Ruthenium catalyzes the synthesis of γ-butenolides fused to cyclohexanones

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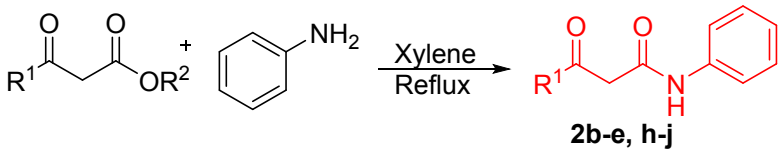
Supplementary Information

TABLE OF CONTENTS

General remarks

All experiments were carried out under nitrogen, unless stated otherwise. Merck precoated silica gel plates (Art. 5554) treated with a fluorescent indicator were used for analytical thin layer chromatography (TLC). Flash column chromatography was performed using silica gel 9385 (Merck). Melting points are uncorrected and were determined using Fisher-Johns Melting Point Apparatus. ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian VNS or DPX (600 or 300 MHz and 150 or 75 MHz, respectively) spectrometers in $CDCl_3$ using δ = 7.24 and 77.00 ppm as the solvent chemical shifts. All chemical shifts (δ) are expressed in units of ppm and J values are given in Hz. Multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or overlap of nonequivalent resonances, and dd = doublet of doublets. Infrared (IR) spectra were recorded on a PerkinElmer Spectrum Two^{TM} IR spectrometer with frequencies expressed in cm^{-1}, and high-resolution mass spectrometry (HRMS) was carried out using a JEOL JMS-700 spectrometer at the Korea Basic Science Institute.

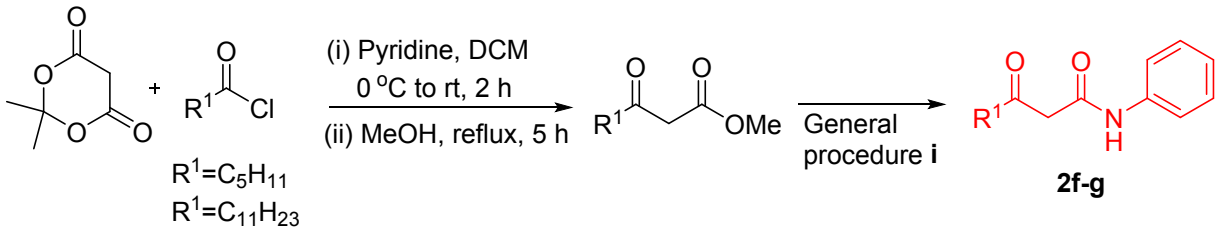
i) General procedure for the synthesis of β-ketoamides (2b-e, h-j).[1]



2b-e, h-j

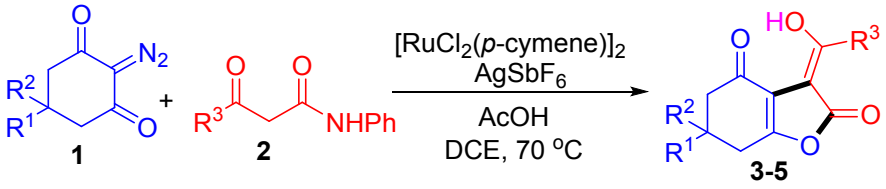
A mixture of β-Ketoester (10 mmol) and aniline (10 mmol) was heated in xylene (5 mL) at 140 ^{o}C for 4h. After the completion of the reaction as indicated by TLC, the reaction mixture was cooled to allow crystallization to take place. To rinse out the xylene in the flask, 10 mL of petroleum ether was added twice. The product was washed with 30 mL of 1:1 petroleum ether and benzene. The washing was repeated three times and collected crystals were directly used for catalytic reaction without any further purification.

ii) General procedure for the synthesis of β-ketoamides (2f-g).[2]



Hexanoyl or Lauroyl chloride (15 mmol) was added to a solution of Meldrum's acid (15 mmol) and pyridine (30 mmol) in DCM (100 mL) at 0 °C over a period of 15 min. The reaction mixture was then allowed to warm to room temperature over 2 h whereupon the solution turned red and a white precipitate was formed. The mixture was then washed with 1.0 M aq. HCl (3X100 mL) and H_2O (50 mL), and then dried, filtered and concentrated *in vacuo*. The residue was re-dissolved in MeOH (100 mL) and the resultant solution was heated at reflux for 5 h. After being allowed to cool to room temperature, the solution was concentrated *in vacuo* to give a white solid which was recrystallized from MeOH. Thus obtained white solid was subjected to the next step following general procedure **i**, and **2f-g** were isolated as white crystalline solids.

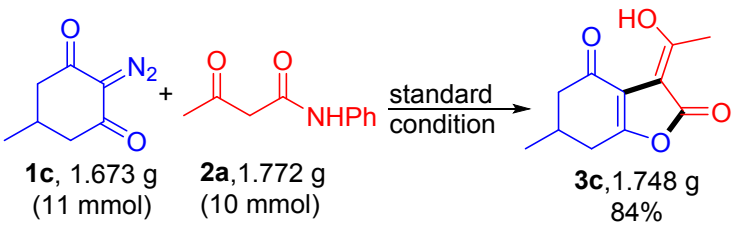
iii) General procedure for the synthesis of cyclohexanone-fused γ-butenolides (3-5)



A mixture of diazo compound **1** (1.1 mmol), β-ketoamide **2** (1 mmol), $[RuCl_2(p\text{-cymene})]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), and AcOH (2 mmol) was stirred in DCE (5 mL) under nitrogen atmosphere at 70 °C for described time. When the reaction was complete as indicated by TLC, water (10 mL) was added and the solution was extracted with ethyl acetate (10 mL x 3) and dried over anhydrous Na_2SO_4. The products were obtained after evaporation of the solvent and purification by column chromatography on silica gel. The same procedure was followed for the construction of quinolinone ring-fused γ-butenolides **5c** and **5d**.

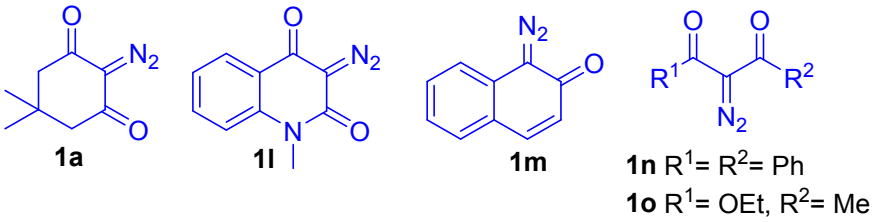
Additional experiments:

(1) Large scale reaction between diazo compound 1c and β-ketoamide 2a:



Scheme S1 Gram scale experiment for **3c**.

(2) Reactivity comparison:



Scheme S2 Reactivity of various diazo compounds towards 3-oxo-*N*-phenylbutanamide (**2a**).

The diazo compounds **1a** and **1l** possessed similar reactivities to give desired products in excellent yields. However, the reactions of other diazo compounds such as 1-diazonaphthalen-2(1*H*)-one (**1m**), 2-diazo-1,3-diphenylpropane-1,3-dione (**1n**), and ethyl 2-diazo-3-oxobutanoate (**1o**) with 3-oxo-*N*-phenylbutanamide (**2a**) were unsuccessful, pointing out that the cyclic carbene motif flanked by two electron acceptors, as is found in **1a** and **1l**, but not present in **1m**-**1o**, is an important requirement.

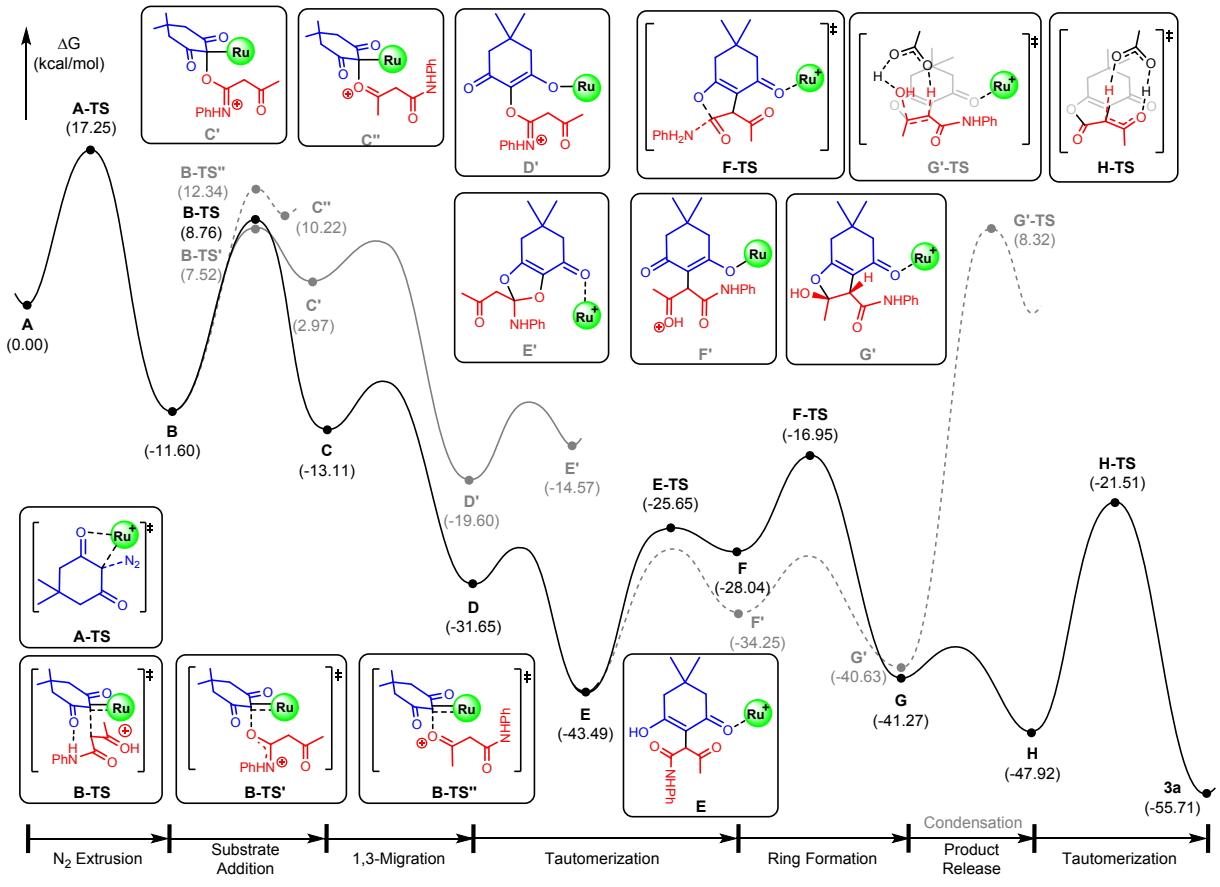
Computational study:

(1) Energy profile diagram:

After the generation of the active Ru(II)-catalyst by the silver salt initiator, the catalytic cycle starts with the addition of the diazo compound **1a** to the Ru(II)-complex to form intermediate **A**, in which the decomposition of the diazo functionality leads to an electrophilic carbene center *via* nitrogen extrusion, traversing **A-TS** located at 17.3 kcal/mol to give **B**. The carbene center in the intermediate **B** could undergo three possible reactions leading to different intermediate products:

(i) C-O bond formation intermediate **C'** through **B-TS'**, (ii) the oxonium ion intermediate **C''**through **B-TS''**, and (iii) C–C coupled intermediate **C** by the addition of **2a'** (**B-TS**) which is generated from the enol tautomer of substrate **2a**.

Due to the higher ability of the iminium ion to stabilize positive charge compared to the oxonium moiety, the transition state **B-TS'** is found to be 4.8 kcal/mol lower in energy than **B-TS''** and the intermediate **C'** is also 7.3 kcal/mol more stable than **C''**. Accordingly, the pathway that produces the oxonium ion intermediate can be ruled out. The C-O bond formation intermediate **C'** could be further stabilized by the 1,3-migration step to afford intermediate **D'**, which is located at -19.6 kcal/mol, which affords the dioxolene complex **E'** found at -14.6 kcal/mol. The transition state **B-TS'** is 1.2 kcal/mol lower in energy than **B-TS** and the immediate intermediate of this reaction step, **C'**, is found at 3.0 kcal/mol, rendering this step



Scheme S3 Reaction energy profile.

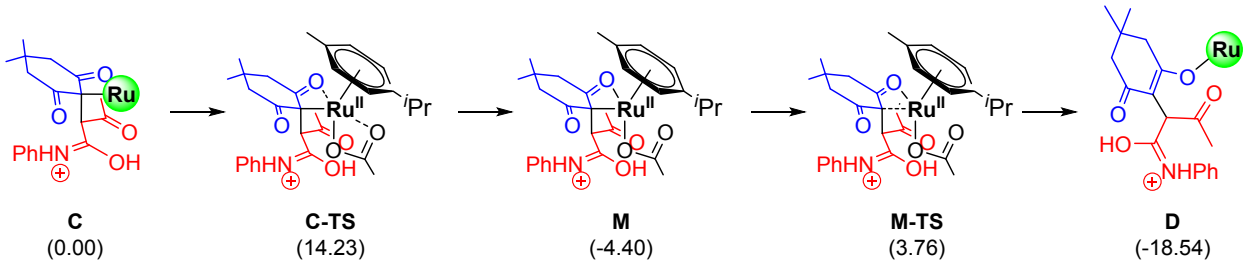
endergonic. However, the back-reaction to reform **B** is much faster since that barrier is only 4.6 kcal/mol. Thus, although the reaction leading to **C** traverses a slightly higher energy transition state **B-TS**, this path is predicted to be the main reaction trajectory, because the intermediate **C** is found at -13.1 kcal/mol. Therefore, the main intermediate formed in this initial substrate engaging step is predicted to be **C**. During this step, the transition state **B-TS** follows a concerted mechanism that forms a C–C bond and shifts a proton asynchronously to yield **C**.[25] This intermediate can be further stabilized by 1,3-migration to give an oxygen-bound intermediate **D** (Scheme S4) and subsequent tautomerization leads to the intermediate **E**, which is located at -43.5 kcal/mol. To test the importance of the amide group, control experiments were carried out employing β-ketoesters **6a** and **6b** as substrates. The reactions of β-ketoesters (**6a-b**) with **1a** did not produce the desired cyclic product as well as C–H insertion product but it resulted into the decomposition of diazo compound **1a** (Scheme S5). The calculation result shows that the exchange of the amide group to ester group increases both transition state barrier for C–H insertion and the energies of the intermediates and therefore, the reaction could not go further with the ester group (See Scheme S6 for details).

To push the catalytic cycle forward, the proton of the hydroxyl group in **E** is shifted to the amide moiety *via* **E-TS** and affords intermediate **F**. This process is associated with the transition state **F-TS** where the heterocycle is formed concomitant to liberation of an equivalent of aniline. As evidence, the eliminated aniline was isolated by column chromatography. The overall barrier of **F-TS** is 26.5 kcal/mol and should be readily overcome under the given condition of slightly elevated temperatures. Finally, the intermediate **G** releases the γ-butenolide isomer **H**, which tautomerizes to product **3a**. Note that the cyclization reaction could also be performed without the Ru catalyst if the dissociation of the Ru catalyst at intermediate **E** is an irreversible process (for details see Scheme S7).

Another possibility that we have considered the formation of furan ring through a condensation-type reaction from **E**. Interestingly, the initial tautomerization from **E** to **F'** and the ring-formation to afford **G'** is more facile according to our calculations, as highlighted in Scheme 6, but the subsequent condensation reaction is highly unlikely and associated with a prohibitive barrier at **G'-TS** of 49.0 kcal/mol. An alternative stepwise condensation was also considered which was eventually rejected due to very high energies. The calculated free energy

of the protonated **G''**, intermediate **H''**, is found at 26.7 kcal/mol (for details see Scheme S8). The low acidity of acetic acid and low polarity of the solvent make the formation of a 2^+ charged intermediate energetically disfavored. Overall, these calculations do not offer any support for the condensation pathway being mechanistically meaningful.

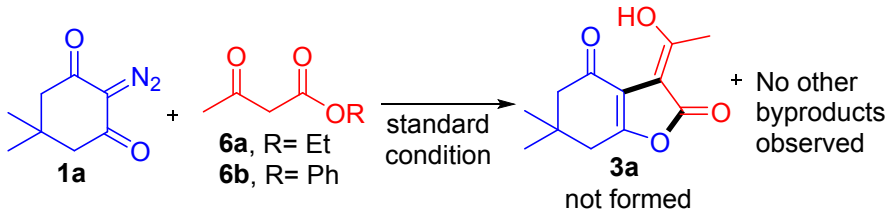
(2) 1,3-Ruthenium migration



Scheme S4 The mechanism of the 1,3-migration.

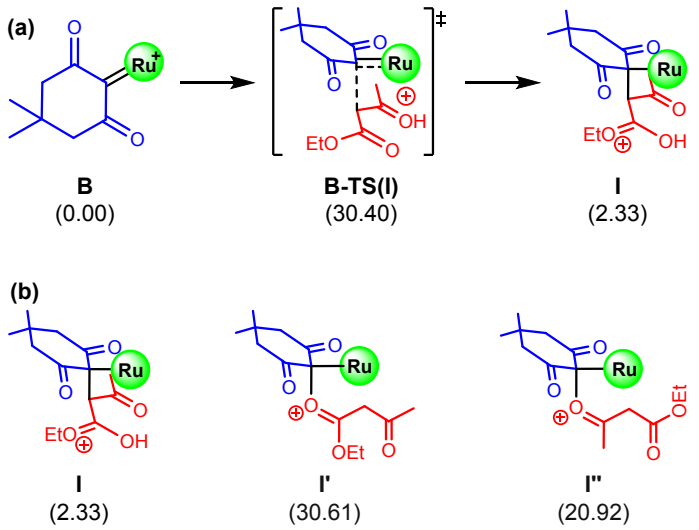
The mechanism of 1,3-migration is examined in detail. First, the oxygen of the intermediate **C** coordinates to the Ru center with the accompanying dissociation of oxygen in acetate through **C-TS** and forms the intermediate **M**. This intermediate severs the Ru–C bonds and yields **D**. The calculated barriers for this transformation are not significant and thus the migration should be easy.

(3) Reactions of β-ketoesters with 1a:



Scheme S5 Control experiments

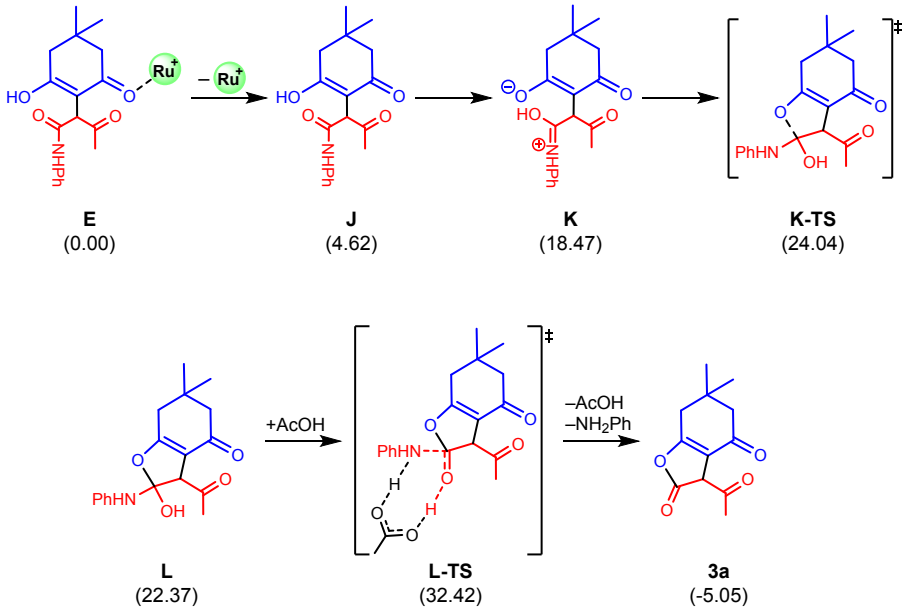
(4) DFT calculations for the reaction with ß-keto ester:



Scheme S6 (a) C–H insertion step with ß-keto ester (b) Three possible ß-keto ester inserted intermediates.

Three possible β-keto ester inserted intermediates are explored by DFT calculations. When the ester group is employed in place of the amide group, the C–H insertion step is expected to require higher energies for two reasons: the reduced electron donating ability of ester makes the substrate an inferior nucleophile and the loss of the hydrogen bonding between N–H--O at the transition state disfavors these substrates. Consistent with these general concerns, the barrier for the C–H insertion step is calculated to be 30.4 kcal/mol. Thus, the ester group is predicted to face difficulty in performing the C–H insertion step in the given condition. Furthermore, the generation of C–O coupled intermediate **I'** and **I''** are highly endergonic and thus, would not be preferred.

(5) DFT calculations for cyclization reaction without the Ru catalyst:

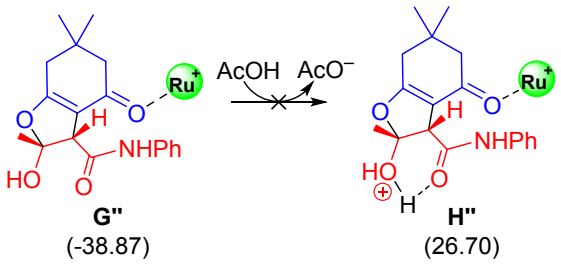


Scheme S7 Cyclization without the Ru catalyst.

The cyclization step without the Ru catalyst has been examined. After the extrusion of the Ru catalyst, the proton of the hydroxyl group in **J** shifts to the oxygen of the amide group and forms **K**. Intermediate **K** undergoes cyclization with an overall barrier of 24.0 kcal/mol and yields **L** that we located at 22.4 kcal/mol. The subsequent proton transfer associated with the aniline dissociation, **L-TS**, leads to the product **3a**. The barrier of **L-TS**, however, is calculated to be 32.4 kcal/mol, which is too high to be overcome with the given experimental conditions. Therefore, the cyclization step is the main reaction pathway.

Note: If the catalyst dissociation step is assumed to be irreversible, the overall cyclization barrier without the catalyst is 27.8 kcal/mol. Only then, the cyclization without the catalyst is possible.

(6) **Stepwise condensation reaction:**

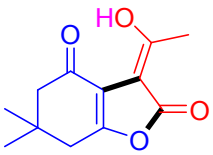


Scheme S8 Stepwise condensation reaction.

The possibility of stepwise condensation reaction is also examined. The calculation result shows that the protonated intermediate **H''** is located at 26.7 kcal/mol and therefore cannot be formed.

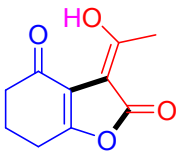
Characterization data of synthesized compounds

(*E*)-3-(1-Hydroxyethylidene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3a)



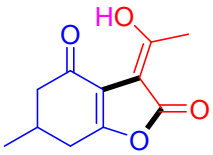
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 94% (209 mg); mp 162-164 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.31 (1H, s), 2.57 (2H, s), 2.41 (2H, s), 2.40 (3H, s), 1.14 (6H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.7, 175.7, 167.0, 166.5, 115.3, 94.4, 49.6, 36.7, 34.5, 28.4, 18.7; IR (ATR) 2962, 1773, 1625, 1264, 1320, 847, 573 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{12}H_{14}O_4Na$: 245.0790. Found: 245.0788.

(*E*)-3-(1-Hydroxyethylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3b)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 92% (179 mg); mp 98-100 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.47 (1H, s), 2.71 (2H, t, J = 6.6 Hz), 2.56 (2H, t, J = 6.6 Hz), 2.41 (3H, s), 2.18-1.13 (2H, m); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.4, 175.9, 167.8, 166.8, 116.6, 94.3, 35.5, 22.8, 21.2, 18.8; IR (ATR) 2958, 1768, 1620, 1312, 866, 567 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{10}H_{10}O_4Na$: 217.0477. Found: 217.0474.

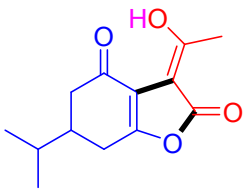
(*E*)-3-(1-Hydroxyethylidene)-6-methyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3c)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 92% (208 mg); mp 84-86 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.41 (1H, s), 2.79-2.74 (1H, m), 2.61 (1H, dd, J = 16.9, 2.4 Hz), 2.41-2.38 (5H, m), 2.28 (1H, dd, J = 17.0, 11.0 Hz), 1.17 (3H, d, J = 6.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.0, 175.9, 167.3, 166.9, 116.3, 94.5, 43.8,

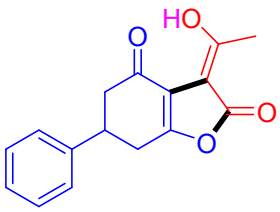
30.88, 29.3, 20.8, 18.8; IR (ATR) 2956, 1766, 1612, 1317, 895, 579 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{11}H_{12}O_4Na$: 231.0634. Found: 231.0630.

(*E*)-3-(1-Hydroxyethylidene)-6-isopropyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3d)



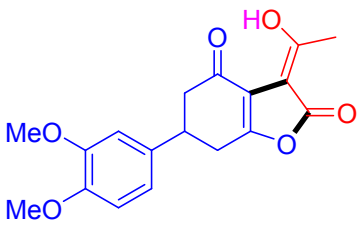
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 90% (213 mg); mp 168-170 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 13.37 (1H, s), 2.71 (1H, dd, J = 18.4, 4.9 Hz), 2.61 (1H, dd, J = 16.9, 3.9 Hz), 2.45 (1H, dd, J = 18.4, 11.3 Hz), 2.39 (3H, s), 2.29 (1H, dd, J = 16.9, 12.8 Hz), 2.10-2.04 (1H, m), 1.71-1.64 (1H, m), 0.95 (6H, d, J = 6.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.4, 175.7, 167.8, 166.9, 116.2, 94.4, 40.9, 39.5, 31.7, 26.5, 19.6, 19.4, 18.7; IR (ATR) 2952, 1714, 1610, 1315, 892, 571 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{13}H_{16}O_4Na$: 259.0947. Found: 259.0943.

(*E*)-3-(1-Hydroxyethylidene)-6-phenyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3e)



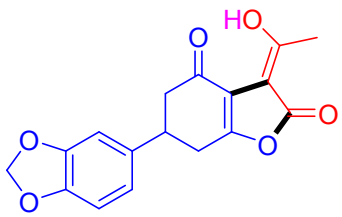
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 78% (212 mg); mp 190-192 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 13.37 (1H, s), 7.36 (2H, t, J = 7.6 Hz), 7.29 (1H, t, J = 7.4 Hz), 7.25 (2H, d, J = 7.5 Hz), 3.57-3.51 (1H, m), 3.01-2.90 (2H, m), 2.83-2.81 (2H, m), 2.44 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.1, 176.2, 166.8, 166.7, 141.1, 129.0, 127.6, 126.6, 116.5, 94.4, 42.7, 40.0, 30.5, 18.8; IR (ATR) 2960, 1769, 1619, 1321, 911, 768, 702 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{16}H_{14}O_4Na$: 293.0790. Found: 293.0787.

(*E*)-6-(3,4-Dimethoxyphenyl)-3-(1-hydroxyethylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3f)



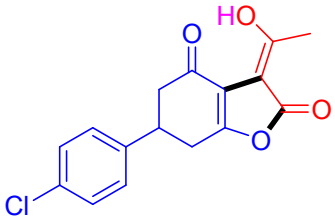
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 74 % (245 mg); mp 208-210 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.37 (1H, s), 6.84 (1H, d, J = 8.3 Hz), 6.79 (1H, dd, J = 8.3, 1.9 Hz), 6.74 (1H, d, J = 2.0 Hz), 3.87 (3H, s), 3.86 (3H, s), 3.49 (1H, m), 2.99 (1H, dd, J = 18.5, 5.3 Hz), 2.90 (1H, dd, J = 18.5, 10.8 Hz), 2.85-2.75 (2H, m), 2.45 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.1, 176.2, 166.8, 166.8, 149.2, 148.5, 133.7, 118.5, 116.5, 111.5, 110.0, 94.4, 55.9, 43.0, 39.7, 30.8, 18.9; IR (ATR) 2965, 1755, 1608, 1519, 1311, 1252, 1022, 761, 574 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{18}O_6Na$: 353.1001. Found: 353.0998.

(*E*)-6-(Benzo[*d*][1,3]dioxol-5-yl)-3-(1-hydroxyethylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3g)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 83% (263 mg); mp 215-217 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.35 (1H, s), 6.77 (1H, d, J = 8.0 Hz), 6.72 (1H, d, J = 1.6 Hz), 6.69 (1H, dd, J = 8.0, 1.6 Hz), 5.94 (2H, s), 3.48-3.42 (1H, m), 2.95 (1H, dd, J = 18.5, 5.2 Hz), 2.85 (1H, dd, J = 18.5, 10.9 Hz), 2.81-2.70 (2H, m), 2.43 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.0, 176.2, 166.8, 166.7, 148.0, 146.9, 135.0, 119.8, 116.4, 108.5, 106.96, 101.2, 94.3, 43.0, 39.8, 30.8, 18.8; IR (ATR) 2907, 1780, 1614, 1311, 1241, 1032, 763, 583 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{14}O_6Na$: 337.0688. Found: 337.0686.

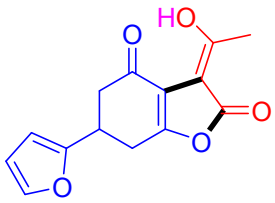
(*E*)-6-(4-Chlorophenyl)-3-(1-hydroxyethylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3h)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 77% (235 mg); mp 197-200 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.31

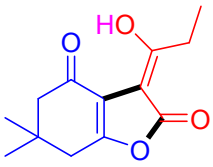
(1H, s), 7.33 (2H, d, J = 8.1 Hz), 7.19 (2H, d, J = 8.1 Hz), 3.55-3.50 (1H, m), 2.98 (1H, dd, J = 18.5, 5.1 Hz,), 2.89 (1H, dd, J = 18.4, 10.8 Hz), 2.83-2.74 (2H, m), 2.43 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.6, 176.3, 166.6, 166.4, 139.5, 133.4, 129.2, 128.0, 116.5, 94.3, 42.6, 39.4, 30.4, 18.8; IR (ATR) 2957, 1766, 1609, 1319, 906, 826, 589 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{16}H_{13}O_4ClNa$: 327.0400. Found: 327.0397.

(*E*)-6-(Furan-2-yl)-3-(1-hydroxyethylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (3i)



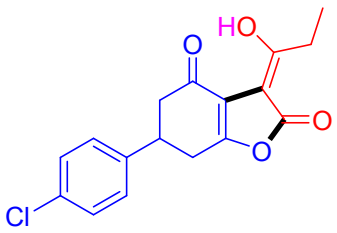
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 81% (212 mg); mp 142-144 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.31 (1H, s), 7.33 (1H, d, J = 1.1 Hz), 6.30 (1H, dd, J = 3.2, 1.9 Hz), 6.09 (1H, d, J = 3.2 Hz), 3.67-3.62 (1H, m), 3.07 (1H, dd, J = 18.5, 5.4 Hz), 2.96 (1H, dd, J = 18.6, 9.2 Hz), 2.90 (1H, dd, J = 17.2, 4.5 Hz), 2.80 (1H, dd, J = 17.2, 10.4 Hz), 2.41 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.4, 176.2, 166.6, 166.0, 154.1, 142.0, 116.5, 110.2, 105.5, 94.3, 40.0, 33.2, 27.9, 18.8; IR (ATR) 3118, 1762, 1623, 1318, 906, 853, 758, 580 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{14}H_{12}O_5Na$: 283.0583. Found: 283.0580.

(*E*)-3-(1-Hydroxypropylidene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4a)



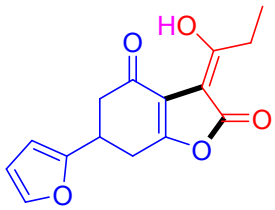
The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow liquid.Yield: 91% (216 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.41 (1H, s), 2.85 (2H, q, J = 7.5 Hz), 2.57 (2H, s), 2.42 (2H, s), 1.18 (3H, t, J = 7.6 Hz), 1.15 (6H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.7, 180.5, 166.6, 115.4, 93.5, 49.7, 36.8, 34.5, 28.5, 25.2, 10.6; IR (ATR) 2961, 1718, 1621, 1452, 1340, 868, 571 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{13}H_{16}O_4Na$: 259.0947. Found: 259.0944.

(*E*)-6-(4-Chlorophenyl)-3-(1-hydroxypropylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4b)



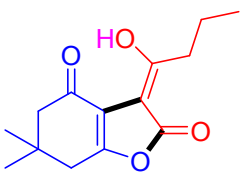
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 87% (280 mg); mp 171-173 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.42 (1H, s), 7.32 (2H, d, J = 8.3 Hz), 7.19 (2H, d, J = 8.4 Hz), 3.55-3.49 (1H, m), 2.97 (1H, dd, J = 18.4, 5.2 Hz), 2.90-2.84 (3H, m), 2.82-2.73 (2H, m), 1.19 (3H, t, J = 7.5 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.6, 181.1, 166.5, 166.3, 139.5, 133.4, 129.1, 128.0, 116.6, 93.3, 42.6, 39.3, 30.4, 25.3, 10.6; IR (ATR) 2980, 1771, 1605, 1319, 821, 590 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{15}ClO_4Na$: 341.0557. Found: 341.0551.

(*E*)-6-(Furan-2-yl)-3-(1-hydroxypropylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4c)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 83% (230 mg); mp 116-118 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.41 (1H, s), 7.33(1H, s), 6.30 (1H, dd, J = 3.0, 1.9 Hz), 6.10 (1H, d, J = 3.2 Hz), 3.67-3.62 (1H, m), 3.07 (1H, dd, J = 18.5, 5.3 Hz), 2.96 (1H, dd, J = 18.5, 9.2 Hz), 2.90 (1H, dd, J = 17.2, 4.5 Hz), 2.86 (2H, q, J = 7.6 Hz), 2.80 (1H, dd, J = 17.1, 10.5 Hz), 1.18 (3H, t, J = 7.5 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.4, 181.0, 166.3, 166.1, 154.2, 142.0, 116.6, 110.2, 105.5, 93.3, 40.0, 33.2, 27.9, 25.3, 10.6; IR (ATR) 2992, 1765, 1612, 1318, 856, 746, 590 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{15}H_{14}O_5Na$: 297.0739. Found: 297.0735.

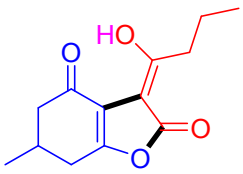
(*E*)-3-(1-Hydroxybutylidene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4d)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow liquid.Yield: 90 % (225 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.37 (1H, s), 2.79 (2H, t, J = 7.2 Hz), 2.56 (2H, s), 2.40 (2H, s), 1.67-1.61 (2H, m), 1.13 (6H, s), 0.96 (3H, t, J = 7.4 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.6, 179.4, 166.7, 166.6, 115.4, 94.0, 49.6, 36.7, 34.4,

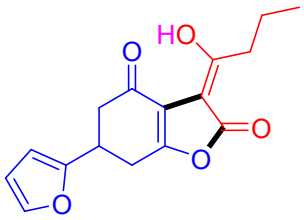
33.4, 28.4, 20.1, 13.7; IR (ATR) 2964, 1726, 1659, 1573, 1216, 748 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{14}H_{18}O_4Na$: 273.1103. Found: 273.1100.

(*E*)-3-(1-Hydroxybutylidene)-6-methyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4e)



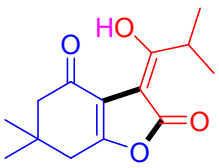
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 92 % (218 mg); mp 80-82 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 13.46 (1H, s), 2.80 (2H, t, J = 7.8 Hz), 2.75 (1H, d, J = 13.5 Hz), 2.60 (1H, dd, J = 17.0, 3.7 Hz), 2.44-2.37 (2H, m), 2.27 (1H, dd, J = 16.9, 11.9 Hz), 1.68-1.62 (2H, m), 1.16 (3H, d, J = 6.2 Hz), 0.96 (3H, t, J = 7.4 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.0, 179.7, 167.3, 166.6, 116.3, 94.1, 43.8, 33.5, 30.9, 29.8, 20.7, 20.1, 13.7; IR (ATR) 2967, 1750, 1599, 1323, 870, 840, 582 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{13}H_{16}O_4Na$: 259.0947. Found: 259.0944.

(*E*)-6-(Furan-2-yl)-3-(1-hydroxybutylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4f)



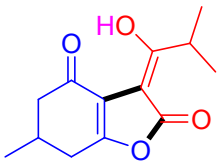
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 82 % (237 mg); mp 104-106 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 13.39 (1H, s), 7.34 (1H, d, J = 1.7 Hz), 6.30 (1H, dd, J = 3.2, 1.9 Hz), 6.10 (1H, d, J = 3.3 Hz), 3.67-3.62 (1H, m), 3.07 (1H, dd, J = 18.5, 5.3 Hz), 2.96 (1H, dd, J = 18.5, 9.3 Hz), 2.91 (1H, dd, J = 17.2, 4.5 Hz), 2.84-2.78 (3H, m), 1.70-1.63 (2H, m), 0.98 (3H, t, J = 7.4 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.4, 180.0, 166.4, 166.1, 154.2, 142.0, 116.5, 110.2, 105.5, 93.9, 40.1, 33.5, 33.2, 27.9, 20.1, 13.7; IR (ATR) 2965, 1764, 1620, 1326, 851, 740, 592 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{16}H_{16}O_5Na$: 311.0896. Found: 311.0893.

(*E*)-3-(1-Hydroxy-2-methylpropylidene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4g)



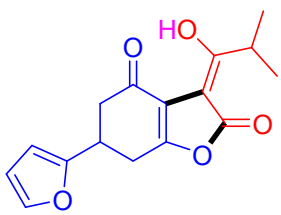
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 89 % (223 mg); mp 101-103 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.53 (1H, s), 3.89-3.83 (1H, m), 2.56 (2H, s), 2.40 (2H, s), 1.14 (3H, s), 1.13 (9H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.7, 183.9, 166.6, 166.4, 115.5, 92.6, 49.7, 36.8, 34.4, 29.4, 28.4, 19.2; IR (ATR) 2967, 1757, 1604, 1304, 858, 579 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{14}H_{18}O_4Na$: 273.1103. Found: 273.1099.

(*E*)-3-(1-Hydroxy-2-methylpropylidene)-6-methyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4h)



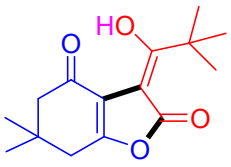
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 90 % (210 mg); mp 117-119 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.67 (1H, s), 3.91-3.84 (1H, m), 2.78-2.73 (1H, m), 2.60 (1H, dd, J = 16.9, 3.8 Hz), 2.44-2.38 (2H, m), 2.37-2.25 (1H, m), 1.16 (3H, d, J = 6.4 Hz), 1.15 (6H, d, J = 6.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.1, 184.2, 167.3, 166.3, 116.4, 92.6, 43.8, 30.9, 29.6, 29.4, 20.8, 19.2, 19.2; IR (ATR) 2965, 1767, 1613, 1314, 843, 583 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{13}H_{16}O_4Na$: 259.0947. Found: 259.0944.

(*E*)-6-(Furan-2-yl)-3-(1-hydroxy-2-methylpropylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4i)



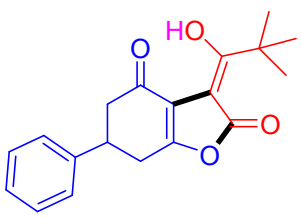
The title compound was prepared according to the general procedure **iii**. The product was obtained as a brown solid.Yield: 86 % (203 mg); mp 85-87 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 13.60 (1H, s), 7.35 (1H, s), 6.31 (1H, dd, J = 3.0, 1.9 Hz), 6.10 (1H, d, J = 2.6 Hz), 3.93-3.84 (1H, m), 3.69-3.59 (1H, m), 3.11-2.93 (2H, m), 2.90-2.75 (2H, m), 1.16 (6H, d, J = 6.8 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 195.5, 184.5, 166.1, 166.1, 154.1, 142.0, 116.6, 110.2, 105.5, 92.5, 40.0, 33.2, 29.5, 27.9, 19.2, 19.2; IR (ATR) 2973, 1767, 1611, 1312, 912, 770 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{16}H_{16}O_5Na$: 311.0896. Found: 311.0892.

(*E*)-3-(1-Hydroxy-2,2-dimethylpropylidene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4j)



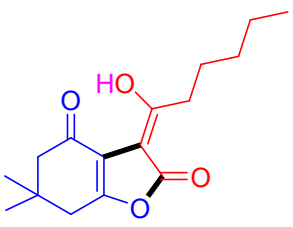
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 78 % (208 mg); mp 109-111 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 14.64 (1H, s), 2.58 (2H, s), 2.44 (2H, s), 1.37 (9H, s), 1.15 (6H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.1, 189.0, 167.2, 165.0, 116.0, 93.3, 49.9, 39.2, 37.1, 34.2, 28.4, 26.1; IR (ATR) 2960, 1759, 1589, 1306, 845, 578 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{15}H_{20}O_4Na$: 287.1260. Found: 287.1258.

(*E*)-3-(1-Hydroxy-2,2-dimethylpropylidene)-6-phenyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4k)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 79 % (247 mg); mp 110-112 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 14.66 (1H, s), 7.30 (2H, t, J = 7.6 Hz), 7.22 (1H, t, J = 7.4 Hz), 7.19 (2H, d, J = 7.7 Hz), 3.50-3.44 (1H, m), 2.94 (1H, dd, J = 18.4, 5.3 Hz), 2.86 (1H, dd, J = 18.4, 10.9 Hz), 2.84-2.73 (2H, m), 1.32 (9H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.5, 189.4, 167.5, 164.8, 141.0, 129.0, 127.6, 126.6, 117.1, 93.2, 42.9, 39.7, 39.2, 30.8, 26.1; IR (ATR) 2941, 1763, 1580, 1309, 867, 769, 698 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{19}H_{20}O_4Na$: 335.1260. Found: 335.1257.

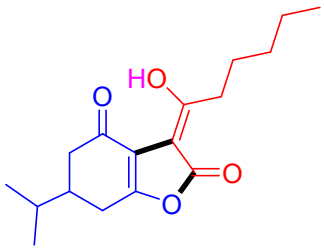
(*E*)-3-(1-Hydroxyhexylidene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4l)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow liquid. Yield: 94 % (262 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.37 (1H, s), 2.82 (2H, t, J = 7.7 Hz), 2.57 (2H, s), 2.41 (2H, s), 1.64-1.59 (2H, m), 1.36-1.28 (4H, m), 1.14

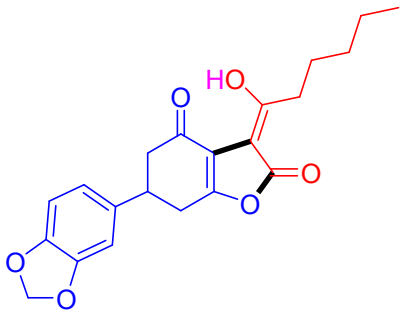
(6H, s), 0.86 (3H, t, J = 6.6 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.6, 179.8, 166.7, 166.6, 115.4, 93.9, 49.7, 36.8, 34.4, 31.6, 31.4, 28.5, 26.4, 22.3, 13.8; IR (ATR) 2957, 1723, 1573, 1453, 755, 573 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{16}H_{22}O_4Na$: 301.1416. Found: 301.1412.

(*E*)-3-(1-Hydroxyhexylidene)-6-isopropyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4m)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a brown solid.Yield: 92 % (270 mg); mp 44-46 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.46 (1H, s), 2.85-2.78 (2H, m), 2.71 (1H, dd, J = 18.4, 4.9 Hz), 2.62 (1H, dd, J = 16.9, 3.9 Hz), 2.45 (1H, dd, J = 18.4, 11.3 Hz), 2.30 (1H, dd, J = 16.9, 12.8 Hz), 2.10-2.04 (1H, m), 1.71-1.66 (1H, m), 1.63-1.59 (2H, m), 1.36-1.27 (4H, m), 0.96 (6H, d, J = 6.8 Hz), 0.86 (3H, t, J = 7.0 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.4, 179.9, 167.9, 166.6, 116.3, 93.9, 40.9, 39.6, 31.8, 31.6, 31.3, 26.6, 26.4, 22.3, 19.6, 19.4, 13.8; IR (ATR) 2956, 1770, 1619, 1336, 826, 590 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{17}H_{24}O_4Na$: 315.1573. Found: 315.1569.

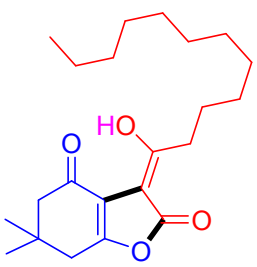
(*E*)-6-(Benzo[*d*][1,3]dioxol-5-yl)-3-(1-hydroxyhexylidene)-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4n)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 83 % (310 mg); mp 144-146 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.43 (1H, s), 6.77 (1H, d, J = 7.8 Hz), 6.72 (1H, s), 6.69 (1H, d, J = 7.9 Hz), 5.94 (2H, s), 3.47-3.42 (1H, m), 2.94 (1H, dd, J = 18.5, 5.1 Hz), 2.87-2.79 (3H, m), 2.79-2.70 (2H, m), 1.66-1.61 (2H, m), 1.36-1.30 (4H, m), 0.88 (3H, t, J = 6.7 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.0, 180.3, 166.7, 166.4, 148.0, 146.9, 135.0, 119.8, 116.5, 108.5, 106.9, 101.2, 93.8, 43.0,

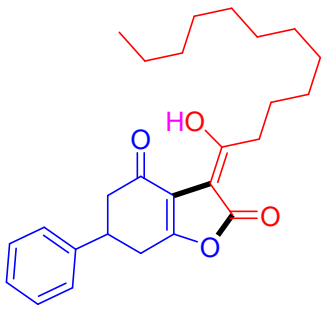
39.8, 31.7, 31.3, 30.9, 26.4, 22.3, 13.8; IR (ATR) 2928, 1765, 1611, 1341, 1239, 1036, 769, 577 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{21}H_{22}O_6Na$: 393.1314. Found: 393.1312.

(*E*)-3-(1-Hydroxydodecylidene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4o)



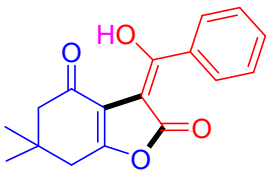
The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow liquid.Yield: 95 % (345 mg); ^1H NMR (600 MHz, $CDCl_3$) δ 13.37 (1H, s), 2.81 (2H, t, J = 7.8 Hz), 2.56 (2H, s), 2.41 (2H, s), 1.63-1.58 (2H, m), 1.37-1.33 (2H, m), 1.27-1.21 (14H, m), 1.14 (6H, s), 0.84 (3H, t, J = 7.0 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.6, 179.8, 166.6, 166.5, 115.4, 93.9, 49.7, 36.8, 34.4, 31.8, 31.7, 29.5, 29.5, 29.4, 29.3, 29.2, 28.4, 26.7, 22.6, 14.0; IR (ATR) 2924, 1727, 1573, 1455, 1215, 754 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{22}H_{34}O_4Na$: 385.2355. Found: 385.2352.

(*E*)-3-(1-Hydroxydodecylidene)-6-phenyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4p)



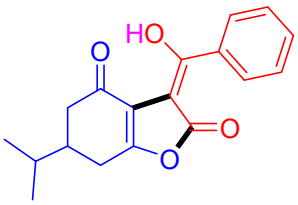
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 91 % (375 mg); mp 112-114 ^oC. ^1H NMR (600 MHz, $CDCl_3$) δ 13.40 (1H, s), 7.31 (2H, t, J = 7.7 Hz), 7.23 (1H, t, J = 6.8 Hz), 7.20 (2H, d, J = 8.6 Hz), 3.52-3.46 (1H, m), 2.94 (1H, dd, J = 18.5, 5.2 Hz), 2.87 (1H, dd, J = 18.5, 10.8 Hz), 2.82-2.73 (4H, m), 1.61-1.56 (2H, m), 1.34-1.31 (2H, m), 1.24-1.19 (14H, m), 0.81 (3H, t, J = 7.0 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.4, 163.0, 148.8, 135.7, 134.9, 130.4, 128.6, 128.3, 128.1, 114.0, 52.1, 51.4, 33.4; IR (ATR) 2918, 1766, 1621, 1336, 914, 697 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{26}H_{34}O_4Na$: 433.2355. Found: 433.2353.

(*E*)-3-(Hydroxy(phenyl)methylene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4q)



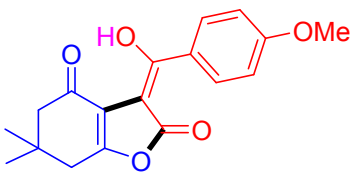
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 90 % (256 mg); mp 177-180 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.94 (1H, s), 7.70 (2H, d, J = 8.0 Hz), 7.48 (1H, t, J = 7.4 Hz), 7.42 (2H, t, J = 7.7 Hz), 2.62 (2H, s), 2.50 (2H, s), 1.19 (6H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.9, 172.7, 168.2, 165.7, 132.5, 131.4, 129.1, 127.7, 115.7, 94.1, 49.8, 37.0, 34.4, 28.5; IR (ATR) 2957, 1773, 1617, 1594, 1326, 1284, 968, 852, 695 cm^{-1}; HRMS (ESI) m/z [M+Na]$^+$ calcd for $C_{17}H_{16}O_4Na$: 307.0947. Found: 307.0944.

(*E*)-3-(Hydroxy(phenyl)methylene)-6-isopropyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4r)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow solid.Yield: 92 % (298 mg); mp 193-195 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (2H, d, J = 8.3 Hz), 7.49-7.46 (1H, m), 7.41 (2H, t, J = 7.8 Hz), 2.75 (1H, dd, J = 18.5, 5.0 Hz), 2.68 (1H, dd, J = 16.9, 3.9 Hz), 2.48 (1H, dd, J = 18.5, 11.3 Hz), 2.35 (1H, dd, J = 16.9, 12.8 Hz), 2.13-2.07 (1H, m), 1.73-1.67 (1H, m), 0.96 (6H, d, J = 6.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.5, 172.7, 169.6, 165.6, 132.6, 131.4, 129.1, 127.7, 116.6, 94.1, 40.7, 39.8, 31.7, 26.8, 19.6, 19.4; IR (ATR) 2967, 1765, 1595, 1328, 760, 696, 596 cm^{-1}; HRMS (ESI) *m/z* [M+Na]$^+$ calcd for $C_{18}H_{18}O_4Na$: 321.1103. Found: 321.1110.

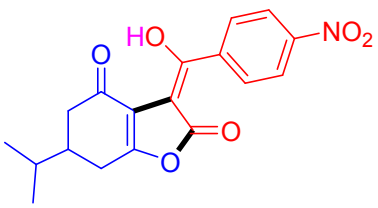
(*E*)-3-(Hydroxy(4-methoxyphenyl)methylene)-6,6-dimethyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4s)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow liquid.Yield: 93 % (292 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.94 (1H, s), 7.76 (2H, d, J = 8.9 Hz), 6.91 (2H, d, J = 8.8 Hz), 3.83 (3H, s), 2.60 (2H, s), 2.48 (2H, s), 1.17 (6H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.8, 172.6, 167.7, 166.0,

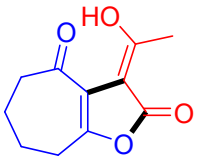
162.3, 131.3, 124.7, 115.9, 113.0, 93.2, 55.3, 49.9, 37.0, 34.3, 28.4; IR (ATR) 2958, 1724, 1673, 1598, 1254, 1165, 1025, 845, 610 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{18}O_5Na$: 337.1052. Found: 337.1048.

(*E*)-3-(Hydroxy(4-nitrophenyl)methylene)-6-isopropyl-3,5,6,7-tetrahydrobenzofuran-2,4-dione (4t)



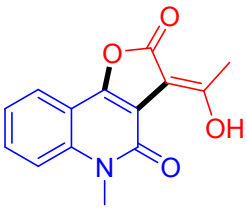
The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow solid.Yield: 72 % (247 mg); mp 159-161 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.24 (2H, d, J = 7.6 Hz), 7.84 (2H, d, J = 7.6 Hz), 2.78 (1H, dd, J = 18.7, 4.9 Hz), 2.72 (1H, dd, J = 17.0, 3.9 Hz), 2.53 (1H, dd, J = 18.6, 11.2 Hz), 2.39 (1H, dd, J = 16.9, 12.9 Hz), 2.17-2.11 (1H, m), 1.76-1.70 (1H, m), 0.99 (6H, d, J = 6.7 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.8, 170.6, 169.2, 165.2, 149.1, 138.6, 130.3, 128.9, 123.0, 120.2, 116.4, 95.8, 40.7, 39.7, 31.7, 26.8, 19.6, 19.4; IR (ATR) 2968, 1767, 1621, 1590, 1516, 1315, 1296, 846 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{18}H_{17}NO_6Na$: 366.0954. Found: 366.0950.

