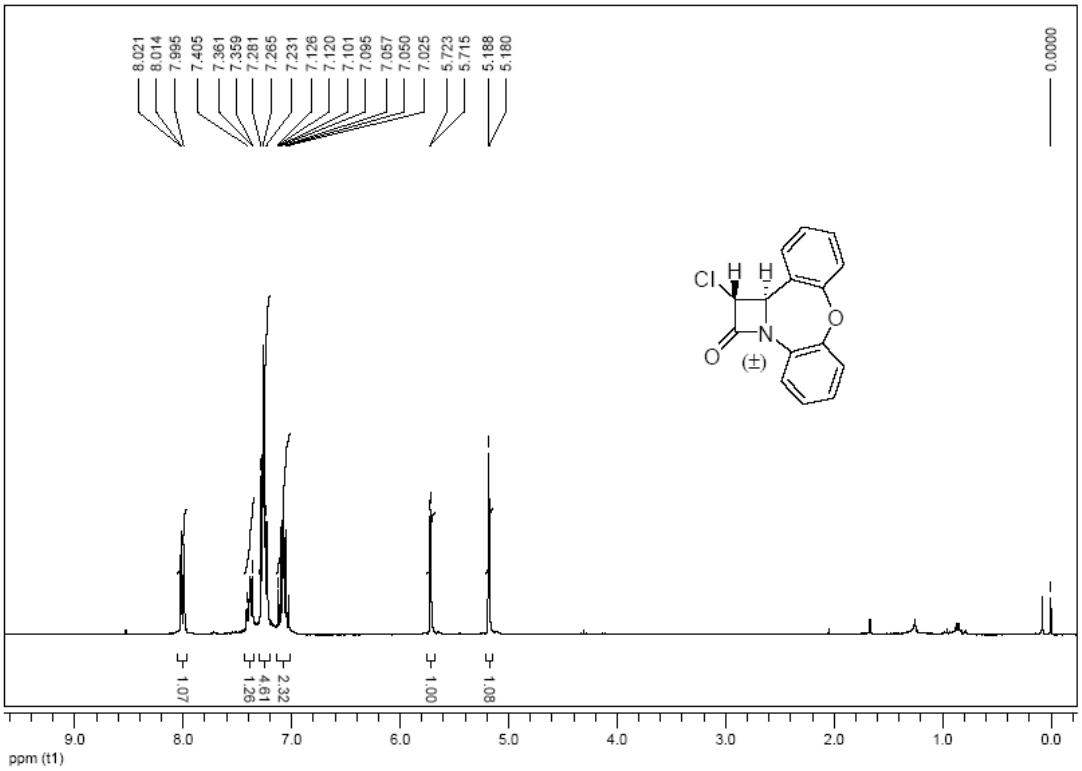


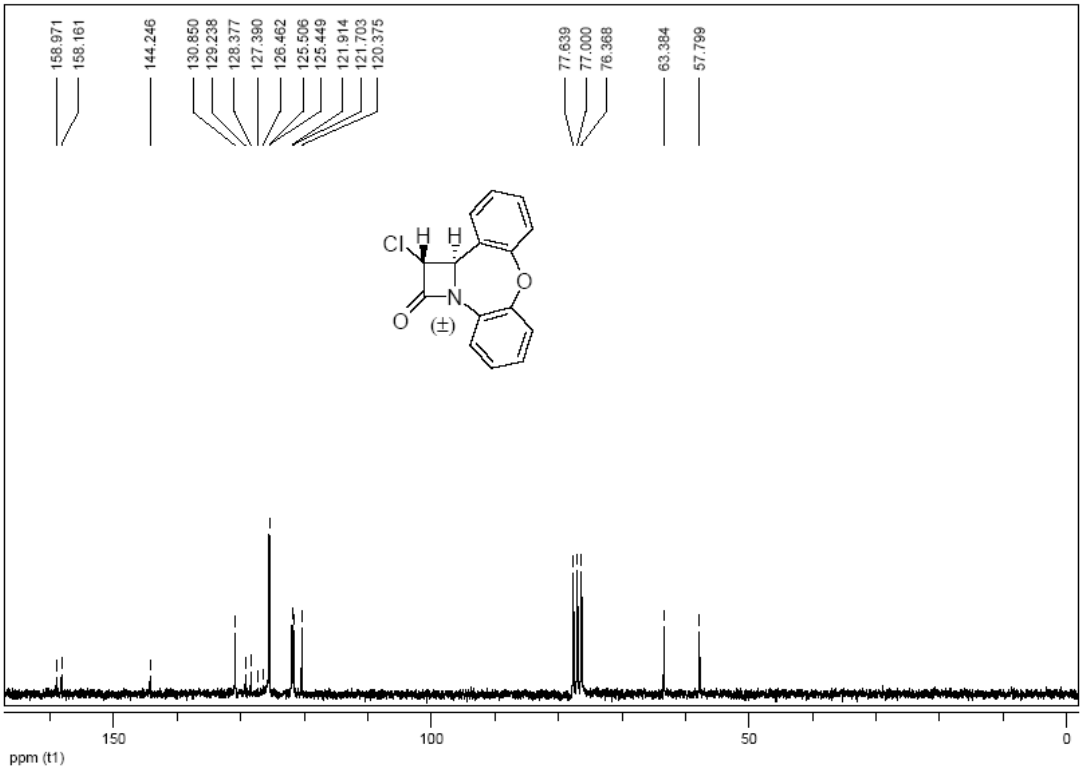
(±)-*trans*-1-Cyano-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one (5g)



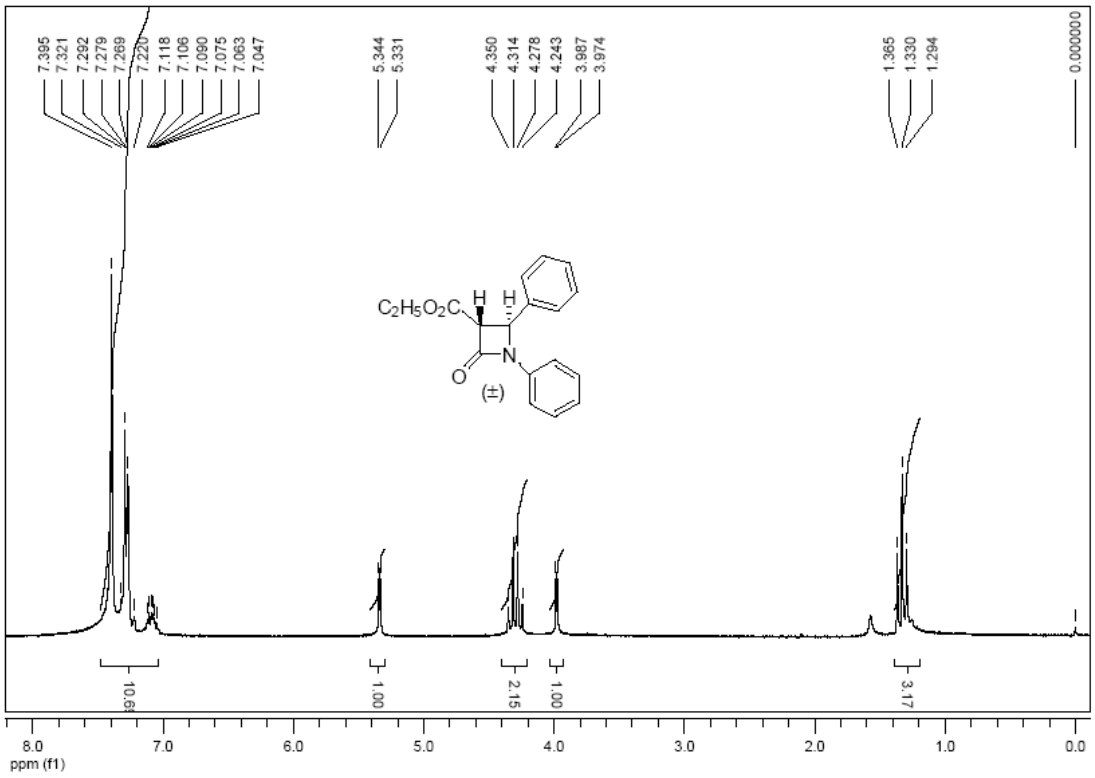


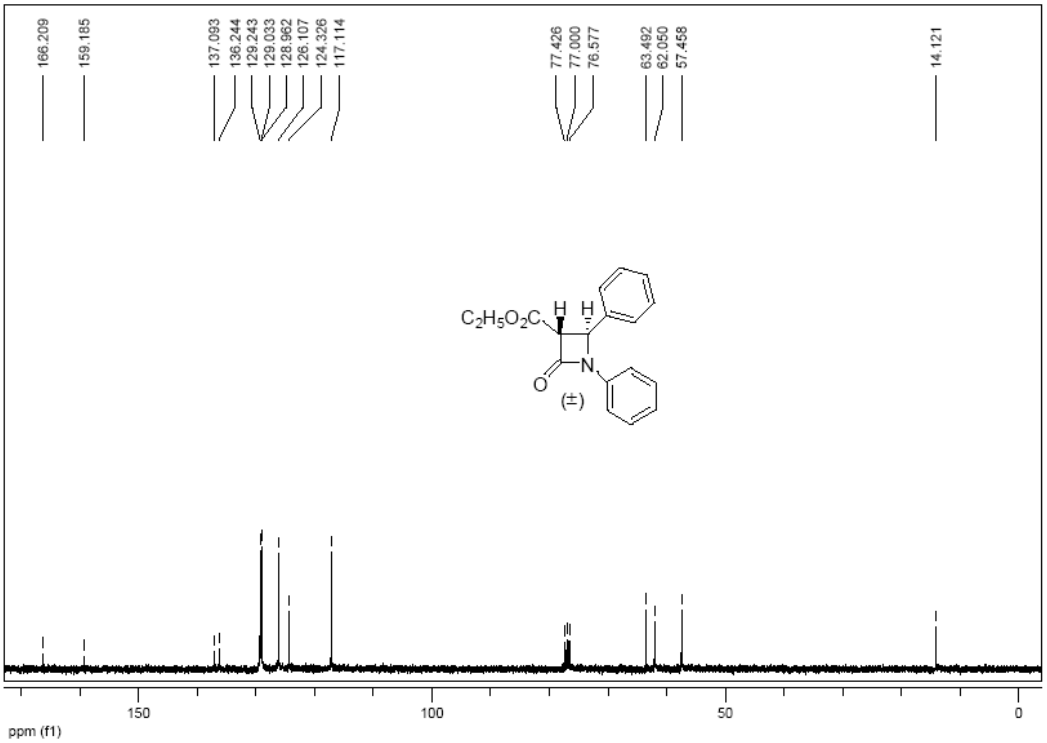
(±)-*trans*-1-Chloro-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one (6h)



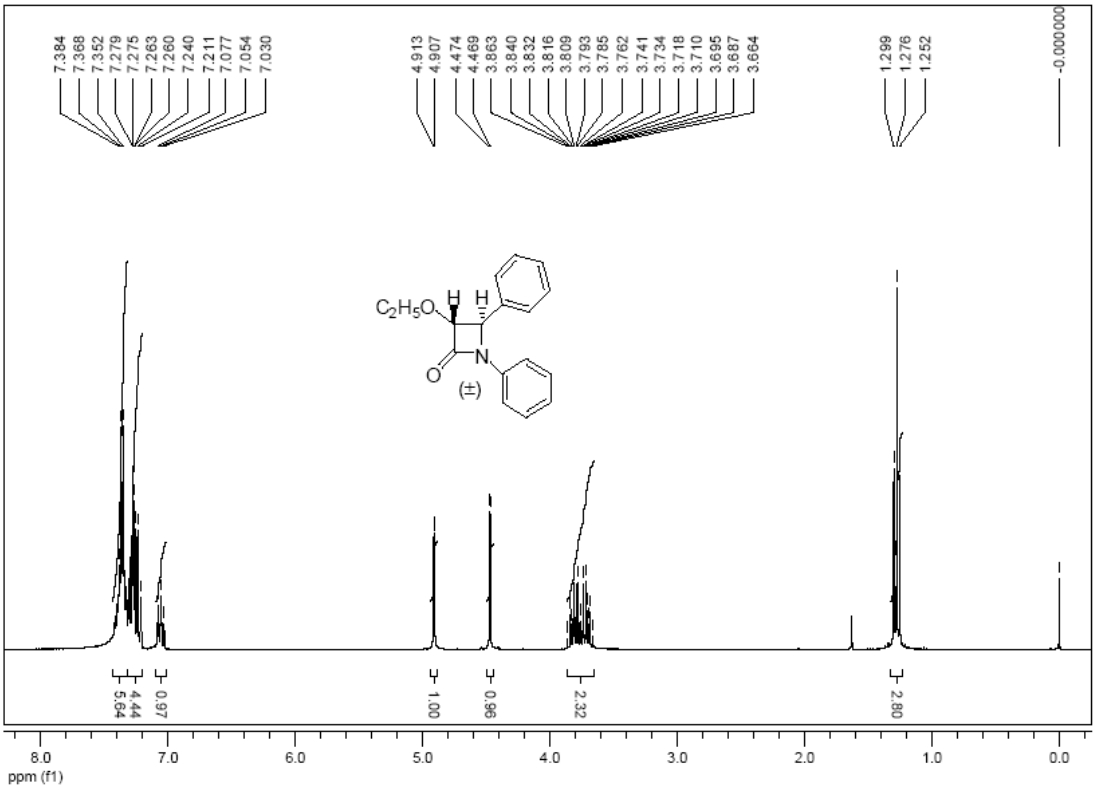


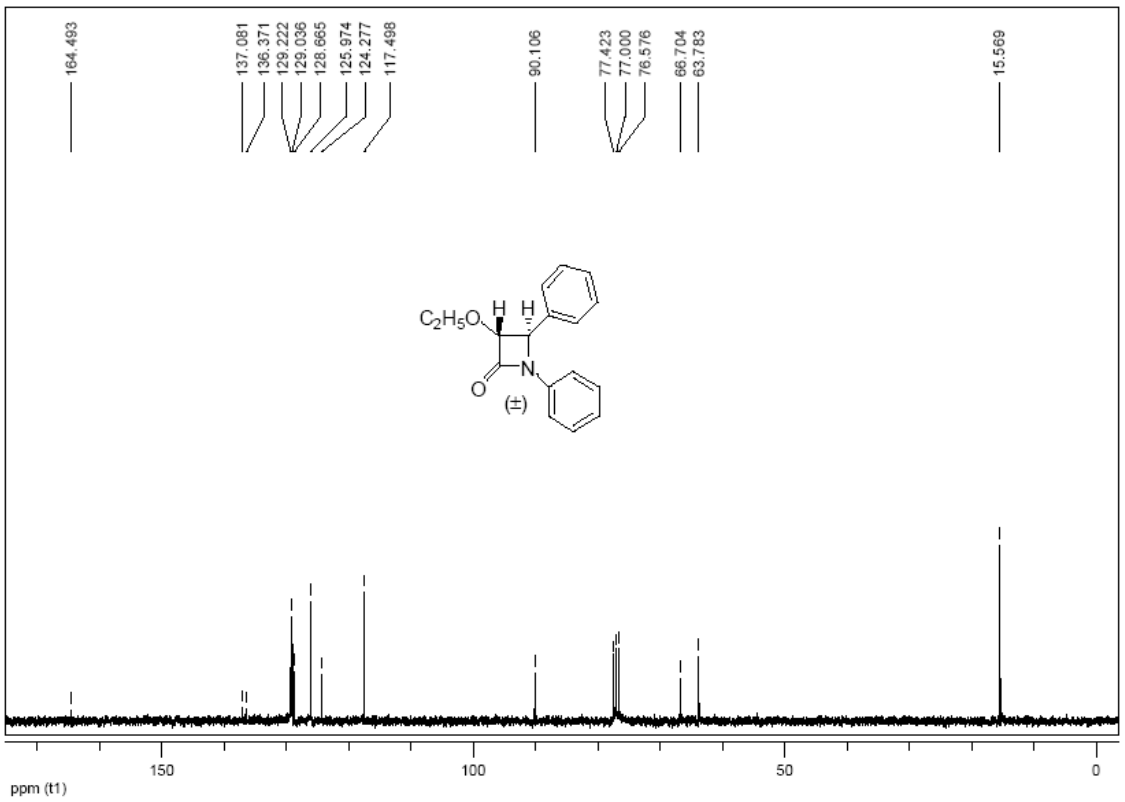
Ethyl (±)-*trans*-1,4-diphenyl-azetidin-2-one-3-carboxylate (11a)



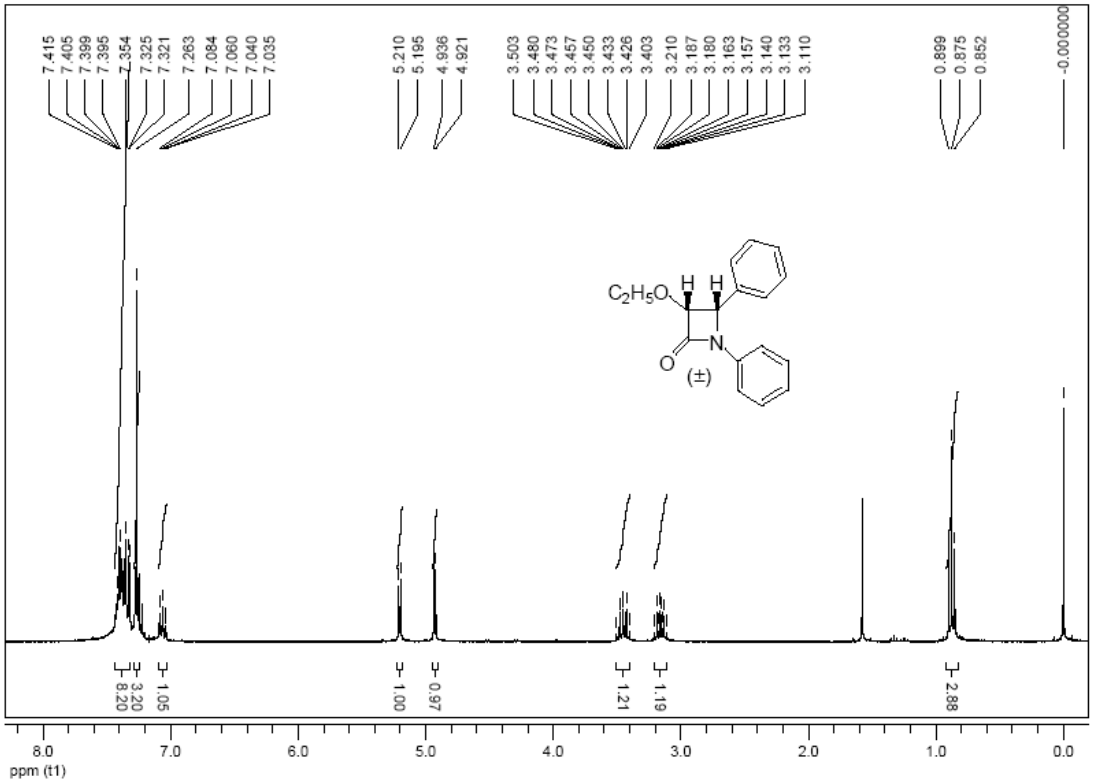


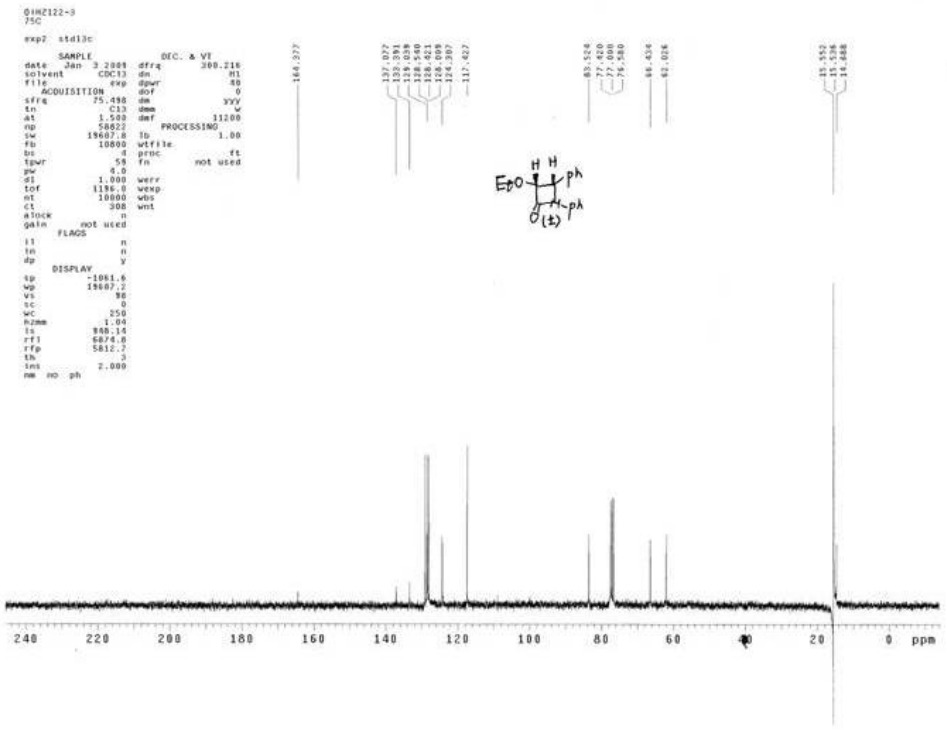
(±)-*trans*-3-Ethoxyl-1,4-diphenyl-2-azetidinone (*trans*-12a)



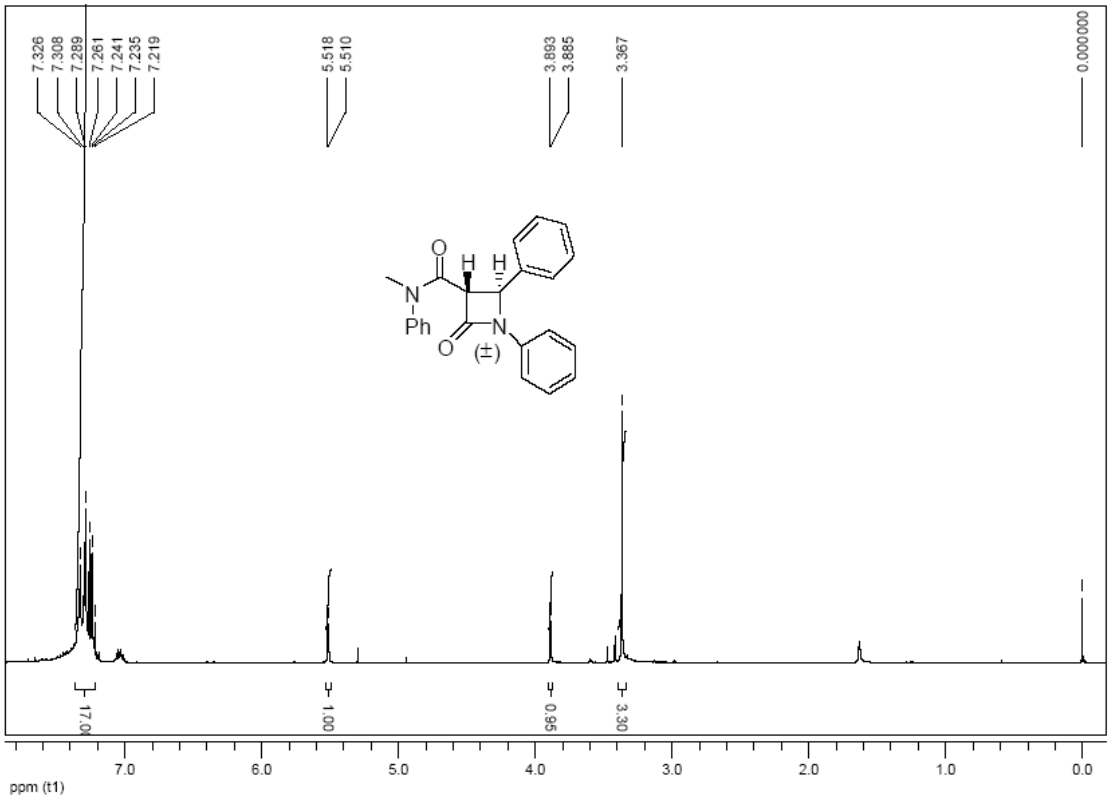


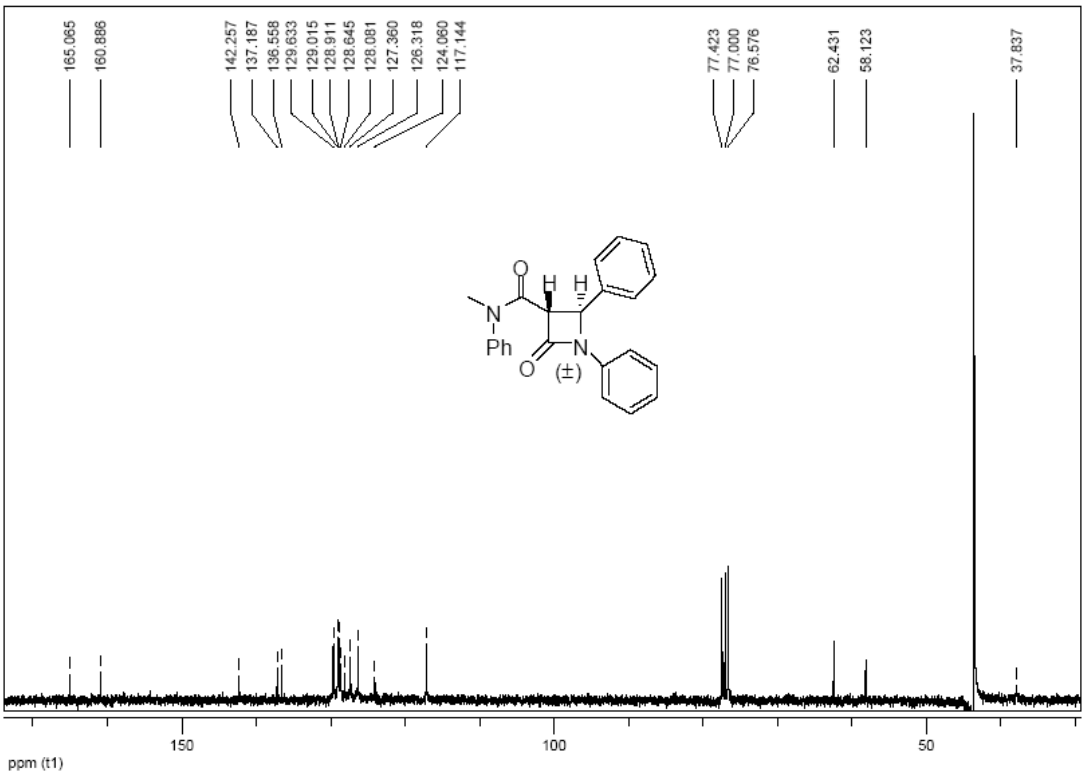
(±)-*cis*-3-Ethoxyl-1,4-diphenyl-2-azetidinone (*cis*-12a)



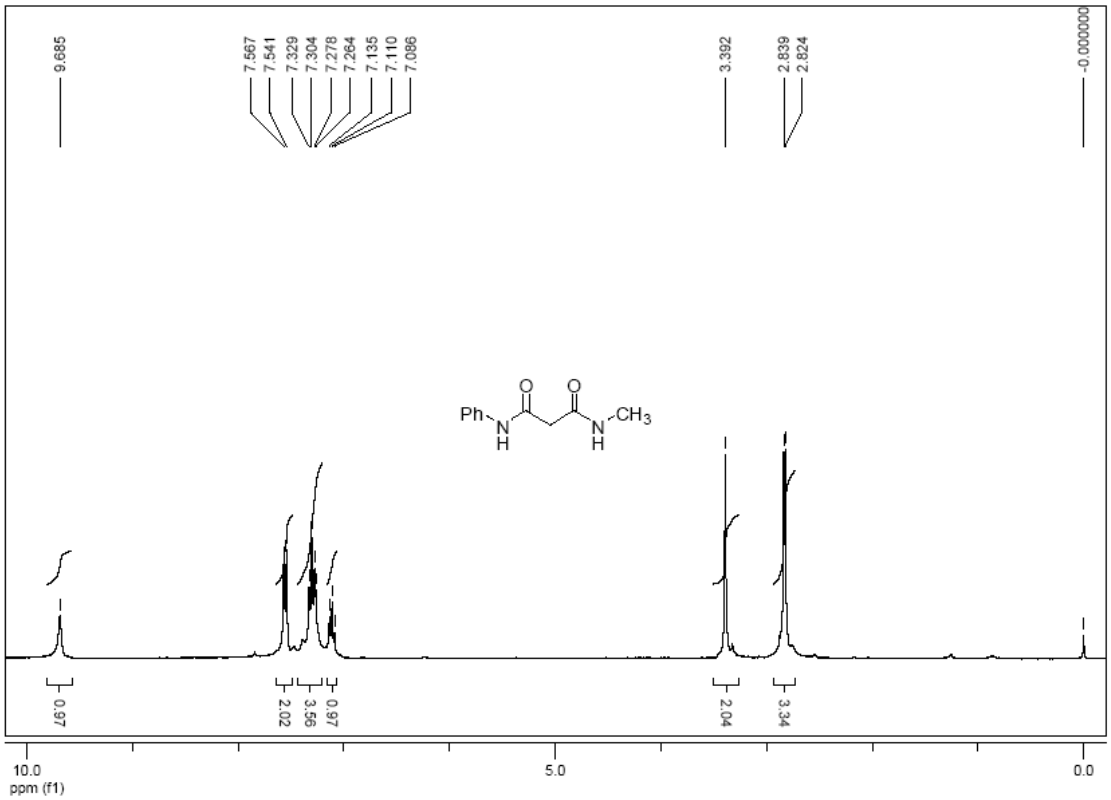


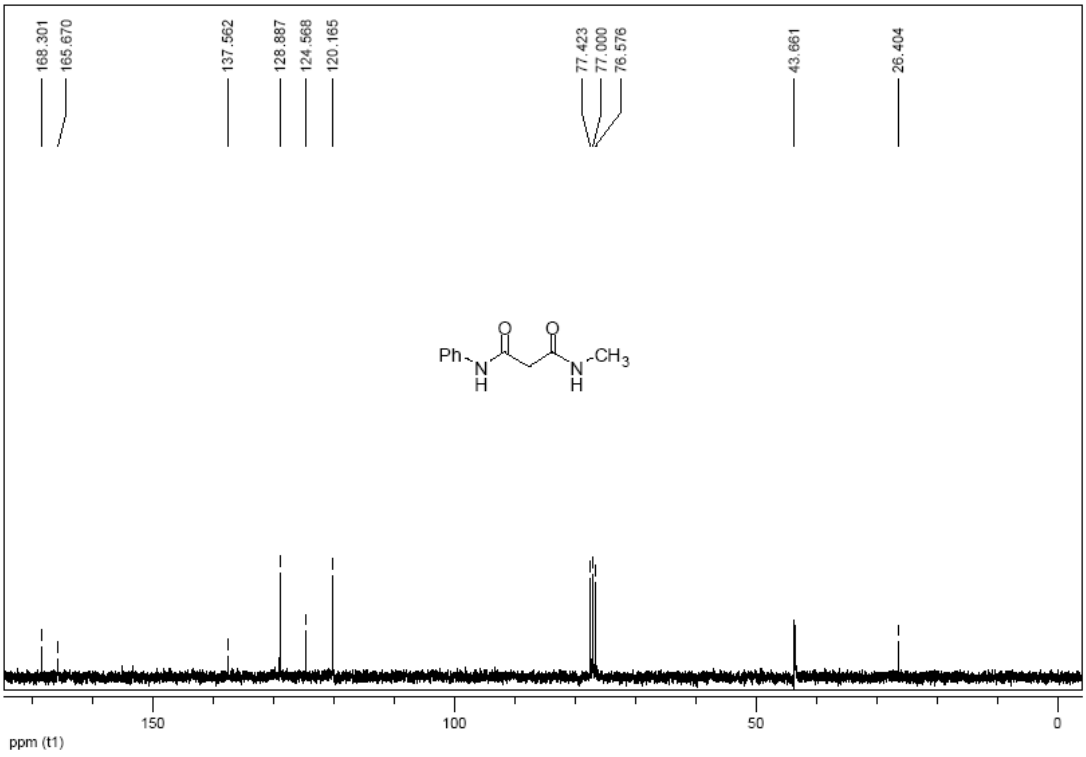
(±)-*trans*-*N*-Methyl-1,4,*N*-triphenyl-azetidin-2-one-3-carboxamide (11b)



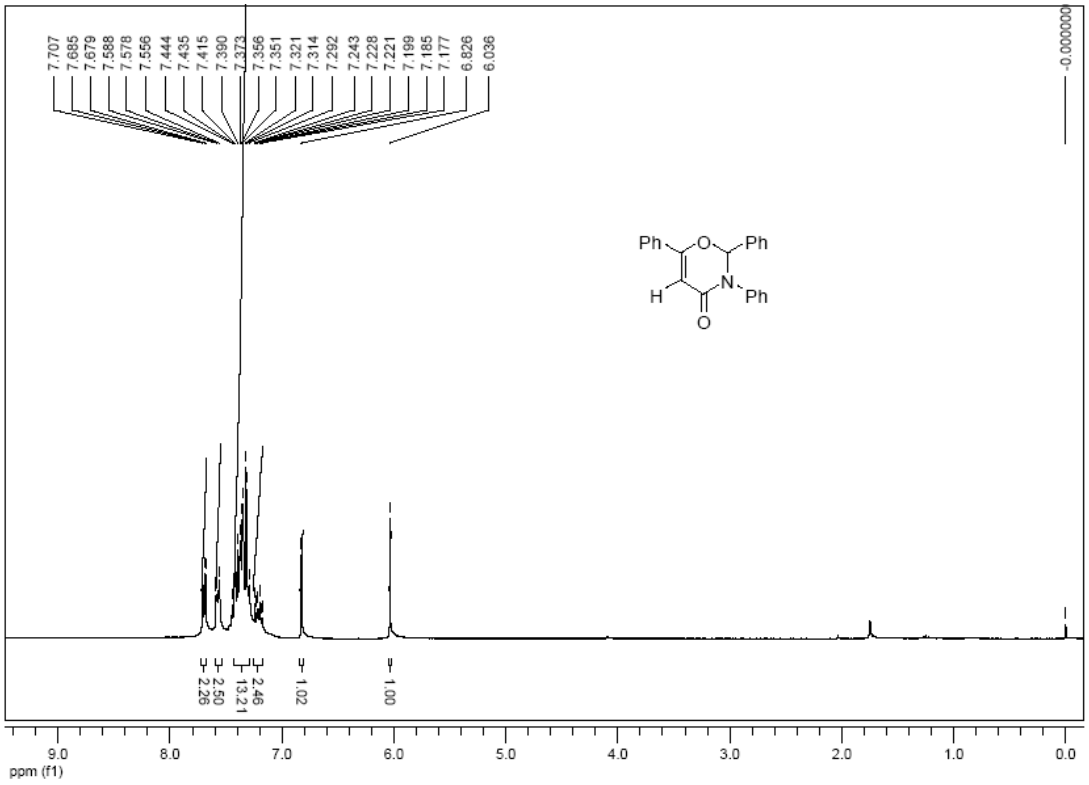


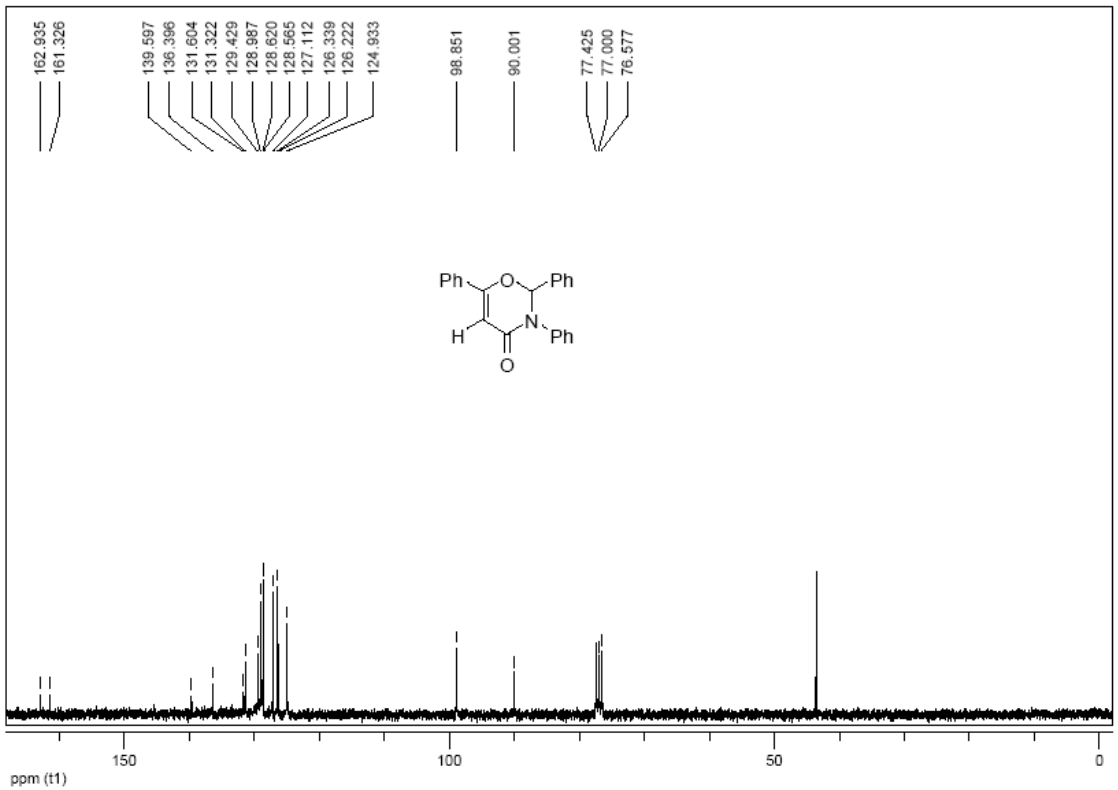
N-Methyl-*N*'-phenylmalonamide



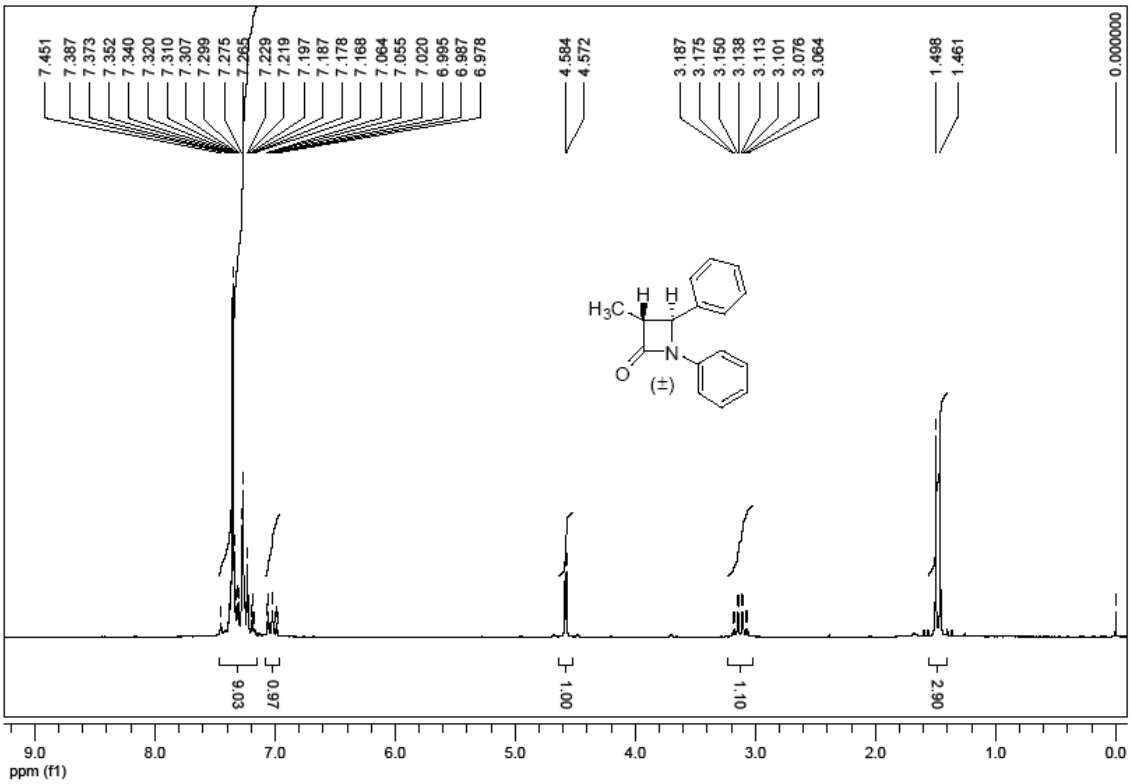


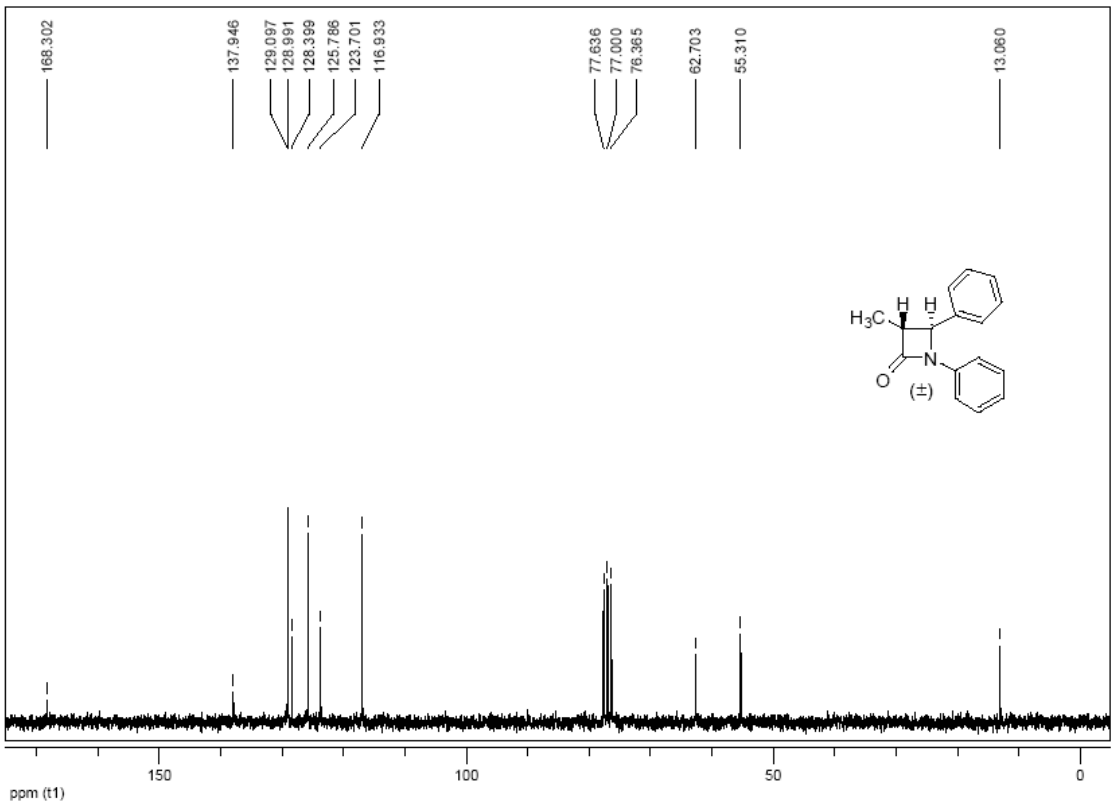
2,3-Dihydro-2,3,6-triphenyl-4*H*-1,3-oxazin-4-one (13d)



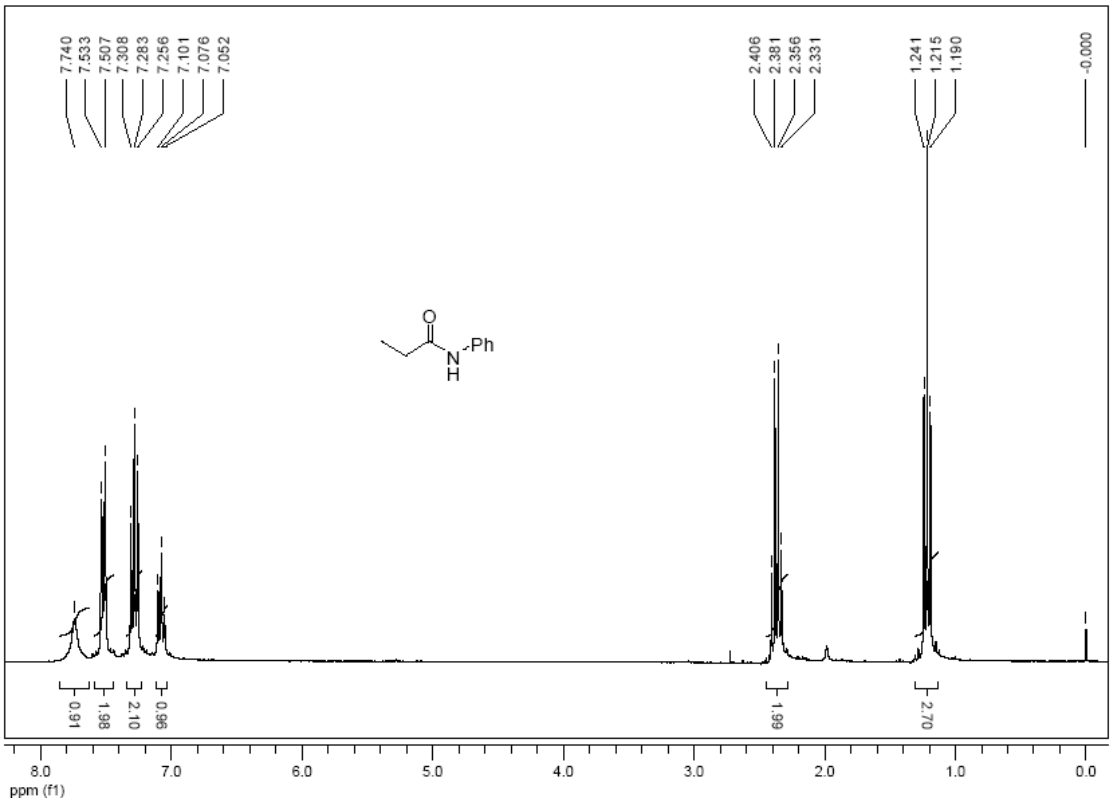


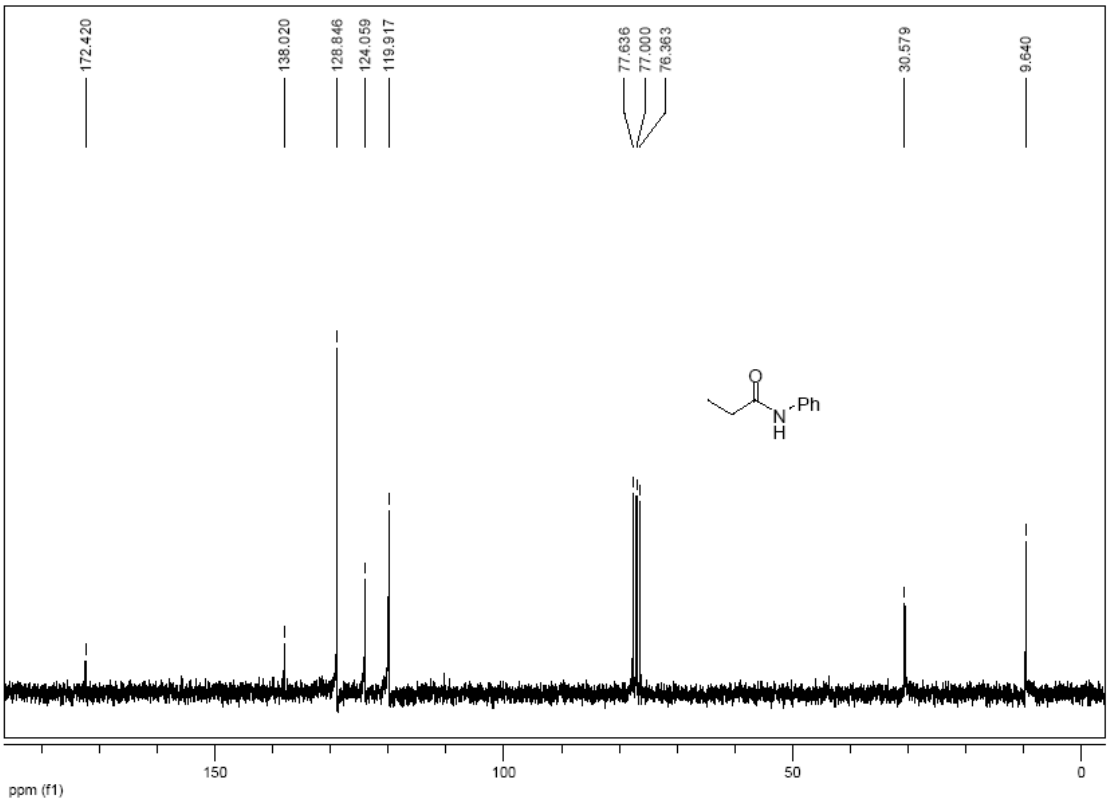
(±)-*trans*-3-Methyl-1,4-diphenyl-2-azetidinone (12e)



