Electronic Supporting Information

for

Selective Photocatalytic C-C Bond Cleavage under Ambient Conditions with Earth Abundant Vanadium Complexes

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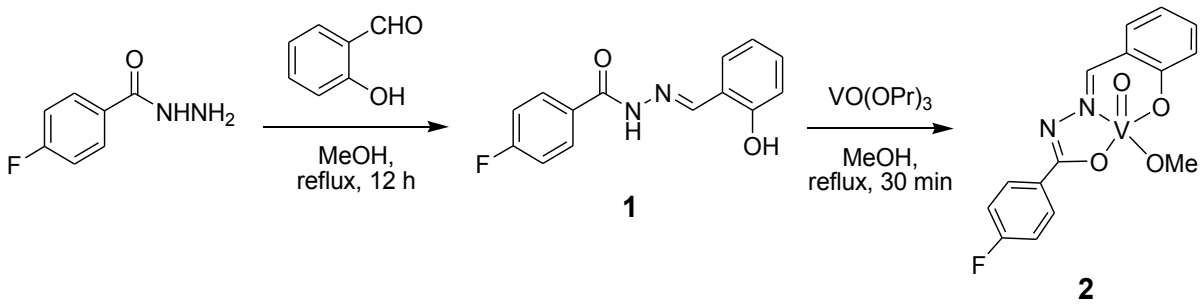
I. General information

The vanadium complexes used in this study were synthesized under dry argon (Ar) using standard Schlenk techniques or in a glovebox under a N_2 atmosphere. Some experiments conducted under anaerobic environments, such as the attempted synthesis of the V^{IV} oxo (**3**), and the control experiments without air are described in further details below. All other reactions were performed under aerobic conditions. Deuterated solvents were purchased from Cambridge Isotope Laboratories and were used as received. The other chemicals were obtained from Sigma-Aldrich and were used as received. The ^{1}H and ^{13}C NMR spectra were recorded at room temperature on a Bruker AVANCE 300 MHz spectrometer, whereas the ^{51}V NMR spectra were obtained at room temperature on a JEOL 400 MHz spectrometer. The ^{1}H and ^{13}C chemical shifts (δ reported in ppm) are referenced to the residual solvent signal(s), and the ^{51}V NMR chemical shift is referenced externally to $V^{V}(O)(Cl)_3$ (0 ppm).

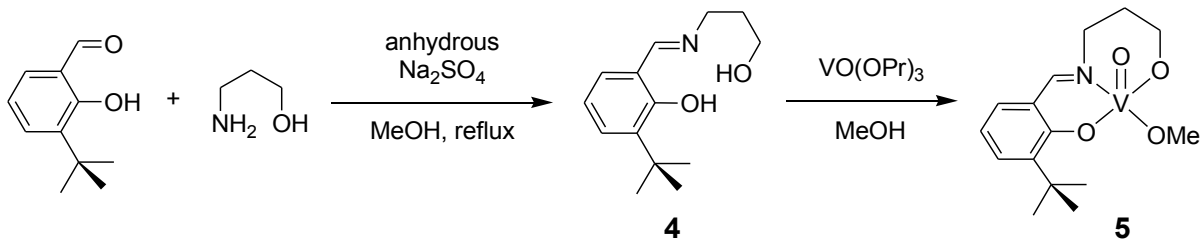
II. Synthesis of vanadium-oxo complexes



Compound 4-fluoro-*N*'-(2-hydroxybenzylidene)benzohydrazide (1). Compound 4-fluorobenzohydrazide[1] (1.54 g, 10 mmol) was dissolved in absolute ethanol (15 mL) and heated to reflux. Salicylaldehyde (1.22 g, 10 mmol) in absolute ethanol (5 mL) was slowly added dropwise into the reaction mixture. After complete addition, the reaction mixture was

heated at reflux overnight. Subsequently, the reaction mixture was cooled to room temperature during which a white precipitate formed. The white solid was filtered off, washed with cold ethanol three times, and dried under vacuum to provide the corresponding hydrazone derivative (**1**) in high yield (2.32 g, 90%). ^{1}H NMR (DMSO–d_6, 300 MHz): δ = 6.89 – 6.95 (m, 2 H), 7.30 (t, J = 6.0 Hz, 1 H), 7.38 (t, J = 9.0 Hz, 2 H), 7.55 (d, J = 6 Hz, 1 H), 8.00 – 8.05 (m, 2 H), 8.64 (s, 1 H) ppm. ^{13}C{^{1}H} NMR (DMSO–d_6, 100 MHz): δ = 115.6, 116.4, 118.7, 119.4, 129.3, 129.5, 130.4, 131.4, 148.3, 157.5, 161.8, 164.3 ppm. ^{19}F{^{1}H} NMR (DMSO–d_6, 282.40 MHz): δ = –108.01 ppm. HRMS (ESI+, m/z) calculated for $C_{14}H_{12}FN_2O_2$ $[M + H]^+$ m/z = 259.0883, found 259.0885.

Vanadium oxo complex (2). The vanadium(V) precursor, $VO(OPr)_3$ (227 μL, 1.0 mmol), was added dropwise to a stirred solution of **1** (0.258 g, 1.0 mmol) in methanol (MeOH, 20 mL), during which the reaction mixture turned dark red. The reaction mixture was heated at reflux for 30 min, followed by hot filtration. The filtrate was then cooled to room temperature and kept aside for crystallization to obtain **2** by slow evaporation (0.248 g, 70%). ^{1}H NMR (MeOD, 300 MHz): δ = 6.94 – 7.04 (m, 2 H), 7.20 (t, J = 9.0 Hz, 2 H), 7.50 (t, J = 7.2 Hz, 1 H), 7.61 (d, J = 7.8 Hz, 1 H), 8.12 – 8.17 (m, 2 H), 8.75 (s, 1 H) ppm. ^{13}C{^{1}H} NMR (MeOD–d_4, 100 MHz): δ = 116.4, 116.6, 117.9, 121.6, 121.9, 132.1, 132.2, 133.8, 135.5, 154.1, 165.2, 167.7 ppm.^{19}F{^{1}H} NMR (MeOD–d_4, 282.40 MHz): δ = –110.6 ppm. ^{51}V NMR (MeOD–d_4, 105.15 MHz): δ = –548.7 ppm. HRMS (ESI+, m/z) calculated for $C_{15}H_{12}FN_2O_4V$ $[M]^+$ = 354.0221, found 354.0205. Elemental analyses for $C_{15}H_{12}FN_2O_4V$ calculated: C, 50.86; H, 3.41; N, 7.91%; found: C, 50.44; H, 3.35; N, 7.90%. UV–vis [acetonitrile, CH_3CN, λ_{max} (ε M^{-1} cm^{-1})]: 270 (9260), 315 (6940), 395 (3300) nm. Melting point: 164 – 166 ºC.



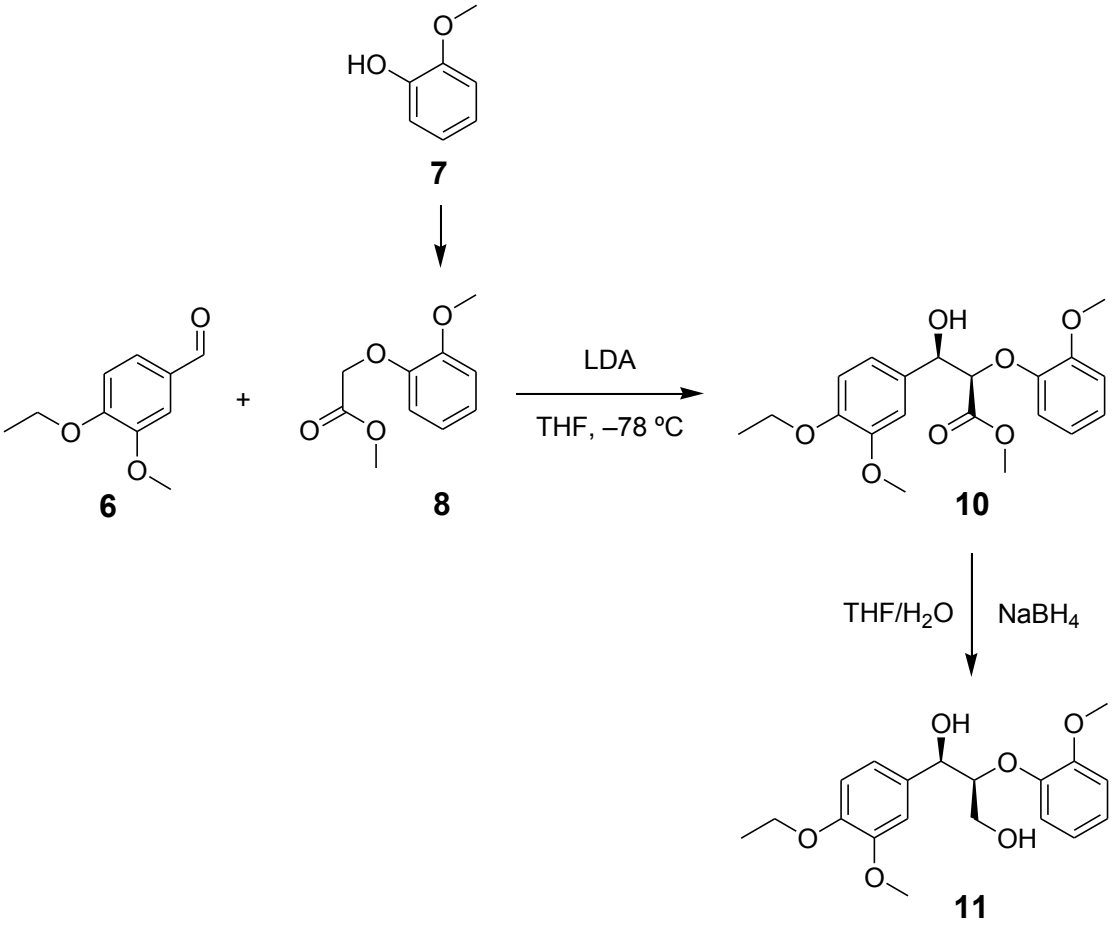
4 **5**

Compound 2-(*tert*-butyl)-6-(((3-hydroxypropyl)imino)methyl)phenol (4). Compound 3-(*tert*-butyl)-2-hydroxybenzaldehyde (0.891 g, 5.0 mmol) and Na_2SO_4 (3.40 g, 24 mmol) were added to a stirred solution of 3-amino-1-propanol (382 μL, 5.0 mmol) in MeOH (20 mL) and the reaction mixture was heated to reflux overnight under nitrogen. The reaction mixture was cooled to roomtemperature, filtered, and concentrated to give **4** as a yellow oil in quantitative yield (1.17 g, 100 %). ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.44 (s, 9 H),1.94 – 2.03 (m, 2 H), 3.71 (t, J = 6 Hz, 2 H), 3.79 (t, J = 6 Hz, 2 H), 6.81 (t, J = 7.5 Hz, 1 H), 7.11 (dd, J = 7.5, 1.5 Hz, 1 H), 7.32 (dd, J = 7.5, 1.5 Hz, 1 H), 8.38 (s, 1 H), 13.99 (bs, 1 H) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ = 29.5, 33.7, 35.0, 55.9, 60.4, 117.9, 118.8, 129.5, 129.8, 137.6, 160.7, 166.2 ppm. HRMS (ESI+, m/z) calculated for $C_{14}H_{22}NO_2$ $[M + H]^+$ *m/z* = 236.1651, found 236.1653.

Vanadium oxo complex (5). The vanadium oxo complex **5** was prepared for control experiments as a mimic of the vanadium catalyst reported by Toste *et al.*[2] The complex was synthesized with **4** and $VO(OPr)_3$ as the vanadium(V) precursor by adopting the procedure described earlier by Toste.[2] ^{1}H NMR (MeOD, 300 MHz): δ = 1.46 (s, 9 H), 2.05 – 1.88 (m, 2 H), 2.29 (d, J = 13.8 Hz, 1 H), 3.35 (s, 3 H), 4.04 (d, J = 10.8 Hz, 1 H), 4.24 (t, J = 12.3 Hz, 1 H), 5.55 (t, J = 9.6 Hz, 1 H), 6.85 (t, J = 7.5 Hz, 1 H), 7.32 (dd, J = 7.5, 1.5 Hz, 1 H), 7.49 (dd, J = 7.5, 1.5 Hz, 1 H), 8.51 (bs, 1 H) ppm. ^{13}C{^{1}H} NMR (MeOD–d_4, 100 MHz): δ = 30.3, 33.8, 36.1, 63.8, 81.2, 119.1, 119.9, 130.4, 131.1, 132.9, 133.1, 165.7 ppm. ^{51}V NMR (MeOD–d_4, 105.15 MHz): δ = –551.1 ppm. HRMS (ESI+, m/z) calculated for $C_{15}H_{23}NO_4V$

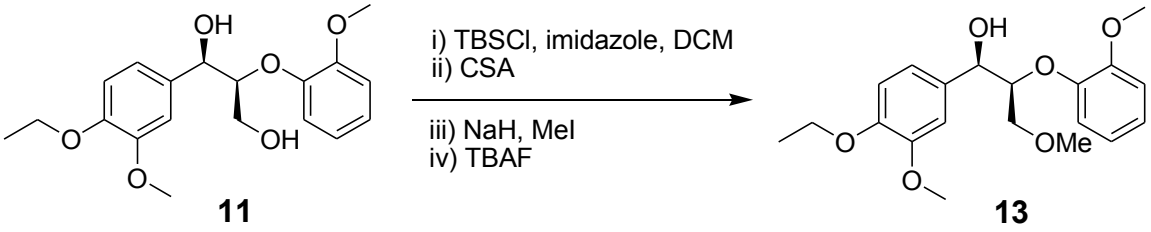
$[M + H]^+$ *m/z* = 332.1067, found 332.1068. Elemental analysis for $C_{15}H_{23}NO_4V$ calculated: C, 54.38; H, 6.69; N, 4.23%; found: C, 54.52; H, 6.34; N, 4.19%. UV–vis [acetonitrile, CH_3CN, λ_{max} (ε M^{-1} cm^{-1})]: 220 (23100), 258 (14500), 336 (5350) nm.

III. Synthesis of lignin model compounds:



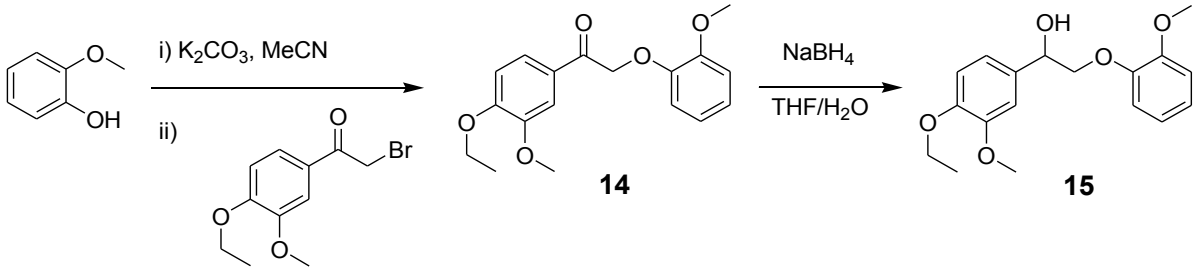
Compound 1-(4-ethoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol (11). The lignin model compound, **11**, was synthesized according to the procedure reported previously.[2] The product identity has been confirmed by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.34 (t, *J* = 6.9 Hz, 3 H), 3.06 (t, *J* = 6.9 Hz, 1 H), 3.60 – 3.75 (m, 2 H), 3.77 (s, 3 H), 3.79 (s, 3 H), 4.01 (q, *J* = 6.9 Hz, 2 H), 4.25 – 4.30 (m, 1 H), 4.82 (t,

J= 4.8 Hz, 1 H), 6.81 – 7.02 (m, 7 H) ppm. HRMS (ESI+, m/z) calculated for $C_{19}H_{25}O_6$ [M + H]$^+$ *m/z* = 349.1651, found 349.1656.



11 **13**

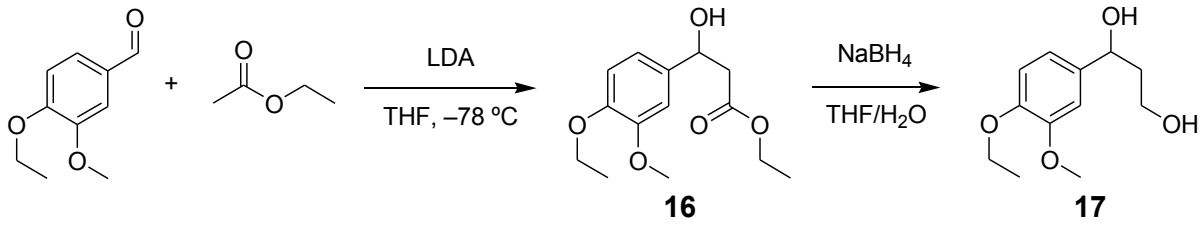
Compound 1-(4-ethoxy-3-methoxyphenyl)-3-methoxy-2-(2-methoxyphenoxy)propan-1-ol (13). The lignin model compound, **13**, was synthesized from **11** by a previously reported procedure.[2] The product identity has been confirmed by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.34 (t, *J* = 6.9 Hz, 3 H), 3.27 (s, 3 H), 3.49 – 3.61 (m, 2 H), 3.78 (s, 3 H), 3.79 (s, 3 H), 4.01 (q, *J* = 6.9 Hz, 2 H,), 4.44 – 4.48 (m, 1 H), 4.80 (d, *J* = 4.8 Hz, 1 H), 6.83 – 7.03 (m, 7 H) ppm. HRMS (ESI+, m/z) calculated for $C_{20}H_{27}O_6$ [M + H]$^+$ *m/z* = 363.1808, found 363.1812.



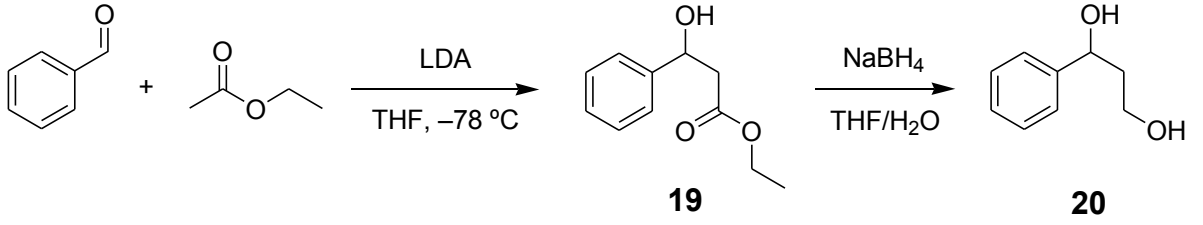
14 **15**

Compound 1-(4-ethoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)ethanone (14). The lignin model compound, **14**, was synthesized according to a previously published procedure.[2] The product has been identified by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.40 (t, *J* = 6.9 Hz, 3 H), 3.83 (s, 3 H), 3.86 (s, 3 H), 4.14 (q, *J* = 6.9 Hz, 2 H), 5.35 (s, 2 H), 6.83 – 6.85 (m, 2 H), 6.91 – 7.02 (m, 3 H), 7.52 (d, *J* = 2.1 Hz, 1 H), 7.65 (dd, *J* = 8.4, 2.1 Hz, 1 H) ppm. HRMS (ESI+, m/z) calculated for $C_{18}H_{21}O_5$ [M + H]$^+$ *m/z* = 317.1389, found 317.1385.

Compound 1-(4-ethoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)ethanol (15). The lignin model compound, **15**, was synthesized by adopting a previously published procedure on a smaller scale.[2] The quantities of reagents used are as follows: **14** (0.316 g, 1.0 mmol) and $NaBH_4$ (0.057 g, 1.50 mmol). The product has been identified by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.36 (t, J = 6.9 Hz, 3 H), 3.64 (bs, 1 H), 3.81 (s, 6 H), 3.97 – 4.09 (m, 4 H), 4.90 – 4.94 (m, 1 H), 6.87 – 7.05(m, 7 H) ppm. HRMS (ESI+, m/z) calculated for $C_{18}H_{22}O_5Na$ $[M + Na]^+$ m/z = 341.1365, found 341.1374.

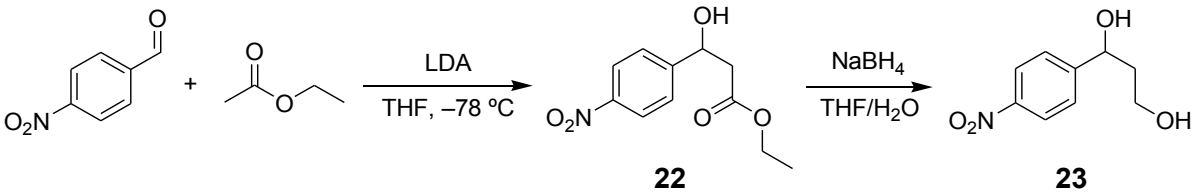


Compound 1-(4-ethoxy-3-methoxyphenyl)propane-1,3-diol (17). The lignin model compound, **17**, was synthesized as reported previously.[2] The product identity has been confirmed by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.35 (t, J = 6.9 Hz, 3 H), 1.81 – 1.89 (m, 2 H), 3.04 (bs, 1 H), 3.64 (bs, 2 H), 3.79 (s, 3 H), 4.01 (q, J = 6.9 Hz, 2 H), 4.74 (bs, 1 H), 6.85 (s, 2 H), 6.95 (s, 1 H) ppm. HRMS (ESI+, m/z) calculated for $C_{12}H_{19}O_4$ $[M + H]^+$ m/z = 227.1283, found 227.1286.



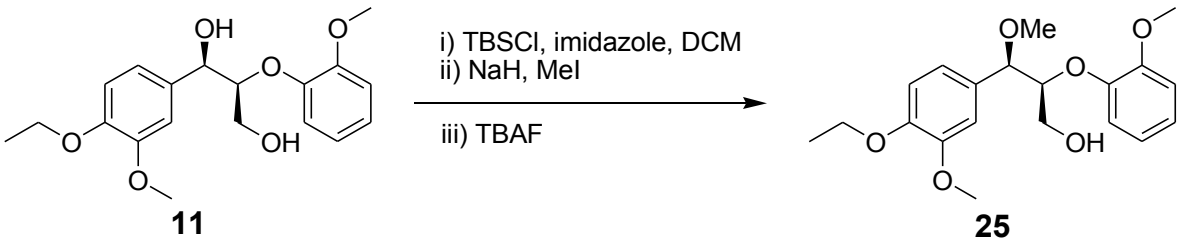
Compound 1-phenylpropane-1,3-diol (20). The lignin model compound, **20**, was synthesized by adopting a previously published procedure on a smaller scale.[2] The quantities of reagents used are as follows: benzaldehyde (1.06 g, 10 mmol), ethyl acetate (1.1 mL, 11 mmol), and 1 M of LDA solution in THF (11 mL, 11 mmol) to synthesize **19** in the first step. The reduction of **19** (0.194 g, 1.0 mmol) was performed with $NaBH_4$ (0.190 g, 5.0 mmol) to

obtain **20** in the second step. The product has been identified by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.79 – 1.87 (m, 2 H), 2.87 (bs, 1 H), 3.57 (bs, 1 H), 3.61 – 3.65 (m, 2 H), 4.80 (t, J = 6.0 Hz, 1 H), 7.24 – 7.27 (m, 1 H), 7.31 – 7.37 (m, 4 H) ppm. HRMS (ESI+, m/z) calculated for $C_9H_{12}O_2Na$ $[M + Na]^+$ m/z = 175.0735, found 175.0737.



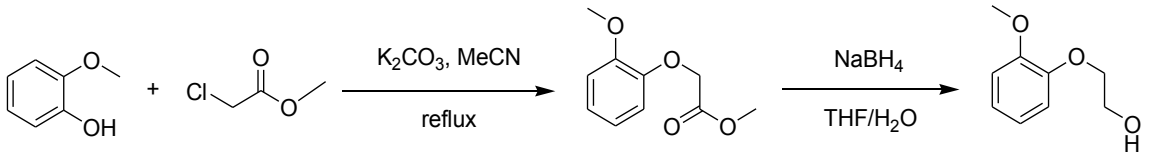
22 **23**

Compound 1-(4-nitrophenyl)propane-1,3-diol (23). The lignin model compound, **23**, was synthesized by adopting a previously published procedure on a smaller scale.[2] The quantities of reagents used are as follows: 4-nitrobenzaldehyde (1.51 g, 10 mmol), ethyl acetate (1.1 mL, 11 mmol), and 1 M of LDA solution in THF (11 mL, 11 mmol) to synthesize **22** in the first step. The reduction of **22** (0.239 g, 1.0 mmol) was conducted with $NaBH_4$ (0.190 g, 5.0 mmol) to give **23** in the second step. The product has been identified by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.80 – 1.87 (m, 2 H), 2.92 (bs, 1 H), 3.58 – 3.71 (m, 2 H), 3.89 (bs, 1 H), 4.95 (t, J = 6.3 Hz, 1 H), 7.58 (d, J = 8.7 Hz, 2 H), 8.18 (d, J = 8.7 Hz, 2 H) ppm. HRMS (ESI+, m/z) calculated for $C_9H_{11}NO_4Na$ $[M + Na]^+$ m/z = 220.0586, found 220.0594.



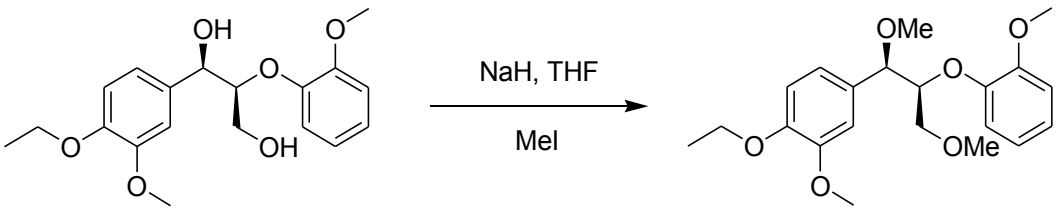
11 **25**

Compound 3-(4-ethoxy-3-methoxyphenyl)-3-methoxy-2-(2-methoxyphenoxy)propan-1-ol (25). The lignin model compound, **25**, was synthesized from **1** by adopting the previously reported procedure.[2] The product identity has been confirmed by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.35 (t, J = 6.9 Hz, 3 H), 2.99 (t, J = 6.3 Hz, 1 H), 3.20 (s, 3 H), 3.69 – 3.73 (m, 2 H), 3.75 (s, 3 H), 3.77 (s, 3 H), 4.01 (q, J = 6.9 Hz, 2 H), 4.29 – 4.34 (m, 1 H), 4.38 (d, J = 6.6 Hz, 1 H), 6.78 – 6.98 (m, 7 H) ppm. HRMS (ESI+, m/z) calculated for $C_{20}H_{26}O_6Na$ $[M + Na]^+$ m/z = 385.1627, found 385.1635.



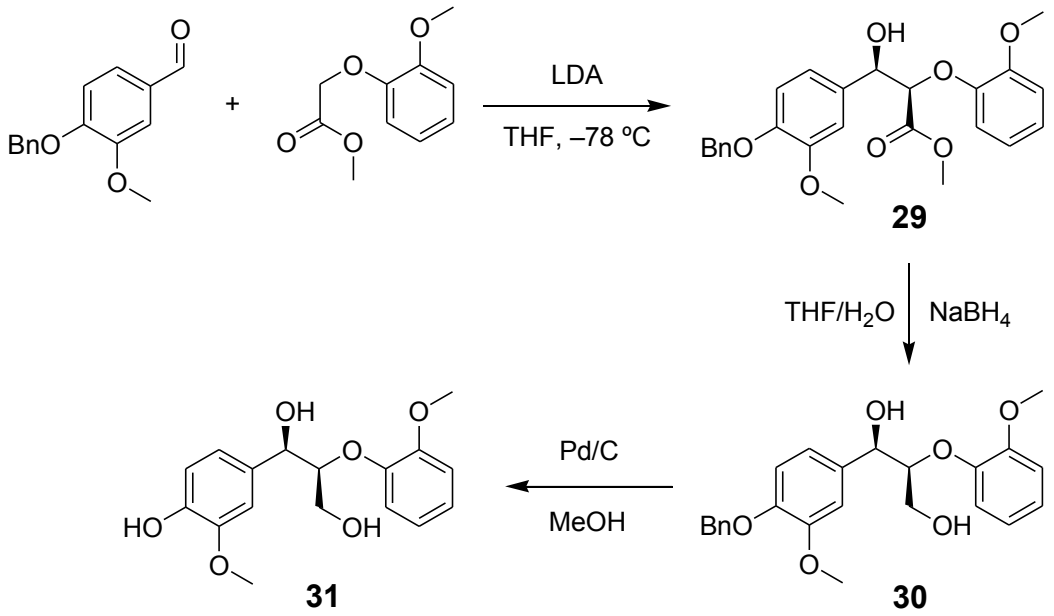
26 **27**

Compound 2-(2-methoxyphenoxy)ethanol (27). The lignin model compound, **27**, was synthesized as reported previously.[2] The product identity has been confirmed by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 3.01 (bs, 1 H), 3.77 – 3.82 (m, 2 H), 3.81 (s, 3 H), 4.00 – 4.03 (m, 2 H), 6.88 – 6.97 (m, 4 H), ppm. HRMS (ESI+, m/z) calculated for $C_9H_{13}O_3$ $[M + H]^+$ m/z = 169.0865, found 169.0868.

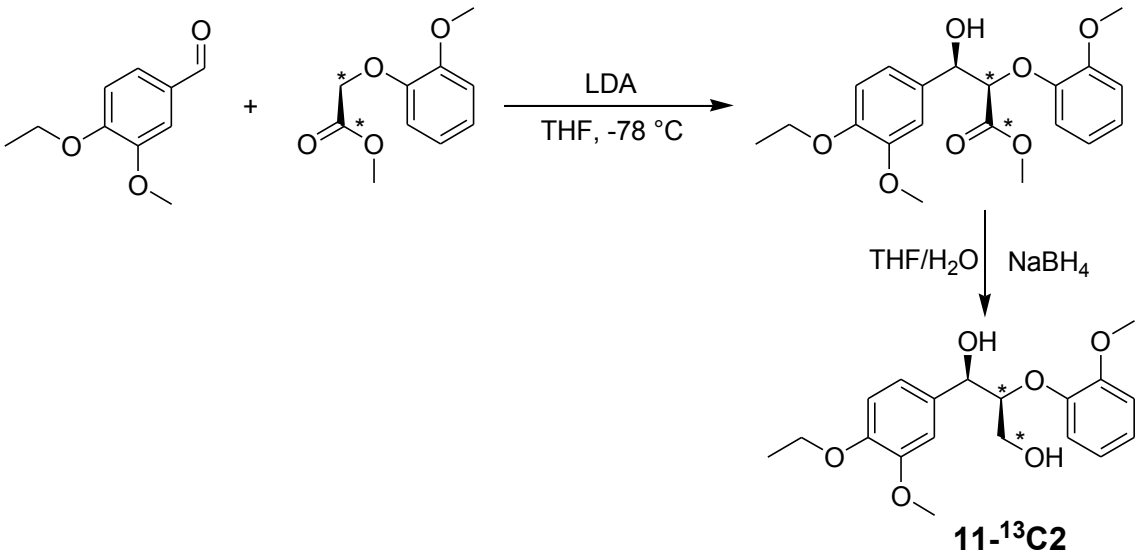


11 **28**

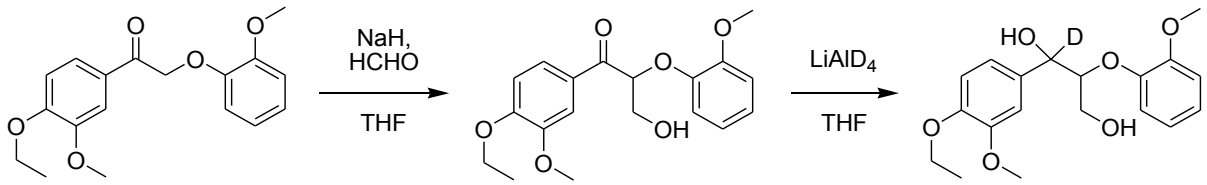
Compound 4-(1,3-dimethoxy-2-(2-methoxyphenoxy)propyl)-1-ethoxy-2-methoxy-benzene (28). The lignin model compound, **28**, was synthesized from **11**. To a stirred solution of **11** (0.348 g, 1.0 mmol) in dry THF (5.0 mL) was added NaH (0.100 g, 2.50 mmol) followed by a 2.0 M solution of iodomethane (MeI, 1.2 mL, 2.4 mmol) in dichloromethane over 10 min. The reaction mixture was stirred at room temperature overnight. After the substrate **11** was consumed, the reaction was quenched by the addition of a saturated aqueous solution of NH_4Cl. The mixture was extracted three times with ethyl acetate (EtOAc, 3 × 30 mL) and the combined organic layers were dried over anhydrous $MgSO_4$, filtered, and concentrated by rotary evaporation. The resulting oily residue was purified by flash column chromatography on silica with hexanes/EtOAc (5:1). The product was isolated as a colorless viscous liquid (0.309 g, 82%) ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.35 (t, J = 6.9 Hz, 3 H), 3.19 (s, 3 H), 3.28 (s, 3 H), 3.59 (d, J = 4.8 Hz, 2 H), 3.73 (s, 3 H), 3.77 (s, 3 H), 4.02 (q, J = 6.9 Hz, 2 H), 4.36 (d, J = 5.7 Hz, 1 H), 4.51 – 4.56 (m, 1 H), 6.76 – 6.97 (m, 7 H) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ = 14.9, 55.9, 56.0, 57.3, 59.4, 64.4, 71.5, 82.5, 82.8, 111.2, 112.2, 112.5, 118.3, 120.5, 120.9, 122,4, 131.0, 148.0, 148.1, 149.2, 150.9 ppm. HRMS (ESI+, m/z) calculated for $C_{21}H_{28}O_6Na$ $[M + Na]^+$ m/z = 399.1784, found 399.1793.



Compound 1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol (31). The lignin model compound, **31**, was synthesized according to the procedure reported previously.[3] The product identity has been confirmed by NMR spectroscopy and HR-MS. ^{1}H NMR (CD_3CN, 300 MHz): δ = 3.06 (t, J = 6.0 Hz, 1 H), 3.73 – 3.78 (m, 2 H), 3.79 (s, 3 H), 3.82 (s, 3 H), 4.24 – 4.29 (m, 1 H), 4.80 (t, J = 4.5 Hz, 1 H), 6.46 (bs, 1 H), 7.03 – 6.74 (m, 7 H) ppm. HRMS (ESI+, m/z) calculated for $C_{17}H_{20}O_6Na$ $[M + Na]^+$ m/z = 343.1158, found 343.1172.

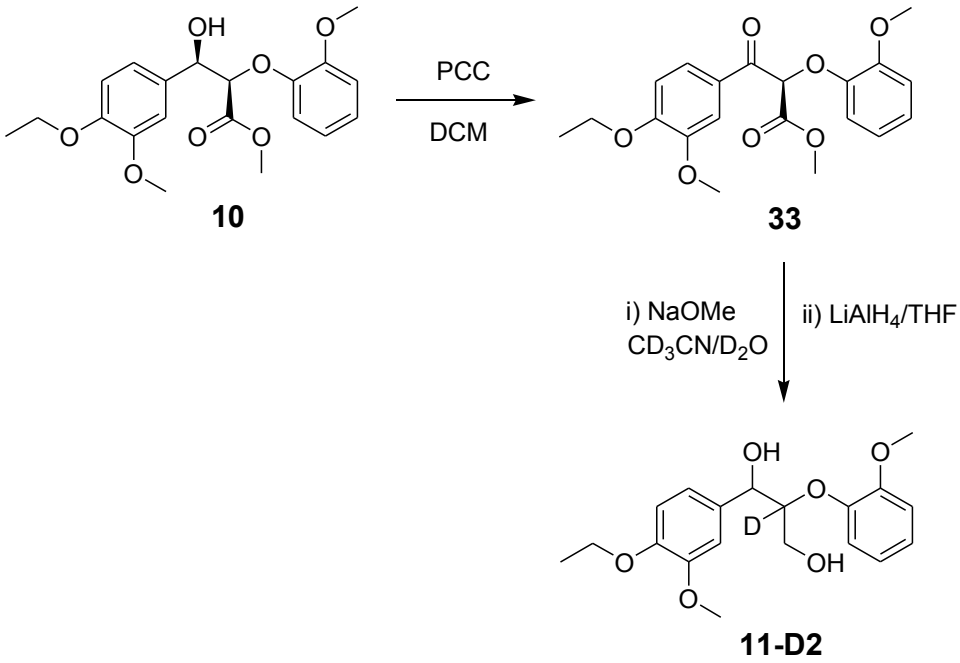


Isotopically ^{13}C-labelled 1-(4-ethoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol (11-^{13}C2). The ^{13}C-labelled congener **11-^{13}C2** was synthesized by adopting a previously published procedure on a smaller scale.[4] The quantities of reagents used are as follows: 4-ethoxy-3-methoxybenzaldehyde (0.90 g, 5.0 mmol), **^{13}C2**-labeled **26** (1.09 g, 5.50 mmol), and 1 M of LDA solution in THF (5.5 mL, 5.5 mmol) in the first step. The reduction of the crude product from first step was conducted with $NaBH_4$ (0.950 g, 25 mmol) to obtain compound **11-^{13}C2** in the second step. The product identity has been confirmed by NMR spectroscopy and HR-MS. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 1.45 (t, J = 6.9 Hz, 3 H), 2.40 (bs, 2 H), 3.40 – 3.71 (m, 1 H), 3.87 (s, 3 H), 3.89 (s, 3 H), 3.90 – 3.93 (m, 1 H), 4.09 (q, J = 6.9 Hz, 2 H), 4.27 (bd, J = 78 Hz, 1 H), 4.98 (d, J = 4.8 Hz, 1 H), 7.09 – 6.82 (m, 7 H), ppm.^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ = 14.9, 56.0, 56.1, 60.9 (d, $^1J_{C\text{-}C}$ = 41.2), 64.5, 72.88 (d, $^1J_{C\text{-}C}$ = 40.5 Hz), 87.3 (d, $^1J_{C\text{-}C}$ = 40.5 Hz), 109.7, 112.3, 112.7, 118.6, 120.9, 121.7, 124.2, 132.8, 147.1, 147.9, 149.4, 151.6 ppm. HRMS (ESI+, m/z) calculated for $C_{17}{}^{13}C_2H_{24}O_6Na$ $[M + Na]^+$ m/z = 373.1538, found 373.1530.



14 **32** **11-D1**

Deuterated 1-(4-ethoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol (11-D1). The deuterated congener **11-D1** was synthesized by adopting a previously published procedure on a smaller scale.[4] The quantities of reagents used are as follows: in the first step, compound **14** (0.632 g, 2.0 mmol), NaH in the form of a 60% dispersion in mineral oil (0.072 g, 1.8 mmol), and paraformaldehyde (0.060 g, 2.0 mmol) were used to synthesize **32**. The reduction of **32** (0.173 g, 0.50 mmol) was performed with $LiAlD_4$ (0.025 g, 0.60 mmol) to give **11-D1**. The product identity has been confirmed by NMR spectroscopy and HR-MS. The ^1H NMR spectrum showed that **11-D1** consisted of two diastereoisomers in a 4:6 ratio. Major diastereoisomer, ^1H NMR (CD_3CN, 300 MHz): δ = 1.35 (t, J = 6.9 Hz, 3 H), 3.05 (bs, 1 H), 3.40 – 3.72 (m, 2 H), 3.47 (bs, 1 H), 3.77 (s, 3 H), 3.84 (s, 3 H), 4.01 (q, J = 6.9 Hz, 2 H), 4.18 (dd, J = 5.4, 3.9 Hz, 1 H), 6.84 – 7.09 (m, 7 H) ppm. Minor diastereoisomer, δ = 1.35 (t, J = 6.9 Hz, 3 H), 3.05 (bs, 1 H), 3.40 – 3.72 (m, 2 H), 3.47 (bs, 1 H), 3.77 (s, 3 H), 3.79 (s, 3 H), 4.01 (q, J = 6.9 Hz, 2 H), 4.27 (dd, J = 5.1, 3.9 Hz, 1 H), 6.84 – 7.09 (m, 7 H) ppm. $^2H\{^1H\}$ NMR (CD_3CN, 400 MHz): δ = 4.83 ppm. HRMS (ESI+, m/z) calculated for $C_{19}H_{23}DO_6Na$ $[M + Na]^+$ m/z = 372.1533, found 372.1542.



10 **33** **11-D2**

Deuterated 1-(4-ethoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol (11-D2). The deuterated congener **11-D2** was synthesized from compound **10.** Compound **10** (0.376 g, 1.0 mmol) in dry DCM (15 mL) was stirred at room temperature overnight with pyridinium chlorochromate (0.259 g, 1.2 mmol) to obtain compound **33**. Purification by flash column chromatography on silica yielded compound **33** as white solid (0.318 g, 85%). The deuteration was carried out under moisture- and air-free conditions. A 50 mL oven-dried RBF was filled with Ar, **33** (0.075 g, 0.20 mmol), and a catalytic amount of NaOMe (0.0011g, 0.020 mmol), following which CD_3CN (1.0 mL) was added. After stirring for 10 min, D_2O (1.0 mL) was injected to the mixture and the solution was stirred at room temperature under Ar for 12 h. The solvent was removed under reduced pressure at 60 ºC, and the residue was dried under vacuum and refilled with Ar. CD_3CN (1.0 mL) followed by D_2O (1.0 mL) were injected to the RBF again and stirred for another 6 h. This sequence of solvent removal and stirring with deuterated solvents was repeated thrice for complete deuteration. Finally, after solvent removal, the reaction mixture was dissolved in of $CDCl_3$ (2.0 mL) and filtered into another dry 50 mL of RBF. The solvent was removed in vacuo and the residue was dried and

stored under Ar. Dry THF (10 mL) was injected and the reaction mixture was cooled in an ice bath under stirring. Excess $LiAlH_4$ (0.038 g, 1.0 mmol) was added slowly to the reaction mixture and stirred at room temperature. After 24 h, aqueous NaOH (10% w/w, 0.50 mL) was added and the reaction mixture was stirred for another 10 min. The solvent was then removed in vacuo. The residue was extracted with $CHCl_3$ (3 × 10 mL) and dried to give the crude **11-D2**. The product was purified by preparative TLC as a colourless oil (0.042 g, 60 %). ^{1}H NMR (CD_3CN, 300 MHz): δ = 1.34 (t, J = 6.9 Hz, 3 H), 3.06 (bs, 1 H), 3.63 – 3.75 (m, 2 H), 3.77 (s, 3 H), 3.79 (s, 3 H), 4.00 (q, J = 6.9 Hz. 2 H), 4.82 (s, 1 H), 6.81 – 7.02 (m, 7 H) ppm. ^{2}H{^{1}H} NMR (CD_3CN, 400 MHz): δ = 4.26 ppm. HRMS (ESI+, m/z) calculated for $C_{19}H_{23}DO_6Na$ $[M + Na]^+$ m/z = 372.1533, found 372.1534.

IV. Single crystal X-ray structure of compounds

Vanadium oxo complex 2

A red block of **2** ($C_{16}H_{16}FN_2O_5V$), with approximate dimensions 0.120× 0.180× 0.360 mm, was used for the single crystal X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 0.39 h. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 21857 reflections to a maximum θ angle of 31.09° (0.69 Å resolution), of which 5189 were independent (average redundancy = 4.212, completeness = 99.8%, R_{int} = 3.70%, R_{sig} = 3.22%) and 4378 (84.37%) were greater than $2\sigma(F^2)$. The final cell constants of $\underline{a}$ = 7.9908(3) Å, $\underline{b}$ = 17.1771(6) Å, $\underline{c}$ = 11.9692(5) Å, β = 100.2079(18)°, volume = 1616.87(11) Å^3, are based upon the refinement of the XYZ-centroids of 5914 reflections above 20 σ(I) with 5.697° < 2θ < 62.13°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to

maximum apparent transmission was 0.881. The calculated minimum and maximum transmission coefficients (based on crystalsize) are 0.7980 and 0.9260. The final anisotropic full-matrix least-squares refinement on F^2 with 232 variables converged at R1 = 3.32%, for the observed data and wR2 = 8.72% for all data. The goodness-of-fit was 1.039. The largest peak in the final difference electron density synthesis was 0.476 $e^-/Å^3$ and the largest hole was -0.374$e^-/Å^3$ with an RMS deviation of 0.068 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.587 g/cm^3 and the F(000) was 792 e^-.

Vanadium oxo complex 5

A red block of $C_{15}H_{22}NO_4V$, with approximate dimensions 0.200 × 0.220 × 0.420 mm, was used for the single crystal X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 0.33 h. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 12950 reflections to a maximum θ angle of 31.07° (0.69 Å resolution), of which4783 were independent (average redundancy = 2.708, completeness = 99.8%, R_{int} = 2.65%, R_{sig} = 3.77%) and 4492 (93.92%) were greater than $2\sigma(F^2)$. The final cell constants of $\underline{a}$ = 14.7897(4) Å, $\underline{b}$ = 13.1867(3) Å, $\underline{c}$ = 7.8841(2) Å, volume = 1537.62(7) $Å^3$, are based upon the refinement of the XYZ-centroids of 5799 reflections above 20 σ(I) with 5.508° < 2θ < 62.11°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.819. The calculated minimum and maximum

transmission coefficients (based on crystal size) are 0.7690 and 0.8790. The final anisotropic full-matrix least-squares refinement on F^2 with 194 variables converged at R1 = 2.89%, for the observed data and wR2 = 7.40% for all data. The goodness-of-fit was 1.072. The largest peak in the final difference electron density synthesis was 0.397 $e^-/Å^3$ and the largest hole was -0.268$e^-/Å^3$ with an RMS deviation of 0.061 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.431 g/cm^3 and the F(000) was 696 e^-.

Vanadium oxo complex 5 (dimer)

A red plate of $C_{30}H_{44}N_2O_8V_2$, with approximate dimensions 0.060 × 0.160 × 0.400 mm, was used for the single crystal X-ray crystallographic analysis. The X-ray intensity data were measured.The total exposure time was 0.46 h. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 18722 reflections to a maximum θ angle of 31.04° (0.69 Å resolution), of which 5001 were independent (average redundancy = 3.744, completeness = 99.4%, R_{int} = 4.40%, R_{sig} = 4.79%) and 3899 (77.96%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.1706(6) Å, b = 11.0345(5) Å, c = 23.8844(12) Å, β = 100.8835(17)°, volume = 3149.9(3) $Å^3$, are based upon the refinement of the XYZ-centroids of 4220 reflections above 20 σ(I) with 5.024° < 2θ < 60.83°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.901. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7830 and 0.9620. The final anisotropic full-matrix least-squares refinement on F^2 with 222 variables converged at R1 = 4.09%, for the observed data and wR2 = 10.48% for all data. The goodness-of-fit was 1.052. The largest peak in the final difference electron density synthesis was 0.432 $e^-/Å^3$ and the largest hole

was -0.434$e^-/Å^3$ with an RMS deviation of 0.076 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.397 g/cm^3 and the F(000) was 1392 e^-.

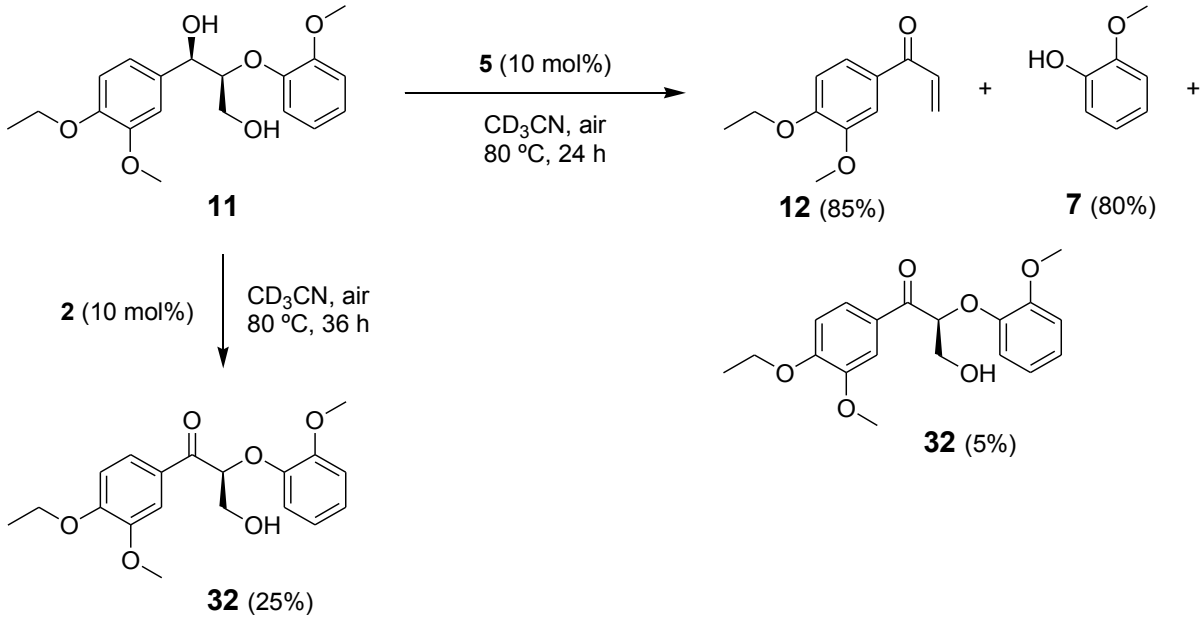
X-ray crystallographic coordinates for structures

2, **5**, and **5 (dimer)** reported herein have been deposited at the Cambridge CrystallographicData Centre (CCDC), under deposition numbers CCDC1058817, 1058818, and 1058819. These data can be obtained free of charge from the Cambridge CrystallographicData Centre via www.ccdc.cam.ac.uk/data_request/cif.

V. Photoluminescence experiments of complex 2

Photoluminescence experiments were performed on methanolic solutions of **2** (1.0 mM).The sample was excited at 360 nm and showed a concentration-dependent emission spectrum with λ_{max} at 480 nm for 1.0 mM of **2** and 466 nm for 0.25mM of **2** (Supporting Information Fig. S2).

VI. Degradation of lignin model compound 11 under thermal conditions

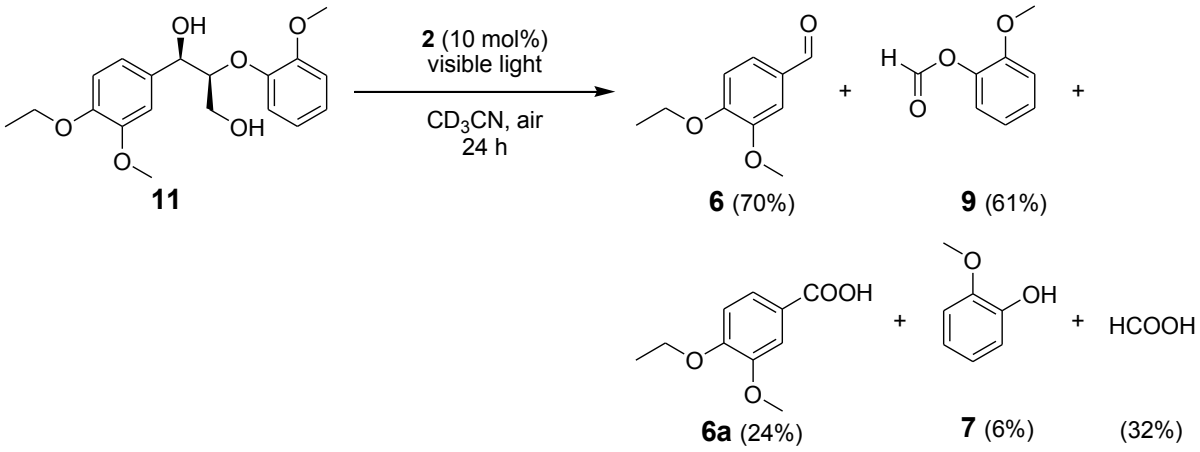


The degradation experiments were carried out in an NMR tube. Compound **11** (0.014 g, 0.040 mmol) in CD_3CN (0.50 mL) with the corresponding catalyst (4.0 μmol) were used in each reaction. An internal standard 1,1,2,2-tetrachloroethane (4.2 μL, 0.040 mmol) was used for calculations of the conversion as well as the yield of the products. The reactions were conducted under air with a balloon to maintain a constant pressure in the sealed tube. The NMR tube was wrapped with aluminium foil during the thermal reactions to minimize the photochemical reactions. The ^{1}H NMR spectra were recorded before and after the reaction. When **5** was used as the catalyst, the reactions were carried out at 25 ºC, 45 ºC, and 80 ºC for 24 h. The conversions and yields were calculated based on the^{1}H NMR spectra. The reaction at 80 ºC gave complete conversion and the major products formed were isolated by preparative TLC and their identities were confirmed by ^{1}H NMR spectroscopy. When **2** was used as the catalyst, the reactions were carried out at 25 ºC and 80 ºC for 36 h. The ^{1}H NMR spectra showed there were no observable changes at room temperature, whereas about 25% of **11** was oxidized to **32** at 80 ºC.