(*E*)-3-(1-hydroxyethylidene)-5,6,7,8-tetrahydro-2*H*-cyclohepta[*b*]furan-2,4(3*H*)-dione (5b)



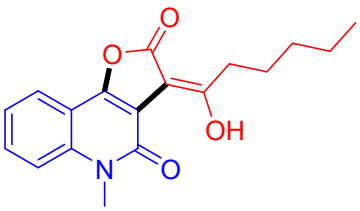
The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 78 % (163 mg); mp 112-114 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 14.39 (1H, s), 2.88 (2H, t, J = 6.3 Hz), 2.80-2.76 (2H, m), 2.44 (3H, s), 1.97-1.93 (2H, m), 1.91-1.87 (2H, m); ^{13}C NMR (150 MHz, $CDCl_3$) δ 201.1, 177.2, 167.1, 166.0, 118.9, 95.6, 42.1, 28.7, 23.0, 21.4, 20.1; IR (ATR) 2960, 1768, 1620, 1315, 866, 567 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{11}H_{12}O_4$: 208.0736. Found: 208.0732.

(*E*)-3-(1-Hydroxyethylidene)-5-methyl-3,5-dihydrofuro[3,2-c]quinoline-2,4-dione (5c)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a white solid.Yield: 85 % (219 mg); mp 213-215 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (1H, d, J = 7.9 Hz), 7.61 (1H, t, J = 7.8 Hz), 7.48 (1H, d, J = 8.6 Hz), 7.36 (1H, t, J = 7.5 Hz), 3.80 (3H, s), 2.51 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.9, 167.1, 160.1, 150.8, 137.9, 130.8, 123.8, 122.6, 115.3, 112.1, 110.4, 95.1, 30.1, 19.5; IR (ATR) 2951, 1755, 1643, 1609, 1609, 1375, 908, 867, 749 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{14}H_{11}NO_4Na$: 280.0586. Found: 280.0583.

(*E*)-3-(1-Hydroxyhexylidene)-5-methyl-3,5-dihydrofuro[3,2-c]quinoline-2,4-dione (5d)



The title compound was prepared according to the general procedure **iii**. The product was obtained as a yellow solid.Yield: 89 % (280 mg); mp 102-104 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (1H, d, J = 8.0 Hz), 7.62-7.59 (1H, m), 7.49 (1H, d, J = 8.6 Hz), 7.37 (1H, t, J = 7.6 Hz), 3.81 (3H, s), 2.94 (2H, t, J = 7.8 Hz), 1.72-1.67 (2H, m), 1.42-1.31 (4H, m), 0.89 (3H, t, J = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$) δ 183.0, 166.9, 160.3, 150.9, 137.9, 130.8, 123.8, 122.6, 115.3, 112.2, 110.6, 94.7, 32.3, 31.4, 30.1, 26.4, 22.4, 13.9; IR (ATR) 2927, 1774, 1638, 1605, 1378, 755, 728 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{18}H_{19}NO_4$: 313.1314. Found: 313.1318.

Computational Detail

All density functional theory (DFT) calculations were conducted using the Jaguar 9.1 of ab initio quantum chemistry software.[3] Geometry optimizations were performed with B3LYP hybrid exchange functional[4,5] along with Grimme's D3[6] dispersion correction (B3LYP-D3) and 6-31G** basis set[7–9] for main group atoms. Ru was described by Los Alamos relativistic effective core potentials (ECP)[10–12] and its corresponding LACVP** basis set. After the geometry optimization, more reliable electronic energies obtained from the single point calculations using Dunning's correlation-consistent triple-ζ basis set, cc-pVTZ(-f),[13] for main group and LACV3P** for Ru. The zero-point energy (ZPE), entropic and solvation contributions to the Gibbs energy are obtained from the same level of theory as the geometry optimizations (B3LYP-

D3/6-31G**/LACVP**). The solvation calculations utilized self-consistent reaction field (SCRF) approach on the gas phase geometry to model the solvation shell of dielectric constant ε = 10.36, which we consider to be an approximate solvation environment offered by the dichloroethane (DCE) solvent.

Table S1. Computed energy components for DFT-optimized structures

	E(SCF)/(eV)	**ZPE/(kcal/mol)**	**S(gas)/(cal/mol)**	**G(solv)/(kcal/mol)**
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
1a	-15537.678	109.51	103.39	-9.27
2a	-16139.798	121.61	111.44	-10.46
2a'	-16139.853	122.12	108.10	-9.39
3a	-20868.953	152.88	118.19	-9.67
6a	-12531.441	97.94	103.90	-9.55
6a'	-12531.652	98.98	97.68	-6.13
Nitrogen	-2981.407	3.52	45.78	0
Aniline	-7828.959	73.65	75.46	-6.98
Acetate	-6220.608	30.14	69.80	-68.63
Acetic Acid	-6236.253	38.91	68.42	-7.73
A	-34911.715	278.17	192.59	-44.35
A-TS	-34911.035	276.58	187.45	-42.99
B	-31930.176	271.58	180.22	-44.29
B-TS	-48070.590	395.33	229.64	-42.44
C	-48071.746	396.97	221.17	-42.24
C-TS	-48070.914	396.91	226.62	-45.24
M	-48071.73	397.19	227.45	-45.04
M-TS	-48071.438	394.77	221.17	-43.38
D	-48072.336	395.66	225.45	-44.38
E	-48072.668	396.89	242.73	-43.77
E-TS	-48072.016	394.19	230.97	-42.72
F	-48072.012	395.75	240.90	-43.31
F-TS	-48071.523	396.45	236.88	-45.23
G	-40242.684	320.97	200.42	-44.39
H	-20868.389	151.97	122.20	-12.58

H-TS	-27104.375	188.42	145.86	-13.18
B-TS'	-48070.617	395.19	236.95	-41.85
C'	-48070.859	396.32	234.82	-42.70
D'	-48071.746	396.44	236.00	-44.53
E'	-48071.57	396.18	238.72	-42.35
B-TS''	-48070.363	395.29	235.73	-43.42
C''	-48070.512	396.16	234.08	-43.55
F'	-48072.496	396.66	229.26	-42.96
G'	-48072.785	398.21	233.77	-42.65
G'-TS	-54307.660	434.03	255.15	-46.50
G''	-48072.699	398.06	233.93	-42.67
H''	-48079.992	403.86	235.46	-128.40
B-TS(I)	-44461.918	372.15	219.25	-41.71
I	-44463.152	373.54	220.79	-42.18
I'	-44461.766	372.54	226.68	-42.81
I''	-44462.223	372.70	227.43	-41.86
J	-28698.283	228.35	156.72	-13.11
K	-28697.623	227.53	153.70	-14.70
K-TS	-28697.467	227.54	149.36	-14.26
L	-28697.539	228.21	151.11	-14.33
L-TS	-34934.109	265.26	178.56	-17.10

Table S2. Cartesian Coordinates of the Optimized Geometries.

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1a

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C 0.982921362 0.249125615 -2.219101429

C 0.987755418 1.472557902 -1.314734101

C 0.192846626 1.310160160 0.001041423

C 0.730438948 0.070955202 0.753537536

C 0.706955552 -1.221357822 -0.048722621

C 0.880995810 -1.036392212 -1.502344847

H 0.615976930 2.312148571 -1.909784913

H 2.039959192 1.687951088 -1.078882456

H 0.172566295 -0.113842808 1.676383734

H 1.777149558 0.246720836 1.041457057

N 0.869188547 -2.131947994 -2.247040272

N 0.860256016 -3.066598177 -2.878528595

C -1.311195612 1.144728422 -0.294894993

H	-1.516924977	0.264085799	-0.911966622
H	-1.875888348	1.035663843	0.636737525
H	-1.699200988	2.020779133	-0.825492442
C	0.402654886	2.558848619	0.873094440
H	-0.130994871	2.463039160	1.824959278
H	1.463761687	2.715085506	1.097604632
H	0.029857736	3.455276966	0.366108716
O	1.071390510	0.319654107	-3.435272694
O	0.572293222	-2.321686506	0.463751733

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2a

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O	2.337485790	0.991839170	-1.002935886
C	1.611075521	1.975168943	-1.009494901
C	1.968056917	3.224889755	-0.240356311
C	0.315788120	2.010281563	-1.812108517
C	-0.589223504	0.760212004	-1.781093717
H	2.958232164	3.120845079	0.204965547
H	1.936539888	4.102241993	-0.896514356
H	1.222711921	3.391487122	0.547035277
H	-0.313310891	2.854405403	-1.524161696
H	0.607128739	2.172301531	-2.859856367
O	-1.805015564	0.898731351	-1.798978686
N	0.082556166	-0.427589118	-1.790793300
H	1.091345549	-0.343323618	-1.685652256
C	-0.444869936	-1.735921621	-1.776669145
C	0.474903464	-2.790236950	-1.657045960
C	-1.814863443	-2.020692587	-1.884041190
C	0.034517843	-4.110269070	-1.645551801
C	-2.238647461	-3.349536657	-1.869151711
C	-1.327438116	-4.399402142	-1.751196504
H	1.536413670	-2.569472313	-1.572431207
H	-2.521923304	-1.208318830	-1.970104933
H	0.759448528	-4.913848400	-1.552023530
H	-3.301077843	-3.561357260	-1.951983094
H	-1.672470093	-5.428884983	-1.741359591

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2a'

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O	-1.489750981	3.478902817	-2.060007334
C	-0.191154361	3.250457287	-1.874540448
C	0.630401433	4.500701904	-1.810779929
C	0.330255061	1.993548155	-1.749441862
C	-0.543092012	0.830526233	-1.817495227
H	0.270012289	5.134911537	-0.993575811
H	1.688871026	4.283169270	-1.655538559
H	0.509835184	5.070069313	-2.738412380
H	1.397289157	1.876003623	-1.600635409
O	-1.778385162	0.935275078	-1.992851377
N	0.078545131	-0.387224883	-1.672630906
H	1.078320384	-0.345005214	-1.536913514
C	-0.455414712	-1.690639377	-1.710320354
C	0.450560659	-2.753844023	-1.557678938
C	-1.819914103	-1.968456268	-1.888454199
C	0.005513273	-4.071652412	-1.583170295
C	-2.248125076	-3.295661449	-1.912301898

C	-1.350110292	-4.352759838	-1.761453986
H	1.509334683	-2.543744087	-1.419075608
H	-2.518359423	-1.152757883	-2.004328966
H	0.722267509	-4.878996372	-1.462984204
H	-3.306148052	-3.500132322	-2.050310373
H	-1.699982762	-5.380269527	-1.781425118
H	-1.922519803	2.574736834	-2.082931042

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3a

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C	0.767037630	0.567446053	-0.000512366
C	0.040876310	-0.336188406	0.930436790
C	-0.583840728	0.018598871	2.091580629
C	-0.582648695	1.389416099	2.532532215
C	0.222953945	2.367096186	1.689324141
C	0.286356509	2.034217358	0.176360294
O	-0.058322333	-1.651894093	0.666432440
C	-0.823208630	-2.272290707	1.726928115
C	-1.174363375	-1.198588729	2.651926994
H	1.845270157	0.498547703	0.206957132
H	1.241225839	2.369520903	2.105107069
O	-1.159348011	1.778650880	3.563549280
C	1.281918645	2.980325460	-0.511674225
H	2.284054518	2.892116070	-0.077312671
H	1.355971932	2.755137205	-1.581226349
H	0.960602403	4.022358894	-0.410355628
C	-1.106648803	2.213856936	-0.460096836
H	-1.460364580	3.240899563	-0.323166728
H	-1.069377899	2.011192560	-1.535692573
H	-1.847270966	1.541938901	-0.016642176
H	-0.185723931	3.368459225	1.854967952
H	0.627652884	0.226894528	-1.032613158
O	-1.027214408	-3.458758116	1.674913883
C	-1.921239138	-1.358045101	3.798681021
C	-2.480023146	-2.665659189	4.267630100
H	-3.567843437	-2.571097851	4.355784893
H	-2.229437590	-3.485327959	3.597999811
H	-2.096608400	-2.870614052	5.273146152
O	-2.224374056	-0.357675344	4.607045650
H	-1.844970226	0.517823458	4.279180050

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Nitrogen

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N	-0.877189517	-1.344226956	1.118046284
N	-0.877189517	-1.344226956	0.013098442

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Aniline

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N	-2.178649426	-0.019033242	-3.268686056
H	-1.586722374	-0.396642685	-2.540171385
H	-1.933559299	-0.410612255	-4.169059753
C	-3.547405243	-0.042476930	-2.975394726
C	-4.502302647	-0.019111544	-4.006223202
C	-3.996041775	-0.022520447	-1.643806458
C	-5.862515926	0.022068555	-3.709228516

C -5.358765125 0.019144893 -1.357871056

C -6.304903030 0.041366179 -2.384997129

H -4.171241283 -0.027458759 -5.042086601

H -3.269473553 -0.036159765 -0.834792972

H -6.582930565 0.037005328 -4.522953987

H -5.682381630 0.031248948 -0.320371658

H -7.366035461 0.072009087 -2.158339024

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Acetate

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O -3.542471647 -7.356662750 -2.415756226

C -2.767788410 -6.534239292 -2.969564199

O -2.940208912 -5.317794800 -3.239475727

C -1.386327744 -7.136989117 -3.436718464

H -1.506558299 -7.595226288 -4.429831505

H -0.611603916 -6.364675522 -3.524384975

H -1.051148415 -7.927827835 -2.753769159

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Acetic Acid

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O -3.564212084 -7.428014278 -2.565527678

C -2.687671423 -6.487030983 -3.000972033

O -2.926274300 -5.301345348 -2.953434944

H -4.342657566 -6.942734718 -2.244539022

C -1.426641345 -7.120657921 -3.532327890

H -1.669547200 -7.778491497 -4.372273445

H -0.736138165 -6.342030048 -3.853871584

H -0.965197325 -7.738824368 -2.756716967

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A

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C -1.270886898 0.564988792 -3.152365685

C -2.435141087 0.785924613 -2.334236145

C -0.040085535 0.335452318 -2.490204334

C -2.350239754 0.776168704 -0.929260790

C 0.043425519 0.337723196 -1.059839845

C -1.098383427 0.558004200 -0.255257934

H -3.407100677 0.869593203 -2.809357643

H 0.839907527 0.083105408 -3.072107315

H -3.263030767 0.854059100 -0.351391733

H 0.990693927 0.097490057 -0.587341070

C -1.400013685 0.487603426 -4.646944046

H -0.522972882 0.019373422 -5.098296165

H -2.284311295 -0.090980403 -4.927140236

H -1.504688144 1.496216893 -5.062467575

C -0.979336083 0.574513495 1.256766677

H -0.126322076 -0.066911519 1.513790965

C -2.219701052 0.039184403 1.986011863

C -0.644111872 2.012319088 1.707982183

H 0.272047520 2.379515409 1.235923052

H -1.458853245 2.698763609 1.453202128

H -0.504652858 2.041578054 2.792543650

H -3.069902420 0.723439276 1.895298243

H -2.003553152 -0.061267871 3.053198814

H -2.527642965 -0.935797632 1.600530982

Ru	-1.496878505	-1.143631458	-1.732328296
C	-0.883197427	-4.862724304	1.848542809
C	-2.099536419	-5.709416389	2.163255215
C	-3.438663721	-4.943272114	2.093694925
C	-3.560199499	-4.291882515	0.695665300
C	-2.399179220	-3.410798550	0.296978831
C	-1.126457691	-3.759101152	0.855578363
H	-1.935457230	-6.151009083	3.150286198
H	-2.105347395	-6.536861897	1.438680530
H	-4.470426083	-3.691007614	0.608688891
H	-3.628510714	-5.076261520	-0.073334441
N	-0.038385123	-3.033467293	0.604187548
N	0.955712020	-2.517664433	0.505242050
C	-3.499937534	-3.863318205	3.193377495
H	-2.690829039	-3.129571199	3.104459047
H	-4.449560165	-3.320629120	3.148108244
H	-3.421379089	-4.320430756	4.184442043
C	-4.599990845	-5.931438923	2.282742023
H	-5.563973427	-5.415331841	2.225424290
H	-4.588530064	-6.715575218	1.517994881
H	-4.536920547	-6.414927006	3.262544394
O	0.218650624	-5.035243034	2.325951099
O	-2.630518198	-2.450672626	-0.477408707
O	-0.388733476	-2.912145853	-2.168013811
C	-1.262673259	-3.285312176	-3.030714989
O	-2.228902578	-2.481276751	-3.240788698
C	-1.166093707	-4.610585690	-3.715600967
H	-1.562394857	-5.384881973	-3.049096823
H	-1.755362630	-4.604126453	-4.633521080
H	-0.121478081	-4.849375725	-3.925773144

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A-TS

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C	-0.103968374	-0.086716473	-2.798862219
C	-1.004689217	0.855788529	-2.239998579
C	0.642948449	-0.875493050	-1.871514082
C	-1.110049844	1.073653936	-0.833969891
C	0.517565489	-0.702409804	-0.472721756
C	-0.353750259	0.295203358	0.073082857
H	-1.662598372	1.408635616	-2.904340982
H	1.294982910	-1.652107596	-2.257280111
H	-1.828892827	1.794744849	-0.465769589
H	1.084280372	-1.337312698	0.200343937
C	0.039677337	-0.273360908	-4.283739090
H	0.237966880	-1.319103122	-4.527913094
H	-0.862972319	0.048571546	-4.809704781
H	0.875821352	0.330408186	-4.654419899
C	-0.463361353	0.437918216	1.577396154
H	-0.293889940	-0.563267827	1.994406700
C	-1.836748481	0.921870589	2.058424234
C	0.674751341	1.360327482	2.068753481
H	1.659330249	0.991638601	1.764149308
H	0.551690578	2.374302387	1.674134970
H	0.656426847	1.416864038	3.160775661
H	-2.032692671	1.957498670	1.760545254
H	-1.870542049	0.891001284	3.150684834
H	-2.634554625	0.281150728	1.673696399

Ru	-1.557644606	-1.143111944	-1.327959299
C	-2.641458511	-4.026428223	-1.440843940
C	-1.983641267	-4.802650928	-0.316673189
C	-0.721109390	-5.553598881	-0.821532369
C	0.260159940	-4.515606403	-1.432150245
C	-0.387495995	-3.699181318	-2.543251038
C	-1.677637696	-3.065429688	-2.102161169
H	-2.731583118	-5.497581005	0.073856503
H	-1.715425253	-4.099146366	0.480653733
H	1.140780210	-4.999643803	-1.862971306
H	0.594321668	-3.828749180	-0.643432915
N	-2.526868105	-2.804994822	-3.681653738
N	-3.017861843	-2.341305017	-4.556177139
C	-1.113368988	-6.596865177	-1.886415243
H	-1.598681569	-6.145768642	-2.760101080
H	-0.229761586	-7.134848595	-2.242753983
H	-1.810417533	-7.328808308	-1.467478395
C	-0.040715221	-6.250890732	0.367083937
H	0.861893475	-6.777920246	0.042071059
H	0.243460447	-5.532827377	1.144043803
H	-0.713870525	-6.987429619	0.816396654
O	-3.792853355	-4.157327652	-1.802320123
O	0.079710737	-3.558588743	-3.657367229
O	-2.933376074	-1.778957367	0.173876718
C	-3.931315899	-1.477168322	-0.575458765
O	-3.629384279	-0.990717649	-1.720384359
C	-5.339675426	-1.735242486	-0.166242763
H	-6.012740612	-1.027939916	-0.653682590
H	-5.596840858	-2.748624563	-0.495483190
H	-5.435050011	-1.683254004	0.919808388

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B

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C	-1.476644397	0.573519289	-0.632230222
C	-1.158206940	-0.546249688	0.183308572
C	-0.656495512	0.787235677	-1.801876068
C	-0.196760938	-1.514420390	-0.221480265
C	0.297009617	-0.146221414	-2.192528009
C	0.487033099	-1.366215587	-1.449954629
H	-1.724048734	-0.729948163	1.089999914
H	-0.848873734	1.651824355	-2.426443100
H	-0.054201897	-2.399287224	0.385244191
H	0.837151289	-0.009851495	-3.124424458
Ru	-1.829663754	-1.325239897	-1.872620106
C	-4.623266697	-1.874205112	-1.019695520
C	-5.530775547	-3.037161350	-1.360950828
C	-5.336028099	-4.190559864	-0.331128418
C	-3.825527668	-4.570178032	-0.278829902
C	-2.953253031	-3.369083405	0.055764399
C	-3.168751240	-2.251112223	-0.924470723
H	-5.279021740	-3.401468754	-2.366699219
H	-6.562556744	-2.675168514	-1.370448351
H	-3.516796112	-4.963044167	-1.257962942
H	-3.631697178	-5.338288307	0.475249827
C	-5.811201096	-3.737095594	1.062631965
H	-5.267926216	-2.857658625	1.426182270
H	-6.874266624	-3.479531288	1.039554715

H	-5.671289444	-4.538433075	1.794181228
C	-6.144328594	-5.416224003	-0.787644446
H	-6.023185730	-6.243112564	-0.080911398
H	-7.210482597	-5.174688339	-0.841276407
H	-5.823551655	-5.763423920	-1.775892377
O	-4.985777855	-0.753097296	-0.715946734
O	-2.213796616	-3.292994976	1.020228505
O	-3.345808744	-0.825283289	-3.296066999
C	-2.823687553	-1.617424130	-4.147787094
O	-1.772291064	-2.246432066	-3.750048399
C	-3.395972013	-1.831400990	-5.508436203
H	-4.109736443	-1.041909456	-5.745972157
H	-2.591696739	-1.863593817	-6.247437954
H	-3.906828403	-2.800349236	-5.532535076
C	1.434168816	-2.414721251	-1.959691525
H	1.312293172	-3.357293844	-1.423118711
H	1.274797440	-2.593961000	-3.026643991
H	2.467302322	-2.073431015	-1.826907516
C	-2.538228273	1.571662545	-0.211844236
H	-3.226171017	1.031372905	0.447750658
C	-3.361849546	2.113161087	-1.389700651
C	-1.861780882	2.705635071	0.587301850
H	-1.314230323	2.323047638	1.454492807
H	-1.160103559	3.265426636	-0.041321244
H	-2.621098042	3.406025410	0.946417451
H	-2.762974501	2.743620157	-2.056642056
H	-4.172718048	2.736304045	-1.003526688
H	-3.806213617	1.300440431	-1.967607379

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B-TS

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C	-1.937515259	0.279288381	-0.225016832
C	-1.831106782	-0.977683365	0.429843038
C	-0.854191959	0.662404060	-1.084004641
C	-0.738135278	-1.855769753	0.195568860
C	0.194265842	-0.212261558	-1.353732347
C	0.266313463	-1.509474874	-0.735847056
H	-2.603712559	-1.279930472	1.128292561
H	-0.899223030	1.612697363	-1.604145408
H	-0.694468558	-2.811079502	0.701501012
H	0.959162056	0.067751266	-2.071033955
Ru	-1.887625456	-1.397313595	-1.826457143
C	-4.452548027	-2.734043837	-2.842324734
C	-5.881082535	-2.896064758	-2.338185787
C	-6.167933941	-2.078196526	-1.063551188
C	-5.212623119	-2.588607788	0.040602662
C	-3.844308853	-3.108217955	-0.412969470
C	-3.369423628	-2.703909636	-1.776679993
H	-6.029972076	-3.967492580	-2.128838539
H	-6.551352978	-2.627334356	-3.158871174
H	-5.657406807	-3.431816816	0.582459331
H	-5.032124043	-1.813395858	0.797059476
C	-5.953019142	-0.581571102	-1.355012774
H	-4.927824497	-0.368178785	-1.668129444
H	-6.617604733	-0.245733321	-2.157676458
H	-6.172561169	0.020131743	-0.466472358
C	-7.622411251	-2.304791212	-0.617989480

H	-7.830480099	-1.768120170	0.313939005
H	-8.322200775	-1.940559149	-1.377052307
H	-7.828949928	-3.367435455	-0.448750436
O	-4.225966454	-2.623789072	-4.034963608
O	-3.189081907	-3.792267561	0.367772698
O	-1.796733737	-4.865237236	-4.694078922
C	-2.745540142	-5.087113380	-3.829406977
C	-4.045014858	-5.518573284	-4.419514179
C	-2.526143789	-4.971717834	-2.447210073
C	-1.128097773	-4.962771893	-1.984881997
H	-3.889102697	-6.460275650	-4.957459927
H	-4.812463284	-5.664482117	-3.657916784
H	-4.386368752	-4.771317959	-5.141180038
H	-3.281542063	-5.384571075	-1.791281104
O	-0.181367680	-4.780738831	-2.789101601
N	-0.950065374	-5.215246201	-0.663856983
H	-1.783552885	-5.075641155	-0.098752931
C	0.255464613	-5.414577484	0.041683208
C	0.225153595	-5.216119289	1.430466294
C	1.444457769	-5.816971302	-0.583266079
C	1.383750319	-5.389723778	2.185651302
C	2.593702793	-5.987062454	0.186252043
C	2.575764179	-5.768938541	1.566038132
H	-0.708792150	-4.939638138	1.915506005
H	1.465595484	-5.974384785	-1.652866006
H	1.350837708	-5.233551979	3.259728670
H	3.513271809	-6.296697617	-0.301492214
H	3.478773594	-5.903353691	2.153021574
H	-0.949406445	-4.693799973	-4.149836540
O	-2.674797773	-0.460036784	-3.521951914
C	-2.002455950	-1.229238868	-4.300043583
O	-1.251431465	-2.079554558	-3.706498384
C	-2.097367048	-1.161257386	-5.782353401
H	-2.603921890	-0.246424481	-6.091865063
H	-1.100714922	-1.224490285	-6.225983620
H	-2.677364111	-2.029282331	-6.109941006
C	1.408961058	-2.429121017	-1.056979179
H	1.696385145	-3.016698599	-0.183134034
H	1.120360136	-3.133548498	-1.843682528
H	2.274423361	-1.859996319	-1.405251145
C	-3.077571630	1.232625365	0.081306569
H	-3.928381681	0.613291740	0.388623089
C	-3.506891966	2.071472883	-1.132834673
C	-2.684142113	2.131546259	1.271555305
H	-2.430621386	1.542144299	2.158243656
H	-1.819416761	2.755002499	1.018057346
H	-3.513287067	2.797476292	1.528467655
H	-2.767188549	2.844386816	-1.368593931
H	-4.445734024	2.586732626	-0.911752760
H	-3.650711060	1.455919862	-2.024253607

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C

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C	-2.224647760	0.406055719	-0.368118078
C	-2.030879498	-0.844329715	0.257814914
C	-1.307379365	0.761561394	-1.412315249
C	-0.899850309	-1.666099191	-0.042922352

C	-0.200897112	-0.048935648	-1.726921916
C	0.045969214	-1.268123746	-1.011770248
H	-2.744981050	-1.193378091	0.995920360
H	-1.492446065	1.649119735	-2.005566359
H	-0.773207366	-2.605247736	0.476840168
H	0.457155287	0.228127643	-2.544427633
Ru	-2.042925119	-1.279324651	-1.987618566
C	-4.534277439	-2.906341076	-3.116190672
C	-5.942461014	-2.548726082	-2.697218657
C	-6.107791424	-1.784525990	-1.377683282
C	-5.229166031	-2.448892117	-0.286291838
C	-3.958992004	-3.191150188	-0.695651770
C	-3.495151043	-3.185787439	-2.090232849
H	-6.434743881	-3.532517910	-2.616104364
H	-6.428487778	-2.033556461	-3.530455589
H	-5.807260513	-3.222796679	0.234688714
H	-4.966684341	-1.725638151	0.494283825
C	-5.735480309	-0.312422186	-1.605006576
H	-4.694515228	-0.204064488	-1.909587741
H	-6.356854439	0.122159734	-2.394844055
H	-5.903231144	0.273532987	-0.696539760
C	-7.581394196	-1.851631403	-0.934262931
H	-7.724788189	-1.323342800	0.014518513
H	-8.233497620	-1.383272648	-1.678861260
H	-7.913788795	-2.886661053	-0.797326267
O	-4.308492661	-3.137286901	-4.305965424
O	-3.380445719	-3.846560001	0.194032952
O	-1.844973087	-4.726852417	-4.726495266
C	-2.816688061	-4.896901608	-3.983067751
C	-3.945218801	-5.796230316	-4.407365799
C	-2.731885195	-4.503987312	-2.481511831
C	-1.285472512	-4.590791225	-2.021963358
H	-3.610497713	-6.830800056	-4.251170635
H	-4.856565475	-5.636601448	-3.830413818
H	-4.145724297	-5.653934956	-5.469560146
H	-3.247768164	-5.304574966	-1.935516953
O	-0.314986765	-4.456550121	-2.860173941
N	-1.082208633	-4.886751652	-0.756618261
H	-1.947245479	-4.731323719	-0.196773231
C	0.121581852	-5.162960052	-0.052776344
C	0.069391616	-5.018284798	1.340016723
C	1.298600078	-5.584766865	-0.683464944
C	1.207881689	-5.268882751	2.102504253
C	2.427706957	-5.834680557	0.095154621
C	2.391469479	-5.672891617	1.481953740
H	-0.859983265	-4.718592644	1.818365574
H	1.335693836	-5.704375744	-1.757671595
H	1.166877747	-5.152403831	3.180896521
H	3.342851639	-6.159523964	-0.390234500
H	3.279186487	-5.866901875	2.075544834
H	-0.762733579	-4.385404110	-3.804820538
O	-3.051151276	-0.542902470	-3.722959995
C	-2.320777416	-1.263519168	-4.485920429
O	-1.445732951	-1.988704920	-3.890670538
C	-2.472324133	-1.283252597	-5.968707561
H	-3.138894558	-0.483691454	-6.293235302
H	-1.493265033	-1.186200023	-6.444952011
H	-2.896624088	-2.251827717	-6.246981144

C	1.265196085	-2.077423573	-1.352794409
H	1.388564348	-2.930605173	-0.688079178
H	1.207975864	-2.445404291	-2.380998611
H	2.153352499	-1.441702127	-1.270804286
C	-3.302777767	1.361801505	0.104918920
H	-4.162290096	0.754520953	0.405602127
C	-3.755703926	2.375934839	-0.955641389
C	-2.779750109	2.089188814	1.363898993
H	-2.514286995	1.384323478	2.157809973
H	-1.892946243	2.687714815	1.128205299
H	-3.548750639	2.765155315	1.749938607
H	-2.983568907	3.131562710	-1.138117075
H	-4.643654823	2.907014370	-0.601789653
H	-4.002413273	1.901130915	-1.908426642

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C-TS

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C	-2.525147915	0.818997324	-0.714312732
C	-2.846121550	-0.133665696	0.281475991
C	-1.216341138	0.776688814	-1.305659175
C	-1.939274192	-1.184659123	0.596991897
C	-0.297586441	-0.212390915	-0.934611559
C	-0.640451550	-1.237032294	0.011027942
H	-3.818547964	-0.104699276	0.751501203
H	-0.974179685	1.449171662	-2.117901802
H	-2.231263638	-1.966911435	1.291267037
H	0.651119769	-0.283325791	-1.457334280
Ru	-2.158454657	-1.284101248	-1.601226926
C	-4.506209850	-2.314252615	-2.515994549
C	-5.936693668	-2.421458244	-2.030999660
C	-6.144098759	-2.229560614	-0.512686312
C	-4.996840477	-2.923879385	0.290858895
C	-3.818706274	-3.549649477	-0.454848379
C	-3.462454557	-3.131501198	-1.821391582
H	-6.252469063	-3.438500881	-2.303103447
H	-6.553766251	-1.724016428	-2.603785992
H	-5.394559860	-3.752489805	0.885460436
H	-4.576417446	-2.236156464	1.031990767
C	-6.217847347	-0.717169106	-0.231608063
H	-5.378782749	-0.189181954	-0.687134802
H	-7.133265495	-0.295748860	-0.659048200
H	-6.229629517	-0.509473801	0.844414592
C	-7.486729622	-2.867533684	-0.106356300
H	-7.693614006	-2.691194773	0.954636872
H	-8.313277245	-2.440761328	-0.684083223
H	-7.479680538	-3.950358391	-0.273232579
O	-4.203841209	-1.651916027	-3.512141466
O	-3.161879301	-4.410616398	0.159124196
O	-2.391280890	-4.150815964	-5.076150894
C	-3.249771357	-4.230160236	-4.201557636
C	-4.688901901	-4.414890766	-4.604466438
C	-2.869421721	-4.298897266	-2.705895901
C	-1.389311075	-4.662143230	-2.520919561
H	-4.721666336	-5.177070141	-5.387915134
H	-5.332093239	-4.714611053	-3.776499271
H	-5.059790611	-3.479115486	-5.032329082
H	-3.394127846	-5.199736595	-2.346180439
O	-0.620658338	-4.925960064	-3.532797813

N	-0.969063759	-4.889281273	-1.303008318
H	-1.719823480	-4.769441128	-0.585530818
C	0.311604142	-5.326347351	-0.854360640
C	0.350827157	-5.885541439	0.428832442
C	1.487310052	-5.153252602	-1.594131351
C	1.570829630	-6.279145718	0.973078251
C	2.700658321	-5.552382946	-1.034019113
C	2.749646902	-6.113557339	0.243282840
H	-0.570205510	-6.010045052	0.992421925
H	1.457691669	-4.712354183	-2.580522060
H	1.598579764	-6.714909077	1.966879845
H	3.614778757	-5.419764996	-1.604719639
H	3.700673342	-6.420169830	0.667308033
H	-1.095395207	-4.572486877	-4.353074551
O	-1.583194852	-0.373123676	-4.076911449
C	-0.965461612	-1.441431165	-4.070106983
O	-0.996609509	-2.244414806	-3.026983261
C	-0.145067021	-1.918093204	-5.245933056
H	0.327950448	-1.061101437	-5.729464531
H	0.607791007	-2.648079872	-4.941799641
H	-0.817853689	-2.385558844	-5.971487522
C	0.363750994	-2.278867483	0.401373386
H	-0.110518463	-3.140754223	0.872299075
H	0.935152650	-2.625320196	-0.461815655
H	1.068201542	-1.846589088	1.122583151
C	-3.514281988	1.883063316	-1.156560659
H	-4.419781685	1.758278012	-0.551846623
C	-3.898468971	1.737262964	-2.641905546
C	-2.940455437	3.283086061	-0.855209708
H	-2.658678293	3.390310049	0.197112113
H	-2.059148550	3.493649483	-1.469942093
H	-3.691986084	4.043851852	-1.085235238
H	-3.024152040	1.802119017	-3.295463562
H	-4.594138145	2.535587788	-2.918154478
H	-4.375553131	0.775403202	-2.846486807

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M

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C	-2.468220472	0.901950657	-1.027308345
C	-2.824794769	0.092116326	0.084734097
C	-1.169468999	0.721573353	-1.593230009
C	-1.945589066	-0.910600901	0.567566633
C	-0.279291064	-0.238910973	-1.064950228
C	-0.642519534	-1.092522502	0.015438138
H	-3.810144901	0.199187368	0.525071442
H	-0.878112555	1.257001042	-2.485147715
H	-2.267212152	-1.570202470	1.368072748
H	0.659020305	-0.403190762	-1.581781149
Ru	-2.208674669	-1.320535541	-1.629443645
C	-4.258632183	-2.010095596	-2.130153418
C	-5.553428650	-1.503895760	-1.523878574
C	-6.117654324	-2.365862846	-0.369985133
C	-4.944395542	-2.805906296	0.532203913
C	-3.868897676	-3.570818901	-0.221477062
C	-3.541211367	-3.168067694	-1.606243372
H	-6.269282341	-1.451019883	-2.354043722
H	-5.402010918	-0.468552709	-1.203708410

H	-5.284298897	-3.454830885	1.344653368
H	-4.490867138	-1.927518725	1.004607201
C	-7.115108013	-1.528082132	0.446092457
H	-6.636518478	-0.637690365	0.870216191
H	-7.947548866	-1.194012046	-0.182183728
H	-7.533027172	-2.111826420	1.272526264
C	-6.840159416	-3.618201256	-0.907771230
H	-7.275033951	-4.193490505	-0.084314890
H	-7.651302338	-3.341705322	-1.589146852
H	-6.163787842	-4.291785717	-1.444570541
O	-3.771272182	-1.435563326	-3.170599699
O	-3.289652824	-4.518315792	0.326609075
O	-2.775463581	-4.385699749	-4.950303078
C	-3.546297312	-4.154475689	-4.022348881
C	-4.992989540	-3.884677649	-4.335539818
C	-3.091552019	-4.310433865	-2.554123878
C	-1.634943604	-4.771999359	-2.443871021
H	-5.334239006	-4.659202099	-5.028685093
H	-5.636381149	-3.871351242	-3.457582235
H	-5.059878826	-2.921060801	-4.847630501
H	-3.667553425	-5.188678741	-2.209628582
O	-0.980729282	-5.195791245	-3.476922750
N	-1.114368796	-4.899146080	-1.248702288
H	-1.797665596	-4.782552719	-0.477557808
C	0.225600466	-5.258789063	-0.917883635
C	0.423334628	-5.948368549	0.281467766
C	1.310415268	-4.859606266	-1.704800844
C	1.720808744	-6.248743534	0.693497837
C	2.602014780	-5.170715332	-1.282534599
C	2.811894655	-5.862269402	-0.087003767
H	-0.431588978	-6.247085094	0.882190466
H	1.144999743	-4.300451756	-2.616055250
H	1.876888275	-6.785897732	1.623854160
H	3.448460579	-4.863784313	-1.889316678
H	3.821517944	-6.097173214	0.235297561
H	-1.516372561	-4.905889511	-4.294155121
O	-0.148604870	-0.582369268	-3.925261974
C	-0.445347935	-1.768662214	-3.965811253
O	-1.199074864	-2.398307562	-3.070260286
C	0.037220288	-2.668335676	-5.092106819
H	0.741916835	-2.114630699	-5.712176323
H	0.516610920	-3.570178509	-4.702599525
H	-0.815297723	-2.982571602	-5.701251507
C	0.311133713	-2.108407021	0.576274335
H	-0.219205141	-2.957611084	1.013034225
H	0.987212539	-2.487417221	-0.191676632
H	0.915524065	-1.648109436	1.366250873
C	-3.422969580	1.947397113	-1.569998980
H	-4.414223194	1.727226853	-1.152052999
C	-3.536354065	1.931505442	-3.103159904
C	-2.985431433	3.331719398	-1.045322299
H	-2.935918331	3.357345343	0.047998622
H	-1.999434948	3.600444555	-1.439133286
H	-3.697997093	4.094263554	-1.373098612
H	-2.592295647	2.210175037	-3.581612349
H	-4.288708210	2.660558224	-3.418267250
H	-3.825843573	0.943985879	-3.468289614

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M-TS

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C	-2.142832518	0.317568749	-0.872552574
C	-2.404179335	-0.702534378	0.068868227
C	-0.954963744	0.190433666	-1.672760487
C	-1.538149834	-1.828737497	0.182490528
C	-0.028652573	-0.868780911	-1.462798834
C	-0.303878516	-1.913620114	-0.535301685
H	-3.330916882	-0.684522033	0.631667674
H	-0.755996287	0.913054645	-2.455344915
H	-1.836319923	-2.665966988	0.806263268
H	0.824810266	-0.967424154	-2.120689631
Ru	-2.029579401	-1.699825168	-1.951286912
C	-4.580760479	-2.041104078	-2.346610308
C	-5.779222965	-1.234937191	-1.877891779
C	-6.755399704	-1.949710965	-0.928359568
C	-5.890464783	-2.658881903	0.126072615
C	-4.847535133	-3.572274923	-0.471306056
C	-4.282829285	-3.327839613	-1.770923018
H	-6.275969028	-0.887638628	-2.792362213
H	-5.379149437	-0.330321580	-1.402626276
H	-6.486208916	-3.262136936	0.818292797
H	-5.366614342	-1.914711714	0.744845510
C	-7.669611931	-0.916834474	-0.251290739
H	-7.089714527	-0.176311225	0.311570704
H	-8.268916130	-0.381272107	-0.994834244
H	-8.359202385	-1.404367924	0.445339531
C	-7.623720169	-2.974502563	-1.685279369
H	-8.321007729	-3.468796253	-1.001416087
H	-8.212558746	-2.481168509	-2.465250015
H	-7.022736073	-3.755357504	-2.162084341
O	-3.846818686	-1.486364961	-3.226482868
O	-4.470674038	-4.545907974	0.247783199
O	-2.922234774	-5.113129616	-4.732193947
C	-3.762715101	-4.543821812	-4.053127766
C	-4.977206230	-3.942847013	-4.707777977
C	-3.685262680	-4.557761192	-2.506497860
C	-2.383429050	-5.097406864	-1.885371447
H	-5.185076237	-4.497317314	-5.624320507
H	-5.853455067	-3.936052084	-4.056347847
H	-4.738601685	-2.907286644	-4.971256733
H	-4.406012058	-5.364096642	-2.269091845
O	-2.305997372	-5.144214630	-0.603082895
N	-1.407628655	-5.554032326	-2.634828329
H	-1.606364727	-5.460587025	-3.639517784
C	-0.138821155	-6.081077576	-2.244854689
C	0.892632067	-5.957956314	-3.182771683
C	0.086701766	-6.708298683	-1.013967872
C	2.162400961	-6.440079212	-2.878726959
C	1.364238739	-7.187410355	-0.725184083
C	2.403519154	-7.051862717	-1.647180200
H	0.709221303	-5.466595173	-4.132225513
H	-0.714987457	-6.819519997	-0.297516137
H	2.962716103	-6.332373142	-3.603916168
H	1.543693781	-7.674293518	0.228484362
H	3.394837856	-7.424896717	-1.409248471
H	-3.306088209	-4.932735920	-0.149731040

O	0.719115496	-2.671176910	-3.558679581
C	-0.339405209	-2.846610546	-4.147830009
O	-1.547193885	-2.718972445	-3.608641148
C	-0.399863720	-3.233258009	-5.612845898
H	0.595002234	-3.507266760	-5.965539932
H	-1.112957954	-4.043223381	-5.780276299
H	-0.758646429	-2.371060610	-6.185556412
C	0.615787029	-3.089022636	-0.369797826
H	0.063480884	-3.975667953	-0.051849809
H	1.124891877	-3.307909727	-1.308882356
H	1.364203334	-2.859240770	0.397529036
C	-3.088470936	1.490409017	-1.041060805
H	-4.026775837	1.217934489	-0.540245950
C	-3.406935453	1.815728307	-2.509529352
C	-2.500786543	2.710418463	-0.300870985
H	-2.316814423	2.494080067	0.756063044
H	-1.554966688	3.023302555	-0.756025314
H	-3.197489500	3.551687479	-0.361463606
H	-2.528463602	2.202710867	-3.036379337
H	-4.174054623	2.594560385	-2.551426649
H	-3.769035816	0.934373736	-3.044803381

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C	-0.368490309	-0.447855860	-3.354629040
C	-1.771540642	-0.582599103	-3.506713629
C	0.124005184	0.459740400	-2.353923082
C	-2.672161341	0.154852182	-2.673308134
C	-0.777919769	1.160960197	-1.523341656
C	-2.206481934	1.046153665	-1.678375721
H	-2.167629004	-1.311051965	-4.205946922
H	1.191520452	0.526222289	-2.170625925
H	-3.733278990	-0.044783339	-2.760291338
H	-0.387011915	1.750917554	-0.699837387
C	0.598287880	-1.281831264	-4.148703098
H	1.401782393	-1.654049873	-3.506923676
H	0.099124551	-2.135154009	-4.613962650
H	1.050148368	-0.673024237	-4.940733433
C	-3.116816998	1.847211838	-0.759130120
H	-2.764373064	1.662816048	0.265386283
C	-4.595441818	1.449832916	-0.841435373
C	-2.944722891	3.352936506	-1.059998870
H	-1.904833078	3.678862333	-0.954602122
H	-3.271121264	3.584151506	-2.080259800
H	-3.552090406	3.943866730	-0.367166013
H	-5.022232056	1.698889971	-1.820003748
H	-4.750611782	0.381745994	-0.662434220
H	-5.166371346	1.998895645	-0.087184004
Ru	-1.243474007	-0.984850943	-1.367837310
C	-3.702487946	-4.918144226	1.464399934
C	-4.270299911	-3.943905115	2.468083858
C	-4.810266018	-2.646205902	1.832962990
C	-3.690002918	-2.064176083	0.947201431
C	-3.057292700	-3.057595730	0.003118941
C	-3.072321892	-4.430988312	0.282581419
H	-3.452150822	-3.704065084	3.164601564
H	-5.040127277	-4.463213921	3.047817469

H	-2.876275063	-1.672345400	1.573086619
H	-4.053685665	-1.218294263	0.354003310
C	-6.068524361	-2.943758488	0.990969896
H	-5.859920502	-3.649046183	0.180040106
H	-6.858639717	-3.375320435	1.615228534
H	-6.460615635	-2.022322893	0.544229805
C	-5.164849758	-1.637482166	2.936671495
H	-5.528229237	-0.697932661	2.503431559
H	-5.953675747	-2.032695293	3.586420536
H	-4.294670582	-1.407497406	3.562938213
O	-3.795140743	-6.150098324	1.745874882
O	-2.482732296	-2.634151936	-1.072972417
O	-0.736158669	-5.513000011	1.342925429
C	-0.823274314	-5.610696793	0.140766487
C	0.351036489	-5.927985191	-0.751702785
C	-2.186590433	-5.305240154	-0.587501109
C	-2.777513266	-6.620936871	-1.041806817
H	0.700686872	-4.972783566	-1.166184068
H	1.153017402	-6.380718231	-0.167218074
H	0.075774506	-6.582232475	-1.584790826
H	-1.925198913	-4.713743210	-1.470161676
O	-3.334626198	-7.413059711	-0.215776876
N	-2.634760380	-6.965502262	-2.319716692
H	-2.196847916	-6.263450146	-2.901958942
C	-3.006295204	-8.157303810	-3.017363071
C	-2.753839970	-8.156200409	-4.395779133
C	-3.573831558	-9.277617455	-2.398122072
C	-3.069047213	-9.274828911	-5.160392761
C	-3.883801937	-10.390169144	-3.180953503
C	-3.636505604	-10.397585869	-4.554020882
H	-2.311233521	-7.282302856	-4.870202065
H	-3.769142866	-9.284651756	-1.336171627
H	-2.870588064	-9.268070221	-6.227626801
H	-4.323721409	-11.260542870	-2.703556299
H	-3.883117199	-11.271875381	-5.148168564
H	-3.491443157	-6.913437366	0.740944564
O	-0.746218204	-1.125305891	0.709497869
C	0.111943126	-2.050566435	0.492041200
O	0.272621036	-2.408161402	-0.725759804
C	0.864799321	-2.688952684	1.617370963
H	0.274658620	-3.521650314	2.017975092
H	1.816237926	-3.087084293	1.255975127
H	1.029278994	-1.959337711	2.414290428

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C	-0.339943886	-0.670201421	-3.555309057
C	-1.745287180	-0.753909767	-3.697795868
C	0.187408566	0.256925315	-2.586985350
C	-2.617964983	0.051960625	-2.894643545
C	-0.681100190	1.038386941	-1.794632554
C	-2.113840580	0.968199313	-1.942510605
H	-2.172693968	-1.496952176	-4.362730503
H	1.256374717	0.282735229	-2.400257587
H	-3.686633587	-0.108241819	-2.974239826
H	-0.265493751	1.653134108	-1.001713753
C	0.591953099	-1.573801637	-4.313904762

H	1.392135739	-1.936565518	-3.662547588
H	0.061421461	-2.434484482	-4.728900909
H	1.053159475	-1.022377014	-5.141548157
C	-2.989488602	1.837947845	-1.055119038
H	-2.594543934	1.737455010	-0.034738641
C	-4.468352795	1.432051301	-1.042188048
C	-2.828491449	3.312645674	-1.486770630
H	-1.784088731	3.640094519	-1.448112488
H	-3.192615509	3.458617687	-2.509724617
H	-3.408832312	3.961799622	-0.823654532
H	-4.940739155	1.601998210	-2.016655922
H	-4.604016781	0.380060196	-0.772928953
H	-5.010066032	2.036416769	-0.308507293
Ru	-1.229209661	-1.080226302	-1.541652799
C	-3.525578976	-5.064857960	1.297613859
C	-4.216365814	-4.142242432	2.263201714
C	-4.820014000	-2.886752367	1.603915334
C	-3.711216211	-2.247592926	0.747284830
C	-3.007835150	-3.209687710	-0.176251933
C	-2.938589334	-4.599029541	0.117097817
H	-3.459756136	-3.848051548	3.006173372
H	-4.974644184	-4.718679905	2.802350521
H	-2.933833122	-1.814482570	1.390787721
H	-4.099227428	-1.422497153	0.141075775
C	-6.032154083	-3.263916016	0.729030132
H	-5.762743473	-3.966405869	-0.066084281
H	-6.816239834	-3.728758335	1.335271716
H	-6.458697796	-2.370484591	0.259937227
C	-5.264400005	-1.896866441	2.691819906
H	-5.677886963	-0.986819804	2.243099689
H	-6.040690899	-2.337748051	3.326005459
H	-4.426908016	-1.605899334	3.335795164
O	-3.509934902	-6.303700924	1.697997212
O	-2.436319590	-2.773074627	-1.232311249
O	-0.549865186	-5.569283962	1.161211967
C	-0.646520436	-5.672979355	-0.042759854
C	0.521976888	-5.991443157	-0.941460133
C	-2.009264469	-5.422145844	-0.759456098
C	-2.552132368	-6.785584927	-1.189774752
H	0.879209757	-5.036254406	-1.348264337
H	1.322664022	-6.457063198	-0.365857512
H	0.232561857	-6.631988049	-1.780261755
H	-1.788181305	-4.817642212	-1.642300248
O	-2.858117104	-7.638875961	-0.338496834
N	-2.623007298	-6.998729229	-2.520976305
H	-2.356420040	-6.219246387	-3.105660439
C	-3.059344292	-8.151704788	-3.235129833
C	-3.090381861	-8.042933464	-4.632063866
C	-3.439272881	-9.346763611	-2.611599207
C	-3.500524759	-9.122665405	-5.407371521
C	-3.849030733	-10.419409752	-3.404806614
C	-3.882984161	-10.317605972	-4.795535088
H	-2.792674065	-7.112837791	-5.112374783
H	-3.414620638	-9.432057381	-1.534956813
H	-3.520186901	-9.028882027	-6.488700867
H	-4.144565105	-11.345701218	-2.921320915
H	-4.204303741	-11.161339760	-5.397995472
H	-3.126343489	-6.933043480	0.997879446

O	-0.855594397	-1.124325156	0.562076449
C	0.016021352	-2.055634260	0.436375141
O	0.263041347	-2.443864107	-0.756660879
C	0.668704808	-2.669816971	1.632163405
H	0.023548545	-3.465298891	2.019213200
H	1.624829650	-3.116371155	1.354619384
H	0.805269301	-1.914555073	2.408801556

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E-TS

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C	-2.042647362	0.012768279	-2.557451010
C	-3.328566551	-0.542020500	-2.344427586
C	-1.584256291	1.029347062	-1.649376154
C	-4.130019665	-0.124106959	-1.236055493
C	-2.385188103	1.432377458	-0.558839023
C	-3.682154417	0.851216435	-0.315490812
H	-3.658580780	-1.366088390	-2.963728189
H	-0.578181505	1.422588825	-1.752210021
H	-5.049135208	-0.661591768	-1.037263036
H	-1.972810149	2.118283987	0.174848899
C	-1.143704414	-0.475073189	-3.658821821
H	-0.117819853	-0.593167424	-3.297975063
H	-1.494047284	-1.427348495	-4.058915138
H	-1.131186247	0.257423818	-4.474186897
C	-4.458343029	1.231023431	0.931995332
H	-3.708387375	1.508594155	1.683876038
C	-5.283199787	0.069574073	1.506603718
C	-5.330869675	2.468549013	0.643670261
H	-4.734883785	3.306048632	0.266749740
H	-6.099626541	2.236084223	-0.101264484
H	-5.832970619	2.794454575	1.559300900
H	-6.141162395	-0.173322394	0.869363248
H	-4.671288013	-0.830123544	1.626615047
H	-5.680852413	0.351690263	2.485509634
Ru	-2.138164282	-0.753054500	-0.448749721
C	-2.627015114	-6.033947945	-0.658638656
C	-3.385561228	-6.675076485	0.477173477
C	-4.500871658	-5.772526741	1.039522886
C	-3.852196693	-4.419853687	1.387459159
C	-3.028113365	-3.796167135	0.272799492
C	-2.415370941	-4.631797791	-0.696701765
H	-2.659646988	-6.903803349	1.271648169
H	-3.775313139	-7.633550644	0.121515132
H	-3.170969725	-4.546831131	2.242071629
H	-4.600666523	-3.683272600	1.695410848
C	-5.618654251	-5.583175182	-0.006213326
H	-5.246067524	-5.131070614	-0.931730747
H	-6.072631836	-6.546181202	-0.262515008
H	-6.409402370	-4.936244488	0.387976289
C	-5.093129158	-6.405074596	2.307900190
H	-5.875164986	-5.766959667	2.733153820
H	-5.541819572	-7.378296852	2.082535267
H	-4.326331139	-6.557044029	3.075597286
O	-2.176353931	-6.821213245	-1.562175155
O	-2.946895599	-2.531899691	0.341823310
O	0.466053069	-4.819598198	-2.878485918
C	-0.086522311	-4.596058369	-1.811544895
C	0.589578211	-4.825700760	-0.489289939

