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# A new access to dihydrotropones through ring expansion of spirocyclohexadienones: Synthesis and mechanism<sup>§</sup>

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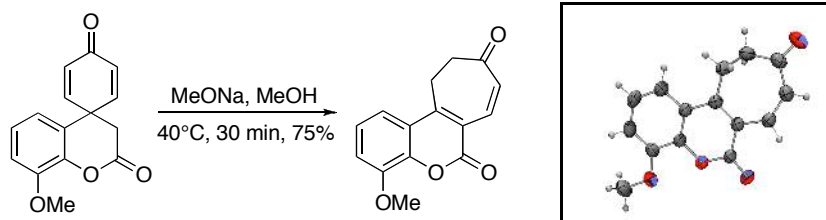
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**ABSTRACT** In this paper we report the rearrangement of spirocyclohexadienones into dihydrotropones in basic conditions as a new method for the preparation of seven-membered ring ketones, which are key building blocks for the synthesis of tropoloalkaloids. DFT calculations and deuterium labeling studies support the mechanism we propose for this rearrangement, involving the ring opening of a spirocyclopropane intermediate followed by successive base-catalyzed 1,3-hydrogen shifts. The X-ray

structure of the resulting dihydropyridone shows near-perfect planarity and the conjugation gain is likely to be the driving force of the reaction.

**KEYWORDS** dienone, dihydropyridone, rearrangement, DFT calculations

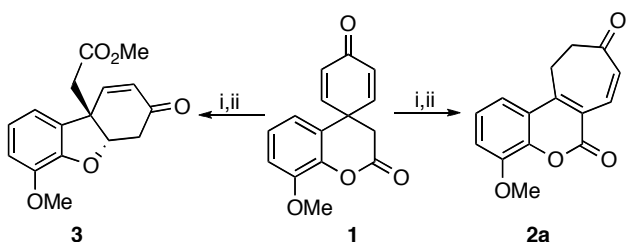
## Introduction

Substituted carbocyclic seven-membered rings are frequently found in natural and medicinally active compounds (e.g. hinokitiol,<sup>1</sup> thapsigargin,<sup>2</sup> colchicine<sup>3,4</sup>), and several methods for their synthesis are available,<sup>5-7</sup> among them, cycloadditions of allyl cations with 1,3-dienes,<sup>8-10</sup> metal-catalyzed cycloadditions,<sup>11-20</sup> electrochemical oxidations,<sup>21</sup> radical,<sup>22-24</sup> acidic<sup>25,26</sup> or thermal<sup>27,28</sup> ring expansion reactions.

We describe here a new method, the rearrangement of spirocyclohexadienones to one-carbon ring expansion products, dihydropyridones, under basic conditions.<sup>29</sup> A mechanism for this reaction is also proposed, which is fully supported by DFT calculations and deuterium labeling studies.

## Results and Discussion

*Reaction conditions.* In basic conditions, we observed conversion of the dienone **1**<sup>30</sup> into two products: a one carbon ring expansion product (**2a**) and a tricyclic ester (**3**) resulting from the lactone ring opening (Scheme 1). These two compounds are obtained in various ratios according to the reaction conditions.



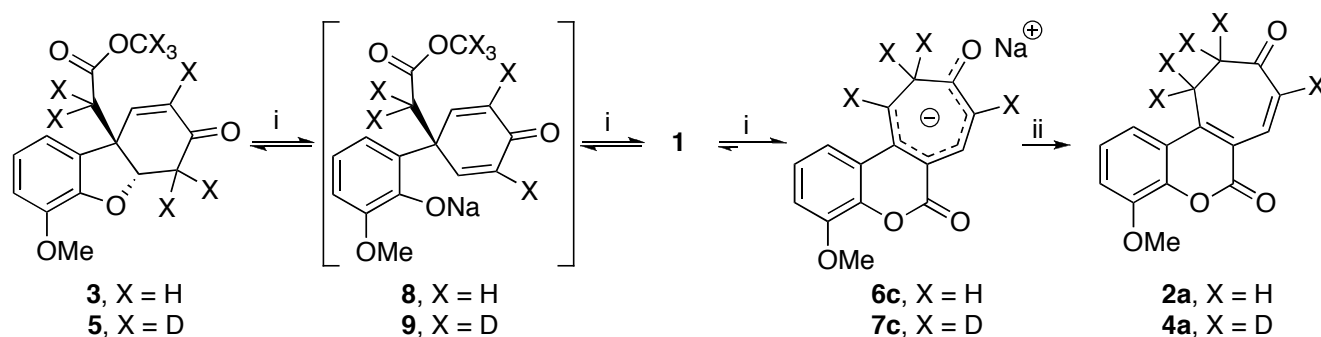
Conditions: i) MeONa, MeOH, 40°C; ii) HCl 1 M

**Scheme 1.** Rearrangement and lactone ring opening products of spirocyclohexadienone **1** in basic conditions. Throughout this study, the following naming system is used: (a) for the keto forms; (b) for the enol forms; (c) for the enolate forms (see Table 1 for more details).

The presence of an efficient protonating agent seems to be essential for the rearrangement of **1** into **2a** to occur. Several systems have been investigated at different temperatures (−78 °C to 75 °C): i) in the absence of protonating agent (NaH/THF) no reaction is observed; ii) in the presence of stoichiometric quantity of

protonating agent (DBU/CH<sub>2</sub>Cl<sub>2</sub>, potassium phthalimide/THF, lithium *N*-methyltoluenesulfonamide/THF) we observed the suppression of the lactone ring opening, a slow reaction rearrangement and low yields of **2a** (5-30 %); iii) when the protonating agent is the solvent (MeONa/MeOH, EtONa/EtOH, *i*-PrONa/*i*-PrOH) we observed a fast reaction and the formation of two compounds: the rearrangement product **2a** and the tricyclic ester **3**. The best results are obtained with MeONa in MeOH at 40 °C for 30 min, the product **2a** being isolated in 75 % yield in these conditions.

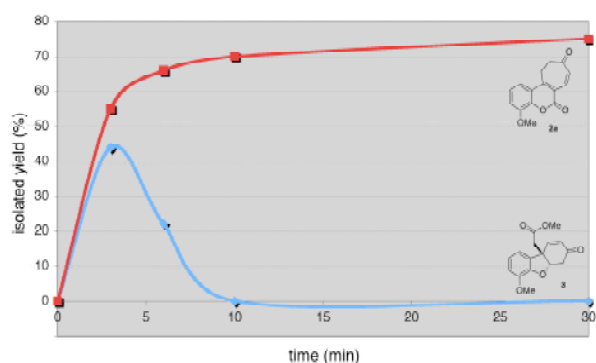
During the study of the reaction of **1** with MeONa in MeOH at 40 °C we evidenced two competitive reactions: i) the rearrangement described above, leading to **2a** after protonation and ii) the intermediate formation of the ester **3**,<sup>31</sup> through the nucleophilic opening of the lactone ring followed by a Michael addition of the resulting phenoxide **8** (Scheme 2).



Conditions: i) CX<sub>3</sub>ONa, CX<sub>3</sub>OX, 40°C; ii) HCl 1 M

**Scheme 2.** Deuterium labeling studies during the rearrangement and lactone ring opening of spirocyclohexadienone **1** in basic conditions.

The formation of compound **3** proved to be reversible and the equilibrium is shifted towards the thermodynamic product **2a** (Figure S1, Supporting information). Figure 1 shows that the ester **3** has completely disappeared after 10 min, but the best yields of **2a** are obtained after 30 min at 40 °C. At lower temperatures (−78 °C to 20 °C), the ester **3** is almost exclusively observed.

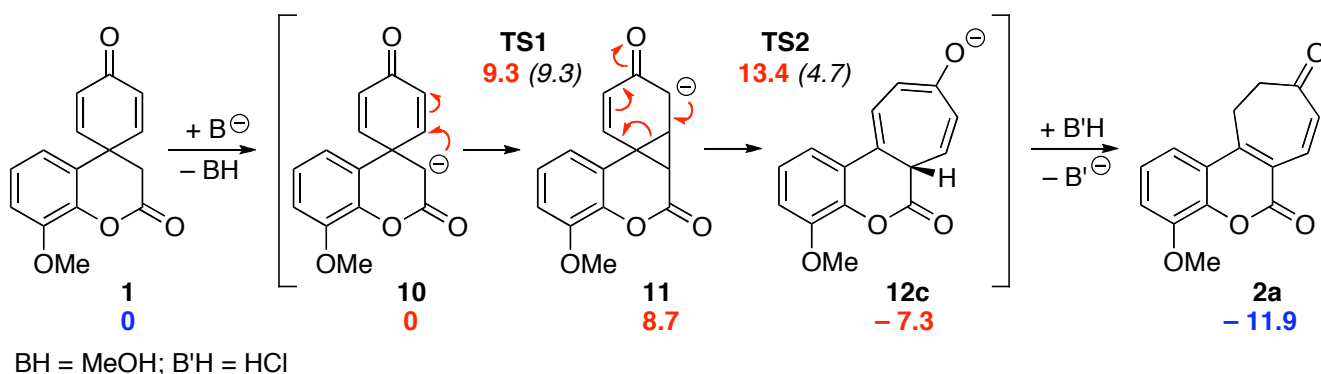


**Figure 1.** Time-dependent formation of compounds **2a** and **3** (MeONa, MeOH, 40 °C)

When the reaction of **1** with CD<sub>3</sub>ONa in CD<sub>3</sub>OD at 40 °C is followed by <sup>1</sup>H-NMR (Figure S2, Supporting information) it is noteworthy that: i) an equilibrium between three species (**5**, **7c** and **9**) is immediately established, which is completely shifted towards the delocalized anion **7c** after 30 min; ii) the deuterium exchange is very fast and all the enolisable positions are completely deuterated after 3 min. The complete incorporation of deuterium into both positions α to the ketone in **5** proves the existence of a dynamic equilibrium between the ester **5** and the open bicyclic phenoxide **9**.<sup>32</sup> Moreover, the reversibility of this process is confirmed by the exclusive formation of the rearrangement product **2a** when the ester **3** is treated with MeONa/MeOH at 40 °C.

The rearrangement product **2a**, in the presence of CD<sub>3</sub>ONa in CD<sub>3</sub>OD at room temperature, is completely deprotonated and immediately forms the enolate **6c**, which then undergoes a slow deuterium exchange, complete after 20 h, leading to the enolate **7c** (Figure S3, Supporting information).

*Reaction mechanism.* In the light of the results presented above, we propose the following mechanism for this rearrangement (Scheme 3): the deprotonation of the lactone **1**, followed by the intramolecular Michael addition of anion **10** leads to the cyclopropyl derivative **11**, which is transformed into the enolate **12c** by a cyclopropane ring opening. The enolate **12c** is then converted into the final protonated product **2a**.



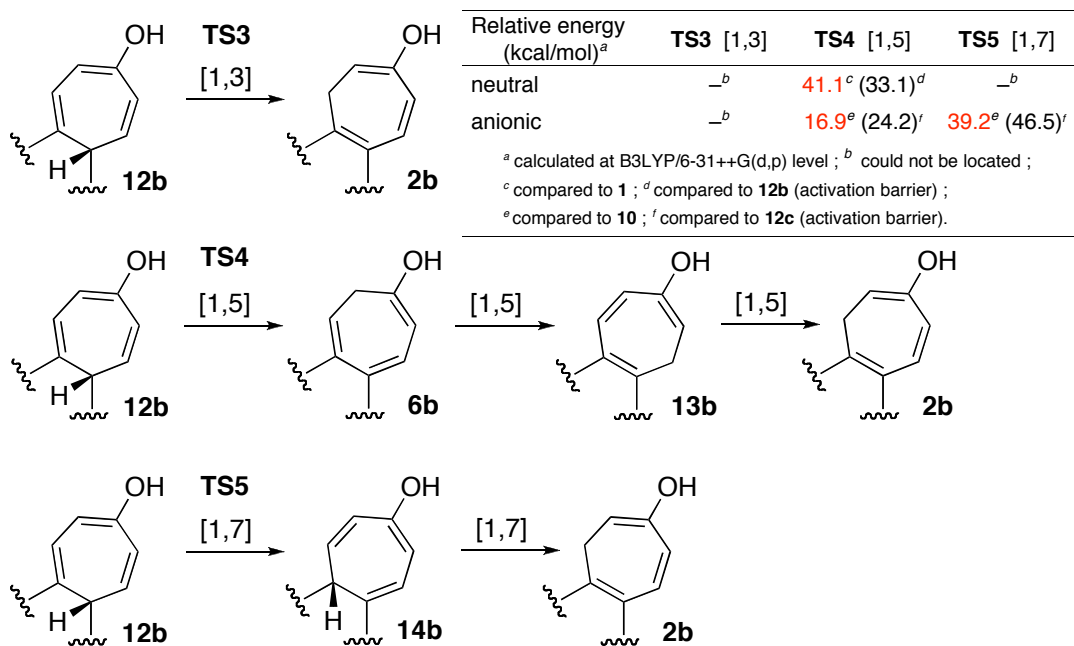
**Scheme 3.** Proposed mechanism for the rearrangement of **1** into **2a**. Calculated relative energies (kcal/mol) of neutral compounds are represented in blue and those of anions and transition states (TS) in red. In brackets are reported the activation barriers (kcal/mol).

In order to support the proposed mechanism, the structures of intermediates and transition states were optimized at the B3LYP level with the 6-31++G(d,p) basis set using Gaussian 03<sup>34</sup> (Scheme 3). Intrinsic

reaction coordinate (IRC) path calculations are in full agreement with a spirocyclopropane intermediate **11**, which rearranges to give a seven-membered ring enolate **12c**. The activation barrier energies for TS1 and TS2 (9.3 and 4.7 kcal/mol, respectively) are not very high, which is consistent with the mild reaction conditions used for this transformation. The driving force of the rearrangement is likely to be the greater extent of conjugation in **2a** than in **1**, confirmed by the near-perfect planarity of the X-ray structure.

Whereas the mechanism for the conversion of **1** into **12c** is relatively intuitive, the second part of the mechanism presented in Scheme 3, the conversion of the enolate **12c** into the rearrangement product **2a**, is not so obvious. We have formulated two hypotheses: a) a sigmatropic hydrogen shift and b) a base-catalyzed 1,3-hydrogen shift.

a) *Sigmatropic hydrogen shift*. Three pathways can be envisaged for the conversion of **12b** into **2b** through a sigmatropic mechanism: i) one direct [1,3] hydrogen shift; ii) three consecutive [1,5] hydrogen shifts; iii) two consecutive [1,7] hydrogen shifts (Scheme 4). These sigmatropic shifts can theoretically take place before or after the protonation step, thus both neutral and anionic forms of the possible intermediates must be considered.



**Scheme 4.** Three different possible pathways for the conversion of **12b** into **2b** through sigmatropic reactions.

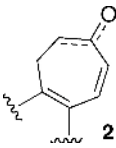
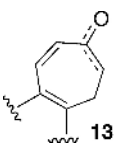
In the cycloheptatrienic systems only the suprafacial hydrogen shifts are possible for steric reasons, thus the [1,3] and [1,7] hydrogen shifts are thermally forbidden, whereas the [1,5] hydrogen shift is allowed.<sup>35-39</sup> In order to evaluate the conditions required for the sigmatropic shift in this rearrangement, we optimized the structures and calculated the energies for all intermediates, as well as for the transition states in the first sigmatropic shift (Scheme 4, Table 1).

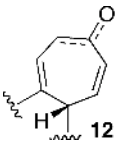
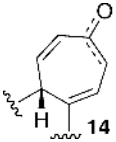
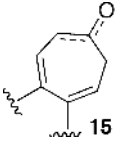
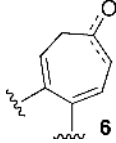
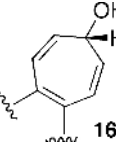
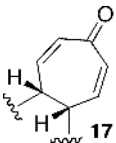
We succeeded in locating valid transition states only in three cases, for neutral **TS4n**, anionic **TS4a** and anionic **TS5a**.<sup>40</sup> The difference of activation barriers between the neutral and anionic forms of **TS4** is almost 9 kcal/mol, so it seems that the sigmatropic rearrangement is more favored in the anionic series. However, in spite of the lower value obtained for **TS4a** (24.2 kcal/mol), this activation barrier is still too high to be compatible with the mild conditions used for this reaction. The activation barrier of the anionic form **TS5a** is higher than that of **TS4a**, as expected for a forbidden sigmatropic shift.

All these calculations data suggest that there is no sigmatropic shift involved in this mechanism; this is further supported by the complete deuterium exchange observed for the two methylene groups in **4a** (Scheme 2), which is not compatible with a sigmatropic shift.

As suggested by one of the referees, in the light of Herndon's studies,<sup>11</sup> we investigated the possibility to convert **2a** into **13a** by two successive thermal [1,5] hydrogen shifts. However, heating **2a** in *p*-xylene at 140 °C for 16 h led only to the partial conversion of **2a** into **13a** and from the mixture of these two compounds (ratio **2a** / **13a** = 3 / 1) **13a** was isolated in 11 % yield. Longer reaction time (3 days) resulted in extensive decomposition. These results are in agreement with an extended delocalized system in our case, a high activation barrier for the thermal [1,5] hydrogen shifts and support the greater stability (1.6 kcal/mol) calculated for **2a** compared to **13a**.

**Table 1.** Calculated relative energies of all possible intermediates in the sigmatropic rearrangement

Structure	Relative energy (kcal/mol) <sup>a</sup>		
	keto ( <b>a</b> ) <sup>b</sup>	enol ( <b>b</b> ) <sup>b</sup>	enolate ( <b>c</b> ) <sup>c</sup>
	- 11.9	- 1.3	- 4.9
	- 10.3	- 0.9	- 3.4

	7.6	8.0	-7.3
	6.0	5.0	-13.8
	-3.7	-0.5	-21.5
	-3.7	0.1	-27.0
	-	2.7 <sup>d</sup>	18.6 <sup>d</sup>
	10.0	-	-

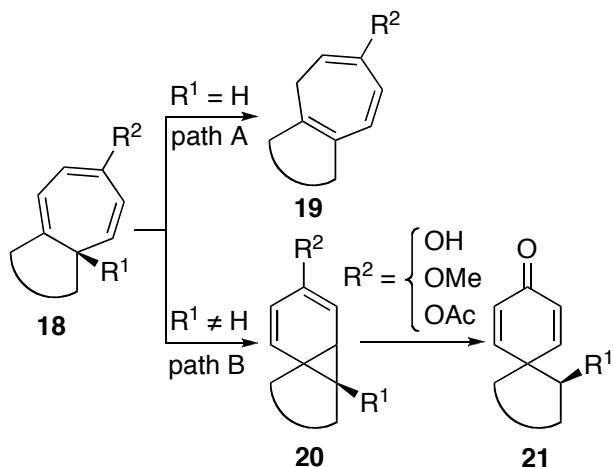
<sup>a</sup> calculated at B3LYP/6-31++G(d,p) level;  
<sup>b</sup> compared to **1**; <sup>c</sup> compared to **10**; <sup>d</sup> in this case, alcohol/alcoholate instead of enol/enolate

However, from the results of the Table 1, it is noteworthy that, with one exception (structures **14**), the keto form is always more stable than the enol, the difference of energies being very important for **2** and **13**. This is in agreement with the experimental results<sup>41</sup> showing that the cycloheptadienone is the major form in this keto-enol equilibrium. Moreover, the energies of compounds **12**, **14** and **17**, bearing ring junction hydrogen atoms, are unusually high, for both keto and enol forms. This is the consequence of the significant geometrical change induced by the presence of these hydrogen atoms, which prevents the conjugation between the 7-membered ring and the other two rings.

