Antimony(V) Cations for the Selective Catalytic Transformation of Aldehydes Into Symmetric Ethers, α,β-Unsaturated Aldehydes, and 1,3,5-Trioxanes

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Supporting Information

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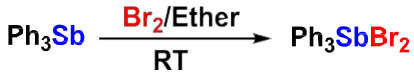
1. General Remarks

All manipulations were carried out under Nitrogen atmosphere using Schlenk or Glove Box and vacuum line techniques. Dichloromethane and Hexanes were dried under nitrogen over CaH and NAC (sodium potassium allow) respectively and distilled prior to use. Aldehydes with 95 to 98% purity have been purchased either from Aldrich, Alfa Aesar laboratories and used as received. The (8-iodonaphthalen-1-yl)diphenylphosphine was synthetized by those reported in the literature.[1] Molecular Sieves were purchased from Aldrich (4Å) were dried prior to use at 130°C. Melting point was recorded on Melt Temp laboratories devices: Temp Range ambient to 400°C. NMR spectra were recorded on a 400 MHz Bruker Spectrometer in $CDCl_3$. All column chromatography was performed on small columns (5 x 60 mm) of Silica Gel (Aldrich), 700-230 mesh, 60A° pore volume 0.75 cm^3/g. Chemical shifts (δ) are given in ppm and are referenced to the residual solvent: ^1H: $CDCl_3$, 7.26 ppm; ^{13}C: 77.0 ppm. Elemental analyses were performed at Midwest Microlabs, LLC (Indianapolis, IN).

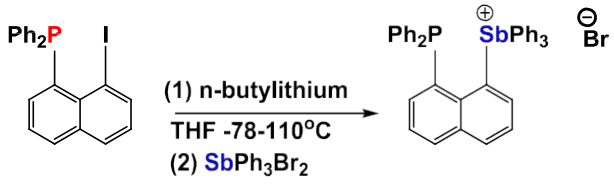
2.0 Experimental Procedures

2.1 Synthesis of the Triphenylstibonium Dibromide



A 250 mL Schlenk flask was charged with triphenylstibine (5 g, 14.16 mmol), 20 mL of diethyl ether, and a magnetic stirbar. Under and atmosphere of nitrogen, bromine (2.48 g, 0.80 mL, 15.57 mmol) diluted in 2 mL of ether was added drop wise. Immediately, the precipitation of a white solid was observed. After all of the bromine had been added, the reaction mixture was stirred for 30 minutes at room temperature, after which time mother liquor was decanted away from the resulting solid. The solid product was then washed with diethyl ether (5 x 50 mL), until the washings were colorless. No further purification was needed in subsequent reactions, and Ph_3SbBr_2 was isolated in 90% yield as a white solid**.**

2.2 Synthesis of [2][Br]

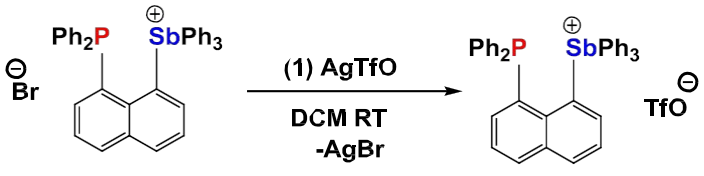


[2][Br]

A 100 mL Schlenk flask was charged with 1-diphenylphosphino-8-iodonaphthalene (1 g, 2.28 mmol) a magnetic stirring bar and 40 mL of tetrahydrofuran. The solution was degassed and cooled to -78 °C followed by the drop wise addition of nBuLi (2.2 M in hexanes, 1.55 mL, 3.42 mmol). After the addition was completed, the solution was stirred for an additional 2 hours at -78 °C during which time the color became dark red. The reaction mixture was then cooled to -110 ° (LN_2/acetone slurry) and a solution of Ph_3SbBr_2

(1.28 g, 2.51 mmol) in THF (5 mL) was added dropwise. The resulting solution was stirred at -110 °C for two hours and was then allowed to warm to room temperature overnight. After that time the color of the solution turned to pale orange. The solvent was then removed in vacuo to yield a brown solid which was washed with a 1:3 DCM:hexanes solvent mixture (3 + 15 mL) to remove traces of any unreacted starting materials and salt byproducts. The residue then was dissolved in DCM and filtered over Celite. The filtrate was then concentrated to afford [2][Br] as a yellow solid in 70% yield which was used in the next step without further purification. Note: [**2**][Br] very air and moisture sensitive, and should be stored under an atmosphere of nitrogen at all times. m.p. 120-122°C. ^{1}H NMR (400 MHz) ($CDCl_3$): 6.56-6.61, 7.08-7.13, 7.3 (m, 10H, PPh), 7.44-7.88(m, 19H, SbPh + H_3 + H_4), 8.33-8.34(d, 1H, H_2, J = 8.4 Hz), 8.41-8.44(d, 1H, H_1, J = 8.4 Hz). ^{13}C NMR (100.61 MHz): δ 128.85, 128.94, 129.81, 130.68, 131.95, 132.40, 132.53, 134.14. ^{31}P NMR (161.9755 MHz) ($CDCl_3$): -38.50. Elemental analysis calculated (%) for $C_{42}H_{35}BrCl_4PSb$ ([**2**][Br] + 2 (CH_2Cl_2)): C: 51.31, H: 3.38. Found: C: 51.42, H: 3.65. $C_{40}H_{31}PSb^+$ HRMS(ESI$^+$) m/z: (M-Br) calculated: 663.1202. Found: 663.1201.

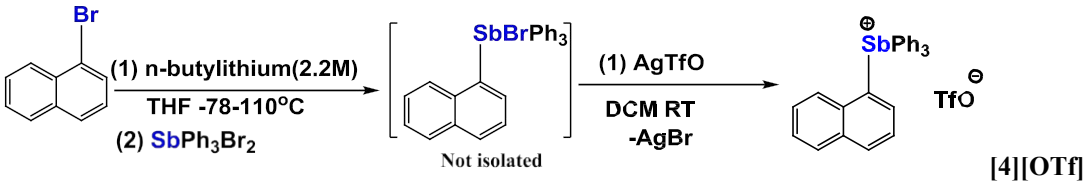
2.3 Synthesis of [2][OTf]



[2][OTf]

A 100 mL Schlenk flask was charged with [**2**][Br] (1 g, 1.34 mmol), silver(I) triflate (370 mg, 1.47 mmol), a magnetic stirring bar, and 50 mL of DCM. The flask was covered with aluminum foil and the reaction was stirred for 5 hours in the dark. The resulting suspension was then filtered over Celite to remove AgBr, and the filtrate was concentrated in vacuo to give a brown oily material that solidified after drying under high vacuum overnight (~80% yield). The resultant brown solid was further purified by dissolving in an excess of diethyl ether (5 mL) followed by the addition of hexanes (50 mL) to precipitate [**2**][OTf] as a white solid that is stable to air and moisture (700 mg, 65% yield). m.p. 94-96 °C ^{1}H NMR (400 MHz) ($CDCl_3$): 6.46-6.51, 7.06-7.10, 7.26-7.29(m, 10H, PPh), 7.43-7.84(m, 19H, SbPh + H_3 + H_4), 8.34(d, 1H, H_2, J = 8.4 Hz), 8.42, 8.44(d, 1H, H_1, J = 8.4 Hz). ^{13}C NMR (100.61 MHz): 128.93, 129.01, 130.94, 132.22, 132.29, 132.30, 132,56, 133.97, 133.98. ^{31}P NMR (161.9755 MHz) ($CDCl_3$): -36.10. ^{19}F NMR (376.49 MHz): -78.50(triflate). Elemental analysis calculated (%) for $C_{42.2}H_{33.4}F_3O_3PCl_{2.4}SSb$ ([**2**][OTf] + 1.2 CH_2Cl_2): C: 55.37, H: 3.68. Found: C: 55.29, H: 3.61. $C_{40}H_{31}PSb^+$ HRMS(ESI$^+$) m/z: (M-OTf) calculated: 663.1202. Found: 663.1201.

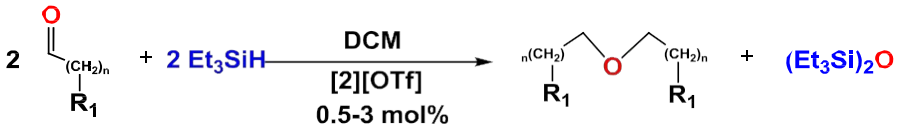
2.4 Synthesis of [4][OTf]



[4][OTf]

A 100 mL Schlenk flask was charged with 1-bromonaphthalene (500 mg, 2.4 mmol) a magnetic stirring bar and 40 mL of tetrahydrofuran. The solution was degassed and cooled to -78 °C followed by the drop wise addition of nBuLi (2.2 M in hexanes, 2.41 mL, 5.31 mmol). The resulting solution became dark and was stirred for 2 hours at -78 °C after which time Ph_3SbBr_2 (1.36 g, 2.65 mmol) in THF (5 mL) was added drop wise. The solution was allowed to warm to room temperature overnight and the color changed from pale yellow to colorless. The reaction mixture was concentrated in vacuo to afford an oily material that was washed with a 1:3 DCM:hexanes solvent mixture (3 x 15 mL). The residue was then dissolved in DCM (50 mL) and then filtered over Celite. The filtrate was then concentrated to dryness to give a white semi-solid material which was used without further purification. The solid was then dissolved in DCM (40 mL) and the solution was transferred to a 100 mL Schlenk flask that was wrapped in aluminum foil. To this solution was added AgOTf (510 mg, 1.96 mmol) and the resulting suspension was allowed to stir at room temperature for 12 hours. The suspension was then filtered over Celite and the filtrate was concentrated to dryness in vacuo to give a brown oily material which was washed with cold hexanes to give a white solid. After drying under high vacuum overnight, [**4**][OTf] was obtained as a white solid that is stable to air and moisture (1.06 g, 70% yield). m.p.90-92°C. ^{1}H NMR (400 MHz) ($CDCl_3$): 7.53-7.57, 8.10-8.14, 8.30-8.35(m, 3H, H_1, H_2, H_5), 7.63-7.84(m, 19H, ShPh + H_3+H_4). ^{13}C NMR (100.61 MHz): 127.66, 129.23, 130.95, 131.35, 131.73, 133.43, 133.86, 135.52, 135.57. ^{19}F NMR(376.4983 MHz) : -78.30(triflate). Elemental analysis calculated (%) for: $C_{31}H_{26}F_3O_3SCl_4Sb$ ([**4**][OTf + 2(CH_2Cl_2)): C: 46.59, H: 3.28. Found: C: 46.07, H: 2.80. $C_{28}H_{22}Sb^+$ HRMS(ESI$^+$) m/z: (M-OTf) calculated: 479.0760. Found: 479.0760.

2.5 General Method (I): Selective reductive coupling of aldehydes catalyzed by [2][OTf] or [4][OTf] to give symmetric ethers (L).



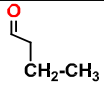
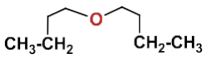
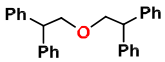
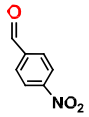
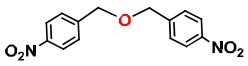
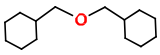
In a typical experiment, 0.10 g. (2 mmol) of the aldehyde {n = 2, 8, R_1 = Me; n = 0, 2, R_1 = Ph; n = 0; R_1 = $(Me)_2CH$, $(Et)_2CH$, cyclohexyl, $(Ph)_2CH$, C_6F_5, (ortho-Br)Ph, (m-Br)Ph, (m-F)Ph, (para-CF_3)Ph, (para-NO_2)Ph, and (para-Me)Ph} and 3 mmol excess of triethylsilane (Et_3SiH) were charged to a Kontes Airless 25ml storage vessel tube, and 0.5-3 mol % of the corresponding stibonium salt [2][OTf] or [4][OTf] together with 2 ml of DCM. The mixture was stirred for 1h to 24 hr at room temperature, except for those with electro

withdrawing group that need to be refluxed on DCM. The reaction was monitored by ^{13}C NMR Spectroscopy analysis by taking aliquots of the crude mixture. When high conversion was observed, then we stopped the reaction and concentrated the solution open to air to avoid losing any volatile component. This solution was transferred for further purification on a silica gel column. Initially the residue was eluted with 100% hexanes to remove completely the hexamethyldisiloxane formed in the process, then it was eluted with 70% dichloromethane and hexane, then the volatiles were removed to leave a nice oily material containing the desired product. Some symmetrical ethers were evaporated to room temperature due to the low boiling point. Before the purification process the final mixture can be concentrated and the catalyst being precipitated with cold hexane for further use with the same aldehyde solution, however we can also pass the residue containing the catalyst **[2][OTf]** by silica gel column washed with DCM and extracted with acetone.

2.5.1 Catalytic comparison of [2][OTf] and [4][OTF] in the synthesis of L

In a typical experiment 0.1 g. of the corresponding aldehyde was added to an NMR tube together with catalytic amount of the stibonium salt and $CDCl_3$ as a solvent. The solution mixture was stirred and leave stood at room temperature for a specific period of time, as show in Table S_1.

Table S_1: Catalytic comparison between [**2**][OTf] and [**4**][OTf].

Entry	Aldehyde	[2][OTf]			[4][OTf]			Symm. ether
		Time (h)	mol% Loading	Selectivity% (Conversion	Time (h)	mol% Loading	Selectivity % (Conversion)%	
1		1	3	100(100)	0.25	3	100(100)	
2		12	5	100(100)	1	5	20(100)	
3		48	5	100(100)	1	5	0(100)	
4		1	0.5	100(100)	1	0.5	20(50)	

Entry 1, shows the higher activity associated with [**4**][OTf] with short periods of time for the reaction. Entry 2 point out the higher selectivity of [**2**][OTf]with a crowded group such as diphenyl acetaldehyde, however longer periods of time were required compared to [**4**][OTf] , **Fig S_1**. Entry 3, shows the enhanced selectivity of [**2**][OTf] over aldehydes with electron withdrawing group such as nitrobenzaldehyde but longer periods of time required compared to [**4**][OTf] in which a no identified product was generated **Fig S_2**. Entry 4, shows interestingly the higher selectivity of [**2**][OTf] at reduced loading of the catalyst compare to [**4**][OTf], **Fig S_3**.

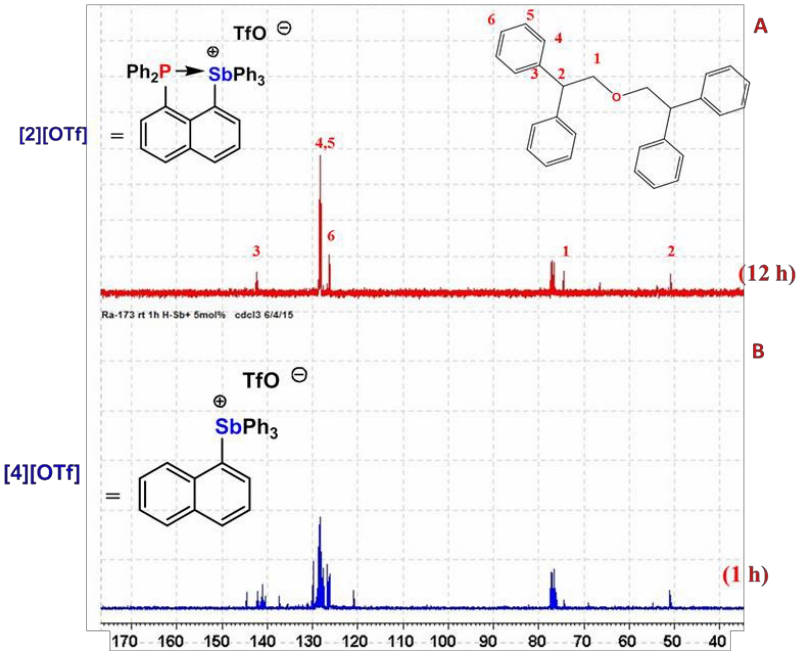


Figure S_1: ^{13}C NMR spectra showing the competitive reactions between (A) [**2**][OTf] and (B) [**4**][OTf] in the reductive coupling of diphenylacetaldehyde to give into 2,2'-oxybis(ethane-2,1,1-triyl)tetrabenzene $\mathbf{L_7}$ (before purification)

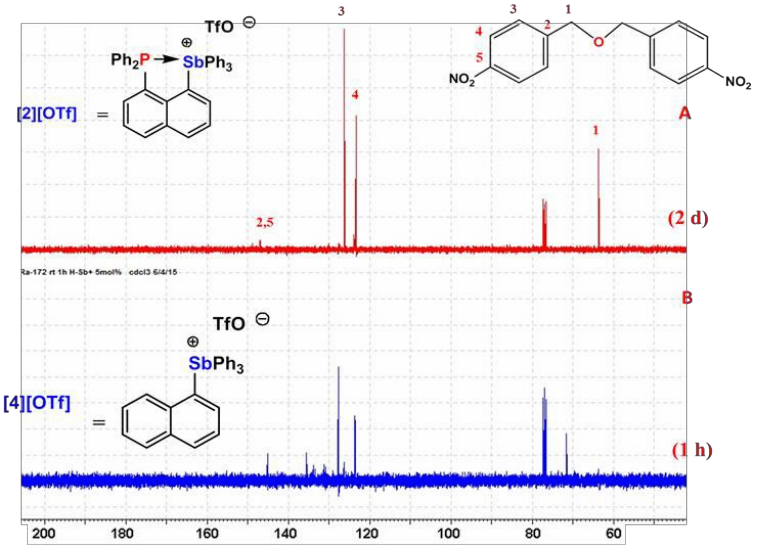


Figure S_2: ^{13}C NMR spectra showing the competitive reactions between (A) [**2**][OTF] and (B) [**4**][OTf] in the reductive coupling of *p*-nitrobenzaldehyde to give 4,4'-oxybis(methylene)bis(nitrobenzene) $\mathbf{L_{14}}$ (before purification)

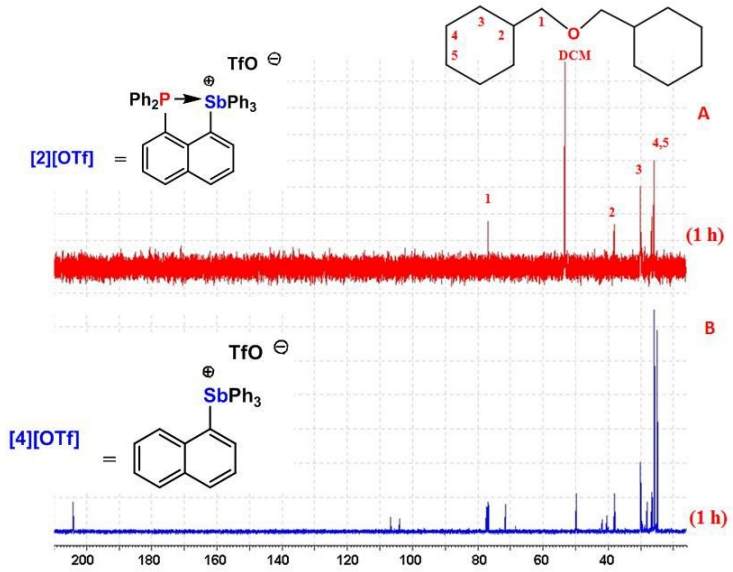
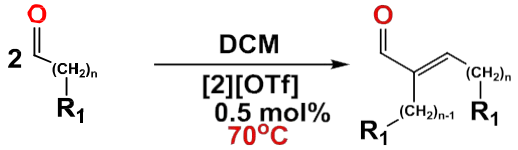


Figure S_3: ^{13}C NMR spectra showing the competitive reactions between (A) [**2**][OTf] and (B) [**4**][OTf] in the reductive coupling of cyclohexanecarbaldehyde to give dicyclohexylmethyl ether $\mathbf{L_6}$ (before purification)

2.6 General Method (II): Selective self Aldol-condensation of aldehydes catalyzed by [2][OTf] or [4][OTf] to the formation of α,β-unsaturated aldehydes M



In a typical experiment, 0.2 g. of the aldehyde (R_1 = Me, n =2, 8; R_1 = Ph, n = 1, 2) was charged to a Kontes Airless 25ml storage vessel tube, together with 2 ml of DCM. Over this mixture 0.5 mol % of the corresponding stibonium salt **[2][OTf] or [4][OTf]** was added under oxygen free conditions. Immediately the mixture was heated to the optimized conditions in pre-heated oil bath (70°C) for 12 h, time after which the solution turn orange indicative that the aldehyde have been transformed, then we stopped the reaction and let it cool to room temperature. The solvent was concentrated at room temperature for further purification on a silica gel column. Initially the residue was eluted with 100% hexanes to remove traces of non-reactive material, then it was eluted with 100% dichloromethane, then the volatiles were removed to leave a nice colorless oily material that correspond to the self Aldol condensation products, no further distillation was needed. The remaining silica gel column can be washed with dichloromethane and the catalyst **[2][OTf]**can be extracted using 100% acetone for further catalysis.

2.6.1 Effect of water on the self Aldol-condensation of aldehydes catalyzed by [2][OTf] or [4][OTf]

In a typical experiment, 0.2 g. of butyraldehyde as a model substrate (2.77 mmol)) was charged to a Kontes Airless 25ml storage vessel tube, together with 2 ml of $CHCl_3$ and some molecular sieves. Over this mixture 0.011 g. (0.5 mol %) of the corresponding stibonium salt was added under oxygen free conditions. Immediately the mixture was heated in pre-heated oil bath (70°C) for 24 h, time after which the reaction was stooped and cooled to room temperature. By ^{1}H NMR Spectroscopy we determine that suppression of the reaction down to 6%, **Fig S$_4$**, implying the strong effect of water on the reaction product.

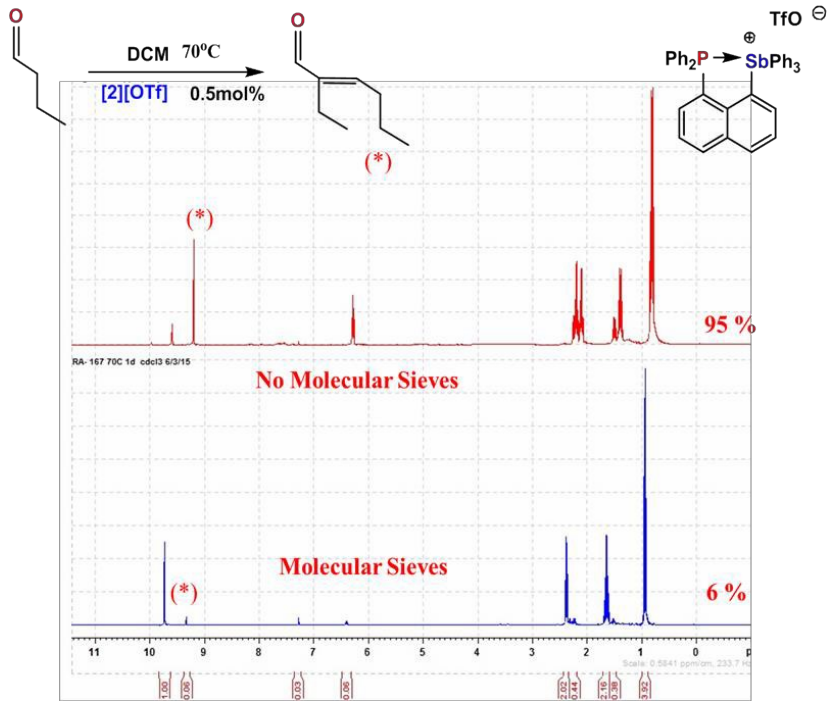
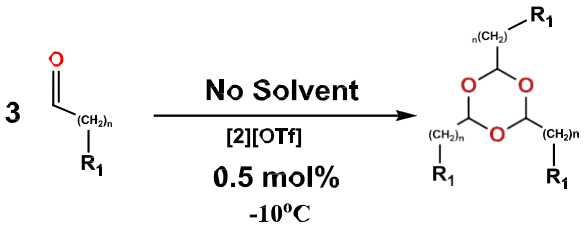


Figure S$_4$: ^{1}H NMR spectra of: self Aldol-condensation of butyraldehyde catalyzed by [**2**]$^+$ in presence of water (top), and butyraldehyde in the presence of [**2**]$^+$ and molecular sieves to scavenge water from the reaction (bottom)

2.7 General Method (III): Selective cyclotrimerization of aldehydes to give 1,3,5-trioxanes N catalyzed by [2][OTf] or [4][OTf]



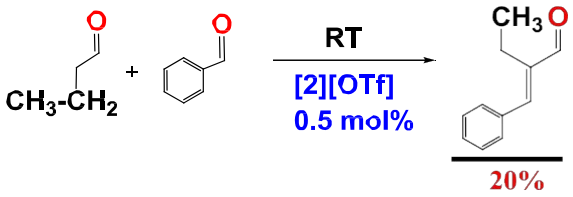
In a typical experiment 0.5 mol % the corresponding stibonium salt [**2**][OTf] or [**4**][OTf] was added to a

Kontes Airless 25ml storage vessel tube and then cooled to -15°C. Over this container, 0.1 g. (3 mmol) of the corresponding aldehyde { n = 2, 8, R_1 = Me; n = 1, 2, R_1 = Ph; n = 0, R_1 = (Et_2)CH, Cyclohexyl, and $(Ph)_2$CH} was added drop wise to this container and then washed slightly with hexamethyldisiloxane (1 ml) to make sure all the aldehyde is completely dissolved on the catalyst. The mixture was stirred at -10°C for the optimized time conditions. After that time 10 ml of cold hexanes was added to precipitate the catalyst, the solution was decanted and reduce on high vacuum to get a nice solid material, that was eventually washed with cold hexanes to removes traces of non-reactive aldehyde or simply re-crystallized on hexane at -30°C. No further purification was needed; however liquid products were purified by silica gel column eluted with 100% DCM, previously washed with 25% DCM to remove trace of non-reactive aldehyde. The catalyst residue can be recycled as mentioned before by silica gel column with 100% acetone.

2.7.1 Retrocyclization of 1,3,5-trioxanes to give starting aldehydes catalyzed by [2][OTf]

In a typical experiment, 0.15g.(0.69 mmol) of 2,4,6-Tripropyl_1,3,5-Trioxane N_1 (isolated from our general system), was charged to a NMR tube together with 1 ml of $CDCl_3$. Over this mixture 0.003g. (0.5 mol %) of the corresponding stibonium salt [2][OTf] was added under oxygen free conditions. Immediately the mixture was mixed at room temperature, and by the time that we run to the NMR room almost 92% of the corresponding aldehyde was formed, and over ten minutes, the reaction reached 100% conversion to the corresponding aldehyde. **Fig S_{70}**. This is a clear example that these species are reversible even at room temperature, that is why low temperatures experiments were performed in order to optimize their formation.

2.8 Cross Aldol-condensation between butyraldehyde and benzaldehyde to give (E)-2- benzylidenebutanal catalyzed by [2][OTf]



In a typical experiment, 0.2 g.. (2.77 mmol) of butyraldehyde and 0.88 g. (8.3 mmol) excess benzaldehyde was charged to a Kontes Airless 25ml storage vessel tube on 3 ml DCM, together with 11.28 mg (0.5 mol %) stibonium salt [2][OTf]. The reaction was heated at 70°C for 12 hr, time after which the solution turn orange. It was cooled to room temperature and the solvent removed under vacuum. Yield 20%. Further purification was eluted on silica gel with 100% DCM to get a colorless oil which was properly characterized by NMR spectroscopy, **Fig $S_{5\text{-}6}$.** The symmetrical self Aldol condensation materials were easily removed under high vacuum because of the low boiling point.

3.0 NMR Characterization data

3.1 NMR spectra of [2][Br]:

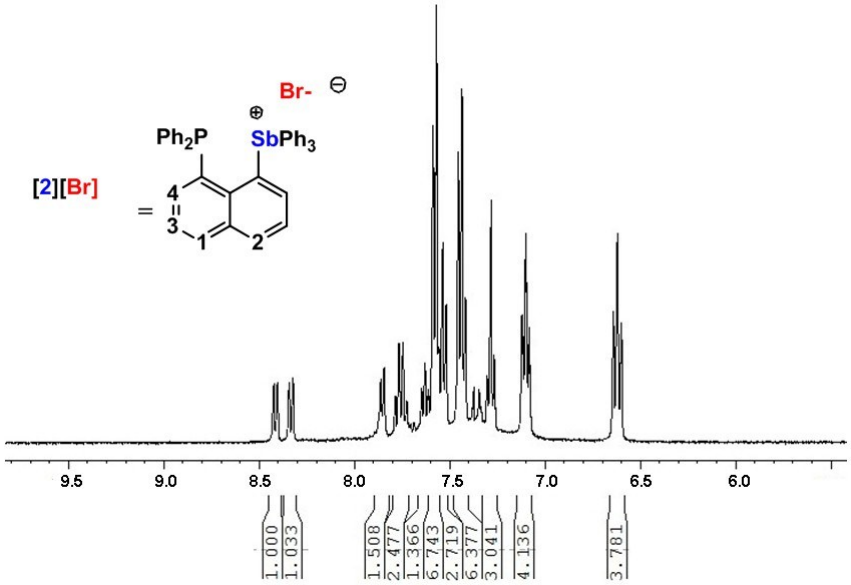


Figure S$_5$: ^{1}H NMR spectrum of [**2**][Br]

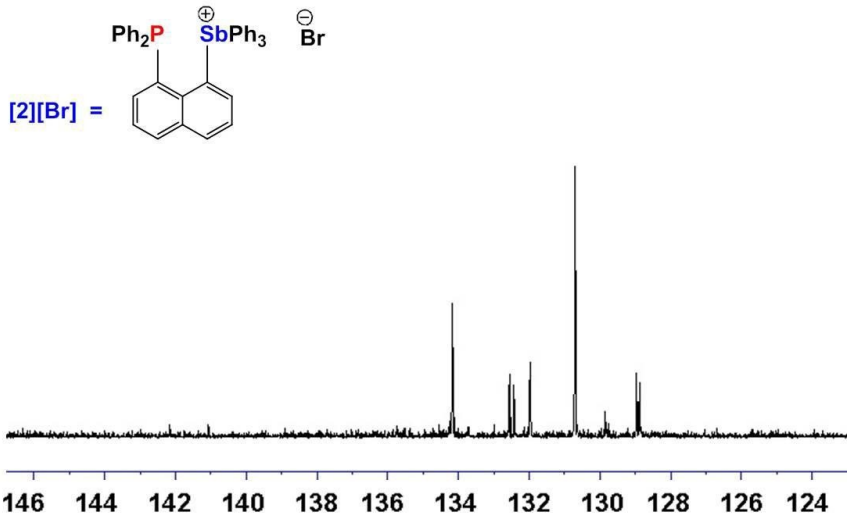


Figure S$_6$: ^{13}C NMR spectrum of [**2**][Br]

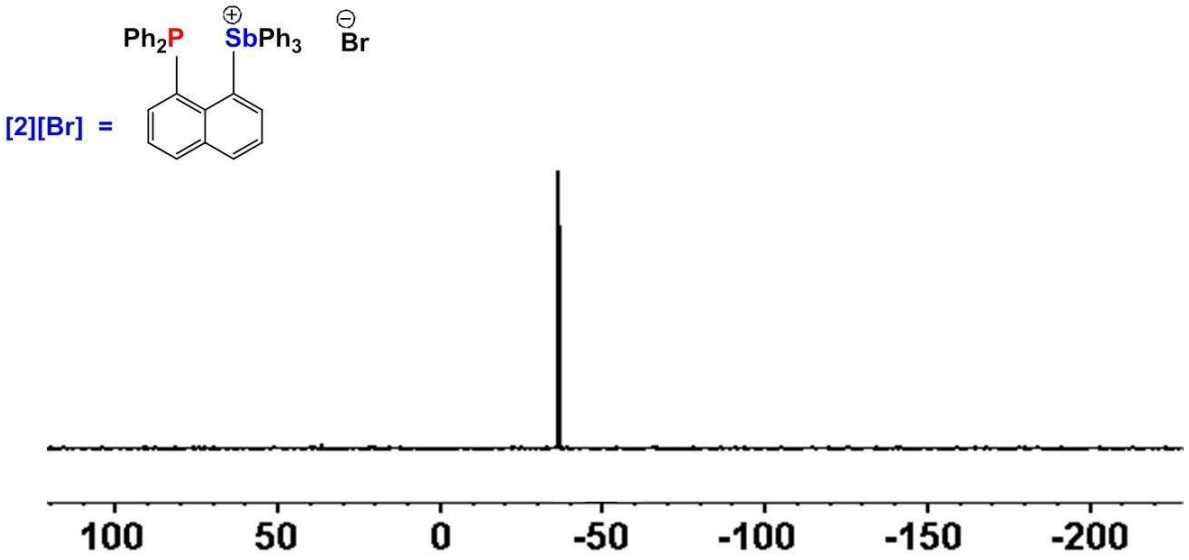


Figure S$_7$: ^{31}P NMR spectrum of [**2**][Br]

3.2 NMR spectra of [2][OTf]:

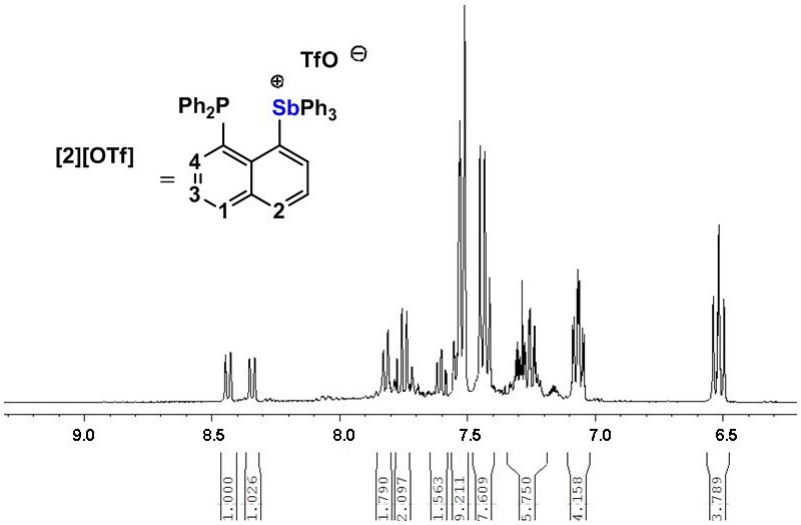


Figure S$_8$: ^{1}H NMR spectrum of [**2**][OTf].