C	-1.528291225	-4.050086975	-1.788889885
C	-2.230263948	-4.207720757	-3.125398159
H	0.296175003	-4.070318222	0.239352152
H	0.273344696	-5.807824135	-0.116963506
H	1.670755744	-4.836605549	-0.632909060
H	-1.426005244	-2.976763010	-1.611442566
O	-2.966195107	-3.418924809	-3.653780222
N	-2.018222332	-5.561681747	-3.715510368
H	-1.023193598	-5.572493553	-3.987320423
C	-2.926528215	-5.948249817	-4.787192345
C	-4.002987385	-6.772844315	-4.468245983
C	-2.719592094	-5.478875637	-6.081547260
C	-4.892505646	-7.138470173	-5.478543758
C	-3.613849401	-5.852986336	-7.084037304
C	-4.698666573	-6.679797173	-6.782970428
H	-4.129199028	-7.132419586	-3.451336145
H	-1.876645327	-4.830155373	-6.301597118
H	-5.732224941	-7.786170006	-5.246885777
H	-3.463594675	-5.497806549	-8.098694801
H	-5.392077446	-6.968528748	-7.566865444
H	-2.050068855	-6.257654190	-2.751549482
O	-1.176800489	-0.701239944	1.473056793
C	-0.179450929	-1.355472326	1.031332970
O	-0.181690902	-1.644794345	-0.218796209
C	0.931934595	-1.800608873	1.932949066
H	0.684146762	-2.785090208	2.346674204
H	1.862931609	-1.888728976	1.369935155
H	1.045977473	-1.102007866	2.763478518

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C	-1.241731167	0.219784483	-2.206774950
C	-2.522961378	-0.310069740	-2.523119926
C	-1.136796355	1.130921960	-1.101142645
C	-3.661545038	0.007438851	-1.722125649
C	-2.275605202	1.426374316	-0.313247889
C	-3.571685314	0.863323987	-0.596099854
H	-2.626529694	-1.044726253	-3.312240601
H	-0.162932813	1.509089112	-0.805629611
H	-4.583928585	-0.529888988	-1.912949324
H	-2.149274111	2.015119791	0.591623783
C	-0.013676957	-0.208120793	-2.963428736
H	0.846071720	-0.294144690	-2.292985678
H	-0.165821597	-1.171298265	-3.459325314
H	0.226754367	0.534633994	-3.732784748
C	-4.737623692	1.140947580	0.337848634
H	-4.299118996	1.307112694	1.331312656
C	-5.712629318	-0.040833220	0.453015447
C	-5.453343391	2.436732531	-0.092551909
H	-4.764891148	3.288141251	-0.125014201
H	-5.900750637	2.321195602	-1.086437464
H	-6.254432201	2.676096201	0.614244878
H	-6.286444187	-0.186173096	-0.470231503
H	-5.180858135	-0.969730616	0.682088196
H	-6.434625626	0.155004412	1.251954317
Ru	-2.051147223	-0.762615085	-0.375259250
C	-2.206957102	-5.964774609	-0.760318816
C	-2.826100349	-6.658504486	0.429034323

C	-4.115793228	-5.952786446	0.901334882
C	-3.761085510	-4.477943420	1.169803023
C	-2.987992287	-3.780105352	0.064309128
C	-2.197858572	-4.540357113	-0.824865222
H	-2.089082718	-6.659588814	1.245463371
H	-3.008515596	-7.702230930	0.157104582
H	-3.133312464	-4.406489849	2.071366072
H	-4.655477524	-3.880797863	1.374797702
C	-5.209436893	-6.054521084	-0.180769607
H	-4.906281948	-5.585349083	-1.122741818
H	-5.446962833	-7.103439808	-0.389402598
H	-6.129790783	-5.564599991	0.153880045
C	-4.621767998	-6.607741833	2.194591045
H	-5.521298885	-6.102017403	2.561942101
H	-4.875546932	-7.659081936	2.022628307
H	-3.864668608	-6.568161011	2.985571146
O	-1.711631298	-6.675220013	-1.687899351
O	-3.145986080	-2.514922380	0.036749091
O	0.320326686	-4.463797569	-3.439630032
C	-0.024086284	-4.367458820	-2.268990040
C	0.892019212	-4.641159534	-1.114804983
C	-1.455212355	-3.883917570	-1.976111650
C	-2.306905031	-4.017222404	-3.218217611
H	0.793498874	-3.858121395	-0.359597355
H	0.596235812	-5.594916821	-0.663173795
H	1.917349458	-4.720468521	-1.477894783
H	-1.371805072	-2.813798904	-1.767532110
O	-3.057630301	-3.221211672	-3.701527834
N	-2.209069490	-5.416998863	-3.847706079
H	-1.380567908	-5.359350204	-4.453452587
C	-3.409340858	-5.864030838	-4.553112507
C	-4.199897289	-6.839930058	-3.949293852
C	-3.749596596	-5.287846088	-5.774311066
C	-5.366108894	-7.249557018	-4.596486092
C	-4.917035103	-5.708437920	-6.410110474
C	-5.725500107	-6.683745861	-5.821365833
H	-3.896244764	-7.282567978	-3.005859852
H	-3.117858887	-4.524438858	-6.216746807
H	-5.989305496	-8.014509201	-4.143926144
H	-5.195346355	-5.271825790	-7.364127636
H	-6.633388519	-7.006877422	-6.321505070
H	-1.924982667	-6.083403111	-3.015677691
O	-1.590491056	-0.963939667	1.718267560
C	-0.606927872	-1.724286079	1.452834129
O	-0.314694107	-1.883305430	0.213680282
C	0.142026782	-2.446724892	2.530272722
H	-0.405642062	-3.360514402	2.788123846
H	1.140470147	-2.721287966	2.186593056
H	0.201784655	-1.826494813	3.426789999

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C	-0.388908923	-0.273305327	-1.919004679
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C	-2.792302370	-0.629307568	-2.347793341
C	-2.106793880	1.122996688	-0.817988098

C	-3.172710419	0.411983758	-1.461062670
H	-1.211568236	-1.862408757	-3.168554544
H	0.033411223	1.330129027	-0.500621080
H	-3.559729338	-1.267991900	-2.762217522
H	-2.352058172	1.861728430	-0.060522459
C	1.043761730	-0.704471529	-2.047558784
H	1.545548558	-0.663190663	-1.077443480
H	1.114604235	-1.724790215	-2.429891586
H	1.570626140	-0.036445197	-2.738550425
C	-4.618736267	0.743638992	-1.141738176
H	-4.632488728	1.081164479	-0.097265288
C	-5.554607868	-0.469285756	-1.250944972
C	-5.093805790	1.910749197	-2.029173136
H	-4.455030918	2.792139769	-1.912935376
H	-5.086017132	1.623049736	-3.086288929
H	-6.115944386	2.195686102	-1.762798190
H	-5.702988625	-0.769524038	-2.295351505
H	-5.162604809	-1.325596213	-0.693238735
H	-6.539559364	-0.213471130	-0.850642562
Ru	-1.805858135	-1.004957914	-0.371891975
C	-3.345317125	-6.297454357	0.259972870
C	-2.849041700	-6.508362770	1.660942912
C	-2.997910261	-5.234636784	2.526069403
C	-2.434850216	-4.020011425	1.745522261
C	-2.962461710	-3.875067234	0.335895181
C	-3.395389080	-5.033015251	-0.328342408
H	-1.789735913	-6.797190189	1.589900136
H	-3.374239683	-7.361023426	2.103037834
H	-1.341785550	-4.090759277	1.670106649
H	-2.662912607	-3.093972683	2.279143572
C	-4.483500957	-5.003545284	2.869416952
H	-5.096719742	-4.877135277	1.971773386
H	-4.885661602	-5.851276398	3.433552504
H	-4.600154877	-4.105741024	3.484972239
C	-2.196577549	-5.405501842	3.826165915
H	-2.289025068	-4.515266418	4.458075523
H	-2.564952374	-6.259982586	4.403305054
H	-1.132221937	-5.570340157	3.622583628
O	-3.686708212	-7.301053524	-0.468369275
O	-3.018051624	-2.751925707	-0.262199759
O	-2.055620193	-4.102897167	-2.753786325
C	-3.267791986	-4.245203972	-2.772717953
C	-4.146568775	-3.692182064	-3.861925602
C	-3.978448868	-5.092368603	-1.706976891
C	-3.965297461	-6.576203346	-2.118236542
H	-4.645822048	-4.532190323	-4.362513542
H	-4.941304684	-3.066857815	-3.439339161
H	-3.557941675	-3.130136013	-4.588187218
H	-5.043916702	-4.831690311	-1.706148028
O	-4.713023663	-7.173819542	-2.817652225
N	-2.181281328	-6.982835293	-2.522930145
H	-1.588694215	-6.211220264	-2.211600304
C	-2.008245468	-7.291306973	-3.919577122
C	-2.566847563	-8.472374916	-4.412832260
C	-1.358942986	-6.391373634	-4.768145561
C	-2.463633776	-8.757175446	-5.773524761
C	-1.261644006	-6.690226078	-6.126599312
C	-1.813827872	-7.868852615	-6.631929398

H	-3.087244749	-9.148782730	-3.743016720
H	-0.942743480	-5.470358372	-4.374116421
H	-2.896149397	-9.673703194	-6.162028313
H	-0.750779808	-5.999305248	-6.790438175
H	-1.736138344	-8.094887733	-7.690873146
H	-2.040790796	-7.792295456	-1.921039343
O	-1.842263460	-0.743420184	1.769601822
C	-0.760154009	-1.407798886	1.897022963
O	-0.249532878	-1.895110250	0.830233335
C	-0.140914351	-1.653050423	3.238932371
H	-0.502505541	-2.613078594	3.624706745
H	0.945458174	-1.711902857	3.147020340
H	-0.428970695	-0.867924809	3.939479351

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G

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C	-0.363177896	-1.205112457	-3.830051422
C	-1.776056170	-1.279432893	-3.856905937
C	0.250057191	-0.399771839	-2.808772802
C	-2.567923546	-0.565080941	-2.901069403
C	-0.543061376	0.273631573	-1.853854418
C	-1.982924223	0.235887051	-1.895740390
H	-2.263680220	-1.939173579	-4.565975666
H	1.330676436	-0.392215669	-2.713286400
H	-3.641182899	-0.708688378	-2.916963339
H	-0.054900993	0.787922680	-1.031864285
C	0.493789941	-2.013235569	-4.761593819
H	1.316218853	-2.482602358	-4.214960575
H	-0.084628478	-2.794544697	-5.258478165
H	0.923461974	-1.359123826	-5.528841496
C	-2.775047779	1.028270721	-0.868128538
H	-2.360675573	0.765972197	0.115126662
C	-4.276179790	0.717308879	-0.863673091
C	-2.538671494	2.536880732	-1.097800732
H	-1.478197217	2.800683498	-1.045924783
H	-2.916983843	2.842795134	-2.079003334
H	-3.065315962	3.117904663	-0.335345894
H	-4.756612301	1.057844639	-1.787528872
H	-4.478570938	-0.351221085	-0.750285387
H	-4.760282516	1.238773465	-0.033509023
Ru	-1.068277001	-1.860873222	-1.805219293
C	-4.215672016	-5.520290852	0.814784527
C	-4.663274765	-4.628236294	1.910808206
C	-4.645331383	-3.145270586	1.449360490
C	-3.321143866	-2.857867956	0.689019024
C	-3.013427019	-3.823044300	-0.433552802
C	-3.488551617	-5.159106731	-0.275408804
H	-3.979422808	-4.776587009	2.759847641
H	-5.657665253	-4.928403854	2.258824825
H	-2.463909626	-2.913161039	1.372949839
H	-3.314509153	-1.839509964	0.291690022
C	-5.856489658	-2.870655060	0.535142064
H	-5.842245579	-3.489579678	-0.367655605
H	-6.792989731	-3.072317839	1.064208388
H	-5.874217987	-1.821552157	0.224966303
C	-4.720610142	-2.233262062	2.683456659
H	-4.720281124	-1.179266334	2.386322021

H	-5.639867783	-2.419999123	3.248333693
H	-3.870910168	-2.395560503	3.355403185
O	-4.497793198	-6.842696667	0.861872911
O	-2.340830803	-3.522843122	-1.452841878
O	-0.892662108	-6.143684864	-0.329857081
C	-1.642954230	-6.733846188	-1.073895454
C	-1.228020072	-7.828795433	-2.016891003
C	-3.166440487	-6.383985043	-1.067856550
C	-3.918267012	-7.463527679	-0.278666705
H	-1.865282178	-8.708602905	-1.872550249
H	-1.371733069	-7.493951321	-3.051513910
H	-0.179885268	-8.081499100	-1.854908586
H	-3.535696983	-6.385130405	-2.099132299
O	-4.032636642	-8.631499290	-0.473652452
O	-0.409186274	-2.238729715	0.196075574
C	0.387389094	-3.157512426	-0.216032222
O	0.441539049	-3.325770140	-1.480404854
C	1.173282623	-3.997240305	0.734883606
H	0.522993624	-4.795825481	1.102225900
H	2.020570517	-4.453319550	0.221476197
H	1.509302378	-3.391681910	1.579424024

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H

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C	-2.143702745	-5.545567036	1.460601807
C	-3.260992289	-5.278298855	2.402902842
C	-4.426486492	-4.554982662	1.666699886
C	-3.854559183	-3.418559074	0.777222335
C	-2.773712635	-3.862043142	-0.209758401
C	-1.909702301	-4.923255920	0.292151362
H	-2.884106874	-4.654020786	3.225642681
H	-3.603165150	-6.216359615	2.854764700
H	-3.394672155	-2.651802540	1.417427778
H	-4.651499748	-2.927910566	0.210779637
C	-5.194213390	-5.564171791	0.789276958
H	-4.542456627	-6.036135674	0.047660440
H	-5.636671066	-6.356225014	1.403001189
H	-6.004515171	-5.062900066	0.249979869
C	-5.384555817	-3.959593296	2.710053205
H	-6.229409695	-3.462926865	2.221482992
H	-5.787601948	-4.743121624	3.361761570
H	-4.878378868	-3.221125841	3.341588736
O	-1.225460410	-6.530711651	1.753027558
O	-2.625678778	-3.354909420	-1.312885761
O	0.519121170	-3.489748955	0.155580267
C	0.503773153	-4.523571968	-0.472558051
C	1.611708760	-4.982385159	-1.387130618
C	-0.688124359	-5.511962414	-0.330518305
C	-0.310953587	-6.592467785	0.694295228
H	1.934215188	-5.986458778	-1.087759852
H	1.237170100	-5.052533150	-2.415055513
H	2.446121216	-4.281758785	-1.343265653
H	-0.867803693	-5.995555401	-1.297467947
O	0.594270051	-7.375786781	0.686762273

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H-TS

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C	-2.073018074	-5.494794369	1.611002564
C	-3.397700310	-5.450892925	2.288192987
C	-4.452134132	-4.780261040	1.370402932
C	-3.830096960	-3.497648478	0.764137685
C	-2.535601854	-3.741021156	-0.016817531
C	-1.633813262	-4.711102486	0.592558146
H	-3.303098917	-4.885856152	3.227257013
H	-3.703720331	-6.465931892	2.565902233
H	-3.602545977	-2.788818836	1.573203564
H	-4.532649994	-3.003065348	0.087180674
C	-4.857686996	-5.749831200	0.241476133
H	-3.995559216	-6.061995983	-0.356319845
H	-5.325071812	-6.650615215	0.653899550
H	-5.578681469	-5.273323536	-0.430892944
C	-5.693608761	-4.415950298	2.196911097
H	-6.460092545	-3.954690456	1.565050840
H	-6.131182194	-5.309092999	2.657051325
H	-5.446720600	-3.710005045	2.997549534
O	-1.170925260	-6.438165665	1.990811586
O	-2.310524464	-3.157515287	-1.072430491
O	0.640536129	-3.598653555	-1.248988986
C	0.811947346	-4.427799702	-0.327901930
C	2.216342688	-4.636057854	0.182305038
C	-0.290383130	-5.229948044	0.195238739
C	-0.007512451	-6.287884235	1.186631083
H	2.258991957	-4.506977081	1.268428564
H	2.530274153	-5.666505337	-0.006692870
H	2.883072376	-3.932684660	-0.317347646
H	-0.722716153	-5.827867508	-1.061311603
O	0.952062905	-6.990622044	1.387151718
O	-1.245357394	-6.204174995	-2.054764748
C	-1.323600292	-5.413368225	-3.046739817
O	-0.787510574	-4.259043217	-3.126000166
C	-2.129214525	-5.853532314	-4.232692719
H	-3.112095833	-5.374615669	-4.164655685
H	-1.655349493	-5.511584282	-5.154574394
H	-2.256431580	-6.935494423	-4.230553627
H	-0.303109556	-3.905675411	-2.237842083

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B-TS'

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C	-2.375036716	-0.919656634	-3.105622292
C	-2.958675861	-0.770425558	-1.829938054
C	-0.955551147	-0.703720868	-3.213756084
C	-2.152448416	-0.533959687	-0.673458278
C	-0.165724143	-0.462823719	-2.089896917
C	-0.745721400	-0.426633269	-0.770833731
H	-4.025310040	-0.915970564	-1.719746470
H	-0.482135683	-0.825294375	-4.183293819
H	-2.614479303	-0.501220465	0.306947023
H	0.909516156	-0.382064581	-2.198273897
C	-3.211041451	-1.238040805	-4.314048767
H	-2.625097752	-1.772048235	-5.066550732
H	-4.066396236	-1.853274465	-4.027509212
H	-3.582388163	-0.314252734	-4.772538185
C	0.099059254	-0.186796308	0.463645637

H	-0.487602443	-0.547654808	1.314566374
C	0.316393733	1.334923387	0.613850534
C	1.432627559	-0.949883580	0.457560062
H	1.276870012	-2.020571709	0.308851421
H	2.113887072	-0.581074834	-0.319024891
H	1.934709549	-0.802687168	1.418162465
H	0.896601439	1.734139204	-0.226430073
H	0.874042749	1.539110065	1.532623410
H	-0.632598937	1.879528284	0.662826955
Ru	-1.403026342	-2.451410055	-1.667020917
C	-4.100122452	-3.754779577	-0.906866789
C	-4.906123161	-4.665457249	0.003788679
C	-4.560482979	-4.552051544	1.506680489
C	-3.028011799	-4.747737408	1.691942811
C	-2.279977083	-3.700798750	0.901414096
C	-2.602174520	-3.555536270	-0.593475997
H	-4.712273598	-5.690721989	-0.333049387
H	-5.963533401	-4.451638699	-0.178239748
H	-2.747856855	-5.747305870	1.349148631
H	-2.746219873	-4.636493206	2.742367029
C	-4.986687183	-3.167254210	2.033319235
H	-4.720157623	-3.052142859	3.088471651
H	-4.505119324	-2.347860098	1.484262943
H	-6.069005966	-3.034723282	1.938341498
C	-5.301698208	-5.653859615	2.280135393
H	-5.084980965	-5.587914944	3.351165295
H	-6.385004044	-5.558986664	2.150113583
H	-5.003558636	-6.649765015	1.934547305
O	-4.604643822	-3.209904432	-1.874547362
O	-1.565419316	-2.865184784	1.427807689
O	-1.462960362	-7.030739307	-4.757070541
C	-2.144669294	-6.032042027	-4.582931519
C	-2.916364908	-5.815806866	-3.275396347
C	-2.200141191	-6.249941349	-2.007402897
H	-3.206130028	-4.772767544	-3.170832157
H	-3.843474865	-6.402865410	-3.356556177
O	-2.323198080	-5.615335941	-0.926681697
O	0.206251264	-3.722564220	-0.986566365
C	0.215645894	-4.346402168	-2.093446970
O	-0.677883923	-3.996767282	-2.953573704
C	1.215337276	-5.414781094	-2.403638840
H	0.870616615	-6.025481701	-3.239267826
H	2.165444136	-4.941191196	-2.674954414
H	1.384223461	-6.033240795	-1.520113349
C	-2.287819147	-4.961483002	-5.628966808
H	-1.734254003	-4.085456848	-5.272353172
H	-1.873204827	-5.303394318	-6.577994823
H	-3.335840464	-4.666169167	-5.750810146
N	-1.489246964	-7.381414890	-2.074670792
H	-1.428331733	-7.767593384	-3.020617247
C	-0.718313575	-8.032465935	-1.072167277
C	-0.281762928	-9.329290390	-1.375469804
C	-0.352718711	-7.432341576	0.141649470
C	0.510625958	-10.027406693	-0.468605667
C	0.441161901	-8.146359444	1.039873838
C	0.874023199	-9.439700127	0.744777143
H	-0.564367831	-9.788722038	-2.319494247
H	-0.659729719	-6.421659470	0.366711259

H	0.843881905	-11.031518936	-0.712503552
H	0.726657033	-7.678020954	1.977306366
H	1.491103768	-9.984481812	1.452386141

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C'

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C	-1.874779582	-0.938109457	-3.393961191
C	-2.782136202	-0.790291131	-2.318802118
C	-0.483441770	-0.652519763	-3.167684078
C	-2.306917667	-0.465170056	-1.009912610
C	-0.026861371	-0.336456180	-1.886217594
C	-0.928775609	-0.263541162	-0.762668073
H	-3.830100536	-1.010799766	-2.460571289
H	0.225844711	-0.784989953	-3.978161335
H	-3.003888607	-0.455321848	-0.181480944
H	1.037445188	-0.217455402	-1.716777444
C	-2.336559772	-1.365324736	-4.760926723
H	-1.609968066	-2.043393850	-5.218654156
H	-3.308768749	-1.862120628	-4.712724209
H	-2.436687231	-0.492536962	-5.416732311
C	-0.410516053	0.099731550	0.615141451
H	-1.216405511	-0.111331366	1.322522044
C	-0.108549580	1.611986518	0.645143092
C	0.811412573	-0.728675246	1.040624261
H	0.600441098	-1.797481894	0.980324328
H	1.690034270	-0.513321280	0.421886295
H	1.076494098	-0.482685417	2.073320150
H	0.696125567	1.868619442	-0.053582847
H	0.214621142	1.907663941	1.647865772
H	-0.989467919	2.206173420	0.381821692
Ru	-1.232520342	-2.298038721	-1.724672675
C	-4.040700436	-3.577575684	-0.647381246
C	-4.732955933	-4.721283436	0.083054885
C	-4.347584724	-4.698555946	1.599707127
C	-2.791403294	-4.659828663	1.749908566
C	-2.253250122	-3.511840820	0.915994704
C	-2.486611366	-3.638092518	-0.624032676
H	-4.446419239	-5.692615509	-0.333273590
H	-5.811876774	-4.597154617	-0.035701469
H	-2.369397402	-5.615168571	1.428044915
H	-2.519118309	-4.483300209	2.793007612
C	-4.970604897	-3.460595131	2.271585941
H	-4.718385696	-3.437389374	3.336066961
H	-4.619086266	-2.524334431	1.827893496
H	-6.060932636	-3.483916283	2.181229115
C	-4.880384445	-5.978762627	2.262602329
H	-4.633445263	-5.990923882	3.328930616
H	-5.969811916	-6.038907051	2.169884920
H	-4.447803974	-6.874774456	1.803754926
O	-4.652910233	-2.612345457	-1.057722569
O	-1.868943572	-2.473119497	1.408823609
O	-2.401783943	-6.889986515	-4.641990662
C	-2.879717588	-5.775040150	-4.498675346
C	-3.076903820	-5.140534878	-3.117649794
C	-2.269966841	-5.708508492	-1.981399179
H	-2.881031275	-4.065745831	-3.166849375
H	-4.144055367	-5.241373062	-2.869178057

O	-2.125082493	-5.080002308	-0.858142734
O	0.391018629	-3.526361465	-0.917879105
C	0.446885705	-4.203684807	-1.990745544
O	-0.440783381	-3.964815140	-2.889060974
C	1.513840199	-5.231815815	-2.226190805
H	1.089194298	-6.114378452	-2.709300518
H	2.264803171	-4.809997559	-2.903114796
H	1.994479656	-5.508377552	-1.287883162
C	-3.332074642	-4.944838047	-5.666756630
H	-2.581965208	-4.164956093	-5.844752789
H	-3.416798353	-5.569817543	-6.556285858
H	-4.281567574	-4.441175938	-5.457576275
N	-1.752256632	-6.915065289	-2.077471256
H	-1.907035232	-7.332963943	-3.007872820
C	-0.990221739	-7.670314789	-1.133763790
C	-0.940808535	-9.050922394	-1.363665581
C	-0.287252009	-7.099785328	-0.063346103
C	-0.201754436	-9.867757797	-0.512434959
C	0.447283924	-7.933267593	0.779417694
C	0.490662903	-9.311850548	0.564940155
H	-1.482534409	-9.481452942	-2.201797009
H	-0.285388589	-6.031237602	0.097378895
H	-0.168458998	-10.937550545	-0.692578256
H	0.995259106	-7.493869305	1.607256055
H	1.066097498	-9.948880196	1.229121447

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D'

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C	-1.980789542	-1.187867403	-3.542508125
C	-3.040289640	-1.698392391	-2.741136789
C	-0.994336247	-0.401946336	-2.870784283
C	-3.158707142	-1.386738896	-1.352534413
C	-1.096736550	-0.086568281	-1.487426519
C	-2.185939789	-0.578728557	-0.706521630
H	-3.741153717	-2.400909424	-3.177350760
H	-0.099735647	-0.106659263	-3.411320210
H	-3.961879253	-1.838238955	-0.786705256
H	-0.295839518	0.462532222	-1.004560590
C	-1.835565209	-1.552933097	-4.994382381
H	-0.782731295	-1.689920545	-5.255974770
H	-2.370707035	-2.479408741	-5.216642857
H	-2.243744373	-0.760052025	-5.631154537
C	-2.239947557	-0.246124655	0.772308409
H	-1.206581950	-0.056594986	1.086633682
C	-2.777724504	-1.386147738	1.645717859
C	-3.049204588	1.053675771	0.959664404
H	-2.633402109	1.874578476	0.367340297
H	-4.092568398	0.911092162	0.657914996
H	-3.037097692	1.355710506	2.011462927
H	-3.830998182	-1.604073286	1.432694674
H	-2.711799860	-1.101014495	2.700359344
H	-2.181457043	-2.286556005	1.488086462
Ru	-1.155754209	-2.301656723	-1.785953522
C	-1.462955475	-6.339909077	1.027511358
C	-0.132759184	-6.963203430	1.406623006
C	0.879805326	-5.948000908	1.984529734
C	1.023791671	-4.767925262	0.993970335

C	-0.280133158	-4.181203365	0.488621622
C	-1.416893125	-4.962969780	0.610691071
H	0.279078782	-7.419123173	0.494218886
H	-0.329082131	-7.781643391	2.105886936
H	1.581287265	-5.089859486	0.101401545
H	1.607718110	-3.951343536	1.432348132
C	0.393855810	-5.437582493	3.356983185
H	1.124676704	-4.749545097	3.793882847
H	-0.559969544	-4.905532837	3.280097961
H	0.258959800	-6.271419048	4.053793430
C	2.242398024	-6.635812759	2.162868023
H	2.985402346	-5.934108257	2.556063890
H	2.165423393	-7.471857071	2.865871429
H	2.619144917	-7.029403210	1.212283611
O	-2.530787468	-6.967309475	1.048789501
O	-0.233352795	-2.999162674	-0.015412375
O	-6.066138744	-3.672322035	2.173337460
C	-5.053026676	-3.935523510	2.803297758
C	-4.896318436	-3.589455128	4.258907318
C	-3.863605261	-4.668590069	2.167422771
H	-5.847436428	-3.241583586	4.662855148
H	-4.532723427	-4.452508450	4.827477932
H	-4.143161297	-2.798041105	4.360309601
C	-3.754445791	-4.581443787	0.672596514
H	-2.920426846	-4.327797413	2.601962328
H	-3.941718817	-5.732826710	2.430230618
O	-2.615309954	-4.461841106	0.052846614
N	-4.843685627	-4.499392509	-0.062452905
H	-5.692217827	-4.338134766	0.492253065
C	-4.949322224	-4.474926472	-1.487552762
C	-5.996015072	-3.721698761	-2.031719208
C	-4.082301617	-5.203597069	-2.304947853
C	-6.169713497	-3.689602852	-3.414313793
H	-6.665495872	-3.168140888	-1.378504634
C	-4.265163422	-5.156825066	-3.685710669
H	-3.273950100	-5.779841900	-1.878360033
C	-5.302021980	-4.405095100	-4.244571209
H	-6.981302261	-3.107808828	-3.839710712
H	-3.590436935	-5.716505051	-4.325259686
H	-5.439118385	-4.381783485	-5.321335316
O	0.593440473	-3.172379017	-2.697924852
C	0.025771394	-4.309737206	-2.762775660
O	-1.197842956	-4.369825840	-2.392286301
C	0.760433078	-5.539385796	-3.204057693
H	1.034580708	-6.123847485	-2.318514347
H	0.111450441	-6.161395073	-3.824835300
H	1.668029189	-5.269711494	-3.745092392

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E'

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C	-3.045253277	-1.516901016	-2.494169712
C	-3.474591494	-2.340034485	-1.399951696
C	-2.076641560	-0.519761980	-2.199703693
C	-3.014043808	-2.137791395	-0.073613837
C	-1.583722591	-0.319778681	-0.873425007
C	-2.049403429	-1.119864941	0.206539333
H	-4.114270687	-3.194219828	-1.599889398

H	-1.631633282	0.041506171	-3.016248465
H	-3.322613001	-2.836104393	0.694178164
H	-0.794033289	0.404202133	-0.702451289
C	-3.528858185	-1.771846890	-3.896017551
H	-2.797765970	-1.428999186	-4.633018494
H	-3.705693245	-2.839351177	-4.056200981
H	-4.470908165	-1.240668774	-4.076678276
C	-1.442485213	-0.912965775	1.583430886
H	-0.361041456	-0.802044809	1.426719427
C	-1.672551632	-2.082035303	2.545823097
C	-1.984043241	0.406144500	2.176198721
H	-1.775931835	1.261591554	1.525436044
H	-3.067725658	0.348008156	2.326496840
H	-1.517163396	0.599052727	3.147045135
H	-2.726300716	-2.175564289	2.826117039
H	-1.099280000	-1.921897292	3.464030266
H	-1.356839180	-3.032833099	2.109876156
Ru	-1.289299369	-2.450015306	-1.478349686
C	-0.748246729	-6.577440262	0.993162572
C	0.466474563	-7.088091850	1.686329484
C	1.393626690	-5.916515350	2.117823124
C	1.544564247	-4.910417557	0.942979038
C	0.241630718	-4.434666634	0.320594221
C	-0.831527531	-5.342571735	0.400488317
H	0.997954011	-7.758441448	0.994963646
H	0.169059396	-7.702140331	2.543641567
H	2.130815029	-5.369598389	0.133468255
H	2.102506399	-4.024209499	1.261673689
C	0.798910081	-5.205402374	3.349189520
H	1.436902761	-4.369565010	3.654147148
H	-0.201045379	-4.808315277	3.151864767
H	0.726508737	-5.895981789	4.195287704
C	2.777772427	-6.478499413	2.480214834
H	3.450161457	-5.676044941	2.800348997
H	2.700521469	-7.196827412	3.303071737
H	3.242205858	-6.988299370	1.628815174
O	-1.864751458	-7.260251522	0.878627896
O	0.216630623	-3.302459478	-0.240198359
O	-4.474814415	-8.549570084	-1.218338847
C	-3.294960737	-8.439646721	-1.510449052
C	-2.447031736	-9.613505363	-1.918079019
C	-2.624688625	-7.061139107	-1.464214325
H	-3.053562403	-10.518017769	-1.972991943
H	-1.960326076	-9.423120499	-2.881858826
H	-1.649330735	-9.743964195	-1.175711274
C	-2.795704365	-6.357454300	-0.118298195
H	-1.557092786	-7.107658386	-1.686081648
H	-3.085033894	-6.421419144	-2.224263430
O	-2.117724895	-5.122964382	-0.063242309
N	-4.089608669	-6.247523308	0.300444335
H	-4.724141598	-6.923655987	-0.120999321
C	-4.539272785	-5.485774994	1.406684637
C	-5.873537540	-5.050072193	1.394462466
C	-3.714196205	-5.166790962	2.494826794
C	-6.377907753	-4.309118748	2.460162878
H	-6.509162903	-5.294704437	0.545517027
C	-4.226161003	-4.412357807	3.551728487
H	-2.691040277	-5.522885799	2.534286499

C	-5.554663181	-3.979467154	3.542557955
H	-7.415819645	-3.984919310	2.441814661
H	-3.580034971	-4.176839828	4.394653320
H	-5.947470188	-3.401690960	4.373315334
O	0.226566643	-2.628107309	-2.986904383
C	-0.095943205	-3.839237928	-3.214137077
O	-1.112382531	-4.297274113	-2.584168673
C	0.698342562	-4.707114697	-4.143213749
H	1.422907233	-5.285080433	-3.558315754
H	0.038366511	-5.408727169	-4.658011913
H	1.244454265	-4.094443798	-4.861831665

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B-TS''

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C	-1.090948462	-1.245822072	-3.895296335
C	-2.355640173	-1.209924459	-3.269166708
C	0.027147638	-0.658164144	-3.204920292
C	-2.490063906	-0.723197341	-1.931773186
C	-0.108927920	-0.179888874	-1.902629256
C	-1.373551250	-0.239730537	-1.208597302
H	-3.217659235	-1.627082467	-3.767481089
H	1.007872105	-0.686837077	-3.668979883
H	-3.454519749	-0.786754072	-1.440621257
H	0.767373621	0.173201486	-1.371179223
C	-0.903096795	-1.836693525	-5.266326427
H	0.011271320	-2.435418844	-5.309715748
H	-1.749832273	-2.467912912	-5.546796799
H	-0.815982044	-1.037457943	-6.011559486
C	-1.517487049	0.288838327	0.204642311
H	-2.433885336	-0.149459019	0.610479832
C	-1.682301044	1.821722865	0.139054015
C	-0.360193968	-0.117293023	1.128886938
H	-0.218297124	-1.199192524	1.129890323
H	0.582410574	0.363310188	0.842185259
H	-0.584489107	0.203452975	2.150168419
H	-0.784281313	2.297051668	-0.271998674
H	-1.839919209	2.220788717	1.145394444
H	-2.536005735	2.113374949	-0.481048286
Ru	-0.938662767	-2.367320538	-1.905312538
C	-3.633219481	-4.087799549	-1.793797970
C	-4.320322990	-5.312592030	-1.222614050
C	-4.450081348	-5.244645596	0.328625023
C	-3.048076630	-4.965232372	0.958029091
C	-2.479741812	-3.711359024	0.337533772
C	-2.264537811	-3.704987764	-1.190416574
H	-3.748388767	-6.205755711	-1.491945744
H	-5.302194595	-5.391089916	-1.696281195
H	-2.389149904	-5.818115711	0.779478312
H	-3.139303923	-4.798788548	2.034191608
C	-5.436877251	-4.126318932	0.715228558
H	-5.543531418	-4.065501690	1.802511096
H	-5.111741543	-3.141275644	0.362874091
H	-6.424453259	-4.324106216	0.287488371
C	-4.967166424	-6.598157883	0.841266334
H	-5.079704285	-6.578700066	1.929958940
H	-5.944877148	-6.828593731	0.405919552
H	-4.279805183	-7.411137104	0.584056675

O	-4.164393425	-3.368379116	-2.624797821
O	-2.402954340	-2.650615454	0.926683009
O	-2.538679361	-7.666054249	-4.120450020
C	-2.656164646	-6.448345661	-4.145435333
C	-1.461709261	-5.538337231	-3.735761642
C	-1.011978507	-5.973769665	-2.367542028
H	-0.658078074	-5.714239597	-4.454845428
H	-1.708864450	-4.476718426	-3.728236675
O	-1.452824950	-5.473858833	-1.313358545
O	0.360383898	-3.118648767	-0.358187228
C	0.981199920	-3.853947639	-1.187580943
O	0.566050649	-3.829948425	-2.405027151
C	2.109992027	-4.738554955	-0.760494173
H	1.696601510	-5.614984035	-0.249744013
H	2.691761732	-5.064704418	-1.623640776
H	2.746474028	-4.210473537	-0.047105178
C	-0.106589079	-7.156455994	-2.276381016
H	0.086582631	-7.433602810	-1.240004420
H	-0.598334908	-7.975097179	-2.819041014
H	0.829695404	-6.937852383	-2.800790787
N	-3.775396109	-5.763852119	-4.495182037
H	-3.751237869	-4.759763241	-4.387816429
C	-5.066364765	-6.292816639	-4.779196739
C	-6.149947166	-5.417031765	-4.622606277
C	-5.272120953	-7.611268520	-5.199847698
C	-7.441863537	-5.861012936	-4.892096519
C	-6.574378014	-8.039410591	-5.459852695
C	-7.659441471	-7.174982548	-5.311185360
H	-5.976202011	-4.401800632	-4.274439335
H	-4.433232784	-8.283906937	-5.311401844
H	-8.278004646	-5.178746700	-4.771073818
H	-6.736641884	-9.062013626	-5.787191391
H	-8.666598320	-7.521434307	-5.520709515

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C''

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C	-1.160103917	-1.192938924	-3.886854887
C	-2.412370920	-1.180188417	-3.229819775
C	-0.028514745	-0.615832388	-3.211094379
C	-2.528130770	-0.700408578	-1.888092518
C	-0.149117589	-0.140036106	-1.901615500
C	-1.403128624	-0.200306520	-1.191286206
H	-3.279219389	-1.610451579	-3.710213900
H	0.945235610	-0.641775787	-3.689182758
H	-3.475700617	-0.796682894	-1.373148680
H	0.736544907	0.202363774	-1.379344821
C	-0.994761705	-1.776593447	-5.264363766
H	-0.095582984	-2.397419930	-5.318713188
H	-1.858731151	-2.383290529	-5.548442841
H	-0.891845286	-0.973886251	-6.003643036
C	-1.523641348	0.319313735	0.228203937
H	-2.461871862	-0.075922035	0.627831578
C	-1.610664964	1.858976603	0.180262864
C	-0.391728103	-0.154333308	1.151549459
H	-0.319655567	-1.242944956	1.155048490
H	0.579964459	0.260183632	0.859511554
H	-0.591229975	0.184343010	2.172453642

H	-0.686915338	2.293413877	-0.219094977
H	-1.755607247	2.254995108	1.189871907
H	-2.443774462	2.200208902	-0.442506909
Ru	-0.952385366	-2.292932987	-1.933089733
C	-3.684162617	-4.086337090	-1.742529631
C	-4.361998081	-5.333896160	-1.208393455
C	-4.497087955	-5.244776249	0.348674327
C	-3.103241682	-4.919826984	0.981906533
C	-2.541372776	-3.686689615	0.305222034
C	-2.242944479	-3.841999769	-1.218898773
H	-3.785640240	-6.229149818	-1.463866115
H	-5.343868256	-5.419486523	-1.679337978
H	-2.434476376	-5.775789261	0.852680147
H	-3.210598230	-4.711541176	2.048746824
C	-5.512504101	-4.147044659	0.718820870
H	-5.625934124	-4.082555294	1.805168509
H	-5.209580421	-3.158644438	0.360009044
H	-6.492741108	-4.373361111	0.288518876
C	-4.981317997	-6.604752064	0.877053499
H	-5.089717865	-6.576251507	1.965965033
H	-5.955517769	-6.860962868	0.448320985
H	-4.277221680	-7.405272484	0.625275791
O	-4.277183056	-3.247704506	-2.397789955
O	-2.532475471	-2.591197252	0.822979093
O	-2.737748146	-7.432501316	-4.031710625
C	-2.785212040	-6.212986946	-4.105463982
C	-1.543396831	-5.348696232	-3.706422329
C	-1.118413806	-5.752799988	-2.338544846
H	-0.743495405	-5.595510483	-4.407893181
H	-1.737063050	-4.275636673	-3.741147041
O	-1.542089581	-5.198501587	-1.272737265
O	0.420846611	-3.073839426	-0.426109076
C	0.995698452	-3.812486887	-1.278322816
O	0.511437476	-3.818713188	-2.474042892
C	2.164644718	-4.676198959	-0.909572423
H	1.810429454	-5.530435085	-0.322154164
H	2.674650431	-5.037277699	-1.803714991
H	2.856347084	-4.112199783	-0.279680610
C	-0.320065796	-6.985837460	-2.161694050
H	-0.135779068	-7.204859734	-1.109999895
H	-0.891135573	-7.794948578	-2.641770363
H	0.621464670	-6.893265724	-2.712234020
N	-3.846138477	-5.474453926	-4.512306213
H	-3.772753716	-4.471890926	-4.411926270
C	-5.162239075	-5.948331833	-4.789384365
C	-6.214070797	-5.051910400	-4.559695721
C	-5.411633492	-7.235569477	-5.274339199
C	-7.523672581	-5.446262360	-4.822340012
C	-6.730513096	-7.615711689	-5.524615288
C	-7.786509991	-6.729856014	-5.305051804
H	-6.004322052	-4.064622402	-4.156372070
H	-4.594159603	-7.924163342	-5.439334393
H	-8.337676048	-4.749994278	-4.644135952
H	-6.929423809	-8.614317894	-5.901570320
H	-8.807544708	-7.037170410	-5.508550167

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C	-0.882886589	-1.302784085	-3.361515999
C	-1.876899004	-0.373055518	-2.973181725
C	0.234078556	-1.495621324	-2.473832607
C	-1.777181745	0.352593154	-1.741723061
C	0.310408354	-0.795475006	-1.250325561
C	-0.690866828	0.165541455	-0.860224247
H	-2.766783237	-0.267089695	-3.582803488
H	0.969686151	-2.259786844	-2.702332497
H	-2.603385210	0.988478959	-1.449373722
H	1.108045816	-1.033492923	-0.553204894
C	-1.023944378	-2.137453556	-4.602775097
H	-0.627490342	-3.142849684	-4.438445568
H	-2.071245432	-2.224376440	-4.897651196
H	-0.461882085	-1.678869843	-5.424791336
C	-0.543575823	0.884698868	0.468791187
H	-0.233305648	0.124605492	1.198487639
C	-1.836385846	1.533666015	0.973690271
C	0.589534760	1.926709175	0.353420436
H	1.533256650	1.470758319	0.038299922
H	0.328245193	2.704895496	-0.371574044
H	0.755259395	2.407139063	1.322085619
H	-2.143839121	2.370858192	0.337187111
H	-2.659919024	0.815100789	1.020954967
H	-1.680841208	1.931808949	1.979828954
Ru	-1.620298147	-1.861746192	-1.331076026
C	-5.847956181	-4.242783070	1.100373983
C	-5.601466179	-3.631086588	2.470018148
C	-5.166641235	-2.148746967	2.451526642
C	-3.976058960	-1.993031859	1.469956040
C	-4.255923748	-2.625524521	0.138661042
C	-5.122582436	-3.670959711	-0.015566461
H	-4.813940048	-4.241374969	2.938114166
H	-6.504229069	-3.778863907	3.070745707
H	-3.072013140	-2.457172871	1.881665349
H	-3.740600586	-0.935917437	1.309945345
C	-6.343774796	-1.259336114	2.005852461
H	-6.705060482	-1.529547572	1.008357406
H	-7.184727669	-1.357472062	2.699266911
H	-6.047829628	-0.205024764	1.985167027
C	-4.714916229	-1.725940466	3.858284235
H	-4.395831585	-0.677794814	3.867171288
H	-5.534794331	-1.830764055	4.576421738
H	-3.877249718	-2.338035107	4.210814476
O	-6.591001987	-5.226614952	0.966025233
O	-3.717816591	-2.139457464	-0.971228600
O	-3.974628210	-3.299594879	-3.324119329
C	-4.804850578	-3.027498007	-2.375650644
C	-5.704371929	-1.852866292	-2.607285976
C	-5.300881863	-4.144900322	-1.448735476
C	-4.617566586	-5.504954338	-1.728358626
H	-6.214216709	-1.554206491	-1.690470457
H	-5.129929543	-1.016602039	-3.007752180
H	-6.453786850	-2.149650335	-3.352129221
H	-6.376647472	-4.269328117	-1.642939091
O	-3.743875504	-5.614669323	-2.617336035
N	-5.034304142	-6.499333382	-0.938591778
H	-5.775513649	-6.237608433	-0.273986578

C	-4.547259331	-7.828835011	-0.829807162
C	-5.087969303	-8.593858719	0.213965386
C	-3.571709156	-8.374132156	-1.675452709
C	-4.655914783	-9.901708603	0.411092639
C	-3.147830248	-9.686292648	-1.459168792
C	-3.682043314	-10.453667641	-0.423964798
H	-5.839918137	-8.157806396	0.867108941
H	-3.163494349	-7.787325859	-2.485854387
H	-5.081074715	-10.488933563	1.219366193
H	-2.393173218	-10.110474586	-2.114911556
H	-3.345087528	-11.474023819	-0.269735664
O	-1.323958635	-3.122020721	0.395303845
C	-1.498895407	-4.166312218	-0.324660599
O	-1.628673911	-3.966837406	-1.580622554
C	-1.621539831	-5.533476830	0.269935399
H	-2.634371042	-5.643031597	0.674662173
H	-1.475666404	-6.297855854	-0.493981123
H	-0.912161767	-5.655774593	1.091196537
H	-3.647114277	-4.278725147	-3.160651922

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C	-0.481891245	-1.897350907	-3.133405209
C	-1.911678791	-1.817980289	-3.153579473
C	0.243961439	-0.834434867	-2.519582748
C	-2.584495783	-0.757410824	-2.507670164
C	-0.456685871	0.226591095	-1.873601913
C	-1.881499529	0.290191352	-1.840668559
H	-2.479693174	-2.635650873	-3.578405857
H	1.324969769	-0.888386250	-2.447038651
H	-3.665581703	-0.804398417	-2.445240974
H	0.112400211	0.953475654	-1.301048160
C	0.206556499	-3.114755630	-3.681469202
H	1.118413091	-3.333427906	-3.120834827
H	-0.457815796	-3.980976105	-3.627903700
H	0.476145416	-2.946680784	-4.730847836
C	-2.590486526	1.424346685	-1.126058340
H	-1.890640140	1.806998253	-0.372110069
C	-3.863703012	0.970953405	-0.396319807
C	-2.883794546	2.555513382	-2.132566929
H	-1.969627500	2.908458233	-2.620712519
H	-3.573427916	2.211617708	-2.911766529
H	-3.346721888	3.405672312	-1.622355938
H	-4.647142887	0.669299304	-1.099999785
H	-3.654980659	0.129206300	0.270251513
H	-4.262365818	1.798531651	0.197586238
Ru	-1.139246583	-1.690607548	-1.034678102
C	-3.790139914	-5.408412457	1.423319101
C	-4.397709370	-5.187798500	2.764592409
C	-4.772595406	-3.697545290	2.974365473
C	-3.585837841	-2.817667484	2.509504080
C	-3.062322140	-3.113904238	1.112809062
C	-3.145400763	-4.460864067	0.659890473
H	-3.658359528	-5.500932217	3.516418695
H	-5.264254570	-5.845775127	2.888871670
H	-2.733365297	-2.960433245	3.190643787
H	-3.843557835	-1.755491018	2.554322958

C	-6.041888714	-3.351907730	2.169550180
H	-5.929710865	-3.563162565	1.100340962
H	-6.897881031	-3.933439493	2.526012659
H	-6.289988518	-2.291004658	2.276657581
C	-5.042886734	-3.444406748	4.466014862
H	-5.321868420	-2.399847269	4.638193607
H	-5.865190506	-4.073087692	4.823332787
H	-4.159897804	-3.663203239	5.076253414
O	-3.857820988	-6.604671955	0.871525824
O	-2.602308750	-2.139381886	0.459957719
O	-1.819182992	-7.206962585	-0.080534689
C	-3.020655632	-6.605722427	-0.391808182
C	-3.835780859	-7.349534988	-1.429322839
C	-2.724586725	-5.094910622	-0.643668652
C	-3.398865223	-4.554428101	-1.909668684
H	-3.291479826	-7.357172489	-2.375400305
H	-4.012963772	-8.376766205	-1.096079946
H	-4.803639412	-6.867119312	-1.582375526
H	-1.653492451	-4.996623039	-0.818896115
O	-2.913351774	-4.782957077	-3.014599800
N	-4.536278725	-3.831661701	-1.691826582
H	-4.773865700	-3.691920280	-0.719802260
C	-5.256020546	-3.028512955	-2.605226994
C	-6.046163559	-2.000662088	-2.066999674
C	-5.193457127	-3.213003397	-3.993024826
C	-6.758732319	-1.153087378	-2.911689043
C	-5.906989098	-2.349158525	-4.825448990
C	-6.685850620	-1.318844557	-4.297096729
H	-6.093130589	-1.863316417	-0.988816202
H	-4.592356682	-4.013660908	-4.401619911
H	-7.369404316	-0.362384588	-2.485992432
H	-5.852809429	-2.491016388	-5.900837421
H	-7.237393856	-0.656258821	-4.956524849
O	0.100335099	-1.652423024	0.729956269
C	0.320849687	-2.902508497	0.633063793
O	-0.154412389	-3.492703915	-0.400442302
C	1.063960075	-3.670616388	1.681632996
H	0.383227766	-4.396090984	2.139030695
H	1.875615478	-4.236196518	1.215720892
H	1.459880114	-2.998839140	2.443546057
H	-1.946569920	-8.164037704	-0.008004084

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C	-2.269034863	-0.861358404	-3.239927292
C	-2.993855238	-0.266553134	-2.183279753
C	-0.834743381	-0.723339200	-3.220363379
C	-2.334437847	0.450541198	-1.137579918
C	-0.179880336	-0.017653625	-2.187777281
C	-0.926368058	0.582151711	-1.112518549
H	-4.061569214	-0.439122260	-2.100574255
H	-0.243954957	-1.243358016	-3.968049526
H	-2.925473452	0.826116979	-0.312506288
H	0.904803872	0.003144076	-2.158740520
C	-2.952314854	-1.658876061	-4.314248562
H	-2.297614336	-2.451191425	-4.686887264
H	-3.870408297	-2.110717297	-3.934497833

H	-3.202665806	-1.003679633	-5.156768322
C	-0.216260478	1.281871796	0.032457154
H	0.860323548	1.143855453	-0.125639156
C	-0.571201384	0.675944924	1.402127743
C	-0.527853847	2.791218758	-0.020013638
H	-0.258185655	3.226048708	-0.987867653
H	-1.593946576	2.973085165	0.152965531
H	0.037718404	3.315264225	0.756340086
H	-1.636523366	0.792989314	1.623392820
H	-0.320289135	-0.388071865	1.436025143
H	-0.008828356	1.189573526	2.187762499
Ru	-1.431762934	-1.603654385	-1.284518361
C	-4.924626350	-4.742776394	1.761042833
C	-4.006544590	-5.581195354	2.569847345
C	-2.661283731	-4.832334042	2.800765276
C	-2.176442385	-4.209638596	1.463029504
C	-3.210620642	-3.375063419	0.741137981
C	-4.587218761	-3.688861132	0.963096321
H	-3.828413486	-6.524924755	2.031445742
H	-4.476245403	-5.852962017	3.522444248
H	-1.903755307	-5.013728142	0.762516141
H	-1.279451013	-3.604222536	1.617865443
C	-2.843445778	-3.723234177	3.857459307
H	-3.606702566	-2.996078014	3.562759161
H	-3.144906282	-4.150645256	4.819158077
H	-1.903475165	-3.183240891	4.011775017
C	-1.604504704	-5.831416607	3.296883345
H	-0.648149788	-5.328364372	3.475090504
H	-1.917756319	-6.292624474	4.239294052
H	-1.437133312	-6.633649826	2.569284916
O	-6.251173973	-5.012214184	1.689284205
O	-2.933611393	-2.465006113	-0.079034679
O	-6.987513065	-5.307226181	-0.543952763
C	-6.813462734	-4.195216179	0.645400882
C	-8.228703499	-3.791108608	0.942855656
C	-5.782378197	-3.229535103	0.227345586
C	-6.155657291	-1.801977158	0.078821309
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H	-8.847031593	-4.660994053	1.178365350
H	-8.225782394	-3.118936539	1.804931760
H	-5.286171913	-3.473777533	-1.304559946
O	-7.048908234	-1.422291160	-0.677096009
N	-5.389681339	-0.931038260	0.839532316
H	-4.781983376	-1.362791419	1.519003749
C	-5.246845722	0.459530681	0.722001374
C	-4.462143421	1.109359503	1.692360401
C	-5.787201405	1.205352783	-0.338670135
C	-4.193315029	2.472487926	1.588580370
C	-5.502171516	2.568224907	-0.431164056
C	-4.702428341	3.210589170	0.517016709
H	-4.061551571	0.539122641	2.528088808
H	-6.427786350	0.715979993	-1.059684515
H	-3.584879637	2.955895424	2.347631216
H	-5.919314384	3.135131836	-1.258627057
H	-4.494350433	4.272623062	0.433332622
O	0.121134408	-2.485784531	-0.067888603
C	0.089665487	-3.562599897	-0.753424048
O	-0.746227562	-3.609886885	-1.719261289