Compound 1-(4-ethoxy-3-methoxyphenyl)prop-2-en-1-one (12)

^{1}H NMR (CD_3CN, 300 MHz): δ = 1.40 (t, J = 6.9 Hz, 3 H), 3.86 (s, 3 H), 4.13 (q, J = 6.9 Hz, 2H), 5.86 (dd, J = 10.5, 2.0 Hz, 1 H), 6.34 (dd, J = 17.1, 2.0 Hz, 1 H), 6.99 (d, J = 8.4 Hz, 1 H), 7.31 (dd, J = 17.1, 10.5 Hz, 1 H), 7.53 (d, J = 2.1 Hz, 1 H), 7.63 (dd, J = 8.4, 2.1 Hz, 1 H) ppm.

VII. Photodegradation of lignin model 11 in the presence of different vanadium oxo complexes



Photodegradation experiments were carried out in an NMR tube. In a typical procedure, **11** (0.014 g, 0.040 mmol) and the vanadium catalyst were dissolved in CD_3CN (0.50 mL) and sealed. Compound 1,1,2,2-tetrachloroethane (4.2 μL, 0.040 mmol) was used as an internal standard to calculate the conversion and yield of the products. A balloon was used to maintain atmospheric conditions via a needle. The reaction mixture was irradiated for 24 h under visible light (> 420 nm) with AM1.5 solar intensity at ambient temperature. A continuous water circulator was used to maintain the temperature below 30 ºC (Supporting Information Fig. S65). The photodegradation experiments were carried out with the different vanadium oxo complexes $VO(OPr)_3$, $VO(acac)_2$, **2**, and **5** with concentrations summarized in Tables 1 and 2 of the main manuscript. Complex **2** was found to be most effective for cleaving **11** into **6** and **9** as the major products through selective C-C bond cleavage. Complete consumption of **11** was observed under optimized conditions. The intermediates formed when stoichiometric amounts of **11** reacted with **2** were detected by ^{1}H NMR spectroscopy (Fig. S68) and ESI-MS (Fig. S69). The ^{1}H NMR spectrum suggests that the solution consists of **2** and at least three new complexes, likely due to diastereomers of **11**

coordinating via the different alcohol groups, in equilibrium at room temperature prior to irradiation.

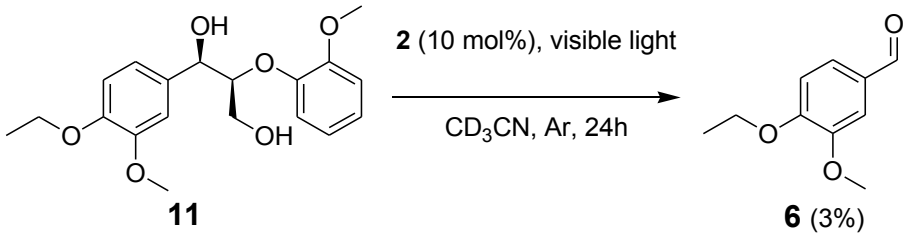
Compound 4-ethoxy-3-methoxybenzaldehyde (6).

^{1}H NMR (CD_3CN, 300 MHz): δ = 1.41 (t, J = 6.9 Hz, 3 H), 3.87 (s, 3 H), 4.15 (q, J = 6.9 Hz, 2 H), 7.07 (d, J = 8.1 Hz, 1 H), 7.40 (d, J= 1.8 Hz, 1 H), 7.49 (dd, J = 8.1, 1.8 Hz, 1 H), 9.83 (s, 1 H) ppm.

2-methoxyphenyl formate (9)

^{1}H NMR (CD_3CN, 300 MHz): δ = 3.82 (s, 3 H), 6.99 (t, J = 7.8 Hz, 1 H), 7.12 (d, J = 7.8 Hz, 2 H), 7.28 (t, J = 7.8 Hz, 1 H), 8.26 (s, 1 H) ppm. $^{13}C\{^1H\}$ NMR (CD_3CN, 75 MHz): δ = 56.9, 114.2, 122.2, 123.9, 128.8, 140.3, 152.5, 161.3 ppm. HRMS (ESI+, m/z) calculated for $C_8H_9O_3$ $[M + H]^+$ m/z = 153.0552, found 153.0547.

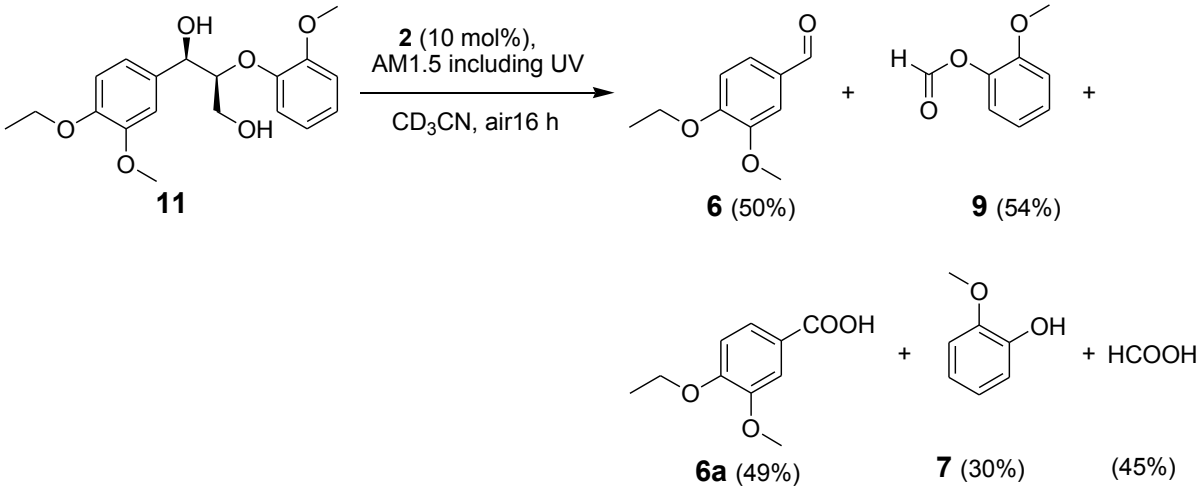
VIII. Photodegradation of 11 with complex 2 under an inert atmosphere



Photodegradation experiments were carried out in a J-Young NMR tube. In a typical procedure, **11** (0.014 g, 0.040 mmol) and the vanadium catalyst were dissolved in CD_3CN (0.50 mL). Compound 1,1,2,2-tetrachloroethane (4.2 μL, 0.040 mmol) was used as an internal standard to calculate the conversion and yield of the products. The dissolved gas in the reaction mixture was removed by six freeze-pump-thaw cycles before the NMR tube was

refilled with argon and sealed. The reaction mixture was irradiated for 24 h under visible light (> 420 nm) with AM1.5 solar intensity at ambient temperature. A continuous water circulator was used to maintain the temperature below 30 ºC (Supporting Information Fig. S65). After 24 h of irradiation, the ^{1}H NMR spectrum was recorded to identify the products and calculate the yields.

IX. Photodegradation of 11 with complex 2 using unfiltered AM1.5 solar irradiation



The photodegradation experiments were carried out in a NMR tube. In a typical procedure, **11** (0.014 g, 0.040 mmol) and **2** (0.0014 g, 4.0 μmol) were dissolved in CD_3CN (0.50 mL) and sealed. A balloon was used to maintain an atmosphere of air via a needle. The reaction mixture was irradiated with AM1.5 solar irradiation without the 420 nm cut-off filter, using a continous water circulator to maintain the temperatures below 30 ºC (Supporting Information Fig. S65). After 16 h of irradiation, the ^{1}H NMR spectrum showed that **11** was completely consumed. The products were identified and quantified with NMR spectroscopy.

X. Photodegradation with isotopically labelled lignin model compounds

The isotopically labelled lignin model compounds **11-^{13}C2**, **11-D1**, and **11-D2** were investigated under the optimized photocatalytic conditions with **2**. In a typical procedure, the substrate (0.014 g, 0.040 mmol) and **2** (0.0014 g, 4.0 μmol) were dissolved in CD_3CN (0.50 mL) in an NMR tube and sealed. A balloon was used to maintain an aerobic environment via a needle. The sample was irradiated for 24 h under visible light (> 420 nm) with AM1.5 solar irradiation with a continuous water circulator used to maintain temperatures below 30 ºC. After 24 h of irradiation, the products were identified and the yields were quantified by ^{1}H NMR spectroscopy.

Deuterated-4-ethoxy-3-methoxybenzaldehyde (6-D).

^{1}H NMR (CD_3CN, 300 MHz): δ = 1.41 (t, J = 6.9 Hz, 3 H), 3.87 (s, 3 H), 4.15 (q, J = 6.9 Hz, 2H), 7.07 (d, J = 8.1 Hz, 1 H), 7.40 (d, J = 1.8 Hz, 1 H), 7.49 (dd, J = 8.1, 1.8 Hz, 1 H). ^{2}H{^{1}H} NMR (CD_3CN, 400 MHz): δ = 9.86 (s, 1 D) ppm. HRMS (ESI+, m/z) calculated for $C_{10}H_{12}DO_3$ $[M + H]^+$ m/z = 182.0927, found 182.0932.

Deuterated-2-methoxyphenyl formate (9-D)

^{1}H NMR (CD_3CN, 300 MHz): δ = 3.82 (s, 3 H), 6.99 (t, J = 7.8 Hz, 1 H), 7.09 – 7.14 (m, 2 H), 7.28 (t, J = 7.8 Hz, 1 H). ^{2}H{^{1}H} NMR (CD_3CN, 400 MHz): δ = 8.31 (s, 1 D). HRMS (ESI+, m/z) calculated for $C_8H_8DO_3$ $[M + H]^+$ m/z = 154.0614, found 154.0610.

^{13}C2-methoxyphenyl formate (9-^{13}C1)

^{1}H NMR (CD_3CN, 300 MHz): δ = 3.82 (s, 3 H), 6.99 (t, J = 7.8 Hz, 1 H), 7.12 (d, J = 8.1 Hz, 2 H), 7.28 (t, J = 8.1 Hz, 1 H), 8.26 (d, J = 234 Hz, 1 H). $^{13}C\{^{1}H\}$ NMR (CD_3CN, 75 MHz): δ = 56.9, 114.3, 122.2, 123.9, 128.8, 140.2, 152.4, 161.3 ppm. HRMS (ESI+, m/z) calculated for $C_7{}^{13}C_1H_9O_3$ $[M + H]^+$ m/z = 154.0585, found 154.0583.

XI. Photodegradation of other lignin model compounds and organic substrates with complex 2

Other lignin model compounds **13**, **15**, **25, 28**, and **31** were also investigated under similar photocatalytic reaction conditions in an NMR tube. Complex **2** was found to be inactive for **28** and **31**, whereas **13** and **15** gave C-C bond cleavage products **6** and **9** at slower rates. These experiments have been summarized in Fig. 6 of the main text. Compound **25** gave a complex product mixture (Supporting Information Fig. S4) containing formic acid and **6** among other products.Other substrates **17**, **20**, **23**, and **27** were also investigated under similar photocatalytic reaction conditions. The ^{1}H NMR spectroscopic analysis revealed that **17**, **20**, and **23** degraded by C-C bond cleavage to the corresponding aldehydes along with benzylic alcohol oxidation to their corresponding ketones. The products were isolated and their identities were confirmed by ^{1}H NMR spectroscopy and HR-MS. Compound **27** gave **9**and formic acid under the photocatalytic conditions. Aliphatic alcohols like glycerol (**35**) and 1-butanol (**36**) were found to convert into formic acid after photolysis with **2**, albeit in low yields. These reaction conditions with aliphatic alcohols have not been optimized.

1-(4-ethoxy-3-methoxyphenyl)-3-hydroxypropan-1-one (18).

^{1}H NMR (CD_3CN, 300 MHz): δ = 1.40 (t, J = 6.9 Hz, 3 H), 3.13 (t, J = 6.0 Hz, 2 H), 3.86 (s, 3 H), 3.87 (t, J = 6.0 Hz, 3 H), 4.13 (q, J = 6.9 Hz, 2 H), 6.98 (d, J = 8.4 Hz, 1 H), 7.50 (d, J = 2.0 Hz, 1 H), 7.62 (dd, J = 8.4, 2.0 Hz, 1 H) ppm. HRMS (ESI+, m/z) calculated for $C_{12}H_{17}O_4$ $[M + H]^+$ m/z = 225.1127, found 225.1124.

3-hydroxy-1-phenylpropan-1-one (21)

^{1}H NMR (CD_3CN, 300 MHz): δ = 3.18 (t, J = 6.0 Hz, 2H), 3.89 (t, J = 6.0 Hz, 3H),7.49 – 7.54 (m, 2H), 7.59 – 7.62 (m, 1H), 7.96 – 7.99 (m, 1H) ppm. HRMS (ESI+, m/z) calculated for $C_9H_{10}O_2Na$ $[M + Na]^+$ m/z =173.0578, found 173.0572.

3-hydroxy-1-(4-nitrophenyl)propan-1-one (24)

^{1}H NMR (CD_3CN, 300 MHz): δ = 3.23 (t, J = 6.0 Hz, 2 H), 3.90 (t, J = 6.0 Hz, 3 H), 8.14 (d, J = 9.0 Hz, 2 H), 8.30 (d, J = 9.0 Hz, 2 H), ppm. HRMS (ESI+, m/z) calculated for $C_9H_{10}NO_4$ $[M + H]^+$ m/z = 196.0610, found 196.0603.

XII. Reduction of vanadium(V) oxo complex (2) to the vanadium(IV) oxo (3)

The reduction of **2** was conducted under moisture- and air-free conditions. An oven-dried Schlenk flask was filled with **2** (0.071 g, 0.20 mmol) and anhydrous DCM (5 mL). Cobaltocene (0.041 g, 0.22 mmol) in anhydrous DCM (5 mL) was injected and the reaction mixture was stirred under N_2. The reaction mixture turned from reddish brown to green slowly. After stirring overnight, hexane (25 mL) was added and a deep green precipitate formed. After deposition of the precipitate, the mother liquor was decanted and the precipitate was washed with hexane (2 × 10 mL). The green solid was dried under vacuum

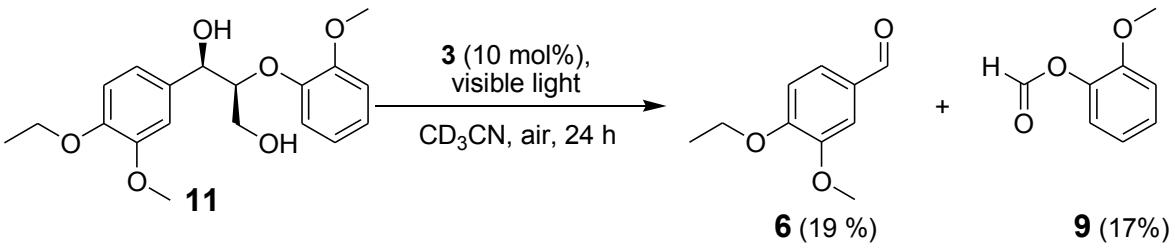
and stored under N_2 (0.050 g). The EPR spectrum (Supporting Information Fig. S5b) of this solid was recorded and exhibited the characteristic signals of a vanadium(IV) species. However, due to poor solubility of the product, **3** could not be isolated in its pure form through crystallization. The as-synthesized **3** was used in photodegradation experiments of the lignin model compound **11**.

XIII. Photodegradation of 11 in the presence of V^{IV} complex 3

Reaction under inert atmosphere

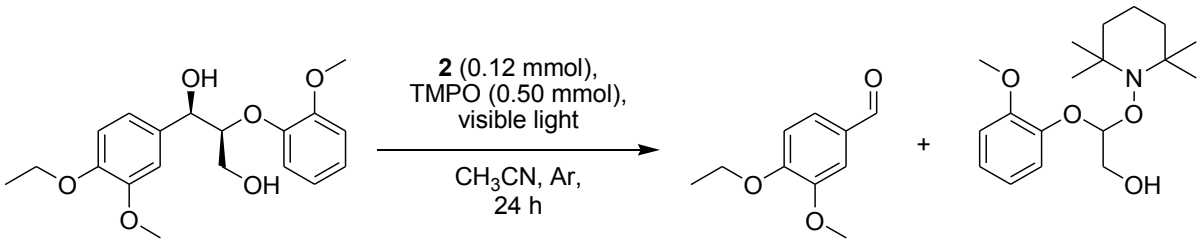
In a glass vial (20 mL), **11** (0.014 g, 0.040 mmol) and **3** (0.0014 g, 4.0 μmol) were dissolved in CH_3CN (5 mL), and the solvent was removed under reduced pressure by rotary evaporation, after which the mixture was dried in vacuo for 1 h. The vial was refilled with Ar and anhydrous CH_3CN (10 mL) was injected. The reaction mixture was stirred in the dark for 10 min with continuous Ar bubbling. The reaction mixture was then sealed and irradiated under visible light (> 420 nm) with AM1.5 solar irradiation. The reaction vial was cooled by a continuous water circulator to keep temperatures below 30 ºC (Supporting Information Fig. S65). After 24 h of irradiation, the solvent was removed by rotary evaporation and the residue was dried in vacuo. The ^1H NMR spectrum showed that **3** was ineffective for thephotocatalytic degradation of **11** under Ar.

Reaction under air



The photodegradation experiments were carried out in a NMR tube. In a typical procedure, **11** (0.014 g, 0.040 mmol) and **3** (0.0014 g, 4.0 μmol) were suspended in CD_3CN (0.50 mL) and sealed. Compound 1,1,2,2-tetrachloroethane (4.2 μL, 0.040 mmol) was added as an internal standard to calculate the conversion and product yields. A balloon was used to maintain an aerobic environment via a needle was passed through the cap into the NMR tube to keep the reaction mixture in contact with air. The sample was irradiated for 24 h under visible light (> 420 nm) with AM1.5 solar irradiation with a continuous water circulator used to maintain temperatures below 30 ºC. After 24 h of irradiation, ^{1}H NMR spectroscopy was used to identify the products (**6** and **9**) and quantify the yields.

XIV. Intermediate trapping by TEMPO



11 (0.10 mmol) **6** **34**

In a glass vial (20 mL), **11** (0.035 g, 0.10 mmol) and **2** (0.042 g, 0.12mmol) were dissolved in MeOH (5 mL) and the solvent was removed by rotary evaporation before being dried in vacuo for 1h. The vial was refilled with Ar and anhydrous CH_3CN (10 mL) was injected to the vial, followed by addition of(2,2,6,6-tetramethylpiperidin-1-yl)oxy (TEMPO, 0.078 g, 0.50 mmol). The solution was stirred in the dark for 10 min and bubbled with Ar. The sample was irradiated for 24 h during which the initially reddish brown solution turned green. The solvent was then removed by rotary evaporation, the residue was dried in vacuo, after which DCM (10 mL) was added. The solution was filtered through a silica plug and rinsed with DCM (90 mL). The solvent was removed at 25 ºC under reduced pressure to yield an oil. The

TEMPO trapped adduct (**34**) was identified by LCMS (m/z 324.2) and was isolated by preparative TLC of the crude product. Compound **34** was identified by ^{1}H, ^{13}C, and DEPT NMR spectroscopy (Supporting Information Fig. S60-63), NOESY (Supporting Information Fig. S64) as well as by mass spectrometry (Supporting Information Fig. S6).

TEMPO-adduct (34).

^{1}H NMR (CD_3CN, 300 MHz): δ = 1.12 (s, 3 H), 1.14 (s, 3 H), 1.18 (s, 3 H), 1.24 (s, 3 H), 1.44 – 1.60 (m, 6 H), 3.07 (dd, J = 4.8, 8.4Hz, 1 H), 3.53 – 3.61 (m, 1 H), 3.66 – 3.72 (m, 1 H), 3.80 (s, 3 H), 5.41 (dd, J = 4.8, 6.6 Hz, 1 H), 6.90 – 7.51 (m, 3 H), 7.53 (d, J = 0.9 Hz, 1 H) ppm. $^{13}C\{^{1}H\}$ NMR (CD_3CN, 100 MHz): δ = 18.3, 20.9, 21.3, 33.4, 33.9, 41.2, 41.5, 56.8, 60.7, 62.3, 63.5, 110.3, 113.8, 120.4, 122.4, 123.9, 149.1, 151.7 ppm. ^{13}C-DEPT-135 (CD_3CN, 100 MHz): δ = 18.3, 20.9, 21.3, 33.4, 33.9, 41.2, 41.5, 56.8, 63.5, 110.3, 113.8, 120.4, 122.4, 123.9 ppm. ^{13}C-DEPT-90 (CD_3CN, 100 MHz): δ = 110.3, 113.8, 120.4, 122.4, 123.9 ppm. HRMS (ESI+, m/z) calculated for $C_{18}H_{30}NO_4$ $[M + H]^+$ m/z = 324.2175, found 324.2176.

XV. Experiments for TEM measurements

Compounnd **11** with complex **2** were dissolved in acetonitrile. To verify the homogeneous reactivity of **2** in this photocatalytic system, transmission electron microscopic (TEM) images were recorded before and after the reaction as illustrated in Supporting Information Fig. S7. Images Fig. S7a and 7b were obtained before irradiation, and shows the presence of amorphous depositions. After irradiation (Supporting Information Fig. 7c and 7d), the images suggested sporadic distribution of irregularly shaped particles, which may be due to

precipitation of the catalyst or substrate after solvent evaporation or oxidation of **2** to vanadium oxides. However, the selectivity of the reactions, especially the isotope labeling experiments, and the DFT calculations do not support the operation of heterogeneous catalysis.

XVI. Measurement of quantum yields

- **Under visible irradiation**

Potassium ferrioxalate ($K_3[Fe(OX)_3].3H_2O$, OX = oxalate) is a standard chemical actinometer for the determination of quantum yields for photochemical reactions under visible light in an aqueous medium.[5] Since the photocatalytic lignin degradation was carried out in CH_3CN, it was necessary to use a chemical actinometer that functions in CH_3CN. Thus, complex (n-$Bu_4N)_3[Fe(OX)_3]$ was synthesized to be used as a chemical actinometer in organic CH_3CN.

The complex (n-$Bu_4N)_3[Fe(OX)_3]$ was synthesized in two steps. The complex (n-$Bu_4N)_3[Fe(OX)_3]$ was crystallized with (n-Bu_4N)Cl as an impurity,since both complexes have very similar solubility properties. Consequently, the Fe content was experimentally determinedin the mixture of (n-$Bu_4N)_3[Fe(OX)_3]$ and (n-Bu_4N)Cl prior to use. A known amount of the mixture (0.040 g) was dissolved in 5 mL of deionized water in the dark. A sample (2 mL) was irradiated under visible light (AM1.5, 420 nm cut-off filter) for 2 h for complete conversion of Fe(III) to Fe(II). After addition of 1,10-phenanthroline (Phen), the Fe(II) was quantified by measuring the absorbance of the $[Fe(Phen)_3]^{2+}$ complex ion. The concentration was determined using the molar extinction coefficient of $[Fe(Phen)_3]^{2+}$ at 510 nm (1.12×10^4 $M^{-1}cm^{-1}$). It was found that 0.040 g of the mixture contains 1.07×10^{-5} mol of

iron. Accordingly, 0.0112 g (1.07×10^{-5} mol) of the complex (n-$Bu_4N)_3[Fe(OX)_3]$ is present in 0.040 g of the mixture.

The quantum yield of (n-$Bu_4N)_3[Fe(OX)_3]$ in CH_3CN is required to determine the quantum yield of the photocatalytic degradation of **11**. Hence, the quantum yield of (n-$Bu_4N)_3[Fe(OX)_3]$ in water was first determined by comparison with the reported quantum yield of $K_3[Fe(OX)_3]$ in water.[5] The quantum yield of (n-$Bu_4N)_3[Fe(OX)_3]$ in CH_3CN was then determined relative to the quantum yield of (n-$Bu_4N)_3[Fe(OX)_3]$ in water. Finally, the quantum yield of the photocatalytic degradation of **11** was determined relative to the quantum yield of (n-$Bu_4N)_3[Fe(OX)_3]$ in CH_3CN.

For each experiment, a 0.60 mL solution containing the respective chemical actinometer and 1,10-phenanthroline (1:3 mole ratio) weredissolved in anoven-dried NMR tube and irradiated under visible light for different lengths of time. The UV-Vis spectrum of each sample was recorded at regular time intervals (Fig. S66). The rate of formation of Fe(II) was then derived from the UV-vis absorption spectra at 510 nm.

Since the quantum yield of $K_3[Fe(OX)_3]$ in water has been reported to be 1.11 at 436 nm in the visible region, all the quantum yields were determined at 436 nm.[5] The quantum yields were calculated using the equation $\phi_2 = (f_1 . \phi_1 . r_2) / (f_2 . r_1)$, where ϕ_1 = known quantum yield of any photoreaction 1, r_1 = rate of reaction 1, f_1 = fraction of light absorbed by the photoactive species used in reaction 1, r_2 = rate of reaction 2, f_2 = fraction of light absorbed by the photoactive species used in reaction 2, and ϕ_2 = quantum yield of the photoreaction 2 to be determined.

Results

$K_3[Fe(OX)_3]$ in water

For $K_3[Fe(OX)_3]$ in water, r_1 = 0.509 s^{-1} (Fig. S66a), $f_1 = (1\text{-}10^{-A}) = 0.995$, since the absorbance at 436 nm is 2.28, and $\phi_1 = 1.11$.

(n-$Bu_4N)_3[Fe(OX)_3]$ in water

For (n-$Bu_4N)_3[Fe(OX)_3]$ in water, r_2 = 0.442 s^{-1} (Fig. S66b), $f_2 = (1\text{-}10^{-A}) = 0.986$, since the absorbance at 436 nm is 1.84, and ϕ_2 = quantum yield to be determined.

(n-$Bu_4N)_3[Fe(OX)_3]$ in CH_3CN

For (n-$Bu_4N)_3[Fe(OX)_3]$ in CH_3CN, r_3 = 0.396 s^{-1} (Fig. S66c), $f_3 = (1\text{-}10^{-A}) = 0.922$, since the absorbance at 436 nm is 1.11, and ϕ_3 = quantum yield to be determined.

Lignin model compound 11 in CH_3CN

Compound **11** (0.028 mmol) in CD_3CN with **2** (0.0028 mmol) were irradiated in the presence of an internal standard (1,1,2,2-tetrachloroethane) in an NMR tube. After 24 h under the standard optimized photocatalytic conditions, **11** was completely consumed. The rate, r_4 = 0.028 mmol / 24 h = 3.24 x 10^{-7} mmol s^{-1}, $f_4 = (1\text{-}10^{-A}) = 0.99$, since the absorbance of **2** at 436 nm is more than 2.0, and ϕ_4 = quantum yield to be determined.

Calculations

$\phi_1 = 1.11$, quantum yield of $K_3[Fe(OX)_3]$ in water

$\phi_2 = (f_1 . \phi_1 . r_2) / (f_2 . r_1)$

$= (0.995 \times 1.11 \times 0.442\ s^{-1}) / (0.986 \times 0.509\ s^{-1})$

$= 0.973$, quantum yield of (n-$Bu_4N)_3[Fe(OX)_3]$ in water

$\phi_3 = (f_2 . \phi_2 . r_3) / (f_3 . r_2)$

$= (0.986 \times 0.973 \times 0.396\ s^{-1}) / (0.922 \times 0.442\ s^{-1})$

= 0.932, quantum yield of (n-$Bu_4N)_3[Fe(OX)_3]$ in CH_3CN

$r_3 = 0.396\ s^{-1}$

= (0.396 / ($1.12 \times 10^4\ M^{-1}\ cm^{-1} \times 1$ cm) of 0.6 mL s^{-1}, since $A = \varepsilon_{510}.c.l$

= 3.54×10^{-5} M of 0.6 mL s^{-1}

= 2.12×10^{-8} mol s^{-1}

= 2.12×10^{-5} mmol s^{-1}

$\phi_4 = (f_3.\ \phi_3.\ r_4) / (f_4.\ r_3)$

= ($0.922 \times 0.932 \times 3.24 \times 10^{-7}$ mmol s^{-1})/($0.99 \times 2.12 \times 10^{-5}$ mmol s^{-1})

= 0.0133, quantum yield for the photocatalytic degradation of **11** in CH_3CN under visible light irradiation

- **Under AM1.5 irradiation**

A 0.60 mL containing the respective chemical actinometer and 1,10-phenanthroline (1:3 mole ratio) were dissolved in an oven-dried NMR tube and irradiated with AM1.5 irradiation. The UV-Vis spectrum of each sample was recorded at regular time intervals (Fig. S66d). Since the quantum yield of $K_3[Fe(OX)_3]$ in water has been reported to be 1.25 at 334 nm, all the quantum yields were determined at 334 nm.[5]

Results

$K_3[Fe(OX)_3]$ in water

For $K_3[Fe(OX)_3]$ in water, $r_1 = 0.777\ s^{-1}$ (Fig. S66d), $f_1 = (1\text{-}10^{-A}) = 0.99$, since the absorbance at 334 nm is 2, and $\phi_1 = 1.25$.

(n-$Bu_4N)_3[Fe(OX)_3]$ in water

For (n-Bu4N)$_3$[Fe(OX)$_3$] in water, $r_2 = 0.674\ s^{-1}$, $f_2 = (1\text{-}10^{-A}) = 0.99$, since the absorbance at 334 nm is more than 2, and ϕ_2 = quantum yield to be determined.

(n-Bu$_4$N)$_3$[Fe(OX)$_3$] in CH$_3$CN

For (n-Bu$_4$N)$_3$[Fe(OX)$_3$] in CH$_3$CN, $r_3 = 0.603\ s^{-1}$, $f_3 = (1\text{-}10^{-A}) = 0.99$, since the absorbance at 334 nm is 2, and ϕ_3 = quantum yield to be determined.

Lignin model compound 11 in CH$_3$CN

Compound **11** (0.028 mmol) in CD$_3$CN with **2** (0.0028 mmol) were irradiated in the presence of an internal standard (1,1,2,2-tetrachloroethane) in an NMR tube. After 16 h under the standard optimized photocatalytic conditions, **11** was completely consumed. The rate, r_4 = 0.028 mmol / 16h = 4.86×10^{-7} mmol s^{-1}, $f_4 = (1\text{-}10^{-A}) = 0.99$, since the absorbance of **2** at 334 nm is more than 2.3, and ϕ_4 = quantum yield to be determined.

Calculations

$\phi_1 = 1.11$, quantum yield of K$_3$[Fe(OX)$_3$] in water

$\phi_2 = (f_1 . \phi_1 . r_2) / (f_2 . r_1)$

$= (0.99 \times 1.25 \times 0.674\ s^{-1})/(0.99 \times 0.777\ s^{-1})$

= 1.08, quantum yield of (n-Bu$_4$N)$_3$[Fe(OX)$_3$] in water

$\phi_3 = (f_2 . \phi_2 . r_3) / (f_3 . r_2)$

$= (0.99 \times 1.084 \times 0.603\ s^{-1})/(0.99 \times 0.674\ s^{-1})$

= 0.966, quantum yield of (n-Bu$_4$N)$_3$[Fe(OX)$_3$] in CH$_3$CN

$r_3 = 0.603\ s^{-1}$

$= (0.603 / (1.12 \times 10^4\ M^{-1}cm^{-1} \times 1\ cm)$ of 0.6 mL s^{-1}

$= 5.38 \times 10^{-5}$ M of 0.6 mL s^{-1}

$= 3.23 \times 10^{-8}$ mol s^{-1}

$= 3.23 \times 10^{-5}$ mmol s^{-1}

$\phi_4 = (f_3 . \phi_3 . r_4) / (f_4 . r_3)$

$= (0.99 \times 0.966 \times 4.86 \times 10^{-7}$ mmol $s^{-1})/(0.99 \times 3.23 \times 10^{-5}$ mmol $s^{-1})$

= 0.0145, quantum yield for the photocatalytic degradation of **11** in CH_3CN under AM1.5 irradiation.

XVII. Photoluminescence experiments

The steady-state photoluminescence measurements were conducted using a fluorescence spectrophotometer (Varian Cary Eclipse). Experiments were conducted with excitation at 360, 375, 420, and 430 nm. The emission intensity with 430 nm excitation was too low to be recorded and have not been shown. The concentration dependence of the emission is consistent with H-type aggregates (Fig. S2). In addition, the absorption spectra of **2** blue-shift and broaden as the concentration increases (Fig. S2e), which is also typical of H-type aggregates. Complex **2** may dimerize in a way that the transition to the higher energy exciton state is favored while the lower exciton energy state has much lower transition dipole moments. Consequently, at higher concentrations, the luminescence quantum yields are reduced and the photoluminescence red-shifts.[19] Another possible cause is the inner filter effect or reabsorption of the photoluminescence due to the overlap of the absorption and emission spectra. The absorption band of **2** overlaps with the blue side of the photoluminescence and some of the light can be reabsorbed.[20-22] Consequently, the emission intensity initially increases and reaches a maximum between 0.2 to 0.4 mM, before beginning to red-shift slightly as concentration increases further.

The photoluminescence lifetimes were measured by a time-correlated single photon counting (TCSPC) method with a spectrofluorimeter (FluoroCube, Horiba Jobin Yvon). A 0.25 mM solution of **2** was used with excitation at 375 nm, and the decay of the signal at 480 nm was detected.

XVIII. Electrochemistry experiments

Cyclic voltammetry (CV) experiments were conducted using a Biologic SP-300 potentiostat with 1.0 mM solutions of the sample and 0.10 M *n*-Bu_4NPF_6 as the electrolyte in CH_3CN at a scan rate of 100 mV s^{-1}. A standard three-electrode electrochemical cell was used with a

glassy carbon working electrode (3 mm in diameter from BAS), a Pt wire as the counter electrode, and another Pt wire as the pseudoreference electrode. The potentials were reported by addition of ferrocene as an internal reference (0 V) after the CV measurements on the compound have been conducted to avoid obscuring signals from our samples. Before each experiment, the working electrode (glassy carbon) was polished using a 0.05 μm alumina solution on a polishing pad, followed by sonication in DI water for 10 min and dried in air. In each experiment, the solutions were prepared by bubbling Ar through the solvents for 10 min. The differential pulse voltammograms (DPV) of each sample measured were conducted with the following parameters: scan rate of 50 mV s^{-1}, pulse-height of 50 mV, pulse-width of 50 ms, step-height of 4 mV, and step-time of 80 ms. The DPVs of compounds **1**, **2**, **4**, and **5** are depicted in Fig. S67. With reduced effects of the charging current, the peaks of the samples are more clearly observed. The ligand **1** shows an asymmetric peak at +1.17 V, corresponding to the multi-electron irreversible oxidation observed in the CV (Fig. 3d). The DPV of **2** has a relatively symmetrical peak at –0.09 V, consistent with the reversible V^{V}/V^{IV} wave detected in the CV (Fig. 3d). The DPV of ligand **4** appears to show a reversible oxidation around +0.55 V, whereas the DPV of **5** is complicated by multiple redox events between –1 to +1.5 V in the electrochemical window measured.

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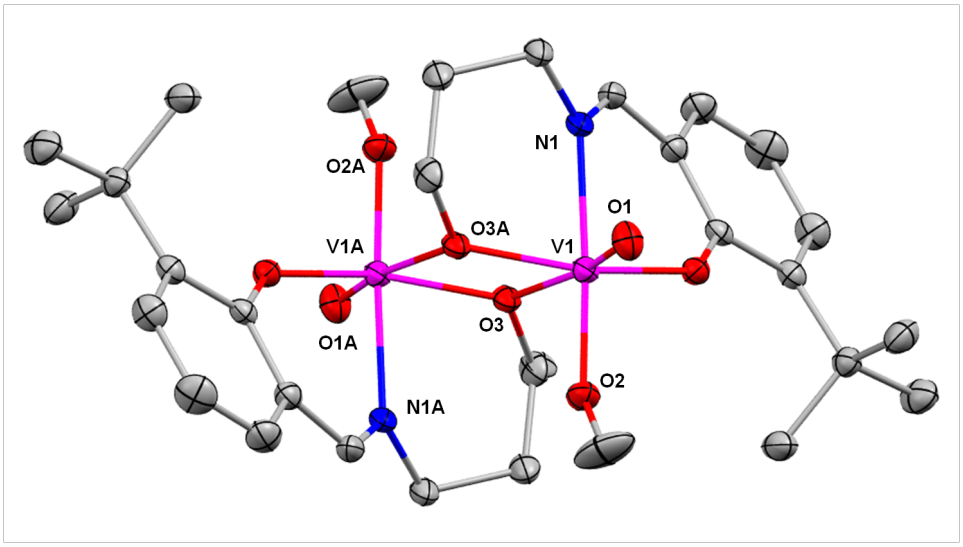


Fig. S1 ORTEP from single crystal X-ray diffraction experiments of dimeric polymorph **5.**

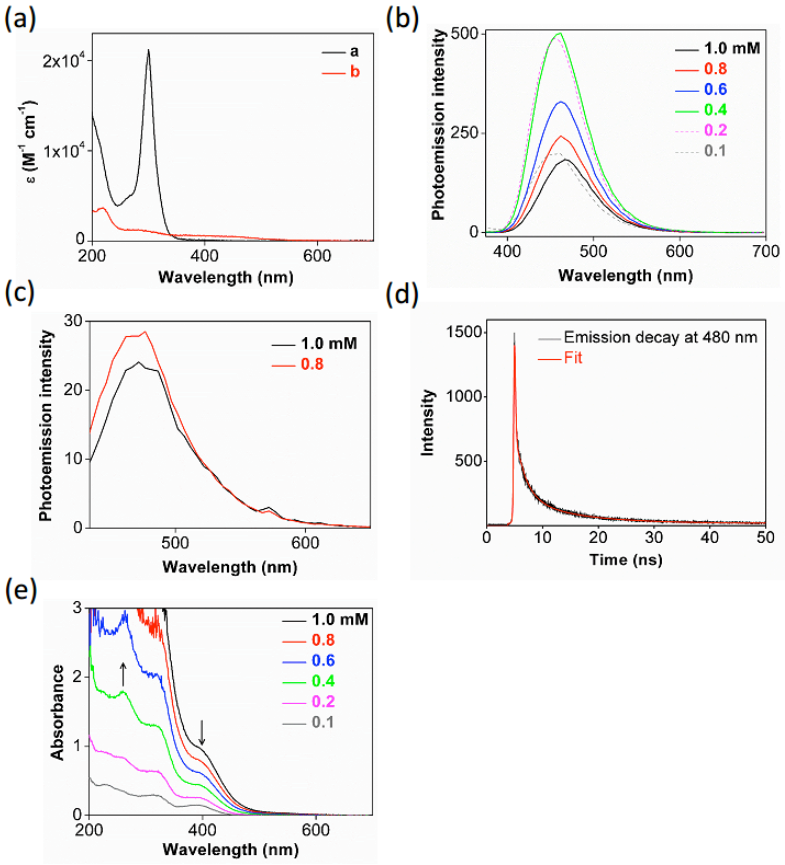


Fig. S2 (a) UV-vis absorption spectra of $VO(acac)_2$ (black) and $VO(OPr)_3$ (red) in CH_3CN (0.10 mM). (b) Photoemission spectra of **2** at different concentrations with excitation at 360 nm in methanol. (c) Photoemission spectra of **2** at different concentrations with excitation at 420 nm in methanol. (d) Decay profile of 0.25 mM **2** after photoexcitation at 375 nm in acetonitrile. The decay profile was monitored at 480 nm. (e) UV-vis absorption spectra of **2** at different concentrations in methanol.

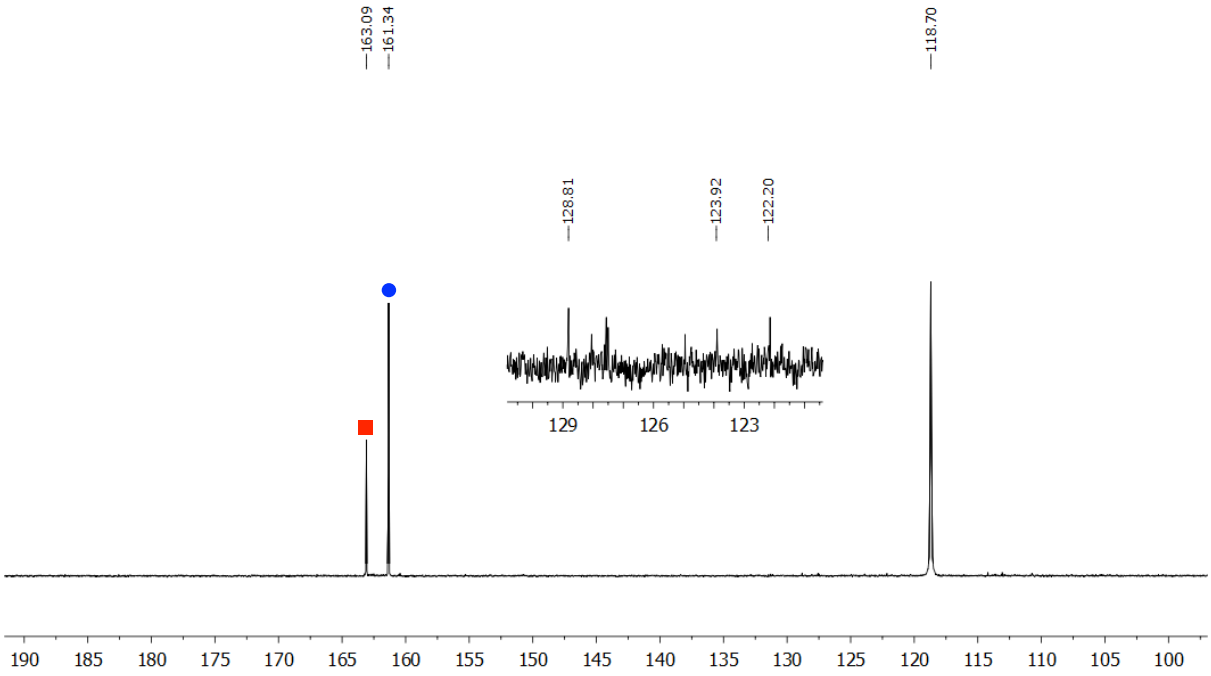


Fig. S3 $^{13}C\{^{1}H\}$ NMR (CD_3CN, 100 MHz) spectrum of the reaction mixture containing **11-^{13}C2** and **2** after 24 h of visible light irradiation. The signal at -118.70 ppm is due to CD_3CN, **9-^{13}C1** is at -161.34 ppm (blue circle), while ^{13}C-labeled formic acid is at 163.39 ppm (red square). The inset shows the unlabeled aryl region corresponding to **9-^{13}C1**.

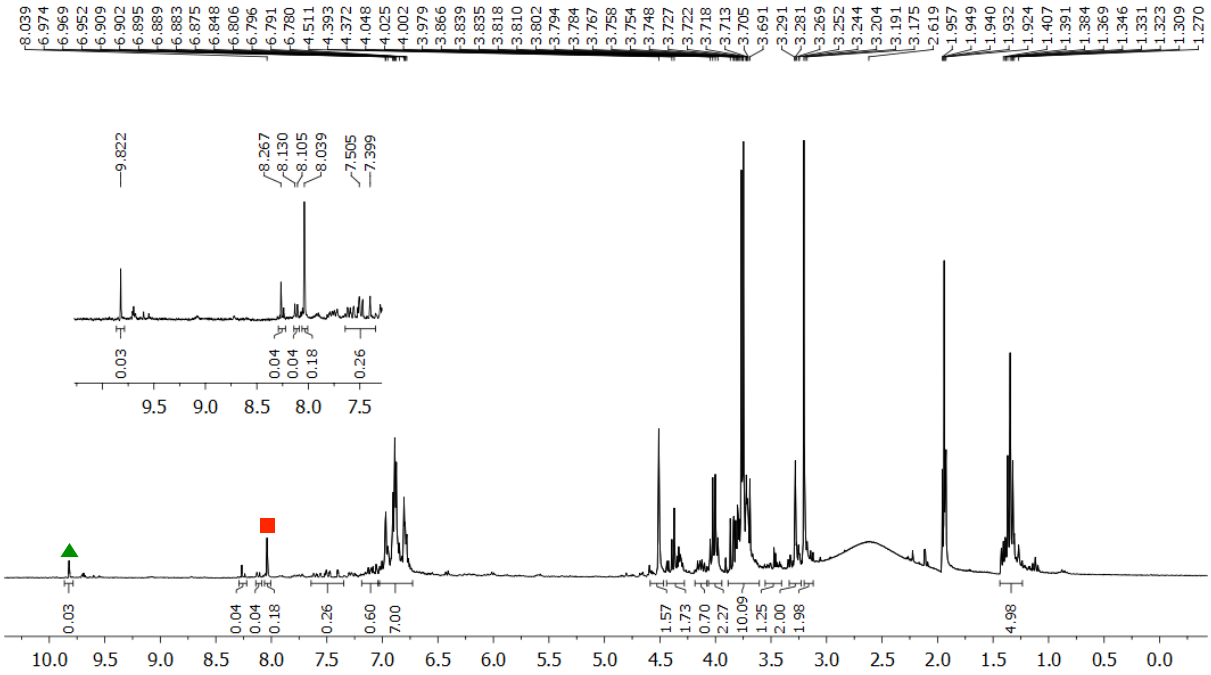


Fig. S4 ^{1}H NMR (CD_3CN, 300 MHz) spectrum of the reaction mixture containing **2** and **25** after 24 h of visible light irradiation. Formic acid (red square) and **6** (green triangle) can be observed, but the remaining signals are unidentified. The products could not be separated readily by preparatory TLC. The solvent residual peak is at 1.94 ppm (quintet).

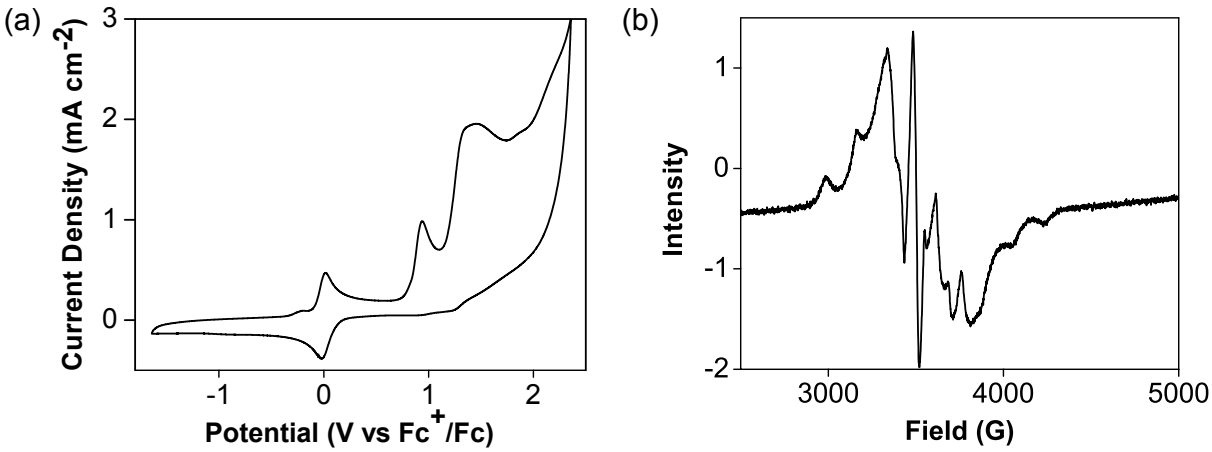


Fig. S5 (a) CV of 1.0 mM **11** with 0.10 M *n*-Bu_4NPF_6 as electrolyte in CH_3CN at a scan rate of 100 mV s^{-1}. The electrochemical wave centered around 0 V is from ferrocene added as the internal standard. (b) EPR spectrum of the V^{IV} oxo **3** recorded in the solid state.

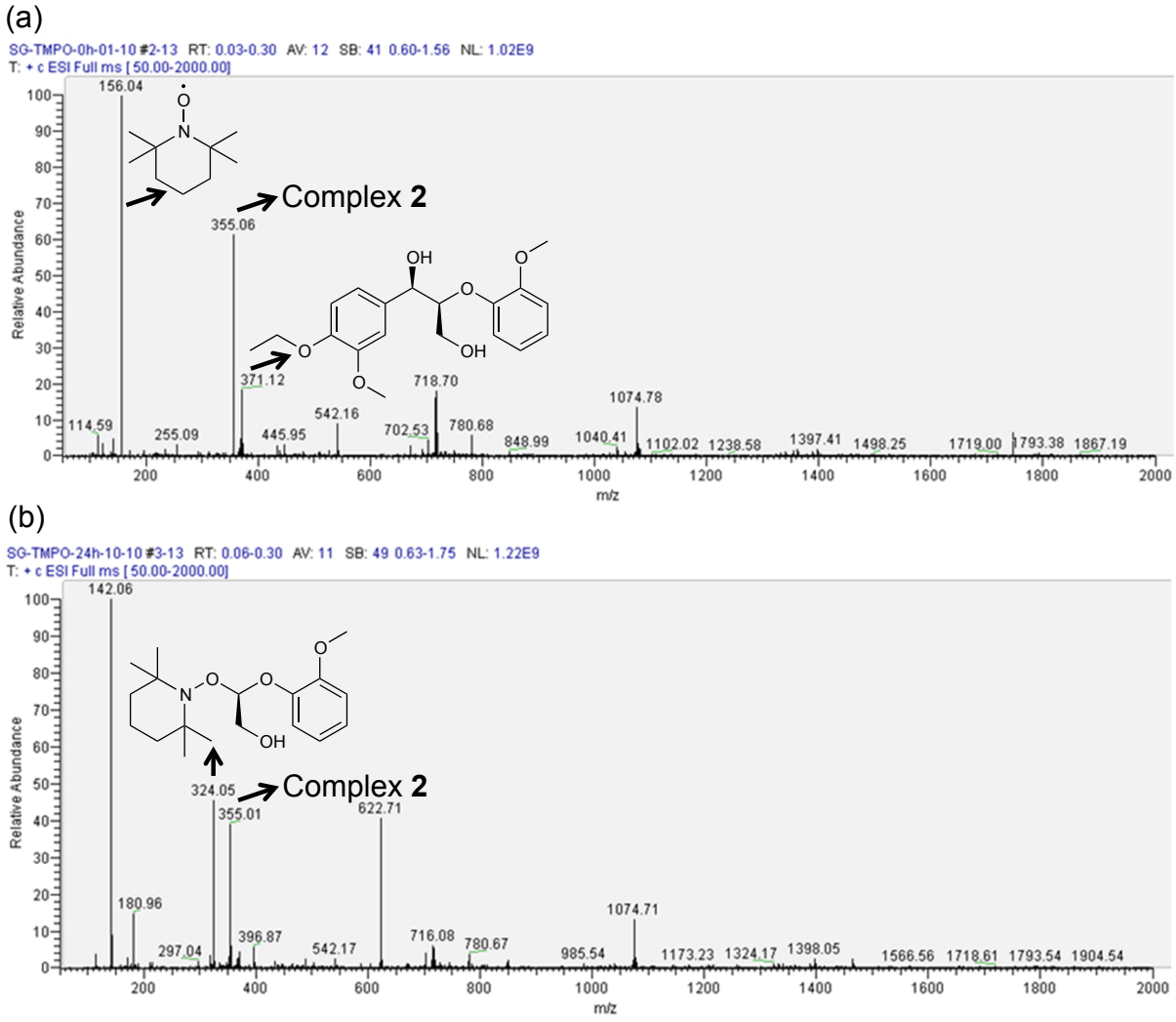


Fig. S6 ESI-mass spectra of the reaction mixtures in intermediate trapping experiments with TEMPO (a) before irradiation, and (b) after irradiation.