*b) Base-catalyzed 1,3-hydrogen shift.* Several examples of this type of transformation are described in cycloheptatrienic systems, catalyzed by triethylamine,<sup>42-45</sup> 1,8-diazabicyclo[5.4.0]undec-7-ene<sup>27,28</sup> or potassium *tert*-butoxide.<sup>46,47</sup> The mechanism and regioselectivity have been studied for cycloheptatrienes bearing electron withdrawing groups.<sup>48-52</sup> There are also a few examples of thermal,<sup>53-57</sup> photochemical<sup>58</sup> or acid-catalyzed<sup>57,58</sup> 1,3-hydrogen shifts. In most cases, the hydrogen atom shifts from a ring-junction

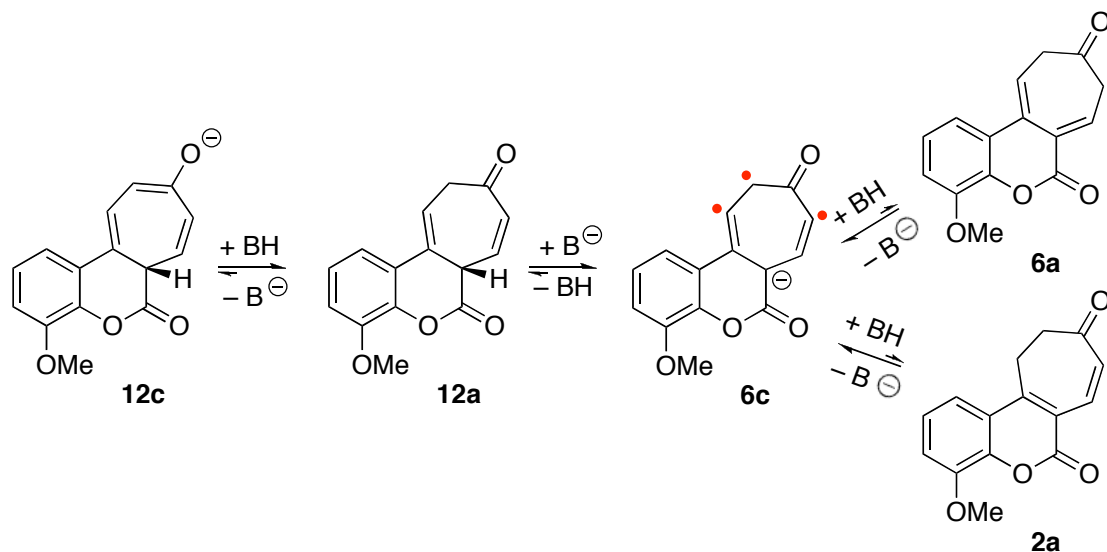


position to the nearest unsubstituted position (path A, Scheme 5).<sup>27,28,42-44,56-58</sup> In the case where cycloheptatriene **18** has  $R^1 \neq H$  (path B, Scheme 5), the 1,3-shift is very unfavored. The system evolves towards the spirodienone **21**<sup>43,53-55</sup> if an oxygenated substituent is present at  $R^2$  or remains in the less constrained norcaradiene form **20**<sup>59</sup> in the other cases. To sum up the above, the pathways and the final products are determined by the stability given by the substituents present on the molecule.



**Scheme 5.** Influence of the ring substituents in the evolution of cycloheptatrienic systems

In our study, the intermediate **12c** is a particular form of **18**, with  $R^1 = H$  and  $R^2 = O^-$ . Following the path A, the enolate **12c** is protonated and the resulting compound **12a** forms the enolate **6c** by deprotonation at the ring-junction position. This deprotonation represents the first step of the base-catalyzed hydrogen shift. In the second step, the delocalized enolate **6c** can be protonated at several positions to give either the compounds **12a**, **6a** or **2a**, which are in equilibrium via **6c** as a common intermediate (Scheme 6).



**Scheme 6.** Proposed mechanism for the conversion of **12c** to **6c**. The red dots represent the positions completely deuterated when the reaction is carried out in  $\text{CD}_3\text{OD}$

This equilibrium is completely shifted towards the enolate **6c**, which is the only species visible in the NMR spectrum. The complete incorporation of deuterium in the positions marked with red dots in Scheme 6 supports the existence of successive base-catalyzed 1,3-hydrogen shifts leading to the enolate **6c**, which is the most stable of all anionic intermediates (Table 1). The protonation of **6c** leads exclusively to the isomer **2a**, the most stable compound among **2a**, **6a** and **12a** (Table 1).

The deuterium labeling results indicate that the mechanism of the rearrangement involves base-catalyzed 1,3-hydrogen shifts. This conclusion is supported by the calculations data.

## Conclusion

In this paper we report the rearrangement of spirocyclohexadienones into dihydrotropones in basic conditions as a new method for the preparation of seven-membered ring ketones, which are key building blocks for the synthesis of tropoloalkaloids. We gained insight into the mechanism that we proposed for this rearrangement by DFT calculations of the possible intermediates and transition states as well as by deuterium labeling. All these data allowed us to choose between two possible paths and thus conclude that the mechanism involves a base-catalyzed 1,3-hydrogen shift in the cycloheptatrienic system obtained from the opening of a fused cyclopropane intermediate.

## Experimental Section

**General Remarks.** Starting materials and reagents were purchased from a commercial supplier and used without further purification with the exception of MeOH, which was distilled over Mg and I<sub>2</sub>.

**Synthesis of methyl 2'-(4-methoxy-7-oxo-5a,6,7,9a-tetrahydrodibenzo[*b,d*]furan-9a-yl)acetate (3).** To a solution of 8-methoxyspiro[chroman-4,1'-cyclohexa[2',5']diene]-2,4'-dione **1**<sup>30</sup> (20 mg, 0.078 mmol) in methanol (0.5 mL) was added trifluoroacetic acid (0.1 mL, 1.3 mmol). After stirring 16 h at room temperature, the mixture was concentrated *in vacuo*. Preparative silica gel TLC (heptane / ethyl acetate 50 / 50) afforded 20 mg of methyl 2'-(4-methoxy-7-oxo-5a,6,7,9a-tetrahydrodibenzo[*b,d*]furan-9a-yl) acetate **3** as a pale yellow oil (87 %): <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 6.94 (dd, *J* = 7.7, 7.8 Hz, 1H), 6.86 (d, *J* = 7.7 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.57 (dd, *J* = 10.3, 2 Hz, 1H), 6.02 (d, *J* = 10.3 Hz, 1H), 5.13 (m, 1H), 3.88 (s, 3H), 3.69 (s, 3H), 3.09 (d, *J* = 14.3 Hz, 1H), 3.13 (dd, *J* = 17.7, 2.8 Hz, 1H), 6.03 (dd, *J* = 17.7, 4.2 Hz, 1H), 2.90 (d, *J* = 15 Hz, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 195.0, 170.3, 146.9, 146.3, 145.1, 131.4, 127.6, 122.6, 115.0, 112.7, 86.0, 56.2, 52.2, 47.4, 41.5, 38.5; IR (CDCl<sub>3</sub>) 1199, 1280, 1492, 1680, 1731 cm<sup>-1</sup>; MS (ESI) *m/z* : 311(M+Na)<sup>+</sup>; HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>16</sub>O<sub>5</sub>Na<sup>+</sup> 311.0895, found 311.0878.

**Synthesis of 4-methoxy-10,11-dihydro-cyclohepta[*c*]chromene-6,9-dione (2a).** A solution of 8-methoxyspiro[chroman-4,1'-cyclohexa[2',5']diene]-2,4'-dione **1**<sup>30</sup> (20 mg, 0.078 mmol) in methanol (0.6 mL) / THF (0.3 mL) is added at 40 °C to a solution of sodium methoxide, freshly prepared from sodium (13 mg, 0.56 mmol) and methanol (0.6 mL). After stirring for 30 min at 40 °C, the reaction is quenched with 1 M hydrochloric acid (2 mL), stirred for 10 min and extracted with dichloromethane (3 x 5 mL). Concentration *in vacuo* of the combined organic layers followed by preparative silica gel TLC (heptane / ethyl acetate 70 / 30) afforded 15 mg of 4-methoxy-10,11-dihydro-cyclohepta[*c*]chromene-6,9-dione **2a** (75 %): <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.59 (d, *J* = 12.9 Hz, 1H), 7.39 (d, *J* = 8.35 Hz, 1H), 7.30 (dd, *J* = 8.35, 8.04 Hz, 1H), 7.18 (d, *J* = 8.04 Hz, 1H), 6.40 (d, *J* = 12.8 Hz, 1H), 4.01 (s, 3H), 3.20 (dd, *J* = 5.5, 6.0 Hz, 2H), 2.83 (dd, *J* = 5.6, 6.1 Hz, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 199.8, 159.7, 155.8, 148.0, 143.4, 135.6, 132.0, 124.7, 121.5, 119.4, 116.7, 115.0, 56.6, 41.2, 22.7; IR (CDCl<sub>3</sub>) 1469, 1662, 1710 cm<sup>-1</sup>; MS (ESI) *m/z* : 279 (M+Na)<sup>+</sup>; HRMS (ESI) *m/z* calcd for C<sub>15</sub>H<sub>12</sub>O<sub>4</sub>Na<sup>+</sup> 279.0633, found 279.0616.

**Synthesis of 4-methoxy-7,8-dihydro-cyclohepta[*c*]chromene-6,9-dione (13a).** A solution of 4-methoxy-10,11-dihydro-cyclohepta[*c*]chromene-6,9-dione **2a** (22 mg, 0.086 mmol) in *p*-xylene (1 mL) is

heated at 140 °C for 16 h, concentrated *in vacuo* and the resulting mixture (ratio **2a** / **13a** = 3 / 1) is purified by preparative silica gel TLC (eluting with heptane / ethyl acetate 40 / 60) to afford 2.5 mg of 4-methoxy-7,8-dihydro-cyclohepta[c]chromene-6,9-dione **13a** (11 %) : <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.42 (d, *J* = 12.8 Hz, 1H), 7.28 (m, 2H), 7.14 (dd, *J* = 7.0, 2.1 Hz, 1H), 6.65 (d, *J* = 12.8 Hz, 1H), 4.01 (s, 3H), 3.17 (m, 2H), 2.84 (m, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) 200.9, 160.6, 147.7, 142.5, 142.1, 136.3, 132.5, 129.3, 124.4, 119.1, 115.0, 113.3, 56.3, 44.1, 20.9; IR (CDCl<sub>3</sub>) 1473, 1671, 1707 cm<sup>-1</sup>; MS (ESI) *m/z* : 279 (M+Na)<sup>+</sup>; HRMS (ESI) *m/z* calcd for C<sub>15</sub>H<sub>12</sub>O<sub>4</sub>Na<sup>+</sup> 279.0633, found 279.0631.

### Computational Methods

Geometry optimization and vibrational frequency calculations were performed at the Density Functional Theory (DFT) level by using the Gaussian 03 program suite.<sup>34</sup> Becke's three-parameter exchange functional (B3)<sup>60,61</sup> was employed in conjunction with the Lee-Yang-Parr correlation functional (LYP),<sup>62</sup> as implemented in Gaussian 03<sup>34</sup> at a 6-31++G(d,p) basis set level. Geometries were optimized without constraint, and vibrational frequencies were then computed to characterize each structure as a minimum or transition structure (TS), via the number of imaginary frequencies (zero for minima and one for saddle points, respectively). After locating a TS, an intrinsic reaction coordinate (IRC)<sup>63-66</sup> calculation was carried out to identify its respective reactant and product.

**Acknowledgment.** We thank the Institut de Chimie des Substances Naturelles (ICSN) and the Centre National de la Recherche Scientifique (CNRS) for the financial support.

**Supporting Information Available.** Spectral characterization of compounds **3**, **2a** and **13a**, equilibrium between different intermediates and deuterium labeling followed by NMR, detailed data for the X-ray structure of compound **2a**, theoretical data for calculated compounds, intermediates and transition states, a movie generated from the IRC calculations showing the first part of the mechanism. This material is available free of charge via the Internet at <http://pubs.acs.org>.

### References

<sup>§</sup> Parts of this work were presented at the 1<sup>st</sup> European Chemistry Congress, 27-31 August 2006, Abstract p. 326.

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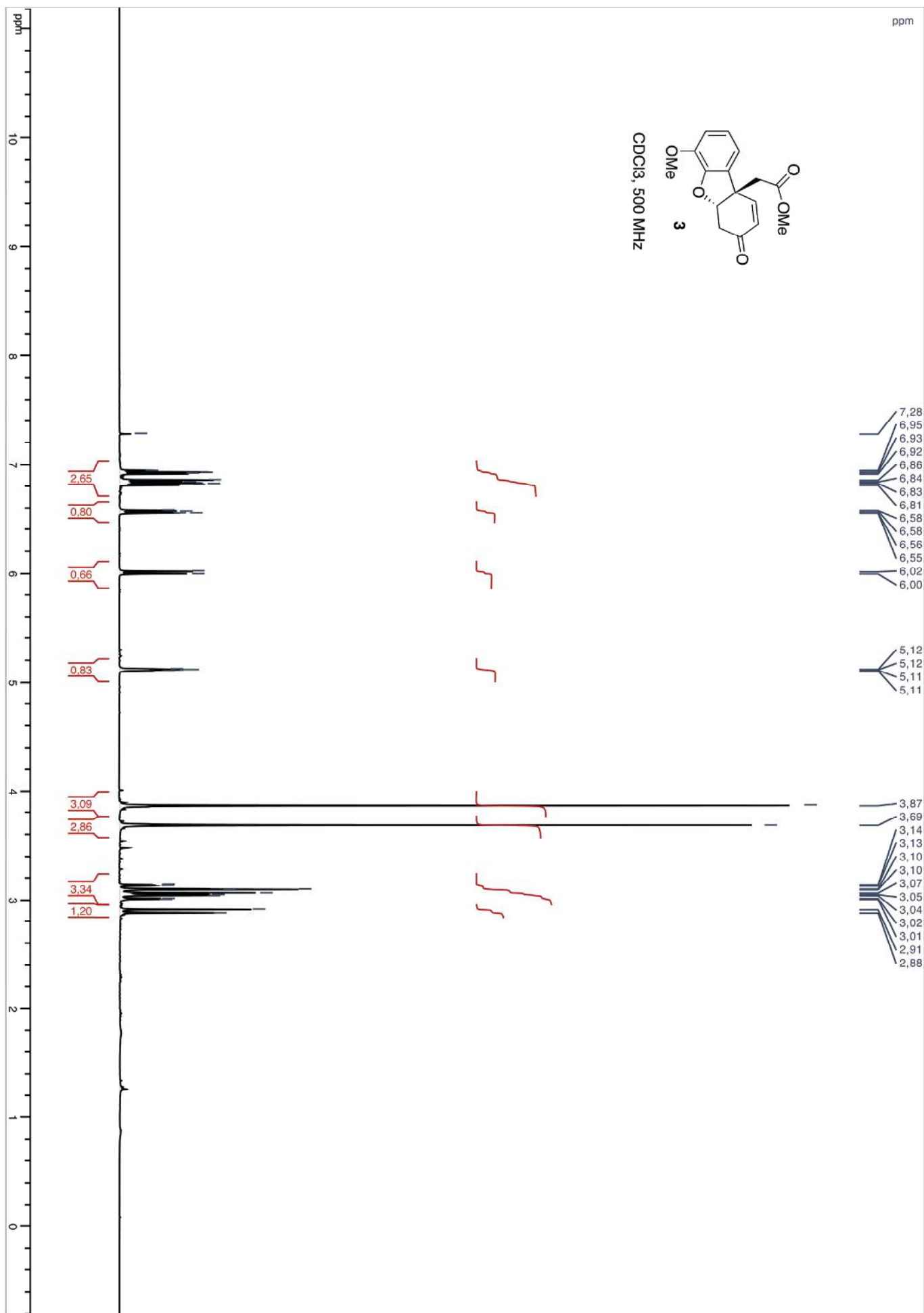
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spirocyclohexadienones: Synthesis and mechanism**