C	0.968770862	-4.729811668	-0.417948127
H	0.424800664	-5.413262844	0.243685201
H	1.234408140	-5.274950981	-1.325680494
H	1.864810824	-4.388135910	0.102759995
H	-7.379835606	-6.119316578	-0.179119900
O	-4.821545601	-5.807720661	-1.542026758
C	-4.350665092	-4.907036781	-2.280889034
O	-4.731628895	-3.668743849	-2.219420433
H	-5.984549522	-5.537641525	-0.969265759
C	-3.266295671	-5.224169254	-3.265584230
H	-3.452022552	-4.702603817	-4.206978321
H	-2.316427708	-4.857760429	-2.859833956
H	-3.209029436	-6.300193787	-3.428612232

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C	-2.551917791	-0.746650577	-2.572290659
C	-0.480858654	0.274777353	-1.819102049
C	-1.905057549	0.310095280	-1.861134648
H	-2.357510567	-2.614606142	-3.642506361
H	1.349209547	-0.798799753	-2.313646317
H	-3.633706808	-0.816656470	-2.564401150
H	0.044045519	1.009134293	-1.214826584
C	0.344703346	-3.026333809	-3.637862682
H	1.270640492	-3.194604397	-3.083292723
H	-0.280063033	-3.920285225	-3.567310095
H	0.597117186	-2.861893415	-4.692195415
C	-2.680016994	1.420041800	-1.177484035
H	-2.026026487	1.825844169	-0.395082593
C	-3.970058203	0.927227020	-0.503587425
C	-2.966655970	2.540394306	-2.197878838
H	-2.044825554	2.922789574	-2.647710800
H	-3.611659288	2.173603296	-3.004441261
H	-3.478358030	3.374892235	-1.708854437
H	-4.712042332	0.600145280	-1.240426421
H	-3.765270948	0.093055300	0.173372954
H	-4.419759274	1.743102908	0.069851123
Ru	-1.167481303	-1.666220903	-1.034562945
C	-3.690331697	-5.407663822	1.547013283
C	-4.189293861	-5.159424782	2.928391695
C	-4.654881954	-3.689340353	3.090743303
C	-3.563894272	-2.759805202	2.506866217
C	-3.094406128	-3.097267628	1.099725246
C	-3.155930042	-4.460634232	0.697587907
H	-3.366907120	-5.374146938	3.626152039
H	-4.989868641	-5.869009495	3.161122084
H	-2.665057659	-2.799055099	3.140861988
H	-3.893381834	-1.716416121	2.508600712
C	-5.990302563	-3.472316504	2.350712299
H	-5.917866707	-3.711384773	1.283493757
H	-6.776745319	-4.104647160	2.774432659
H	-6.314630985	-2.430540323	2.438561201
C	-4.851520538	-3.377997398	4.582828045
H	-5.184953213	-2.344687223	4.723088264

H	-5.610013485	-4.036015034	5.019593239
H	-3.921977282	-3.512463331	5.146676064
O	-3.752045155	-6.623749733	1.052230358
O	-2.685889721	-2.135491133	0.394321084
O	-4.337872982	-6.997873306	-1.169311285
C	-3.273684263	-6.615982533	-0.389370292
C	-2.194494724	-7.666348457	-0.503884494
C	-2.767513990	-5.136025429	-0.595808983
C	-3.339173794	-4.548535824	-1.887892842
H	-1.814061403	-7.660439014	-1.528647304
H	-1.375822663	-7.450175285	0.186028004
H	-2.613477707	-8.649739265	-0.281088412
H	-1.686138153	-5.134324551	-0.734683871
O	-2.765792131	-4.701352119	-2.957917452
N	-4.544725418	-3.905401707	-1.729543209
H	-4.804943562	-3.728536606	-0.768107057
C	-5.207736492	-3.084245920	-2.677500010
C	-5.986090660	-2.028263807	-2.181056738
C	-5.101422310	-3.292575598	-4.058201313
C	-6.645846367	-1.174194455	-3.062673330
C	-5.760212898	-2.422111750	-4.928278923
C	-6.528969288	-1.363603711	-4.441910744
H	-6.064248085	-1.871772528	-1.107169390
H	-4.507631779	-4.114316940	-4.434945107
H	-7.249303818	-0.361064106	-2.670125246
H	-5.674204350	-2.582640409	-5.998834610
H	-7.039417267	-0.697077036	-5.129874229
O	0.007439297	-1.626399875	0.769706905
C	0.243059486	-2.874626875	0.683480859
O	-0.206771642	-3.478392601	-0.352514714
C	0.982620656	-3.621117353	1.752128482
H	0.302956313	-4.340837955	2.220650673
H	1.802395105	-4.189311981	1.303699851
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H	-4.997220516	-6.289653778	-1.224905849

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C	-2.652217627	-0.635201514	-2.824702024
C	-1.083527446	0.412368864	-1.272556543
C	-2.427442789	0.140020087	-1.633277178
H	-1.780566692	-1.784134746	-4.430139542
H	1.027029395	0.075893603	-1.704493523
H	-3.656708002	-0.942703068	-3.089063883
H	-0.876468122	0.931031764	-0.340877116
C	0.919581890	-1.427783370	-4.027029037
H	1.831831813	-1.506909013	-3.430900097
H	0.655793667	-2.419072628	-4.404933929
H	1.131416917	-0.781913579	-4.887025833
C	-3.567192078	0.648670018	-0.768921673
H	-3.189150095	0.677450895	0.262289405
C	-4.816672325	-0.244526863	-0.798679709
C	-3.901089430	2.096080542	-1.193979144
H	-3.028995514	2.752746344	-1.115350723

H	-4.260158539	2.125180244	-2.228579044
H	-4.689541340	2.499748468	-0.551444590
H	-5.326673031	-0.195044875	-1.766973019
H	-4.573132515	-1.290580273	-0.590699792
H	-5.532065868	0.099987909	-0.046202376
Ru	-1.253842115	-1.792792082	-1.495715737
C	-3.897261143	-5.226873398	1.947707891
C	-3.939509869	-4.464995384	3.216642141
C	-3.878173351	-2.929141998	2.943948269
C	-2.796418905	-2.621697903	1.864164352
C	-2.947278500	-3.438912868	0.607875466
C	-3.421571493	-4.779516220	0.759809971
H	-3.078381538	-4.783347130	3.823457003
H	-4.834735870	-4.730254650	3.789204597
H	-1.789676189	-2.835115671	2.253062725
H	-2.807537794	-1.561300635	1.594864964
C	-5.252886295	-2.438083887	2.447773457
H	-5.565853596	-2.940469265	1.525738597
H	-6.023213387	-2.614751816	3.204241991
H	-5.225191116	-1.362680674	2.248228312
C	-3.509680033	-2.207741261	4.249182224
H	-3.483147144	-1.124195814	4.098001957
H	-4.250944614	-2.415529728	5.027248859
H	-2.529224873	-2.522557735	4.622189999
O	-4.324468613	-6.519250393	1.890856266
O	-2.680209875	-3.031782627	-0.543358684
O	-5.725398064	-6.569183826	0.051005986
C	-4.341351986	-6.920154095	0.531430662
C	-4.096348286	-8.400027275	0.389038771
C	-3.403172493	-5.937440872	-0.223827586
C	-3.805990696	-5.654147148	-1.680849552
H	-4.185614586	-8.699478149	-0.659426510
H	-3.090008497	-8.637647629	0.743476510
H	-4.809295177	-8.968424797	0.994391084
H	-2.402034044	-6.388383865	-0.236635342
O	-4.991002083	-5.901362419	-2.074933290
N	-2.854650497	-5.162607670	-2.460620403
H	-1.951915026	-4.939496040	-2.029564381
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C	-1.789702654	-4.663210869	-4.557579041
C	-4.165603161	-4.177252293	-4.326764584
C	-1.810849667	-4.152579308	-5.854504108
C	-4.168454647	-3.660506010	-5.623807907
C	-2.999368191	-3.646401405	-6.389782429
H	-0.868950486	-5.046169758	-4.128665924
H	-5.076395512	-4.199117184	-3.741930008
H	-0.902163625	-4.159142494	-6.448919773
H	-5.094887733	-3.277006388	-6.040470600
H	-3.017942667	-3.255819798	-7.402451515
O	0.041411314	-2.570755482	0.018754523
C	0.213348389	-3.674627304	-0.593732059
O	-0.379083693	-3.807306051	-1.726757288
C	1.044442058	-4.776005745	-0.012087217
H	0.389950931	-5.587086678	0.328718692
H	1.704586744	-5.186967373	-0.780558169
H	1.628435493	-4.409245014	0.832721233
H	-6.389521599	-7.248896122	0.307792842
H	-5.584233284	-6.377210617	-1.020962715

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C	-1.958256602	0.274020612	-0.253101021
C	-1.884276509	-0.976146162	0.411365330
C	-0.860771418	0.631424487	-1.111789346
C	-0.813308418	-1.885050893	0.179891691
C	0.171808317	-0.265631855	-1.359886050
C	0.212025821	-1.561904550	-0.731881738
H	-2.667845726	-1.257634401	1.105243087
H	-0.883730412	1.577454805	-1.640313029
H	-0.825827777	-2.858095646	0.655167878
H	0.947265923	-0.010988202	-2.075931072
Ru	-1.912757158	-1.394091845	-1.848094463
C	-4.425174236	-2.864720345	-2.849706173
C	-5.850381851	-2.969889164	-2.325873613
C	-6.111137867	-2.088831425	-1.088920236
C	-5.144394398	-2.557872295	0.024478102
C	-3.792550087	-3.142292738	-0.411659777
C	-3.324087381	-2.827418089	-1.800516367
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H	-4.936357975	-1.744770408	0.731356978
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H	-6.565587521	-0.306528568	-2.260313511
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H	-8.268741608	-1.941633701	-1.378105879
H	-7.777435303	-3.330116272	-0.392235667
O	-4.205200672	-2.823181629	-4.048025131
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C	-2.652642727	-5.084444046	-3.684465408
C	-3.864577532	-5.733739853	-4.257636547
C	-2.439220428	-4.947832108	-2.289981127
C	-1.037504196	-4.782965183	-1.874762535
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H	-3.122438908	-5.479172230	-1.643332243
O	-0.215470344	-4.256920338	-2.633517742
H	-1.007917643	-4.278944016	-4.036253452
O	-2.884425640	-0.423273861	-3.440343618
C	-2.193291903	-1.071709037	-4.307100296
O	-1.340765357	-1.891253948	-3.823771954
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H	-1.456051826	-1.077875733	-6.304831028
H	-3.123698711	-1.656025171	-6.088840008
C	1.391722322	-2.458948374	-0.966785073
H	1.213493705	-3.466185570	-0.593732238
H	1.626054883	-2.528569460	-2.030556917
H	2.258899212	-2.030759811	-0.448122859
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H	-3.948422670	0.651730359	0.337405026

C	-3.474981785	2.119077921	-1.157410383
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H	-2.708896637	2.869503498	-1.381828904
H	-4.396017075	2.663497925	-0.930824220
H	-3.638763905	1.518531322	-2.055004597
O	-0.607283592	-5.195348740	-0.682313323
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H	0.554941475	-6.938591480	0.904078841
H	-0.885041296	-7.349871159	1.860116482

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C	-0.046839997	-1.766268969	-1.114821196
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Ru	-2.110522509	-1.280909538	-1.906017065
C	-4.545612812	-2.935414076	-2.725618839
C	-5.831622601	-2.210643291	-2.419842720
C	-6.060415745	-1.761148334	-0.955624938
C	-5.359013081	-2.743554831	0.004775241
C	-3.945993185	-3.194846630	-0.325978220
C	-3.504558802	-3.172033548	-1.744009852
H	-6.613312244	-2.916255951	-2.729517221
H	-5.900533676	-1.361423254	-3.107975006
H	-5.916601658	-3.693742514	0.024161797
H	-5.367230892	-2.373498201	1.034577608
C	-5.537525654	-0.332849741	-0.736868739
H	-4.474965572	-0.263458014	-0.962065458
H	-6.058966637	0.377846301	-1.385708928
H	-5.696777821	-0.021456052	0.301526487
C	-7.573010921	-1.777132869	-0.665246129
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H	-8.104955673	-1.101801991	-1.343886018
H	-7.995529175	-2.780838013	-0.786949575
O	-4.397222996	-3.409193277	-3.876883745
O	-3.242607117	-3.692313433	0.552430153
O	-3.821478367	-6.190753460	-1.258832812
C	-2.764892340	-5.565648556	-1.228635311
C	-1.606862903	-5.996842384	-0.379943550
C	-2.601110697	-4.367888927	-2.195137739
C	-3.010443449	-4.821608067	-3.606310129
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H	-1.962916136	-6.644264221	0.421832383
H	-1.554039836	-4.081756592	-2.269917727
O	-3.810060740	-5.840978622	-3.779786587
H	-4.199566841	-6.079380989	-2.892633677
O	-3.486772537	-0.372766435	-3.307078838
C	-2.923212051	-0.976335168	-4.284516335
O	-1.942371249	-1.739318609	-3.990803719
C	-3.430202723	-0.841476738	-5.684755802
H	-3.933984995	0.117542483	-5.816765785
H	-2.611368895	-0.945880890	-6.399179935
H	-4.151727200	-1.647765517	-5.855074406
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H	0.558442712	-3.841266632	-1.077220321
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H	1.886759996	-2.684391022	-1.203959346
C	-2.670046329	1.600682020	-0.002576306
H	-3.517233610	1.190420628	0.556996644
C	-3.219700813	2.398428202	-1.196313262
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H	-1.515933990	1.955492854	1.835433245
H	-0.987002254	2.925880671	0.447460264
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H	-2.432774544	2.980478287	-1.688400984
H	-3.969419479	3.112122297	-0.843260169
H	-3.682041645	1.747197986	-1.941944003
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C	-2.501945257	-4.949529648	-5.921173573
H	-3.519779682	-4.592721939	-6.099613667
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H	-0.476023853	-4.664400578	-6.619896412
H	-1.491865396	-3.209228277	-6.684421539
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C	-0.094878003	-0.355666488	-2.005618572
C	-0.902184486	-0.266807348	-0.815742970
H	-3.949024200	-0.891418457	-2.297966480
H	-0.025117202	-0.751442432	-4.123106003
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H	0.983253658	-0.280597121	-1.918756366
C	-2.686244965	-1.142140746	-4.725121975
H	-1.970533133	-1.643221736	-5.381650925
H	-3.576579809	-1.768014312	-4.623582840
H	-2.986762524	-0.209447905	-5.216859341
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H	-1.031078815	-0.115029581	1.285847187
C	0.082097732	1.571572065	0.531683028
C	0.948479056	-0.799946129	0.856403172
H	0.695621967	-1.860634208	0.822382808
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H	1.303490520	-0.556902826	1.862444520

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H	0.484053999	1.852817416	1.509731650
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Ru	-1.318267107	-2.283885956	-1.794507265
C	-4.059693336	-3.658075333	-0.682853281
C	-4.737073898	-4.730247974	0.167948559
C	-4.330901146	-4.596871376	1.669341087
C	-2.773050547	-4.574420452	1.789442778
C	-2.242551804	-3.467497349	0.898321033
C	-2.497026205	-3.640564442	-0.635056794
H	-4.469648838	-5.736006737	-0.175314561
H	-5.816897869	-4.612312794	0.049750246
H	-2.366496801	-5.546892643	1.499782681
H	-2.477744102	-4.356462002	2.818232536
C	-4.928386211	-3.300438881	2.249660015
H	-4.650978565	-3.189013481	3.302081823
H	-4.581024647	-2.406902552	1.721943617
H	-6.020635605	-3.321380377	2.186465263
C	-4.875040054	-5.810005665	2.440067530
H	-4.618840694	-5.736886024	3.501651764
H	-5.966026306	-5.862521172	2.361362934
H	-4.458133698	-6.747214317	2.054938078
O	-4.698456287	-2.802007437	-1.257590771
O	-1.845751405	-2.413119316	1.345111966
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C	-2.161386967	-5.759607315	-4.279757977
C	-3.070525885	-5.457396507	-3.042807341
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H	-3.284632921	-4.391043663	-2.999778986
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O	-2.110929966	-5.118963718	-0.807924151
O	0.332886010	-3.509833097	-1.100667357
C	0.267427921	-4.246781349	-2.130794764
O	-0.648758054	-3.964966297	-2.989011765
C	1.196945429	-5.401700497	-2.349466801
H	0.668677628	-6.213915348	-2.853727102
H	2.018367529	-5.082544327	-3.000520706
H	1.615341902	-5.733851910	-1.398383141
C	-2.380069256	-4.841143608	-5.448488712
H	-1.901783824	-3.888280630	-5.204556942
H	-1.916159034	-5.266373158	-6.339151382
H	-3.444987535	-4.652744770	-5.621033192
O	-2.175773382	-7.131630898	-1.483584046
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H	0.545787811	0.214905649	-1.624742866
C	-1.146755099	-2.096768618	-5.349048138
H	-0.172681779	-2.586934566	-5.437088013
H	-1.932464004	-2.833496809	-5.535453320
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H	-2.579286098	-0.153047815	0.474165976
C	-1.920769691	1.816919804	-0.122906111
C	-0.496519238	-0.008871986	0.933207810
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H	0.420837283	0.482257724	0.588468492
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Ru	-1.003149390	-2.406309605	-1.971305370
C	-3.695425272	-4.269449711	-1.592718005
C	-4.307421207	-5.502958775	-0.949161470
C	-4.343489170	-5.349164009	0.606475472
C	-2.913962126	-4.989079952	1.130712748
C	-2.434810877	-3.771244764	0.370266736
C	-2.227123260	-3.968712807	-1.162815452
H	-3.734483242	-6.395204067	-1.214104414
H	-5.319330215	-5.620840549	-1.343347907
H	-2.243859053	-5.840320110	0.981453001
H	-2.949140072	-4.743573189	2.194449186
C	-5.343923092	-4.245477676	0.999135911
H	-5.384283066	-4.133671761	2.086806297
H	-5.079200268	-3.271070957	0.577619016
H	-6.348241329	-4.499904633	0.647136211
C	-4.777916908	-6.689314842	1.221239328
H	-4.819223404	-6.615818501	2.312725544
H	-5.774074554	-6.971502781	0.865553081
H	-4.082157135	-7.493623734	0.959027410
O	-4.346088409	-3.482945442	-2.251573563
O	-2.440643072	-2.653607368	0.839874506
O	-3.249175787	-6.983135223	-3.601635456
C	-2.813230991	-5.947309971	-4.062765598
C	-1.459187746	-5.354634285	-3.663993120
C	-1.062860131	-5.835741997	-2.307697058
H	-0.711396277	-5.664245605	-4.399004459
H	-1.526157022	-4.266239643	-3.665673971
O	-1.509433985	-5.323479652	-1.233915806
O	0.384957433	-3.022190094	-0.394600242
C	0.986680388	-3.813249826	-1.175907493
O	0.531885684	-3.908338785	-2.380352497
C	2.143909216	-4.648321152	-0.717104614
H	1.766283870	-5.478210449	-0.108920939
H	2.695073843	-5.046843052	-1.569795489
H	2.802773476	-4.052229404	-0.081916369
C	-0.281147599	-7.083856583	-2.157806396
H	-0.008883690	-7.271136761	-1.119226217
H	-0.931648612	-7.891978741	-2.524180889

H 0.603752494 -7.058351517 -2.799419641

O -3.399564981 -5.158713818 -4.955530167

C -4.742422104 -5.510369301 -5.432611942

H -5.168622494 -6.248703957 -4.751368523

H -4.613127708 -5.966872215 -6.418124676

C -5.546134472 -4.226465225 -5.482535362

H -5.068317890 -3.491410494 -6.137391090

H -5.645016670 -3.802277088 -4.479491711

H -6.545695782 -4.434445381 -5.876229763

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6a

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O 1.446541190 1.116838217 0.097672433

C 1.365281820 1.983120561 -0.747387767

C 2.182805061 3.258931875 -0.687455297

C 0.412474602 1.862940192 -1.945795655

C -0.516556621 0.676731825 -1.795946360

H 2.933536291 3.177202702 0.099763386

H 2.663074255 3.468720675 -1.649347544

H 1.519140124 4.103950500 -0.467137784

H -0.183627084 2.775811434 -2.034368515

H 1.021822691 1.762455106 -2.851514816

O -1.651854992 0.738827407 -1.379649162

O 0.099987470 -0.460705429 -2.163275957

C -0.650407135 -1.678746462 -1.941636682

H -1.573746443 -1.638042450 -2.529274225

H -0.932404757 -1.726916671 -0.885129213

C 0.242231682 -2.834109306 -2.351114273

H 1.158214927 -2.842994213 -1.753605366

H 0.518761873 -2.756865740 -3.406768322

H -0.281341285 -3.783139944 -2.199216366

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6a'

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O -1.478828788 3.454176903 -2.080392361

C -0.189519063 3.200103760 -1.857712984

C 0.647611976 4.436124802 -1.751303911

C 0.309822291 1.933886886 -1.739376307

C -0.580981970 0.800171494 -1.857996464

H 0.273708254 5.065175533 -0.936339378

H 1.697232962 4.197665215 -1.571015835

H 0.561690629 5.019488335 -2.674293995

H 1.362199664 1.765297890 -1.559100270

O -1.802774668 0.889087498 -2.063914061

H -1.933807850 2.565976143 -2.131992817

O 0.033414524 -0.387960523 -1.723875999

C -0.805586517 -1.559812069 -1.829349756

H -1.302725196 -1.554742932 -2.805035353

H -1.586104155 -1.507808685 -1.062923074

C 0.094214022 -2.766987324 -1.650357723

H 0.583736837 -2.744469166 -0.672359824

H 0.868649304 -2.791549206 -2.422552109

H -0.496554792 -3.685423374 -1.721818209

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J

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C	-3.090728760	-5.095524788	1.304849505
C	-4.135151863	-4.261217594	1.994779944
C	-5.011981010	-3.454933643	1.007709146
C	-4.075761318	-2.705205679	0.033438820
C	-3.073460340	-3.619816065	-0.651450455
C	-2.491986990	-4.699688911	0.139302164
H	-3.617479563	-3.571585417	2.676278830
H	-4.751980782	-4.918324471	2.616104126
H	-3.500267506	-1.953133345	0.592787087
H	-4.641273975	-2.176696777	-0.739359379
C	-5.936100960	-4.407166004	0.222059056
H	-5.368464470	-5.153815746	-0.342096567
H	-6.609036922	-4.941020012	0.901431441
H	-6.550554752	-3.846361876	-0.490061849
C	-5.867977142	-2.447087288	1.789576769
H	-6.498466492	-1.863880157	1.109553814
H	-6.526373386	-2.961354017	2.498617887
H	-5.243528843	-1.746471524	2.355128050
O	-2.832598925	-6.238846779	1.942106724
O	-2.773622274	-3.466698647	-1.841444850
O	-0.027876906	-5.211076736	1.464128375
C	-0.137793347	-5.723289013	0.369875371
C	0.932908297	-6.614006996	-0.224817976
C	-1.372721314	-5.473817348	-0.518195570
C	-1.982679605	-6.770798206	-1.031297088
H	1.150881767	-6.331850529	-1.261088133
H	1.837297916	-6.554574966	0.381637841
H	0.563625038	-7.644844055	-0.238126218
H	-1.022915721	-4.869090557	-1.364469051
O	-2.028714895	-7.769962311	-0.298871994
N	-2.541842937	-6.663887501	-2.265410185
H	-2.521860600	-5.723477364	-2.650187016
C	-3.335391283	-7.600358009	-2.966320753
C	-3.944961786	-7.158326626	-4.149897575
C	-3.523252726	-8.921543121	-2.535065651
C	-4.735097885	-8.027118683	-4.896776676
C	-4.318357944	-9.778207779	-3.296093225
C	-4.926700592	-9.343930244	-4.474123478
H	-3.800547123	-6.132030487	-4.479255676
H	-3.056783676	-9.257851601	-1.620201111
H	-5.202068806	-7.671494007	-5.810602188
H	-4.461484909	-10.800271988	-2.957063437
H	-5.542978764	-10.022179604	-5.056318760
H	-2.314977407	-6.854349613	1.379514694

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C	-2.962555647	-4.999981880	1.474594951
C	-4.100564480	-4.181562424	2.051652670
C	-5.066087246	-3.660309076	0.955855787
C	-4.242182732	-2.910807371	-0.119647250
C	-3.082752228	-3.732204914	-0.664737284
C	-2.372729540	-4.554186344	0.268423736
H	-3.666639566	-3.327263832	2.589720488
H	-4.631415367	-4.796537399	2.784712553
H	-3.821674109	-1.994958997	0.319620758

H	-4.873510361	-2.608003855	-0.960828245
C	-5.813813210	-4.844325066	0.309072852
H	-5.126102924	-5.557837009	-0.156597927
H	-6.400366306	-5.387461662	1.057536960
H	-6.500540733	-4.490104198	-0.467469454
C	-6.087367058	-2.701278448	1.585599422
H	-6.778923035	-2.314857006	0.828324854
H	-6.680824280	-3.211746454	2.352470875
H	-5.591167450	-1.845577478	2.057071447
O	-2.598620653	-6.076107979	2.044481516
O	-2.792902231	-3.706277609	-1.885138988
O	0.276798964	-4.648079872	1.476360202
C	-0.034942269	-5.546629429	0.727407098
C	0.729764104	-6.851585865	0.648171365
C	-1.188917756	-5.332836151	-0.272884667
C	-1.914234638	-6.526329041	-0.787518620
H	0.968907833	-7.100955486	-0.392557591
H	1.644024134	-6.772309780	1.237068892
H	0.112209864	-7.665975094	1.040121794
H	-0.769157112	-4.769032478	-1.114042521
O	-2.262959957	-7.492286205	0.016932800
N	-2.348445177	-6.502076149	-2.046677589
H	-2.250794172	-5.561698914	-2.449506521
C	-3.387729168	-7.301784515	-2.605605125
C	-4.325676441	-6.649473190	-3.414669752
C	-3.467346430	-8.679327011	-2.386708260
C	-5.349902153	-7.385017872	-4.006347656
C	-4.502760410	-9.400742531	-2.980837345
C	-5.442779064	-8.762197495	-3.791914463
H	-4.258122444	-5.572947979	-3.546578407
H	-2.734860182	-9.172651291	-1.760445714
H	-6.080022335	-6.877761841	-4.629696846
H	-4.569523335	-10.470971107	-2.809958696
H	-6.242851734	-9.333262444	-4.252588272
H	-2.285419941	-7.102684975	0.937642813

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C	-3.464880943	-5.779279709	0.345669508
C	-4.807671070	-5.405566216	0.915162146
C	-5.140633106	-3.909251213	0.672664464
C	-3.936117887	-3.044208765	1.113841295
C	-2.584827662	-3.460780859	0.526983142
C	-2.443220377	-4.855618477	0.227175683
H	-4.787462234	-5.609466076	1.995205402
H	-5.572911263	-6.059067726	0.483192384
H	-3.832560539	-3.097768068	2.207667351
H	-4.095606327	-1.989879608	0.865540564
C	-5.440980434	-3.675218582	-0.822070539
H	-4.585124969	-3.939606905	-1.450991511
H	-6.296869755	-4.277060986	-1.146947026
H	-5.677684307	-2.622001648	-1.007238507
C	-6.379670143	-3.524405003	1.496578455
H	-6.637061119	-2.471017838	1.340319633
H	-7.247213840	-4.128555298	1.207268596
H	-6.206908226	-3.672874212	2.568432093
O	-3.244106054	-6.974798679	-0.092058584

O	-1.680014610	-2.632544994	0.360516816
O	-0.171071291	-6.983395100	1.269605637
C	-0.261046410	-5.841029644	0.821832657
C	0.531505883	-4.702820301	1.402976513
C	-1.198358297	-5.507616997	-0.341204673
C	-1.699136257	-6.761964321	-1.088124275
H	-0.044728432	-3.774719954	1.417208672
H	0.904893994	-4.977643490	2.390732050
H	1.389289379	-4.525585175	0.739060640
H	-0.683654070	-4.832366943	-1.036330462
O	-1.082428455	-7.926870823	-0.943644762
N	-2.132090092	-6.497085571	-2.357806206
H	-2.420234919	-5.536689758	-2.495368481
C	-2.739015818	-7.432682037	-3.240079403
C	-2.864129066	-7.056888580	-4.582751274
C	-3.227782488	-8.671524048	-2.810346365
C	-3.473437786	-7.915807724	-5.494865894
C	-3.821877718	-9.527699471	-3.736574411
C	-3.950039864	-9.159287453	-5.076959133
H	-2.474736691	-6.095285892	-4.907796860
H	-3.152638912	-8.949398041	-1.767541289
H	-3.567039490	-7.613906384	-6.534084320
H	-4.199208260	-10.489003181	-3.399635553
H	-4.418595314	-9.832939148	-5.787979126
H	-0.748099625	-7.930651188	-0.009418650

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C	-2.626277685	-5.734008312	0.640187562
C	-3.934484243	-5.018372059	0.729618967
C	-3.718980551	-3.488433123	0.889277279
C	-2.668121576	-3.237244129	1.999236584
C	-1.349295020	-4.000310421	1.840854049
C	-1.454719305	-5.272842407	1.165216088
H	-4.487161636	-5.410041809	1.595173359
H	-4.534319401	-5.244841576	-0.158200830
H	-3.086835861	-3.538640022	2.970709562
H	-2.427587986	-2.172470570	2.078495979
C	-3.232648134	-2.884901524	-0.444075316
H	-2.291536570	-3.334857225	-0.773128271
H	-3.973932505	-3.038860321	-1.235359788
H	-3.068796873	-1.807531118	-0.339514732
C	-5.049694061	-2.828234911	1.280472159
H	-4.925879478	-1.745733023	1.392286420
H	-5.812835217	-3.000499487	0.513126731
H	-5.428320408	-3.223675251	2.229456425
O	-2.543715239	-6.877618313	-0.024329605
O	-0.293539554	-3.550189495	2.290805101
O	-0.631280780	-8.086739540	2.468572855
C	-0.055524431	-7.042325497	2.185724735
C	0.957475185	-6.408905983	3.098673582
C	-0.366169959	-6.290691853	0.887414455
C	-1.025712132	-7.178585529	-0.218700379
H	0.790089846	-5.329588413	3.166151047
H	0.930685639	-6.889565468	4.077313423
H	1.952013373	-6.551161766	2.655069828
H	0.552550435	-5.829511166	0.510029316

O	-0.886626899	-8.525856972	-0.120940968
N	-0.638717532	-6.714382648	-1.494714975
H	-0.379382849	-5.737303257	-1.479334950
C	-1.287457585	-7.077732563	-2.697743654
C	-1.045943975	-6.282328606	-3.828365326
C	-2.140232563	-8.185135841	-2.808834791
C	-1.647451401	-6.584002018	-5.047149658
C	-2.736916304	-8.474185944	-4.035186291
C	-2.500594378	-7.682801247	-5.159963608
H	-0.379252344	-5.426054001	-3.749063015
H	-2.333719730	-8.805602074	-1.944748640
H	-1.447683454	-5.954584122	-5.909924984
H	-3.400972843	-9.331370354	-4.105607986
H	-2.971531153	-7.919128895	-6.109161377
H	-1.018380404	-8.740064621	0.827378154

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C	-2.882754326	-5.455306053	0.018168006
C	-4.319946289	-5.261558056	0.356771886
C	-4.492186546	-4.122461319	1.397800803
C	-3.447293282	-4.307667732	2.527246952
C	-1.995311379	-4.413927555	2.049342871
C	-1.820030212	-5.103248596	0.785774648
H	-4.710441113	-6.207863331	0.758094847
H	-4.889369011	-5.053211689	-0.556350350
H	-3.670423746	-5.232864857	3.078659773
H	-3.500486374	-3.486264944	3.248036623
C	-4.288266659	-2.755404472	0.713814855
H	-3.300607920	-2.677428246	0.249396399
H	-5.041381836	-2.594789267	-0.065572701
H	-4.380094528	-1.944306016	1.443464756
C	-5.908390999	-4.185057163	1.989885807
H	-6.060595989	-3.379978418	2.716794968
H	-6.665799141	-4.075359821	1.205343604
H	-6.086127281	-5.138111591	2.500577927
O	-2.560387135	-6.020921230	-1.167503238
O	-1.064007521	-3.967281103	2.716518879
O	1.700959086	-5.851096153	-0.278077573
C	0.751843870	-5.880290508	0.494482130
C	0.811922371	-6.459072590	1.873180270
C	-0.572804153	-5.331000805	-0.031864841
C	-1.120694399	-6.364645481	-1.051367640
H	0.055045228	-7.249267578	1.937770009
H	1.805259228	-6.862569809	2.073136806
H	0.541370273	-5.683813572	2.597885370
H	-0.317314804	-4.396493435	-0.542607665
O	-0.935017467	-7.616218567	-0.728877366
N	-0.548622310	-6.143493652	-2.477026701
H	0.428932905	-6.424147606	-2.360225439
C	-0.638816833	-4.827046394	-3.082913160
C	0.431961060	-3.939771175	-2.970731735
C	-1.809659600	-4.480155945	-3.754951000
C	0.323659569	-2.674580336	-3.548604727
C	-1.904924512	-3.211531401	-4.325501442
C	-0.842791498	-2.309681892	-4.223698616
H	1.319749117	-4.236393929	-2.418245077

H	-2.614843607	-5.202164650	-3.830012321
H	1.150073886	-1.975285769	-3.466876030
H	-2.809827328	-2.928741932	-4.854763985
H	-0.924159884	-1.323558450	-4.671116352
H	-1.635767221	-8.369387627	-1.391875505
O	-1.958106399	-7.796587944	-3.831439257
C	-2.505601168	-8.771890640	-3.249270201
H	-1.091159940	-6.904991150	-3.088159084
O	-2.337607861	-9.097630501	-2.023745537
C	-3.465815783	-9.625885010	-4.048263550
H	-3.044268370	-9.828196526	-5.035592556
H	-3.691480637	-10.555592537	-3.525686026
H	-4.393206120	-9.062275887	-4.196316242

Table S3. Vibrational Frequencies (in cm^{-1}) of the Optimized Geometries

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73.24 87.74 121.67 129.38 221.80 238.92

262.20 299.78 304.47 344.59 360.49 405.91

423.83 449.08 483.24 524.14 574.72 594.91

640.25 645.37 716.06 820.48 903.20 930.53

952.46 964.70 991.65 1041.67 1057.26 1135.59

1151.26 1162.36 1204.46 1278.72 1297.01 1310.02

1315.30 1344.85 1363.50 1424.39 1444.51 1461.47

1475.84 1501.40 1509.24 1522.41 1528.35 1754.95

1779.45 2273.80 3025.91 3028.10 3035.63 3044.11

3106.13 3106.59 3110.17 3111.13 3116.32 3118.59

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2a

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30.48 46.29 73.06 83.37 119.40 166.53

216.93 260.90 297.06 352.45 389.56 419.02

471.36 518.70 535.52 576.79 610.06 631.67

705.14 722.56 757.51 773.63 830.00 850.66

859.94 914.56 918.46 956.52 971.73 1000.64

1002.42 1013.58 1044.78 1060.75 1122.27 1180.86

1195.90 1204.44 1216.43 1242.26 1290.32 1345.17

1356.58 1369.55 1401.39 1456.98 1473.32 1485.89

1488.86 1542.71 1603.68 1657.00 1664.07 1782.86

1797.11 3039.01 3042.96 3105.34 3139.13 3168.28

3170.12 3181.35 3191.63 3206.54 3265.63 3493.92

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2a'

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40.87 48.09 104.96 124.44 149.88 189.51

247.85 264.23 272.60 387.93 410.70 417.58

509.51 519.36 545.33 573.18 608.66 631.47

704.51 739.32 767.89 770.39 798.73 843.22

845.82 912.29 945.86 967.36 968.65 999.66

1011.15 1015.38 1051.04 1064.22 1066.74 1124.44

1195.88 1199.65 1217.59 1261.91 1279.07 1353.32

1368.84 1414.74 1433.71 1461.57 1481.45 1489.53

1504.71 1540.88 1580.58 1650.45 1661.63 1681.92

1708.98 3051.01 3113.18 3128.95 3152.87 3160.21

3182.24 3191.75 3207.92 3210.98 3269.81 3627.83

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3a

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63.22 76.46 104.33 120.12 137.05 191.50

199.68 211.75 247.35 260.97 289.77 304.60

316.84 358.55 365.40 379.27 404.23 414.57

466.13 494.03 534.29 576.44 581.74 620.03

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1003.17 1013.25 1041.26 1049.96 1060.49 1069.51

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1423.82 1444.72 1462.59 1471.81 1480.90 1489.16

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3024.45 3036.03 3046.14 3053.70 3084.25 3105.11

3108.49 3109.62 3111.95 3117.97 3125.04 3198.10

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Nitrogen

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2460.69

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Aniline

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224.60 287.18 392.50 417.91 509.21 537.41

634.27 637.69 704.18 763.86 827.98 835.07

881.21 955.60 980.06 1009.12 1057.01 1079.12

1147.12 1193.31 1214.65 1313.64 1368.08 1371.58

1513.44 1546.28 1643.71 1662.07 1680.45 3165.68

3167.43 3182.70 3187.97 3206.36 3558.24 3659.59

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Acetate

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32.25 424.64 585.72 624.93 857.50 987.37

1020.75 1317.48 1370.62 1479.53 1493.58 1753.53

2993.83 3057.86 3083.10

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AceticAcid

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89.28 422.60 540.89 583.72 677.16 866.87

1003.16 1070.03 1218.21 1354.72 1422.11 1482.55

1488.55 1857.63 3065.97 3132.84 3184.83 3756.23

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A

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13.50 25.18 36.53 41.11 49.40 64.73

69.94 84.65 95.19 103.79 106.06 118.16

125.60 126.61 141.97 162.33 171.32 183.35

213.59 228.13 239.45 242.43 244.20 248.17

266.52 273.71 288.36 301.81 303.40 316.16

321.15 350.72 360.28 366.25 388.51 400.54

410.26 412.03 429.81 440.33 449.96 453.14

494.07 498.03 522.62 530.09 563.64 573.77

599.19 613.80 638.61 641.74 647.97 663.68

693.41 694.63 719.05 811.61 817.48 882.23

897.59 899.92 911.66 927.44 948.95 952.09

955.27 966.61 967.11 969.37 978.05 992.13

1009.93 1020.08 1022.06 1043.15 1056.07 1056.55

1068.98 1079.18 1110.37 1133.99 1139.55 1151.45

1158.85 1179.44 1201.52 1205.59 1225.65 1241.15

1243.90 1285.52 1309.67 1310.16 1321.92 1337.26

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1457.38 1471.45 1477.93 1483.29 1495.63 1497.09

1500.20 1503.42 1507.67 1509.15 1515.79 1519.28

1523.55 1526.21 1527.39 1539.83 1557.77 1579.26

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3041.89 3046.00 3047.88 3055.46 3057.87 3062.14

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3126.12 3127.05 3128.72 3133.46 3137.35 3150.30

3153.42 3177.85 3211.91 3219.11 3225.19 3242.33

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A-TS

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252.82 262.94 272.09 285.52 290.13 290.98

297.15 317.99 332.60 341.44 355.72 361.19

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447.84 466.56 506.42 519.51 528.69 563.05

585.59 613.74 618.43 632.64 635.33 647.71

678.34 697.60 706.05 794.12 808.28 880.82

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952.51 966.78 967.13 969.26 974.57 980.27

984.26 1003.59 1019.23 1023.29 1029.07 1047.08

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1426.42 1429.36 1434.49 1442.18 1450.68 1453.79

1467.71 1471.48 1481.31 1490.47 1495.05 1500.64

1505.18 1509.63 1509.79 1515.54 1520.26 1521.33

1523.63 1524.60 1527.14 1538.56 1544.49 1583.73

1767.55 1807.48 2424.00 3040.99 3041.63 3042.22

3046.31 3048.18 3053.99 3054.13 3061.00 3062.16

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3126.32 3130.25 3133.90 3134.82 3141.35 3145.64

3156.94 3176.84 3208.80 3212.39 3224.16 3246.17

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B

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32.99 39.00 43.32 47.00 57.46 71.60

76.98 92.31 98.97 109.75 120.99 138.57

142.78 147.30 164.63 169.89 195.29 205.39

222.85 235.26 242.89 258.40 261.72 270.58

276.16 293.87 296.72 319.57 341.62 347.05

359.27 361.52 372.57 398.74 404.41 406.10

429.68 449.79 472.33 512.17 527.61 537.39

555.73 575.91 613.79 634.69 640.30 655.86

678.61 692.62 695.38 704.21 800.61 807.48

866.52 867.12 897.91 912.77 916.77 924.77

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988.03 999.25 1006.06 1008.79 1018.14 1018.99

1046.23 1054.90 1063.44 1068.75 1078.72 1103.09

1110.79 1141.12 1180.86 1194.04 1205.37 1216.79

1226.13 1230.18 1240.55 1248.98 1285.53 1304.13

1319.75 1329.16 1334.70 1352.49 1396.87 1410.98

1422.82 1426.05 1429.07 1433.56 1448.06 1449.74

1450.83 1467.81 1473.21 1479.74 1480.48 1494.37

1495.81 1496.49 1501.55 1503.02 1506.62 1509.22

1518.87 1521.45 1523.24 1524.62 1539.10 1555.66

1601.35 1738.21 1780.37 3030.66 3034.10 3043.48

3043.92 3048.09 3051.55 3054.52 3063.54 3071.81

3115.53 3117.32 3117.41 3119.84 3123.14 3123.89

3125.06 3126.06 3133.76 3133.94 3136.49 3157.67

3160.90 3179.45 3212.48 3233.60 3238.78 3256.41

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B-TS

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-130.58 28.12 35.47 40.86 42.45 54.45

55.70 61.20 71.34 78.78 85.36 87.22

92.61 96.49 111.74 113.21 119.15 126.48

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188.05 189.28 198.14 204.03 211.98 224.26

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330.45 342.70 348.86 373.92 376.21 384.19

387.68 401.76 405.71 417.90 421.82 424.81

447.65 455.25 469.63 517.75 522.74 524.66

525.50 534.83 538.78 560.88 588.02 591.06

595.06 602.50 606.40 629.70 638.85 660.98

676.00 677.50 699.29 700.68 711.63 748.53

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858.30 865.93 881.07 891.05 900.58 909.15

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973.10 978.04 980.82 982.50 987.15 1004.49

1005.16 1008.80 1013.65 1014.64 1018.23 1020.21

1023.53 1026.45 1046.79 1047.94 1055.74 1062.06

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1209.66 1211.11 1217.22 1220.41 1226.91 1241.69

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1662.74 1690.08 1716.31 1760.89 2826.96 3006.56

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3131.79 3135.53 3147.09 3147.16 3157.97 3163.72

3168.88 3176.75 3193.09 3201.41 3213.31 3215.69

3222.33 3230.89 3232.62 3256.14 3263.27 3522.36

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C

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7.08 30.84 39.61 42.65 47.32 54.38

63.34 75.47 86.85 96.43 102.19 104.39

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140.55 159.40 173.04 175.42 182.93 186.37

203.48 207.07 212.37 219.64 222.79 233.29

258.74 263.31 271.31 274.95 283.13 290.20

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398.88 406.79 412.79 418.22 424.20 447.89

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1010.43 1015.71 1016.77 1021.74 1024.23 1025.34

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1078.94 1083.60 1106.99 1128.28 1140.05 1152.94

1177.62 1182.40 1191.49 1201.14 1203.99 1209.17

1221.34 1224.68 1235.63 1239.15 1259.21 1286.86

1304.06 1309.28 1311.00 1318.66 1327.18 1331.52

1337.62 1360.67 1362.12 1369.52 1374.30 1376.43

1392.57 1408.78 1409.70 1423.37 1425.41 1425.86

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C-TS

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541.54 544.22 546.00 567.17 596.24 610.13

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673.62 696.52 701.32 704.07 761.07 779.73

798.60 805.88 835.74 845.72 849.90 865.51

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3163.57 3169.66 3170.62 3185.19 3197.01 3204.74

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M

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14.08 30.14 35.04 49.00 55.15 56.29

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3126.56 3131.38 3139.94 3144.11 3149.44 3156.81

3161.45 3176.79 3187.70 3190.50 3197.06 3202.91

3206.69 3217.11 3217.90 3240.25 3250.13 3278.13

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M-TS

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189.49 202.58 206.84 217.02 219.00 231.89

242.66 246.40 253.99 262.28 275.32 283.33

287.33 304.98 310.29 310.89 322.43 341.10

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405.35 413.30 415.85 422.29 426.98 429.68

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931.96 937.41 945.12 947.34 955.07 957.56

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1012.08 1016.12 1017.53 1020.76 1022.37 1028.91

1045.40 1059.01 1061.81 1065.93 1075.97 1076.72

1086.81 1091.20 1115.17 1131.47 1138.10 1153.40

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3222.20 3222.93 3233.22 3259.26 3259.52 3315.77

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D

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54.83 57.78 59.40 66.15 82.14 90.31

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290.61 309.03 313.72 319.21 325.78 331.83

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545.11 566.02 573.06 607.15 614.11 622.95

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940.83 942.33 950.42 952.07 960.29 964.74

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E

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E-TS

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534.43 542.00 558.29 563.98 602.62 607.51

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F

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F-TS

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G

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H

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H-TS

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B-TS'

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C'

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D'

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3039.04 3042.30 3044.90 3045.33 3045.48 3051.07

3051.44 3055.48 3060.31 3090.63 3105.73 3108.99

3110.17 3112.00 3115.30 3116.52 3120.71 3121.87

3122.02 3123.62 3127.83 3133.09 3143.76 3162.24

3176.26 3176.77 3185.74 3197.47 3206.81 3210.06

3218.27 3224.42 3240.32 3256.42 3268.60 3366.06

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E'

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15.00 18.06 31.60 35.14 35.95 44.80

48.43 51.05 56.67 59.32 69.49 86.00

86.87 91.57 101.75 106.20 116.05 130.82

144.03 148.71 154.03 163.50 167.74 176.29

184.02 193.63 220.51 232.84 238.77 248.58

252.18 259.18 265.14 267.01 277.52 281.28

301.42 308.65 312.14 324.19 330.96 339.54

355.80 360.40 370.69 374.97 394.34 396.88

407.14 410.19 421.22 426.59 443.23 453.83

471.08 478.18 488.51 499.64 504.63 518.23

525.19 547.92 559.44 588.81 597.56 604.89

614.27 626.40 638.50 640.40 650.75 655.23

659.82 689.53 695.80 703.11 704.70 714.82

775.49 804.01 809.58 811.62 821.48 845.82

853.42 886.72 896.67 901.20 904.34 911.71

915.70 918.25 920.35 948.89 951.28 954.35

964.76 964.90 968.08 976.32 981.73 995.88

1004.89 1011.97 1012.46 1014.32 1019.76 1022.49

1047.10 1049.65 1057.59 1060.77 1069.16 1088.02

1098.68 1111.63 1120.15 1137.60 1148.23 1151.70

1164.33 1172.95 1179.95 1190.31 1199.53 1201.54

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1406.84 1407.88 1412.94 1426.80 1427.83 1432.59

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3169.17 3174.07 3174.31 3175.89 3188.28 3206.48

3210.13 3210.99 3221.51 3226.39 3245.58 3490.37

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B-TS"

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134.17 143.87 151.08 157.00 170.68 177.43

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1326.80 1334.29 1347.37 1361.71 1364.90 1371.44

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3214.81 3222.97 3227.79 3244.50 3264.63 3277.53

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95.48 101.34 109.11 116.93 123.44 136.35

150.92 157.25 164.92 178.39 181.08 192.53

219.77 225.17 232.42 240.13 245.06 256.53

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410.20 419.76 426.64 427.72 435.79 444.90

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617.94 628.95 635.58 640.97 652.23 662.02

675.86 687.24 696.51 702.41 709.47 728.31

771.28 782.47 812.65 818.88 828.36 852.28

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1474.13 1475.45 1480.07 1480.71 1482.86 1495.91

1496.67 1502.19 1506.00 1507.27 1507.80 1511.25

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1528.74 1540.65 1564.65 1566.90 1577.13 1598.81

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3169.34 3177.51 3192.90 3200.54 3204.26 3215.39

3223.05 3231.54 3248.49 3257.40 3611.86 3794.88

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163.06 176.31 179.31 182.49 194.38 195.39

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445.87 454.43 471.29 485.74 489.57 511.38

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585.97 589.76 604.29 615.05 621.70 627.55

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3220.13 3225.67 3252.55 3253.98 3638.11 3743.93

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19.68 22.28 25.81 37.21 41.33 50.21

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96.00 100.94 115.28 115.99 120.41 130.96

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3222.52 3230.50 3248.19 3255.33 3598.06 3767.35

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385.58 403.32 407.50 426.42 446.80 453.06

465.73 508.82 515.30 524.01 529.17 539.67

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3135.49 3137.31 3140.47 3143.68 3147.61 3153.37

3165.17 3167.01 3173.28 3189.46 3210.59 3228.94

3235.08 3250.14 3254.03

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79.11 85.15 89.32 94.00 99.91 102.47

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1209.83 1222.60 1240.56 1256.65 1274.75 1282.32

1294.99 1305.70 1309.74 1319.11 1323.41 1334.78

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556.96 560.17 575.94 619.52 625.25 641.82

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1129.48 1138.31 1173.34 1177.07 1182.02 1193.22

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1821.00 1831.92 3039.88 3040.95 3049.57 3051.01

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3170.18 3172.35 3175.48 3177.23 3197.80 3212.95

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62.21 69.62 79.47 83.70 88.58 93.60

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291.87 297.10 300.34 307.70 318.52 331.99

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413.16 424.59 429.78 435.01 448.78 450.34

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746.31 804.50 808.80 825.01 837.89 843.85

867.80 878.47 899.42 903.19 911.11 926.03

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963.94 969.63 977.26 981.33 1005.31 1011.27

1018.97 1021.39 1026.22 1033.56 1046.02 1051.26

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893.52 916.31 919.93 935.47 951.00 963.98

973.46 975.71 995.48 1001.47 1003.68 1014.27

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K

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K-TS

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98.68 120.40 138.11 142.07 155.14 194.38

235.96 246.50 251.57 262.93 279.89 297.22

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417.43 423.72 437.45 469.06 488.42 506.01

514.93 552.93 569.73 593.60 598.05 617.91

629.22 637.36 641.38 652.42 703.94 759.38

777.62 801.40 817.76 832.68 845.29 848.24

895.95 913.21 917.55 924.96 941.68 951.47

961.26 970.07 991.40 994.88 1002.18 1016.70

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L

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313.55 331.76 341.15 361.64 391.39 418.10

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1667.46 1731.32 1777.91 3022.45 3028.37 3034.93

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L-TS

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303.68 314.38 331.96 365.07 388.35 393.44

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3184.78 3190.90 3201.29 3211.68 3227.49 3464.85