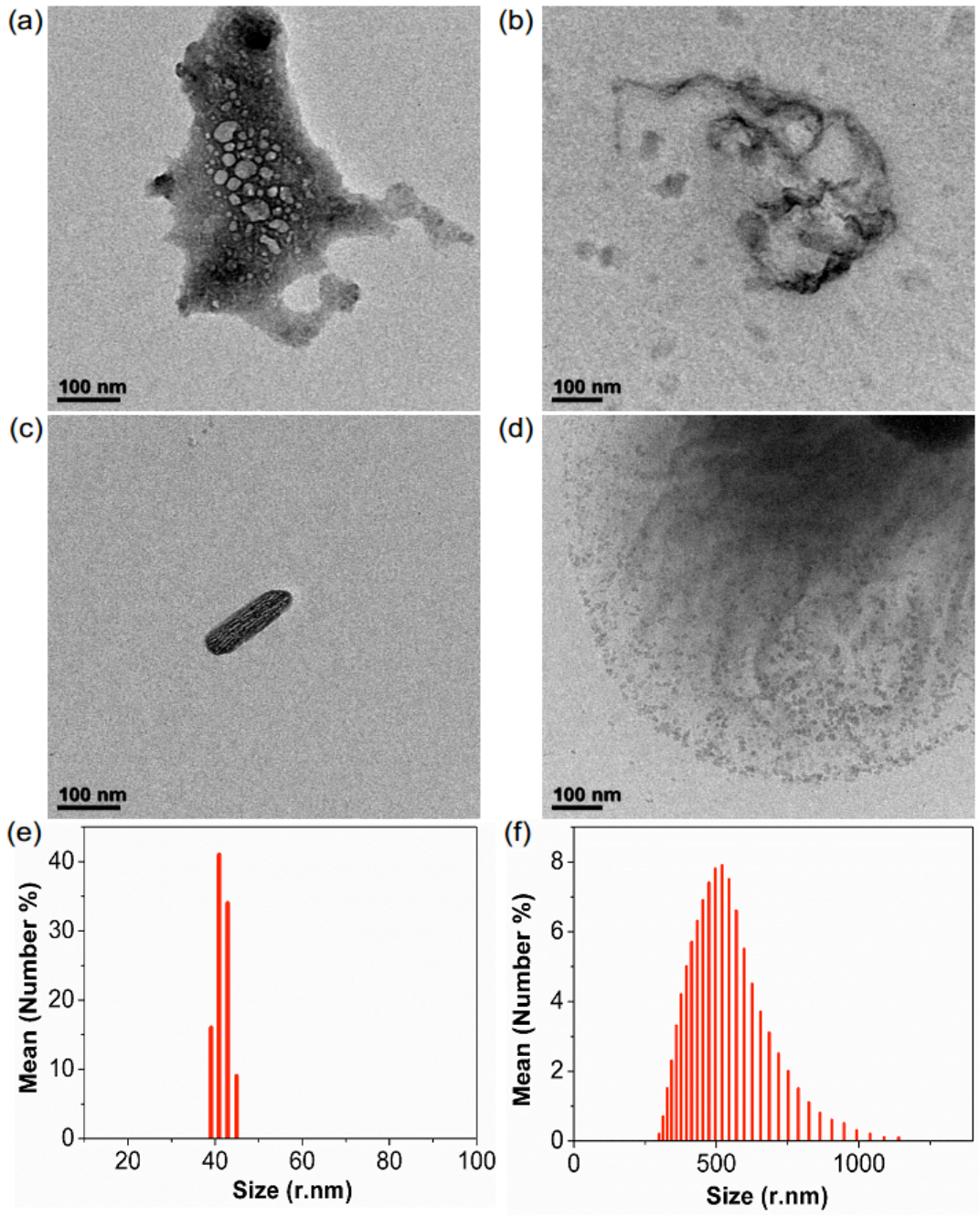


Fig. S7 TEM images of the reaction mixture containing **2** and **11** in CH_3CN before ((a) and (b)) and after visible-light irradiation ((c) and (d)). The amorphous and sporadic deposition in all the samples could have arisen due to precipitation of the catalyst or substrate after solvent evaporation. DLS profiles of the reaction mixture containing **2** and **11** (e) before visible light irradiation and (f) after 24 h of visible light irradiation.

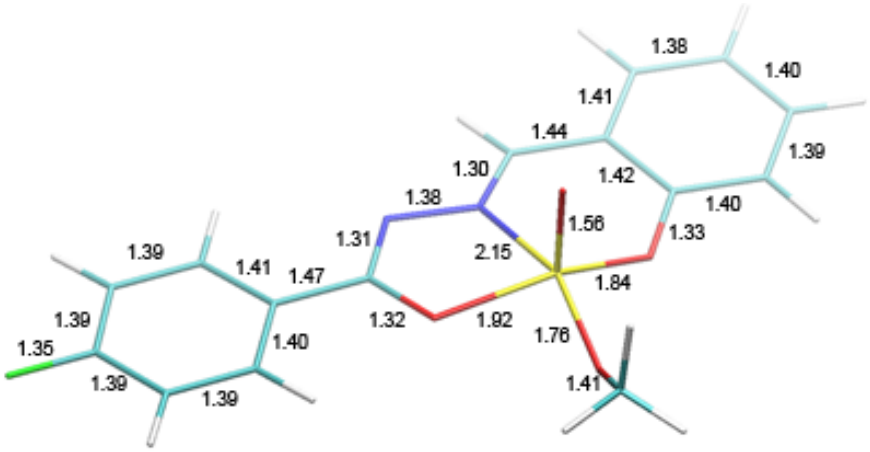


Fig. S8 B3LYP/6-31G*-optimized geometry of **2** (without a methanol ligand). Bond distances are shown in Å.

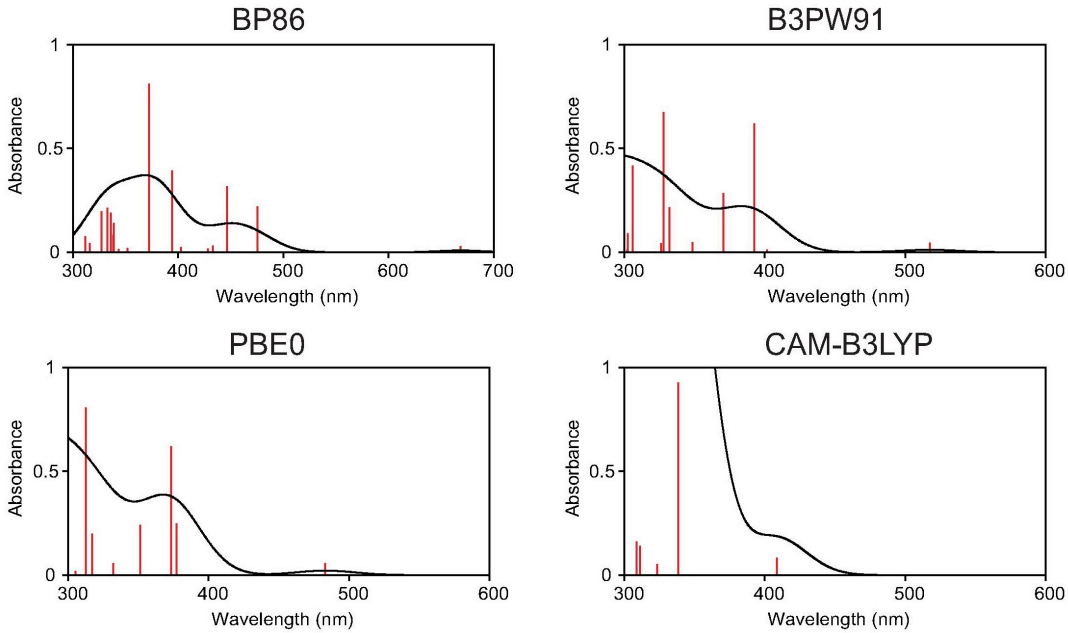


Fig. S9 Absorption spectra obtained with different functionals. All the absorption curves are scaled so that the absorbance at 396 nm is 0.2. The oscillator strengths of all excitations (red lines) are multiplied by 4 for ease of viewing.

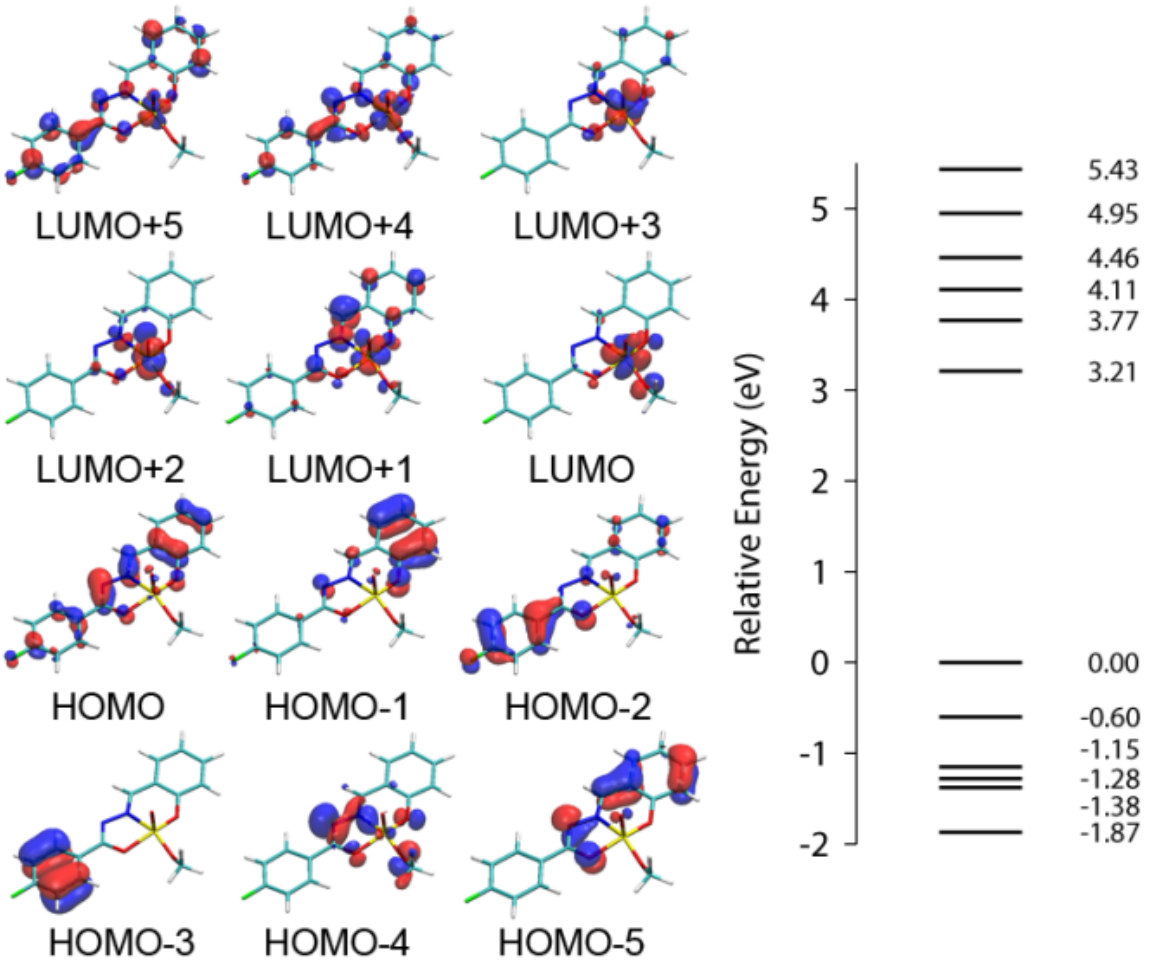


Fig. S10 Illustration of select frontier molecular orbitals (B3LYP/6-31G*) and their relative energy levels at the valence edge.

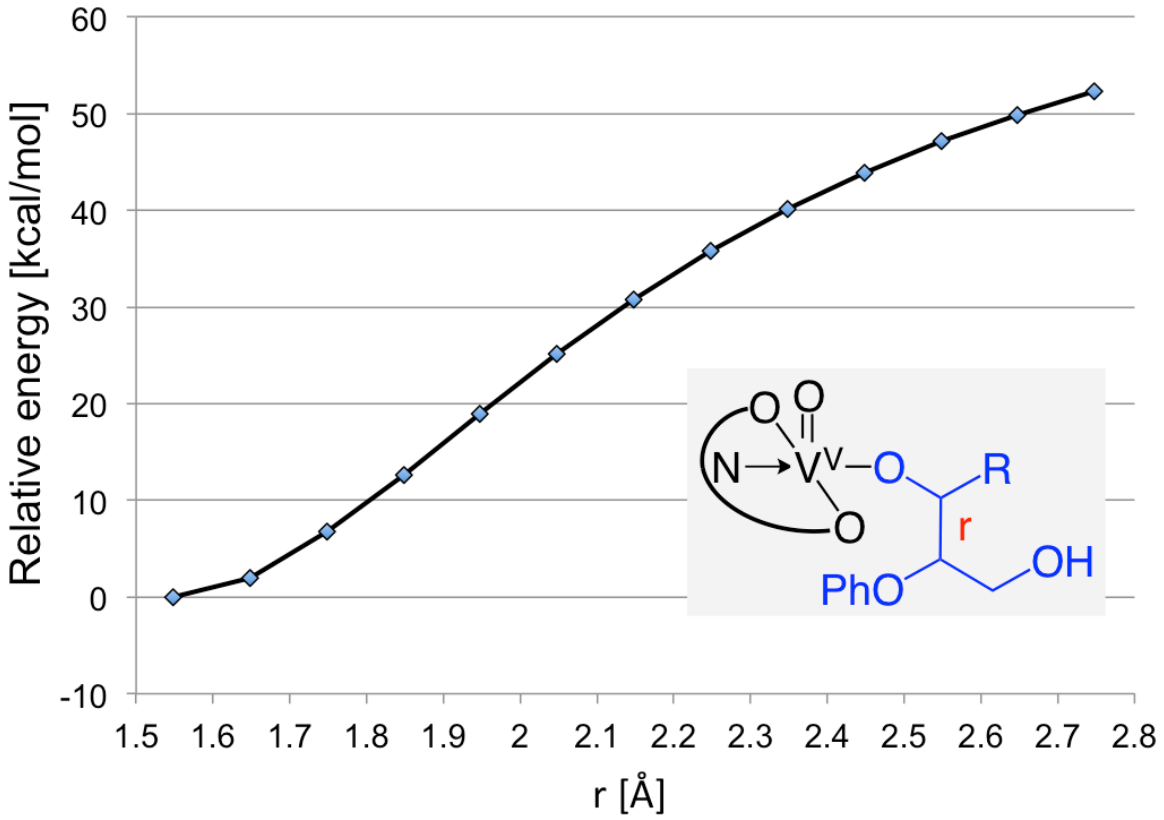


Fig. S11 Change in energy with increasing C–C bond distance in the S_0 state (B3LYP/6-31G*) for a substrate bound via the benzylic alcohol to the vanadium photocatalyst.

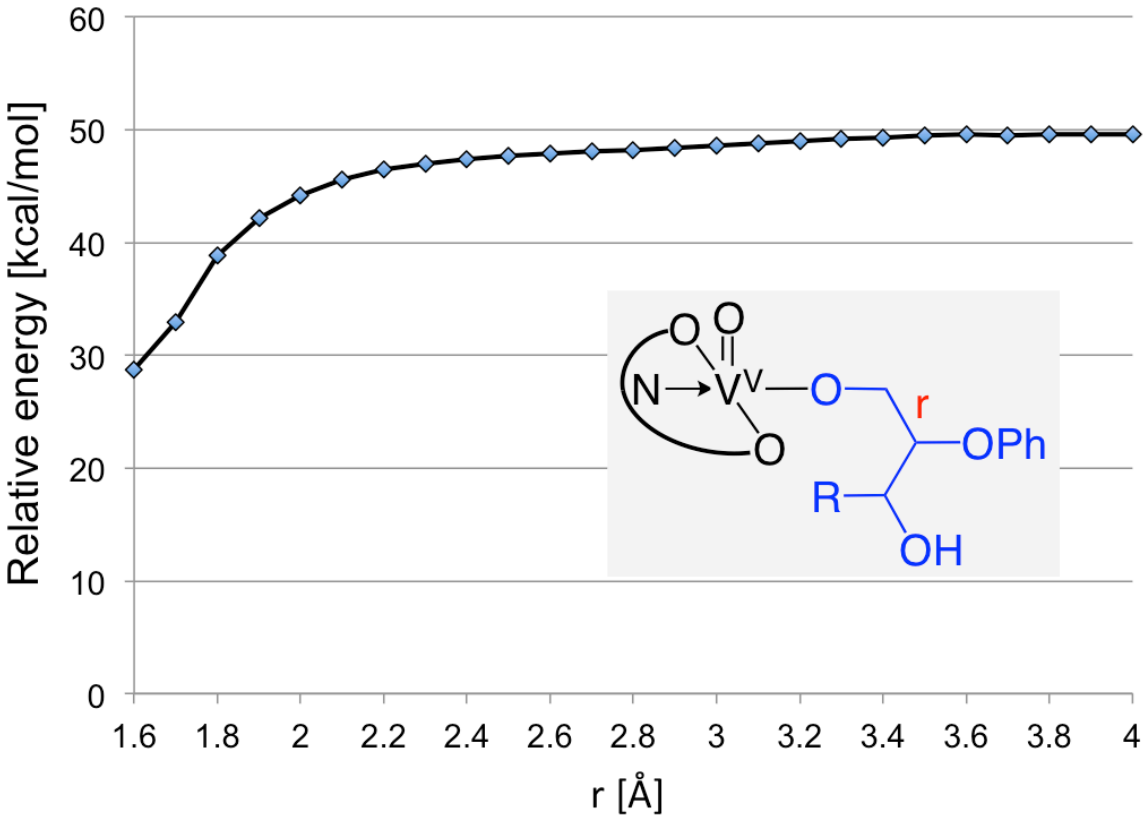


Fig. S12 Change in energy with increasing C–C bond distance in the T_1 state (B3LYP/6-31G*), for the case in which the substrate is bound to the vanadium center via the primary alcohol.

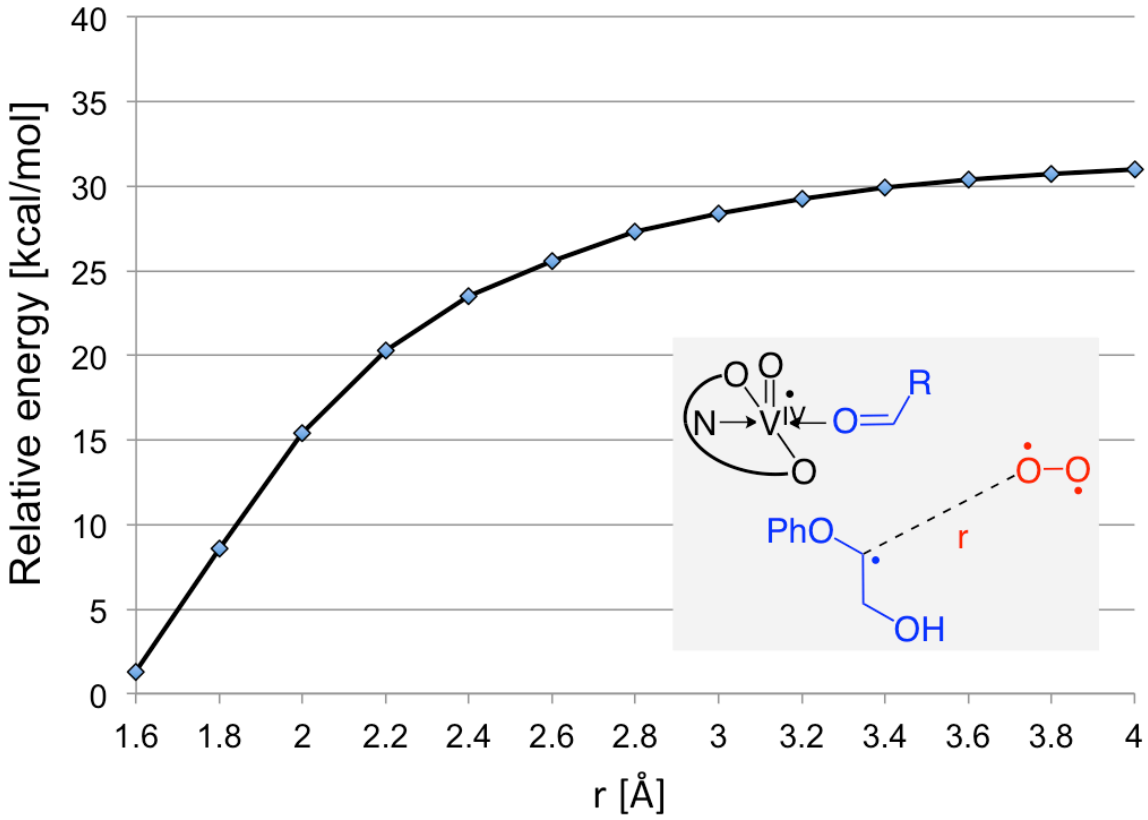


Fig. S13 Change in energy in the attack of O_2 on the substrate radical in the **Int1** state (B3LYP/6-31G*). In these broken-symmetry calculations, at large distances, there are two β-spin electrons on O_2 and two α-spin electrons on **Int1**. Thus, overall, the system has a singlet spin state. The energy is relative to ^{3}**Int2**.

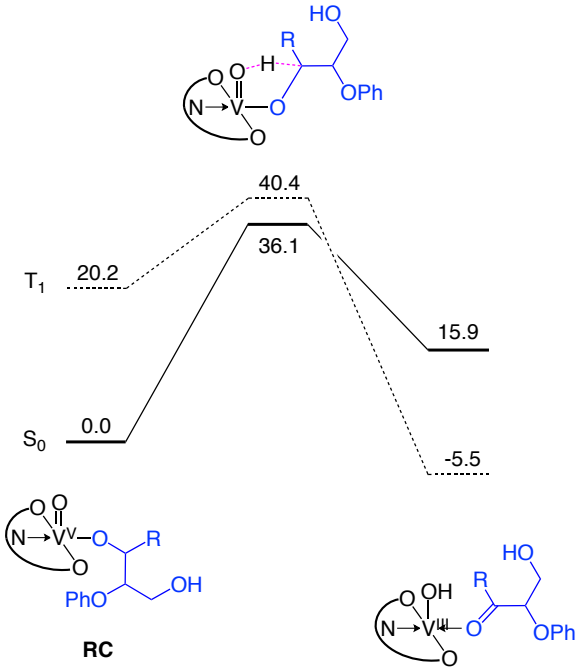


Fig. S14 Energy profile (kcal mol^{-1}) for the H-abstraction reaction from the benzyl carbon in the S_0 and T_1 states, as obtained at the B3LYP(SCRF)/6-311+G(d,p)//B3LYP/6-31G* level with zero-point energy corrections.

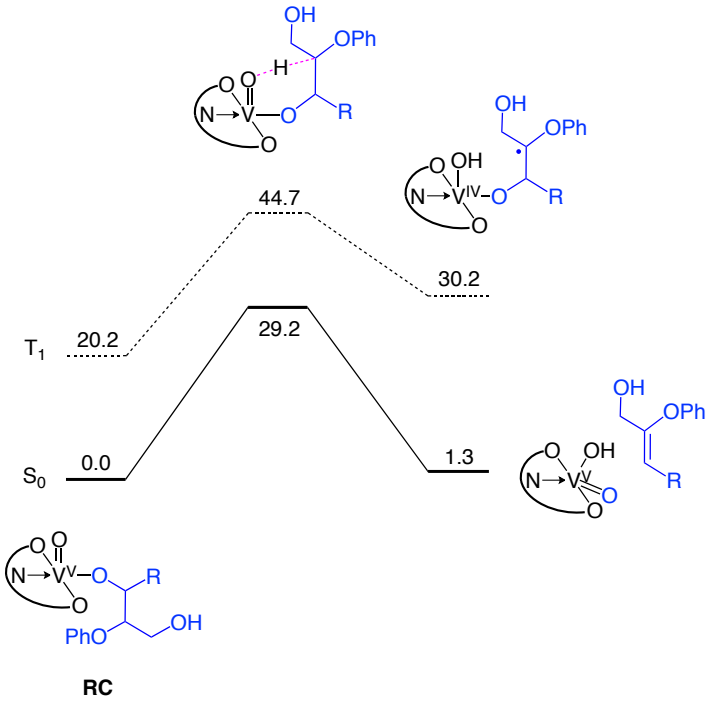


Fig. S15 Energy profile (kcal mol^{-1}) for the H-abstraction reaction from the carbon next to the hydroxymethyl group in the S_0 and T_1 states, as obtained at the B3LYP(SCRF)/6-311+G(d,p)//B3LYP/6-31G* level with zero-point energy corrections.

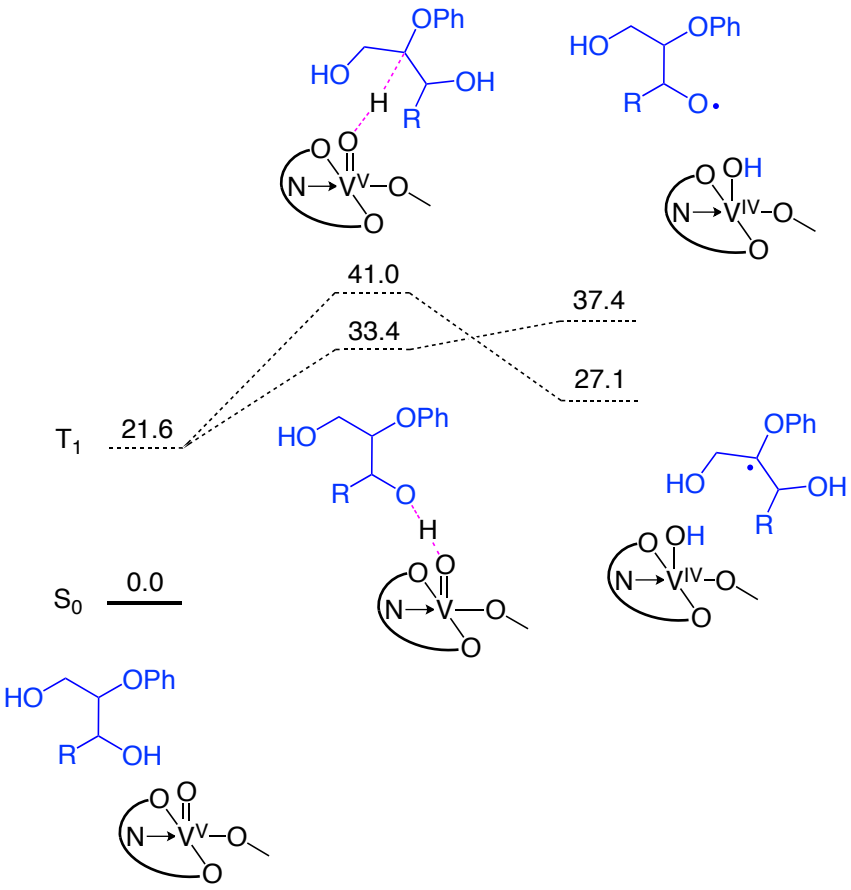
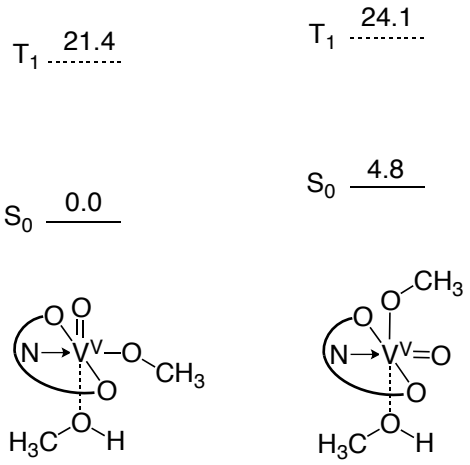


Fig. S16 Energy profile (kcal mol^{-1}) for outer-sphere HAT reactions between **2** and substrates, as obtained at the B3LYP(SCRF)/6-311+G(d,p)//B3LYP/6-31G* level with zero-point energy corrections.

(a)



(b)

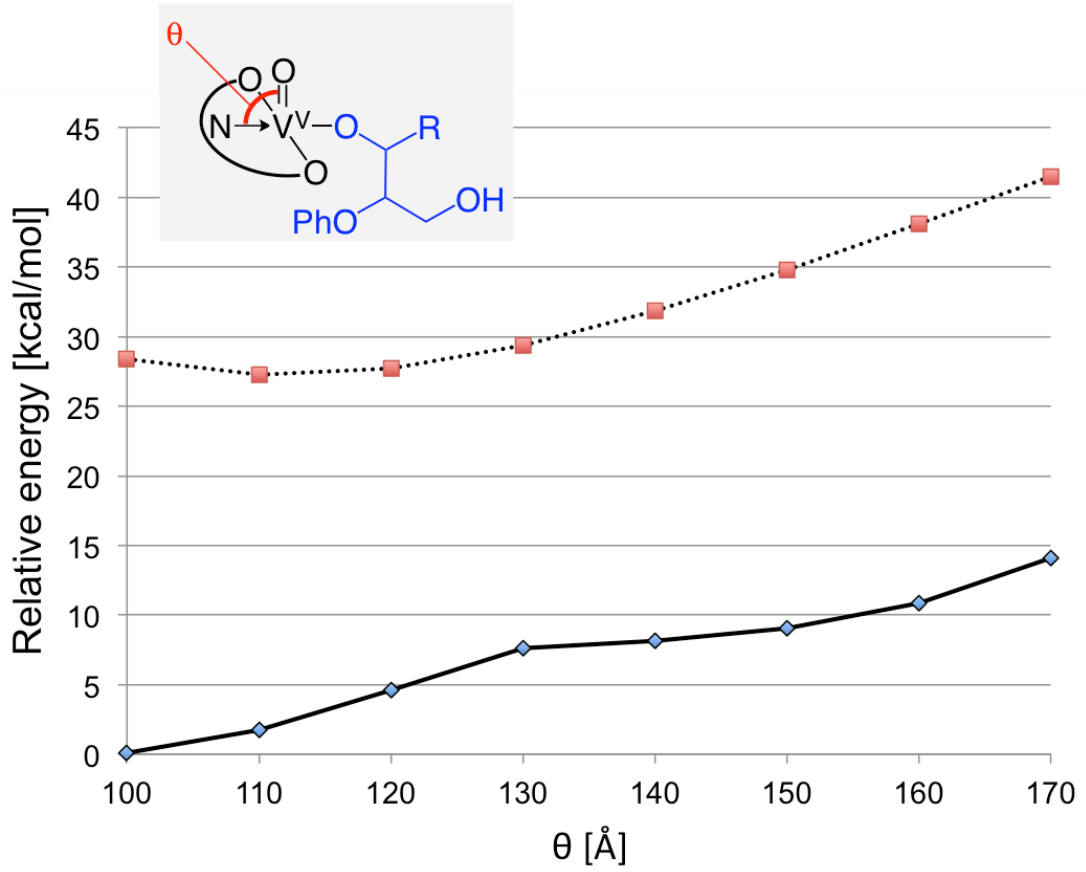


Fig. S17 (a) Relative stability of the axial and equatorial isomers of **2** (with an axial methanol ligand), as calculated at the B3LYP(SCRF)/6-311+G(d,p)//B3LYP/6-31G* level with zero-point energy corrections. (b) Changes in energy with increasing O-V-N angle of **RC** (B3LYP/6-31G*). The solid and dotted lines indicate the data for the S_0 and T_1 states, respectively.

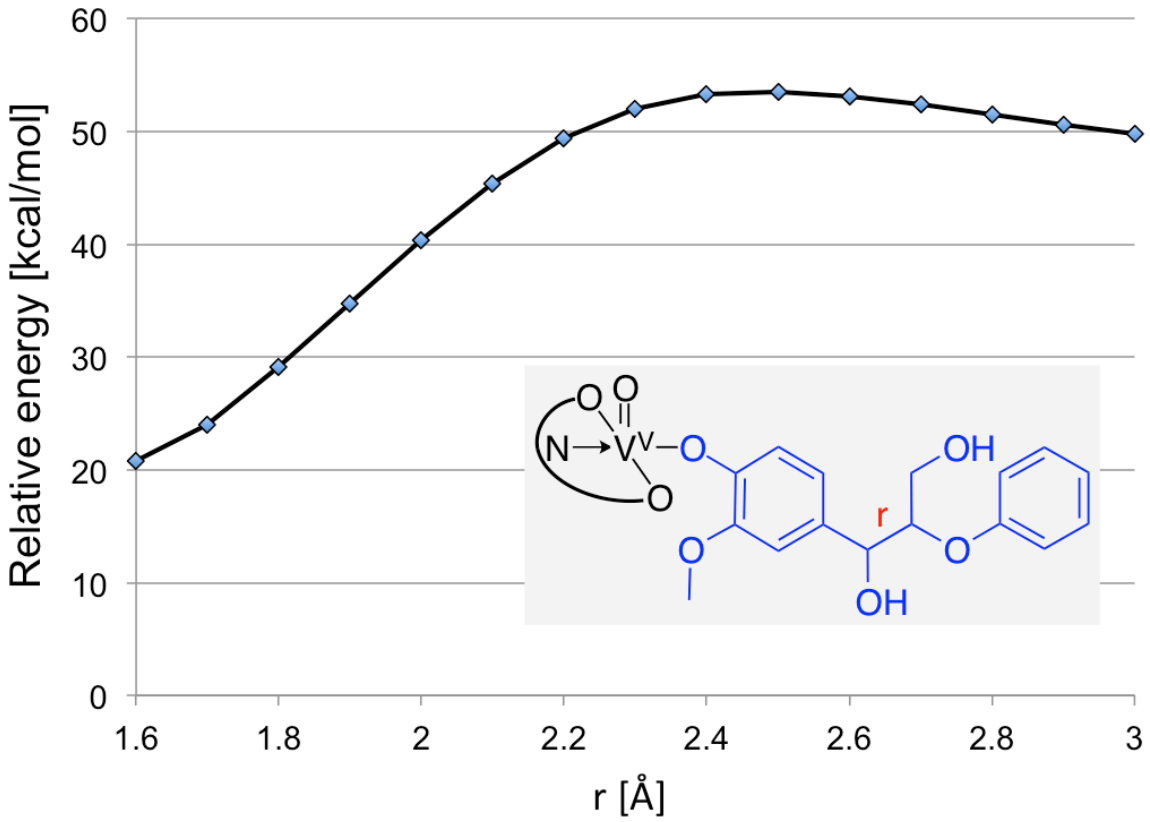


Fig. S18 Change in energy with increasing C–C bond distance in the reaction of a phenol-type substate in the T_1 state (B3LYP/6-31G*).

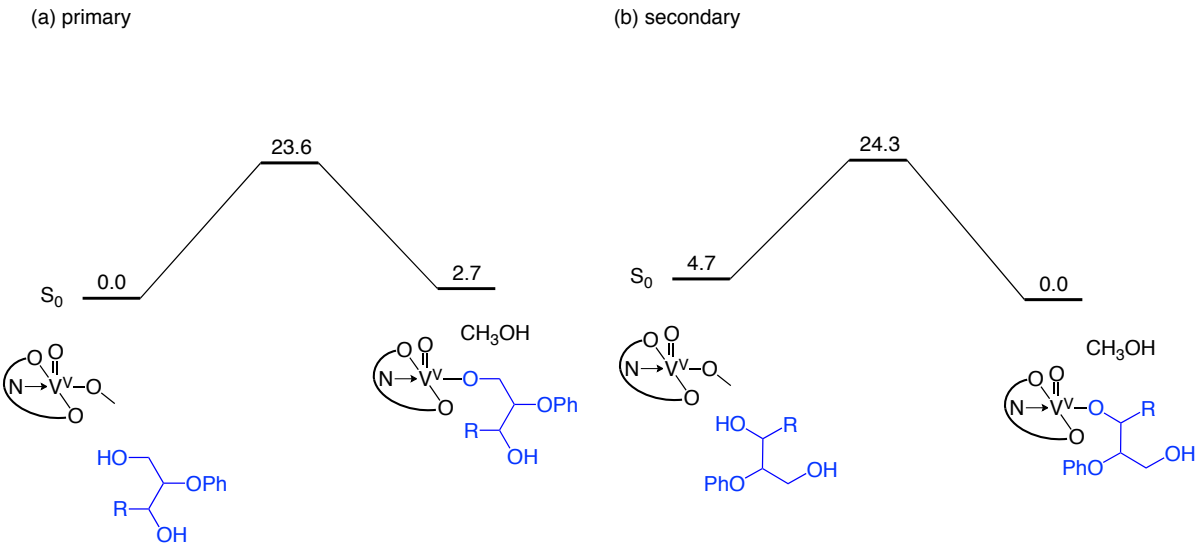


Fig. S19 Energy profile (kcal mol^{-1}) for ligand exchange reactions of **11** with the methoxide on **2**, as obtained at the B3LYP(SCRF)/6-311+G(d,p)//B3LYP/6-31G* level with zero-point energy corrections.

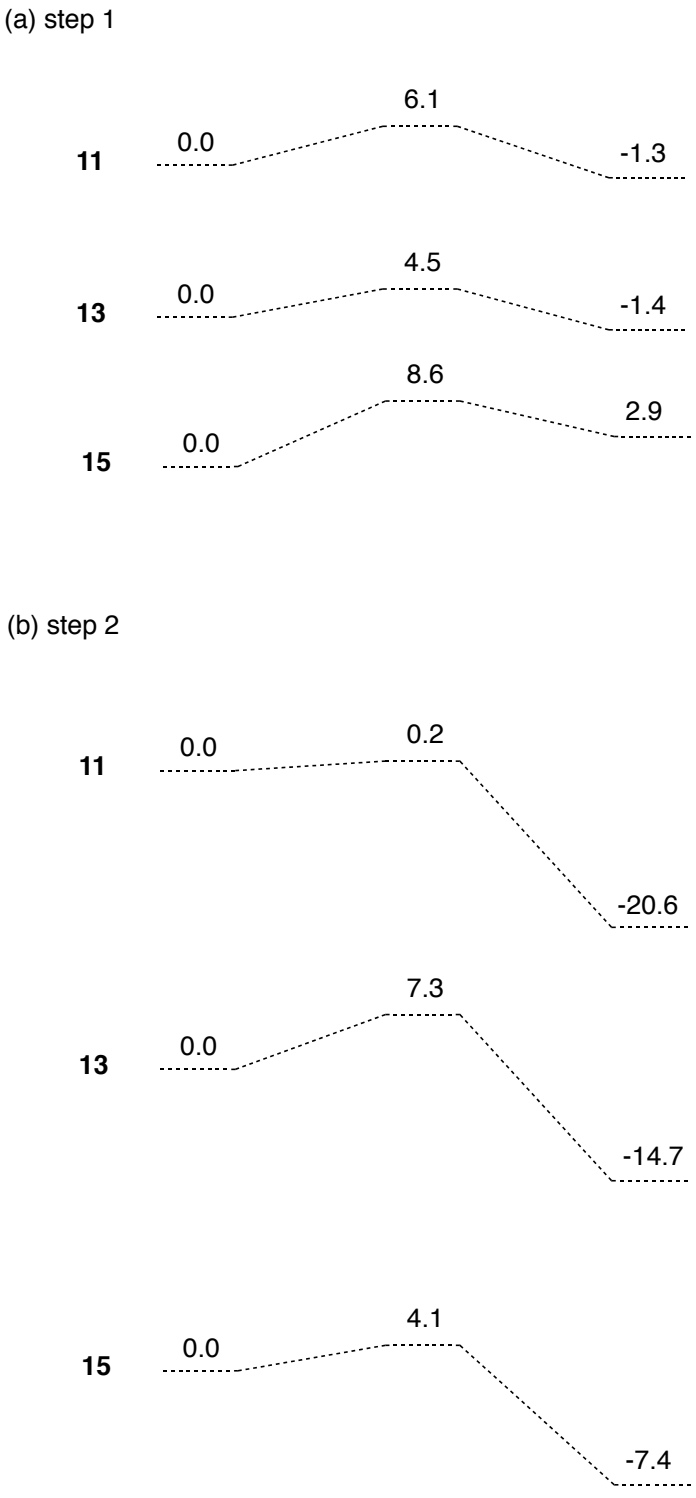


Fig. S20 The relative energies (kcal mol^{-1}) on the triplet energy surface for **TS1** and **TS4** of Fig. 8 respectively (and the corresponding analogs for substrates **13** and **15**), as obtained at the B3LYP(SCRF)/6-311+G(d,p)//B3LYP/6-31G* level with zero-point energy corrections.

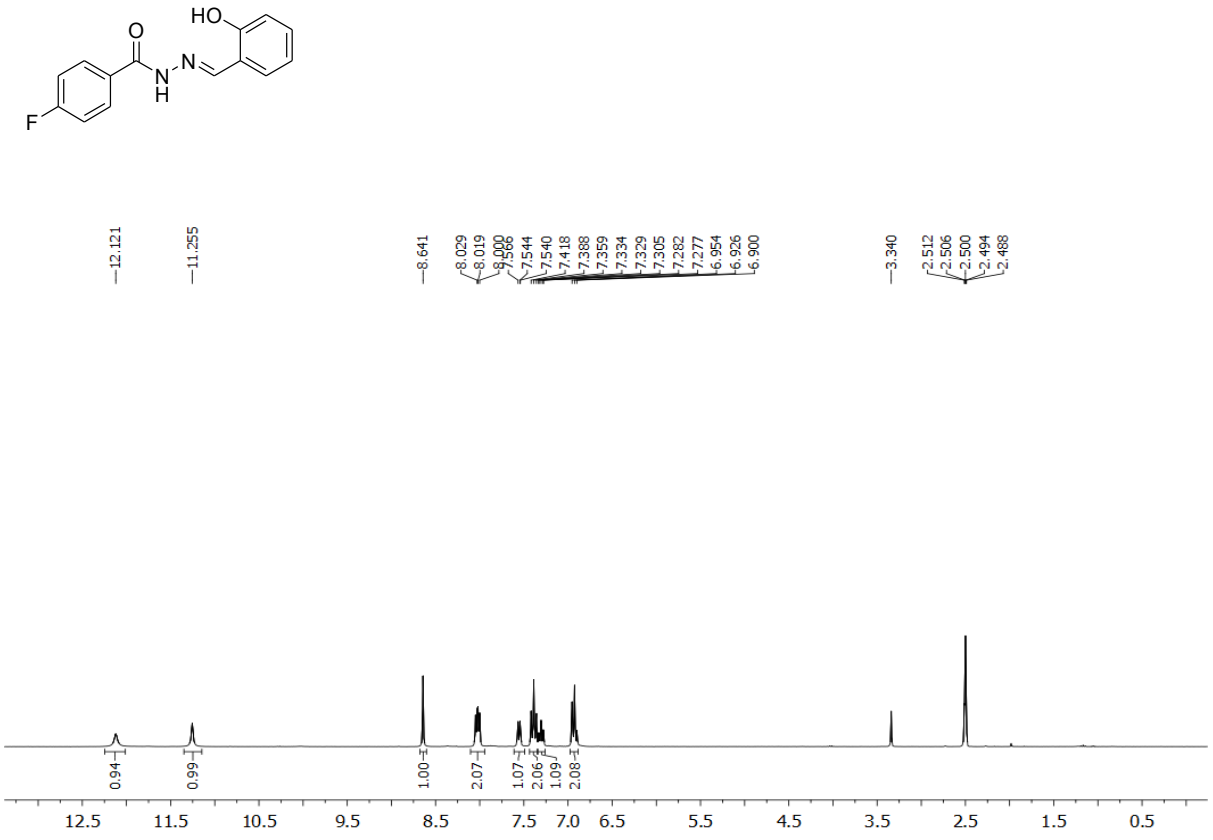


Fig. S21 The ^{1}H NMR (DMSO-d_6, 300 MHz) spectrum of **1**.The solvent residual peak is at 2.50 ppm (quintet). The peak at 3.34 ppm is due to water present in the NMR solvent.

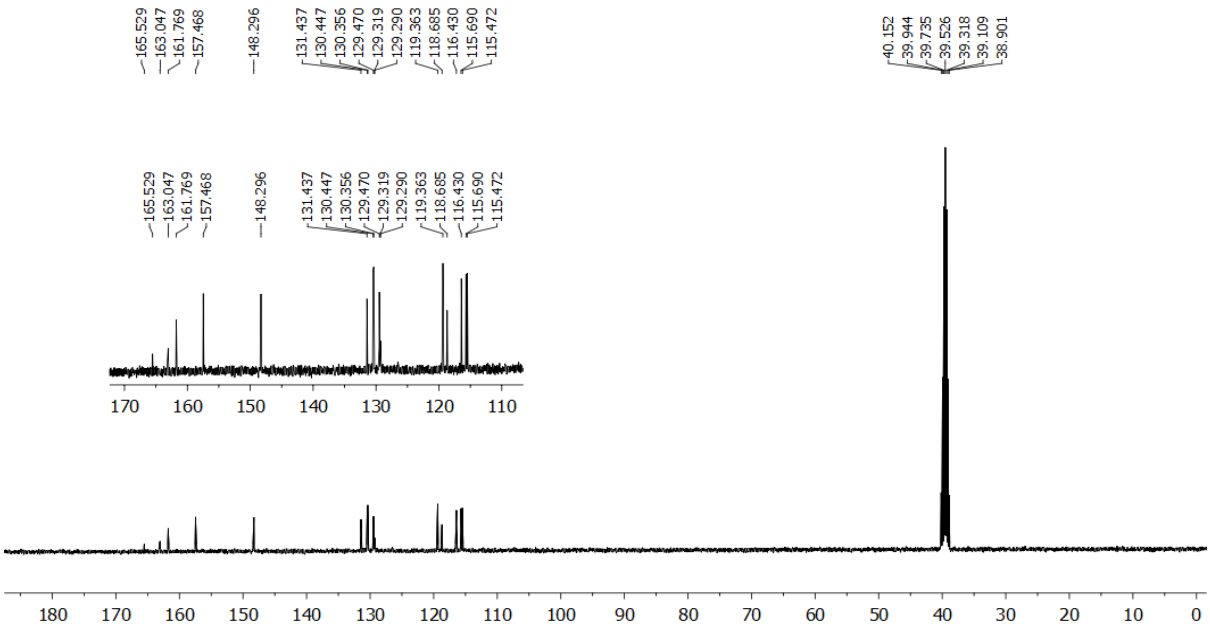


Fig. S22 The $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 300 MHz) spectrum of **1**. The solvent residual peak is at 39.5 ppm (septet). Inset: Magnification of the aromatic region.

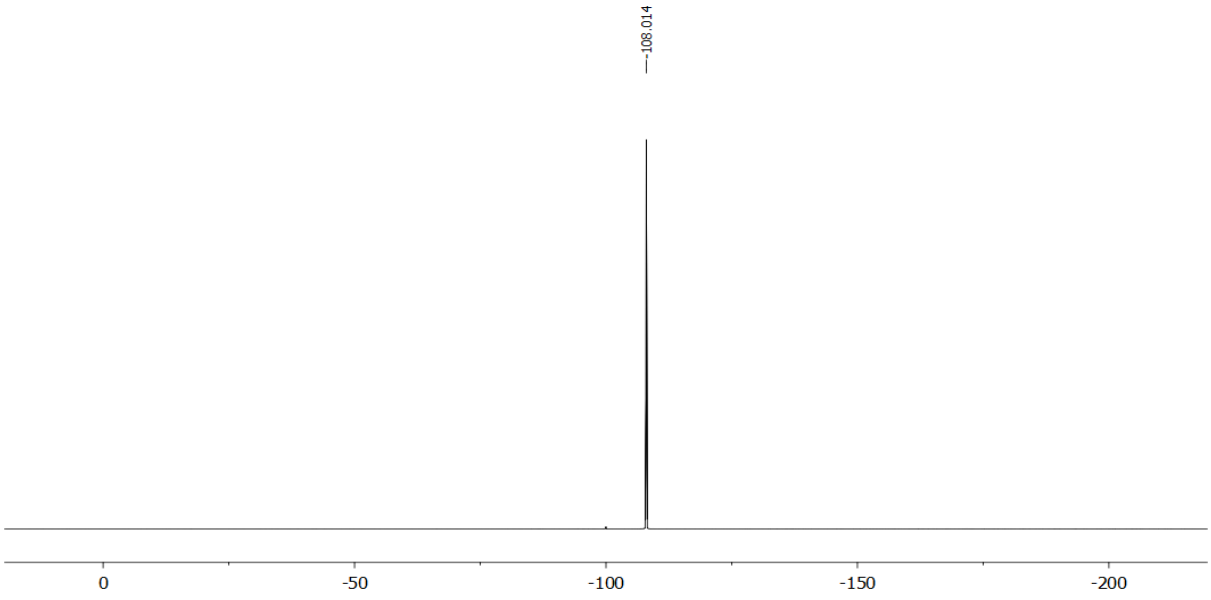


Fig. S23 The $^{19}F\{^{1}H\}$ NMR (DMSO-d_6, 282.40 MHz) spectrum of **1**.

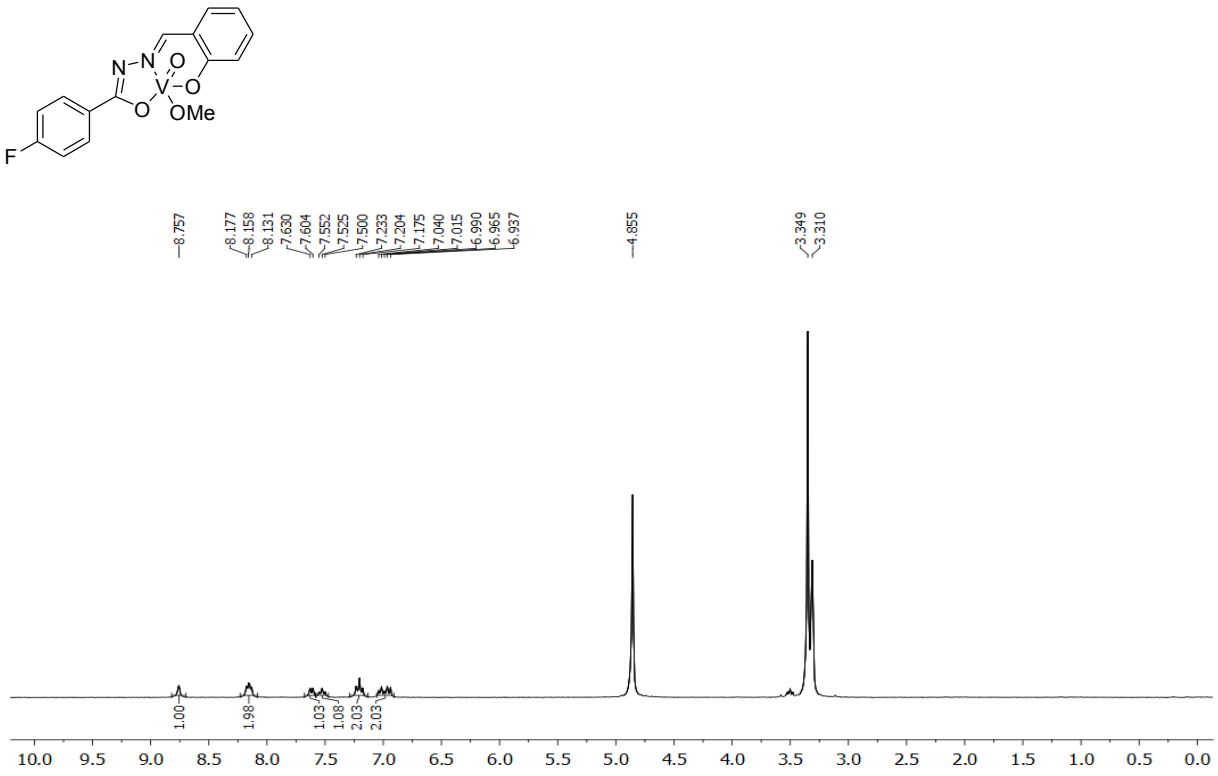


Fig. S24 The ^{1}H NMR (MeOD-d_4, 300 MHz) spectrum of **2**. The solvent residual peak is at 3.31 ppm (quintet). The peaks at 3.35 and 4.85 ppm are due to methanol and waterpresent in the NMR solvent, respectively.

