**SUPPORTING INFORMATION**

# Chain propagation determines the chemo- and regioselectivity of alkyl radical additions to C–O vs. C–C double bonds

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**Content**

# 1 General considerations

## *1.1 Synthetic methodology*

Unless otherwise noted, all reactions were conducted under argon atmosphere in dried glassware. The solvents were either purified via distillation over standard drying agents or purchased dry and stored over molecular sieves. Solvents used for extraction or chromatography were flash-distilled prior to use. All commercial chemicals and reagents were purchased from *Sigma Aldrich, Alfa Aesar, ABCR, Acros Organics, TCI Europe, Merck, Fluorochem, ChemPur* and *Combi-Blocks* and were used without further purification. The used photocatalysts were purchased from commercial suppliers or synthesized according to literature procedures. For thin layer chromatography, *Merck* 60 $F_{254}$ aluminum plates with a fluorescent indicator were used. Substances were visualized either by exposure to UV light (λ = 254 nm) or by oxidation with a $KMnO_4$ stain solution. Flash column chromatography was performed using *Acros* silica gel (35–70 µm, 60 Å) with a positive overpressure of argon (approx. 0.5 bar).

## *1.2 Photochemical reaction setup*

The standard setup for carrying out photochemical reactions was a custom made “light box” (see Figure S1): Six LED (5W, 455 nm) were arranged around the reaction vessels in a distance of approx. 3 cm. A fan attached to the apparatus was used to maintain the temperature inside the “light box” at no more than 9 °C above room temperature. Emission spectra of the used LED (400 nm, 420 nm, 455 nm) are shown in Figure S2.

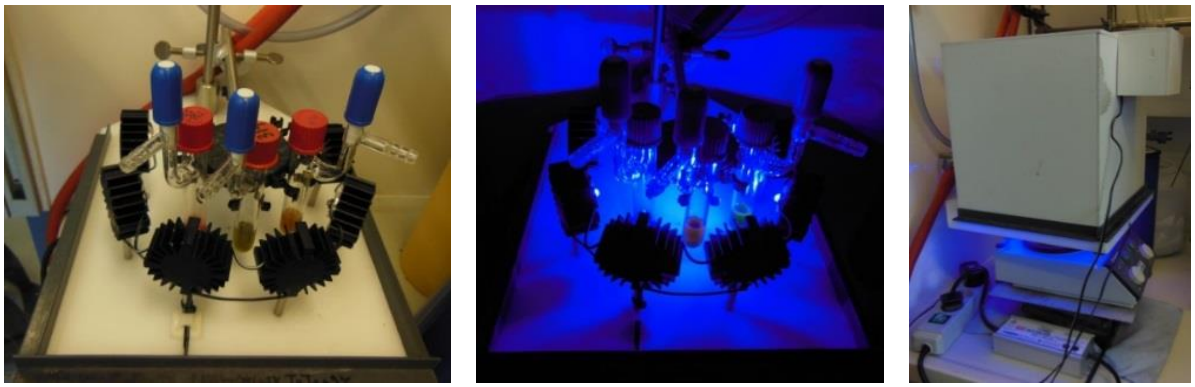


**Figure S1:** Photographs of the custom-made “light box” with six LED.

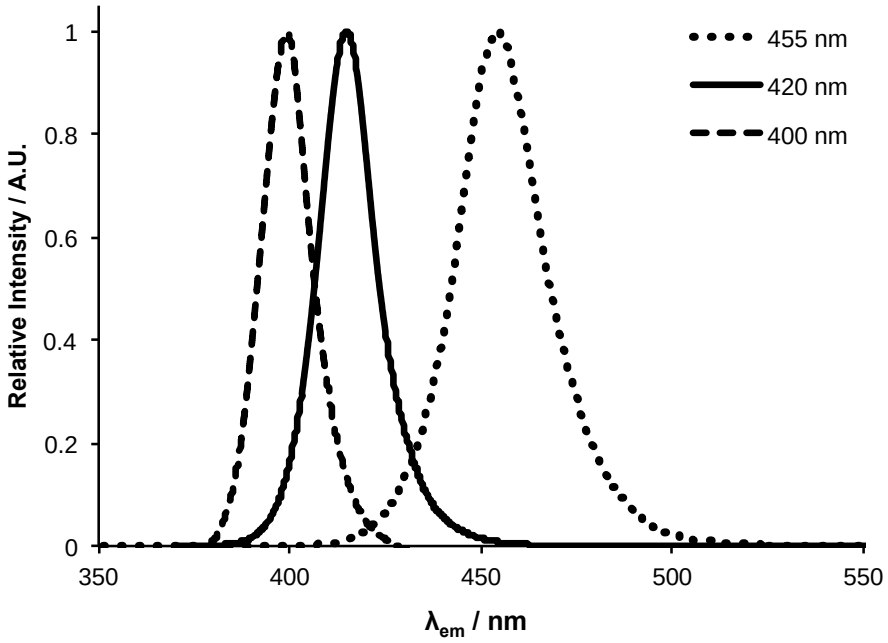
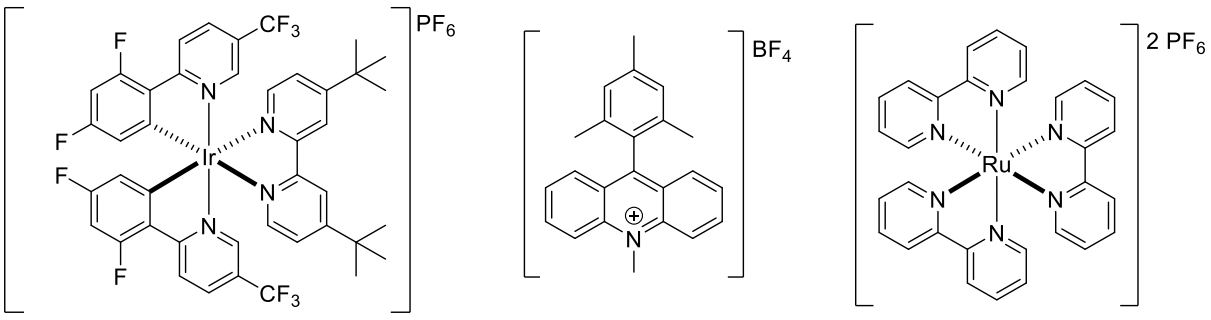