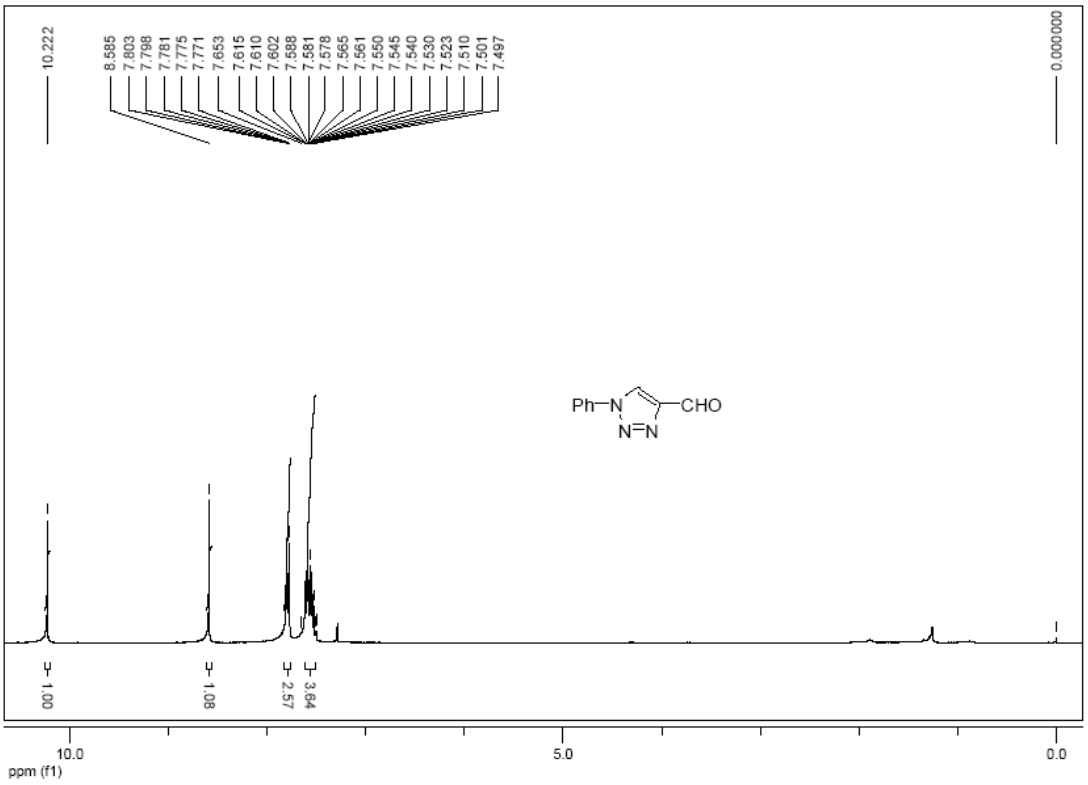


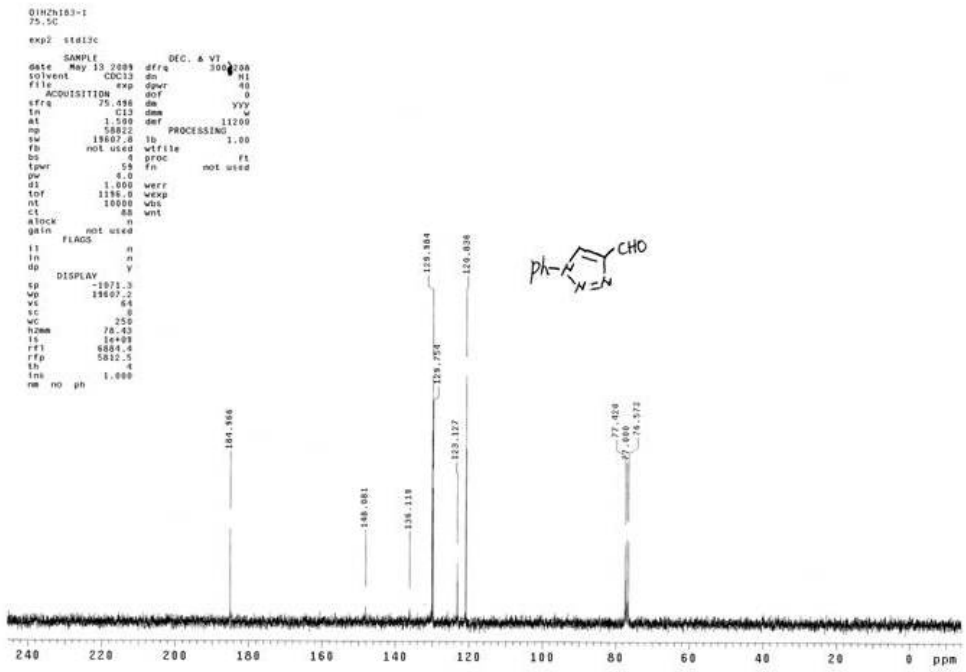
N-Phenylpropanamide



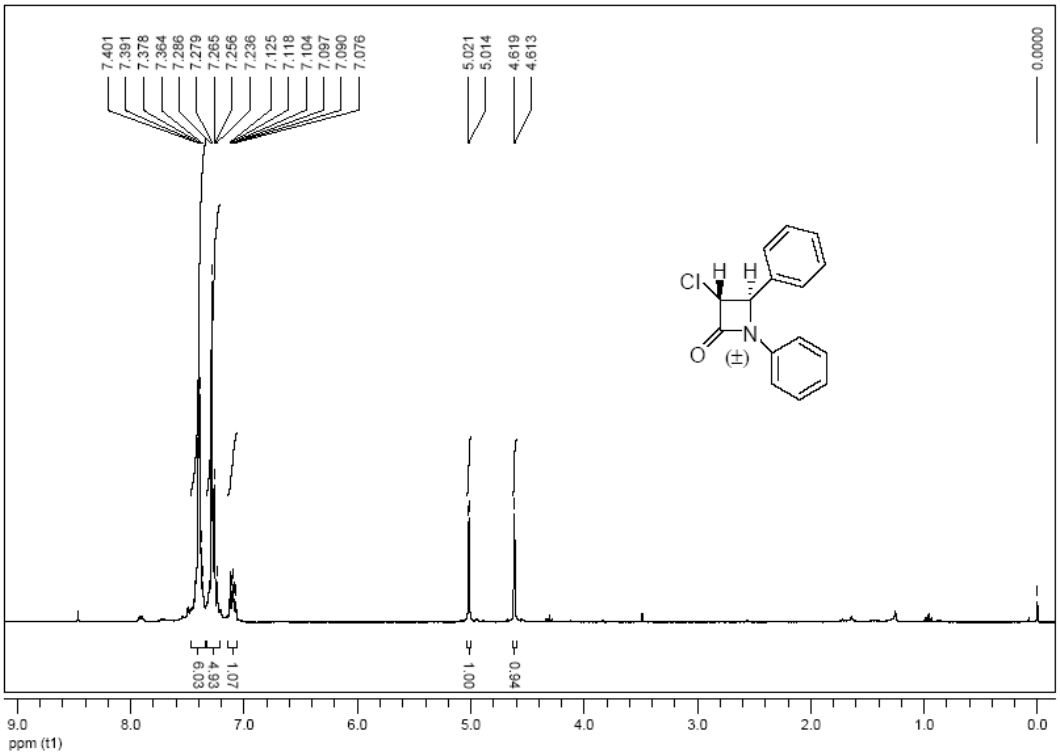


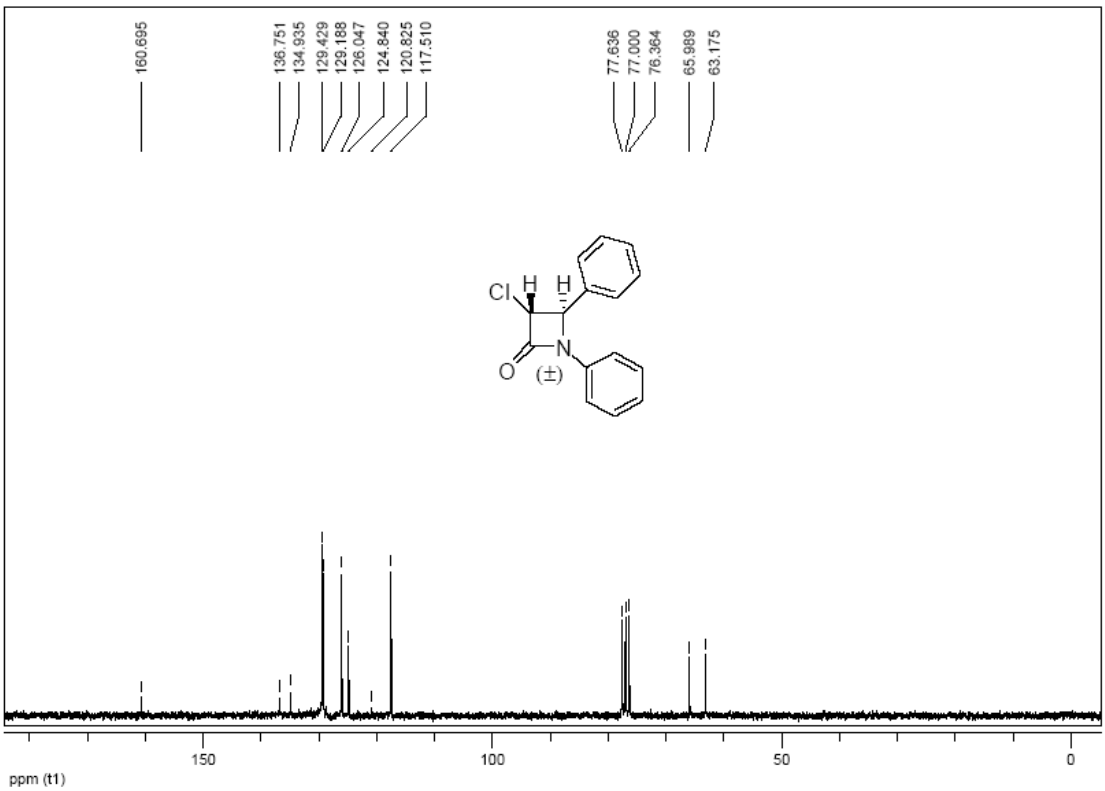
1-Phenyl-1*H*-1,2,3-triazole-4-carboxaldehyde (14)



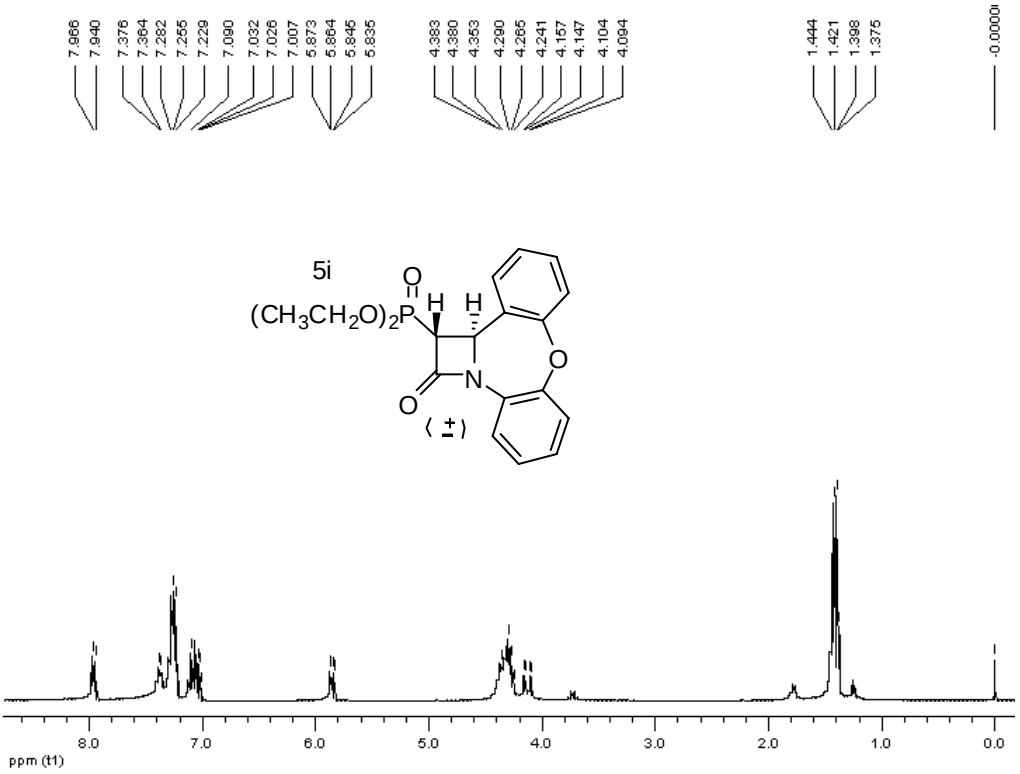


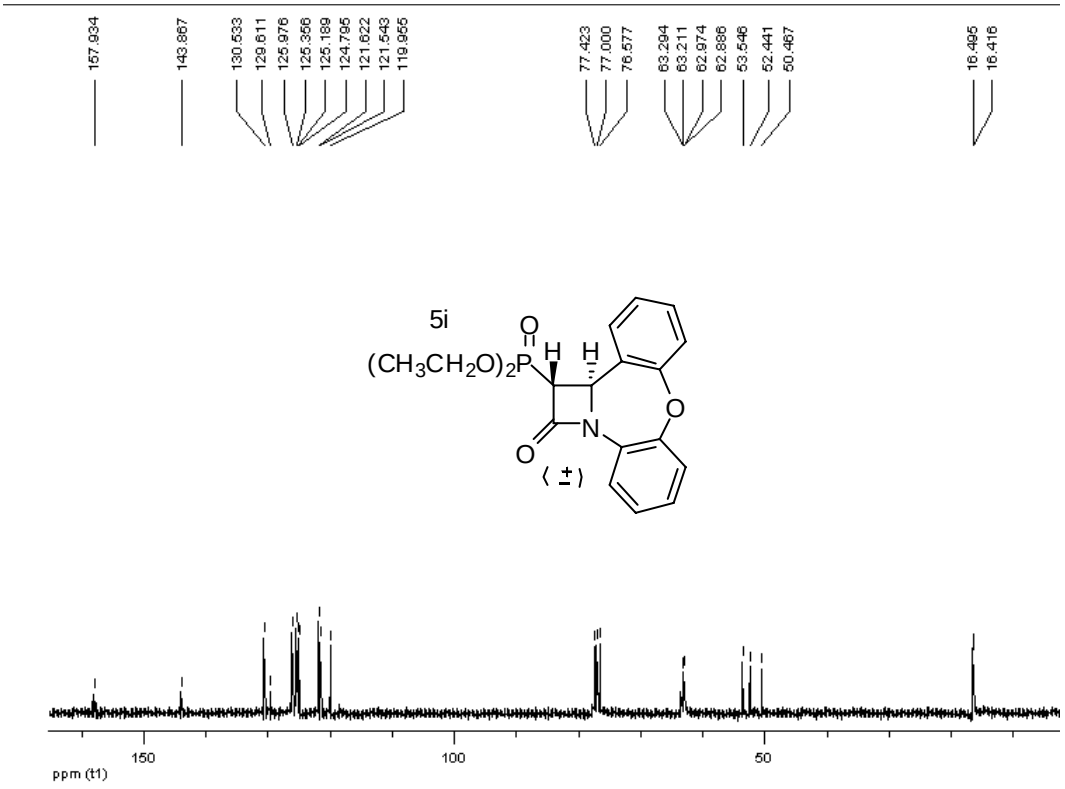
(±)-*trans*-3-Chloro-1,4-diphenyl-2-azetidinone (12h)



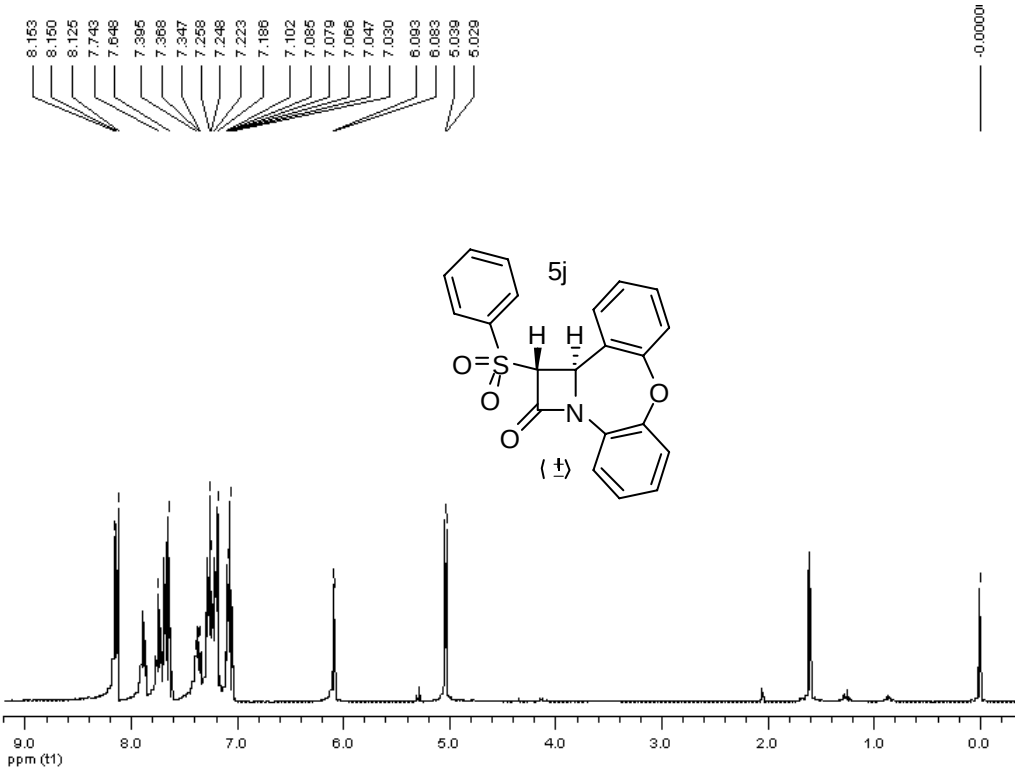


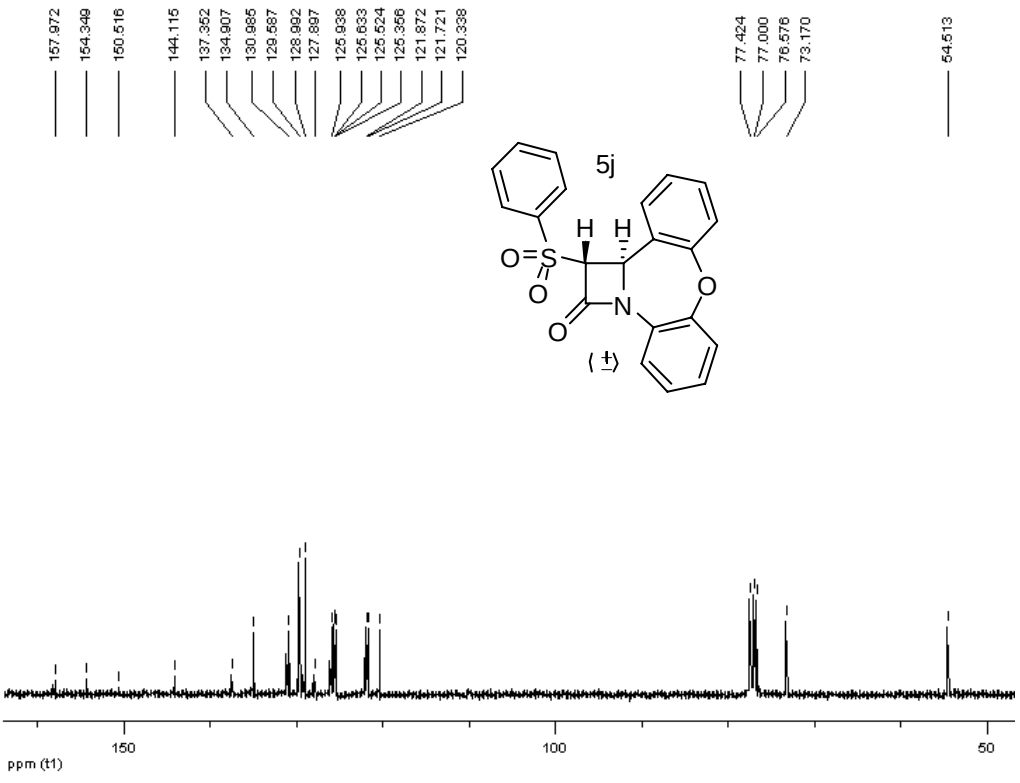
Diethyl (±)-*trans*-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-phosphonate (5i)



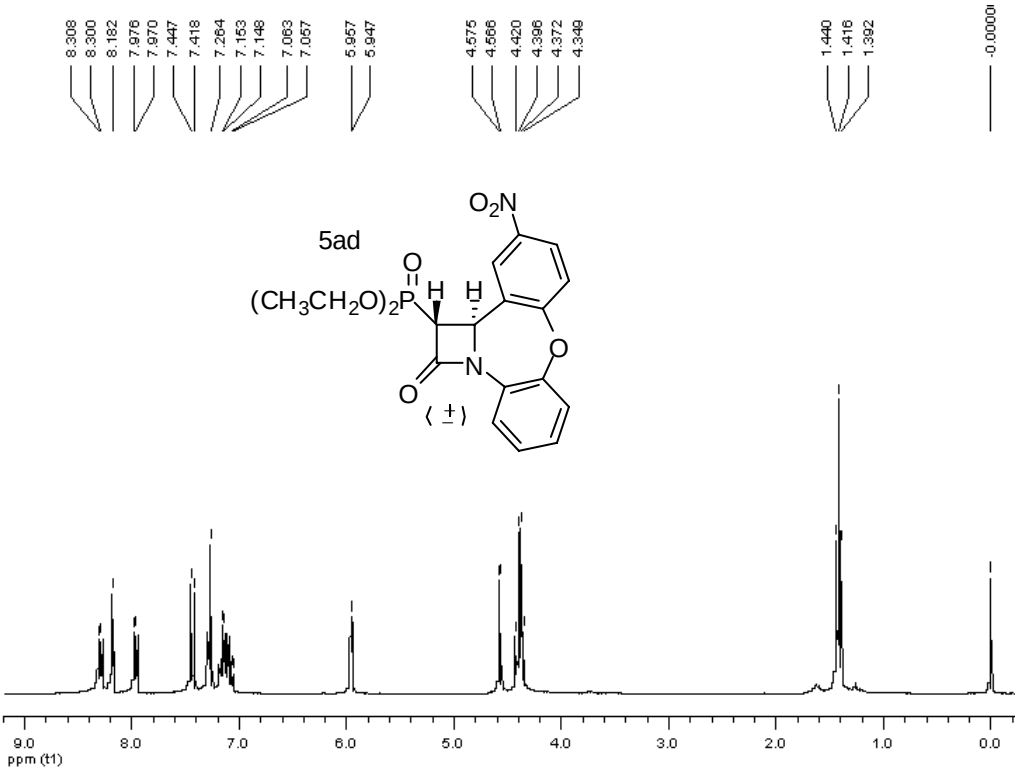


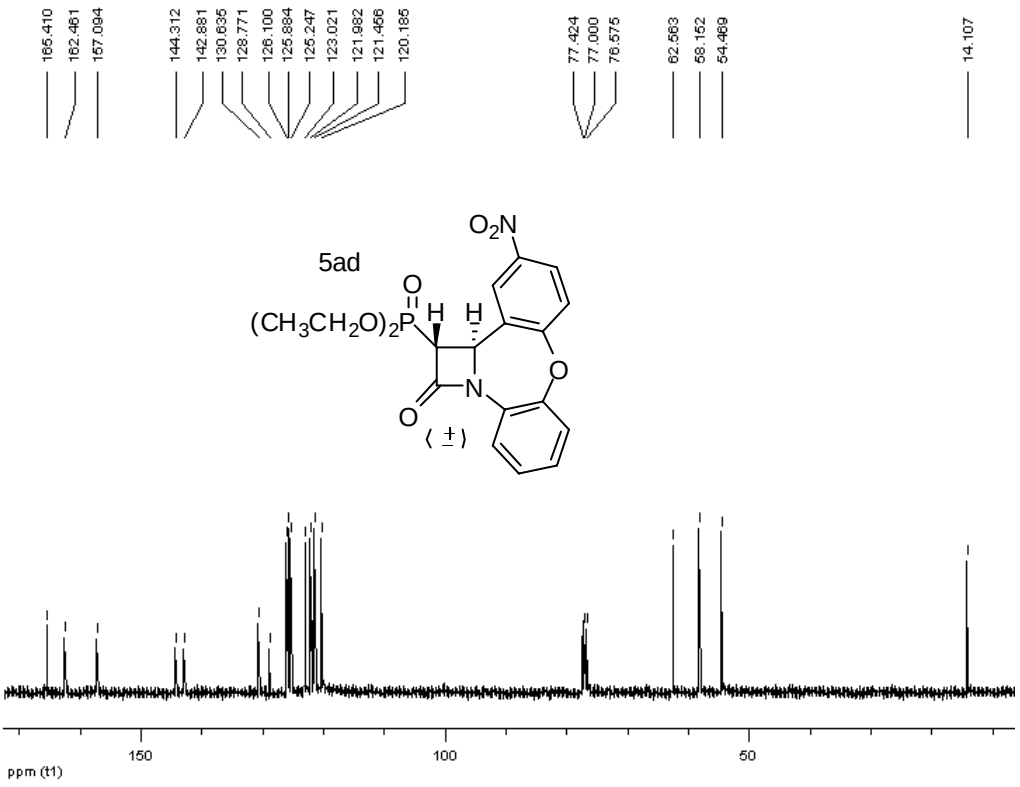
(±)-*trans*-1-Benzenesulfonyl-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one (5j)



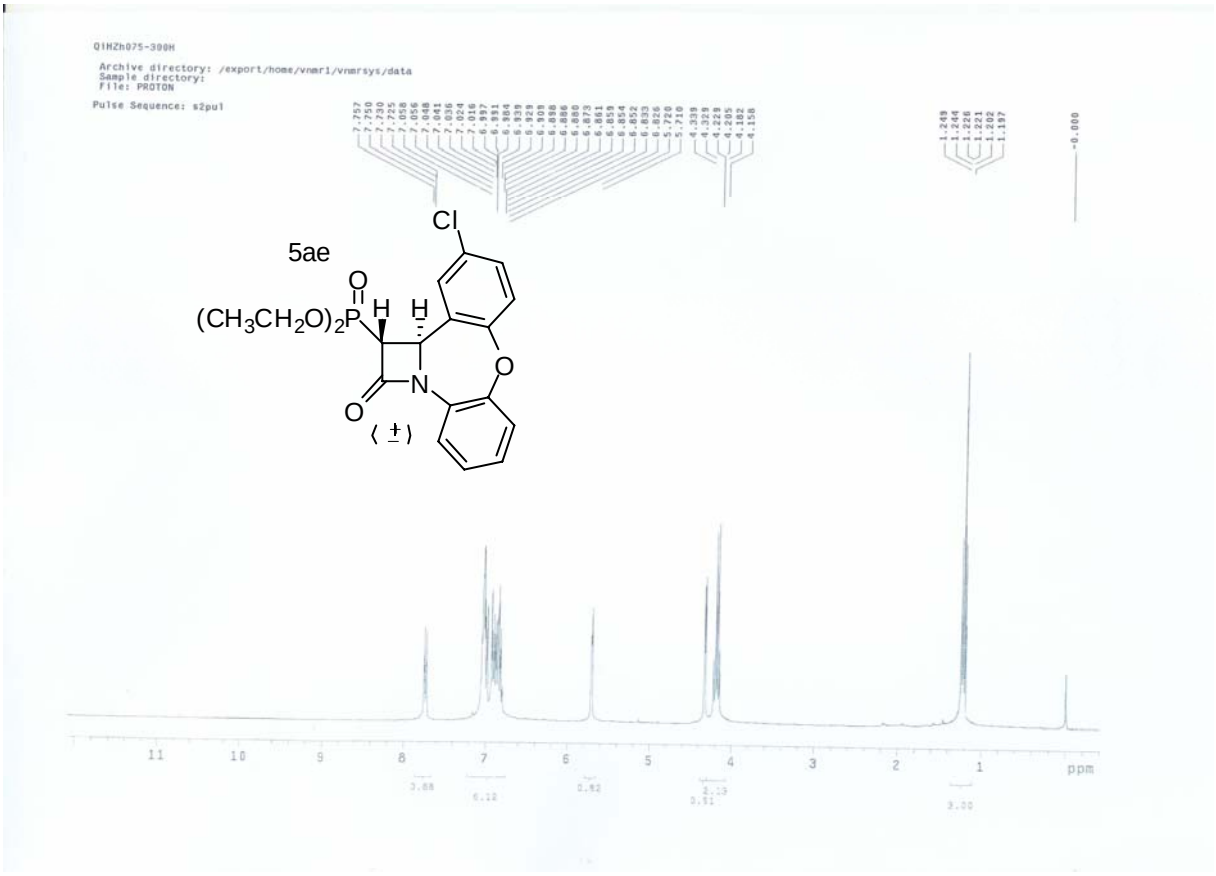


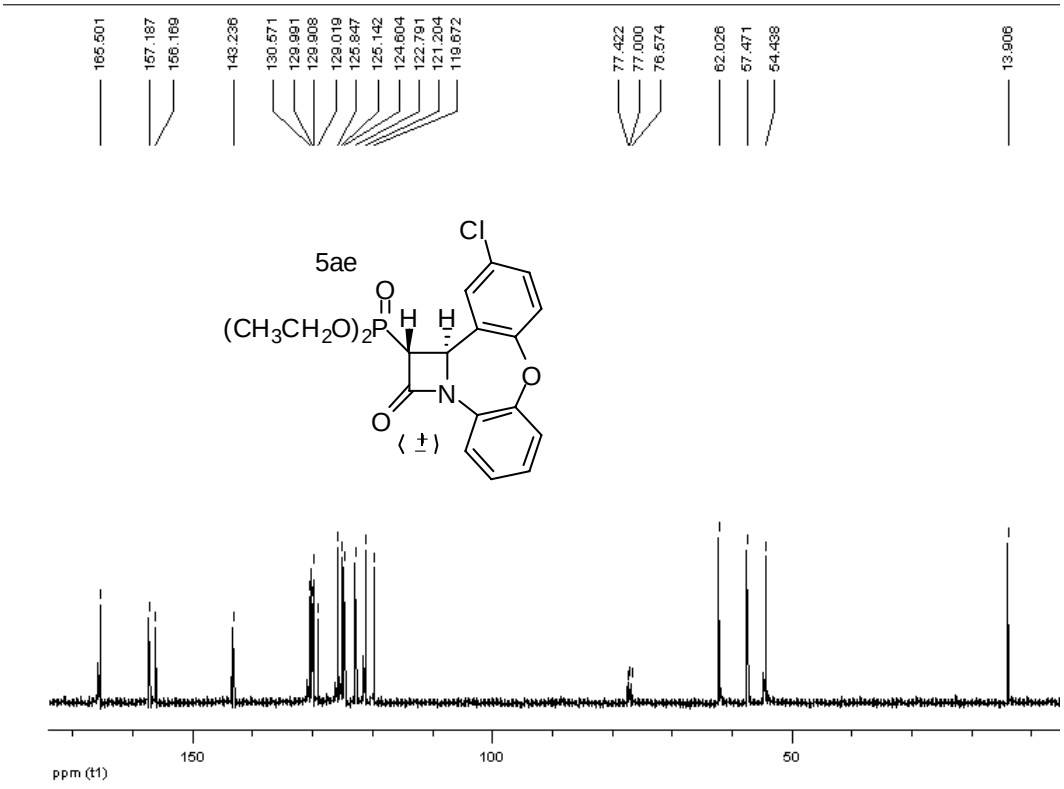
Ethyl (±)-*trans*-1,12b-dihydro-11-nitro-azeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepin-2-one-1-carboxylate (5ad).



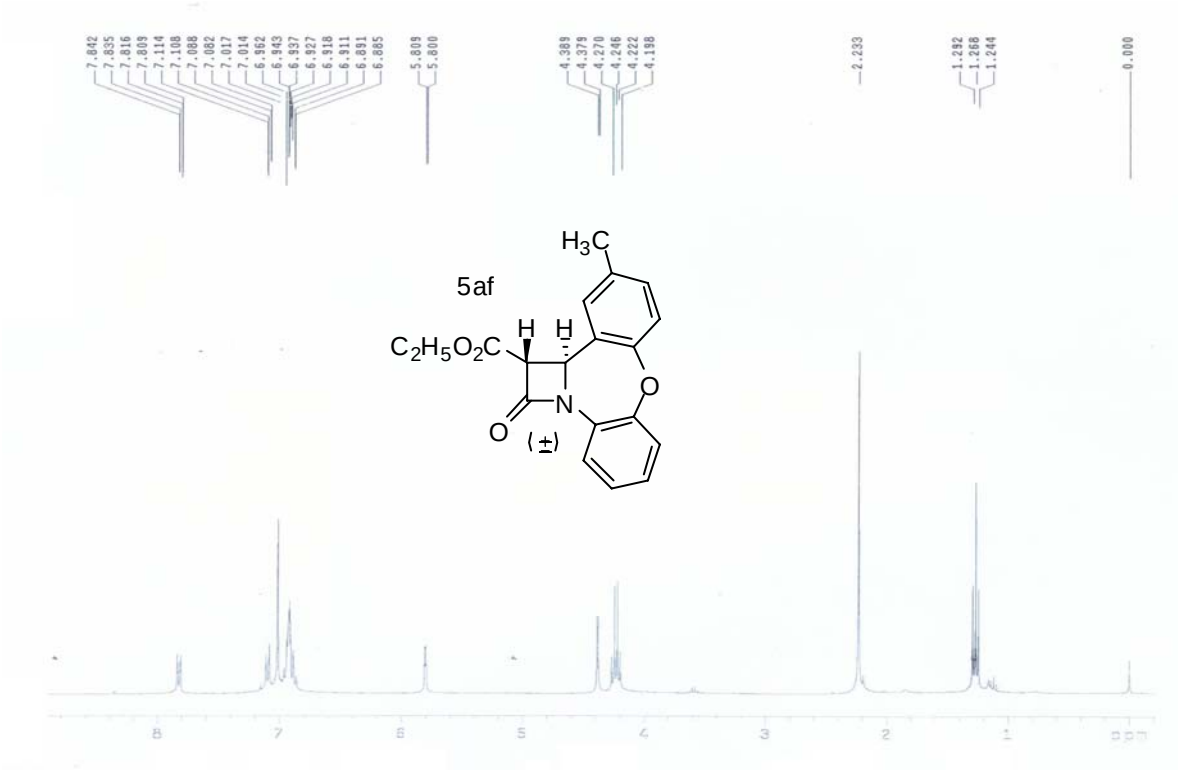


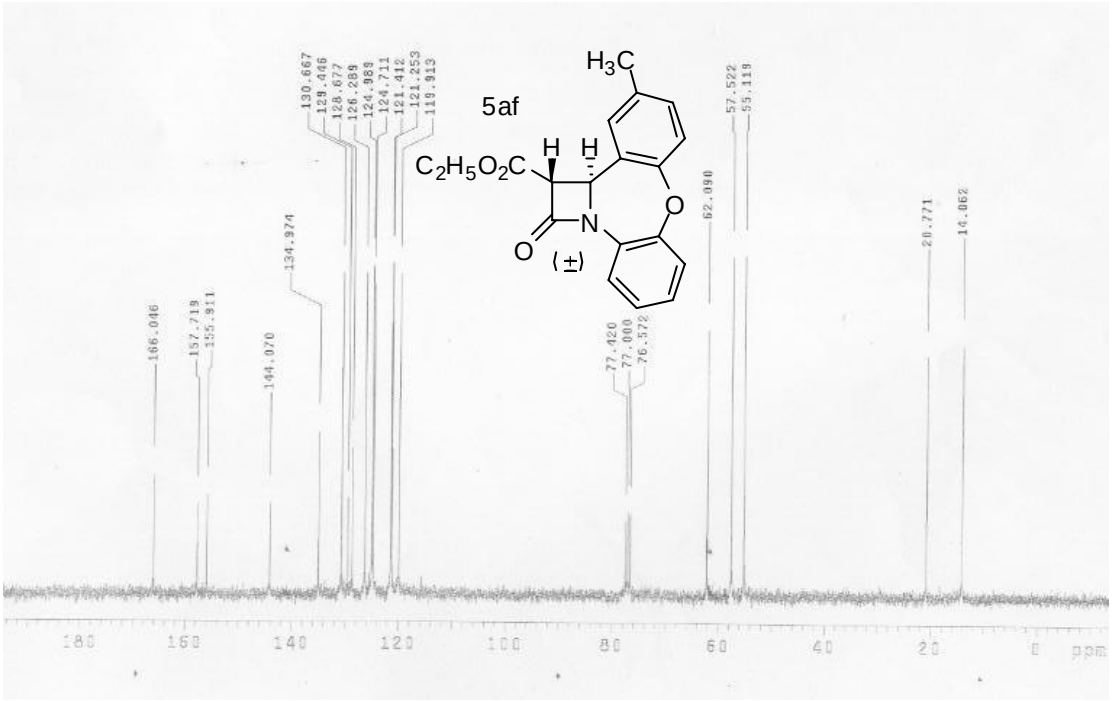
Ethyl (±)-*trans*-11-chloro-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-carboxylate (5ae)



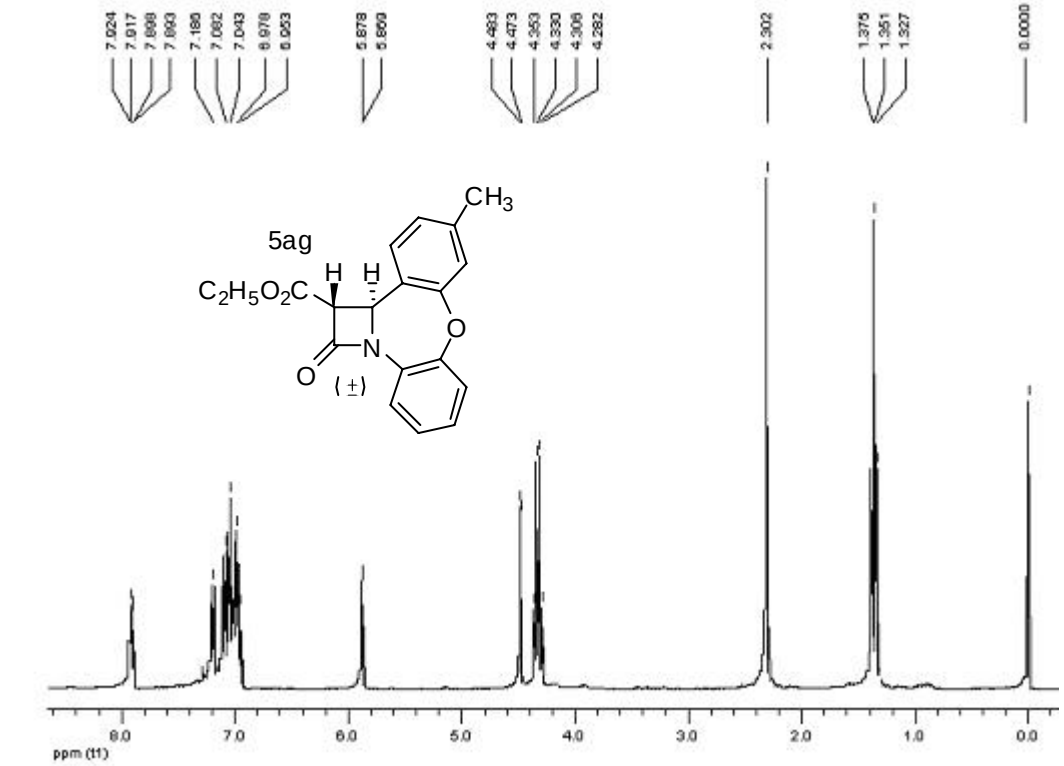


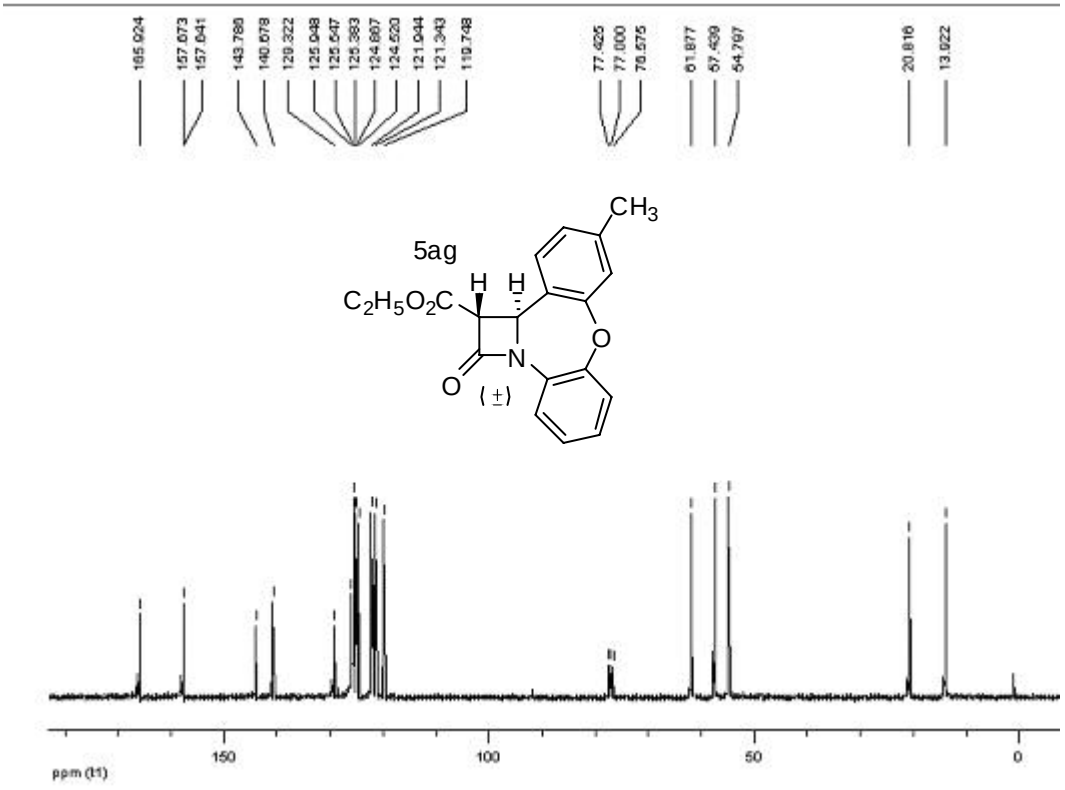
Ethyl (±)-*trans*-11-methyl-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepin-2-one-1-carboxylate (5af)



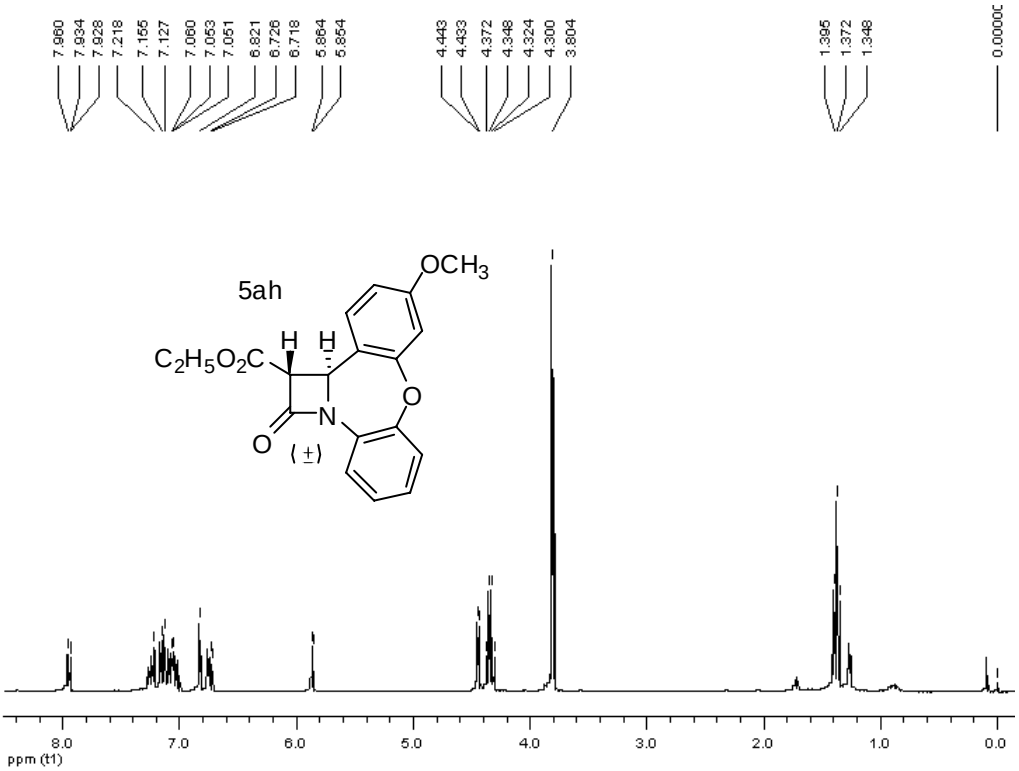


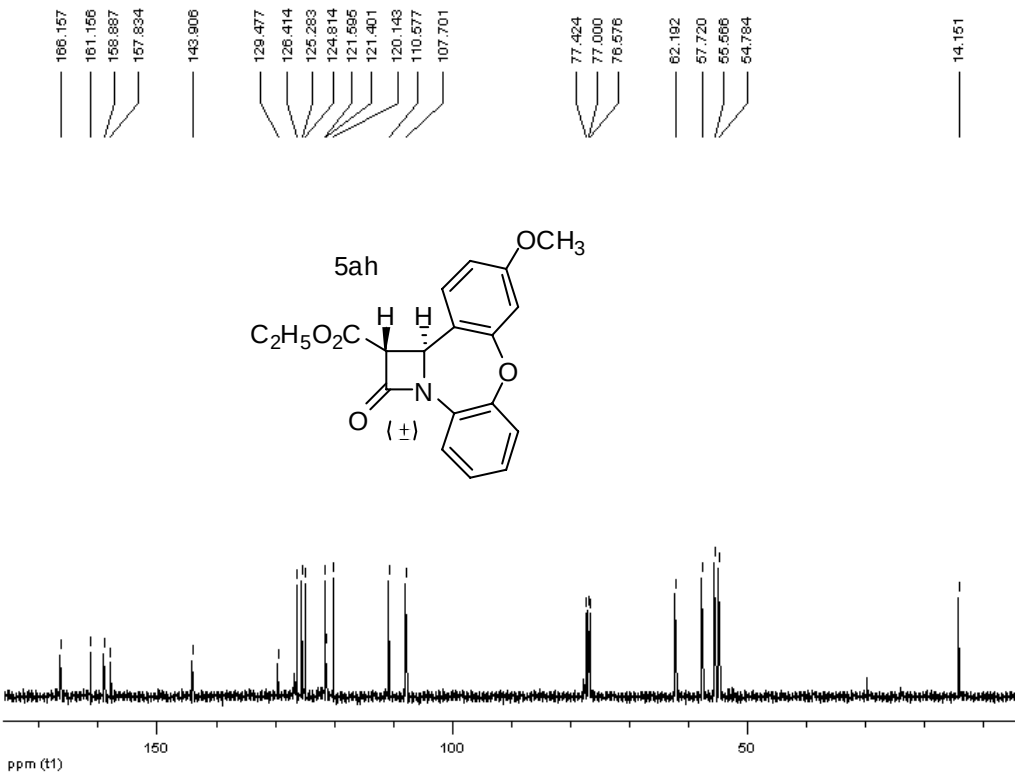
Ethyl (±)-*trans*-10-methyl-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepin-2-one-1-carboxylate (5ag)