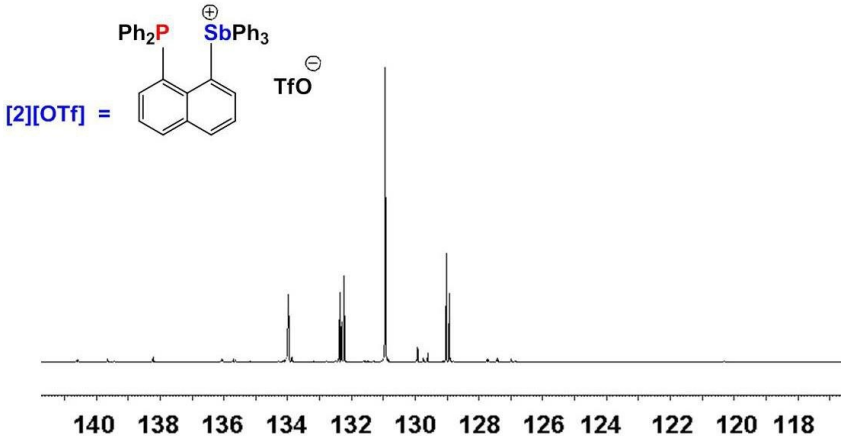


Figure S_9: ^{13}C NMR spectrum of [**2**][OTf].

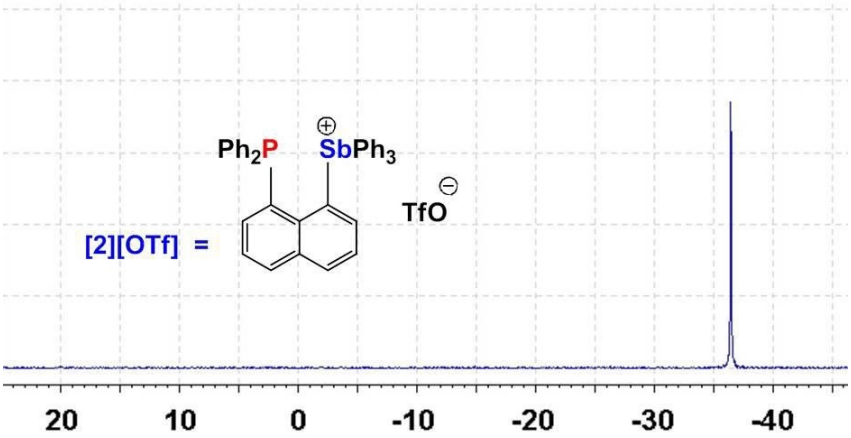


Figure S_{10}: ^{31}P NMR spectrum of [**2**][OTf].

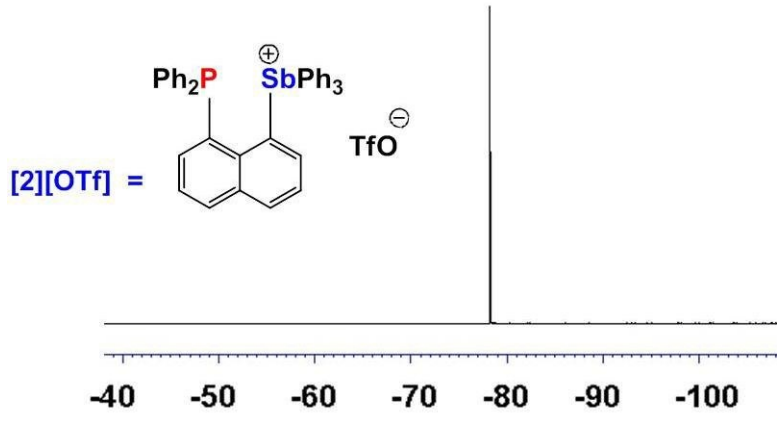


Figure S_{11}: ^{19}F NMR spectrum of [**2**][OTf].

3.3 NMR spectra of [4][OTf]:

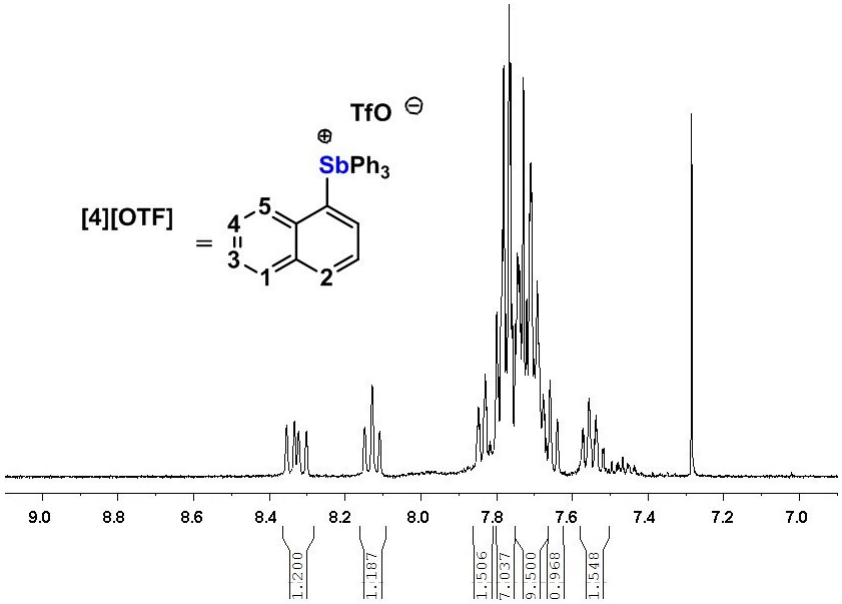


Figure S_{12}: ^{1}H NMR spectrum of [**4**][OTf]

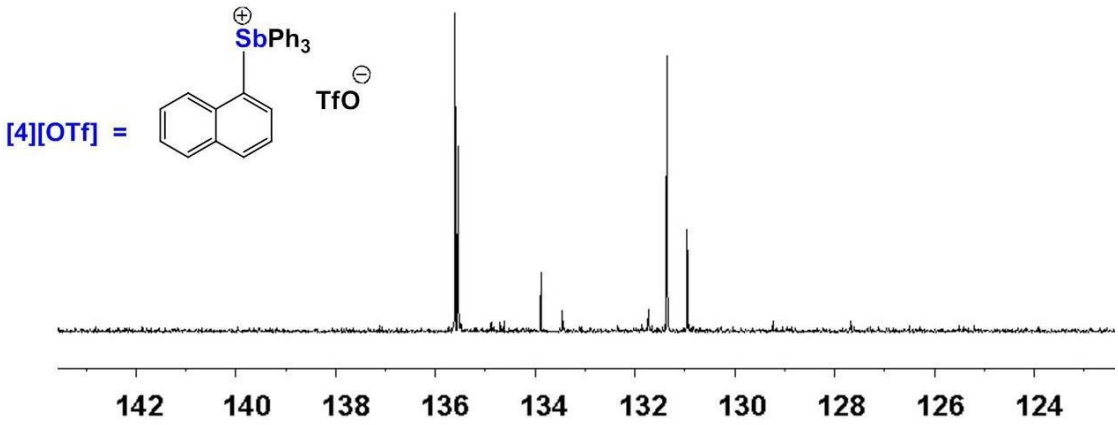


Figure S_{13}: ^{13}C NMR spectrum of [**4**][OTf]

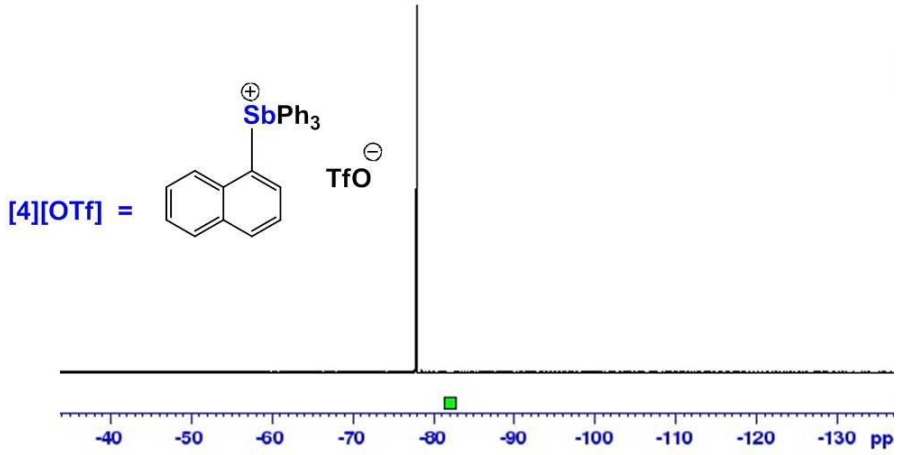


Figure S_{14}: ^{19}F NMR spectrum of [**4**][OTf]

3.4 NMR spectra of (*E*)-2-benzylidenebutanal synthesized from the cross Aldol-condensation reaction catalyzed by [2][OTf] (0.5 mol%):

^{1}H NMR (400 MHz) ($CDCl_3$): □.1.15-1.19(t, 3H, H_1, J = 7.6 Hz); 2.56-2.61(m, 2H, H_2); 7.22(s, 1H, H_4); 7.41-7.54(m, 5H, H_{6-8}); 9.56(s, 1H, H_9). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □12.76(C_1, CH_3); 17.97(C_2, CH_2); 128.70, 129.46, 129.53(C_{6-8}, CH); 134.81(C_5, C); 144.34(C_3, C(CO)); 149.45(C_4, CH(=C)); 195.43(C_9, CHO).

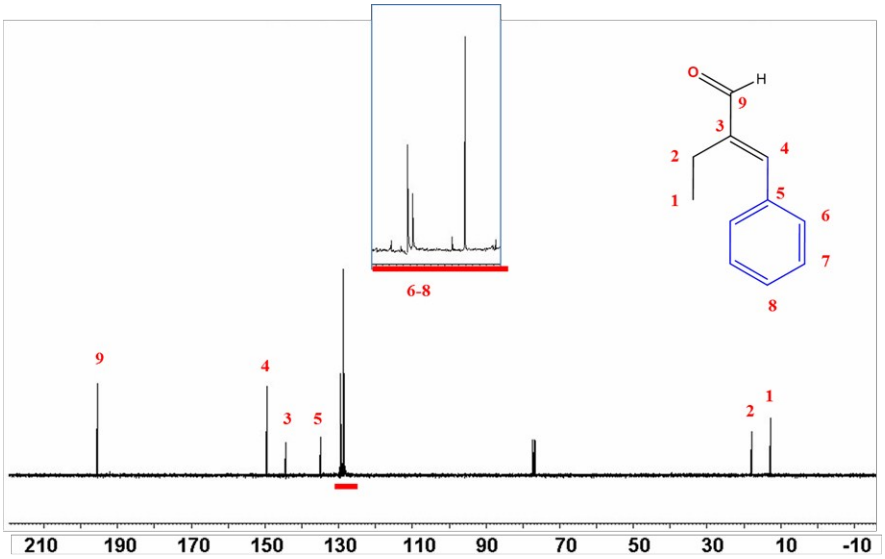


Figure S_{15}: ^{13}C NMR spectrum of isolated (*E*)-2-benzylidenebutanal

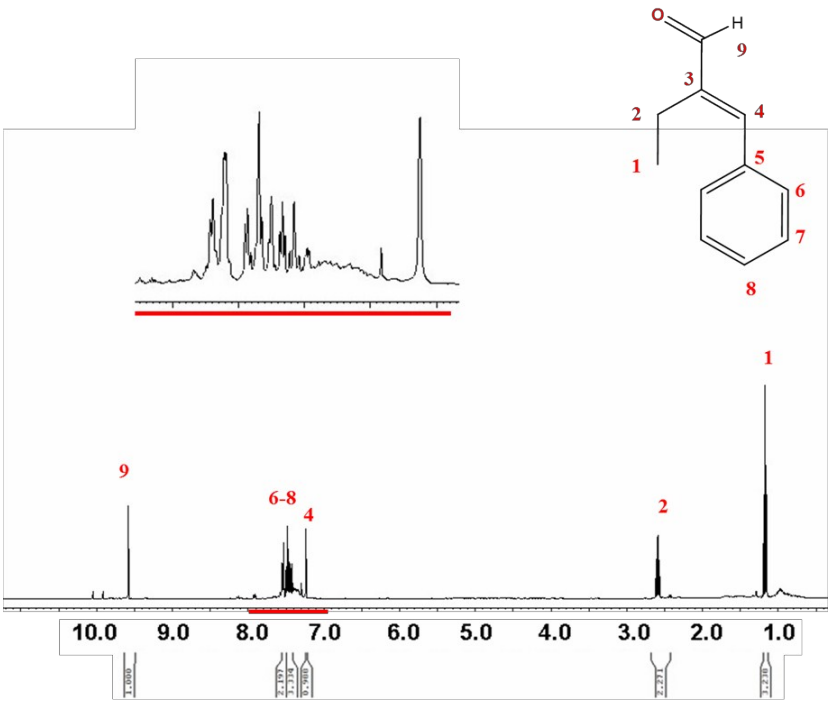


Figure S_{16}: ^{1}H NMR spectrum of isolated (*E*)-2-benzylidenebutanal

3.5 NMR spectra of isolated didecyl ether L_2

^{1}H NMR (400 MHz) ($CDCl_3$): 0.88-0.91(t, 6H, H10, J = 6.8 Hz); 1.28-1.32, 1.54-1.63(m, 32H, $H_{2\text{-}9}$); 3.39-3.42(t, 4H, H_1, J = 6.8 Hz). ^{13}C NMR (100.61 MHz) ($CDCl_3$): 14.08(C_{10},CH_3); 22.67(C_9, CH2); 26.20 29.32, 29.51, 29.57, 29.62, 29.79, 31.90($C_{2\text{-}8}$, CH_2); 70.96 (C_1, CH_2O).

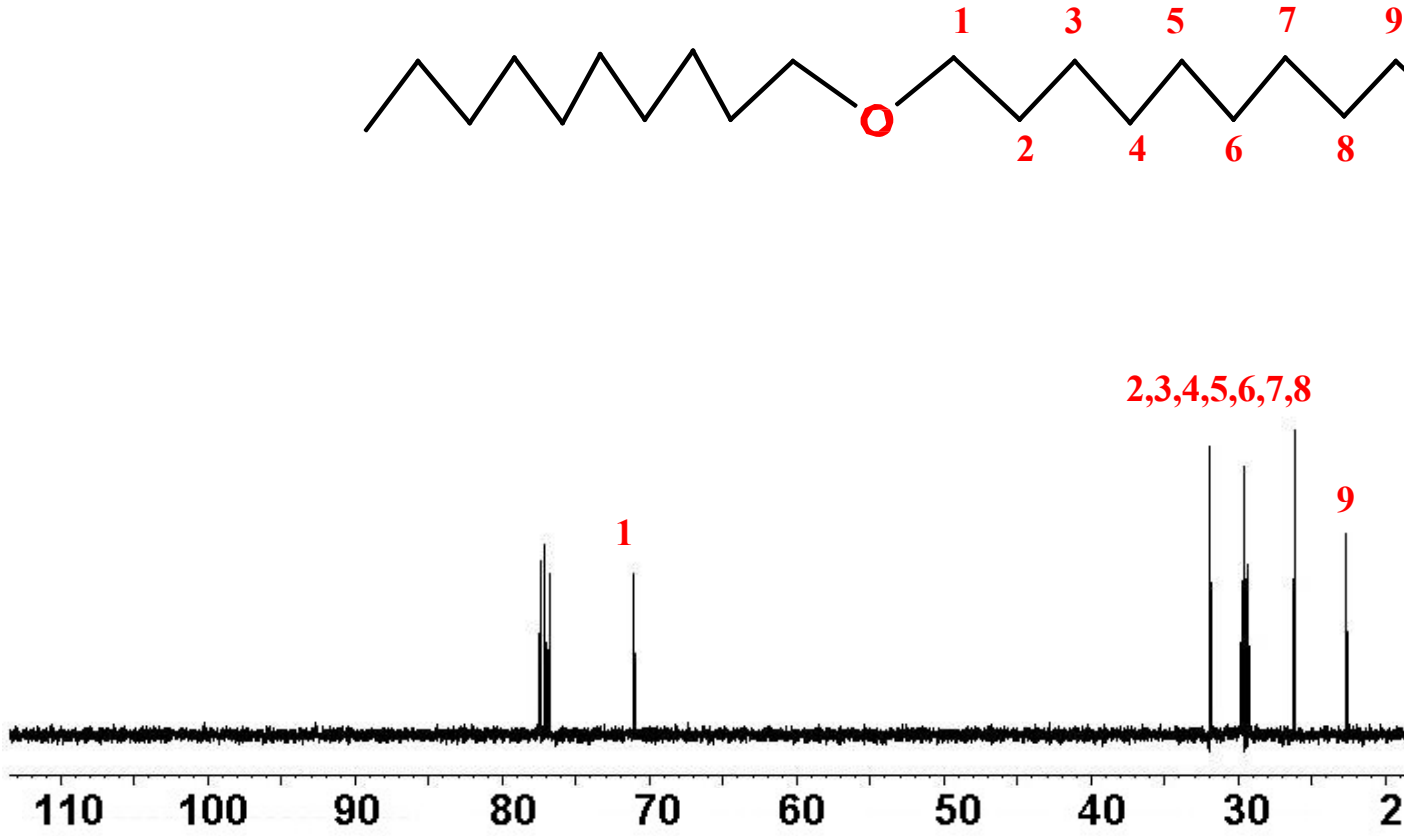


Figure S_{17}: ^{13}C NMR spectrum of isolated didecyl ether (L_2)

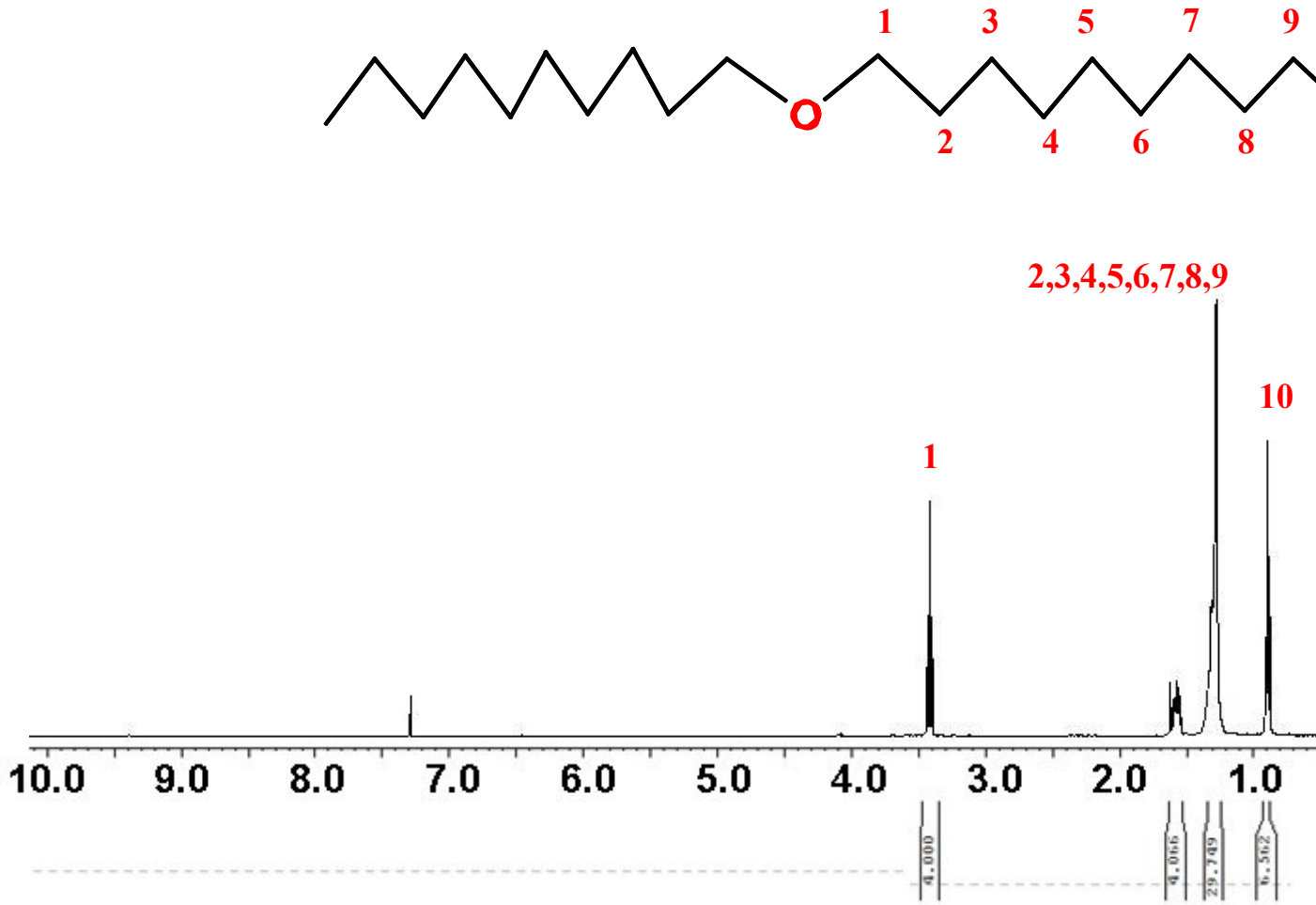


Figure S_{18}: ^{1}H NMR spectrum of isolated didecyl ether (**L_2**)

3.6 NMR spectra of isolated bis(3-phenylpropyl) ether (L_3): ^{1}H NMR (400 MHz) ($CDCl_3$): □1.94-2.01(m, 4H, H2); 2.76-2.79(t, 4H, H3, J = 7.2 Hz); 3.47-3.50(t, 4H, H1, J = 6.8 Hz). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □31.3, 32.3(C_{2-3}, CH_2); 69.92(C_1, CH_2); 125.71, 128.27, 128.44(C_{5-7}, CH); 142.0(C_4, C).

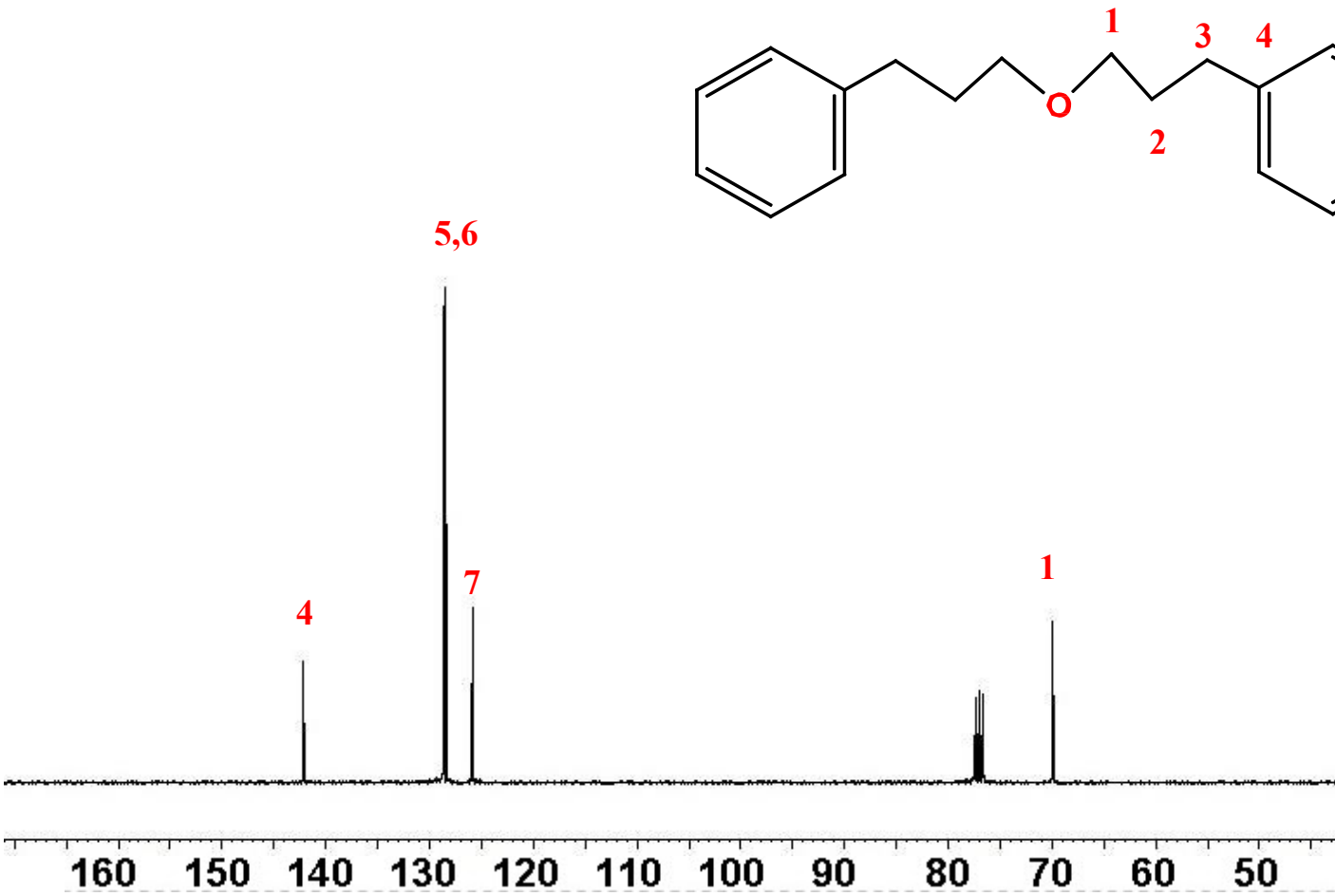


Figure S_{19}: ^{13}C NMR spectrum of isolated bis(3-phenylpropyl) ether L_3

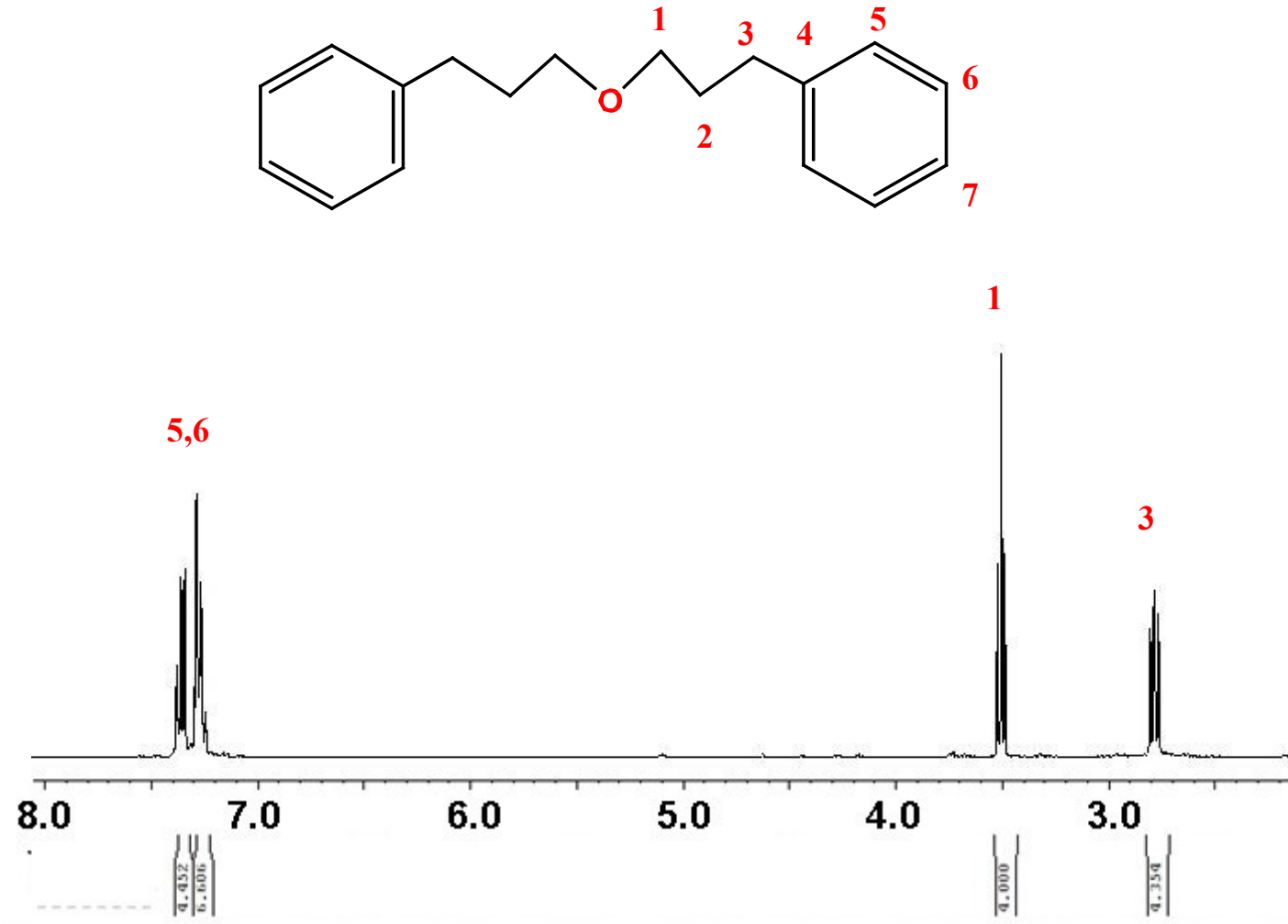


Figure S_{20}: ^{1}H NMR spectrum of isolated bis(3-phenylpropyl) ether **L_3**

3. 7 NMR spectra of isolated 3-((2-ethylbutoxy)methyl)pentane (L_5): ^{1}H NMR (400 MHz) ($CDCl_3$): □ 0.87-0.91(t, 12H, H4, J = 7.2 Hz); 1.31-1.48(m, 10H, H2-3); 3.27-3.29(d, 4H, H1, J = 5.60 Hz). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □11.11(C_4,CH_3); 23.4(C_3, CH_2); 41.2(C_2,CH); 73.5(C_1,CH_2O).