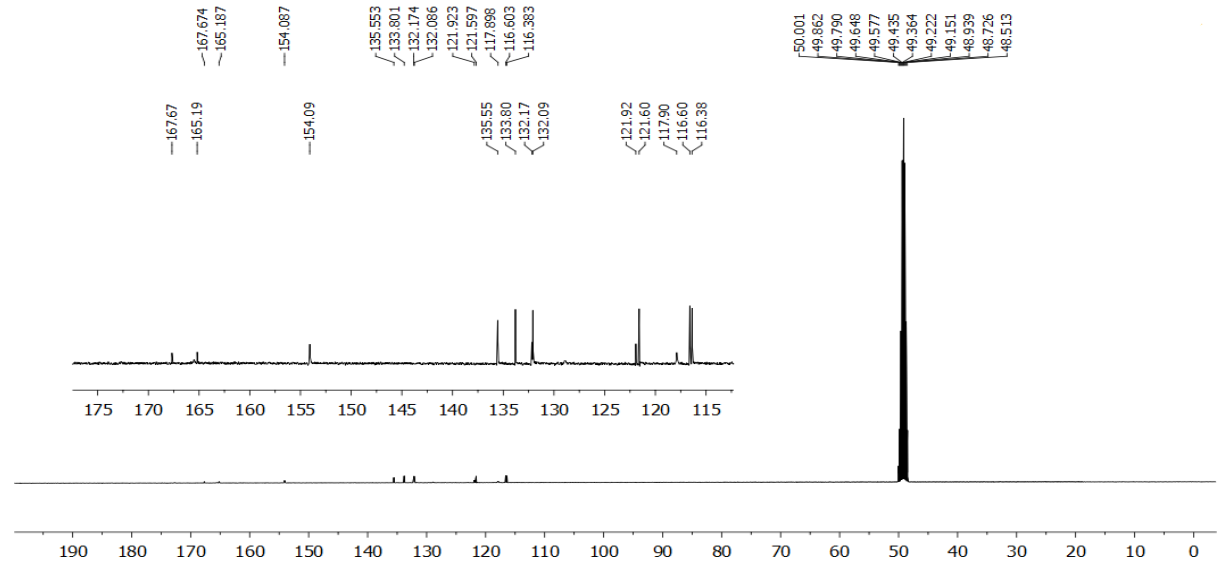


Fig. S25 The ^{13}C{^{1}H} NMR (MeOD-d_4, 100 MHz) spectrum of **2**. The solvent residual peak is at 49.4 ppm (septet). Inset: Magnification of the aromatic region.

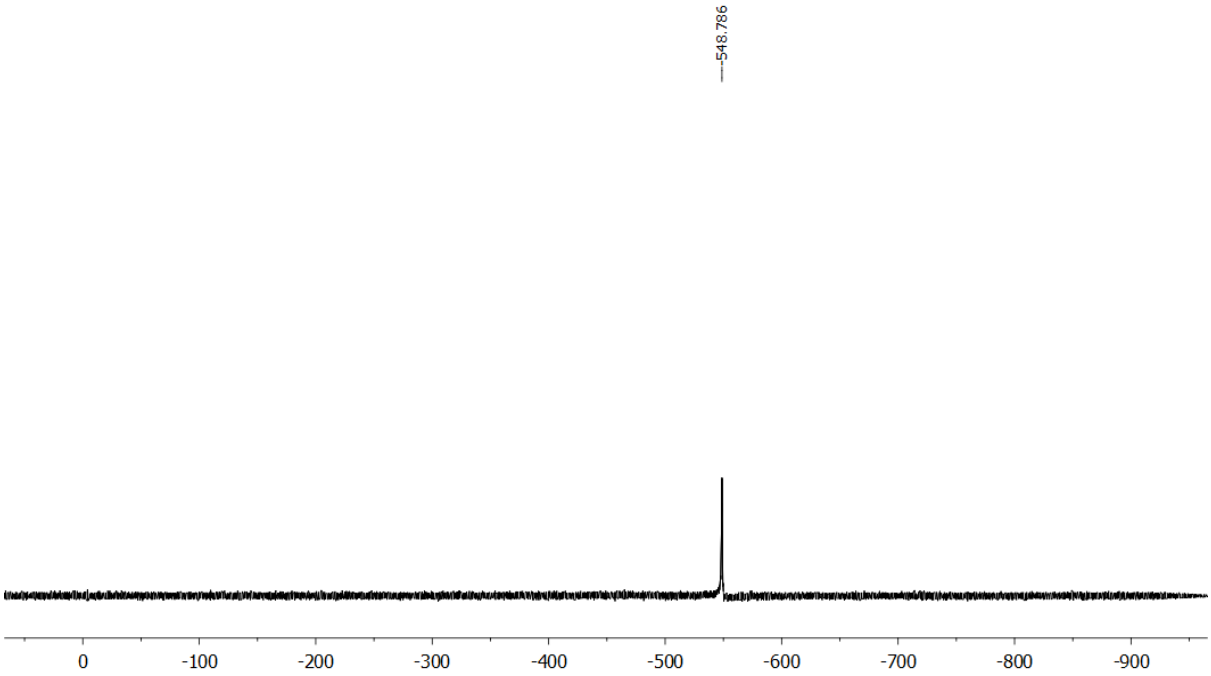


Fig. S26 The ^{51}V NMR (MeOD-d_4, 105.15 MHz) spectrum of **2**.

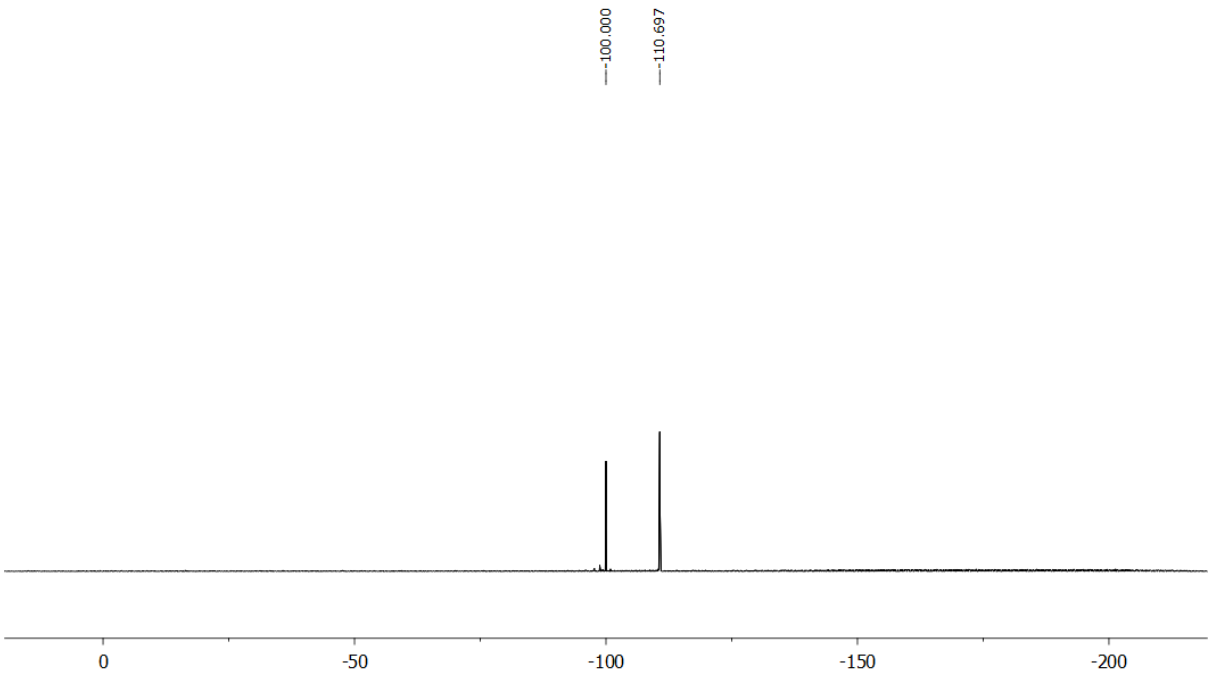


Fig. S27 The ^{19}F{^{1}H} NMR (MeOD-d_4, 282.40 MHz) spectrum of **2**.

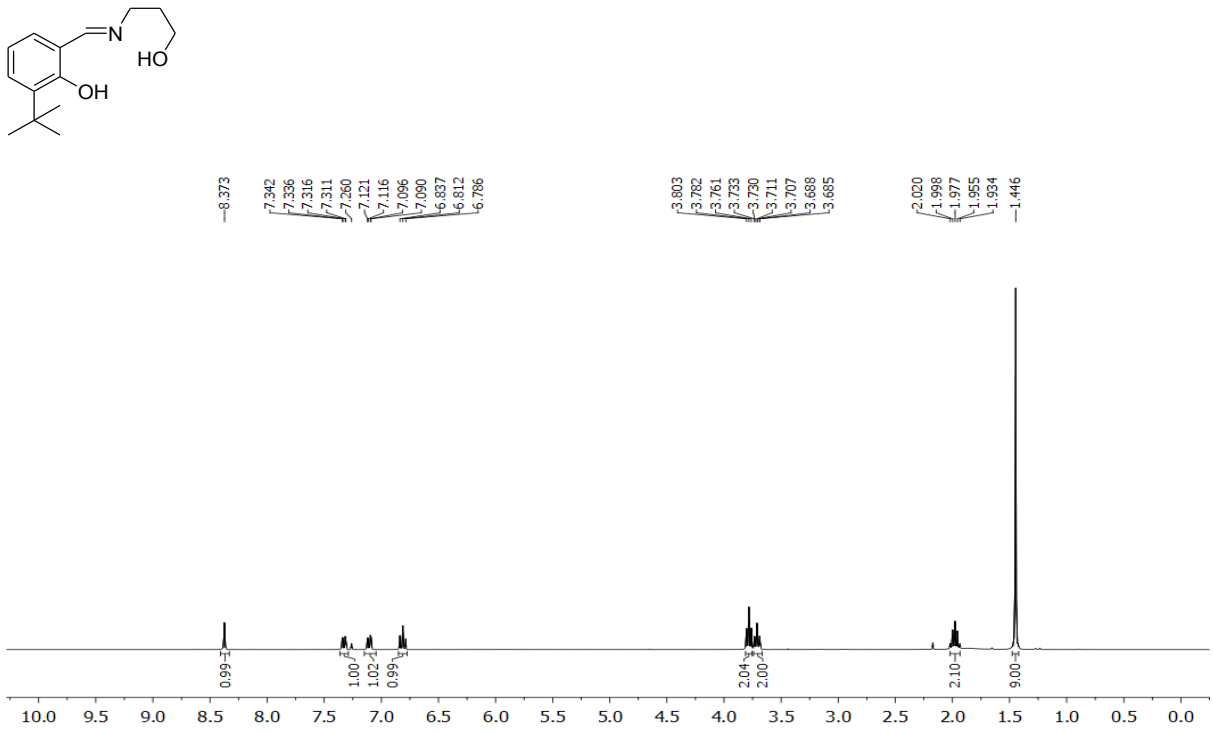


Fig. S28 The ^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **4**. The solvent residual peak is at 7.26 ppm.

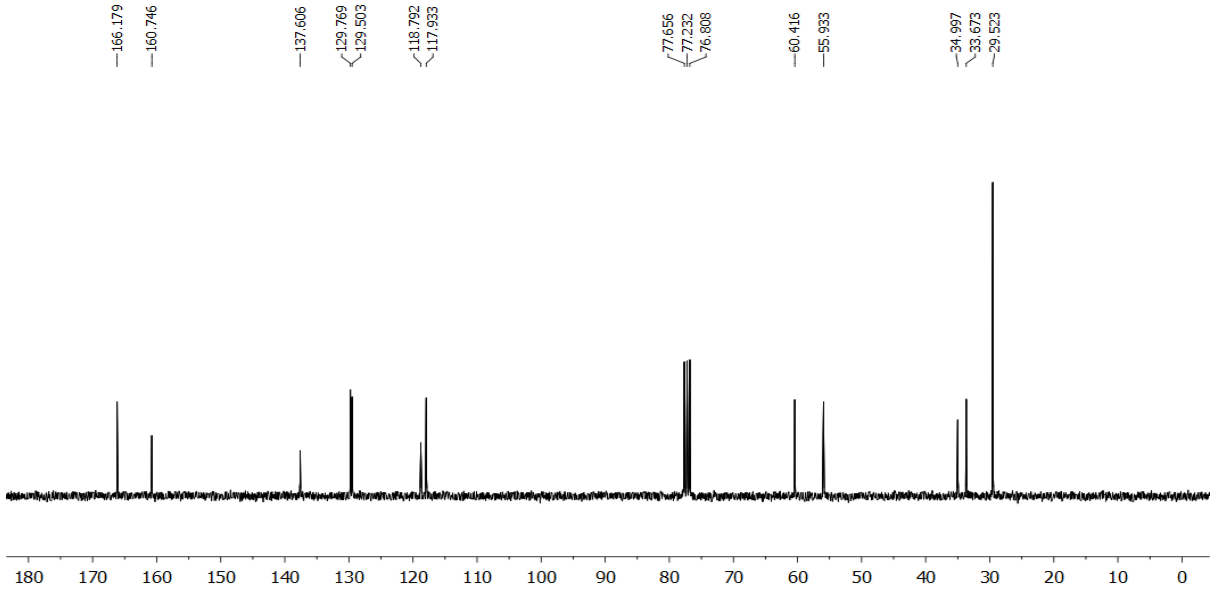


Fig. S29 The $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75 MHz) spectrum of **4**. The solvent residual peak is at 77.2 ppm (triplet).

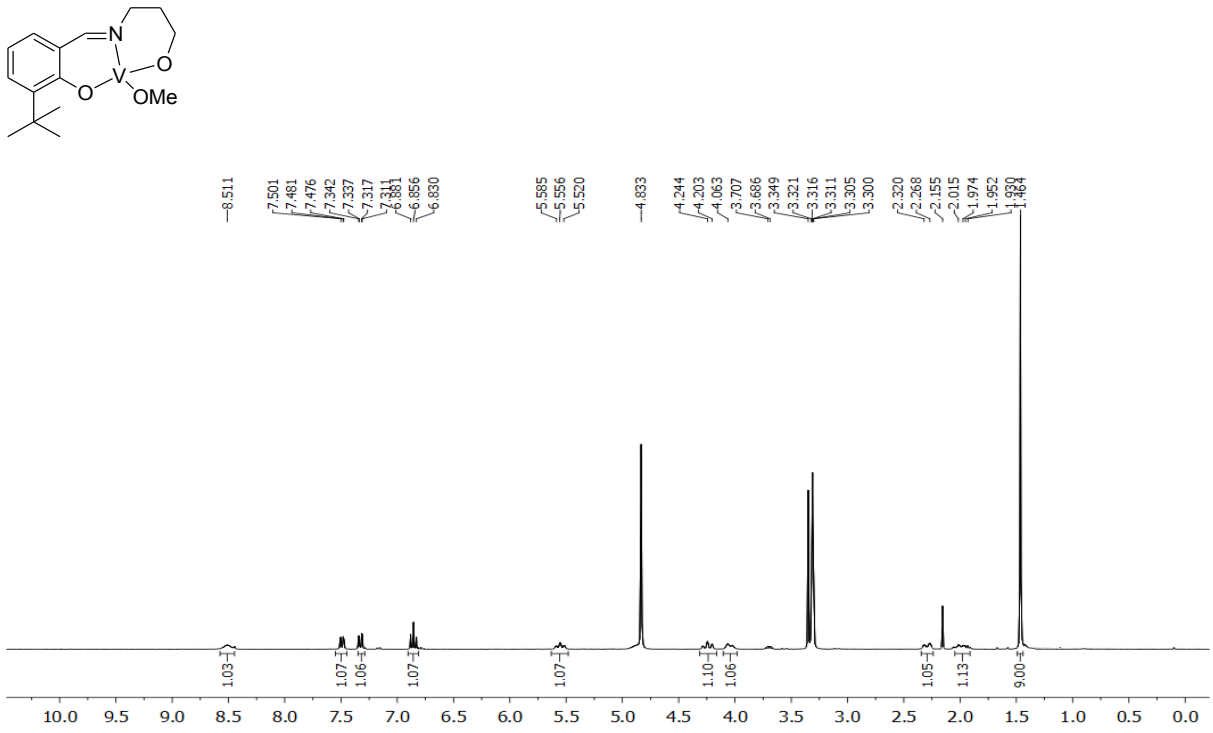


Fig. S30 The ^{1}H NMR (MeOD-d_4, 300 MHz) spectrum of **5**. The solvent residual peak is at 3.31 ppm (quintet). The peaks at 3.35 and 4.83 ppm are due to methanol and water present in the NMR solvent, respectively.

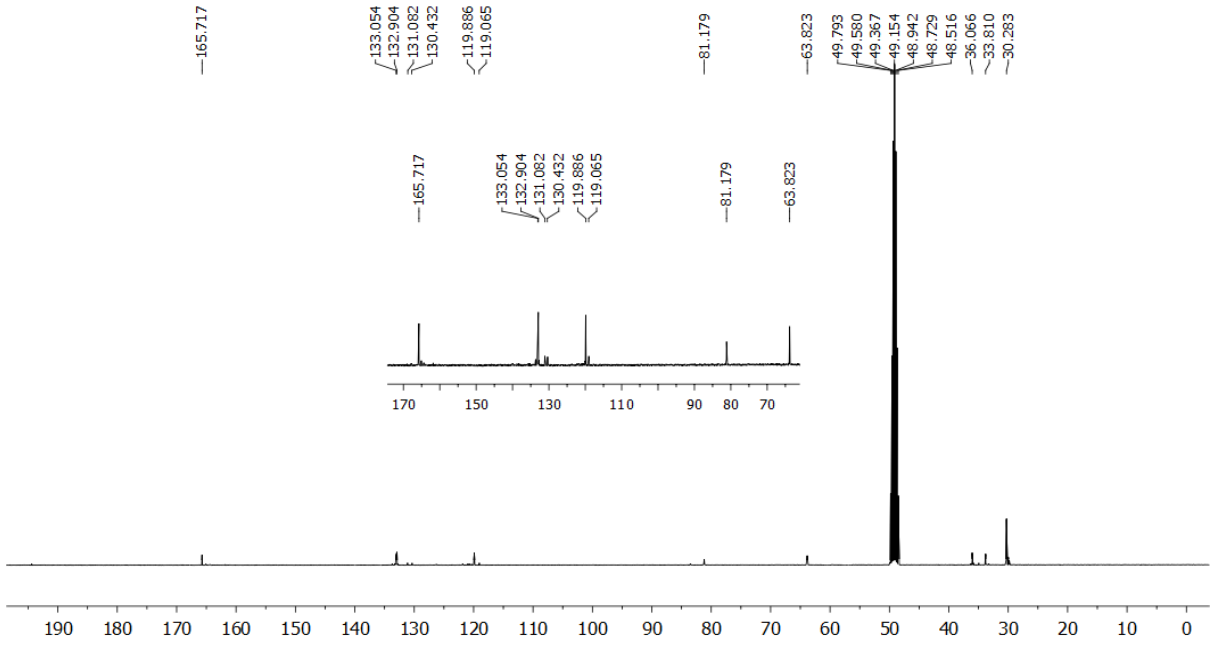


Fig. S31 The ^{13}C{^{1}H} NMR (MeOD-d_4, 100 MHz) spectrum of **5**. The solvent residual peak is at 49.1 ppm (multiplet). Inset: Magnification of the aromatic region.

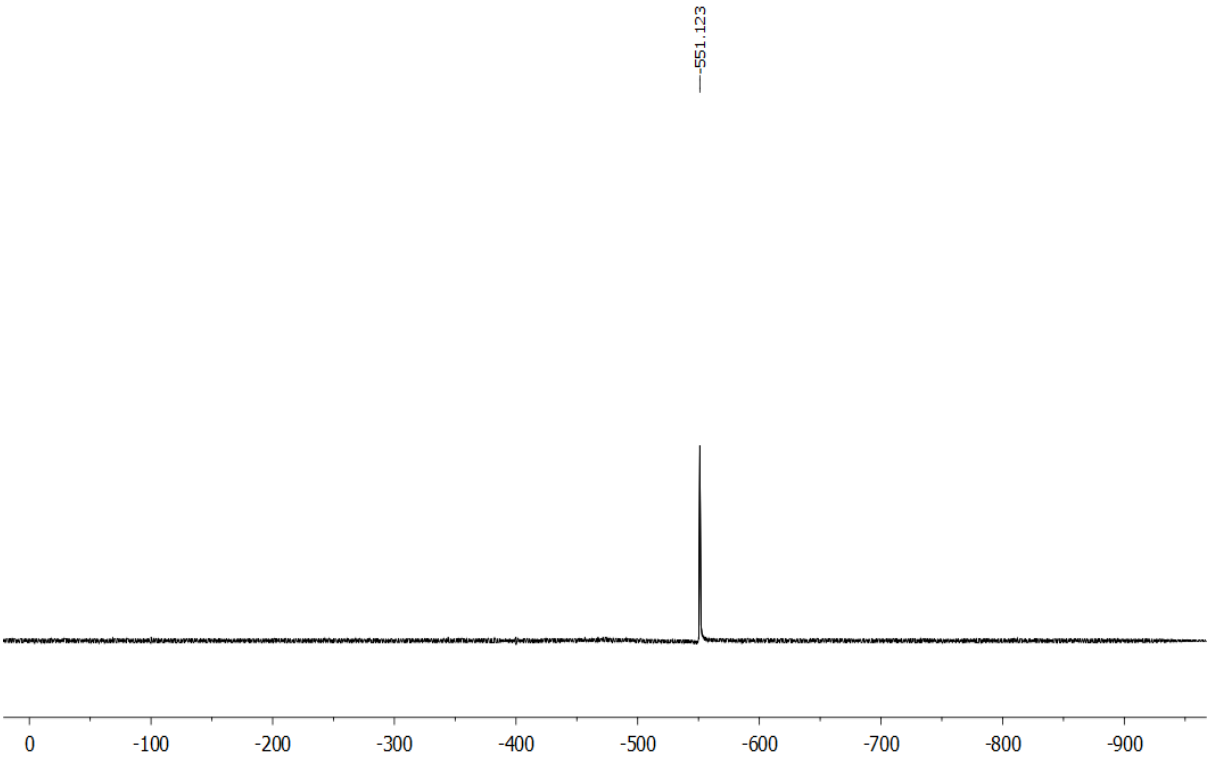


Fig. S32 The ^{51}V NMR (MeOD-d_4, 105.15 MHz) spectrum of **5**.

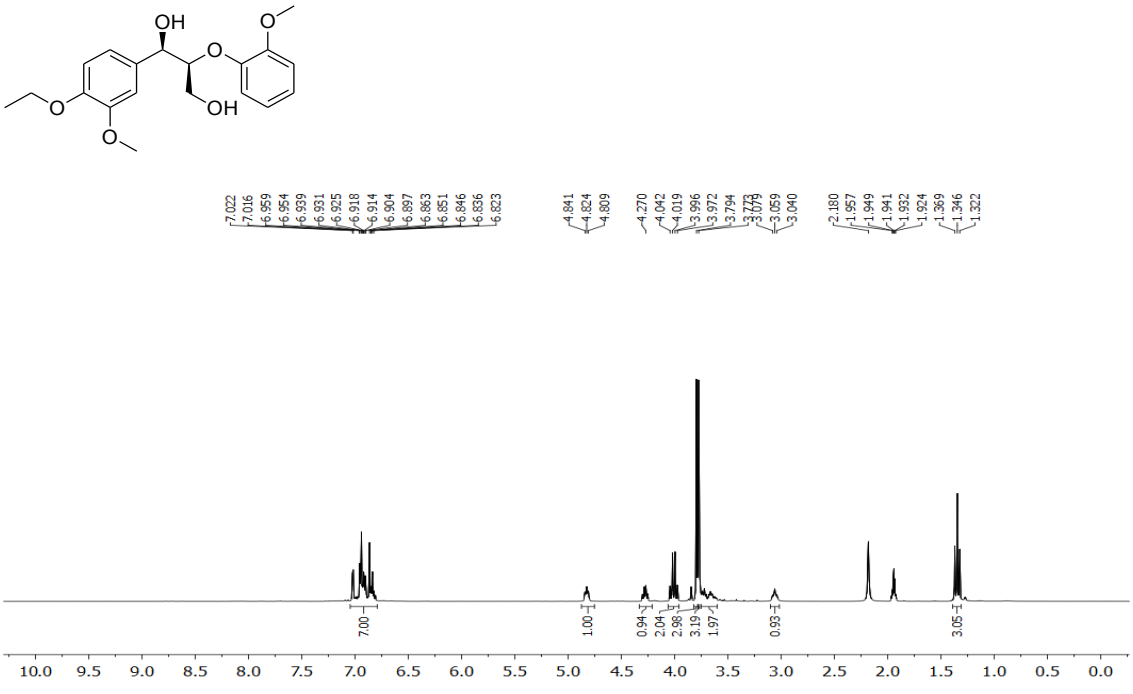


Fig. S33 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **11**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.18 ppm is due to water present in the NMR solvent.

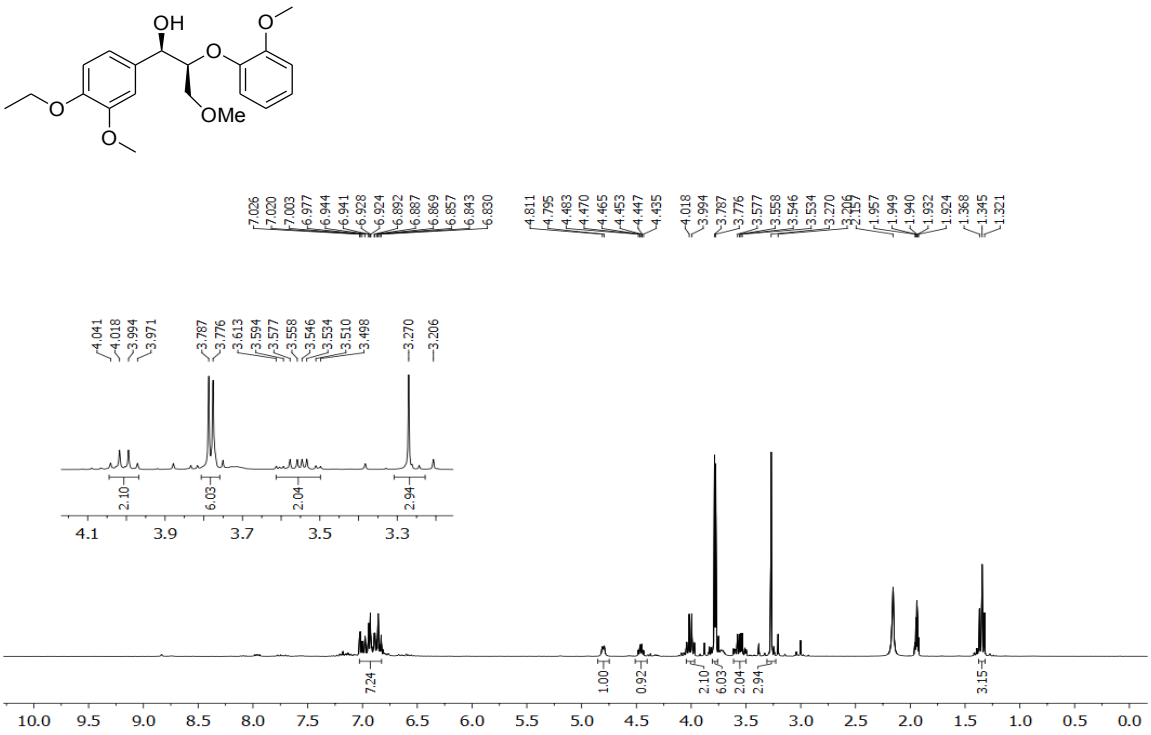


Fig. S34 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **13**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.16 ppm is due to water present in the NMR solvent.

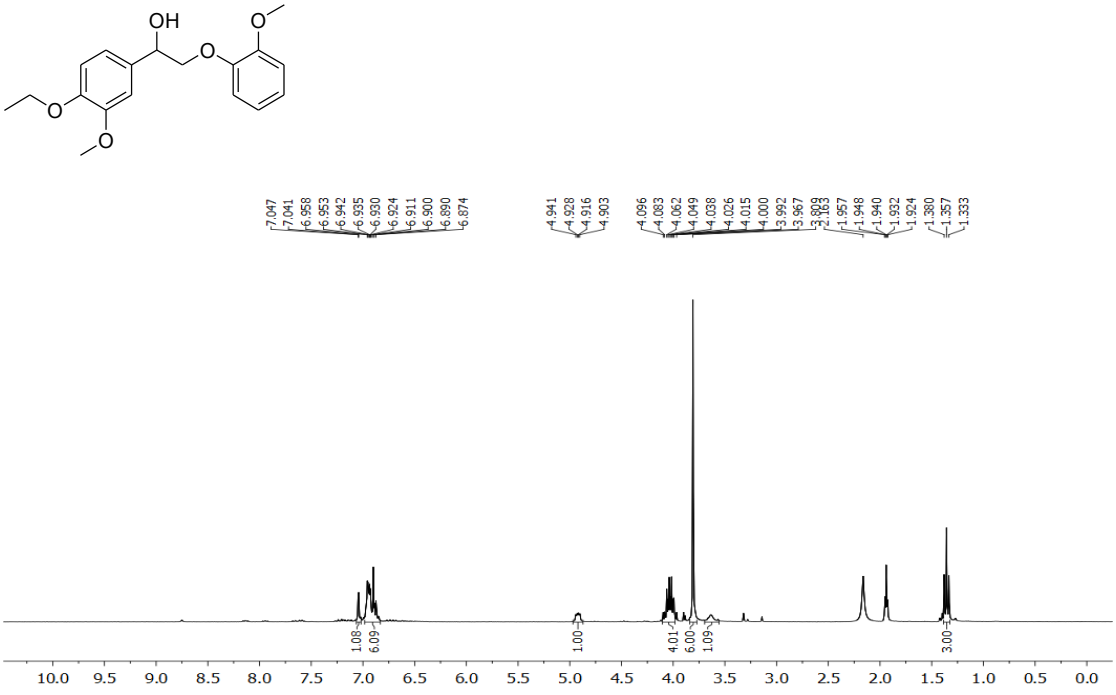


Fig. S35 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **15**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.16 ppm is due to water present in the NMR solvent.

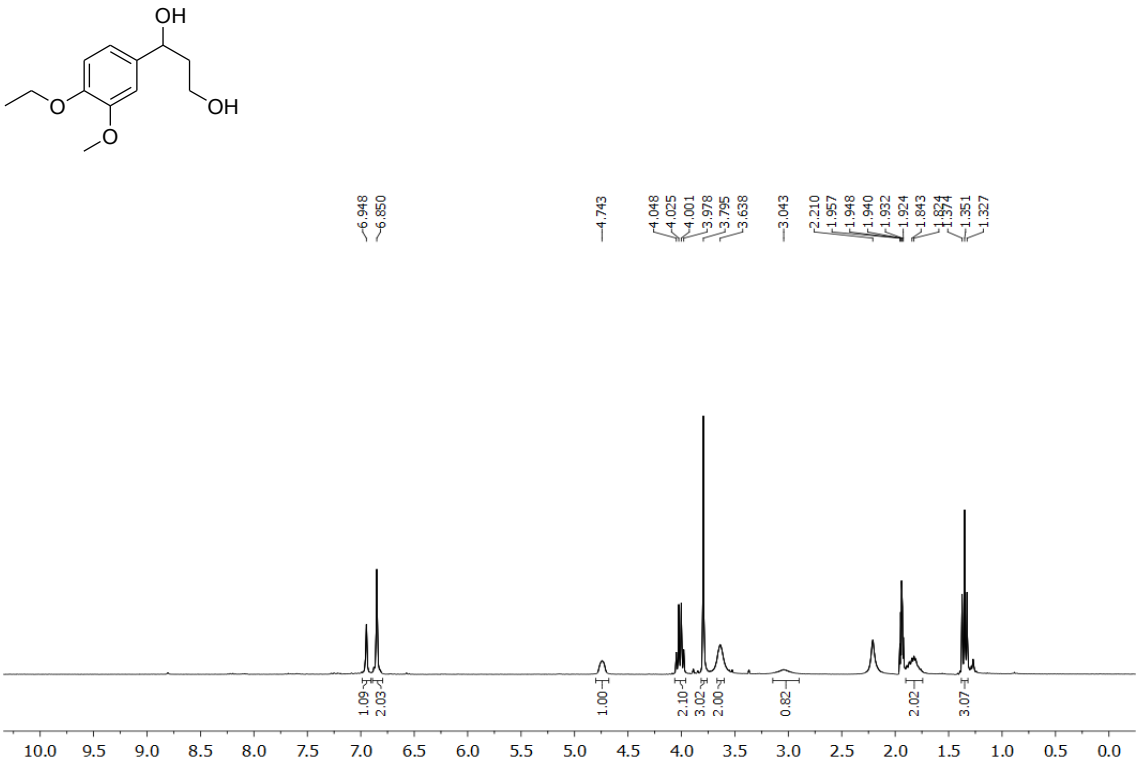


Fig. S36 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **17**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.21 ppm is due to water present in the NMR solvent.

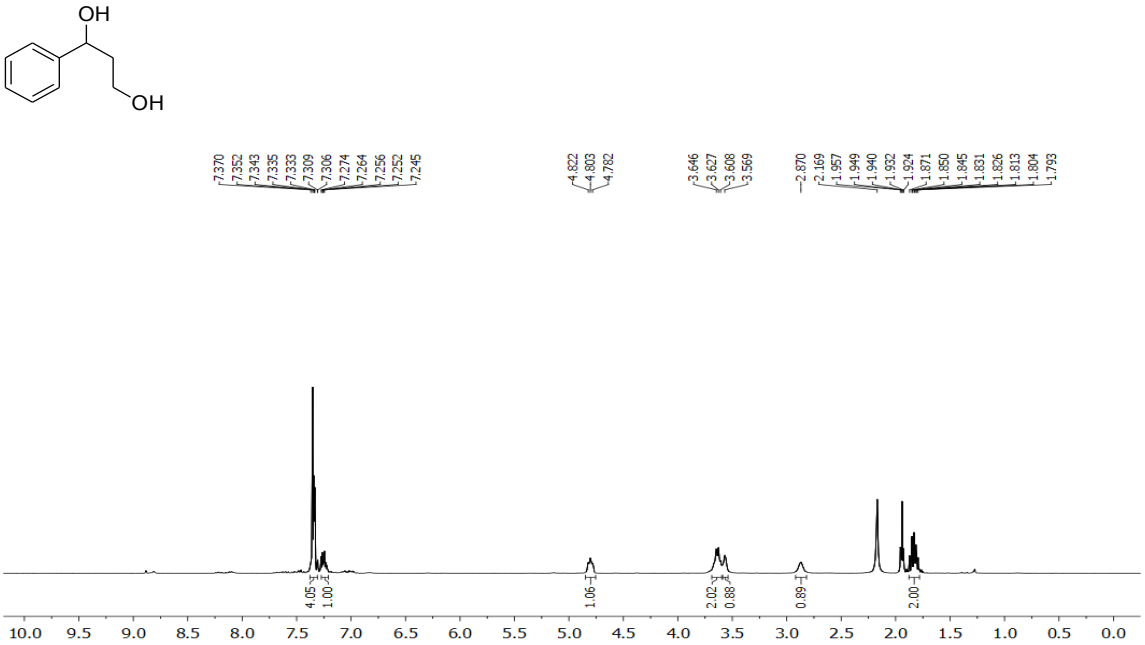


Fig. S37 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **20**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.17 ppm is due to water present in the NMR solvent.

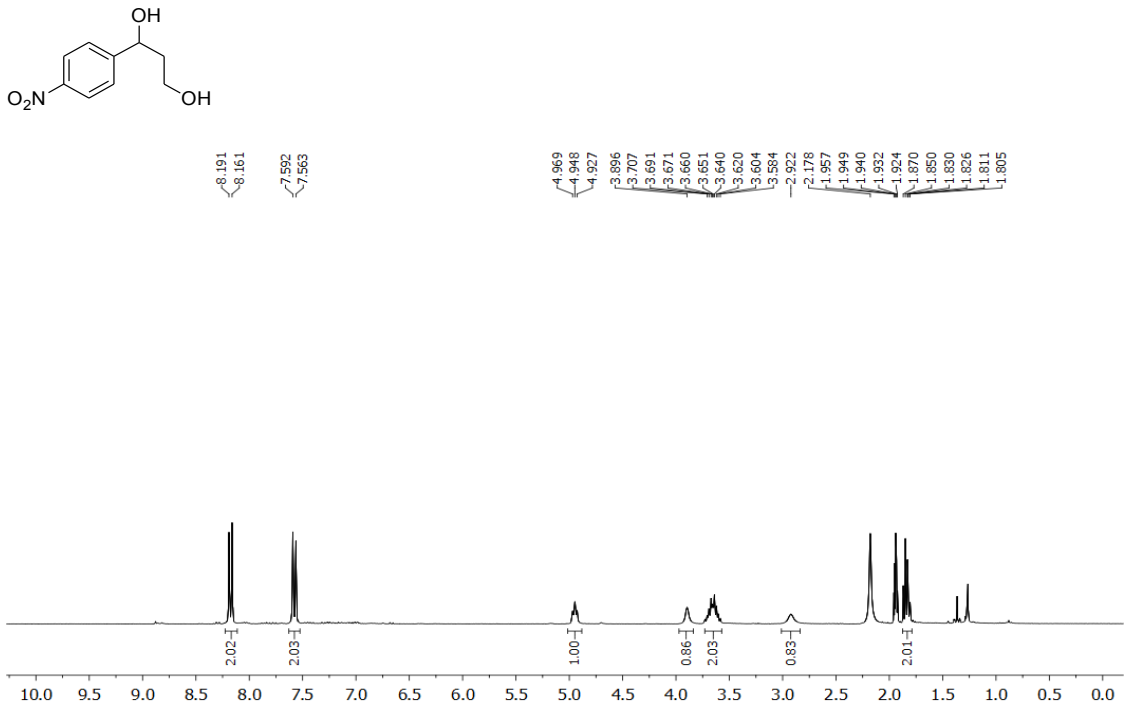


Fig. S38 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **23**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.18 ppm is due to water present in the NMR solvent.

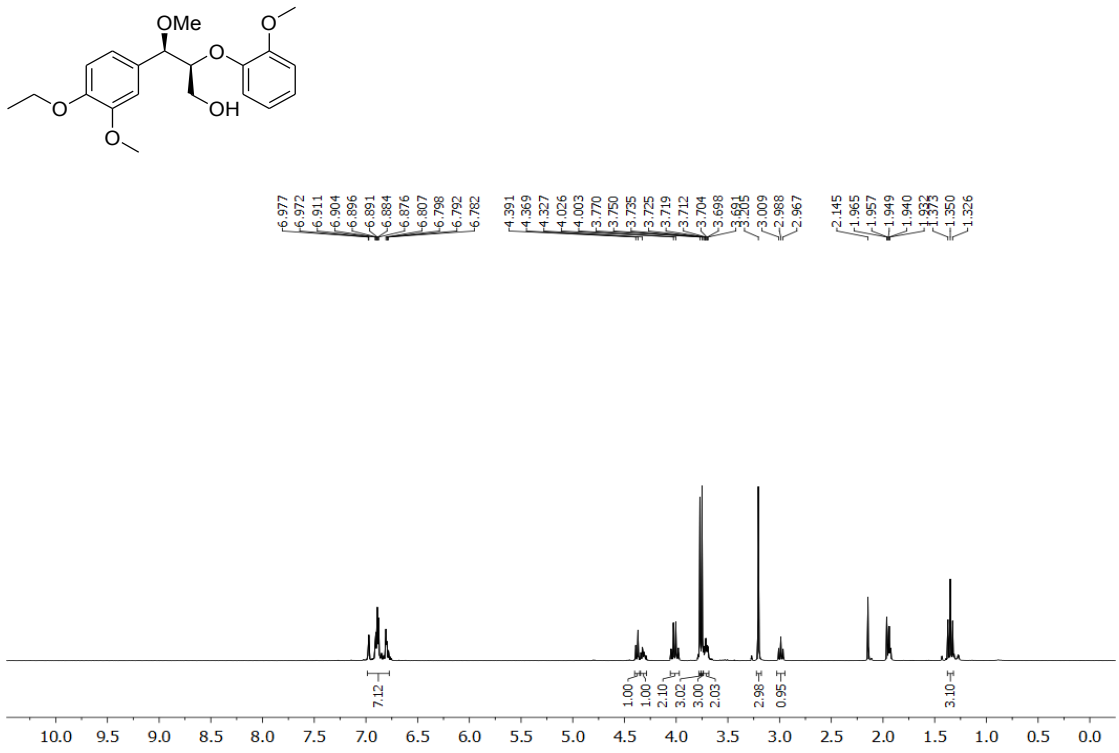


Fig. S39 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **25**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.15 ppm is due to water present in the NMR solvent.

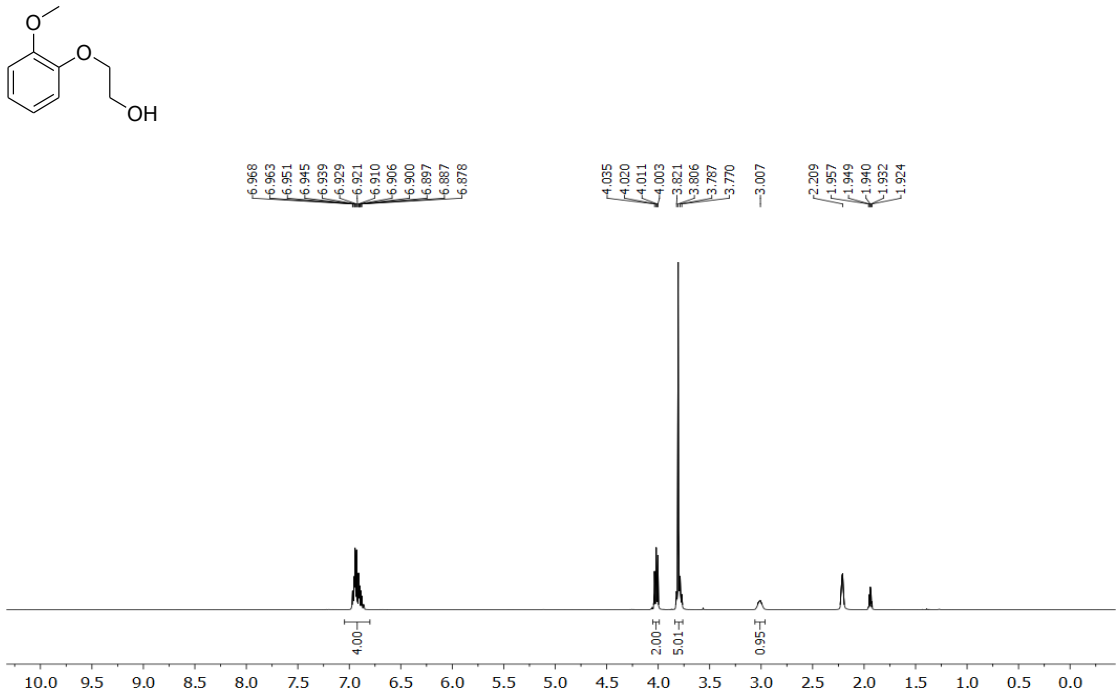


Fig. S40 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **27**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.21 ppm is due to water present in the NMR solvent.

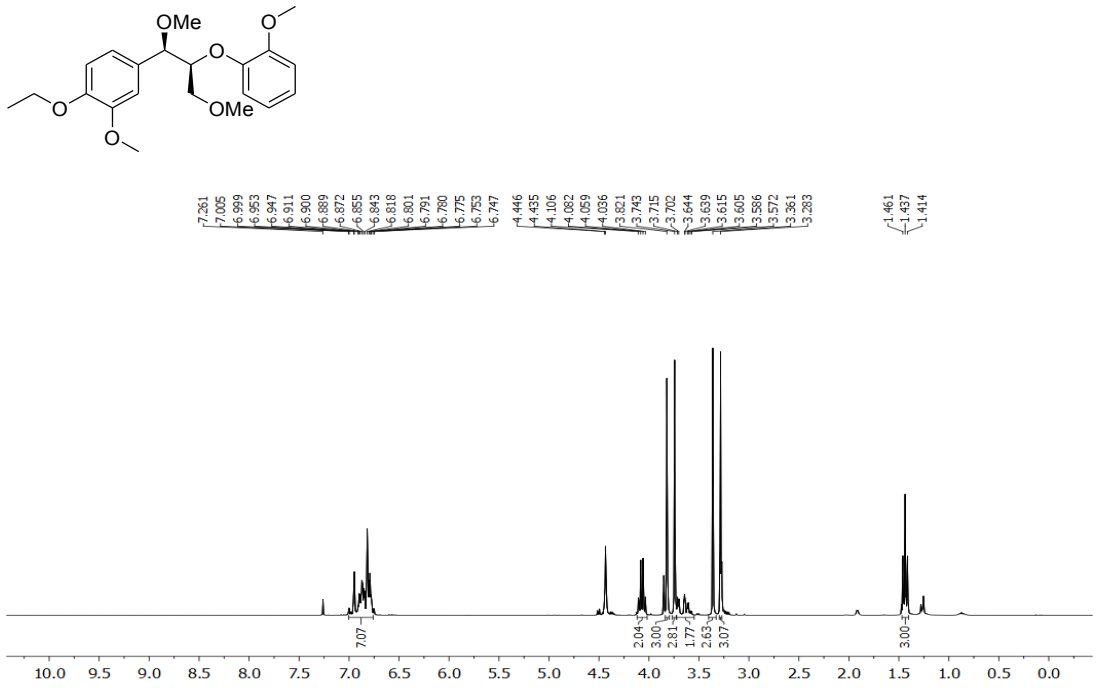


Fig. S41 The ^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **28**. The solvent residual peak is at 7.26 ppm.

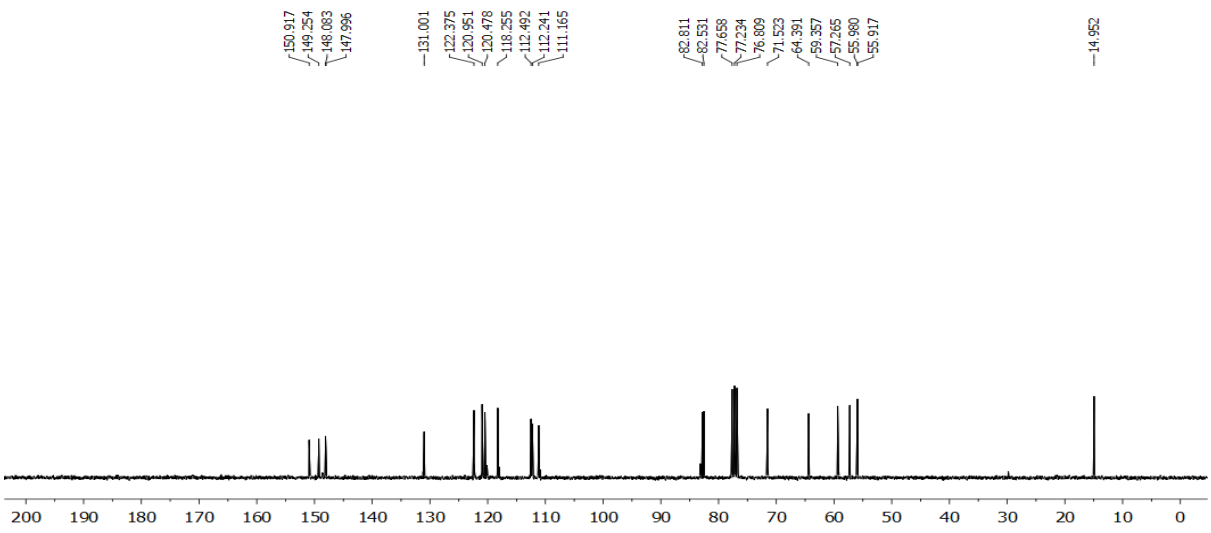


Fig. S42 The $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75 MHz) spectrum of **28**. The solvent residual is peak at 77.2 ppm (triplet).

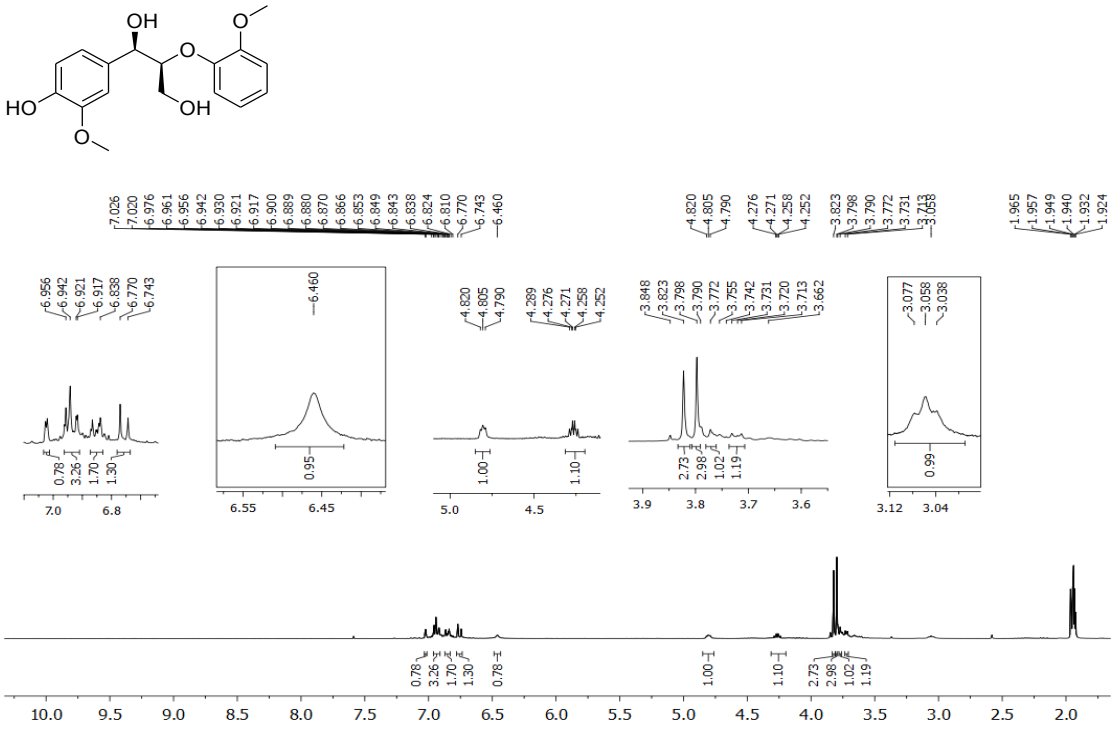


Fig. S43 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **31**. The solvent residual peak is at 1.94 ppm (quintet).