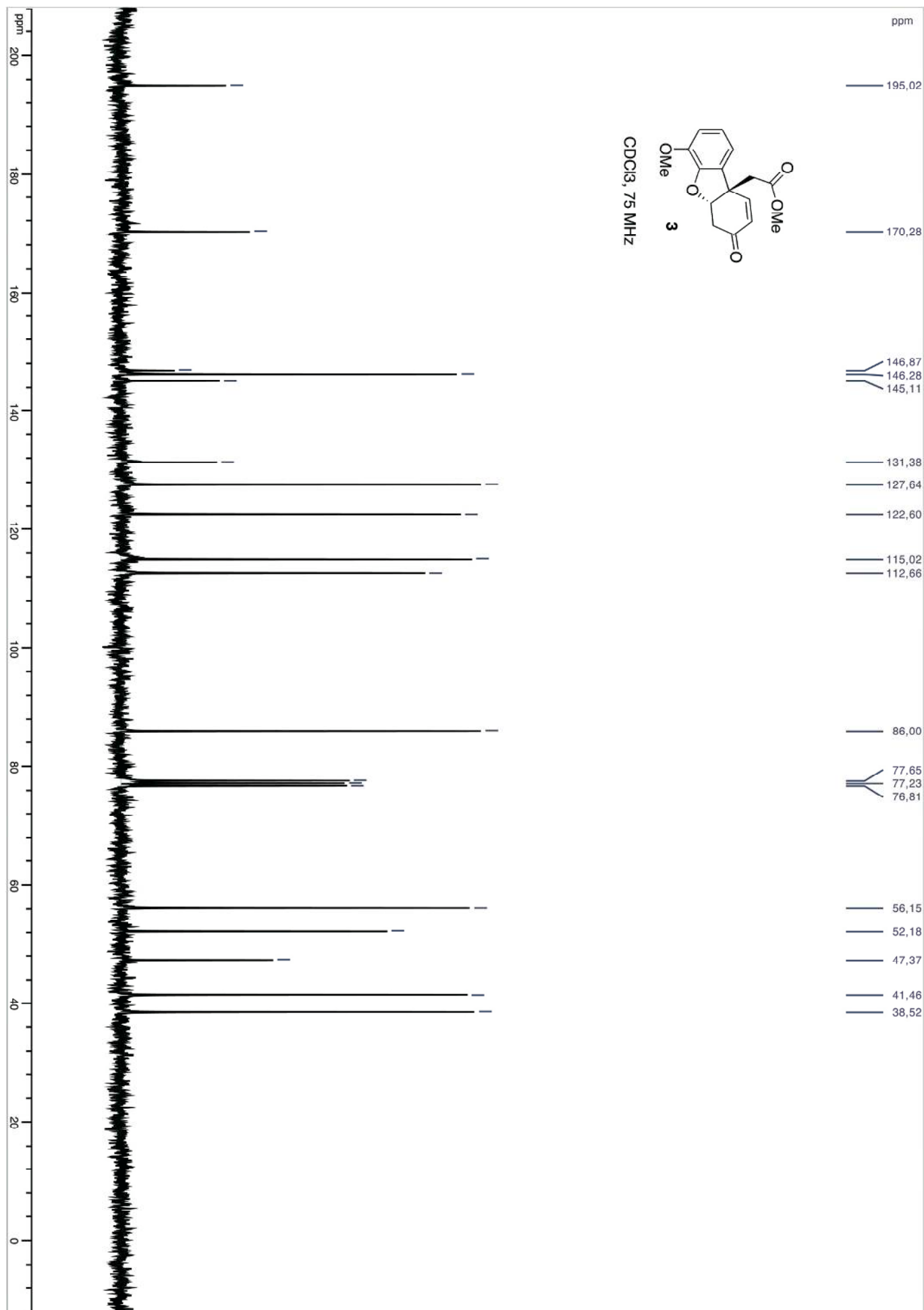
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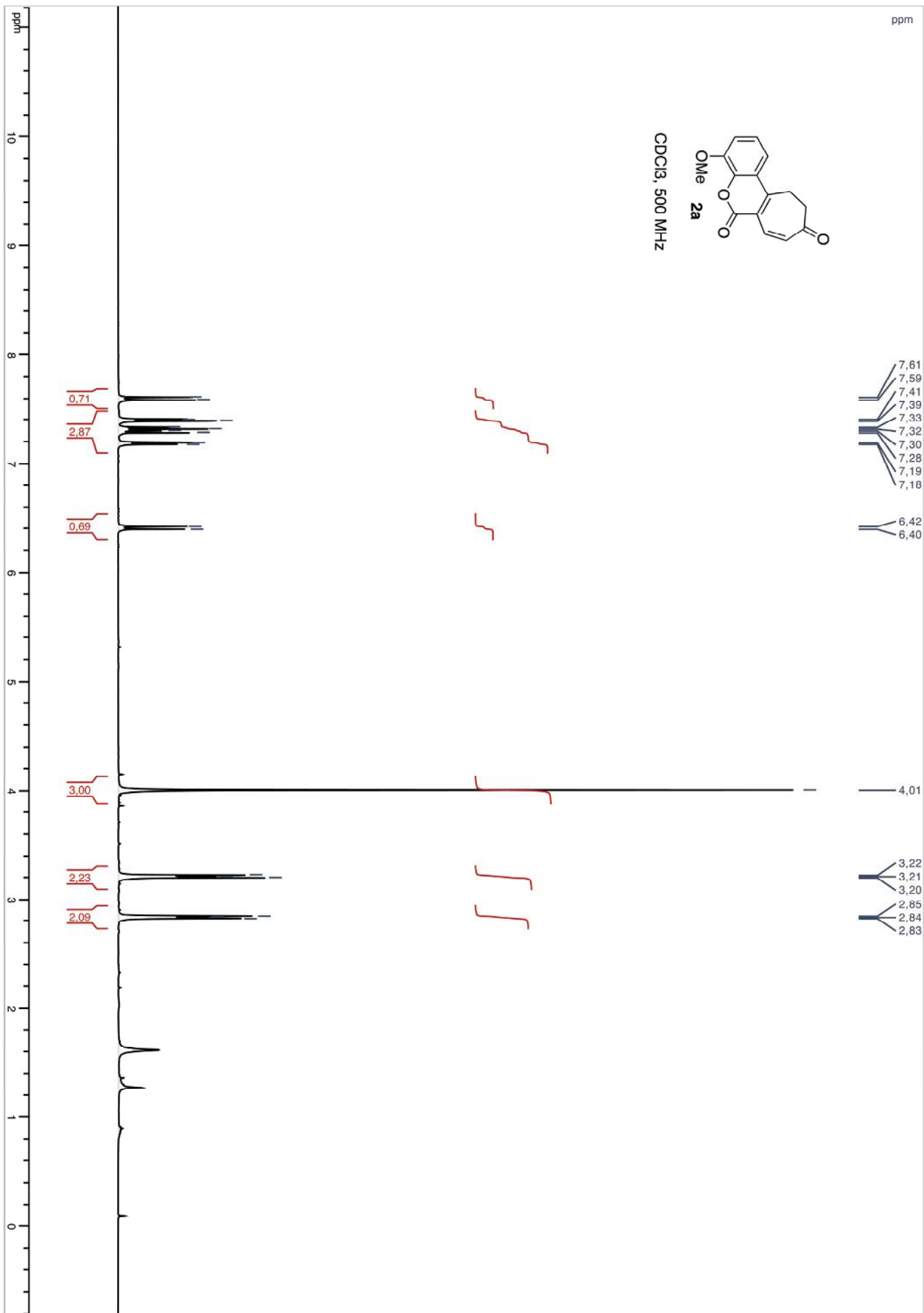
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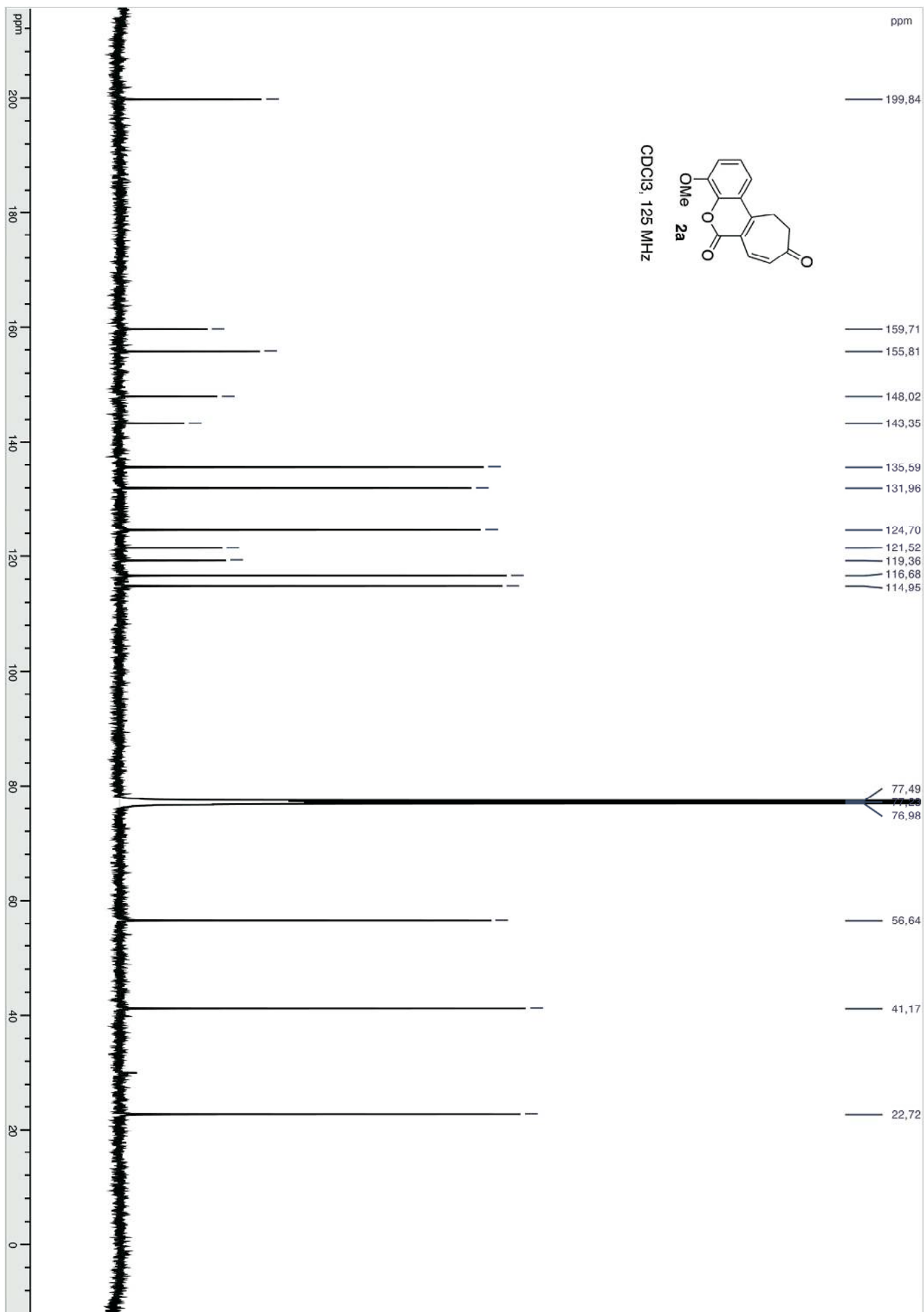
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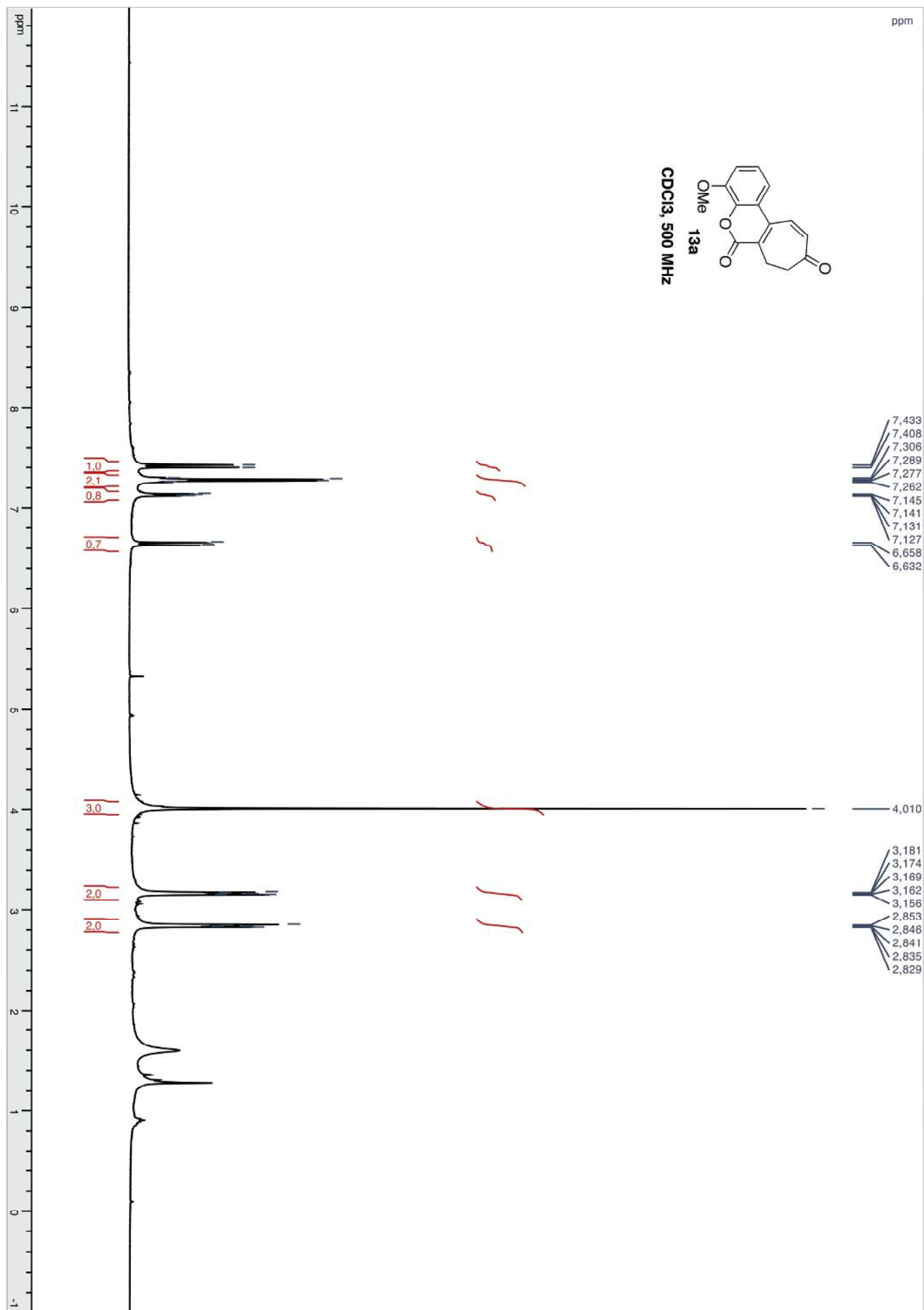
<sup>1</sup> H and <sup>13</sup> C-NMR spectra of compound <b>3</b>	S2
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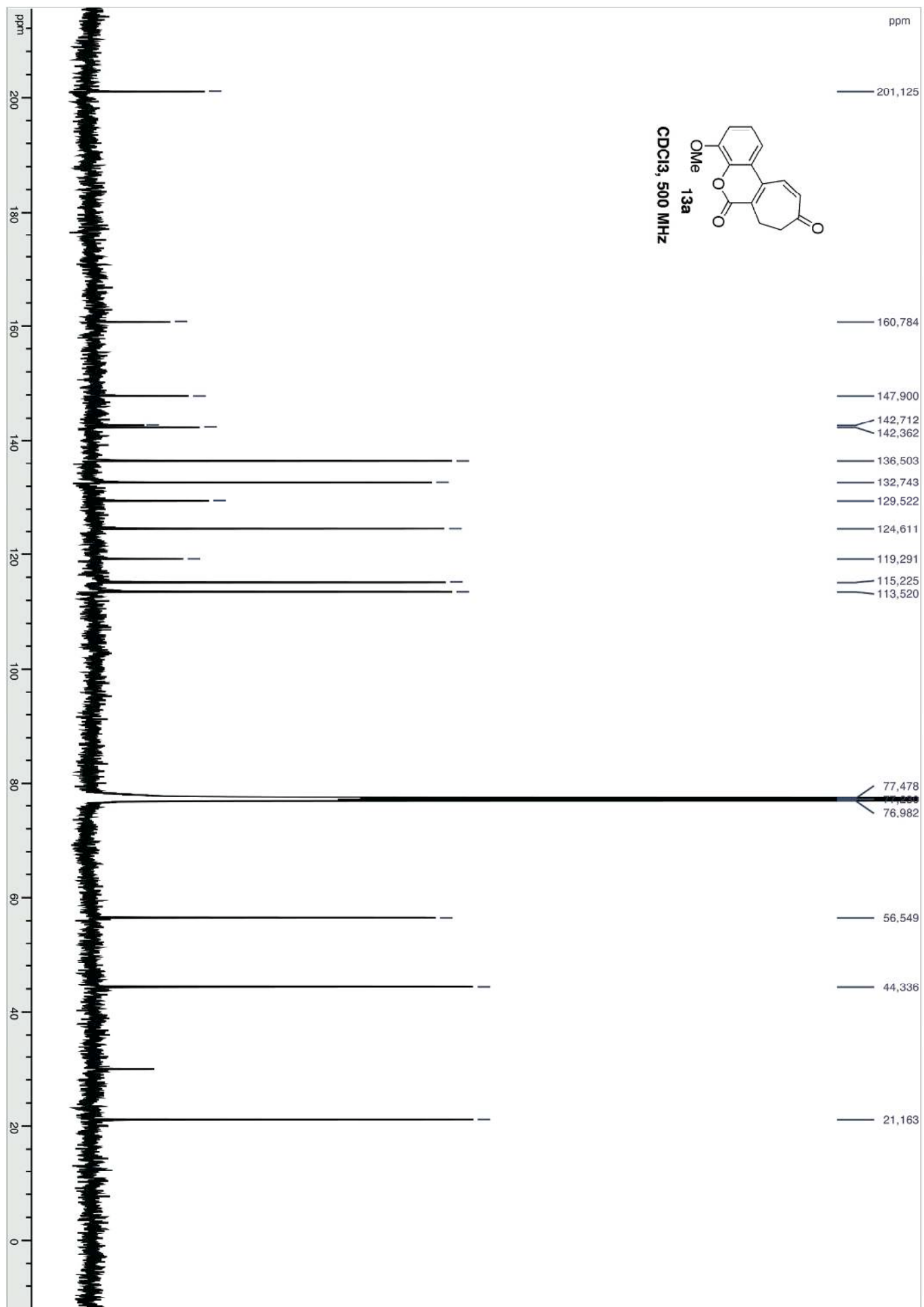