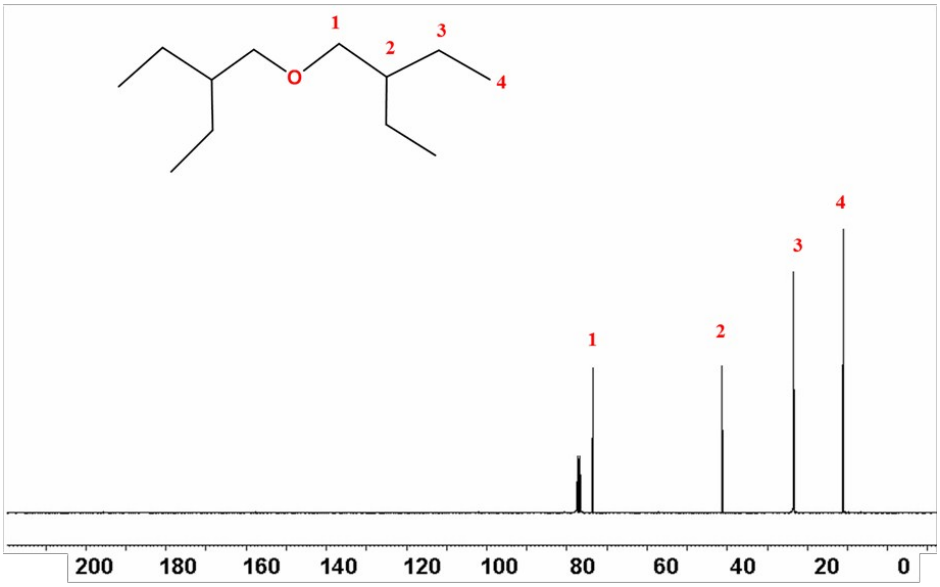


Figure S_{21}: ^{13}C NMR spectrum of isolated 3-((2-ethylbutoxy)methyl)pentane **L_5**

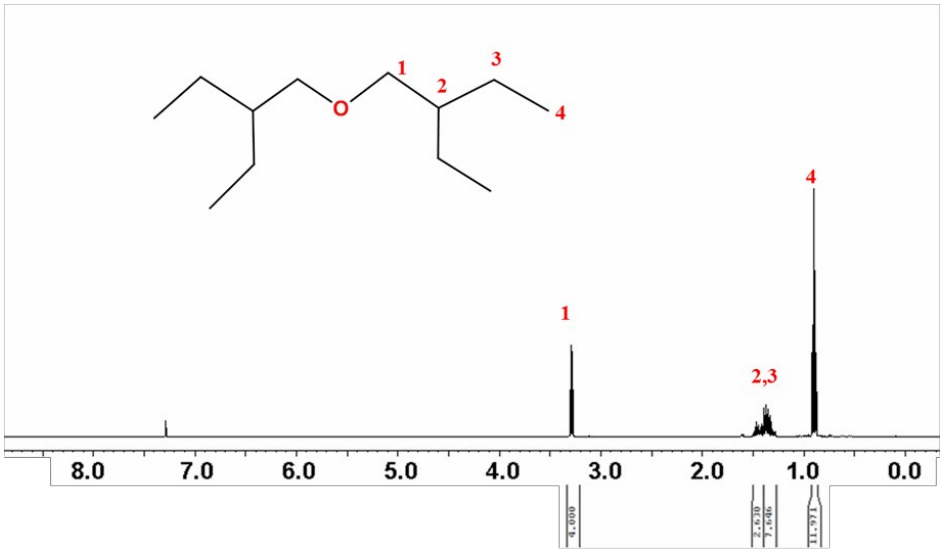


Figure S_{22}: ^{1}H NMR spectrum of isolated 3-((2-ethylbutoxy)methyl)pentane **L_5**

3.8 NMR spectra of isolated dicyclohexylmethyl ether (L_6): : ^{1}H NMR (400 MHz) ($CDCl_3$): □0.88-0.97,1.15-1.28,1.69-1.79(m, 20H, H_{3-5}); 1.58-1.60(m, 2H, H_2); 3.18, 3.20(d, 4H, H_1, J = 6.40Hz). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □25.90,26.69(C_{4-5}, CH_2); 30.15(C_3, CH_2); 38.04(C_2, CH); 76.9(C_1, CHO).

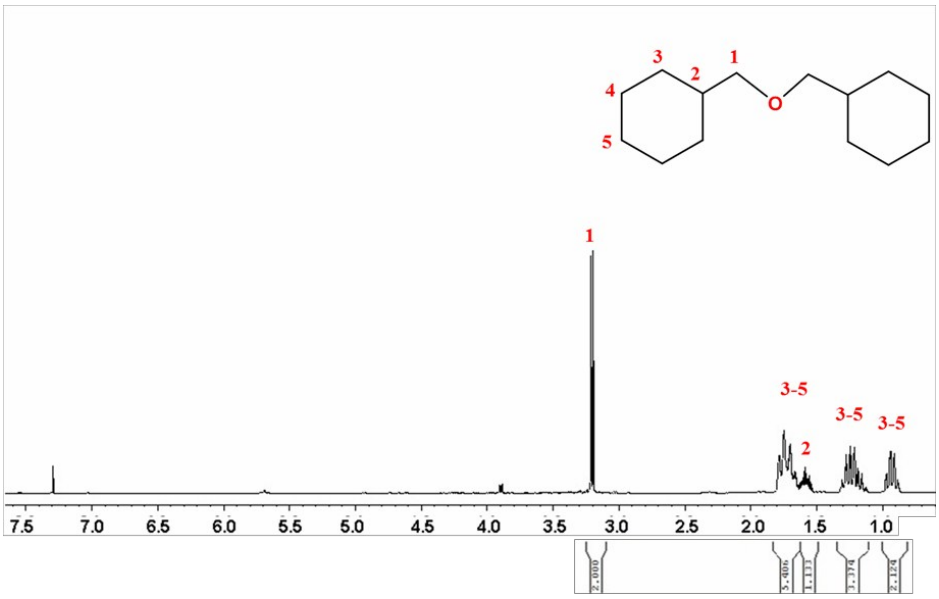
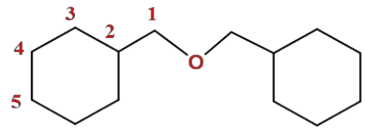


Figure S_{23}: ^{1}H NMR spectrum of isolated dicyclohexylmethyl ether **L_6**



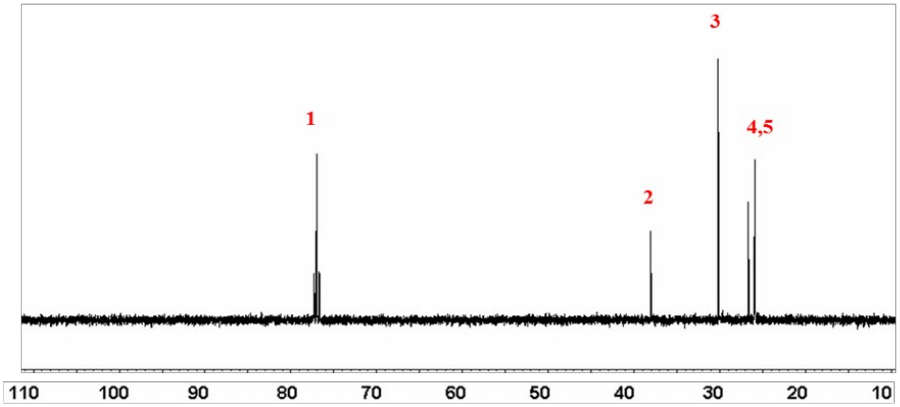


Figure S_{24}: ^{13}C NMR spectrum of isolated dicyclohexylmethyl ether **L_6**

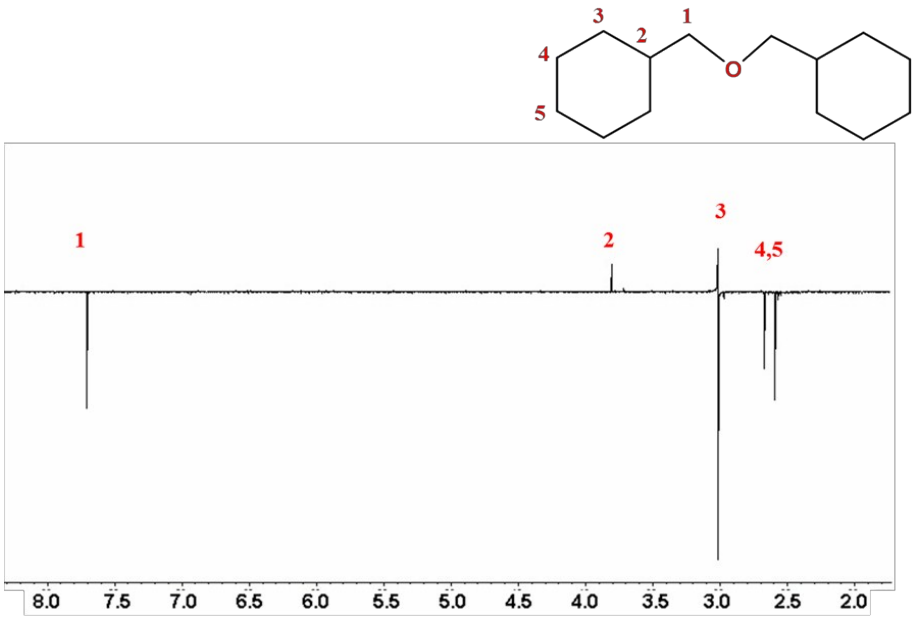


Figure S_{25}: DEPT 135 NMR spectrum of isolated dicyclohexylmethyl ether **L_6**

3.9 NMR spectra of isolated of 2,2'-oxybis(ethane-2,1,1-triyl)tetrabenzene L_7 : (L_7) ^{1}H NMR (400 MHz) ($CDCl_3$): □. 4.01, 4.03(d, 4H, H1, J = 6.8Hz); 4.26-4.29(t, 2H, H2, J = 7.2 Hz); 7.17-7.28(m, 20H, H_{4-6}). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □50.79(C_1, CH_2); 74.41(C_2, CH); 126.31(C_6, CH); 128.24-128.40(C4-5, CH); 142.18(C_3, C).

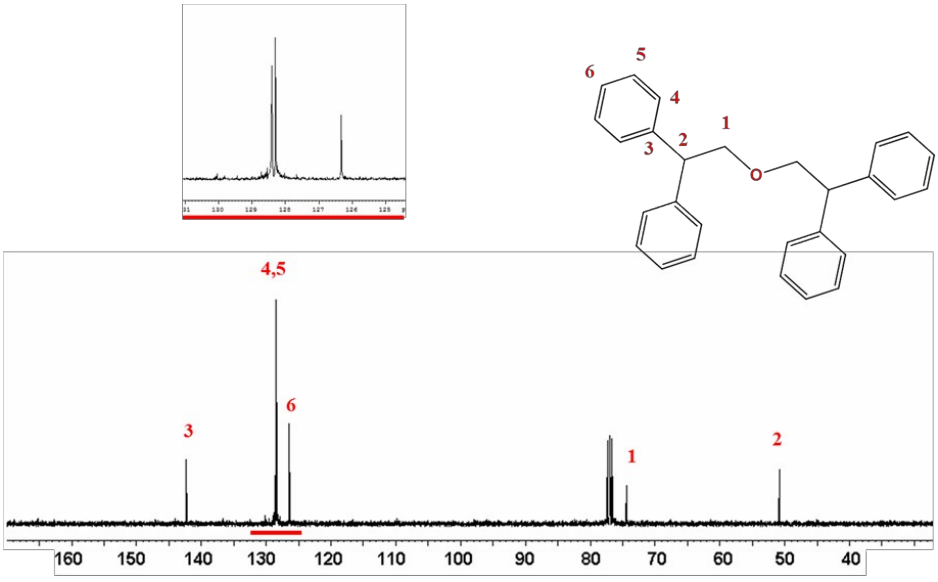


Figure S_{26}: ^{13}C NMR spectrum of isolated 2,2'-oxybis(ethane-2,1,1-triyl)tetrabenzene **L_7**

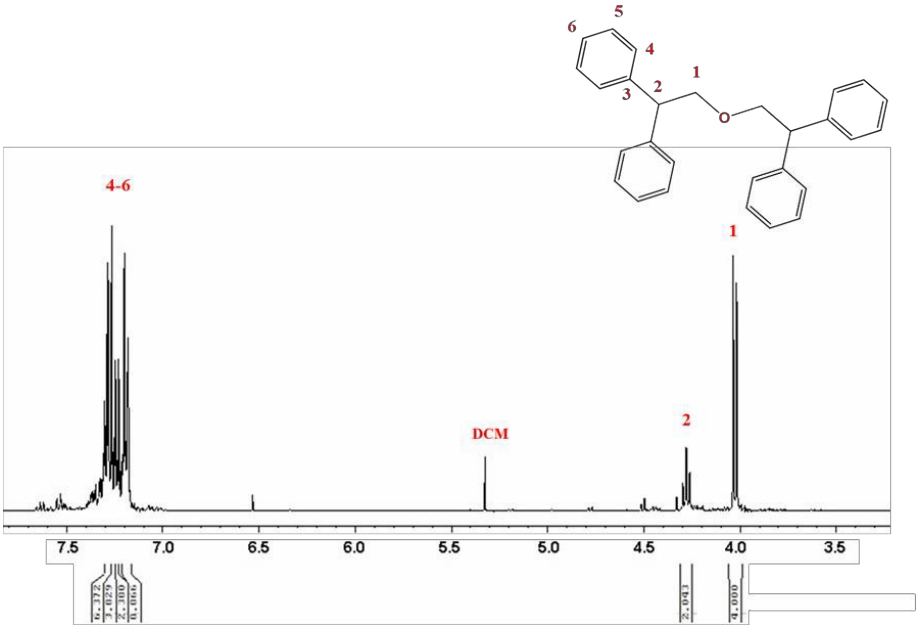


Figure S_{27}: ^{1}H NMR spectrum of isolated 2,2'-oxybis(ethane-2,1,1-triyl)tetrabenzene **L_7**

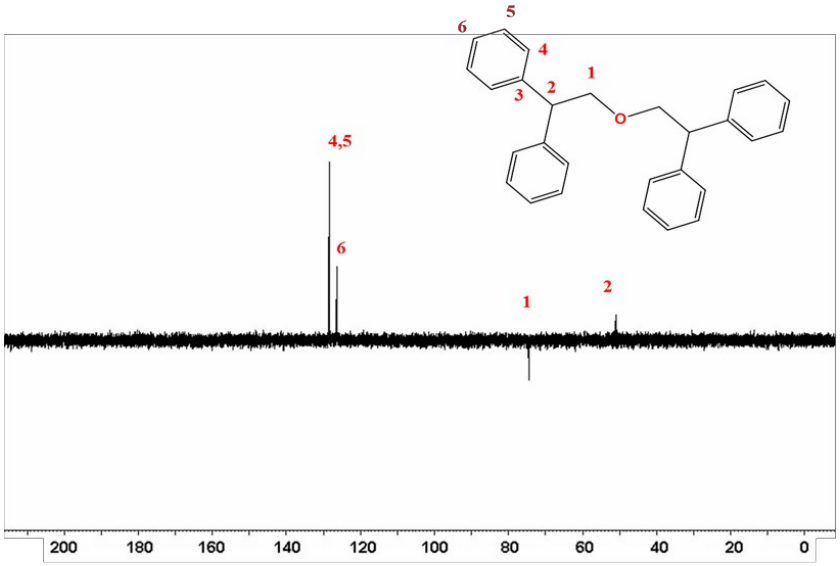


Figure S_{28}: DEPT 135 NMR spectrum of isolated 2,2'-oxybis(ethane-2,1,1-triyl)tetrabenzene **L_7**

3.10 NMR spectra of isolateed dibenzyl ether (L_8): ^{1}H NMR (400 MHz) ($CDCl_3$): □. 4.62(s, 4H, H1); 7.36-7.42(m, 10H, $H_{3\text{-}5}$). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □72.08(C_1, CH_2); 127.58,127.74, 128.36($C_{3\text{-}5}$, CH); 138.26(C_2, C).

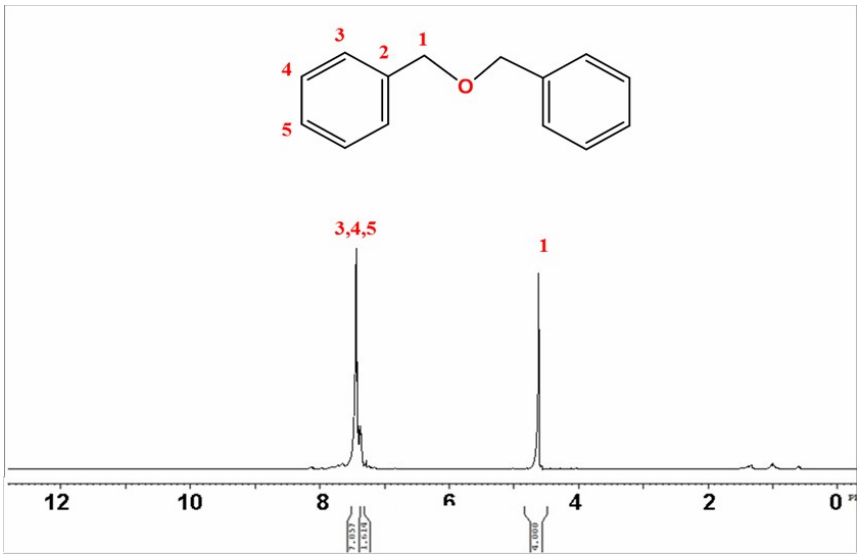


Figure S_{29}: ^{1}H NMR spectrum of isolated dibenzyl ether **L_8**

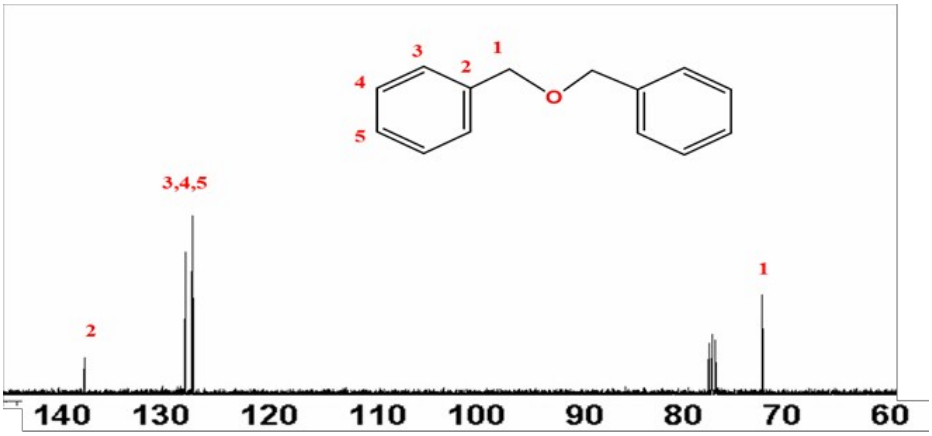


Figure S_{30}: ^{13}C NMR spectrum of isolated dibenzyl ether **L_8**

3.11 NMR spectra of isolated bis(2-bromobenzyl) ether (L_{10}): ^{1}H NMR (400 MHz) ($CDCl_3$): □.4.74(s, 4H, H1); 7.16-7.21; 7.34-7.36; 7.57-7.59(m, 8H, $H_{3\text{-}5}$). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □72.07(C_1, CH_2); 127.42, 128.97, 132.52($C_{3\text{-}5}$, CH); 137.46(C_2, C).

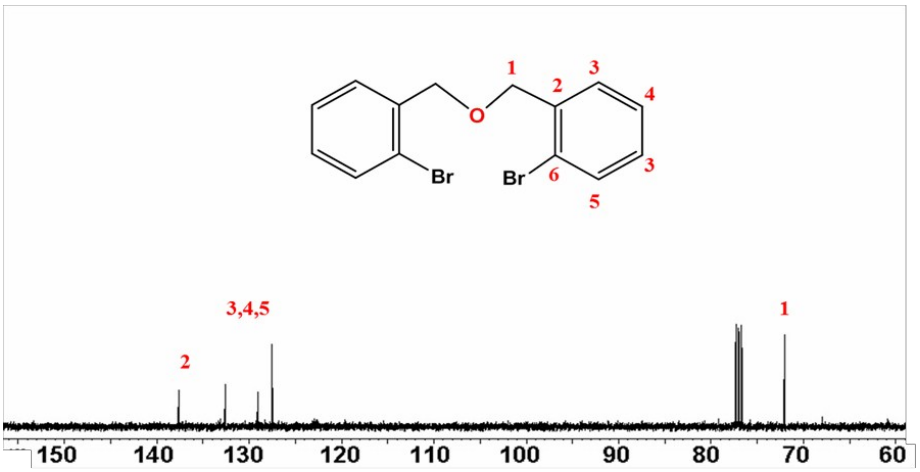


Figure S_{31}: ^{13}C NMR spectrum of isolated bis(2-bromobenzyl) ether **L_{10}**

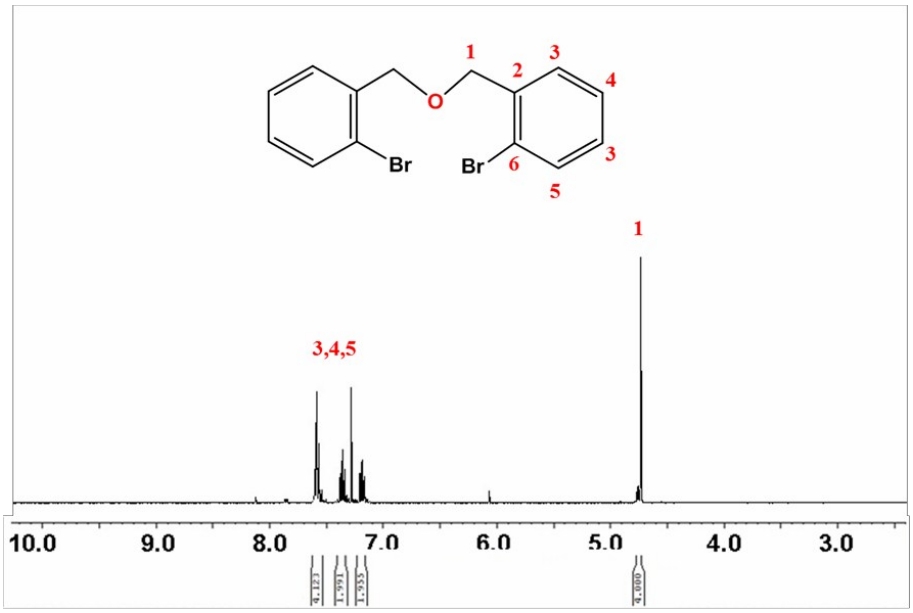


Figure S_{32}: ^{1}H NMR spectrum of isolated bis(2-bromobenzyl) ether **L_{10}**

3.12 NMR spectra of isolated bis(3-bromobenzyl) ether (L_{11}) : ^{1}H NMR (400 MHz) ($CDCl_3$): □.4.54(s, 4H, H_1); 7.25-7.29; 7.44-7.47; 7.54(m, 8H, $H_{3\text{-}5}$). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □ 71.47(C_1, CH_2); 122.56(C_6, CBr); 126.12, 130.0, 130.6, 131.0($C_{3\text{-}5}$, CH); 140.23(C_2, C).

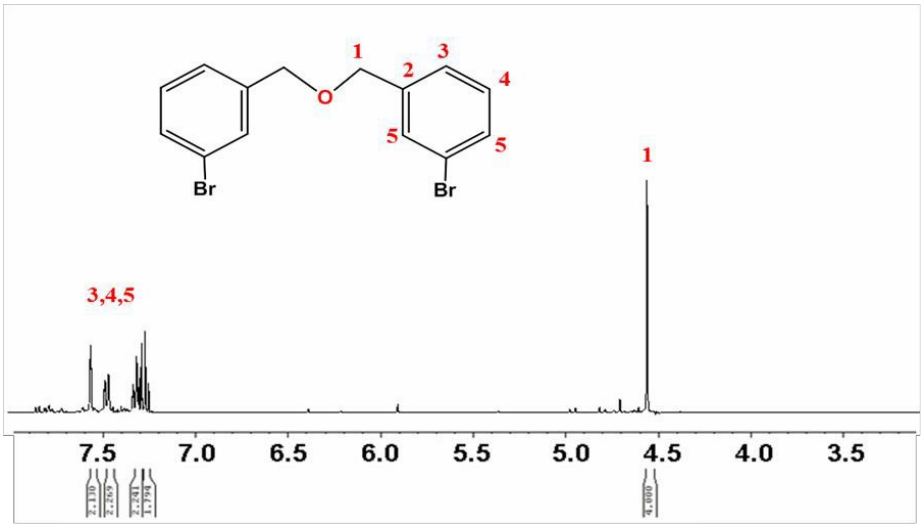


Figure S_{33}: ^{1}H NMR spectrum of isolated bis(3-bromobenzyl) ether **L_{11}**

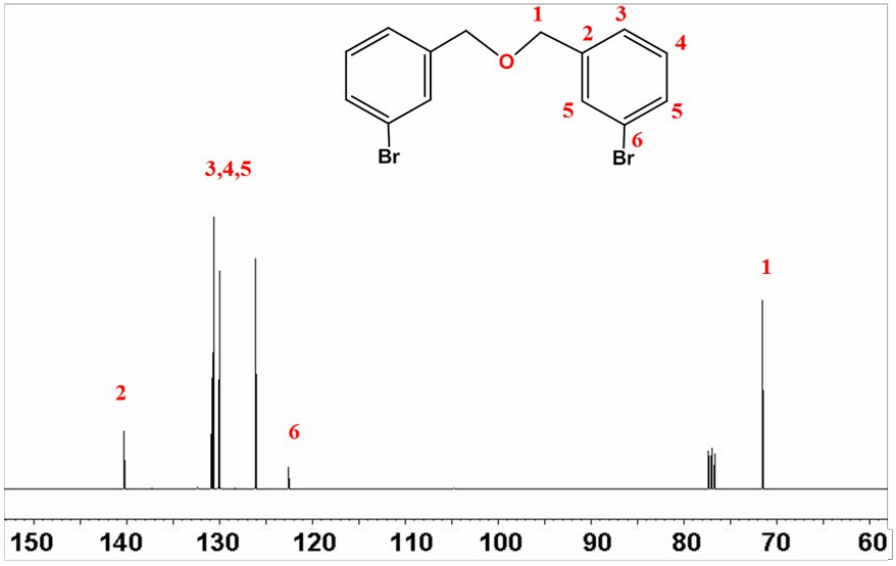


Figure S_{34}: ^{13}C NMR spectrum of isolated bis(3-bromobenzyl) ether **L_{11}**

3.13 NMR spectra of bis(3-fluorobenzyl) ether (L_{12}) : ^{1}H NMR (400 MHz) ($CDCl_3$): □. 4.59(s, 4H, H_1); 7.01-7.04; 7.11-7.17; 7.32-7.37(m, 8H, $H_{3\text{-}5}$). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □71.49(C_1, CH_2); 114.2, 114.41, 114.42, 114.6, 122.97, 129.96($C_{3\text{-}5}$, CH); 140.7(C_2, C); 165.1(C_6, CF). ^{19}F NMR (376.4983 MHz) ($CDCl_3$): □-113.14. Elemental analysis calculated (%) for $C_{14}H_{12}F_2O$: C.71.78, H.5.16. Found: C. 71.66, H. 5.19.

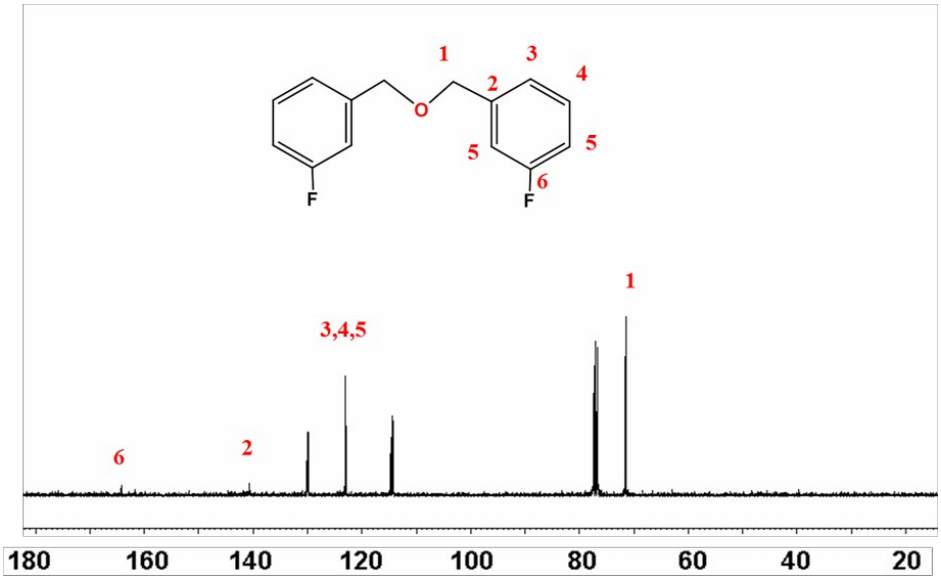


Figure S_{35}: ^{13}C NMR spectrum of isolated bis(3-fluorobenzyl) ether $\mathbf{L_{12}}$

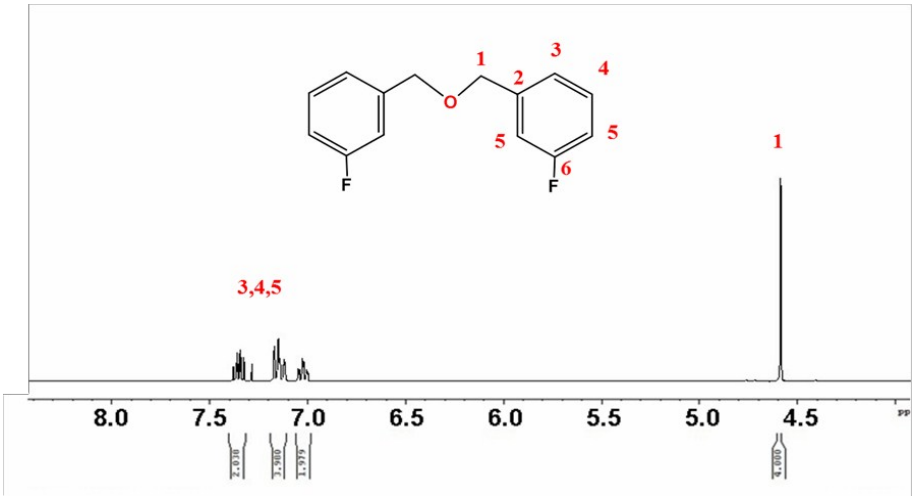


Figure S_{36}: ^{1}H NMR spectrum of isolated bis(3-fluorobenzyl) ether $\mathbf{L_{12}}$

Figure S_{37}: ^{19}F NMR spectrum of isolated bis(3-fluorobenzyl) ether **L_{12}**

3.14 NMR spectra of isolated 4,4'-oxybis(methylene)bis((trifluoromethyl)benzene) L_{13} : ^{1}H NMR (400 MHz) ($CDCl_3$): □.4.66(s, 4H, H_1); 7.50-7.52; 7.64-7.66 (m, 8H, H_{3-4}). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □71.66(C_1, CH_2); 125.41, 125.45, 125.48, 127.60(C_{3-6}), 141.97(C_2, C). ^{19}F NMR (376.4983 MHz) ($CDCl_3$): □-62.51.