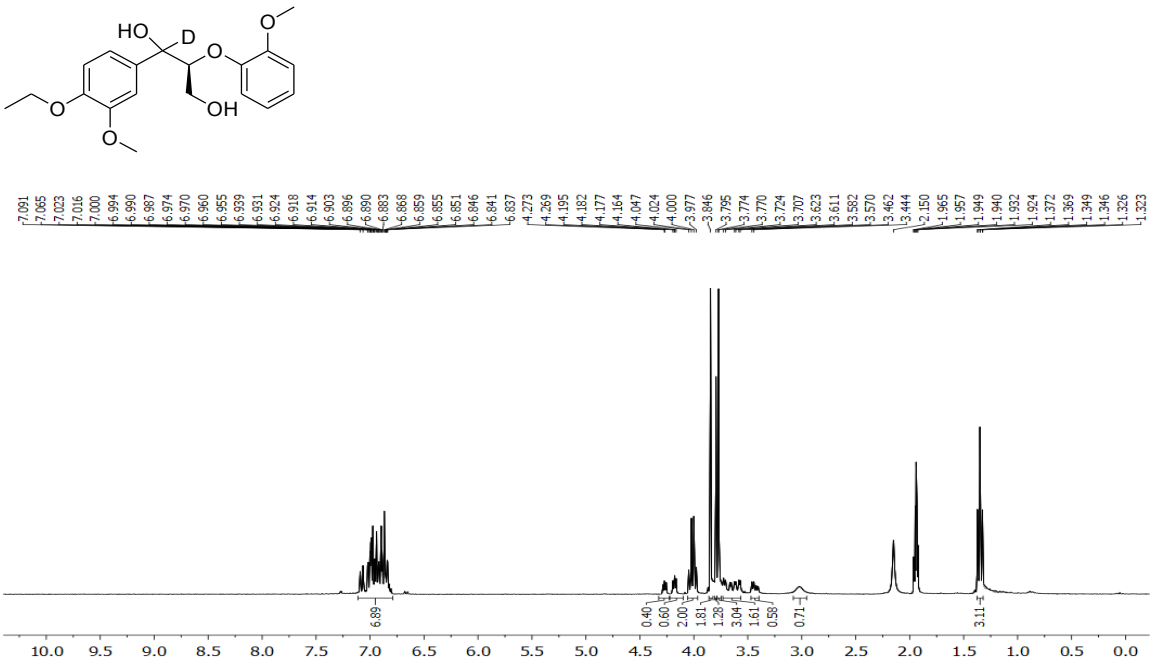


Fig. S44 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **11-D1**. The solvent residual peak is at 1.94 ppm (multiplet).The peak at 2.15 ppm is due to water present in the NMR solvent.

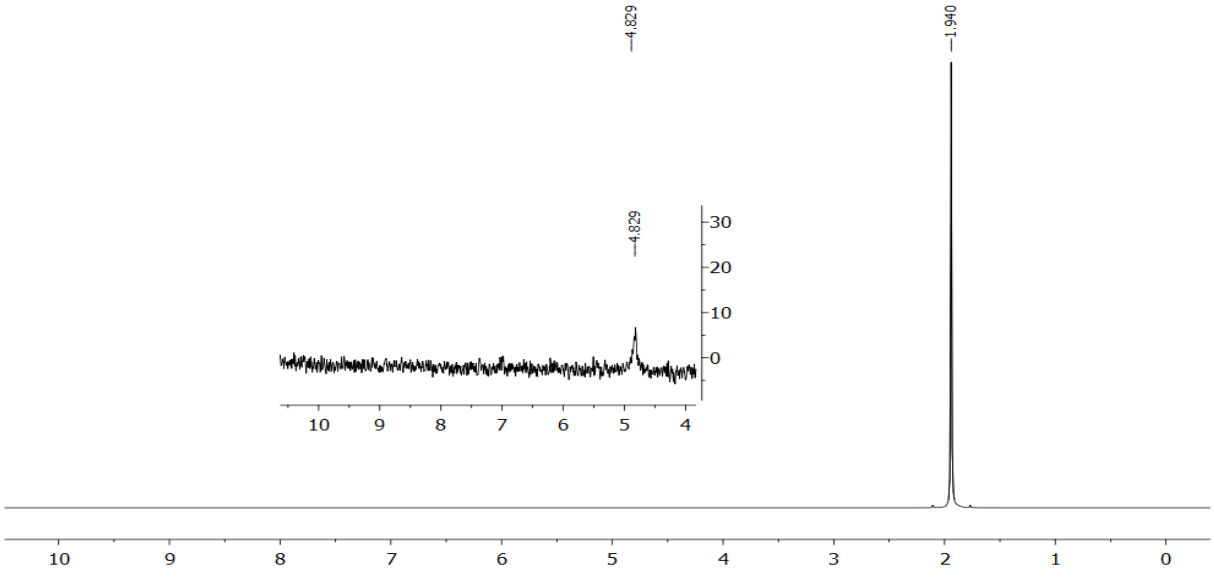


Fig. S45 The $^{2}H\{^{1}H\}$ NMR (CD_3CN, 400 MHz) spectrum of **11-D1**. Inset: Magnification of the region corresponding to the signal from **11-D1**, with the peak at -1.94 ppm derived from CD_3CN.

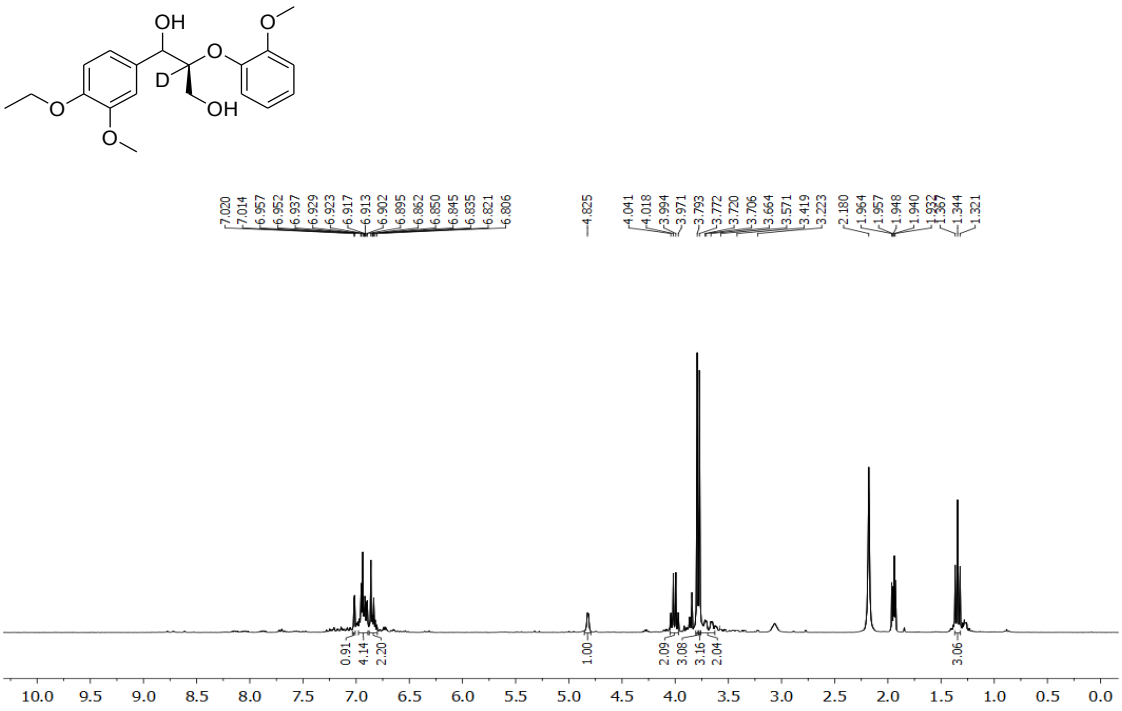


Fig. S46 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **11-D2**. The solvent residual peak is at 1.94 ppm (quintet).The peak at 2.18 ppm is due to water present in the NMR solvent.

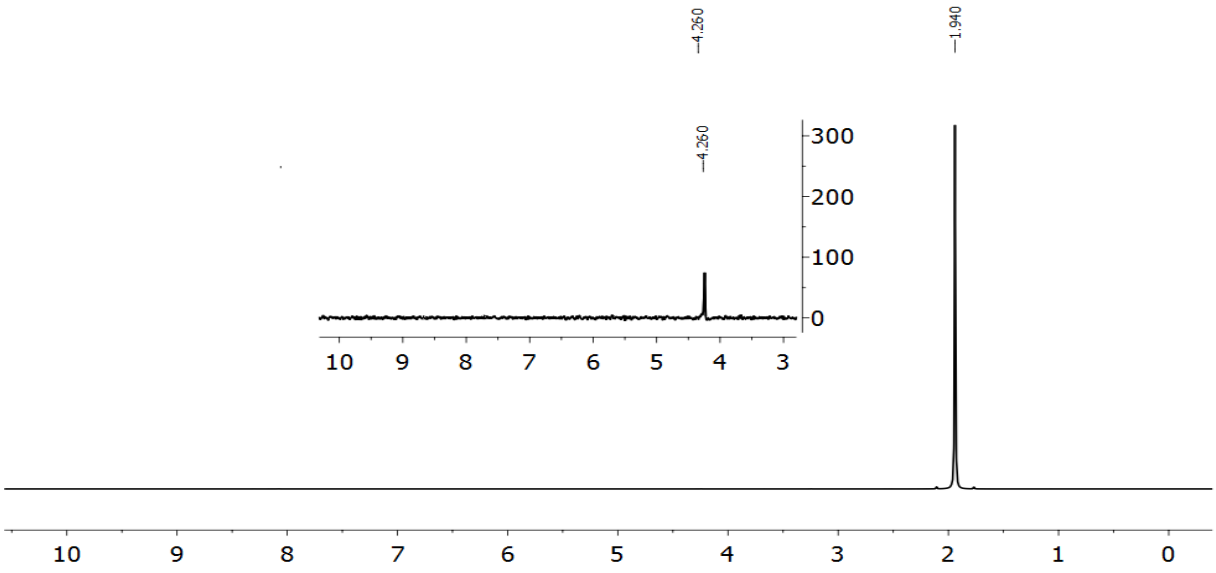


Fig. S47 The $^{2}H\{^{1}H\}$ NMR (CD_3CN, 400 MHz) spectrum of **11-D2**. Inset: Magnification of the region corresponding to the signal from **11-D2**, with the peak at -1.94 ppm derived from CD_3CN.

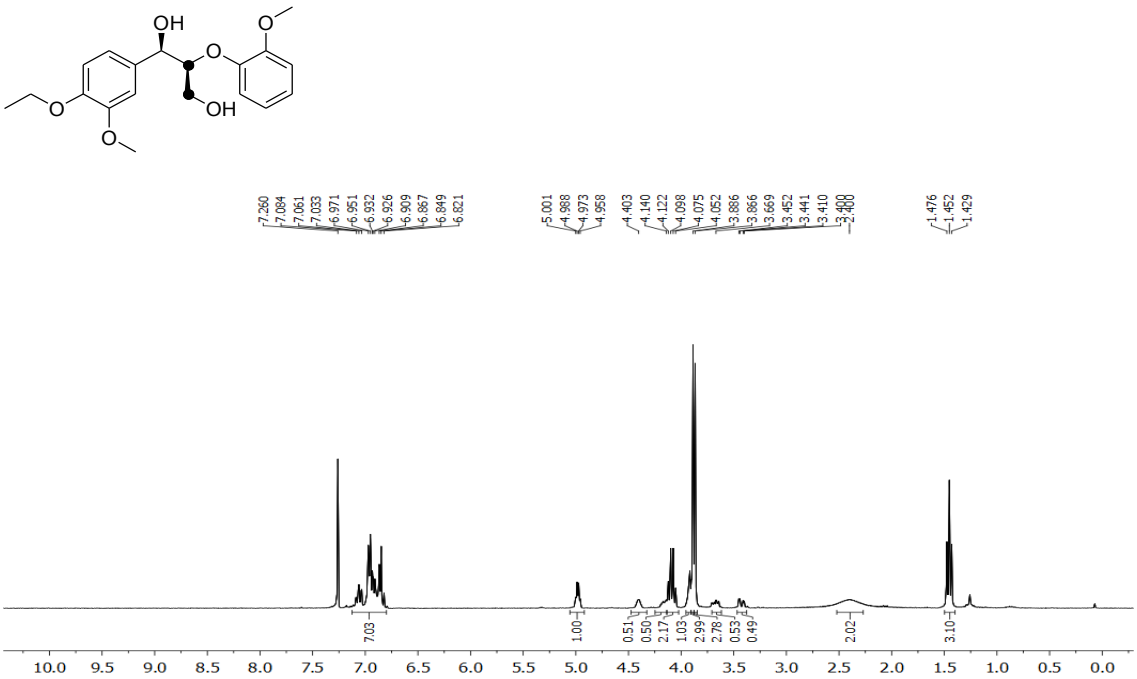


Fig. S48 The ^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **11-^{13}C2**. The solvent residual peak is at 7.26 ppm.

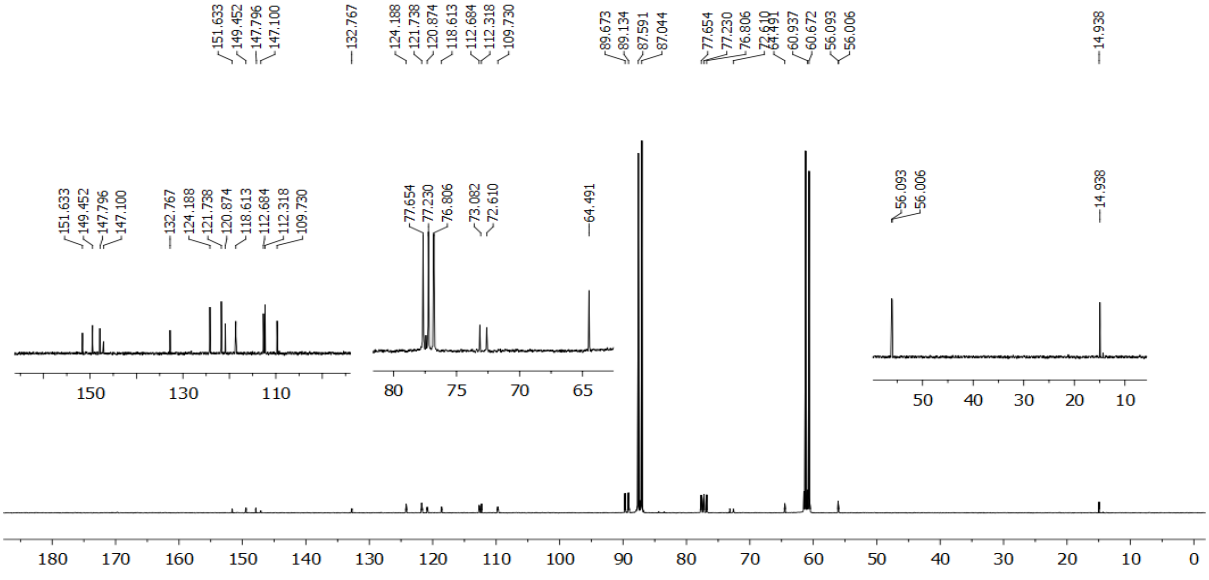


Fig. S49 The ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz) spectrum of **11-^{13}C2**. The solvent residual peak is at 77.2 (triplet) ppm. Inset (left): Magnification of the aromatic region. (middle): Magnification of the ethereal carbon region. (right): Magnification of the aliphatic carbon region.

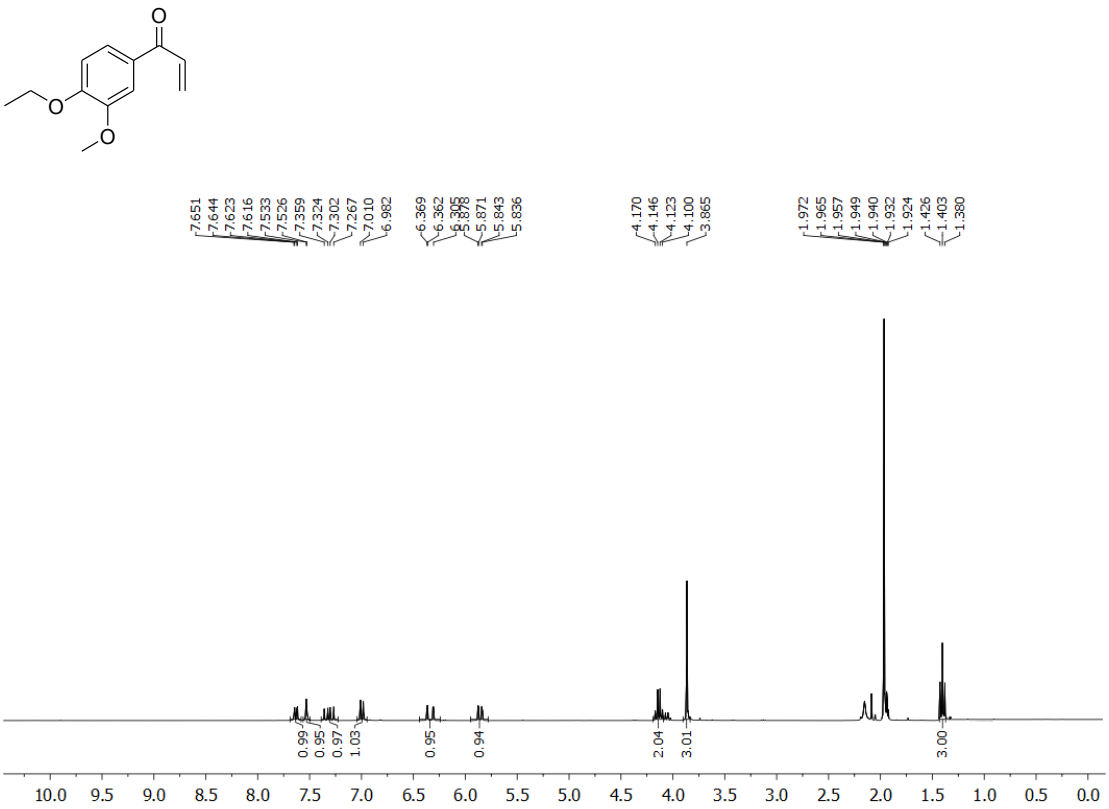


Fig. S50 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **12**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.21 ppm is due to water present in the NMR solvent.

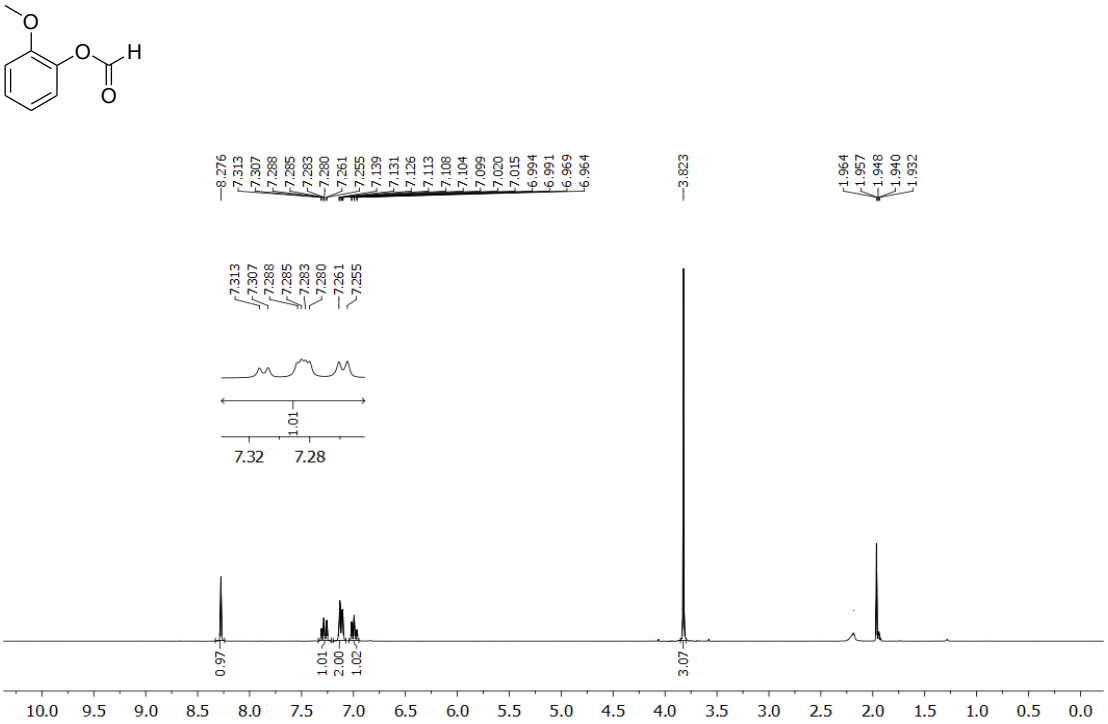


Fig. S51 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **9**. The solvent residual peak is at 1.94 ppm (quintet).

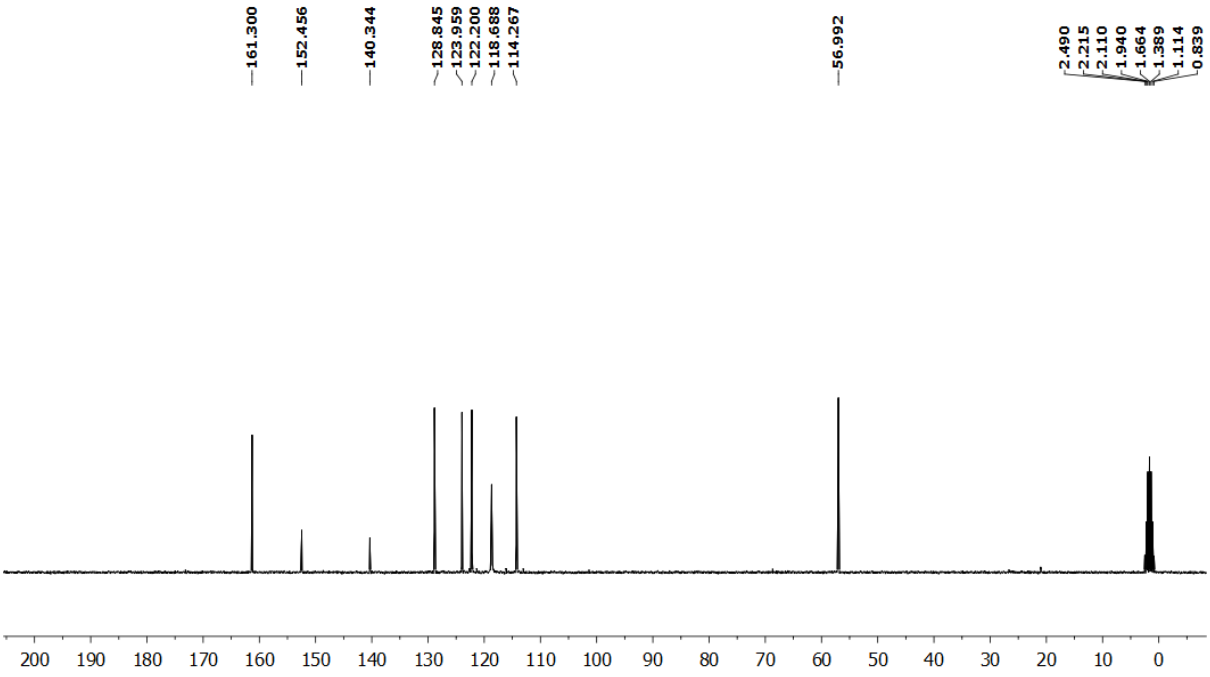


Fig. S52 The $^{13}C\{^{1}H\}$ NMR (CD_3CN, 75 MHz) spectrum of **9**. The solvent residual peak is at 1.39 ppm (septet).

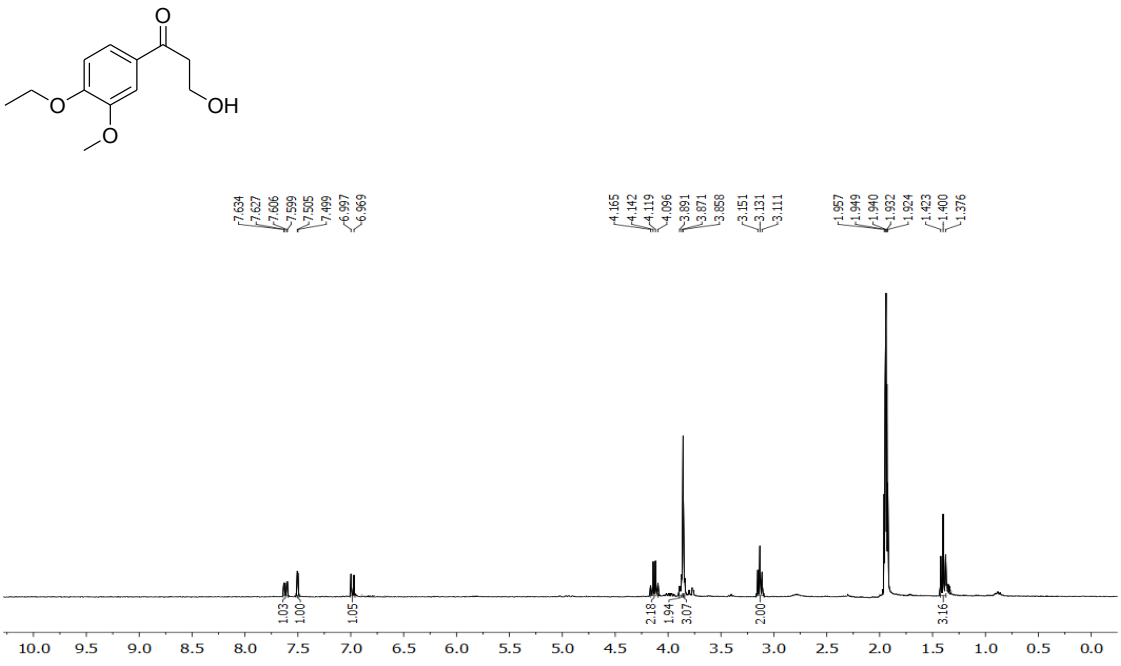


Fig. S53 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **18**. The solvent residual peak is at 1.94 ppm (quintet).

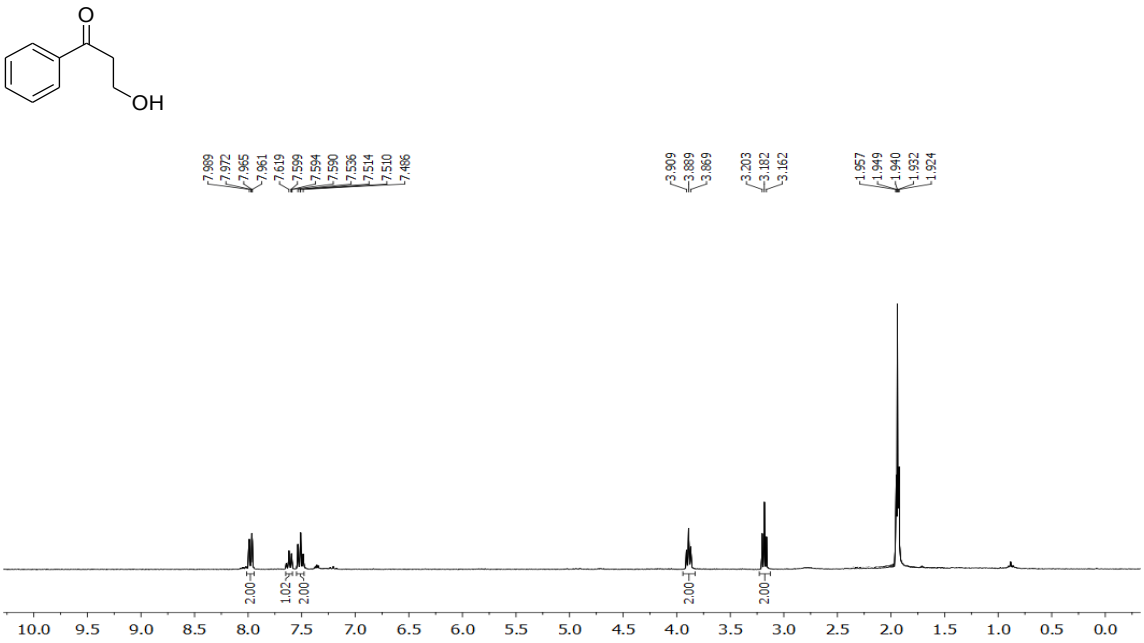


Fig. S54 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **21**. The solvent residual peak is at 1.94 ppm (quintet).

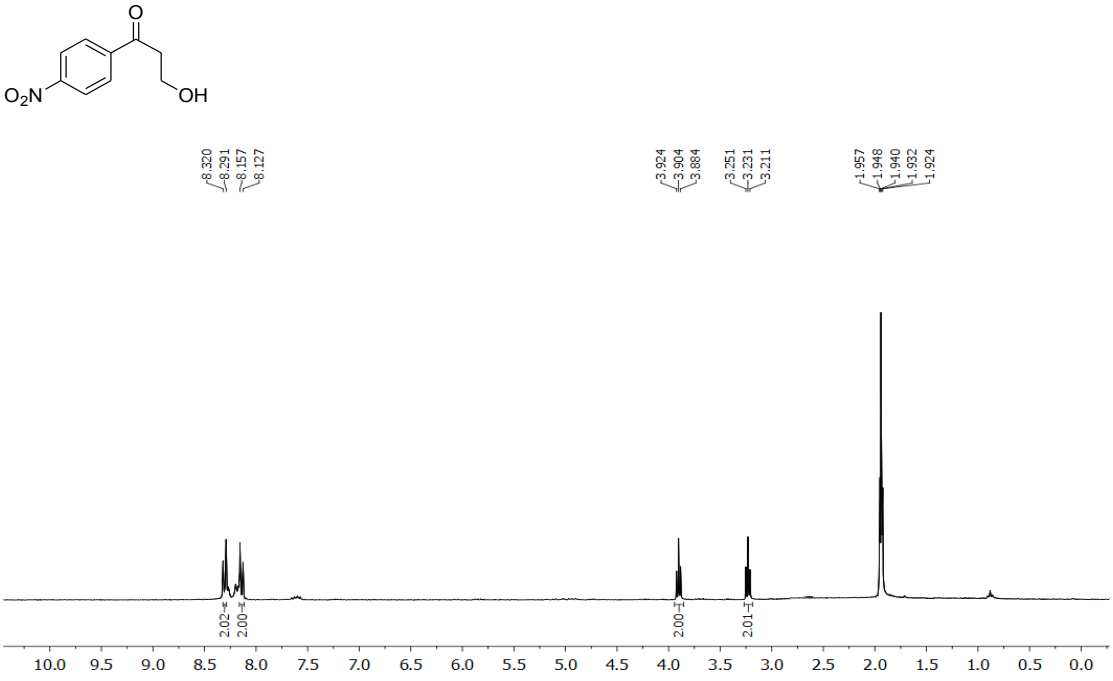


Fig. S55 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **24**. The solvent residual peak is at 1.94 ppm (quintet).

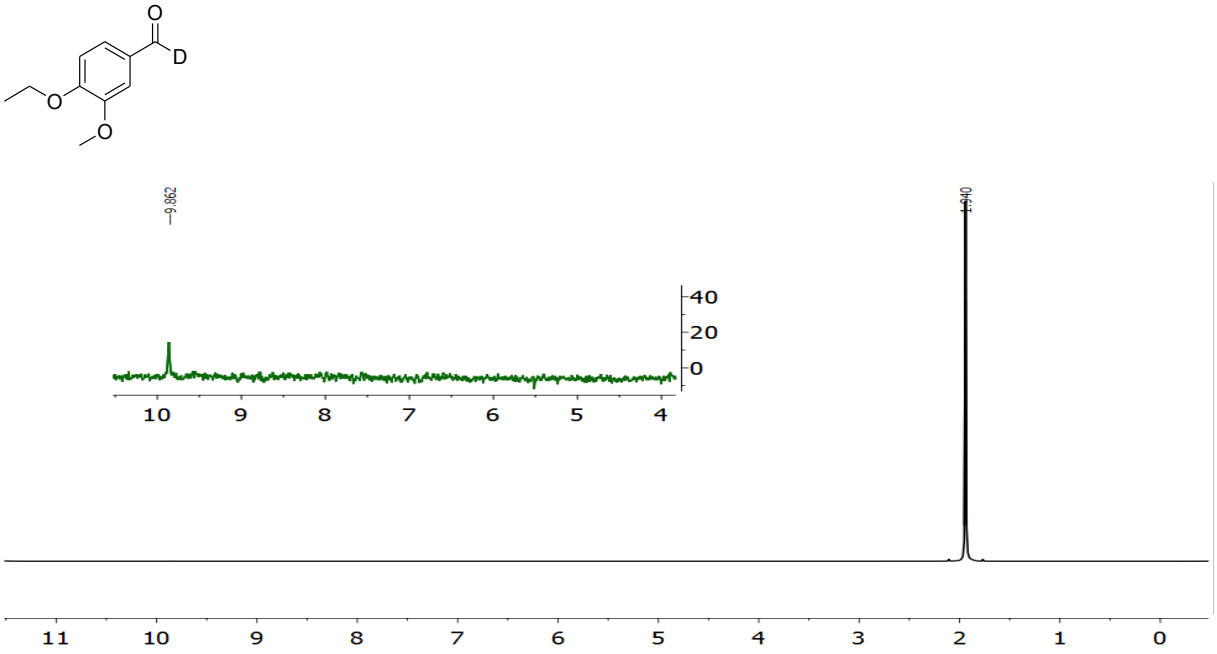


Fig. S56 The $^{2}H\{^{1}H\}$ NMR (CD_3CN, 400 MHz) spectrum of **6-D**. Inset: Magnification of the region corresponding to the signal from **6-D**, with the peak at -1.94 ppm derived from CD_3CN.

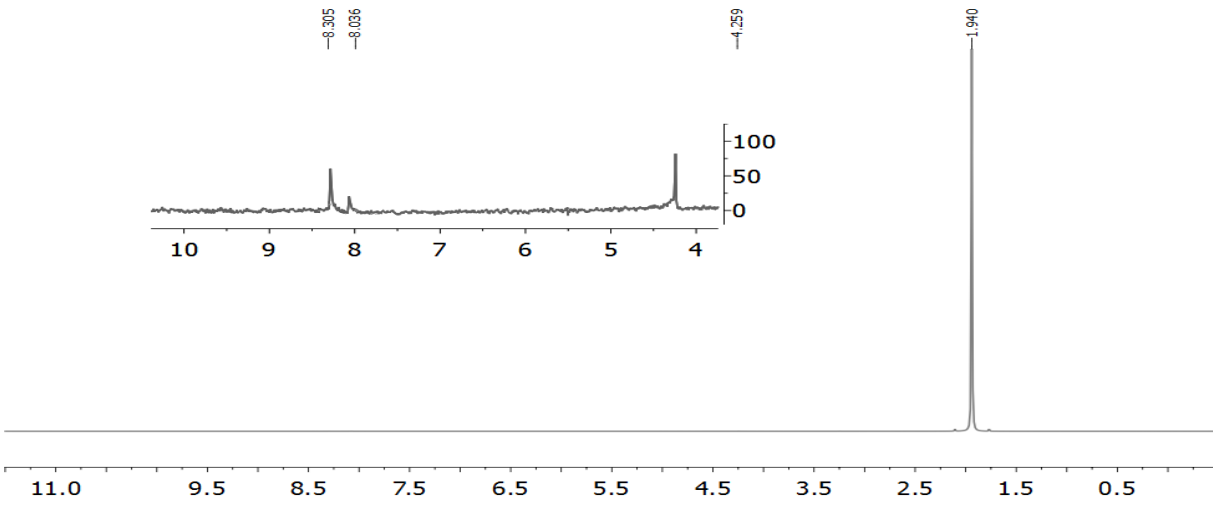


Fig. S57 The $^{2}H\{^{1}H\}$ NMR (CD_3CN, 400 MHz) spectrum of the photocatalytic reaction mixture containing **11-D2** and **2** in CD_3CN after 24 h of visible light irradiation. Inset: Magnification of the region corresponding to the signal from the products **9-D** and deuterated formic acid, with the peak at -1.94 ppm derived from CD_3CN. Unreacted **11-D2** remained after 24 h due to the slower reaction rate.

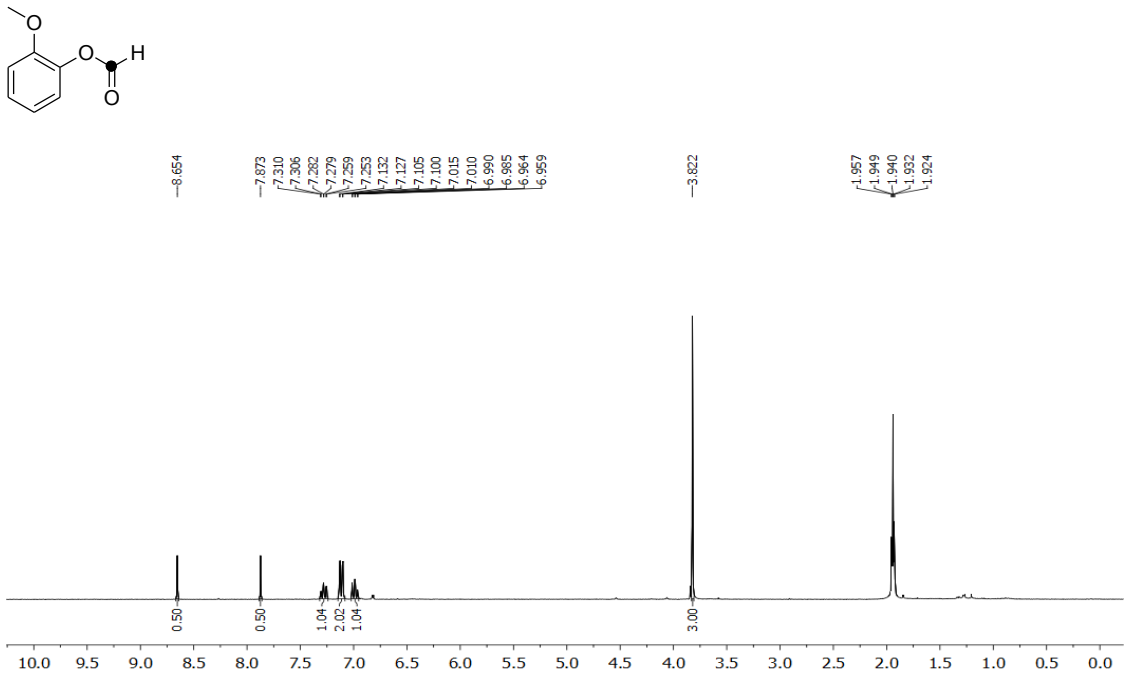


Fig. S58 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **9-^{13}C1**. The solvent residual peak is at 1.94 ppm (quintet).

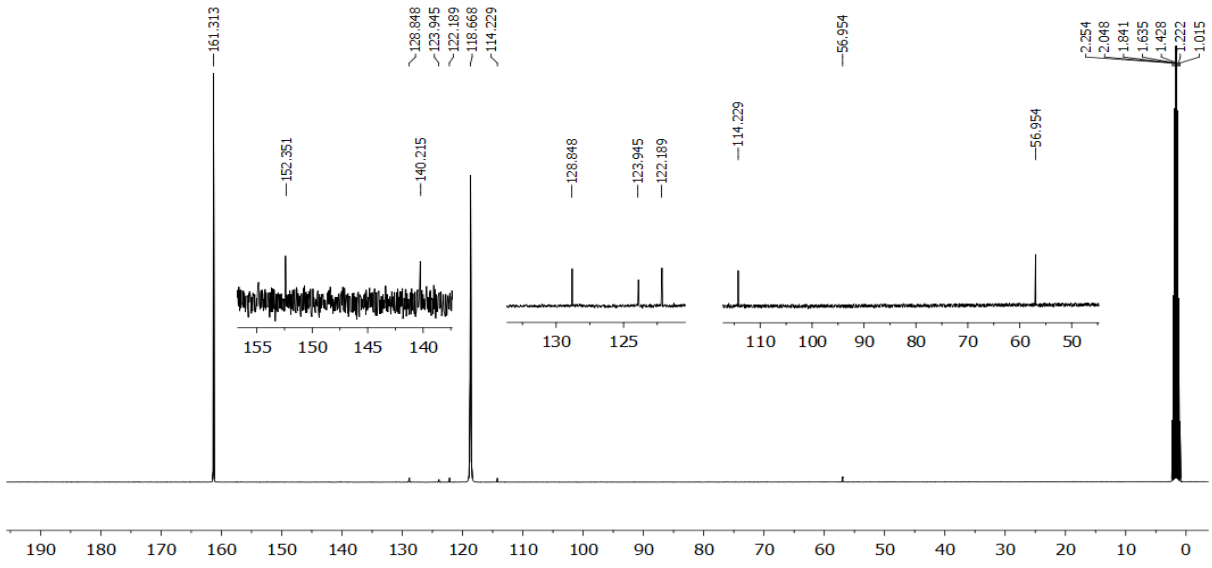


Fig. S59 The ^{13}C{^{1}H} NMR (CD_3CN, 75 MHz) spectrum of **9-^{13}C1**. The solvent residual peaks are at 1.39 (septet) and 118.6 ppm. Inset (left and middle): Magnification of the aromatic region. (right): Magnification of the remainder.

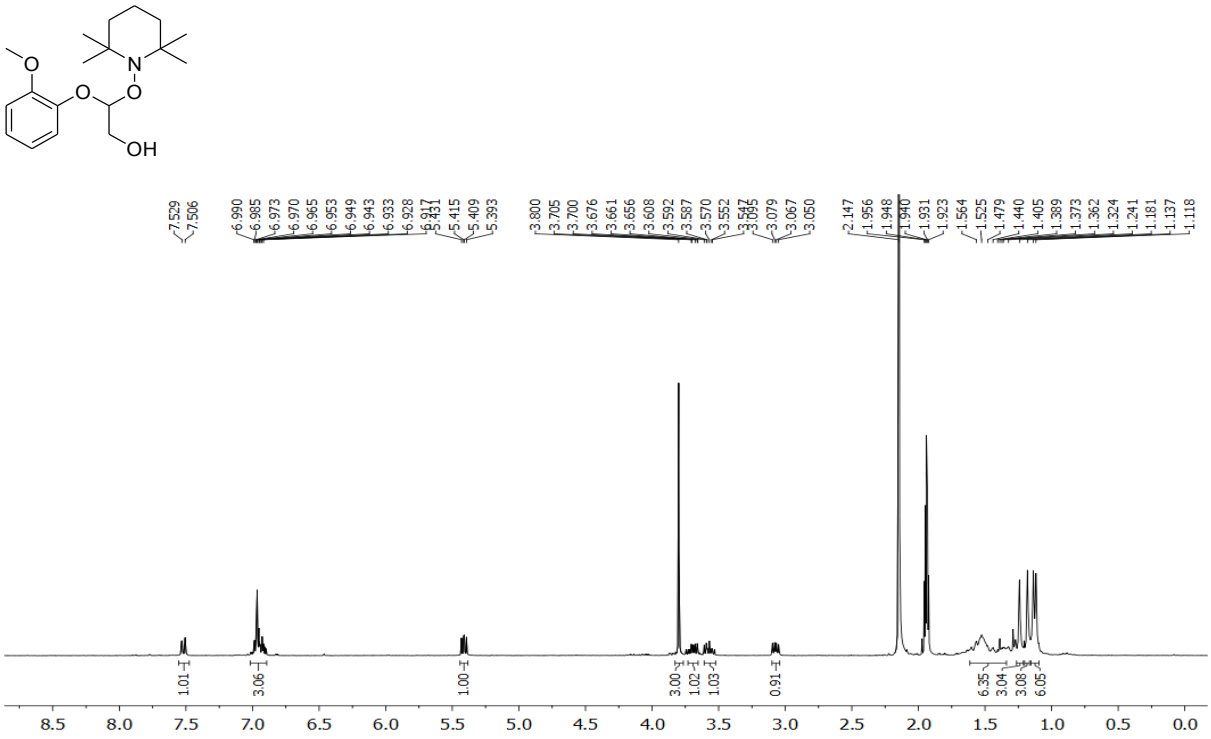


Fig. S60 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of **34**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.15 ppm is due to water present in the NMR solvent.

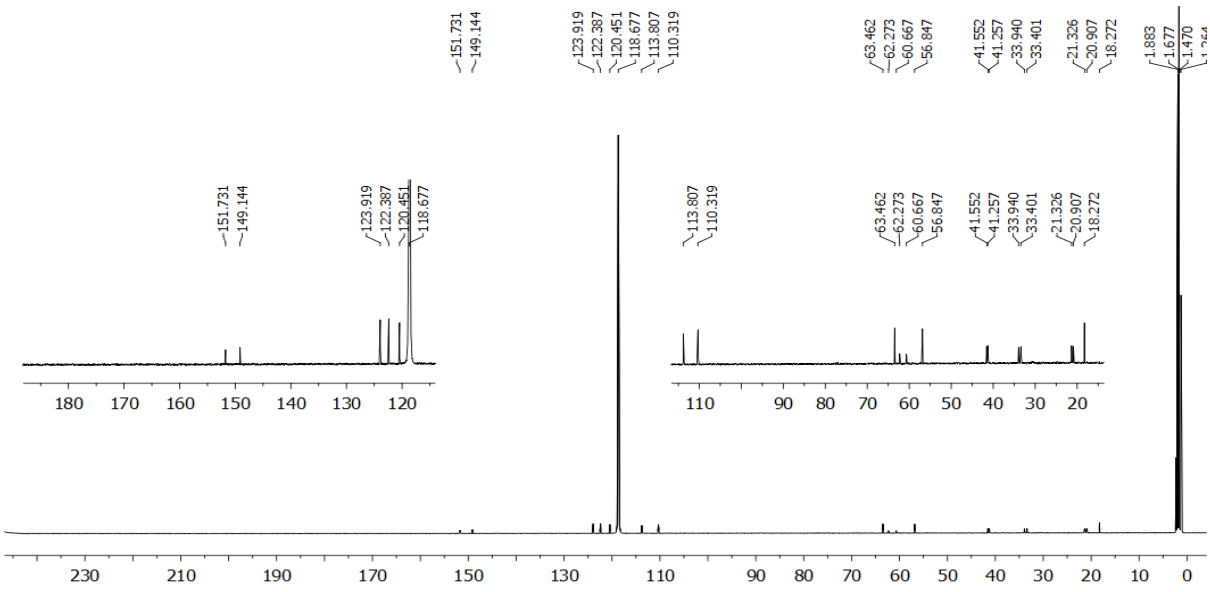


Fig. S61 The $^{13}C\{^{1}H\}$ NMR (CD_3CN, 100 MHz) spectrum of **34**. The solvent residual peaksare at 1.39 (septet) and 118.6 ppm. Inset (left): Magnification of the aromatic region. (right): Magnification of the remainder.

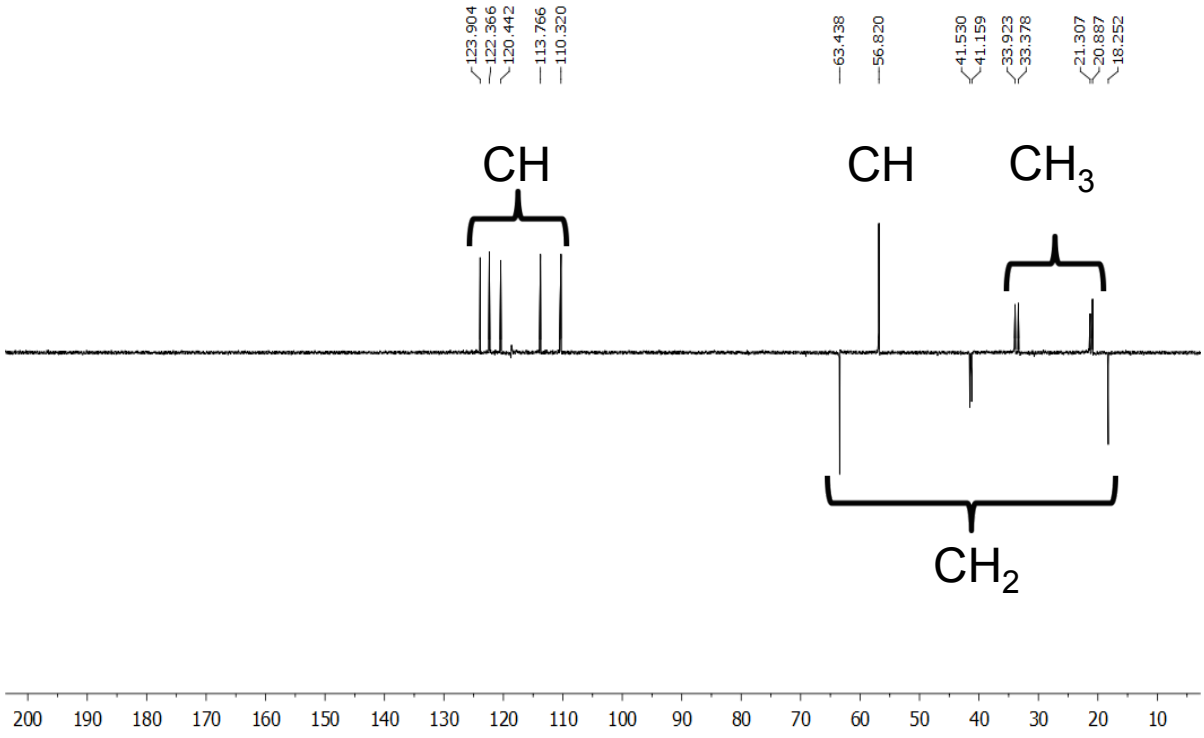


Fig. S62 The ^{13}C-DEPT-135 NMR (CD_3CN, 100 MHz) spectrum of **34**. The signals with positive phase correspond to the CH and CH_3 carbons, whereas the signals with the opposite phase belong to the CH_2 carbons.

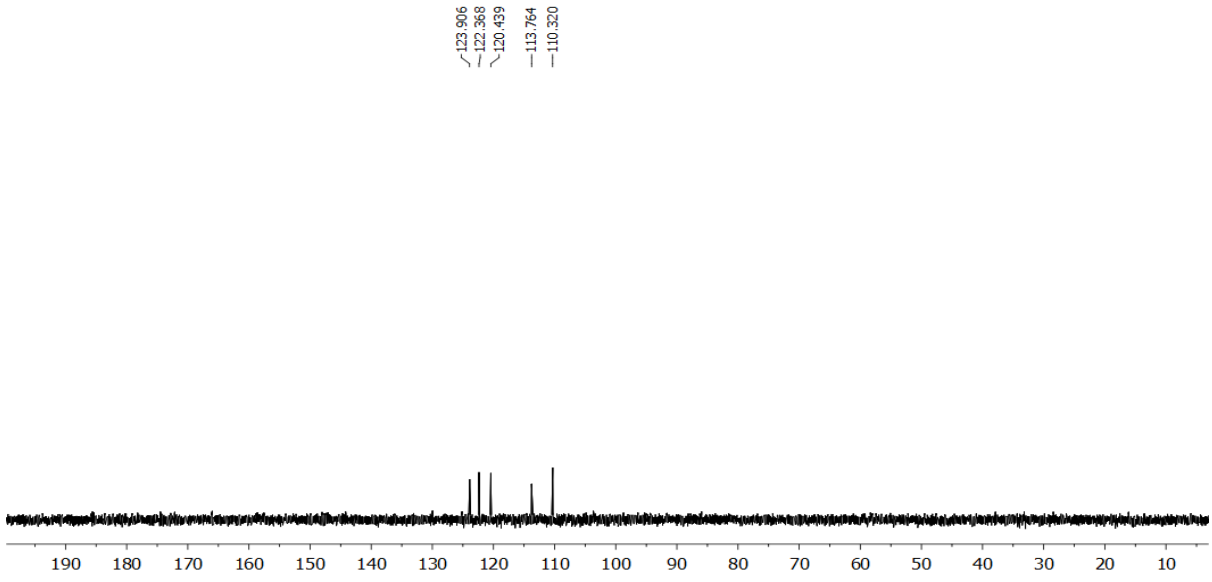


Fig. S63 The ^{13}C-DEPT-90 NMR (CD_3CN, 100 MHz) spectrum of **34**. The signals with positive phase correspond to the CH carbons.