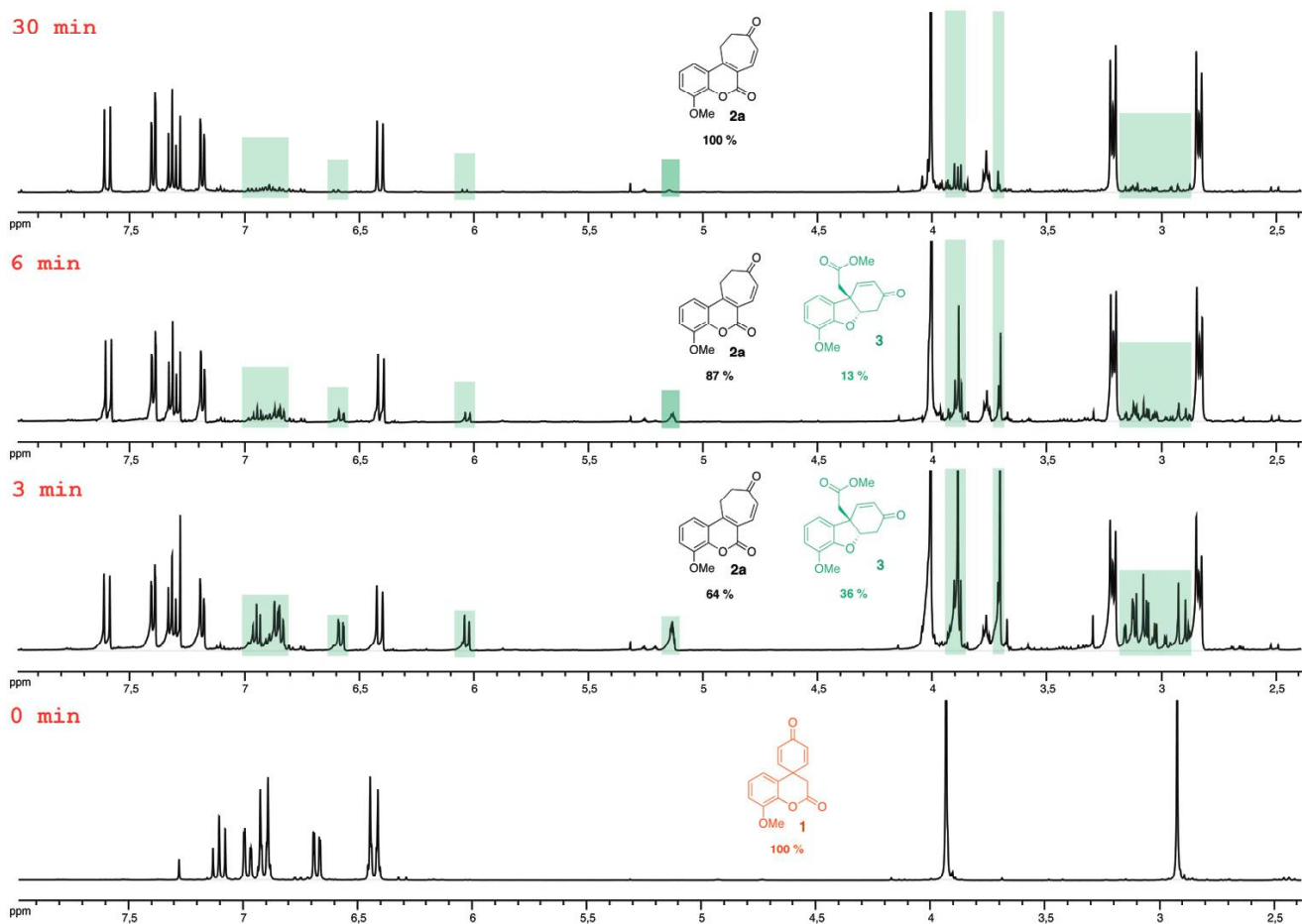






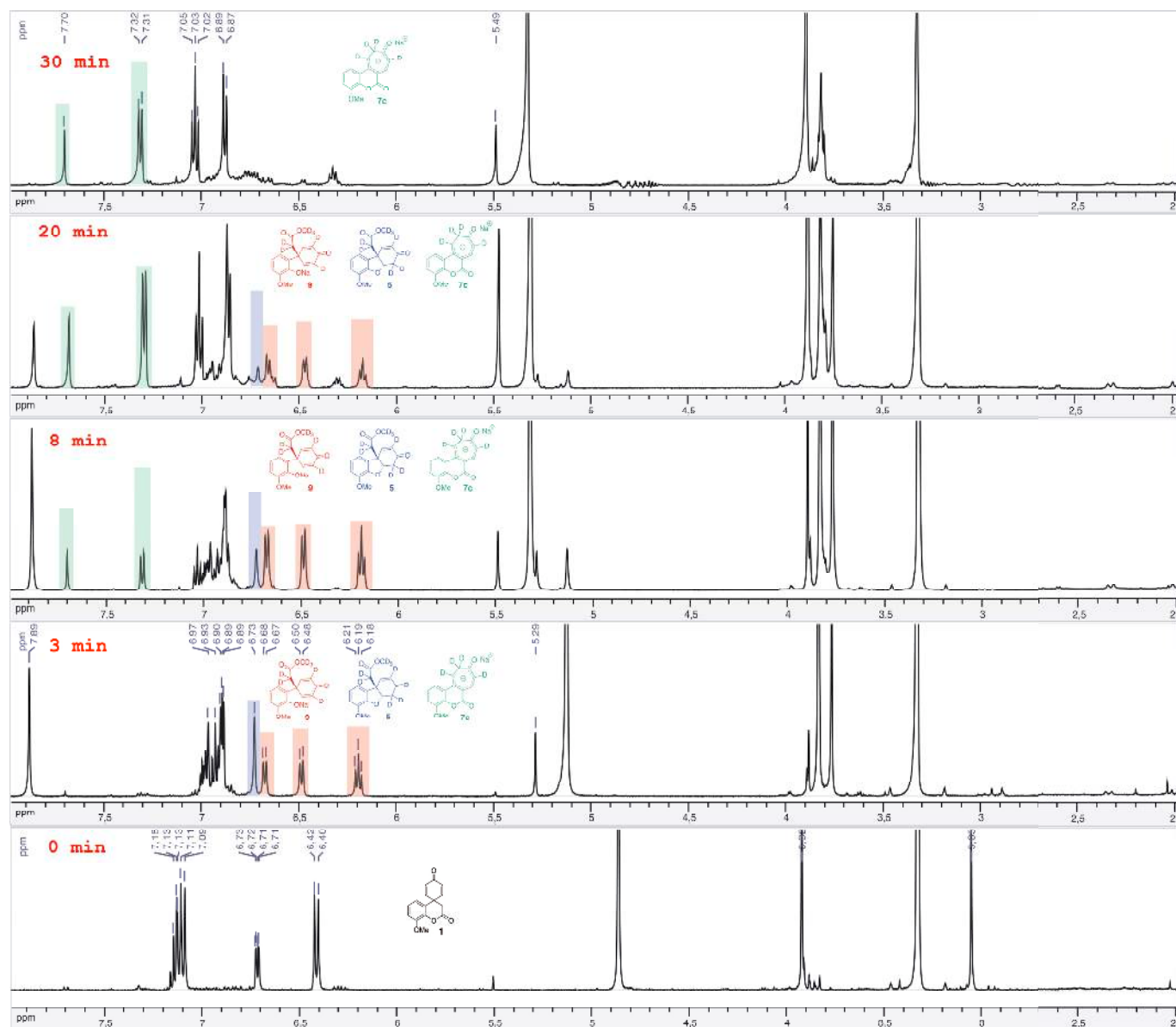




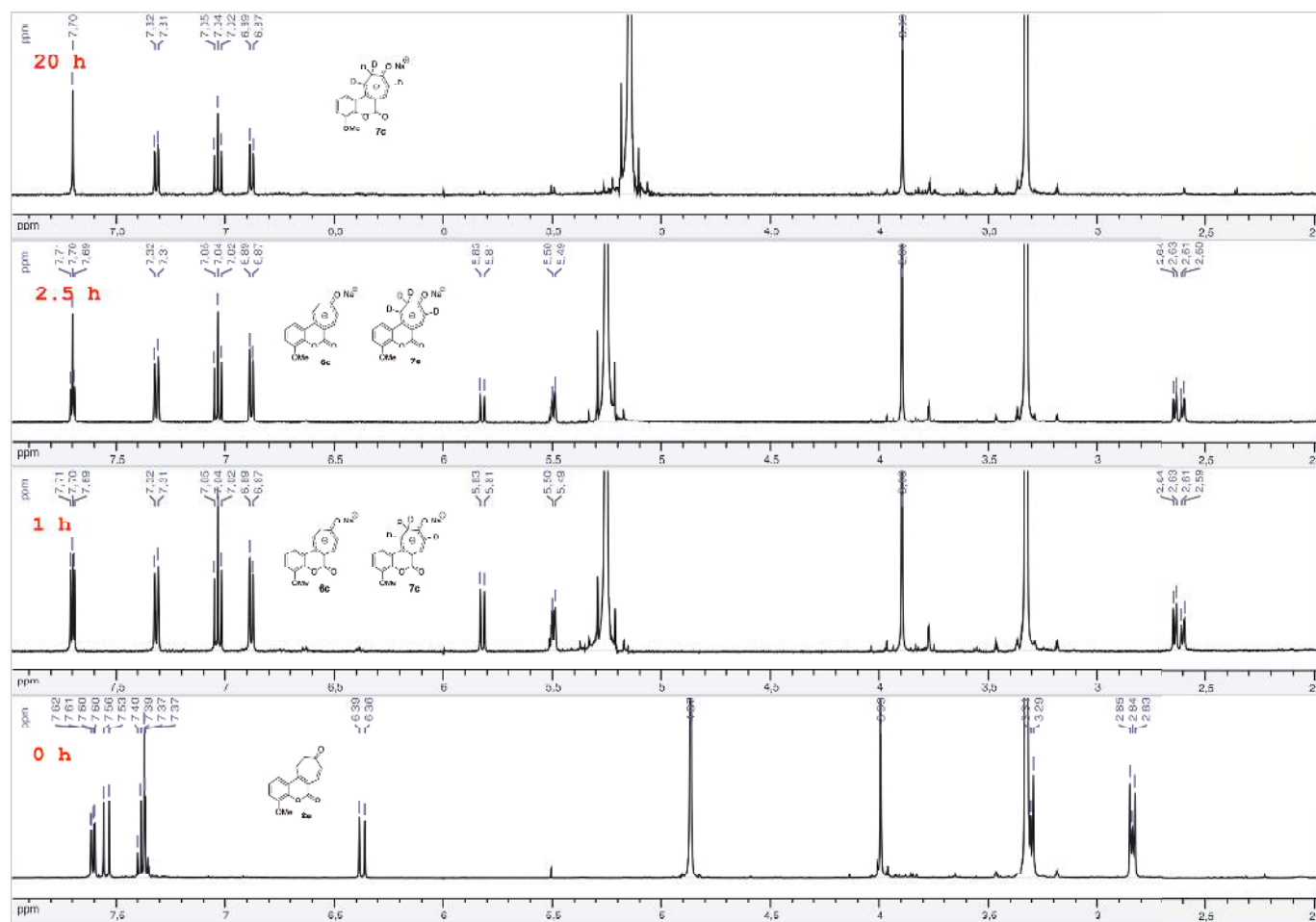


**Figure S1.** Superposed  $^1\text{H-NMR}$  spectra (500 MHz,  $\text{CDCl}_3$ ) of reaction mixture (from the reaction of **1** with MeONa in MeOH at  $40^\circ\text{C}$ ) after acidic quench at different times. The competitive formation of **2a** and **3** (green) is observed, then the conversion of **3** in **2a**. The rearrangement product **2a** is obtained almost exclusively after 30 min.



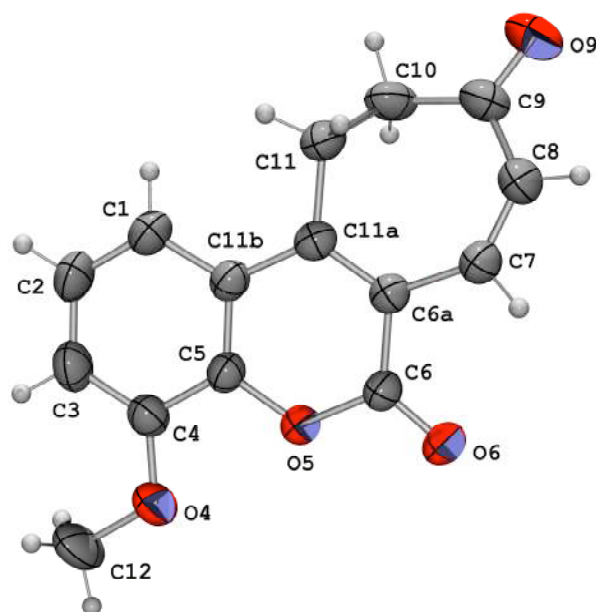


**Figure S2.** Superposed  $^1\text{H-NMR}$  spectra (500 MHz,  $\text{CD}_3\text{OD}$ ) of intermediates from the reaction of **1** with  $\text{CD}_3\text{ONa}$  in  $\text{CD}_3\text{OD}$  at  $40^\circ\text{C}$ . The competitive formation of the ester **5**, phenoxide **9** and 7-membered ring anion **7c** is observed. The equilibrium is shifted almost completely towards the more thermodynamically stable anion **7c** after 30 min.

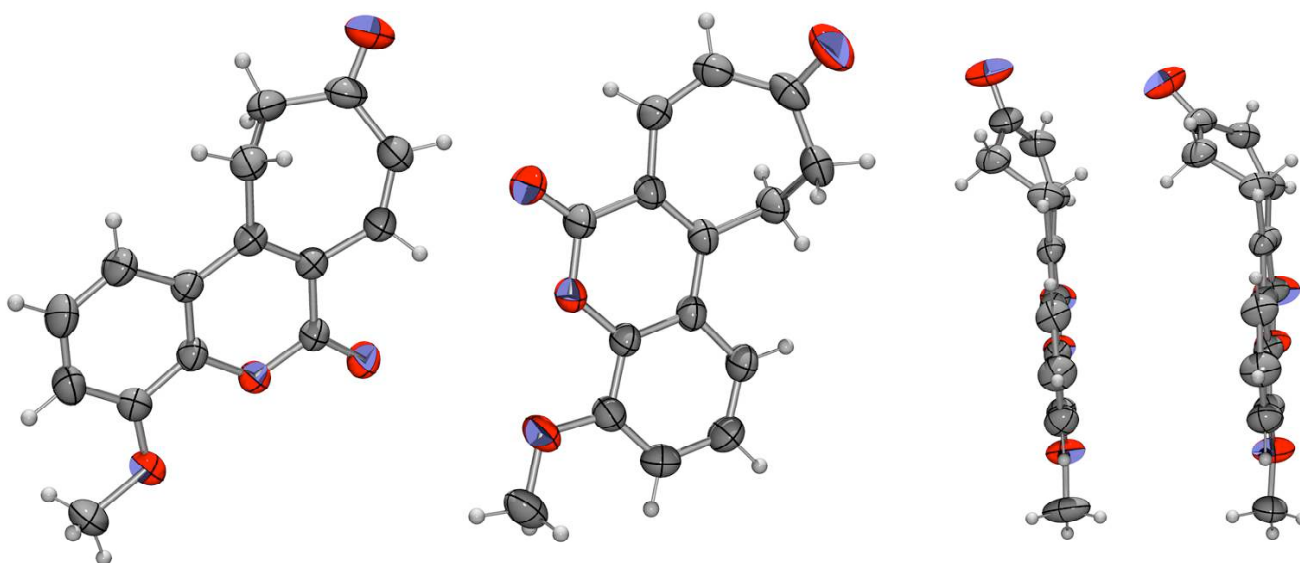


**Figure S3.** Superposed <sup>1</sup>H-NMR spectra (500 MHz, CD<sub>3</sub>OD) of intermediates from the reaction of **2a** with CD<sub>3</sub>ONa in CD<sub>3</sub>OD at room temperature. We observe the immediate formation of the anion **6c**, which is progressively deuterated, leading to the complete formation of the anion **7c** after 20 h.

## X-RAY STRUCTURE ANALYSIS OF COMPOUND 2A



**Figure S4.** ORTEP drawing of the X-ray structure of **2a** shown as displacement ellipsoids at the 30% probability level



**Figure S5.** ORTEP drawing of the asymmetric unit (left) and deviations of the atoms C8, C9, C10 and O9 from the molecule plane for the two molecules in the asymmetric unit. Displacement ellipsoids are shown at the 30 % probability level.

Crystals suitable for an X-ray study have been obtained for the 6,7-dihydrotropone **2a** and the tridimensional structure is shown in Figure S4. All atoms are coplanar except the atoms C8, C9, C10 and O9. There are two independent molecules in the asymmetric unit, the main difference between them being the degree of deviation of the atoms C8, C9, C10 and O9 from the molecule plane (Figure S5).

*Crystallographic results.* Data were obtained from a small colorless crystal plate (0.55 x 0.50 x 0.20 mm). Empirical formula : C<sub>15</sub> H<sub>12</sub> O<sub>4</sub>, M<sub>w</sub> = 256.25. The compound crystallizes in the triclinic system, space group P-1, racemic. There are four molecules in the unit-cell (Z= 4) and so, two independent molecules in the asymmetric unit. Cell parameters : a = 7.510(5), b = 12.824(5), c = 13.261(7) Å, α = 73.61(3), β = 78.80(3), γ = 87.33(3)°, V = 1202 Å<sup>3</sup>; d<sub>c</sub> = 1.416 g cm<sup>-3</sup>, F(000) = 536, λ (Mo Kα) = 0.71073 Å, μ = 0.103 mm<sup>-1</sup>. Data were measured with a Nonius Kappa-CCD linear area-detector diffractometer, using graphite monochromated Mo Kα radiation, according to the phi and omega scan method, up to θ = 27.50°. A total of 9306 intensity data was collected reduced to 7000 triclinic reflections of which 5273 were unique (Rint = 0.020).<sup>1</sup> Structure was solved with program *SHELXS86*<sup>2</sup> and refined by full-matrix least-squares, upon all unique F<sup>2</sup> with program *SHELXL97*.<sup>3</sup> All the hydrogen atoms were located in difference Fourier maps. They were fitted at theoretical positions and treated as riding, assigned of an isotropic displacement parameter equivalent to 1.12 the one of the bonded atom, 1.15 for those of the methyl groups. Refinement of 345 parameters converged to R1(F) = 0.0486 with the 3639 observed reflections having I ≥ 2 sigma (I) and wR2(F<sup>2</sup>) = 0.1272 with all the 5273 unique data ; goodness-of-fit S factor of 1.024. The residual electron density was found between -0.18 and 0.19 eÅ<sup>-3</sup>. All the crystallographic results are given in Cif file and Tables S1 to S6.

*Comparison of molecular conformations.* The two independent molecules of the asymmetric unit named respectively, \* and \*\*, appear in Figure S5, showing the same diastereoisomer. In both molecules, bond distance and angle values are nearly the same with double bonds C6a-C11a (1.362 Å) and C7-C8 (av. 1.341Å) clearly precised. However, differences appear in torsion angle values of the seven membered rings principally along the bonds: C8-C9 (-6.1 in \*, -28.1° in \*\*), C9-C10 (-43.7 and -19.0°) and C10-C11 (76.9 and 86.2), indicating differences in the ring conformations. Fitting the two structures, atoms C7 and C11 are quietly coplanar with the bicyclic aromatic part in each molecule, while atoms C8, C9 and C10 are respectively deviated by 0.226(2), 0.885(2) and 1.183(2) Å in \*, by 0.500(2), 1.372(2) and 1.284(2) Å in \*\*, from the mean plane of the other twelve atoms. If atom C8 is included in the aromatic mean plane, deviations of atoms C9 and C10 become : 0.800(2) and 1.114(2) Å in \*, 1.180(2) and 1.144 (2) Å - nearly the same - in \*\*. So, the angles between the planes [C11, C11a, C6a, C7, C8] and [C8, C9, C10, C11] in the seven membered rings, are respectively 136.3° in \*, 131.0° in \*\*. More, if we consider only the mean plane of the double bonds involving atoms [C11a, C6a, C7, C8, C9], atoms C10 and C11 are deviated from this plane by respectively 0.327(2) and -0.620(2) Å in \*, while atom C10 lies in this plane in \*\*, with C11 situated below by -0.890(2) Å. The crystal packing study shows that only van der Waals contacts exist between the molecules.

<sup>1</sup> *Collect* (Nonius BV, 1997-2000); *HKL Denzo and Scalepack* (Otinowski & Minor, 1997).

<sup>2</sup> Sheldrick, G.M. (1990). *SHELXS86*. *Acta Cryst. A* **46**, 467-473.

<sup>3</sup> Sheldrick, G.M. (1997). *SHELXL97*. Program for the Refinement of Crystal Structures, Univ. of Göttingen, Germany.

**Table S1.** Crystal data and structure refinement for compound **2a**.

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Identification code	'VARIN051'
Empirical formula	C15 H12 O4
Formula weight	256.25
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 7.510(5) Å    alpha = 73.61(3) deg. b = 12.824(5) Å    beta = 78.80(3) deg. c = 13.261(7) Å    gamma = 87.33(3) deg.
Volume	1201.9(11) Å <sup>3</sup>
Z, Z', Calculated density	4, 2, 1.416 Mg/m <sup>3</sup>
Absorption coefficient	0.103 mm <sup>-1</sup>
F(000)	536
Crystal size	0.55 x 0.50 x 0.20 mm
Theta range for data collection	2.76 to 27.50 deg.
Limiting indices	-9<=h<=9, -16<=k<=16, -16<=l<=17
Reflections collected / unique	9306 - 7000 / 5273 [R(int) = 0.0199]
Completeness to theta = 27.50	95.3 %
Absorption correction	Not measured
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	5273 / 0 / 345
Goodness-of-fit on F <sup>2</sup>	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0486, wR2 = 0.1101 (3639 Fo)
R indices (all data)	R1 = 0.0779, wR2 = 0.1272 (5273 data)
Largest diff. peak and hole	0.187 and -0.177 e.Å <sup>-3</sup>

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**Table S2.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2a**.  
 $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.  
 (\* Molecule 1, \*\* Molecule 2)

	x	y	z	U(eq)
* C1	5205(3)	3658(2)	2140(2)	54(1)
C2	4806(3)	2587(2)	2304(2)	62(1)
C3	5442(3)	2054(2)	1534(2)	57(1)
C4	6506(3)	2600(1)	571(1)	48(1)
C5	6902(2)	3696(1)	402(1)	41(1)
O5	7928(2)	4211(1)	-580(1)	46(1)
C6	8399(2)	5287(1)	-854(1)	41(1)
C6a	7777(2)	5888(1)	-64(1)	40(1)
C7	8222(3)	7045(1)	-455(1)	49(1)
C8	8325(3)	7798(2)	62(2)	58(1)
C9	8167(3)	7658(2)	1207(2)	58(1)
C10	7663(3)	6568(2)	1970(2)	59(1)
C11	6121(3)	6017(2)	1708(1)	54(1)
C11a	6766(2)	5385(1)	910(1)	41(1)
C11b	6285(2)	4246(1)	1170(1)	42(1)
C12	6884(4)	1034(2)	-73(2)	85(1)
O4	7196(2)	2168(1)	-249(1)	62(1)
O6	9313(2)	5647(1)	-1733(1)	56(1)
O9	8478(3)	8426(1)	1518(1)	90(1)
** C1	9034(3)	1683(2)	3263(1)	53(1)
C2	8869(3)	922(2)	2744(2)	60(1)
C3	8165(3)	-106(2)	3296(2)	56(1)
C4	7624(3)	-378(1)	4389(1)	47(1)
C5	7810(2)	394(1)	4922(1)	42(1)
O5	7255(2)	74(1)	6015(1)	50(1)
C6	7373(3)	757(1)	6629(1)	48(1)
C6a	8072(2)	1858(1)	6080(1)	42(1)
C7	8174(3)	2531(1)	6792(1)	49(1)
C8	8020(3)	3609(2)	6606(2)	53(1)
C9	7519(3)	4385(1)	5663(2)	53(1)
C10	7904(3)	4170(1)	4592(2)	58(1)
C11	9339(3)	3317(1)	4460(1)	50(1)
C11a	8623(2)	2182(1)	4997(1)	40(1)
C11b	8504(2)	1432(1)	4377(1)	41(1)
C12	6606(3)	-2132(2)	4486(2)	66(1)
O4	6921(2)	-1359(1)	5015(1)	64(1)
O6	6862(2)	398(1)	7580(1)	72(1)
O9	6781(2)	5233(1)	5757(1)	83(1)