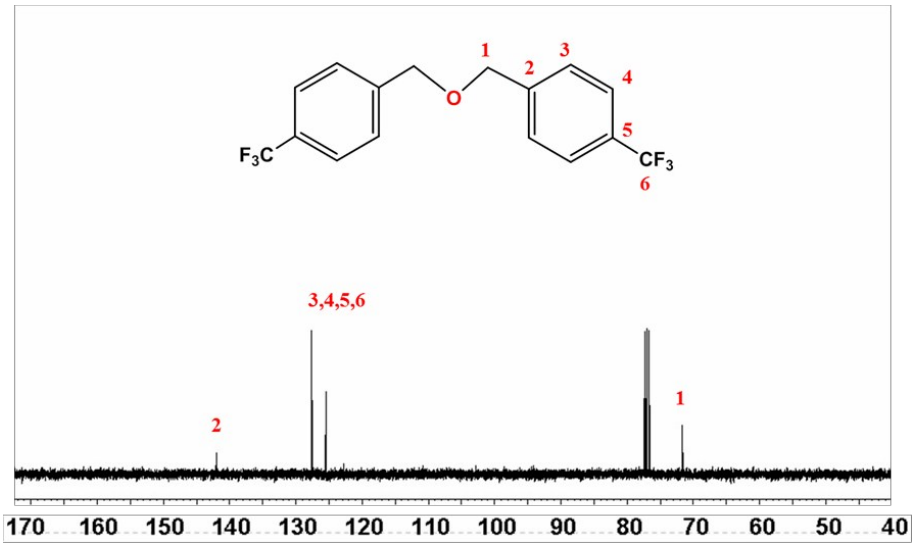


Figure S_{38}: ^{13}C NMR spectrum of isolated 4,4'-oxybis(methylene)bis((trifluoromethyl)benzene) **L_{13}**

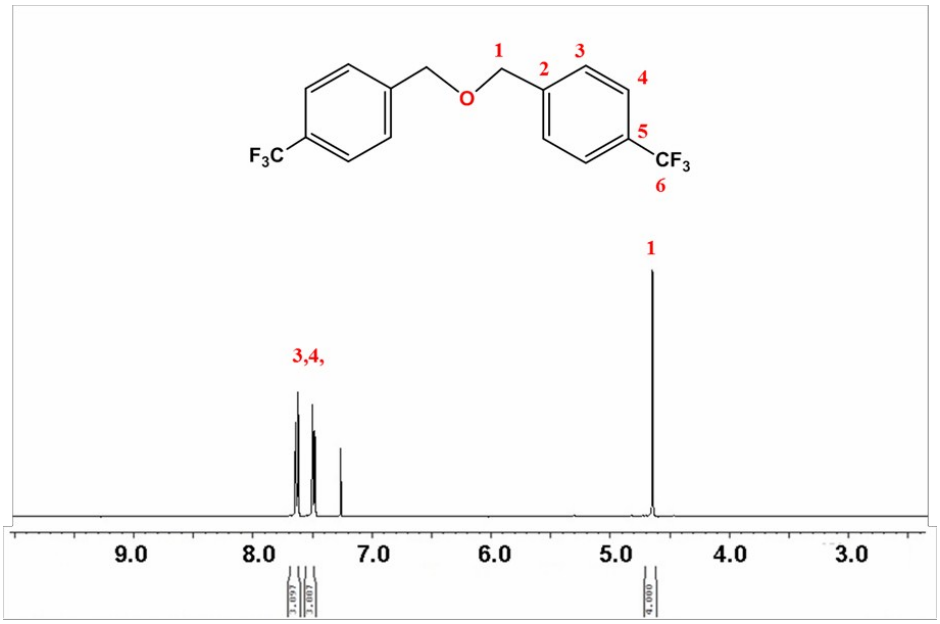


Figure S_{39}: ^{1}H NMR spectrum of isolated 4,4'-oxybis(methylene)bis((trifluoromethyl)benzene) **L_{13}**

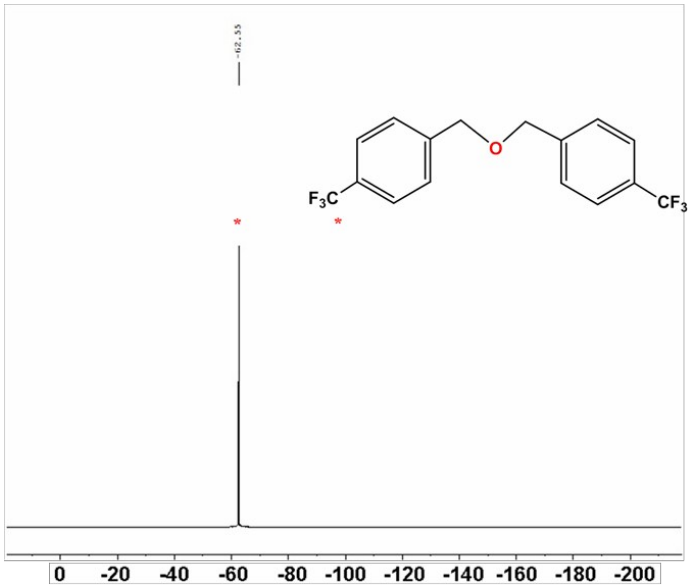


Figure S_{40}: ^{19}F NMR spectrum of isolated 4,4'-oxybis(methylene)bis((trifluoromethyl)benzene) **L_{13}**

3.15 NMR spectra of isolated 4,4'-oxybis(methylene)bis(nitrobenzene) (L_{14}): ^{1}H NMR (400 MHz) ($CDCl_3$): □. 4.86(s, 4H, H_1); 7.51,7.53(d, 4H, H_3, J =8.8 Hz); 8.20, 8.22(d, 4H, H_4, J = 8.8 Hz). ^{13}C NMR (100.61) ($CDCl_3$): □63.68(C_1, CH_2O); 123.45, 126.27($C_{3\text{-}4}$, CH_2); 148.9($C_{2,5}$, C).

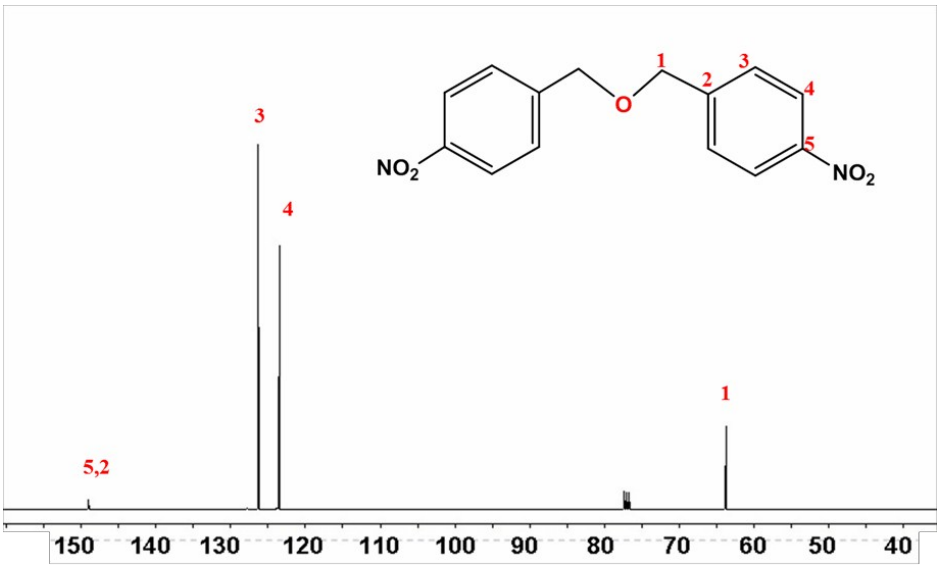


Figure S_{41}: ^{13}C NMR spectrum of isolated 4,4'-oxybis(methylene)bis(nitrobenzene) **L_{14}**

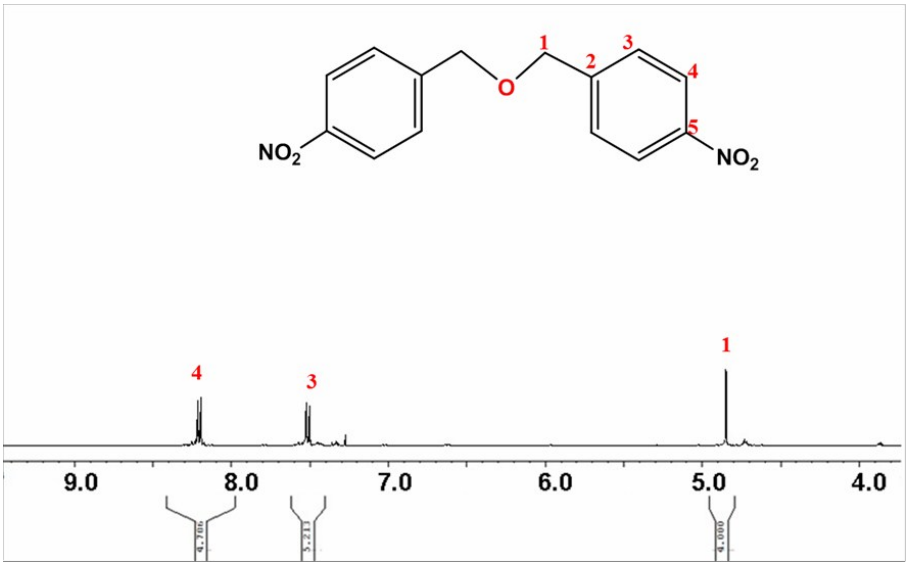


Figure S_{42}: ^{1}H NMR spectrum of isolated 4,4'-oxybis(methylene)bis(nitrobenzene) **L_{14}**

3.16 NMR spectra of isolated bis(*p*-methylbenzyl) ether (L_{15}) : ^{1}H NMR (400 MHz) ($CDCl_3$): □.2.37(s, 6H, H_6); 4.52(s, 4H, H_1); 7.17,7.19, 7.28, 7.29(m, 8H, H_{3-4}). ^{13}C NMR (100.61) ($CDCl_3$): □ 21.09(C_6, CH_3); 71.77(C_1, CH_2); 127.87, 129.04(C_{3-4}, CH); 135.1, 137.1($C_{2,5}$, C).

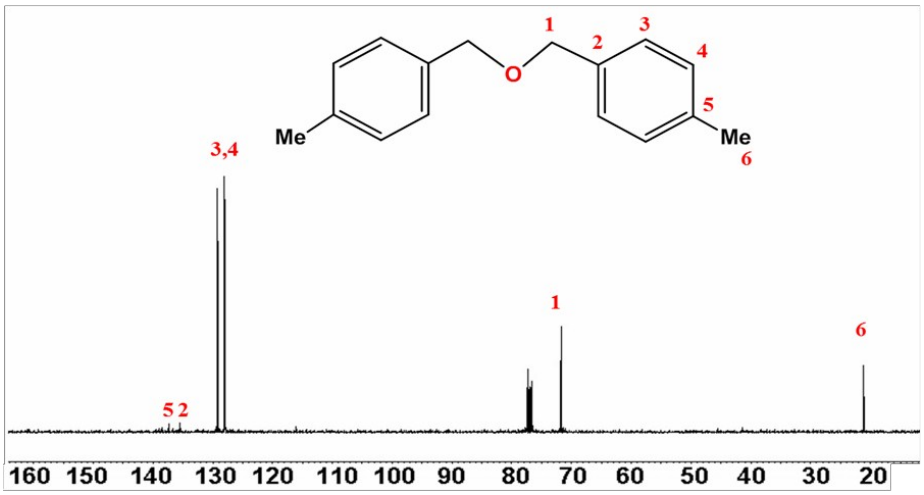


Figure S_{43}: ^{13}C NMR spectrum of isolated bis(*p*-methylbenzyl) ether **L_{15}**

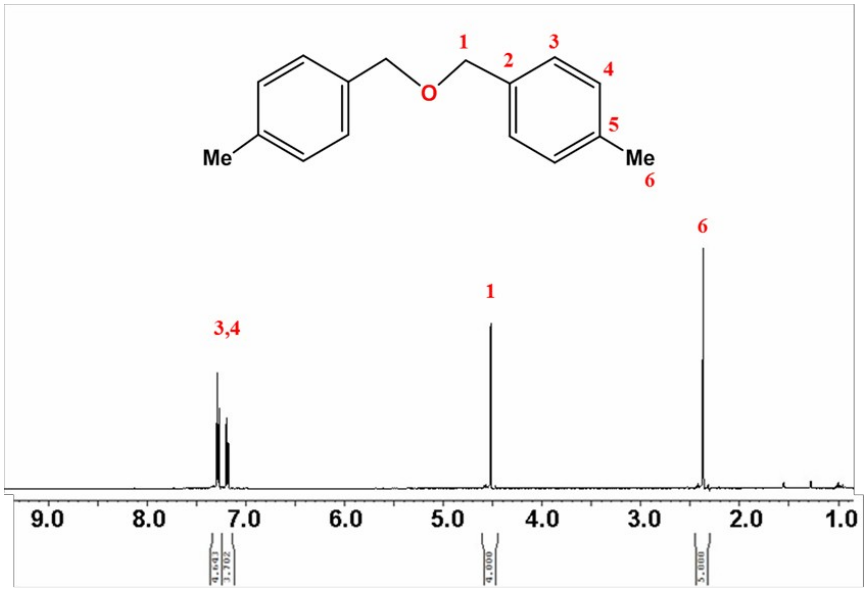


Figure S_{44}: ^{1}H NMR spectrum of isolated bis(*p*-methylbenzyl) ether **L_{15}**

3.17 NMR spectra of isolated (*E*)-2-ethyl-2-hexenal (M_1) : ^{1}H NMR (400 MHz) ($CDCl_3$): □. 0.80-0.84(m, 6H, $H_{7,8}$); 1.36-1.42(m, 2H, H6); 2.07-2.25(m, 4H, $H_{4,5}$); 6.28(m, 1H, H_3); 9.19(s, 1H, H1). ^{13}C NMR (100.61) ($CDCl_3$): □12.8, 13.4(C_{7-8}, CH_3); 16.85(C_4, CH_2); 21.58(C_6, CH_2); 30.27(C_5, CH_2); 144.98(C_2, C); 154.07(C_3, CH); 194.51(C_1, CHO).

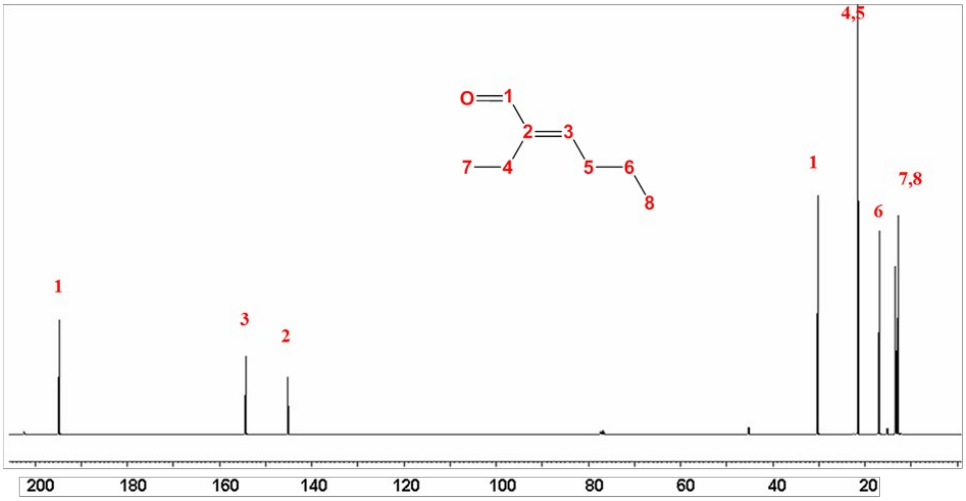


Figure S_{45}: ^{13}C NMR spectrum of isolated (*E*)-2-ethyl-2-hexenal **M_1**

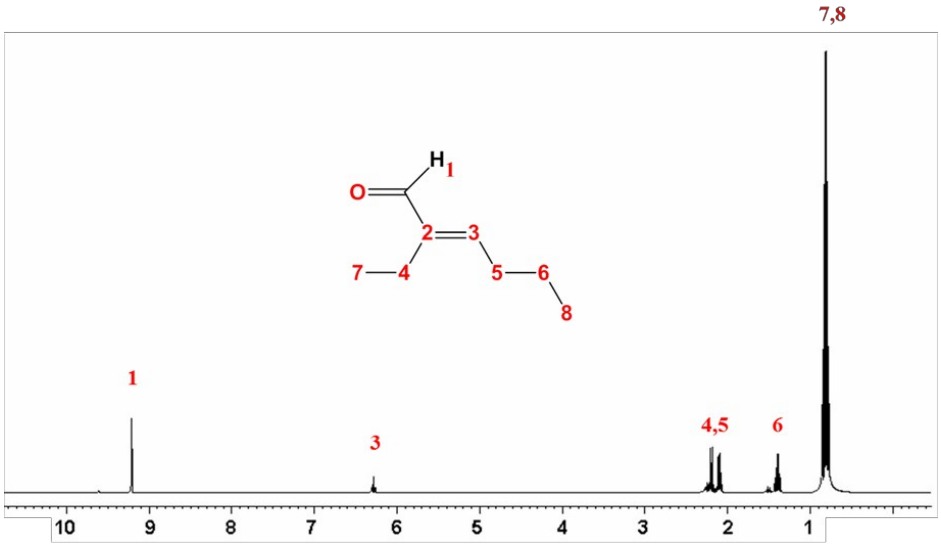


Figure S_{46}: ^{1}H NMR spectrum of isolated (*E*)-2-ethyl-2-hexenal **M_1**

3.18 NMR spectra of isolated (*E*)-2-octyl-3-nonylacrolein M_2 : ^{1}H NMR (400 MHz) ($CDCl_3$): □. 0.86-0.90(m, 6H, H_{19-20}); 1.26(s, 24H, H_{7-18}); 1.5(m, 2H, H_6); 2.25(m, 2H, H_4); 2.41(m, 2H, H_5); 6.42-6.45(t, 1H, H_3, J = 7.2 Hz); 9.36(s, 1H, H_1). ^{13}C NMR(100.61 MHz) ($CDCl_3$): □14.03(C_{19-20}, CH_3); 22.64, 24.00, 28.67, 28.89, 29.21, 29.25, 29.36, 29.39, 29.45, 29.65, 31.83(C_{4-18}, CH_2); 143.8(C_2, C); 155.14(C_3, CH); 195.18(C_1, CHO).

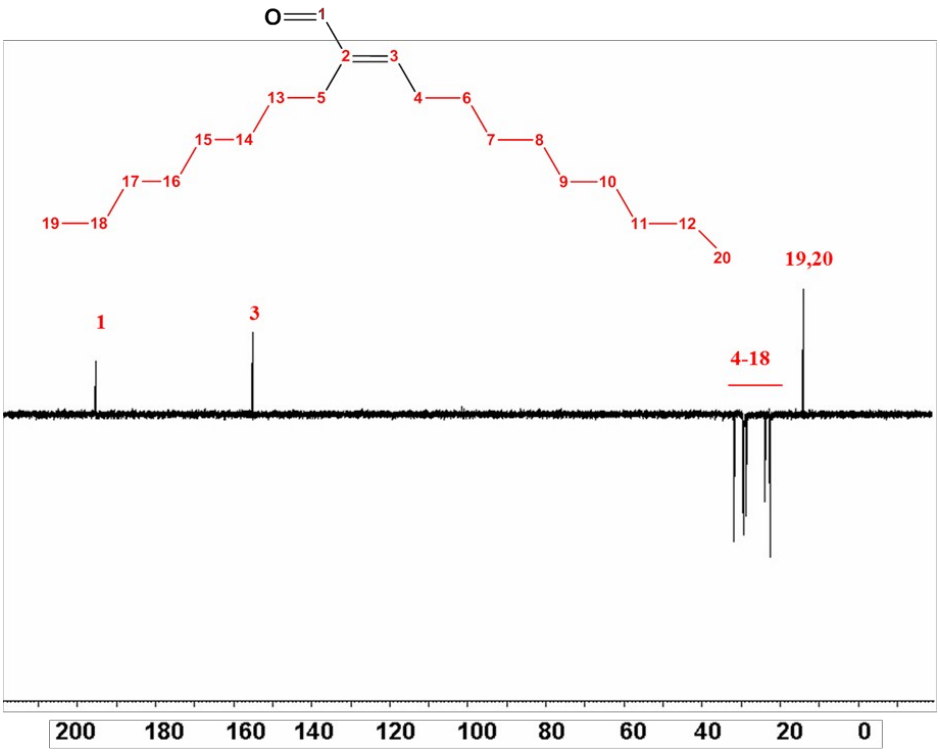


Figure S_{47}: DEPT 135 NMR spectrum of isolated (*E*)-2-octyl-3-nonylacrolein **M_2**

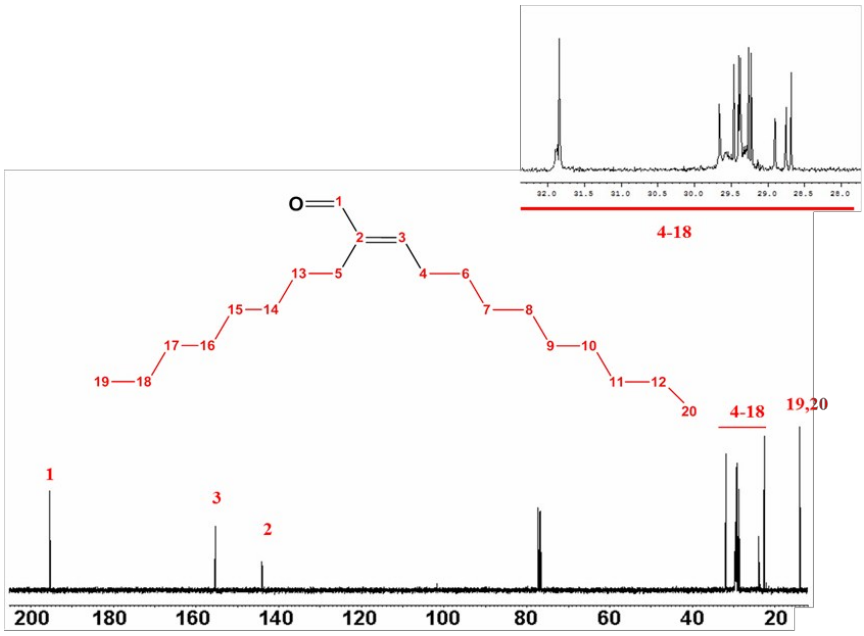


Figure S_{48}: ^{13}C NMR spectrum of isolated (*E*)-2-octyl-3-nonylacrolein **M_2**

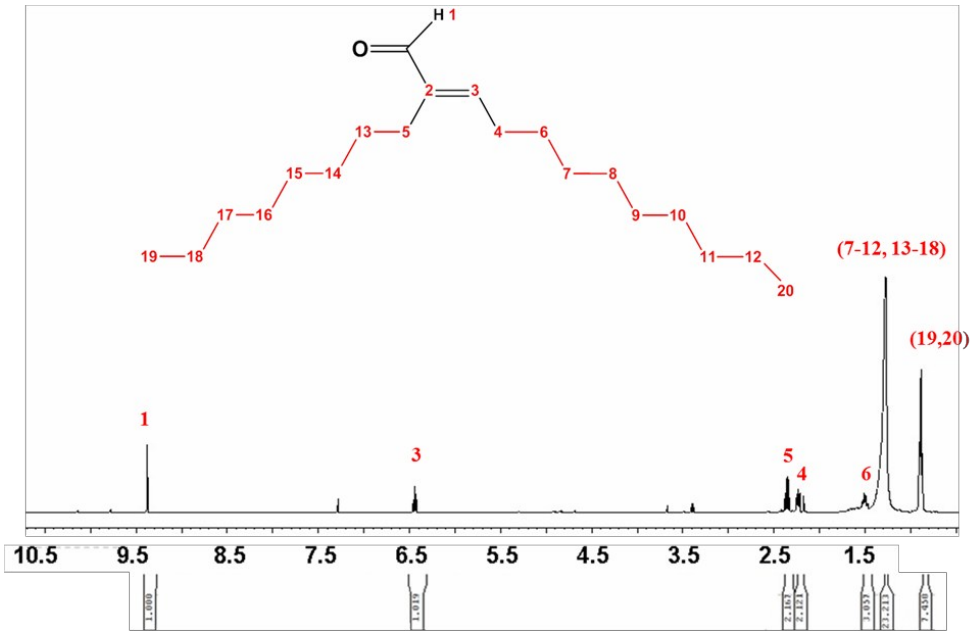


Figure S_{49}: ^{1}H NMR spectrum of isolated (*E*)-2-octyl-3-nonylacrolein **M_2**

3.19 NMR spectra of isolated (*E*)-2-benzyl-5-phenyl-pent-2-enal (M_3) : ^{1}H NMR (400 MHz) ($CDCl_3$): □. 2.78-2.81(m, 4H, H_{5-6}); 3.65(s, 2H, H4); 6.65-6.67(m, 1H, H_3); 7.17-7.34(m, 10H, H_{9-14}); 9.51(s, 1H, H_1). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □29.57(C_5, CH_2); 30.95(C_4, CH_2); 34.34(C_6, CH_2); 126.02, 126.31, 128.24, 128.28, 128.38, 128.52(C_{9-14}, CH); 138.98, 140.36($C_{7,8}$, C); 142.74(C_2, C); 154.60(C_3, CH); 194.44(C_1, CHO).

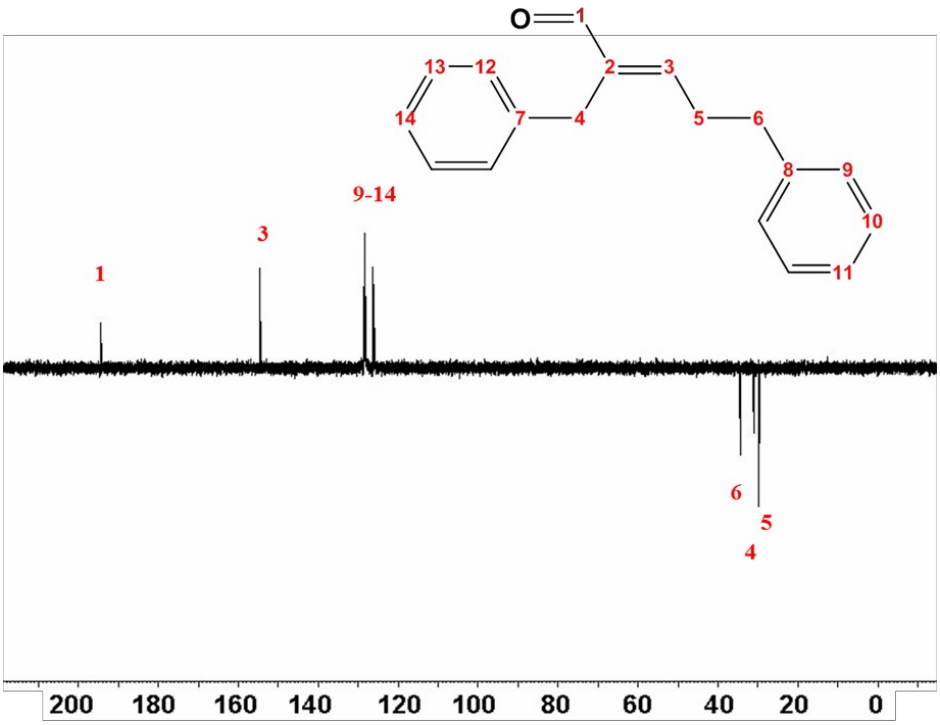


Figure S_{50}: DEPT 135 NMR spectrum of isolated (*E*)-2-benzyl-5-phenyl-pent-2-enal **M_3**

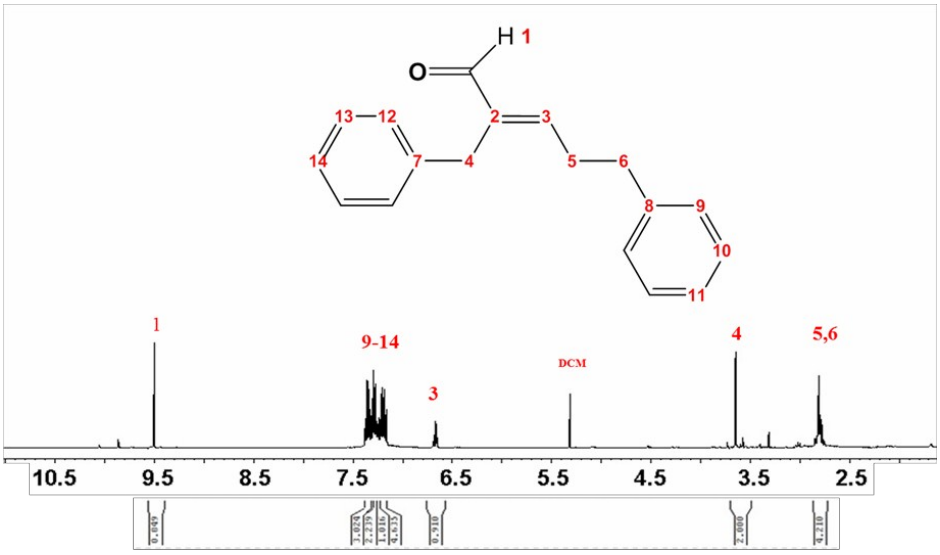


Figure S_{51}: ^{1}H NMR spectrum of isolated (*E*)-2-benzyl-5-phenyl-pent-2-enal **M_3**

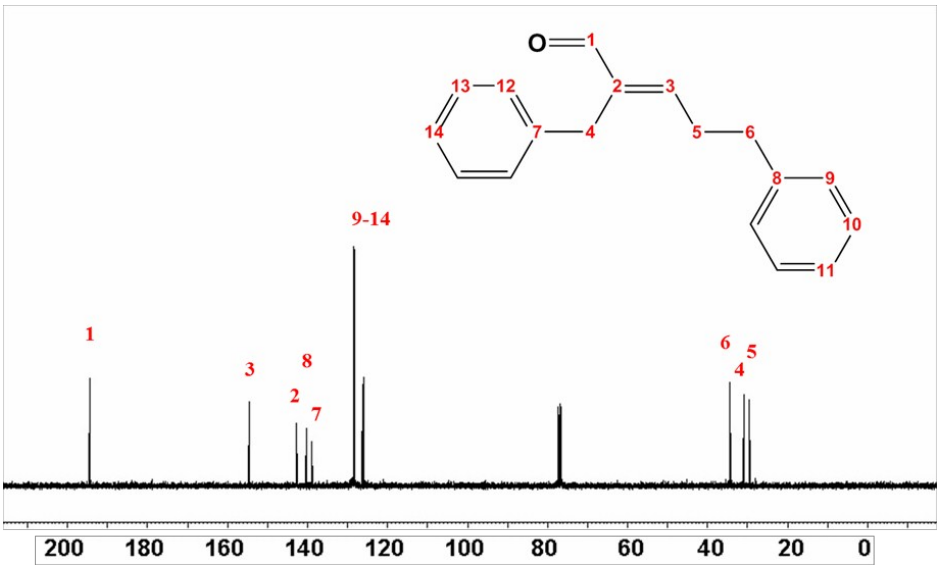


Figure S_{52}: ^{13}C NMR spectrum of isolated (*E*)-2-benzyl-5-phenyl-pent-2-enal **M_3**

3.20 NMR spectra of isolated (*E*)-2,4-diphenyl-but-2-enal (M_4): ^{1}H NMR (400 MHz) ($CDCl_3$): □.3.74, 3.76(d, 2H, H_5, J = 7.6 Hz); 6.90-6.94(t, 1H, H_3, J = 7.6 Hz); 7.21-7.51(m, 10H, H_{7-12}); 9.71(s, 1H, H_1). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □35.72(C_5, CH_2); 126.71, 128.09, 128.29, 128.38, 129.37(C_{7-12}, CH); 132.1, 137.99($C_{4,6}$, C); 144.04(C_2, C(=CH_2)); 153.27(C_3, CH); 193.35(C_1, CHO).