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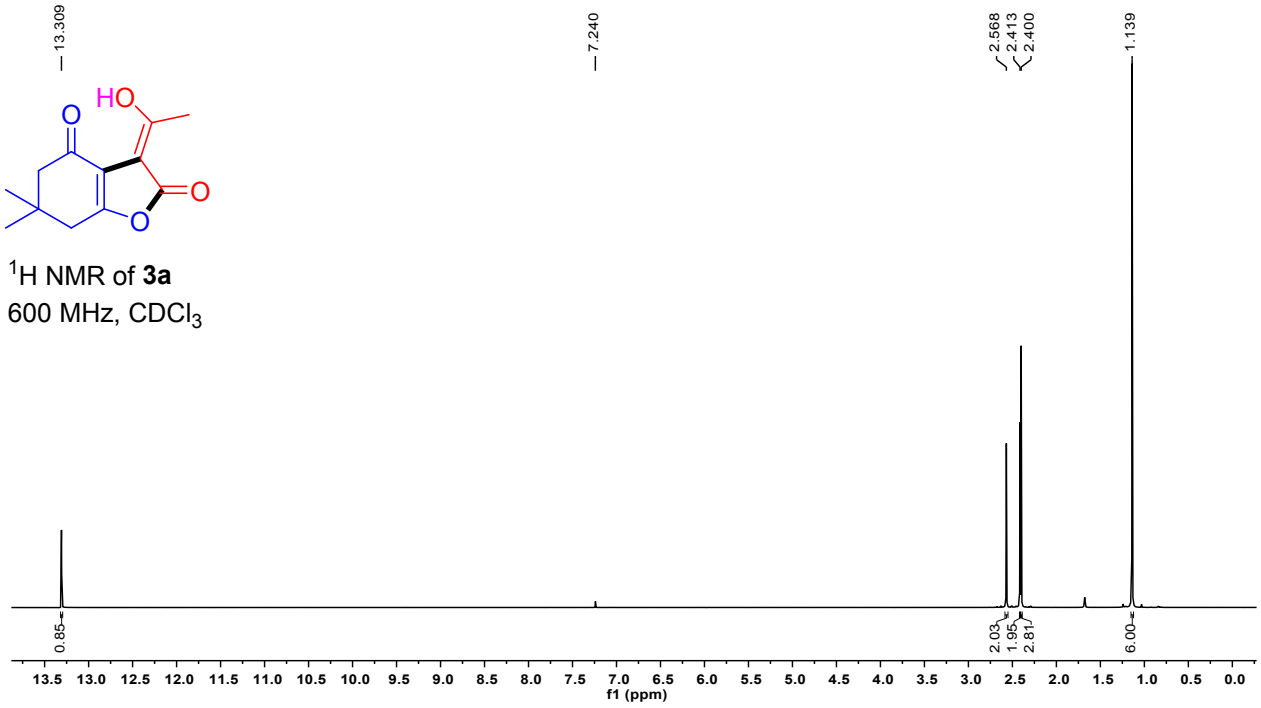
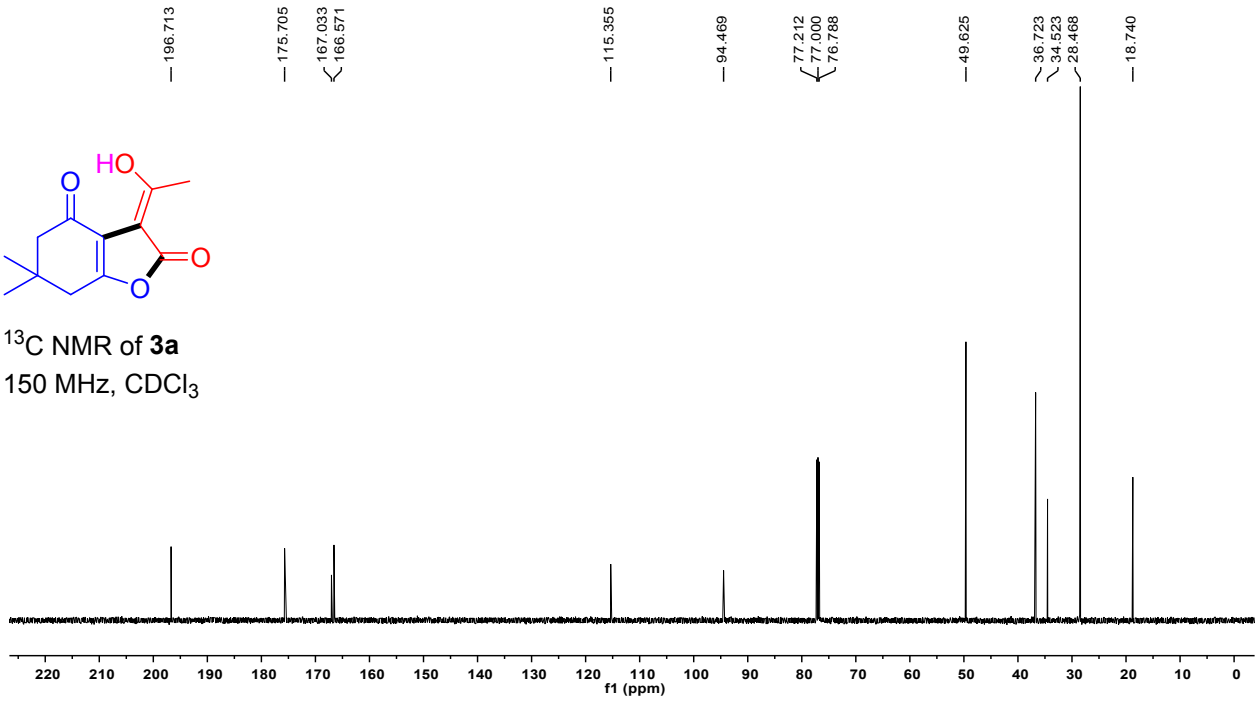
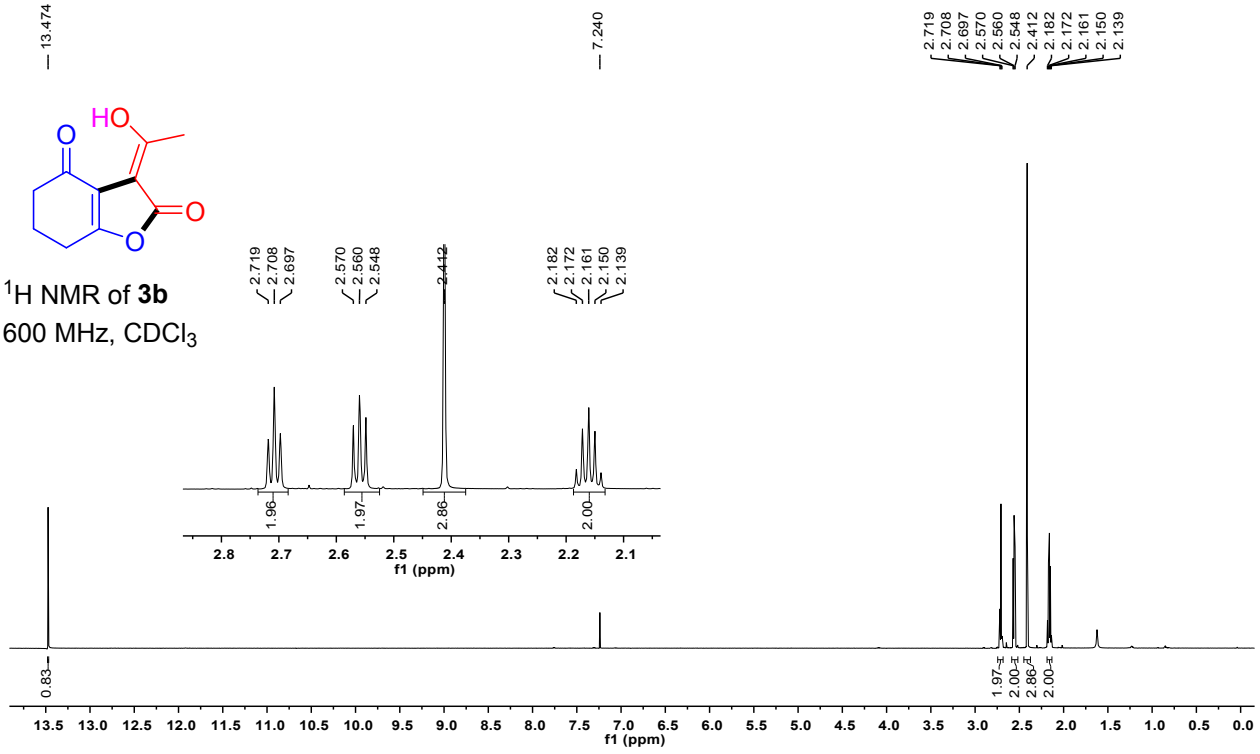
^{1}H NMR and ^{13}C NMR spectra of synthesized compounds



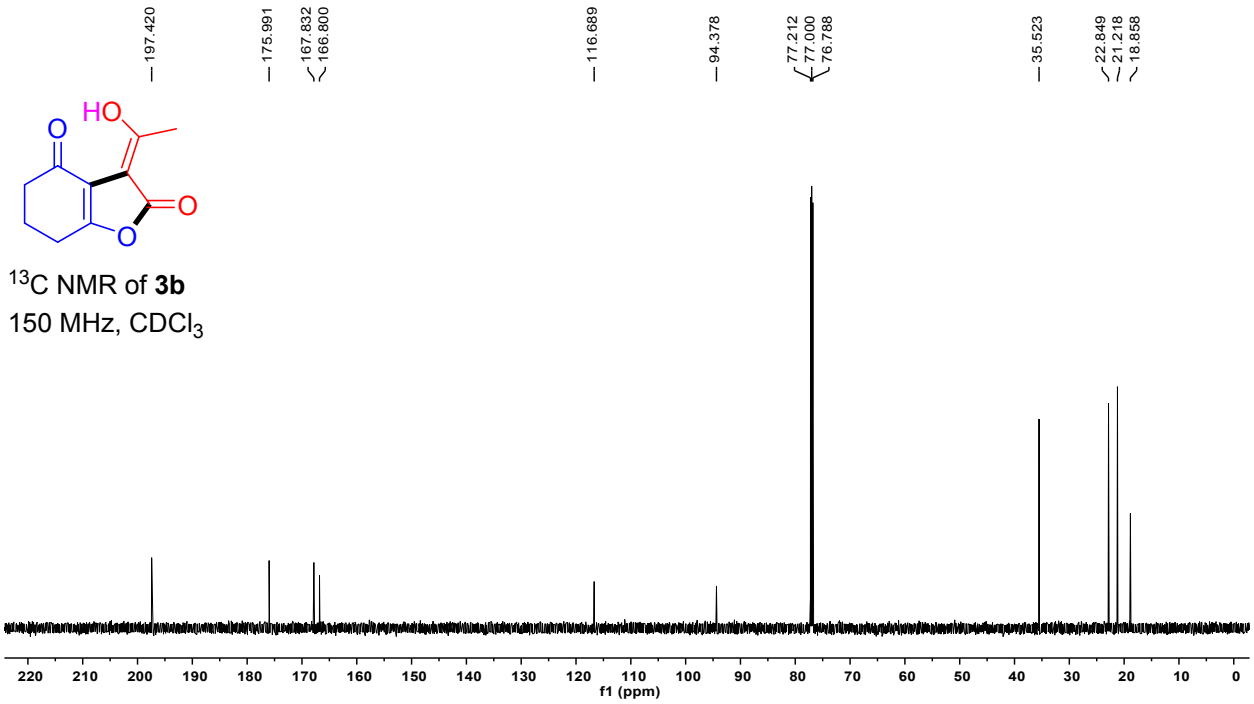
^{1}H NMR of **3a**
600 MHz, $CDCl_3$



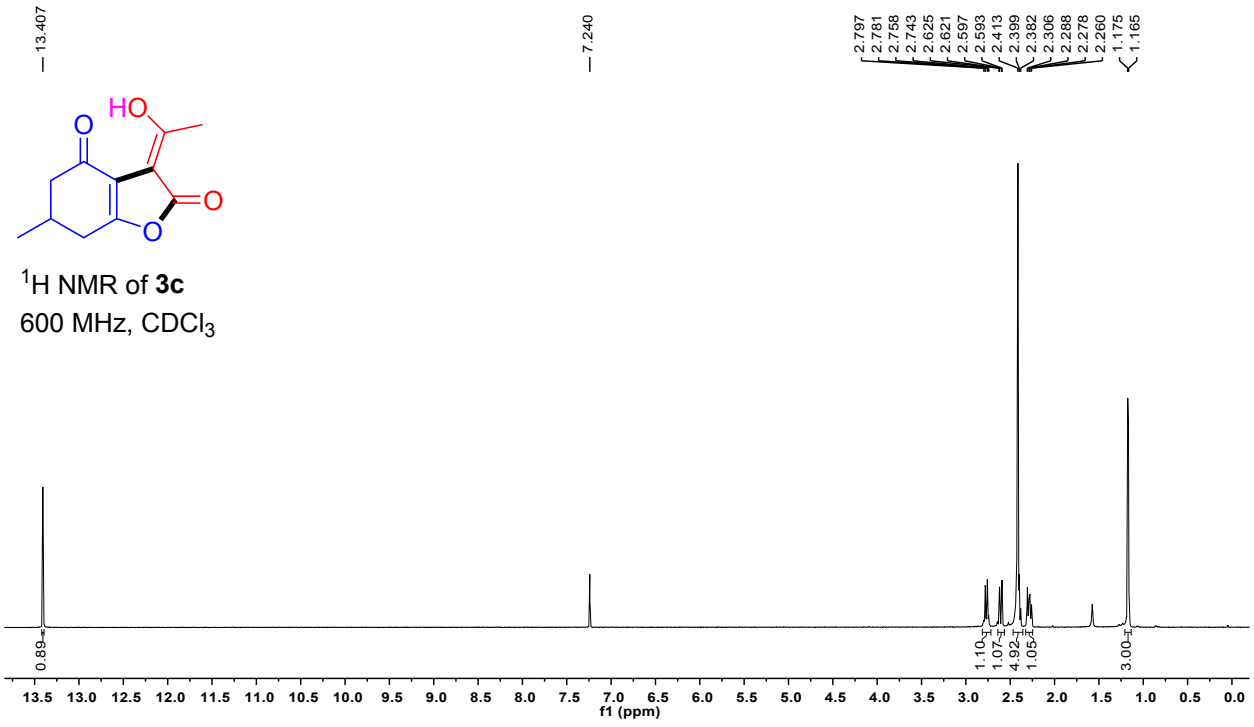
^{13}C NMR of **3a**
150 MHz, $CDCl_3$



^{1}H NMR of **3b**
600 MHz, $CDCl_3$



^{13}C NMR of **3b**
150 MHz, $CDCl_3$



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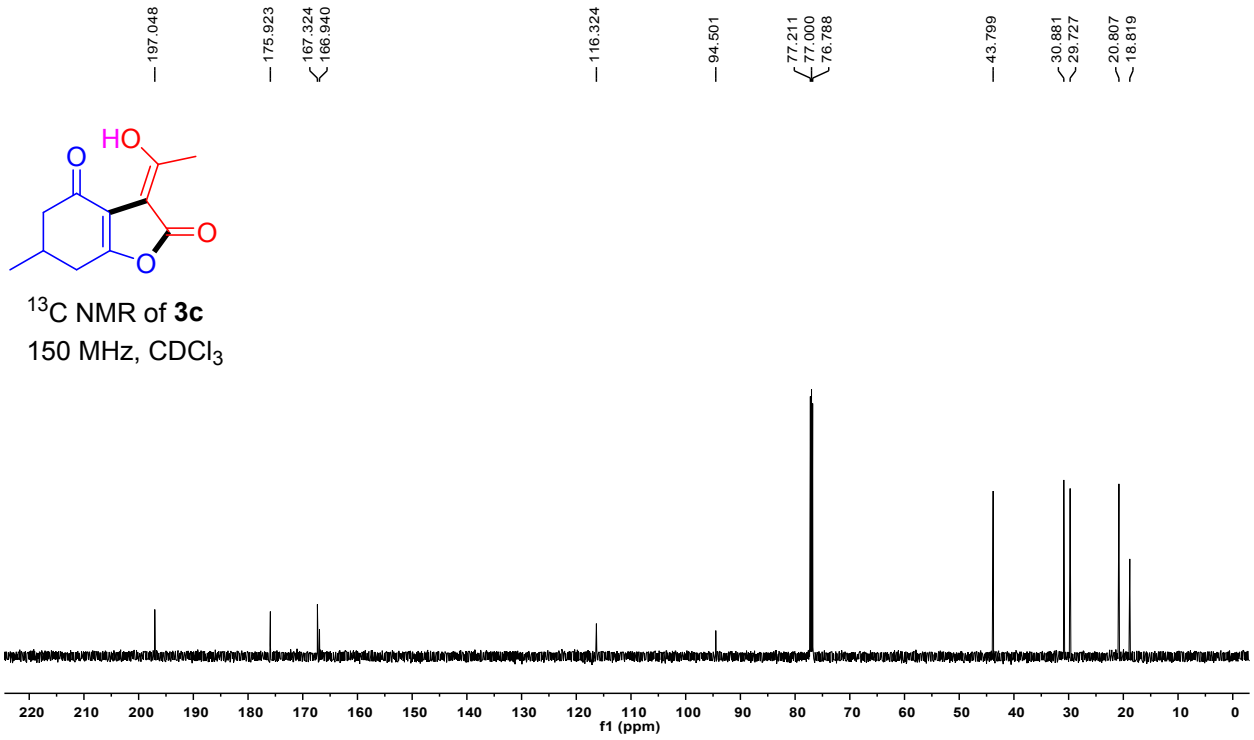

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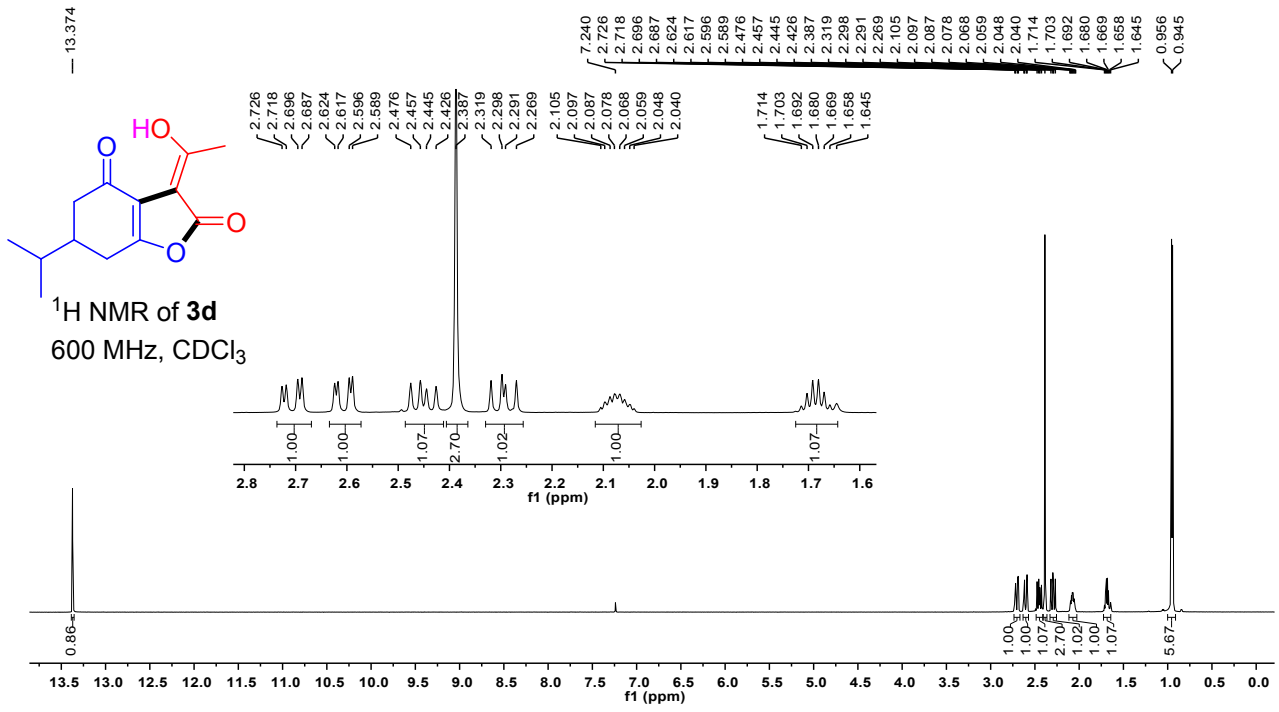

^{1}H NMR of **3d**
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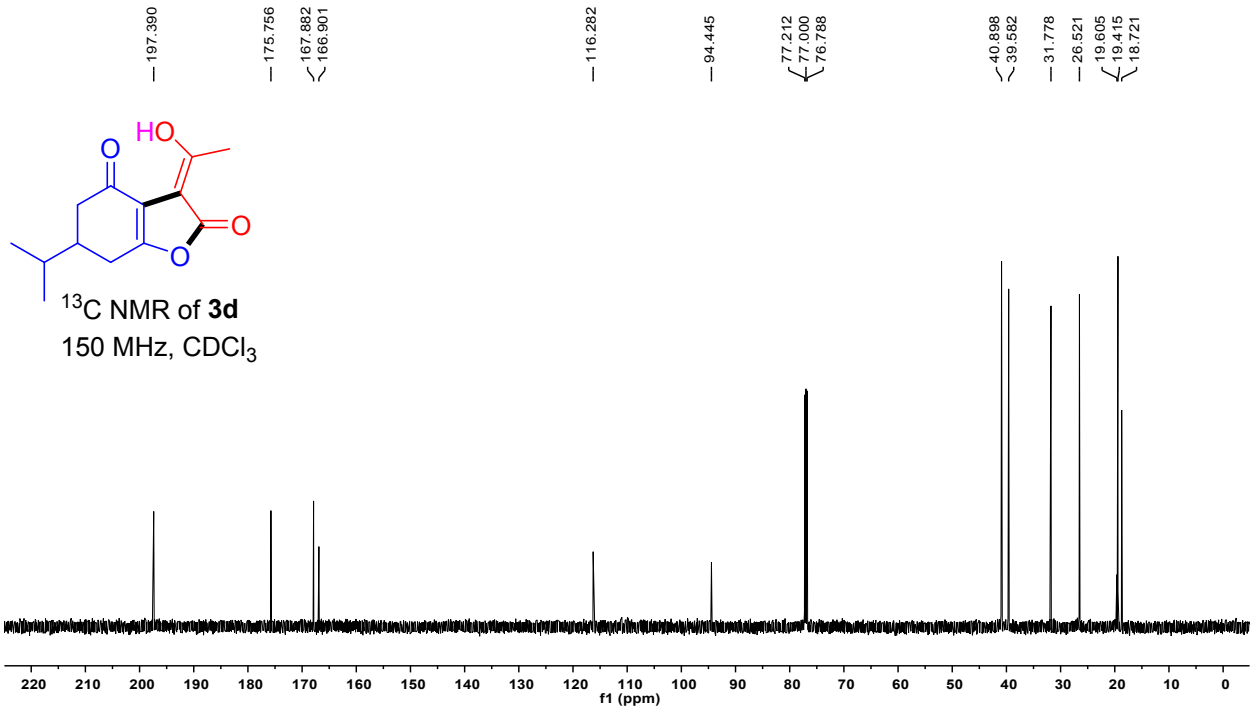
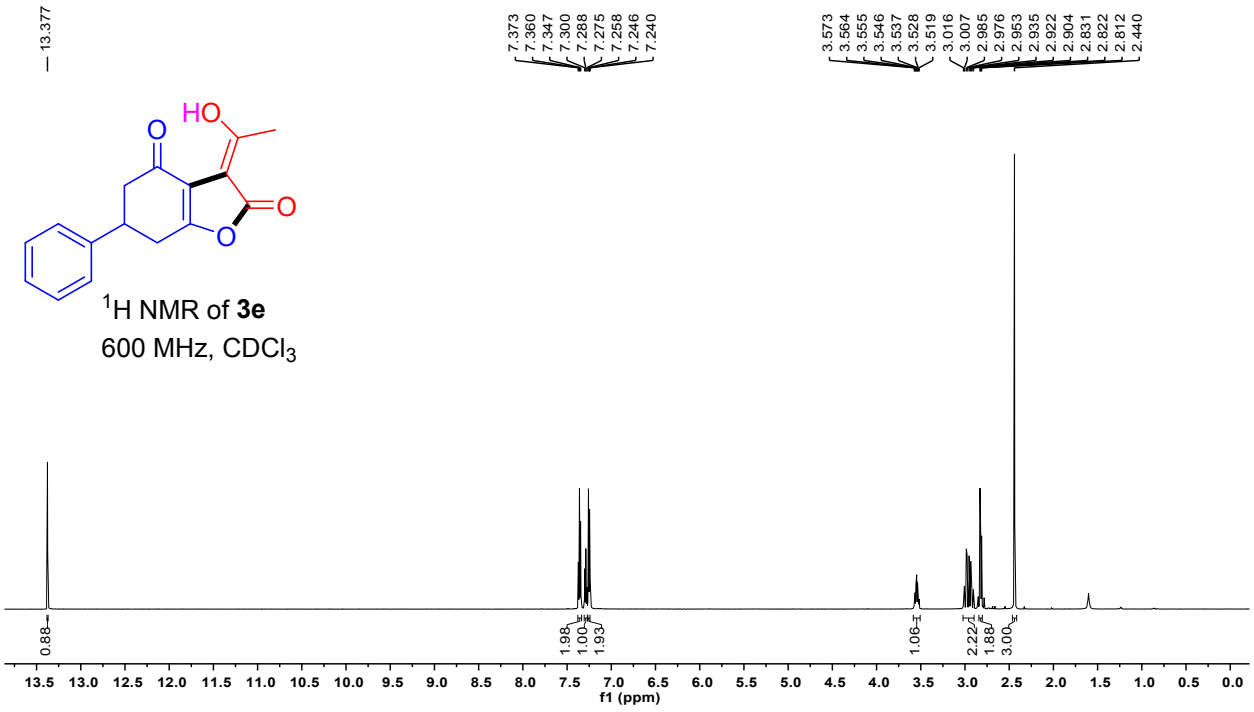
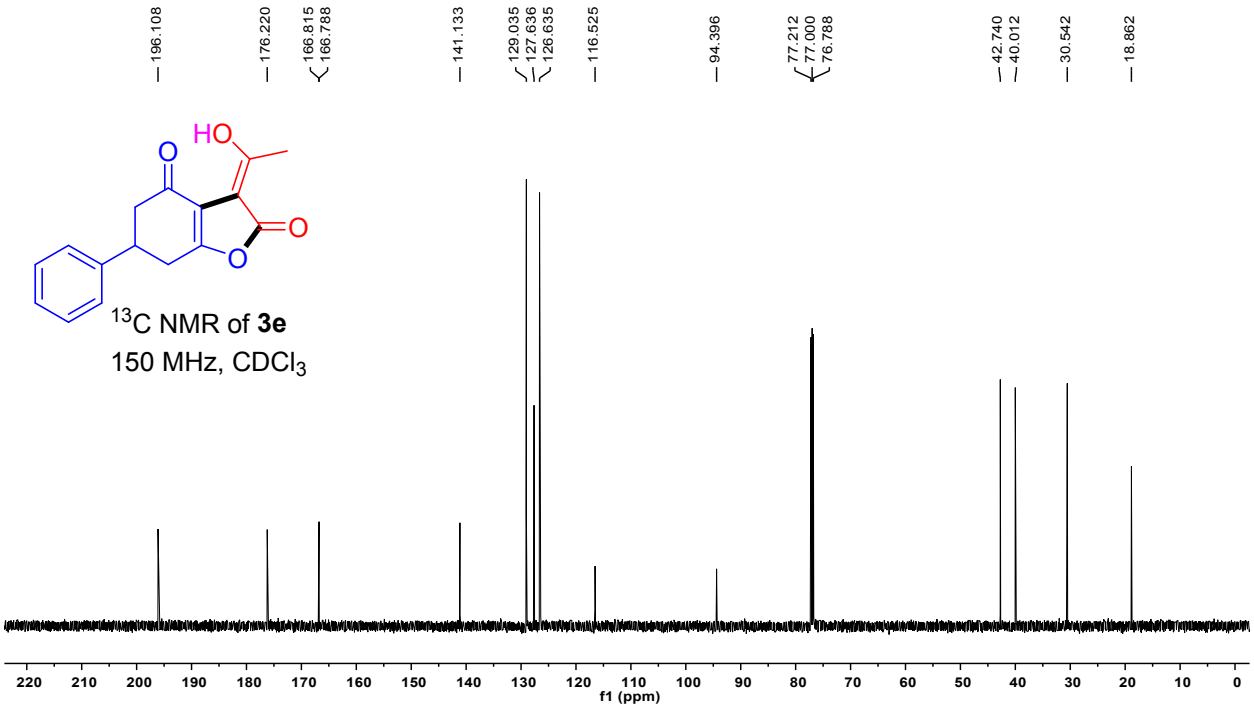
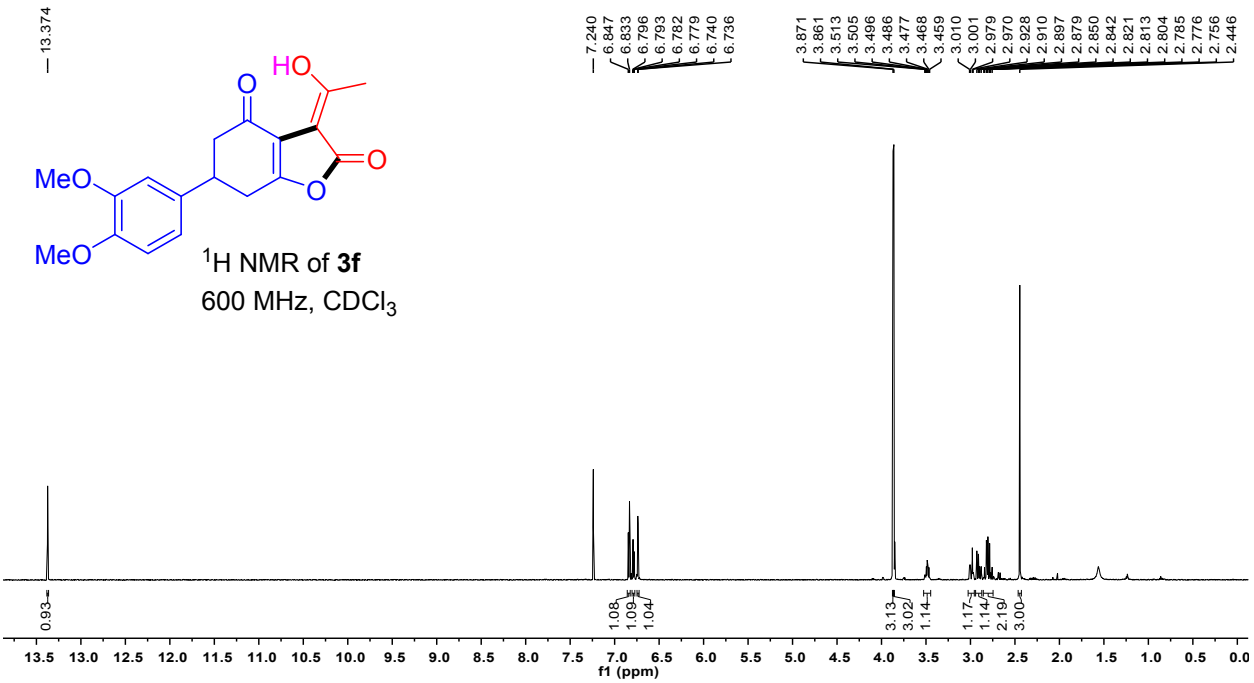


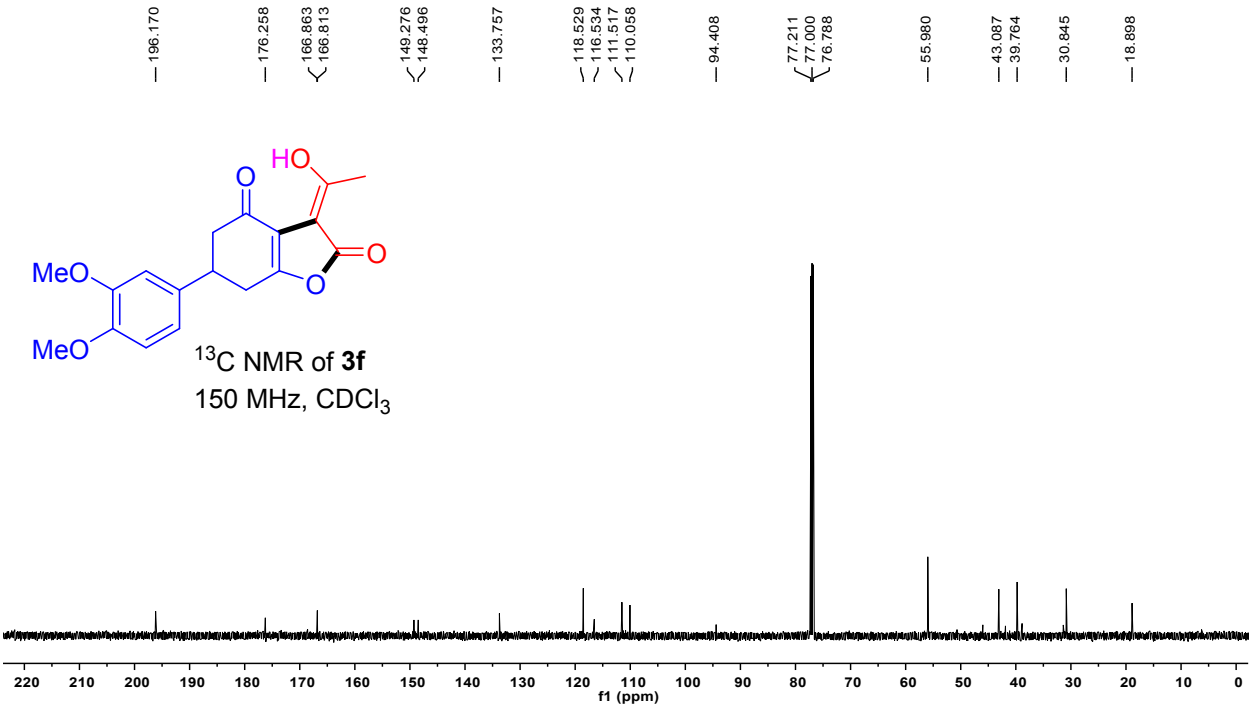
^{13}C NMR of **3d**
150 MHz, $CDCl_3$

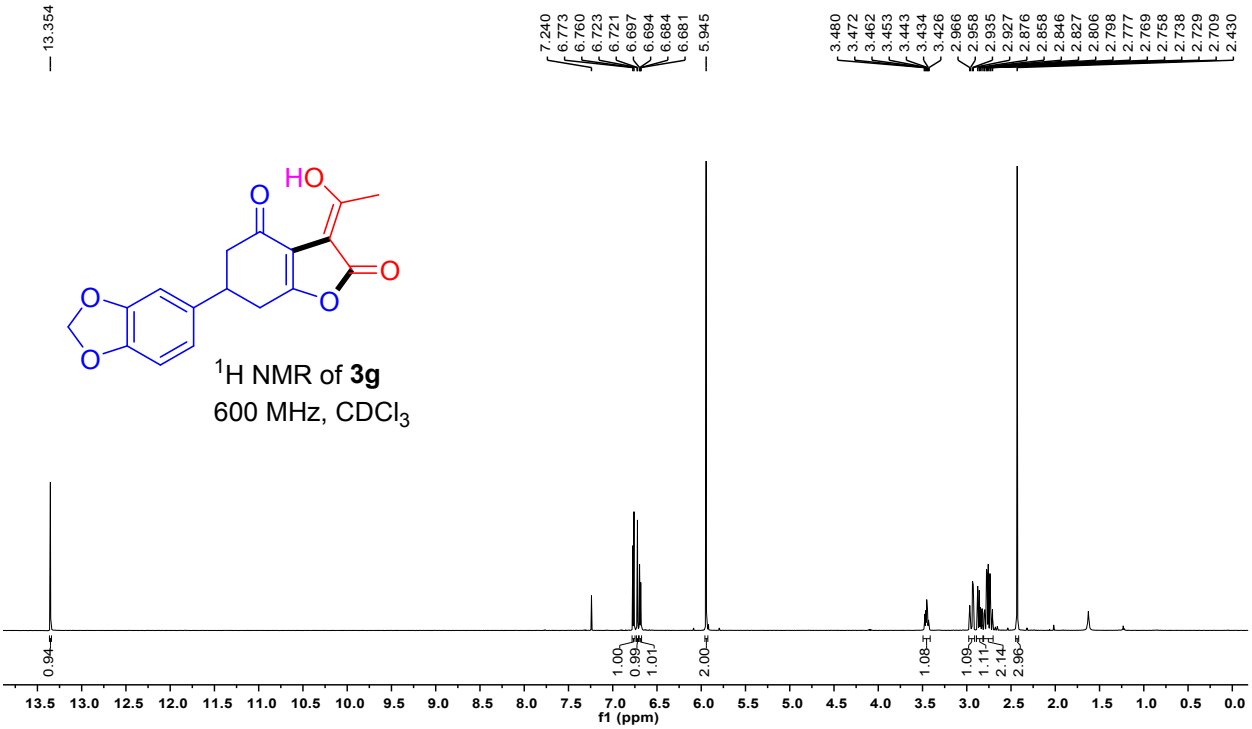


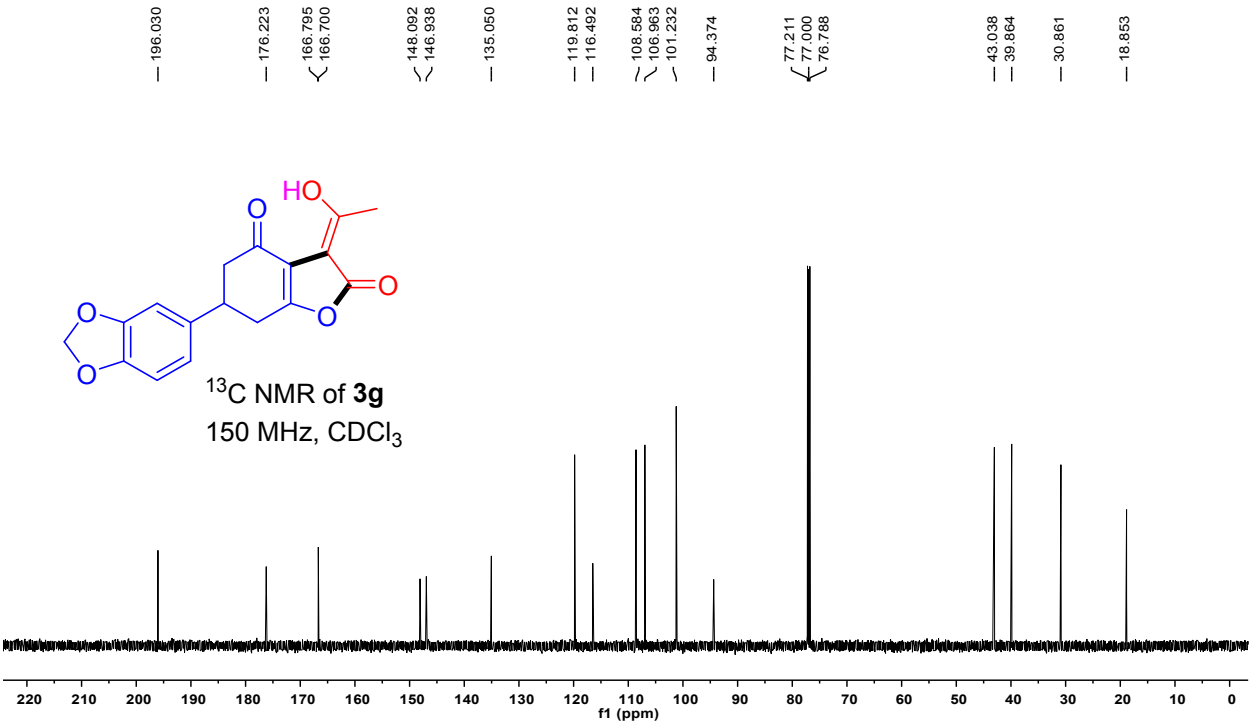
^{1}H NMR of **3e**
600 MHz, $CDCl_3$

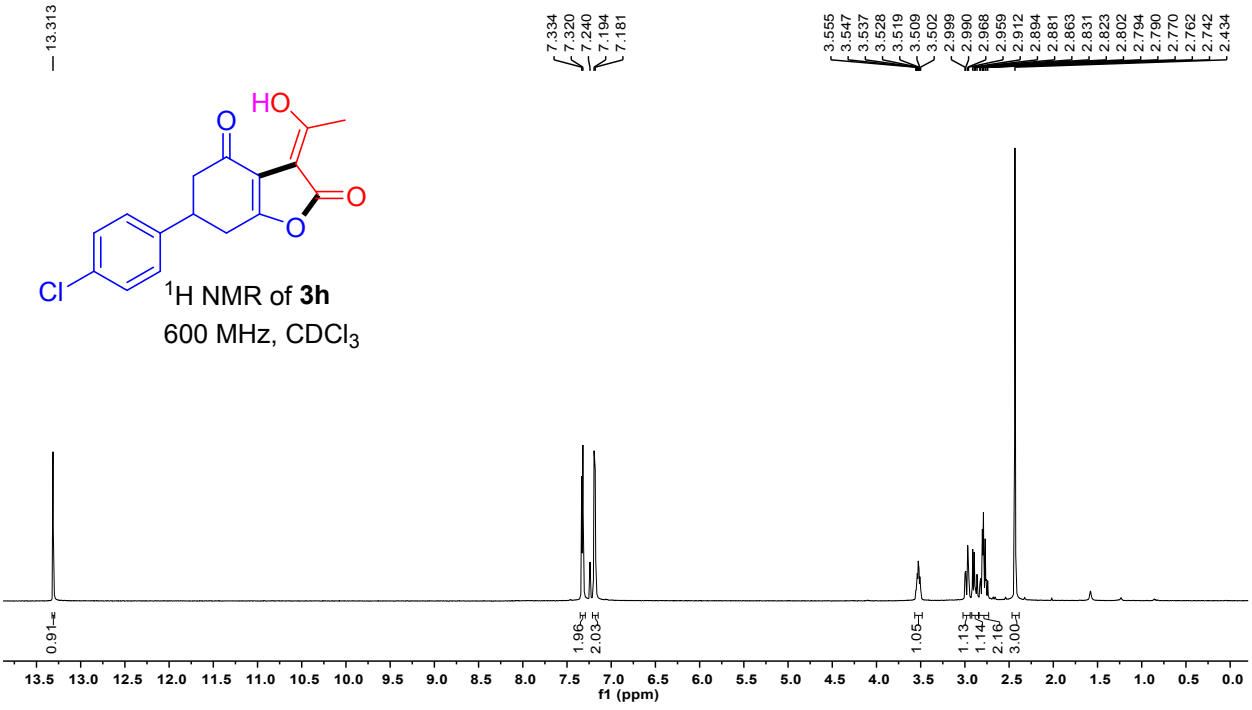

196.108
176.220
166.815
166.788
141.133
129.035
127.636
126.635
116.525
94.396
77.212
77.000
76.788
42.740
40.012
30.542
18.862
HO
O
O
O
^{13}C NMR of **3e**
150 MHz, $CDCl_3$
f1 (ppm)

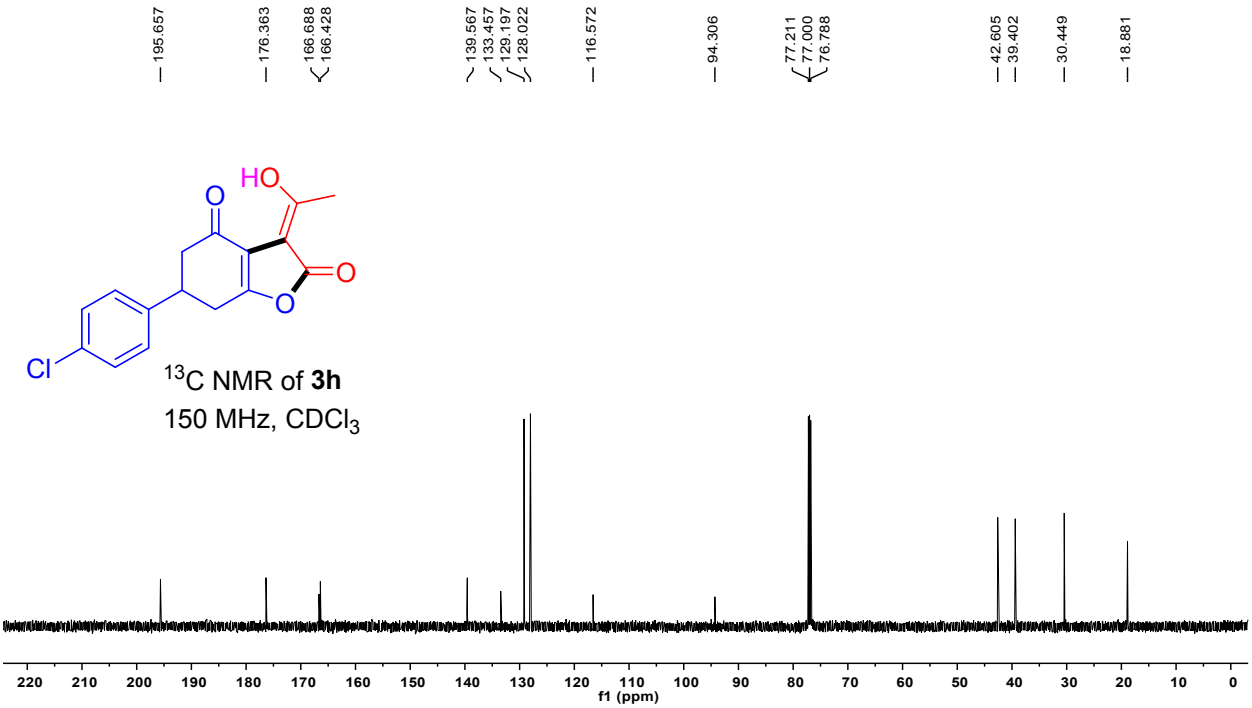

13.374
7.240
6.847
6.833
6.796
6.793
6.782
6.779
6.740
6.736
3.871
3.861
3.513
3.505
3.496
3.486
3.477
3.468
3.459
3.010
3.001
2.979
2.970
2.928
2.910
2.897
2.879
2.850
2.842
2.821
2.813
2.804
2.785
2.776
2.756
2.446
HO
O
O
O
MeO
MeO
^{1}H NMR of **3f**
600 MHz, $CDCl_3$
0.93
1.08
1.09
1.04
3.13
3.02
1.14
1.17
1.14
2.19
3.00
f1 (ppm)

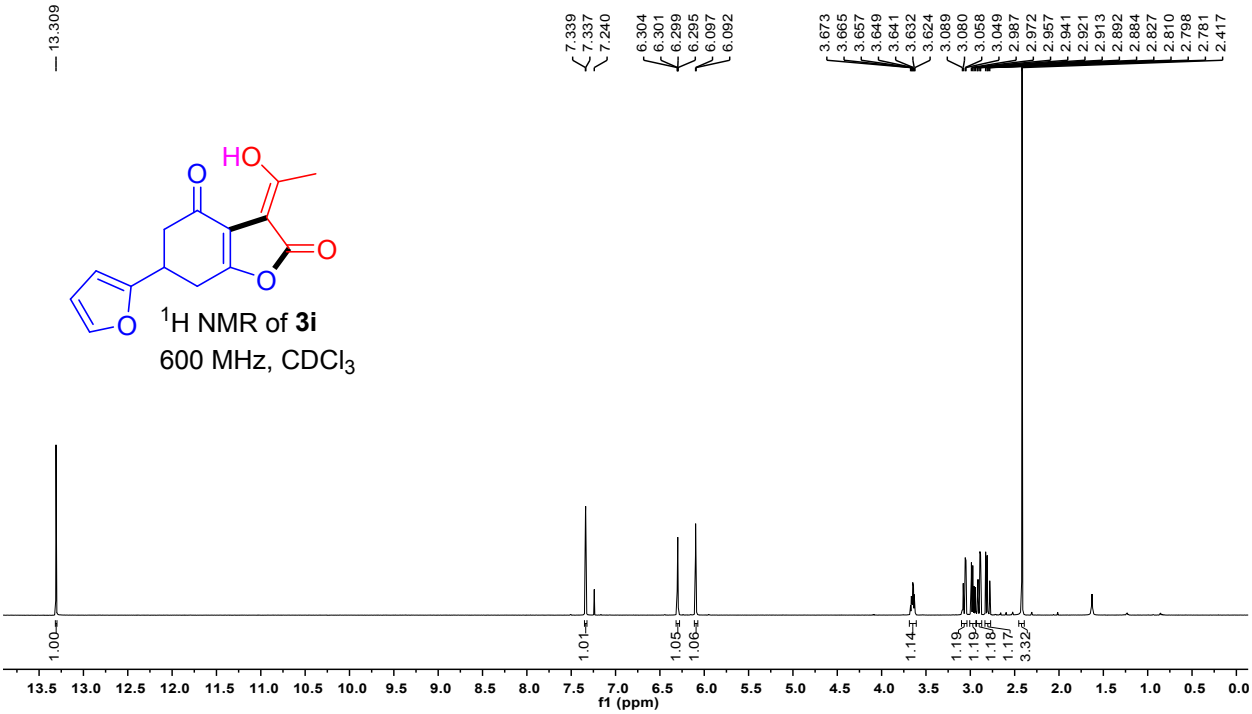

196.170
176.258
166.863
166.813
149.276
148.496
133.757
118.529
116.534
111.517
110.058
94.408
77.211
77.000
76.788
55.980
43.087
39.764
30.845
18.898
HO
O
O
O
MeO
MeO
13C NMR of 3f
150 MHz, CDCl3
f1 (ppm)

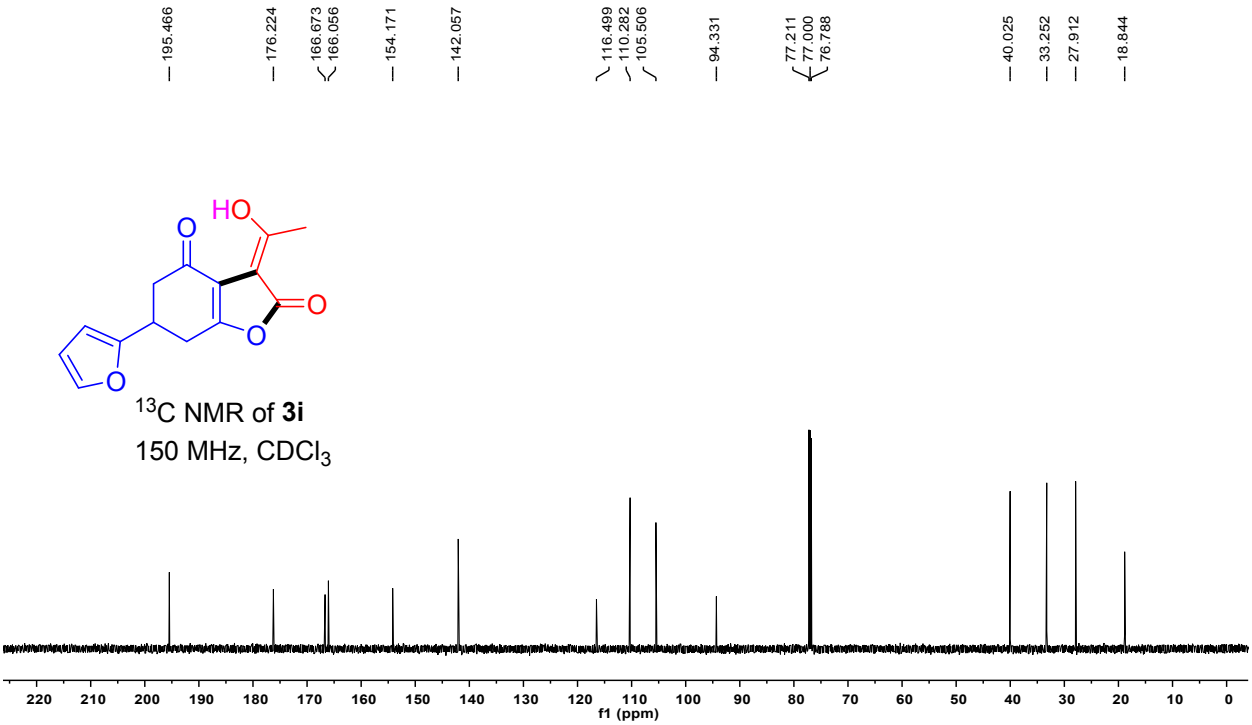

13.354
7.240
6.773
6.760
6.723
6.721
6.697
6.694
6.684
6.681
5.945
3.480
3.472
3.462
3.453
3.443
3.434
3.426
2.966
2.958
2.935
2.927
2.876
2.858
2.846
2.827
2.806
2.798
2.777
2.769
2.758
2.738
2.729
2.709
2.430
HO
O
O
O
O
O
1H NMR of 3g
600 MHz, CDCl3
0.94
1.00
0.99
1.01
2.00
1.08
1.09
1.11
2.14
2.96
f1 (ppm)

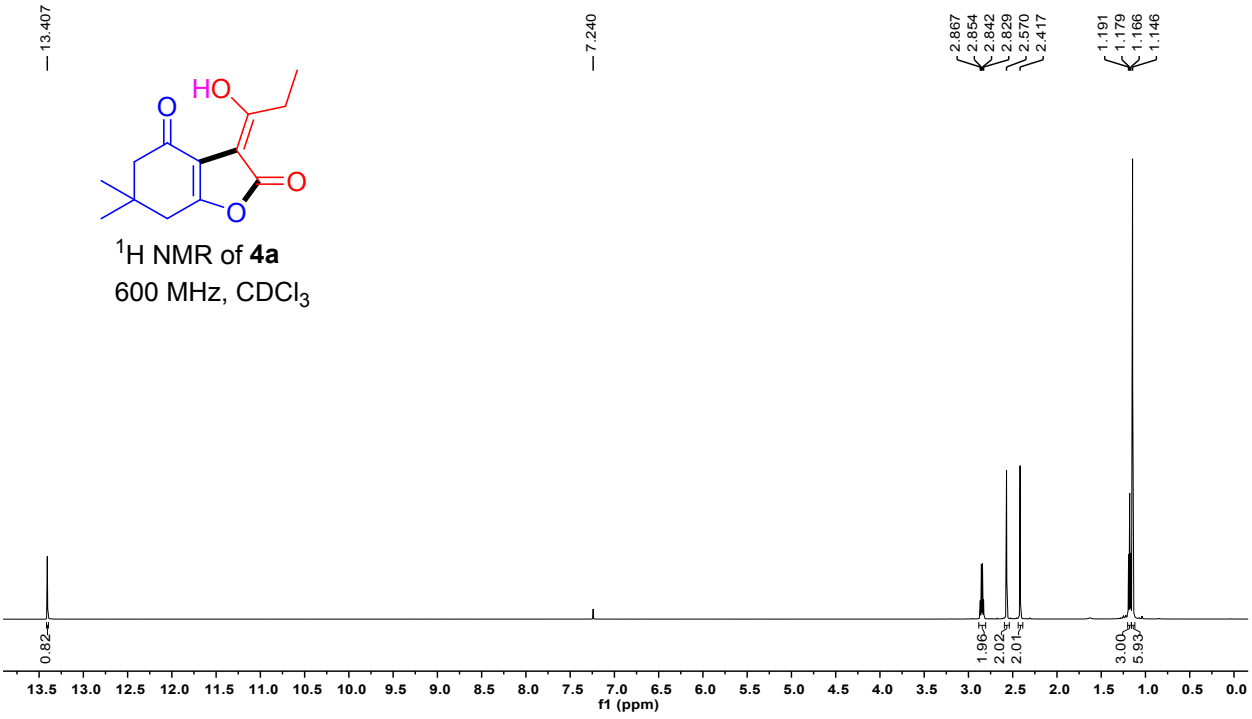

196.030
176.223
166.795
166.700
148.092
146.938
135.050
119.812
116.492
108.584
106.963
101.232
94.374
77.211
77.000
76.788
43.038
39.864
30.861
18.853
HO
O
O
O
O
O
13C NMR of 3g
150 MHz, CDCl3
f1 (ppm)