**Table S3.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2a**.

	x	y	z	U(eq)
* H1	4763	3999	2670	61
H2	4091	2208	2947	69
H3	5153	1324	1664	63
H7	8482	7311	-1197	55
H8	8525	8508	-371	65
H10A	7304	6646	2687	66
H10B	8721	6104	1961	66
H11A	5471	5529	2363	60
H11B	5276	6567	1427	60
H12A	5603	897	49	97
H12B	7362	627	542	97
H12C	7477	817	-690	97
** H1	9498	2370	2875	59
H2	9238	1096	2005	68
H3	8059	-610	2926	63
H7	8373	2156	7471	55
H8	8259	3898	7135	60
H10A	8286	4846	4052	65
H10B	6782	3941	4455	65
H11A	9768	3397	3703	56
H11B	10364	3438	4761	56
H12A	7735	-2305	4089	76
H12B	5788	-1834	4006	76
H12C	6081	-2779	5006	76

**Table S4.** Comparison of selected torsion angles [deg] for compound **2a**.

* O6-C6-C6a-C7	5.3(3)
C11a-C6a-C7-C8	24.3(3)
C6a-C7-C8-C9	6.0(4)
C7-C8-C9-C10	-6.1(3)
O9-C9-C10-C11	137.5(2)
C8-C9-C10-C11	-43.7(3)
C9-C10-C11-C11a	86.2(2)
C7-C6a-C11a-C11	-4.3(3)
C10-C11-C11a-C6a	-56.2(2)
C10-C11-C11a-C11b	124.8(2)
C11-C11a-C11b-C1	0.8(3)
C3-C4-O4-C12	-4.1(3)
** O6-C6-C6a-C7	1.8(3)
C11a-C6a-C7-C8	32.1(3)
C6a-C7-C8-C9	6.9(3)
C7-C8-C9-C10	-28.1(3)
O9-C9-C10-C11	160.4(2)
C8-C9-C10-C11	-19.0(3)
C9-C10-C11-C11a	76.9(2)
C7-C6a-C11a-C11	-2.1(3)
C10-C11-C11a-C6a	-63.8(2)
C10-C11-C11a-C11b	115.9(2)
C11-C11a-C11b-C1	0.4(3)
C3-C4-O4-C12	-4.7(2)

**Table S5.** Bond lengths [Å] and angles [deg] for compound **2a**.

---

* C1-C2	1.367(3)
C1-C11b	1.409(3)
C2-C3	1.383(3)
C3-C4	1.382(3)
C4-O4	1.361(2)
C4-C5	1.397(2)
C5-O5	1.378(2)
C5-C11b	1.393(2)
O5-C6	1.369(2)
C6-O6	1.207(2)
C6-C6a	1.464(2)
C6a-C11a	1.362(2)
C6a-C7	1.458(2)
C7-C8	1.345(2)
C8-C9	1.460(3)
C9-O9	1.218(2)
C9-C10	1.491(3)
C10-C11	1.526(3)
C11-C11a	1.504(2)
C11a-C11b	1.449(2)
C12-O4	1.429(2)
* C2-C1-C11b	120.08(18)
C1-C2-C3	121.49(18)
C4-C3-C2	120.31(17)
O4-C4-C3	125.72(16)
O4-C4-C5	116.13(16)
C3-C4-C5	118.15(16)
O5-C5-C11b	121.67(15)
O5-C5-C4	115.90(15)
C11b-C5-C4	122.42(16)
C6-O5-C5	121.93(13)
O6-C6-O5	116.09(14)
O6-C6-C6a	126.08(15)
O5-C6-C6a	117.83(14)
C11a-C6a-C7	125.30(15)
C11a-C6a-C6	120.60(15)
C7-C6a-C6	113.93(15)
C8-C7-C6a	131.71(17)
C7-C8-C9	129.12(18)
O9-C9-C8	119.4(2)
O9-C9-C10	121.46(19)
C8-C9-C10	119.08(16)
C9-C10-C11	113.17(17)
C11a-C11-C10	113.11(16)
C6a-C11a-C11b	120.06(15)
C6a-C11a-C11	119.97(15)
C11b-C11a-C11	119.96(15)
C5-C11b-C1	117.54(16)
C5-C11b-C11a	117.90(15)
C1-C11b-C11a	124.55(16)
C4-O4-C12	117.01(16)

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** C1-C2	1.365 (3)
C1-C11b	1.400 (2)
C2-C3	1.386 (3)
C3-C4	1.374 (3)
C4-O4	1.361 (2)
C4-C5	1.395 (2)
C5-O5	1.374 (2)
C5-C11b	1.394 (2)
O5-C6	1.370 (2)
C6-O6	1.204 (2)
C6-C6a	1.463 (2)
C6a-C11a	1.361 (2)
C6a-C7	1.461 (2)
C7-C8	1.337 (3)
C8-C9	1.463 (3)
C9-O9	1.224 (2)
C9-C10	1.493 (3)
C10-C11	1.521 (3)
C11-C11a	1.502 (2)
C11a-C11b	1.447 (2)
C12-O4	1.417 (2)

** C2-C1-C11b	120.13 (17)
C1-C2-C3	121.47 (18)
C4-C3-C2	119.96 (17)
O4-C4-C3	125.29 (16)
O4-C4-C5	116.01 (16)
C3-C4-C5	118.69 (16)
O5-C5-C11b	121.93 (14)
O5-C5-C4	116.12 (15)
C11b-C5-C4	121.95 (16)
C6-O5-C5	121.70 (13)
O6-C6-O5	116.64 (15)
O6-C6-C6a	125.63 (16)
O5-C6-C6a	117.73 (15)
C11a-C6a-C7	124.68 (15)
C11a-C6a-C6	120.93 (15)
C7-C6a-C6	114.34 (15)
C8-C7-C6a	129.16 (17)
C7-C8-C9	127.37 (17)
O9-C9-C8	118.98 (19)
O9-C9-C10	119.53 (19)
C8-C9-C10	121.49 (16)
C9-C10-C11	115.53 (17)
C11a-C11-C10	112.11 (16)
C6a-C11a-C11b	119.72 (15)
C6a-C11a-C11	119.55 (15)
C11b-C11a-C11	120.73 (15)
C5-C11b-C1	117.79 (15)
C5-C11b-C11a	117.97 (15)
C1-C11b-C11a	124.24 (15)
C4-O4-C12	117.02 (16)

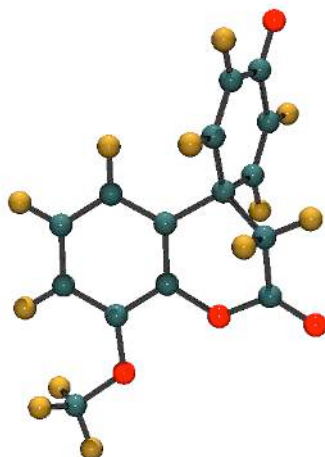
**Table S6.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )  
for compound **2a**.

The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
* C1	59(1)	57(1)	41(1)	-11(1)	0(1)	-9(1)
C2	71(1)	58(1)	46(1)	-2(1)	1(1)	-18(1)
C3	68(1)	44(1)	53(1)	-3(1)	-12(1)	-13(1)
C4	57(1)	43(1)	44(1)	-12(1)	-13(1)	-5(1)
C5	43(1)	42(1)	35(1)	-7(1)	-5(1)	-5(1)
O5	56(1)	40(1)	38(1)	-12(1)	0(1)	-5(1)
C6	46(1)	40(1)	34(1)	-7(1)	-4(1)	-2(1)
C6a	43(1)	40(1)	37(1)	-11(1)	-7(1)	0(1)
C7	61(1)	44(1)	39(1)	-9(1)	-3(1)	-2(1)
C8	74(1)	43(1)	54(1)	-15(1)	-3(1)	-5(1)
C9	68(1)	54(1)	60(1)	-30(1)	-10(1)	0(1)
C10	83(2)	56(1)	43(1)	-23(1)	-14(1)	7(1)
C11	64(1)	50(1)	43(1)	-16(1)	4(1)	0(1)
C11a	42(1)	45(1)	36(1)	-12(1)	-7(1)	1(1)
C11b	43(1)	44(1)	36(1)	-8(1)	-6(1)	-2(1)
C12	145(2)	44(1)	68(1)	-21(1)	-15(2)	-18(1)
O4	91(1)	41(1)	54(1)	-17(1)	-7(1)	-10(1)
O6	70(1)	48(1)	40(1)	-10(1)	7(1)	-4(1)
O9	134(2)	68(1)	81(1)	-44(1)	-11(1)	-15(1)
** C1	67(1)	46(1)	39(1)	-5(1)	-2(1)	-6(1)
C2	82(2)	58(1)	38(1)	-12(1)	-5(1)	-6(1)
C3	69(1)	53(1)	52(1)	-23(1)	-12(1)	0(1)
C4	53(1)	40(1)	48(1)	-12(1)	-6(1)	-2(1)
C5	47(1)	38(1)	36(1)	-8(1)	-3(1)	-1(1)
O5	68(1)	38(1)	39(1)	-7(1)	2(1)	-11(1)
C6	58(1)	41(1)	39(1)	-10(1)	1(1)	-6(1)
C6a	44(1)	36(1)	40(1)	-8(1)	-3(1)	-2(1)
C7	57(1)	48(1)	40(1)	-11(1)	-4(1)	-5(1)
C8	57(1)	50(1)	56(1)	-23(1)	-4(1)	-8(1)
C9	50(1)	37(1)	70(1)	-18(1)	-1(1)	-7(1)
C10	73(1)	36(1)	61(1)	-5(1)	-14(1)	-2(1)
C11	60(1)	39(1)	44(1)	-7(1)	3(1)	-11(1)
C11a	40(1)	35(1)	41(1)	-6(1)	-2(1)	0(1)
C11b	43(1)	37(1)	38(1)	-6(1)	-3(1)	1(1)
C12	68(1)	49(1)	90(2)	-25(1)	-25(1)	-6(1)
O4	88(1)	42(1)	59(1)	-16(1)	0(1)	-18(1)
O6	112(1)	57(1)	37(1)	-8(1)	10(1)	-26(1)
O9	101(1)	46(1)	97(1)	-24(1)	-2(1)	11(1)

## Theoretical data for compound 1 :

Final Energy in Hartrees: HF = - 879.7282735 (B3LYP/6-31++G(D,P))



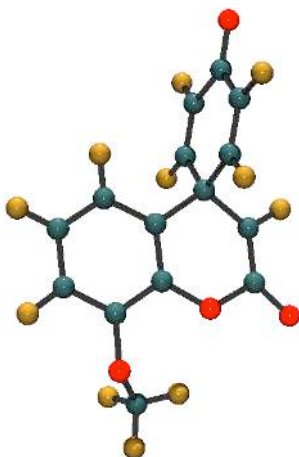
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.430375	-2.624924	.213216
2	6	0	2.621041	-1.922539	-.002833
3	6	0	2.603370	-.527822	-.102583
4	6	0	1.368559	.143881	.022208
5	6	0	.180569	-.551790	.249198
6	6	0	.219787	-1.951149	.338540
7	8	0	3.690478	.256180	-.315312
8	6	0	4.962127	-.369795	-.457047
9	8	0	1.413634	1.520834	-.149536
10	6	0	.385244	2.322836	.266576
11	6	0	-.746564	1.629288	.991570
12	6	0	-1.122870	.252859	.360784
13	6	0	-2.109260	-.417821	1.284057
14	6	0	-3.357675	-.758168	.928875
15	6	0	-3.870456	-.529416	-.441128
16	6	0	-2.933292	.107363	-1.390807
17	6	0	-1.690638	.463430	-1.028670
18	8	0	-5.011154	-.852488	-.767131
19	8	0	.446034	3.507930	.056338
20	1	0	5.670075	.442406	-.622930
21	1	0	4.977208	-1.049835	-1.317395
22	1	0	5.239930	-.917561	.451778
23	1	0	-3.304543	.271909	-2.398013
24	1	0	-4.046438	-1.221414	1.629455
25	1	0	-1.025817	.928860	-1.754349
26	1	0	-1.600472	2.307732	1.011579
27	1	0	-.417967	1.462243	2.026169
28	1	0	-1.756578	-.606753	2.296725
29	1	0	1.457016	-3.707770	.283683
30	1	0	-.700312	-2.502051	.501309
31	1	0	3.554074	-2.464804	-.094619

		1	2	3
		A	A	A
Frequencies --		37.9740	43.9304	80.4251
Red. masses --		5.8775	6.0358	4.2839
Frc consts --		.0050	.0069	.0163
IR Inten --		1.4632	1.7113	4.0625

### Theoretical data for compound 10 :

Final Energy in Hartrees: HF = - 879.1713081 (B3LYP/6-31++G(D,P))



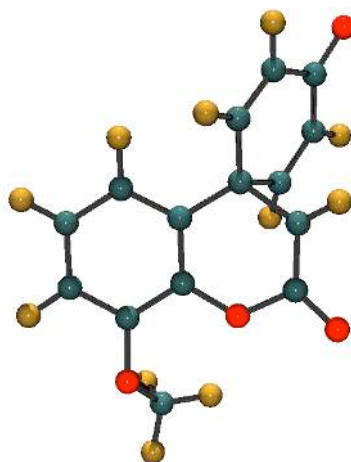
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.099823	-2.852971	.067652
2	6	0	-2.382061	-2.323520	-.112456
3	6	0	-2.568667	-.946705	-.215622
4	6	0	-1.456732	-.068011	-.152804
5	6	0	-.171113	-.599612	.052513
6	6	0	-.009651	-1.988789	.155230
7	8	0	-1.706282	1.247676	-.317863
8	6	0	-.685634	2.260225	.026098
9	6	0	.584949	1.782350	.281556
10	6	0	1.040592	.337881	.110827
11	6	0	1.818158	.255868	-1.185026
12	6	0	3.149086	.036962	-1.268887
13	6	0	3.956172	-.240459	-.072257
14	6	0	3.235488	-.250753	1.217840
15	6	0	1.910831	-.017958	1.292528
16	8	0	5.175445	-.458782	-.133048
17	8	0	-1.154866	3.403836	.040157
18	8	0	-3.848313	-.491805	-.457807
19	6	0	-4.385441	.456529	.474592
20	1	0	-5.418225	.626898	.159525
21	1	0	-3.824605	1.393258	.457413
22	1	0	-4.381607	.035402	1.489925
23	1	0	3.837077	-.447814	2.101758
24	1	0	3.680910	.063099	-2.216596
25	1	0	1.399192	-.019641	2.252713
26	1	0	1.352664	2.517073	.492073
27	1	0	1.233079	.457160	-2.079765
28	1	0	-.957141	-3.927409	.143763
29	1	0	.991046	-2.388123	.297472
30	1	0	-3.257177	-2.963526	-.180502

	1	2	3
	A	A	A
Frequencies --	23.6524	50.0833	77.0913
Red. masses --	5.1137	8.2316	3.8149
Frc consts --	.0017	.0122	.0134
IR Inten --	.1974	2.6776	3.0598

## Theoretical data for transition state TS1 :

Final Energy in Hartrees: HF = - 879.1565668 (B3LYP/6-31++G(D,P))



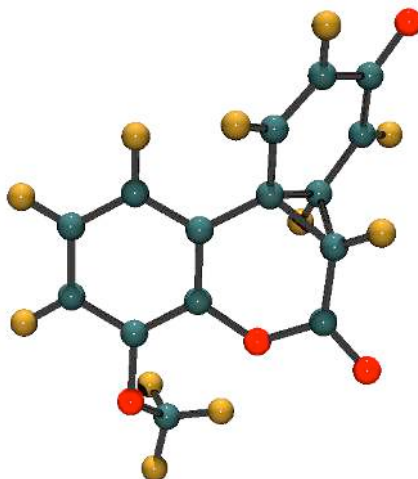
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.762037	2.812218	-.089311
2	6	0	2.882876	1.989731	.035655
3	6	0	2.743113	.600062	.021253
4	6	0	1.462768	.027827	-.127712
5	6	0	.328060	.850609	-.234145
6	6	0	.494473	2.241037	-.217040
7	8	0	1.393892	-1.341116	-.153544
8	6	0	.242067	-2.020849	-.673900
9	6	0	-.966746	-1.285037	-.689980
10	6	0	-1.027367	.208614	-.334931
11	6	0	-2.091101	.992244	-1.026739
12	6	0	-3.378996	.932594	-.641946
13	6	0	-3.872450	.133695	.524643
14	6	0	-2.875262	-.564137	1.249143
15	6	0	-1.507795	-.551482	.858863
16	8	0	-5.107060	.159937	.789692
17	8	0	.439835	-3.184879	-1.001810
18	8	0	3.892712	-.159296	.074873
19	6	0	4.001168	-1.094708	1.154339
20	1	0	5.003775	-1.522315	1.076342
21	1	0	3.251179	-1.884599	1.074182
22	1	0	3.900847	-.578728	2.119345
23	1	0	-3.175830	-1.148391	2.113975
24	1	0	-4.145830	1.488939	-1.177672
25	1	0	-.750657	-.833117	1.584782
26	1	0	-1.804899	-1.721033	-1.214428
27	1	0	-1.786970	1.601024	-1.877644
28	1	0	1.874710	3.892732	-.072820
29	1	0	-.385208	2.873298	-.287786
30	1	0	3.882775	2.400510	.138889

	1	2	3
	A	A	A
Frequencies --	-306.1658	47.2981	70.6809
Red. masses --	10.1525	5.5042	7.5343
Frc consts --	.5607	.0073	.0222
IR Inten --	679.7455	1.4875	5.1084

Theoretical data for compound 11 :

Final Energy in Hartrees: HF = - 879.1575149 (B3LYP/6-31++G(D,P))



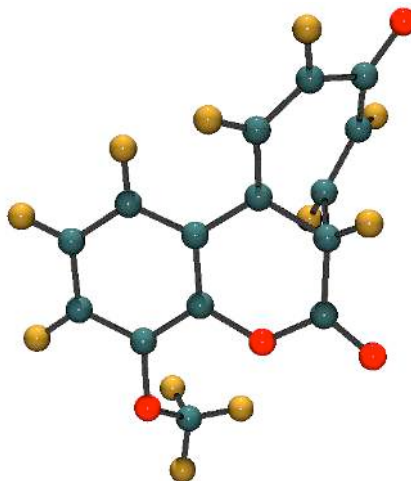
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.830040	2.797463	-.071724
2	6	0	2.932000	1.949851	.050594
3	6	0	2.757611	.563768	.022794
4	6	0	1.465679	.028664	-.139005
5	6	0	.346388	.872614	-.239086
6	6	0	.549154	2.259542	-.207675
7	8	0	1.371328	-1.345710	-.197197
8	6	0	.208904	-1.988554	-.679070
9	6	0	-1.022991	-1.249849	-.603895
10	6	0	-1.017239	.273691	-.341464
11	6	0	-2.088583	1.067370	-.991238
12	6	0	-3.378785	.956625	-.615073
13	6	0	-3.869451	.118146	.524238
14	6	0	-2.872787	-.587109	1.222433
15	6	0	-1.482653	-.602843	.805574
16	8	0	-5.110250	.150989	.795114
17	8	0	.360958	-3.135659	-1.066143
18	8	0	3.884996	-.228376	.074596
19	6	0	3.972050	-1.151124	1.166408
20	1	0	4.958058	-1.615034	1.085956
21	1	0	3.195582	-1.917220	1.104707
22	1	0	3.897988	-.618852	2.124710
23	1	0	-3.152015	-1.154191	2.106032
24	1	0	-4.151057	1.527222	-1.128143
25	1	0	-.737753	-.805479	1.573245
26	1	0	-1.840061	-1.655617	-1.186229
27	1	0	-1.795939	1.735808	-1.800652
28	1	0	1.967395	3.874928	-.044685
29	1	0	-.315072	2.912970	-.270753
30	1	0	3.940597	2.335985	.161980