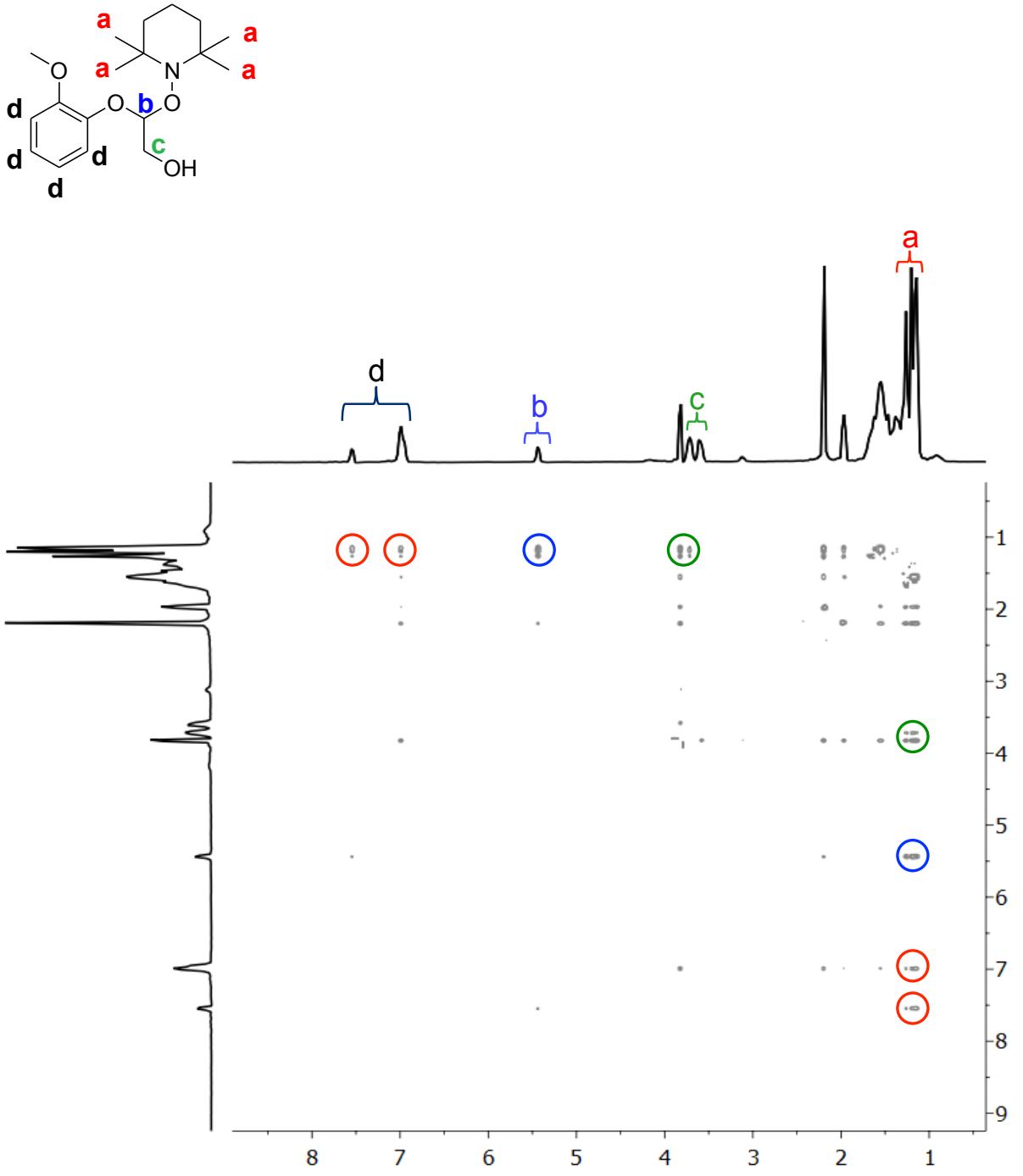


Fig. S64 The NOESY (CD_3CN, 400 MHz) data from **34**. The solvent residual peak is at 1.94 ppm (quintet). The peak at 2.15 ppm is due to water present in the NMR solvent. The correlated signals between the tetramethyl groups on the TEMPO fragment and the remainder of the molecule are highlighted with green (aliphatic primary alcohol, c), blue (methine, b), and red (aryl, d) circles.

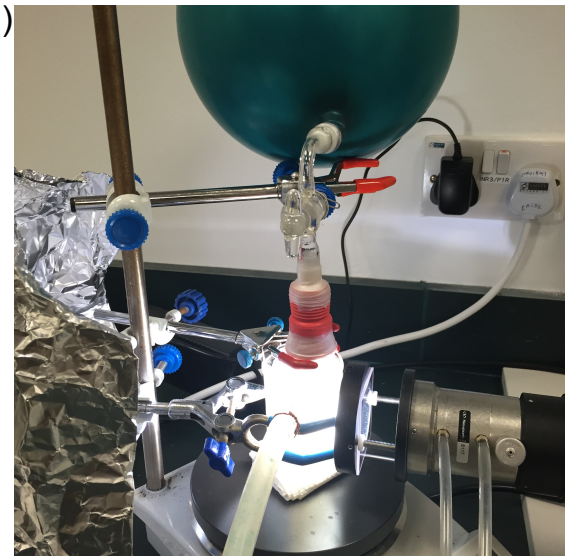
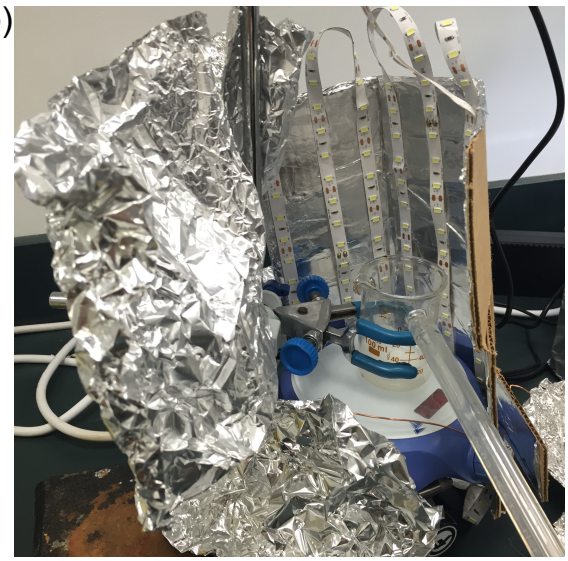
(a)  (b) 

Fig. S65 Photos of the AM1.5 solar simulator (a) and white light LED (b) setup with a water regulator for the photocatalytic experiments. Vials or NMR tubes can be rested within the water-jacketed Pyrex beakers and the temperatures have been maintained below 30 ºC throughout the experiments.

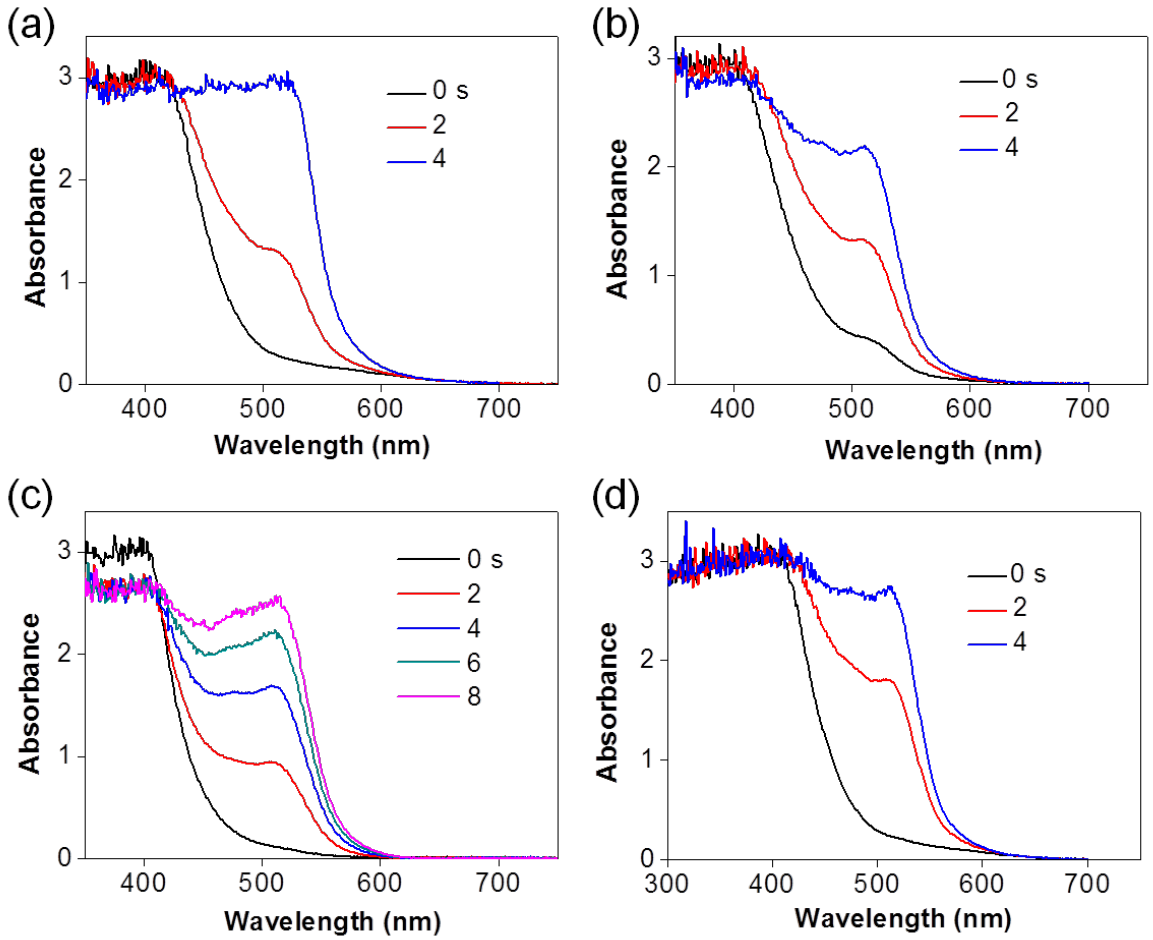


Fig. S66 UV-Vis absorption spectra containing a chemical actinometer and 1,10-phenanthroline at different irradiation time. (a) $K_3[Fe(OX)_3]$ and 1,10-phenanthroline (1:3 mole ratio) in water under visible light irradiation (with 420 nm cut-off filter). (b) $(n\text{-}Bu_4N)_3[Fe(OX)_3]$ and 1,10-phenanthroline (1:3 mole ratio) in water under visible light irradiation. (c) $(n\text{-}Bu_4N)_3[Fe(OX)_3]$ and 1,10-phenanthroline (1:3 mole ratio) in CH_3CN under visible light irradiation. (d) $K_3[Fe(OX)_3]$ and 1,10-phenanthroline (1:3 mole ratio) in water under AM1.5 irradiation (without 420 nm cut-off filter).

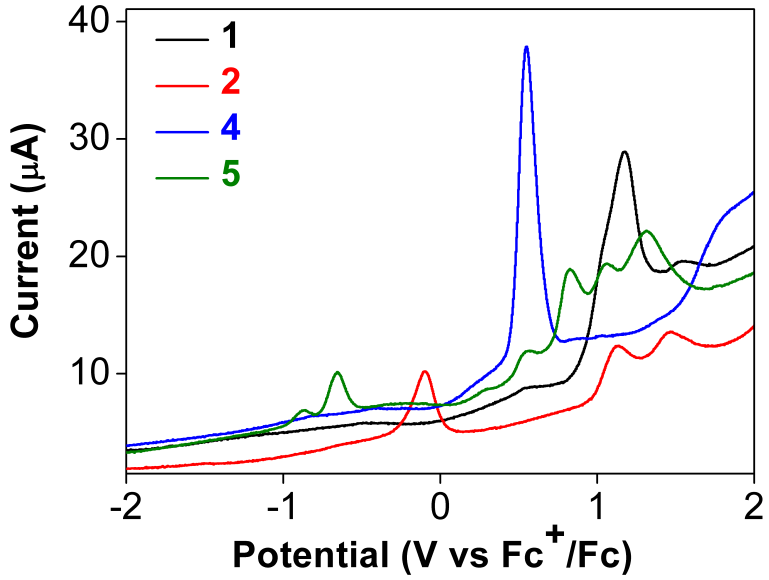


Fig. S67 Differential pulse voltammograms (DPV) of compounds **1** (black), **2** (red), **4** (blue), and **5** (green) in CH_3CN. (with scan rate 50 mV s^{-1}, pulse-height 50 mV, pulse-width 50 ms, step-height 4 mV, and step-time 80 ms).

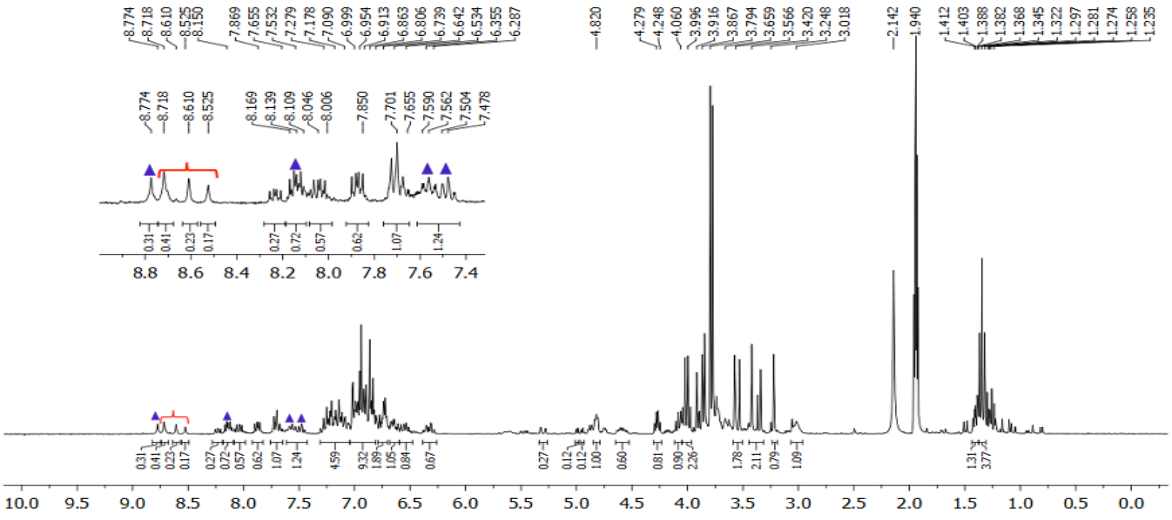


Fig. S68 The ^1H NMR (CD_3CN, 300 MHz) spectrum of a solution containing **2** and **9** (each 0.020 mmol). The solvent residual peak is at 1.94 ppm (quintet). The characteristic peaks of **2** are indicated by blue triangles. The peaks between 8.5 to 8.8 ppm are characteristic of the aldimine peak. The spectrum suggests that the solution consists of **2** and at least three new complexes, likely due to diastereomers of **11** coordinating via the different alcohol groups existing in equilibrium at room temperature in the absence of light.

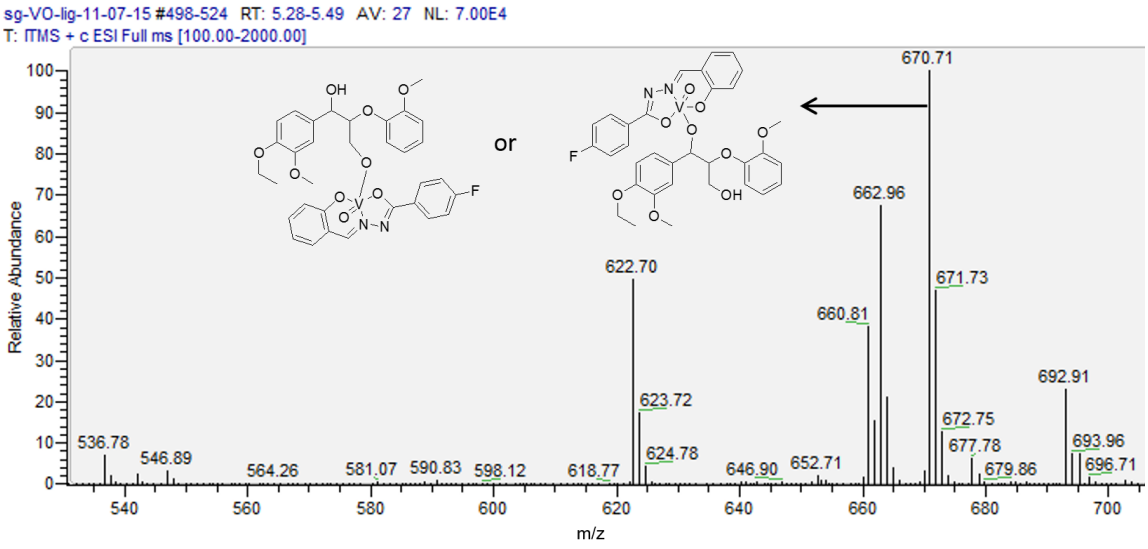


Fig. S69 ESI-mass spectrum of an equimolar mixture of **2** and **11**.

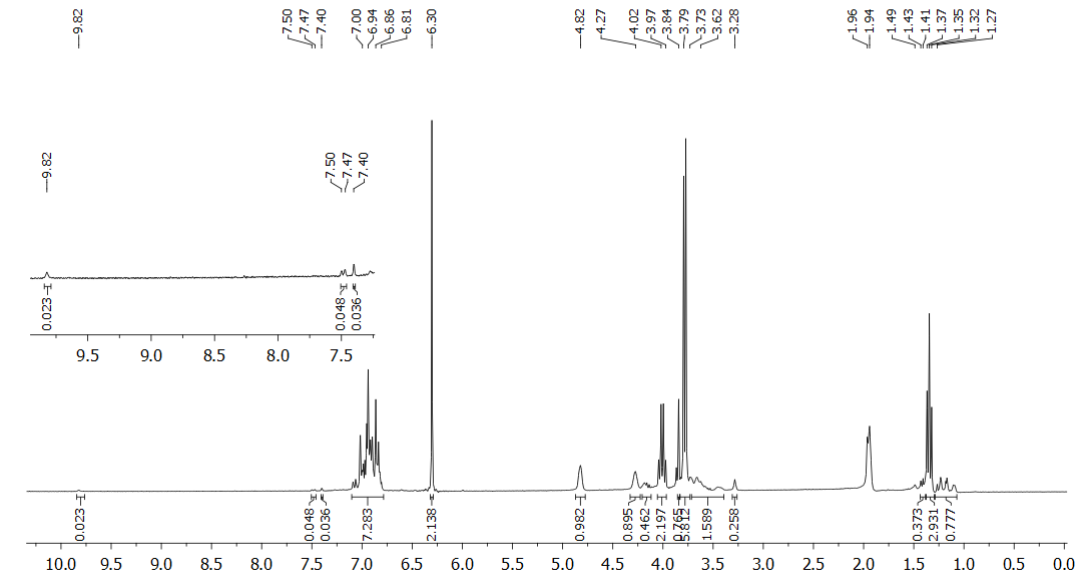


Fig. S70 The ^{1}H NMR (CD_3CN, 300 MHz) spectrum of the reaction mixture containing **2** and **11** after 24 h of visible light irradiation under argon. The solvent residual peak is at 1.94 ppm and the internal standard is 1,1,2,2-dichloroethane at 6.30 ppm.

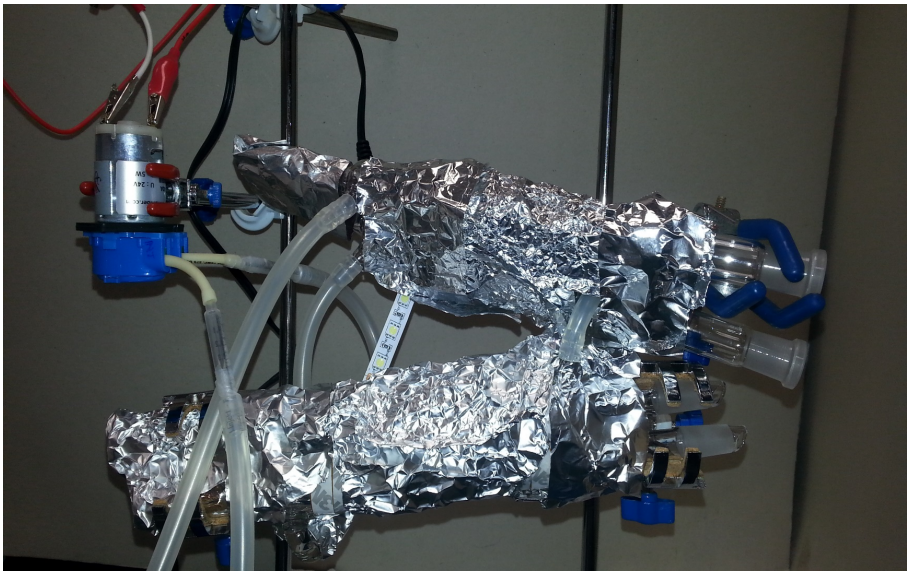


Fig. S71 Photo of the homemade continuous flow photoreactor with a white-light LED strip used as the visible light source.

Table S1. Crystal data and structure refinement for complex **2**

Chemical formula	$C_{16}H_{16}FN_2O_5V$
Formula weight	386.25
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal size	0.120 x 0.180 x 0.360 mm
Crystal habit	red block
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 7.9908(3) Å α = 90°
	b = 17.1771(6) Å β = 100.2079(18)°
	c = 11.9692(5) Å γ = 90°
Volume	1616.87(11) $Å^3$
Z	4
Density (calculated)	1.587 g/cm^3
Absorption coefficient	0.655 mm^{-1}
F(000)	792
Theta range for data collection	2.59 to 31.09°
Index ranges	-11<=h<=11, -24<=k<=24, -17<=l<=14
Reflections collected	21857
Independent reflections	5189 [R(int) = 0.0370]
Coverage of independent reflections	99.8%
Absorption correction	multi-scan
Max. and min. transmission	0.9260 and 0.7980
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2013 (Sheldrick, 2013)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	5189 / 0 / 232
Goodness-of-fit on F^2	1.039
Δ/σ_{max}	0.001
Final R indices	4378 data; I>2σ(I) R1 = 0.0332, wR2 = 0.0816
	all data R1 = 0.0426, wR2 = 0.0872
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0387P)^2+0.7994P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.476 and -0.374 $eÅ^{-3}$
R.M.S. deviation from mean	0.068 $eÅ^{-3}$

Table S2. Selectbond lengths (Å) for complex **2**

V1-O1	1.5893(11)	V1-O5	1.7630(10)
V1-O3	1.8552(10)	V1-O2	1.9584(9)
V1-N1	2.1307(11)	V1-O4	2.3443(10)
C1-O2	1.3027(15)	C1-N2	1.3131(16)
C1-C2	1.4768(17)	C10-O3	1.3330(16)
C8-N1	1.2939(16)	C15-O5	1.4164(16)
C16-O4	1.4250(17)	N1-N2	1.3967(14)

Table S3. Select bond angles (°) for complex **2**

O1-V1-O5	103.83(5)	O1-V1-O3	99.87(5)
O5-V1-O3	102.24(4)	O1-V1-O2	96.95(5)
O5-V1-O2	93.78(4)	O3-V1-O2	153.17(4)
O1-V1-N1	95.50(5)	O5-V1-N1	158.25(5)
O3-V1-N1	83.88(4)	O2-V1-N1	73.80(4)
O1-V1-O4	174.45(4)	O5-V1-O4	81.29(4)
O3-V1-O4	80.91(4)	O2-V1-O4	80.42(4)
N1-V1-O4	79.10(4)	O2-C1-N2	122.55(11)
O2-C1-C2	116.42(11)	N2-C1-C2	121.04(11)
N1-C8-C9	123.44(12)	N1-C8-H8	118.3
C9-C8-H8	118.3	C14-C9-C10	118.93(12)
O3-C10-C11	118.78(12)	C10-C9-C8	121.93(12)
C11-C10-C9	119.48(12)	O3-C10-C9	121.64(11)
C8-N1-N2	116.89(11)	C12-C11-C10	120.38(13)
C8-N1-V1	126.58(9)	N2-N1-V1	116.36(8)
C1-N2-N1	108.09(10)	C1-O2-V1	119.08(8)
C10-O3-V1	131.51(8)	C16-O4-V1	122.63(9)
C16-O4-H1O	111.4(15)	V1-O4-H1O	115.9(15)
C15-O5-V1	133.54(9)		

Table S4. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for complex **2**

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
V1	0.29301(3)	0.48136(2)	0.24810(2)	0.01207(6)
C1	0.11554(16)	0.38112(7)	0.08001(10)	0.0114(2)
C2	0.02016(16)	0.30961(7)	0.04105(11)	0.0116(2)
C3	0.98986(18)	0.25580(8)	0.12268(11)	0.0166(3)
C4	0.8979(2)	0.18839(8)	0.09199(12)	0.0195(3)
C5	0.83732(18)	0.17613(8)	0.97820(12)	0.0163(3)
C6	0.86642(18)	0.22720(8)	0.89492(11)	0.0165(3)
C7	0.95903(18)	0.29429(8)	0.92659(11)	0.0152(2)
C8	0.30797(17)	0.54480(7)	0.00919(11)	0.0124(2)
C9	0.40923(17)	0.60950(7)	0.05931(11)	0.0126(2)
C10	0.42714(17)	0.62719(7)	0.17598(11)	0.0137(2)
C11	0.52345(19)	0.69198(8)	0.21951(12)	0.0179(3)
C12	0.59922(19)	0.73885(8)	0.14869(12)	0.0189(3)
C13	0.57995(18)	0.72240(8)	0.03310(12)	0.0180(3)
C14	0.48592(18)	0.65863(8)	0.98908(12)	0.0152(2)
C15	0.3299(2)	0.43053(8)	0.48442(12)	0.0193(3)
C16	0.8913(2)	0.50962(11)	0.28031(13)	0.0252(3)
F1	0.74566(12)	0.11129(5)	0.94675(8)	0.0246(2)
N1	0.24585(14)	0.49242(6)	0.06794(9)	0.0111(2)
N2	0.14783(14)	0.43386(6)	0.00730(9)	0.0115(2)
O1	0.47743(13)	0.44468(6)	0.25660(8)	0.0187(2)
O2	0.16460(13)	0.38854(5)	0.18922(8)	0.01443(19)
O3	0.34672(13)	0.58632(6)	0.24502(8)	0.0167(2)
O4	0.01724(13)	0.53318(6)	0.21661(8)	0.01466(19)
O5	0.24758(13)	0.47009(6)	0.38605(8)	0.01517(19)

Table S5. Anisotropic atomic displacement parameters ($Å^2$) for complex **2**

The anisotropic atomic displacement factor exponent takes the form:

$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.01440(12)	0.01274(10)	0.00850(10)	-0.00128(7)	0.00048(7)	0.00099(8)
C1	0.0115(6)	0.0118(5)	0.0105(5)	-0.0006(4)	0.0010(4)	0.0007(4)
C2	0.0113(6)	0.0104(5)	0.0131(5)	-0.0004(4)	0.0018(4)	-0.0003(4)
C3	0.0200(7)	0.0174(6)	0.0118(6)	0.0012(4)	0.0014(5)	-0.0045(5)
C4	0.0245(7)	0.0171(6)	0.0169(6)	0.0024(5)	0.0038(5)	-0.0075(5)
C5	0.0153(6)	0.0130(6)	0.0205(6)	-0.0027(5)	0.0032(5)	-0.0050(5)
C6	0.0200(7)	0.0154(6)	0.0133(6)	-0.0032(4)	0.0007(5)	-0.0026(5)
C7	0.0198(7)	0.0125(5)	0.0130(6)	-0.0002(4)	0.0019(5)	-0.0027(5)
C8	0.0134(6)	0.0122(5)	0.0118(5)	-0.0017(4)	0.0029(4)	-0.0004(5)
C9	0.0117(6)	0.0116(5)	0.0143(6)	-0.0017(4)	0.0022(4)	-0.0011(4)
C10	0.0136(6)	0.0122(5)	0.0148(6)	-0.0011(4)	0.0014(5)	-0.0008(5)
C11	0.0209(7)	0.0161(6)	0.0153(6)	-0.0028(5)	-0.0010(5)	-0.0031(5)
C12	0.0180(7)	0.0133(6)	0.0234(7)	-0.0011(5)	-0.0013(5)	-0.0047(5)
C13	0.0171(7)	0.0139(6)	0.0231(7)	0.0012(5)	0.0040(5)	-0.0027(5)
C14	0.0160(6)	0.0136(6)	0.0169(6)	-0.0006(5)	0.0050(5)	-0.0014(5)
C15	0.0249(7)	0.0196(6)	0.0133(6)	0.0037(5)	0.0033(5)	0.0048(6)
C16	0.0187(7)	0.0425(9)	0.0156(7)	0.0047(6)	0.0066(5)	-0.0011(7)
F1	0.0303(5)	0.0185(4)	0.0252(5)	-0.0048(3)	0.0055(4)	-0.0135(4)
N1	0.0120(5)	0.0103(4)	0.0105(5)	-0.0017(4)	0.0010(4)	-0.0007(4)
N2	0.0125(5)	0.0102(4)	0.0111(5)	-0.0016(4)	0.0003(4)	-0.0022(4)
O1	0.0167(5)	0.0232(5)	0.0145(4)	-0.0030(4)	-0.0015(4)	0.0021(4)
O2	0.0198(5)	0.0130(4)	0.0096(4)	0.0000(3)	0.0001(3)	-0.0029(4)
O3	0.0227(5)	0.0157(4)	0.0121(4)	-0.0033(3)	0.0042(4)	-0.0056(4)
O4	0.0149(5)	0.0185(4)	0.0107(4)	0.0022(3)	0.0027(3)	-0.0002(4)
O5	0.0194(5)	0.0163(4)	0.0090(4)	0.0000(3)	0.0006(3)	0.0012(4)

Table S6. Crystal data and structure refinement for complex **5**

Chemical formula	$C_{15}H_{22}NO_4V$
Formula weight	331.27 g/mol
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal size	0.200 x 0.220 x 0.420 mm
Crystal habit	red block
Crystal system	orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 14.7897(4) Å α = 90°
	b = 13.1867(3) Å β = 90°
	c = 7.8841(2) Å γ = 90°
Volume	1537.62(7) $Å^3$
Z	4
Density (calculated)	1.431 g/cm^3
Absorption coefficient	0.660 mm^{-1}
F(000)	696
Theta range for data collection	2.75 to 31.07°
Index ranges	-21<=h<=20, -15<=k<=19, -11<=l<=11
Reflections collected	12950
Independent reflections	4783 [R(int) = 0.0265]
Coverage of independent reflections	99.8%
Absorption correction	multi-scan
Max. and min. transmission	0.8790 and 0.7690
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4783 / 1 / 194
Goodness-of-fit on F^2	1.072
Δ/σ_{max}	0.002
Final R indices	4492 data; I>2σ(I) R1 = 0.0289, wR2 = 0.0725
	all data R1 = 0.0317, wR2 = 0.0740
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0407P)^2]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	0.0(0)
Largest diff. peak and hole	0.397 and -0.268 $eÅ^{-3}$
R.M.S. deviation from mean	0.061 $eÅ^{-3}$

Table S7. Select bond lengths (Å) for complex **5**

V1-O1	1.5984(15)	V1-O3	1.7983(15)
V1-O4	1.8085(15)	V1-O2	1.8676(13)
V1-N1	2.1476(16)	C1-O2	1.329(2)
C11-N1	1.286(2)	C15-O4	1.407(2)
C12-N1	1.477(2)		

Table S8. Select bond angles (°) for complex **5.**

O1-V1-O3	103.46(8)	O1-V1-O4	107.70(8)
O3-V1-O4	92.31(7)	O1-V1-O2	110.70(8)
O3-V1-O2	144.24(8)	O4-V1-O2	87.28(6)
O1-V1-N1	96.68(7)	O3-V1-N1	84.33(6)
O4-V1-N1	155.48(7)	O2-V1-N1	81.58(6)
O2-C1-C10	119.27(16)	O2-C1-C2	119.95(16)
C10-C1-C2	120.77(16)	C7-C2-C1	116.47(18)
C7-C2-C3	122.58(17)	C1-C2-C3	120.90(16)
C5-C3-C4	109.36(16)	C5-C3-C2	111.66(17)
C4-C3-C2	109.36(16)	C5-C3-C6	107.39(17)
C4-C3-C6	108.45(18)	C2-C3-C6	110.55(16)
N1-C11-C10	126.31(17)	C1-C10-C11	120.83(16)
C10-C11-H11	116.8	N1-C11-H11	116.8
C11-N1-V1	127.75(14)	C11-N1-C12	116.01(17)
C1-O2-V1	141.49(12)	C12-N1-V1	116.21(12)
C15-O4-V1	123.09(13)	C14-O3-V1	128.34(13)

Table S9. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for complex **5**

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
V1	0.93022(2)	0.87770(2)	0.92650(6)	0.01050(8)
C1	0.80690(12)	0.05997(13)	0.9019(2)	0.0111(3)
C2	0.71513(13)	0.08592(14)	0.8709(3)	0.0123(3)
C3	0.64153(13)	0.00364(15)	0.8625(3)	0.0137(4)
C4	0.65759(15)	0.93649(16)	0.7059(3)	0.0185(4)
C5	0.64119(14)	0.93725(16)	0.0224(3)	0.0167(4)
C6	0.54702(14)	0.05233(17)	0.8471(3)	0.0221(5)
C7	0.69690(14)	0.18813(15)	0.8424(3)	0.0169(4)
C8	0.76330(15)	0.26329(15)	0.8464(3)	0.0181(4)
C9	0.85170(14)	0.23727(15)	0.8796(3)	0.0160(4)
C10	0.87433(13)	0.13523(13)	0.9066(3)	0.0123(4)
C11	0.96725(13)	0.10935(14)	0.9438(3)	0.0129(4)
C12	0.09603(13)	0.01278(16)	0.0076(3)	0.0154(4)
C13	0.15192(13)	0.95496(16)	0.8772(3)	0.0162(4)
C14	0.12177(13)	0.84534(15)	0.8623(3)	0.0172(4)
C15	0.88114(16)	0.68208(16)	0.8099(3)	0.0236(5)
N1	0.99989(11)	0.01934(12)	0.95814(19)	0.0121(3)
O1	0.94923(11)	0.83484(12)	0.11276(19)	0.0181(3)
O2	0.82984(8)	0.96364(9)	0.9268(2)	0.0137(2)
O3	0.02939(9)	0.84116(11)	0.80954(19)	0.0150(3)
O4	0.86052(9)	0.78613(11)	0.8167(2)	0.0164(3)

Table S10. Anisotropic atomic displacement parameters ($Å^2$) for complex **5**

The anisotropic atomic displacement factor exponent takes the form:

$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.01046(13)	0.00944(14)	0.01159(13)	0.00032(13)	-0.00076(14)	-0.00018(10)
C1	0.0135(8)	0.0099(8)	0.0098(9)	-0.0013(6)	0.0012(7)	0.0010(6)
C2	0.0127(8)	0.0116(9)	0.0127(7)	-0.0005(7)	0.0008(7)	0.0005(7)
C3	0.0106(8)	0.0136(9)	0.0169(8)	-0.0007(7)	0.0000(7)	-0.0003(7)
C4	0.0182(10)	0.0183(10)	0.0190(9)	-0.0043(8)	-0.0011(8)	-0.0033(8)
C5	0.0145(9)	0.0159(10)	0.0196(10)	0.0027(8)	0.0019(7)	-0.0014(7)
C6	0.0118(9)	0.0209(11)	0.0337(13)	0.0004(9)	-0.0026(9)	0.0012(8)
C7	0.0155(9)	0.0154(10)	0.0198(10)	0.0022(8)	0.0015(8)	0.0033(7)
C8	0.0212(10)	0.0090(9)	0.0241(11)	0.0024(8)	0.0031(9)	0.0017(7)
C9	0.0182(9)	0.0107(9)	0.0192(9)	0.0001(7)	0.0031(7)	-0.0026(7)
C10	0.0145(8)	0.0114(8)	0.0111(10)	-0.0020(7)	0.0011(7)	-0.0009(6)
C11	0.0143(8)	0.0132(8)	0.0113(10)	-0.0017(7)	0.0005(8)	-0.0036(6)
C12	0.0114(8)	0.0174(10)	0.0172(9)	-0.0003(7)	-0.0037(7)	-0.0021(7)
C13	0.0106(8)	0.0193(10)	0.0187(9)	-0.0001(7)	-0.0013(7)	-0.0017(7)
C14	0.0123(9)	0.0162(10)	0.0230(9)	-0.0005(8)	-0.0021(8)	0.0015(7)
C15	0.0218(10)	0.0127(10)	0.0363(12)	-0.0048(9)	-0.0021(10)	0.0012(8)
N1	0.0107(7)	0.0148(7)	0.0106(8)	0.0001(6)	-0.0001(5)	-0.0015(6)
O1	0.0204(7)	0.0187(8)	0.0153(7)	0.0055(6)	-0.0016(6)	-0.0021(6)
O2	0.0122(5)	0.0084(5)	0.0206(6)	0.0004(7)	0.0003(6)	-0.0006(4)
O3	0.0129(6)	0.0146(7)	0.0176(6)	-0.0022(6)	0.0004(6)	0.0014(5)
O4	0.0138(7)	0.0116(7)	0.0238(7)	-0.0044(6)	-0.0032(6)	0.0009(5)

Table S11. Crystal data and structure refinement for complex **5-dimer**

Chemical formula	$C_{30}H_{44}N_2O_8V_2$	
Formula weight	662.55 g/mol	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal size	0.060 x 0.160 x 0.400 mm	
Crystal habit	red plate	
Crystal system	monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 12.1706(6) Å	α = 90°
	b = 11.0345(5) Å	β = 100.8835(17)°
	c = 23.8844(12) Å	γ = 90°
Volume	3149.9(3) $Å^3$	
Z	4	
Density (calculated)	1.397 g/cm^3	
Absorption coefficient	0.644 mm^{-1}	
F(000)	1392	
Theta range for data collection	2.55 to 31.04°	
Index ranges	-17<=h<=17, -15<=k<=15, -14<=l<=34	
Reflections collected	18722	
Independent reflections	5001 [R(int) = 0.0440]	
Coverage of independent reflections	99.4%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9620 and 0.7830	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5001 / 83 / 222	
Goodness-of-fit on F^2	1.052	
Δ/σ_{max}	0.001	
Final R indices	3899 data; I>2σ(I)	R1 = 0.0409, wR2 = 0.0942
	all data	R1 = 0.0602, wR2 = 0.1048
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0418P)^2+2.8598P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.432 and -0.434 $eÅ^{-3}$	
R.M.S. deviation from mean	0.076 $eÅ^{-3}$	

Table S12. Select bond lengths (Å) for complex **5-dimer**

V1-O1	1.5984(13)	V1-O4	1.7920(12)
V1-O3	1.8787(12)	V1-O2	1.8950(11)
V1-N1	2.1639(14)	V1-O3	2.3152(12)
C1-O2	1.3254(18)	C1-C10	1.412(2)
C11-N1	1.280(2)	C10-C11	1.453(2)
C12-N1	1.490(7)	C12-C13	1.526(7)
C13-C14	1.510(13)	C14-O3	1.439(7)
C12A-C13A	1.516(13)	C12A-N1	1.480(11)
C14A-O3	1.434(12)	C13A-C14A	1.53(2)
C15-O4	1.404(2)	O3-V1	1.8787(12)

Table S13. Select bond angles (°) for complex **5-dimer**

O1-V1-O4	99.06(6)	O1-V1-O3	99.95(6)
O4-V1-O3	98.58(5)	O1-V1-O2	101.80(6)
O4-V1-O2	94.29(5)	O3-V1-O2	152.58(5)
O1-V1-N1	92.47(6)	O4-V1-N1	168.40(6)
O3-V1-N1	80.59(5)	O2-V1-N1	81.99(5)
O1-V1-O3	171.98(6)	O4-V1-O3	85.34(5)
O3-V1-O3	72.65(5)	O2-V1-O3	84.45(5)
N1-V1-O3	83.37(5)	O2-C1-C10	120.18(15)
O2-C1-C2	119.73(14)	C10-C1-C2	120.06(14)
C11-N1-C12A	116.0(5)	C11-N1-C12	118.0(3)
C11-N1-V1	124.03(11)	C12A-N1-V1	119.3(5)
C12-N1-V1	117.9(3)	C1-O2-V1	134.59(10)
C14A-O3-V1	124.0(9)	C14-O3-V1	119.7(6)
C14A-O3-V1	122.3(9)	C14-O3-V1	124.7(6)
V1-O3-V1	107.34(5)	C15-O4-V1	129.28(14)
N1-C12-C13	114.4(5)	N1-C11-C10	125.99(15)
C14-C13-C12	113.0(6)	C12A-C13A-C14A	113.7(10)
O3-C14-C13	112.5(8)	O3-C14A-C13A	111.4(13)
N1-C12A-C13A	112.4(9)		

Table S14. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for complex **5-dimer**

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
V1	0.13740(2)	0.98492(2)	0.02923(2)	0.01615(8)
C1	0.12344(13)	0.79535(13)	0.11642(7)	0.0160(3)
C2	0.13581(14)	0.77544(14)	0.17617(7)	0.0174(3)
C3	0.20419(15)	0.86260(14)	0.21965(7)	0.0193(3)
C4	0.32630(16)	0.86241(18)	0.21177(8)	0.0278(4)
C5	0.15698(17)	0.99264(15)	0.21245(8)	0.0263(4)
C6	0.20294(18)	0.82519(17)	0.28130(8)	0.0294(4)
C7	0.08627(16)	0.67190(15)	0.19359(8)	0.0242(4)
C8	0.02752(17)	0.58863(17)	0.15516(9)	0.0300(4)
C9	0.01916(16)	0.60665(16)	0.09771(8)	0.0253(4)
C10	0.06670(14)	0.70943(14)	0.07759(7)	0.0183(3)
C11	0.06946(15)	0.71693(14)	0.01713(7)	0.0203(3)
C12	0.1294(6)	0.7867(7)	0.9336(3)	0.0223(12)
C13	0.0705(3)	0.8749(3)	0.88856(12)	0.0241(7)
C14	0.9148(12)	0.9943(12)	0.0930(4)	0.0228(19)
C12A	0.1061(12)	0.7899(13)	0.9304(5)	0.025(2)
C13A	0.1505(5)	0.9002(4)	0.9040(2)	0.0248(12)
C14A	0.9209(18)	0.986(2)	0.0948(6)	0.018(3)
C15	0.2182(2)	0.2206(2)	0.07130(10)	0.0484(6)
N1	0.10507(12)	0.80688(12)	0.99177(6)	0.0186(3)
O1	0.25800(11)	0.99207(11)	0.01211(6)	0.0245(3)
O2	0.16815(10)	0.89304(10)	0.09743(5)	0.0173(2)
O3	0.95302(10)	0.97128(10)	0.04054(5)	0.0173(2)
O4	0.13822(11)	0.12748(10)	0.06525(5)	0.0231(3)

Table S15. Anisotropic atomic displacement parameters ($Å^2$) for **5-dimer**

The anisotropic atomic displacement factor exponent takes the form:

$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.01764(15)	0.01423(12)	0.01662(13)	0.00007(10)	0.00332(10)	0.00147(10)
C1	0.0141(8)	0.0137(6)	0.0203(7)	0.0005(5)	0.0035(6)	0.0027(5)
C2	0.0168(8)	0.0165(7)	0.0196(8)	0.0006(6)	0.0049(6)	0.0021(6)
C3	0.0237(9)	0.0189(7)	0.0153(7)	0.0004(6)	0.0035(6)	0.0004(6)
C4	0.0247(10)	0.0345(9)	0.0227(8)	-0.0070(7)	0.0010(7)	-0.0028(8)
C5	0.0372(11)	0.0192(8)	0.0218(8)	-0.0029(6)	0.0040(8)	0.0020(7)
C6	0.0440(12)	0.0268(9)	0.0181(8)	0.0007(7)	0.0071(8)	-0.0004(8)
C7	0.0254(10)	0.0231(8)	0.0252(8)	0.0041(7)	0.0076(7)	-0.0020(7)
C8	0.0320(11)	0.0233(8)	0.0363(10)	0.0048(8)	0.0106(9)	-0.0086(7)
C9	0.0228(9)	0.0204(8)	0.0312(9)	-0.0023(7)	0.0016(7)	-0.0051(7)
C10	0.0166(8)	0.0165(7)	0.0212(8)	-0.0012(6)	0.0017(6)	0.0015(6)
C11	0.0202(9)	0.0163(7)	0.0217(8)	-0.0040(6)	-0.0028(7)	0.0032(6)
C12	0.027(3)	0.0232(17)	0.0167(18)	-0.0020(14)	0.0026(17)	0.0103(18)
C13	0.0288(18)	0.0278(13)	0.0159(12)	-0.0018(10)	0.0050(11)	0.0091(11)
C14	0.029(4)	0.025(3)	0.015(2)	0.006(2)	0.007(2)	0.005(3)
C12A	0.030(4)	0.024(3)	0.021(3)	-0.007(2)	0.001(3)	0.011(3)
C13A	0.028(3)	0.032(2)	0.015(2)	-0.0004(17)	0.0064(19)	0.0097(19)
C14A	0.015(4)	0.021(4)	0.020(5)	-0.003(4)	0.008(3)	0.008(3)
C15	0.0711(18)	0.0368(11)	0.0394(12)	-0.0164(10)	0.0155(12)	-0.0307(12)
N1	0.0202(7)	0.0182(6)	0.0168(6)	-0.0027(5)	0.0015(5)	0.0070(5)
O1	0.0212(7)	0.0281(6)	0.0246(6)	0.0061(5)	0.0050(5)	0.0022(5)
O2	0.0203(6)	0.0148(5)	0.0162(5)	0.0009(4)	0.0023(5)	-0.0011(4)
O3	0.0198(6)	0.0171(5)	0.0158(5)	0.0000(4)	0.0054(4)	0.0042(4)
O4	0.0304(7)	0.0150(5)	0.0223(6)	-0.0013(5)	0.0009(5)	-0.0019(5)

Table S16. The six lowest singlet excitations obtained by TDDFT/B3LYP/6-31G* calculations.

Excitation from S_0 to	S_1	S_2	S_3	S_4	S_5	S_6
Wavelength (nm)	535.68	414.67	401.34	379.03	354.75	337.83
Oscillator strength	0.0088	0.0011	0.1088	0.0819	0.0108	0.0761
Main contribution	HOMO →LUMO	HOMO-1 →LUMO	HOMO →LUMO+1	HOMO →LUMO+2	HOMO-4 →LUMO+1	HOMO →LUMO+3

Table S17. XYZ coordinates of DFT-optimized geometries.