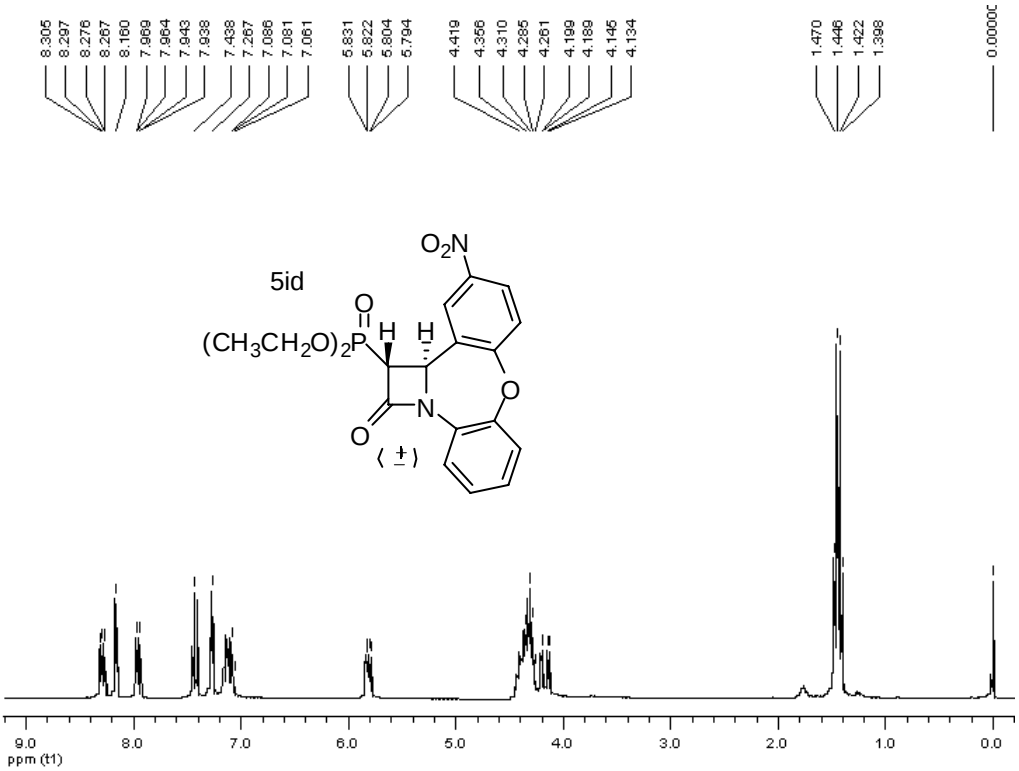


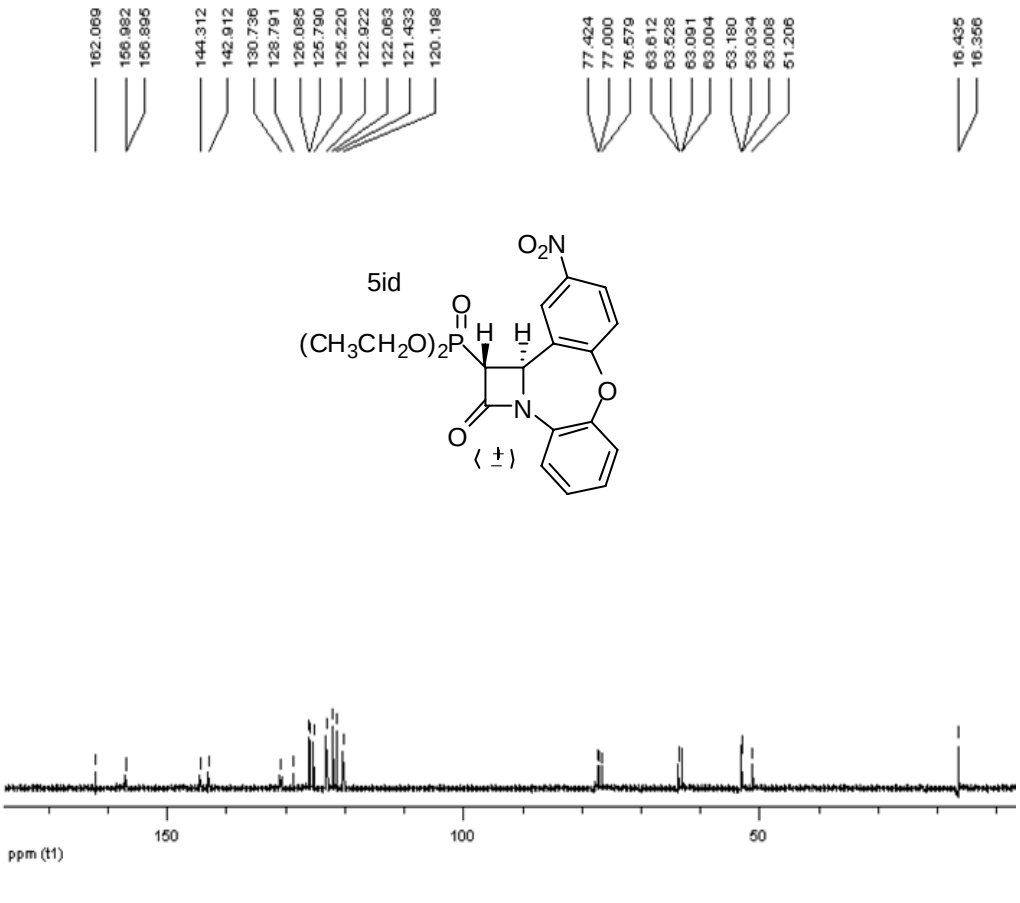
Ethyl (±)-*trans*-11-methoxy-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-carboxylate (5ah)



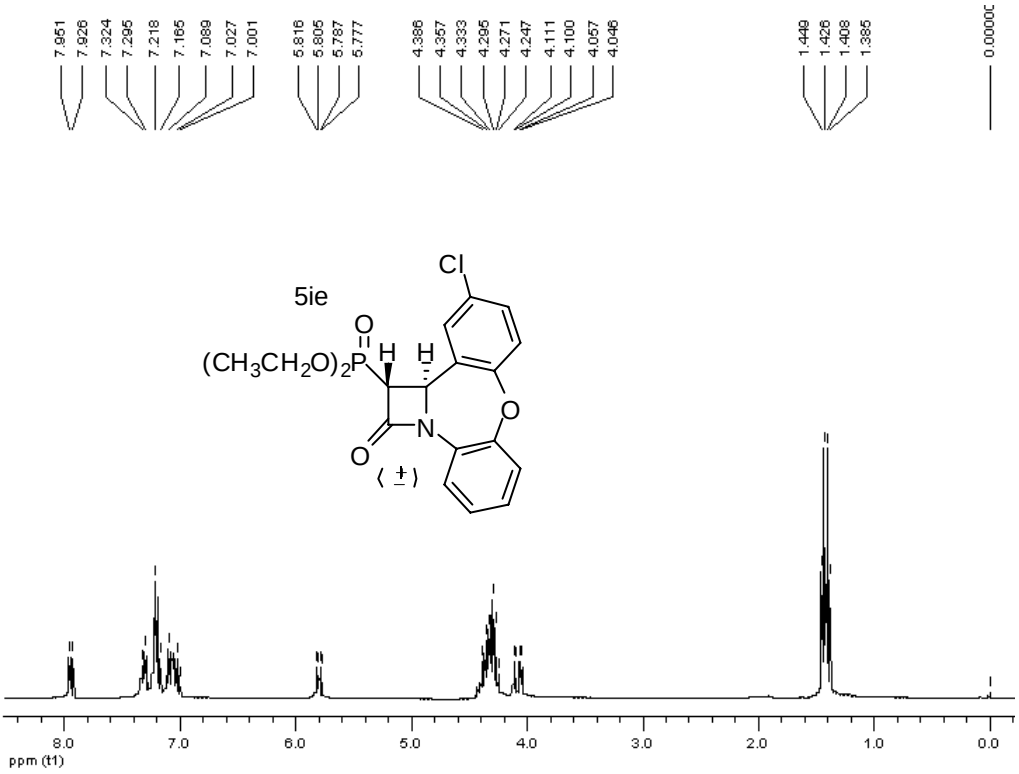


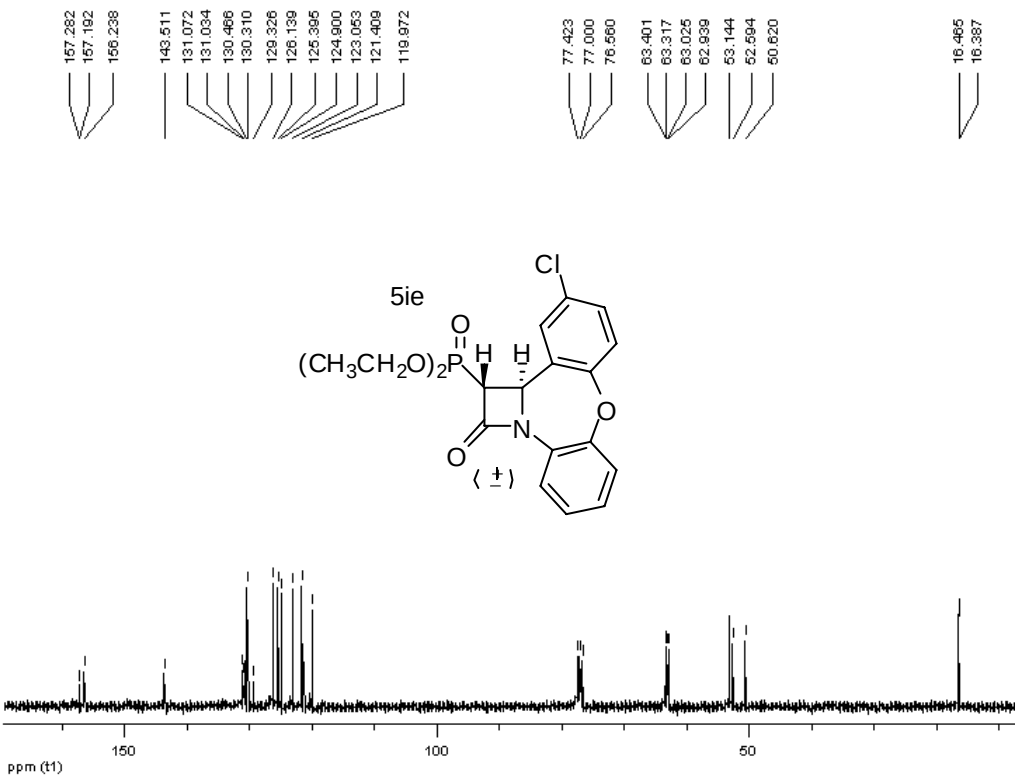
Diethyl (±)-*trans*-1,12b-dihydro-11-nitro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-phosphonate (5id)



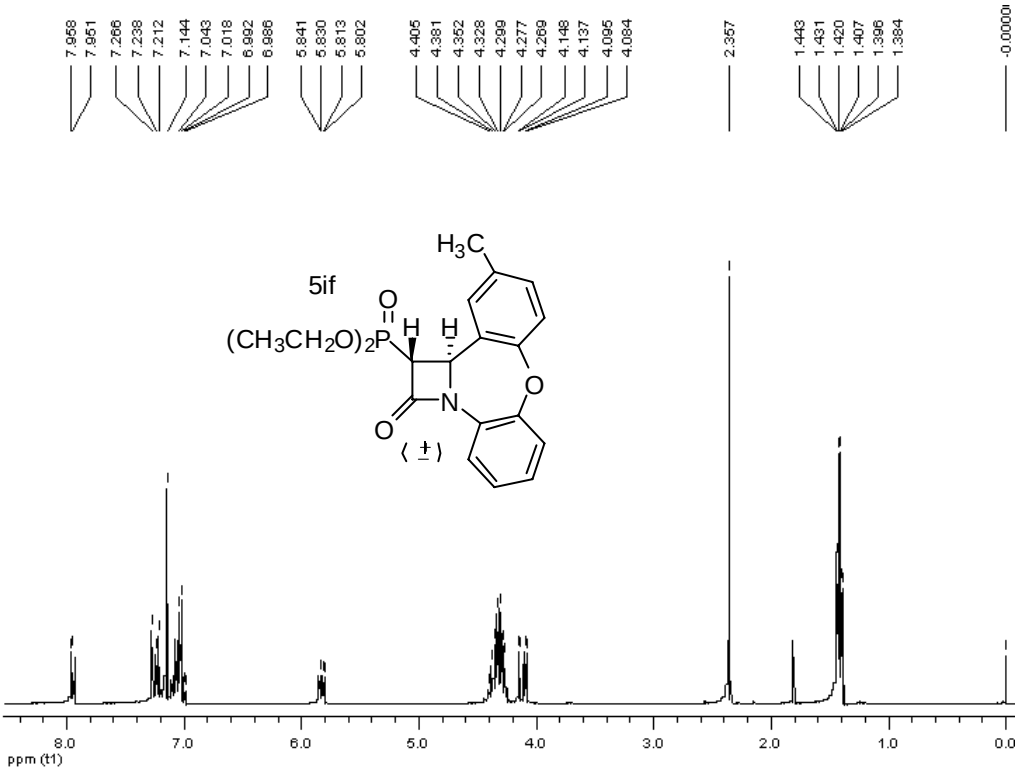


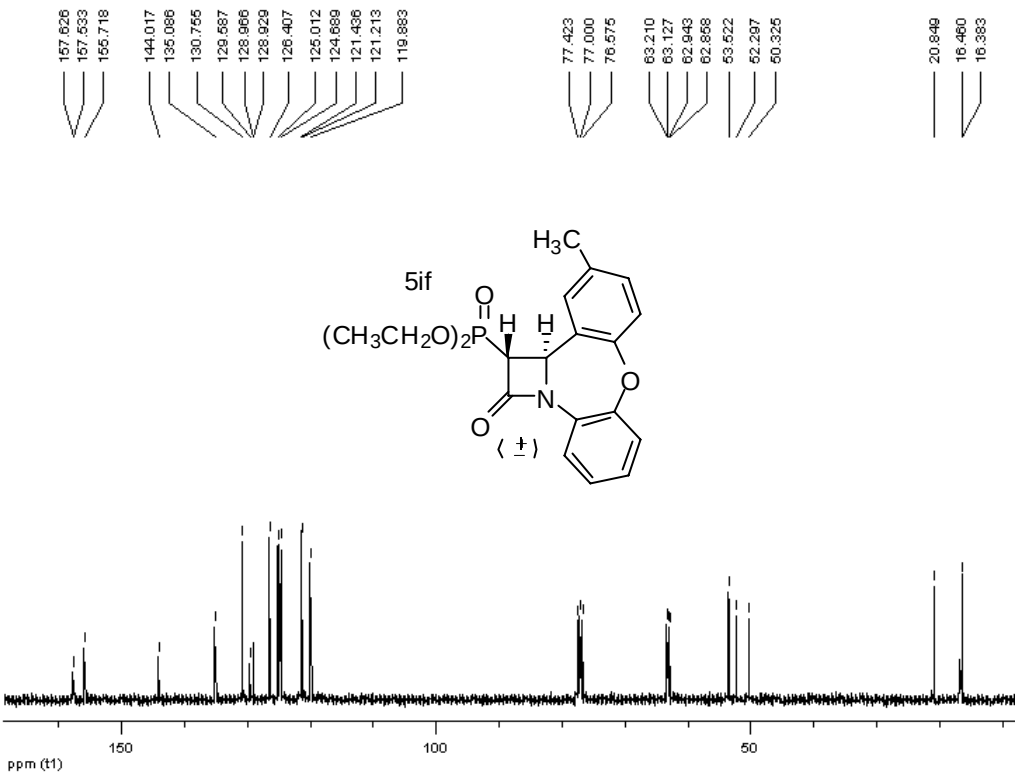
Diethyl (±)-*trans*-11-chloro-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-phosphonate (5ie)



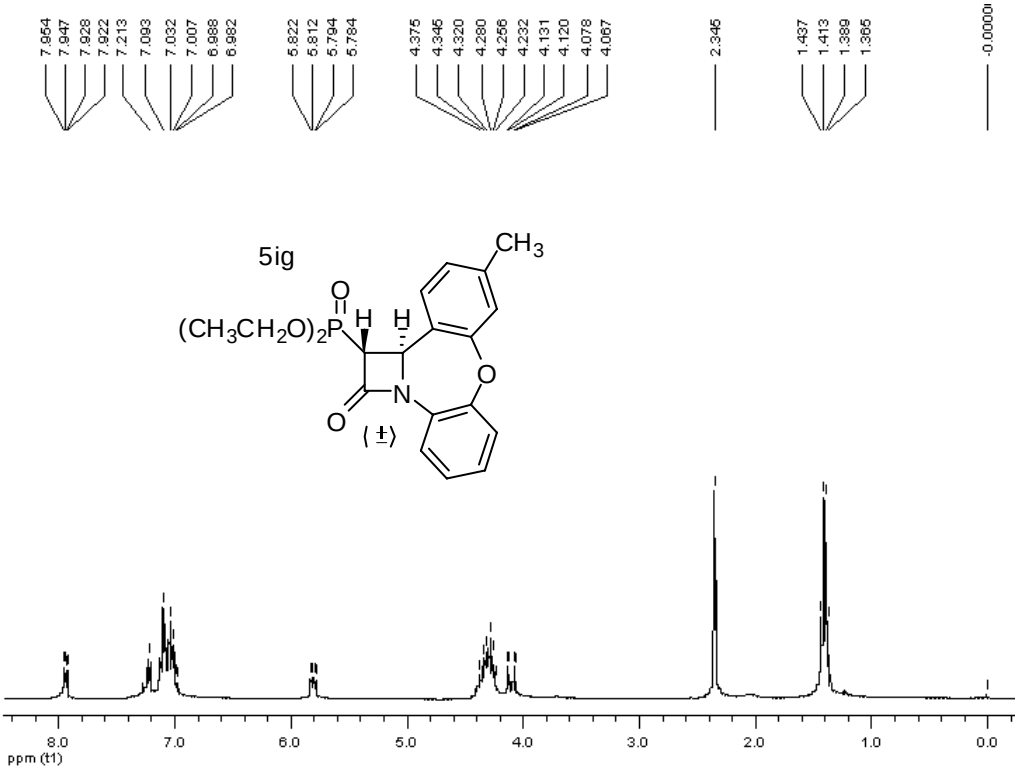


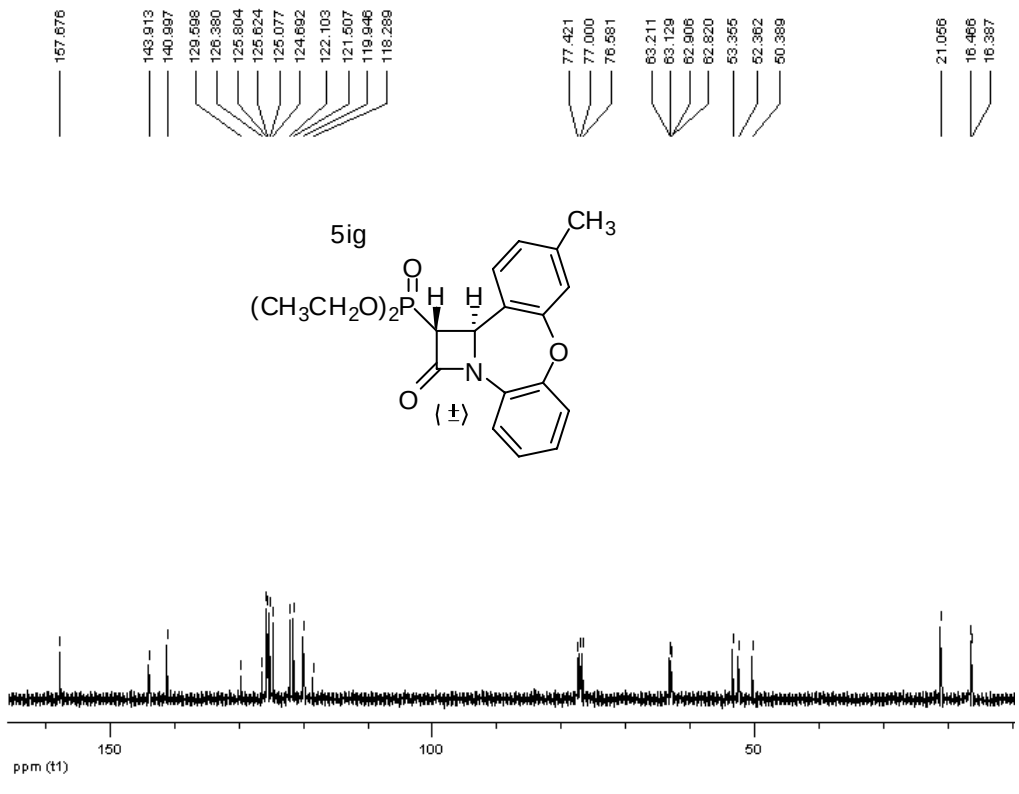
Diethyl (±)-*trans*-11-methyl-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-phosphonate (5if)



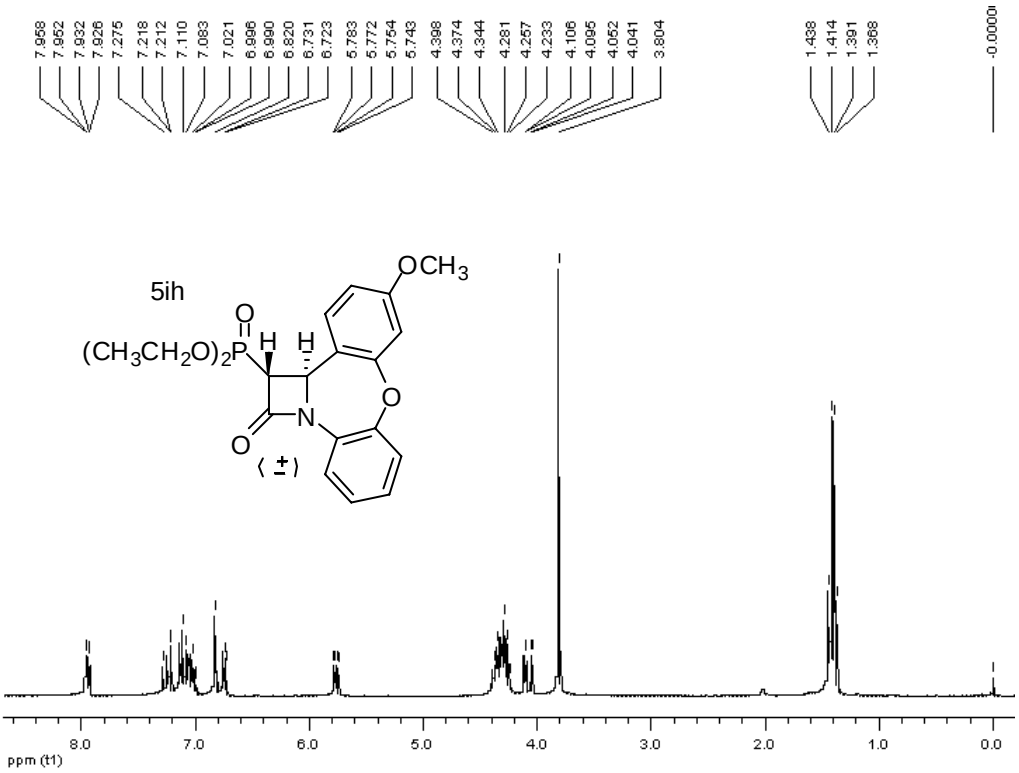


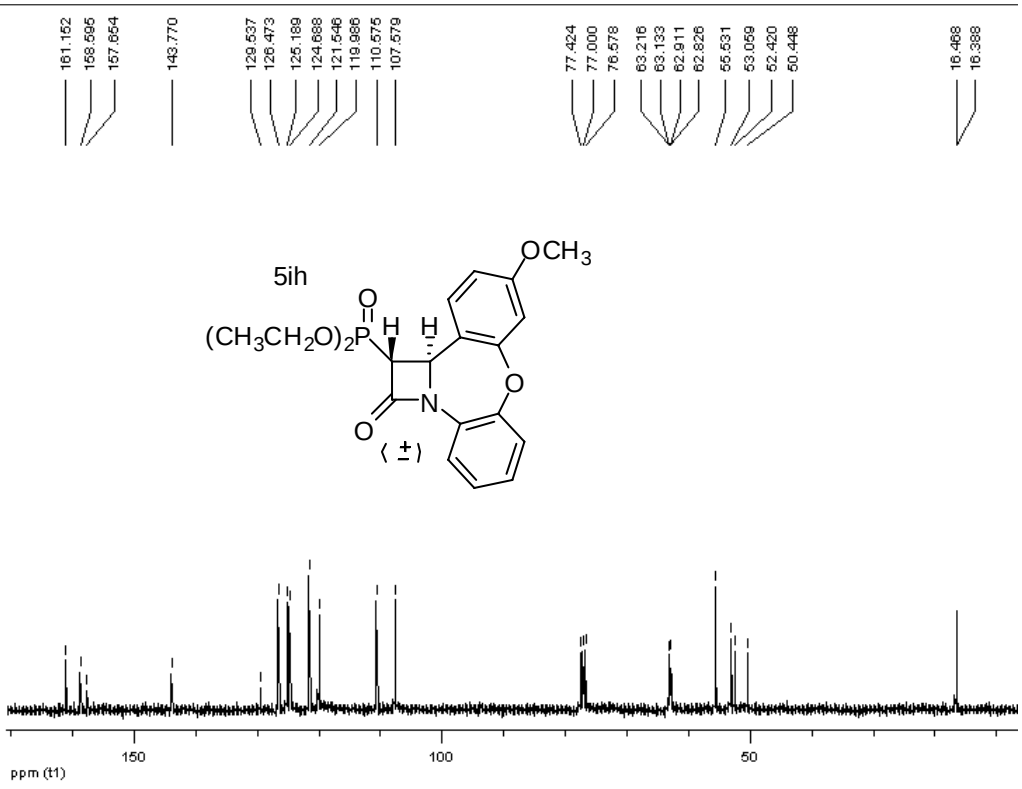
Diethyl (±)-*trans*-10-methyl-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b,f*][1,4]oxazepin-2-one-1-phosphonate (5ig)



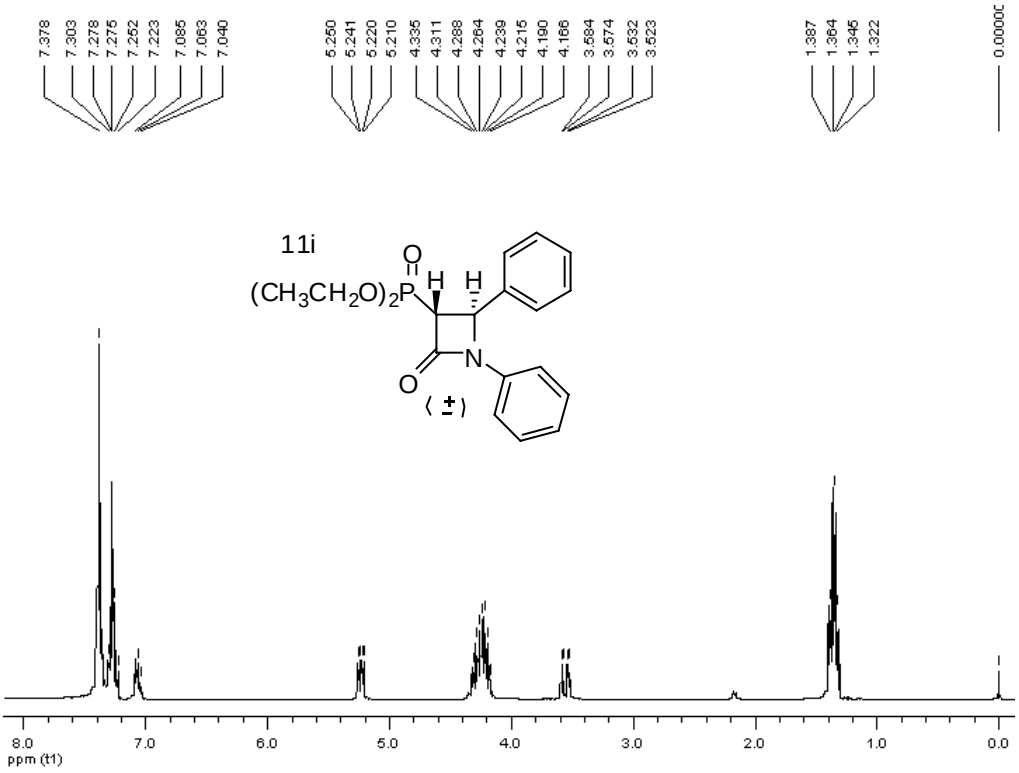


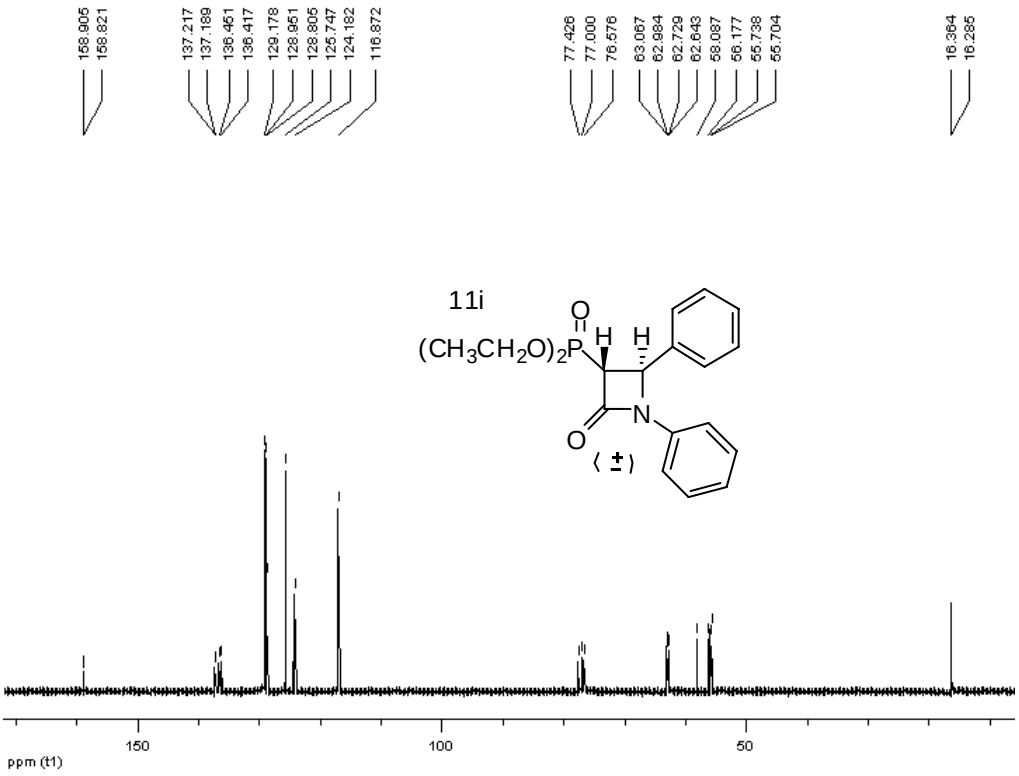
Diethyl (±)-*trans*-11-methoxy-1,12b-dihydro-azeto[1,2-*d*]dibenzo[*b*,*f*][1,4]oxazepin-2-one-1-phosphonate (5ih)



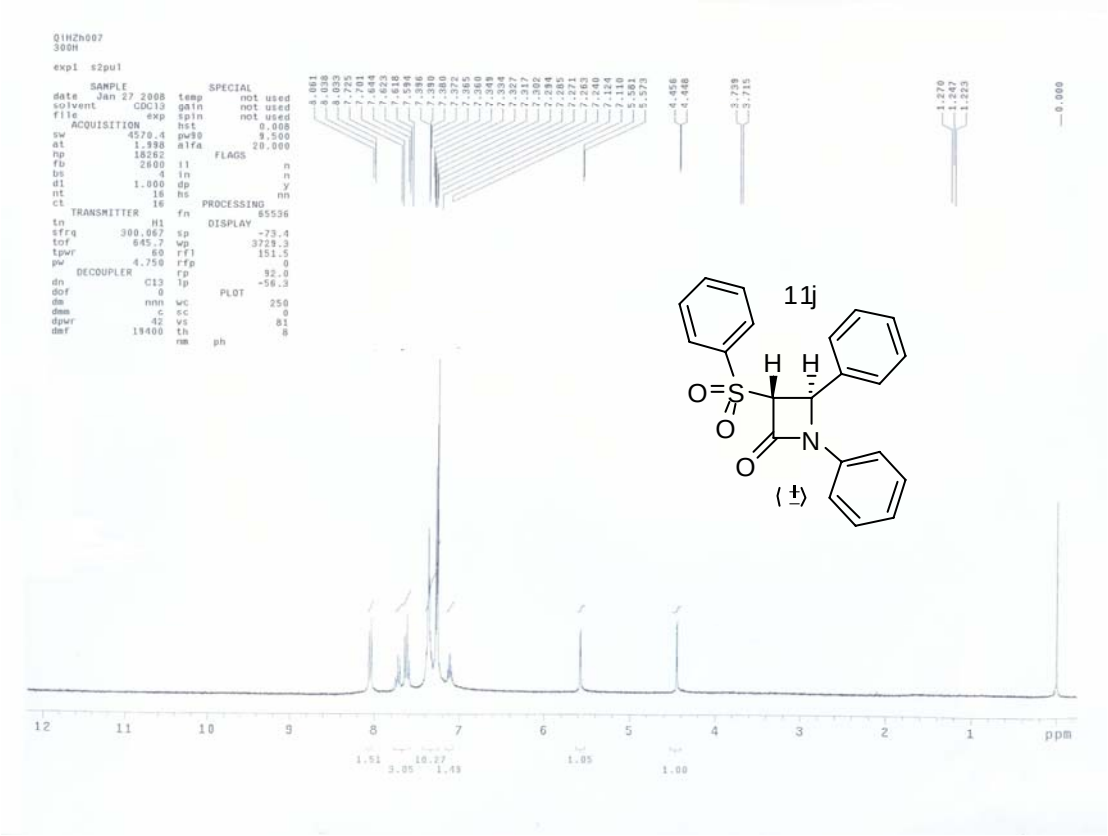


Diethyl (±)-*trans*-1,4-diphenyl-azetidin-2-one-3-phosphonate (11i)

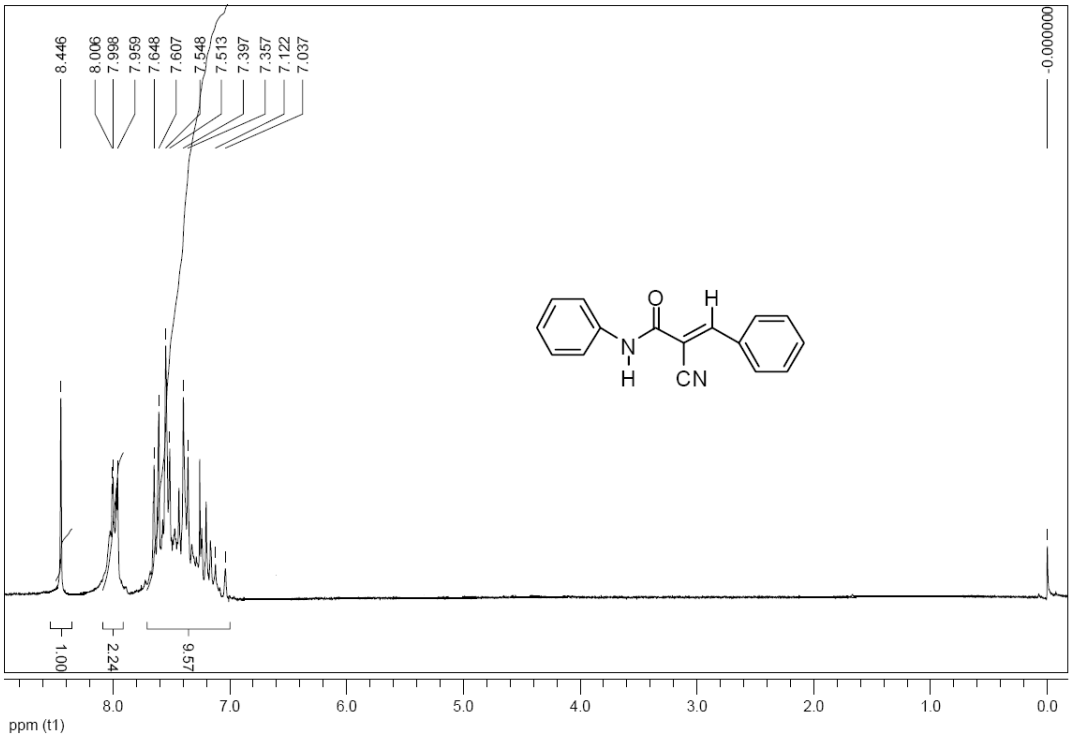




(±)-*trans*-3-Benzenesulfonyl-1,4-diphenyl-azetidin-2-one (11j)

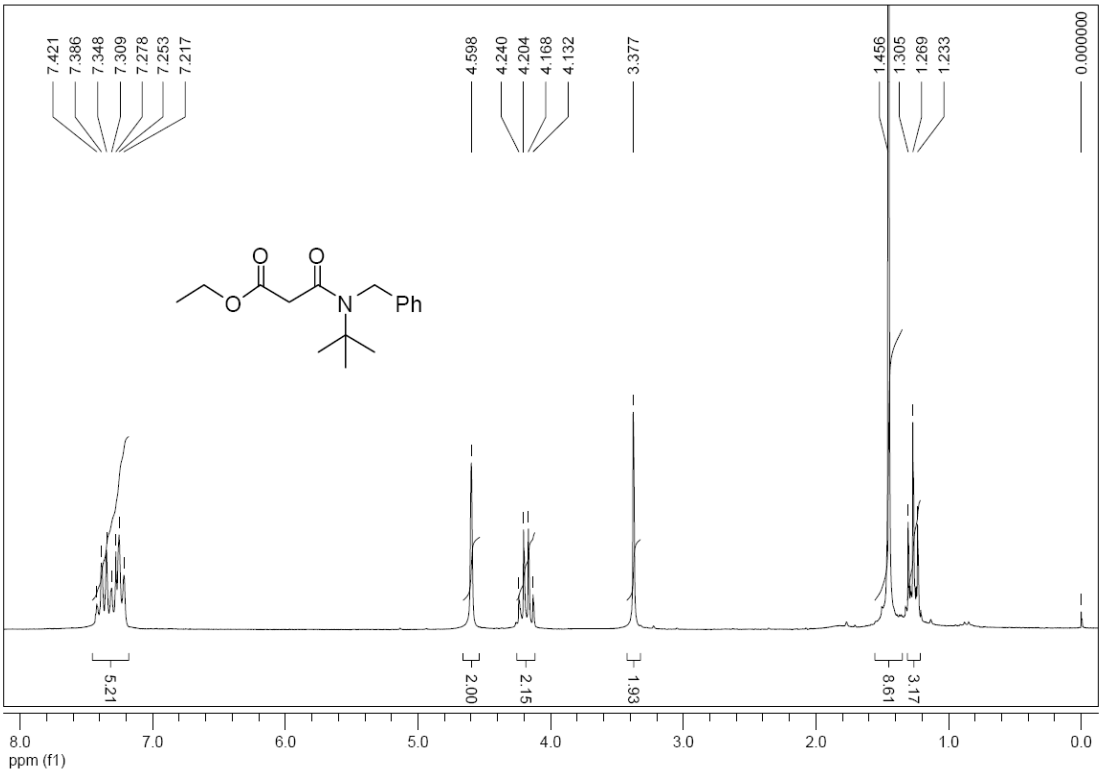


2-Cyano-*N*-phenylcinnamamide (15)

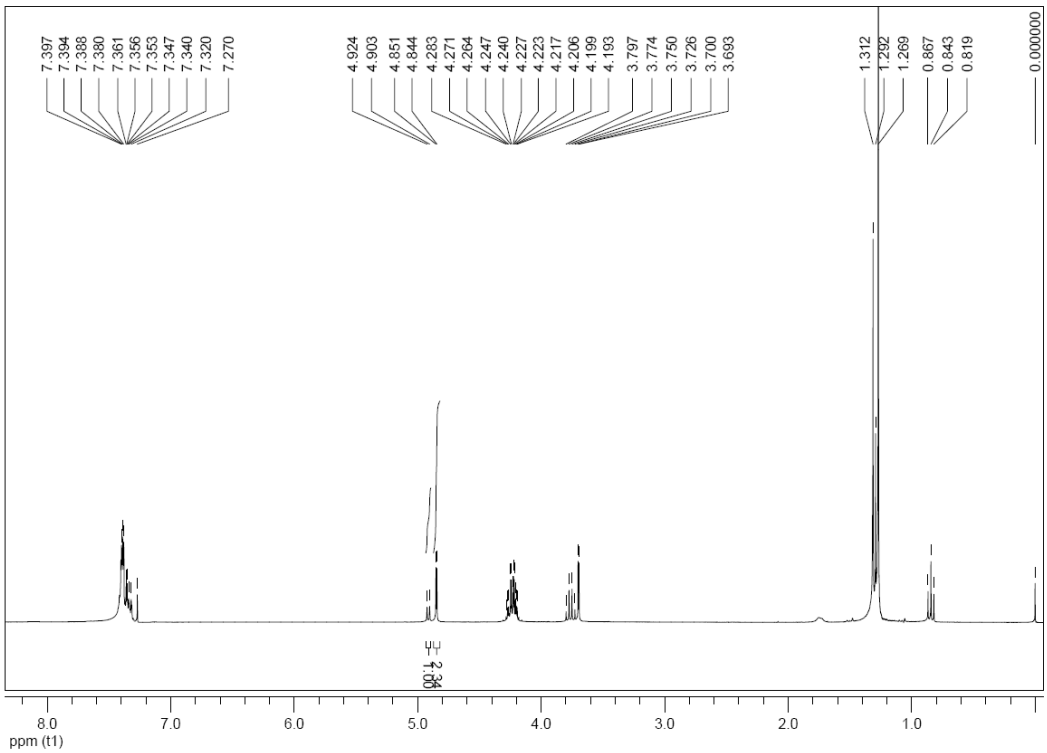


Copies of ^{1}H NMR spectra for the determination of the epimerization

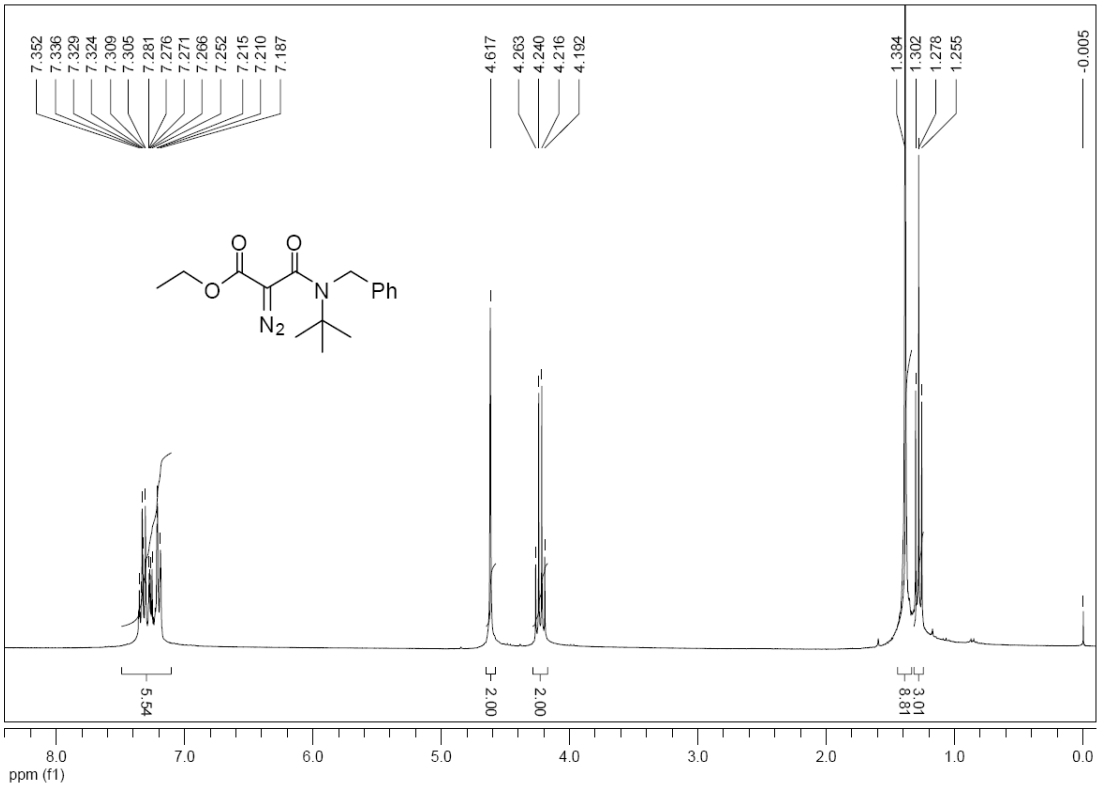
N-benzyl-*N*-*tert*-butyl-3-ethoxy-3-oxopropanamide

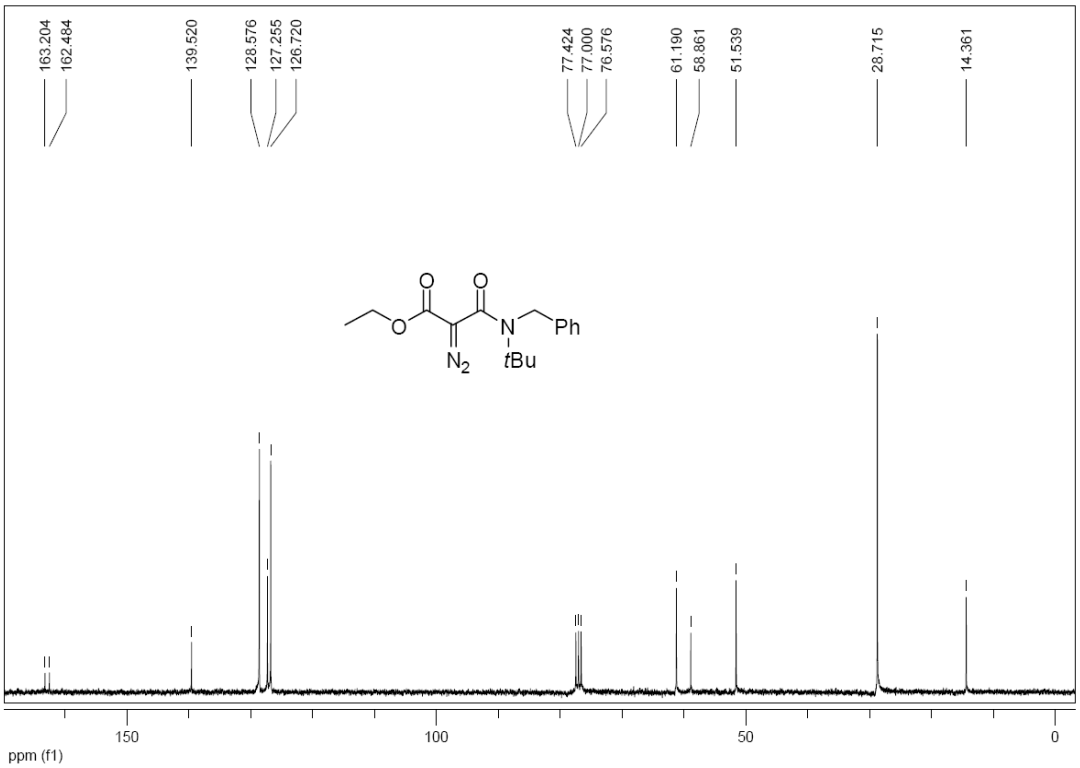


ethyl 1-*tert*-butyl-4-phenyl-2-azetidinone-3-carboxylate (11m)