	1	2	3
	A	A	A
Frequencies --	48.2311	70.1956	82.0859
Red. masses --	5.6904	7.1232	2.1130
Frc consts --	.0078	.0207	.0084
IR Inten --	1.5936	4.5749	2.4441

Theoretical data for transition state TS2 :

Final Energy in Hartrees: HF = - 879.1498774 (B3LYP/6-31++G(D,P))



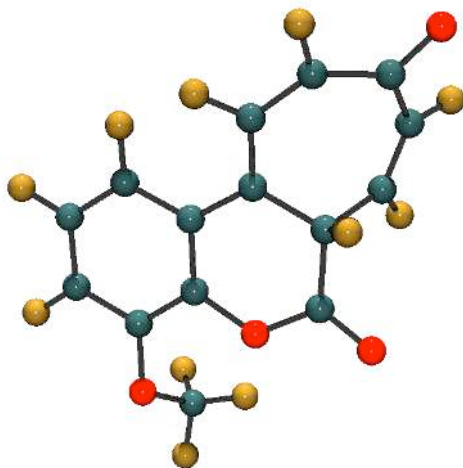
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.991332	2.759143	.028772
2	6	0	3.054286	1.856076	.107168
3	6	0	2.801733	.482672	.004455
4	6	0	1.490466	.032580	-.194103
5	6	0	.400029	.925571	-.257191
6	6	0	.684811	2.301430	-.133744
7	8	0	1.332975	-1.343693	-.345028
8	6	0	.117357	-1.919713	-.663535
9	6	0	-1.102501	-1.100030	-.511240
10	6	0	-.956278	.404500	-.408237
11	6	0	-2.049201	1.221933	-.891606
12	6	0	-3.364550	.969723	-.625544
13	6	0	-3.886536	.085363	.441455
14	6	0	-2.893935	-.532625	1.256949
15	6	0	-1.537099	-.701408	.874813
16	8	0	-5.131875	.082607	.687464
17	8	0	.137008	-3.076820	-1.028650
18	8	0	3.880871	-.379087	.021835
19	6	0	3.923296	-1.316361	1.101854
20	1	0	4.873879	-1.846231	1.002370
21	1	0	3.097461	-2.030844	1.045665
22	1	0	3.898385	-.792178	2.067086
23	1	0	-3.164653	-.766447	2.283432
24	1	0	-4.125681	1.592774	-1.092193
25	1	0	-.798758	-.880922	1.655018
26	1	0	-1.905465	-1.460601	-1.150695
27	1	0	-1.785898	2.093272	-1.492571
28	1	0	2.181389	3.825697	.117190
29	1	0	-.141325	3.004531	-.147085
30	1	0	4.079582	2.183773	.245220

	1	2	3
	A	A	A
Frequencies --	-490.6418	45.5429	69.6040
Red. masses --	5.3992	5.8733	3.8492
Frc consts --	.7658	.0072	.0110
IR Inten --	192.1547	1.7354	5.4452

Theoretical data for compound 12c :

Final Energy in Hartrees: HF = - 879.1830086 (B3LYP/6-31++G(D,P))



Standard orientation:

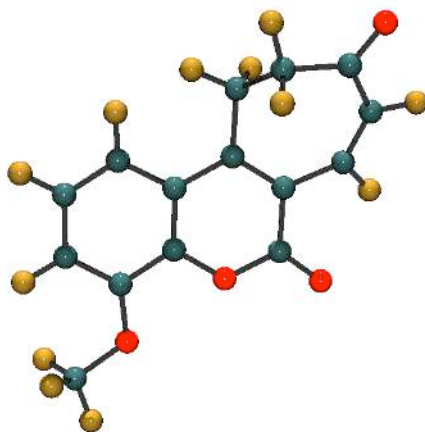
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.335577	2.677858	.251889
2	6	0	3.320110	1.687280	.145429
3	6	0	2.924765	.363419	-.074728
4	6	0	1.566548	.056256	-.205162
5	6	0	.546117	1.031948	-.100438
6	6	0	.985961	2.359914	.153063
7	8	0	1.270963	-1.277981	-.477378
8	6	0	.000414	-1.775410	-.507299
9	6	0	-1.175356	-.831733	-.346487
10	6	0	-.827778	.640135	-.267227
11	6	0	-1.875458	1.538939	-.453509
12	6	0	-3.256571	1.288041	-.465608
13	6	0	-3.993232	.222438	.160908
14	6	0	-3.278597	-.771295	1.011439
15	6	0	-2.035032	-1.250326	.833021
16	8	0	-5.252903	.172737	.137627
17	8	0	-.122864	-2.970504	-.679653
18	8	0	3.909685	-.595509	-.232150
19	6	0	3.951887	-1.618693	.765245
20	1	0	2.629018	3.708089	.439438
21	1	0	4.378441	1.909370	.232365
22	1	0	.243072	3.138436	.288234
23	1	0	-1.791455	-.990033	-1.251905
24	1	0	-1.593787	2.572195	-.664226
25	1	0	-3.899675	2.072967	-.860299
26	1	0	-3.874991	-1.140038	1.844359
27	1	0	-1.618152	-1.963356	1.543020
28	1	0	4.830967	-2.226972	.536677
29	1	0	3.055942	-2.245485	.736111
30	1	0	4.065440	-1.177740	1.765442

	1	2	3
	A	A	A
Frequencies --	35.6304	62.8939	78.0753
Red. masses --	6.7930	3.5666	6.1076
Frc consts --	.0051	.0083	.0219
IR Inten --	.2839	.3609	3.1001



Theoretical data for compound 2a :

Final Energy in Hartrees: HF = - 879.7472803 (B3LYP/6-31++G(D,P))



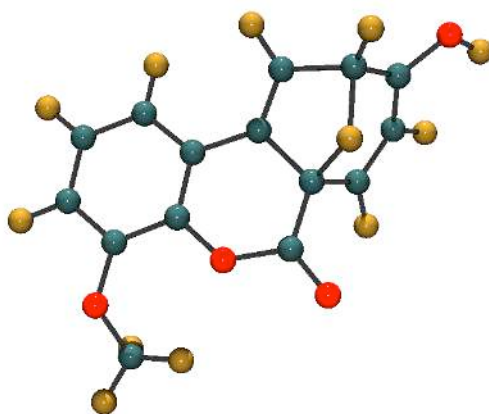
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.349150	-2.507020	-.140323
2	6	0	3.310763	-1.496038	.021122
3	6	0	2.917250	-.160087	.074401
4	6	0	1.540855	.145310	-.038901
5	6	0	.566571	-.854500	-.204577
6	6	0	1.004075	-2.202037	-.250928
7	8	0	3.747390	.900227	.228288
8	6	0	5.145697	.654887	.347793
9	8	0	1.219489	1.464892	.017180
10	6	0	-.079672	1.920359	-.070011
11	6	0	-1.139629	.904328	-.225502
12	6	0	-.823046	-.433999	-.310222
13	8	0	-.255921	3.118293	-.015285
14	6	0	-2.474584	1.483322	-.363343
15	6	0	-3.709570	.954388	-.180142
16	6	0	-4.085459	-.382297	.318918
17	6	0	-3.010718	-1.432930	.550618
18	6	0	-1.918926	-1.445294	-.537072
19	8	0	-5.262011	-.636784	.557367
20	1	0	5.605419	1.636875	.459401
21	1	0	5.541581	.165065	-.550198
22	1	0	5.368002	.043875	1.231139
23	1	0	-3.519087	-2.399541	.599453
24	1	0	-2.563546	-1.255830	1.538860
25	1	0	-4.566968	1.602253	-.342670
26	1	0	2.671876	-3.542588	-.176273
27	1	0	.290442	-3.006791	-.368260
28	1	0	4.357227	-1.762248	.105044
29	1	0	-2.441191	2.538150	-.623357
30	1	0	-1.508287	-2.450502	-.613372
31	1	0	-2.383598	-1.232090	-1.511147

	1	2	3
	A	A	A
Frequencies --	31.7646	53.9631	71.6721
Red. masses --	6.0848	3.7000	6.2170
Frc consts --	.0036	.0063	.0188
IR Inten --	.5194	1.4801	10.6039

### Theoretical data for transition state **TS4n** :

Final Energy in Hartrees: HF = - 879.662717 (B3LYP/6-31++G(D,P))



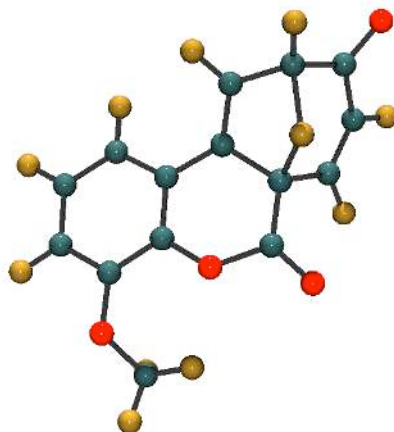
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.424677	2.655365	.403496
2	6	0	3.365309	1.636139	.230276
3	6	0	2.958324	.333511	-.071641
4	6	0	1.583637	.072055	-.209371
5	6	0	.627554	1.086422	-.036927
6	6	0	1.064765	2.383114	.280003
7	8	0	3.925313	-.606824	-.304929
8	6	0	3.920715	-1.789692	.511612
9	8	0	1.226437	-1.217005	-.577833
10	6	0	-.045409	-1.718288	-.387352
11	6	0	-1.134013	-.736911	-.117287
12	6	0	-.765191	.714782	-.272374
13	8	0	-.198716	-2.916255	-.461189
14	6	0	-1.978092	-1.095991	.997645
15	6	0	-3.218478	-.519000	1.190716
16	6	0	-3.804525	.229514	.145843
17	6	0	-3.044839	.683018	-.964734
18	6	0	-1.796930	1.458880	-.711085
19	8	0	-5.150946	.383565	.076332
20	1	0	2.757488	3.659527	.647334
21	1	0	4.429509	1.826154	.323039
22	1	0	.329525	3.166585	.433258
23	1	0	4.839297	-2.321641	.259030
24	1	0	3.055701	-2.420834	.297554
25	1	0	3.937192	-1.518258	1.574473
26	1	0	-1.678539	-1.919488	1.641991
27	1	0	-3.830841	-.829895	2.034151
28	1	0	-3.653422	1.001031	-1.812975
29	1	0	-2.200999	-.527817	-1.028892
30	1	0	-1.755042	2.523330	-.919649
31	1	0	-5.591618	-.144047	.758723

	1	2	3
	A	A	A
Frequencies --	-1503.8333	43.5221	58.9796
Red. masses --	1.1994	6.1536	2.0421
Frc consts --	1.5982	.0069	.0042
IR Inten --	247.0457	1.7397	2.5080

### Theoretical data for transition state **TS4a** :

Final Energy in Hartrees: HF = - 879.1443616 (B3LYP/6-31++G(D,P))



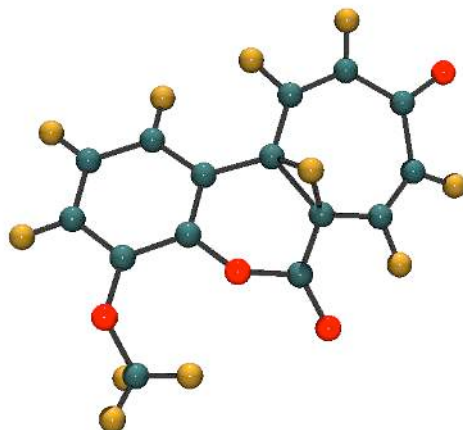
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.412460	2.644924	.430127
2	6	0	3.353816	1.631956	.216492
3	6	0	2.928919	.336883	-.097623
4	6	0	1.554657	.070975	-.209893
5	6	0	.593066	1.077694	.015001
6	6	0	1.049229	2.369535	.344228
7	8	0	1.183408	-1.199535	-.595416
8	6	0	-.101695	-1.709630	-.334994
9	6	0	-1.180581	-.741945	-.100597
10	6	0	-.794613	.703235	-.184137
11	6	0	-1.821465	1.471174	-.645435
12	6	0	-3.061427	.760480	-.968287
13	6	0	-3.948442	.241275	.087218
14	6	0	-3.329051	-.586567	1.137662
15	6	0	-2.095239	-1.130402	.998668
16	8	0	-5.191362	.388298	.058649
17	8	0	-.199449	-2.923404	-.361573
18	8	0	3.896761	-.610292	-.363527
19	6	0	3.872910	-1.797787	.437693
20	1	0	4.767889	-2.360594	.160465
21	1	0	2.980158	-2.396043	.241864
22	1	0	3.922400	-1.540547	1.504732
23	1	0	-3.983720	-.895326	1.949330
24	1	0	-3.650773	1.196020	-1.780067
25	1	0	-1.763393	-1.907039	1.687927
26	1	0	-2.174153	-.523676	-1.033214
27	1	0	-1.694158	2.522276	-.900780
28	1	0	2.748341	3.647488	.682622
29	1	0	.316535	3.147455	.536826
30	1	0	4.420739	1.818642	.288487

	1 A	2 A	3 A
Frequencies --	-1437.1718	45.6003	70.2999
Red. masses --	1.1704	6.5841	2.5285
Frc consts --	1.4243	.0081	.0074
IR Inten --	543.4094	.0748	2.2404

### Theoretical data for transition state **TS5a** :

Final Energy in Hartrees: HF = - 879.1087276 (B3LYP/6-31++G(D,P))



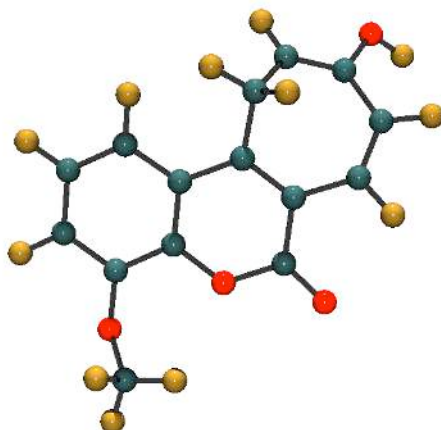
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.271007	2.709654	.412532
2	6	0	3.280412	1.758013	.255286
3	6	0	2.938058	.439209	-.073108
4	6	0	1.593226	.103722	-.276729
5	6	0	.557432	1.048560	-.114176
6	6	0	.928901	2.358775	.257300
7	8	0	1.304502	-1.173721	-.725645
8	6	0	.121902	-1.800965	-.236434
9	6	0	-1.031494	-.957562	-.148758
10	6	0	-.818397	.598188	-.318788
11	6	0	-1.903230	1.513478	-.407375
12	6	0	-3.273487	1.380259	-.328964
13	6	0	-4.074749	.252673	.124351
14	6	0	-3.505940	-1.062873	.520750
15	6	0	-2.249085	-1.546704	.376251
16	8	0	-5.312659	.383026	.221195
17	8	0	.208365	-3.003177	-.010553
18	8	0	3.964686	-.461151	-.272376
19	6	0	3.934253	-1.650263	.528321
20	1	0	4.855368	-2.189669	.292622
21	1	0	3.066320	-2.270654	.293977
22	1	0	3.929500	-1.390359	1.595948
23	1	0	-4.261567	-1.726661	.932504
24	1	0	-3.873832	2.257354	-.555164
25	1	0	-2.089282	-2.579159	.685042
26	1	0	-1.006246	-.291395	-1.249489
27	1	0	-1.571081	2.529177	-.623978
28	1	0	2.529493	3.729904	.685401
29	1	0	.159734	3.102305	.435730
30	1	0	4.329586	2.004359	.383673

	1	2	3
	A	A	A
Frequencies --	-1653.2005	47.5290	56.5620
Red. masses --	1.2708	6.4905	4.2436
Frc consts --	2.0463	.0086	.0080
IR Inten --	1805.7267	1.0927	.2551

Theoretical data for compound 2b :

Final Energy in Hartrees: HF = - 879.7303913 (B3LYP/6-31++G(D,P))



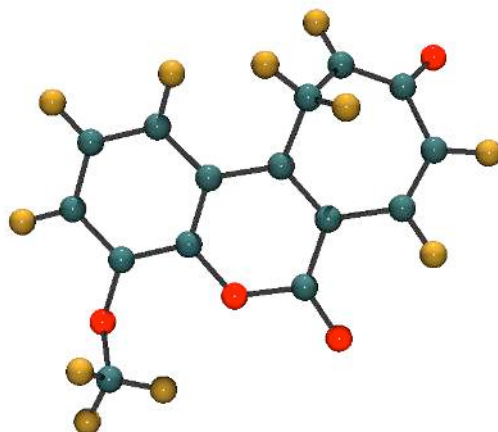
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.193964	-2.717996	-.005408
2	6	0	-3.183343	-1.780092	.316443
3	6	0	-2.885688	-.419421	.358380
4	6	0	-1.566146	-.008887	.083528
5	6	0	-.559332	-.933911	-.259383
6	6	0	-.902507	-2.303378	-.299425
7	8	0	-3.861281	.453962	.751821
8	6	0	-4.260214	1.473597	-.181669
9	8	0	-1.309616	1.329381	.163424
10	6	0	-.056619	1.873325	-.060454
11	6	0	1.030405	.932030	-.368538
12	6	0	.769101	-.413274	-.534670
13	8	0	.043640	3.080134	.006075
14	6	0	2.345896	1.538691	-.480753
15	6	0	3.539090	.966586	-.157270
16	6	0	3.728781	-.381598	.348203
17	6	0	2.944743	-1.431612	.015834
18	6	0	1.888528	-1.292406	-1.048564
19	8	0	4.794868	-.595389	1.197666
20	1	0	-2.441307	-3.774498	-.027519
21	1	0	-4.197940	-2.086821	.548413
22	1	0	-.147791	-3.042299	-.539317
23	1	0	-5.107797	1.978518	.283644
24	1	0	-4.579714	1.018045	-1.126881
25	1	0	-3.455128	2.189550	-.360269
26	1	0	2.343896	2.596619	-.725695
27	1	0	4.424396	1.601378	-.186119
28	1	0	3.099226	-2.386695	.508575
29	1	0	2.310219	-.812661	-1.943087
30	1	0	1.521640	-2.271618	-1.354825
31	1	0	5.057025	.235852	1.613668

	1	2	3
	A	A	A
Frequencies --	40.4893	59.3426	72.3116
Red. masses --	6.2660	3.8561	2.0836
Frc consts --	.0061	.0080	.0064
IR Inten --	.6649	.9673	3.7119

### Theoretical data for compound 2c :

Final Energy in Hartrees: HF = - 879.1790705 (B3LYP/6-31++G(D,P))



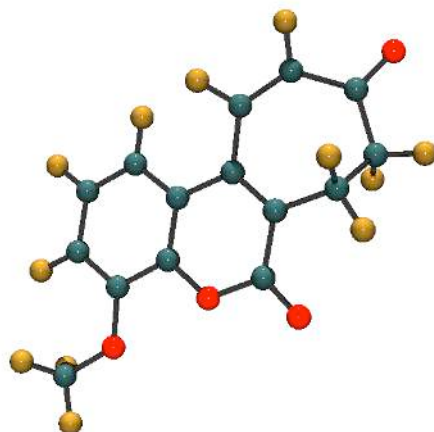
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.091416	-2.728786	-.000267
2	6	0	3.101241	-1.811241	-.318604
3	6	0	2.817364	-.446930	-.358420
4	6	0	1.508025	-.006515	-.085982
5	6	0	.483096	-.912349	.260714
6	6	0	.807200	-2.287085	.294118
7	8	0	3.820644	.416465	-.742965
8	6	0	4.204153	1.421210	.203778
9	8	0	1.279156	1.335755	-.157830
10	6	0	.011239	1.902344	.055428
11	6	0	-1.074543	.991141	.370540
12	6	0	-.828761	-.368908	.569537
13	8	0	-.034073	3.119157	-.021290
14	6	0	-2.405141	1.566952	.409224
15	6	0	-3.566346	.937933	.055781
16	6	0	-3.758193	-.441988	-.466559
17	6	0	-2.894069	-1.443923	.017289
18	6	0	-1.931538	-1.205736	1.148695
19	8	0	-4.693550	-.627021	-1.312390
20	1	0	2.314592	-3.792003	.015484
21	1	0	4.111739	-2.132980	-.550448
22	1	0	.030166	-3.007145	.522049
23	1	0	5.065622	1.929692	-.235713
24	1	0	4.502029	.957717	1.154353
25	1	0	3.398073	2.138483	.375701
26	1	0	-2.438202	2.639878	.582453
27	1	0	-4.458515	1.557923	-.030460
28	1	0	-2.956021	-2.434598	-.427673
29	1	0	-2.387801	-.659269	1.989299
30	1	0	-1.549957	-2.149261	1.549116