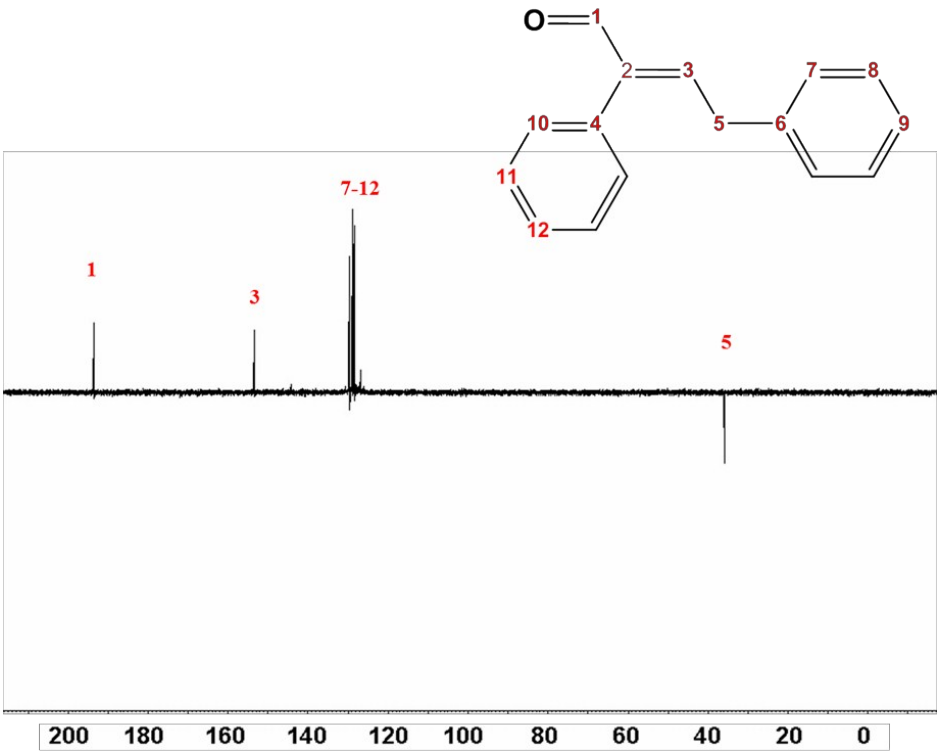


Figure S_{53}: DEPT 135 NMR spectrum of isolated (*E*)-2,4-diphenyl-but-2-enal **M_4**

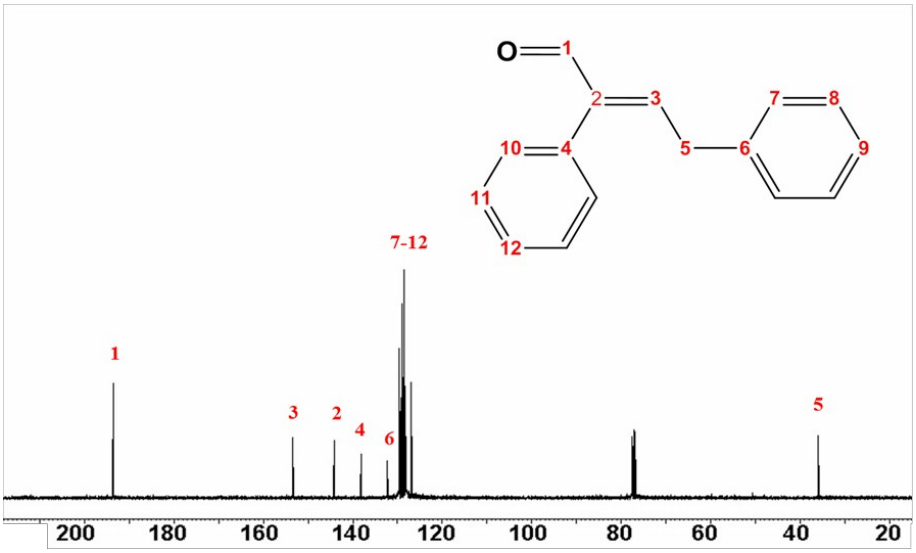


Figure S_{54}: ^{13}C NMR spectrum of isolated (*E*)-2,4-diphenyl-but-2-enal **M_4**

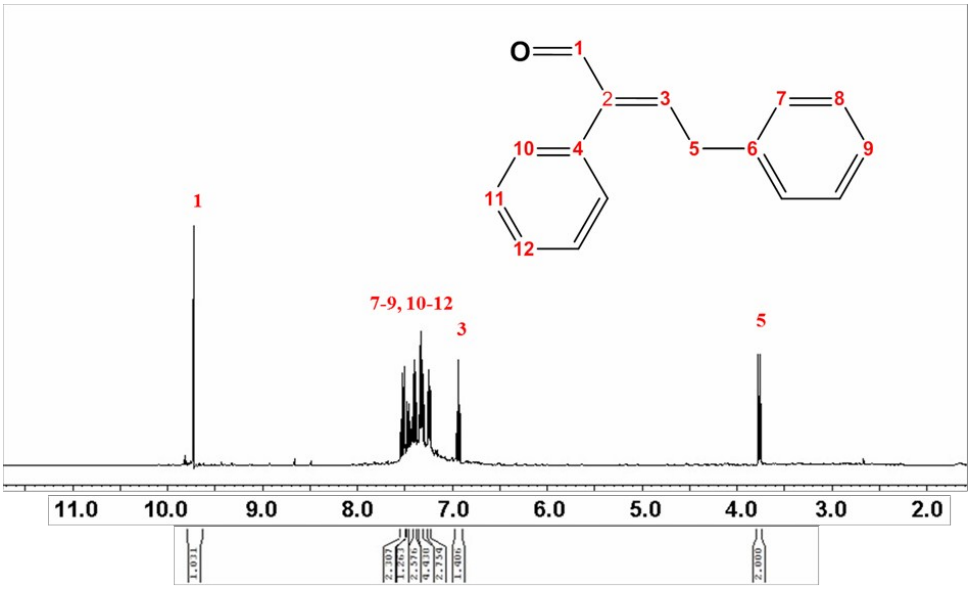


Figure S_{55}: ^{1}H NMR spectrum of isolated (*E*)-2,4-diphenyl-but-2-enal **M_4**

3.21 NMR spectra of isolated 2,4,6-tripropyl-1,3,5-Trioxane (N_1): ^{1}H NMR (400 MHz) ($CDCl_3$): □.0.91-0.95(t, 9H, H_4, J = 7.6 Hz); 1.41-1.47; 1.63-1,68(m, 12H, H_{2-3}); 4.84, 4.86, 4.87(t, 3H, H_1, J = 5.2 Hz). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □13.82(C_4, CH_3); 16.87(C_3, CH_2); 36.42(C_2, CH_2); 101.41 (C_1, CHO).

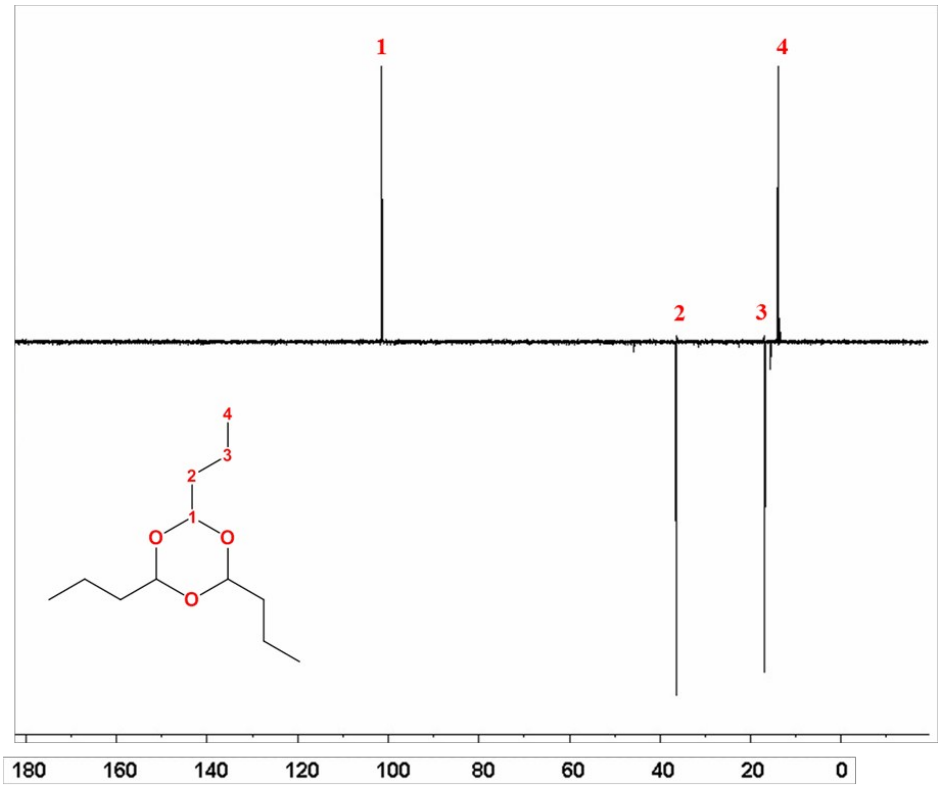


Figure S_{56}: DEPT 135 NMR spectrum of isolated 2,4,6-tripropyl-1,3,5-trioxane $\mathbf{N_1}$

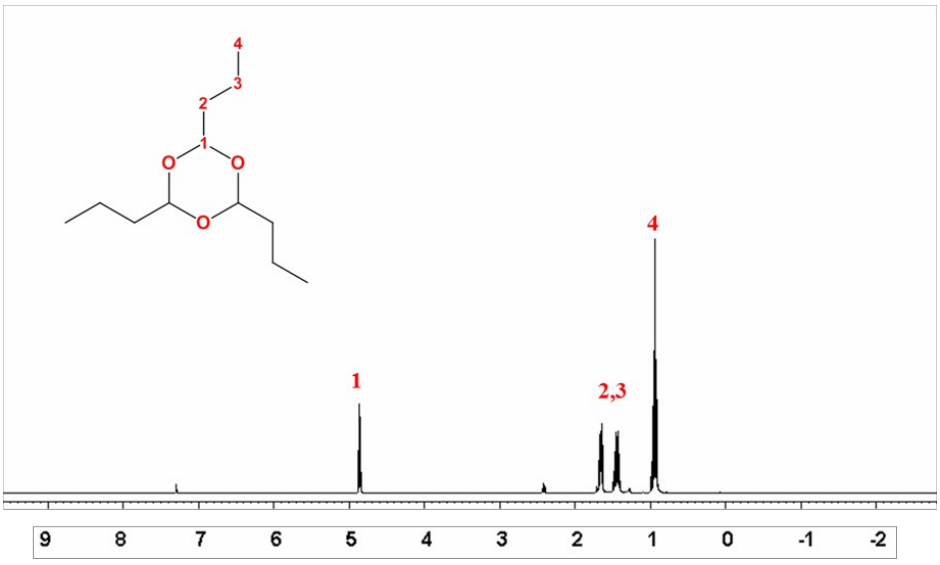


Figure S_{57}: ^{1}H NMR spectrum of isolated 2,4,6-tripropyl-1,3,5-trioxane $\mathbf{N_1}$

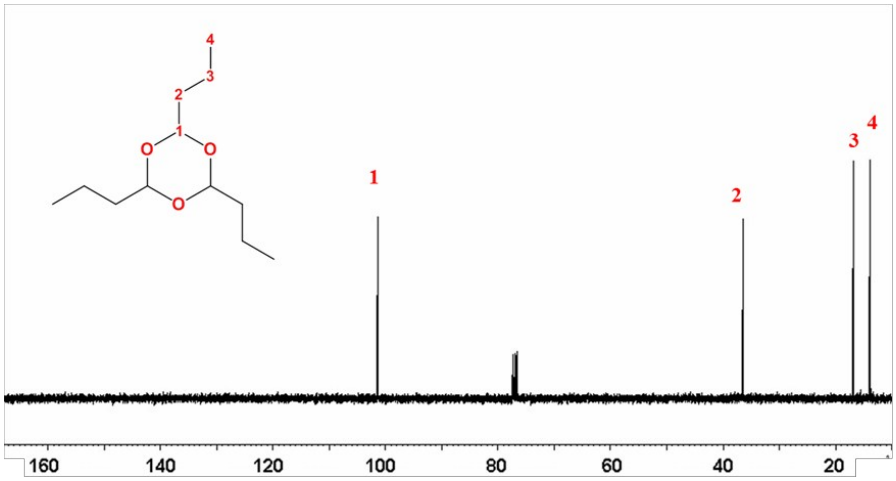


Figure S_{58}: ^{13}C NMR spectrum of isolated 2,4,6-tripropyl-1,3,5-trioxane **N_1**

3.22 NMR spectra of isolated 2,4,6-trinonyl-1,3,5-trioxane (N_2) : ^{1}H NMR (400 MHz) ($CDCl_3$): □.0.88-0.91(t, 9H, H_{10}, J = 6.4 Hz).; 1.28(s, 36H, $H_{4\text{-}9}$); 1.39-1.43(m, 6H, H_3); 1.60-1.71(m, 6H, H_2); 4.83-4.86(t, 3H, H_1, J = 5.20 Hz). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □14.09(C_{10}, CH_3); 22.67, 23.56, 29.29, 29.37, 29.50, 31.88, 34.42($C_{2\text{-}7}$, CH_2); 101.71(C_1, CHO). MP 39^{o}C.

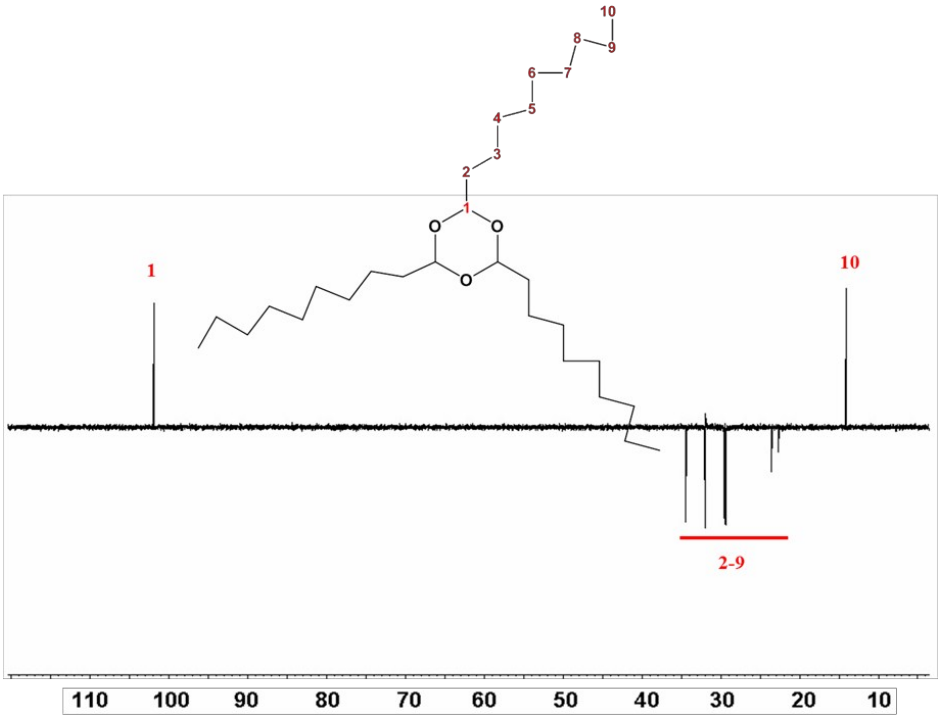


Figure S_{59}: DEPT 135 NMR spectrum of isolated 2,4,6-trinonyl-1,3,5-trioxane **N_2**

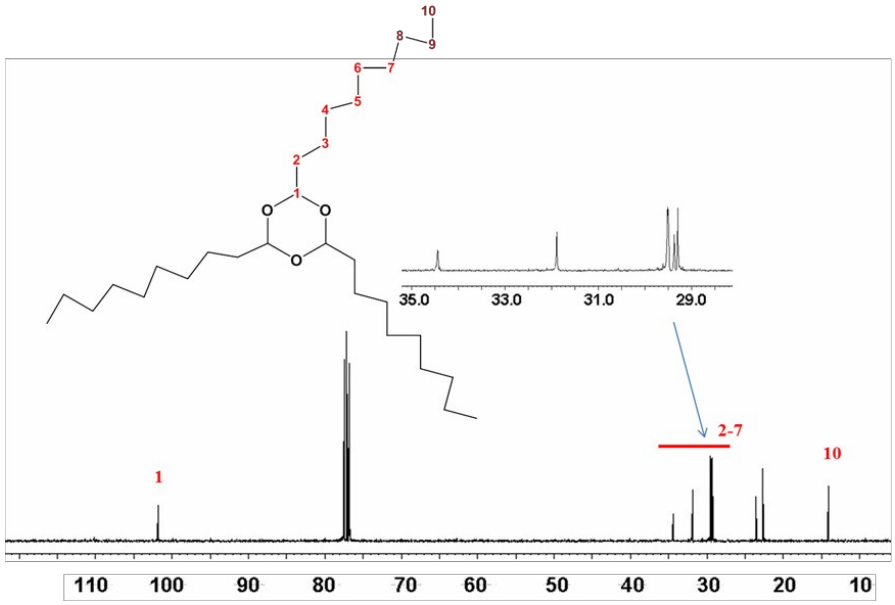


Figure S_{60}: ^{13}C NMR spectrum of isolated 2,4,6-trinonyl-1,3,5-trioxane **N_2**

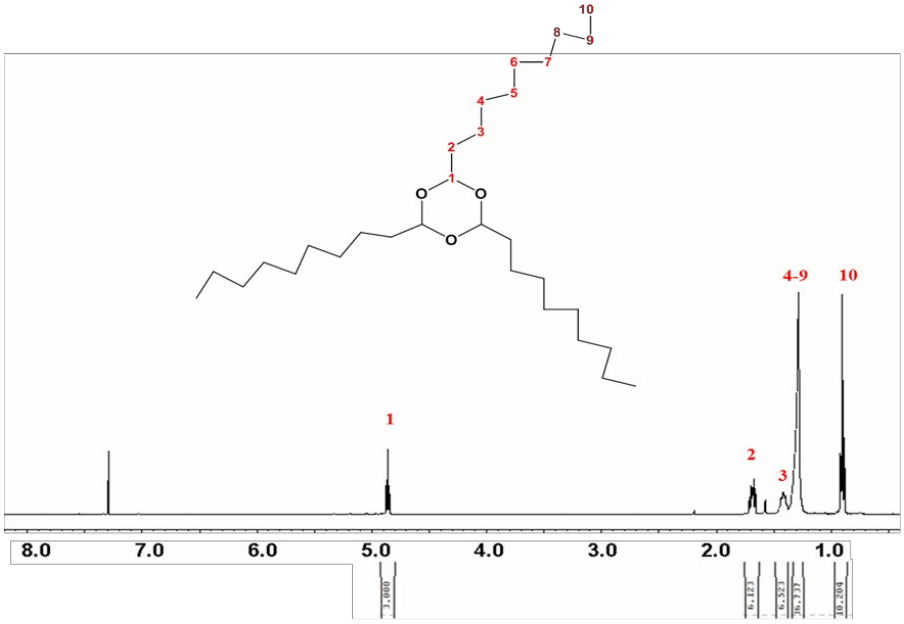


Figure S_{61}: ^{1}H NMR spectrum of isolated 2,4,6-trinonyl-1,3,5-trioxane **N_2**

3.23 NMR of isolated 2,4,6-tribenzyl-1,3,5-trioxane (N_3) : ^{1}H NMR (400 MHz) ($CDCl_3$): □.3.04, 3.05(d, 6H, H_2, J = 5.2 Hz); 4.97-4.99(t, 3H, H_1, J = 5.6Hz); 7.24-7.28(m, 15H, H_{4-6}). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □ 41.01(C_2, CH_2); 101.70(C_1, CHO); 126.57(C_6, CH); 128.13(C_4, CH); 129.8(C_5, CH); 135.5(C_3, C). Mp. 161^{o}C.

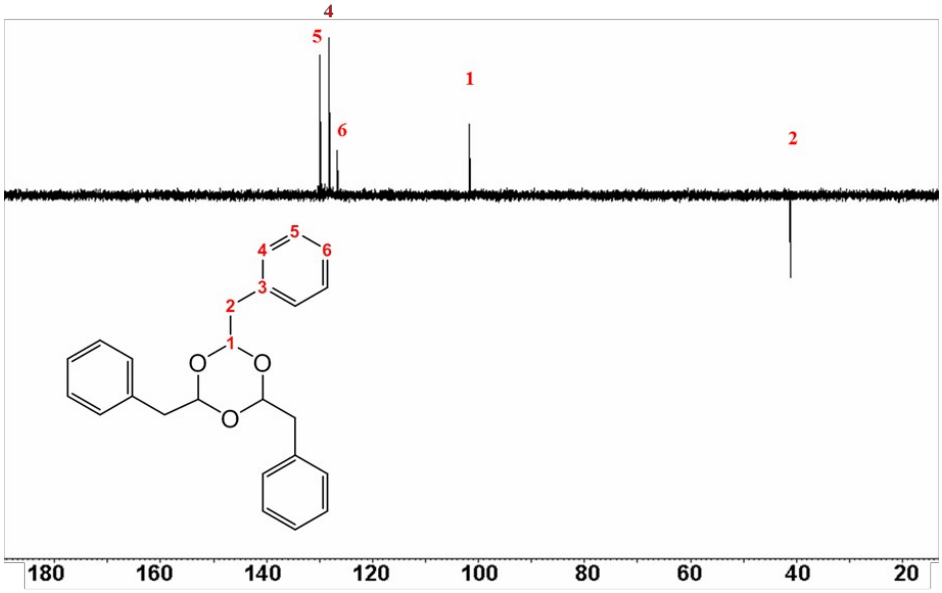


Figure S_{62}: DEPT 135 NMR spectrum of isolated 2,4,6-tribenzyl-1,3,5-trioxane **N_3**

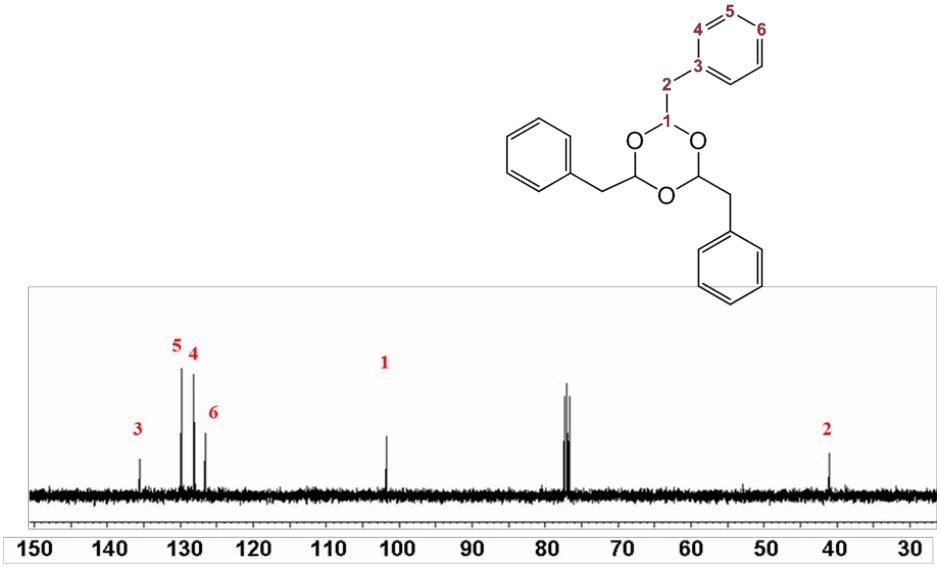


Figure S_{63}: ^{13}C NMR spectrum of isolated 2,4,6-tribenzyl-1,3,5-trioxane **N_3**

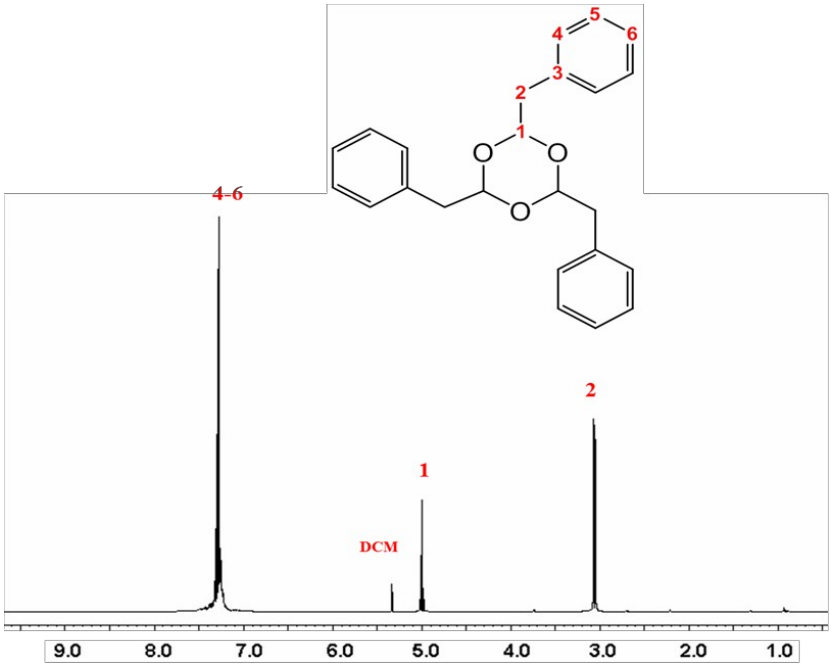


Figure S_{64}: ^{1}H NMR spectrum of isolated 2,4,6-tribenzyl-1,3,5-trioxane **N_3**

3.24 NMR spectra of isolated 2,4,6-tri-(2-phenylethyl)-1,3,5-trioxane (N_4) : ^{1}H NMR (400 MHz) ($CDCl_3$): □.2.04-2.09(m, 6H, H_2); 2.78-2.82(t, 6H, H_3, J = 7.2 Hz); 4.83-4.86(t, 3H, H_1, J = 5.20 Hz); 7.22-7.32(m, 15H, H_{5-7}). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □29.57(C_3, CH_2); 35.62(C_2, CH_2); 100.60(C_1, CHO); 125.91, 128.38, 128.43(C_{5-7}, CH); 141.32(C_4, C). Mp. 61^{o}C.

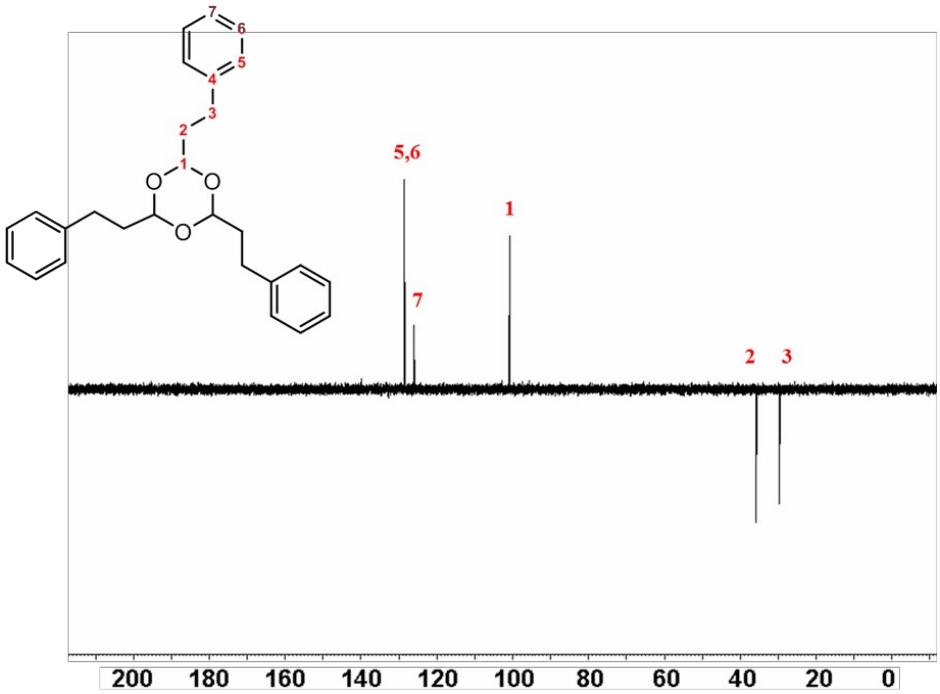


Figure S_{65}: DEPT 135 NMR spectrum of isolated 2,4,6-tri-(2-phenylethyl)-1,3,5-trioxane **N_4**

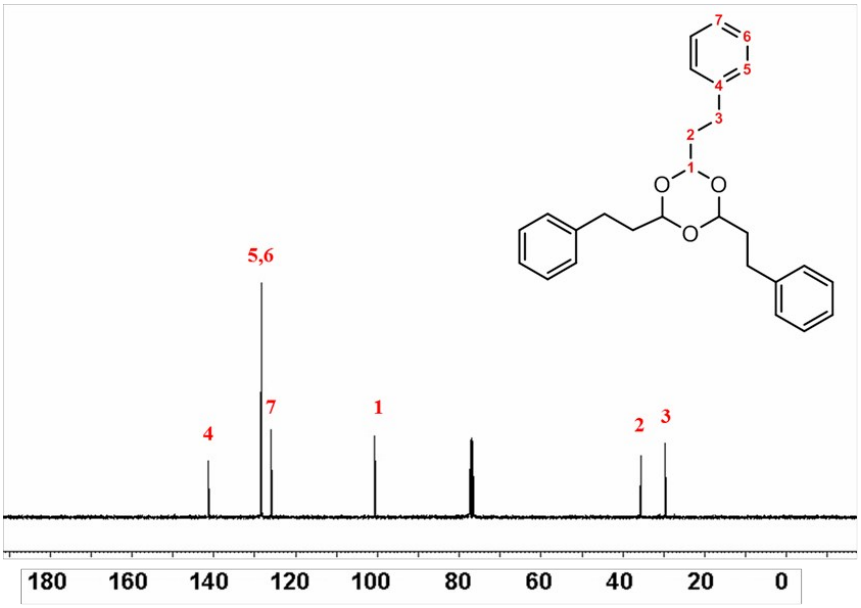


Figure S_{66}: ^{13}C NMR spectrum of isolated 2,4,6-tri-(2-phenylethyl)-1,3,5-trioxane **N_4**

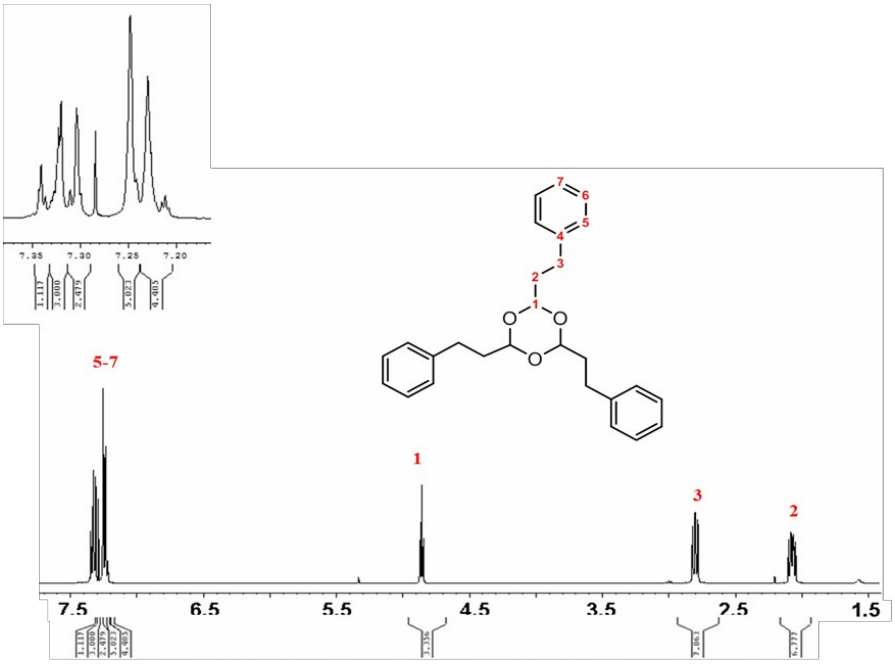


Figure S_{67}: ^{1}H NMR spectrum of isolated 2,4,6-tri-(2-phenylethyl)-1,3,5-trioxane **N_4**

3.25 NMR spectra of 2,4,6-tri-(pentan-3-yl)-1,3,5-trioxane (N_5) : ^{1}H NMR (400 MHz) ($CDCl_3$): □.0.91-0.97(m, 18H, H_4); 1.37-1.42; 1.47-1.58(m, 15H, H_{2-3}); 4.75, 474(d, 3H, H_1, J = 4.80Hz). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □ 11.33(C_4, CH_3); 20.77(C_3, CH_2); 44.88(C_2, CH); 103.16(C_1, CHO). Elemental analysis calculated (%) for $C_{18}H_{36}O_3$: C. 71.95, H 12.08. Found: C. 72.00, H. 12.17.