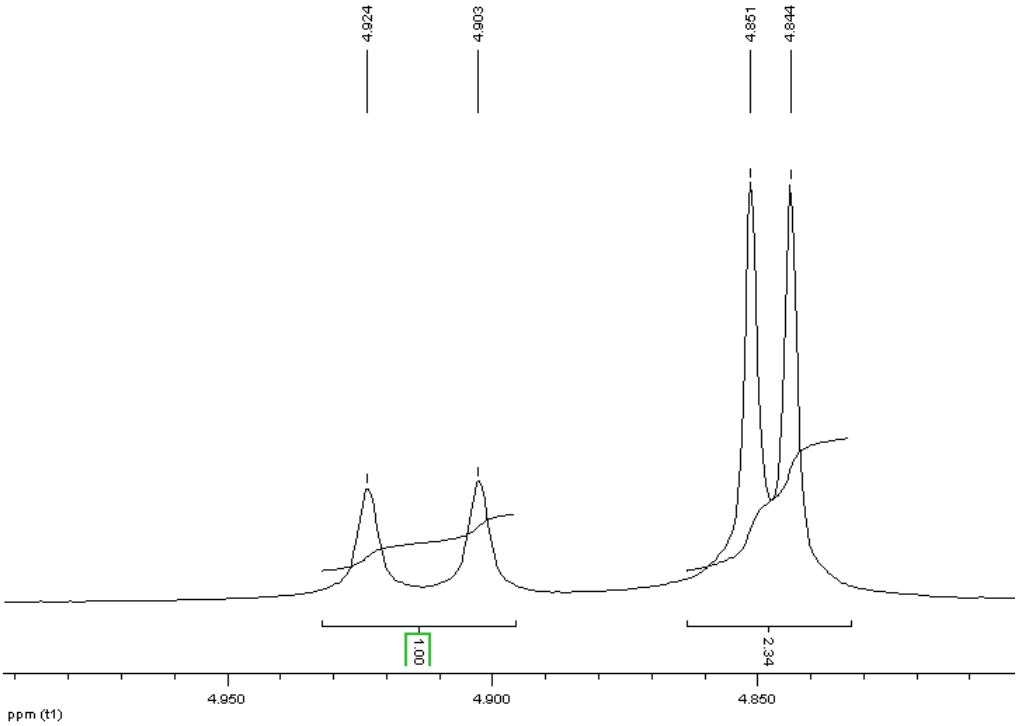
N-benzyl-*N*-*tert*-butyl-2-diazo-3-ethoxy-3-oxopropanamide



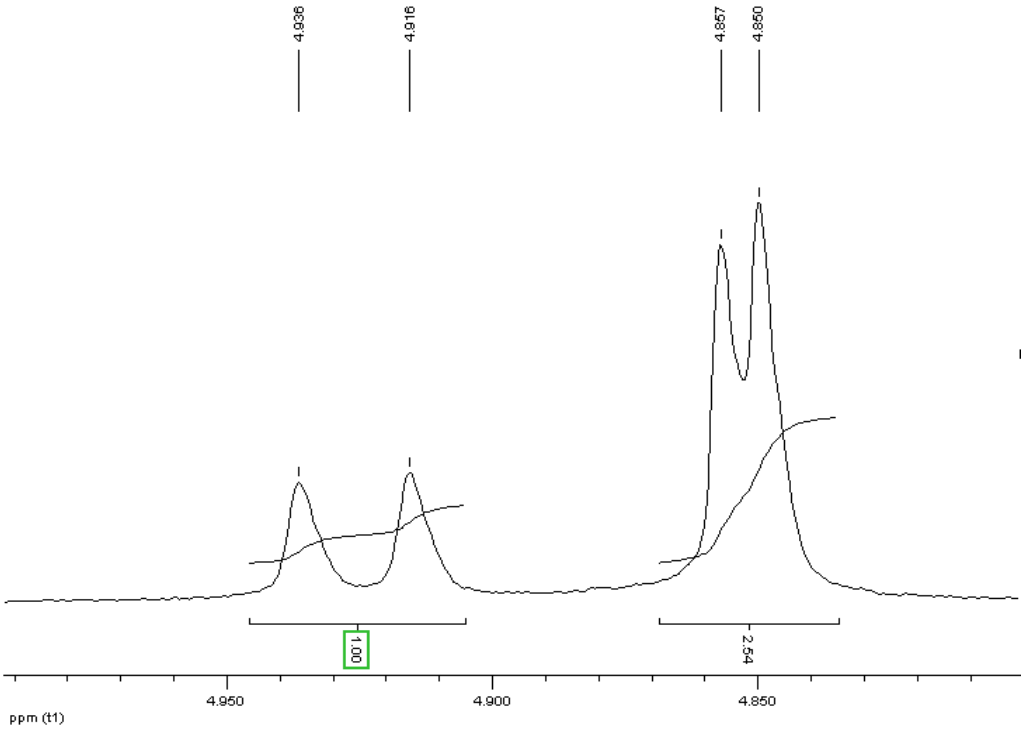


Copies of ^{1}H NMR spectra for the determination of the epimerization of ethyl *cis*-1-*tert*-butyl-4-phenyl-azetidin-2-one-3-carboxylate (*cis*-11m)

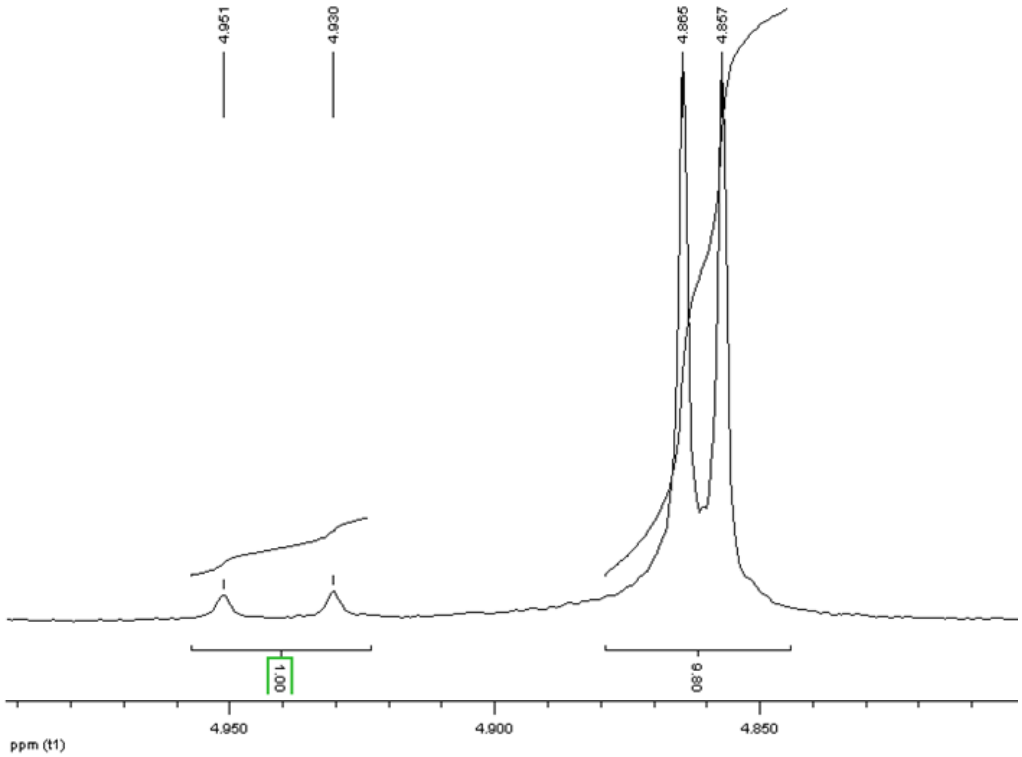
Diastereomeric mixture (Cis/trans = 1:2.34, 30:70)



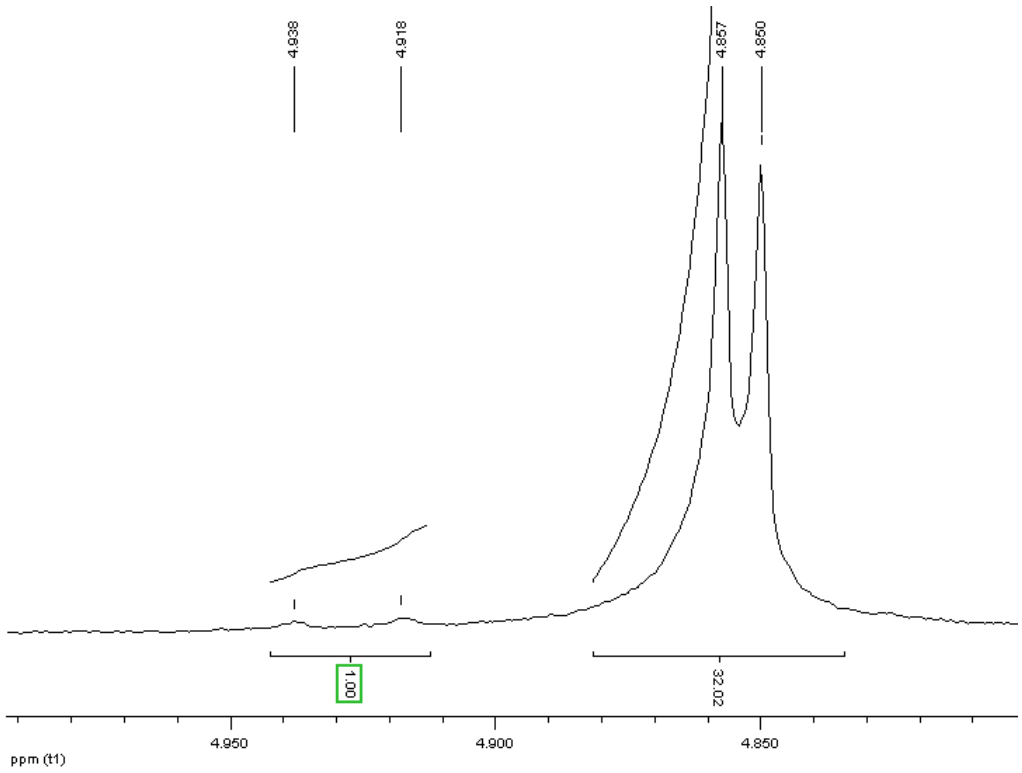
Ethyl hydrogen malonate/ Diastereomeric mixture = 1:1（5 h）(Cis/trans = 1:2.54, 28:72)



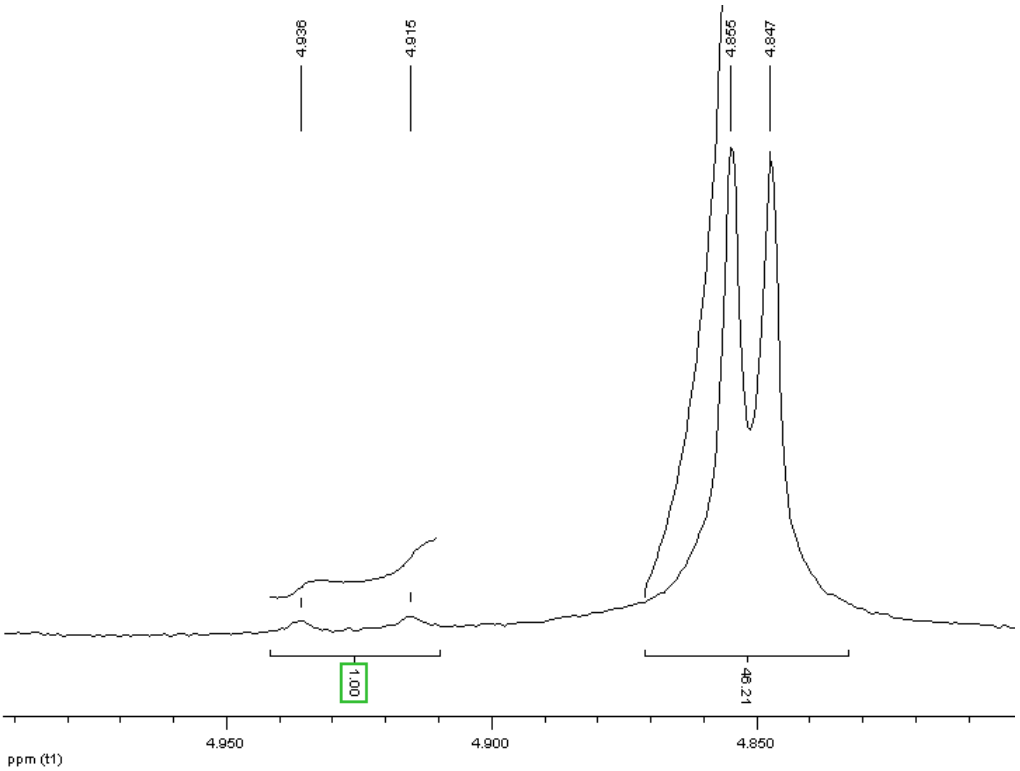
CDI/ Diastereomeric mixture = 1 : 1（5 h）(Cis/trans = 1 : 9.80, 9:91)



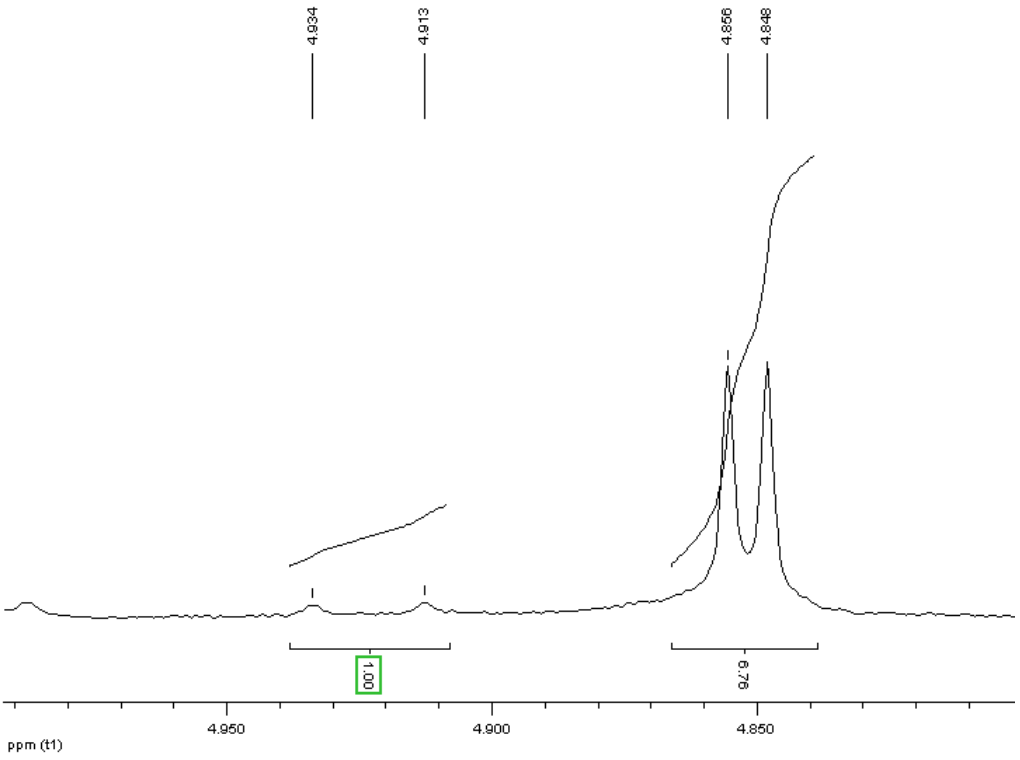
Imidazole/ Diastereomeric mixture = 1:1（5 h）(Cis/trans = 1 : 32.02, 3:97)



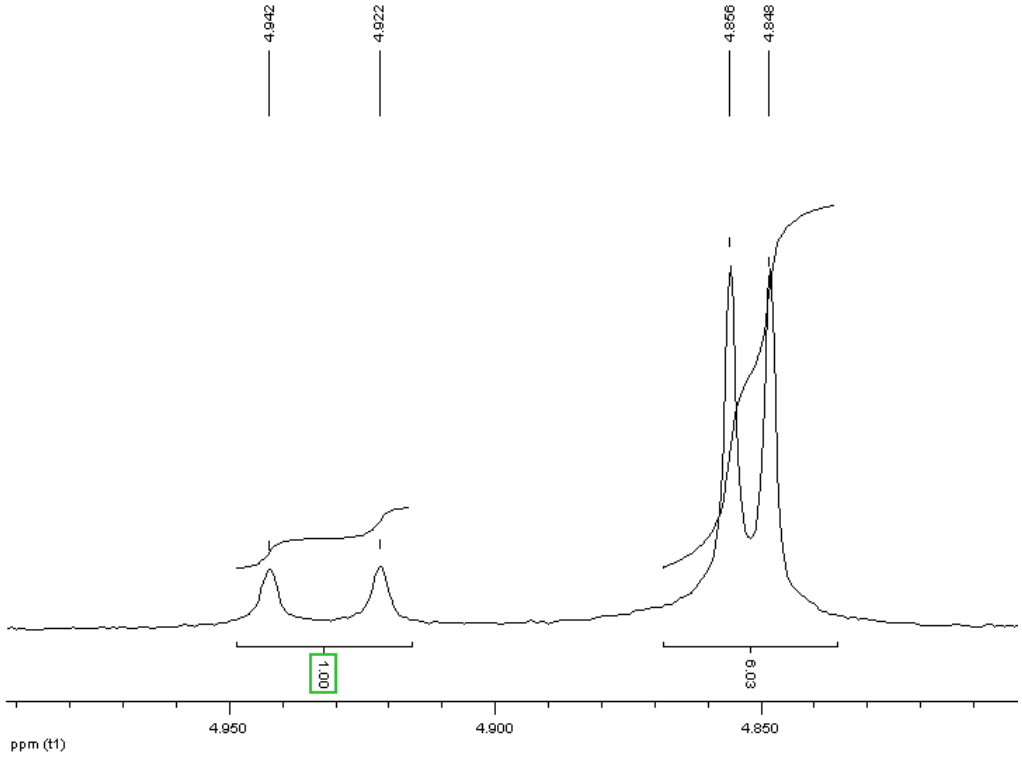
CDI/Ethyl hydrogen malonate / Diastereomeric mixture = 1:1:1（5h）(Cis/trans = 1:46.21, 2:98)



Imidazole/ Diastereomeric mixture = 2:1（3 h）(Cis/trans = 1 : 6.76, 13:87)

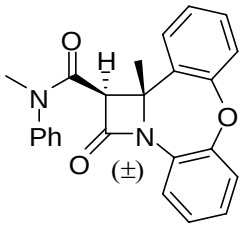


Imidazole/Ethyl hydrogen malonate/Diastereomeric mixture = 2.2:2.3:1（3 h）(Cis/trans = 1:6.03, 14:86)



XRD analysis of product 5bb

Chemical structure of **5bb**



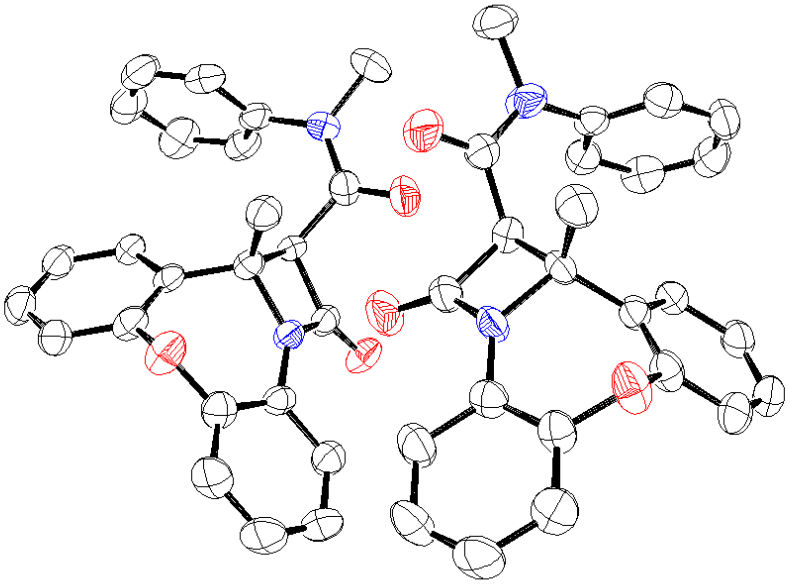


Figure 1. ORTEP drawing of product 5bb (shown with 50% probability ellipsoids).

Cif format file of product 5bb

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and
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C14 C 0.28804(13) 1.1875(3) 0.70400(7) 0.0215(3) Uani 1 1 d . . .
H14 H 0.2378 1.2140 0.7334 0.026 Uiso 1 1 calc R . .
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C9 0.0171(7) 0.0164(7) 0.0146(7) 0.0021(6) 0.0028(6) 0.0022(6)
C10 0.0178(7) 0.0152(7) 0.0139(7) 0.0019(6) -0.0011(6) 0.0031(6)
C11 0.0176(7) 0.0192(7) 0.0206(8) 0.0011(6) 0.0033(6) 0.0020(6)
C12 0.0197(8) 0.0188(8) 0.0259(8) 0.0004(7) -0.0018(6) -0.0012(6)
C13 0.0274(9) 0.0186(8) 0.0185(8) -0.0031(6) 0.0002(7) 0.0029(6)
C14 0.0239(8) 0.0244(8) 0.0166(7) -0.0016(6) 0.0052(6) 0.0036(7)
C15 0.0188(8) 0.0206(8) 0.0169(7) -0.0004(6) 0.0033(6) -0.0009(6)
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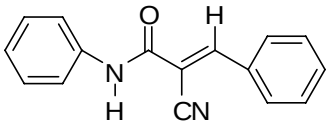
XRD analysis of product 15

Chemical structure of product **15**



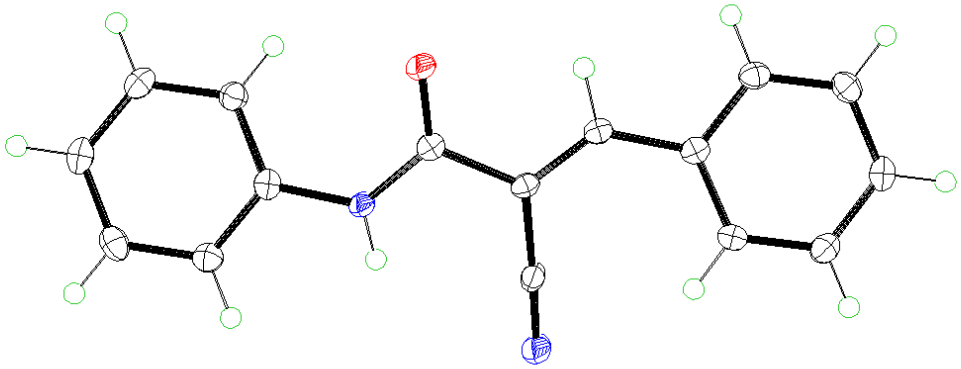


Figure 2. ORTEP drawing of product 15 (shown with 50% probability ellipsoids).

Cif format file of product 15

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and
is
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based
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R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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O6 O 0.25156(18) 0.76020(19) 0.21192(15) 0.0657(8) Uani 1 1 d . . .
N1 N 0.22603(14) 0.5106(2) 0.30010(12) 0.0381(6) Uani 1 1 d . . .
N2 N 0.30117(19) 0.8432(2) 0.31116(16) 0.0537(8) Uani 1 1 d . . .
N3 N 0.49153(13) 0.5030(2) 0.12774(13) 0.0340(6) Uani 1 1 d . . .
N4 N 0.55383(17) 0.8393(2) 0.13108(16) 0.0467(7) Uani 1 1 d . . .
C1 C 0.45851(16) 0.4018(2) 0.12674(15) 0.0343(7) Uani 1 1 d . . .
C2 C 0.41205(18) 0.3674(3) 0.06796(18) 0.0431(8) Uani 1 1 d . . .
C3 C 0.3765(2) 0.2695(3) 0.0712(2) 0.0513(9) Uani 1 1 d . . .
H3 H 0.339(3) 0.260(3) 0.032(3) 0.098(17) Uiso 1 1 d . . .
C4 C 0.3888(2) 0.2031(3) 0.1297(2) 0.0594(10) Uani 1 1 d . . .
H4 H 0.3654(17) 0.139(2) 0.1296(16) 0.040(8) Uiso 1 1 d . . .
C5 C 0.4371(3) 0.2348(3) 0.1869(2) 0.0590(11) Uani 1 1 d . . .
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C6 C 0.4718(2) 0.3329(3) 0.18546(18) 0.0448(8) Uani 1 1 d . . .
H6 H 0.5076(18) 0.351(2) 0.2217(16) 0.035(8) Uiso 1 1 d . . .
C7 C 0.45704(18) 0.4760(3) -0.03261(16) 0.0417(8) Uani 1 1 d . . .
C8 C 0.50128(17) 0.5592(2) -0.00267(15) 0.0343(7) Uani 1 1 d . . .
C9 C 0.5578(2) 0.6046(3) -0.04794(17) 0.0379(8) Uani 1 1 d . . .
H9 H 0.5907(17) 0.651(2) -0.0279(15) 0.029(8) Uiso 1 1 d . . .
C10 C 0.5703(2) 0.5702(3) -0.11969(17) 0.0458(8) Uani 1 1 d . . .
H10 H 0.609(2) 0.604(3) -0.1465(18) 0.056(10) Uiso 1 1 d . . .
C11 C 0.5266(2) 0.4886(3) -0.14813(19) 0.0509(9) Uani 1 1 d . . .
H11 H 0.5370(16) 0.470(2) -0.2008(16) 0.047(9) Uiso 1 1 d . . .
C12 C 0.4693(2) 0.4405(3) -0.10454(18) 0.0493(9) Uani 1 1 d . . .
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H12 H 0.436(2) 0.377(3) -0.1167(19) 0.064(11) Uiso 1 1 d . . .
C13 C 0.59055(18) 0.8483(2) 0.05924(17) 0.0402(7) Uani 1 1 d . . .
C14 C 0.6702(2) 0.8263(3) 0.0512(2) 0.0492(9) Uani 1 1 d . . .
H14 H 0.697(2) 0.806(3) 0.092(2) 0.066(11) Uiso 1 1 d . . .
C15 C 0.7027(3) 0.8284(3) -0.0190(2) 0.0620(11) Uani 1 1 d . . .
H15 H 0.754(3) 0.838(4) -0.022(3) 0.13(2) Uiso 1 1 d . . .
C16 C 0.6574(3) 0.8544(3) -0.0795(2) 0.0633(11) Uani 1 1 d . . .
H16 H 0.6773(18) 0.850(2) -0.1319(19) 0.048(9) Uiso 1 1 d . . .
C17 C 0.5798(3) 0.8824(3) -0.0702(2) 0.0587(10) Uani 1 1 d . . .
H17 H 0.537(2) 0.906(3) -0.115(2) 0.086(13) Uiso 1 1 d . . .
C18 C 0.5459(2) 0.8781(3) -0.0009(2) 0.0478(9) Uani 1 1 d . . .
H18 H 0.4942(19) 0.900(3) 0.0108(18) 0.047(9) Uiso 1 1 d . . .
C19 C 0.5347(3) 0.9394(3) 0.1705(2) 0.0830(15) Uani 1 1 d . . .
C20 C 0.5362(2) 0.7464(2) 0.1631(2) 0.0424(9) Uani 1 1 d . . .
C21 C 0.55352(19) 0.6462(2) 0.11895(16) 0.0332(7) Uani 1 1 d . . .
H21 H 0.605(2) 0.645(3) 0.0861(19) 0.068(11) Uiso 1 1 d . . .
C22 C 0.55392(19) 0.5460(3) 0.16543(16) 0.0356(7) Uani 1 1 d . . .
C23 C 0.48270(16) 0.5943(2) 0.07536(16) 0.0341(7) Uani 1 1 d . . .
C24 C 0.40478(17) 0.6528(3) 0.08001(17) 0.0451(8) Uani 1 1 d . . .
H24A H 0.3952 0.6736 0.1303 0.080 Uiso 1 1 calc R . .
H24B H 0.3629 0.6075 0.0635 0.080 Uiso 1 1 calc R . .
H24C H 0.4069 0.7145 0.0491 0.080 Uiso 1 1 calc R . .
C25 C 0.19714(17) 0.4069(3) 0.30289(16) 0.0406(7) Uani 1 1 d . . .
C26 C 0.15184(18) 0.3713(3) 0.36206(17) 0.0426(8) Uani 1 1 d . . .
C27 C 0.1232(2) 0.2689(3) 0.3648(2) 0.0541(10) Uani 1 1 d . . .
H27 H 0.092(2) 0.246(3) 0.412(2) 0.055(10) Uiso 1 1 d . . .
C28 C 0.1423(2) 0.1990(3) 0.3073(2) 0.0618(10) Uani 1 1 d . . .
H28 H 0.1248(19) 0.121(3) 0.313(2) 0.070(11) Uiso 1 1 d . . .
C29 C 0.1885(3) 0.2327(3) 0.2499(2) 0.0614(11) Uani 1 1 d . . .
H29 H 0.2052(18) 0.182(3) 0.210(2) 0.055(9) Uiso 1 1 d . . .
C30 C 0.2164(2) 0.3351(3) 0.2460(2) 0.0527(9) Uani 1 1 d . . .
H30 H 0.2476(18) 0.361(2) 0.2032(19) 0.048(9) Uiso 1 1 d . . .
C31 C 0.19271(17) 0.4800(3) 0.46166(16) 0.0410(7) Uani 1 1 d . . .
C32 C 0.23866(17) 0.5602(2) 0.43320(15) 0.0341(7) Uani 1 1 d . . .
C33 C 0.2968(2) 0.6031(3) 0.47804(17) 0.0401(8) Uani 1 1 d . . .
H33 H 0.331(2) 0.665(3) 0.4580(19) 0.060(10) Uiso 1 1 d . . .
C34 C 0.3087(2) 0.5648(3) 0.54954(16) 0.0454(9) Uani 1 1 d . . .
H34 H 0.3528(18) 0.595(2) 0.5795(18) 0.049(9) Uiso 1 1 d . . .
C35 C 0.2624(2) 0.4841(3) 0.57546(19) 0.0505(9) Uani 1 1 d . . .
H35 H 0.2739(17) 0.454(2) 0.6230(17) 0.047(9) Uiso 1 1 d . . .
C36 C 0.2046(2) 0.4420(3) 0.53183(19) 0.0518(9) Uani 1 1 d . . .
H36 H 0.174(2) 0.393(3) 0.5495(19) 0.061(11) Uiso 1 1 d . . .
C37 C 0.33642(18) 0.8437(2) 0.38317(16) 0.0367(7) Uani 1 1 d . . .
C38 C 0.4147(2) 0.8166(3) 0.39169(17) 0.0447(8) Uani 1 1 d . . .
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H38 H 0.4472(18) 0.799(3) 0.3459(18) 0.049(9) Uiso 1 1 d . . .
C39 C 0.4476(2) 0.8169(3) 0.4613(2) 0.0545(9) Uani 1 1 d . . .
H39 H 0.5055(19) 0.797(2) 0.4674(15) 0.044(8) Uiso 1 1 d . . .
C40 C 0.4047(3) 0.8460(3) 0.52120(19) 0.0558(10) Uani 1 1 d . . .
H40 H 0.436(2) 0.849(3) 0.5661(19) 0.063(10) Uiso 1 1 d . . .
C41 C 0.3270(3) 0.8761(3) 0.5127(2) 0.0581(12) Uani 1 1 d . . .
H41 H 0.2995(19) 0.897(3) 0.5419(17) 0.042(11) Uiso 1 1 d . . .
C42 C 0.2927(2) 0.8756(3) 0.4433(2) 0.0462(8) Uani 1 1 d . . .
H42 H 0.2399(17) 0.895(2) 0.4396(15) 0.033(8) Uiso 1 1 d . . .
C43 C 0.2985(5) 0.9459(9) 0.2697(5) 0.060(2) Uani 0.60 1 d PU . .
C43' C 0.2633(8) 0.9500(14) 0.2858(9) 0.060(2) Uani 0.40 1 d PU . .
C44 C 0.2796(2) 0.7551(3) 0.2732(2) 0.0435(9) Uani 1 1 d . . .
C45 C 0.29236(19) 0.6501(3) 0.31081(18) 0.0366(8) Uani 1 1 d . . .
H45 H 0.3438(16) 0.645(2) 0.3361(13) 0.022(7) Uiso 1 1 d . . .
C46 C 0.28673(19) 0.5538(3) 0.25991(18) 0.0419(8) Uani 1 1 d . . .
C47 C 0.22181(16) 0.5996(2) 0.35529(15) 0.0345(7) Uani 1 1 d . . .
C48 C 0.14491(18) 0.6619(3) 0.35030(18) 0.0508(9) Uani 1 1 d . . .
H48A H 0.1370 0.6850 0.3002 0.080 Uiso 1 1 calc R . .
H48B H 0.1477 0.7222 0.3824 0.080 Uiso 1 1 calc R . .
H48C H 0.1016 0.6177 0.3651 0.080 Uiso 1 1 calc R . .

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N1 0.0460(15) 0.0333(15) 0.0351(13) -0.0110(11) 0.0042(11) -0.0028(12)
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N3 0.0377(13) 0.0326(13) 0.0317(12) 0.0042(11) -0.0019(11) -0.0026(11)
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C1 0.0339(15) 0.0308(17) 0.0383(16) 0.0054(14) 0.0078(14) 0.0005(13)
C2 0.0401(17) 0.047(2) 0.0425(18) 0.0010(16) 0.0034(15) -0.0034(15)
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C4 0.065(2) 0.041(2) 0.073(3) 0.002(2) 0.006(2) -0.0222(19)
C5 0.078(3) 0.038(2) 0.060(3) 0.0105(19) 0.008(2) -0.008(2)
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C6 0.051(2) 0.043(2) 0.0398(19) 0.0023(16) -0.0004(17) -0.0051(17)
C7 0.0415(17) 0.0427(19) 0.0408(18) 0.0093(15) -0.0075(14) -0.0043(14)
C8 0.0364(17) 0.0337(18) 0.0327(15) 0.0081(13) -0.0065(13) 0.0045(14)
C9 0.0445(19) 0.0373(19) 0.0317(17) 0.0072(15) 0.0004(15) 0.0013(16)
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C12 0.063(2) 0.044(2) 0.0405(18) -0.0013(16) -0.0159(17) -0.0003(18)
C13 0.051(2) 0.0283(17) 0.0415(18) 0.0059(14) -0.0039(15) -0.0059(14)
C14 0.050(2) 0.047(2) 0.050(2) 0.0111(16) -0.0149(18) -0.0074(17)
C15 0.052(2) 0.068(3) 0.067(3) 0.013(2) 0.005(2) -0.020(2)
C16 0.079(3) 0.060(3) 0.051(2) 0.0160(19) 0.005(2) -0.022(2)
C17 0.074(3) 0.048(2) 0.053(2) 0.0171(18) -0.013(2) -0.010(2)
C18 0.047(2) 0.035(2) 0.062(2) 0.0101(17) -0.0090(18) -0.0006(16)
C19 0.141(4) 0.035(2) 0.072(3) -0.015(2) 0.012(3) 0.008(2)
C20 0.045(2) 0.046(3) 0.037(2) -0.0037(14) 0.0008(17) -0.0037(15)
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C22 0.0379(17) 0.0385(19) 0.0304(15) 0.0067(14) 0.0045(14) 0.0026(15)
C23 0.0359(16) 0.0323(17) 0.0341(15) 0.0055(13) 0.0011(13) -0.0034(13)
C24 0.0422(18) 0.049(2) 0.0438(18) 0.0061(15) 0.0036(14) 0.0108(15)
C25 0.0400(17) 0.0389(19) 0.0430(18) -0.0055(15) -0.0062(15) -0.0062(14)
C26 0.0382(17) 0.047(2) 0.0426(18) -0.0078(16) 0.0002(15) -0.0097(16)
C27 0.050(2) 0.056(2) 0.056(2) -0.004(2) -0.0080(19) -0.0161(19)
C28 0.071(3) 0.044(3) 0.070(3) -0.009(2) -0.016(2) -0.016(2)
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C30 0.064(2) 0.050(3) 0.045(2) -0.0140(18) 0.0001(18) -0.0058(19)
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 are estimated using the full covariance matrix.  The cell esds are taken
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(isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Stereoselective Control in the Staudinger Reactions Involving Monosubstituted Ketenes with Electron Acceptor Substituents: Experimental Investigation and Theoretical Rationalization

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Calculational part

1. Details of Calculation

All of the DFT calculations were performed with the Gaussian 03 program package.[1] The geometry optimization of all the minima and transition states involved were performed at the B3LYP levels of theory[2] with the 6−31G(d) basis set.[3] The vibrational frequencies were computed at the same level of theory to check whether every optimized geometrical structure is an energy minimum or a transition state, and to evaluate its zero-point vibration energy (ZPVE). IRC calculations[4] were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. Solvent effects were computed by the CPCM model[5] at the B3LYP/6−31G(d) level using the gas phase optimized structures. In some cases, transition states **TS1** and intermediates **INT** were not located, which were less important.

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople *Gaussian 03*, Revision B.02; Gaussian, Inc.: Wallingford, CT, 2004.
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3 Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.
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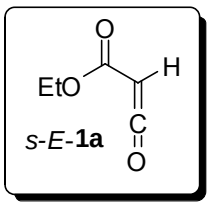
5 (a) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995. (b) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669. (c) Takano, Y.; Houk, K. N. *J. Chem. Theory Comput.* **2005**, *1*, 70.

2. Coordinates of All Stationary Points



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.208187	1.009203	0.000000
2	6	0	-1.648346	0.720052	0.000038
3	6	0	-2.106875	-0.525580	0.000010
4	8	0	-2.517006	-1.614545	-0.000019
5	8	0	0.266783	2.124753	0.000023
6	1	0	-2.352625	1.542240	0.000066
7	8	0	0.522923	-0.134913	-0.000054
8	6	0	1.959293	0.034160	-0.000065
9	6	0	2.579555	-1.350288	0.000066
10	1	0	2.245902	0.613309	0.883557
11	1	0	2.245901	0.613133	-0.883806
12	1	0	3.671680	-1.266053	0.000038
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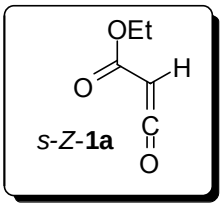

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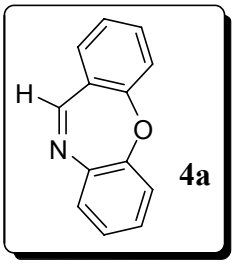
3	6	0	-2.535628	-0.361869	0.000017
4	8	0	-3.640447	-0.001518	0.000053
5	8	0	-0.326299	1.403502	-0.000003

6	1	0	-1.089531	-1.855470	-0.000046
7	8	0	1.007995	-0.437410	-0.000095
8	6	0	2.167758	0.427020	-0.000008
9	6	0	3.395989	-0.463517	0.000077
10	1	0	2.126694	1.072453	0.883209
11	1	0	2.126821	1.072447	-0.883232
12	1	0	4.300994	0.153693	0.000110
13	1	0	3.415518	-1.103778	0.887844
14	1	0	3.415606	-1.103810	-0.887666

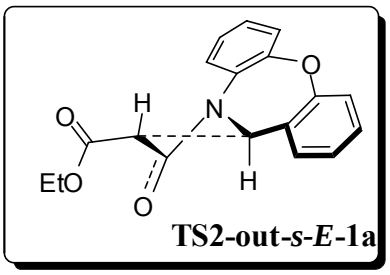


4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.706615	1.936002	0.424427
2	6	0	-0.575655	1.909923	0.408424
3	6	0	-1.503317	0.803097	0.123918
4	6	0	-2.774515	1.094200	-0.398074
5	6	0	-3.690675	0.083793	-0.677861
6	6	0	-3.350612	-1.245681	-0.416874
7	6	0	-2.099131	-1.559021	0.115389
8	6	0	-1.187621	-0.541650	0.385460
9	8	0	-0.009994	-0.888974	1.021910
10	6	0	1.179476	-0.529124	0.393798
11	6	0	1.511684	0.819034	0.150382
12	6	0	2.784636	1.088371	-0.381590
13	6	0	3.680251	0.066867	-0.684508
14	6	0	3.328418	-1.260691	-0.432966
15	6	0	2.077010	-1.554180	0.109980
16	1	0	-1.064099	2.873315	0.585236
17	1	0	-3.034840	2.133263	-0.585955
18	1	0	-4.666346	0.330532	-1.085746
19	1	0	-4.062344	-2.041459	-0.618210
20	1	0	-1.820254	-2.581890	0.346905
21	1	0	3.041679	2.130042	-0.546709
22	1	0	4.654625	0.306720	-1.100240

23	1	0	4.025399	-2.065984	-0.646828
24	1	0	1.780145	-2.574393	0.332418

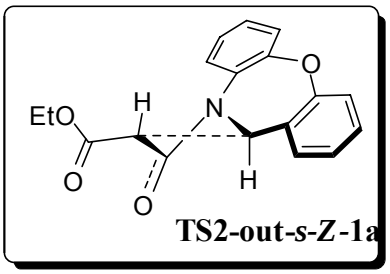


TS2-out-*s*-*E*-1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.117127	0.645318	-0.255371
2	6	0	-0.158041	-0.661671	-0.645119
3	6	0	-1.286845	-1.540820	-0.476825
4	6	0	-1.256926	-2.790397	-1.138769
5	6	0	-2.271795	-3.720986	-0.979879
6	6	0	-3.355749	-3.420134	-0.146561
7	6	0	-3.421929	-2.190774	0.506951
8	6	0	-2.403796	-1.253790	0.344767
9	8	0	-2.517273	-0.094902	1.075611
10	6	0	-2.405166	1.143625	0.447189
11	6	0	-1.216473	1.538610	-0.177345
12	6	0	-1.102971	2.837678	-0.684161
13	6	0	-2.174963	3.722560	-0.567949
14	6	0	-3.363313	3.315779	0.040243
15	6	0	-3.479541	2.021034	0.548317
16	1	0	0.594492	-0.983856	-1.351971
17	1	0	-0.401508	-3.018473	-1.769304
18	1	0	-2.221363	-4.676492	-1.492204
19	1	0	-4.155249	-4.142545	-0.009482
20	1	0	-4.255563	-1.937162	1.153291
21	1	0	-0.165594	3.137762	-1.136179
22	1	0	-2.077773	4.731710	-0.956898
23	1	0	-4.198446	4.004341	0.128595
24	1	0	-4.382364	1.682902	1.046566
25	6	0	3.114647	-0.721318	0.794740
26	8	0	3.491737	-1.671943	1.464942
27	8	0	3.941694	-0.005123	-0.007404
28	6	0	5.327876	-0.393656	0.022126
29	6	0	6.086760	0.562003	-0.880334

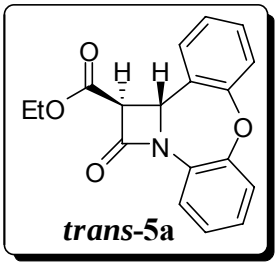
30	1	0	5.416699	-1.433279	-0.313422
31	1	0	5.688245	-0.354606	1.055705
32	1	0	7.152015	0.305053	-0.885703
33	1	0	5.713234	0.509001	-1.908227
34	1	0	5.979042	1.593531	-0.530819
35	6	0	1.719152	-0.292306	0.712006
36	6	0	1.245140	0.958390	0.150508
37	8	0	1.769922	2.043561	-0.018501
38	1	0	1.068991	-0.790817	1.421041



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.467382	-0.877339	-0.462582
2	6	0	0.084621	0.349225	-0.920241
3	6	0	0.750250	1.590553	-0.615496
4	6	0	0.383626	2.738031	-1.356444
5	6	0	0.930930	3.982576	-1.086129
6	6	0	1.871109	4.111239	-0.056824
7	6	0	2.264461	2.996027	0.681063
8	6	0	1.717718	1.744280	0.406935
9	8	0	2.113600	0.710849	1.222507
10	6	0	2.597440	-0.471870	0.665840
11	6	0	1.785598	-1.284654	-0.133773
12	6	0	2.266236	-2.525081	-0.567296
13	6	0	3.548947	-2.935458	-0.204044
14	6	0	4.358991	-2.111743	0.578811
15	6	0	3.882224	-0.874259	1.014130
16	1	0	-0.588246	0.365384	-1.766901
17	1	0	-0.358085	2.627553	-2.143280
18	1	0	0.627890	4.849450	-1.664763
19	1	0	2.304377	5.081623	0.167919
20	1	0	2.994995	3.074016	1.479365
21	1	0	1.614436	-3.156120	-1.158908

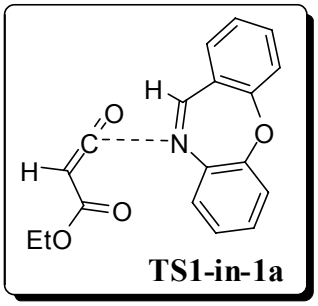
22	1	0	3.913516	-3.902331	-0.537708
23	1	0	5.358293	-2.431220	0.859339
24	1	0	4.479674	-0.221712	1.642563
25	6	0	-3.160917	-0.929139	-0.151204
26	8	0	-3.658731	-1.723281	-0.929669
27	8	0	-3.902680	-0.037665	0.575119
28	6	0	-5.324211	-0.097921	0.358591
29	6	0	-5.968562	0.943839	1.255419
30	1	0	-5.678843	-1.108912	0.586441
31	1	0	-5.535199	0.087576	-0.700818
32	1	0	-7.056148	0.931206	1.122934
33	1	0	-5.747351	0.742251	2.308632
34	1	0	-5.603607	1.947876	1.014658
35	6	0	-1.735928	-0.726830	0.099962
36	6	0	-0.727183	-1.693248	-0.291073
37	8	0	-0.761641	-2.892887	-0.484509
38	1	0	-1.473865	-0.034802	0.891672



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.312243	-0.860793	-0.105161
2	6	0	0.238426	0.409071	0.440215
3	6	0	-0.555514	1.626577	0.048602
4	6	0	-0.017691	2.752229	-0.579950
5	6	0	-0.818136	3.857757	-0.876875
6	6	0	-2.172620	3.846331	-0.544441
7	6	0	-2.727513	2.731827	0.086746
8	6	0	-1.919866	1.635667	0.375897
9	8	0	-2.475073	0.586855	1.099510
10	6	0	-2.656883	-0.662546	0.513899
11	6	0	-1.601395	-1.401929	-0.051817
12	6	0	-1.861870	-2.681107	-0.567581
13	6	0	-3.146158	-3.215301	-0.498863
14	6	0	-4.184732	-2.487583	0.084424