Species 2

=== B3LYP ===

C	4.972502	-2.117550	-3.138241
C	3.806610	-1.828899	-2.396700
C	2.767348	-1.077704	-3.008242
C	2.917859	-0.642108	-4.335331
C	4.072020	-0.951316	-5.043379
C	5.107077	-1.691939	-4.449068
H	5.766337	-2.687282	-2.661018
H	2.116094	-0.062032	-4.780507
H	4.173439	-0.611283	-6.070531
H	6.004860	-1.927089	-5.012092
O	1.674153	-0.733742	-2.329867
C	3.706859	-2.240161	-1.025158
H	4.581027	-2.672016	-0.536495
N	2.627144	-2.113888	-0.311246
C	1.558252	-2.222969	1.581602
N	2.707820	-2.482258	1.011346
O	0.571794	-1.658806	0.915538
C	1.345176	-2.534169	3.005605
C	0.119024	-2.226188	3.614308
C	2.361685	-3.137075	3.766402
C	-0.094940	-2.512929	4.959786
H	-0.661074	-1.760429	3.022833
C	2.158480	-3.427551	5.110371
H	3.306954	-3.372378	3.290266
C	0.930419	-3.109518	5.685334
H	-1.035267	-2.283004	5.449565
H	2.928818	-3.893156	5.716059
F	0.730534	-3.390155	6.987872
V	0.674901	-1.521195	-0.998974
O	0.183743	-2.902552	-1.543948
O	-0.692246	-0.420405	-1.025917
C	-2.078808	-0.605422	-1.210167
H	-2.465222	0.213488	-1.828391
H	-2.286468	-1.565463	-1.698926
H	-2.582554	-0.576513	-0.235688

=== BP86 ===

C	4.977099	-2.136173	-3.153180
C	3.808530	-1.838501	-2.402877
C	2.770048	-1.065491	-3.015497
C	2.927738	-0.617210	-4.345969
C	4.085564	-0.936314	-5.060499
C	5.116548	-1.698631	-4.468242
H	5.770390	-2.724206	-2.676122
H	2.126209	-0.019305	-4.790239
H	4.191825	-0.586318	-6.093439
H	6.018884	-1.942546	-5.037770
O	1.675998	-0.711176	-2.332049
C	3.708596	-2.253253	-1.031841
H	4.584110	-2.703952	-0.541381
N	2.621791	-2.109045	-0.303268
C	1.545419	-2.218128	1.596103
N	2.710751	-2.475492	1.019335
O	0.550753	-1.653482	0.927553
C	1.340001	-2.532734	3.022024
C	0.107823	-2.229144	3.641604
C	2.369728	-3.135909	3.781202
C	-0.098961	-2.520092	4.994649
H	-0.683166	-1.762054	3.048287
C	2.174343	-3.430671	5.133012
H	3.320877	-3.367169	3.293346
C	0.939806	-3.117049	5.719280
H	-1.045801	-2.292936	5.493073
H	2.957126	-3.897440	5.738037
F	0.746854	-3.401765	7.030138
V	0.668906	-1.512076	-0.998883
O	0.179972	-2.909243	-1.557160
O	-0.709928	-0.400625	-1.021716
C	-2.094056	-0.606096	-1.242485
H	-2.477589	0.211708	-1.881020
H	-2.282685	-1.579769	-1.733049
H	-2.629151	-0.573374	-0.273958

=== B3PW91 ===

C	4.960574	-2.125087	-3.131029
C	3.797693	-1.833213	-2.390526
C	2.763180	-1.076772	-2.997502
C	2.916388	-0.636550	-4.320801
C	4.067457	-0.948769	-5.028651
C	5.097170	-1.696299	-4.438661
H	5.751819	-2.700607	-2.655490
H	2.117381	-0.050779	-4.764411
H	4.170453	-0.604929	-6.054757
H	5.993877	-1.934130	-5.002870
O	1.676046	-0.733990	-2.319517
C	3.696551	-2.242909	-1.021964
H	4.568433	-2.678471	-0.531696
N	2.619583	-2.110945	-0.307147
C	1.553370	-2.221076	1.575872
N	2.702750	-2.476975	1.007063
O	0.569081	-1.662862	0.912220
C	1.343895	-2.531681	2.996985
C	0.119892	-2.226687	3.605946
C	2.361610	-3.130509	3.754730
C	-0.091134	-2.512426	4.949816
H	-0.662292	-1.762929	3.014343
C	2.161912	-3.420111	5.097215
H	3.307019	-3.363613	3.276132
C	0.935482	-3.105328	5.673977
H	-1.031799	-2.284142	5.440502
H	2.935178	-3.883472	5.701551
F	0.739170	-3.384228	6.971739
V	0.681150	-1.519470	-0.994785
O	0.198790	-2.894535	-1.540246
O	-0.685636	-0.429309	-1.022236
C	-2.064558	-0.613075	-1.210559
H	-2.449706	0.207563	-1.827576
H	-2.273875	-1.571210	-1.702492
H	-2.572553	-0.586133	-0.238176

=== PBE0 ===

C	4.957678	-2.132198	-3.131961
C	3.798330	-1.833391	-2.392849
C	2.770407	-1.070581	-2.996998
C	2.925862	-0.630513	-4.318064
C	4.073087	-0.949828	-5.025742
C	5.096894	-1.703946	-4.437836
H	5.744624	-2.713026	-2.656241
H	2.130590	-0.038775	-4.759907

H	4.178013	-0.605730	-6.051216
H	5.991497	-1.947067	-5.002433
O	1.688053	-0.722248	-2.318682
C	3.694987	-2.243107	-1.025032
H	4.564288	-2.683166	-0.534470
N	2.620553	-2.106713	-0.312737
C	1.552279	-2.213610	1.562727
N	2.699274	-2.475321	0.997995
O	0.574157	-1.649984	0.900354
C	1.338114	-2.523902	2.981471
C	0.114833	-2.214601	3.584695
C	2.350494	-3.125654	3.740076
C	-0.101188	-2.499545	4.926276
H	-0.662472	-1.747861	2.989023
C	2.145707	-3.414398	5.080273
H	3.295836	-3.361304	3.262736
C	0.919980	-3.095564	5.652429
H	-1.041837	-2.268482	5.415150
H	2.914418	-3.880437	5.687903
F	0.719356	-3.373070	6.945480
V	0.693272	-1.507060	-1.002328
O	0.209776	-2.875731	-1.544769
O	-0.674039	-0.425589	-1.024460
C	-2.051172	-0.642973	-1.155953
H	-2.487986	0.184953	-1.726004
H	-2.254745	-1.590554	-1.670261
H	-2.514570	-0.664682	-0.161645

=== CAM-B3LYP ===

C	4.960921	-2.118441	-3.133664
C	3.801795	-1.825859	-2.396262
C	2.770605	-1.077831	-2.999682
C	2.917364	-0.643346	-4.321911
C	4.063575	-0.955352	-5.028996
C	5.094417	-1.696463	-4.439813
H	5.753107	-2.688969	-2.656703
H	2.115858	-0.062026	-4.763528
H	4.163920	-0.616178	-6.055470
H	5.989440	-1.933903	-5.004128
O	1.680786	-0.735930	-2.320025
C	3.699183	-2.236027	-1.022895
H	4.570959	-2.665598	-0.530110
N	2.625247	-2.111323	-0.320688
C	1.564203	-2.221773	1.565262
N	2.703083	-2.488298	1.002075
O	0.584960	-1.653706	0.901644
C	1.343018	-2.529770	2.988307
C	0.120177	-2.219122	3.584445
C	2.350604	-3.130358	3.748764
C	-0.100892	-2.502464	4.924405
H	-0.653404	-1.753029	2.986001
C	2.141050	-3.417769	5.087293
H	3.296121	-3.366920	3.275292
C	0.915669	-3.097525	5.651954
H	-1.041719	-2.270899	5.410307
H	2.905433	-3.883468	5.698683
F	0.709473	-3.374559	6.947626
V	0.692424	-1.511769	-0.997503
O	0.196179	-2.875202	-1.535319
O	-0.665741	-0.426694	-1.019924
C	-2.050123	-0.630496	-1.162184
H	-2.469559	0.190530	-1.751618
H	-2.253297	-1.584484	-1.661679
H	-2.520485	-0.630637	-0.172956

Aerobic reaction

=== 1RC (S0) ===

C	1.071878	-6.050575	1.456070
C	0.724978	-4.769189	0.974726
C	-0.546905	-4.577982	0.369228
C	-1.431915	-5.664348	0.264456
C	-1.067500	-6.909506	0.759762
C	0.186832	-7.110639	1.360102
H	2.049198	-6.189794	1.912029
H	-2.394640	-5.501661	-0.209017
H	-1.764640	-7.739040	0.677648
H	0.459867	-8.089060	1.742606
O	-0.888208	-3.400448	-0.147966
C	1.676582	-3.698009	1.036246
H	2.700554	-3.916254	1.340076
N	1.404042	-2.461916	0.731635
C	1.995259	-0.393110	0.396430
N	2.445389	-1.564350	0.768427
O	0.738588	-0.230652	0.034909
C	2.888125	0.776964	0.369930
C	2.380375	2.039336	0.027613
C	4.250166	0.643894	0.690043
C	3.213659	3.154266	0.003614
H	1.328225	2.138295	-0.213697
C	5.091240	1.750065	0.667023
H	4.636322	-0.333914	0.955079
C	4.556945	2.989336	0.322794
H	2.840634	4.139550	-0.255235
H	6.145580	1.670255	0.910037
F	5.369931	4.063610	0.299488
V	-0.511810	-1.658877	0.337806
O	-0.995215	-1.539144	1.822738
O	-0.070604	-1.750045	-2.839609
C	-1.341362	-1.105040	-3.045812
H	-1.333827	-0.573280	-4.002616
O	-1.692151	-0.795977	-0.667246
C	-1.610299	-0.104125	-1.895996
H	-0.738253	0.562893	-1.833486
C	-2.359807	-2.242580	-3.140717
H	-2.381915	-2.791741	-2.190537
H	-3.352035	-1.823144	-3.324971
O	-2.064947	-3.096806	-4.233267
H	-1.165311	-3.426950	-4.076023
C	-2.862023	0.726996	-2.136731
C	-4.051502	0.452679	-1.442908
C	-2.845533	1.758885	-3.069934
C	-5.205692	1.194070	-1.681569
H	-4.047638	-0.336700	-0.702213
C	-4.001823	2.507000	-3.326186
H	-1.930713	2.004135	-3.604769
C	-5.185687	2.236203	-2.644215
H	-3.964452	3.307397	-4.056274
O	-6.360824	2.904599	-2.813193
O	-6.396583	1.003744	-1.049991
C	1.095419	-1.190580	-3.311649
C	2.246706	-1.966741	-3.118498
C	1.192968	0.049856	-3.951293
C	3.481681	-1.505434	-3.562455
H	2.148696	-2.928539	-2.624293
C	2.441332	0.498476	-4.394047
H	0.321053	0.673364	-4.108696
C	3.588319	-0.268507	-4.205729
H	4.365695	-2.117796	-3.406167
H	2.506727	1.463652	-4.889398
H	4.553006	0.090868	-4.551239
C	-6.469501	-0.011983	-0.062170

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H        -6.264777   -1.003870   -0.486771
H        -5.770561    0.176407    0.763231
H        -7.493141    0.014966    0.315717
C        -6.394341    3.957191   -3.760976
H        -7.413995    4.346120   -3.738724
H        -5.693746    4.761463   -3.498098
H        -6.165095    3.597972   -4.773482

=== 3RC (T1) ===
C         0.849670   -5.986816    1.748009
C         0.431919   -4.706395    1.284831
C        -0.955346   -4.529307    0.853555
C        -1.819638   -5.675054    0.909302
C        -1.367079   -6.883336    1.368928
C        -0.017779   -7.049732    1.796964
H         1.882411   -6.107213    2.065457
H        -2.843135   -5.530132    0.580142
H        -2.044322   -7.732312    1.409481
H         0.318693   -8.017004    2.156513
O        -1.424652   -3.424981    0.421689
C         1.393637   -3.677476    1.216284
H         2.426205   -3.906254    1.482222
N         1.152061   -2.435124    0.820481
C         1.862918   -0.403910    0.301499
N         2.225492   -1.630244    0.760316
O         0.660266   -0.118360   -0.016465
C         2.918074    0.611862    0.192045
C         2.581006    1.911486   -0.225806
C         4.255705    0.310949    0.510279
C         3.556184    2.895925   -0.323054
H         1.547927    2.132776   -0.467970
C         5.238578    1.287972    0.413809
H         4.508915   -0.691752    0.833594
C         4.870648    2.565624   -0.001617
H         3.319725    3.906269   -0.639256
H         6.275894    1.081255    0.654557
F         5.818767    3.514640   -0.094366
V        -0.728313   -1.524059    0.467792
O        -1.371146   -0.970782    1.800067
O         0.094531   -1.580638   -3.286367
C        -1.201946   -0.961103   -3.403570
H        -1.188665   -0.244998   -4.232082
O        -1.709314   -1.211227   -1.074093
C        -1.583533   -0.247414   -2.072186
H        -0.757894    0.446729   -1.844518
C        -2.143298   -2.105536   -3.773345
H        -2.154581   -2.836262   -2.954822
H        -3.155917   -1.714424   -3.900814
O        -1.772199   -2.698044   -5.009899
H        -0.849464   -2.979040   -4.898352
C        -2.860634    0.570111   -2.242598
C        -4.022785    0.200805   -1.551110
C        -2.897839    1.691371   -3.073730
C        -5.200284    0.931637   -1.683163
H        -3.967598   -0.662363   -0.900754
C        -4.074477    2.432868   -3.223076
H        -2.006018    2.011500   -3.607793
C        -5.232881    2.065540   -2.538988
H        -4.077299    3.301006   -3.872350
O        -6.426279    2.716589   -2.610354
O        -6.365826    0.649535   -1.042012
C         1.247806   -0.875520   -3.489830
C         2.433108   -1.600275   -3.285194
C         1.320058    0.465232   -3.889746
C         3.669197   -0.994271   -3.484048
H         2.356622   -2.639391   -2.979124
C         2.569934    1.059752   -4.085506
H         0.422525    1.050578   -4.048657
C         3.748258    0.342353   -3.886808
H         4.576678   -1.570788   -3.324254
H         2.613000    2.100114   -4.397728
H         4.713529    0.815505   -4.040455
C        -6.379335   -0.453273   -0.146748
H        -6.164271   -1.395821   -0.666755
H        -5.655637   -0.319459    0.667206
H        -7.389966   -0.487375    0.264216
C        -6.513289    3.856589   -3.447768
H        -7.540728    4.214121   -3.358649
H        -5.823810    4.648522   -3.125391
H        -6.305766    3.604452   -4.496463

=== 3TS1 (T1) ===
C         1.228299   -6.182593    1.231101
C         0.795646   -4.865439    0.949108
C        -0.540832   -4.648542    0.478120
C        -1.376483   -5.778797    0.317936
C        -0.924985   -7.054011    0.615809
C         0.386906   -7.268343    1.077050
H         2.248816   -6.327187    1.579638
H        -2.388103   -5.608170   -0.037930
H        -1.596024   -7.900336    0.489629
H         0.732913   -8.271410    1.306802
O        -1.005772   -3.458739    0.154011
C         1.738729   -3.791962    1.071002
H         2.787866   -4.031702    1.254247
N         1.431660   -2.533635    0.940348
C         1.998134   -0.428724    0.667868
N         2.471401   -1.617527    0.970442
O         0.741905   -0.219812    0.351525
C         2.925204    0.725228    0.651566
C         2.428878    2.012980    0.401293
C         4.300301    0.554168    0.885938
C         3.282963    3.113417    0.381143
H         1.365639    2.140063    0.231623
C         5.163517    1.644704    0.865279
H         4.677874   -0.442182    1.087030
C         4.638360    2.909193    0.612129
H         2.915992    4.117358    0.194343
H         6.227865    1.533082    1.044922
F         5.473142    3.969484    0.590860
V        -0.461196   -1.722817    0.820952
O        -0.993004   -1.532571    2.292526
O        -0.080522   -1.741955   -2.891232
C        -1.359514   -1.288319   -2.999800
H        -1.519842   -0.585360   -3.816208
O        -1.846538   -0.911982   -0.423506
C        -1.672329   -0.093198   -1.404694
H        -0.676904    0.360271   -1.518865
C        -2.367813   -2.403069   -2.848576
H        -2.169656   -2.955878   -1.924431
H        -3.372363   -1.977156   -2.807348
O        -2.316688   -3.231122   -4.008561
H        -1.530458   -3.793248   -3.920378
C        -2.809180    0.735316   -1.856098
C        -4.102944    0.493997   -1.350752
C        -2.608139    1.775909   -2.768880
C        -5.174712    1.280231   -1.745754
H        -4.223988   -0.300930   -0.625457
C        -3.677928    2.574302   -3.175311
H        -1.612225    1.976110   -3.156705
C        -4.962609    2.338920   -2.679199
H        -3.505259    3.383849   -3.874616
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O        -6.064570    3.051197   -3.006275
O        -6.450463    1.142026   -1.309445
C         0.948744   -1.118249   -3.592969
C         2.149735   -0.928962   -2.910023
C         0.808823   -0.766320   -4.937563
C         3.221782   -0.344622   -3.582831
H         2.231276   -1.236543   -1.873766
C         1.892168   -0.181403   -5.594994
H        -0.113481   -0.979494   -5.468875
C         3.095453    0.036813   -4.921078
H         4.155671   -0.183064   -3.052720
H         1.795380    0.090497   -6.642319
H         3.934129    0.492386   -5.439264
C        -6.721801    0.115778   -0.362008
H        -6.494886   -0.876736   -0.771537
H        -6.151605    0.264520    0.563336
H        -7.789345    0.186578   -0.149000
C        -5.926715    4.133546   -3.917612
H        -6.926625    4.555478   -4.027199
H        -5.246756    4.901045   -3.526819
H        -5.565915    3.789867   -4.895376

=== 1TS1 (S1) ===
C         1.153808   -6.320253    0.556154
C         0.751757   -4.965859    0.484743
C        -0.569762   -4.646762    0.033480
C        -1.424776   -5.715585   -0.321463
C        -1.004194   -7.032289   -0.225846
C         0.293700   -7.347528    0.215801
H         2.164616   -6.542122    0.891930
H        -2.425777   -5.467457   -0.661343
H        -1.689299   -7.831801   -0.497402
H         0.615191   -8.382067    0.286133
O        -1.002074   -3.408156   -0.104314
C         1.712394   -3.945004    0.787122
H         2.756671   -4.229684    0.927715
N         1.428090   -2.677120    0.868820
C         2.030708   -0.569039    0.948432
N         2.485886   -1.798197    1.040768
O         0.771736   -0.295650    0.695228
C         2.973614    0.560309    1.104080
C         2.494914    1.877697    1.052145
C         4.346819    0.336418    1.302017
C         3.365103    2.956534    1.191205
H         1.433177    2.043298    0.908508
C         5.225673    1.405511    1.440435
H         4.710865   -0.683955    1.347318
C         4.718127    2.700850    1.381559
H         3.012592    3.982218    1.157893
H         6.288965    1.253618    1.594875
F         5.568092    3.740462    1.514064
V        -0.454878   -1.832725    0.870287
O        -1.014988   -1.939654    2.338269
O        -0.044740   -1.583542   -2.881435
C        -1.290644   -1.056484   -2.996574
H        -1.390165   -0.236362   -3.705163
O        -1.768933   -0.737451   -0.177340
C        -1.571151    0.164261   -1.051358
H        -0.543038    0.493228   -1.242140
C        -2.388006   -2.071925   -2.881746
H        -2.247487   -2.669960   -1.975221
H        -3.349560   -1.556398   -2.828714
O        -2.426013   -2.883005   -4.062342
H        -1.684533   -3.505794   -3.996294
C        -2.653817    1.053639   -1.471671
C        -3.974314    0.826887   -1.026108
C        -2.382665    2.148400   -2.298454
C        -5.002336    1.677103   -1.402465
H        -4.153348   -0.016299   -0.370480
C        -3.409750    3.010163   -2.685030
H        -1.366960    2.336373   -2.637515
C        -4.718906    2.788180   -2.251244
H        -3.184757    3.857741   -3.321556
O        -5.783717    3.559875   -2.568198
O        -6.299248    1.553994   -1.024932
C         1.032011   -0.974404   -3.522273
C         2.215760   -0.851967   -2.795485
C         0.947591   -0.567084   -4.855264
C         3.329639   -0.285351   -3.414275
H         2.254826   -1.196954   -1.767904
C         2.071696   -0.000454   -5.458119
H         0.031660   -0.721289   -5.417323
C         3.260646    0.146786   -4.741168
H         4.252080   -0.178632   -2.851041
H         2.017349    0.313909   -6.496660
H         4.131824    0.587722   -5.216689
C        -6.639667    0.476303   -0.161456
H        -6.429280   -0.493818   -0.629538
H        -6.101354    0.542001    0.792374
H        -7.711845    0.569137    0.017291
C        -5.576463    4.690251   -3.404622
H        -6.557055    5.153469   -3.522177
H        -4.886178    5.408215   -2.943830
H        -5.191739    4.394840   -4.389090

=== 3Int1 (T1) ===
C         1.237791   -5.790233    0.182246
C         0.857300   -4.427888    0.189874
C        -0.485097   -4.075903   -0.158483
C        -1.378108   -5.109053   -0.517056
C        -0.973693   -6.435213   -0.501512
C         0.339362   -6.788922   -0.144831
H         2.263744   -6.041025    0.442543
H        -2.382696   -4.825171   -0.813749
H        -1.685444   -7.210840   -0.773477
H         0.646137   -7.830276   -0.135524
O        -0.909707   -2.818901   -0.197658
C         1.864150   -3.437059    0.447948
H         2.910005   -3.746397    0.484290
N         1.614311   -2.168825    0.590973
C         2.250783   -0.070042    0.595600
N         2.690924   -1.302708    0.682700
O         0.974637    0.222601    0.431898
C         3.222216    1.043563    0.651588
C         2.769547    2.370748    0.630376
C         4.603362    0.792536    0.725201
C         3.670536    3.431941    0.679421
H         1.703451    2.560600    0.582199
C         5.512980    1.843269    0.773252
H         4.948774   -0.234936    0.745082
C         5.029680    3.148852    0.748755
H         3.338008    4.464735    0.667488
H         6.582513    1.669298    0.829794
F         5.908870    4.170825    0.793996
V        -0.227251   -1.297527    0.776614
O        -0.623066   -1.376092    2.299846
O        -0.591695   -1.558963   -3.276602
C        -1.536365   -2.516064   -3.542157
H        -1.191659   -3.548033   -3.549880
O        -1.750737   -0.251556   -0.133534
C        -1.830447    0.937360   -0.497891
H        -0.943227    1.581013   -0.409371
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C	-2.918530	-2.155913	-3.135429
H	-3.039816	-1.068499	-3.251052
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O	-3.299679	-2.570457	-1.811333
H	-2.523652	-2.466336	-1.220418
C	-3.040990	1.503562	-1.030856
C	-4.194537	0.695618	-1.182633
C	-3.072898	2.856868	-1.392000
C	-5.361649	1.237908	-1.687352
H	-4.123813	-0.356212	-0.929126
C	-4.242884	3.412433	-1.901036
H	-2.186029	3.473568	-1.274523
C	-5.388822	2.621648	-2.052304
H	-4.264829	4.459294	-2.178478
O	-6.566107	3.061105	-2.532785
O	-6.518786	0.565911	-1.880131
C	0.708439	-1.739562	-3.698004
C	1.678454	-0.973362	-3.043935
C	1.062763	-2.602112	-4.739434
C	3.013071	-1.087442	-3.424314
H	1.374264	-0.307532	-2.242568
C	2.406121	-2.705834	-5.107439
H	0.299680	-3.163812	-5.266956
C	3.385012	-1.956482	-4.454650
H	3.764462	-0.499470	-2.904782
H	2.682412	-3.374951	-5.918171
H	4.427375	-2.044760	-4.746984
C	-6.579136	-0.789826	-1.432191
H	-5.825894	-1.416295	-1.921952
H	-6.437611	-0.847336	-0.345774
H	-7.580262	-1.136514	-1.691408
C	-6.684641	4.425110	-2.926403
H	-7.710947	4.539899	-3.276448
H	-6.507968	5.099419	-2.079811
H	-5.990113	4.665323	-3.740372

=== Int1 (S1) ===

C	1.277490	-5.803361	0.199864
C	0.899795	-4.440237	0.196776
C	-0.439419	-4.087612	-0.162950
C	-1.332104	-5.121020	-0.521551
C	-0.930579	-6.447892	-0.495257
C	0.379235	-6.802137	-0.127402
H	2.301107	-6.054694	0.468681
H	-2.334040	-4.836836	-0.826815
H	-1.642066	-7.223674	-0.767474
H	0.683751	-7.844044	-0.109746
O	-0.861079	-2.829972	-0.212441
C	1.906870	-3.449891	0.455879
H	2.951853	-3.761002	0.500952
N	1.658597	-2.180368	0.589925
C	2.299342	-0.082891	0.586224
N	2.736367	-1.315863	0.683849
O	1.024946	0.211257	0.411788
C	3.272505	1.029196	0.642336
C	2.822462	2.357078	0.610903
C	4.652679	0.776064	0.726223
C	3.725087	3.416872	0.659991
H	1.757059	2.548631	0.554727
C	5.563922	1.825387	0.774414
H	4.996051	-0.251915	0.753917
C	5.083224	3.131698	0.739673
H	3.394553	4.450187	0.640256
H	6.632741	1.649761	0.838799
F	5.963993	4.152293	0.785016
V	-0.182476	-1.304202	0.757250
O	-0.589412	-1.372645	2.278026
O	-0.517580	-1.588012	-3.296760
C	-1.462028	-2.545408	-3.562154
H	-1.119014	-3.577965	-3.560942
O	-1.697135	-0.260482	-0.169925
C	-1.772222	0.926700	-0.540854
H	-0.884675	1.569424	-0.448866
C	-2.846547	-2.180149	-3.168431
H	-2.964888	-1.093282	-3.292055
H	-3.558611	-2.671655	-3.842329
O	-3.238432	-2.585393	-1.844560
H	-2.466013	-2.479760	-1.249218
C	-2.977907	1.492195	-1.085449
C	-4.131814	0.685526	-1.241302
C	-3.004873	2.843758	-1.453466
C	-5.294381	1.227381	-1.756849
H	-4.064795	-0.365131	-0.981943
C	-4.170254	3.398854	-1.973442
H	-2.117759	3.459490	-1.332769
C	-5.316510	2.609335	-2.128839
H	-4.188386	4.444373	-2.256161
O	-6.489612	3.048478	-2.619712
O	-6.451394	0.556540	-1.954356
C	0.784979	-1.773621	-3.708507
C	1.752255	-1.005519	-3.052633
C	1.144322	-2.642893	-4.742604
C	3.089080	-1.124472	-3.423676
H	1.444239	-0.334391	-2.257171
C	2.489823	-2.751459	-5.101250
H	0.383522	-3.206135	-5.271779
C	3.465961	-2.000247	-4.446490
H	3.838263	-0.534899	-2.902763
H	2.770009	-3.425836	-5.906267
H	4.510022	-2.092272	-4.731518
C	-6.517396	-0.796827	-1.500130
H	-5.762080	-1.427142	-1.981696
H	-6.383299	-0.849252	-0.412516
H	-7.517419	-1.142889	-1.764390
C	-6.602965	4.410761	-3.020751
H	-7.626594	4.525642	-3.378522
H	-6.431005	5.088848	-2.176207
H	-5.902333	4.645810	-3.830982

=== 1Int2 ===

C	1.401003	-5.644734	-0.113776
C	0.986190	-4.294063	-0.058150
C	-0.361941	-3.963099	-0.403201
C	-1.229115	-5.005162	-0.795985
C	-0.791663	-6.321071	-0.826066
C	0.529210	-6.653615	-0.480404
H	2.431862	-5.879053	0.142229
H	-2.243260	-4.739126	-1.076206
H	-1.484253	-7.104538	-1.123771
H	0.862467	-7.686449	-0.507484
O	-0.814677	-2.713699	-0.404768
C	1.965231	-3.288451	0.247269
H	3.019280	-3.569474	0.269132
N	1.678297	-2.036937	0.451461
C	2.250220	0.078367	0.553508
N	2.728519	-1.143597	0.581787
O	0.965960	0.336998	0.398858
C	3.184930	1.217381	0.675803
C	2.692125	2.530165	0.694714
C	4.570769	1.004848	0.776672
C	3.558323	3.614956	0.808744

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H         1.622268    2.690198    0.626337
C         5.445944    2.079317    0.889968
H         4.947366   -0.011726    0.766565
C         4.923342    3.369877    0.903240
H         3.194638    4.637046    0.828073
H         6.518474    1.935213    0.968845
F         5.768935    4.414745    1.012422
V        -0.190399   -1.230687    0.663848
O        -0.597767   -1.399524    2.176620
O        -0.699733   -1.650856   -3.539178
C        -1.754141   -2.425346   -3.998009
H        -1.570754   -3.498488   -3.875413
O        -1.737745   -0.182841   -0.206204
C        -1.841279    1.020237   -0.517308
H        -0.961244    1.671816   -0.418292
C        -3.035867   -1.977681   -3.297373
H        -3.059687   -0.879649   -3.319699
H        -3.885523   -2.349581   -3.878139
O        -3.171146   -2.502045   -1.995010
H        -2.358840   -2.333641   -1.468096
C        -3.068948    1.590548   -1.002499
C        -4.223227    0.780325   -1.138827
C        -3.117678    2.950744   -1.334793
C        -5.406154    1.326518   -1.599357
H        -4.142689   -0.273132   -0.897694
C        -4.302599    3.509887   -1.803233
H        -2.230755    3.569395   -1.229126
C        -5.448602    2.716654   -1.939735
H        -4.335928    4.561282   -2.061467
O        -6.639176    3.158121   -2.380683
O        -6.567283    0.654889   -1.769196
C         0.607485   -2.039048   -3.789944
C         1.581265   -1.349999   -3.061830
C         0.972645   -3.027264   -4.707156
C         2.925728   -1.666775   -3.236040
H         1.272408   -0.576829   -2.365848
C         2.326587   -3.336092   -4.868050
H         0.228898   -3.533870   -5.310888
C         3.305737   -2.665682   -4.137027
H         3.673748   -1.135958   -2.654270
H         2.609232   -4.104845   -5.582200
H         4.354848   -2.912613   -4.271558
C        -6.606372   -0.713076   -1.363169
H        -5.877091   -1.320499   -1.910906
H        -6.414491   -0.808048   -0.287212
H        -7.617332   -1.054887   -1.588017
C        -6.773221    4.526891   -2.754857
H        -7.808284    4.640722   -3.078096
H        -6.578795    5.191224   -1.904388
H        -6.099849    4.779052   -3.582610
O        -1.918640   -2.297803   -5.457543
O        -2.164325   -1.042287   -5.810452

=== 3Int2 ===
C         1.401232   -5.644316   -0.115073
C         0.986304   -4.293715   -0.058926
C        -0.361936   -3.962779   -0.403589
C        -1.229113   -5.004830   -0.796509
C        -0.791507   -6.320693   -0.827094
C         0.529484   -6.653177   -0.481828
H         2.432168   -5.878589    0.140630
H        -2.243365   -4.738802   -1.076397
H        -1.484085   -7.104138   -1.124889
H         0.862841   -7.685964   -0.509302
O        -0.814818   -2.713405   -0.404669
C         1.965305   -3.288099    0.246580
H         3.019373   -3.569052    0.268078
N         1.678352   -2.036679    0.451255
C         2.250183    0.078609    0.553905
N         2.728557   -1.143338    0.581555
O         0.965864    0.337218    0.399880
C         3.184870    1.217638    0.676287
C         2.691953    2.530364    0.696303
C         4.570793    1.005175    0.776157
C         3.558122    3.615171    0.810447
H         1.622035    2.690337    0.628727
C         5.445941    2.079659    0.889542
H         4.947479   -0.011357    0.765203
C         4.923224    3.370163    0.903926
H         3.194350    4.637213    0.830642
H         6.518534    1.935612    0.967646
F         5.768791    4.415044    1.013205
V        -0.190394   -1.230653    0.664278
O        -0.597783   -1.400361    2.176932
O        -0.699821   -1.650905   -3.539251
C        -1.754377   -2.425433   -3.997686
H        -1.571065   -3.498560   -3.874894
O        -1.737631   -0.182430   -0.205435
C        -1.841169    1.020543   -0.516879
H        -0.961123    1.672153   -0.418074
C        -3.035992   -1.977450   -3.297004
H        -3.059493   -0.879410   -3.319367
H        -3.885752   -2.349147   -3.877745
O        -3.171352   -2.501739   -1.994614
H        -2.358932   -2.333525   -1.467781
C        -3.068856    1.590752   -1.002186
C        -4.223152    0.780506   -1.138216
C        -3.117540    2.950815   -1.335058
C        -5.406051    1.326523   -1.599028
H        -4.142634   -0.272865   -0.896712
C        -4.302433    3.509777   -1.803816
H        -2.230611    3.569504   -1.229616
C        -5.448445    2.716501   -1.940042
H        -4.335715    4.561056   -2.062534
O        -6.638984    3.157793   -2.381282
O        -6.567185    0.654845   -1.768613
C         0.607329   -2.039416   -3.789900
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C         0.972312   -3.027890   -4.706900
C         2.925663   -1.667460   -3.236101
H         1.272533   -0.577025   -2.366070
C         2.326177   -3.337022   -4.867745
H         0.228445   -3.534508   -5.310491
C         3.305454   -2.666632   -4.136886
H         3.673806   -1.136680   -2.654454
H         2.608673   -4.105976   -5.581724
H         4.354518   -2.913765   -4.271377
C        -6.606293   -0.712967   -1.362052
H        -5.876955   -1.320608   -1.909467
H        -6.414519   -0.807503   -0.286035
H        -7.617233   -1.054872   -1.586855
C        -6.772899    4.526344   -2.756315
H        -7.807918    4.640039   -3.079744
H        -6.578524    5.191198   -1.906242
H        -6.099414    4.777942   -3.584154
O        -1.919095   -2.298170   -5.457297
O        -2.164289   -1.042632   -5.810440

=== 1TS2 ===
C         0.472247   -4.691643    1.540479
C         0.368358   -3.402098    0.970604
C        -0.876246   -2.983504    0.414437
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C	-1.966446	-3.877213	0.450958
C	-1.834031	-5.132462	1.025298
C	-0.611400	-5.550332	1.579035
H	1.430033	-4.999359	1.954148
H	-2.903666	-3.557068	0.006794
H	-2.690051	-5.802412	1.041809
H	-0.517656	-6.535641	2.024984
O	-1.025814	-1.804166	-0.165000
C	1.535798	-2.570537	0.926636
H	2.484764	-2.989775	1.262876
N	1.563139	-1.335861	0.514105
C	2.651936	0.517896	0.081780
N	2.796324	-0.705687	0.528504
O	1.495995	0.979619	-0.330583
C	3.824572	1.413779	0.014129
C	3.677804	2.716545	-0.484534
C	5.089983	0.979458	0.443042
C	4.771595	3.575920	-0.556745
H	2.698412	3.045462	-0.813553
C	6.189116	1.828739	0.375624
H	5.196377	-0.028428	0.828273
C	6.010191	3.115738	-0.124710
H	4.678613	4.587187	-0.938897
H	7.174510	1.513284	0.702530
F	7.074481	3.942528	-0.191886
V	-0.051409	-0.144999	0.019422
O	-0.505734	0.334922	1.454818
O	-0.057558	-3.068884	-4.151538
C	-0.303281	-1.729686	-3.896370
H	0.162776	-1.078975	-4.649287
O	-1.756802	0.969478	-0.751533
C	-2.570060	1.602918	-0.061242
H	-2.249415	2.008702	0.910779
C	-1.810870	-1.461847	-3.814936
H	-1.946611	-0.371849	-3.814462
H	-2.250143	-1.864620	-4.733849
O	-2.466248	-2.079357	-2.733340
H	-2.015277	-1.831265	-1.898591
C	-3.947360	1.798891	-0.456353
C	-4.470863	1.100701	-1.570306
C	-4.775300	2.636396	0.299002
C	-5.803003	1.236139	-1.916527
H	-3.820263	0.424091	-2.110948
C	-6.112350	2.801083	-0.056467
H	-4.375113	3.162566	1.161405
C	-6.638167	2.110883	-1.153828
H	-6.746351	3.457645	0.527034
O	-7.917687	2.186588	-1.570467
O	-6.418804	0.590458	-2.935360
C	1.163325	-3.445690	-4.685376
C	1.180899	-4.696207	-5.309904
C	2.322331	-2.669059	-4.613001
C	2.363567	-5.166643	-5.873924
H	0.264040	-5.276128	-5.343103
C	3.499360	-3.152430	-5.191723
H	2.324755	-1.719644	-4.089604
C	3.528302	-4.395011	-5.822920
H	2.373259	-6.138778	-6.359476
H	4.401274	-2.549282	-5.132452
H	4.449422	-4.763289	-6.265102
C	-5.629716	-0.287221	-3.735842
H	-4.844665	0.266377	-4.267096
H	-5.166133	-1.080354	-3.137668
H	-6.320528	-0.723259	-4.458811
C	-8.823572	3.019340	-0.854550
H	-9.781721	2.916653	-1.365204
H	-8.926454	2.692189	0.187316
H	-8.505378	4.068794	-0.880177
O	0.339706	-1.447884	-2.610781
O	-0.151655	-0.278851	-2.112897

=== 3TS2 ===

C	1.533194	-4.703176	2.470294
C	1.269360	-3.570398	1.663644
C	0.151564	-3.592130	0.766435
C	-0.648661	-4.757099	0.726478
C	-0.369470	-5.842231	1.540017
C	0.727260	-5.824364	2.422941
H	2.390213	-4.673064	3.139682
H	-1.486823	-4.766506	0.036817
H	-1.006360	-6.722176	1.491967
H	0.938094	-6.681635	3.054823
O	-0.129547	-2.594124	-0.044069
C	2.175251	-2.462686	1.714193
H	3.099523	-2.563754	2.285027
N	1.990054	-1.330104	1.094371
C	2.698683	0.620019	0.379814
N	2.998191	-0.388504	1.170885
O	1.615085	0.648626	-0.354495
C	3.634392	1.762065	0.292901
C	3.328435	2.849563	-0.538379
C	4.830027	1.776731	1.030666
C	4.195952	3.934943	-0.636840
H	2.403252	2.832206	-1.103383
C	5.704169	2.854744	0.940527
H	5.061130	0.934075	1.672525
C	5.371039	3.917957	0.105681
H	3.976165	4.785744	-1.273448
H	6.632048	2.885248	1.502261
F	6.217071	4.965643	0.015131
V	0.292094	-0.736451	0.133714
O	-0.585551	-0.133334	1.302962
O	-0.583762	-2.702186	-4.794801
C	-0.211950	-1.519242	-4.205508
H	0.783584	-1.174881	-4.510034
O	-2.035566	0.023001	-1.148900
C	-2.795436	0.642141	-0.392716
H	-2.475596	0.780972	0.651697
C	-1.284312	-0.447434	-4.418359
H	-0.887565	0.498523	-4.025242
H	-1.427554	-0.343704	-5.498942
O	-2.519658	-0.789845	-3.842886
H	-2.427193	-0.660221	-2.874171
C	-4.087473	1.207820	-0.753396
C	-4.595202	1.153382	-2.071980
C	-4.840635	1.818201	0.254863
C	-5.837913	1.687194	-2.366481
H	-4.000547	0.689216	-2.848616
C	-6.092260	2.362199	-0.030082
H	-4.450162	1.863198	1.267904
C	-6.602733	2.303050	-1.329373
H	-6.666891	2.829908	0.760351
O	-7.799824	2.794897	-1.713204
O	-6.422048	1.681974	-3.590409
C	0.377346	-3.673107	-5.048806
C	0.004795	-4.641280	-5.984233
C	1.627225	-3.719794	-4.428637
C	0.896288	-5.659944	-6.309009
H	-0.977168	-4.575929	-6.441770
C	2.513445	-4.745336	-4.771826
H	1.908211	-2.996339	-3.672112
C	2.157465	-5.714291	-5.708134

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H         0.605260   -6.411487   -7.037691
H         3.485342   -4.784520   -4.287944
H         2.852144   -6.508880   -5.963834
C        -5.702217    1.081092   -4.662189
H        -4.763676    1.614242   -4.859323
H        -5.474071    0.028605   -4.456898
H        -6.355870    1.155969   -5.532551
C        -8.623701    3.421709   -0.737301
H        -9.525471    3.729382   -1.268227
H        -8.891786    2.724484    0.066113
H        -8.133237    4.304005   -0.307555
O        -0.118117   -1.800539   -2.742604
O         0.366106   -0.738460   -2.113422

=== 1Int3 ===
C         3.893730   -4.300713    2.473960
C         3.179755   -3.420365    1.632443
C         2.003186   -3.886660    0.986512
C         1.570794   -5.205688    1.197655
C         2.288211   -6.044197    2.041199
C         3.453820   -5.596618    2.685109
H         4.797031   -3.940469    2.960479
H         0.673962   -5.541847    0.687743
H         1.941123   -7.061444    2.201145
H         4.005762   -6.261975    3.341558
O         1.334038   -3.102682    0.142592
C         3.678097   -2.097112    1.385204
H         4.667690   -1.825842    1.753779
N         3.025110   -1.189335    0.719525
C         2.890577    0.747982   -0.264290
N         3.664692    0.006184    0.488216
O         1.734054    0.291571   -0.703165
C         3.296902    2.103715   -0.664692
C         2.430036    2.899060   -1.432559
C         4.549919    2.612711   -0.280823
C         2.810234    4.183260   -1.814071
H         1.460195    2.512562   -1.727862
C         4.936129    3.892998   -0.658345
H         5.211967    1.992951    0.313685
C         4.056411    4.657976   -1.420866
H         2.156082    4.815650   -2.404812
H         5.898238    4.306174   -0.374268
F         4.428392    5.899747   -1.788732
V         1.005440   -1.301500    0.067178
O         0.316893   -0.898925    1.407720
O        -1.503673   -1.258788   -3.724912
C        -0.126689   -1.163502   -3.529563
H         0.430137   -1.713329   -4.303923
O        -1.269394    1.412992   -0.125531
C        -2.365562    1.159847    0.359512
H        -2.468041    1.079826    1.461545
C         0.298499    0.310495   -3.578579
H         1.349911    0.343520   -3.262482
H         0.249641    0.619256   -4.629006
O        -0.498240    1.225114   -2.868169
H        -0.512304    1.018654   -1.911878
C        -3.605848    0.943436   -0.390793
C        -3.628374    1.074345   -1.795147
C        -4.770461    0.591440    0.294350
C        -4.798770    0.849606   -2.499224
H        -2.709782    1.328407   -2.309681
C        -5.953716    0.353381   -0.406122
H        -4.754955    0.493614    1.377095
C        -5.981020    0.474430   -1.797979
H        -6.850847    0.074660    0.133936
O        -7.072458    0.263053   -2.572389
O        -4.924576    0.945971   -3.851709
C        -2.071054   -2.468732   -4.085821
C        -3.420112   -2.405063   -4.453769
C        -1.390461   -3.690096   -4.103685
C        -4.078778   -3.562297   -4.859736
H        -3.938536   -1.452512   -4.412112
C        -2.066617   -4.840409   -4.521225
H        -0.363783   -3.762339   -3.767319
C        -3.405467   -4.786450   -4.903510
H        -5.125661   -3.503784   -5.145677
H        -1.533642   -5.787629   -4.533242
H        -3.922175   -5.687082   -5.222628
C        -3.826390    1.508804   -4.569908
H        -3.600428    2.519820   -4.208496
H        -2.928812    0.888270   -4.484117
H        -4.152262    1.554030   -5.610706
C        -8.283596   -0.124615   -1.940037
H        -9.011339   -0.245649   -2.743997
H        -8.169611   -1.075607   -1.404091
H        -8.636717    0.645309   -1.241842
O         0.318433   -1.868951   -2.365542
O        -0.311481   -1.315048   -1.188218

=== 3Int3 ===
C         2.695531   -4.823491    2.312638
C         2.200819   -3.772987    1.504559
C         1.393781   -4.088727    0.363167
C         1.125391   -5.448236    0.087654
C         1.613320   -6.450868    0.909411
C         2.404031   -6.145409    2.032995
H         3.315383   -4.569324    3.169595
H         0.518850   -5.674718   -0.783546
H         1.382339   -7.488065    0.679866
H         2.783494   -6.938808    2.669435
O         0.925652   -3.166616   -0.459327
C         2.604490   -2.427546    1.793619
H         3.392368   -2.256587    2.528931
N         2.122759   -1.381990    1.183845
C         2.256370    0.713240    0.558026
N         2.706730   -0.157136    1.437272
O         1.399951    0.390124   -0.384805
C         2.745827    2.105800    0.608489
C         2.270694    3.043991   -0.320115
C         3.683977    2.508278    1.574339
C         2.720036    4.361818   -0.290830
H         1.546575    2.726888   -1.062061
C         4.139487    3.821461    1.613367
H         4.047574    1.779028    2.289464
C         3.648407    4.727824    0.677283
H         2.364587    5.102069   -1.000051
H         4.863160    4.152485    2.350955
F         4.088402    6.002428    0.711978
V         0.520973   -1.331847   -0.094142
O        -0.777852   -1.154033    0.785728
O        -1.121680   -3.214870   -4.629132
C        -0.742642   -1.998648   -4.132741
H         0.264253   -1.691110   -4.438930
O        -3.271568   -1.291599   -1.477115
C        -3.562099   -0.423383   -0.657130
H        -3.239153   -0.552795    0.390285
C        -1.789165   -0.922268   -4.451868
H        -1.501666   -0.021076   -3.888751
H        -1.685519   -0.702159   -5.520662
O        -3.110397   -1.318417   -4.228474
H        -3.253198   -1.381095   -3.255899
C        -4.307907    0.802489   -0.947098
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C	-4.755485	1.091651	-2.255313
C	-4.579720	1.693919	0.092435
C	-5.463879	2.252934	-2.513531
H	-4.523808	0.394666	-3.051632
C	-5.292228	2.868313	-0.154858
H	-4.232926	1.473320	1.098585
C	-5.738856	3.159324	-1.445676
H	-5.496764	3.553191	0.659447
O	-6.435041	4.265085	-1.793977
O	-5.938868	2.627992	-3.729146
C	-0.152497	-4.197454	-4.832516
C	-0.353197	-5.013001	-5.947061
C	0.929292	-4.399492	-3.973534
C	0.550429	-6.039293	-6.214208
H	-1.211734	-4.828628	-6.584831
C	1.830944	-5.428572	-4.261895
H	1.055628	-3.802021	-3.077320
C	1.649473	-6.247127	-5.376317
H	0.396829	-6.674230	-7.082407
H	2.672790	-5.591950	-3.594857
H	2.354593	-7.045634	-5.588282
C	-5.730253	1.739403	-4.820225
H	-4.662227	1.576464	-5.010638
H	-6.210402	0.768866	-4.643139
H	-6.187516	2.222448	-5.685189
C	-6.746048	5.216258	-0.784241
H	-7.300925	6.009232	-1.287609
H	-7.371423	4.775192	0.002210
H	-5.836742	5.634958	-0.334843
O	-0.635002	-2.163456	-2.640904
O	0.006644	-1.122905	-2.123838

=== 1Int3’ (S0) ===

C	3.941079	-4.263799	2.502511
C	3.203932	-3.410976	1.652007
C	2.041997	-3.914888	1.008395
C	1.644882	-5.242783	1.228950
C	2.383721	-6.053381	2.081414
C	3.535699	-5.568904	2.723670
H	4.832980	-3.874885	2.987728
H	0.758386	-5.608023	0.721181
H	2.064112	-7.078107	2.250005
H	4.103746	-6.213642	3.386744
O	1.354152	-3.153710	0.158284
C	3.664280	-2.077640	1.394175
H	4.644371	-1.775004	1.763191
N	2.991394	-1.190357	0.717849
C	2.832997	0.751385	-0.268118
N	3.609527	0.016710	0.485199
O	1.675886	0.280295	-0.706376
C	3.244274	2.108870	-0.660764
C	2.436708	2.887027	-1.506726
C	4.459940	2.636951	-0.188308
C	2.834809	4.169710	-1.875075
H	1.499630	2.492359	-1.884403
C	4.863910	3.915277	-0.551550
H	5.079194	2.032404	0.464678
C	4.041211	4.662647	-1.391417
H	2.224739	4.785887	-2.526921
H	5.796869	4.340761	-0.197273
F	4.429824	5.902082	-1.745280
V	0.995479	-1.362532	0.052121
O	0.244970	-0.949386	1.356258
O	-1.508874	-1.267943	-3.700079
C	-0.128283	-1.184874	-3.585455
H	0.382293	-1.746183	-4.383612
C	0.299215	0.284255	-3.652501
H	1.398073	0.303057	-3.594243
H	0.003104	0.662201	-4.636662
O	-0.294889	1.129175	-2.695746
H	0.061799	0.867213	-1.829337
C	-2.102518	-2.457326	-4.078936
C	-3.422981	-2.340851	-4.525809
C	-1.476969	-3.706544	-4.034131
C	-4.114620	-3.475218	-4.940180
H	-3.881400	-1.357171	-4.542596
C	-2.183080	-4.834562	-4.463147
H	-0.472601	-3.810572	-3.642114
C	-3.496599	-4.729107	-4.917016
H	-5.139729	-3.377786	-5.287543
H	-1.695662	-5.805377	-4.426897
H	-4.036982	-5.613235	-5.242728
O	0.383773	-1.883256	-2.432201
O	-0.271348	-1.402047	-1.240994

=== 3Int3’ (T1) ===

C	1.234579	-4.835661	3.157956
C	1.031345	-3.869879	2.144493
C	0.030554	-4.113396	1.143150
C	-0.716026	-5.311884	1.213566
C	-0.501749	-6.223629	2.232162
C	0.477534	-5.990349	3.216891
H	2.003735	-4.648078	3.903267
H	-1.457771	-5.492640	0.442050
H	-1.096151	-7.132612	2.267768
H	0.640062	-6.713007	4.010340
O	-0.183502	-3.285946	0.129423
C	1.903979	-2.732610	2.101705
H	2.791268	-2.722346	2.736103
N	1.721123	-1.711014	1.311864
C	2.363184	0.144211	0.341067
N	2.685305	-0.736218	1.275013
O	1.273865	0.042910	-0.376598
C	3.267100	1.280761	0.089006
C	2.912285	2.251875	-0.860733
C	4.481053	1.408912	0.786760
C	3.749638	3.334193	-1.113335
H	1.973612	2.146604	-1.392793
C	5.325379	2.485435	0.541511
H	4.749013	0.656339	1.519583
C	4.944012	3.431685	-0.406666
H	3.493459	4.097033	-1.840999
H	6.266504	2.604221	1.068028
F	5.759712	4.476378	-0.646675
V	0.024124	-1.341337	0.217097
O	-1.052280	-0.750487	1.196540
O	-0.347196	-3.321707	-4.381093
C	-1.142706	-2.685875	-3.461161
H	-1.722565	-1.853737	-3.878940
C	-2.034463	-3.696261	-2.723813
H	-2.666906	-3.114399	-2.036106
H	-2.677043	-4.172191	-3.471700
O	-1.304374	-4.696716	-2.075028
H	-0.818058	-4.262487	-1.341199
C	0.253583	-2.581607	-5.391185
C	0.725514	-3.332505	-6.470720
C	0.406537	-1.193671	-5.361170
C	1.348064	-2.686167	-7.534457
H	0.592989	-4.409519	-6.456105
C	1.028436	-0.560063	-6.441451
H	0.075784	-0.608353	-4.510962
C	1.498691	-1.295860	-7.527454

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H         1.713640   -3.270949   -8.373949
H         1.150114    0.519296   -6.419661
H         1.983110   -0.793711   -8.359598
O        -0.221520   -2.084473   -2.466573
O        -0.918110   -1.263542   -1.647258

=== 1Int3” (S1) ===
C        -0.027390   -6.139426    2.725944
C         0.313617   -5.135810    1.793364
C        -0.306762   -5.144944    0.515725
C        -1.241464   -6.141880    0.199720
C        -1.567361   -7.107065    1.144526
C        -0.963425   -7.110562    2.412892
H         0.454911   -6.133907    3.700254
H        -1.692965   -6.135054   -0.786781
H        -2.298394   -7.870703    0.893744
H        -1.226473   -7.871319    3.140919
O         0.033434   -4.239477   -0.404024
C         1.334654   -4.176927    2.101479
H         1.937308   -4.313661    2.999024
N         1.622892   -3.151038    1.351594
C         2.881737   -1.469045    0.797187
N         2.702279   -2.386367    1.714575
O         2.103157   -1.415028   -0.264365
C         3.965706   -0.482954    0.915689
C         4.134301    0.492108   -0.079977
C         4.837370   -0.506256    2.018267
C         5.155623    1.432313    0.019614
H         3.458868    0.504290   -0.928042
C         5.860647    0.427692    2.125967
H         4.701940   -1.261948    2.784033
C         6.002091    1.383315    1.122199
H         5.303980    2.194815   -0.737561
H         6.545463    0.429394    2.967332
F         6.992579    2.289288    1.224255
V         0.510257   -2.482055   -0.310693
O        -0.603377   -1.707720    0.490775
O        -1.349797   -0.877883   -4.122420
C        -1.518926   -1.074026   -2.746151
H        -1.043442   -0.217183   -2.266379
C        -2.971082   -1.212655   -2.267099
H        -3.579566   -0.494528   -2.824793
H        -3.343194   -2.221766   -2.499393
O        -3.098100   -0.887242   -0.901645
H        -2.440474   -1.393811   -0.392476
C        -2.036230   -1.677312   -5.029095
C        -1.896142   -3.068463   -5.063874
C        -2.821788   -1.018519   -5.977854
C        -2.572651   -3.794897   -6.045657
H        -1.261027   -3.563956   -4.339375
C        -3.482296   -1.755553   -6.960630
H        -2.898333    0.063567   -5.934362
C        -3.365223   -3.146603   -6.994805
H        -2.466682   -4.876263   -6.073103
H        -4.091903   -1.239955   -7.697850
H        -3.881897   -3.720184   -7.759117
O         0.549995   -1.983682   -2.073785
O        -0.855641   -2.269578   -2.285223

=== 1TS3 (S0) ===
C         0.141287   -6.374896    2.872932
C         0.379723   -5.396850    1.882662
C        -0.343509   -5.454284    0.659581
C        -1.285168   -6.483318    0.469230
C        -1.506178   -7.424010    1.465419
C        -0.793791   -7.376312    2.676147
H         0.705929   -6.324800    3.801121
H        -1.821429   -6.517049   -0.473676
H        -2.238887   -8.210166    1.302456
H        -0.973974   -8.118527    3.447598
O        -0.119333   -4.594638   -0.324543
C         1.379389   -4.391979    2.096754
H         2.011769   -4.456131    2.983337
N         1.594236   -3.396824    1.286069
C         2.728887   -1.637587    0.682342
N         2.630563   -2.552357    1.613790
O         1.943862   -1.637123   -0.371631
C         3.753157   -0.581751    0.785754
C         3.870181    0.381036   -0.227956
C         4.619624   -0.528544    1.890832
C         4.833228    1.383396   -0.145043
H         3.200753    0.332032   -1.079352
C         5.585087    0.467443    1.983486
H         4.524703   -1.275946    2.670612
C         5.675012    1.408949    0.961271
H         4.940619    2.136775   -0.918371
H         6.263930    0.527115    2.827763
F         6.609760    2.376576    1.048291
V         0.411925   -2.813831   -0.428805
O        -0.778033   -1.971748    0.234246
O        -1.400600   -0.532693   -4.329838
C        -1.298508   -0.729967   -2.972276
H        -0.627408    0.031172   -2.565462
C        -2.809281   -0.247419   -2.023230
H        -3.026055    0.691614   -2.535920
H        -3.522264   -1.048361   -2.225684
O        -2.415409   -0.048729   -0.765202
H        -2.049051   -0.880472   -0.349768
C        -1.993431   -1.499829   -5.146116
C        -1.531919   -2.817255   -5.187447
C        -3.015746   -1.060620   -5.987531
C        -2.129775   -3.705338   -6.082971
H        -0.726089   -3.134746   -4.536415
C        -3.598825   -1.959838   -6.880080
H        -3.333905   -0.023627   -5.939613
C        -3.160186   -3.284794   -6.926733
H        -1.780057   -4.733167   -6.121237
H        -4.394329   -1.622531   -7.538689
H        -3.615405   -3.984881   -7.621449
O         0.336487   -2.674417   -2.115792
O        -1.350763   -1.889177   -2.428317