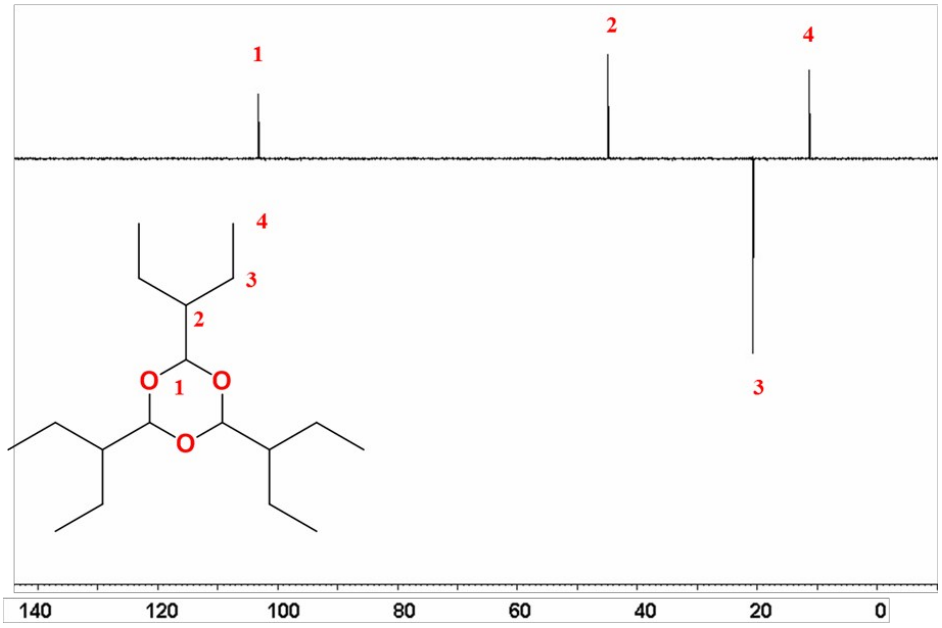


Figure S_{68}: DEPT 135 NMR spectrum of isolated 2,4,6-tri-(pentan-3-yl)-1,3,5-trioxane **N_5**

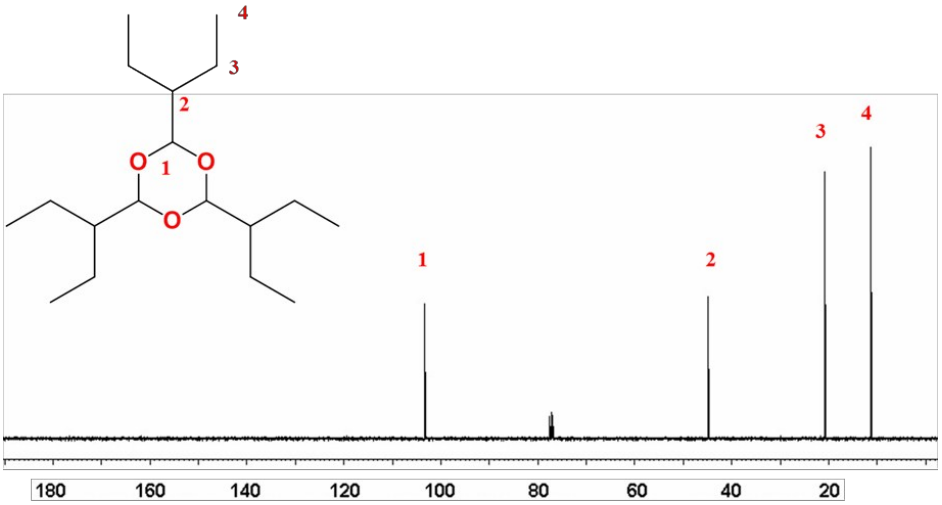


Figure S_{69}: ^{13}C NMR spectrum of isolated 2,4,6-tri-(pentan-3-yl)-1,3,5-trioxane **N_5**

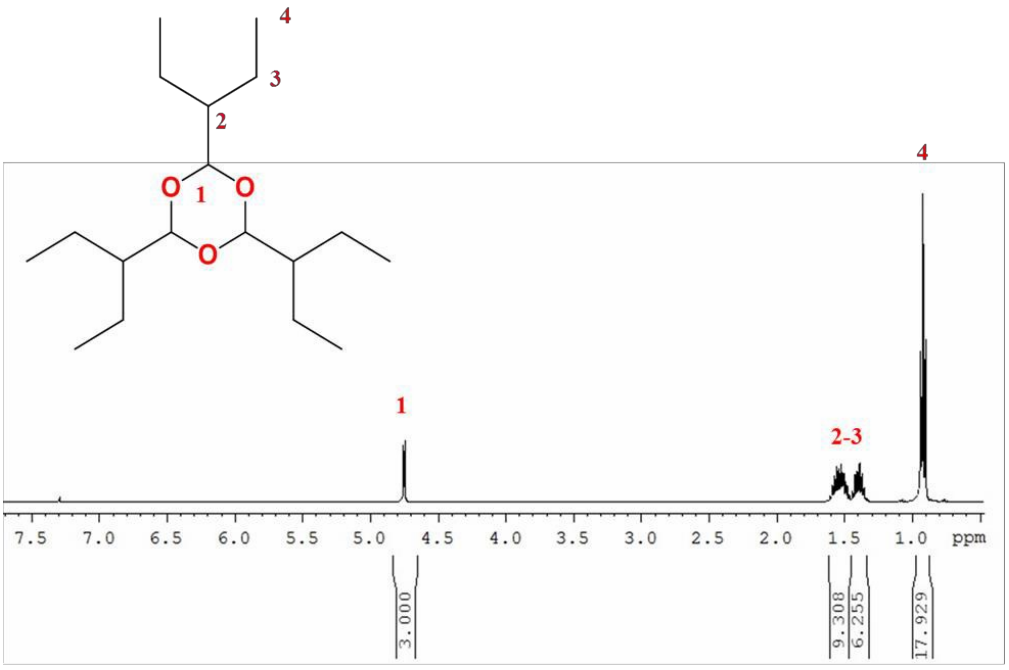


Figure S_{70}: ^{1}H NMR spectrum of isolated 2,4,6-tri-(pentan-3-yl)-1,3,5-trioxane **N_5**

3.26 NMR spectra of isolated 2,4,6-tricyclohexyl-1,3,5-trioxane (N_6) : ^{1}H NMR (400 MHz) ($CDCl_3$): □. 1.06-1.10; 1.85-1.86(m, 12H, H_3); 1.18-1.23; 1.72-1.82(m, 12H, H_4); 1.56-1.68(m, 6H, $H_{2,5}$).; 4.50-4.52(d, 3H, H_1, J = 6.0 HZ). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □25.6(C_3, CH_2); 26.48(C_5, CH_2); 27.05(C_4, CH_2); 41.8(C_2, CH); 104.20(C_1, CHO). MP. 196^{o}C.

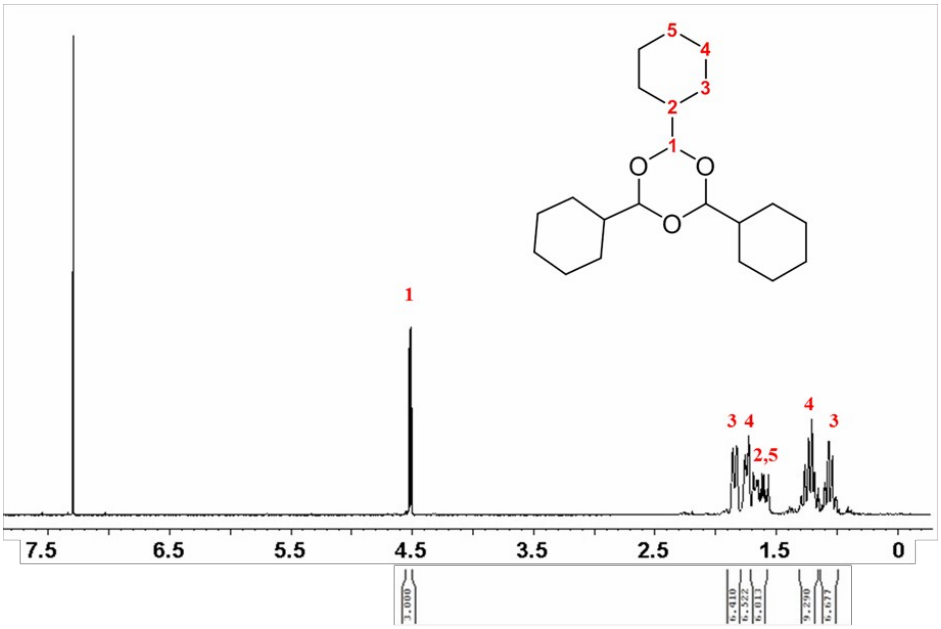


Figure S_{71}: ^{1}H NMR spectrum of isolated 2,4,6-tricyclohexyl-1,3,5-trioxane **N_6**

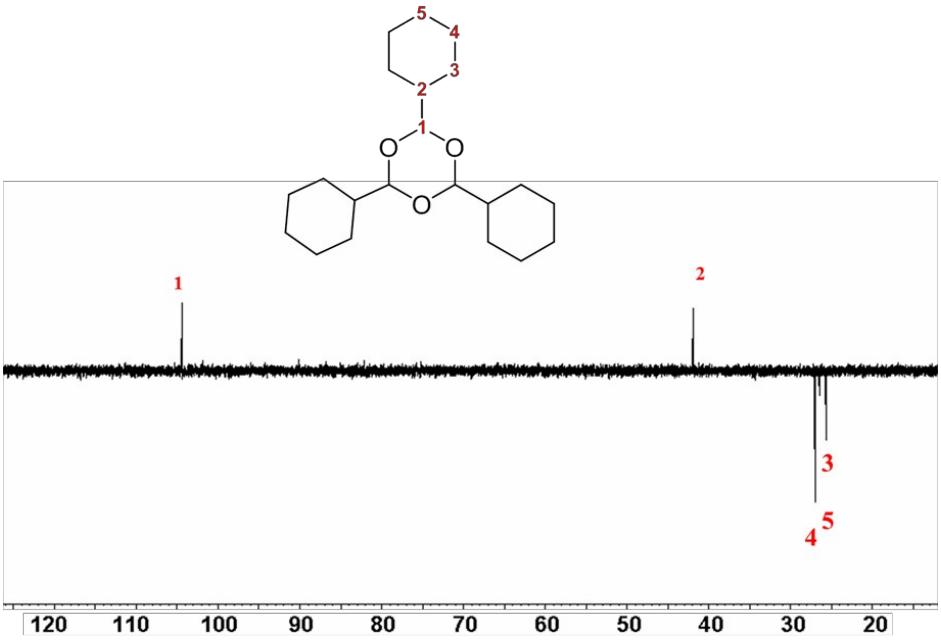


Figure S_{72}: DEPT 135 NMR spectrum of isolated 2,4,6-tricyclohexyl-1,3,5-trioxane **N_6**

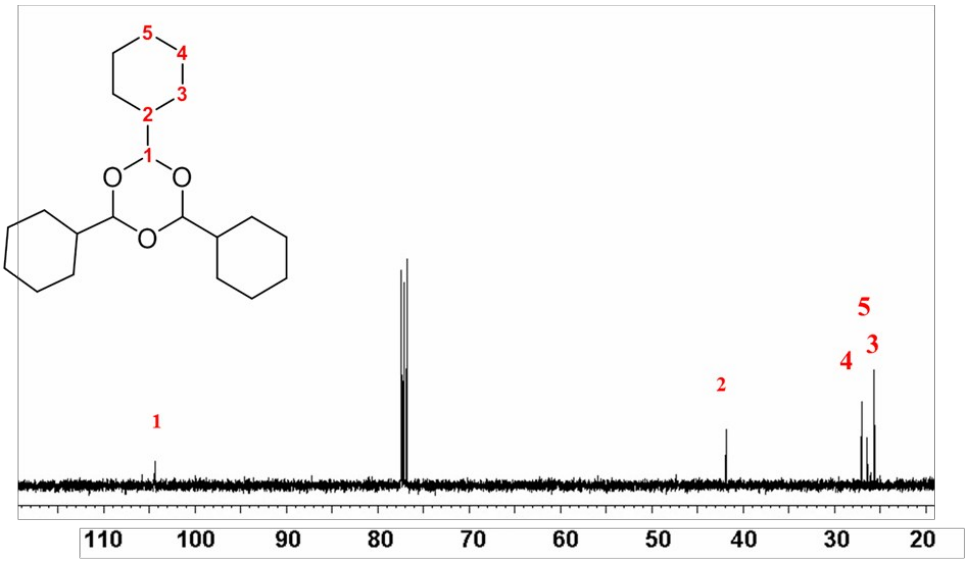


Figure S_{73}: ^{13}C NMR spectrum of isolated 2,4,6-tricyclohexyl-1,3,5-trioxane **N_6**

3.27 NMR spectra of isolated 2,4,6-tris-(diphenylmethyl)-1,3,5-trioxane (N_7) : ^{1}H NMR (400 MHz) ($CDCl_3$): □.4.24-4.25(d, 3H, H_2, J = 4.01 Hz); 5.44-5.45(d, 3H, H_1, J = 4.40 Hz); 7.10-7.28(m, 30H, H_{4-6}). ^{13}C NMR (100.61 MHz) ($CDCl_3$): □ 54.7(C_2, CH); 102.5(C_1, CHO); 126.35, 127.95, 129.57(C_{4-6}, CH); 139.30(C_3, C). Mp. 171°C.

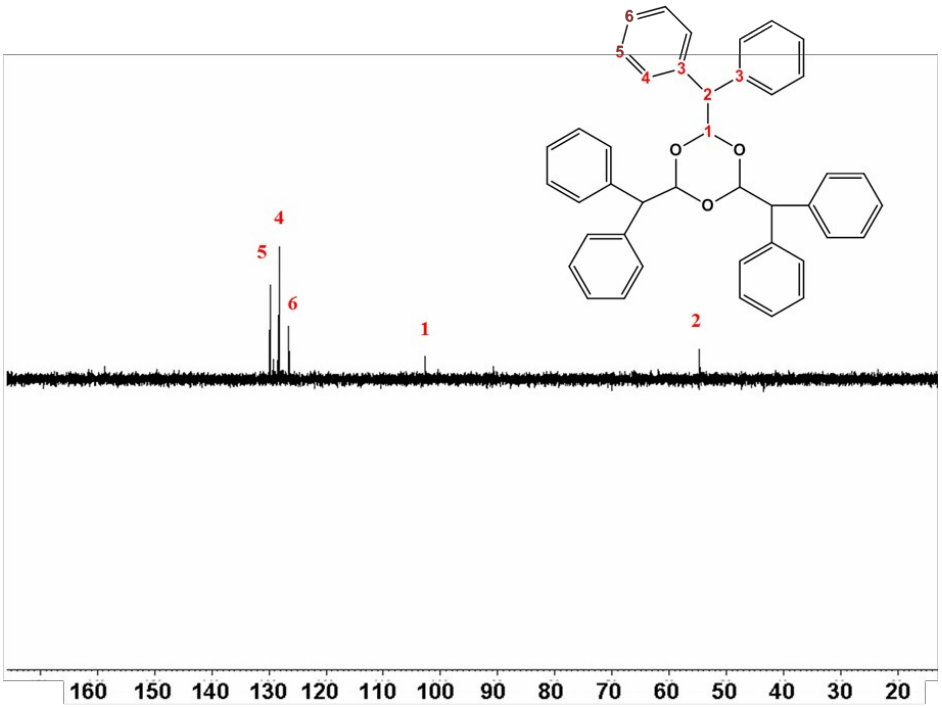


Figure S_{74}: DEPT 135 NMR spectrum of isolated 2,4,6-tris-(diphenylmethyl)-1,3,5-trioxane **N_7**

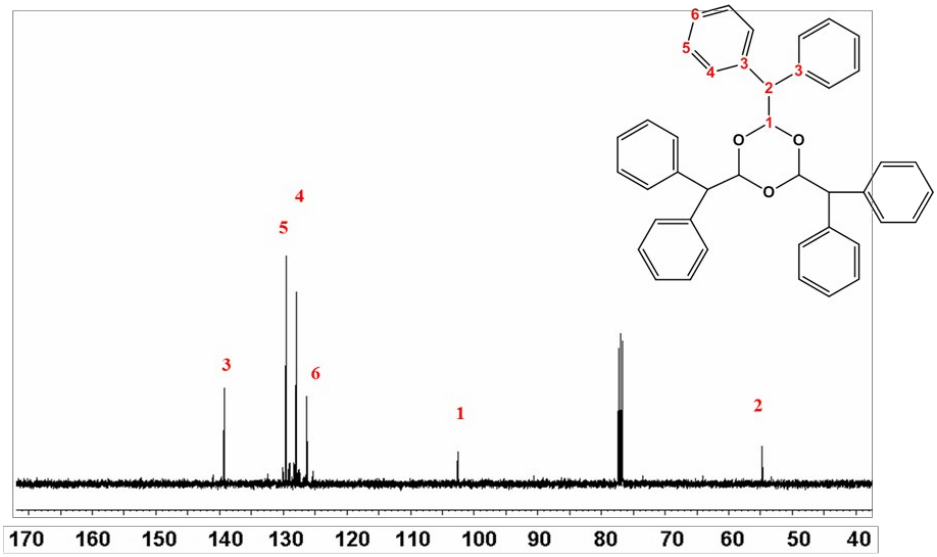


Figure S_{75}: ^{13}C NMR spectrum of isolated 2,4,6-tris-(diphenylmethyl)-1,3,5-trioxane **N_7**

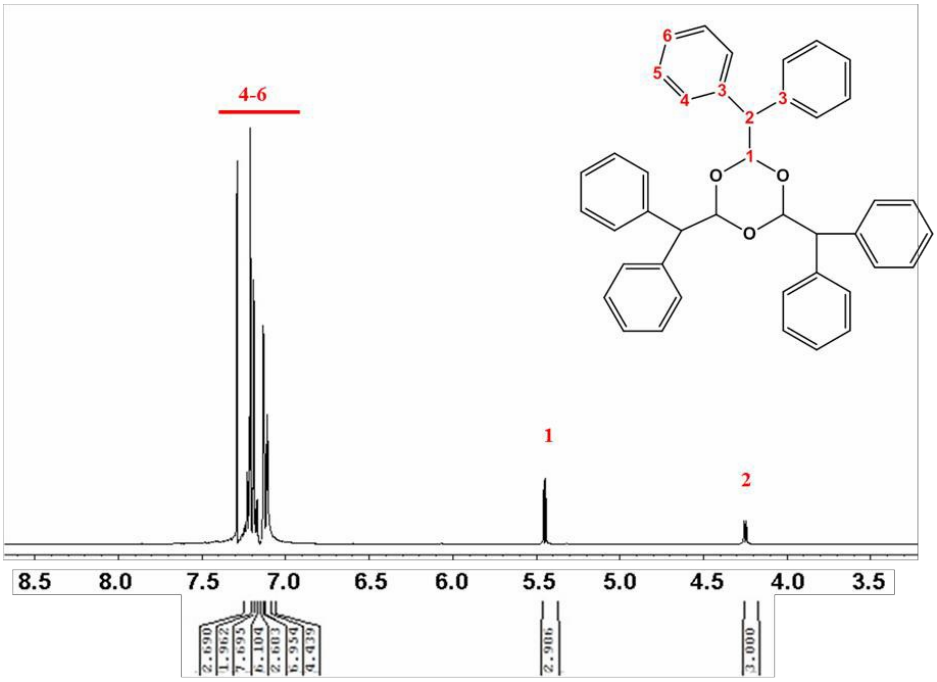


Figure S_{76}:^{1}H NMR spectrum of isolated 2,4,6-tris-(diphenylmethyl)-1,3,5-trioxane **N_7**

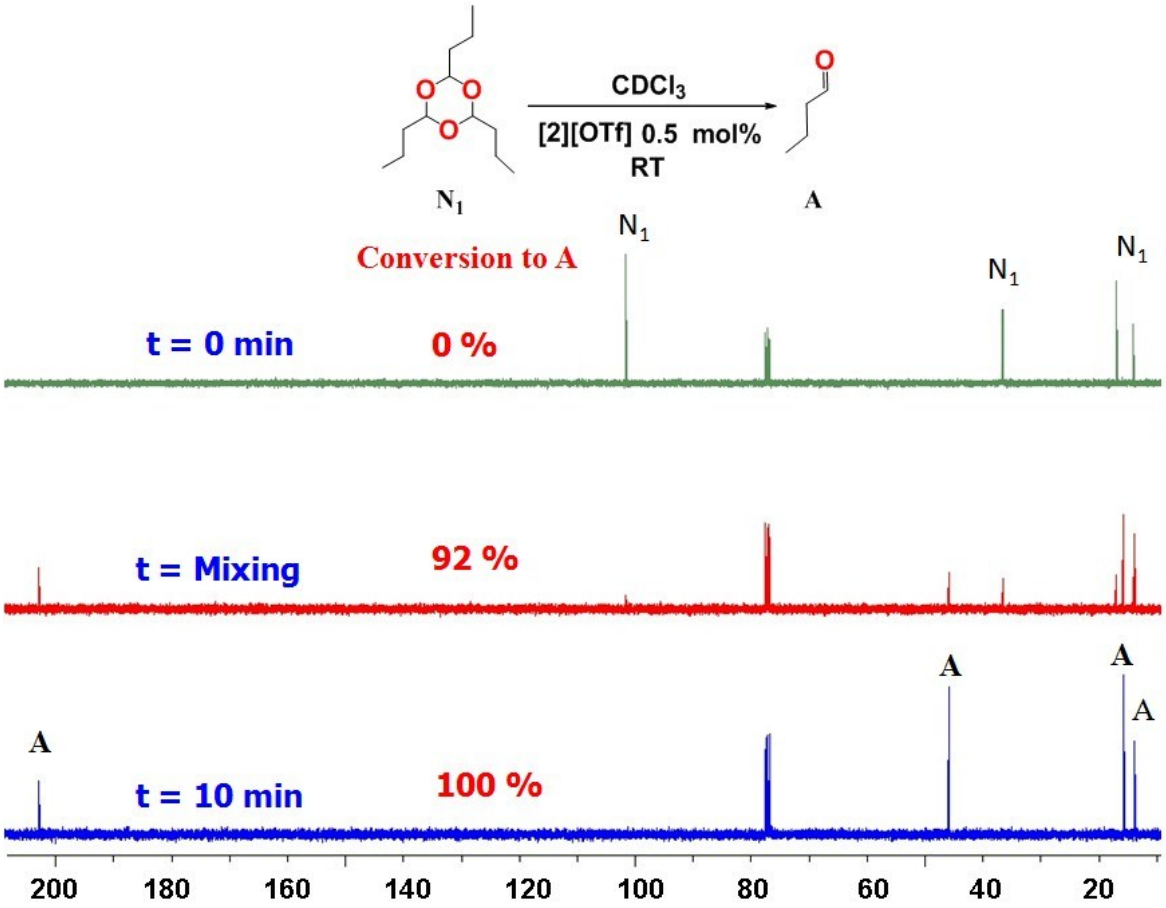
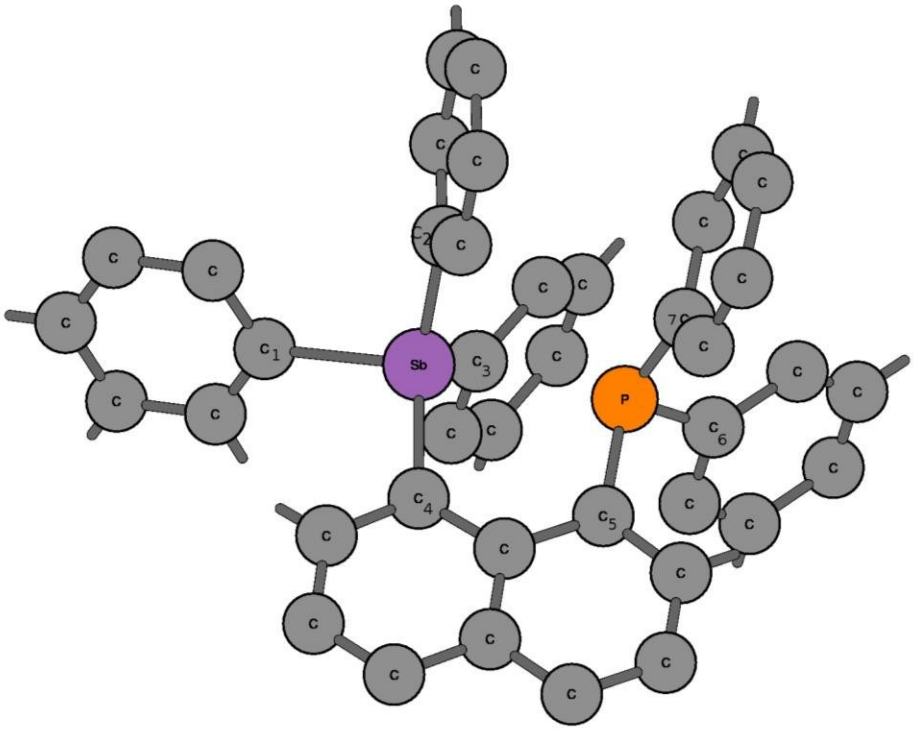


Figure S$_{77}$: ^{13}C NMR spectra showing the conversion of 2,4,6-tripropyl-1,3,5-trioxane (**N$_1$**) into butyraldehyde (**A**) over a period of 10 minutes. Reaction conditions: 0.5 mol% [**2**][OTf] in $CDCl_3$ at room temperature.

4. Computational Details:

All geometries were optimized using the M06[1] density functional method with LANL2DZ basis/pseudopotential for antimony and 6-31G(d,p) basis set for other atoms. Stationary points were characterized as minima by vibrational frequency analysis from the Hessian matrix. Solvent effect was included using the SMD implicit solvent model for dichloromethane. This method was chosen for geometry optimization since, the computed bond parameters of the catalyst [**2**]$^+$ are in good agreement with the experimental values (Figure S$_{78}$). The energies were further refined using M06/6-31+G(2d,2p)[LANL2DZdp] electronic energies. All calculations were performed using Gaussian 09[2]. In the catalytic cycle II dimeric H_2O species was included, in order to correctly model the hydrogen bonding interactions and solvation effects of the hydronium ion and water molecules in the solution. Propanal was used as the model aldehyde in the computational study. The enthalpy energies in the main articles were reported in kcal/mol.

NBO Calculations: A Natural Bond Orbital (NBO) analysis[3] was conducted on the crystal structure geometry of [**2**][OTf] using Density Functional Theory (DFT) methods with the Gaussian 09 program[2] and the following level of theory: B3LYP functional;[4] mixed basis set: Sb, aug-cc-pVTZ-PP;[5] C/N/O/H, 6-31g).[6] The Natural Bond Orbitals were visualized and plotted in Jimp 2 program.[7]



Sb-C1	2.155 (2.157)	Sb-P	2.909 (2.924)
Sb-C2	2.113 (2.109)	P-C5	1.816 (1.810)
Sb-C3	2.127 (2.161)	P-C6	1.826 (1.823)
Sb-C4	2.144 (2.145)	P-C7	1.822 (1.826)

Figure S$_{78}$: M06/6-31G(d,p)[LANL2DZ] optimized structure of the catalyst [**2**]$^{+}$, bond lengths are given in angstroms. Experimental bond lengths from the crystal structure of [**2**][OTf] are shown in the parentheses.

XYZ coordinates and energies (in Hartree) of the optimized structures

[2]$^{+}$

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -1888.29723837

Electronic and Zero-Point Energy = -1887.716163

Enthalpy = -1887.679261

Free Energy = -1887.784344

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -1888.37795432

Sb	2.94006800	2.24775600	14.63566100
P	3.90125900	0.96946300	12.20534400
C	3.54925100	2.23485900	9.74638800
H	4.15665800	1.42382400	9.34573000
C	3.27753100	2.26969300	11.10154500
C	1.43950400	4.56723100	13.48100700
H	1.21968300	4.69897200	14.53843600
C	1.98728500	4.31684200	10.75680800
C	1.89057000	0.42698000	14.85736800
C	2.22683800	3.51398100	13.05892400
C	2.51008700	3.33680500	11.66359900
C	5.62162100	0.90400400	15.23025300
H	5.04370600	-0.01174800	15.09828900
C	2.18601700	-0.69387300	10.66798600
H	1.92898400	0.18214400	10.07583800
C	2.25274500	5.21457400	17.85644500
H	2.65468800	6.18993900	18.12169600

C	5.68307500	0.87111200	11.82053500
C	3.42259400	-1.73530900	12.46234900
H	4.12724900	-1.66618800	13.29230200
C	6.41538400	2.06469000	11.87185800
H	5.90546100	3.01222600	12.05162100
C	3.13244000	-0.60031600	11.69189100
C	0.90429500	5.50146100	12.57134000
H	0.28452100	6.31424200	12.94044700
C	5.01433600	2.15503100	15.09576100
C	1.86951900	-3.03680700	11.15792000
H	1.37722900	-3.98388500	10.94929500
C	0.86541400	0.12440700	13.95877200
H	0.61292900	0.81404000	13.15288700
C	5.76890900	3.32253400	15.22612500
H	5.31197300	4.30248200	15.09473500
C	2.20209800	3.30758700	16.36075100
C	2.71278500	4.56318900	16.71712300
H	3.46113800	5.05245900	16.09390400
C	1.27744000	4.61918800	18.65367600
H	0.91884100	5.12802600	19.54555000
C	6.35060900	-0.33436500	11.59403100
H	5.79604200	-1.26958700	11.54293300
C	2.22257400	-0.46105300	15.88392200
H	3.01365000	-0.21815600	16.59384500
C	1.55726200	-1.90835400	10.40635300
H	0.82103600	-1.97098800	9.60819700
C	1.18560600	5.38063800	11.23846800
H	0.79973400	6.10007700	10.51829000

C	1.52514800	-1.66081300	16.00221400
H	1.77919000	-2.35565800	16.79927300
C	0.17200100	-1.07575200	14.08719400
H	-0.62332100	-1.31718800	13.38539800
C	0.75968800	3.37618000	18.30549500
H	-0.00540800	2.91024500	18.92264300
C	2.80533800	-2.94932300	12.18628700
H	3.04557100	-3.82529000	12.78457200
C	1.21807600	2.72206100	17.16335600
H	0.80084500	1.74927900	16.90579300
C	0.50235000	-1.96506400	15.10707900
H	-0.03938100	-2.90312800	15.20401200
C	7.13105700	3.23386600	15.50614000
H	7.72048000	4.14285600	15.60115400
C	7.73336800	-0.34421300	11.42748000
H	8.24466400	-1.28752500	11.24846500
C	6.98118000	0.82447000	15.51538000
H	7.45365600	-0.14938400	15.62244800
C	7.73380000	1.98848700	15.65553000
H	8.79701800	1.92318700	15.87442400
C	3.05095700	3.21627300	8.87260900
H	3.27704600	3.16320800	7.81101200
C	2.27332000	4.22825100	9.37427600
H	1.86293700	4.99240200	8.71609700
C	7.79384800	2.04892400	11.70203600
H	8.35298800	2.98114700	11.74243500
C	8.45675600	0.84249800	11.48379200
H	9.53654300	0.82946900	11.35551000

Propanal

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -193.020432680

Electronic and Zero-Point Energy = -192.936692

Enthalpy = -192.930608

Free Energy = -192.964361

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -193.034845574

O	4.74167500	4.57146600	14.04909200
C	4.39393600	5.24974000	13.10856200
C	5.30083500	5.77322600	12.03933200
C	5.00931900	7.23033900	11.70897300
H	5.21752800	7.88363300	12.56382700
H	5.62181700	7.57188300	10.86901200
H	3.95720800	7.36941400	11.43116000
H	6.34023700	5.60810000	12.34574800
H	5.11642900	5.15176700	11.14887500
H	3.31953100	5.52922400	12.97280800

H_2O dimer

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -152.792707527

Electronic and Zero-Point Energy = -152.745681

Enthalpy = -152.739249

Free Energy = -152.771493

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -152.823094916

O	3.21608600	5.29435400	0.80799000
H	3.78600600	5.34903400	0.02152000
H	3.18264500	6.19948800	1.13046700
O	4.93777500	5.54688200	-1.44608300
H	5.83284000	5.68804000	-1.11446300
H	4.73391300	6.35232700	-1.93656500