15	6	0	-3.934258	-1.211245	0.586956
16	1	0	0.354820	0.345026	1.527396
17	1	0	1.039581	2.774968	-0.828880
18	1	0	-0.381485	4.724497	-1.364314
19	1	0	-2.799766	4.703345	-0.773206
20	1	0	-3.775574	2.699419	0.366629
21	1	0	-1.044551	-3.237842	-1.010786
22	1	0	-3.330372	-4.208090	-0.898889
23	1	0	-5.185389	-2.905053	0.144532
24	1	0	-4.718558	-0.616847	1.044860
25	6	0	2.780897	-0.123630	0.590037
26	8	0	2.743962	-0.320442	1.786442
27	8	0	3.906149	-0.090132	-0.143475
28	6	0	5.138410	-0.365623	0.570136
29	6	0	6.267780	-0.322080	-0.440702
30	1	0	5.049877	-1.344759	1.050509
31	1	0	5.258647	0.383424	1.359254
32	1	0	7.219878	-0.528197	0.060193
33	1	0	6.119816	-1.072276	-1.223712
34	1	0	6.333796	0.663120	-0.913448
35	6	0	1.565902	0.073610	-0.287409
36	6	0	0.853285	-1.244418	-0.727367
37	8	0	1.169524	-2.220977	-1.365326
38	1	0	1.800089	0.696744	-1.152656

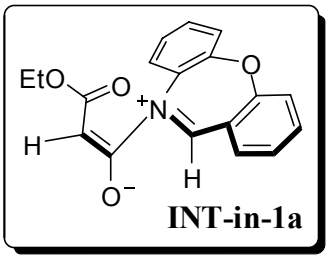


TS1-in-1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.207978	-0.908289	0.566054
2	6	0	1.306937	-1.439711	0.170470
3	6	0	2.570545	-0.799924	-0.190861
4	6	0	3.761561	-1.539000	-0.079434
5	6	0	4.985912	-0.987197	-0.441835
6	6	0	5.031095	0.313861	-0.950428

7	6	0	3.860131	1.060377	-1.085181
8	6	0	2.639367	0.507096	-0.707670
9	8	0	1.497124	1.237977	-0.958694
10	6	0	0.664984	1.496607	0.125539
11	6	0	0.018515	0.464320	0.826015
12	6	0	-0.863280	0.813070	1.859043
13	6	0	-1.093972	2.146845	2.185331
14	6	0	-0.451232	3.159967	1.472405
15	6	0	0.430800	2.830240	0.443186
16	1	0	1.303277	-2.531071	0.145428
17	1	0	3.711714	-2.556403	0.300357
18	1	0	5.896633	-1.569697	-0.342901
19	1	0	5.980034	0.748029	-1.252433
20	1	0	3.870357	2.064355	-1.496418
21	1	0	-1.371805	0.017269	2.391729
22	1	0	-1.781431	2.392267	2.989232
23	1	0	-0.636169	4.203467	1.710296
24	1	0	0.938480	3.594061	-0.137035
25	6	0	-2.636903	-1.016658	-0.559525
26	8	0	-1.843555	-0.324851	-1.178800
27	8	0	-3.988876	-0.948078	-0.766519
28	6	0	-4.431638	-0.001434	-1.757174
29	6	0	-4.602266	1.389803	-1.161442
30	1	0	-5.386333	-0.400912	-2.111418
31	1	0	-3.717387	0.013635	-2.584418
32	1	0	-5.003231	2.076217	-1.916866
33	1	0	-5.295985	1.367145	-0.314106
34	1	0	-3.638809	1.777642	-0.818901
35	6	0	-2.365698	-2.027613	0.444552
36	6	0	-1.179445	-2.413172	0.968812
37	8	0	-0.540224	-3.205246	1.573442
38	1	0	-3.193429	-2.661247	0.748832

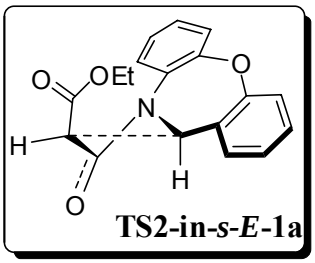


INT-in-1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	0.166124	-0.488706	1.002063
2	6	0	1.143985	-1.292356	0.750581
3	6	0	2.378422	-1.024180	0.038866
4	6	0	3.487826	-1.855642	0.288434
5	6	0	4.686412	-1.672508	-0.389769
6	6	0	4.783029	-0.666549	-1.356468
7	6	0	3.691533	0.156211	-1.635216
8	6	0	2.496662	-0.019491	-0.942973
9	8	0	1.415226	0.738670	-1.327398
10	6	0	0.794386	1.497940	-0.343131
11	6	0	0.153806	0.909965	0.756410
12	6	0	-0.497818	1.733302	1.683491
13	6	0	-0.521978	3.114237	1.505379
14	6	0	0.101723	3.687412	0.397014
15	6	0	0.765351	2.875996	-0.523302
16	1	0	1.018803	-2.290442	1.166647
17	1	0	3.393976	-2.645057	1.029536
18	1	0	5.534949	-2.315783	-0.179927
19	1	0	5.710311	-0.527052	-1.904768
20	1	0	3.740441	0.926563	-2.397347
21	1	0	-0.976860	1.280362	2.543463
22	1	0	-1.033045	3.737605	2.232340
23	1	0	0.073115	4.762229	0.244627
24	1	0	1.252440	3.289771	-1.400110
25	6	0	-2.497283	-0.766325	-0.105402
26	8	0	-1.670978	-0.409211	-0.943749
27	8	0	-3.828723	-0.866761	-0.417374
28	6	0	-4.174912	-0.545062	-1.772189
29	6	0	-5.678218	-0.714016	-1.909201
30	1	0	-3.629353	-1.205496	-2.456028
31	1	0	-3.860758	0.480798	-1.995949
32	1	0	-5.992907	-0.477151	-2.931973
33	1	0	-5.977235	-1.743482	-1.685753
34	1	0	-6.209452	-0.047699	-1.221467
35	6	0	-2.272665	-1.136948	1.266613
36	6	0	-1.059817	-1.174646	1.917298
37	8	0	-0.637644	-1.579321	2.981969
38	1	0	-3.113019	-1.515277	1.836075

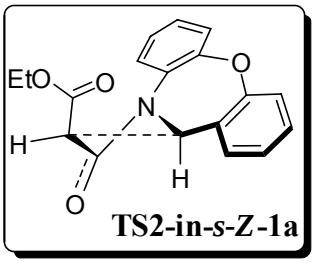


TS2-in-*s*-*E*-1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.799579	-0.630247	-1.063879
2	6	0	-0.241533	0.084858	-1.570884
3	6	0	-0.776966	1.295078	-1.011676
4	6	0	-1.743033	1.991315	-1.777684
5	6	0	-2.373772	3.127264	-1.298330
6	6	0	-2.046112	3.605457	-0.023592
7	6	0	-1.086830	2.953878	0.747959
8	6	0	-0.448917	1.811021	0.266360
9	8	0	0.437330	1.219575	1.127620
10	6	0	1.699932	0.809811	0.712011
11	6	0	1.894826	-0.112962	-0.322839
12	6	0	3.191159	-0.556426	-0.610956
13	6	0	4.272627	-0.084091	0.131564
14	6	0	4.071839	0.842017	1.155338
15	6	0	2.782780	1.290776	1.442456
16	1	0	-0.535757	-0.138102	-2.586731
17	1	0	-2.001236	1.597456	-2.757155
18	1	0	-3.118743	3.635245	-1.902268
19	1	0	-2.534358	4.493219	0.368104
20	1	0	-0.813067	3.315375	1.733570
21	1	0	3.321628	-1.289384	-1.397319
22	1	0	5.272243	-0.442237	-0.095432
23	1	0	4.911864	1.212907	1.735120
24	1	0	2.591171	1.997391	2.243484
25	6	0	-0.851142	-2.232029	-1.357342
26	6	0	0.585838	-2.034831	-1.347074
27	8	0	1.479950	-2.819458	-1.617317
28	1	0	-1.228906	-3.003682	-2.023951
29	6	0	-1.766962	-1.953118	-0.250737
30	8	0	-2.965354	-2.187392	-0.303095
31	8	0	-1.160474	-1.429981	0.855863
32	6	0	-2.018656	-1.142463	1.979687

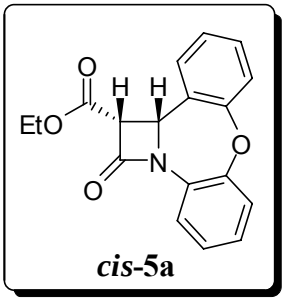
33	6	0	-2.225685	-2.374627	2.848968
34	1	0	-2.973817	-0.758291	1.612399
35	1	0	-1.492485	-0.353710	2.523519
36	1	0	-2.813350	-2.113052	3.737186
37	1	0	-2.765584	-3.146267	2.293411
38	1	0	-1.264631	-2.782669	3.179285



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.876248	-0.931637	0.810241
2	6	0	-0.015791	-0.056227	1.403940
3	6	0	0.212945	1.292284	0.980801
4	6	0	1.072409	2.083439	1.784465
5	6	0	1.464976	3.353505	1.404037
6	6	0	0.997726	3.875762	0.189131
7	6	0	0.132327	3.137643	-0.609920
8	6	0	-0.276052	1.857209	-0.225567
9	8	0	-1.125279	1.243317	-1.095421
10	6	0	-2.208751	0.472033	-0.701775
11	6	0	-2.110218	-0.602067	0.189659
12	6	0	-3.239828	-1.386613	0.448654
13	6	0	-4.449872	-1.102228	-0.183039
14	6	0	-4.543794	-0.025286	-1.064640
15	6	0	-3.422259	0.762894	-1.320561
16	1	0	0.359444	-0.326759	2.381883
17	1	0	1.445353	1.651900	2.709867
18	1	0	2.132770	3.933500	2.032963
19	1	0	1.300850	4.869356	-0.128868
20	1	0	-0.252608	3.534001	-1.543373
21	1	0	-3.136978	-2.229632	1.120729
22	1	0	-5.316525	-1.724985	0.017299
23	1	0	-5.483880	0.201672	-1.558769
24	1	0	-3.458413	1.596411	-2.014439
25	6	0	1.140787	-2.048990	0.786961

26	6	0	-0.294718	-2.251256	0.850696
27	8	0	-0.932474	-3.279893	1.001220
28	1	0	1.760261	-2.798635	1.273701
29	6	0	1.789826	-1.340311	-0.317672
30	8	0	1.271647	-0.705750	-1.224696
31	8	0	3.146887	-1.485063	-0.213376
32	6	0	3.919396	-0.846367	-1.245770
33	1	0	3.608964	-1.236418	-2.221098
34	1	0	3.706132	0.228405	-1.243751
35	6	0	5.383291	-1.133065	-0.962479
36	1	0	5.578127	-2.210413	-0.969233
37	1	0	6.012005	-0.663868	-1.727525
38	1	0	5.677590	-0.738128	0.015577

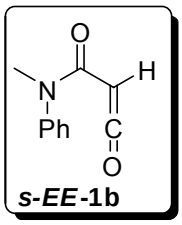


***cis*-5a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.469904	-0.967246	0.545304
2	6	0	0.065641	0.247855	1.216084
3	6	0	-0.317079	1.532003	0.530147
4	6	0	0.593130	2.503053	0.105877
5	6	0	0.151848	3.686336	-0.490932
6	6	0	-1.213346	3.909659	-0.668811
7	6	0	-2.138261	2.952403	-0.248554
8	6	0	-1.686003	1.776564	0.343336
9	8	0	-2.632229	0.892218	0.847783
10	6	0	-2.810622	-0.362161	0.271843
11	6	0	-1.768852	-1.300039	0.145845
12	6	0	-2.049287	-2.565632	-0.392475
13	6	0	-3.347946	-2.890965	-0.776045
14	6	0	-4.382326	-1.965575	-0.627237
15	6	0	-4.106950	-0.702437	-0.104777
16	1	0	-0.219365	0.263513	2.273505
17	1	0	1.657454	2.343274	0.254175

18	1	0	0.874653	4.430314	-0.812721
19	1	0	-1.562034	4.828079	-1.132535
20	1	0	-3.206630	3.104010	-0.364398
21	1	0	-1.238052	-3.276773	-0.495286
22	1	0	-3.549172	-3.875904	-1.187128
23	1	0	-5.396697	-2.219709	-0.919939
24	1	0	-4.886425	0.042086	0.022566
25	6	0	2.480778	-0.173442	-0.097689
26	8	0	2.218386	0.290025	-1.187566
27	8	0	3.705994	-0.565906	0.289831
28	6	0	4.773518	-0.356164	-0.669337
29	6	0	6.063354	-0.821174	-0.021838
30	1	0	4.800939	0.705834	-0.931468
31	1	0	4.539633	-0.918341	-1.579002
32	1	0	6.898114	-0.676899	-0.716266
33	1	0	6.269839	-0.251700	0.889675
34	1	0	6.011500	-1.883357	0.238056
35	6	0	1.484434	-0.347902	1.025649
36	6	0	0.754541	-1.576555	0.396163
37	8	0	1.100147	-2.642384	-0.056860
38	1	0	1.877755	-0.910301	1.874647

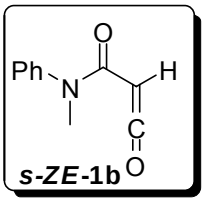


***s-EE*-1b**

Standard orientation:

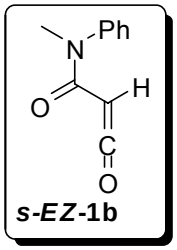
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.065202	0.234706	0.000045
2	6	0	1.529889	1.618198	0.000021
3	6	0	0.284324	2.073405	0.000000
4	8	0	-0.765582	2.585739	-0.000121
5	8	0	3.279606	0.063805	0.000094
6	1	0	2.295123	2.388543	0.000061
7	7	0	1.173016	-0.825053	0.000015
8	6	0	1.694020	-2.190670	-0.000144
9	1	0	1.353725	-2.734130	-0.889756
10	1	0	2.782024	-2.130601	-0.000624
11	1	0	1.354569	-2.734095	0.889820

12	6	0	-0.245270	-0.656559	0.000076
13	6	0	-0.945295	-0.591244	-1.212452
14	6	0	-0.945365	-0.591262	1.212560
15	6	0	-2.330729	-0.434161	-1.210211
16	1	0	-0.392432	-0.652149	-2.145600
17	6	0	-2.330802	-0.434171	1.210212
18	1	0	-0.392609	-0.652137	2.145768
19	6	0	-3.023178	-0.351364	-0.000018
20	1	0	-2.869135	-0.371935	-2.151706
21	1	0	-2.869267	-0.371948	2.151672
22	1	0	-4.102079	-0.223790	-0.000050



Standard orientation:

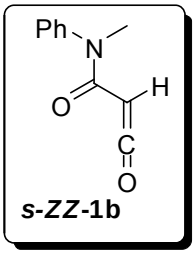
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.205350	1.004041	-0.091947
2	6	0	-2.695118	0.903374	-0.075128
3	6	0	-3.461024	-0.168396	-0.195576
4	8	0	-4.156792	-1.100900	-0.303405
5	8	0	-0.705108	2.061607	-0.450017
6	1	0	-3.204321	1.856837	-0.174518
7	7	0	-0.452333	-0.094268	0.302816
8	6	0	-1.056439	-1.297271	0.875559
9	1	0	-1.416067	-2.007710	0.119572
10	1	0	-0.306923	-1.802663	1.487338
11	1	0	-1.887863	-1.022306	1.529549
12	6	0	0.969295	-0.101102	0.113854
13	6	0	1.763802	1.007114	0.439695
14	6	0	1.581263	-1.265486	-0.370714
15	6	0	3.146422	0.940420	0.274651
16	1	0	1.298202	1.911194	0.806744
17	6	0	2.966548	-1.325177	-0.522145
18	1	0	0.974323	-2.123742	-0.643361
19	6	0	3.756347	-0.221346	-0.202303
20	1	0	3.751199	1.806338	0.530447
21	1	0	3.423433	-2.235874	-0.900078
22	1	0	4.835070	-0.264874	-0.323708



***s-EZ*-1b**

Standard orientation:

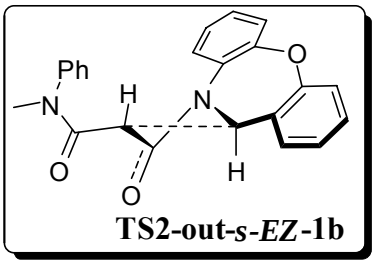
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.518406	0.615824	0.040001
2	6	0	-1.611612	-0.839846	-0.196984
3	6	0	-2.823177	-1.382142	-0.220138
4	8	0	-3.873626	-1.881432	-0.241494
5	8	0	-2.524452	1.309955	0.176734
6	1	0	-0.763981	-1.490096	-0.373807
7	7	0	-0.239655	1.148438	0.071452
8	6	0	-0.089923	2.593073	0.246142
9	1	0	0.520725	3.015472	-0.559526
10	1	0	-1.085236	3.035967	0.226013
11	1	0	0.392503	2.819759	1.204742
12	6	0	0.956085	0.363002	0.035952
13	6	0	1.774025	0.385738	-1.100613
14	6	0	1.336991	-0.399461	1.147468
15	6	0	2.958851	-0.349938	-1.125079
16	1	0	1.470309	0.974871	-1.961370
17	6	0	2.516650	-1.144450	1.114192
18	1	0	0.702475	-0.402863	2.028999
19	6	0	3.331008	-1.118341	-0.019620
20	1	0	3.587317	-0.329278	-2.011210
21	1	0	2.802984	-1.737861	1.978202
22	1	0	4.252151	-1.693981	-0.042056



***s-ZZ*-1b**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.328057	-0.096140	-0.003132
2	6	0	-2.660460	0.548167	0.039898
3	6	0	-3.708648	-0.243027	-0.171921
4	8	0	-4.641571	-0.912123	-0.350033
5	8	0	-1.225255	-1.290780	-0.271589
6	1	0	-2.863722	1.601620	0.181882
7	7	0	-0.237210	0.719131	0.267947
8	6	0	-0.400034	2.135740	0.599302
9	1	0	-0.658039	2.752015	-0.272584
10	1	0	-1.172245	2.262233	1.363466
11	1	0	0.537573	2.503850	1.016883
12	6	0	1.093484	0.215879	0.101160
13	6	0	1.471282	-1.028645	0.623913
14	6	0	2.045818	0.997503	-0.566719
15	6	0	2.783296	-1.474265	0.474899
16	1	0	0.737845	-1.640463	1.131731
17	6	0	3.359945	0.548159	-0.699688
18	1	0	1.758795	1.953066	-0.995799
19	6	0	3.734857	-0.690939	-0.181617
20	1	0	3.063455	-2.441208	0.884170
21	1	0	4.085844	1.167551	-1.219769
22	1	0	4.756679	-1.043944	-0.289206

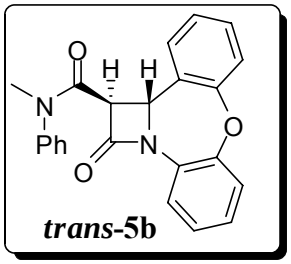


TS2-out-*s*-*EZ*-1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.183546	-0.890487	-0.720951
2	6	0	1.029536	0.318692	-1.326099
3	6	0	1.670895	1.540700	-0.916221
4	6	0	1.599631	2.652199	-1.788214
5	6	0	2.139944	3.881521	-1.443405

6	6	0	2.773504	4.031861	-0.204095
7	6	0	2.872300	2.951168	0.671126
8	6	0	2.333268	1.715056	0.323056
9	8	0	2.415286	0.719670	1.269111
10	6	0	2.953835	-0.518512	0.923873
11	6	0	2.335412	-1.341175	-0.025038
12	6	0	2.837086	-2.627662	-0.252958
13	6	0	3.948900	-3.073378	0.461844
14	6	0	4.569923	-2.241572	1.394509
15	6	0	4.071318	-0.958447	1.625051
16	1	0	0.578378	0.315348	-2.308652
17	1	0	1.093224	2.526335	-2.741695
18	1	0	2.066762	4.720732	-2.127984
19	1	0	3.197175	4.991039	0.079430
20	1	0	3.362030	3.045626	1.634668
21	1	0	2.329018	-3.261883	-0.968685
22	1	0	4.329572	-4.074713	0.283980
23	1	0	5.436584	-2.589033	1.949156
24	1	0	4.518850	-0.295919	2.358890
25	6	0	-2.358425	-0.848465	-1.559145
26	8	0	-2.410146	-1.397660	-2.660472
27	6	0	-1.096313	-0.677674	-0.827282
28	6	0	-0.041809	-1.662182	-0.889683
29	8	0	-0.059788	-2.870540	-1.052109
30	1	0	-1.040717	0.043543	-0.021319
31	7	0	-3.488374	-0.225082	-1.018703
32	6	0	-4.696693	-0.213797	-1.844427
33	1	0	-5.287881	-1.128492	-1.702302
34	1	0	-5.315236	0.647202	-1.580014
35	1	0	-4.401874	-0.157210	-2.892157
36	6	0	-3.629602	0.050709	0.372856
37	6	0	-3.348223	-0.931920	1.333883
38	6	0	-4.084917	1.308355	0.794698
39	6	0	-3.501330	-0.650487	2.691651
40	1	0	-3.014400	-1.912571	1.008729
41	6	0	-4.255015	1.577256	2.151915
42	1	0	-4.292646	2.075600	0.054054
43	6	0	-3.959470	0.601140	3.106316
44	1	0	-3.275308	-1.419585	3.425386
45	1	0	-4.607863	2.556558	2.464595
46	1	0	-4.087223	0.814309	4.163988

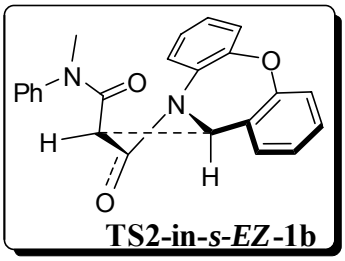


***trans*-5b**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.297190	-0.835562	0.146769
2	6	0	0.785299	0.497084	-0.280847
3	6	0	1.726447	1.628408	0.035593
4	6	0	1.372271	2.770201	0.758514
5	6	0	2.294692	3.795642	0.978413
6	6	0	3.589468	3.687591	0.471445
7	6	0	3.961204	2.557093	-0.257907
8	6	0	3.032975	1.541281	-0.468520
9	8	0	3.401271	0.481938	-1.289754
10	6	0	3.547996	-0.801957	-0.775863
11	6	0	2.516318	-1.477380	-0.097431
12	6	0	2.730606	-2.795378	0.335274
13	6	0	3.943103	-3.429360	0.075792
14	6	0	4.954832	-2.763422	-0.618023
15	6	0	4.751972	-1.449859	-1.039195
16	1	0	0.511021	0.492346	-1.339837
17	1	0	0.360101	2.870882	1.140235
18	1	0	1.998774	4.676298	1.540970
19	1	0	4.311414	4.481831	0.639130
20	1	0	4.957621	2.451619	-0.674892
21	1	0	1.933903	-3.303047	0.866187
22	1	0	4.091420	-4.450802	0.413816
23	1	0	5.898769	-3.257941	-0.826972
24	1	0	5.517534	-0.901578	-1.579036
25	6	0	-1.797178	0.214161	-0.121745
26	8	0	-1.847830	0.402685	-1.331063
27	6	0	-0.453883	0.233744	0.613632
28	6	0	0.205223	-1.140616	0.920059
29	8	0	-0.093500	-2.112344	1.583461
30	1	0	-0.489273	0.852110	1.515093
31	7	0	-2.905594	-0.034412	0.654330
32	6	0	-2.804099	-0.264814	2.104727

33	1	0	-3.774999	-0.601632	2.466428
34	1	0	-2.059479	-1.029906	2.334995
35	1	0	-2.556230	0.663663	2.637061
36	6	0	-4.205862	-0.062646	0.044636
37	6	0	-5.036467	-1.171505	0.241045
38	6	0	-4.660349	1.015012	-0.723426
39	6	0	-6.317670	-1.194342	-0.310522
40	1	0	-4.673713	-2.021132	0.812638
41	6	0	-5.936847	0.980303	-1.282380
42	1	0	-4.010992	1.866816	-0.888395
43	6	0	-6.772345	-0.119100	-1.074529
44	1	0	-6.954001	-2.060573	-0.150957
45	1	0	-6.280823	1.820891	-1.878936
46	1	0	-7.768000	-0.139104	-1.508830

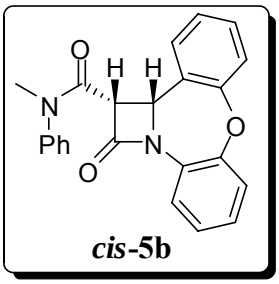


TS2-in-*s*-*EZ*-1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.264354	-1.019901	-0.720874
2	6	0	0.612135	0.078920	-1.188442
3	6	0	0.917477	1.436365	-0.846149
4	6	0	0.192294	2.450240	-1.521941
5	6	0	0.309430	3.786180	-1.182772
6	6	0	1.175241	4.150649	-0.141849
7	6	0	1.924370	3.185409	0.521013
8	6	0	1.817149	1.834633	0.175951
9	8	0	2.610130	0.998673	0.900636
10	6	0	3.267564	-0.101933	0.373111
11	6	0	2.639717	-1.100853	-0.380387
12	6	0	3.375758	-2.222043	-0.781550
13	6	0	4.718558	-2.344967	-0.427550
14	6	0	5.340482	-1.342708	0.316918
15	6	0	4.613406	-0.220987	0.713140
16	1	0	-0.045392	-0.069759	-2.034521
17	1	0	-0.486559	2.147707	-2.315647

18	1	0	-0.266123	4.539732	-1.710914
19	1	0	1.276121	5.194008	0.143446
20	1	0	2.614052	3.451499	1.314896
21	1	0	2.865096	-2.996308	-1.340728
22	1	0	5.274217	-3.225308	-0.736415
23	1	0	6.386389	-1.431239	0.595766
24	1	0	5.062996	0.567495	1.307924
25	6	0	-1.036819	-0.559471	1.026427
26	8	0	-0.077916	-0.229128	1.729506
27	6	0	-0.941112	-1.432110	-0.157945
28	6	0	0.303702	-2.080104	-0.522561
29	8	0	0.533194	-3.260902	-0.729481
30	1	0	-1.841357	-1.975302	-0.434676
31	7	0	-2.332687	-0.148350	1.361576
32	6	0	-2.524550	0.625280	2.585362
33	1	0	-2.793281	1.665462	2.357837
34	1	0	-3.323748	0.188668	3.195114
35	1	0	-1.585312	0.609101	3.137347
36	6	0	-3.464309	-0.297083	0.503901
37	6	0	-3.546547	0.418096	-0.698303
38	6	0	-4.526403	-1.129946	0.879700
39	6	0	-4.666022	0.287181	-1.520537
40	1	0	-2.729492	1.079003	-0.972522
41	6	0	-5.649570	-1.249866	0.061358
42	1	0	-4.457545	-1.689052	1.808576
43	6	0	-5.721347	-0.544937	-1.142210
44	1	0	-4.718290	0.843273	-2.452980
45	1	0	-6.465455	-1.902636	0.359946
46	1	0	-6.594878	-0.643414	-1.780755



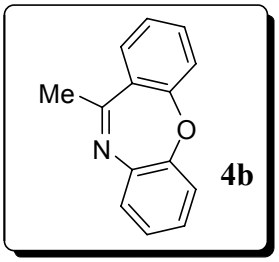
***cis*-5b**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.047372	-0.966128	-0.137488

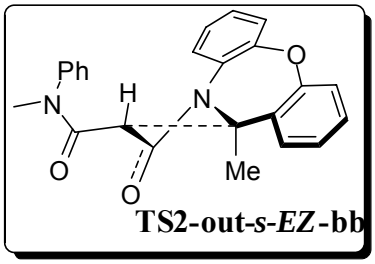
2	6	0	0.557259	0.287409	-0.772407
3	6	0	1.339790	1.536624	-0.450884
4	6	0	0.784462	2.758579	-0.060279
5	6	0	1.584171	3.889834	0.106824
6	6	0	2.958479	3.817723	-0.119567
7	6	0	3.529789	2.614407	-0.531113
8	6	0	2.721008	1.493519	-0.699793
9	8	0	3.309969	0.361746	-1.258004
10	6	0	3.439760	-0.815641	-0.533001
11	6	0	2.331280	-1.508323	-0.015612
12	6	0	2.532459	-2.736417	0.633596
13	6	0	3.816193	-3.265015	0.745628
14	6	0	4.912305	-2.581031	0.217245
15	6	0	4.717794	-1.355896	-0.419829
16	1	0	0.564375	0.163142	-1.864396
17	1	0	-0.279973	2.831340	0.121188
18	1	0	1.129519	4.825939	0.417730
19	1	0	3.584749	4.695307	0.014614
20	1	0	4.590881	2.528803	-0.742296
21	1	0	1.672110	-3.259989	1.033122
22	1	0	3.955575	-4.217862	1.247994
23	1	0	5.913365	-2.993419	0.301811
24	1	0	5.546521	-0.798327	-0.844683
25	6	0	-1.472622	0.641070	0.949773
26	8	0	-0.754856	1.090824	1.835531
27	6	0	-0.872234	-0.093638	-0.244723
28	6	0	-0.195857	-1.401194	0.244533
29	8	0	-0.591766	-2.415436	0.780447
30	1	0	-1.589085	-0.249506	-1.050698
31	7	0	-2.848191	0.742856	0.991516
32	6	0	-3.452012	1.392953	2.159934
33	1	0	-4.243261	2.076271	1.838064
34	1	0	-3.886036	0.646503	2.836018
35	1	0	-2.672186	1.942732	2.684916
36	6	0	-3.747150	0.039779	0.120376
37	6	0	-3.782034	-1.360584	0.107724
38	6	0	-4.634726	0.767228	-0.682199
39	6	0	-4.689374	-2.022429	-0.721582
40	1	0	-3.083080	-1.920871	0.722376
41	6	0	-5.548718	0.098694	-1.495787
42	1	0	-4.597740	1.853051	-0.670663
43	6	0	-5.577171	-1.297700	-1.518311
44	1	0	-4.704012	-3.108657	-0.736342
45	1	0	-6.232887	0.669035	-2.118106

46	1	0	-6.286983	-1.817358	-2.155906



Standard orientation:

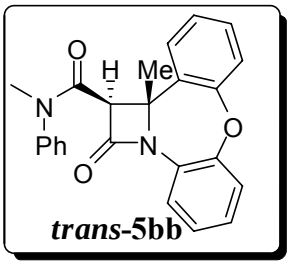
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.615610	1.794132	0.234918
2	6	0	-0.666729	1.681831	0.234271
3	6	0	-1.451446	0.437264	-0.001944
4	6	0	-2.695189	0.477858	-0.657456
5	6	0	-3.450361	-0.674621	-0.859776
6	6	0	-2.982802	-1.902990	-0.388829
7	6	0	-1.754733	-1.972578	0.266675
8	6	0	-1.001729	-0.815456	0.453566
9	8	0	0.171444	-0.927084	1.181327
10	6	0	1.323165	-0.581441	0.478650
11	6	0	1.511374	0.737845	0.027490
12	6	0	2.731169	1.042883	-0.600918
13	6	0	3.708229	0.070668	-0.794955
14	6	0	3.500255	-1.230629	-0.330756
15	6	0	2.303994	-1.553825	0.310511
16	1	0	-3.073601	1.428410	-1.019154
17	1	0	-4.404313	-0.612083	-1.375163
18	1	0	-3.571857	-2.805025	-0.529214
19	1	0	-1.367694	-2.909727	0.653495
20	1	0	2.884852	2.067549	-0.925203
21	1	0	4.639004	0.331933	-1.290427
22	1	0	4.266499	-1.989942	-0.458601
23	1	0	2.115252	-2.552353	0.692543
24	6	0	-1.447751	2.957664	0.463991
25	1	0	-1.984073	3.270480	-0.441224
26	1	0	-2.196579	2.829188	1.254331
27	1	0	-0.752995	3.752474	0.740457



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.242155	-0.968943	-0.642544
2	6	0	1.079481	0.141378	-1.425003
3	6	0	1.626230	1.435259	-1.025586
4	6	0	1.666808	2.497170	-1.964243
5	6	0	2.079387	3.775604	-1.619994
6	6	0	2.469507	4.047668	-0.305613
7	6	0	2.464733	3.027115	0.640532
8	6	0	2.063458	1.738540	0.292474
9	8	0	2.065122	0.825954	1.322956
10	6	0	2.765418	-0.364313	1.154548
11	6	0	2.349991	-1.280583	0.187589
12	6	0	2.979875	-2.525593	0.098293
13	6	0	4.026150	-2.829661	0.970494
14	6	0	4.448488	-1.898379	1.921109
15	6	0	3.817325	-0.656129	2.015059
16	1	0	1.354482	2.309154	-2.983664
17	1	0	2.090021	4.559847	-2.370599
18	1	0	2.786338	5.046778	-0.020570
19	1	0	2.773288	3.202005	1.665788
20	1	0	2.619738	-3.241865	-0.630297
21	1	0	4.511006	-3.799119	0.904682
22	1	0	5.264543	-2.137837	2.596614
23	1	0	4.109890	0.079126	2.757721
24	6	0	-2.330389	-1.145932	-1.336307
25	8	0	-2.377655	-1.795590	-2.384490
26	6	0	-1.055012	-0.849821	-0.680243
27	6	0	0.032575	-1.791225	-0.689775
28	8	0	0.059226	-3.009326	-0.738534
29	1	0	-0.977969	-0.011925	0.000400
30	7	0	-3.483680	-0.538309	-0.819435
31	6	0	-4.681227	-0.533692	-1.659598
32	1	0	-5.561682	-0.766431	-1.053980

33	1	0	-4.835187	0.438268	-2.147632
34	1	0	-4.545457	-1.293339	-2.429168
35	6	0	-3.579438	-0.005101	0.491762
36	6	0	-3.083112	-0.715292	1.598021
37	6	0	-4.225659	1.222013	0.708031
38	6	0	-3.200254	-0.187319	2.882489
39	1	0	-2.619789	-1.684027	1.442821
40	6	0	-4.356876	1.733353	1.998783
41	1	0	-4.616987	1.779329	-0.137665
42	6	0	-3.838678	1.037012	3.091811
43	1	0	-2.808037	-0.749206	3.726050
44	1	0	-4.859769	2.685547	2.146973
45	1	0	-3.939063	1.438878	4.096152
46	6	0	0.680807	-0.061682	-2.874183
47	1	0	0.269374	-1.057009	-3.036334
48	1	0	-0.068104	0.661705	-3.205820
49	1	0	1.572968	0.060237	-3.509770

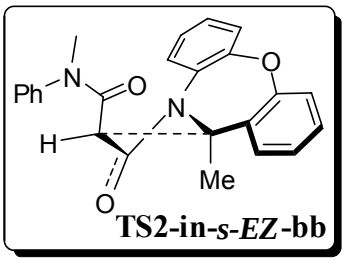


***trans*-5bb**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.350741	0.975656	0.621953
2	8	0	0.244979	-2.435921	-0.950533
3	8	0	1.460488	-1.542267	2.516648
4	7	0	-1.238197	-0.934076	0.132895
5	7	0	3.127171	-0.747608	1.182484
6	6	0	-2.555437	-1.168943	-0.283971
7	6	0	-3.562602	-0.211761	-0.066685
8	6	0	-4.872166	-0.468190	-0.467087
9	6	0	-5.194332	-1.661815	-1.110061
10	6	0	-4.193491	-2.603628	-1.355192
11	6	0	-2.885033	-2.363948	-0.944469
12	6	0	-2.329758	1.853612	0.276400
13	6	0	-0.978803	1.523641	0.474228
14	6	0	-0.024167	2.517987	0.235778

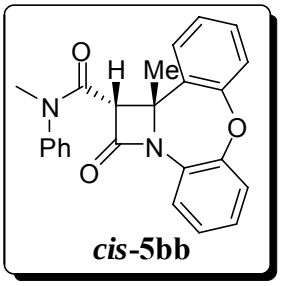
15	6	0	-0.395163	3.792602	-0.197027
16	6	0	-1.741298	4.093391	-0.399161
17	6	0	-2.711590	3.120904	-0.158177
18	6	0	3.607712	-0.297813	-0.092462
19	6	0	3.341191	-1.027184	-1.258646
20	6	0	3.846507	-0.584648	-2.482562
21	6	0	4.636934	0.563776	-2.548000
22	6	0	4.912399	1.283290	-1.382785
23	6	0	4.396860	0.857988	-0.159058
24	6	0	1.796963	-0.954048	1.494360
25	6	0	0.771416	-0.415904	0.505719
26	6	0	-0.040525	-1.485571	-0.251461
27	6	0	-0.628992	0.136985	0.989007
28	6	0	-0.986433	-0.001834	2.473034
29	1	0	-5.622868	0.289375	-0.265155
30	1	0	-6.217685	-1.848816	-1.421727
31	1	0	-4.429156	-3.535022	-1.861793
32	1	0	-2.099748	-3.088384	-1.124458
33	1	0	1.027169	2.300179	0.401750
34	1	0	0.368037	4.544854	-0.374268
35	1	0	-2.039483	5.081211	-0.738924
36	1	0	-3.768847	3.327764	-0.289955
37	1	0	2.718903	-1.915999	-1.206994
38	1	0	3.625460	-1.147627	-3.384845
39	1	0	5.035239	0.898510	-3.501781
40	1	0	5.522606	2.181329	-1.426636
41	1	0	4.597213	1.420652	0.748748
42	1	0	1.225566	0.259306	-0.219324
43	1	0	-0.806122	-1.016917	2.824296
44	1	0	-2.035528	0.268137	2.620556
45	1	0	-0.367966	0.678630	3.066739
46	6	0	4.132772	-1.277556	2.110129
47	1	0	4.961606	-0.570252	2.198021
48	1	0	3.661002	-1.425760	3.080331
49	1	0	4.526198	-2.237123	1.752123



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.274230	-1.035035	-0.564891
2	6	0	0.634765	0.002794	-1.192613
3	6	0	0.927128	1.381417	-0.862482
4	6	0	0.237191	2.406330	-1.569222
5	6	0	0.301157	3.738307	-1.205947
6	6	0	1.077646	4.110518	-0.099917
7	6	0	1.802656	3.151317	0.589687
8	6	0	1.760410	1.801863	0.215713
9	8	0	2.581692	1.019119	0.963613
10	6	0	3.271145	-0.075472	0.478315
11	6	0	2.657215	-1.097569	-0.246303
12	6	0	3.406603	-2.215798	-0.628196
13	6	0	4.753314	-2.307267	-0.276876
14	6	0	5.361610	-1.277712	0.442279
15	6	0	4.619888	-0.158039	0.817486
16	1	0	-0.382769	2.127805	-2.412312
17	1	0	-0.253503	4.483385	-1.767656
18	1	0	1.132080	5.150739	0.208563
19	1	0	2.439080	3.415686	1.427247
20	1	0	2.905224	-3.013631	-1.162254
21	1	0	5.323038	-3.185518	-0.565626
22	1	0	6.410247	-1.343885	0.717303
23	1	0	5.059493	0.651842	1.390584
24	6	0	-1.014284	-0.419003	1.166954
25	8	0	-0.059292	0.038668	1.802963
26	6	0	-0.912904	-1.450523	0.127860
27	6	0	0.332861	-2.082799	-0.236492
28	8	0	0.578875	-3.273879	-0.361686
29	1	0	-1.796483	-2.063137	-0.032516
30	7	0	-2.319202	-0.000880	1.464363
31	6	0	-2.517364	0.941120	2.561678
32	1	0	-2.715742	1.956392	2.190466
33	1	0	-3.367041	0.628718	3.178856
34	1	0	-1.605969	0.954866	3.158841
35	6	0	-3.443452	-0.259552	0.622469
36	6	0	-3.574271	0.391992	-0.611633
37	6	0	-4.452078	-1.134580	1.045333
38	6	0	-4.687503	0.155437	-1.419058
39	1	0	-2.802722	1.092479	-0.918906
40	6	0	-5.568384	-1.363108	0.240286

41	1	0	-4.345008	-1.639887	2.001067
42	6	0	-5.687280	-0.722207	-0.994908
43	1	0	-4.779105	0.663797	-2.375457
44	1	0	-6.342264	-2.048785	0.574804
45	1	0	-6.555371	-0.904365	-1.622441
46	6	0	-0.112418	-0.311461	-2.477281
47	1	0	-0.195306	-1.390070	-2.608911
48	1	0	-1.118386	0.111888	-2.509765
49	1	0	0.453216	0.095783	-3.330116

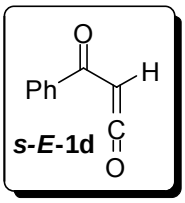


***cis*-5bb**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.074193	-1.007347	-0.190892
2	6	0	0.530051	0.236415	-0.826437
3	6	0	1.231172	1.514164	-0.415831
4	6	0	0.550830	2.695765	-0.102939
5	6	0	1.237080	3.879642	0.163410
6	6	0	2.631014	3.903037	0.116578
7	6	0	3.329073	2.745890	-0.222091
8	6	0	2.631134	1.570694	-0.496278
9	8	0	3.380266	0.512073	-1.001960
10	6	0	3.488614	-0.708462	-0.351904
11	6	0	2.375002	-1.489111	0.001767
12	6	0	2.584992	-2.751883	0.580725
13	6	0	3.878540	-3.225686	0.782360
14	6	0	4.980677	-2.453450	0.411548
15	6	0	4.778522	-1.195938	-0.154097
16	1	0	-0.533136	2.694226	-0.071318
17	1	0	0.681377	4.779356	0.411080
18	1	0	3.174046	4.819386	0.330266
19	1	0	4.411385	2.736117	-0.301678
20	1	0	1.721451	-3.342044	0.862428
21	1	0	4.021012	-4.205213	1.229550

22	1	0	5.990732	-2.821889	0.564556
23	1	0	5.610649	-0.567209	-0.454802
24	6	0	-1.415479	0.511101	1.008518
25	8	0	-0.663207	0.883374	1.900264
26	6	0	-0.871886	-0.188430	-0.235035
27	6	0	-0.149533	-1.479807	0.209513
28	8	0	-0.508518	-2.508034	0.746181
29	1	0	-1.628115	-0.336084	-1.005061
30	7	0	-2.783599	0.691143	1.080784
31	6	0	-3.311332	1.330280	2.292678
32	1	0	-4.191652	1.924444	2.035716
33	1	0	-3.597831	0.579299	3.039563
34	1	0	-2.535768	1.968118	2.714656
35	6	0	-3.735392	0.007096	0.252588
36	6	0	-3.776898	-1.393001	0.214512
37	6	0	-4.665032	0.751648	-0.483931
38	6	0	-4.732949	-2.036034	-0.573856
39	1	0	-3.047812	-1.968413	0.778611
40	6	0	-5.628105	0.101792	-1.254743
41	1	0	-4.622275	1.836962	-0.454757
42	6	0	-5.663275	-1.293836	-1.303084
43	1	0	-4.752885	-3.121763	-0.608009
44	1	0	-6.345101	0.686367	-1.824716
45	1	0	-6.411086	-1.799144	-1.907896
46	6	0	0.522046	0.125199	-2.363181
47	1	0	0.059181	-0.814915	-2.683082
48	1	0	-0.042590	0.960002	-2.792201
49	1	0	1.542722	0.164009	-2.752764

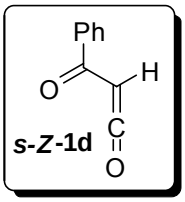


***s-E*-1d**

Standard orientation:

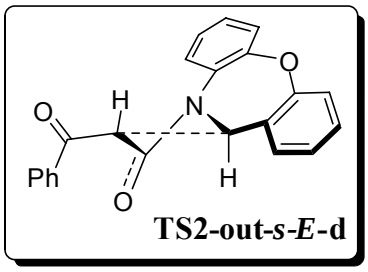
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.649644	0.483178	0.512315
2	6	0	1.412499	1.112842	0.415491
3	6	0	0.308993	0.430015	-0.118847
4	6	0	0.475104	-0.880212	-0.588833
5	6	0	1.719396	-1.506012	-0.501853

6	6	0	2.804863	-0.829244	0.055656
7	1	0	3.495428	1.014306	0.940149
8	1	0	1.274719	2.135327	0.751448
9	1	0	-0.349543	-1.405091	-1.061571
10	1	0	1.841414	-2.517678	-0.878420
11	1	0	3.772069	-1.319437	0.126785
12	6	0	-0.992095	1.171319	-0.193948
13	8	0	-1.017570	2.392187	-0.271365
14	6	0	-2.271361	0.424781	-0.151495
15	1	0	-3.175828	0.998849	-0.326919
16	6	0	-2.432434	-0.833194	0.236114
17	8	0	-2.595668	-1.935576	0.578980



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.809577	0.992868	0.081994
2	6	0	-1.433153	1.195770	0.061901
3	6	0	-0.553022	0.104585	-0.012264
4	6	0	-1.081316	-1.192751	-0.077618
5	6	0	-2.461019	-1.395436	-0.063801
6	6	0	-3.327209	-0.304036	0.019847
7	1	0	-3.481130	1.844761	0.144948
8	1	0	-1.008946	2.193337	0.102971
9	1	0	-0.426656	-2.055010	-0.159599
10	1	0	-2.858655	-2.404926	-0.120718
11	1	0	-4.402121	-0.463242	0.033917
12	6	0	0.915300	0.411617	-0.031073
13	8	0	1.318580	1.565889	-0.149391
14	6	0	1.860306	-0.712438	0.108954
15	1	0	1.570287	-1.739983	0.287054
16	6	0	3.163694	-0.450284	0.055858
17	8	0	4.301819	-0.225178	0.005470

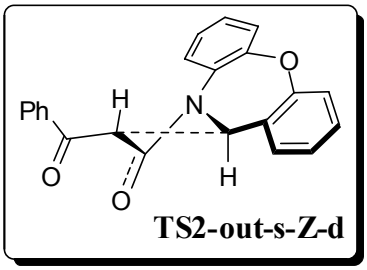


TS2-out-*s*-*E*-d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.645080	-0.667769	-0.193329
2	6	0	0.656060	0.633377	-0.611611
3	6	0	1.775838	1.528891	-0.495620
4	6	0	1.701074	2.772069	-1.167104
5	6	0	2.704273	3.720917	-1.050198
6	6	0	3.820764	3.446293	-0.251252
7	6	0	3.930991	2.224415	0.410577
8	6	0	2.925095	1.268628	0.290411
9	8	0	3.083717	0.117408	1.025166
10	6	0	2.968374	-1.126472	0.409426
11	6	0	1.762558	-1.545953	-0.163128
12	6	0	1.653958	-2.845437	-0.668279
13	6	0	2.747139	-3.709009	-0.598171
14	6	0	3.950988	-3.279227	-0.038120
15	6	0	4.063258	-1.982612	0.465472
16	1	0	-0.130606	0.936107	-1.289464
17	1	0	0.820118	2.980284	-1.768490
18	1	0	2.619617	4.671133	-1.567704
19	1	0	4.611417	4.183799	-0.147487
20	1	0	4.790212	1.991713	1.030695
21	1	0	0.706058	-3.164992	-1.083076
22	1	0	2.654296	-4.719350	-0.984962
23	1	0	4.802305	-3.951388	0.014745
24	1	0	4.979793	-1.626117	0.924223
25	6	0	-2.494650	0.886095	0.929168
26	8	0	-2.530092	2.006444	1.455934
27	6	0	-1.163379	0.268766	0.823635
28	6	0	-0.675959	-0.992171	0.290521
29	8	0	-1.158855	-2.113289	0.199079
30	1	0	-0.447016	0.804364	1.438876
31	6	0	-3.759321	0.323501	0.341741
32	6	0	-4.795295	1.243377	0.097518

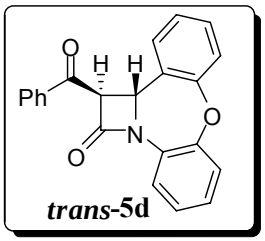
33	6	0	-3.980471	-1.035549	0.072190
34	6	0	-6.011979	0.821811	-0.427160
35	1	0	-4.618825	2.287431	0.333244
36	6	0	-5.208678	-1.455967	-0.443220
37	1	0	-3.202459	-1.761731	0.274128
38	6	0	-6.222790	-0.533712	-0.699723
39	1	0	-6.799414	1.546034	-0.620027
40	1	0	-5.371108	-2.512520	-0.640570
41	1	0	-7.175194	-0.867069	-1.104692