	1	2	3
	A	A	A
Frequencies --	41.5043	60.1134	82.1901
Red. masses --	6.9013	4.6347	2.1725
Frc consts --	.0070	.0099	.0086
IR Inten --	1.8849	2.3228	4.8168

Theoretical data for compound 13a :

Final Energy in Hartrees: HF = - 879.7447082 (B3LYP/6-31++G(D,P))



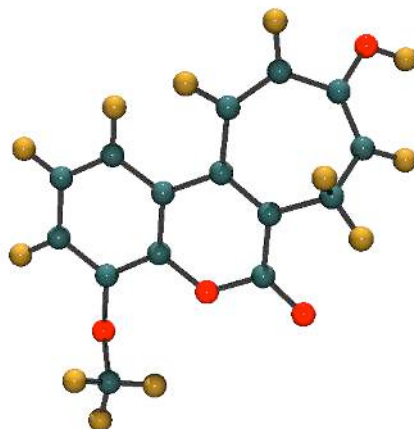
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.313421	-2.530857	.059514
2	6	0	-3.285576	-1.522069	.151148
3	6	0	-2.907587	-.181313	.096624
4	6	0	-1.536649	.129297	-.059679
5	6	0	-.559558	-.868676	-.174515
6	6	0	-.973105	-2.219105	-.097839
7	8	0	-3.748446	.878694	.185674
8	6	0	-5.141028	.626915	.347323
9	8	0	-1.221952	1.454816	-.086491
10	6	0	.075777	1.909311	-.185967
11	6	0	1.136599	.899564	-.326087
12	6	0	.831284	-.437298	-.341383
13	8	0	.253130	3.110256	-.167064
14	6	0	2.538257	1.432610	-.462934
15	6	0	3.495093	.914964	.624067
16	6	0	4.013841	-.489613	.374859
17	6	0	3.171645	-1.490677	-.331164
18	6	0	1.846527	-1.469861	-.598601
19	8	0	5.136678	-.820998	.737536
20	1	0	-5.611636	1.609062	.393986
21	1	0	-5.341184	.080480	1.277109
22	1	0	-5.545671	.067202	-.504807
23	1	0	2.997377	.923972	1.604415
24	1	0	4.372134	1.562471	.714992
25	1	0	3.728810	-2.385153	-.599243
26	1	0	-2.622066	-3.569685	.119166
27	1	0	-.243862	-3.018370	-.141877
28	1	0	-4.327137	-1.792752	.272819
29	1	0	2.490689	2.521517	-.420468
30	1	0	2.937119	1.167176	-1.453275
31	1	0	1.457562	-2.367225	-1.072250

	1	2	3
	A	A	A
Frequencies --	31.8613	57.6338	67.2632
Red. masses --	6.5382	4.7245	4.5207
Frc consts --	.0039	.0092	.0121
IR Inten --	1.2865	10.3222	.5703

Theoretical data for compound 13b :

Final Energy in Hartrees: HF = - 879.7297326 (B3LYP/6-31++G(D,P))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.248134	2.721570	.047005
2	6	0	3.232827	1.763404	.315882
3	6	0	2.913285	.407731	.338178
4	6	0	1.580361	.023099	.087420
5	6	0	.582571	.967972	-.215226
6	6	0	.941194	2.332397	-.216162
7	8	0	3.883699	-.488664	.692121
8	6	0	4.229686	-1.508309	-.261214
9	8	0	1.300316	-1.311232	.179952
10	6	0	.034690	-1.828936	-.031864
11	6	0	-1.013467	-.883574	-.417937
12	6	0	-.769066	.467197	-.482597
13	8	0	-.104522	-3.029056	.095036
14	6	0	-2.361594	-1.459645	-.780408
15	6	0	-3.402190	-1.027401	.221718
16	6	0	-3.760053	.270682	.336952
17	6	0	-3.130832	1.352801	-.403503
18	6	0	-1.831047	1.423356	-.792789
19	8	0	-4.779326	.723650	1.144955
20	1	0	2.508494	3.775256	.046406
21	1	0	4.257577	2.049665	.528494
22	1	0	.190204	3.089319	-.405542
23	1	0	5.084895	-2.031332	.168999
24	1	0	4.521986	-1.052304	-1.215060
25	1	0	3.406041	-2.208979	-.414248
26	1	0	-2.288795	-2.546981	-.805958
27	1	0	-2.638084	-1.113113	-1.786898
28	1	0	-3.883656	-1.783489	.839478
29	1	0	-3.764543	2.218699	-.582316
30	1	0	-1.526733	2.338920	-1.290520
31	1	0	-5.235721	-.027320	1.547929

	1	2	3
	A	A	A
Frequencies --	40.4855	56.5587	67.6228
Red. masses --	5.8898	3.3867	2.1990
Frc consts --	.0057	.0064	.0059
IR Inten --	.6914	1.3699	3.4663



### Theoretical data for compound 13c :

Final Energy in Hartrees: HF = - 879.1767698 (B3LYP/6-31++G(D,P))



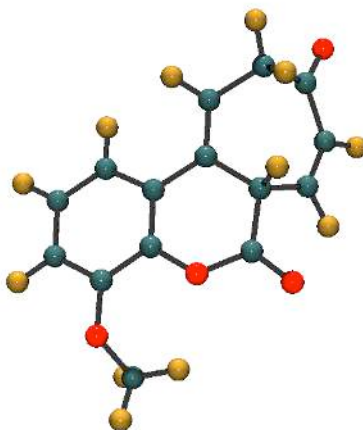
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.258180	2.707007	0.020072
2	6	0	3.231437	1.737316	0.291916
3	6	0	2.876416	0.390133	0.334611
4	6	0	1.537128	0.021285	0.103438
5	6	0	0.549392	0.977626	-0.210645
6	6	0	0.941767	2.334915	-0.226086
7	8	0	3.844411	-0.527165	0.682609
8	6	0	4.130179	-1.556921	-0.271412
9	8	0	1.237509	-1.305211	0.212909
10	6	0	-0.049744	-1.810920	-0.021620
11	6	0	-1.071330	-0.860311	-0.421099
12	6	0	-0.806211	0.502121	-0.485060
13	8	0	-0.165325	-3.019487	0.091486
14	6	0	-2.416753	-1.398903	-0.834223
15	6	0	-3.422328	-1.028501	0.223719
16	6	0	-3.838275	0.292863	0.449848
17	6	0	-3.170167	1.354633	-0.350169
18	6	0	-1.866125	1.455685	-0.753797
19	8	0	-4.755895	0.667790	1.255531
20	1	0	2.533361	3.758052	0.006535
21	1	0	4.264092	2.004643	0.492800
22	1	0	0.198601	3.099770	-0.415266
23	1	0	4.977987	-2.112324	0.136529
24	1	0	4.415113	-1.116069	-1.236542
25	1	0	3.277618	-2.226949	-0.404985
26	1	0	-2.350537	-2.484499	-0.932205
27	1	0	-2.669477	-0.984370	-1.825194
28	1	0	-3.873543	-1.816649	0.822042
29	1	0	-3.793879	2.238733	-0.485798
30	1	0	-1.566325	2.404077	-1.195161

	1	2	3
	A	A	A
Frequencies --	40.4683	54.8517	75.6483
Red. masses --	6.5766	4.4953	2.0564
Frc consts --	.0063	.0080	.0069
IR Inten --	1.6994	.4552	3.7086

Theoretical data for compound 12a :

Final Energy in Hartrees: HF = - 879.7161544 (B3LYP/6-31++G(D,P))



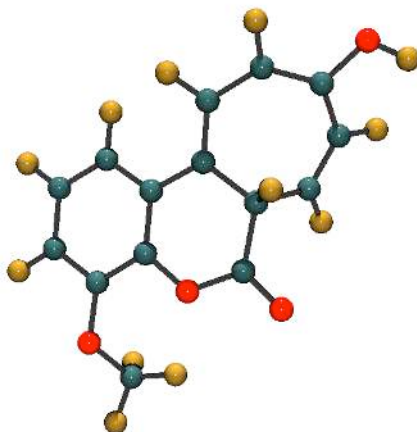
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.157522	2.747102	.304289
2	6	0	3.192667	1.809808	.232235
3	6	0	2.906108	.469345	-.022237
4	6	0	1.566299	.088695	-.221535
5	6	0	.513486	1.012111	-.170525
6	6	0	.838087	2.352963	.115694
7	8	0	3.940772	-.416923	-.154972
8	6	0	4.049180	-1.450060	.838862
9	8	0	1.367028	-1.258275	-.497477
10	6	0	.140743	-1.842796	-.471446
11	6	0	-1.103106	-.958751	-.455747
12	6	0	-.859600	.549213	-.431108
13	8	0	.073917	-3.047539	-.503295
14	6	0	-2.057941	-1.461385	.617351
15	6	0	-3.242224	-.925692	.962084
16	6	0	-3.917847	.243304	.349868
17	6	0	-3.307689	.880705	-.900324
18	6	0	-1.899120	1.368021	-.672412
19	8	0	-4.964042	.666374	.822475
20	1	0	-1.569801	-1.198179	-1.427171
21	1	0	4.967708	-1.989312	.603310
22	1	0	3.199584	-2.136317	.795824
23	1	0	4.129897	-1.008294	1.839577
24	1	0	-3.808846	-1.380906	1.770604
25	1	0	4.229957	2.095412	.371394
26	1	0	-3.965978	1.695855	-1.204408
27	1	0	-3.325635	.122272	-1.700434
28	1	0	-1.752655	2.443225	-.684839
29	1	0	2.384498	3.786451	.519588
30	1	0	.045851	3.088026	.199879
31	1	0	-1.735367	-2.362810	1.132520

	1	2	3
	A	A	A
Frequencies --	34.8250	54.7312	61.2133
Red. masses --	6.6370	3.9926	5.0008
Frc consts --	.0047	.0070	.0110
IR Inten --	.5916	3.8859	3.0258

Theoretical data for compound 12b :

Final Energy in Hartrees: HF = - 879.7154875 (B3LYP/6-31++G(D,P))



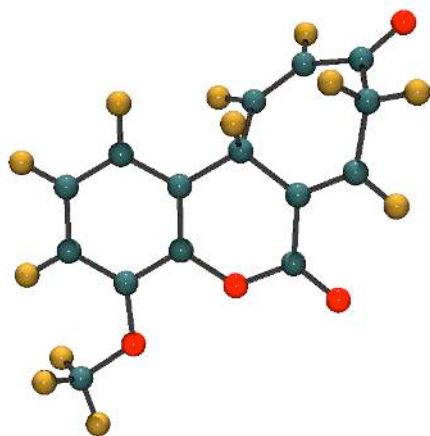
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.355393	2.675332	.304424
2	6	0	3.330982	1.682857	.169081
3	6	0	2.957362	.361762	-.080352
4	6	0	1.591801	.055642	-.214580
5	6	0	.594053	1.037413	-.093902
6	6	0	1.007427	2.355002	.190512
7	8	0	3.938588	-.574831	-.272336
8	6	0	4.024765	-1.639471	.688602
9	8	0	1.302453	-1.272899	-.495412
10	6	0	.036340	-1.780125	-.479620
11	6	0	-1.136400	-.828857	-.325685
12	6	0	-.803824	.649941	-.288121
13	8	0	-.104210	-2.972799	-.602175
14	6	0	-1.948359	-1.164472	.903202
15	6	0	-3.214621	-.715932	1.041459
16	6	0	-3.856810	.209998	.132292
17	6	0	-3.224435	1.220778	-.547366
18	6	0	-1.824927	1.533098	-.500044
19	8	0	-5.230750	.197458	.072648
20	1	0	2.651848	3.697912	.516212
21	1	0	4.388609	1.908175	.256270
22	1	0	.258887	3.126335	.333113
23	1	0	4.911672	-2.212559	.414156
24	1	0	3.143847	-2.285175	.649820
25	1	0	4.151239	-1.231337	1.699081
26	1	0	-1.775744	-1.015828	-1.202860
27	1	0	-1.496203	-1.770462	1.683527
28	1	0	-3.791788	-1.025441	1.912186
29	1	0	-3.877518	1.925239	-1.056915
30	1	0	-1.575588	2.577962	-.667630
31	1	0	-5.570374	-.628041	.441821

	1	2	3
	A	A	A
Frequencies --	35.8372	58.2511	74.5111
Red. masses --	6.3175	2.8679	3.0436
Frc consts --	.0048	.0057	.0100
IR Inten --	1.1746	.9009	2.3515

Theoretical data for compound 14a :

Final Energy in Hartrees: HF = - 879.7186584 (B3LYP/6-31++G(D,P))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.428058	-2.456413	-.439943
2	6	0	-3.335544	-1.427260	-.158211
3	6	0	-2.873763	-.125515	.049658
4	6	0	-1.483439	.126354	-.024507
5	6	0	-.579180	-.894124	-.294561
6	6	0	-1.065417	-2.194729	-.509551
7	8	0	-3.657574	.947661	.323635
8	6	0	-5.065721	.755571	.408334
9	8	0	-1.109903	1.439257	.192651
10	6	0	.167082	1.892607	-.006218
11	6	0	1.211134	.891339	-.353420
12	6	0	.905001	-.600395	-.362595
13	8	0	.372206	3.077921	.125298
14	6	0	2.447623	1.337071	-.629574
15	6	0	3.598602	.420356	-.935892
16	6	0	4.019127	-.453416	.254711
17	6	0	3.006911	-1.271852	.962699
18	6	0	1.686197	-1.347735	.712463
19	8	0	5.191367	-.494386	.600906
20	1	0	1.259157	-.989829	-1.332635
21	1	0	-5.481221	1.737634	.635133
22	1	0	-5.324933	.054488	1.211217
23	1	0	-5.476791	.395216	-.542765
24	1	0	3.425874	-1.863149	1.773218
25	1	0	4.482129	.973159	-1.257628
26	1	0	3.317828	-.268174	-1.750519
27	1	0	2.630032	2.407375	-.599854
28	1	0	-4.395096	-1.645595	-.108062
29	1	0	-2.798814	-3.462735	-.607626
30	1	0	-.365599	-2.994784	-.734698
31	1	0	1.095335	-2.018382	1.333952

	1	2	3
	A	A	A
Frequencies --	37.1078	61.5411	64.4137
Red. masses --	5.8085	6.9639	4.5436
Frc consts --	.0047	.0155	.0111
IR Inten --	.4599	6.3032	.4052

### Theoretical data for compound **14b** :

Final Energy in Hartrees: HF = - 879.7203451 (B3LYP/6-31++G(D,P))



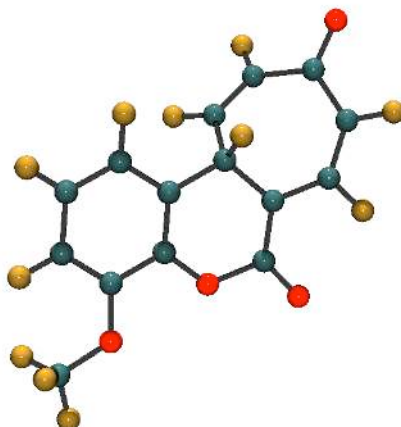
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.302087	-2.519815	-.434298
2	6	0	-3.267516	-1.530642	-.205651
3	6	0	-2.876941	-.204986	-.000965
4	6	0	-1.498893	.113357	-.025110
5	6	0	-.538042	-.867962	-.244336
6	6	0	-.951528	-2.193519	-.455033
7	8	0	-3.724581	.832651	.224377
8	6	0	-5.122593	.570978	.249799
9	8	0	-1.193800	1.444316	.183881
10	6	0	.075745	1.949155	.028450
11	6	0	1.168273	.988245	-.225547
12	6	0	.927832	-.506104	-.239028
13	8	0	.211671	3.151788	.109336
14	6	0	2.410888	1.485001	-.488270
15	6	0	3.618654	.723579	-.604243
16	6	0	3.897724	-.447497	.062072
17	6	0	3.021944	-1.111704	1.005160
18	6	0	1.673840	-1.090359	.943216
19	8	0	5.142422	-1.011227	.019009
20	1	0	-2.618586	-3.545216	-.598372
21	1	0	-4.316721	-1.799204	-.193540
22	1	0	-.202908	-2.960084	-.634677
23	1	0	-5.597285	1.534260	.438612
24	1	0	-5.383890	-.128761	1.053513
25	1	0	-5.471973	.173316	-.711268
26	1	0	1.396544	-.906992	-1.152292
27	1	0	2.494262	2.562413	-.608988
28	1	0	4.443738	1.199189	-1.134619
29	1	0	3.521378	-1.626693	1.821728
30	1	0	1.091573	-1.511459	1.759483
31	1	0	5.734387	-.477373	-.529699

		1		2		3
		A		A		A
Frequencies	--	39.4168		64.6039		85.0857
Red. masses	--	4.9099		4.5417		4.3780
Frc consts	--	.0045		.0112		.0187
IR Inten	--	1.8318		2.3416		1.1459

Theoretical data for compound 14c :

Final Energy in Hartrees: HF = - 879.1933354 (B3LYP/6-31++G(D,P))



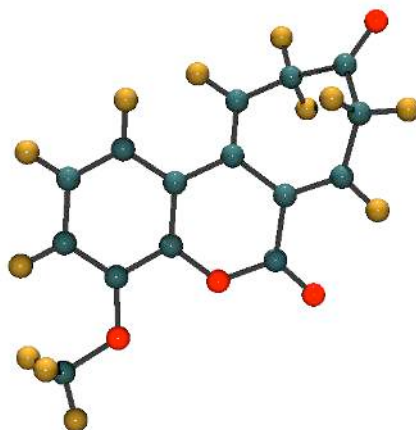
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.256912	-2.517871	-.424628
2	6	0	-3.229952	-1.530435	-.206917
3	6	0	-2.841695	-.205508	-.004271
4	6	0	-1.465666	.136787	-.016755
5	6	0	-.498777	-.848630	-.223588
6	6	0	-.910031	-2.176345	-.432213
7	8	0	-3.711672	.831001	.213157
8	6	0	-5.095874	.546112	.224565
9	8	0	-1.173144	1.451728	.184275
10	6	0	.151900	1.958763	.035699
11	6	0	1.201216	1.012257	-.166304
12	6	0	.967110	-.482513	-.219164
13	8	0	.224094	3.181355	.097216
14	6	0	2.491843	1.486971	-.437165
15	6	0	3.682689	.767606	-.539034
16	6	0	4.022863	-.516361	.027532
17	6	0	3.072434	-1.184897	.963098
18	6	0	1.729359	-1.165589	.903116
19	8	0	5.165646	-1.023801	-.107814
20	1	0	-2.564965	-3.547179	-.586924
21	1	0	-4.278877	-1.803509	-.201590
22	1	0	-.151311	-2.936975	-.597251
23	1	0	-5.594895	1.500216	.406185
24	1	0	-5.360708	-.159042	1.025354
25	1	0	-5.435418	.137060	-.737713
26	1	0	1.413699	-.846133	-1.163969
27	1	0	2.554611	2.558221	-.625899
28	1	0	4.542887	1.282882	-.963156
29	1	0	3.566209	-1.737341	1.761090
30	1	0	1.146338	-1.652549	1.685374