$[H_3O]^+$ $[H_2O]$

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -153.219264095

Electronic and Zero-Point Energy = -153.160669

Enthalpy = -153.155274

Free Energy = -153.185181

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -153.232703357

H	6.74502200	5.95305800	12.09527200
O	3.92389500	5.86746200	11.21600800
H	3.70500200	5.09117700	10.67008300
H	3.46089500	5.77375300	12.06726400
O	6.27191900	6.30710000	11.32149900
H	6.48428200	7.25500700	11.25075900

H	5.09787000	6.07689400	11.30741900

H_2O trimer

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -229.203595934

Electronic and Zero-Point Energy = -229.128859

Enthalpy = -229.121104

Free Energy = -229.157397

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -229.240073268

O	3.12939400	5.42884200	0.79045100
H	3.51769800	5.57943500	-0.09541300
H	3.03265400	6.30988500	1.16904000
O	4.89237200	5.49660800	-1.34959500
H	5.42055100	5.06428400	-0.64803100
H	5.30180300	6.36136500	-1.46599300
O	5.69287700	4.39886700	1.06790900
H	6.23592600	5.00102900	1.58879100
H	4.77146400	4.67219300	1.25237200

Et_3SiH

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -527.570727172

Electronic and Zero-Point Energy = -527.365502

Enthalpy = -527.353584

Free Energy = -527.401174

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -527.585727520

Si	0.13858500	-0.53856000	-0.06353600
C	1.75872200	0.14574500	0.62091200
H	1.57472100	1.17157000	0.97461600
H	2.03894000	-0.43178800	1.51439500
C	-1.15802000	-0.66427700	1.30293400
H	-2.07854300	-1.09457500	0.88198800
H	-0.80680600	-1.38896500	2.05189400
C	-0.47927900	0.55192800	-1.47777200
H	0.27025000	0.52524900	-2.28232000
H	-0.50583900	1.59723100	-1.13385100
C	-1.84309800	0.12963100	-2.01632500
H	-2.14714300	0.72126900	-2.88922500
H	-1.84499200	-0.92488800	-2.32457200
H	-2.63041400	0.24352100	-1.25965000
C	-1.45505700	0.67724500	1.96844500
H	-2.23182400	0.59441700	2.73918200
H	-0.56244900	1.09175900	2.45523300
H	-1.80180200	1.42423000	1.24148400
C	2.89541600	0.13860500	-0.39751400
H	3.83535800	0.51674400	0.02424300
H	3.09252800	-0.87424400	-0.77319100
H	2.65958500	0.76421900	-1.26837500

H	0.39092100	-1.90846500	-0.61835700

α,β-unsaturated aldehyde

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -309.647996428

Electronic and Zero-Point Energy = -309.502140

Enthalpy = -309.492719

Free Energy = -309.535225

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -309.665935453

O	4.03740400	4.12646000	14.47073000
C	5.02359300	4.79476800	14.71932300
C	6.73328100	6.66003600	14.41590000
H	7.48221800	6.76539200	13.62174200
H	6.51134700	7.66802700	14.78871500
H	7.20639000	6.10946500	15.23773400
H	5.65582600	4.55155100	15.60650700
C	5.50146300	5.95104900	13.93581300
C	5.12493500	7.39731500	11.89502400
H	4.20970800	7.96994500	11.68838600
H	5.84580900	8.09635200	12.33683900
C	5.67389000	6.84536600	10.57917400
H	4.96598200	6.14662400	10.11733100
H	5.86774500	7.65182600	9.86367600
H	6.61370300	6.30442100	10.74464600

C	4.80379000	6.29210600	12.83732500
H	3.93758900	5.67221100	12.59165800

Dipropyl ether

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -312.066743839

Electronic and Zero-Point Energy = -311.873147

Enthalpy = -311.863366

Free Energy = -311.906287

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -312.081243847

C	4.75489200	6.85693000	11.16923900
C	4.87464800	6.82162200	9.65581000
C	5.57419700	8.04908400	9.09899500
H	6.57388800	8.16357000	9.53472500
H	5.68452400	7.99783500	8.01000200
H	5.00981200	8.96125300	9.33438100
H	5.40177600	5.90567400	9.34889000
H	3.85995200	6.73996800	9.24032900
H	4.20542200	7.76096500	11.47107500
C	7.94438300	5.72347700	10.98973000
O	5.99399400	6.91858000	11.84341400
H	7.63358600	5.83496100	9.94112000
H	8.54263200	6.61249100	11.23525700
C	8.77036800	4.46019900	11.16228800

H	9.65731000	4.46220900	10.51968600
H	9.11403600	4.34805900	12.19893000
H	8.18438900	3.56565600	10.91312800
C	6.72036600	5.70730700	11.88557100
H	6.07081100	4.85293300	11.62405200
H	7.04144700	5.54656100	12.92824200
H	4.17134200	5.98980000	11.52545800

$(Et_3Si)_2O$

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -1129.25492888

Electronic and Zero-Point Energy = -1128.853783

Enthalpy = -1128.830264

Free Energy = -1128.902745

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -1129.28987322

O	-0.75268900	2.69921100	0.68001300
Si	0.26909500	3.35088400	-0.45535200
C	1.47170600	1.99224900	-0.94683300
H	2.15643800	2.39916500	-1.70695800
H	2.10109700	1.74418100	-0.07890900
C	1.18551800	4.80731200	0.30604900
H	0.45165600	5.57581100	0.59198000
H	1.64591700	4.47165900	1.24769700
C	-0.69154700	3.90243000	-1.98264000

H	-1.37395900	3.08749300	-2.27002600
H	0.02942400	3.98309300	-2.81206400
C	-1.46574100	5.20859500	-1.83466000
H	-2.00832100	5.47587800	-2.75042300
H	-2.21181400	5.15210400	-1.02952400
H	-0.80122900	6.04966100	-1.59665900
C	2.24199900	5.39960500	-0.62355200
H	2.73218000	6.28098100	-0.19118400
H	3.03174300	4.67101500	-0.84869300
H	1.80788400	5.71068900	-1.58406100
C	0.78006400	0.73945300	-1.47888300
H	1.49503300	-0.04409300	-1.76012200
H	0.10203600	0.30833600	-0.73088100
H	0.17798000	0.96089400	-2.37077200
Si	-2.17453700	2.98380600	1.49210000
C	-3.62789100	2.65673500	0.34069100
C	-2.20889800	4.75888500	2.12015100
C	-2.20846000	1.77274700	2.92997500
H	-4.55770200	2.83277800	0.90367100
H	-3.62339100	3.40814100	-0.46445000
C	-3.62889200	1.24592600	-0.24270400
H	-1.28567800	4.94639000	2.69001800
H	-2.17409500	5.44352700	1.25867700
C	-3.43415300	5.06532600	2.97890400
H	-2.04018200	0.76636300	2.51786900
H	-3.22108700	1.75214800	3.36165900
C	-1.16967500	2.08046700	4.00507900
H	-4.45891400	1.08312300	-0.94174600

H	-2.69907900	1.03283500	-0.78810600
H	-3.71831300	0.48668500	0.54550300
H	-3.43401200	6.09834800	3.34854300
H	-4.36651900	4.92598400	2.41581700
H	-3.48788100	4.40801100	3.85724300
H	-1.14247300	1.31561400	4.79138100
H	-0.15988800	2.14326400	3.57726800
H	-1.36984700	3.04207100	4.49594000

1,3,5-trioxane

M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -579.113288967

Electronic and Zero-Point Energy = -578.846651

Enthalpy = -578.832508

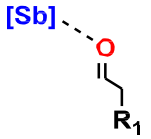
Free Energy = -578.886122

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -579.138932256

O	-0.11259200	2.15372700	-0.56265800
O	1.69751300	1.12745800	0.45298400
O	-0.28279600	-0.02710300	0.18002900
C	-0.87553700	1.26045300	0.20739000
H	-0.89111100	1.61754500	1.25596000
C	1.15764200	2.36048800	0.00377000
H	1.06281500	2.99203400	0.90862600
C	1.08781900	0.01833500	-0.15844700

H	1.18113300	0.10087600	-1.25766000
C	2.04241000	3.02027100	-1.02538400
H	3.04408500	3.10296800	-0.58473100
H	2.12370400	2.34458200	-1.88899700
C	1.52352500	4.38314200	-1.44725300
H	1.41088500	5.04758500	-0.58069800
H	2.20901600	4.86814400	-2.14984200
H	0.54530500	4.30176400	-1.93333400
C	-2.27206800	1.17971900	-0.35763500
H	-2.83406600	0.47180300	0.26536600
H	-2.74443300	2.16259100	-0.22879900
C	-2.29661700	0.74892600	-1.81373500
H	-3.32453600	0.65738000	-2.18008000
H	-1.77632600	1.47244600	-2.45064800
H	-1.80600600	-0.22318300	-1.93999600
C	1.75400200	-1.24451900	0.32989400
H	1.25658600	-2.08572100	-0.17034500
H	2.79159700	-1.23041800	-0.02766900
C	1.70378900	-1.41170700	1.83809000
H	0.66854000	-1.41841200	2.19590100
H	2.17317000	-2.35281500	2.14380200
H	2.22783900	-0.59407600	2.34478000



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2081.33557889

Electronic and Zero-Point Energy = -2080.668098

Enthalpy = -2080.625121

Free Energy = -2080.743313

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

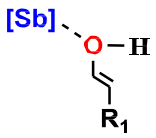
Electronic Energy = -2081.42533835

Sb	3.03245400	2.24723700	14.71963600
P	4.07652600	1.22934600	12.26099800
C	3.86130000	2.79451200	9.95034800
H	4.66820900	2.18338100	9.54694800
C	3.43110900	2.58397100	11.24441400
O	4.68978300	4.34639100	13.87428100
C	0.86933400	4.02856600	13.59075800
H	0.55001700	3.98160800	14.63134400
C	1.71558800	4.30213200	10.93906200
C	1.92516600	0.45481200	14.99394400
C	1.95488100	3.29633500	13.16174400
C	2.37480700	3.36838400	11.79979900
C	5.54359500	0.54148700	15.26077700
H	5.01082100	-0.20789700	14.67456100
C	2.19227700	-0.18435600	10.70146000
H	1.96397000	0.76191800	10.21392700
C	2.25482800	5.57833900	17.55006600
H	2.45873100	6.64656400	17.58352900
C	5.83730300	1.07478400	11.83224000
C	3.47877400	-1.48310300	12.28279600

H	4.26481100	-1.55621600	13.03507200
C	6.72137500	2.00765400	12.39197300
H	6.34466500	2.78655400	13.05741500
C	3.20557400	-0.25613100	11.66188600
C	0.16723600	4.88195600	12.70961700
H	-0.69359900	5.43676200	13.07405700
C	4.98549400	1.79877700	15.48925200
C	1.74402400	-2.53881400	10.98346500
H	1.17194500	-3.42606700	10.72204300
C	0.81073500	0.19816100	14.18979300
H	0.50245600	0.91145800	13.42489600
C	5.68363700	2.74866400	16.23507200
H	5.25619500	3.73288300	16.41944100
C	2.38213300	3.46052500	16.38022600
C	2.63712200	4.83579400	16.43655200
H	3.14245100	5.33439300	15.61020200
C	1.61511800	4.95479000	18.61881000
H	1.31692900	5.53607300	19.48860400
C	6.32620700	0.07339900	10.98923200
H	5.64563800	-0.65236600	10.54740400
C	2.30634700	-0.47435400	15.96836000
H	3.17057700	-0.28259200	16.60465300
C	1.46592900	-1.32393100	10.36589800
H	0.68025900	-1.25814800	9.61672300
C	0.60663300	5.03994000	11.42208000
H	0.11227600	5.73276600	10.74325500
C	1.58139400	-1.65226100	16.12870900
H	1.88218500	-2.37153400	16.88712800

C	0.09032900	-0.98240900	14.35306300
H	-0.77131100	-1.18196100	13.71973400
C	1.35938700	3.58829700	18.57289800
H	0.85764800	3.09727700	19.40411500
C	2.75610400	-2.61820800	11.93869100
H	2.97575500	-3.56542600	12.42578400
C	1.74156600	2.84288700	17.45853200
H	1.52776100	1.77427600	17.43860400
C	0.47759800	-1.90762500	15.31899700
H	-0.08337800	-2.83122700	15.44273400
C	6.94922900	2.44317200	16.72924600
H	7.49954800	3.19076100	17.29626500
C	7.68853900	0.00653400	10.70955400
H	8.06480800	-0.77280000	10.05089400
C	6.80091300	0.23310100	15.77408600
H	7.23046800	-0.75057400	15.59836600
C	7.50744000	1.18834700	16.49891500
H	8.49569700	0.95359100	16.88761100
C	3.24654900	3.76237700	9.13218600
H	3.59996000	3.91256000	8.11538700
C	2.17947200	4.47975200	9.61303400
H	1.66542600	5.20217000	8.98090000
C	8.07896500	1.93598200	12.10495200
H	8.76197400	2.66035300	12.54283200
C	8.56401400	0.93374100	11.26672200
H	9.62780700	0.87569400	11.04814600
C	4.39873400	5.26024700	13.11715200
C	5.31141000	5.79864600	12.07287200

C	4.99306500	7.23015800	11.68001400
H	5.14262400	7.91907700	12.51859000
H	5.63277600	7.56079100	10.85689100
H	3.95085200	7.32326300	11.34936500
H	6.34952400	5.65435800	12.39764100
H	5.16571500	5.12587000	11.20751500
H	3.38403100	5.71999200	13.16306900



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2081.31418061

Electronic and Zero-Point Energy = -2080.646353

Enthalpy = -2080.603107

Free Energy = -2080.721963

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

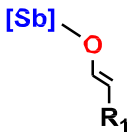
Electronic Energy = -2081.40461875

Sb	2.83517400	2.59874500	14.34971000
P	3.95084500	1.30294700	12.03465400
C	2.50791400	1.41699500	9.64506700
H	3.13062100	0.58124600	9.32630100
C	2.64257800	1.91078300	10.92791000
O	4.40726900	4.86093300	13.80724900
C	1.18589100	4.72919000	12.97089500

H	1.22728800	5.16359100	13.96871100
C	0.98455600	3.63368900	10.40804000
C	1.66805000	0.82420100	14.49264500
C	1.91673100	3.59824600	12.67371100
C	1.86759200	3.03108200	11.36188000
C	5.91106100	2.06302200	14.68978900
H	5.99464200	2.28333300	13.62773600
C	2.70281600	-1.21804200	11.74226100
H	1.88756000	-0.70654000	11.23453400
C	2.08882500	5.57002500	17.55541500
H	2.64815600	6.37680900	18.02438800
C	5.47415900	1.67300800	11.08941200
C	4.86179000	-1.17551200	12.82929500
H	5.73983400	-0.62511200	13.16980600
C	5.92910700	2.99718300	11.09921600
H	5.40387000	3.74938500	11.68939200
C	3.83272400	-0.50613200	12.15185800
C	0.35685200	5.34259200	12.00660500
H	-0.20195200	6.23661400	12.27138700
C	4.67970000	2.14546400	15.33796600
C	3.63862600	-3.24602600	12.65756600
H	3.56193900	-4.31277200	12.85485300
C	0.38104500	0.79157900	13.94440000
H	-0.02630900	1.66651300	13.43578200
C	4.59460400	1.88861100	16.70939400
H	3.63928600	1.95111100	17.23055200
C	1.96674200	3.78006300	15.92927600
C	2.67476500	4.82141600	16.53835200

H	3.69070700	5.05300500	16.22271500
C	0.79056800	5.28636200	17.97203400
H	0.33369500	5.87117800	18.76730900
C	6.16161100	0.71460600	10.34046600
H	5.81997200	-0.31867900	10.32203200
C	2.17801400	-0.30751900	15.13521400
H	3.18388900	-0.30014200	15.55487400
C	2.60775400	-2.58300400	11.99896100
H	1.72045600	-3.12796100	11.68432700
C	0.24389500	4.78893700	10.76015100
H	-0.41420700	5.22699000	10.01149400
C	1.40495300	-1.46135100	15.22852400
H	1.81064400	-2.34380000	15.71897000
C	-0.39234300	-0.36175600	14.05090700
H	-1.39491400	-0.38062500	13.62958600
C	0.07878800	4.25182000	17.37180500
H	-0.93477700	4.02473700	17.69545400
C	4.76741100	-2.54072700	13.07039700
H	5.57446500	-3.05380200	13.58818100
C	0.66344600	3.50184600	16.35403000
H	0.09322800	2.69369600	15.89529300
C	0.12026700	-1.48726800	14.69090100
H	-0.48195000	-2.38984400	14.76709300
C	5.74021900	1.53564800	17.42018200
H	5.66819500	1.32369900	18.48447800
C	7.29126100	1.08139100	9.61345700
H	7.82281000	0.33037100	9.03359000
C	7.05517600	1.72480900	15.40772600

H	8.01488600	1.67551200	14.89828100
C	6.96908200	1.45696700	16.77106200
H	7.86225500	1.18871100	17.33066600
C	1.59802800	1.98407200	8.73576900
H	1.50109700	1.56808100	7.73638500
C	0.86343800	3.08033000	9.11177900
H	0.17595300	3.55450800	8.41344400
C	7.05461400	3.35898500	10.36904100
H	7.39971600	4.39066500	10.38531300
C	7.73854800	2.39917100	9.62643500
H	8.62240100	2.67836100	9.05767500
C	5.69937700	5.23476900	14.08949400
C	6.46979000	5.98906500	13.30926500
C	7.86844600	6.36221000	13.66760200
H	8.58631900	5.99506500	12.92216300
H	7.99870800	7.45072000	13.71870200
H	8.15361600	5.94349400	14.63966600
H	6.03087800	4.82706200	15.04413700
H	6.06484100	6.35494500	12.36143100
H	4.09638700	5.31786500	13.00825700



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2080.85584100

Electronic and Zero-Point Energy = -2080.201512

Enthalpy = -2080.158702

Free Energy = -2080.277223

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

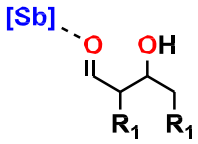
Electronic Energy = -2080.95108429

Sb	3.07620800	2.63345400	14.36930800
P	3.96647800	1.33895500	12.00273200
C	3.11041700	2.19633000	9.49489400
H	3.92322600	1.58496700	9.10309800
C	2.92476500	2.29276800	10.85994200
O	4.25214100	4.17339900	13.48688800
C	0.58565900	4.03016800	13.21969500
H	0.40894700	4.18599900	14.28372000
C	0.98427500	3.72978000	10.47490900
C	1.96985300	0.79135400	14.81038900
C	1.67899300	3.30272200	12.80042800
C	1.87690000	3.09966600	11.40210300
C	5.93933700	1.33263000	14.86681700
H	5.95099600	1.15605000	13.79217500
C	2.54400300	-0.85415000	10.87004500
H	2.12805900	-0.15887300	10.14320600
C	1.98578900	6.13430500	16.85773800
H	2.17221700	7.20572400	16.81531400
C	5.63346200	1.44021000	11.26233800
C	3.95576200	-1.30923500	12.77652100
H	4.64416400	-0.96058400	13.54784800
C	6.28529200	2.67770200	11.33471900

H	5.78377000	3.52012900	11.81004400
C	3.44789400	-0.40370500	11.83534400
C	-0.32408800	4.60960100	12.30591700
H	-1.17454300	5.17444100	12.68171000
C	4.86075500	1.98134100	15.47018400
C	2.68128700	-3.08993000	11.76991100
H	2.38021100	-4.13481200	11.74538700
C	0.87163300	0.41728200	14.02872800
H	0.52241400	1.06722900	13.22549200
C	4.90951600	2.20426100	16.85049900
H	4.08761000	2.71349400	17.35352700
C	2.28641700	3.91977300	15.91552700
C	2.51866200	5.29941300	15.87837300
H	3.10737200	5.72917100	15.06833900
C	1.21267800	5.60066200	17.88597100
H	0.79585600	6.25383200	18.64988300
C	6.27507000	0.35166500	10.66721300
H	5.77673400	-0.61456900	10.60446600
C	2.38728400	-0.08031000	15.82324200
H	3.24397000	0.17600400	16.44668800
C	2.16409500	-2.19348700	10.83987900
H	1.45890200	-2.53616900	10.08588800
C	-0.11412900	4.48090800	10.95961100
H	-0.78526600	4.94437900	10.23789100
C	1.72837800	-1.28735600	16.04834000
H	2.06805800	-1.94858300	16.84365000
C	0.21875300	-0.79563500	14.24025000
H	-0.62665100	-1.07188500	13.61243600

C	0.97132900	4.23053200	17.93134700
H	0.36489700	3.80855000	18.73054900
C	3.57990600	-2.64655800	12.73837400
H	3.98162900	-3.34215700	13.47190700
C	1.50308600	3.39619500	16.94915300
H	1.30350200	2.32495200	16.99548300
C	0.64601900	-1.65084600	15.25151100
H	0.13803600	-2.59880200	15.41744800
C	5.99927500	1.77546400	17.60746500
H	6.01382900	1.95541500	18.68082500
C	7.55707300	0.50546800	10.14322500
H	8.05139900	-0.34270100	9.67450200
C	7.03333800	0.90649800	15.61850600
H	7.86468400	0.40704000	15.12452300
C	7.06450300	1.12503100	16.99238500
H	7.91786800	0.79442700	17.58077800
C	2.25098200	2.85669300	8.59672800
H	2.41461400	2.76498200	7.52581400
C	1.20064300	3.59315900	9.08316600
H	0.50897600	4.08918700	8.40337800
C	7.56368800	2.82294000	10.81252000
H	8.06366000	3.78767300	10.87945200
C	8.20217400	1.73641100	10.21617500
H	9.20467900	1.84957500	9.80929700
C	5.32551600	4.73086400	14.05123500
C	6.10353500	5.64961800	13.45414400
C	7.30053400	6.25608500	14.10979400
H	8.22691000	6.05981800	13.54977800

H	7.22415900	7.34926600	14.20152000
H	7.44111200	5.85248700	15.12108300
H	5.85056900	5.96385700	12.43837400
H	5.58030000	4.41022500	15.07357400



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2274.37564016

Electronic and Zero-Point Energy = -2273.617588

Enthalpy = -2273.569976

Free Energy = -2273.697249

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

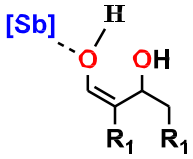
Electronic Energy = -2274.47567544

Sb	2.82713100	2.39347800	14.41565600
P	3.88940300	1.37962700	11.99240000
C	2.88092500	2.14023700	9.51804700
H	3.68485600	1.53482400	9.10064400
C	2.75229500	2.25167100	10.89007000
O	4.34170600	4.29190700	13.50861800
C	0.49457000	4.01582000	13.32335700
H	0.34623000	4.17062000	14.39007700
C	0.80733200	3.69561000	10.56850700

C	1.76836400	0.57521500	14.78047500
C	1.55499400	3.26210900	12.86750100
C	1.72455500	3.05814100	11.46631600
C	5.87488900	1.56075500	14.74536200
H	5.87520600	1.39447400	13.67079200
C	2.65216600	-0.93365100	10.91488100
H	2.18887400	-0.28665500	10.17288300
C	1.88618500	5.84004300	17.06149800
H	2.12448600	6.90157600	17.08031200
C	5.52772200	1.65187000	11.22969400
C	4.08727300	-1.24427500	12.83642600
H	4.75086700	-0.83396800	13.59867800
C	5.91925400	2.97016700	10.96074000
H	5.23496900	3.79426300	11.16406800
C	3.51962600	-0.40062200	11.87158000
C	-0.42496500	4.61531300	12.43420800
H	-1.25019100	5.19951500	12.83391600
C	4.72032100	1.97443000	15.40932600
C	2.94222200	-3.13107300	11.87050700
H	2.71240700	-4.19398400	11.87126700
C	0.67202200	0.23080900	13.98446800
H	0.36418800	0.87343700	13.15934400
C	4.77299500	2.18923200	16.79020600
H	3.89196300	2.52064700	17.33733700
C	2.08248200	3.67366300	15.99455200
C	2.38134000	5.04089600	16.03435600
H	2.98481800	5.50542700	15.25452800
C	1.08564600	5.28510000	18.05687000

H	0.69874600	5.91172000	18.85744400
C	6.41083500	0.60212600	10.96721700
H	6.11972400	-0.42694100	11.17055600
C	2.15673600	-0.27419200	15.82140700
H	3.01564600	-0.02577200	16.44542200
C	2.36841300	-2.29636700	10.91636400
H	1.69029200	-2.70450300	10.17054700
C	-0.25963200	4.47022900	11.08403800
H	-0.94550300	4.93872700	10.38019100
C	1.44453600	-1.44403400	16.07354400
H	1.74775700	-2.09570600	16.89014300
C	-0.03458800	-0.94311600	14.23447600
H	-0.88674500	-1.20539000	13.61111400
C	0.77832000	3.92876100	18.02235700
H	0.14939600	3.49059700	18.79456600
C	3.80506200	-2.60486500	12.82902400
H	4.24859200	-3.25229800	13.58172000
C	1.27310400	3.12647100	16.99485900
H	1.02221500	2.06556000	16.98231000
C	0.34948400	-1.77790100	15.28033300
H	-0.20433600	-2.69326400	15.47715500
C	5.96247800	1.98868600	17.48965000
H	5.98660600	2.15684800	18.56409300
C	7.67022600	0.86940600	10.43487600
H	8.34921700	0.04614900	10.22567100
C	7.06609800	1.37219900	15.44278900
H	7.95869100	1.06001100	14.90478500
C	7.11240700	1.58994200	16.81646300

H	8.04332200	1.44809500	17.36062300
C	1.98432600	2.78703300	8.64938000
H	2.10048000	2.67917500	7.57421300
C	0.96388100	3.54103200	9.17157800
H	0.24885600	4.03749100	8.51723800
C	7.17640700	3.22839700	10.42755400
H	7.46891800	4.25461700	10.21158500
C	8.05518900	2.17853800	10.16590300
H	9.03862300	2.38227600	9.74889400
C	5.27908000	4.76458200	14.13941200
C	7.39420800	6.01189800	14.51703800
H	8.21630300	6.55177600	14.03669600
H	7.00966000	6.62993400	15.33619900
H	7.81029700	5.09357600	14.95002100
H	5.40442100	4.51967200	15.21707500
C	6.28946200	5.68303800	13.52789000
H	6.69392500	5.14532500	12.65446400
C	6.39287800	7.95339100	12.35166700
H	5.73612300	8.78086900	12.04361200
H	7.08106800	8.36948800	13.10070800
C	7.15316700	7.42305000	11.14806300
H	6.47582000	6.92164000	10.44246900
H	7.65507600	8.23079500	10.60551300
H	7.92434400	6.69944300	11.44278300
C	5.51706800	6.90237900	13.00624200
H	4.79665500	6.52802200	12.25511300
O	4.82537500	7.41633600	14.13448700
H	4.30615900	8.17918000	13.84794600



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2274.36068235

Electronic and Zero-Point Energy = -2273.602076

Enthalpy = -2273.554386

Free Energy = -2273.681130

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

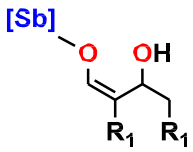
Electronic Energy = -2274.46468134

Sb	3.03335700	2.28372400	14.57605300
P	4.18551300	1.26152600	12.16054100
C	3.88587800	2.68482200	9.77427600
H	4.72964200	2.10248300	9.40551800
C	3.47817800	2.53581800	11.08386100
O	4.51160400	4.41947300	13.65514900
C	0.82621300	3.95109500	13.34664000
H	0.50069100	3.93754000	14.38554700
C	1.65022400	4.11265000	10.67902200
C	2.00756100	0.44474100	14.84737700
C	1.95381800	3.25642100	12.95956400
C	2.37268500	3.28188000	11.59469300
C	5.73229300	0.86181400	15.16647500
H	5.39111800	0.13868100	14.42629700

C	2.38470400	-0.30499800	10.63396200
H	2.15049600	0.59539000	10.06872100
C	1.95716600	5.65873300	17.25758800
H	2.08633700	6.73894700	17.25664700
C	5.94191900	1.14693900	11.69611200
C	3.62627600	-1.45119200	12.35977700
H	4.36866100	-1.44696100	13.15731800
C	6.77212200	2.22527200	12.02994700
H	6.35655400	3.09248600	12.54384800
C	3.35827300	-0.28011200	11.63765300
C	0.08105800	4.71538300	12.42228700
H	-0.80784100	5.24306000	12.75847400
C	4.96479400	1.98445500	15.47633100
C	1.97591000	-2.64399100	11.07080500
H	1.43482000	-3.56178900	10.85235100
C	0.93040800	0.12706900	14.01463100
H	0.59222600	0.82902400	13.25203700
C	5.41802200	2.88705500	16.44165100
H	4.82578200	3.75989800	16.71356200
C	2.25405500	3.51727600	16.16453400
C	2.41068400	4.90875500	16.17624700
H	2.89372200	5.42017700	15.34325000
C	1.34266700	5.02771100	18.33692500
H	0.98845800	5.61564400	19.18077000
C	6.48029800	0.03202300	11.04988500
H	5.84463000	-0.81113300	10.78571100
C	2.43347300	-0.47316600	15.81354200
H	3.27301900	-0.23698900	16.46800900

C	1.69764300	-1.48382800	10.35568100
H	0.94208300	-1.49222300	9.57340400
C	0.50490100	4.81614900	11.12353700
H	-0.03219100	5.43427300	10.40607300
C	1.78641500	-1.69997800	15.93978100
H	2.11941400	-2.40989500	16.69363200
C	0.29470200	-1.10526900	14.13786900
H	-0.53497800	-1.35333100	13.47942300
C	1.18484700	3.64574800	18.33498900
H	0.70293400	3.14899600	19.17444600
C	2.94409100	-2.62648500	12.07288100
H	3.16192500	-3.52795400	12.64104600
C	1.64088100	2.89242100	17.25407900
H	1.50702400	1.81057500	17.26901800
C	0.72223700	-2.01722700	15.09964400
H	0.22471300	-2.97982700	15.19491600
C	6.64415800	2.67678700	17.06925200
H	6.99742700	3.38979000	17.81087300
C	7.83715500	-0.00004500	10.73708300
H	8.25177500	-0.86955700	10.23230600
C	6.94946300	0.64599200	15.80750900
H	7.53745500	-0.23605300	15.56401500
C	7.40943800	1.55807200	16.75281100
H	8.36449300	1.39451000	17.24695300
C	3.19656900	3.54227200	8.89474800
H	3.52952100	3.63944700	7.86473300
C	2.08721600	4.21875200	9.33599200
H	1.51834400	4.85486500	8.65976100

C	8.12256000	2.18974300	11.70704800
H	8.76037300	3.03205500	11.96454500
C	8.65731100	1.07508100	11.06331400
H	9.71595700	1.04624900	10.81628800
C	5.43582600	5.33664700	14.10406900
C	6.51296600	7.52175100	14.38336500
H	7.00076400	8.08315200	13.57487100
H	6.12454400	8.26369200	15.09049100
H	7.28088900	6.92905800	14.89194500
H	6.21170400	4.85549400	14.69669900
C	5.41810700	6.64868100	13.85641500
C	4.80964600	7.53685500	11.57861100
H	4.05615400	8.16865800	11.08397400
H	5.74421400	8.11522800	11.59350600
C	4.97770700	6.24638500	10.79781200
H	4.03520200	5.68028900	10.77154300
H	5.26442900	6.44124900	9.75899600
H	5.74781400	5.59731100	11.23568400
C	4.35010500	7.30603900	13.01848600
H	3.44906800	6.65140200	12.97122200
O	4.01336700	8.52127400	13.65539800
H	3.40487100	8.99625600	13.07482800
H	3.90626200	4.84586400	13.02613000



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2273.90335217

Electronic and Zero-Point Energy = -2273.159200

Enthalpy = -2273.111456

Free Energy = -2273.239915

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

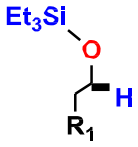
Electronic Energy = -2274.01235987

Sb	3.16122600	2.53060400	14.44830300
P	4.10955500	1.39694100	12.04359300
C	3.54795600	2.64544100	9.60873700
H	4.40111100	2.09463300	9.21343800
C	3.22751200	2.54350100	10.94703300
O	4.30209300	4.10506400	13.59061300
C	0.63790300	3.88594500	13.29573900
H	0.36927400	3.88715600	14.35247100
C	1.29706700	4.00129400	10.58383000
C	2.09144500	0.66810200	14.84926800
C	1.78714100	3.25064300	12.87891800
C	2.11341600	3.25376500	11.49100900
C	5.87451900	0.99826200	15.02574700
H	5.70277600	0.52675100	14.05853300
C	2.50882300	-0.44989200	10.60314500
H	2.21029000	0.38167700	9.96786100
C	1.96147800	5.94264600	17.00361500
H	2.08182500	7.02369800	16.95716500
C	5.83949100	1.43041000	11.46795000