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.070106	-0.936158	-0.436692
2	6	0	0.595130	0.214693	-0.994143
3	6	0	1.121437	1.531860	-0.748410
4	6	0	0.675511	2.588673	-1.576714
5	6	0	1.082051	3.896798	-1.365780
6	6	0	1.955924	4.183730	-0.310020
7	6	0	2.425039	3.162006	0.514114
8	6	0	2.020359	1.846446	0.300013
9	8	0	2.478560	0.909922	1.195753
10	6	0	3.102149	-0.248400	0.733196
11	6	0	2.409096	-1.187323	-0.039230
12	6	0	3.031017	-2.393839	-0.378938
13	6	0	4.334415	-2.644913	0.049906
14	6	0	5.025011	-1.696306	0.805343
15	6	0	4.407055	-0.492310	1.147064
16	1	0	-0.046583	0.108772	-1.858354
17	1	0	-0.014810	2.354641	-2.382927
18	1	0	0.720529	4.691356	-2.010761
19	1	0	2.278656	5.205475	-0.131838
20	1	0	3.106617	3.363170	1.333895
21	1	0	2.471629	-3.123420	-0.951272
22	1	0	4.808913	-3.585907	-0.211667

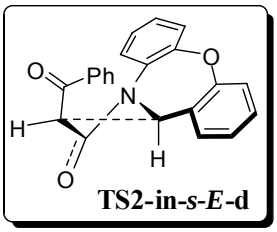
23	1	0	6.040424	-1.891933	1.136990
24	1	0	4.910215	0.255535	1.751419
25	6	0	-2.532699	-1.318039	-0.469790
26	8	0	-2.736384	-2.134669	-1.373324
27	6	0	-1.182319	-1.002996	-0.018094
28	6	0	-0.039459	-1.865936	-0.280847
29	8	0	0.074059	-3.071309	-0.379964
30	1	0	-1.030773	-0.249176	0.744929
31	6	0	-3.692531	-0.549730	0.113927
32	6	0	-4.912209	-0.593215	-0.579336
33	6	0	-3.624060	0.173429	1.314167
34	6	0	-6.029639	0.081123	-0.096043
35	1	0	-4.954899	-1.171130	-1.496817
36	6	0	-4.745539	0.843956	1.803793
37	1	0	-2.703714	0.197103	1.889718
38	6	0	-5.948916	0.804080	1.097825
39	1	0	-6.966293	0.042317	-0.646209
40	1	0	-4.680153	1.392996	2.739539
41	1	0	-6.821320	1.329037	1.478462



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.750710	-0.819273	0.061854
2	6	0	-0.358625	0.537474	0.536951
3	6	0	-1.238626	1.637662	0.006666
4	6	0	-0.766858	2.768667	-0.664404
5	6	0	-1.644493	3.768462	-1.089697
6	6	0	-3.011915	3.645324	-0.844171
7	6	0	-3.502024	2.525069	-0.171068
8	6	0	-2.617138	1.534986	0.246307
9	8	0	-3.122233	0.486756	1.007345
10	6	0	-3.144070	-0.809059	0.502787
11	6	0	-1.986234	-1.477348	0.063139
12	6	0	-2.089170	-2.806274	-0.377165
13	6	0	-3.320031	-3.457366	-0.356976

14	6	0	-4.461278	-2.798023	0.102619
15	6	0	-4.367190	-1.473707	0.528629
16	1	0	-0.302504	0.571970	1.629174
17	1	0	0.298848	2.881596	-0.842860
18	1	0	-1.257681	4.641289	-1.607426
19	1	0	-3.699335	4.419842	-1.172332
20	1	0	-4.559264	2.408263	0.044444
21	1	0	-1.194359	-3.308547	-0.725507
22	1	0	-3.381798	-4.486797	-0.697615
23	1	0	-5.420864	-3.305870	0.124859
24	1	0	-5.234546	-0.929739	0.889010
25	6	0	2.226616	0.345378	0.868975
26	8	0	2.051524	0.666117	2.035660
27	6	0	1.036697	0.281179	-0.088630
28	6	0	0.472570	-1.114745	-0.487160
29	8	0	0.903312	-2.082597	-1.076900
30	1	0	1.241240	0.869751	-0.988650
31	6	0	3.586802	0.046639	0.335946
32	6	0	4.693718	0.378629	1.135551
33	6	0	3.792645	-0.554240	-0.915997
34	6	0	5.985013	0.130410	0.683897
35	1	0	4.513724	0.831697	2.105026
36	6	0	5.089947	-0.811933	-1.359424
37	1	0	2.948271	-0.864628	-1.522537
38	6	0	6.184770	-0.464332	-0.566512
39	1	0	6.837368	0.396360	1.303051
40	1	0	5.244252	-1.288872	-2.323208
41	1	0	7.194048	-0.660722	-0.918820

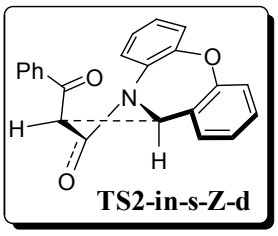


TS2-in-*s*-*E*-d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.978830	-0.392680	-1.238092
2	6	0	-0.067192	0.312924	-1.762235
3	6	0	-0.728987	1.416055	-1.129069
4	6	0	-1.711788	2.104708	-1.882131

5	6	0	-2.457965	3.134357	-1.333972
6	6	0	-2.233733	3.510981	-0.003648
7	6	0	-1.261670	2.866056	0.758018
8	6	0	-0.509049	1.829878	0.208756
9	8	0	0.385114	1.225857	1.052771
10	6	0	1.696074	0.976542	0.664725
11	6	0	2.010989	0.156078	-0.424590
12	6	0	3.351006	-0.139967	-0.698704
13	6	0	4.358068	0.377577	0.115576
14	6	0	4.037793	1.200301	1.195884
15	6	0	2.703534	1.502174	1.468419
16	1	0	-0.274536	0.173570	-2.813683
17	1	0	-1.889336	1.787671	-2.906231
18	1	0	-3.213701	3.637688	-1.928341
19	1	0	-2.813606	4.315214	0.440090
20	1	0	-1.069536	3.147919	1.787746
21	1	0	3.577182	-0.795729	-1.529811
22	1	0	5.394398	0.135549	-0.100107
23	1	0	4.820920	1.604489	1.830510
24	1	0	2.420037	2.125309	2.310335
25	6	0	-1.629728	-1.926759	-1.039579
26	8	0	-2.768204	-2.016321	-1.511276
27	6	0	-0.475512	-2.069105	-1.933371
28	6	0	0.921293	-1.761459	-1.688878
29	8	0	1.908538	-2.452546	-1.898602
30	1	0	-0.673114	-2.717925	-2.784891
31	6	0	-1.459793	-1.740306	0.445910
32	6	0	-2.521327	-1.152644	1.151626
33	6	0	-0.346478	-2.209383	1.158488
34	6	0	-2.454978	-1.000456	2.533501
35	1	0	-3.393844	-0.831158	0.591987
36	6	0	-0.287542	-2.070283	2.546225
37	1	0	0.462709	-2.713841	0.639797
38	6	0	-1.335185	-1.458170	3.234734
39	1	0	-3.279035	-0.534709	3.068126
40	1	0	0.575221	-2.447656	3.088721
41	1	0	-1.286116	-1.348153	4.315140

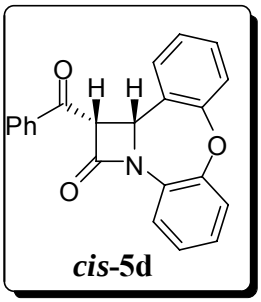


TS2-in-s-Z-d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.297131	-0.985777	-0.754531
2	6	0	0.485356	-0.081409	-1.374127
3	6	0	0.356948	1.295446	-1.008606
4	6	0	-0.481391	2.102088	-1.820644
5	6	0	-0.790442	3.406249	-1.484191
6	6	0	-0.258581	3.949764	-0.305247
7	6	0	0.587855	3.197299	0.499595
8	6	0	0.913774	1.880666	0.159257
9	8	0	1.761551	1.264597	1.027919
10	6	0	2.771022	0.394623	0.646473
11	6	0	2.569239	-0.712718	-0.184312
12	6	0	3.632758	-1.587254	-0.434059
13	6	0	4.879180	-1.360123	0.147835
14	6	0	5.075907	-0.250436	0.969867
15	6	0	4.021088	0.627600	1.215622
16	1	0	0.066040	-0.372681	-2.328274
17	1	0	-0.907451	1.654942	-2.715077
18	1	0	-1.445027	3.996709	-2.117087
19	1	0	-0.497304	4.970582	-0.020494
20	1	0	1.023206	3.609163	1.403671
21	1	0	3.450850	-2.453693	-1.057931
22	1	0	5.693018	-2.052792	-0.044205
23	1	0	6.044556	-0.067165	1.425437
24	1	0	4.137460	1.490074	1.863767
25	6	0	-1.365890	-1.112052	0.457488
26	8	0	-0.693974	-0.611147	1.366625
27	6	0	-0.800870	-1.935059	-0.613688
28	6	0	0.617206	-2.254956	-0.681789
29	8	0	1.171935	-3.337503	-0.748998
30	1	0	-1.465202	-2.662738	-1.074864
31	6	0	-2.858333	-0.883890	0.434857
32	6	0	-3.450193	-0.352457	1.590509
33	6	0	-3.668730	-1.144308	-0.680335
34	6	0	-4.819190	-0.103241	1.637662
35	1	0	-2.808318	-0.143615	2.439965
36	6	0	-5.039363	-0.887519	-0.637364
37	1	0	-3.231355	-1.533372	-1.594993
38	6	0	-5.618817	-0.370997	0.523006
39	1	0	-5.265523	0.300417	2.542898

40	1	0	-5.654424	-1.090222	-1.510346
41	1	0	-6.687728	-0.176650	0.558039

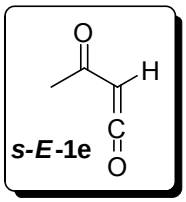


***cis*-5d**

Standard orientation:

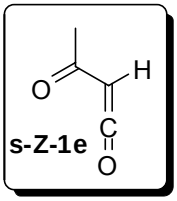
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.220188	-1.061633	0.392606
2	6	0	-0.311382	-0.033451	0.958542
3	6	0	-0.442364	1.338685	0.344652
4	6	0	0.618724	2.116050	-0.127904
5	6	0	0.404789	3.408708	-0.610209
6	6	0	-0.881025	3.947257	-0.620419
7	6	0	-1.951152	3.197129	-0.132665
8	6	0	-1.725867	1.910193	0.347468
9	8	0	-2.791719	1.256022	0.955513
10	6	0	-3.348267	0.114356	0.388370
11	6	0	-2.597003	-1.048692	0.145838
12	6	0	-3.243807	-2.187035	-0.360909
13	6	0	-4.615752	-2.162181	-0.599845
14	6	0	-5.360158	-1.010314	-0.339938
15	6	0	-4.719943	0.126378	0.152870
16	1	0	-0.469659	0.052116	2.042292
17	1	0	1.628744	1.723491	-0.109421
18	1	0	1.245781	3.990290	-0.976030
19	1	0	-1.053142	4.951269	-0.997930
20	1	0	-2.959889	3.596295	-0.102386
21	1	0	-2.654827	-3.075758	-0.553598
22	1	0	-5.102134	-3.051745	-0.989472
23	1	0	-6.430409	-0.991515	-0.522918
24	1	0	-5.266558	1.039464	0.366609
25	6	0	1.867373	-0.731746	-0.446089
26	8	0	1.464476	-0.665082	-1.596791
27	6	0	0.873651	-1.034717	0.675275
28	6	0	-0.237740	-2.006479	0.199935

29	8	0	-0.262800	-3.152587	-0.183280
30	1	0	1.362037	-1.370756	1.591214
31	6	0	3.319577	-0.551204	-0.128217
32	6	0	4.216611	-0.495547	-1.209514
33	6	0	3.817640	-0.413109	1.177218
34	6	0	5.578016	-0.318933	-0.989410
35	1	0	3.816888	-0.597490	-2.212969
36	6	0	5.182354	-0.225492	1.395953
37	1	0	3.147319	-0.435198	2.030584
38	6	0	6.064080	-0.183258	0.315065
39	1	0	6.263400	-0.286236	-1.831762
40	1	0	5.556024	-0.114719	2.409970
41	1	0	7.127972	-0.044491	0.487639



Standard orientation:

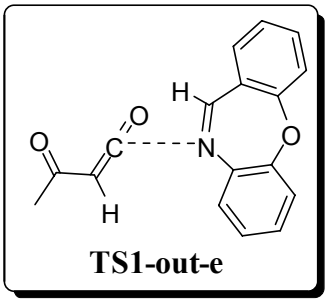
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.923015	1.396491	0.000000
2	6	0	-1.000561	-0.121835	-0.000001
3	6	0	0.274959	-0.878788	0.000000
4	6	0	1.468742	-0.302329	0.000000
5	8	0	2.507545	0.227817	0.000000
6	8	0	-2.062983	-0.717900	0.000001
7	1	0	-0.386167	1.758859	-0.885297
8	1	0	-0.386167	1.758858	0.885298
9	1	0	-1.935222	1.804094	0.000001
10	1	0	0.230304	-1.962381	0.000001



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.231730	-0.469262	0.000000
2	6	0	-0.854664	0.173724	-0.000001
3	6	0	0.280080	-0.775377	0.000002
4	6	0	1.524176	-0.305693	0.000001
5	8	0	2.606394	0.116322	0.000001
6	8	0	-0.698553	1.384856	-0.000003
7	1	0	-2.360136	-1.106184	0.883786
8	1	0	-2.360135	-1.106187	-0.883784
9	1	0	-2.992202	0.313499	-0.000002
10	1	0	0.142573	-1.850905	0.000004

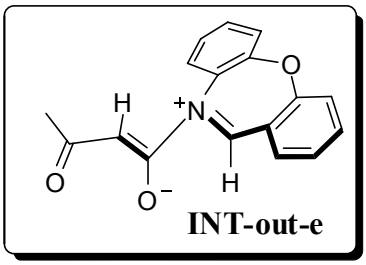


TS1-out-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.280847	-0.343059	0.270526
2	6	0	0.585723	-1.300432	0.204459
3	6	0	2.041760	-1.228548	0.083235
4	6	0	2.820717	-2.304445	0.556098
5	6	0	4.210175	-2.295130	0.431101
6	6	0	4.843711	-1.214238	-0.196750
7	6	0	4.089544	-0.144305	-0.691133
8	6	0	2.704141	-0.157858	-0.549466
9	8	0	1.980136	0.884423	-1.164425
10	6	0	1.086662	1.646395	-0.371790
11	6	0	-0.001678	1.046752	0.292466
12	6	0	-0.873236	1.877455	1.020674
13	6	0	-0.670665	3.258057	1.072417
14	6	0	0.403638	3.835031	0.385288
15	6	0	1.286637	3.023459	-0.335145
16	1	0	0.155920	-2.300381	0.279990
17	1	0	2.319817	-3.145705	1.025321
18	1	0	4.794532	-3.127468	0.806776
19	1	0	5.922307	-1.207714	-0.311774

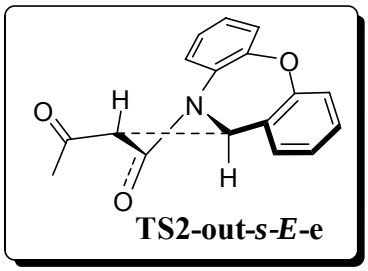
20	1	0	4.553319	0.690913	-1.201589
21	1	0	-1.705829	1.418339	1.538788
22	1	0	-1.355728	3.879690	1.637730
23	1	0	0.555039	4.908640	0.406902
24	1	0	2.126722	3.438780	-0.878805
25	6	0	-4.514311	-0.504371	-0.464127
26	8	0	-5.210308	0.441426	-0.897763
27	6	0	-3.074731	-0.315397	-0.256826
28	6	0	-2.279802	-1.295812	0.203888
29	8	0	-2.013780	-2.411597	0.572206
30	1	0	-2.670024	0.651518	-0.507028
31	6	0	-5.139727	-1.851577	-0.146055
32	1	0	-4.690913	-2.649101	-0.750438
33	1	0	-4.989850	-2.121396	0.906306
34	1	0	-6.209125	-1.798936	-0.356005



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.128841	-0.173205	-0.528296
2	8	0	2.587300	0.372652	-1.552395
3	6	0	2.612230	-0.897136	0.538416
4	6	0	-0.180126	-1.132259	-0.458105
5	7	0	0.490273	-0.014474	-0.359924
6	6	0	-0.049733	1.301212	-0.186662
7	6	0	0.609966	2.395499	-0.777187
8	6	0	0.123594	3.691030	-0.591667
9	6	0	-1.021675	3.916936	0.179414
10	6	0	-1.691607	2.835110	0.758773
11	6	0	-1.209570	1.543271	0.572283
12	8	0	-1.894072	0.502279	1.249963
13	6	0	-2.434573	-0.549620	0.492319
14	6	0	-1.604412	-1.358924	-0.310611
15	6	0	-3.786552	-0.838273	0.654465
16	6	0	-4.335163	-1.951550	0.008333

17	6	0	-2.175209	-2.491694	-0.933604
18	6	0	-3.530793	-2.778465	-0.789510
19	1	0	0.430939	-1.999480	-0.691655
20	1	0	1.491122	2.203852	-1.375376
21	1	0	0.645706	4.522672	-1.050893
22	1	0	-1.392651	4.924463	0.331376
23	1	0	-2.575203	2.971315	1.370311
24	1	0	-4.382549	-0.202549	1.297422
25	1	0	-5.387366	-2.180295	0.138004
26	1	0	-1.541169	-3.136282	-1.534243
27	1	0	-3.957229	-3.645329	-1.280684
28	1	0	1.946036	-1.209927	1.331068
29	6	0	4.007234	-1.260571	0.722032
30	8	0	4.355301	-1.928152	1.731826
31	6	0	5.040618	-0.839349	-0.307807
32	1	0	6.019204	-1.201186	0.013824
33	1	0	4.801121	-1.242505	-1.298413
34	1	0	5.063476	0.250268	-0.421950

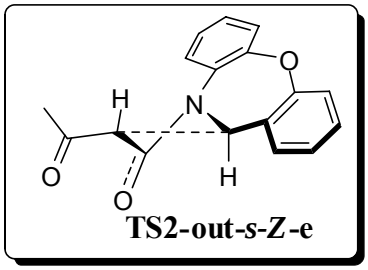


TS2-out-*s*-*E*-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.451295	-0.692675	0.329701
2	6	0	0.477906	0.621341	0.718226
3	6	0	-0.573876	1.573161	0.467949
4	6	0	-0.494305	2.831273	1.109912
5	6	0	-1.427382	3.828267	0.873246
6	6	0	-2.478961	3.587493	-0.019084
7	6	0	-2.595234	2.351804	-0.653134
8	6	0	-1.658998	1.348202	-0.413885
9	8	0	-1.818969	0.184137	-1.128398
10	6	0	-1.824363	-1.048648	-0.480873
11	6	0	-0.698948	-1.514576	0.208238
12	6	0	-0.698618	-2.810846	0.733237
13	6	0	-1.820296	-3.624070	0.570665

14	6	0	-2.946171	-3.146262	-0.101545
15	6	0	-2.949212	-1.853585	-0.627963
16	1	0	1.184171	0.888207	1.493443
17	1	0	0.337061	3.011950	1.786304
18	1	0	-1.337909	4.788689	1.370799
19	1	0	-3.214783	4.361612	-0.216881
20	1	0	-3.406519	2.143420	-1.342637
21	1	0	0.192157	-3.167311	1.236168
22	1	0	-1.811433	-4.632274	0.973790
23	1	0	-3.820532	-3.778325	-0.225326
24	1	0	-3.800985	-1.462868	-1.175207
25	6	0	3.811757	0.496369	-0.481009
26	8	0	4.200289	1.548273	-0.987591
27	6	0	2.384524	0.155049	-0.519895
28	6	0	1.797426	-1.075047	-0.021581
29	8	0	2.266971	-2.189242	0.154969
30	1	0	1.804560	0.724406	-1.239293
31	6	0	4.777311	-0.441099	0.225024
32	1	0	4.838333	-1.395664	-0.308374
33	1	0	5.761608	0.030302	0.264503
34	1	0	4.433523	-0.681713	1.237783

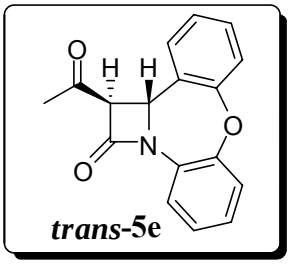


TS2-out-*s*-*Z*-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.370033	-0.766492	-0.359035
2	6	0	-0.532561	0.533578	-0.737973
3	6	0	0.410665	1.593329	-0.487138
4	6	0	0.217119	2.824952	-1.155442
5	6	0	1.041261	3.914852	-0.922155
6	6	0	2.092754	3.797971	-0.005121
7	6	0	2.318842	2.592563	0.657424
8	6	0	1.493590	1.495556	0.419923
9	8	0	1.746073	0.365584	1.160585
10	6	0	1.908079	-0.863336	0.521785

11	6	0	0.861825	-1.451253	-0.198605
12	6	0	1.022639	-2.740554	-0.718109
13	6	0	2.223247	-3.422091	-0.518721
14	6	0	3.268027	-2.821960	0.185403
15	6	0	3.110622	-1.536683	0.706476
16	1	0	-1.280444	0.730395	-1.494114
17	1	0	-0.611219	2.906696	-1.854563
18	1	0	0.868454	4.851245	-1.443138
19	1	0	2.743347	4.645761	0.189385
20	1	0	3.131740	2.480067	1.367069
21	1	0	0.193298	-3.194542	-1.246284
22	1	0	2.339196	-4.424956	-0.918587
23	1	0	4.203111	-3.352667	0.338093
24	1	0	3.896420	-1.052562	1.277290
25	6	0	-3.883225	-0.048925	0.312662
26	8	0	-4.550903	-0.714869	-0.474161
27	6	0	-2.434660	-0.198496	0.450388
28	6	0	-1.684377	-1.329845	-0.074120
29	8	0	-1.979300	-2.489255	-0.284240
30	1	0	-1.936521	0.375437	1.226486
31	6	0	-4.533558	1.031332	1.173590
32	1	0	-3.968833	1.971033	1.139752
33	1	0	-5.555844	1.203212	0.830049
34	1	0	-4.561168	0.708699	2.222734

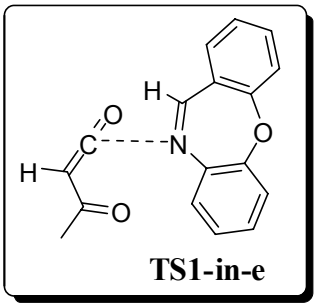


***trans*-5e**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.217669	-0.914741	-0.067909
2	6	0	0.906908	0.296203	0.462632
3	6	0	0.255697	1.587686	0.046731
4	6	0	0.923891	2.638039	-0.587167
5	6	0	0.257022	3.822586	-0.907823
6	6	0	-1.094061	3.967628	-0.593572
7	6	0	-1.777985	2.931105	0.043756

8	6	0	-1.102376	1.755041	0.356803
9	8	0	-1.781268	0.786839	1.087883
10	6	0	-2.096027	-0.443430	0.520298
11	6	0	-1.125298	-1.306610	-0.020950
12	6	0	-1.522759	-2.556843	-0.519905
13	6	0	-2.859422	-2.942689	-0.457834
14	6	0	-3.815062	-2.093060	0.101980
15	6	0	-3.427660	-0.844564	0.587077
16	1	0	1.012252	0.241631	1.551308
17	1	0	1.980711	2.539677	-0.819098
18	1	0	0.794584	4.628816	-1.398235
19	1	0	-1.618013	4.886680	-0.840337
20	1	0	-2.825973	3.021063	0.311029
21	1	0	-0.769142	-3.208830	-0.945901
22	1	0	-3.150143	-3.914922	-0.844828
23	1	0	-4.856895	-2.394285	0.157005
24	1	0	-4.144694	-0.158143	1.026167
25	6	0	3.391265	-0.551881	0.618188
26	8	0	3.393011	-0.346179	1.816410
27	6	0	2.187548	-0.205001	-0.248942
28	6	0	1.332118	-1.428203	-0.687342
29	8	0	1.545568	-2.443688	-1.313110
30	1	0	2.491925	0.378027	-1.124537
31	6	0	4.540927	-1.207919	-0.114081
32	1	0	5.307941	-1.519866	0.597270
33	1	0	4.169760	-2.070427	-0.682107
34	1	0	4.977171	-0.510547	-0.840935

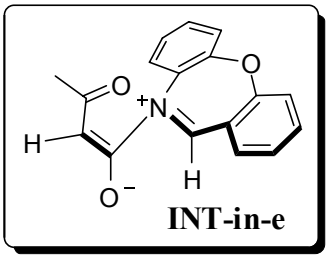


TS1-in-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.433872	-0.703047	-0.465806
2	6	0	-0.622164	-1.408070	-0.284864
3	6	0	-1.998258	-0.977260	-0.036405

4	6	0	-3.052870	-1.836303	-0.391772
5	6	0	-4.377615	-1.487658	-0.149229
6	6	0	-4.665554	-0.274188	0.481444
7	6	0	-3.634613	0.587429	0.857370
8	6	0	-2.311332	0.238028	0.600029
9	8	0	-1.322535	1.067840	1.085602
10	6	0	-0.400834	1.555914	0.165403
11	6	0	0.463401	0.703036	-0.542351
12	6	0	1.414156	1.282455	-1.395112
13	6	0	1.501554	2.664156	-1.541625
14	6	0	0.641987	3.496051	-0.822938
15	6	0	-0.310467	2.937167	0.029284
16	1	0	-0.475835	-2.486564	-0.373811
17	1	0	-2.815978	-2.785562	-0.865949
18	1	0	-5.179503	-2.160856	-0.436312
19	1	0	-5.695652	0.000469	0.690531
20	1	0	-3.834416	1.524507	1.366503
21	1	0	2.087532	0.624711	-1.933676
22	1	0	2.245805	3.088758	-2.208798
23	1	0	0.712475	4.575698	-0.918507
24	1	0	-0.986522	3.556428	0.610082
25	6	0	3.110091	-0.672035	1.104324
26	8	0	2.113510	-0.168926	1.614249
27	6	0	3.122275	-1.547569	-0.062465
28	6	0	2.102977	-2.006140	-0.825324
29	8	0	1.647183	-2.758481	-1.612505
30	1	0	4.061594	-2.032720	-0.321504
31	6	0	4.489978	-0.423740	1.710470
32	1	0	4.952441	-1.367182	2.026741
33	1	0	5.161505	0.036609	0.974971
34	1	0	4.387926	0.235936	2.574165

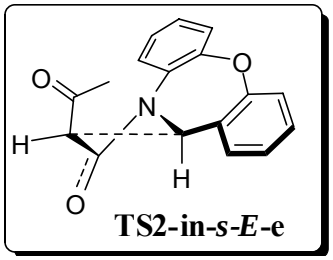


INT-in-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

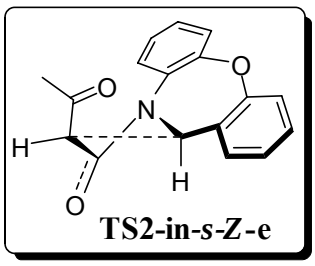
1	7	0	0.522366	-0.657075	-0.617399
2	6	0	-0.553624	-1.365572	-0.537894
3	6	0	-1.896400	-0.937892	-0.196964
4	6	0	-2.977342	-1.736076	-0.620120
5	6	0	-4.285295	-1.405757	-0.288388
6	6	0	-4.529929	-0.279565	0.503761
7	6	0	-3.474445	0.515282	0.950518
8	6	0	-2.165441	0.191397	0.603389
9	8	0	-1.155716	0.941989	1.156730
10	6	0	-0.240019	1.522704	0.289423
11	6	0	0.596733	0.760037	-0.536686
12	6	0	1.527931	1.414084	-1.352962
13	6	0	1.635214	2.802464	-1.327414
14	6	0	0.814653	3.551219	-0.483857
15	6	0	-0.127706	2.908057	0.318746
16	1	0	-0.418602	-2.415930	-0.788066
17	1	0	-2.772129	-2.619013	-1.219769
18	1	0	-5.107525	-2.026322	-0.630051
19	1	0	-5.547499	-0.022674	0.784028
20	1	0	-3.642839	1.379984	1.583525
21	1	0	2.154846	0.824887	-2.011872
22	1	0	2.363534	3.293905	-1.964888
23	1	0	0.903962	4.632894	-0.447554
24	1	0	-0.775662	3.461193	0.990625
25	6	0	2.729307	-1.035687	1.220505
26	8	0	1.724469	-0.488896	1.702177
27	6	0	2.839523	-1.520365	-0.129583
28	6	0	1.858077	-1.494688	-1.103566
29	8	0	1.723457	-1.941346	-2.227014
30	1	0	3.750379	-2.027093	-0.433359
31	6	0	3.962565	-1.239371	2.100177
32	1	0	4.193646	-2.306578	2.207397
33	1	0	4.844217	-0.761518	1.655228
34	1	0	3.776628	-0.809818	3.086875



TS2-in-*s*-*E*-e

Standard orientation:

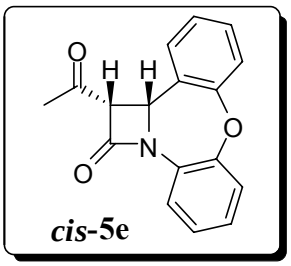
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.602333	0.912365	-0.552135
2	6	0	0.613472	0.518479	-1.035546
3	6	0	1.282240	-0.708411	-0.707649
4	6	0	2.465828	-1.020898	-1.419942
5	6	0	3.210836	-2.151917	-1.128805
6	6	0	2.783687	-3.014263	-0.111600
7	6	0	1.613049	-2.744821	0.595670
8	6	0	0.863088	-1.608632	0.303536
9	8	0	-0.242318	-1.389918	1.090684
10	6	0	-1.478633	-1.113447	0.510914
11	6	0	-1.687292	0.035505	-0.259662
12	6	0	-2.974686	0.327335	-0.724210
13	6	0	-4.033515	-0.525716	-0.413281
14	6	0	-3.815678	-1.674437	0.348119
15	6	0	-2.532876	-1.970388	0.809790
16	1	0	1.001699	1.061040	-1.885253
17	1	0	2.796391	-0.333772	-2.194188
18	1	0	4.121072	-2.362400	-1.681048
19	1	0	3.360760	-3.902679	0.128030
20	1	0	1.262512	-3.403573	1.383137
21	1	0	-3.127106	1.233546	-1.296248
22	1	0	-5.030719	-0.287805	-0.771037
23	1	0	-4.640483	-2.338081	0.590088
24	1	0	-2.333465	-2.845770	1.419280
25	6	0	0.688330	2.836685	-0.266449
26	6	0	-0.663953	2.353934	-0.474155
27	8	0	-1.685248	2.998874	-0.661292
28	1	0	0.922823	3.780088	-0.757183
29	6	0	1.656043	2.489072	0.779140
30	8	0	2.786582	2.975854	0.735152
31	6	0	1.257337	1.636412	1.977911
32	1	0	0.386074	0.999973	1.820756
33	1	0	2.113304	1.028251	2.283947
34	1	0	1.027666	2.319185	2.805624



TS2-in-*s*-*Z*-e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.681300	0.884807	-0.675563
2	6	0	0.535854	0.526055	-1.172702
3	6	0	1.258172	-0.655036	-0.814307
4	6	0	2.471955	-0.902990	-1.505919
5	6	0	3.321686	-1.931701	-1.146441
6	6	0	2.973624	-2.756177	-0.065531
7	6	0	1.779653	-2.559142	0.616402
8	6	0	0.908830	-1.527623	0.249561
9	8	0	-0.230305	-1.459611	0.989663
10	6	0	-1.476486	-1.136289	0.475794
11	6	0	-1.727126	-0.000563	-0.302173
12	6	0	-3.039770	0.289328	-0.691637
13	6	0	-4.087780	-0.543028	-0.300815
14	6	0	-3.830441	-1.677790	0.468498
15	6	0	-2.523454	-1.974441	0.852898
16	1	0	0.886916	1.066035	-2.042270
17	1	0	2.737686	-0.236426	-2.322548
18	1	0	4.249795	-2.092141	-1.685605
19	1	0	3.633391	-3.564601	0.236716
20	1	0	1.486302	-3.200019	1.440844
21	1	0	-3.217631	1.187150	-1.270666
22	1	0	-5.103042	-0.300596	-0.599943
23	1	0	-4.641920	-2.330851	0.775809
24	1	0	-2.293043	-2.839860	1.465667
25	6	0	0.661881	2.693792	-0.183747
26	6	0	-0.707452	2.316649	-0.492628
27	8	0	-1.696338	3.011255	-0.652211
28	1	0	0.962821	3.687691	-0.515431
29	6	0	1.409272	2.155947	0.959539
30	8	0	1.028714	1.243099	1.692832
31	6	0	2.744762	2.847621	1.231493
32	1	0	3.282781	3.085718	0.306576
33	1	0	2.570227	3.793219	1.761339
34	1	0	3.359166	2.205421	1.866489

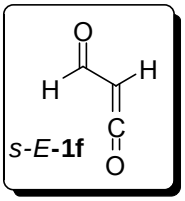


***cis*-5e**

Standard orientation:

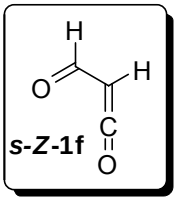
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.110877	-1.043639	0.385295
2	6	0	0.791823	-0.015434	0.975338
3	6	0	0.686498	1.364497	0.371644
4	6	0	1.762358	2.155162	-0.042729
5	6	0	1.561504	3.463264	-0.486575
6	6	0	0.277555	4.006203	-0.516897
7	6	0	-0.806904	3.242631	-0.086486
8	6	0	-0.594854	1.940682	0.358161
9	8	0	-1.681990	1.273801	0.918266
10	6	0	-2.225737	0.150047	0.310739
11	6	0	-1.478697	-1.018986	0.085087
12	6	0	-2.115328	-2.147527	-0.453965
13	6	0	-3.476733	-2.107349	-0.745780
14	6	0	-4.217825	-0.948530	-0.508467
15	6	0	-3.586635	0.177633	0.018816
16	1	0	0.572129	0.076621	2.048320
17	1	0	2.762437	1.744706	-0.032313
18	1	0	2.413247	4.054154	-0.810446
19	1	0	0.117923	5.022593	-0.865900
20	1	0	-1.815945	3.641905	-0.071150
21	1	0	-1.530640	-3.043424	-0.626018
22	1	0	-3.956976	-2.989383	-1.159223
23	1	0	-5.279603	-0.916979	-0.733996
24	1	0	-4.132678	1.093942	0.219513
25	6	0	3.042678	-1.004940	-0.267827
26	8	0	3.045254	-0.222768	-1.196418
27	6	0	1.956418	-1.052122	0.805661
28	6	0	0.840483	-2.029167	0.328627
29	8	0	0.817755	-3.196415	0.003096
30	1	0	2.391169	-1.361467	1.761335
31	6	0	4.062398	-2.118608	-0.135177
32	1	0	3.539617	-3.083813	-0.116430

33	1	0	4.755294	-2.085216	-0.977973
34	1	0	4.618008	-2.029857	0.806621



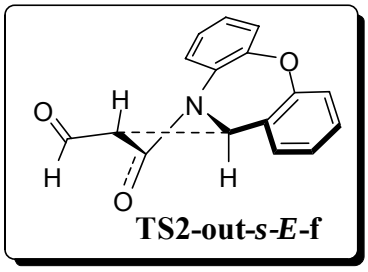
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.131227	-0.372232	0.000000
2	6	0	-0.006779	0.573067	0.000000
3	6	0	1.251505	0.147104	0.000000
4	8	0	2.340606	-0.262861	0.000000
5	8	0	-2.294853	-0.022644	0.000000
6	1	0	-0.198928	1.640748	0.000000
7	1	0	-0.848091	-1.444343	0.000000



Standard orientation:

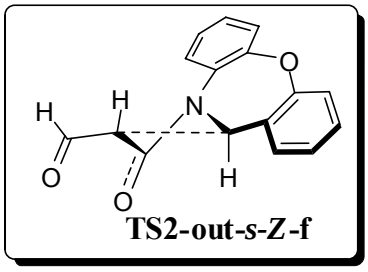
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.343823	0.283843	-0.000001
2	6	0	0.022189	0.921685	0.000002
3	6	0	-1.079268	0.172460	0.000001
4	8	0	-2.028158	-0.495322	0.000001
5	8	0	1.552236	-0.915354	-0.000003
6	1	0	-0.088725	2.000322	0.000004
7	1	0	2.175643	1.017157	0.000000



TS2-out-*s*-*E*-f

Standard orientation:

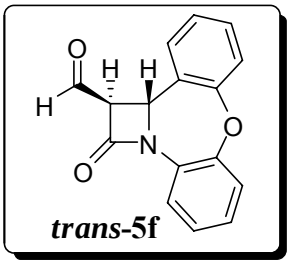
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.195532	-1.001326	0.335852
2	6	0	0.954176	0.075460	0.723665
3	6	0	0.619727	1.450505	0.457484
4	6	0	1.393981	2.452688	1.088785
5	6	0	1.186239	3.798881	0.834929
6	6	0	0.183097	4.181764	-0.063868
7	6	0	-0.609845	3.219509	-0.686219
8	6	0	-0.403798	1.865459	-0.429636
9	8	0	-1.196225	0.987812	-1.130306
10	6	0	-1.889974	-0.026196	-0.474137
11	6	0	-1.217802	-1.039143	0.218733
12	6	0	-1.942170	-2.110228	0.751203
13	6	0	-3.327397	-2.155455	0.592885
14	6	0	-3.993544	-1.131666	-0.082353
15	6	0	-3.273099	-0.062365	-0.616907
16	1	0	1.674372	-0.092140	1.514028
17	1	0	2.181700	2.141407	1.769903
18	1	0	1.800848	4.547844	1.324024
19	1	0	0.012244	5.233494	-0.274738
20	1	0	-1.397699	3.496564	-1.378671
21	1	0	-1.403035	-2.902384	1.256719
22	1	0	-3.884266	-2.993173	1.001686
23	1	0	-5.072311	-1.165356	-0.202418
24	1	0	-3.761207	0.735684	-1.166883
25	6	0	3.617111	-1.934825	-0.336382
26	8	0	4.638339	-1.411536	-0.769741
27	6	0	2.287165	-1.368950	-0.485527
28	6	0	1.100158	-2.065790	-0.015480
29	8	0	0.876455	-3.254115	0.140780
30	1	0	2.163044	-0.591153	-1.232927
31	1	0	3.664898	-2.876681	0.249398



TS2-out-*s*-*Z*-f

Standard orientation:

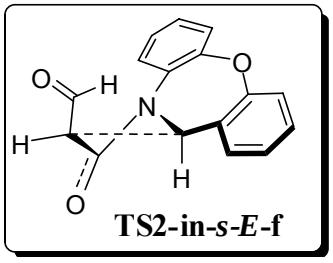
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.922081	0.277718	-0.241846
2	6	0	0.432173	-0.952414	-0.578963
3	6	0	-0.927214	-1.382564	-0.377539
4	6	0	-1.339068	-2.586970	-0.995228
5	6	0	-2.609694	-3.104951	-0.800412
6	6	0	-3.511009	-2.422374	0.025715
7	6	0	-3.140494	-1.225045	0.635539
8	6	0	-1.865130	-0.700919	0.436117
9	8	0	-1.561801	0.451160	1.120827
10	6	0	-1.047518	1.553415	0.439140
11	6	0	0.192922	1.494584	-0.206014
12	6	0	0.731377	2.655257	-0.771854
13	6	0	0.025208	3.855585	-0.691809
14	6	0	-1.218974	3.902486	-0.061438
15	6	0	-1.758771	2.746524	0.504762
16	1	0	1.017389	-1.535373	-1.277473
17	1	0	-0.624988	-3.114428	-1.622400
18	1	0	-2.899985	-4.034183	-1.280257
19	1	0	-4.508414	-2.819943	0.189915
20	1	0	-3.826672	-0.678638	1.273982
21	1	0	1.705947	2.601223	-1.241237
22	1	0	0.451606	4.754548	-1.126593
23	1	0	-1.768899	4.836977	-0.001551
24	1	0	-2.713693	2.756441	1.020199
25	6	0	3.509640	-2.094536	0.669045
26	8	0	4.496561	-1.938399	-0.040171
27	6	0	2.358485	-1.213550	0.730347
28	6	0	2.314253	0.123247	0.146633
29	8	0	3.167007	0.967189	-0.037319
30	1	0	1.609964	-1.428681	1.487964
31	1	0	3.411933	-3.008221	1.299429



***trans*-5f**

Standard orientation:

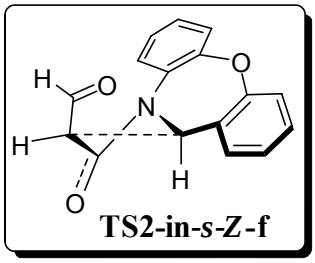
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.009446	-1.090876	0.030653
2	6	0	1.088649	-0.250540	0.570816
3	6	0	1.040042	1.184541	0.115446
4	6	0	2.093621	1.853068	-0.512474
5	6	0	1.972554	3.197880	-0.870037
6	6	0	0.790902	3.887884	-0.599815
7	6	0	-0.271008	3.236802	0.030499
8	6	0	-0.139588	1.896455	0.380535
9	8	0	-1.168872	1.298967	1.100342
10	6	0	-1.945489	0.301492	0.516959
11	6	0	-1.396154	-0.893291	0.016212
12	6	0	-2.252376	-1.876692	-0.502674
13	6	0	-3.630477	-1.675099	-0.500136
14	6	0	-4.172340	-0.498221	0.019247
15	6	0	-3.324882	0.487344	0.524475
16	1	0	1.103607	-0.296869	1.668435
17	1	0	3.022723	1.327475	-0.713053
18	1	0	2.802030	3.702613	-1.356271
19	1	0	0.692612	4.933686	-0.876602
20	1	0	-1.197444	3.752189	0.262527
21	1	0	-1.818257	-2.787421	-0.898337
22	1	0	-4.280534	-2.446480	-0.902349
23	1	0	-5.246906	-0.342313	0.027389
24	1	0	-3.712434	1.415140	0.933192
25	6	0	3.000812	-2.001322	0.855749
26	8	0	4.157233	-2.261256	0.616844
27	6	0	2.095336	-1.243080	-0.084429
28	6	0	0.824191	-2.020475	-0.552639
29	8	0	0.620043	-3.033565	-1.178079
30	1	0	2.670286	-0.848643	-0.924475
31	1	0	2.520454	-2.326887	1.805705



TS2-in-*s*-*E*-f

Standard orientation:

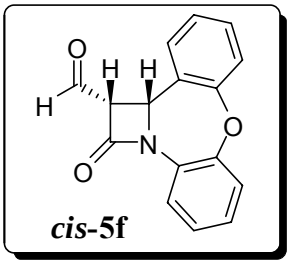
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.717477	0.929337	-0.493088
2	6	0	0.577501	0.835118	-0.936217
3	6	0	1.472076	-0.252368	-0.637110
4	6	0	2.696063	-0.315397	-1.343111
5	6	0	3.639810	-1.293361	-1.071840
6	6	0	3.377994	-2.245467	-0.079521
7	6	0	2.173272	-2.220403	0.621540
8	6	0	1.224114	-1.239379	0.347475
9	8	0	0.090575	-1.246570	1.127288
10	6	0	-1.167379	-1.241114	0.528596
11	6	0	-1.598453	-0.157261	-0.244320
12	6	0	-2.910090	-0.131253	-0.728535
13	6	0	-3.773783	-1.187990	-0.439907
14	6	0	-3.332891	-2.273166	0.318784
15	6	0	-2.024453	-2.301274	0.803778
16	1	0	0.848523	1.449312	-1.784710
17	1	0	2.895675	0.440133	-2.098413
18	1	0	4.576341	-1.314716	-1.619821
19	1	0	4.111812	-3.013884	0.145773
20	1	0	1.950131	-2.951622	1.391209
21	1	0	-3.238206	0.729333	-1.298412
22	1	0	-4.793500	-1.159759	-0.811861
23	1	0	-4.005827	-3.095740	0.541913
24	1	0	-1.659976	-3.120961	1.414359
25	6	0	0.233517	2.948728	0.042369
26	6	0	-1.032244	2.322275	-0.314937
27	8	0	-2.132522	2.815065	-0.493484
28	1	0	0.388495	3.985364	-0.253704
29	6	0	1.040787	2.499196	1.170375
30	8	0	1.997620	3.122574	1.612605
31	1	0	0.728449	1.537322	1.629507



TS2-in-*s*-*Z*-f

Standard orientation:

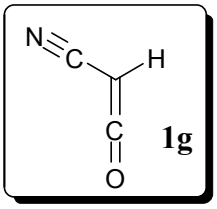
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.767942	0.945668	-0.512253
2	6	0	0.513169	0.973005	-0.986969
3	6	0	1.510594	-0.008551	-0.702642
4	6	0	2.769367	0.146347	-1.340278
5	6	0	3.852405	-0.649034	-1.021272
6	6	0	3.703803	-1.640353	-0.038231
7	6	0	2.479036	-1.839213	0.585132
8	6	0	1.373779	-1.046494	0.257268
9	8	0	0.231788	-1.365553	0.923536
10	6	0	-1.034872	-1.332271	0.360729
11	6	0	-1.554207	-0.220249	-0.310211
12	6	0	-2.879532	-0.243170	-0.757640
13	6	0	-3.676002	-1.364694	-0.529530
14	6	0	-3.149549	-2.474318	0.132177
15	6	0	-1.827288	-2.457845	0.574509
16	1	0	0.725463	1.670479	-1.787157
17	1	0	2.872853	0.939293	-2.076637
18	1	0	4.807601	-0.501675	-1.514841
19	1	0	4.547619	-2.269016	0.231767
20	1	0	2.342517	-2.615014	1.330710
21	1	0	-3.272714	0.637798	-1.250056
22	1	0	-4.706823	-1.366787	-0.870654
23	1	0	-3.764583	-3.351284	0.311144
24	1	0	-1.394739	-3.298087	1.107745
25	6	0	0.061297	2.963486	0.222241
26	6	0	-1.168238	2.284590	-0.168790
27	8	0	-2.304309	2.711985	-0.266731
28	1	0	0.116736	4.030075	0.004139
29	6	0	0.912947	2.517056	1.316294
30	8	0	0.830050	1.479352	1.968055
31	1	0	1.721181	3.248520	1.544004



***cis*-5f**

Standard orientation:

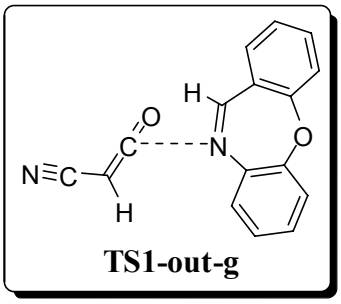
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.381475	-1.099515	0.342426
2	6	0	0.848162	-0.524384	0.943251
3	6	0	1.288248	0.792624	0.353134
4	6	0	2.588082	1.077295	-0.076922
5	6	0	2.925717	2.345724	-0.553439
6	6	0	1.963067	3.353790	-0.595516
7	6	0	0.666877	3.097221	-0.148061
8	6	0	0.340786	1.828905	0.325039
9	8	0	-0.914429	1.659489	0.895863
10	6	0	-1.869805	0.825032	0.326433
11	6	0	-1.641818	-0.542318	0.092045
12	6	0	-2.685109	-1.334549	-0.412399
13	6	0	-3.933911	-0.769788	-0.659509
14	6	0	-4.160429	0.584665	-0.409007
15	6	0	-3.124292	1.377443	0.082990
16	1	0	0.719530	-0.407585	2.027409
17	1	0	3.355706	0.311417	-0.025034
18	1	0	3.940640	2.541972	-0.885789
19	1	0	2.219549	4.341926	-0.966608
20	1	0	-0.096716	3.868340	-0.143706
21	1	0	-2.497345	-2.385920	-0.595220
22	1	0	-4.732331	-1.396228	-1.046159
23	1	0	-5.134840	1.025211	-0.597448
24	1	0	-3.265947	2.433163	0.291336
25	6	0	2.556383	-1.967819	-0.496619
26	8	0	3.630403	-2.517460	-0.400092
27	6	0	1.555304	-1.893414	0.637659
28	6	0	0.147946	-2.359009	0.164909
29	8	0	-0.317036	-3.399223	-0.240450
30	1	0	1.953892	-2.414774	1.510371
31	1	0	2.225415	-1.511858	-1.452628