	1	2	3
	A	A	A
Frequencies --	39.7482	61.4077	76.6007
Red. masses --	4.7705	4.6043	5.4395
Frc consts --	.0044	.0102	.0188
IR Inten --	.1498	1.2772	7.0362

Theoretical data for compounds 15a and 6a :

Final Energy in Hartrees: HF = - 879.7342275 (B3LYP/6-31++G(D,P))



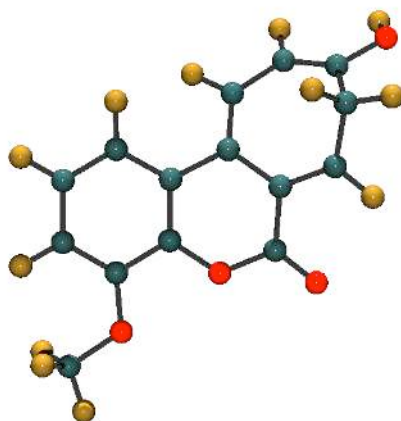
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.311009	-2.527939	.324768
2	6	0	3.281105	-1.518780	.251171
3	6	0	2.895084	-.192142	.043963
4	6	0	1.520691	.101334	-.091232
5	6	0	.549101	-.902342	-.036371
6	6	0	.962739	-2.229983	.185741
7	8	0	3.742321	.865232	-.043142
8	6	0	5.139882	.625065	.080462
9	8	0	1.212119	1.429041	-.322150
10	6	0	-.064550	1.918322	-.213411
11	6	0	-1.136157	.920373	.065785
12	6	0	-.856974	-.493196	-.220746
13	8	0	-.236746	3.108099	-.344168
14	6	0	-2.291527	1.372462	.610468
15	6	0	-3.394678	.498049	1.119018
16	6	0	-4.095316	-.401148	.087301
17	6	0	-3.213951	-.895691	-1.062952
18	6	0	-1.821990	-1.321696	-.693894
19	8	0	-5.264521	-.696550	.189425
20	1	0	5.614512	1.600938	-.024627
21	1	0	5.500787	-.044179	-.710296
22	1	0	5.386654	.202343	1.062216
23	1	0	-4.161394	1.070634	1.643938
24	1	0	-2.971324	-.224324	1.837361
25	1	0	-2.394614	2.446478	.740402
26	1	0	-3.157621	-.026904	-1.741269
27	1	0	-3.753540	-1.688865	-1.583330
28	1	0	-1.567796	-2.357364	-.900217
29	1	0	2.623756	-3.552154	.502580
30	1	0	.220555	-3.016380	.269789
31	1	0	4.327838	-1.772926	.363310

	1	2	3
	A	A	A
Frequencies --	37.3845	49.5040	76.5492
Red. masses --	6.7381	5.4742	4.4583
Frc consts --	.0055	.0079	.0154
IR Inten --	1.3950	4.8171	1.1114

### Theoretical data for compound **15b** :

Final Energy in Hartrees: HF = - 879.7291446 (B3LYP/6-31++G(D,P))



Standard orientation:

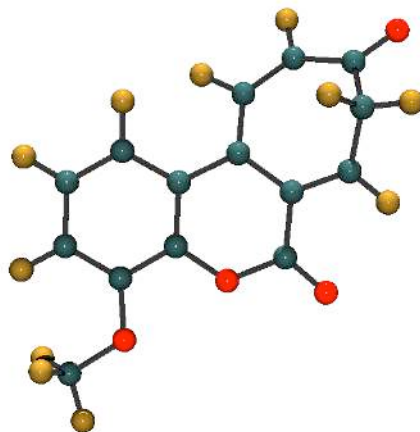
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.452177	-2.471743	.301562
2	6	0	3.376013	-1.425507	.170925
3	6	0	2.922618	-.116454	-.009047
4	6	0	1.532521	.120608	-.063124
5	6	0	.602907	-.918013	.049285
6	6	0	1.087206	-2.227568	.247458
7	8	0	3.719796	.976315	-.143208
8	6	0	5.129619	.793586	-.096146
9	8	0	1.156693	1.431383	-.271378
10	6	0	-.139784	1.857279	-.141651
11	6	0	-1.163184	.823822	.190349
12	6	0	-.827234	-.576796	-.033439
13	8	0	-.367624	3.036014	-.296596
14	6	0	-2.368943	1.276494	.624110
15	6	0	-3.428831	.352932	1.150660
16	6	0	-3.937662	-.412519	-.036760
17	6	0	-3.155154	-1.306813	-.705647
18	6	0	-1.752794	-1.496706	-.482072
19	8	0	-5.238088	-.159078	-.343281
20	1	0	5.558258	1.788282	-.221923
21	1	0	5.475320	.141417	-.907981
22	1	0	5.446701	.378378	.868685
23	1	0	-3.624222	-1.949613	-1.449853
24	1	0	-4.247186	.902722	1.618551
25	1	0	-3.001893	-.346426	1.882264
26	1	0	-2.560444	2.345003	.591755
27	1	0	-1.359379	-2.453114	-.817727
28	1	0	2.814963	-3.482589	.460764
29	1	0	.385244	-3.042283	.387485
30	1	0	4.437019	-1.636710	.220276
31	1	0	-5.467440	-.557752	-1.195382

	1	2	3
	A	A	A
Frequencies --	40.5628	78.1995	86.3837
Red. masses --	4.9080	4.5149	4.1037
Frc consts --	.0048	.0163	.0180
IR Inten --	2.9038	.5360	1.7504



### Theoretical data for compound 15c :

Final Energy in Hartrees: HF = - 879.2055479 (B3LYP/6-31++G(D,P))



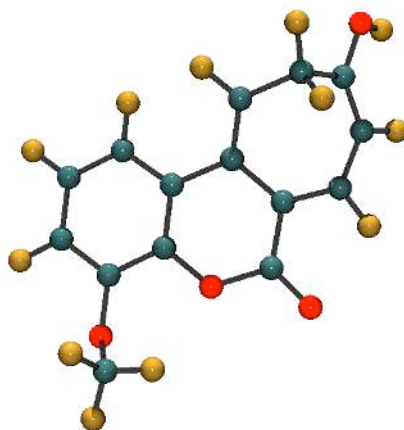
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.390492	-2.488787	.253725
2	6	0	3.337309	-1.455913	.166428
3	6	0	2.888422	-.138110	.019958
4	6	0	1.508911	.123409	-.047024
5	6	0	.544693	-.899304	.039652
6	6	0	1.029889	-2.222583	.201784
7	8	0	3.715588	.953953	-.081024
8	6	0	5.111041	.733664	-.041981
9	8	0	1.151601	1.439179	-.248596
10	6	0	-.156242	1.877657	-.168009
11	6	0	-1.192217	.867665	.138319
12	6	0	-.861061	-.536695	-.034373
13	8	0	-.336711	3.068720	-.345286
14	6	0	-2.425266	1.333980	.502878
15	6	0	-3.490545	.449728	1.067919
16	6	0	-4.097018	-.418521	-.051232
17	6	0	-3.198306	-1.358384	-.659633
18	6	0	-1.821369	-1.475951	-.466997
19	8	0	-5.309909	-.321441	-.329933
20	1	0	5.571413	1.718727	-.145046
21	1	0	5.445055	.089451	-.867620
22	1	0	5.426867	.284869	.910499
23	1	0	-3.688222	-2.134703	-1.244825
24	1	0	-4.299193	1.032836	1.515533
25	1	0	-3.058480	-.213151	1.834018
26	1	0	-2.622078	2.396647	.398796
27	1	0	-1.400211	-2.421288	-.812415
28	1	0	2.734202	-3.512162	.383788
29	1	0	.318616	-3.033377	.316397
30	1	0	4.395101	-1.682254	.221121

	1	2	3
	A	A	A
Frequencies --	39.8844	77.0514	81.3043
Red. masses --	4.6962	4.2661	4.4123
Frc consts --	.0044	.0149	.0172
IR Inten --	.4875	3.6547	.9263

Theoretical data for compound 6b :

Final Energy in Hartrees: HF = - 879.7281245 (B3LYP/6-31++G(D,P))



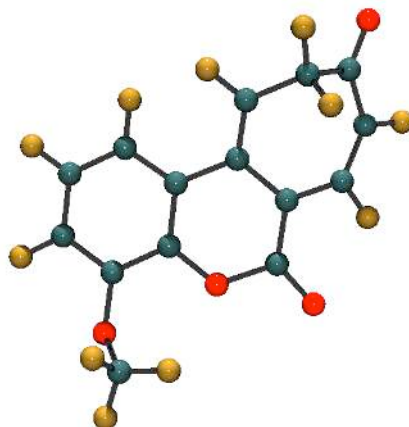
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.156982	-2.741821	-.383779
2	6	0	3.197051	-1.808231	-.431506
3	6	0	2.930417	-.449733	-.267431
4	6	0	1.599094	-.038200	-.059659
5	6	0	.548367	-.962563	.022299
6	6	0	.850160	-2.325031	-.154006
7	8	0	3.961138	.442011	-.401720
8	6	0	4.288813	1.247751	.742391
9	8	0	1.394338	1.320254	.068330
10	6	0	.141566	1.890041	-.000246
11	6	0	-1.017614	.970414	-.032739
12	6	0	-.813478	-.442862	.281663
13	8	0	.081709	3.100619	-.016327
14	6	0	-2.187066	1.510666	-.525386
15	6	0	-3.434384	.852616	-.747499
16	6	0	-3.867534	-.219079	-.020772
17	6	0	-3.143094	-.687464	1.206783
18	6	0	-1.807881	-1.230920	.769667
19	8	0	-5.001748	-.908645	-.293609
20	1	0	2.370731	-3.796165	-.529112
21	1	0	4.223597	-2.110031	-.611112
22	1	0	.051522	-3.058214	-.132446
23	1	0	5.180076	1.809913	.459434
24	1	0	4.517963	.608531	1.604126
25	1	0	3.479310	1.938216	.989882
26	1	0	-2.113743	2.541348	-.863889
27	1	0	-4.088692	1.269367	-1.511733
28	1	0	-3.735047	-1.453220	1.711339
29	1	0	-3.009920	.160082	1.892764
30	1	0	-1.643788	-2.296794	.889977
31	1	0	-5.363877	-.640438	-1.151309

	1	2	3
	A	A	A
Frequencies --	44.2913	59.7389	70.4787
Red. masses --	5.6905	2.0570	3.4938
Frc consts --	.0066	.0043	.0102
IR Inten --	1.7936	3.8444	.9854

Theoretical data for compound 6c :

Final Energy in Hartrees: HF = - 879.2136405 (B3LYP/6-31++G(D,P))



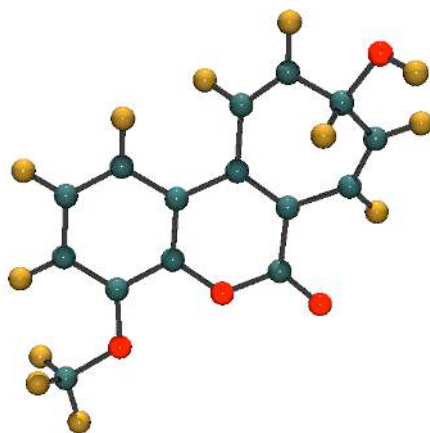
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.185309	-2.715628	-.451150
2	6	0	3.217872	-1.771403	-.431789
3	6	0	2.923821	-.423348	-.232175
4	6	0	1.583825	-.021499	-.051986
5	6	0	.540493	-.964032	-.025046
6	6	0	.868203	-2.315249	-.244550
7	8	0	3.964942	.479378	-.298058
8	6	0	4.182045	1.301041	.854313
9	8	0	1.353882	1.316620	.103115
10	6	0	.054628	1.868787	-.057101
11	6	0	-1.051207	.949796	-.049098
12	6	0	-.829713	-.466556	.231270
13	8	0	.038906	3.088231	-.168476
14	6	0	-2.285405	1.469457	-.524359
15	6	0	-3.525127	.871852	-.677860
16	6	0	-4.016501	-.305670	-.006674
17	6	0	-3.154680	-.817968	1.157600
18	6	0	-1.813531	-1.295886	.678651
19	8	0	-5.105635	-.851162	-.266622
20	1	0	2.412757	-3.763479	-.628204
21	1	0	4.254602	-2.054259	-.586565
22	1	0	.074104	-3.053745	-.268230
23	1	0	5.095695	1.864704	.649285
24	1	0	4.333271	.677344	1.746501
25	1	0	3.348777	1.988128	1.018177
26	1	0	-2.197677	2.485931	-.906055
27	1	0	-4.268355	1.394281	-1.277253
28	1	0	-3.705123	-1.625502	1.647432
29	1	0	-3.021895	.003113	1.879168
30	1	0	-1.623113	-2.363224	.745801

	1	2	3
	A	A	A
Frequencies --	45.9306	64.3066	76.7101
Red. masses --	6.0821	4.1244	2.0953
Frc consts --	.0076	.0100	.0073
IR Inten --	.1810	.4962	4.3992

### Theoretical data for compound **16b** :

Final Energy in Hartrees: HF = - 879.7239323 (B3LYP/6-31++G(D,P))



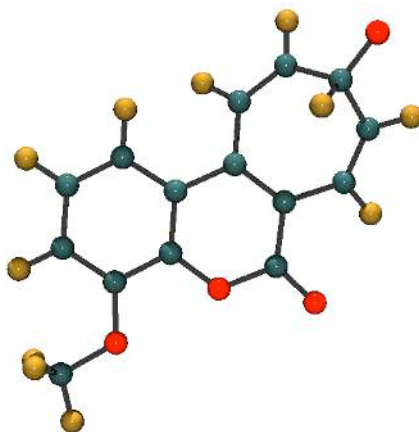
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.313636	-2.524717	-.034579
2	6	0	3.287402	-1.521575	.099172
3	6	0	2.910343	-.179384	.103795
4	6	0	1.540311	.140186	-.039847
5	6	0	.562022	-.850188	-.191302
6	6	0	.973919	-2.203104	-.173513
7	8	0	3.754516	.875101	.236832
8	6	0	5.145914	.612520	.383549
9	8	0	1.228656	1.467777	-.018631
10	6	0	-.066495	1.926123	-.115389
11	6	0	-1.143896	.922561	-.248391
12	6	0	-.835171	-.431947	-.327156
13	8	0	-.237690	3.126823	-.095946
14	6	0	-2.461224	1.502454	-.452011
15	6	0	-3.636450	.915388	-.146100
16	6	0	-3.710013	-.397449	.595603
17	6	0	-3.132057	-1.428045	-.328228
18	6	0	-1.828763	-1.442453	-.672601
19	8	0	-5.042575	-.786329	.918070
20	1	0	-5.402617	-.160838	1.560309
21	1	0	-3.095492	-.338933	1.508982
22	1	0	5.620201	1.590181	.471624
23	1	0	5.547183	.088860	-.492954
24	1	0	5.347403	.025226	1.287983
25	1	0	4.328959	-1.798242	.207039
26	1	0	2.621108	-3.565625	-.020080
27	1	0	.236486	-2.993098	-.246137
28	1	0	-1.478040	-2.262664	-1.292258
29	1	0	-2.464268	2.502364	-.875807
30	1	0	-3.821710	-2.173319	-.717202
31	1	0	-4.579352	1.376884	-.432097

	1	2	3
	A	A	A
Frequencies --	38.5875	70.4761	86.3899
Red. masses --	5.0287	4.4451	4.4096
Frc consts --	.0044	.0130	.0194
IR Inten --	1.2567	1.2303	7.4491

Theoretical data for compound 16c :

Final Energy in Hartrees: HF = - 879.1417281 (B3LYP/6-31++G(D,P))



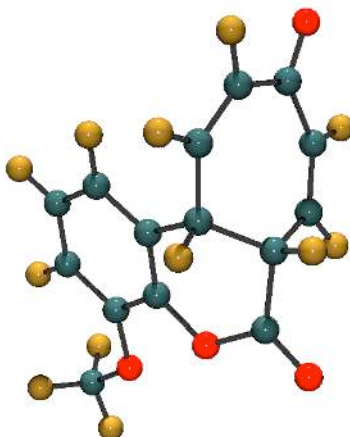
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.281582	-2.524999	-.035969
2	6	0	3.261516	-1.525346	.089227
3	6	0	2.878583	-.184698	.093915
4	6	0	1.511165	.142633	-.042844
5	6	0	.525904	-.843638	-.185644
6	6	0	.942042	-2.196024	-.165001
7	8	0	3.737053	.873108	.221239
8	6	0	5.116740	.594821	.373757
9	8	0	1.202955	1.469012	-.024553
10	6	0	-.107562	1.928751	-.112176
11	6	0	-1.184774	.933225	-.210600
12	6	0	-.874951	-.430643	-.306307
13	8	0	-.243814	3.138224	-.114622
14	6	0	-2.506742	1.491459	-.388863
15	6	0	-3.682335	.871297	-.103912
16	6	0	-3.860251	-.452074	.665997
17	6	0	-3.185835	-1.396347	-.342675
18	6	0	-1.864998	-1.423881	-.663443
19	8	0	-5.115891	-.766033	.983134
20	1	0	-3.142960	-.385738	1.533909
21	1	0	5.607119	1.565853	.463721
22	1	0	5.521859	.063080	-.498288
23	1	0	5.312953	.003492	1.278647
24	1	0	4.303681	-1.803029	.192161
25	1	0	2.583543	-3.568496	-.018447
26	1	0	.195891	-2.979095	-.225125
27	1	0	-1.504932	-2.244669	-1.282131
28	1	0	-2.523449	2.508271	-.774003
29	1	0	-3.870579	-2.116700	-.792319
30	1	0	-4.626040	1.335332	-.392471

	1	2	3
	A	A	A
Frequencies --	37.4928	67.5092	80.6873
Red. masses --	5.1564	4.8778	4.1550
Frc consts --	.0043	.0131	.0159
IR Inten --	1.7583	3.0955	9.7902

Theoretical data for compound 17a :

Final Energy in Hartrees: HF = - 879.7122644 (B3LYP/6-31++G(D,P))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.407365	-2.617793	-.353510
2	6	0	-2.511180	-1.883921	.091888
3	6	0	-2.462644	-.484794	.108218
4	6	0	-1.287271	.148718	-.338407
5	6	0	-.185980	-.577743	-.788277
6	6	0	-.249333	-1.976054	-.787739
7	8	0	-3.465389	.330273	.524896
8	6	0	-4.678081	-.263920	.977631
9	8	0	-1.299485	1.539981	-.344698
10	6	0	-.139932	2.263966	-.352519
11	6	0	1.164359	1.466933	-.334175
12	6	0	1.005148	.244309	-1.265935
13	8	0	-.200152	3.467952	-.361076
14	6	0	1.539576	1.167927	1.104427
15	6	0	2.433881	.279614	1.565513
16	6	0	3.336691	-.627133	.816218
17	6	0	3.248774	-.862338	-.648456
18	6	0	2.270067	-.540443	-1.509397
19	8	0	4.215835	-1.221420	1.442351
20	1	0	.722069	.661193	-2.245052
21	1	0	1.916690	2.147923	-.750374
22	1	0	-5.326816	.568478	1.251051
23	1	0	-4.507617	-.898531	1.855855
24	1	0	-5.153477	-.852466	.183552
25	1	0	4.088711	-1.448926	-1.012734
26	1	0	2.607253	.229950	2.637474
27	1	0	-3.399649	-2.403535	.429164
28	1	0	2.386401	-.900909	-2.530410
29	1	0	-1.456377	-3.702220	-.353650
30	1	0	.606695	-2.554914	-1.116441
31	1	0	1.049379	1.795701	1.846893

	1	2	3
	A	A	A
Frequencies --	25.4191	48.0998	70.2939
Red. masses --	8.2299	4.7776	4.2892
Frc consts --	.0031	.0065	.0125
IR Inten --	4.0869	1.8111	2.6267