C	3.78290900	-1.33593600	12.45101800
H	4.47644400	-1.19372800	13.27976000
C	6.51608400	2.65696100	11.51503700
H	5.98326900	3.55561900	11.82546800
C	3.43277200	-0.25225400	11.63377100
C	-0.20561300	4.57116400	12.39073000
H	-1.10719800	5.05521100	12.76037200
C	4.96824800	1.93123100	15.53123100
C	2.32455100	-2.78390900	11.19106200
H	1.89043200	-3.76663600	11.02106900
C	0.98107300	0.29724500	14.08389100
H	0.63381700	0.94231500	13.27550700
C	5.23778100	2.51078300	16.77603200
H	4.55800600	3.25173200	17.19642100
C	2.33737300	3.75727300	16.02194800
C	2.47842100	5.14905000	15.98260600
H	2.99442200	5.62289200	15.14909300
C	1.29627900	5.35465900	18.07686800
H	0.89230100	5.97489200	18.87455800
C	6.52333800	0.27963800	11.06936300
H	6.00966300	-0.67949800	11.02973200
C	2.51225900	-0.18941700	15.87203700
H	3.37685800	0.07339500	16.48298600
C	1.95633200	-1.70945100	10.38806300
H	1.23452300	-1.84879500	9.58639100
C	0.13451200	4.65159400	11.06634200
H	-0.48049800	5.20846700	10.36078800
C	1.83935500	-1.38313600	16.12727100

H	2.17842200	-2.03530600	16.93020600
C	0.30965600	-0.89880800	14.33086600
H	-0.55048600	-1.17320000	13.72257300
C	1.14909300	3.97112500	18.12607300
H	0.62929400	3.50602300	18.96169800
C	3.24182800	-2.59550400	12.22282400
H	3.52668300	-3.42864400	12.86142700
C	1.66747100	3.17763600	17.10369200
H	1.54665600	2.09498300	17.15812300
C	0.73741300	-1.74038900	15.35443200
H	0.21325800	-2.67405200	15.54884000
C	6.38121400	2.16164800	17.49375500
H	6.57307300	2.62648800	18.45916300
C	7.86888300	0.35559300	10.71801000
H	8.39447700	-0.54410600	10.40552000
C	7.01942500	0.64643800	15.73802600
H	7.71252900	-0.08253600	15.32220300
C	7.27468200	1.22893100	16.97607900
H	8.16831600	0.95891400	17.53503200
C	2.76672800	3.42969800	8.73698600
H	3.03572300	3.49761100	7.68570700
C	1.65432900	4.07501800	9.21575200
H	1.02010500	4.65773700	8.54867400
C	7.85678400	2.72575400	11.15701300
H	8.37329900	3.68289000	11.19094600
C	8.53724500	1.57498700	10.76271400
H	9.58837100	1.63023800	10.48863600
C	5.30881300	4.78966400	14.13488100

C	6.69603200	6.81104700	14.51973400
H	7.36305900	7.19695500	13.73233100
H	6.40893600	7.67634100	15.13239700
H	7.29226200	6.13618400	15.14630800
H	6.03868300	4.22012900	14.73186400
C	5.49680100	6.11302500	13.95923600
C	5.09348300	7.51344500	11.88777300
H	4.30712300	8.10666600	11.39494800
H	5.89698700	8.21907600	12.14660400
C	5.60248200	6.44442700	10.93719000
H	4.82322600	5.69500600	10.73323500
H	5.91560500	6.86839400	9.97650300
H	6.46365900	5.91444000	11.36534500
C	4.51212300	6.92792700	13.17184700
H	3.67330600	6.26512300	12.88971500
O	4.04233700	7.97339400	14.02625100
H	3.43806800	8.51704100	13.50497200



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -720.655421966

Electronic and Zero-Point Energy = -720.359194

Enthalpy = -720.341959

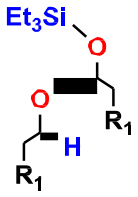
Free Energy = -720.402025

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -720.679873768

C	-1.55445200	2.24040700	1.62586400
C	-0.79327500	1.65708400	2.79835200
H	-0.07459300	0.91927800	2.41464700
H	-0.20042800	2.45578300	3.26881900
C	-1.72589300	1.01956900	3.81284700
H	-1.17529600	0.59881700	4.66094400
H	-2.44018200	1.75114200	4.21297300
H	-2.30804100	0.20663900	3.36007000
H	-2.17745900	1.45872500	1.15985600
O	-0.66883100	2.75661300	0.65297300
Si	-0.62348600	4.37117100	0.21384000
C	0.94121900	4.55473700	-0.80676500
H	1.07120400	5.62095200	-1.04882400
H	1.79147200	4.29207100	-0.15925900
C	-0.50437000	5.44896400	1.75504200
H	-1.26477400	5.14751300	2.49075000
H	0.46742500	5.23806200	2.22721100
C	-2.13254900	4.84243700	-0.80879200
H	-2.16118900	4.20063000	-1.70194200
H	-1.96150400	5.86351600	-1.18667400
C	-3.46644100	4.76680200	-0.06980600
H	-4.30311100	5.12034600	-0.68561300
H	-3.70053900	3.73625100	0.22761600
H	-3.46086600	5.37249200	0.84678100
C	-0.62824500	6.94071800	1.45144400

H	-0.47297200	7.55994300	2.34364300
H	0.10895200	7.26610000	0.70471200
H	-1.62008100	7.19143500	1.05295100
C	0.97097000	3.72044000	-2.08383200
H	1.91940300	3.82875600	-2.62532200
H	0.83940100	2.65226500	-1.86904500
H	0.17048700	4.01298400	-2.77559900
H	-2.25393400	3.01353400	1.99376400



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -913.699545367

Electronic and Zero-Point Energy = -913.312905

Enthalpy = -913.291180

Free Energy = -913.360958

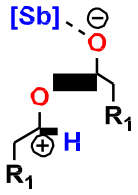
M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -913.731545451

O	3.82780700	5.94868700	11.68658500
C	4.72383700	6.91767700	11.22441500
C	4.87023200	6.77031400	9.72139500
C	5.62938600	7.93035900	9.10375600
H	6.61268200	8.05915400	9.57143200

H	5.78322300	7.78381200	8.02927700
H	5.08102300	8.87229500	9.23432400
H	5.35593600	5.80942100	9.49860300
H	3.85843800	6.70877500	9.30030500
H	4.34044800	7.93085600	11.44793300
C	7.93391200	5.78749800	11.01247400
O	5.94753600	6.87815800	11.92284500
H	7.65987100	5.99588900	9.96844300
H	8.50542300	6.65785100	11.36527600
C	8.77822000	4.52758900	11.09185600
Si	3.22830700	5.96125900	13.26563100
H	9.68967300	4.61209400	10.49045700
H	9.08164400	4.31667900	12.12557200
H	8.22258400	3.65300200	10.72905200
C	2.89221100	7.73255000	13.80274600
C	4.43217100	5.12914700	14.44862700
C	1.63012400	4.98217200	13.14727000
H	2.59134300	7.70702300	14.86123100
H	3.83562100	8.29873000	13.78122500
C	1.81951700	8.43421900	12.97319000
H	4.75415400	4.17102200	14.01302300
H	5.33722400	5.75146100	14.51329600
C	3.84494900	4.90251800	15.84049000
H	1.01250200	5.45064400	12.36683300
H	1.06690000	5.10472400	14.08555200
C	1.83776600	3.50257100	12.83393000
H	1.68377700	9.48170800	13.27011500
H	2.06399300	8.42892600	11.90207900

H	0.84571900	7.93932200	13.08093300
H	4.56688400	4.43456000	16.52137200
H	3.53033200	5.84467100	16.30877300
H	2.96252100	4.24981500	15.80921500
H	0.88747100	2.96698600	12.71478100
H	2.40539700	3.36771500	11.90402600
H	2.39724800	2.99422300	13.63000500
C	6.67810300	5.65975100	11.85216200
H	6.04050300	4.84407000	11.47860200
H	6.95289200	5.38766600	12.88408200



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2274.37210131

Electronic and Zero-Point Energy = -2273.617493

Enthalpy = -2273.568717

Free Energy = -2273.699449

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2274.47087902

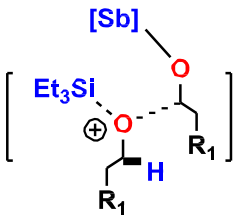
Sb	2.85336000	2.53092400	14.39692400
P	4.09569700	1.30735100	12.14917800
C	3.75005200	2.44686300	9.61458300

H	4.63777400	1.88963300	9.31708900
C	3.31109700	2.38720100	10.92123000
O	4.32586200	4.45014900	13.34726700
C	0.48630300	3.78072300	12.97239000
H	0.12562900	3.82830200	13.99956600
C	1.40166800	3.79853500	10.32955900
C	1.89022000	0.70156500	14.91728000
C	1.68369000	3.16322500	12.68168500
C	2.14430400	3.10064600	11.33363200
C	5.46439500	1.11603300	15.28798500
H	5.05719300	0.27708900	14.72235500
C	2.32313600	-0.52833700	10.94339500
H	1.92628300	0.31182100	10.37590900
C	1.52705500	6.21352900	16.51006100
H	1.42592900	7.26871300	16.26124200
C	5.86818800	1.27704700	11.73355200
C	3.90051800	-1.44436000	12.52835500
H	4.74963500	-1.32116500	13.20014300
C	6.67736300	2.31350600	12.21935000
H	6.24672700	3.09838200	12.84241000
C	3.40884400	-0.34806800	11.80593500
C	-0.28409600	4.39946200	11.96179700
H	-1.22718800	4.87339300	12.22227400
C	4.76127900	2.31603100	15.37379400
C	2.23112600	-2.86765300	11.52838800
H	1.77113400	-3.84740700	11.42193800
C	0.85831400	0.19980600	14.11796500
H	0.52159800	0.75252800	13.24077900

C	5.28698900	3.37725600	16.11089100
H	4.74253700	4.31798900	16.19504400
C	2.07700300	3.95397900	15.82396700
C	1.93454400	5.31287700	15.52819500
H	2.14155900	5.69080600	14.52899700
C	1.25882300	5.76404300	17.80081800
H	0.93718600	6.46557100	18.56736000
C	6.43115300	0.27431600	10.93774500
H	5.81129100	-0.53255900	10.55100200
C	2.30863900	-0.02702000	16.03627800
H	3.11694500	0.34449300	16.66592500
C	1.73860500	-1.78475200	10.80800700
H	0.89569400	-1.91445800	10.13320800
C	0.18597200	4.43895600	10.67591600
H	-0.36732000	4.95562500	9.89337400
C	1.70113400	-1.23976100	16.35078300
H	2.02884700	-1.79854100	17.22466700
C	0.25859200	-1.01731400	14.43072200
H	-0.53666000	-1.40430800	13.79693900
C	1.40506900	4.41372300	18.10784400
H	1.19816400	4.05743300	19.11481500
C	3.31769600	-2.69695900	12.38419700
H	3.71100600	-3.54203600	12.94431300
C	1.81574900	3.51411300	17.12629500
H	1.92927400	2.46138000	17.38927100
C	0.67974500	-1.73682100	15.54585500
H	0.20980300	-2.68754300	15.78753900
C	6.52200000	3.24074400	16.73999200

H	6.93308500	4.07370900	17.30799100
C	7.78863900	0.30860500	10.63254500
H	8.21995300	-0.47331800	10.01183600
C	6.69302700	0.97615000	15.92934800
H	7.23372200	0.03476800	15.86185900
C	7.22583800	2.04245800	16.64821600
H	8.18958500	1.93786000	17.14148900
C	3.04654900	3.19287600	8.64911700
H	3.41023300	3.22894200	7.62556300
C	1.88492900	3.83429500	8.99933700
H	1.30627300	4.37918000	8.25518900
C	8.03178000	2.34183400	11.90690600
H	8.65546000	3.14742200	12.28760400
C	8.58912500	1.33922000	11.11690800
H	9.65006500	1.36055100	10.87877100
C	4.99077500	5.86024200	11.53428100
C	4.50530400	7.11873900	10.84286800
H	4.37904000	7.93599500	11.56042600
H	5.21270600	7.44309700	10.07405200
H	3.53771100	6.94934500	10.35322600
H	5.96156300	5.98742500	12.03291200
H	5.13666500	5.04695200	10.80020900
C	4.01765500	5.29595900	12.51034200
H	2.95566700	5.58765300	12.36850300
O	4.02444200	7.33278500	13.99739300
C	4.79734800	7.04156800	14.88948500
C	5.05296400	7.86541100	16.10605600
H	4.28301700	8.64195100	16.18286400

H	6.01519600	8.37354500	15.93377200
H	5.38241200	6.09102200	14.83293400
C	5.14983000	7.00151300	17.35654100
H	5.93128500	6.23804500	17.24705100
H	5.40057400	7.60877200	18.23137300
H	4.20044800	6.48952800	17.56287600



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2802.00797229

Electronic and Zero-Point Energy = -2801.039790

Enthalpy = -2800.980440

Free Energy = -2801.131325

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2802.12006579

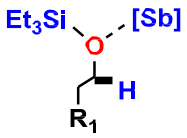
Sb	1.80170100	3.95901500	10.92616500
P	3.26249700	3.58368800	8.48348000
C	3.69001800	5.75956400	6.78510600
H	4.43534200	5.13150200	6.29818800
C	2.99960400	5.27520000	7.87841100
O	3.81530500	5.78715200	11.18657800

C	0.32460600	6.49721500	10.22884800
H	-0.21638600	6.20524800	11.12745400
C	1.73483100	7.36734500	7.97920300
C	0.45776800	2.45879300	10.25830100
C	1.31332500	5.68772900	9.71319100
C	2.01751400	6.07833100	8.53448100
C	3.90357300	1.72831700	11.26228100
H	3.49849200	1.37600900	10.31303600
C	1.62785900	3.03336900	6.24264700
H	1.53797200	4.10993700	6.10962700
C	0.70787300	6.15831600	14.62004400
H	1.11353900	6.99762200	15.18384700
C	5.05645700	3.29999100	8.31111900
C	2.52272600	1.12241000	7.41888500
H	3.14706500	0.69913300	8.20608100
C	5.90198900	3.86708100	9.27487100
H	5.47712700	4.41920600	10.11581000
C	2.43026700	2.51253000	7.26185800
C	0.00769500	7.73942500	9.63481200
H	-0.78152400	8.35134800	10.06406400
C	3.41834700	2.89326900	11.85411400
C	1.03537900	0.79896000	5.54921000
H	0.49257400	0.13251600	4.88295300
C	-0.35944600	2.71643700	9.15422200
H	-0.30558100	3.67843400	8.64347900
C	3.93877400	3.32045900	13.07646700
H	3.56318600	4.21956300	13.56281200
C	0.84756500	4.64536400	12.73348300

C	1.35797800	5.72240200	13.46909800
H	2.27214800	6.22535300	13.14397000
C	-0.45764300	5.52683400	15.04827300
H	-0.96499800	5.87188300	15.94634700
C	5.60686100	2.57539000	7.25017000
H	4.96026000	2.13036600	6.49592900
C	0.38988700	1.21750500	10.89914900
H	1.01739400	1.00384800	11.76464800
C	0.93367200	2.17710200	5.39185500
H	0.31288400	2.59258400	4.60137700
C	0.72305500	8.17640600	8.55295700
H	0.52540600	9.14854400	8.10444300
C	-0.49093900	0.24410000	10.43485700
H	-0.54531200	-0.71906100	10.93743400
C	-1.23520400	1.73799200	8.69065400
H	-1.85887400	1.93981900	7.82216800
C	-0.97159000	4.45638900	14.32416600
H	-1.88271900	3.96080900	14.65254500
C	1.83450000	0.27248200	6.56224300
H	1.92067900	-0.80429000	6.68747700
C	-0.32308800	4.01794200	13.17040700
H	-0.74467100	3.18292900	12.61112900
C	-1.29998300	0.50328800	9.33133000
H	-1.98346700	-0.26081800	8.96785900
C	4.95849800	2.59429700	13.68732500
H	5.36976300	2.94108600	14.63408600
C	6.98782800	2.42642100	7.15023200
H	7.40899900	1.86103000	6.32214000

C	4.91509100	0.99783300	11.88133000
H	5.28785600	0.08876100	11.41498700
C	5.44894400	1.43618800	13.09001700
H	6.24657700	0.87367100	13.56987400
C	3.43348100	7.04575500	6.27436000
H	3.98979300	7.40504000	5.41256800
C	2.46457000	7.82439000	6.85590400
H	2.23231600	8.81147800	6.45886200
C	7.28020800	3.72958300	9.15715300
H	7.93329600	4.18492900	9.89956200
C	7.82484800	3.00620600	8.09816900
H	8.90318200	2.89364000	8.01367600
C	4.00204900	6.97691700	10.97380000
C	5.06634000	7.48294000	10.05849700
C	5.21890800	8.98926700	10.06322100
H	5.56643500	9.34350600	11.04115500
H	5.94282000	9.31439300	9.31005200
H	4.26318400	9.48079800	9.83792300
H	6.00190900	6.95829100	10.29689500
H	4.77953500	7.11748800	9.05797600
H	3.30491200	7.73374100	11.40327400
C	7.65939900	6.07702500	12.70105700
O	5.67291000	7.43157900	13.08621300
H	7.67515800	6.44600000	11.66441600
H	8.29109200	6.76309000	13.28410800
C	8.20264300	4.66017100	12.76795700
Si	5.41382700	8.40800000	14.43724500
H	9.23000900	4.59988900	12.39208000

H	8.20480900	4.28166300	13.79896300
H	7.58776500	3.97332500	12.16803600
C	5.11668000	10.14484500	13.78619700
C	6.94680900	8.39135400	15.53088900
C	3.89837400	7.80339500	15.37417000
H	5.33624000	10.84837500	14.60386300
H	5.87922700	10.34743000	13.01875500
C	3.71610100	10.40999800	13.24235000
H	7.28978100	7.35771600	15.68485300
H	7.75359800	8.89555800	14.97695000
C	6.72717400	9.07655700	16.87817500
H	3.05321200	7.82110700	14.66662600
H	3.65656900	8.56104900	16.13709000
C	4.02454600	6.42422600	16.01520800
H	3.63008200	11.40530900	12.78845400
H	3.42899800	9.68007800	12.47281800
H	2.96154800	10.35043900	14.03693800
H	7.64707400	9.11563900	17.47437800
H	6.37993900	10.11170800	16.75909700
H	5.97312300	8.55392700	17.48048600
H	3.13878200	6.15470400	16.60455500
H	4.15661100	5.63840600	15.25785600
H	4.89035600	6.36664700	16.68880300
C	6.23813900	6.13758500	13.22212100
H	5.60949600	5.42540900	12.66212600
H	6.22422400	5.79888400	14.27396300



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2608.96890651

Electronic and Zero-Point Energy = -2608.088332

Enthalpy = -2608.034424

Free Energy = -2608.174115

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2609.07351790

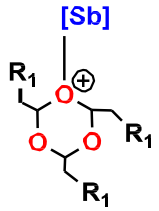
Sb	2.49439100	1.48755600	14.85838100
P	3.47131600	0.71842000	12.29337700
C	3.10440200	2.36935900	10.07351600
H	3.82043000	1.71994400	9.56998100
C	2.79732400	2.13973600	11.40113700
C	0.60465000	3.69048700	14.04514100
H	0.36487800	3.61266400	15.10350300
C	1.21453800	4.00120100	11.33711200
C	1.37316400	-0.30251700	14.88573000
C	1.57744200	2.88395500	13.48971500
C	1.87766500	2.98242200	12.09552100
C	5.11860300	-0.12447900	15.06733000
H	4.57854900	-0.84400300	14.45328500
C	1.81631200	-0.70009700	10.48485000
H	1.58645100	0.25486800	10.01759000

C	2.12758600	4.46878600	18.08750800
H	2.46326200	5.49371100	18.23465100
C	5.26088300	0.73892100	11.97037800
C	2.99014300	-2.00990600	12.13977800
H	3.68421200	-2.08275900	12.97671900
C	5.97640100	1.86153300	12.41218800
H	5.45886200	2.72331400	12.84526800
C	2.72995100	-0.76859900	11.54116800
C	-0.08855200	4.64750300	13.27384800
H	-0.85218700	5.26163200	13.74410500
C	4.50652400	1.06204200	15.47483600
C	1.46693700	-3.08560100	10.61292700
H	0.97507600	-3.98546500	10.25106800
C	0.25950500	-0.43281200	14.05174000
H	-0.05066000	0.39111000	13.40803400
C	5.20137000	1.95629700	16.28823800
H	4.72716000	2.87105900	16.63812200
C	1.94742200	2.50875000	16.67315300
C	2.36758100	3.83049700	16.87500200
H	2.88875500	4.36810700	16.07911400
C	1.45838800	3.79362300	19.10672300
H	1.26783200	4.29235500	20.05447700
C	5.94400800	-0.34666900	11.41994400
H	5.39653100	-1.22115300	11.07221300
C	1.76824300	-1.36070100	15.70897500
H	2.63442300	-1.26032500	16.36320500
C	1.19122600	-1.85565100	10.02462600
H	0.48348800	-1.79042500	9.20147100

C	0.23211300	4.81405100	11.95315800
H	-0.26085800	5.57431000	11.34934900
C	1.04816900	-2.55237900	15.69019800
H	1.35247900	-3.37798200	16.32936600
C	-0.45394700	-1.62797200	14.03890200
H	-1.31846900	-1.73311800	13.38755000
C	1.03312200	2.48302200	18.91261500
H	0.50695500	1.95762700	19.70678700
C	2.37071500	-3.16162600	11.67059000
H	2.58706700	-4.11902300	12.13900400
C	1.28029400	1.83878900	17.70043800
H	0.94561800	0.81016600	17.56331200
C	-0.05766400	-2.68533300	14.85439500
H	-0.61611300	-3.61843600	14.83962800
C	6.51369300	1.67580400	16.66578900
H	7.05300700	2.38211100	17.29477700
C	7.33282100	-0.31462400	11.31840800
H	7.85900800	-1.16164000	10.88424000
C	6.42469400	-0.40661500	15.45335600
H	6.89409800	-1.33258000	15.12857100
C	7.12717800	0.50063000	16.24346500
H	8.15264400	0.28643300	16.53513900
C	2.48551700	3.40720900	9.35354600
H	2.73968900	3.56866200	8.30928400
C	1.54349700	4.18980100	9.97351600
H	1.02880100	4.97927400	9.42778300
C	7.36151700	1.88392700	12.30941600
H	7.91160700	2.75739900	12.65648800

C	8.04251800	0.79432100	11.76789600
H	9.12728800	0.81277500	11.69463600
C	6.11367800	5.52130100	16.41920500
C	7.37183200	5.65850700	17.25715300
H	8.05785000	6.40023100	16.82651200
H	7.14574900	5.97168500	18.28182000
H	7.91930900	4.70769400	17.31507000
H	5.59689500	6.49072700	16.33819500
H	5.39834200	4.83598300	16.89849700
O	5.25998000	4.97650200	14.21563200
C	6.41701200	5.01765800	15.02097600
H	6.83136400	3.99638200	15.07118200
H	7.19979600	5.64891300	14.56228800
Si	4.76656100	6.20389700	13.17668200
C	5.94814000	7.67061600	13.12561800
H	6.95289700	7.32042400	12.84570500
H	5.60370500	8.25272500	12.25350500
C	3.04983400	6.71406800	13.74426400
H	2.43843600	5.79779800	13.79153600
H	3.11970900	7.07647800	14.78230800
C	4.71986500	5.42321600	11.47006100
H	4.15325600	4.48590500	11.57753000
H	4.14173300	6.04896700	10.77439400
C	2.37080000	7.75422400	12.85710900
H	2.26540400	7.39854800	11.82281400
H	1.36443600	8.01057700	13.21276200
H	2.94375200	8.69049800	12.81412800
C	6.10552900	5.13457200	10.89841200

H	6.75357600	4.63423100	11.63289000
H	6.06296300	4.48287400	10.01468500
H	6.61633000	6.05816400	10.59761400
C	6.02802200	8.57489500	14.35159100
H	6.51953700	8.07235600	15.19442900
H	6.60104000	9.48804500	14.14735800
H	5.03482400	8.88908400	14.69968900



M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2467.42149206

Electronic and Zero-Point Energy = -2466.572183

Enthalpy = -2466.520320

Free Energy = -2466.658483

M06/6-31+G(2d,2p)[LANL2DZdp] // M06/6-31G(d,p)[LANL2DZ]

Electronic Energy = -2467.52644792

P	3.56154500	0.57007300	12.06912900
C	3.49940800	2.38449500	9.95050000
H	4.09076200	1.64264800	9.41417300
C	3.12222800	2.13274500	11.25685100
C	1.22921800	3.95362400	13.97701200

H	0.95026600	3.86490600	15.02483000
C	1.95723400	4.28142900	11.30307500
C	1.37896400	-0.33683900	14.51226500
C	2.00096700	2.97949100	13.37589800
C	2.36450800	3.09421700	11.99377200
C	5.12684200	-0.30900500	15.01979400
H	4.49068300	-1.10573300	14.63129100
C	1.84837100	-0.54124600	10.09395000
H	1.71198100	0.46383500	9.70035800
C	2.17838100	3.78591500	18.37030500
H	2.61396100	4.70452000	18.76071400
C	5.34873900	0.38322200	11.75177100
C	2.83921900	-2.06642300	11.68424800
H	3.47342000	-2.25373200	12.55185800
C	6.17779200	1.43553800	12.15958500
H	5.74156300	2.33629900	12.59416400
C	2.70269400	-0.76594100	11.17680000
C	0.79202200	5.09122500	13.26733200
H	0.18031800	5.83474400	13.77106900
C	4.63054300	0.98706800	15.17133200
C	1.32749000	-2.89700600	10.00089800
H	0.79537700	-3.72545200	9.53920400
C	0.32906600	-0.32765700	13.59008900
H	0.14531300	0.54811800	12.96626700
C	5.45763200	2.00939300	15.64092300
H	5.08058000	3.02719800	15.75201300
C	1.96324500	2.16198100	16.58388600
C	2.52135200	3.34217700	17.09715400

H	3.21226600	3.93709500	16.49613300
C	1.27544800	3.05959600	19.14376800
H	1.00828900	3.40675100	20.13937300
C	5.92142200	-0.77526900	11.22412300
H	5.29243600	-1.60148000	10.89842800
C	1.62086700	-1.46474100	15.30123100
H	2.43237300	-1.46979500	16.02884800
C	1.16433600	-1.60484400	9.51133800
H	0.50316600	-1.41953500	8.66796900
C	1.16589200	5.25495300	11.96161400
H	0.86748500	6.13837700	11.39966100
C	0.81033400	-2.58818700	15.15528500
H	0.99836200	-3.47025000	15.76301200
C	-0.48287700	-1.45086400	13.46030500
H	-1.29970200	-1.44642500	12.74221700
C	0.71177600	1.89219600	18.63998700
H	0.00204100	1.32517000	19.23846400
C	2.16760700	-3.12704400	11.08833600
H	2.28924300	-4.13300900	11.48345600
C	1.05335200	1.44375100	17.36478300
H	0.60325300	0.52597800	16.98755200
C	-0.23727000	-2.58010400	14.23773800
H	-0.86771900	-3.45957300	14.12973000
C	6.78436700	1.72657400	15.96119600
H	7.43329300	2.52469300	16.31811400
C	7.30617900	-0.87627500	11.10690600
H	7.74386700	-1.78107200	10.69115700
C	6.44751800	-0.58719300	15.36026500

H	6.83193600	-1.59859000	15.25006000
C	7.27551900	0.43038700	15.82911600
H	8.30957500	0.21259700	16.08571800
C	3.12097700	3.56870000	9.29444100
H	3.42618300	3.74033400	8.26568700
C	2.35014400	4.48860500	9.95972500
H	2.02529400	5.40342500	9.46688700
C	7.55695000	1.33240000	12.03709300
H	8.19023100	2.15475500	12.36522000
C	8.12483000	0.17221300	11.51303000
H	9.20514300	0.08702400	11.42264800
Sb	2.59721000	1.38243700	14.67637000
O	4.74326600	5.39076400	15.46397900
O	6.45975500	6.60265200	14.48177200
O	5.48558400	7.38157300	16.41274900
C	5.71065900	7.65027500	15.04881100
H	4.73934100	7.74175400	14.52528500
C	5.74034000	5.38808500	14.46047300
H	6.48856400	4.59385200	14.65169300
C	5.10934000	6.03879600	16.66409500
H	4.18475200	6.05838900	17.26461000
C	6.19974100	5.31460500	17.42820200
H	5.87804300	4.26941000	17.55504400
H	7.11759600	5.31281800	16.82396100
C	6.45449700	5.95427800	18.78133000
H	7.22674800	5.41332400	19.33762900
H	6.78437200	6.99273900	18.66876700
H	5.54312400	5.95678800	19.39415300

C	5.03711000	5.14378100	13.14674800
H	4.49085200	4.19237200	13.24499500
H	4.27675800	5.92742800	13.01461400
C	5.98989700	5.10530700	11.96767200
H	6.47066500	6.07825400	11.81819500
H	6.78675000	4.36374800	12.11592200
H	5.46026300	4.84074000	11.04452900
C	6.49986100	8.92654600	14.92729400
H	6.70525800	9.08162100	13.86040100
H	7.46612800	8.76788900	15.42491000
C	5.76897000	10.11873000	15.51669400
H	5.59858200	9.98621200	16.59041100
H	6.34227400	11.04087200	15.37721900
H	4.79086200	10.26027200	15.03907000

5. CRYSTALLOGRAPHY

General Considerations: The crystallographic measurement of [**2**][OTf] was carried out on a Rigaku Mini CCD area detector diffractometer using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 223 K using an Oxford Cryostream low-temperature device. A sample of suitable size and quality was selected and mounted onto a nylon loop. Data reductions were performed using Crystal Clear Expert 2.0. The structures were solved by direct methods, which successfully located most of the non-hydrogen atoms. Subsequent refinements on F^2 using the SHELXTL/PC package (version 5.1) allowed location of the remaining non-hydrogen. Colorless, single crystals of [**2**][OTf] were obtained by slow vapor diffusion of diethyl ether into a dichloromethane solution saturated with [**2**][OTf]. This compound crystallized in the monoclinic space group $P2_{1/n}$. Key details of the crystal and structure refinement data are summarized in Table S2. Further crystallographic details may be found in the respective CIF file which was deposited at the Cambridge Crystallographic Data Centre, Cambridge, UK. The CCDC reference number for [2][OTf]was assigned as 1453179.

Table S2. Crystal Data, Data Collection and Structure Refinement for [**2**][OTf]

	[**2**][OTf]	
Empirical Formula	$C_{41}H_{31}F_3O_3P_1S_1Sb_1$	
Formula Weight	813.44	
Temperature	150(2) K	
Wavelength	0.71075 Å	
Crystal System	Monoclinic	
Space Group	$P2_1/n$	
Unit Cell Dimensions	a = 9.8944(12) Å	□= 90°
	b = 21.026(3) Å	□=96.354(3)°
	c = 17.789(2) Å	□= 90°
Volume	3677.1(8) $Å^3$	
Z	4	
Density (calculated)	1.469 Mg/m3	
Absorption coefficient	0.903 mm^{-1}	
F(000)	1640	
Crystal size	0.2 x 0.2 x 0.2 mm^3	
Theta range for data collections	3.011 to 24.997°	
Index ranges	-11<=h<=11, -25<=k<=25, -21<=l<=21	
Reflections collected	30243	
Independent reflections	6463 [R(int) = 0.0590]	
Completeness to theta =	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parame	6463 / 0 / 575	
GooF on F^2	1.007	
Final R indices	R1 = 0.0421, wR2 = 0.0947	
R indices (all data)	R1 = 0.0611, wR2 = 0.1059	
Largest diff. peak and	1.081and -0.395 e.$Å^{-3}$	

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