1g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.127851	0.038815	0.000000
2	8	0	-2.124135	-0.558638	0.000000
3	6	0	0.000000	0.745474	0.000000
4	1	0	-0.083079	1.828460	0.000000
5	6	0	1.268430	0.111934	0.000000
6	7	0	2.318954	-0.390956	0.000000

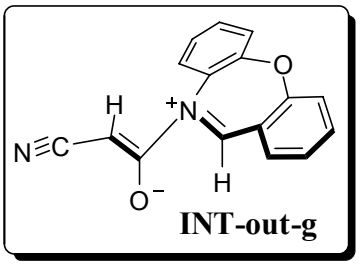


TS1-out-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.763372	-0.261342	0.237495
2	6	0	0.034897	-1.273475	0.256060
3	6	0	1.489725	-1.293605	0.164959
4	6	0	2.195331	-2.358261	0.754555
5	6	0	3.582383	-2.422210	0.678396
6	6	0	4.281898	-1.431801	-0.017553
7	6	0	3.599898	-0.378856	-0.629663
8	6	0	2.213565	-0.313514	-0.538554
9	8	0	1.556727	0.668315	-1.255652
10	6	0	0.757358	1.544260	-0.527473
11	6	0	-0.381287	1.098299	0.168326
12	6	0	-1.194982	2.050903	0.804048
13	6	0	-0.877878	3.404732	0.744940

14	6	0	0.249565	3.832516	0.041781
15	6	0	1.067721	2.898363	-0.592830
16	1	0	-0.454351	-2.238738	0.389993
17	1	0	1.639504	-3.129948	1.280777
18	1	0	4.115616	-3.243916	1.145753
19	1	0	5.363983	-1.484288	-0.095788
20	1	0	4.123104	0.383822	-1.196655
21	1	0	-2.064356	1.710312	1.353522
22	1	0	-1.518298	4.124875	1.244523
23	1	0	0.491838	4.889323	-0.018839
24	1	0	1.942868	3.199435	-1.159384
25	6	0	-2.996006	-1.138247	-0.709218
26	6	0	-2.605910	-0.703669	0.522009
27	8	0	-2.902064	-0.502661	1.658258
28	1	0	-2.321673	-1.103799	-1.551812
29	6	0	-4.318525	-1.608370	-0.899111
30	7	0	-5.399779	-2.006471	-1.085635

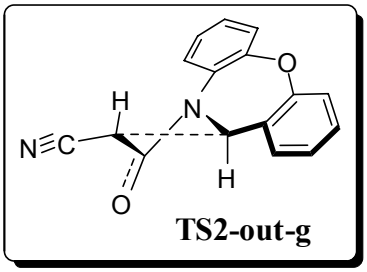


INT-out-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.704996	-0.580082	0.164577
2	6	0	0.296804	-1.409715	0.221848
3	6	0	1.708385	-1.115940	0.136441
4	6	0	2.629395	-2.021095	0.702527
5	6	0	3.997292	-1.812173	0.582363
6	6	0	4.468740	-0.711934	-0.142210
7	6	0	3.576792	0.182782	-0.735408
8	6	0	2.208407	-0.017929	-0.594008
9	8	0	1.346860	0.821439	-1.275587
10	6	0	0.448236	1.513777	-0.470386
11	6	0	-0.569430	0.840032	0.219677
12	6	0	-1.441111	1.580269	1.032717
13	6	0	-1.322838	2.965692	1.109662
14	6	0	-0.331154	3.628293	0.384228

15	6	0	0.562492	2.898371	-0.398406
16	1	0	-0.029332	-2.442726	0.346573
17	1	0	2.250510	-2.884546	1.242322
18	1	0	4.695515	-2.509643	1.033849
19	1	0	5.537360	-0.555059	-0.256802
20	1	0	3.923882	1.026556	-1.322268
21	1	0	-2.210330	1.058718	1.588893
22	1	0	-2.010050	3.524581	1.736887
23	1	0	-0.245896	4.709690	0.432528
24	1	0	1.351740	3.381445	-0.964919
25	6	0	-3.128402	-0.540917	-0.405238
26	6	0	-2.145989	-1.347039	0.132852
27	8	0	-2.071671	-2.501709	0.514353
28	1	0	-2.916625	0.460465	-0.749795
29	6	0	-4.437482	-1.036298	-0.590223
30	7	0	-5.533448	-1.406259	-0.752579

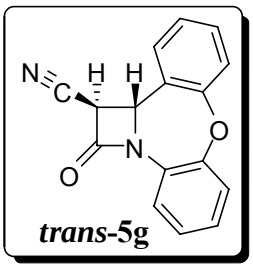


TS2-out-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.957115	0.334995	0.308860
2	6	0	-0.514457	-0.909330	0.673839
3	6	0	0.809925	-1.414520	0.420935
4	6	0	1.186818	-2.626355	1.046592
5	6	0	2.417510	-3.215797	0.804652
6	6	0	3.313936	-2.599391	-0.076851
7	6	0	2.979270	-1.395474	-0.694475
8	6	0	1.744109	-0.800024	-0.448755
9	8	0	1.473122	0.355527	-1.143471
10	6	0	1.044133	1.495893	-0.467472
11	6	0	-0.174346	1.516698	0.219856
12	6	0	-0.634442	2.713447	0.777568
13	6	0	0.128785	3.873984	0.647832
14	6	0	1.351965	3.842432	-0.023442
15	6	0	1.812861	2.649171	-0.582048

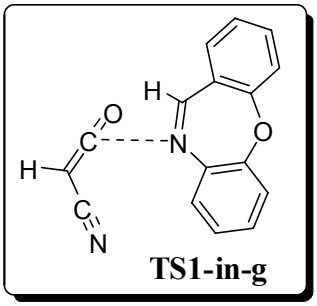
16	1	0	-1.087597	-1.429575	1.430067
17	1	0	0.475932	-3.103009	1.716535
18	1	0	2.680006	-4.150076	1.290609
19	1	0	4.279870	-3.053452	-0.278185
20	1	0	3.663125	-0.898586	-1.374490
21	1	0	-1.594163	2.718835	1.280035
22	1	0	-0.235950	4.802814	1.075726
23	1	0	1.946775	4.745640	-0.121730
24	1	0	2.748683	2.599898	-1.129210
25	6	0	-2.459501	-1.111925	-0.582643
26	6	0	-2.353373	0.234722	-0.034444
27	8	0	-3.190046	1.092396	0.172982
28	1	0	-1.744312	-1.390106	-1.349348
29	6	0	-3.676531	-1.830497	-0.568474
30	7	0	-4.651020	-2.472705	-0.516305



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.152268	-1.105887	-0.022489
2	6	0	1.089010	-0.494901	0.514306
3	6	0	1.304582	0.932724	0.088674
4	6	0	2.459555	1.404735	-0.539581
5	6	0	2.590443	2.755653	-0.869183
6	6	0	1.562079	3.648850	-0.569107
7	6	0	0.403326	3.195561	0.063785
8	6	0	0.283188	1.847184	0.385911
9	8	0	-0.829660	1.439243	1.111544
10	6	0	-1.787264	0.612423	0.530997
11	6	0	-1.479744	-0.653902	0.001186
12	6	0	-2.513487	-1.454532	-0.507768
13	6	0	-3.830150	-1.002300	-0.469377
14	6	0	-4.133508	0.246032	0.076407
15	6	0	-3.108120	1.049721	0.573185
16	1	0	1.127171	-0.586161	1.606127

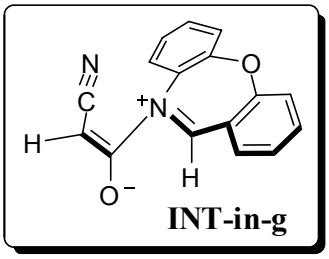
17	1	0	3.274261	0.720197	-0.758978
18	1	0	3.495865	3.106468	-1.355110
19	1	0	1.659706	4.700327	-0.823423
20	1	0	-0.406630	3.870887	0.319762
21	1	0	-2.265345	-2.424971	-0.921264
22	1	0	-4.620050	-1.634552	-0.863703
23	1	0	-5.160282	0.597301	0.112555
24	1	0	-3.308709	2.025687	1.003508
25	6	0	1.874731	-1.644833	-0.197936
26	6	0	0.463971	-2.188485	-0.606139
27	8	0	0.060780	-3.149215	-1.213106
28	1	0	2.423537	-1.309911	-1.083238
29	6	0	2.714127	-2.495026	0.629167
30	7	0	3.377278	-3.171102	1.300932



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.690132	-0.808690	-0.211099
2	6	0	-0.425255	-1.436895	-0.094035
3	6	0	-1.787062	-0.911358	-0.017486
4	6	0	-2.854560	-1.725124	-0.436790
5	6	0	-4.169380	-1.277606	-0.361891
6	6	0	-4.436976	-0.010181	0.163496
7	6	0	-3.395096	0.807289	0.603173
8	6	0	-2.080599	0.358084	0.513564
9	8	0	-1.088412	1.145106	1.061922
10	6	0	-0.057875	1.529946	0.208912
11	6	0	0.813478	0.587925	-0.365796
12	6	0	1.879333	1.059973	-1.146764
13	6	0	2.065262	2.422252	-1.358545
14	6	0	1.194956	3.343006	-0.772713
15	6	0	0.132808	2.893197	0.011071
16	1	0	-0.341230	-2.525536	-0.104860

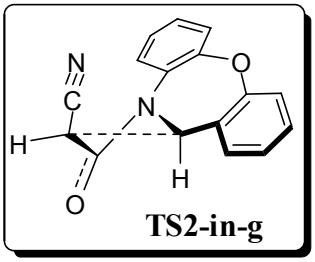
17	1	0	-2.635349	-2.715309	-0.828414
18	1	0	-4.981705	-1.915098	-0.696768
19	1	0	-5.461882	0.341316	0.241679
20	1	0	-3.582828	1.784631	1.035236
21	1	0	2.560922	0.334068	-1.577073
22	1	0	2.898001	2.763590	-1.965702
23	1	0	1.345361	4.409089	-0.914930
24	1	0	-0.551887	3.584438	0.491677
25	6	0	3.249204	-1.843099	0.484413
26	6	0	2.281327	-2.303964	-0.335158
27	8	0	1.818558	-3.102273	-1.068506
28	1	0	4.138367	-2.469539	0.510664
29	6	0	3.187406	-0.732114	1.350175
30	7	0	3.194043	0.165506	2.095017



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.608232	-1.010551	-0.183315
2	6	0	-0.593341	-1.503921	-0.145565
3	6	0	-1.852327	-0.800793	-0.061553
4	6	0	-3.021665	-1.452263	-0.505227
5	6	0	-4.263640	-0.842609	-0.387429
6	6	0	-4.360263	0.417649	0.213575
7	6	0	-3.220745	1.070890	0.683835
8	6	0	-1.974917	0.467341	0.545063
9	8	0	-0.881578	1.084455	1.112062
10	6	0	0.153407	1.385858	0.229027
11	6	0	0.904223	0.372060	-0.378293
12	6	0	1.944360	0.723261	-1.249142
13	6	0	2.242139	2.062517	-1.478252
14	6	0	1.508485	3.064261	-0.840726
15	6	0	0.455802	2.724109	0.007562
16	1	0	-0.603951	-2.591878	-0.203191
17	1	0	-2.934417	-2.439981	-0.949618

18	1	0	-5.154859	-1.348997	-0.743875
19	1	0	-5.331371	0.890814	0.327323
20	1	0	-3.280261	2.036605	1.174276
21	1	0	2.522864	-0.061324	-1.721718
22	1	0	3.057932	2.320802	-2.145766
23	1	0	1.753866	4.109769	-1.000723
24	1	0	-0.132646	3.479009	0.518279
25	6	0	2.918981	-1.814568	0.477377
26	6	0	1.761982	-2.171283	-0.187147
27	8	0	1.383346	-3.198052	-0.727052
28	1	0	3.680047	-2.587924	0.501334
29	6	0	3.148721	-0.661067	1.251499
30	7	0	3.377687	0.275298	1.914170

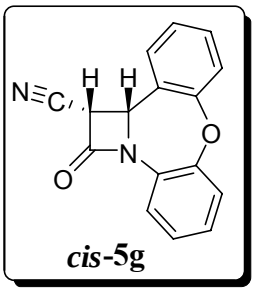


TS2-in-g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.784707	0.962559	-0.485006
2	6	0	0.498038	0.979150	-0.976066
3	6	0	1.490736	-0.010889	-0.691188
4	6	0	2.729692	0.083657	-1.372361
5	6	0	3.785347	-0.761401	-1.080135
6	6	0	3.627104	-1.736931	-0.086076
7	6	0	2.416307	-1.870316	0.587330
8	6	0	1.347608	-1.025452	0.290021
9	8	0	0.210996	-1.221717	1.028080
10	6	0	-1.048003	-1.276729	0.440796
11	6	0	-1.577116	-0.197372	-0.274374
12	6	0	-2.894113	-0.251296	-0.739060
13	6	0	-3.670427	-1.382784	-0.487499
14	6	0	-3.132355	-2.463362	0.212872
15	6	0	-1.817443	-2.411664	0.677591
16	1	0	0.696363	1.644752	-1.806584
17	1	0	2.844141	0.861095	-2.123273
18	1	0	4.728633	-0.662168	-1.607483

19	1	0	4.449962	-2.402253	0.159057
20	1	0	2.273617	-2.626086	1.352132
21	1	0	-3.295830	0.606880	-1.264563
22	1	0	-4.696247	-1.416629	-0.841716
23	1	0	-3.735211	-3.345524	0.406946
24	1	0	-1.380803	-3.227107	1.244900
25	6	0	0.080415	2.972300	0.213069
26	6	0	-1.166624	2.306550	-0.171928
27	8	0	-2.282855	2.771343	-0.307158
28	1	0	0.128517	4.047514	0.041068
29	6	0	0.873145	2.495791	1.284833
30	7	0	1.542975	2.098443	2.157179

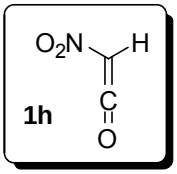


***cis*-5g**

Standard orientation:

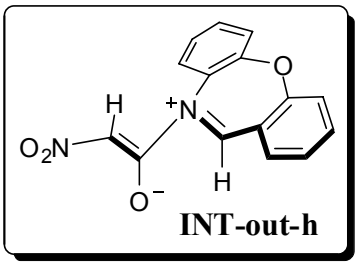
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.389617	-1.123578	0.350207
2	6	0	0.850054	-0.602059	0.983346
3	6	0	1.364369	0.674419	0.363463
4	6	0	2.652792	0.885558	-0.135098
5	6	0	3.025479	2.135259	-0.636647
6	6	0	2.116691	3.192078	-0.637717
7	6	0	0.830037	3.004058	-0.130711
8	6	0	0.466778	1.755620	0.362445
9	8	0	-0.780805	1.629264	0.968175
10	6	0	-1.776477	0.872546	0.359748
11	6	0	-1.614382	-0.495770	0.080734
12	6	0	-2.682025	-1.215895	-0.475695
13	6	0	-3.894855	-0.578522	-0.727290
14	6	0	-4.058439	0.775355	-0.429776
15	6	0	-2.995087	1.497181	0.111802
16	1	0	0.689672	-0.441244	2.056656
17	1	0	3.376518	0.080080	-0.135311
18	1	0	4.030176	2.276646	-1.023421

19	1	0	2.406000	4.164221	-1.026597
20	1	0	0.105105	3.811079	-0.100701
21	1	0	-2.543647	-2.267452	-0.697518
22	1	0	-4.714448	-1.147992	-1.155313
23	1	0	-5.005151	1.271211	-0.621837
24	1	0	-3.088012	2.551044	0.354000
25	6	0	1.470538	-2.030612	0.749540
26	6	0	0.080940	-2.393512	0.125660
27	8	0	-0.402399	-3.390682	-0.350760
28	1	0	1.643486	-2.560446	1.692207
29	6	0	2.610898	-2.239831	-0.126969
30	7	0	3.515626	-2.456570	-0.821990



Standard orientation:

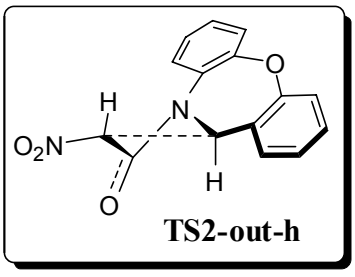
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376399	-0.276168	0.000000
2	8	0	-2.443074	0.173871	0.000000
3	6	0	-0.164317	-0.835071	0.000000
4	1	0	0.003415	-1.901314	0.000000
5	7	0	0.951689	0.062223	0.000000
6	8	0	2.074699	-0.430928	0.000000
7	8	0	0.690757	1.273705	0.000000



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.379239	-0.466874	0.235762

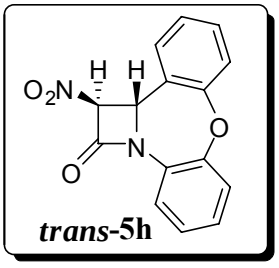
2	6	0	0.554670	-1.357849	0.212566
3	6	0	1.988387	-1.167121	0.093200
4	6	0	2.855041	-2.149874	0.608632
5	6	0	4.232342	-2.026680	0.469152
6	6	0	4.761949	-0.932935	-0.223392
7	6	0	3.920680	0.039934	-0.765351
8	6	0	2.544253	-0.077399	-0.605398
9	8	0	1.728995	0.838954	-1.243044
10	6	0	0.881753	1.564071	-0.411158
11	6	0	-0.160930	0.934895	0.288274
12	6	0	-0.997742	1.718021	1.098422
13	6	0	-0.811697	3.095165	1.182566
14	6	0	0.210243	3.710324	0.457205
15	6	0	1.062425	2.941024	-0.334448
16	1	0	0.179445	-2.377922	0.315228
17	1	0	2.430006	-3.006163	1.125263
18	1	0	4.890730	-2.784818	0.880918
19	1	0	5.836409	-0.841625	-0.353550
20	1	0	4.312107	0.881275	-1.327260
21	1	0	-1.793493	1.233101	1.651352
22	1	0	-1.471523	3.685502	1.810308
23	1	0	0.347485	4.786256	0.507398
24	1	0	1.867861	3.389137	-0.906954
25	6	0	-2.880480	-0.369815	-0.301365
26	6	0	-2.011723	-1.272417	0.245279
27	8	0	-1.905782	-2.387083	0.663524
28	1	0	-2.600660	0.599942	-0.669242
29	7	0	-4.252876	-0.696314	-0.473717
30	8	0	-4.952606	0.172379	-1.021270
31	8	0	-4.679179	-1.789054	-0.080823



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.464899	-0.705731	-0.392037

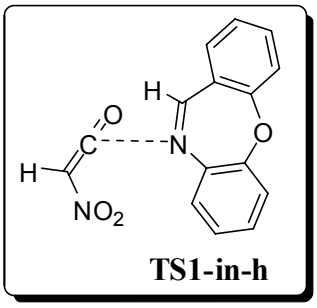
2	6	0	-0.516037	0.609527	-0.752901
3	6	0	0.516014	1.578174	-0.489352
4	6	0	0.429191	2.828804	-1.144867
5	6	0	1.341401	3.841487	-0.895107
6	6	0	2.372222	3.624580	0.027484
7	6	0	2.491811	2.398460	0.679748
8	6	0	1.578859	1.377825	0.425306
9	8	0	1.727135	0.224507	1.156739
10	6	0	1.788345	-1.008415	0.509116
11	6	0	0.703037	-1.497206	-0.225754
12	6	0	0.753723	-2.788868	-0.759496
13	6	0	1.888010	-3.575218	-0.557259
14	6	0	2.973524	-3.075445	0.163384
15	6	0	2.925134	-1.786554	0.697181
16	1	0	-1.238990	0.879188	-1.511320
17	1	0	-0.386800	2.989155	-1.844577
18	1	0	1.251597	4.795522	-1.404345
19	1	0	3.089965	4.412550	0.236601
20	1	0	3.286107	2.212462	1.394777
21	1	0	-0.105731	-3.163216	-1.302202
22	1	0	1.919753	-4.580123	-0.966916
23	1	0	3.856722	-3.687666	0.319078
24	1	0	3.744925	-1.379574	1.280082
25	6	0	-2.394060	0.071562	0.464960
26	6	0	-1.816698	-1.146411	-0.083999
27	8	0	-2.240045	-2.262779	-0.287078
28	1	0	-1.900981	0.565082	1.291362
29	7	0	-3.800746	0.319290	0.447511
30	8	0	-4.216056	1.207128	1.210749
31	8	0	-4.504022	-0.300371	-0.359351



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.092022	-0.969349	-0.110137

2	6	0	0.967439	0.101422	0.439637
3	6	0	0.542577	1.494002	0.058045
4	6	0	1.371576	2.431773	-0.562343
5	6	0	0.904865	3.716261	-0.849732
6	6	0	-0.401262	4.073966	-0.515540
7	6	0	-1.241673	3.151107	0.109292
8	6	0	-0.766776	1.873316	0.389064
9	8	0	-1.584997	1.010182	1.108134
10	6	0	-2.106971	-0.134759	0.514508
11	6	0	-1.298516	-1.134361	-0.056790
12	6	0	-1.898595	-2.290955	-0.577123
13	6	0	-3.280206	-2.450858	-0.508495
14	6	0	-4.077218	-1.466595	0.078502
15	6	0	-3.485969	-0.310476	0.586443
16	1	0	1.074679	-0.005985	1.523909
17	1	0	2.395905	2.168359	-0.811048
18	1	0	1.563139	4.433491	-1.330566
19	1	0	-0.768632	5.071786	-0.737295
20	1	0	-2.257694	3.406870	0.391923
21	1	0	-1.266955	-3.051098	-1.021717
22	1	0	-3.730974	-3.352862	-0.911331
23	1	0	-5.154023	-1.592636	0.138105
24	1	0	-4.076696	0.474018	1.048439
25	6	0	2.139148	-0.573891	-0.313120
26	6	0	1.102304	-1.663231	-0.728798
27	8	0	1.151513	-2.688810	-1.361900
28	1	0	2.581697	-0.031946	-1.145362
29	7	0	3.259962	-1.084490	0.536142
30	8	0	2.965564	-1.553789	1.632702
31	8	0	4.386835	-1.023015	0.057514

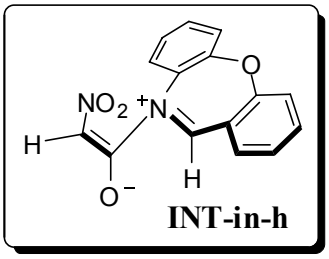


TS1-in-h

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.420134	-0.714043	-0.399700

2	6	0	-0.648822	-1.402368	-0.236362
3	6	0	-2.032153	-0.952531	-0.061245
4	6	0	-3.081721	-1.799056	-0.457373
5	6	0	-4.410731	-1.423418	-0.287955
6	6	0	-4.708758	-0.195520	0.309060
7	6	0	-3.683018	0.653663	0.726072
8	6	0	-2.355591	0.276226	0.542157
9	8	0	-1.374712	1.091473	1.071475
10	6	0	-0.406167	1.562331	0.191391
11	6	0	0.467224	0.689631	-0.483815
12	6	0	1.466009	1.252053	-1.294042
13	6	0	1.592132	2.631491	-1.430930
14	6	0	0.723918	3.480210	-0.742928
15	6	0	-0.276412	2.941443	0.066499
16	1	0	-0.511491	-2.486295	-0.275876
17	1	0	-2.838369	-2.759513	-0.905114
18	1	0	-5.209073	-2.087008	-0.605652
19	1	0	-5.743081	0.099869	0.460905
20	1	0	-3.891808	1.600709	1.212657
21	1	0	2.142530	0.580079	-1.811374
22	1	0	2.374809	3.040938	-2.062257
23	1	0	0.825689	4.558119	-0.827981
24	1	0	-0.960208	3.575076	0.622154
25	6	0	3.289375	-1.545691	-0.047377
26	6	0	2.224365	-2.215253	-0.524777
27	8	0	1.646257	-3.082479	-1.056568
28	1	0	4.265177	-1.795643	-0.441089
29	7	0	3.268904	-0.575673	0.993336
30	8	0	4.320662	0.054318	1.159169
31	8	0	2.253374	-0.440511	1.684414

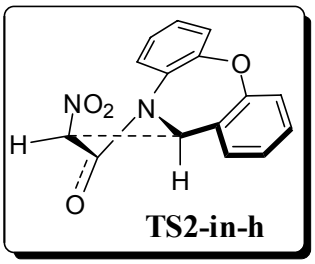


INT-in-h

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.555225	-0.658321	-0.577903
2	6	0	-0.531947	-1.359139	-0.535722

3	6	0	-1.874767	-0.916913	-0.232493
4	6	0	-2.952374	-1.706967	-0.682223
5	6	0	-4.263807	-1.364639	-0.380905
6	6	0	-4.516211	-0.237466	0.408219
7	6	0	-3.465343	0.547583	0.882669
8	6	0	-2.152074	0.213825	0.564694
9	8	0	-1.147682	0.950623	1.145668
10	6	0	-0.207892	1.529044	0.303018
11	6	0	0.643820	0.762173	-0.502171
12	6	0	1.602520	1.405080	-1.295046
13	6	0	1.722839	2.791887	-1.261887
14	6	0	0.887791	3.546731	-0.437819
15	6	0	-0.082558	2.913044	0.338357
16	1	0	-0.396823	-2.410600	-0.778865
17	1	0	-2.741113	-2.591050	-1.277858
18	1	0	-5.083647	-1.976830	-0.742318
19	1	0	-5.537715	0.027072	0.665764
20	1	0	-3.641737	1.410657	1.515545
21	1	0	2.237901	0.812289	-1.942813
22	1	0	2.472705	3.277301	-1.878217
23	1	0	0.988663	4.626991	-0.395644
24	1	0	-0.741096	3.471901	0.994826
25	6	0	2.837304	-1.552474	-0.022481
26	6	0	1.858350	-1.464161	-0.999752
27	8	0	1.812713	-1.890196	-2.142887
28	1	0	3.767084	-2.041751	-0.267722
29	7	0	2.738524	-1.127393	1.307508
30	8	0	3.729660	-1.301847	2.035362
31	8	0	1.678512	-0.602533	1.727021

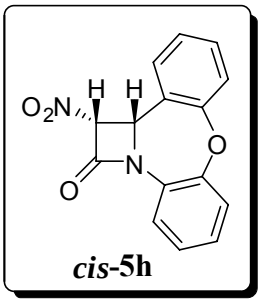


TS2-in-h

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.707173	0.871282	-0.655705
2	6	0	0.538210	0.595392	-1.147516
3	6	0	1.331580	-0.535646	-0.794609

4	6	0	2.581206	-0.672838	-1.456032
5	6	0	3.497932	-1.637536	-1.087736
6	6	0	3.184457	-2.507287	-0.031710
7	6	0	1.960291	-2.419794	0.619918
8	6	0	1.022579	-1.453287	0.246143
9	8	0	-0.133677	-1.478463	0.960421
10	6	0	-1.390378	-1.224891	0.431104
11	6	0	-1.701986	-0.089404	-0.323623
12	6	0	-3.021959	0.125362	-0.733484
13	6	0	-4.020267	-0.782709	-0.383052
14	6	0	-3.702588	-1.916668	0.364664
15	6	0	-2.386551	-2.138211	0.768439
16	1	0	0.865810	1.174179	-2.001249
17	1	0	2.818211	0.030768	-2.249575
18	1	0	4.452572	-1.712231	-1.597902
19	1	0	3.898329	-3.265601	0.276981
20	1	0	1.698608	-3.096191	1.426260
21	1	0	-3.248766	1.022806	-1.296064
22	1	0	-5.043650	-0.599478	-0.695686
23	1	0	-4.475212	-2.628016	0.640674
24	1	0	-2.111926	-3.001765	1.365237
25	6	0	0.546528	2.735017	-0.124264
26	6	0	-0.812130	2.278499	-0.394793
27	8	0	-1.830699	2.934165	-0.503196
28	1	0	0.831124	3.750412	-0.373259
29	7	0	1.301949	2.240615	0.982647
30	8	0	2.405634	2.778463	1.168946
31	8	0	0.857482	1.316566	1.685742

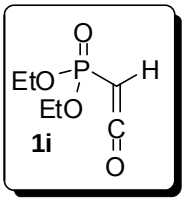


***cis*-5h**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.420500	-1.063233	-0.421392
2	6	0	-0.739320	-0.351992	-1.023505

3	6	0	-1.070955	0.983850	-0.406541
4	6	0	-2.343520	1.385116	0.012022
5	6	0	-2.556916	2.672179	0.508617
6	6	0	-1.500432	3.578815	0.584337
7	6	0	-0.229960	3.204894	0.146325
8	6	0	-0.025921	1.920067	-0.347712
9	8	0	1.212846	1.635320	-0.912862
10	6	0	2.077637	0.713202	-0.336530
11	6	0	1.720225	-0.630140	-0.129267
12	6	0	2.670395	-1.524040	0.387554
13	6	0	3.959832	-1.081283	0.671714
14	6	0	4.316832	0.249281	0.446154
15	6	0	3.371664	1.142776	-0.056604
16	1	0	-0.584122	-0.220124	-2.102620
17	1	0	-3.186162	0.707357	-0.064117
18	1	0	-3.551821	2.961157	0.833307
19	1	0	-1.663726	4.579955	0.972764
20	1	0	0.605979	3.896574	0.164966
21	1	0	2.381014	-2.554909	0.553486
22	1	0	4.686509	-1.783594	1.069000
23	1	0	5.323017	0.594417	0.664100
24	1	0	3.616181	2.183451	-0.243969
25	6	0	-1.555991	-1.666564	-0.788491
26	6	0	-0.225561	-2.265037	-0.260480
27	8	0	0.119212	-3.354138	0.129122
28	1	0	-2.008151	-2.118215	-1.668688
29	7	0	-2.612567	-1.625959	0.275251
30	8	0	-2.243196	-1.419643	1.425026
31	8	0	-3.774151	-1.787600	-0.091387

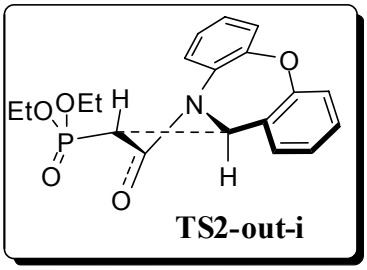


1i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.641581	-0.722948	1.864675
2	6	0	0.283005	1.703460	0.646631
3	1	0	0.995477	2.176200	1.313438
4	6	0	-0.527425	2.458593	-0.071148

5	8	0	-1.251212	3.117963	-0.703632
6	15	0	0.194820	-0.080198	0.603598
7	8	0	-1.331090	-0.261704	0.115943
8	8	0	0.986818	-0.612348	-0.711538
9	6	0	-1.824526	-1.572527	-0.262533
10	6	0	-3.315360	-1.450838	-0.514152
11	1	0	-1.613757	-2.276081	0.550220
12	1	0	-1.287929	-1.899357	-1.158996
13	1	0	-3.722676	-2.423811	-0.810791
14	1	0	-3.834874	-1.117393	0.389373
15	1	0	-3.515750	-0.732443	-1.315353
16	6	0	2.304031	-1.204352	-0.600370
17	6	0	3.399096	-0.156720	-0.729990
18	1	0	2.356141	-1.927808	-1.419294
19	1	0	2.374675	-1.741625	0.349597
20	1	0	4.381212	-0.643787	-0.738995
21	1	0	3.285378	0.411517	-1.658661
22	1	0	3.378095	0.544159	0.111285

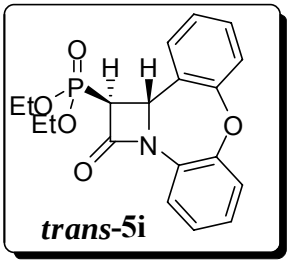


TS2-out-i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.918475	-0.795031	-0.401442
2	6	0	0.987647	0.444921	-0.967730
3	6	0	2.027567	1.408400	-0.716220
4	6	0	2.073941	2.558025	-1.539150
5	6	0	3.005650	3.562712	-1.328702
6	6	0	3.924922	3.439900	-0.280031
7	6	0	3.913272	2.311908	0.539363
8	6	0	2.979296	1.300856	0.326809
9	8	0	2.994110	0.254053	1.219805
10	6	0	3.052979	-1.058179	0.755074
11	6	0	2.018100	-1.604692	-0.012452
12	6	0	2.055503	-2.960046	-0.356930
13	6	0	3.123986	-3.751306	0.065109

14	6	0	4.159782	-3.196474	0.818061
15	6	0	4.125485	-1.844326	1.162453
16	1	0	0.358392	0.625272	-1.828798
17	1	0	1.343677	2.647834	-2.339015
18	1	0	3.016554	4.439104	-1.968886
19	1	0	4.657483	4.222098	-0.102660
20	1	0	4.620122	2.196542	1.354323
21	1	0	1.232918	-3.372451	-0.928089
22	1	0	3.144631	-4.804110	-0.200016
23	1	0	4.992180	-3.812825	1.144545
24	1	0	4.905667	-1.389023	1.763869
25	8	0	-2.938855	0.647239	-1.993746
26	6	0	-1.144762	0.094422	0.000906
27	6	0	-0.478053	-1.152030	-0.264740
28	8	0	-0.908908	-2.286893	-0.437265
29	1	0	-0.693471	0.759973	0.729141
30	15	0	-2.818816	0.442423	-0.527599
31	8	0	-3.231629	1.754029	0.326525
32	8	0	-3.813120	-0.670247	0.103296
33	6	0	-3.514547	1.695843	1.739213
34	6	0	-3.805651	3.107631	2.215654
35	1	0	-2.651477	1.272491	2.271085
36	1	0	-4.369448	1.032872	1.903121
37	1	0	-4.034532	3.102622	3.287451
38	1	0	-2.943630	3.761029	2.046691
39	1	0	-4.663122	3.524359	1.678181
40	6	0	-4.153770	-1.868202	-0.645899
41	6	0	-5.268300	-2.576219	0.101680
42	1	0	-3.257548	-2.489906	-0.720770
43	1	0	-4.467945	-1.570816	-1.650977
44	1	0	-5.552195	-3.489155	-0.434392
45	1	0	-4.944169	-2.855993	1.109420
46	1	0	-6.152259	-1.935355	0.186125



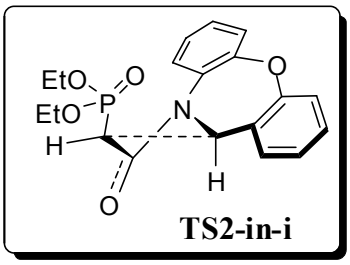
***trans*-5i**

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	7	0	-1.044911	-0.905317	-0.066525
2	6	0	-0.390684	0.385559	0.270304
3	6	0	-1.123268	1.596434	-0.239660
4	6	0	-0.530611	2.600056	-1.010094
5	6	0	-1.267451	3.712982	-1.421271
6	6	0	-2.609527	3.832465	-1.060127
7	6	0	-3.214371	2.845111	-0.280675
8	6	0	-2.470410	1.739946	0.123517
9	8	0	-3.066039	0.838330	0.997331
10	6	0	-3.341455	-0.469265	0.611999
11	6	0	-2.357854	-1.350273	0.125458
12	6	0	-2.714282	-2.673770	-0.177709
13	6	0	-4.021369	-3.110369	0.021985
14	6	0	-4.988195	-2.239350	0.526978
15	6	0	-4.642545	-0.920465	0.818173
16	1	0	-0.221800	0.454400	1.351388
17	1	0	0.521786	2.524040	-1.268477
18	1	0	-0.790845	4.484742	-2.018566
19	1	0	-3.187513	4.695376	-1.378767
20	1	0	-4.251925	2.920271	0.028592
21	1	0	-1.951818	-3.340578	-0.562675
22	1	0	-4.279694	-4.138552	-0.213986
23	1	0	-6.006662	-2.579342	0.689312
24	1	0	-5.369144	-0.216188	1.210736
25	6	0	0.864940	-0.139243	-0.490273
26	6	0	0.061772	-1.447222	-0.677630
27	8	0	0.279560	-2.531630	-1.175006
28	1	0	1.044152	0.353495	-1.449835
29	15	0	2.422538	-0.240602	0.448325
30	8	0	2.277132	-0.758458	1.833135
31	8	0	3.457843	-1.037712	-0.498643
32	8	0	2.934579	1.280878	0.273876
33	6	0	3.601121	-2.485790	-0.391374
34	6	0	4.891064	-2.872799	-1.088564
35	1	0	2.729161	-2.946527	-0.864327
36	1	0	3.615039	-2.756728	0.668378
37	1	0	5.023411	-3.959649	-1.043288
38	1	0	4.870373	-2.571984	-2.140906
39	1	0	5.753234	-2.398645	-0.608286
40	6	0	4.130780	1.714958	0.973726
41	6	0	4.223398	3.223666	0.848615
42	1	0	4.995048	1.220969	0.516268

43	1	0	4.059800	1.401347	2.020253
44	1	0	5.123538	3.584610	1.358473
45	1	0	4.277775	3.523943	-0.202725
46	1	0	3.351475	3.704176	1.303429

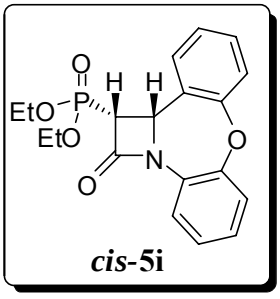


TS2-in-i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.986610	-0.745086	1.025534
2	6	0	-0.641750	0.539380	1.337507
3	6	0	-1.085566	1.706928	0.630467
4	6	0	-0.779560	2.964840	1.203171
5	6	0	-1.067485	4.152210	0.552414
6	6	0	-1.682225	4.107908	-0.706260
7	6	0	-2.023016	2.888383	-1.282809
8	6	0	-1.742749	1.690466	-0.624508
9	8	0	-2.115013	0.556582	-1.285216
10	6	0	-2.762534	-0.491197	-0.647030
11	6	0	-2.222069	-1.160180	0.457241
12	6	0	-2.890615	-2.269938	0.986208
13	6	0	-4.082220	-2.706986	0.408703
14	6	0	-4.619357	-2.033357	-0.688454
15	6	0	-3.959491	-0.922389	-1.213311
16	1	0	-0.251824	0.709441	2.331349
17	1	0	-0.283384	2.980891	2.170520
18	1	0	-0.813693	5.103913	1.008420
19	1	0	-1.908398	5.029896	-1.234477
20	1	0	-2.512295	2.835986	-2.249417
21	1	0	-2.444375	-2.790445	1.824374
22	1	0	-4.587471	-3.575612	0.820227
23	1	0	-5.546827	-2.371001	-1.141533
24	1	0	-4.342611	-0.386807	-2.075765
25	8	0	0.956252	0.405176	-1.278496
26	6	0	1.305889	-0.819620	1.227831
27	6	0	0.100749	-1.616949	1.384263

28	8	0	-0.037192	-2.752975	1.810097
29	1	0	2.124301	-1.125278	1.884947
30	15	0	1.908104	-0.277857	-0.368557
31	8	0	2.595778	-1.549770	-1.096657
32	8	0	3.244891	0.571606	0.030528
33	6	0	3.542818	-2.418312	-0.442346
34	6	0	4.031699	-3.425440	-1.467961
35	1	0	3.047606	-2.923769	0.395840
36	1	0	4.372635	-1.818626	-0.050854
37	1	0	4.749002	-4.113441	-1.006026
38	1	0	3.193894	-4.008954	-1.862005
39	1	0	4.522797	-2.917598	-2.303901
40	6	0	3.111404	1.949122	0.428861
41	6	0	4.495243	2.574099	0.441030
42	1	0	2.654778	1.991223	1.427350
43	1	0	2.447426	2.463354	-0.273992
44	1	0	4.432852	3.623248	0.752084
45	1	0	5.154466	2.045114	1.137078
46	1	0	4.943108	2.533147	-0.556746

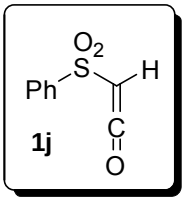


***cis*-5i**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.159759	-0.877128	-0.531849
2	6	0	0.464810	0.336243	-1.042437
3	6	0	0.800583	1.603895	-0.294170
4	6	0	-0.124628	2.503815	0.239630
5	6	0	0.297717	3.682367	0.858407
6	6	0	1.655827	3.983433	0.944194
7	6	0	2.595037	3.109624	0.395804
8	6	0	2.163040	1.938471	-0.218382
9	8	0	3.118376	1.161915	-0.870220
10	6	0	3.455140	-0.093783	-0.380817
11	6	0	2.507950	-1.123292	-0.243903

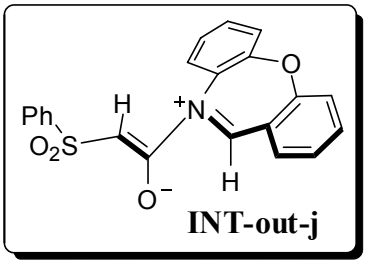
12	6	0	2.930123	-2.389693	0.189409
13	6	0	4.276775	-2.620857	0.460558
14	6	0	5.216314	-1.600290	0.305850
15	6	0	4.799154	-0.337302	-0.113292
16	1	0	0.710316	0.484147	-2.102460
17	1	0	-1.183723	2.299847	0.156522
18	1	0	-0.440682	4.362800	1.272188
19	1	0	1.987103	4.898190	1.427687
20	1	0	3.658511	3.324384	0.422748
21	1	0	2.192002	-3.175050	0.299086
22	1	0	4.589301	-3.606893	0.791756
23	1	0	6.266671	-1.781072	0.514034
24	1	0	5.501861	0.479489	-0.244283
25	6	0	-0.870570	-0.488063	-0.935389
26	6	0	0.032102	-1.656040	-0.473589
27	8	0	-0.150696	-2.816841	-0.169400
28	1	0	-1.324132	-0.672817	-1.914056
29	15	0	-2.248776	-0.195404	0.233579
30	8	0	-1.885633	0.058130	1.649723
31	8	0	-3.058926	0.962997	-0.554351
32	8	0	-3.193879	-1.477863	-0.026579
33	6	0	-4.350288	1.394277	-0.048496
34	6	0	-4.815761	2.565038	-0.893142
35	1	0	-4.241919	1.675693	1.004489
36	1	0	-5.045138	0.550536	-0.116605
37	1	0	-5.796822	2.907292	-0.545384
38	1	0	-4.113100	3.401373	-0.822155
39	1	0	-4.903137	2.273963	-1.944634
40	6	0	-3.258120	-2.584856	0.920676
41	6	0	-3.438594	-3.869265	0.135885
42	1	0	-4.106175	-2.389889	1.585347
43	1	0	-2.346099	-2.608831	1.520139
44	1	0	-3.555558	-4.710826	0.828561
45	1	0	-4.329298	-3.818963	-0.499243
46	1	0	-2.560265	-4.051478	-0.488631



Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	8	0	-1.422554	0.098928	1.571308
2	6	0	-1.792358	0.103935	-1.011006
3	1	0	-1.676764	0.559863	-1.985787
4	6	0	-2.658504	-0.870121	-0.791217
5	8	0	-3.415695	-1.729321	-0.587763
6	16	0	-0.880042	0.754331	0.372952
7	8	0	-0.855969	2.213327	0.224102
8	6	0	0.800852	0.162302	0.125821
9	6	0	1.698490	0.947695	-0.599741
10	6	0	1.176877	-1.066212	0.672916
11	6	0	2.999252	0.480822	-0.791043
12	1	0	1.384861	1.911953	-0.985643
13	6	0	2.480827	-1.519559	0.475974
14	1	0	0.464341	-1.640648	1.255624
15	6	0	3.387725	-0.750262	-0.257768
16	1	0	3.710446	1.082774	-1.349351
17	1	0	2.790008	-2.470212	0.900764
18	1	0	4.402557	-1.108094	-0.407634

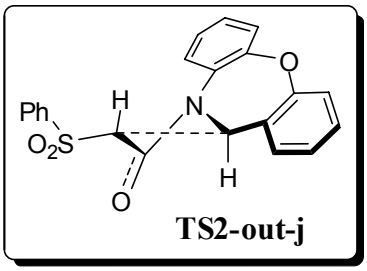


INT-out-j

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.989798	0.039500	-0.547440
2	6	0	-1.579681	-1.101644	-0.723460
3	6	0	-2.937722	-1.472642	-0.388887
4	6	0	-3.550895	-2.528925	-1.091484
5	6	0	-4.831488	-2.953670	-0.760039
6	6	0	-5.505304	-2.351672	0.308179
7	6	0	-4.907167	-1.322229	1.036193
8	6	0	-3.633756	-0.885839	0.687615
9	8	0	-3.020908	0.059162	1.487906
10	6	0	-2.653856	1.234168	0.838101
11	6	0	-1.646651	1.235728	-0.138186

12	6	0	-1.311038	2.446142	-0.764108
13	6	0	-1.943835	3.628488	-0.389005
14	6	0	-2.918823	3.618281	0.609897
15	6	0	-3.280758	2.416299	1.217260
16	1	0	-0.928129	-1.840441	-1.192527
17	1	0	-3.007846	-3.002615	-1.904691
18	1	0	-5.298271	-3.759731	-1.316971
19	1	0	-6.498600	-2.693287	0.584588
20	1	0	-5.404170	-0.861391	1.883196
21	1	0	-0.547177	2.447392	-1.531885
22	1	0	-1.666990	4.557627	-0.876695
23	1	0	-3.401958	4.541852	0.914265
24	1	0	-4.039881	2.373881	1.991315
25	6	0	1.332101	0.959839	-0.302029
26	6	0	0.644381	-0.027123	-0.951042
27	8	0	0.887605	-0.975833	-1.670969
28	1	0	0.895947	1.642509	0.409218
29	16	0	3.062793	1.158760	-0.527204
30	8	0	3.398811	1.135702	-1.960359
31	8	0	3.434959	2.314309	0.312877
32	6	0	3.832531	-0.299941	0.207572
33	6	0	4.333116	-0.218729	1.508165
34	6	0	3.923796	-1.480287	-0.534693
35	6	0	4.930352	-1.343519	2.078154
36	1	0	4.264535	0.720530	2.046897
37	6	0	4.518380	-2.599696	0.048506
38	1	0	3.536168	-1.511006	-1.546427
39	6	0	5.019922	-2.532820	1.350903
40	1	0	5.330868	-1.289425	3.087032
41	1	0	4.597127	-3.523482	-0.518532
42	1	0	5.486914	-3.407063	1.797254