=== Int4 (S1) ===
C         0.102394   -6.279634    0.089336
C         0.170889   -4.886626    0.306323
C        -1.033397   -4.135312    0.373119
C        -2.265750   -4.794651    0.217473
C        -2.301828   -6.165249   -0.005328
C        -1.116669   -6.917444   -0.072225
H         1.029239   -6.846867    0.047016
H        -3.174863   -4.205559    0.279258
H        -3.262202   -6.659767   -0.124595
H        -1.156472   -7.988814   -0.242710
O        -1.021875   -2.830456    0.626590
C         1.442578   -4.252489    0.508609
H         2.334800   -4.872669    0.602103
N         1.601240   -2.964918    0.598580
C         2.839657   -1.209184    0.944970
N         2.875545   -2.514982    0.853064
O         1.708799   -0.545069    0.842026
C         4.072068   -0.442348    1.193743
C         4.014131    0.955237    1.306739
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C	5.309796	-1.095871	1.321092
C	5.170464	1.693664	1.542991
H	3.056080	1.453215	1.208006
C	6.470008	-0.367771	1.557356
H	5.347370	-2.175915	1.232913
C	6.379789	1.017987	1.664453
H	5.147993	2.774492	1.633710
H	7.436116	-0.850900	1.658898
F	7.503095	1.726234	1.892991
V	0.122811	-1.431745	0.229463
O	-0.893750	-0.139964	0.821830
O	-0.943393	-1.394886	-4.488453
C	-1.640149	-0.648072	-3.613895
H	-1.105111	0.293970	-3.441946
C	-3.277530	0.733159	-1.238334
H	-4.018610	1.100836	-1.965939
H	-3.527304	-0.202494	-0.713458
O	-2.261917	1.362477	-0.997280
H	-1.303696	0.495867	0.176599
C	-1.385299	-2.700413	-4.772436
C	-1.327479	-3.684134	-3.789438
C	-1.791902	-2.980128	-6.072040
C	-1.701737	-4.985537	-4.124237
H	-0.990995	-3.429552	-2.790425
C	-2.158717	-4.288188	-6.394781
H	-1.813506	-2.185273	-6.810808
C	-2.117090	-5.289790	-5.423196
H	-1.664575	-5.760630	-3.364021
H	-2.476776	-4.520957	-7.407179
H	-2.404335	-6.305968	-5.678368
O	0.190981	-1.370467	-1.336601
O	-2.695478	-0.945254	-3.103408

=== 3TS4 (T1) ===

C	2.114991	-3.743222	2.290413
C	1.939601	-2.803382	1.231114
C	1.145330	-3.191692	0.065466
C	0.572952	-4.505534	0.045903
C	0.764757	-5.362779	1.096499
C	1.543767	-4.987490	2.233540
H	2.710747	-3.447359	3.149984
H	-0.015275	-4.775991	-0.824514
H	0.315125	-6.351664	1.068612
H	1.678899	-5.691528	3.048476
O	0.961875	-2.421171	-0.935576
C	2.568886	-1.552834	1.328337
H	3.208974	-1.347080	2.186432
N	2.458102	-0.574549	0.429995
C	2.991173	1.447217	-0.288474
N	3.184215	0.512536	0.693493
O	2.206864	1.244550	-1.262780
C	3.734830	2.704833	-0.177402
C	3.559284	3.693390	-1.164198
C	4.618089	2.938484	0.894343
C	4.250738	4.894259	-1.085887
H	2.876191	3.501849	-1.984322
C	5.313892	4.137409	0.980294
H	4.748095	2.173844	1.651041
C	5.118008	5.095232	-0.012716
H	4.132835	5.672141	-1.832472
H	5.999510	4.343691	1.795012
F	5.788927	6.254696	0.067304
V	1.117371	-0.487674	-1.277840
O	-0.308206	0.061926	-0.895022
O	-1.207957	-2.165558	-4.028820
C	0.031705	-1.959179	-4.697736
H	0.194351	-2.775586	-5.427901
C	-0.084840	-0.649293	-5.502383
H	0.895536	-0.501621	-5.985394
H	-0.833735	-0.800126	-6.287139
O	-0.494471	0.463102	-4.753932
H	0.108782	0.495834	-3.988857
C	-1.529782	-3.414409	-3.576809
C	-2.822141	-3.542782	-3.045136
C	-0.688853	-4.535318	-3.629412
C	-3.273090	-4.776496	-2.588328
H	-3.451982	-2.659480	-3.008986
C	-1.162248	-5.772228	-3.177507
H	0.329105	-4.450573	-3.989366
C	-2.448748	-5.905109	-2.656218
H	-4.278209	-4.858958	-2.182505
H	-0.505993	-6.637779	-3.235131
H	-2.806089	-6.870570	-2.309004
O	1.131437	-2.064907	-3.879080
O	1.333097	-0.552874	-2.985193

=== 3Int5 (T1) ===

C	2.396092	-5.256662	-0.311466
C	1.653353	-4.059392	-0.097030
C	0.198672	-4.142988	0.004068
C	-0.410841	-5.433151	-0.128530
C	0.351705	-6.553338	-0.327395
C	1.772761	-6.473197	-0.419420
H	3.477611	-5.183391	-0.389414
H	-1.492363	-5.473785	-0.058918
H	-0.130718	-7.522810	-0.418190
H	2.353483	-7.375884	-0.580152
O	-0.556046	-3.131488	0.196154
C	2.348252	-2.837599	-0.037516
H	3.428342	-2.834503	-0.189398
N	1.767801	-1.663215	0.171176
C	1.859452	0.530091	0.334135
N	2.579444	-0.610815	0.126456
O	0.609082	0.518513	0.552609
C	2.585512	1.804893	0.294201
C	1.880894	3.003629	0.508488
C	3.970760	1.846246	0.047915
C	2.543115	4.223788	0.476958
H	0.814486	2.958238	0.699813
C	4.641584	3.062539	0.014726
H	4.506966	0.918566	-0.113557
C	3.914780	4.231354	0.229889
H	2.023037	5.161593	0.640070
H	5.708460	3.122234	-0.171874
F	4.559947	5.409347	0.198544
V	-0.362148	-1.242680	0.706116
O	-0.279723	-1.404702	2.278258
O	-0.806859	-2.734474	-3.110172
C	-0.713790	-1.325120	-2.894173
H	-0.369703	-0.831483	-3.825050
C	-2.313547	-0.811117	-2.817217
H	-2.217466	0.264793	-2.629931
H	-2.694675	-1.026696	-3.818621
O	-3.039036	-1.492025	-1.897331
H	-2.751325	-1.186871	-0.990625
C	0.222243	-3.327939	-3.794113
C	-0.063641	-4.566588	-4.385817
C	1.508559	-2.780675	-3.902658
C	0.929343	-5.250322	-5.079740
H	-1.067742	-4.967202	-4.287865
C	2.492070	-3.476336	-4.611908
H	1.748501	-1.836217	-3.426708

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C         2.213254   -4.707784   -5.202383
H         0.697610   -6.209654   -5.535254
H         3.486513   -3.045128   -4.695436
H         2.983848   -5.240183   -5.752426
O        -0.086859   -0.933304   -1.829255
O        -1.852584   -0.722140    0.327931

=== 1Int5 (S1) ===
C         2.418561   -5.243437   -0.288106
C         1.670321   -4.048377   -0.080300
C         0.215323   -4.137567    0.015855
C        -0.388228   -5.430842   -0.115415
C         0.379484   -6.548406   -0.308615
C         1.800605   -6.462768   -0.395367
H         3.500114   -5.166122   -0.361739
H        -1.469827   -5.475662   -0.049662
H        -0.098679   -7.520035   -0.398899
H         2.385604   -7.363516   -0.551424
O        -0.544474   -3.129284    0.203233
C         2.360946   -2.824099   -0.020811
H         3.442097   -2.818320   -0.165061
N         1.775431   -1.650800    0.179397
C         1.858287    0.543312    0.335124
N         2.584090   -0.596239    0.139493
O         0.605840    0.528959    0.540651
C         2.580977    1.820040    0.296838
C         1.870952    3.017600    0.499661
C         3.968310    1.864438    0.063038
C         2.529878    4.239551    0.469030
H         0.802984    2.969851    0.681442
C         4.635860    3.082540    0.030797
H         4.508627    0.937671   -0.089626
C         3.903716    4.250102    0.234370
H         2.005632    5.176501    0.623483
H         5.704213    3.144611   -0.146325
F         4.545705    5.429843    0.203886
V        -0.360413   -1.235293    0.700346
O        -0.279305   -1.388149    2.273307
O        -0.808027   -2.747352   -3.108501
C        -0.702847   -1.337725   -2.899037
H        -0.353626   -0.851499   -3.831856
C        -2.302444   -0.809843   -2.829806
H        -2.196639    0.265574   -2.645338
H        -2.680646   -1.026071   -3.832142
O        -3.034820   -1.482289   -1.910387
H        -2.746254   -1.178057   -1.003156
C         0.209686   -3.349645   -3.801710
C        -0.093283   -4.582372   -4.397159
C         1.501393   -2.816169   -3.914853
C         0.888245   -5.273892   -5.099686
H        -1.101195   -4.972302   -4.295240
C         2.473185   -3.519291   -4.632741
H         1.754108   -1.876702   -3.435603
C         2.177333   -4.744875   -5.227153
H         0.643499   -6.228587   -5.558117
H         3.471951   -3.098932   -4.719812
H         2.938926   -5.283286   -5.783841
O        -0.080390   -0.945837   -1.833015
O        -1.852325   -0.721991    0.318517

=== Int6’ (T1) ===
C         3.247886   -5.144100    2.701388
C         2.318945   -4.308893    2.013306
C         1.021043   -4.863046    1.636042
C         0.756785   -6.231000    1.966102
C         1.684543   -6.988505    2.632473
C         2.947310   -6.445690    3.010270
H         4.210739   -4.721539    2.976763
H        -0.208802   -6.628383    1.672471
H         1.456796   -8.021993    2.879334
H         3.665379   -7.066364    3.536646
O         0.117290   -4.202659    1.016072
C         2.715565   -2.999450    1.683563
H         3.726095   -2.672635    1.932669
N         1.938918   -2.129543    1.051150
C         1.607073   -0.186276    0.078399
N         2.502501   -0.963451    0.760094
O         0.420116   -0.568812   -0.159709
C         2.063733    1.121296   -0.399915
C         1.198317    1.905088   -1.187912
C         3.350002    1.599830   -0.085054
C         1.610603    3.147462   -1.651660
H         0.212055    1.522093   -1.437716
C         3.766173    2.843765   -0.541830
H         4.008916    0.988292    0.520149
C         2.887263    3.596546   -1.317930
H         0.966665    3.770734   -2.262864
H         4.749411    3.238885   -0.310209
F         3.286709    4.799438   -1.762883
V        -0.249104   -2.323075    0.600059
O        -0.775249   -1.808323    2.003981
O         1.274035   -3.282156   -3.696252
C         0.776023   -2.708525   -2.587698
H         0.064588   -1.890305   -2.754498
C        -2.236628    0.273985   -2.364766
H        -2.603297    0.555463   -1.379739
H        -2.506932    0.874671   -3.228163
O        -2.117052   -1.055069   -2.641287
H        -2.019911   -1.560841   -1.793843
C         0.874453   -2.844572   -4.966541
C        -0.433563   -2.459206   -5.258922
C         1.865093   -2.873090   -5.946640
C        -0.734795   -2.075199   -6.568345
H        -1.203201   -2.436573   -4.494976
C         1.542808   -2.498001   -7.249696
H         2.867553   -3.188533   -5.675900
C         0.242614   -2.094946   -7.563624
H        -1.749200   -1.767308   -6.805229
H         2.310305   -2.519881   -8.018272
H        -0.007214   -1.801493   -8.579123
O         1.117648   -3.101214   -1.492540
O        -1.508542   -2.421934   -0.409226

=== 1Int6 (S1) ===
C         2.725634   -5.131424    0.428153
C         1.951058   -3.966870    0.239740
C         0.645055   -4.084008   -0.308518
C         0.146006   -5.357513   -0.633824
C         0.923917   -6.488283   -0.417802
C         2.221211   -6.382078    0.111021
H         3.727537   -5.031211    0.838782
H        -0.853648   -5.425931   -1.050266
H         0.519760   -7.467199   -0.662245
H         2.820851   -7.272059    0.274780
O        -0.093605   -3.007155   -0.568376
C         2.501474   -2.678013    0.551484
H         3.560928   -2.596922    0.795733
N         1.805411   -1.580064    0.553578
C         1.641843    0.583533    0.711898
N         2.483489   -0.412526    0.812587
O         0.383414    0.391165    0.368784
C         2.087663    1.965986    0.959009
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C	1.152093	3.012102	0.966049
C	3.443908	2.250898	1.192881
C	1.558418	4.323465	1.199338
H	0.105072	2.785107	0.797991
C	3.860201	3.556657	1.424882
H	4.161247	1.437892	1.187649
C	2.907840	4.573063	1.423549
H	0.850847	5.145749	1.214104
H	4.902156	3.799511	1.604969
F	3.308677	5.839777	1.647353
V	-0.314362	-1.412934	0.355612
O	-0.688833	-1.791464	1.825113
O	1.669763	-2.854500	-3.959194
C	0.950186	-1.791068	-3.542647
H	-0.134443	-1.888767	-3.708760
C	-0.394527	1.057002	-2.851614
H	0.117007	1.269399	-1.901227
H	0.026728	1.522734	-3.759880
O	-1.398423	0.367904	-2.908535
H	-1.727686	-0.416108	-1.323852
C	1.017490	-3.869627	-4.667565
C	1.191365	-5.176873	-4.219646
C	0.276561	-3.581594	-5.812645
C	0.597912	-6.217104	-4.933951
H	1.776340	-5.361325	-3.325332
C	-0.321736	-4.632885	-6.510904
H	0.186788	-2.558067	-6.164060
C	-0.162334	-5.948769	-6.075355
H	0.727456	-7.240392	-4.593247
H	-0.903527	-4.418371	-7.402682
H	-0.624145	-6.763270	-6.625647
O	1.477989	-0.830902	-3.038552
O	-1.775562	-0.861695	-0.440747

Anaerobic reaction

=== 2Int1’ ===			
C	1.527021	-5.847389	-0.095390
C	1.059962	-4.515513	0.001272
C	-0.312782	-4.227908	-0.292604
C	-1.149321	-5.302708	-0.670671
C	-0.663361	-6.598068	-0.740504
C	0.683857	-6.883095	-0.451467
H	2.574631	-6.044762	0.121902
H	-2.185864	-5.074680	-0.898912
H	-1.334281	-7.404669	-1.026243
H	1.055950	-7.901245	-0.511242
O	-0.813722	-3.007439	-0.265442
C	1.999094	-3.474046	0.300968
H	3.065430	-3.706586	0.300666
N	1.660696	-2.237905	0.529160
C	2.147225	-0.104752	0.657773
N	2.676519	-1.304884	0.655820
O	0.851540	0.102501	0.538789
C	3.033445	1.072365	0.780659
C	2.478645	2.355084	0.897360
C	4.431144	0.927355	0.785189
C	3.296452	3.476700	1.015291
H	1.399626	2.460524	0.904340
C	5.258236	2.039399	0.900253
H	4.854987	-0.066668	0.697301
C	4.675001	3.298628	1.013150
H	2.885137	4.476157	1.112176
H	6.339435	1.947775	0.904343
F	5.474283	4.380228	1.124478
V	-0.241862	-1.515172	0.792693
O	-0.626660	-1.724431	2.306289
O	-1.806968	-0.442511	-0.043904
C	-1.749110	0.595868	-0.727665
H	-0.763778	1.028911	-0.952236
C	-2.916106	1.272306	-1.239542
C	-4.215232	0.779128	-0.971657
C	-2.749858	2.430025	-2.008606
C	-5.326687	1.436469	-1.465341
H	-4.307644	-0.119505	-0.374241
C	-3.861669	3.099890	-2.512910
H	-1.751611	2.807262	-2.213122
C	-5.148981	2.618867	-2.251517
H	-3.726177	3.994938	-3.107854
O	-6.287045	3.188444	-2.689177
O	-6.614113	1.062236	-1.274947
C	-6.857245	-0.103602	-0.494784
H	-6.406618	-0.992202	-0.954240
H	-6.472866	0.012648	0.526178
H	-7.941582	-0.217458	-0.466137
C	-6.204028	4.369338	-3.482108
H	-7.234897	4.638214	-3.714461
H	-5.727369	5.186937	-2.928051
H	-5.653926	4.184569	-4.412585

=== 2Int1A ===			
C	3.364594	-2.226775	-3.382782
C	2.574229	-1.850942	-2.275370
C	1.553705	-0.879615	-2.453227
C	1.351652	-0.312069	-3.722768
C	2.142937	-0.705759	-4.795331
C	3.152482	-1.668933	-4.632477
H	4.147001	-2.967807	-3.237797
H	0.576732	0.439338	-3.834015
H	1.980283	-0.253985	-5.770366
H	3.763830	-1.969478	-5.477493
O	0.817041	-0.457032	-1.428118
C	2.847523	-2.399673	-0.977689
H	3.728072	-3.028869	-0.843930
N	2.111844	-2.176915	0.071810
C	1.729547	-2.336310	2.209565
N	2.549516	-2.711973	1.260625
O	0.713234	-1.535733	1.960551
C	1.938782	-2.780892	3.597573
C	1.055229	-2.367916	4.606620
C	3.019448	-3.618000	3.925317
C	1.242213	-2.780661	5.922836
H	0.223242	-1.722661	4.348405
C	3.215533	-4.035027	5.236489
H	3.698412	-3.934000	3.141243
C	2.321121	-3.607954	6.215153
H	0.570566	-2.473807	6.717563
H	4.042467	-4.681035	5.511941
F	2.508407	-4.010623	7.486684
V	0.200368	-1.190265	0.142752
O	-0.727178	-2.403782	-0.238425
O	-3.975896	-3.352385	-3.517720
C	-3.655539	-2.585039	-2.431608
H	-3.383266	-1.548104	-2.624440
C	-4.329048	-2.983840	-1.161666
H	-5.349664	-2.576510	-1.082706
H	-4.423452	-4.081663	-1.138945
O	-3.637097	-2.480887	-0.024563
H	-2.698172	-2.726935	-0.117809
C	-3.298184	-3.168135	-4.703296
C	-3.947814	-3.608957	-5.860374
C	-2.020435	-2.606097	-4.771214

C	-3.315707	-3.476056	-7.093904
H	-4.938142	-4.044666	-5.772443
C	-1.401398	-2.478128	-6.016463
H	-1.509407	-2.301831	-3.863885
C	-2.041446	-2.906544	-7.179611
H	-3.822621	-3.816829	-7.992754
H	-0.403995	-2.049583	-6.065745
H	-1.551949	-2.804518	-8.143958
O	-0.793349	0.145719	0.657091
C	-2.115052	0.318262	1.138924
H	-2.437497	1.336945	0.895841
H	-2.794514	-0.414409	0.689906
H	-2.111469	0.200786	2.229882

=== 2TS1A ===

C	3.906590	-2.878669	-3.327649
C	2.863771	-2.530325	-2.441708
C	1.651744	-2.005551	-2.968895
C	1.516567	-1.855643	-4.360466
C	2.556231	-2.217991	-5.206999
C	3.759734	-2.731473	-4.696395
H	4.832276	-3.271406	-2.913453
H	0.586347	-1.453673	-4.747570
H	2.433542	-2.098554	-6.280311
H	4.566082	-3.009698	-5.367830
O	0.664215	-1.613093	-2.167929
C	3.059698	-2.660303	-1.026674
H	4.048868	-2.928926	-0.654334
N	2.128635	-2.463182	-0.138384
C	1.476622	-2.254454	1.930994
N	2.506565	-2.560965	1.182498
O	0.329946	-1.885667	1.403670
C	1.592621	-2.298977	3.400390
C	0.477145	-2.016285	4.202821
C	2.815493	-2.625435	4.011632
C	0.573863	-2.056660	5.591360
H	-0.465743	-1.769138	3.728492
C	2.924027	-2.666982	5.396820
H	3.674107	-2.844012	3.386752
C	1.798173	-2.380858	6.164964
H	-0.277740	-1.843397	6.228790
H	3.858734	-2.915657	5.888396
F	1.900020	-2.420214	7.508348
V	0.060492	-2.147837	-0.498009
O	-0.475007	-3.643858	-0.631934
O	-3.285825	-3.383738	-3.402873
C	-3.075656	-3.279918	-2.090989
H	-2.846094	-2.315181	-1.654090
C	-3.452860	-4.466561	-1.268828
H	-4.547321	-4.600397	-1.285961
H	-3.027120	-5.378262	-1.724241
O	-3.083320	-4.303488	0.079746
H	-2.108694	-4.221372	0.081671
C	-3.089864	-2.317050	-4.274506
C	-3.722546	-2.447609	-5.511812
C	-2.313702	-1.199247	-3.963996
C	-3.589472	-1.430971	-6.454382
H	-4.312553	-3.336284	-5.711540
C	-2.197530	-0.187918	-4.921676
H	-1.785915	-1.115486	-3.020937
C	-2.829960	-0.294855	-6.161462
H	-4.083383	-1.526609	-7.417166
H	-1.597329	0.687297	-4.688906
H	-2.728840	0.498799	-6.895880
O	-1.337507	-1.034436	-0.373935
C	-2.281798	-0.792182	0.649689
H	-2.894965	0.071998	0.366328
H	-2.928850	-1.668165	0.791852
H	-1.764818	-0.568042	1.590391

=== 2Int2A ===

C	4.028948	-2.093486	-3.448727
C	2.935699	-1.802309	-2.598370
C	1.874454	-0.979687	-3.078496
C	1.941503	-0.489711	-4.398849
C	3.020632	-0.801662	-5.210731
C	4.075732	-1.606285	-4.740720
H	4.834619	-2.715483	-3.065737
H	1.130480	0.140001	-4.749737
H	3.053006	-0.412860	-6.225165
H	4.916084	-1.839948	-5.386668
O	0.852412	-0.634222	-2.315164
C	2.927408	-2.320659	-1.268118
H	3.796692	-2.877416	-0.916709
N	1.944763	-2.180245	-0.416900
C	1.129136	-2.456045	1.599219
N	2.155570	-2.728916	0.838932
O	0.122053	-1.721068	1.158205
C	1.080517	-2.952439	2.986727
C	0.009561	-2.603765	3.824267
C	2.102821	-3.779131	3.485105
C	-0.047265	-3.071459	5.134698
H	-0.778785	-1.963380	3.444968
C	2.056999	-4.249691	4.791829
H	2.928202	-4.045440	2.834539
C	0.979207	-3.887396	5.596493
H	-0.867872	-2.813829	5.795767
H	2.835093	-4.889299	5.194974
F	0.931561	-4.343386	6.862896
V	0.069734	-1.352666	-0.765413
O	-1.093249	-2.532587	-1.340237
O	-2.850116	-3.575234	-2.428671
C	-2.501631	-2.683758	-1.408213
H	-2.947558	-1.695191	-1.582587
C	-3.003749	-3.294390	-0.094512
H	-4.090743	-3.400490	-0.155025
H	-2.564260	-4.297498	0.005051
O	-2.726298	-2.466586	1.015275
H	-1.762323	-2.446706	1.160278
C	-2.891911	-3.131485	-3.736088
C	-3.616904	-3.939467	-4.618292
C	-2.257794	-1.972782	-4.193908
C	-3.717307	-3.581576	-5.959801
H	-4.095096	-4.834361	-4.232418
C	-2.376533	-1.623600	-5.542384
H	-1.659124	-1.362200	-3.528573
C	-3.101346	-2.417913	-6.429433
H	-4.284334	-4.212251	-6.639386
H	-1.884503	-0.721442	-5.896377
H	-3.183195	-2.137821	-7.475676
O	-0.752897	0.184721	-0.420331
C	-1.424056	0.640599	0.743566
H	-1.834333	1.633582	0.526021
H	-2.238220	-0.038610	1.019146
H	-0.723758	0.720368	1.583336

=== 2Int2A’ ===

C	3.790800	-2.340405	-3.502204
C	2.801311	-1.965803	-2.564581
C	1.810214	-1.014124	-2.940986
C	1.838313	-0.481757	-4.245185

C	2.815194	-0.878279	-5.146474
C	3.801117	-1.811851	-4.780314
H	4.548065	-3.059834	-3.199251
H	1.081903	0.249167	-4.512741
H	2.820167	-0.454797	-6.147478
H	4.563255	-2.111906	-5.492691
O	0.884038	-0.586637	-2.093358
C	2.837570	-2.518178	-1.243488
H	3.680066	-3.150443	-0.960127
N	1.926718	-2.304563	-0.335254
C	1.218389	-2.447144	1.721138
N	2.159355	-2.857574	0.908607
O	0.284797	-1.608555	1.320621
C	1.199408	-2.901465	3.123522
C	0.186928	-2.462693	3.989868
C	2.188594	-3.775047	3.607123
C	0.156313	-2.884798	5.316489
H	-0.574874	-1.789737	3.613013
C	2.168693	-4.201796	4.929918
H	2.968620	-4.110971	2.933141
C	1.149989	-3.748114	5.764174
H	-0.618444	-2.557233	6.001721
H	2.923013	-4.875194	5.323225
F	1.127715	-4.160303	7.047181
V	0.079875	-1.306805	-0.574080
O	-1.066450	-2.487362	-1.183576
C	-2.095997	-2.300800	-2.142056
H	-2.706062	-1.425975	-1.884954
O	-0.887405	0.157387	-0.231010
C	-1.763261	0.398043	0.849546
H	-2.210323	1.391674	0.723861
H	-2.570474	-0.348311	0.886691
H	-1.219873	0.369138	1.801852
H	-1.665474	-2.154758	-3.140273
H	-2.728522	-3.195101	-2.151135

=== 1Int3A ===

C	4.936545	-3.626088	-3.766001
C	3.858522	-2.970134	-3.135909
C	2.926274	-2.252565	-3.931409
C	3.089656	-2.219227	-5.325274
C	4.154670	-2.886399	-5.919699
C	5.085411	-3.593836	-5.143474
H	5.649633	-4.168227	-3.149467
H	2.368615	-1.663772	-5.916603
H	4.264856	-2.856218	-7.000401
H	5.913781	-4.111110	-5.617239
O	1.934726	-1.560276	-3.366486
C	3.743410	-2.995018	-1.702797
H	4.564306	-3.405598	-1.114423
N	2.710698	-2.556396	-1.047441
C	1.638710	-2.170167	0.812190
N	2.769296	-2.616433	0.325471
O	0.678379	-1.728720	0.030442
C	1.413116	-2.143319	2.267716
C	0.178180	-1.711043	2.775201
C	2.423337	-2.546620	3.157581
C	-0.049527	-1.678678	4.148274
H	-0.599691	-1.406303	2.083936
C	2.206688	-2.516446	4.530223
H	3.374596	-2.880756	2.758785
C	0.970774	-2.081644	5.002871
H	-0.997366	-1.350235	4.561371
H	2.972480	-2.821856	5.235445
F	0.758080	-2.051180	6.332977
V	0.866864	-1.900083	-1.872624
O	-0.469795	-0.755810	-2.247359
O	-1.671613	1.191545	-1.816370
C	-0.457555	0.642951	-2.263432
H	-0.276627	0.954656	-3.306325
C	0.625339	1.186087	-1.325422
H	0.802193	2.252166	-1.509312
H	0.302051	1.048431	-0.292763
O	1.820270	0.417830	-1.472589
H	2.176093	0.538308	-2.369758
C	-2.747598	1.232077	-2.682201
C	-3.729765	2.181233	-2.381668
C	-2.891707	0.385874	-3.785545
C	-4.854975	2.290932	-3.194644
H	-3.590929	2.820982	-1.515649
C	-4.022138	0.515966	-4.596943
H	-2.154660	-0.382206	-3.989093
C	-5.004946	1.462764	-4.310607
H	-5.614776	3.030928	-2.957458
H	-4.134599	-0.143765	-5.453263
H	-5.882190	1.551484	-4.944927
O	0.280086	-3.319911	-2.159185

=== 3Int3A ===

C	4.779085	-3.356015	-3.696883
C	3.616420	-2.823951	-3.060772
C	2.623626	-2.126006	-3.879677
C	2.880375	-2.020265	-5.283345
C	4.007776	-2.563649	-5.844794
C	4.974931	-3.241292	-5.048609
H	5.512293	-3.866976	-3.078088
H	2.135646	-1.502697	-5.878941
H	4.168755	-2.477749	-6.916148
H	5.860333	-3.661575	-5.514648
O	1.566326	-1.572714	-3.402372
C	3.526743	-2.945181	-1.659899
H	4.370239	-3.367472	-1.112829
N	2.480257	-2.565453	-0.932285
C	1.458993	-2.281781	1.016518
N	2.614706	-2.686846	0.384404
O	0.428774	-1.912338	0.384897
C	1.471550	-2.299337	2.484349
C	0.314778	-1.901569	3.180404
C	2.612369	-2.703650	3.203436
C	0.293394	-1.905207	4.568418
H	-0.557408	-1.593795	2.614120
C	2.599805	-2.710675	4.592703
H	3.499291	-3.010379	2.661894
C	1.439273	-2.310557	5.251324
H	-0.585561	-1.604028	5.128120
H	3.464479	-3.018113	5.170945
F	1.423657	-2.315857	6.594093
V	0.574915	-2.013798	-1.679467
O	-0.769676	-0.705544	-1.893351
O	-1.649885	1.439321	-2.093638
C	-0.525275	0.583952	-2.283890
H	-0.237732	0.634447	-3.352798
C	0.578945	1.192104	-1.408358
H	0.893972	2.179269	-1.766943
H	0.209384	1.278309	-0.385039
O	1.694937	0.286087	-1.358806
H	2.087996	0.259678	-2.247657
C	-2.689054	1.366984	-2.987153
C	-3.562836	2.461868	-2.996260
C	-2.909963	0.284973	-3.848247
C	-4.646888	2.479385	-3.869719
H	-3.370757	3.286043	-2.315804

C	-3.997064	0.323128	-4.724987
H	-2.265212	-0.584649	-3.802570
C	-4.868444	1.412129	-4.744866
H	-5.318818	3.334144	-3.869745
H	-4.166540	-0.520765	-5.389255
H	-5.713662	1.427591	-5.427337
O	-0.022068	-3.425356	-2.041718

=== 3Int3A’ ===

C	4.199206	-3.117826	-3.834724
C	3.121925	-2.636119	-3.034370
C	2.057808	-1.857211	-3.677626
C	2.172409	-1.608193	-5.088105
C	3.225844	-2.101553	-5.808426
C	4.254798	-2.868292	-5.182040
H	4.984267	-3.692135	-3.349759
H	1.381099	-1.023690	-5.544955
H	3.285984	-1.908827	-6.876091
H	5.080291	-3.246860	-5.776335
O	1.058168	-1.378057	-3.050717
C	3.162473	-2.877464	-1.649063
H	4.031303	-3.382926	-1.226783
N	2.222586	-2.501335	-0.786852
C	1.477863	-2.265648	1.281549
N	2.491083	-2.742740	0.500763
O	0.456785	-1.685182	0.787758
C	1.606438	-2.433432	2.731055
C	0.562487	-1.993214	3.566926
C	2.749083	-3.030890	3.298363
C	0.654002	-2.144536	4.943628
H	-0.314575	-1.539832	3.118676
C	2.849015	-3.185161	4.674706
H	3.547777	-3.369317	2.648977
C	1.798368	-2.738527	5.474205
H	-0.137244	-1.816409	5.608922
H	3.717136	-3.641590	5.137783
F	1.891797	-2.887002	6.804611
V	0.272203	-1.770957	-1.235244
O	-0.531877	-0.115301	-1.271435
O	-1.565730	1.862428	-0.698824
C	-1.479821	0.463421	-0.439084
H	-1.225778	0.307958	0.620897
C	-2.885171	-0.091308	-0.714288
H	-3.610366	0.482601	-0.129109
H	-3.108442	0.053547	-1.781941
O	-3.009306	-1.441317	-0.312390
H	-2.481188	-1.994881	-0.913752
C	-0.578864	2.690490	-0.241356
C	-0.811329	4.062215	-0.418543
C	0.602260	2.260793	0.379160
C	0.121930	4.992928	0.026387
H	-1.732430	4.370973	-0.903300
C	1.526546	3.208936	0.825742
H	0.806748	1.204180	0.499396
C	1.298437	4.573760	0.655584
H	-0.072843	6.053005	-0.115917
H	2.439810	2.867239	1.307321
H	2.025966	5.301395	1.003969
O	-0.730305	-2.963730	-1.529848

=== 3TS2A ===

C	4.571885	-2.627868	-3.470201
C	3.458120	-2.287013	-2.665804
C	2.489986	-1.353927	-3.165861
C	2.691864	-0.807681	-4.455191
C	3.784524	-1.175232	-5.220341
C	4.736606	-2.092545	-4.732734
H	5.302609	-3.328755	-3.072819
H	1.956997	-0.096294	-4.818131
H	3.910946	-0.746021	-6.211075
H	5.591488	-2.370778	-5.341158
O	1.448836	-0.956929	-2.465583
C	3.376830	-2.814246	-1.338463
H	4.229026	-3.360945	-0.931877
N	2.352000	-2.640934	-0.549608
C	1.430686	-2.655255	1.437851
N	2.465546	-3.086560	0.751585
O	0.489005	-1.911098	0.897513
C	1.322523	-2.997109	2.870055
C	0.183138	-2.620322	3.596474
C	2.349115	-3.702678	3.521485
C	0.063585	-2.937456	4.947071
H	-0.610580	-2.083614	3.089619
C	2.242162	-4.023193	4.870087
H	3.227055	-3.993731	2.955959
C	1.098131	-3.633784	5.561858
H	-0.812075	-2.658627	5.523870
H	3.024229	-4.565809	5.390804
F	0.990596	-3.942465	6.869735
V	0.521372	-1.855460	-1.059210
O	-0.708772	-0.281256	-0.962729
O	-2.332067	1.123895	-0.285729
C	-1.744950	-0.150630	-0.187720
H	-1.634724	-0.490193	0.854341
C	-2.994067	-1.207245	-0.753621
H	-3.877636	-0.859452	-0.213938
H	-3.018474	-0.974932	-1.823163
O	-2.733067	-2.496148	-0.431403
H	-2.008677	-2.855612	-1.008851
C	-2.986535	1.624468	0.818317
C	-4.246300	2.196853	0.609399
C	-2.400539	1.628410	2.091426
C	-4.929133	2.760934	1.684197
H	-4.665193	2.193215	-0.391916
C	-3.100497	2.189887	3.159263
H	-1.399510	1.233854	2.234722
C	-4.363160	2.753093	2.962670
H	-5.907249	3.205422	1.523679
H	-2.646859	2.200313	4.146243
H	-4.898956	3.193433	3.798340
O	-0.399900	-3.020425	-1.660953

=== 3Int4A ===

C	4.083850	-3.209187	-3.506449
C	3.101922	-2.666662	-2.645903
C	2.242090	-1.630498	-3.135913
C	2.408651	-1.204891	-4.471433
C	3.369532	-1.771574	-5.294544
C	4.218629	-2.783388	-4.815642
H	4.739541	-3.983991	-3.115074
H	1.762160	-0.408438	-4.827931
H	3.470261	-1.421210	-6.318844
H	4.973254	-3.221190	-5.461888
O	1.322335	-1.024798	-2.391312
C	3.066510	-3.113136	-1.277848
H	3.898560	-3.705130	-0.891735
N	2.114308	-2.793298	-0.453141
C	1.453783	-2.402610	1.604841
N	2.285974	-3.116107	0.885220
O	0.634796	-1.501600	1.084081
C	1.441801	-2.587616	3.072540
C	0.596809	-1.807683	3.874953

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C         2.269359   -3.545599    3.683620
C         0.570897   -1.973802    5.257927
H        -0.039974   -1.067341    3.404469
C         2.253404   -3.721486    5.062803
H         2.920515   -4.147385    3.059937
C         1.401586   -2.930457    5.829050
H        -0.078162   -1.379894    5.893128
H         2.884258   -4.457350    5.550556
F         1.382096   -3.098044    7.167752
V         0.432281   -1.701450   -0.855524
O        -1.000276   -0.078391   -0.836735
O        -2.480242    1.222939    0.172960
C        -1.626624    0.203311    0.172544
H        -1.522258   -0.345221    1.116303
C        -2.213208   -1.109690   -3.688879
H        -2.645776   -0.575686   -4.557829
H        -1.111875   -1.122687   -3.615860
O        -2.923727   -1.643495   -2.863322
H        -1.671266   -2.586569   -1.631921
C        -3.098344    1.567953    1.389716
C        -4.488843    1.586871    1.417173
C        -2.328857    1.925102    2.493585
C        -5.127084    1.966349    2.598031
H        -5.047014    1.307362    0.529711
C        -2.983436    2.295039    3.670787
H        -1.244867    1.934641    2.427657
C        -4.377830    2.315798    3.724612
H        -6.212188    1.984712    2.636756
H        -2.397764    2.575850    4.541094
H        -4.880942    2.608660    4.641249
O        -0.820411   -2.923462   -1.285093

=== 3Int5A ===
C         3.880444   -3.199406   -3.579233
C         2.945672   -2.649411   -2.673634
C         2.091197   -1.588470   -3.115587
C         2.216642   -1.143700   -4.448894
C         3.133034   -1.718135   -5.317918
C         3.974519   -2.756284   -4.887247
H         4.534263   -3.993405   -3.225150
H         1.579979   -0.322694   -4.766239
H         3.204777   -1.351449   -6.338890
H         4.694228   -3.200641   -5.567858
O         1.206511   -0.978293   -2.329189
C         2.954075   -3.112242   -1.308417
H         3.793914   -3.715201   -0.957726
N         2.034157   -2.789813   -0.450686
C         1.435767   -2.398042    1.620336
N         2.245847   -3.117431    0.879349
O         0.608200   -1.496453    1.113738
C         1.453257   -2.570816    3.087241
C         0.593627   -1.807614    3.891215
C         2.320462   -3.495186    3.694616
C         0.593422   -1.959224    5.275801
H        -0.074492   -1.097110    3.418021
C         2.329853   -3.654860    5.075776
H         2.982513   -4.082588    3.068490
C         1.463623   -2.881882    5.844736
H        -0.065243   -1.379065    5.913686
H         2.991400   -4.363305    5.563442
F         1.469988   -3.034312    7.185047
V         0.334730   -1.681256   -0.794193
C        -1.586069   -1.279968   -4.095965
H        -1.703742   -1.425135   -5.185393
H        -1.219885   -2.132802   -3.501669
O        -1.867021   -0.211071   -3.583521
H        -1.848541   -2.581257   -1.167945
O        -0.938692   -2.909417   -1.272447
O        -1.179037   -0.158312   -0.911917
H        -1.460812   -0.073506   -1.856799
C        -0.873909    1.144041   -0.384188
H        -0.092003    1.633464   -0.976119
H        -1.775962    1.764242   -0.373820
H        -0.521354    0.993208    0.636890

=== 3TS3A ===
C         4.450755   -3.238916   -3.738680
C         3.443891   -2.713928   -2.899459
C         2.424210   -1.897781   -3.472463
C         2.455344   -1.650470   -4.856436
C         3.450453   -2.193883   -5.659029
C         4.458235   -2.994815   -5.102320
H         5.229695   -3.851349   -3.290509
H         1.673235   -1.026756   -5.279714
H         3.445465   -1.992791   -6.727112
H         5.236435   -3.416484   -5.730819
O         1.465215   -1.320398   -2.733333
C         3.528382   -2.965738   -1.482416
H         4.444510   -3.401311   -1.080640
N         2.583282   -2.681516   -0.637705
C         1.811277   -2.425838    1.396532
N         2.833655   -2.885681    0.702273
O         0.767062   -1.866882    0.837624
C         1.843100   -2.521536    2.869880
C         0.754250   -2.048196    3.617664
C         2.946887   -3.079690    3.536511
C         0.761524   -2.127782    5.007757
H        -0.093769   -1.620384    3.094891
C         2.964936   -3.164077    4.924351
H         3.784693   -3.444241    2.952869
C         1.868975   -2.685004    5.637377
H        -0.070578   -1.768592    5.604258
H         3.806628   -3.591407    5.459372
F         1.883602   -2.764677    6.983727
V         0.657575   -2.085274   -1.099153
O        -0.751789   -0.601021   -1.102668
O        -2.245290    0.796289   -2.061390
C        -1.035602    0.113613   -2.121006
H        -0.810181   -0.283465   -3.122526
C         0.168226    1.534152   -2.154185
H         0.006241    1.838945   -3.195765
H        -0.242764    2.215913   -1.411703
O         1.398267    1.119482   -1.823193
H         1.657982    0.342430   -2.391568
C        -2.879026    1.097820   -3.254976
C        -3.348668    2.403836   -3.418944
C        -3.104083    0.122446   -4.233048
C        -4.035568    2.739959   -4.583538
H        -3.173339    3.130762   -2.632253
C        -3.786016    0.477126   -5.397846
H        -2.786542   -0.902596   -4.068269
C        -4.249612    1.781464   -5.578469
H        -4.403116    3.753691   -4.714668
H        -3.968686   -0.277133   -6.157824
H        -4.785602    2.047864   -6.484592
O        -0.126583   -3.392013   -1.488130

=== 3Int6A ===
C         5.362166   -3.076016   -3.394294
C         4.242959   -2.514399   -2.738615
C         3.494435   -1.491306   -3.395133
C         3.898144   -1.084658   -4.682154
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C         4.994061   -1.666805   -5.303762
C         5.736958   -2.670472   -4.662836
H         5.929926   -3.846094   -2.877145
H         3.330137   -0.302533   -5.176132
H         5.278973   -1.333976   -6.298461
H         6.595146   -3.119345   -5.153053
O         2.454229   -0.881820   -2.818138
C         3.950957   -2.945921   -1.398527
H         4.677824   -3.571791   -0.878517
N         2.883085   -2.605734   -0.740360
C         1.758163   -2.385285    1.126460
N         2.792510   -2.989126    0.585167
O         0.993691   -1.550506    0.455934
C         1.443046   -2.627386    2.548635
C         0.365430   -1.956845    3.146312
C         2.207561   -3.522434    3.316297
C         0.051294   -2.171186    4.485961
H        -0.219109   -1.266499    2.548800
C         1.902577   -3.745106    4.654457
H         3.039030   -4.038339    2.849448
C         0.826722   -3.063587    5.217590
H        -0.777180   -1.661488    4.966672
H         2.479339   -4.432732    5.264198
F         0.527973   -3.276947    6.515279
V         1.247740   -1.596184   -1.471895
O         0.159755    0.147449   -1.602896
O        -1.571137    1.423382   -2.119410
C        -0.945695    0.249696   -2.145968
H        -1.508989   -0.603652   -2.530875
C        -0.015112    0.193677   -4.665028
H         0.030407   -0.894670   -4.641936
H        -0.688187    0.690035   -5.357007
O         1.096548    0.892668   -4.375962
H         1.669619    0.338952   -3.783039
C        -2.864376    1.497384   -2.658852
C        -3.082064    2.440958   -3.658289
C        -3.888463    0.693695   -2.164331
C        -4.366680    2.571567   -4.185801
H        -2.255015    3.052435   -4.003558
C        -5.167364    0.830705   -2.708858
H        -3.696089   -0.006958   -1.357269
C        -5.407497    1.765499   -3.716958
H        -4.552449    3.303627   -4.966272
H        -5.976161    0.210716   -2.333533
H        -6.405310    1.871169   -4.132312
O         0.273655   -2.639646   -2.145303

=== 3Int7A ===
C         5.290367   -3.359055   -3.486891
C         4.188959   -2.763131   -2.830637
C         3.390296   -1.812845   -3.535065
C         3.732104   -1.511443   -4.868400
C         4.811634   -2.124673   -5.488831
C         5.602757   -3.056762   -4.800123
H         5.894630   -4.073553   -2.932799
H         3.126833   -0.788312   -5.406589
H         5.044117   -1.873380   -6.520342
H         6.447754   -3.531439   -5.288744
O         2.358163   -1.175856   -2.971126
C         3.965022   -3.097111   -1.450917
H         4.717697   -3.689530   -0.928586
N         2.934923   -2.711570   -0.758230
C         1.923714   -2.389978    1.162108
N         2.923001   -3.022292    0.590328
O         1.117921   -1.591283    0.496700
C         1.705342   -2.557750    2.613570
C         0.652978   -1.880781    3.247195
C         2.542383   -3.390778    3.375882
C         0.434245   -2.026342    4.614774
H         0.008618   -1.239302    2.657190
C         2.334051   -3.544556    4.741831
H         3.353923   -3.913164    2.882204
C         1.280720   -2.857453    5.339671
H        -0.374741   -1.510951    5.121813
H         2.968834   -4.183339    5.346990
F         1.075978   -3.003302    6.664118
V         1.261996   -1.742315   -1.450292
C         0.776466    1.346775   -4.093989
H         0.103463    2.080558   -4.527985
H         1.762274    1.676522   -3.757141
O         0.678371    0.119458   -4.655417
H         1.322756   -0.472145   -4.185339
O         0.227267   -2.807708   -1.968017
O         0.354903    0.120922   -1.500384
H         0.388668    0.643818   -2.350678
C        -0.901162    0.349783   -0.829023
H        -1.727282   -0.066766   -1.414005
H        -0.831398   -0.152489    0.134105
H        -1.040975    1.424502   -0.681642

=== 1Int7A ===
C         5.292055   -3.359451   -3.486829
C         4.191343   -2.762192   -2.830774
C         3.394816   -1.810353   -3.535137
C         3.737248   -1.508774   -4.868086
C         4.816106   -2.123237   -5.488505
C         5.605490   -3.056744   -4.799812
H         5.894929   -4.075330   -2.932994
H         3.132615   -0.784661   -5.405772
H         5.049369   -1.871938   -6.519823
H         6.449978   -3.532483   -5.288280
O         2.363390   -1.172205   -2.971296
C         3.965126   -3.096835   -1.451455
H         4.715916   -3.691499   -0.928941
N         2.935253   -2.709656   -0.759354
C         1.924300   -2.387198    1.161010
N         2.921579   -3.022431    0.588627
O         1.122154   -1.584220    0.497043
C         1.705166   -2.556599    2.612259
C         0.656275   -1.875421    3.247106
C         2.537994   -3.395163    3.373098
C         0.436849   -2.022212    4.614441
H         0.015222   -1.229646    2.658187
C         2.328923   -3.550254    4.738802
H         3.346877   -3.920802    2.878502
C         1.279116   -2.858850    5.337871
H        -0.369484   -1.503584    5.122404
H         2.960481   -4.193295    5.342831
F         1.073682   -3.005934    6.662100
V         1.264671   -1.734050   -1.451338
C         0.764843    1.335577   -4.083206
H         0.083951    2.067259   -4.508570
H         1.755262    1.668767   -3.763855
O         0.660701    0.107384   -4.641110
H         1.314648   -0.481462   -4.181167
O         0.226011   -2.797244   -1.965725
O         0.362446    0.124618   -1.500172
H         0.397279    0.651319   -2.351480
C        -0.896750    0.351183   -0.833653
H        -1.718806   -0.074373   -1.417813
H        -0.826866   -0.143338    0.133475
H        -1.042588    1.426312   -0.695324
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=== 1TS4A ===

C	5.302954	-3.370652	-3.490261
C	4.207306	-2.756908	-2.842236
C	3.426266	-1.801084	-3.554577
C	3.778006	-1.506258	-4.886070
C	4.853643	-2.134184	-5.499241
C	5.627090	-3.075085	-4.802899
H	5.894179	-4.092246	-2.931331
H	3.185460	-0.773604	-5.426689
H	5.096592	-1.888098	-6.529545
H	6.468543	-3.562412	-5.285140
O	2.396332	-1.155057	-2.999859
C	3.962600	-3.082637	-1.464012
H	4.689543	-3.704498	-0.939598
N	2.944763	-2.661998	-0.773368
C	1.935412	-2.344783	1.147746
N	2.920782	-2.992977	0.569246
O	1.156731	-1.514315	0.494439
C	1.705463	-2.532039	2.595218
C	0.672993	-1.832101	3.236583
C	2.510504	-3.406692	3.345061
C	0.442812	-1.995944	4.600196
H	0.053900	-1.158531	2.655313
C	2.290256	-3.579065	4.706988
H	3.306556	-3.946736	2.845150
C	1.257407	-2.868451	5.312935
H	-0.350990	-1.463264	5.113339
H	2.900190	-4.250068	5.302777
F	1.041129	-3.032364	6.633580
V	1.287582	-1.626415	-1.460806
C	0.660859	1.188860	-3.825165
H	-0.114844	1.907310	-4.093098
H	1.668316	1.614839	-3.726003
O	0.566364	0.048972	-4.561631
H	1.283345	-0.548550	-4.224193
O	0.218465	-2.674797	-1.937829
O	0.445739	0.156263	-1.486497
H	0.491789	0.777884	-2.570392
C	-0.848434	0.362394	-0.908758
H	-1.622104	-0.159373	-1.483314
H	-0.814051	-0.035636	0.107678
H	-1.062656	1.435747	-0.873471

=== 1Int8A ===

C	5.094456	-3.357837	-3.497567
C	4.067633	-2.773587	-2.724215
C	3.164556	-1.872592	-3.346437
C	3.300672	-1.584169	-4.714426
C	4.313458	-2.185834	-5.450811
C	5.216811	-3.076328	-4.847656
H	5.787134	-4.041853	-3.013117
H	2.602604	-0.885163	-5.164926
H	4.405682	-1.958667	-6.509468
H	6.004155	-3.538983	-5.434455
O	2.215108	-1.247328	-2.639711
C	3.982991	-3.053209	-1.319308
H	4.786855	-3.614232	-0.841404
N	2.996667	-2.667216	-0.564511
C	2.039347	-2.460556	1.380233
N	3.089907	-2.954990	0.778118
O	1.127796	-1.776336	0.714053
C	1.851948	-2.633886	2.829635
C	0.715901	-2.100943	3.458048
C	2.802773	-3.330873	3.595241
C	0.526440	-2.259065	4.828113
H	-0.014485	-1.564231	2.863083
C	2.623394	-3.493302	4.963760
H	3.678219	-3.740174	3.103643
C	1.485149	-2.953348	5.558009
H	-0.344750	-1.856102	5.333598
H	3.344004	-4.027507	5.573958
F	1.308506	-3.109641	6.884048
V	1.147538	-1.763948	-1.191896
C	1.375546	2.005956	-4.011977
H	0.933407	2.693093	-4.739424
H	2.469102	2.035563	-4.133966
O	0.838505	0.717220	-4.268966
H	1.238760	0.100847	-3.627727
O	0.373977	-3.040144	-1.657508
O	0.065869	-0.393356	-1.300192
H	1.129658	2.367494	-3.002290
C	-1.233075	-0.202958	-1.838461
H	-1.741024	-1.165375	-1.972308
H	-1.808472	0.429968	-1.153858
H	-1.125931	0.299037	-2.806685