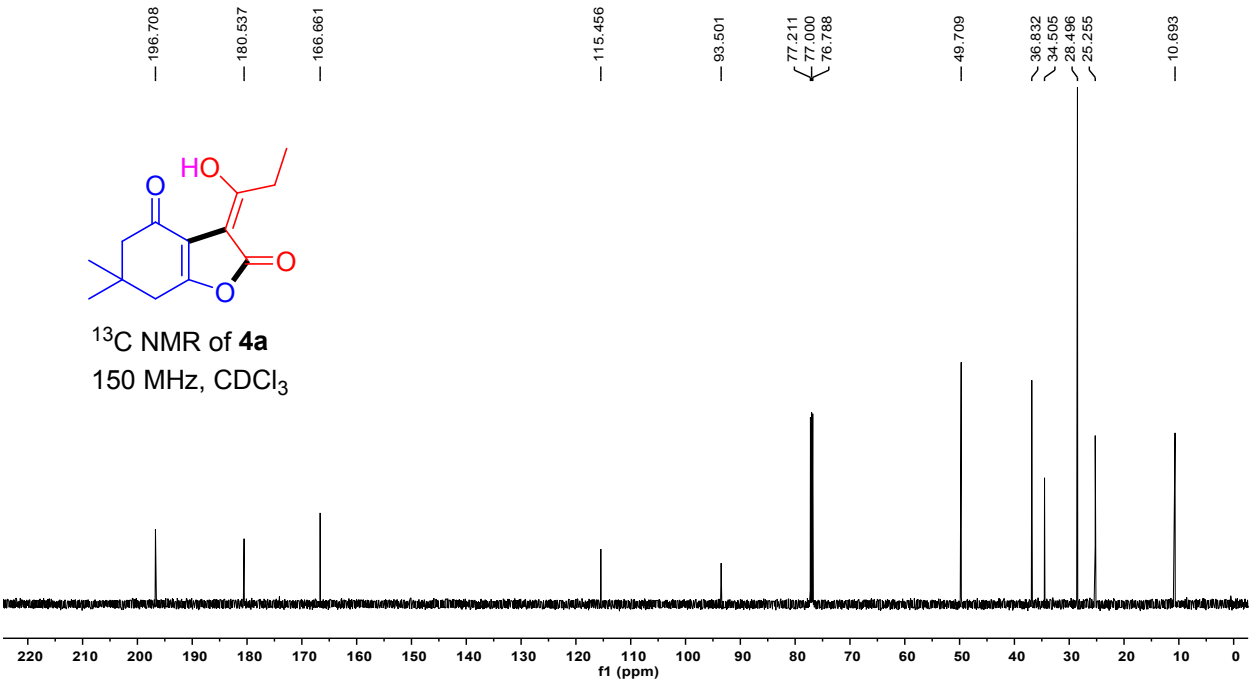

13.313
7.334
7.320
7.240
7.194
7.181
3.555
3.547
3.537
3.528
3.519
3.509
3.502
2.999
2.990
2.968
2.959
2.912
2.894
2.881
2.863
2.831
2.823
2.802
2.794
2.790
2.770
2.762
2.742
2.434
HO
O
O
O
Cl
1H NMR of 3h
600 MHz, CDCl3
0.91
1.96
2.03
1.05
1.13
1.14
2.16
3.00
f1 (ppm)


195.657
176.363
166.688
166.428
139.567
133.457
129.197
128.022
116.572
94.306
77.211
77.000
76.788
42.605
39.402
30.449
18.881
HO
O
O
O
Cl
13C NMR of 3h
150 MHz, CDCl3
f1 (ppm)

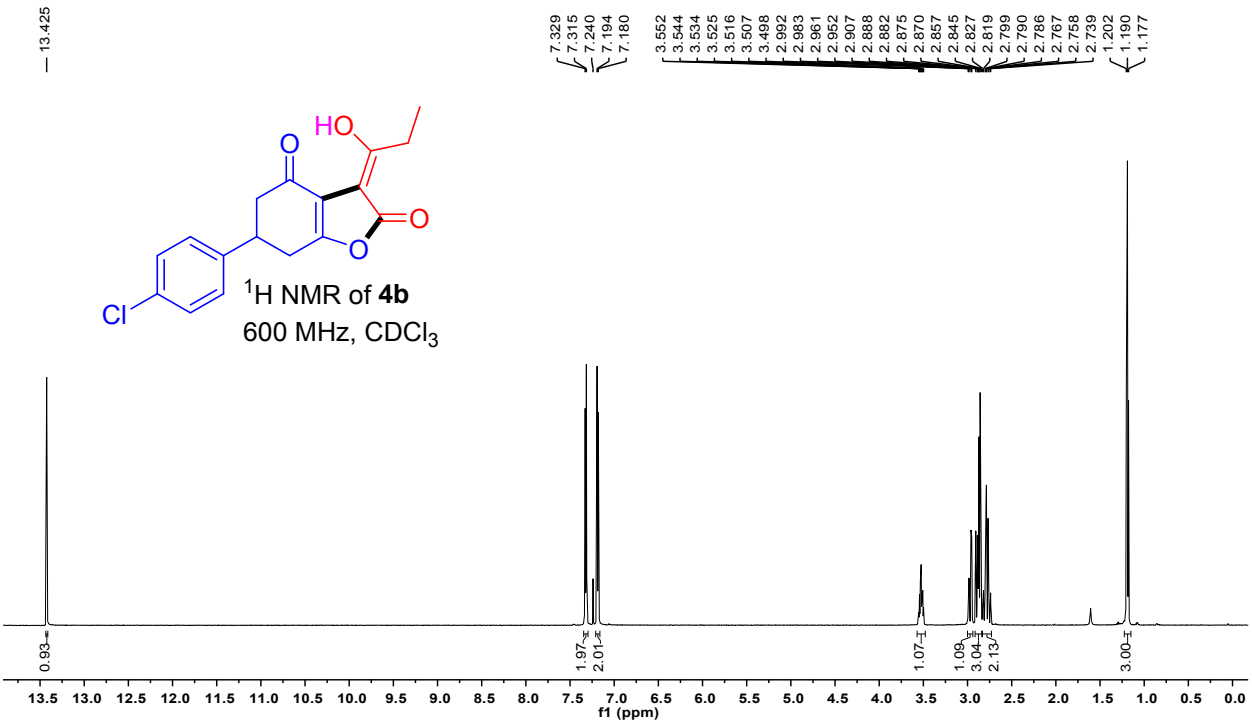

13.309
7.339
7.337
7.240
6.304
6.301
6.299
6.295
6.097
6.092
3.673
3.665
3.657
3.649
3.641
3.632
3.624
3.089
3.080
3.058
3.049
2.987
2.972
2.957
2.941
2.921
2.913
2.892
2.884
2.827
2.810
2.798
2.781
2.417
HO
O
O
O
O
1H NMR of 3i
600 MHz, CDCl3
1.00
1.01
1.05
1.06
1.14
1.19
1.19
1.18
1.17
3.32
f1 (ppm)


195.466
176.224
166.673
166.056
154.171
142.057
116.499
110.282
105.506
94.331
77.211
77.000
76.788
40.025
33.252
27.912
18.844
HO
O
O
O
O
^{13}C NMR of **3i**
150 MHz, $CDCl_3$
f1 (ppm)

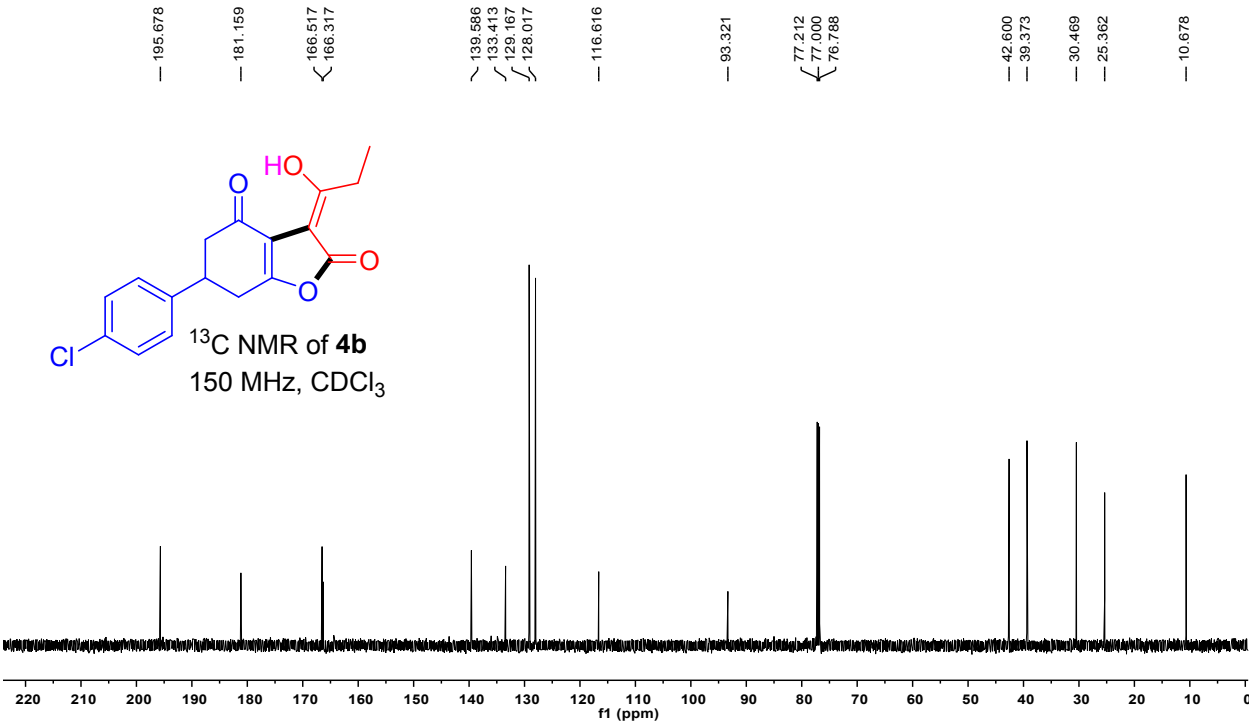

13.407
7.240
2.867
2.854
2.842
2.829
2.570
2.417
1.191
1.179
1.166
1.146
HO
O
O
O
^{1}H NMR of **4a**
600 MHz, $CDCl_3$
0.82
1.96
2.02
2.01
3.00
5.93
f1 (ppm)

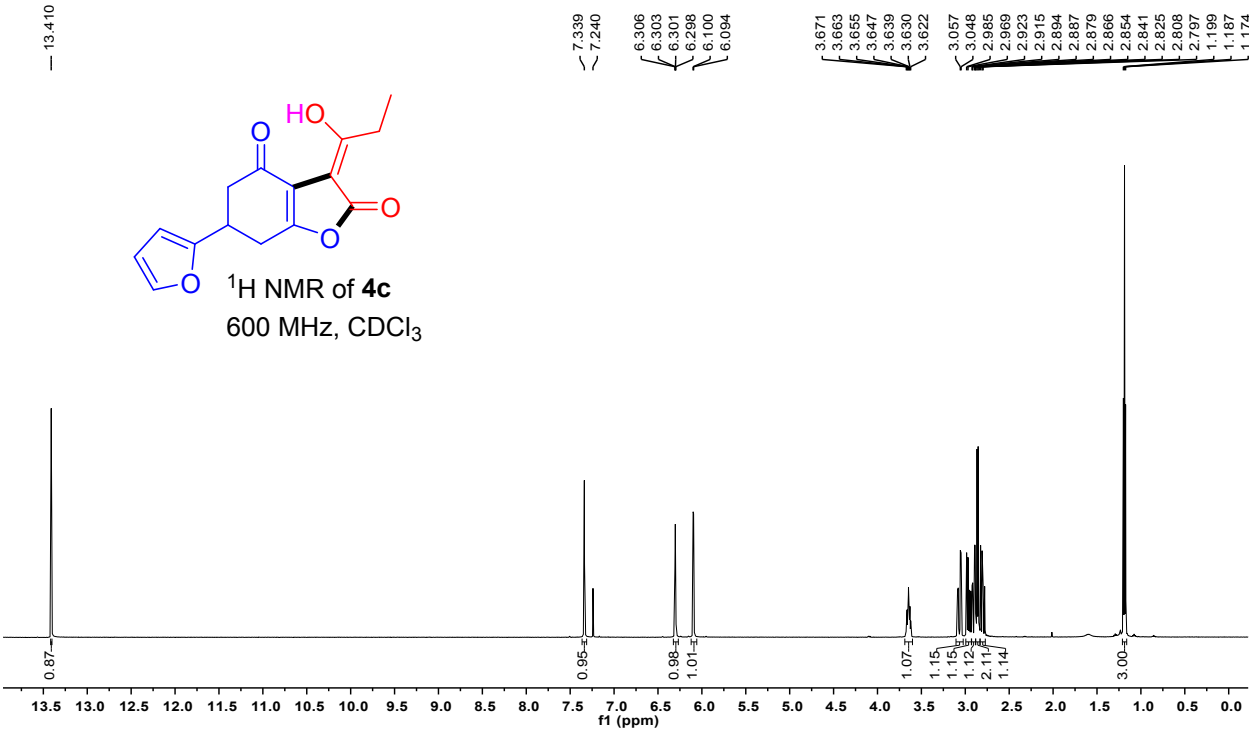


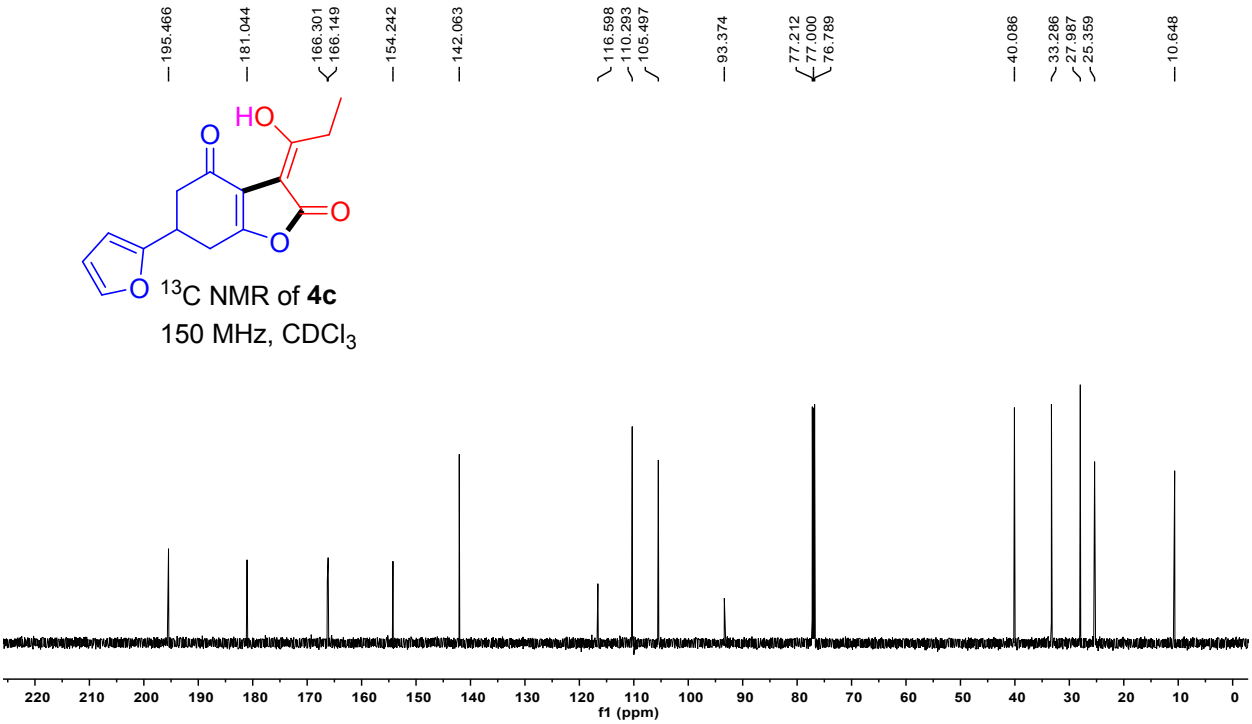
^{13}C NMR of **4a**
150 MHz, $CDCl_3$



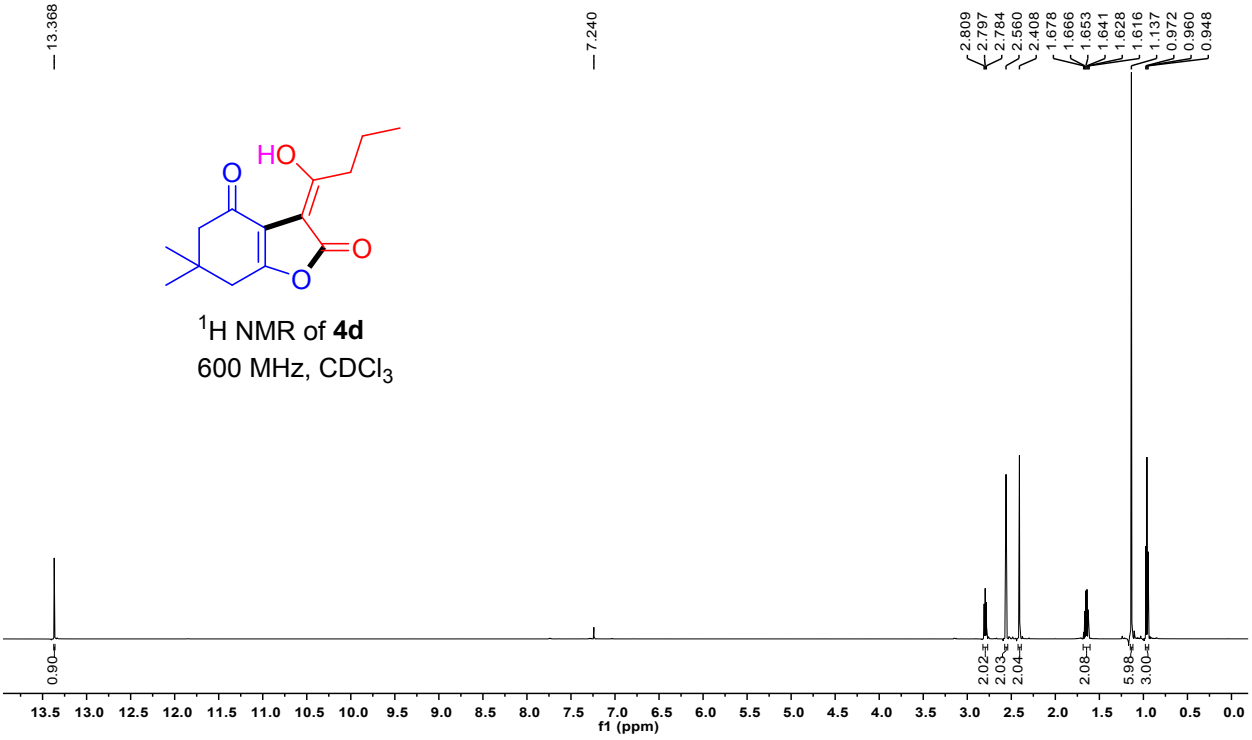
^{1}H NMR of **4b**
600 MHz, $CDCl_3$


195.678
181.159
166.517
166.317
139.586
133.413
129.167
128.017
116.616
93.321
77.212
77.000
76.788
42.600
39.373
30.469
25.362
10.678
HO
O
O
O
Cl
^{13}C NMR of **4b**
150 MHz, $CDCl_3$
f1 (ppm)

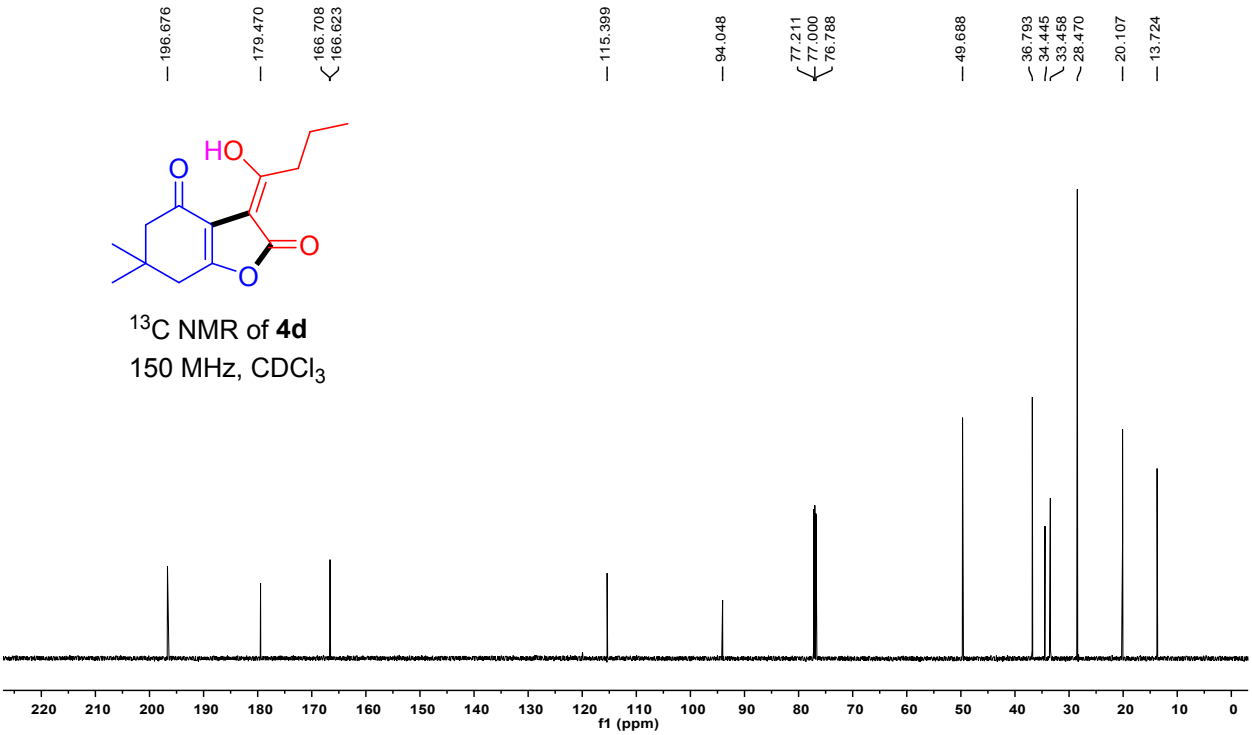

13.410
7.339
7.240
6.306
6.303
6.301
6.298
6.100
6.094
3.671
3.663
3.655
3.647
3.639
3.630
3.622
3.057
3.048
2.985
2.969
2.923
2.915
2.894
2.887
2.879
2.866
2.854
2.841
2.825
2.808
2.797
1.199
1.187
1.174
HO
O
O
O
O
^{1}H NMR of **4c**
600 MHz, $CDCl_3$
0.87
0.95
0.98
1.01
1.07
1.15
1.15
1.12
2.11
1.14
3.00
f1 (ppm)