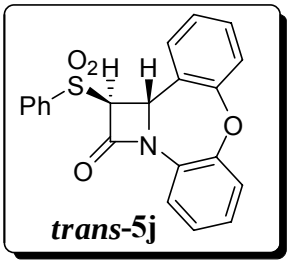


TS2-out-j

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	1.342549	-0.839152	-0.495600
2	6	0	0.737925	0.292328	-0.950094
3	6	0	1.160682	1.635973	-0.646802
4	6	0	0.592041	2.691998	-1.396041
5	6	0	0.897434	4.017340	-1.128299
6	6	0	1.789112	4.321377	-0.092721
7	6	0	2.375954	3.301816	0.655139
8	6	0	2.072561	1.969667	0.383596
9	8	0	2.640481	1.029191	1.209950
10	6	0	3.344885	-0.041870	0.662051
11	6	0	2.710280	-0.991710	-0.146118
12	6	0	3.418550	-2.119584	-0.574161
13	6	0	4.751303	-2.282596	-0.196419
14	6	0	5.382917	-1.322912	0.595808
15	6	0	4.678055	-0.197291	1.025315
16	1	0	0.063376	0.179882	-1.787326
17	1	0	-0.110633	2.442611	-2.186756
18	1	0	0.443983	4.811132	-1.713283
19	1	0	2.033046	5.356136	0.130071
20	1	0	3.071576	3.517416	1.459231
21	1	0	2.903602	-2.860075	-1.174029
22	1	0	5.294330	-3.163291	-0.525499
23	1	0	6.420851	-1.450085	0.888614
24	1	0	5.135897	0.554018	1.660529
25	8	0	-2.652042	-2.290959	-1.416007
26	6	0	-0.830564	-1.112517	0.089811
27	6	0	0.328155	-1.873970	-0.322491
28	8	0	0.504559	-3.053025	-0.554633
29	1	0	-0.721578	-0.434311	0.929726
30	8	0	-2.721919	-2.725384	1.106131
31	16	0	-2.453896	-1.826368	-0.032184
32	6	0	-3.488124	-0.362589	0.201811
33	6	0	-3.877396	0.002441	1.491828
34	6	0	-3.898741	0.367073	-0.915289
35	6	0	-4.677189	1.132895	1.664434
36	1	0	-3.573963	-0.606782	2.337288
37	6	0	-4.701979	1.493017	-0.732247
38	1	0	-3.607350	0.034739	-1.906504
39	6	0	-5.085415	1.877738	0.555216
40	1	0	-4.990631	1.425346	2.662784
41	1	0	-5.036518	2.064625	-1.593756
42	1	0	-5.712795	2.754268	0.693563

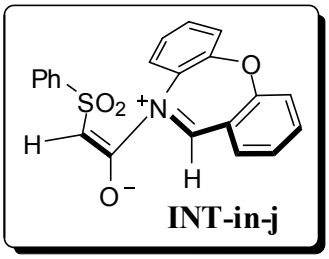


***trans*-5j**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.409043	-0.922851	-0.204278
2	6	0	-0.257819	-0.036866	0.103354
3	6	0	-0.457570	1.393590	-0.324808
4	6	0	0.419566	2.103292	-1.148421
5	6	0	0.173815	3.440187	-1.469470
6	6	0	-0.956744	4.081890	-0.964106
7	6	0	-1.840382	3.390594	-0.133709
8	6	0	-1.586241	2.058118	0.178276
9	8	0	-2.420037	1.426992	1.092664
10	6	0	-3.255531	0.388182	0.688963
11	6	0	-2.772331	-0.785585	0.082283
12	6	0	-3.674230	-1.812010	-0.238676
13	6	0	-5.026901	-1.672136	0.061118
14	6	0	-5.498004	-0.515012	0.683772
15	6	0	-4.607949	0.512753	0.993342
16	1	0	-0.005051	-0.097045	1.168156
17	1	0	1.314585	1.618783	-1.527960
18	1	0	0.867117	3.976819	-2.110302
19	1	0	-1.152623	5.121255	-1.211850
20	1	0	-2.720899	3.868347	0.283599
21	1	0	-3.293700	-2.707881	-0.714798
22	1	0	-5.711698	-2.476920	-0.189280
23	1	0	-6.551518	-0.407563	0.923882
24	1	0	-4.940308	1.426235	1.476177
25	6	0	0.608004	-0.991703	-0.763116
26	6	0	-0.685628	-1.835403	-0.941871
27	8	0	-0.980809	-2.855270	-1.513642
28	1	0	0.990444	-0.585862	-1.701240
29	16	0	1.980075	-1.854320	0.076990
30	8	0	1.480982	-2.281073	1.393527
31	8	0	2.540834	-2.805490	-0.890321
32	6	0	3.194092	-0.548067	0.339611

33	6	0	3.232809	0.116530	1.566946
34	6	0	4.084199	-0.235475	-0.691415
35	6	0	4.174405	1.129044	1.755773
36	1	0	2.551976	-0.174974	2.359825
37	6	0	5.018577	0.780429	-0.490506
38	1	0	4.057207	-0.798241	-1.619178
39	6	0	5.059867	1.462815	0.728548
40	1	0	4.220235	1.651503	2.706896
41	1	0	5.720901	1.031136	-1.280290
42	1	0	5.791650	2.251210	0.881308

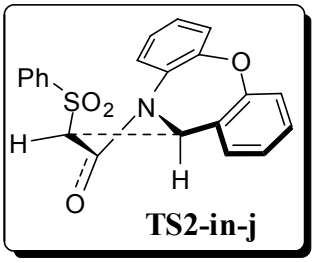


INT-in-j

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.889419	0.060224	1.089120
2	6	0	1.579714	-1.032949	1.143745
3	6	0	2.788526	-1.381861	0.430442
4	6	0	3.612996	-2.389368	0.971520
5	6	0	4.761806	-2.803256	0.310373
6	6	0	5.085725	-2.235447	-0.926668
7	6	0	4.273745	-1.252433	-1.492083
8	6	0	3.132850	-0.824542	-0.818459
9	8	0	2.304602	0.064458	-1.457568
10	6	0	2.004026	1.243621	-0.784429
11	6	0	1.279717	1.253407	0.415893
12	6	0	0.959596	2.482349	1.006968
13	6	0	1.348958	3.675619	0.404972
14	6	0	2.055394	3.654711	-0.797079
15	6	0	2.387067	2.435244	-1.387313
16	1	0	1.196725	-1.754386	1.862691
17	1	0	3.337952	-2.835281	1.923666
18	1	0	5.393141	-3.572335	0.743568
19	1	0	5.971783	-2.567152	-1.460395
20	1	0	4.497630	-0.817682	-2.460316
21	1	0	0.397050	2.493409	1.932435

22	1	0	1.085217	4.618892	0.872112
23	1	0	2.342944	4.582817	-1.281807
24	1	0	2.923379	2.385174	-2.329046
25	6	0	-1.588215	0.415747	1.519148
26	6	0	-0.396569	0.053885	2.103081
27	8	0	-0.077271	-0.282430	3.231522
28	1	0	-2.437231	0.522816	2.184323
29	16	0	-1.973418	0.638160	-0.162214
30	8	0	-2.386939	2.030270	-0.431583
31	8	0	-0.913410	0.026355	-0.998028
32	6	0	-3.459369	-0.369845	-0.374323
33	6	0	-4.714688	0.219929	-0.220810
34	6	0	-3.329948	-1.721704	-0.698369
35	6	0	-5.858759	-0.564500	-0.377889
36	1	0	-4.784271	1.280345	-0.001513
37	6	0	-4.478699	-2.495856	-0.858047
38	1	0	-2.341468	-2.147008	-0.837683
39	6	0	-5.741367	-1.919736	-0.693157
40	1	0	-6.841155	-0.114644	-0.262144
41	1	0	-4.389610	-3.547722	-1.116178
42	1	0	-6.634209	-2.526681	-0.817967

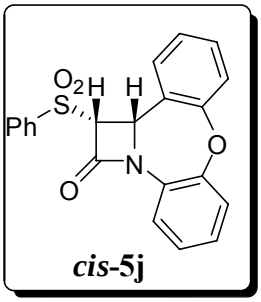


TS2-in-j

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.909473	0.733088	1.129451
2	6	0	1.172844	-0.580545	1.401332
3	6	0	1.959217	-1.458318	0.585831
4	6	0	2.234292	-2.744793	1.111332
5	6	0	2.899636	-3.706163	0.371522
6	6	0	3.315535	-3.397945	-0.930404
7	6	0	3.081997	-2.135309	-1.467576
8	6	0	2.416327	-1.162285	-0.722541
9	8	0	2.220636	0.029578	-1.358202
10	6	0	2.424934	1.251497	-0.735541

11	6	0	1.779683	1.629631	0.448027
12	6	0	1.973958	2.919517	0.955926
13	6	0	2.795009	3.821289	0.280096
14	6	0	3.438182	3.438197	-0.896805
15	6	0	3.254766	2.151072	-1.400698
16	1	0	0.994653	-0.911812	2.414069
17	1	0	1.876726	-2.977174	2.110777
18	1	0	3.084655	-4.689819	0.790660
19	1	0	3.832613	-4.143819	-1.527432
20	1	0	3.406970	-1.877478	-2.469766
21	1	0	1.450128	3.202615	1.860221
22	1	0	2.929481	4.822321	0.678681
23	1	0	4.078915	4.136734	-1.426823
24	1	0	3.729160	1.826829	-2.321159
25	8	0	-0.668002	-0.705210	-0.953203
26	6	0	-1.156592	-0.162413	1.613749
27	6	0	-0.392276	1.074458	1.631340
28	8	0	-0.698786	2.169213	2.075655
29	1	0	-1.958759	-0.247998	2.346664
30	8	0	-1.899138	-2.410808	0.506810
31	16	0	-1.615759	-1.012463	0.133552
32	6	0	-3.195852	-0.268278	-0.328749
33	6	0	-4.383136	-0.883292	0.071809
34	6	0	-3.204088	0.914712	-1.071658
35	6	0	-5.600919	-0.296106	-0.274268
36	1	0	-4.342787	-1.813900	0.628150
37	6	0	-4.426708	1.492866	-1.410293
38	1	0	-2.267119	1.360585	-1.388947
39	6	0	-5.622718	0.890673	-1.010056
40	1	0	-6.531939	-0.768599	0.026648
41	1	0	-4.446064	2.411139	-1.990583
42	1	0	-6.573035	1.345181	-1.276877

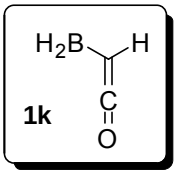


***cis*-5j**

Standard orientation:

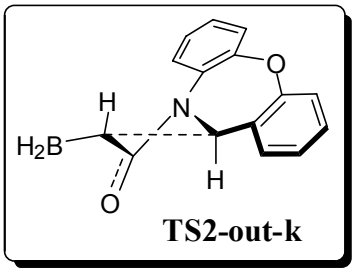
Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	7	0	0.948619	-0.914827	-0.455522
2	6	0	0.708353	0.439399	-1.030038
3	6	0	1.490057	1.545953	-0.357653
4	6	0	0.970754	2.740571	0.149678
5	6	0	1.816234	3.708982	0.696401
6	6	0	3.194095	3.505221	0.733657
7	6	0	3.734039	2.332134	0.205982
8	6	0	2.885128	1.373108	-0.335771
9	8	0	3.470712	0.280054	-0.973688
10	6	0	3.375685	-0.985667	-0.412018
11	6	0	2.136196	-1.606958	-0.183304
12	6	0	2.105727	-2.915443	0.322630
13	6	0	3.297520	-3.591202	0.574915
14	6	0	4.526538	-2.976593	0.329678
15	6	0	4.560222	-1.671977	-0.162204
16	1	0	0.961584	0.439351	-2.098498
17	1	0	-0.092259	2.937802	0.101507
18	1	0	1.387579	4.625959	1.089632
19	1	0	3.850855	4.257974	1.160639
20	1	0	4.803946	2.150735	0.192597
21	1	0	1.145489	-3.383844	0.501509
22	1	0	3.260466	-4.604879	0.962922
23	1	0	5.455287	-3.504783	0.523745
24	1	0	5.497787	-1.163974	-0.364403
25	6	0	-0.826489	0.116173	-0.890912
26	6	0	-0.373488	-1.264160	-0.361392
27	8	0	-0.937722	-2.275461	-0.004534
28	1	0	-1.349644	0.087919	-1.850009
29	16	0	-1.946693	1.020253	0.246972
30	8	0	-1.419134	0.889124	1.611737
31	8	0	-2.198252	2.346033	-0.349763
32	6	0	-3.475351	0.082978	0.115724
33	6	0	-4.445124	0.509069	-0.795339
34	6	0	-3.677920	-1.021487	0.946166
35	6	0	-5.643852	-0.198397	-0.880406
36	1	0	-4.265895	1.389113	-1.403832
37	6	0	-4.882352	-1.717665	0.849758
38	1	0	-2.909444	-1.325059	1.646545
39	6	0	-5.859451	-1.309281	-0.061151
40	1	0	-6.410673	0.122412	-1.579585
41	1	0	-5.056713	-2.578881	1.487860
42	1	0	-6.795559	-1.856668	-0.129942



Standard orientation:

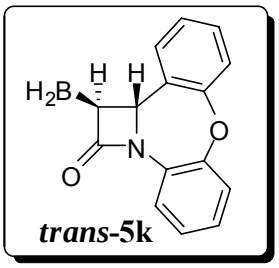
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.729264	-0.466995	0.000000
2	1	0	1.810461	-0.357051	0.000000
3	6	0	0.000000	0.648642	0.000000
4	8	0	-0.675181	1.593432	0.000000
5	5	0	-0.028397	-1.778075	0.000000
6	1	0	-1.223908	-1.784616	0.000000
7	1	0	0.581299	-2.805302	0.000000



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.809522	0.897567	0.247661
2	6	0	-0.489122	1.178008	0.584477
3	6	0	-1.605998	0.292952	0.373460
4	6	0	-2.840580	0.632503	0.975527
5	6	0	-3.982296	-0.125385	0.770231
6	6	0	-3.916241	-1.259009	-0.049175
7	6	0	-2.710754	-1.630839	-0.641000
8	6	0	-1.561158	-0.871087	-0.432324
9	8	0	-0.432681	-1.280031	-1.099618
10	6	0	0.769648	-1.455730	-0.416974
11	6	0	1.411235	-0.386479	0.217889
12	6	0	2.677833	-0.580212	0.779251
13	6	0	3.284061	-1.834260	0.708320

14	6	0	2.628598	-2.900419	0.090484
15	6	0	1.365899	-2.711242	-0.472857
16	1	0	-0.644865	1.968243	1.305951
17	1	0	-2.882500	1.524210	1.595595
18	1	0	-4.919511	0.161662	1.236348
19	1	0	-4.804561	-1.859975	-0.221248
20	1	0	-2.636984	-2.510086	-1.272252
21	1	0	3.177407	0.264740	1.237448
22	1	0	4.270523	-1.975375	1.139698
23	1	0	3.099298	-3.877673	0.037911
24	1	0	0.841370	-3.514985	-0.979367
25	6	0	0.309416	2.924558	-0.727158
26	6	0	1.428222	2.123299	-0.223202
27	8	0	2.617067	2.357589	-0.136646
28	1	0	-0.333730	2.375285	-1.416382
29	5	0	0.175771	4.424381	-0.559807
30	1	0	1.039305	5.067449	-0.036553
31	1	0	-0.838921	4.971216	-0.893324

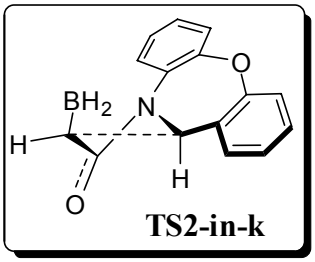


***trans*-5k**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.571519	1.098145	0.136649
2	6	0	-0.802784	1.096105	0.699298
3	6	0	-1.657354	-0.034743	0.188205
4	6	0	-2.909689	0.131234	-0.408542
5	6	0	-3.660130	-0.973198	-0.818979
6	6	0	-3.161402	-2.262290	-0.632863
7	6	0	-1.913840	-2.448929	-0.034857
8	6	0	-1.175086	-1.340222	0.367598
9	8	0	0.013722	-1.559117	1.054666
10	6	0	1.232226	-1.220548	0.472848
11	6	0	1.533923	0.084831	0.042049
12	6	0	2.807009	0.352735	-0.485038
13	6	0	3.762471	-0.658059	-0.556610

14	6	0	3.466653	-1.944751	-0.103624
15	6	0	2.198957	-2.220185	0.407668
16	1	0	-0.768418	1.076813	1.795506
17	1	0	-3.311870	1.131264	-0.542404
18	1	0	-4.632241	-0.823791	-1.279651
19	1	0	-3.740859	-3.124766	-0.949899
20	1	0	-1.505511	-3.440538	0.132060
21	1	0	3.025099	1.356733	-0.829427
22	1	0	4.743613	-0.433026	-0.964447
23	1	0	4.212456	-2.732512	-0.152701
24	1	0	1.933287	-3.210144	0.764845
25	6	0	-0.986254	2.535564	0.133821
26	6	0	0.485647	2.363851	-0.398014
27	8	0	1.257586	3.043665	-1.031934
28	1	0	-1.652689	2.593783	-0.734033
29	5	0	-1.106883	3.759470	1.093233
30	1	0	-0.949518	3.630028	2.272449
31	1	0	-1.312121	4.847042	0.645381

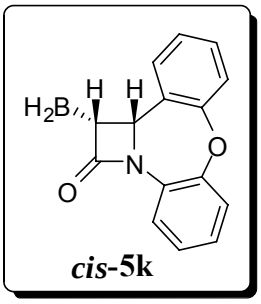


TS2-in-k

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.829779	1.038095	-0.267246
2	6	0	0.492426	1.305196	-0.562238
3	6	0	1.581498	0.359834	-0.393651
4	6	0	2.794498	0.622334	-1.066049
5	6	0	3.900978	-0.201438	-0.914179
6	6	0	3.816538	-1.321688	-0.080890
7	6	0	2.624574	-1.616471	0.580185
8	6	0	1.515775	-0.789593	0.423974
9	8	0	0.389636	-1.110151	1.147558
10	6	0	-0.807528	-1.300184	0.463209
11	6	0	-1.431933	-0.248134	-0.218017
12	6	0	-2.682480	-0.460385	-0.809227
13	6	0	-3.292340	-1.710989	-0.716922

14	6	0	-2.658319	-2.757328	-0.045740
15	6	0	-1.410273	-2.551644	0.542705
16	1	0	0.661898	2.032425	-1.346276
17	1	0	2.856501	1.504926	-1.697626
18	1	0	4.825364	0.026985	-1.435368
19	1	0	4.676900	-1.971862	0.049089
20	1	0	2.533229	-2.483600	1.225838
21	1	0	-3.171502	0.367667	-1.306538
22	1	0	-4.266131	-1.863932	-1.172440
23	1	0	-3.133112	-3.731436	0.026094
24	1	0	-0.898558	-3.340115	1.085053
25	6	0	-0.453194	3.172369	0.521352
26	6	0	-1.503515	2.255953	0.082407
27	8	0	-2.705595	2.435092	-0.012002
28	1	0	-0.618601	4.218314	0.254929
29	5	0	0.718352	2.730927	1.358430
30	1	0	1.653667	3.469653	1.500609
31	1	0	0.704471	1.703145	1.969255



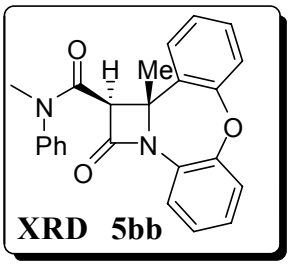
***cis*-5k**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.635478	1.086758	0.312094
2	6	0	-0.728410	1.059822	0.890462
3	6	0	-1.640531	0.007476	0.317549
4	6	0	-2.937060	0.257054	-0.138443
5	6	0	-3.756049	-0.778846	-0.590056
6	6	0	-3.281799	-2.090924	-0.585112
7	6	0	-1.995790	-2.365008	-0.119327
8	6	0	-1.189893	-1.321301	0.329719
9	8	0	0.027204	-1.653549	0.911901
10	6	0	1.238050	-1.270790	0.344517
11	6	0	1.572609	0.071315	0.087833
12	6	0	2.850022	0.373955	-0.409862

13	6	0	3.774810	-0.643538	-0.630833
14	6	0	3.443381	-1.972169	-0.360259
15	6	0	2.173277	-2.278999	0.126058
16	1	0	-0.665404	0.925488	1.979018
17	1	0	-3.319300	1.274730	-0.128621
18	1	0	-4.759461	-0.559624	-0.942731
19	1	0	-3.911801	-2.902578	-0.937796
20	1	0	-1.607106	-3.377686	-0.084556
21	1	0	3.097647	1.410317	-0.606713
22	1	0	4.759780	-0.391457	-1.012787
23	1	0	4.164228	-2.766686	-0.528460
24	1	0	1.881974	-3.300420	0.349653
25	6	0	-0.855053	2.579608	0.540450
26	6	0	0.653339	2.449049	0.118809
27	8	0	1.509250	3.217740	-0.257037
28	1	0	-0.996978	3.229447	1.408138
29	5	0	-1.551507	3.066098	-0.772674
30	1	0	-1.918869	4.198898	-0.862997
31	1	0	-1.632575	2.348024	-1.721391

Structural data of product 5bb from XRD analysis

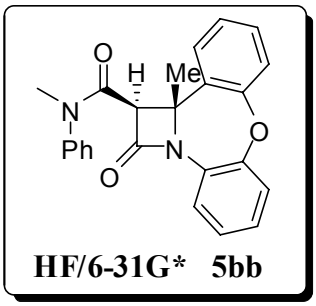


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.568645	1.300429	-1.181964
2	8	0	0.919699	-2.471602	1.919939
3	8	0	-1.060532	-3.241607	-0.587958
4	7	0	1.451205	-0.964165	0.197934
5	7	0	-2.807313	-1.795180	-0.458016
6	6	0	2.828324	-0.720690	0.173636
7	6	0	3.360495	0.382329	-0.484965
8	6	0	4.728912	0.542179	-0.557429
9	6	0	5.579102	-0.332546	0.058872
10	6	0	5.061428	-1.400672	0.757539

11	6	0	3.701404	-1.592897	0.818198
12	6	0	1.521864	1.928500	-0.489825
13	6	0	0.360912	1.219211	-0.152634
14	6	0	-0.669295	1.939605	0.426422
15	6	0	-0.569309	3.299255	0.660340
16	6	0	0.573989	3.978543	0.327311
17	6	0	1.635208	3.293643	-0.253594
18	6	0	-3.365916	-0.525802	-0.057913
19	6	0	-3.669547	-0.296044	1.272663
20	6	0	-4.116081	0.958549	1.645092
21	6	0	-4.289464	1.949836	0.707475
22	6	0	-4.064253	1.684131	-0.618729
23	6	0	-3.585919	0.449898	-1.003125
24	6	0	-1.531897	-2.150003	-0.225903
25	6	0	-0.628001	-1.121593	0.451815
26	6	0	0.653218	-1.707253	1.026107
27	6	0	0.310832	-0.255963	-0.473968
28	6	0	0.174333	-0.511893	-1.961169
29	1	0	4.973887	1.243459	-1.163501
30	1	0	6.469412	-0.188660	0.005876
31	1	0	5.601276	-2.123909	1.118733
32	1	0	3.361576	-2.263148	1.351098
33	1	0	-1.362067	1.488449	0.748231
34	1	0	-1.293662	3.711388	1.051793
35	1	0	0.563752	4.961200	0.486542
36	1	0	2.550064	3.645880	-0.484872
37	1	0	-3.496530	-0.959645	1.860058
38	1	0	-4.577477	1.011389	2.390441
39	1	0	-4.525355	2.899019	0.946058
40	1	0	-4.180472	2.403493	-1.477256
41	1	0	-3.457195	0.167889	-1.892381
42	1	0	-1.054671	-0.512724	1.200598
43	1	0	0.147812	-1.458007	-2.121979
44	1	0	0.924765	-0.130179	-2.421720
45	1	0	-0.637743	-0.109697	-2.282035
46	6	0	-3.698909	-2.727949	-1.162216
47	1	0	-3.364121	-2.848194	-2.171354
48	1	0	-3.686135	-3.676264	-0.666803
49	1	0	-4.695456	-2.338342	-1.161074

Structural data of product 5bb from calculation



HF/6-31G* 5bb

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.282135	0.925504	0.712372
2	8	0	0.181983	-2.410184	-1.010233
3	8	0	1.475230	-1.749086	2.332645
4	7	0	-1.245997	-0.960083	0.141382
5	7	0	3.108281	-0.791514	1.143226
6	6	0	-2.563803	-1.150781	-0.295132
7	6	0	-3.536791	-0.190350	-0.044033
8	6	0	-4.834810	-0.374182	-0.480641
9	6	0	-5.179700	-1.511274	-1.187802
10	6	0	-4.213104	-2.466705	-1.453260
11	6	0	-2.915210	-2.292591	-1.009465
12	6	0	-2.298315	1.814410	0.364730
13	6	0	-0.957620	1.478484	0.528637
14	6	0	-0.010197	2.463004	0.288240
15	6	0	-0.382462	3.734971	-0.120579
16	6	0	-1.719546	4.038872	-0.296111
17	6	0	-2.682512	3.074170	-0.048310
18	6	0	3.591229	-0.268168	-0.096071
19	6	0	3.473144	-0.996965	-1.271181
20	6	0	3.974304	-0.481410	-2.456714
21	6	0	4.609818	0.748970	-2.470529
22	6	0	4.736902	1.472010	-1.294393
23	6	0	4.225603	0.967156	-0.110881
24	6	0	1.798654	-1.064817	1.401040
25	6	0	0.756530	-0.476552	0.464255
26	6	0	-0.079556	-1.501945	-0.288391
27	6	0	-0.615088	0.073402	0.999373
28	6	0	-0.924374	-0.094113	2.487102
29	1	0	-5.559461	0.384746	-0.251077
30	1	0	-6.190579	-1.647109	-1.526198
31	1	0	-4.465844	-3.355639	-2.002044

32	1	0	-2.165406	-3.030964	-1.210539
33	1	0	1.033497	2.247191	0.426110
34	1	0	0.371755	4.479321	-0.300426
35	1	0	-2.016490	5.020957	-0.616773
36	1	0	-3.729626	3.287381	-0.156339
37	1	0	2.973283	-1.948399	-1.260548
38	1	0	3.869528	-1.045707	-3.365493
39	1	0	5.002101	1.143174	-3.390573
40	1	0	5.227664	2.428635	-1.298795
41	1	0	4.315072	1.523625	0.805060
42	1	0	1.190678	0.202244	-0.249763
43	1	0	-0.777070	-1.114522	2.801524
44	1	0	-1.946539	0.202413	2.679857
45	1	0	-0.268938	0.543248	3.070539
46	6	0	4.092500	-1.411906	2.027791
47	1	0	5.038837	-0.907472	1.898697
48	1	0	3.769333	-1.319467	3.052380
49	1	0	4.218031	-2.464490	1.797824

3. Computed Energies

Table 1S. Reaction of **1a** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGE	Gs
s-*E*-1a	-419.694339	-419.684894	-419.728567	0.071199	-419.728676
s-*Z*-1a	-419.727366	-419.683794	-419.693268	0.071261	-419.728019
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
TS2-out-s-*E*-a	-1050.236125	-1050.216291	-1050.28498	0.245783	-1050.294708
TS2-out-s-*Z*-a	-1050.235619	-1050.215771	-1050.284413	0.245741	-1050.295689
***trans*-5a**	-1050.297433	-1050.277594	-1050.346393	0.248812	-1050.350408
TS1-in-a	-1050.256803	-1050.256803	-1050.306772	0.243713	-1050.308893
INT-in-a	-1050.257484	-1050.236757	-1050.308021	0.244329	-1050.317768
TS2-in-s-*E*-a	-1050.23461	-1050.214946	-1050.282553	0.246885	-1050.29114
TS2-in-s-*Z*-a	-1050.235965	-1050.216146	-1050.284993	0.245578	-1050.29307
***cis*-5a**	-1050.28969	-1050.269909	-1050.338379	0.249114	-1050.34339

Table 2S. Reaction of **1a** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
s-*E*-1a	0	0	0	0
s-*Z*-1a	-20.72	0.69	22.15	0.41
TS2-out-s-*E*-a	17.40	16.84	31.02	28.64
TS2-out-s-*Z*-a	17.72	17.17	31.37	28.02
***trans*-5a**	-21.07	-21.62	-7.52	-6.31
TS1-in-a	4.43	-8.58	17.34	19.74
INT-in-a	4.00	4.00	16.56	14.17
TS2-in-s-*E*-a	18.35	17.69	32.54	30.88
TS2-in-s-*Z*-a	17.50	16.94	31.01	29.67
***cis*-5a**	-16.21	-16.80	-2.49	-1.91

Table 3S. Reaction of **1b** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGFE	Gs
***s-EE*-1b**	-591.48863	-591.475702	-591.52817	0.130105	-591.532541
***s-ZE*-1b**	-591.490855	-591.477849	-591.531041	0.129537	-591.533949
***s-EZ*-1b**	-591.481816	-591.469227	-591.520749	0.131293	-591.525323
***s-ZZ*-1b**	-591.485314	-591.472532	-591.524476	0.130901	-591.529158
4a	-630.56952	-630.558241	-630.60584	0.150059	-630.611673
TS2-out-*s-EZ*-b	-1222.0316	-1222.00813	-1222.0867	0.303782	-1222.09694
***trans*-5b**	-1222.0929	-1222.06969	-1222.1462	0.309163	-1222.15232

TS2-in-*s*-*EZ*-b	-1222.030953	-1222.007577	-1222.084766	0.305088	-1222.081793
***cis*-5b**	-1222.0885	-1222.06514	-1222.1424	0.308421	-1222.1471

Table 4S. Reaction of **1b** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
***s*-*EE*-1b**	1.40	1.35	1.80	0.88
***s*-*ZE*-1b**	5.67	5.41	6.46	5.41
***s*-*EZ*-1b**	0.00	0.00	0.00	0.00
***s*-*ZZ*-1b**	3.48	3.34	4.12	3.01
TS2-out-*s*-*EZ*-b	18.06	17.55	31.51	30.55
***trans*-5b**	-20.38	-21.08	-5.87	-4.20
TS2-in-*s*-*EZ*-b	18.46	17.89	32.71	33.11
***cis*-5b**	-17.63	-18.23	-3.47	-0.93

Table 5S. Reaction of **1b** with **4b**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGFE	Gs
***s*-*EZ*-1b**	-591.490855	-591.477849	-591.531041	0.129537	-591.533949
4b	-669.86115	-669.848238	-669.899258	0.176032	-669.901277
TS2-out-*s*-*EZ*-bb	-1261.314882	-1261.290211	-1261.370173	0.331871	-1261.375704
***trans*-5bb**	-1261.381748	-1261.357795	-1261.435133	0.336829	-1261.434196
TS2-in-*s*-*EZ*-bb	-1261.31289	-1261.288104	-1261.368122	0.331709	-1261.372929
***cis*-5bb**	-1261.376666	-1261.351926	-1261.431246	0.3355	-1261.431036

Table 6S. Reaction of **1b** with **4b**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
TS2-out-*s*-*EZ*-bb	23.30	22.51	37.73	37.35
***trans*-5bb**	-18.66	-19.90	-3.03	0.65
TS2-in-*s*-*EZ*-bb	24.55	23.83	39.02	39.09
***cis*-5bb**	-15.48	-16.21	-0.59	2.63

Table 7S. Reaction of **1d** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGE	Gs
***s*-*E*-1d**	-496.862945	-496.852932	-496.898152	0.089646	-496.903325
***s*-*Z*-1d**	-496.864903	-496.854747	-496.900832	0.088851	-496.906523
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
TS2-out- *s*-*E*-d	-1127.405445	-1127.385059	-1127.455204	0.264731	-1127.467317
TS2-out- *s*-*Z*-d	-1127.405631	-1127.385061	-1127.456065	0.263523	-1127.471231

***trans*-5d**	-1127.469047	-1127.448593	-1127.518638	0.267667	-1127.525965
TS2-in- *s-E*-d	-1127.403229	-1127.382819	-1127.451907	0.265289	-1127.464097
TS2-in- *s-Z*-d	-1127.407429	-1127.386954	-1127.457156	0.264351	-1127.469173
***cis*-5d**	-1127.457159	-1127.436683	-1127.507181	0.267143	-1127.516918

Table 8S. Reaction of **1d** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
***s-E*-1d**	1.23	1.14	1.68	2.01
***s-Z*-1d**	0	0	0	0
TS2-out- *s-E*-d	18.18	17.53	32.30	31.93
TS2-out- *s-Z*-d	18.07	17.52	31.76	29.47
***trans*-5d**	-21.73	-22.34	-7.51	-4.88
TS2-in- *s-E*-d	19.57	18.93	34.37	33.95
TS2-in- *s-Z*-d	16.94	16.34	31.07	30.76
***cis*-5d**	-14.27	-14.87	-0.32	0.80

Table 9S. Reaction of **1e** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGE	Gs
***s-E*-1e**	-305.179538	-305.172131	-305.210461	0.040052	-305.212205
***s-Z*-1e**	-305.179697	-305.172321	-305.210226	0.040493	-305.212123
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
TS1-out-e	-935.747402*	-935.728565*	-935.794641*	0.214253**	-935.797643*
IN1-out-e	-935.738181*	-935.720094*	-935.783096*	0.216184**	-935.798472*
TS2-out-*s-E*-e	-935.724321	-935.706752	-935.769265	0.215636	-935.779441
TS2-out-*s-Z*-e	-935.719834	-935.702083	-935.765422	0.214597	-935.778106
***trans*-5e**	-935.782992	-935.765476	-935.827813	0.218682	-935.832732
TS1-in-e	-935.742695	-935.724252	-935.789927	0.211768	-935.793618
IN2-in-e	-935.744099	-935.726358	-935.790003	0.214746	-935.800674
TS2-in-*s-E*-e	-935.718394	-935.700871	-935.763211	0.215807	-935.775987
TS2-in-*s-Z*-e	-935.721302	-935.703666	-935.766391	0.215294	-935.776423
***cis*-5e**	-935.772597	-935.755082	-935.817827	0.218284	-935.823233

* Calculated at the B3LYP/6-31G*//B3LYP/6-31G level of theory.

** Calculated at the B3LYP/6-31G level of theory.

Table 10S. Reaction of **1e** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
***s-E*-1e**	0	0	0	0
***s-Z*-1e**	-0.10	-0.12	0.15	0.05
TS1-out-e	1.04	1.13	13.59	16.46

IN1-out-e	6.82	6.45	20.84	15.94
TS2-out-*s*-*E*-e	15.52	14.82	29.52	27.88
TS2-out-*s*-*Z*-e	18.34	17.75	31.93	28.72
***trans*-5e**	-21.30	-22.03	-7.22	-5.56
TS1-in-e	3.99	3.84	16.55	18.99
IN2-in-e	3.11	2.52	16.50	14.56
TS2-in-*s*-*E*-e	19.24	18.51	33.32	30.05
TS2-in-*s*-*Z*-e	17.42	16.76	31.32	29.78
***cis*-5e**	-14.77	-15.51	-0.96	0.40

Table 11S. Reaction of **1f** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGE	Gs
***s*-*E*-1f**	-265.882807	-265.876975	-265.910562	0.015219	-265.916141
***s*-*Z*-1f**	-265.882447	-265.876689	-265.910327	0.015201	-265.915303
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
TS2-out-*s*-*E*-f	-896.4288	-896.412801	-896.471619	0.189628	-896.485592
TS2-out-*s*-*Z*-f	-896.424415	-896.408408	-896.467278	0.189463	-896.483482
***trans*-5f**	-896.480668	-896.464594	-896.523903	0.191906	-896.533408
TS2-in-*s*-*E*-f	-896.428688	-896.412913	-896.471067	0.190575	-896.485789
TS2-in-*s*-*Z*-f	-896.426436	-896.410553	-896.468828	0.190159	-896.482908
***cis*-5f**	-896.476709	-896.460741	-896.519612	0.192477	-896.528784

Table 12S. Reaction of **1f** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
***s*-*E*-1f**	0	0	0	0
***s*-*Z*-1f**	0.23	0.18	0.15	0.53
TS2-out-*s*-*E*-f	14.76	14.07	28.10	26.49
TS2-out-*s*-*Z*-f	17.51	16.82	30.83	27.82
***trans*-5f**	-17.79	-18.43	-4.70	-3.51
TS2-in-*s*-*E*-f	14.83	14.00	28.45	26.37
TS2-in-*s*-*Z*-f	16.25	15.48	29.86	28.18
***cis*-5f**	-15.30	-16.02	-2.01	-0.61

Table 13S. Reaction of **1g** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Structure	E	H	G	TCGFE	Gs
1g	-244.804947	-244.799352	-244.832394	0.004675	-244.838654
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
TS1-out-g	-875.375254	-875.358863	-875.419944	0.176373	-875.43456

INT-out-g	-875.379531	-875.363132	-875.42278	0.179187	-875.442738
TS2-out-g	-875.360049	-875.344348	-875.402419	0.179422	-875.417741
***trans*-5g**	-875.412144	-875.396447	-875.454549	0.182354	-875.46493
TS1-in-g	-875.377618	-875.361016	-875.422064	0.175794	-875.43106
INT-in-g	-875.377775	-875.361294	-875.421198	0.178695	-875.438483
TS2-in-g	-875.356241	-875.340522	-875.398671	0.179297	-875.412846
***cis*-5g**	-875.40837	-875.39272	-875.450667	0.182596	-875.46054

Table 14S. Reaction of **1g** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Structure	ΔE	ΔH	ΔG	ΔG_S
TS1-out-g	-0.50	-0.80	11.48	9.89
INT-out-g	-3.18	-3.48	9.70	4.76
TS2-out-g	9.05	8.31	22.48	20.45
***trans*-5g**	-23.64	-24.38	-10.24	-9.16
TS1-in-g	-1.98	-2.15	10.15	12.09
INT-in-g	-2.08	-2.32	10.69	7.43
TS2-in-g	11.44	10.71	24.83	23.52
***cis*-5g**	-21.28	-22.04	-7.80	-6.41

Table 15S. Reaction of **1h** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Structure	E	H	G	TCGE	Gs
1h	-357.053837	-357.047594	-357.082937	0.007135	-357.088788
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
IN1-out-h	-987.630303	-987.612636	-987.676656	0.179506	-987.694916
TS2-out-h	-987.608017	-987.591502	-987.652108	0.18173	-987.670786
***trans*-5h**	-987.665456	-987.648905	-987.709836	0.184489	-987.718107
TS1-in-h	-987.621979	-987.604537	-987.667916	0.178005	-987.676009
IN2-in-h	-987.630144	-987.61291	-987.675799	0.180898	-987.695644
TS2-in-h	-987.606416	-987.589948	-987.650089	0.182117	-987.666417
***cis*-5h**	-987.65933	-987.642901	-987.702914	0.185473	-987.711998

Table 16S. Reaction of **1h** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Structure	ΔE	ΔH	ΔG	ΔG_S
IN1-out-b	-4.36	-4.27	7.61	3.48
TS2-out-b	9.62	8.99	23.01	18.62
trans-b	-26.42	-27.03	-13.21	-11.07
TS1-in-b	0.86	0.81	13.09	15.34
IN2-in-b	-4.26	-4.44	8.15	3.02
TS2-in-b	10.63	9.97	24.28	21.36

cis-b	-22.57	-23.26	-8.87	-7.24

Table 17S. Reaction of **1i** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGFE	Gs
1i	-877.374822	-877.360279	-877.417177	0.130901	-877.417138
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
TS2-out-i	-1507.914331	-1507.88926	-1507.971006	0.305616	-1507.977396
***trans*-5i**	-1507.982327	-1507.957277	-1508.039085	0.308803	-1508.039311
TS2-in-i	-1507.909752	-1507.884667	-1507.967619	0.304362	-1507.966
***cis*-5i**	-1507.973804	-1507.948917	-1508.029264	0.310283	-1508.030654

Table 18S. Reaction of **1i** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
TS2-out-i	18.83	18.36	32.64	32.26
***trans*-5i**	-23.84	-24.32	-10.08	-6.59
TS2-in-i	21.70	21.24	34.77	33.98
***cis*-5i**	-18.49	-19.07	-3.92	-1.16

Table 19S. Reaction of **1j** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGFE	Gs
1j	-932.092296	-932.080662	-932.130313	0.086986	-932.13986
4a	-630.569518	-630.558241	-630.605844	0.150059	-630.611673
IN1-out-j	-1562.662156	-1562.639308	-1562.715576	0.261262	-1562.737236
TS2-out-j	-1562.635976	-1562.613863	-1562.688454	0.261573	-1562.708674
***trans*-5j**	-1562.700045	-1562.677994	-1562.752024	0.265311	-1562.765102
IN2-in-j	-1562.655231	-1562.632312	-1562.709468	0.26024	-1562.728507
TS2-in-j	-1562.638586	-1562.616581	-1562.690902	0.262049	-1562.705628
***cis*-5j**	-1562.695983	-1562.674081	-1562.746977	0.266646	-1562.758845

Table 20S. Reaction of **1j** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
IN1-out-j	-0.21	-0.25	12.91	8.97
TS2-out-j	16.21	15.71	29.93	26.89
***trans*-5j**	-23.99	-24.53	-9.96	-8.51
IN2-in-j	4.13	4.14	16.75	14.45
TS2-in-j	14.58	14.01	28.40	28.81
***cis*-5j**	-21.44	-22.07	-6.79	-4.59

Table 21S. Reaction of **1k** with **4a**. Sum of electronic and zero-point energies (E, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.), thermal correction to Gibbs free energy (TCGFE, in a.u.), total free energy in solution (G_S, in a.u., solvent =dichloromethane)

Struture	E	H	G	TCGFE	Gs
1k	-178.0185	-178.0131	-178.0447	0.018749	-178.0411
4a	-630.5695	-630.5582	-630.6058	0.150059	-630.6117
TS2-out-k	-808.5481	-808.5325	-808.5898	0.19226	-808.5973
***trans*-5k**	-808.5994	-808.5837	-808.6413	0.194632	-808.6441
TS2-in-k	-808.5585	-808.5434	-808.5994	0.194196	-808.6067
***cis*-5k**	-808.5955	-808.5799	-808.6372	0.195061	-808.6404

Table 22S. Reaction of **1k** with **4a**. Electronic energies (ΔE, in kcal/mol), enthalpies (ΔH, in kcal/mol), Gibbs free energies at 298 K (ΔG, in kcal/mol), Gibbs free energies in solution (ΔG_S, in kcal/mol)

Struture	ΔE	ΔH	ΔG	ΔG_S
TS2-out-k	25.00	24.35	38.15	34.84
***trans*-5k**	-7.20	-7.79	5.83	5.49
TS2-in-k	18.49	17.53	32.08	28.92
***cis*-5k**	-4.74	-5.40	8.40	7.78

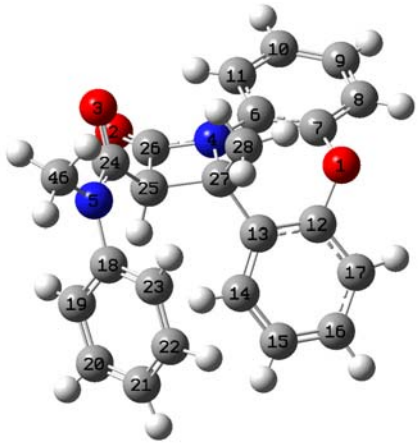
Table 23S. Calculated Transition State Energies ($\Delta G^{\neq}$) for the Reactions of Ketenes **1** with Imines **4** in the gas and solution phases (in kcal/mol).

Entry	Ketene	Imine	Gas phase			Solution phase		
			$\Delta G^{\neq}$ (TS2-out)	$\Delta G^{\neq}$ (TS2-in)	$-\Delta\Delta G^{\neq}$ (TS2out-in)	$\Delta G^{\neq}$(TS2-out)	$\Delta G^{\neq}$ (TS2-in)	$-\Delta\Delta G^{\neq}$ (TS2out-in)
1	s-*E*-**1a**	4a	31.0	32.5	1.5	28.6	30.9	2.3
2	s-*Z*-**1a**	4a	31.4	31.0	-0.4	28.0	29.7	1.7
3	s-*EZ*-**1b**	4a	31.5	32.7	1.2	30.5	33.1	2.6
4	s-*EZ*-**1b**	4b	37.7	39.0	1.3	37.4	39.1	1.7
5	s-*E*-**1d**	4a	32.3	34.4	2.1	31.9	33.9	2.0
6	s-*Z*-**1d**	4a	31.8	31.1	-0.7	29.5	30.8	1.3
7	s-*E*-**1e**	4a	29.5	33.3	3.8	27.9	30.1	2.2
8	s-*Z*-**1e**	4a	31.9	31.3	-0.6	28.7	29.8	1.1
9	s-*E*-**1f**	4a	28.1	28.5	0.4	26.5	26.4	-0.1
10	s-*Z*-**1f**	4a	30.8	29.9	-0.9	27.8	28.2	0.4
11	1g	4a	22.5	24.8	2.3	20.4	23.5	3.1
12	1h	4a	23.0	24.3	1.3	18.6	21.4	2.8

13	1i	4a	32.6	34.8	2.2	32.3	34.0	1.7
14	1j	4a	29.9	28.4	-1.5	26.9	28.8	1.9
15	1k	4a	38.2	32.1	-6.1	34.8	28.9	-5.9

4. Comparison on the structural parameters of 5bb.

Table 24S. Comparison on the structural parameters of **5bb** betweem XRD, HF/6-31G* and B3LYP/6-31G*



	N_4-C_{26}	N_4-C_{27}	C_{25}-C_{27}	C_{24}.C_{25}	C_{24}-C_{25}-C_{27}-C_{28}	O_3-C_{24}-N_5-C_{46}	C_{18}-N_5-C_{24}-C_{25}
XRD	1.369 Å	1.501 Å	1.577 Å	1.528 Å	2.063°	0.337°	-2.348°
HF/6-31G*	1.356 Å	1.484 Å	1.572 Å	1.520 Å	-4.545°	2.124°	-15.401°
B3LYP/6-31G*	1.373 Å	1.500 Å	1.581 Å	1.523 Å	-5.627°	0.958°	-12.098°

5. Main two-electron interactions in the different TS2 structures

Table 25S. Main two-electron interactions in the different **TS2** structures.*

Entry	Ketene	Imine	ΔE (2)-out (kcal/mol)	ΔE(2)-in (kcal/mol)
			π5,6—> **σ***3,4	**π**5,6—> **σ***3,4
1	s-*E*-**1a**	**4a**	-5.42	-3.12
2	s-*Z*-**1a**	**4a**	-5.14	-0.53
3	s-*EZ*-**1b**	**4a**	-4.81	--
4	s-*EZ*-**1b**	**4b**	-4.58	--
5	s-*E*-**1d**	**4a**	-6.92	-2.74
6	s-*Z*-**1d**	**4a**	-6.50	-1.89
7	s-*E*-**1e**	**4a**	-6.60	-3.90

8	s-*Z*-**1e**	**4a**	-6.46	-2.05
9	s-*E*-**1f**	**4a**	-6.77	-3.82
10	s-*Z*-**1f**	**4a**	-6.75	-2.32
11	**1g**	**4a**	-10.34	-5.47
12	**1h**	**4a**	-5.14	-3.32

* The two-electron interaction of **π**5,6—> **σ***3,4 is not conspicuous in **TS2-i** and **TS2-j**, while no existence in **TS2-k**.

6. Dipole moments of the different TS2 structures

Table 26S. Dipole moments of the different **TS2** structures.

Entry	Ketene	Imine	**μ(**out**)**/D	**μ(**in**)**/D
1	s-*E*-**1a**	**4a**	6.6934	7.0671
2	s-*Z*-**1a**	**4a**	7.8724	5.9805
3	s-*EZ*-**1b**	**4a**	7.5933	5.6439
4	s-*EZ*-**1b**	**4b**	7.6716	5.7315
5	s-*E*-**1d**	**4a**	7.2378	7.3098
6	s-*Z*-**1d**	**4a**	8.6211	6.1632
7	s-*E*-**1e**	**4a**	5.5638	7.6329
8	s-*Z*-**1e**	**4a**	8.8047	5.7790
9	s-*E*-**1f**	**4a**	8.1435	7.6373
10	s-*Z*-**1f**	**4a**	9.2319	6.1211
11	**1g**	**4a**	9.8375	6.7294
12	**1h**	**4a**	10.9177	7.5803
13	**1i**	**4a**	7.0734	5.2627
14	**1j**	**4a**	11.5720	3.6732
15	**1k**	**4a**	7.6888	5.8993