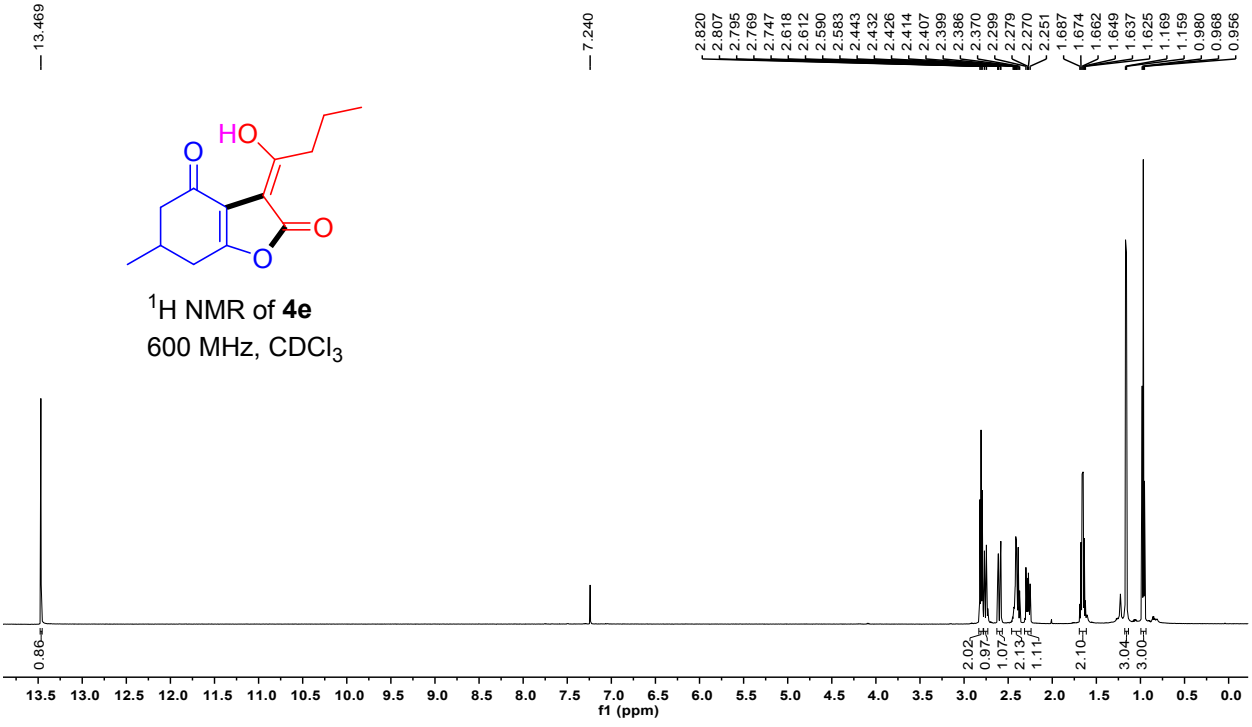
^{13}C NMR of **4c**
150 MHz, $CDCl_3$



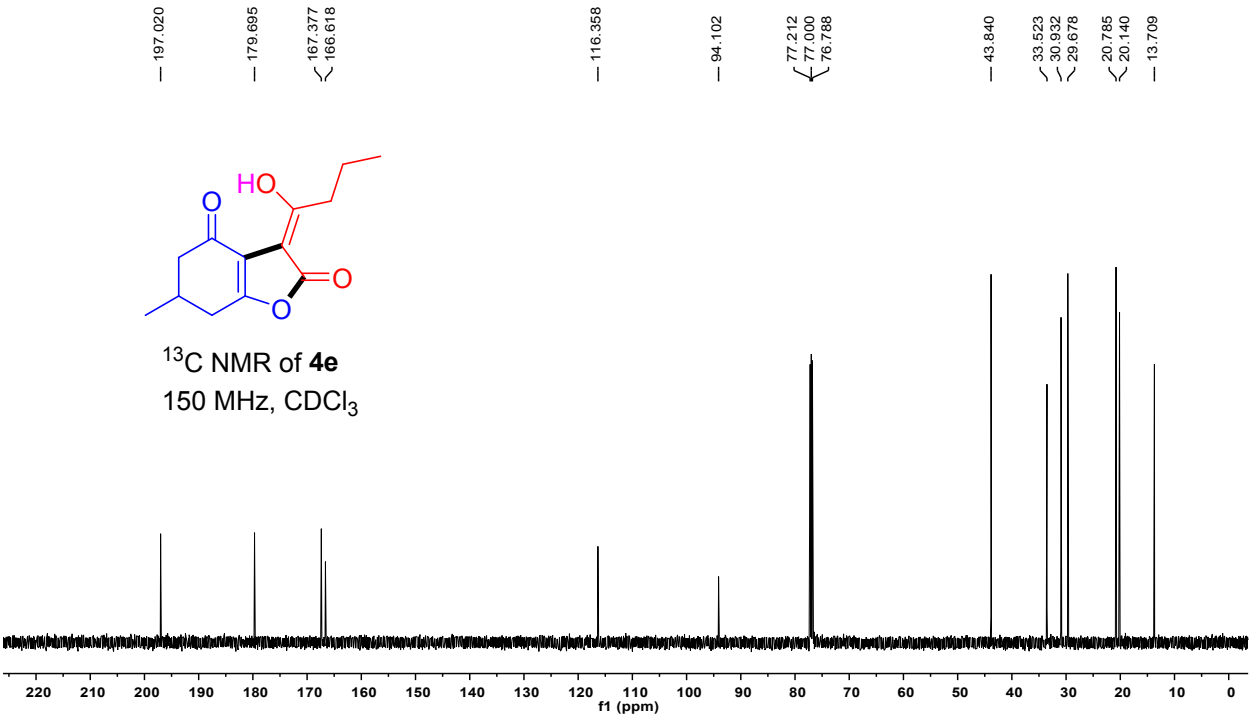
^{1}H NMR of **4d**
600 MHz, $CDCl_3$



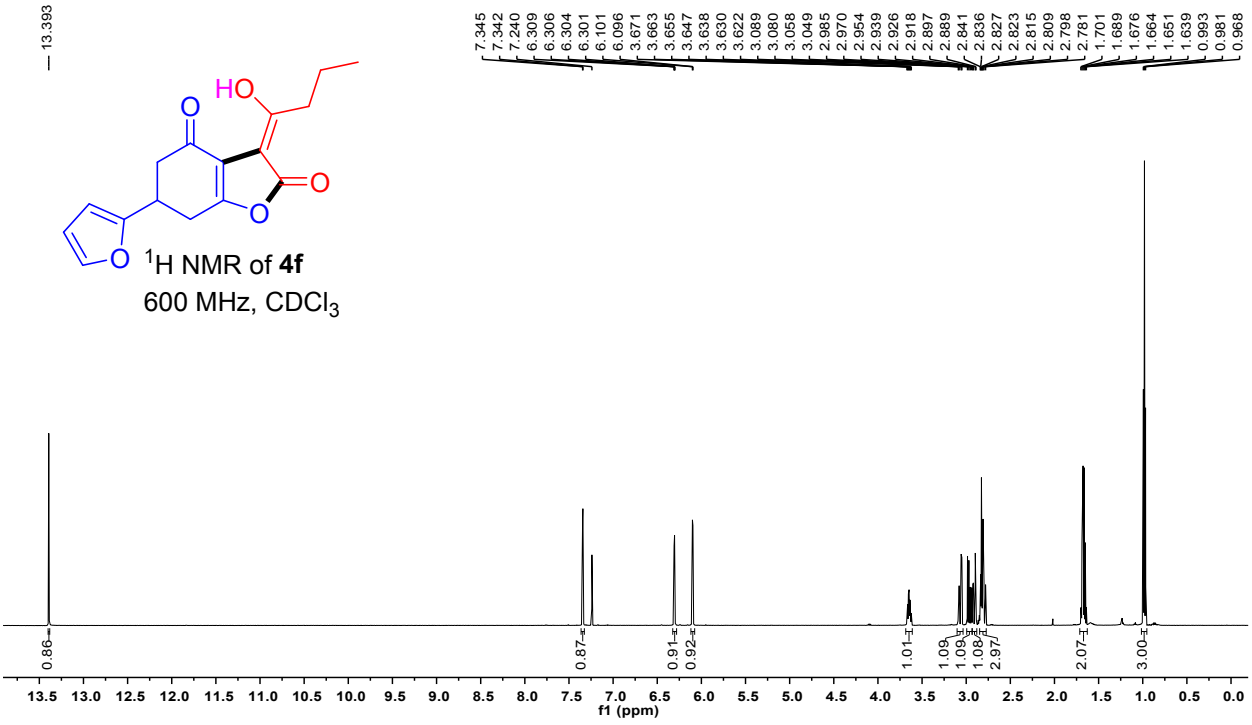
^{13}C NMR of **4d**
150 MHz, $CDCl_3$



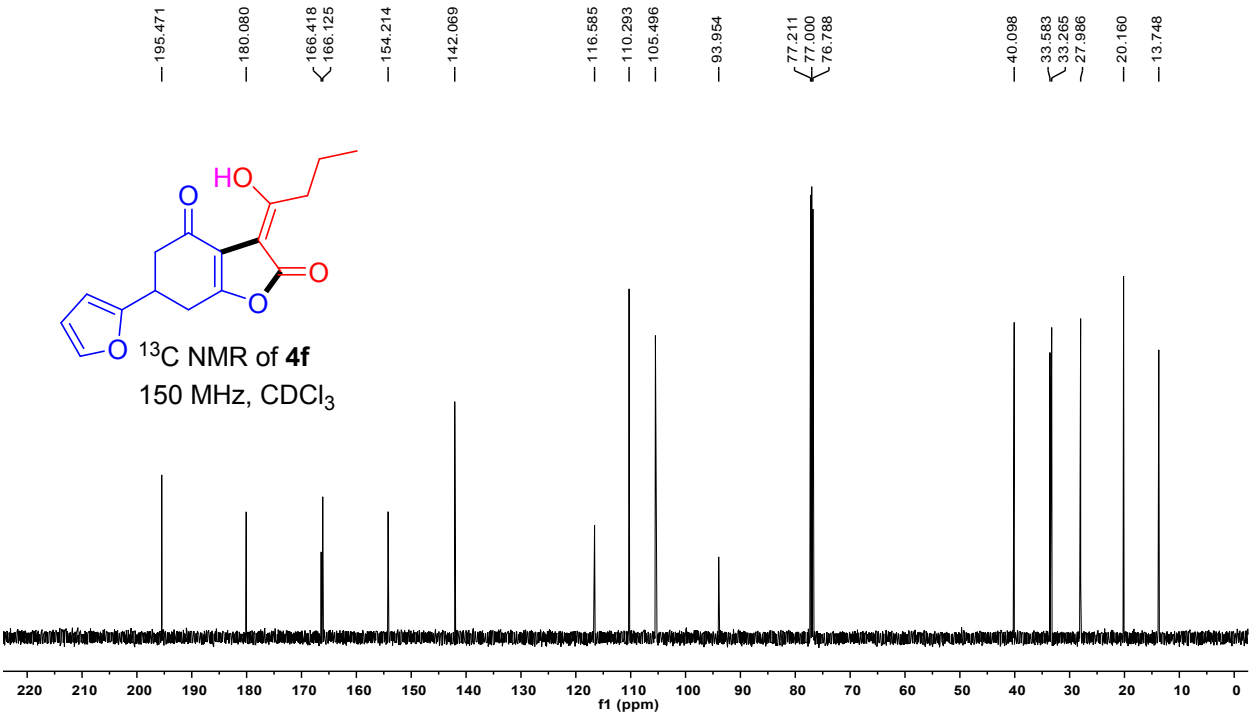
^{1}H NMR of **4e**
600 MHz, $CDCl_3$



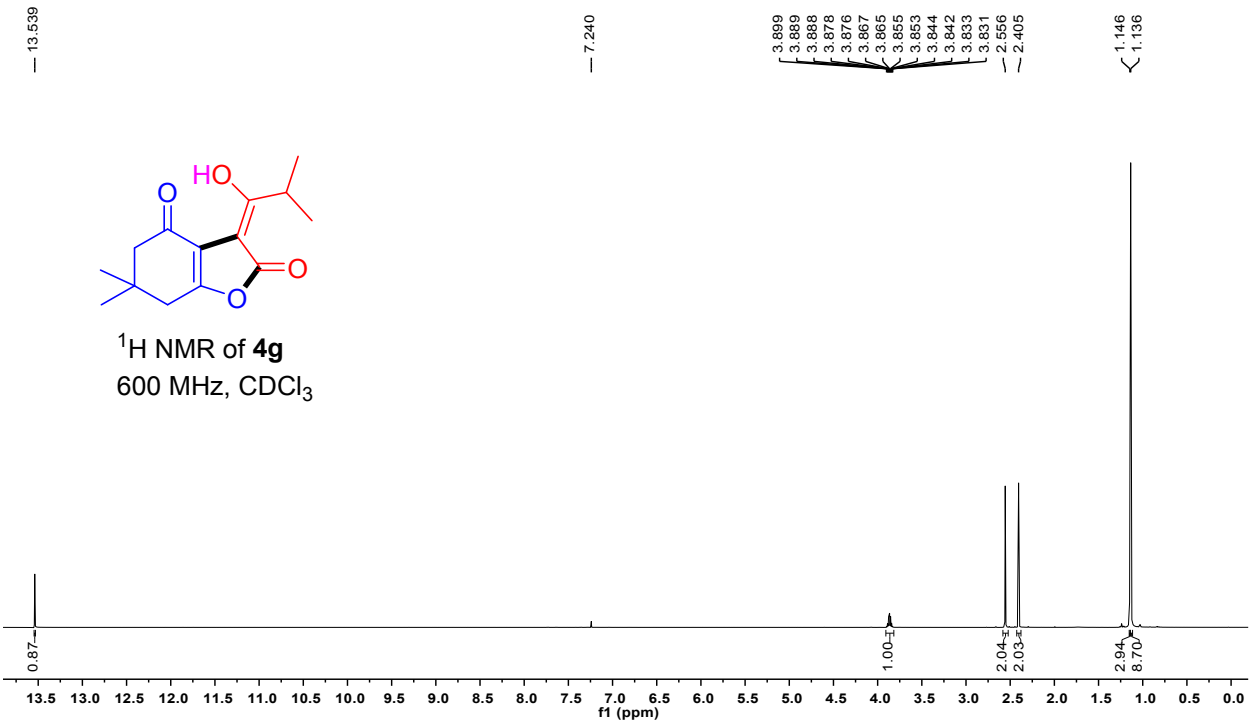
^{13}C NMR of **4e**
150 MHz, $CDCl_3$



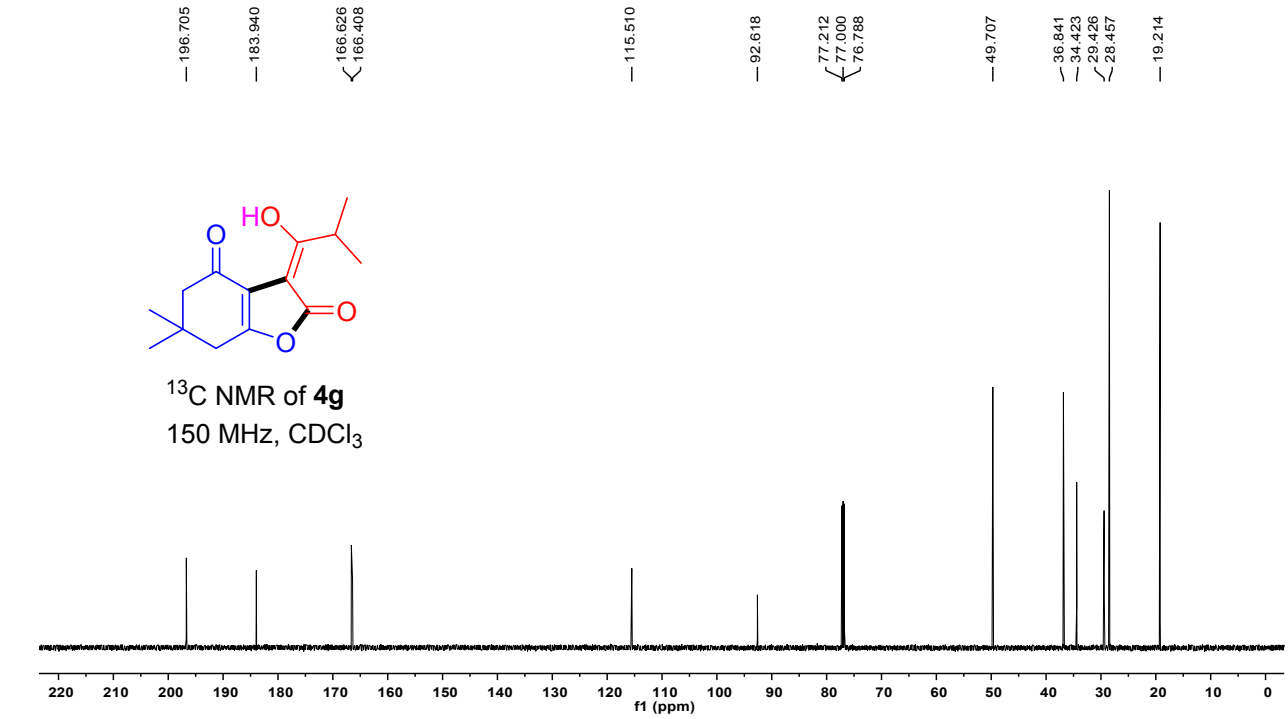
^{1}H NMR of **4f**
600 MHz, $CDCl_3$



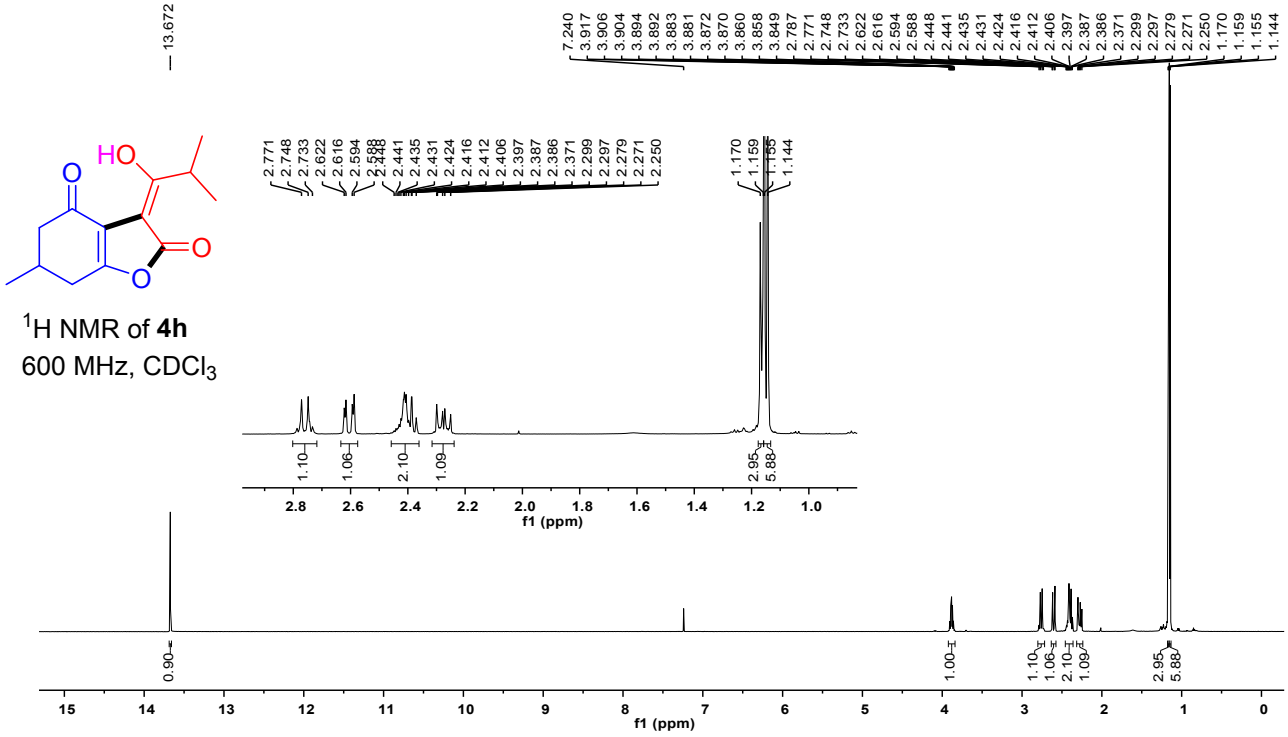
^{13}C NMR of **4f**
150 MHz, $CDCl_3$



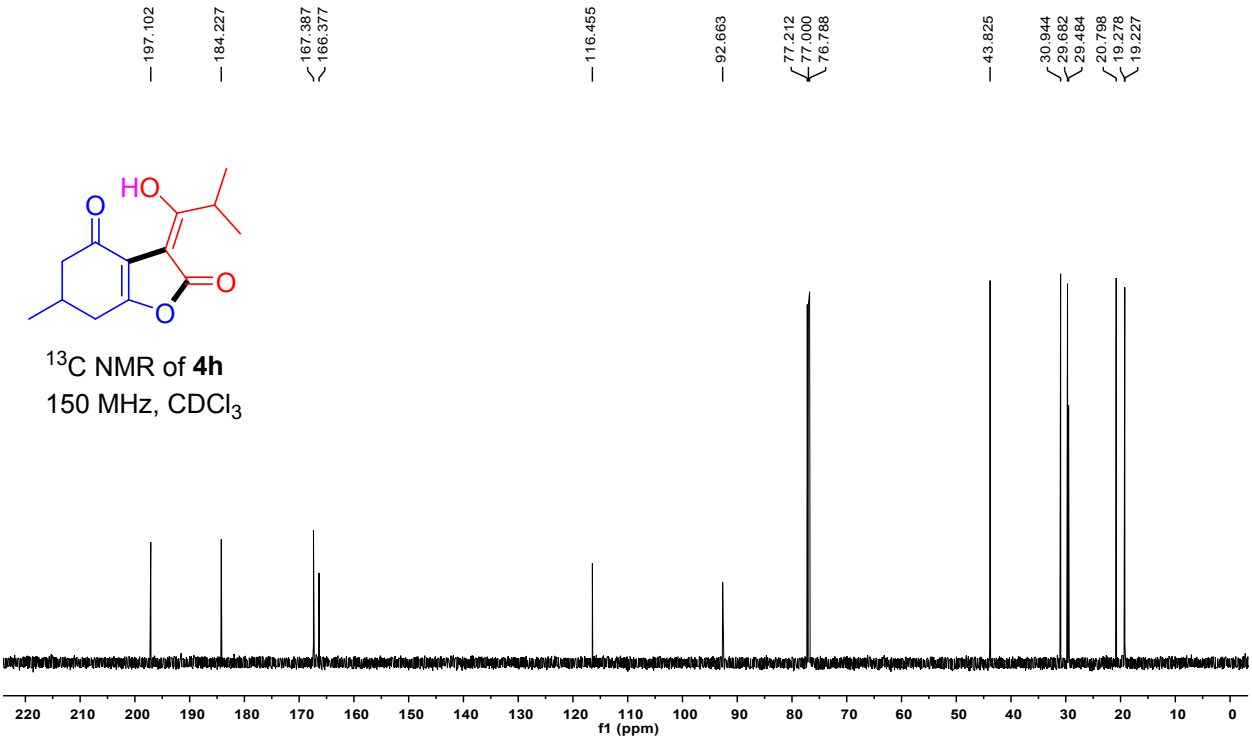
^{1}H NMR of **4g**
600 MHz, $CDCl_3$



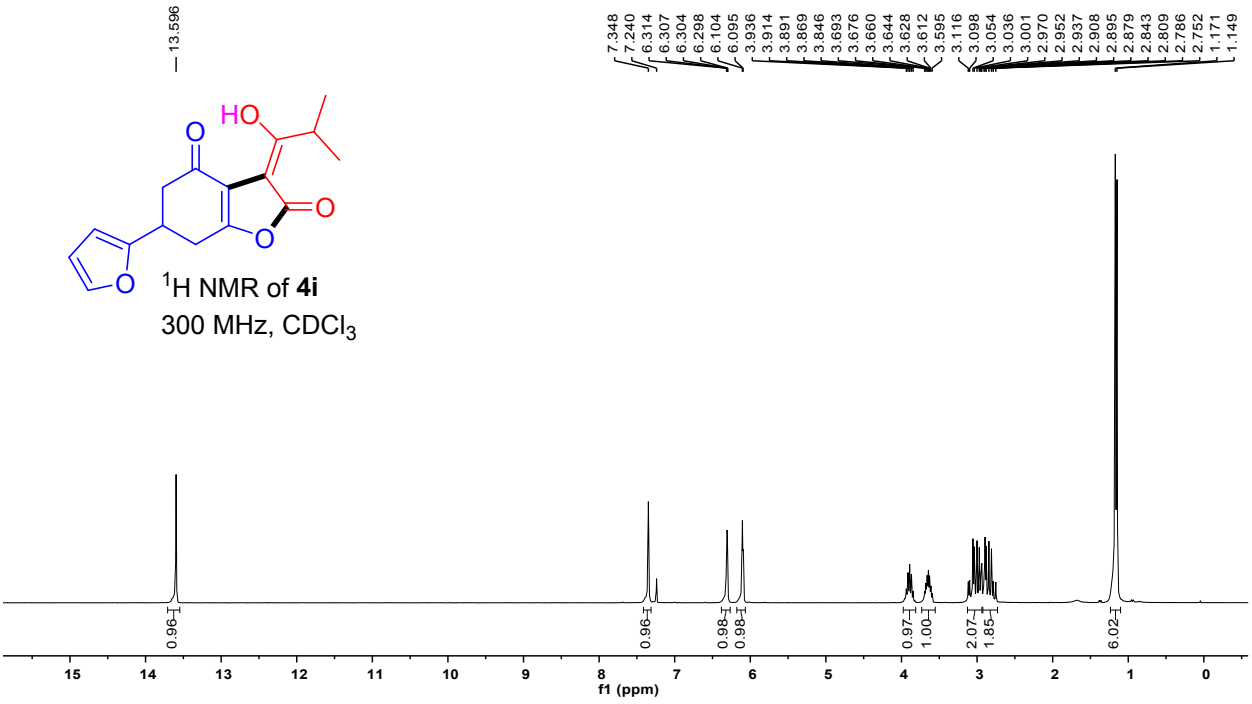
^{13}C NMR of **4g**
150 MHz, $CDCl_3$



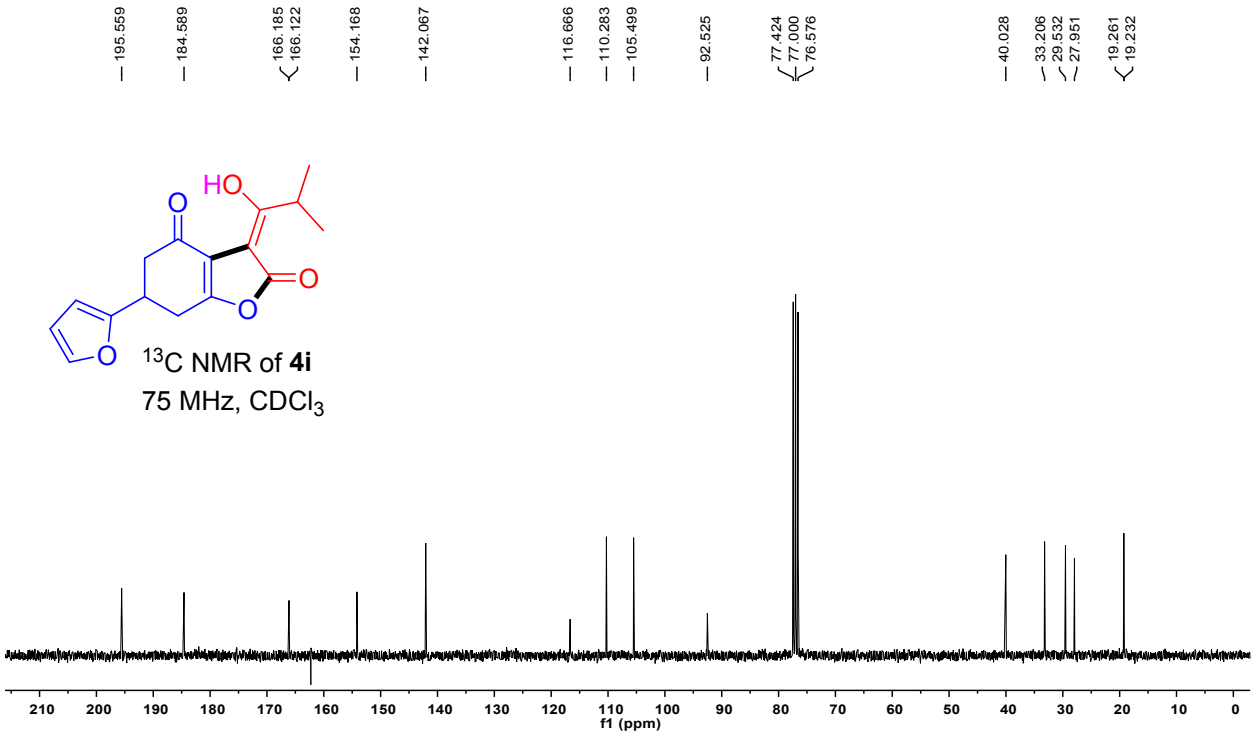
^{1}H NMR of **4h**
600 MHz, $CDCl_3$



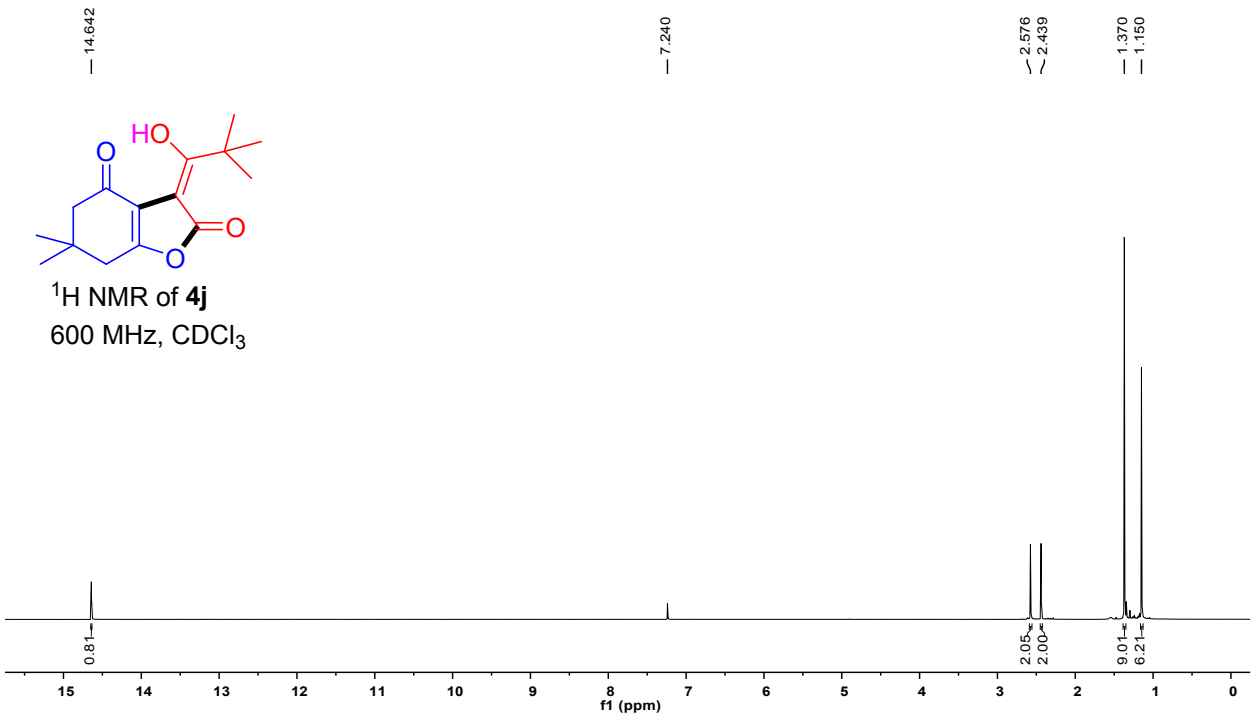
^{13}C NMR of **4h**
150 MHz, $CDCl_3$



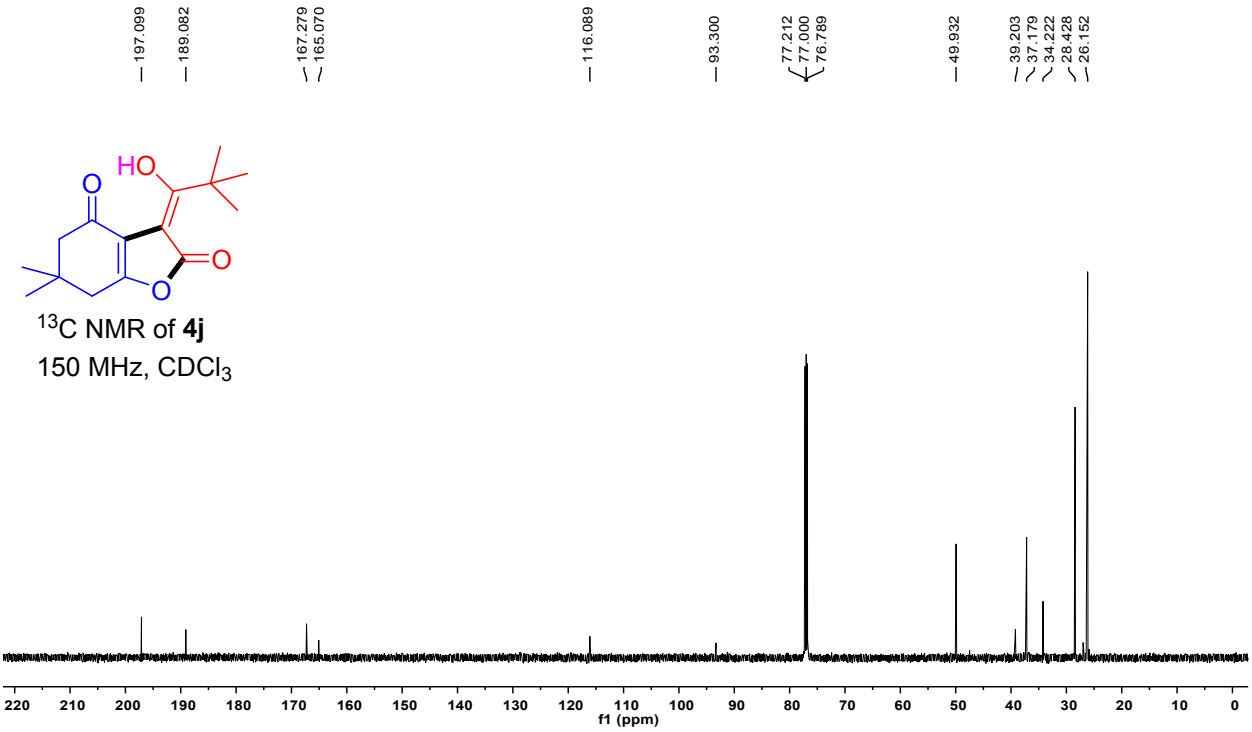
^{1}H NMR of **4i**
300 MHz, $CDCl_3$



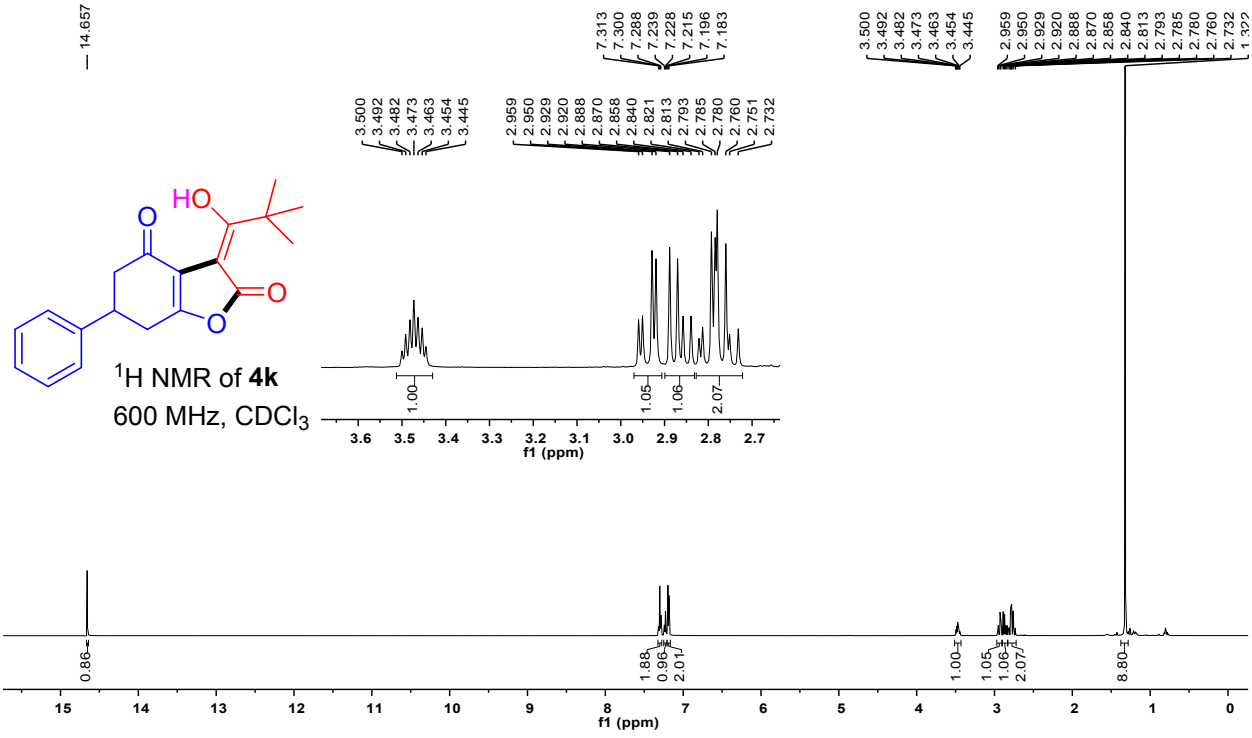
^{13}C NMR of **4i**
75 MHz, $CDCl_3$



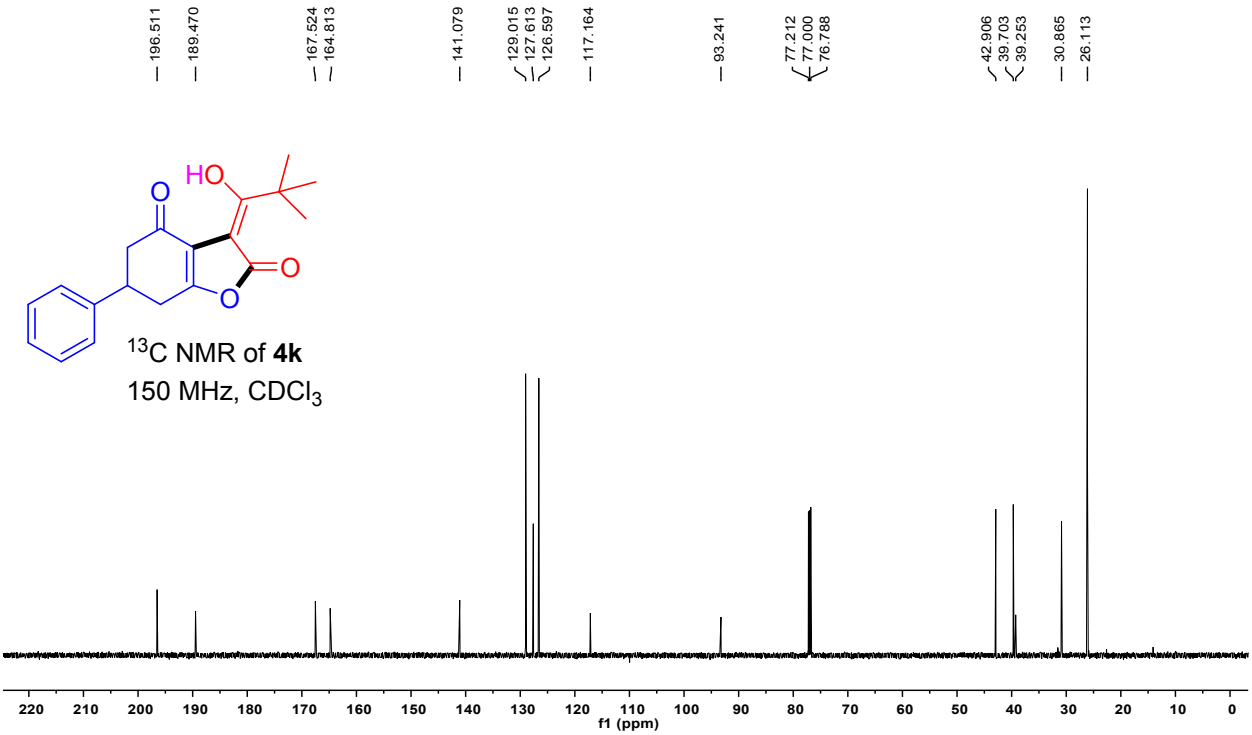
^{1}H NMR of **4j**
600 MHz, $CDCl_3$



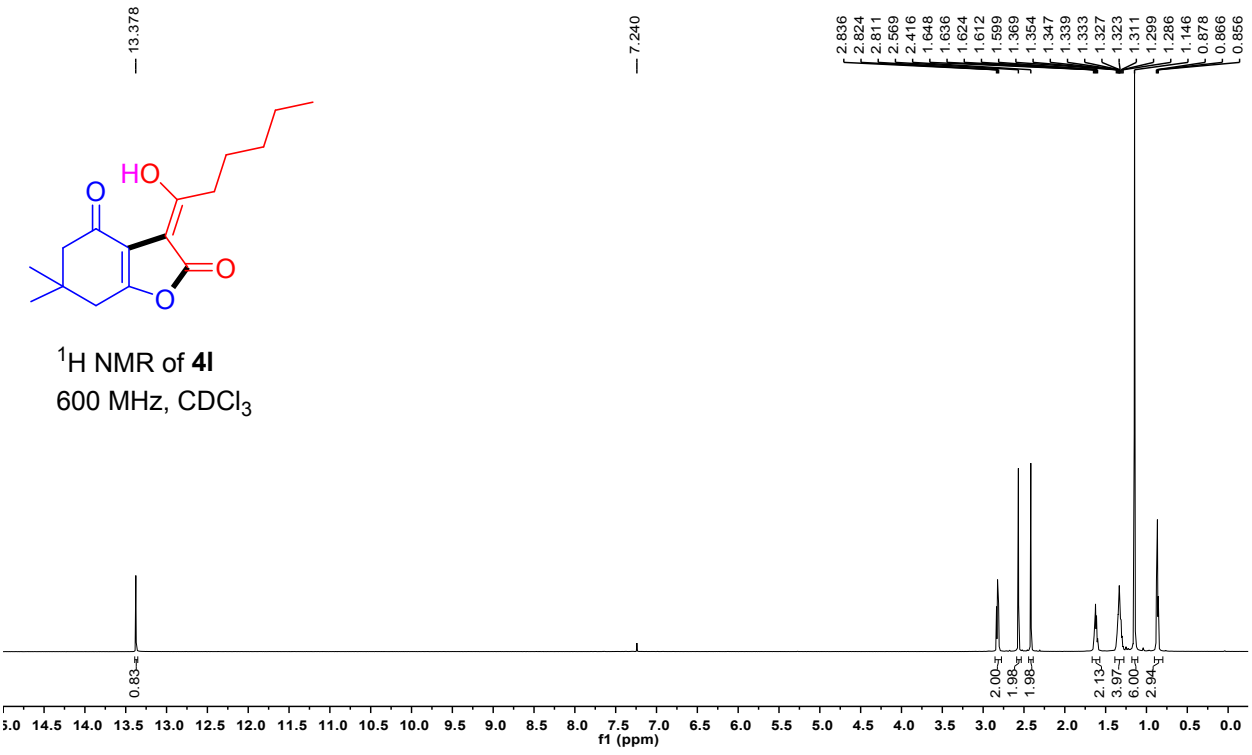
^{13}C NMR of **4j**
150 MHz, $CDCl_3$



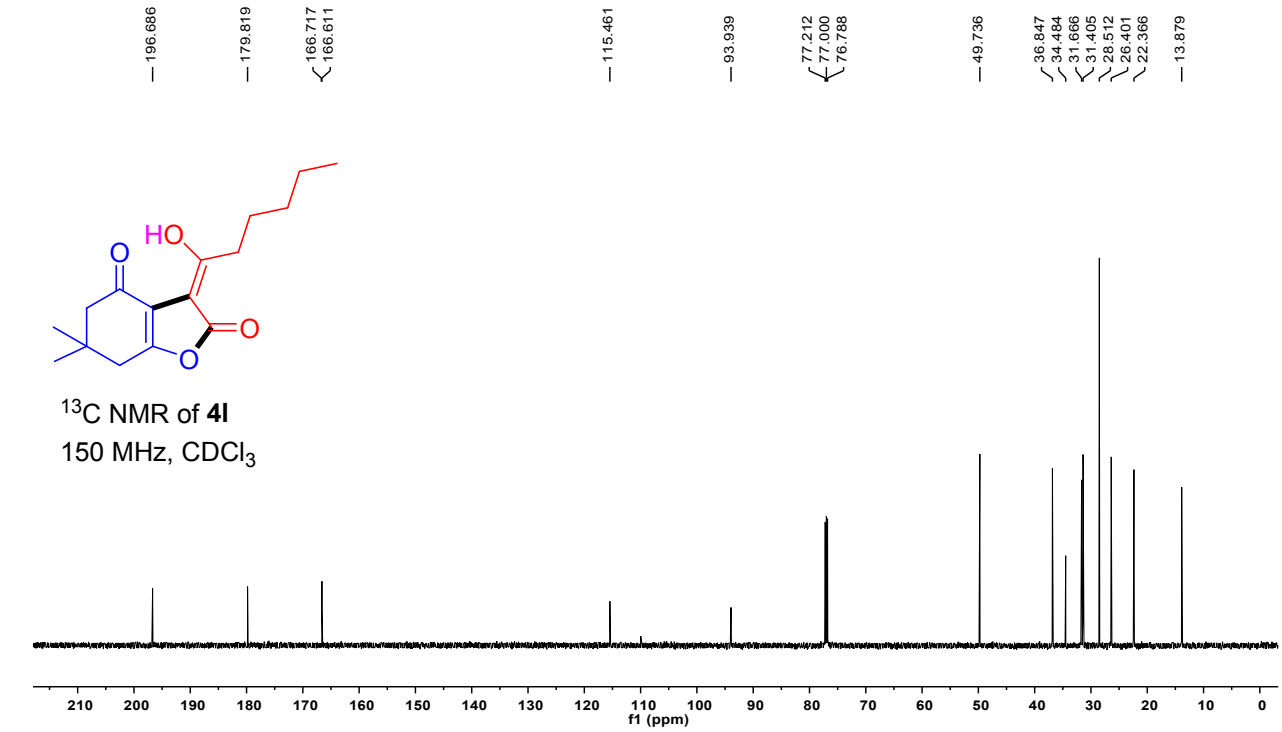
^{1}H NMR of **4k**
600 MHz, $CDCl_3$

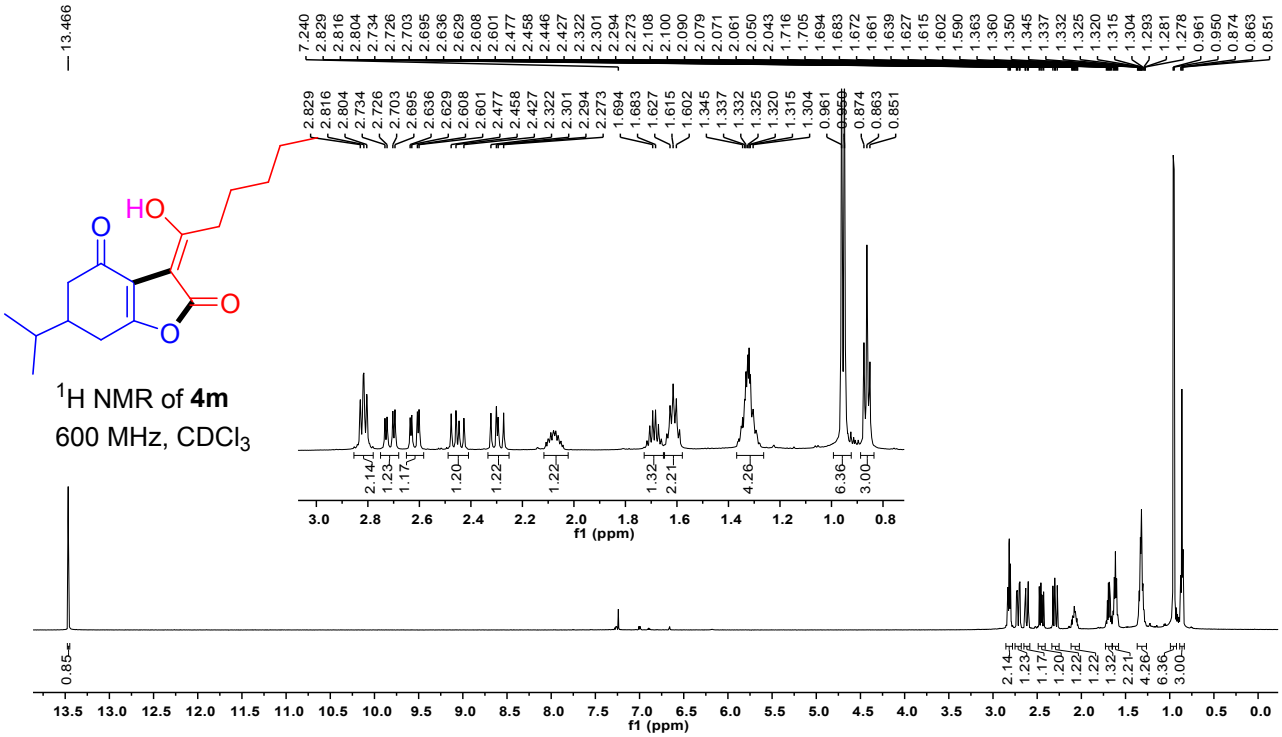


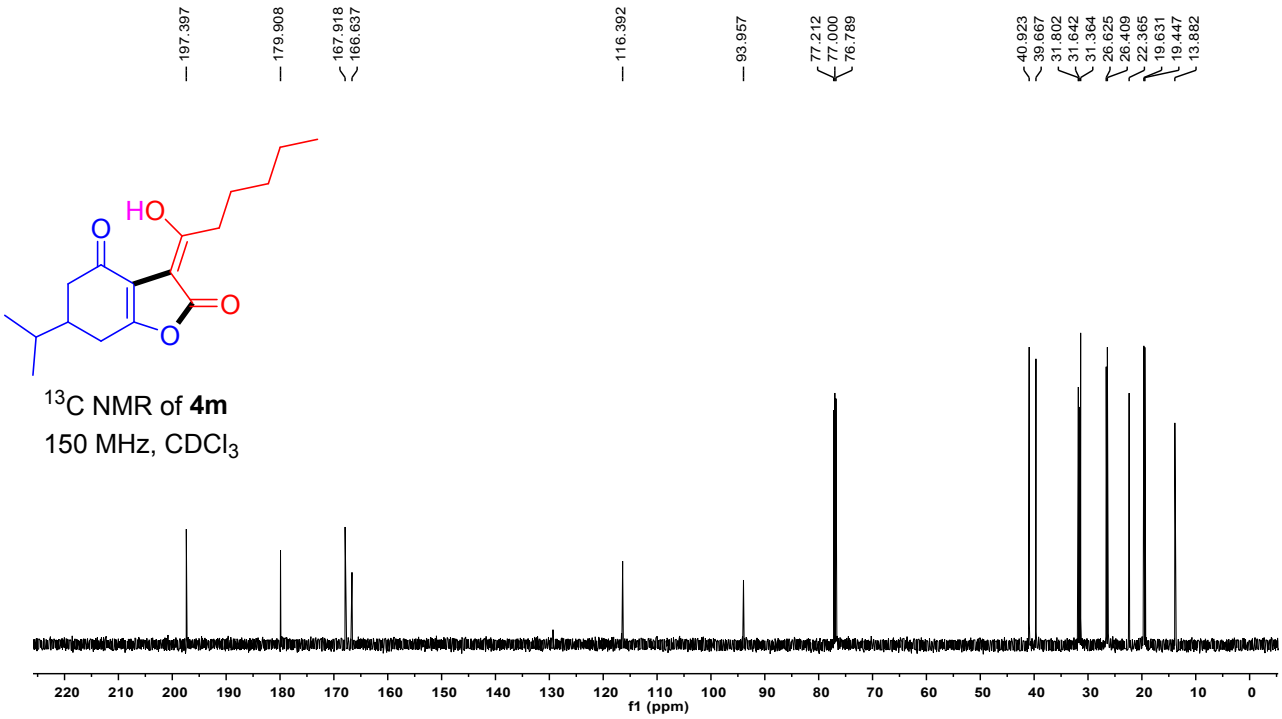
^{13}C NMR of **4k**
150 MHz, $CDCl_3$



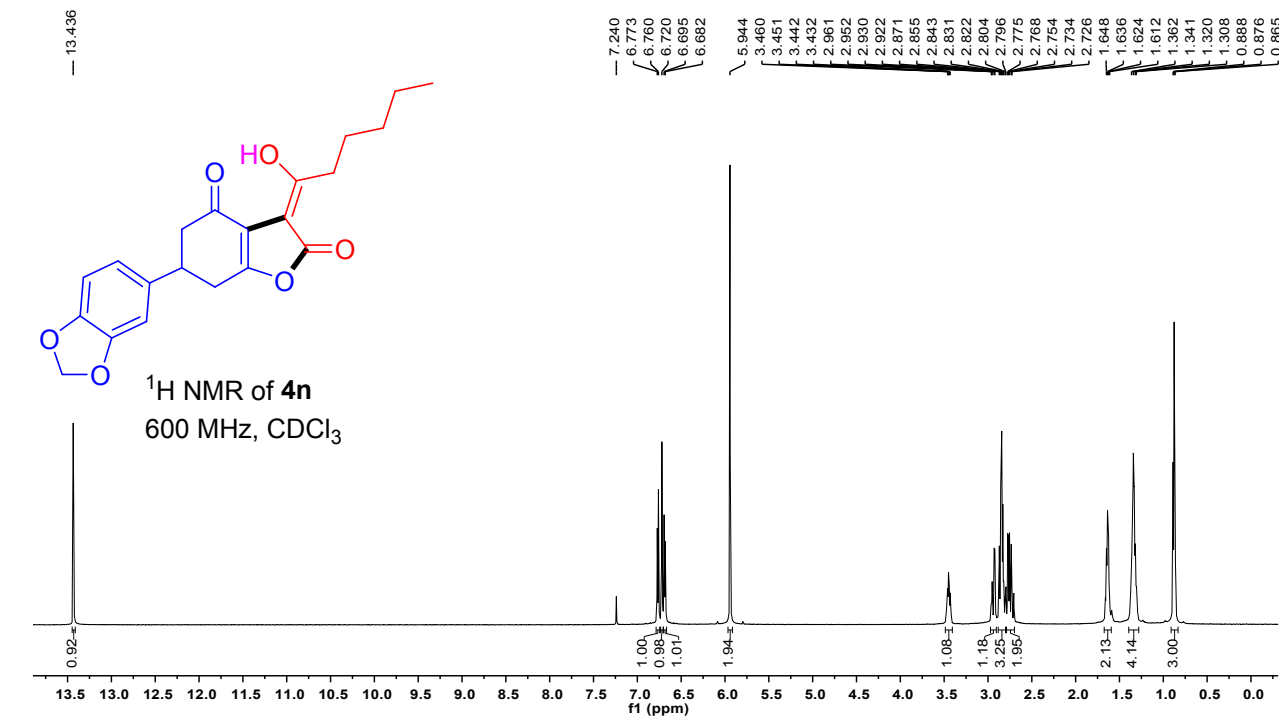
^{1}H NMR of **4l**
600 MHz, $CDCl_3$


196.686
179.819
166.717
166.611
115.461
93.939
77.212
77.000
76.788
49.736
36.847
34.484
31.666
31.405
28.512
26.401
22.366
13.879
HO
O
O
O
13C NMR of 4l
150 MHz, CDCl3
f1 (ppm)

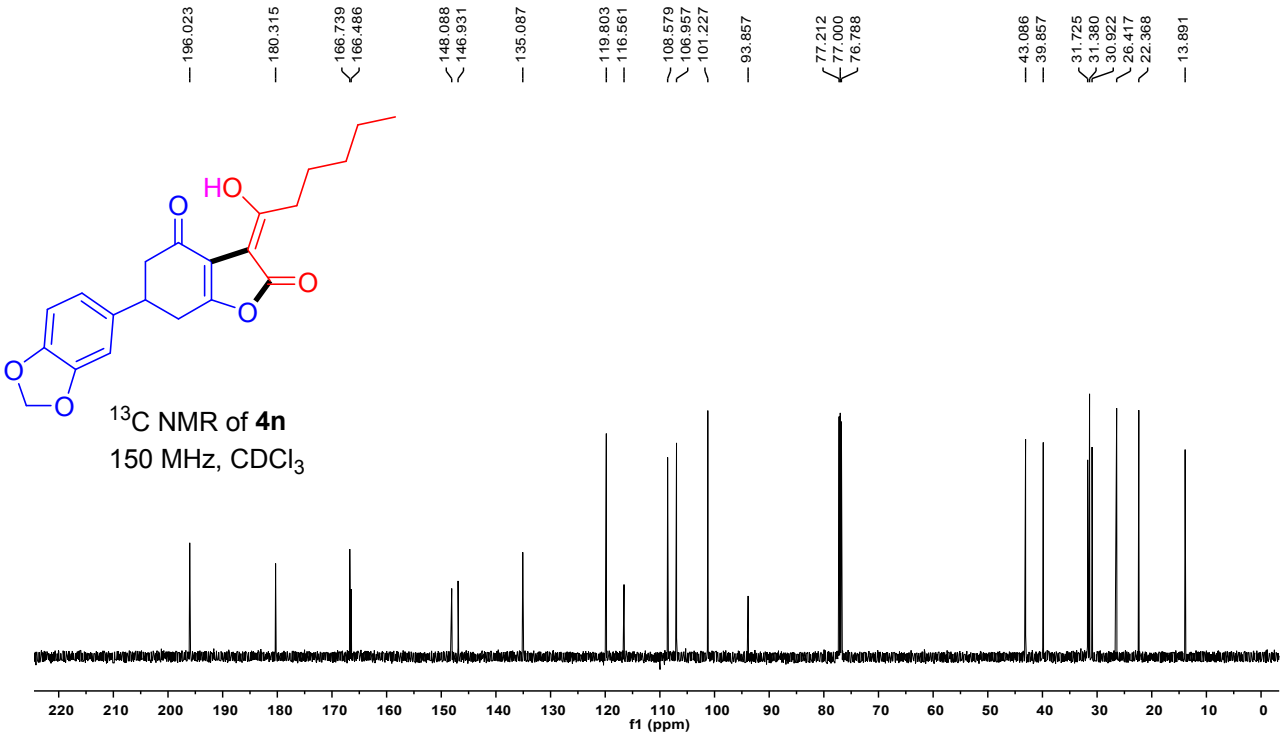

13.466
HO
O
O
O
1H NMR of 4m
600 MHz, CDCl3
f1 (ppm)

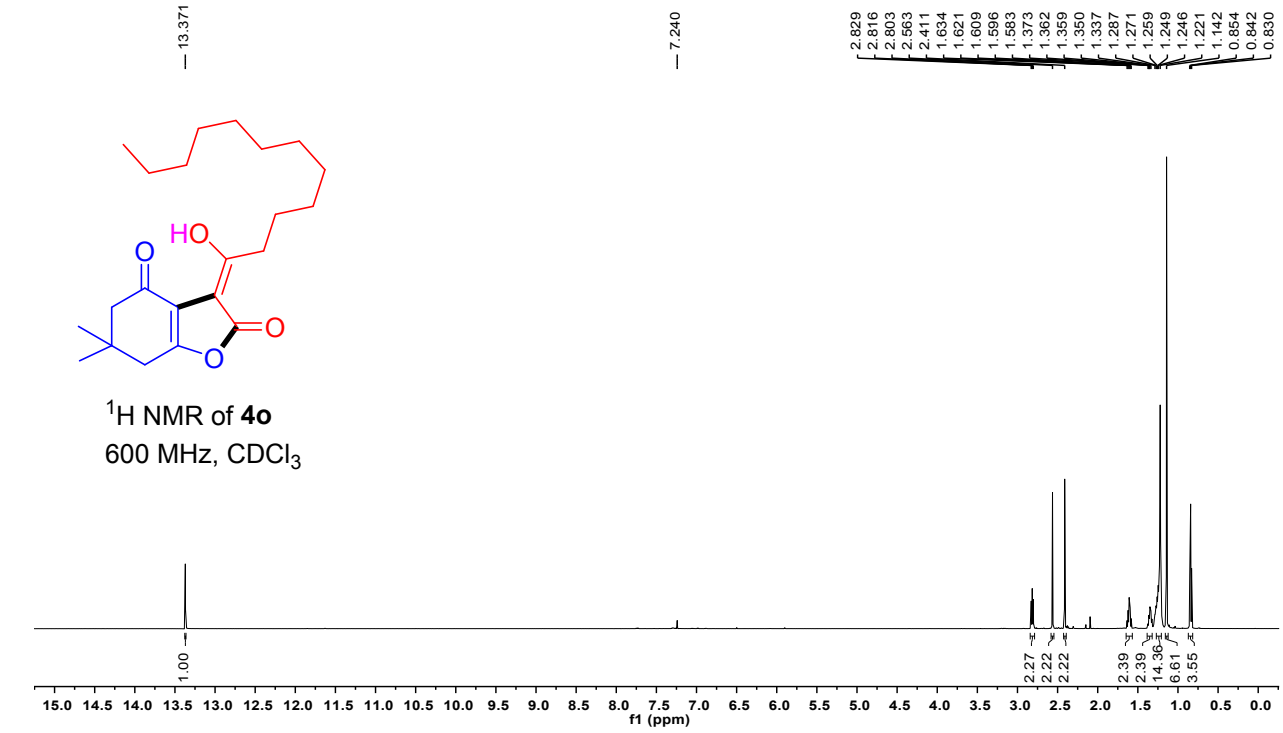


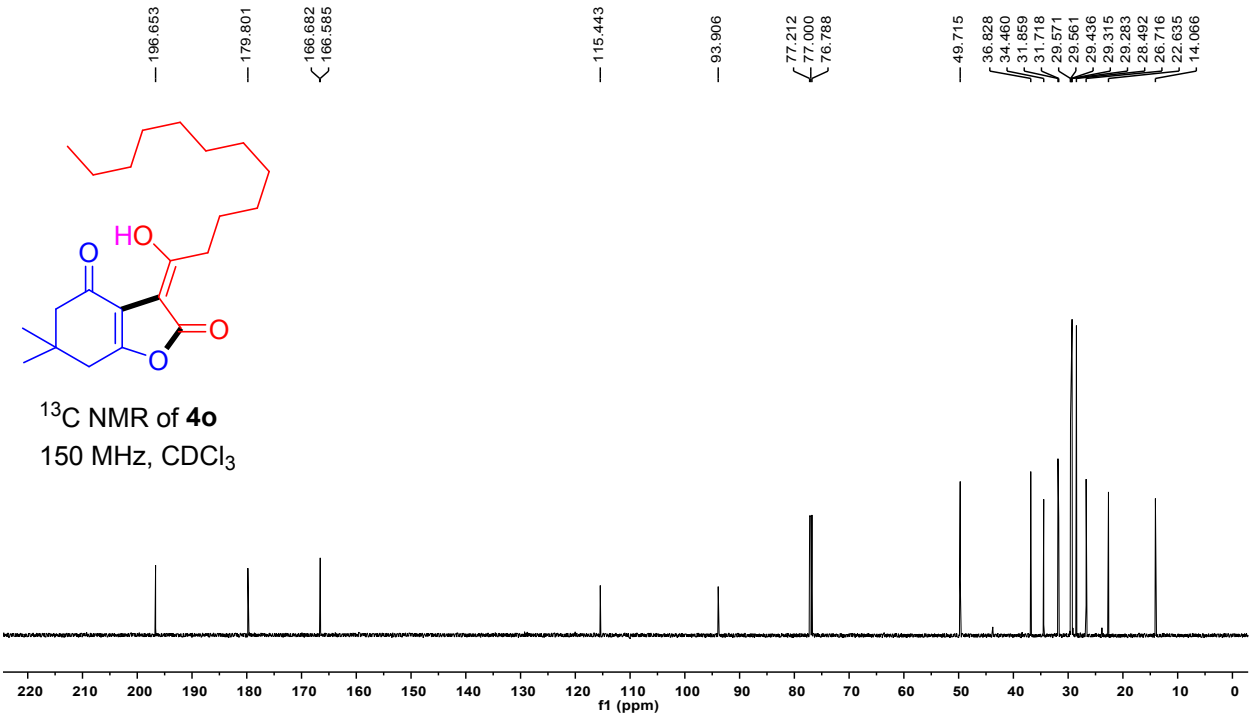
^{13}C NMR of **4m**
150 MHz, $CDCl_3$



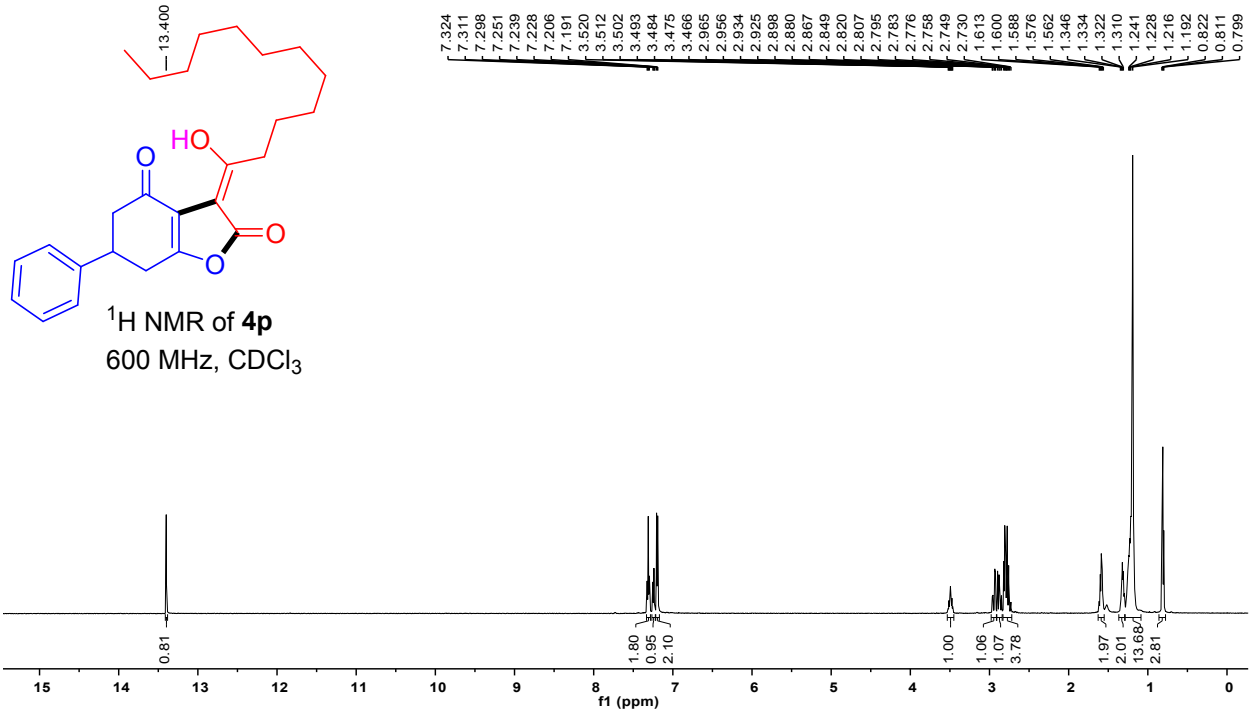
^{1}H NMR of **4n**
600 MHz, $CDCl_3$


196.023
180.315
166.739
166.486
148.088
146.931
135.087
119.803
116.561
108.579
106.957
101.227
93.857
77.212
77.000
76.788
43.086
39.857
31.725
31.380
30.922
26.417
22.368
13.891
HO
O
O
O
O
O
13C NMR of 4n
150 MHz, CDCl3
f1 (ppm)

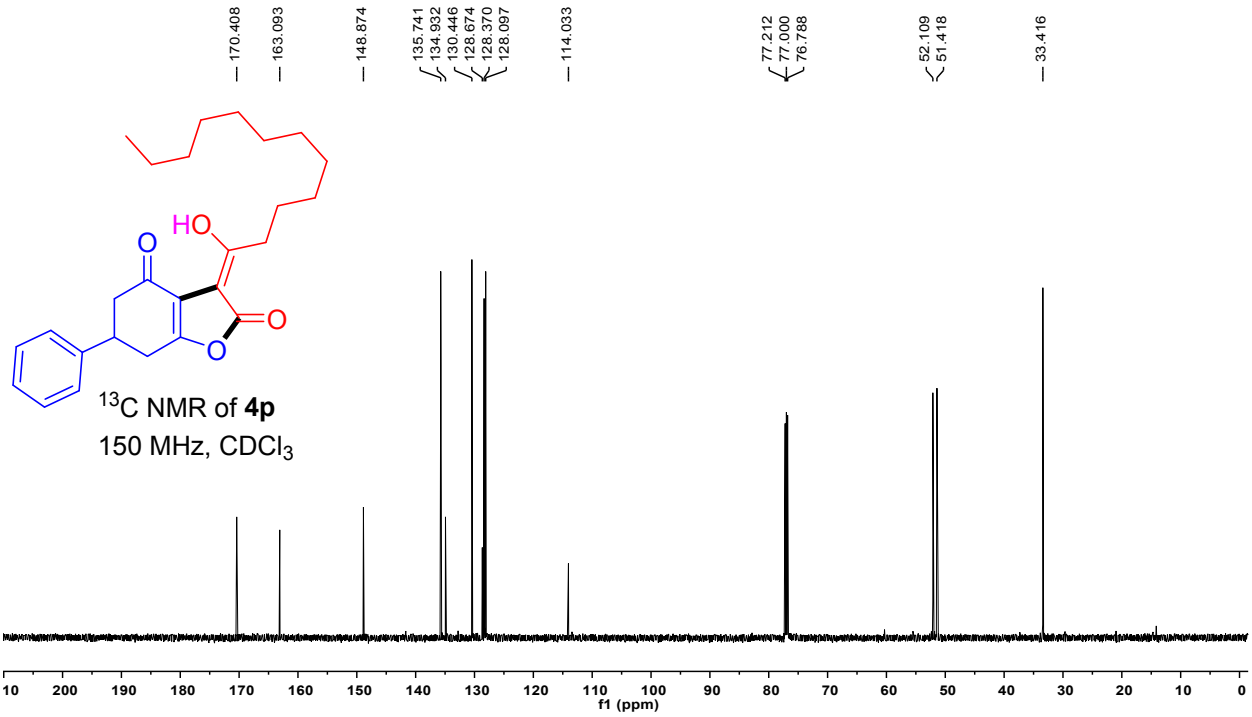

13.371
7.240
2.829
2.816
2.803
2.583
2.411
1.634
1.621
1.609
1.596
1.583
1.373
1.362
1.359
1.350
1.337
1.287
1.271
1.259
1.249
1.246
1.221
1.142
0.854
0.842
0.830
HO
O
O
O
1H NMR of 4o
600 MHz, CDCl3
1.00
2.27
2.22
2.22
2.39
2.39
14.36
6.61
3.55
f1 (ppm)

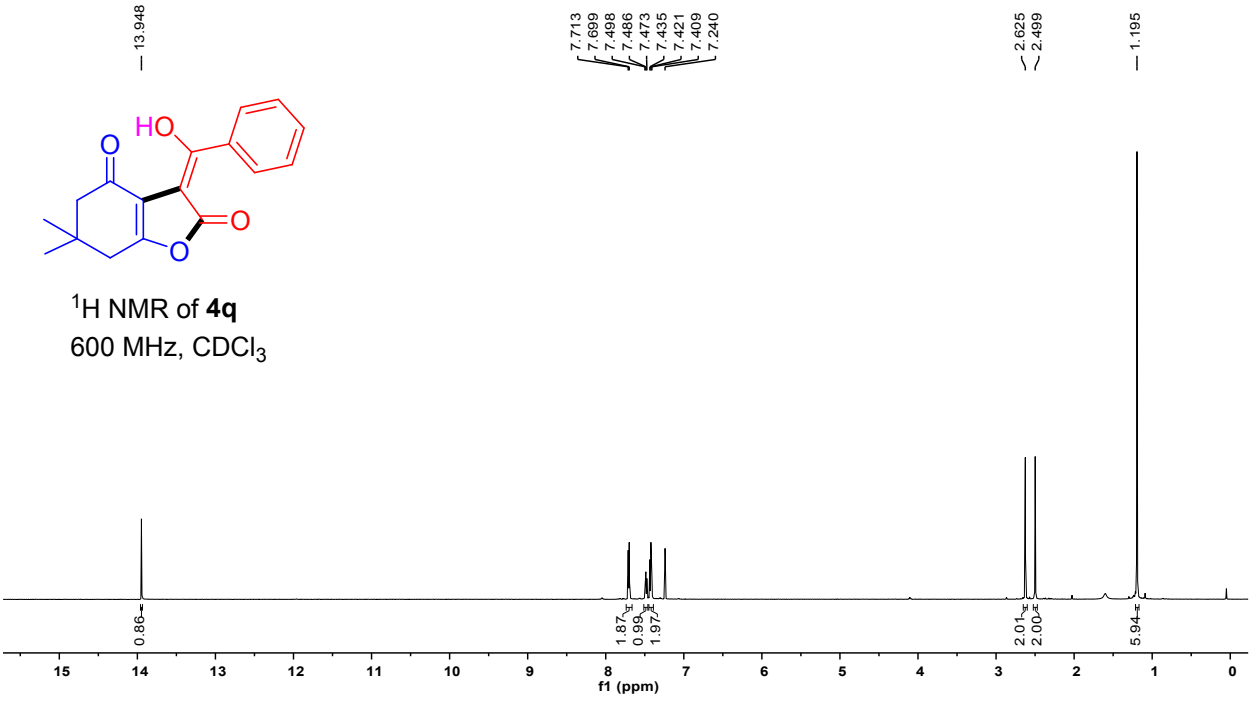


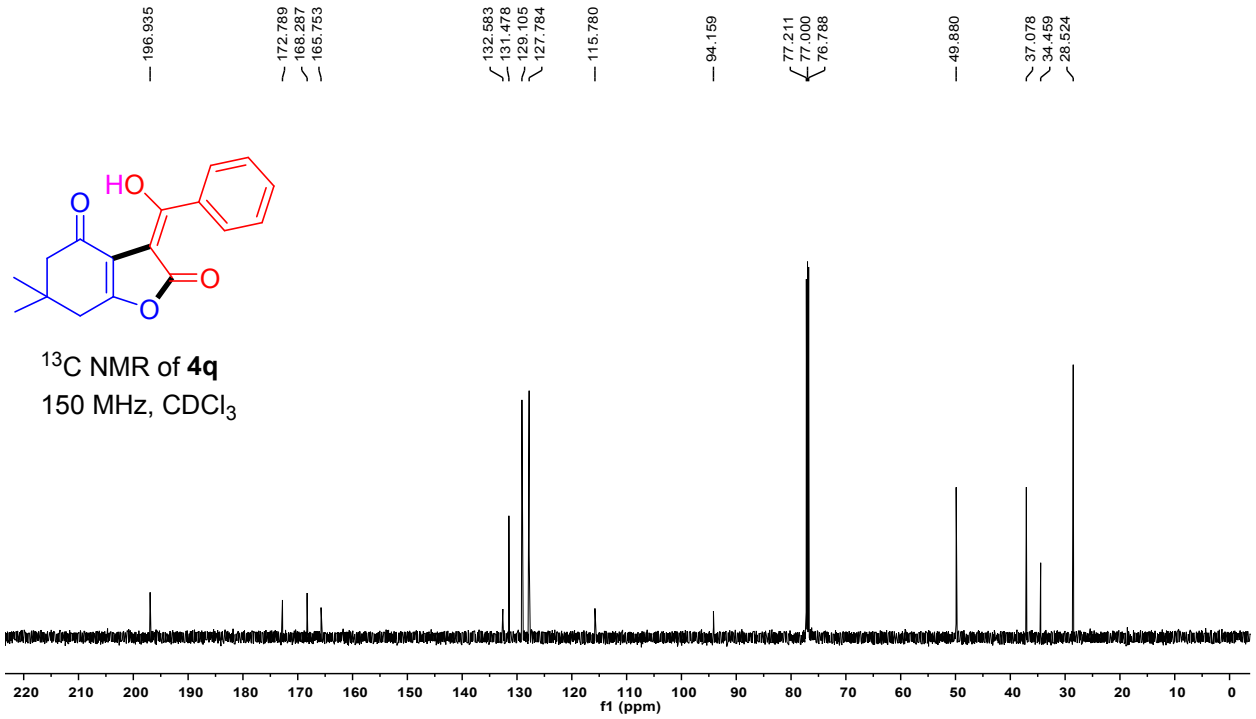
^{13}C NMR of **4o**
150 MHz, $CDCl_3$



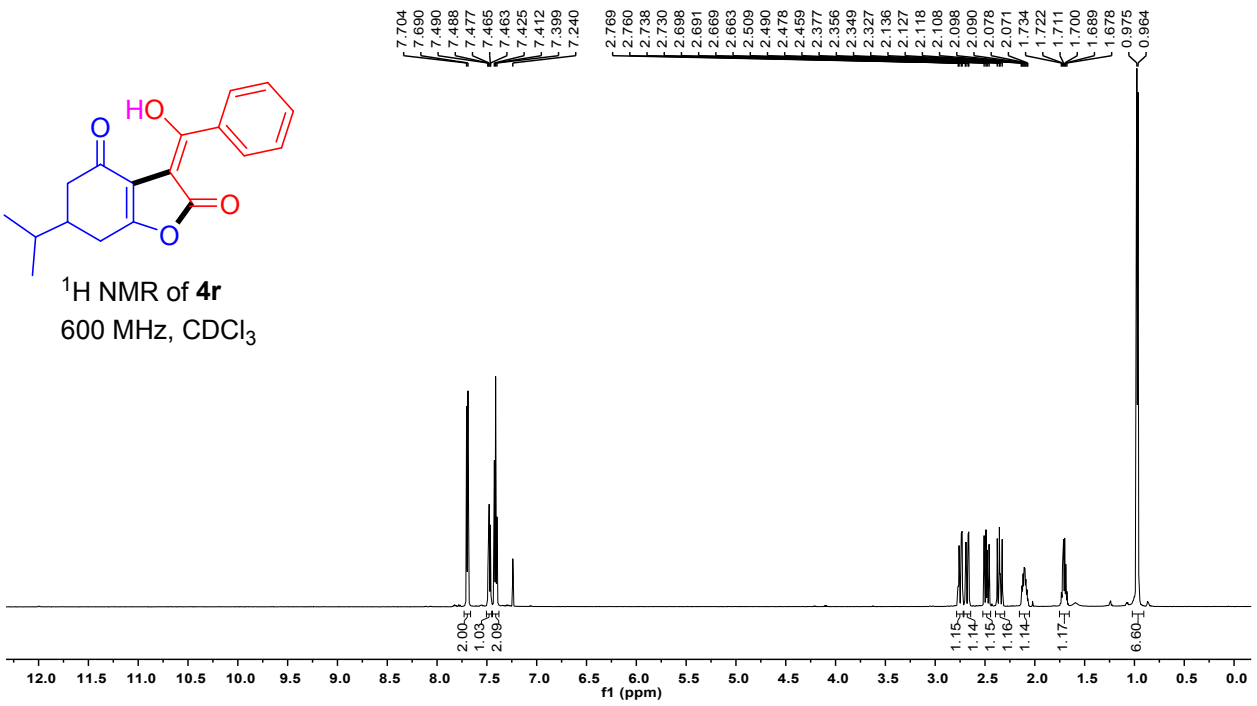
^{1}H NMR of **4p**
600 MHz, $CDCl_3$


170.408
163.093
148.874
135.741
134.932
130.446
128.674
128.370
128.097
114.033
77.212
77.000
76.788
52.109
51.418
33.416
HO
O
O
O
13C NMR of 4p
150 MHz, CDCl3
f1 (ppm)

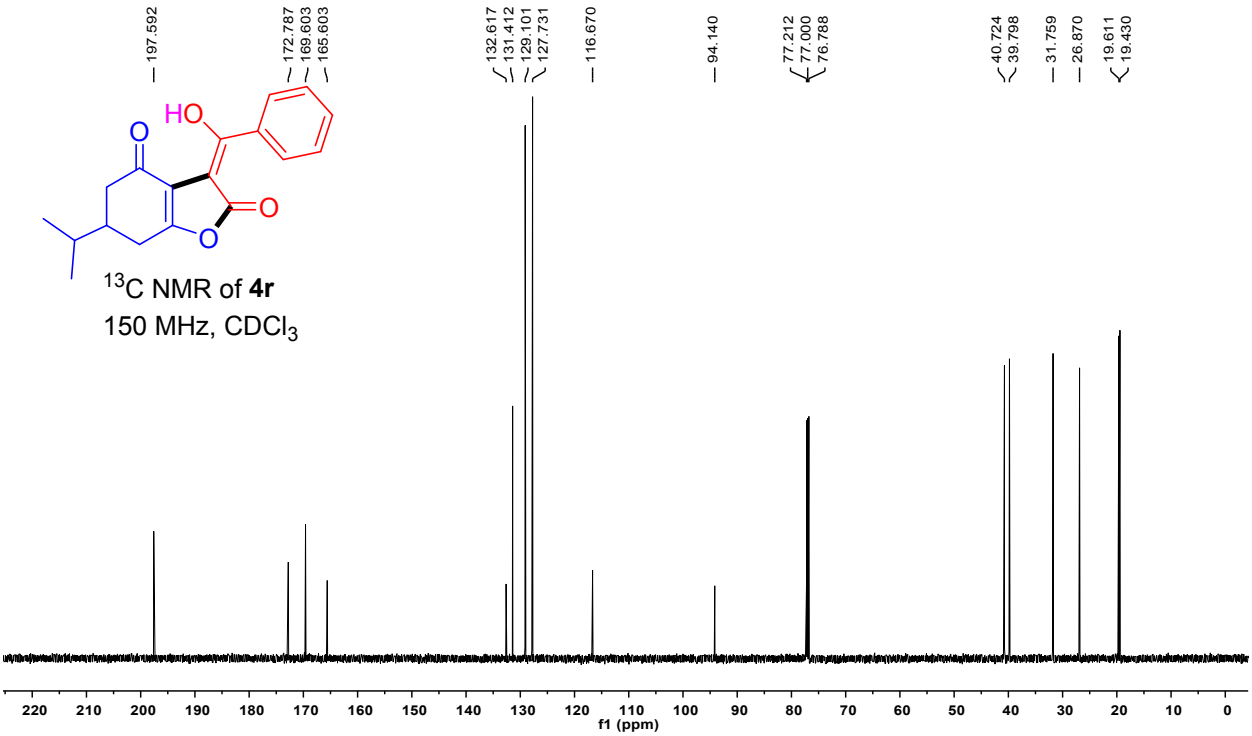

13.948
7.713
7.699
7.498
7.486
7.473
7.435
7.421
7.409
7.240
2.625
2.499
1.195
HO
O
O
O
1H NMR of 4q
600 MHz, CDCl3
0.86
1.87
0.99
1.97
2.01
2.00
5.94
f1 (ppm)



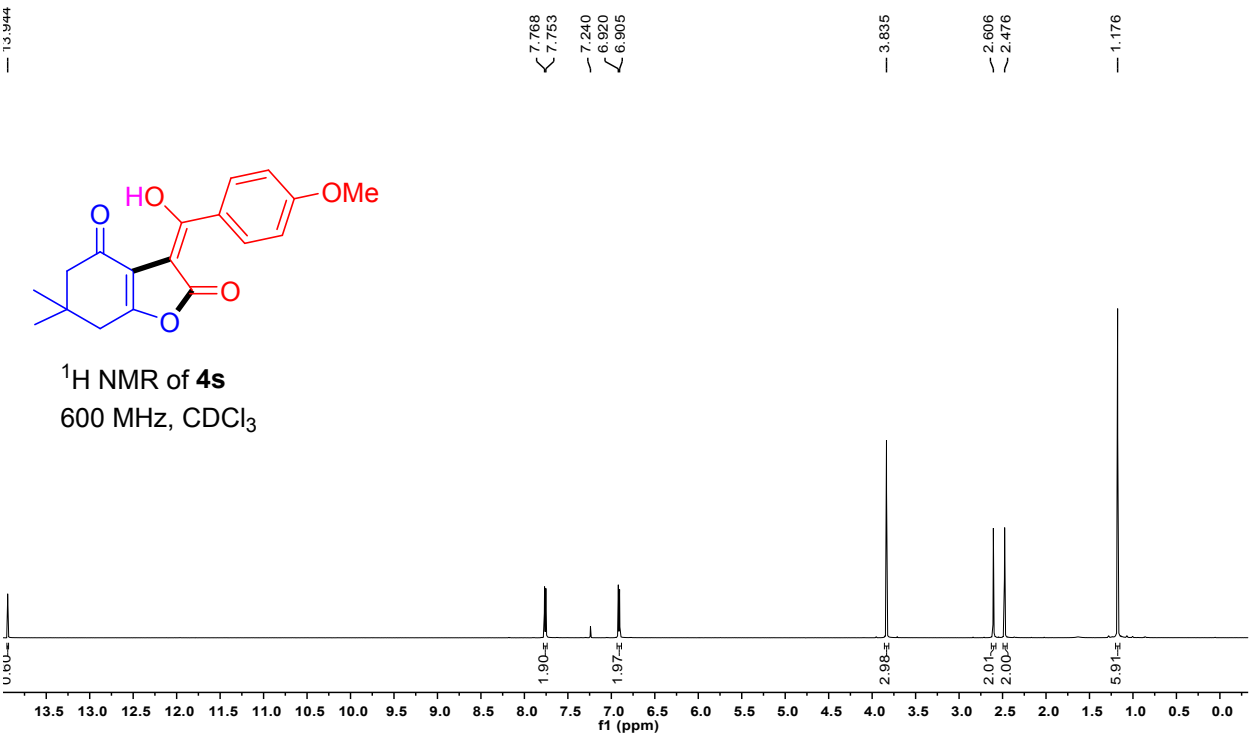
^{13}C NMR of **4q**
150 MHz, $CDCl_3$



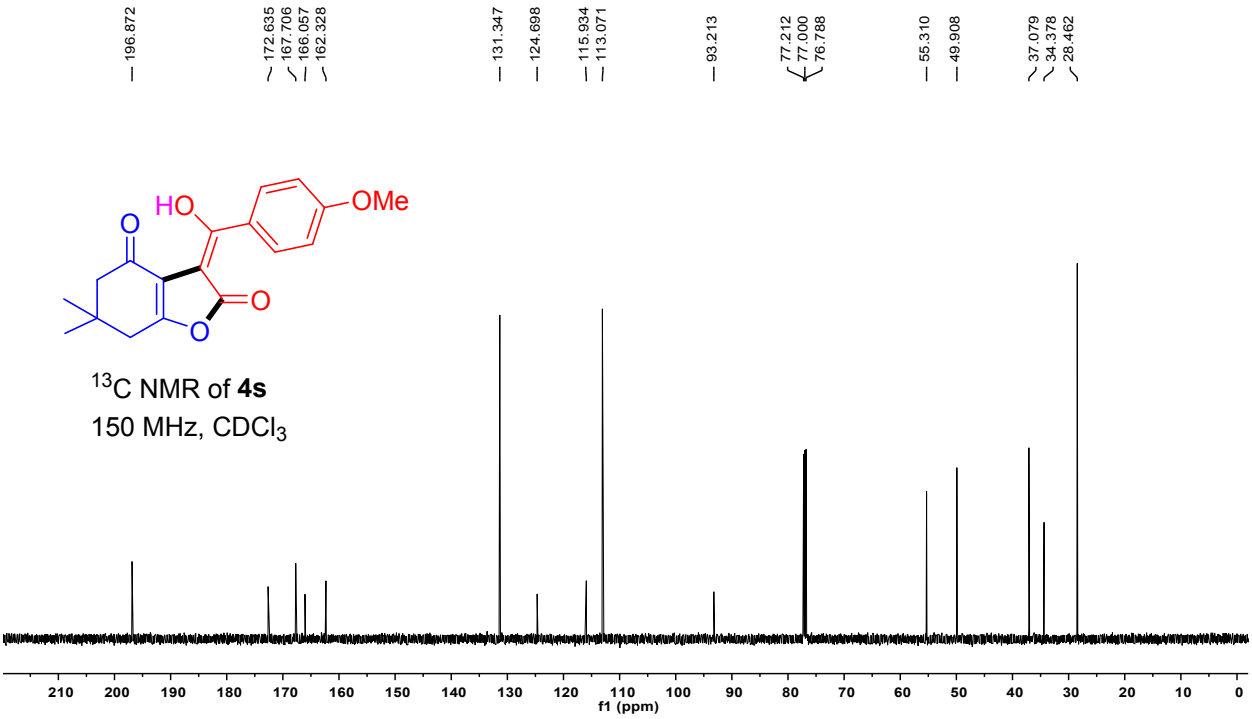
^{1}H NMR of **4r**
600 MHz, $CDCl_3$



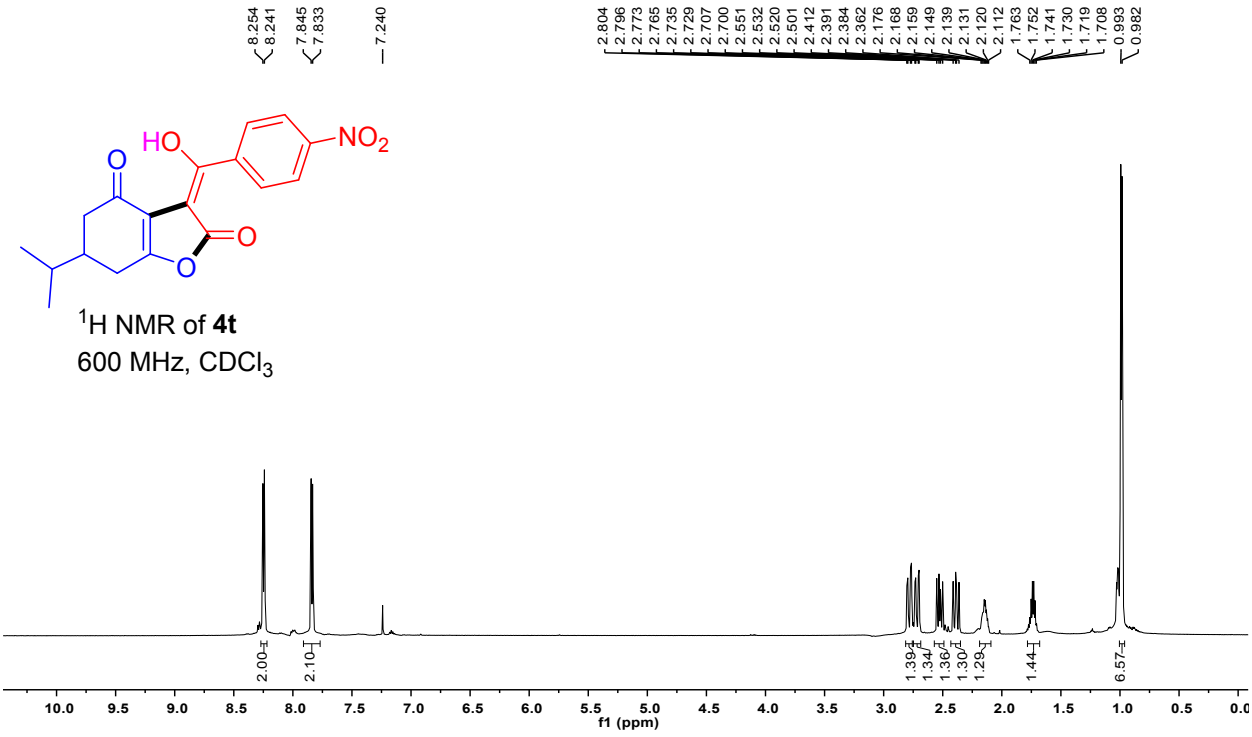
^{13}C NMR of **4r**
150 MHz, $CDCl_3$



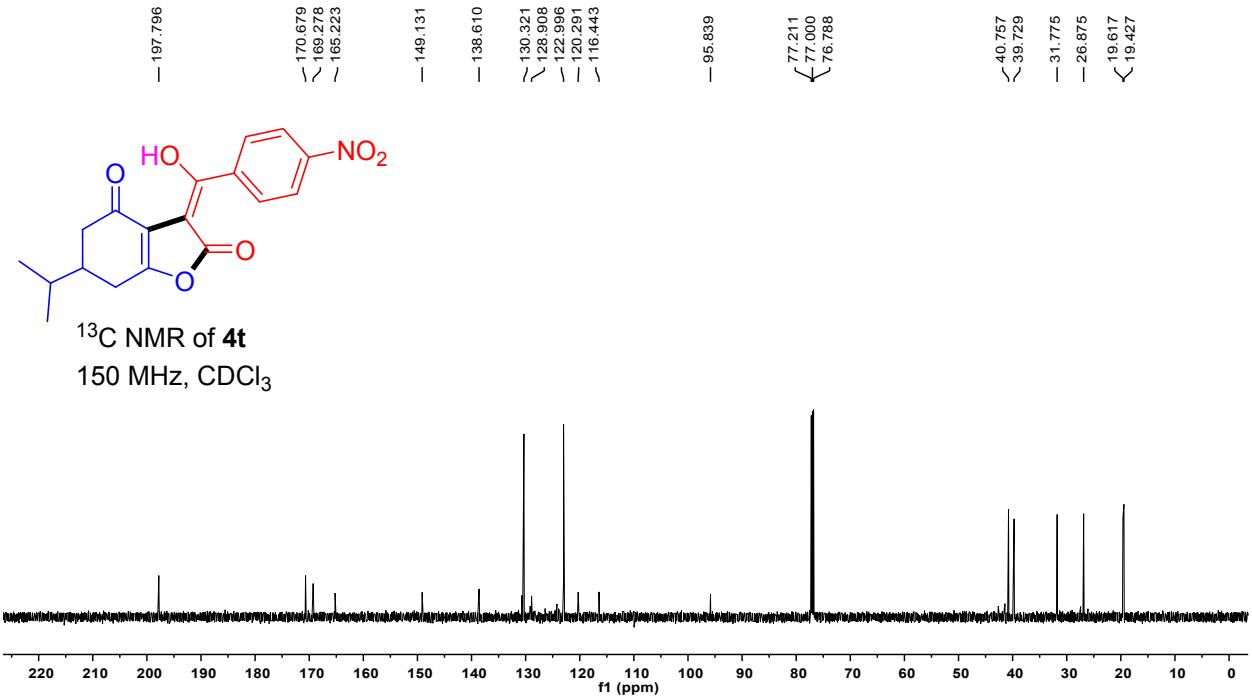
^{1}H NMR of **4s**
600 MHz, $CDCl_3$

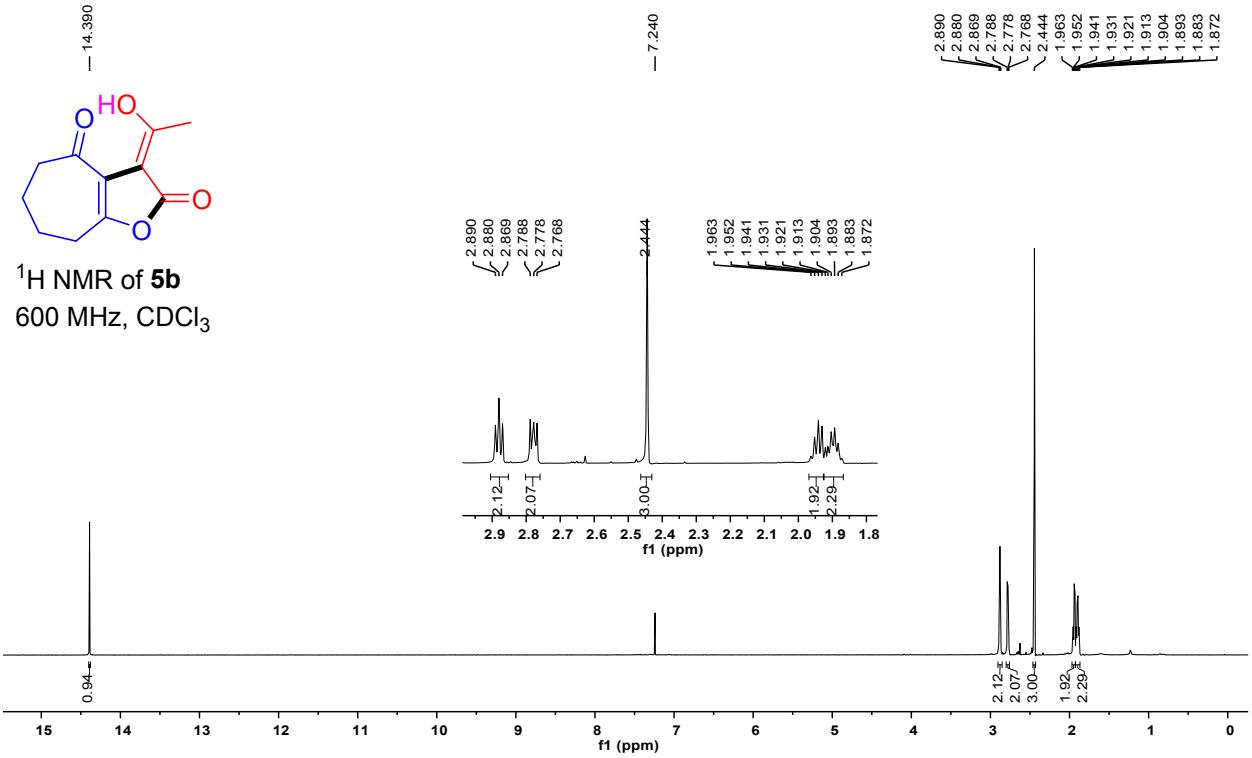


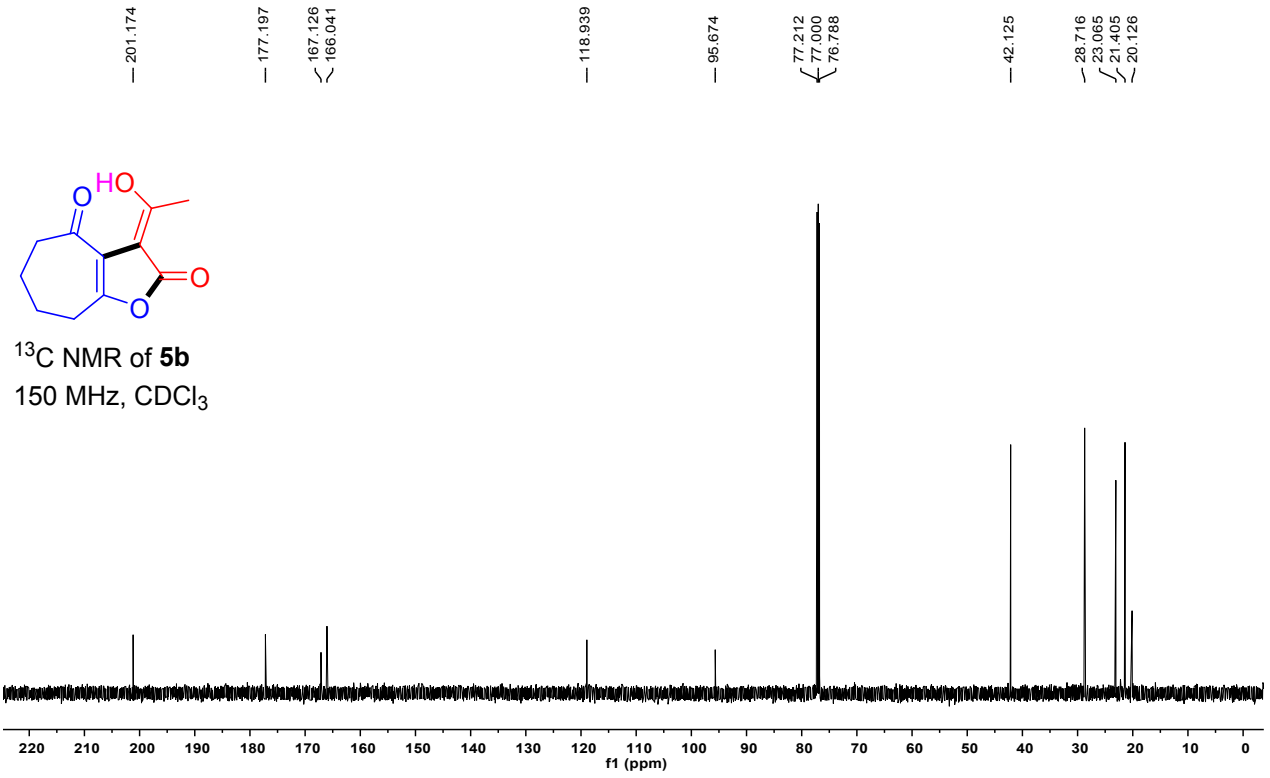
^{13}C NMR of **4s**
150 MHz, $CDCl_3$



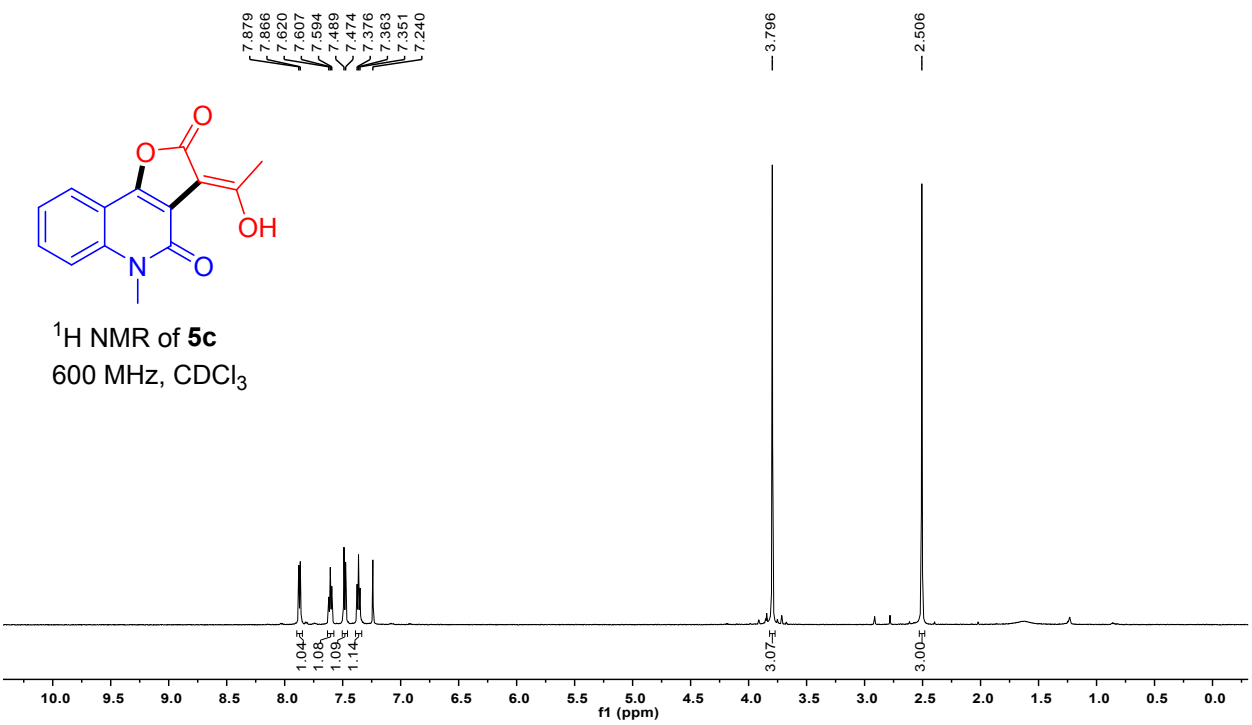
^{1}H NMR of **4t**
600 MHz, $CDCl_3$


197.796
170.679
169.278
165.223
149.131
138.610
130.321
128.908
122.996
120.291
116.443
95.839
77.211
77.000
76.788
40.757
39.729
31.775
26.875
19.617
19.427
HO
NO2
O
O
O
13C NMR of 4t
150 MHz, CDCl3
f1 (ppm)

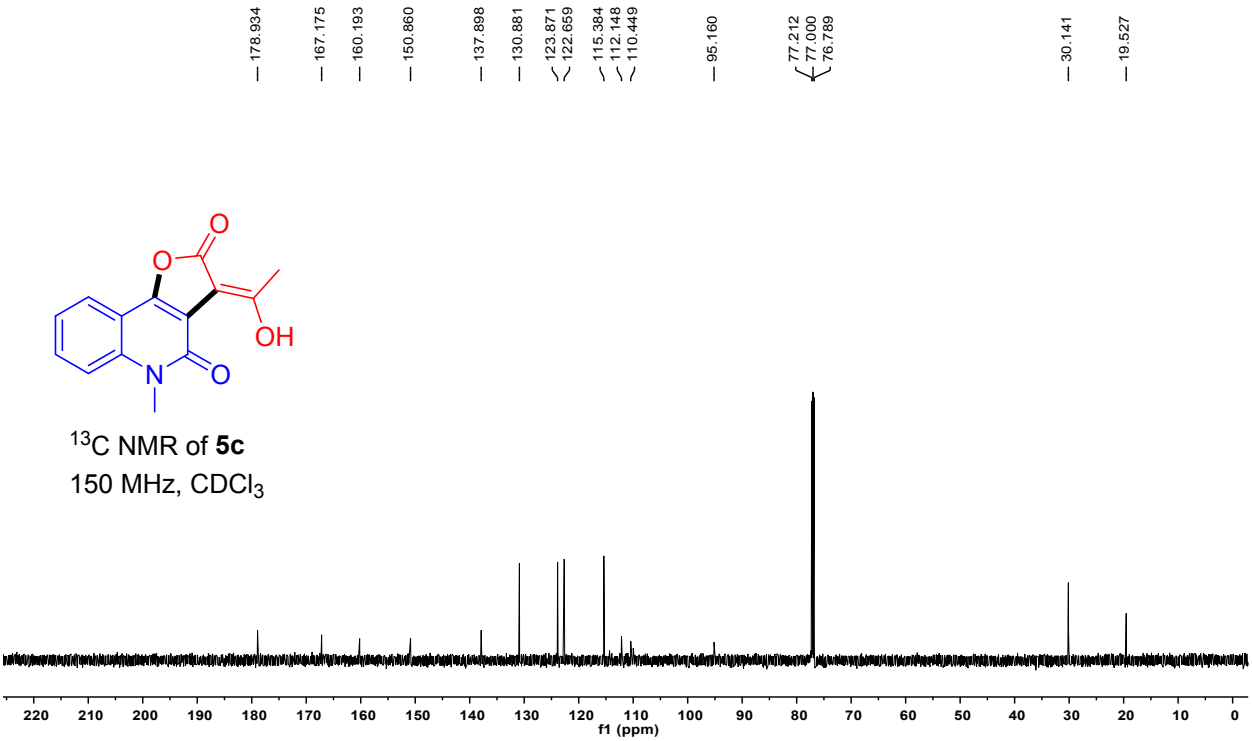

14.390
7.240
2.890
2.880
2.869
2.788
2.778
2.768
2.444
1.963
1.952
1.941
1.931
1.921
1.913
1.904
1.893
1.883
1.872
HO
O
O
O
1H NMR of 5b
600 MHz, CDCl3
0.94
2.12
2.07
3.00
1.92
2.29
f1 (ppm)

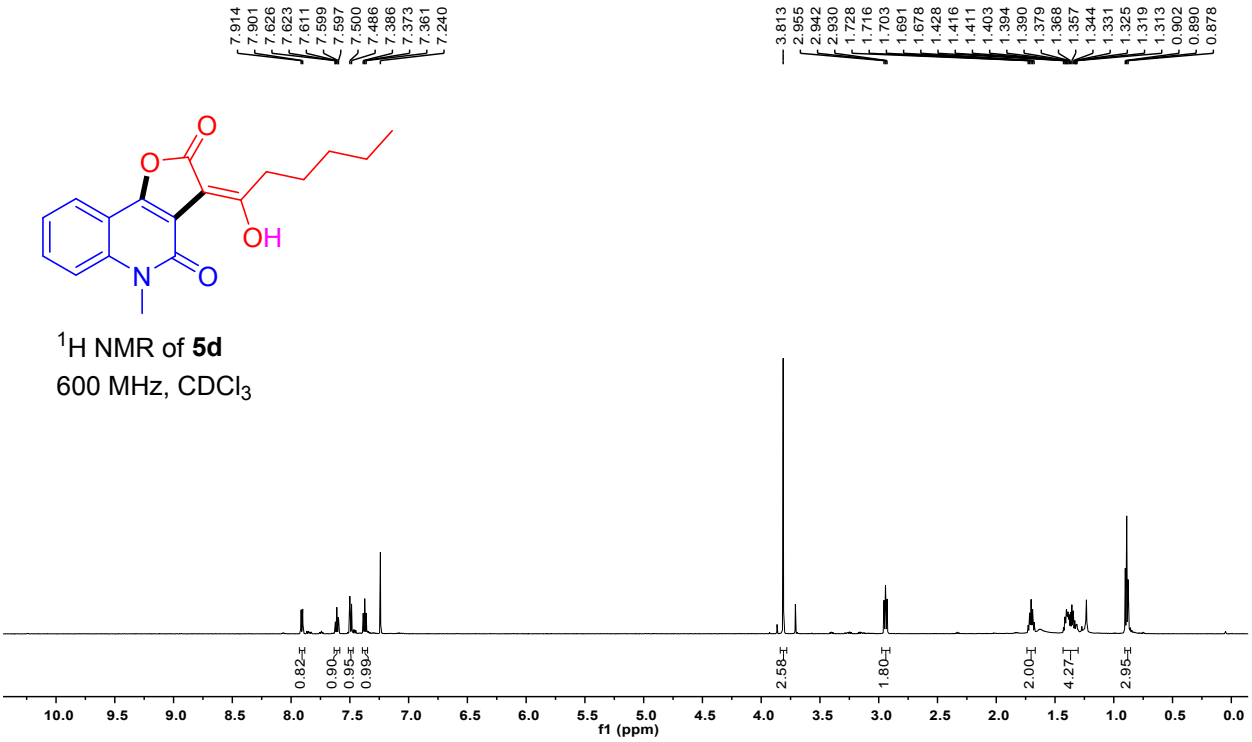


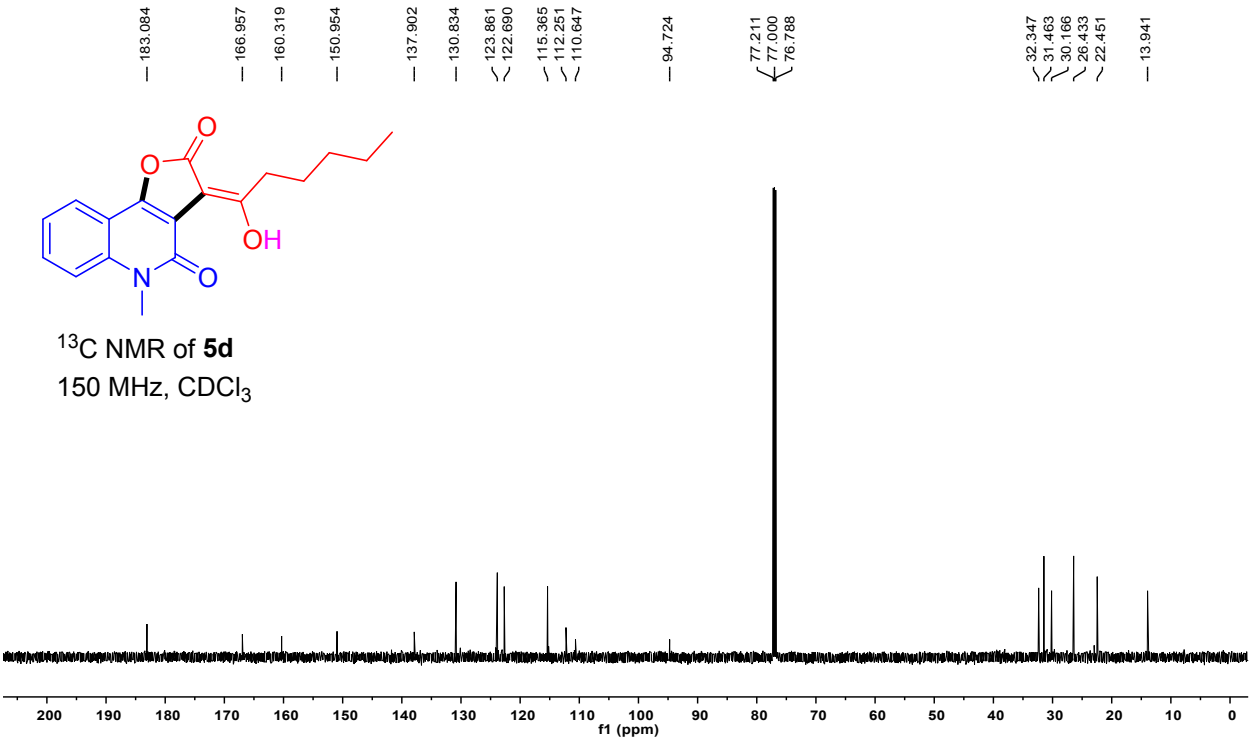
^{13}C NMR of **5b**
150 MHz, $CDCl_3$



^{1}H NMR of **5c**
600 MHz, $CDCl_3$


178.934
167.175
160.193
150.860
137.898
130.881
123.871
122.659
115.384
112.148
110.449
95.160
77.212
77.000
76.789
30.141
19.527
O
O
OH
N
O
13C NMR of 5c
150 MHz, CDCl3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.914
7.901
7.626
7.623
7.611
7.599
7.597
7.500
7.486
7.386
7.373
7.361
7.240
3.813
2.955
2.942
2.930
1.728
1.716
1.703
1.691
1.678
1.428
1.416
1.411
1.403
1.394
1.390
1.379
1.368
1.357
1.344
1.331
1.325
1.319
1.313
0.902
0.890
0.878
O
O
OH
N
O
1H NMR of 5d
600 MHz, CDCl3
0.82
0.90
0.95
0.99
2.58
1.80
2.00
4.27
2.95
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



^{13}C NMR of **5d**
150 MHz, $CDCl_3$

Crystal refinement data for compound 3c: Empirical Formula- $C_{11}H_{12}O_4$, M= 208.21, Monoclinic, Space group P_{bca}, a = 18.4754(11) Å, b = 10.1860(6) Å, c = 10.7954(6) Å, V = 2012.5(2) $Å^3$, Z = 8, T = 223(2) K, ρ_{calcd} = 1.374 Mg/m^3, $2\Theta_{max.}$ = 25.24^0, Refinement of 277 parameters on 3988 independent reflections out of 3988 collected reflections (R_{int} = 0.1049) led to R_1 = 0.1139 [I >2σ(I)], wR_2 = 0.1616 (all data) and S = 1.043 with the largest difference peak and hole of 0.458 and -0.196 $e.A^{o-3}$ respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1851023). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

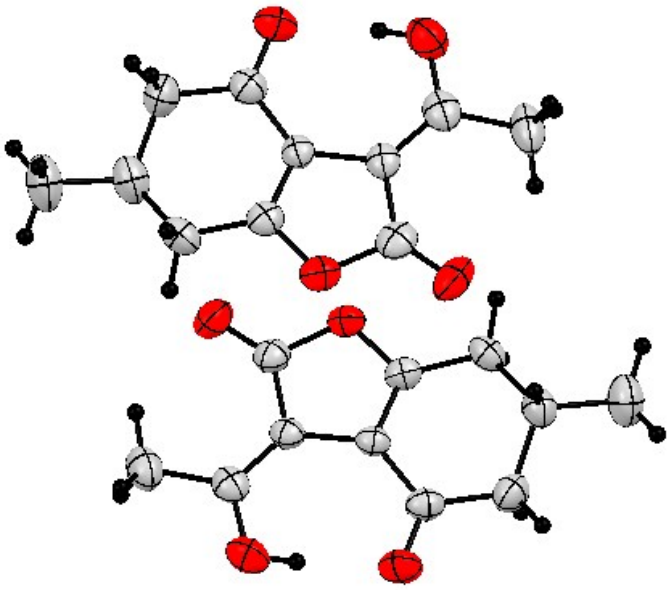


Figure S1. X-ray structure of compound **3c**.

Table S4. Crystal data and structure refinement for No 2.

Identification code	No2
Empirical formula	C_{11} H_{12} O_4
Formula weight	208.21
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	$P2_1/c$
Unit cell dimensions	a = 18.4754(11) Å □ a = 90°.
	b = 10.1860(6) b=97.8576(18)°.
	c = 10.7954(6) Å □√= 90°.
Volume	2012.5(2) $Å^3$
Z	8
Density (calculated)	1.374 Mg/m^3
Absorption coefficient	0.105 mm^{-1}
F(000)	880
Crystal size	0.300 x 0.250 x 0.130 mm^3
Theta range for data collection	2.226 to 26.080°.
Index ranges	-22<=h<=22, -12<=k<=12, -13<=l<=13
Reflections collected	54311
Independent reflections	3988 [R(int) = 0.1049]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7453 and 0.7068
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	3988 / 0 / 277
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0614, wR2 = 0.1372
R indices (all data)	R1 = 0.1139, wR2 = 0.1616
Extinction coefficient	n/a
Largest diff. peak and hole	0.458 and -0.196 e.Å-3

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for No 2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2751(1)	4577(2)	4976(2)	40(1)
C(1)	3187(2)	5243(3)	5971(3)	39(1)
C(2)	2736(1)	6268(3)	6390(2)	34(1)
C(3)	2038(1)	6168(2)	5587(2)	31(1)
C(4)	1377(2)	6927(3)	5492(3)	38(1)
C(5)	801(2)	6604(3)	4413(3)	45(1)
C(6)	767(2)	5162(3)	4038(3)	44(1)
C(7)	1516(2)	4676(3)	3812(3)	39(1)
C(8)	2085(2)	5164(3)	4793(2)	34(1)
O(2)	3803(1)	4880(2)	6272(2)	55(1)
C(9)	2959(2)	7107(3)	7343(3)	41(1)
O(3)	2530(1)	8053(2)	7672(2)	55(1)
C(10)	3688(2)	7088(3)	8117(3)	55(1)
O(4)	1292(1)	7828(2)	6234(2)	53(1)
C(11)	197(2)	4928(4)	2914(3)	64(1)
O(5)	2333(1)	3024(2)	7428(2)	45(1)
C(12)	1870(2)	2372(3)	6435(3)	46(1)
C(13)	2307(2)	1307(3)	6003(2)	36(1)
C(14)	3007(1)	1386(3)	6798(2)	33(1)
C(15)	3650(2)	588(3)	6871(3)	41(1)

C(16)	4246(2)	881(3)	7930(3)	54(1)
C(17)	4297(2)	2302(3)	8340(3)	54(1)
C(18)	3567(2)	2836(3)	8578(3)	43(1)
C(19)	2984(2)	2396(3)	7596(3)	37(1)
O(6)	1265(1)	2759(2)	6157(2)	60(1)
C(20)	2050(2)	460(3)	5086(3)	46(1)
O(7)	2458(1)	-523(2)	4743(2)	59(1)
C(21)	1302(2)	495(4)	4368(3)	62(1)
O(8)	3706(1)	-332(2)	6134(2)	55(1)
C(22)	4878(2)	2473(4)	9473(3)	69(1)

Table S6. Bond lengths [Å] and angles [°] for No2.

O(1)-C(8)	1.358(3)
O(1)-C(1)	1.422(3)
C(1)-O(2)	1.200(3)
C(1)-C(2)	1.447(4)
C(2)-C(9)	1.358(4)
C(2)-C(3)	1.455(4)
C(3)-C(8)	1.345(4)
C(3)-C(4)	1.438(4)
C(4)-O(4)#1	1.242(3)
C(4)-O(4)	1.242(3)
C(4)-C(5)	1.503(4)
C(5)-C(6)	1.522(4)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(6)-C(11)	1.514(4)
C(6)-C(7)	1.520(4)
C(6)-H(6)	0.9900
C(7)-C(8)	1.473(4)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(9)-O(3)	1.327(3)
C(9)-C(10)	1.484(4)
O(3)-H(3)	0.8300

C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(10)-H(10C)	0.9700
O(4)-O(4)#1	0.000(5)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(11)-H(11C)	0.9700
O(5)-C(19)	1.353(3)
O(5)-C(12)	1.439(4)
C(12)-O(6)	1.185(4)
C(12)-C(13)	1.466(4)
C(13)-C(20)	1.350(4)
C(13)-C(14)	1.454(4)
C(14)-C(19)	1.346(4)
C(14)-C(15)	1.432(4)
C(15)-O(8)#1	1.243(3)
C(15)-O(8)	1.243(3)
C(15)-C(16)	1.505(4)
C(16)-C(17)	1.513(4)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(17)-C(18)	1.510(4)
C(17)-C(22)	1.523(4)
C(17)-H(17)	0.9900
C(18)-C(19)	1.473(4)

C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(20)-O(7)	1.335(4)
C(20)-C(21)	1.490(4)
O(7)-H(7)	0.8300
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(21)-H(21C)	0.9700
O(8)-O(8)#1	0.000(6)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(22)-H(22C)	0.9700
C(8)-O(1)-C(1)	108.0(2)
O(2)-C(1)-O(1)	118.5(3)
O(2)-C(1)-C(2)	134.7(3)
O(1)-C(1)-C(2)	106.9(2)
C(9)-C(2)-C(1)	124.3(3)
C(9)-C(2)-C(3)	130.4(3)
C(1)-C(2)-C(3)	105.3(2)
C(8)-C(3)-C(4)	119.5(3)
C(8)-C(3)-C(2)	107.7(2)
C(4)-C(3)-C(2)	132.8(2)
O(4)#1-C(4)-C(3)	122.2(3)
O(4)-C(4)-C(3)	122.2(3)
O(4)#1-C(4)-C(5)	121.5(3)

O(4)-C(4)-C(5)	121.5(3)
C(3)-C(4)-C(5)	116.2(2)
C(4)-C(5)-C(6)	114.6(2)
C(4)-C(5)-H(5A)	108.6
C(6)-C(5)-H(5A)	108.6
C(4)-C(5)-H(5B)	108.6
C(6)-C(5)-H(5B)	108.6
H(5A)-C(5)-H(5B)	107.6
C(11)-C(6)-C(7)	111.6(3)
C(11)-C(6)-C(5)	111.3(3)
C(7)-C(6)-C(5)	110.6(2)
C(11)-C(6)-H(6)	107.7
C(7)-C(6)-H(6)	107.7
C(5)-C(6)-H(6)	107.7
C(8)-C(7)-C(6)	110.5(2)
C(8)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(3)-C(8)-O(1)	112.2(2)
C(3)-C(8)-C(7)	127.8(3)
O(1)-C(8)-C(7)	120.0(2)
O(3)-C(9)-C(2)	122.0(3)
O(3)-C(9)-C(10)	112.8(3)

C(2)-C(9)-C(10) 125.2(3)

C(9)-O(3)-H(3) 109.5

C(9)-C(10)-H(10A) 109.5

C(9)-C(10)-H(10B) 109.5

H(10A)-C(10)-H(10B) 109.5

C(9)-C(10)-H(10C) 109.5

H(10A)-C(10)-H(10C) 109.5

H(10B)-C(10)-H(10C) 109.5

C(6)-C(11)-H(11A) 109.5

C(6)-C(11)-H(11B) 109.5

H(11A)-C(11)-H(11B) 109.5

C(6)-C(11)-H(11C) 109.5

H(11A)-C(11)-H(11C) 109.5

H(11B)-C(11)-H(11C) 109.5

C(19)-O(5)-C(12) 108.0(2)

O(6)-C(12)-O(5) 118.6(3)

O(6)-C(12)-C(13) 134.9(3)

O(5)-C(12)-C(13) 106.4(2)

C(20)-C(13)-C(14) 131.6(3)

C(20)-C(13)-C(12) 123.6(3)

C(14)-C(13)-C(12) 104.8(2)

C(19)-C(14)-C(15) 119.8(3)

C(19)-C(14)-C(13) 108.5(2)

C(15)-C(14)-C(13) 131.7(3)

O(8)#1-C(15)-C(14) 122.3(3)

O(8)-C(15)-C(14) 122.3(3)

O(8)#1-C(15)-C(16) 121.3(3)

O(8)-C(15)-C(16) 121.3(3)

C(14)-C(15)-C(16) 116.4(3)

C(15)-C(16)-C(17) 115.0(3)

C(15)-C(16)-H(16A) 108.5

C(17)-C(16)-H(16A) 108.5

C(15)-C(16)-H(16B) 108.5

C(17)-C(16)-H(16B) 108.5

H(16A)-C(16)-H(16B) 107.5

C(18)-C(17)-C(16) 111.8(3)

C(18)-C(17)-C(22) 111.7(3)

C(16)-C(17)-C(22) 110.7(3)

C(18)-C(17)-H(17) 107.4

C(16)-C(17)-H(17) 107.4

C(22)-C(17)-H(17) 107.4

C(19)-C(18)-C(17) 110.5(2)

C(19)-C(18)-H(18A) 109.5

C(17)-C(18)-H(18A) 109.5

C(19)-C(18)-H(18B) 109.5

C(17)-C(18)-H(18B) 109.5

H(18A)-C(18)-H(18B) 108.1

C(14)-C(19)-O(5) 112.4(3)

C(14)-C(19)-C(18) 127.5(3)

O(5)-C(19)-C(18) 120.1(3)

O(7)-C(20)-C(13) 121.9(3)

O(7)-C(20)-C(21) 113.1(3)

C(13)-C(20)-C(21) 125.0(3)

C(20)-O(7)-H(7) 109.5

C(20)-C(21)-H(21A) 109.5

C(20)-C(21)-H(21B) 109.5

H(21A)-C(21)-H(21B) 109.5

C(20)-C(21)-H(21C) 109.5

H(21A)-C(21)-H(21C) 109.5

H(21B)-C(21)-H(21C) 109.5

C(17)-C(22)-H(22A) 109.5

C(17)-C(22)-H(22B) 109.5

H(22A)-C(22)-H(22B) 109.5

C(17)-C(22)-H(22C) 109.5

H(22A)-C(22)-H(22C) 109.5

H(22B)-C(22)-H(22C) 109.5

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z

Table S7. Anisotropic displacement parameters ($Å^2$x 10^3) for No2. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U11	U22	U33	U23	U13	U12
O(1)	42(1)	34(1)	45(1)	-5(1)	8(1)	6(1)
C(1)	40(2)	34(2)	44(2)	5(1)	5(1)	0(1)
C(2)	38(2)	29(1)	34(2)	3(1)	6(1)	0(1)
C(3)	35(2)	27(1)	32(1)	1(1)	9(1)	-1(1)
C(4)	41(2)	33(2)	43(2)	2(1)	12(1)	1(1)
C(5)	36(2)	47(2)	52(2)	5(2)	4(1)	4(1)
C(6)	43(2)	48(2)	40(2)	0(1)	1(1)	-4(1)
C(7)	48(2)	38(2)	33(2)	-4(1)	6(1)	-7(1)
C(8)	37(2)	33(2)	33(2)	4(1)	10(1)	3(1)
O(2)	40(1)	51(1)	72(2)	3(1)	1(1)	10(1)
C(9)	48(2)	37(2)	38(2)	5(1)	6(1)	-5(1)
O(3)	64(2)	49(1)	51(1)	-18(1)	8(1)	2(1)
C(10)	61(2)	53(2)	47(2)	4(2)	-8(2)	-10(2)
O(4)	54(1)	45(1)	62(1)	-16(1)	14(1)	10(1)
C(11)	56(2)	83(3)	48(2)	-4(2)	-6(2)	-7(2)
O(5)	47(1)	39(1)	51(1)	1(1)	11(1)	4(1)
C(12)	49(2)	39(2)	49(2)	16(2)	9(2)	-1(2)
C(13)	40(2)	35(2)	32(2)	9(1)	3(1)	-5(1)
C(14)	37(2)	32(2)	31(1)	5(1)	2(1)	-2(1)
C(15)	44(2)	39(2)	41(2)	3(1)	8(1)	-3(1)

C(16)	41(2)	56(2)	62(2)	0(2)	-3(2)	3(2)
C(17)	50(2)	65(2)	47(2)	-5(2)	1(2)	-12(2)
C(18)	54(2)	38(2)	38(2)	-5(1)	9(1)	-9(1)
C(19)	40(2)	35(2)	37(2)	7(1)	9(1)	-2(1)
O(6)	43(1)	63(2)	72(2)	19(1)	2(1)	12(1)
C(20)	54(2)	43(2)	41(2)	9(2)	2(2)	-10(2)
O(7)	67(2)	54(1)	53(1)	-11(1)	2(1)	-4(1)
C(21)	61(2)	63(2)	54(2)	13(2)	-17(2)	-22(2)
O(8)	61(2)	47(1)	57(1)	-13(1)	8(1)	8(1)
C(22)	56(2)	95(3)	52(2)	-6(2)	-6(2)	-17(2)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for No2.

	x	y	z	U(eq)
H(5A)	891	7128	3689	55
H(5B)	324	6863	4632	55
H(6)	622	4654	4746	53
H(7A)	1520	3714	3808	47
H(7B)	1618	4982	2992	47
H(3)	2129	8023	7219	82
H(10A)	3989	7780	7842	82
H(10B)	3919	6245	8027	82
H(10C)	3631	7227	8987	82
H(11A)	-277	5217	3101	95
H(11B)	176	3999	2715	95
H(11C)	325	5417	2204	95
H(16A)	4715	620	7678	65
H(16B)	4167	338	8650	65
H(17)	4455	2817	7646	65
H(18A)	3460	2532	9396	52
H(18B)	3584	3797	8593	52
H(7)	2863	-515	5182	88
H(21A)	1330	340	3490	93
H(21B)	1084	1349	4468	93

H(21C)	1003	-180	4680	93
H(22A)	4742	1973	10170	104
H(22B)	4919	3395	9698	104
H(22C)	5345	2160	9273	104

Table S9. Torsion angles [°] for No2.

C(8)-O(1)-C(1)-O(2)	-179.2(2)
C(8)-O(1)-C(1)-C(2)	0.6(3)
O(2)-C(1)-C(2)-C(9)	-1.1(5)
O(1)-C(1)-C(2)-C(9)	179.1(2)
O(2)-C(1)-C(2)-C(3)	179.0(3)
O(1)-C(1)-C(2)-C(3)	-0.8(3)
C(9)-C(2)-C(3)-C(8)	-179.2(3)
C(1)-C(2)-C(3)-C(8)	0.7(3)
C(9)-C(2)-C(3)-C(4)	2.9(5)
C(1)-C(2)-C(3)-C(4)	-177.2(3)
C(8)-C(3)-C(4)-O(4)#1	176.8(3)
C(2)-C(3)-C(4)-O(4)#1	-5.5(5)
C(8)-C(3)-C(4)-O(4)	176.8(3)
C(2)-C(3)-C(4)-O(4)	-5.5(5)
C(8)-C(3)-C(4)-C(5)	-5.3(4)
C(2)-C(3)-C(4)-C(5)	172.4(3)
O(4)#1-C(4)-C(5)-C(6)	-148.7(3)
O(4)-C(4)-C(5)-C(6)	-148.7(3)
C(3)-C(4)-C(5)-C(6)	33.4(4)
C(4)-C(5)-C(6)-C(11)	-177.6(3)
C(4)-C(5)-C(6)-C(7)	-52.9(3)
C(11)-C(6)-C(7)-C(8)	167.8(3)
C(5)-C(6)-C(7)-C(8)	43.2(3)

C(4)-C(3)-C(8)-O(1)	177.9(2)
C(2)-C(3)-C(8)-O(1)	-0.4(3)
C(4)-C(3)-C(8)-C(7)	-2.3(4)
C(2)-C(3)-C(8)-C(7)	179.5(3)
C(1)-O(1)-C(8)-C(3)	-0.2(3)
C(1)-O(1)-C(8)-C(7)	180.0(2)
C(6)-C(7)-C(8)-C(3)	-17.9(4)
C(6)-C(7)-C(8)-O(1)	161.9(2)
C(1)-C(2)-C(9)-O(3)	178.3(3)
C(3)-C(2)-C(9)-O(3)	-1.9(5)
C(1)-C(2)-C(9)-C(10)	-1.4(4)
C(3)-C(2)-C(9)-C(10)	178.5(3)
C(3)-C(4)-O(4)-O(4)#1	0.0(6)
C(5)-C(4)-O(4)-O(4)#1	0.0(5)
C(19)-O(5)-C(12)-O(6)	178.5(3)
C(19)-O(5)-C(12)-C(13)	-1.0(3)
O(6)-C(12)-C(13)-C(20)	-0.6(5)
O(5)-C(12)-C(13)-C(20)	178.9(2)
O(6)-C(12)-C(13)-C(14)	-178.5(3)
O(5)-C(12)-C(13)-C(14)	1.0(3)
C(20)-C(13)-C(14)-C(19)	-178.3(3)
C(12)-C(13)-C(14)-C(19)	-0.6(3)
C(20)-C(13)-C(14)-C(15)	-0.5(5)
C(12)-C(13)-C(14)-C(15)	177.2(3)
C(19)-C(14)-C(15)-O(8)#1	-178.0(3)

C(13)-C(14)-C(15)-O(8)#1	4.4(5)
C(19)-C(14)-C(15)-O(8)	-178.0(3)
C(13)-C(14)-C(15)-O(8)	4.4(5)
C(19)-C(14)-C(15)-C(16)	4.8(4)
C(13)-C(14)-C(15)-C(16)	-172.8(3)
O(8)#1-C(15)-C(16)-C(17)	151.7(3)
O(8)-C(15)-C(16)-C(17)	151.7(3)
C(14)-C(15)-C(16)-C(17)	-31.0(4)
C(15)-C(16)-C(17)-C(18)	50.6(4)
C(15)-C(16)-C(17)-C(22)	175.9(3)
C(16)-C(17)-C(18)-C(19)	-42.4(4)
C(22)-C(17)-C(18)-C(19)	-167.1(3)
C(15)-C(14)-C(19)-O(5)	-178.2(2)
C(13)-C(14)-C(19)-O(5)	-0.1(3)
C(15)-C(14)-C(19)-C(18)	1.3(4)
C(13)-C(14)-C(19)-C(18)	179.3(3)
C(12)-O(5)-C(19)-C(14)	0.7(3)
C(12)-O(5)-C(19)-C(18)	-178.8(2)
C(17)-C(18)-C(19)-C(14)	18.5(4)
C(17)-C(18)-C(19)-O(5)	-162.1(2)
C(14)-C(13)-C(20)-O(7)	-0.6(5)
C(12)-C(13)-C(20)-O(7)	-178.0(3)
C(14)-C(13)-C(20)-C(21)	178.6(3)
C(12)-C(13)-C(20)-C(21)	1.2(4)
C(14)-C(15)-O(8)-O(8)#1	0.0(2)

C(16)-C(15)-O(8)-O(8)#1 0.0(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z

Table S10. Hydrogen bonds for No2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7)-H(7)...O(8)#1	0.83	1.75	2.581(3)	174.4
O(3)-H(3)...O(4)#1	0.83	1.76	2.593(3)	175.5

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z