**Figure S2:** Emission Spectra of the LED used for reaction irradiation.

## *1.3 Photocatalysts*

All employed photocatalysts were purchased from the abovementioned commercial suppliers or prepared according to literature procedures: [1, 2, 3]




$[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ (**PC-1**) $MesAcrBF_4$ $[Ru(bpy)_3](PF_6)_2$

**Figure S3**: Photocatalysts utilized for screening or reaction optimization studies.

## *1.4 Analytical methods*

NMR-spectra were recorded on a Bruker ARX-300, AV-300 or AV-400 MHz. Chemical shifts (δ) are quoted in ppm downfield of tetramethylsilane. As references for $^1H$ and $^{13}C$ NMR-spectra $CDCl_3$ ($\delta_H$ = 7.26 ppm; $\delta_C$ = 77.16 ppm) was used. Coupling constants (*J*) are quoted in Hz. Multiplicities are reported as: s (singlet), d (doublet), t (triplet), q (quartet), p (quintet), hept (septet), m (multiplet) or a combination of these. Coupling constants (*J*) are quoted in Hz.

ESI mass spectra were recorded on a *Bruker* MicrOTof or a *Thermo Scientific* Orbitrap LTQ XL spectrometer. GC-MS chromatograms were recorded on an *Agilent Technologies* 7890A GC system with an HP5-MS column. A standard separation method (50°C for 3 min, heated to 290 °C by 40 °C/min, 290 °C for 3 min) was used. The GC system is coupled with an *Agilent* 5975C VL mass selective detector (MSD) or an *Agilent* 5975 inert mass selective detector for recording EI mass spectra. The major signals of are quoted as *m*/*z* with the relative intensity in parentheses.

UV/Vis spectra were recorded on a *Jasco* V750 photometer using the following set of parameters: bandwidth = 1.0 nm, scan speed = 400 nm/min, response time = 0.24 sec. All samples were measured in *Hellma* fluorescence QS quartz cuvettes (chamber volume = 1.4 mL, dimensions: 46 mm × 12.5 mm × 12.5 mm) fitted with a PTFE stopper.

All luminescence spectra were recorded on a *Jasco* FP-8300 spectrofluorometer with the following parameter set excitation bandwidth = 5.0 nm, data interval = 0.2 nm, scan speed = 500 nm/min, response time = 0.2 sec.

## *1.5 Photophysical methods*

UV/Vis absorption spectra between 220 and 800 nm were measured with a PerkinElmer Lambda2 dual beam absorption spectrometer with a scan rate of 480 nm/min and a resolution of 1 nm.

Steady state emission measurements were carried out using a Fluoromax-3-spectrometer from HORIBA Jobin Yvon. The measurement parameters include a slit width of 2 nm for both, excitation slit and the emission slit, and an integration time of 0.1 s.

Nanosecond transient absorption experiments were carried out with a Clark MXR CPA-2101 amplified Ti:Sapphire fs laser system (output ~775 nm, ~1 kHz repetition rate, and 150 fs pulse width) using a transient absorption pump/probe detection system (Ultrafast Systems EOS). The excitation wavelengths were generated by a second harmonic generator (387 nm, Clark MXR Storc harmonic generator) or by a noncollinear optical parametric amplifier with subsequent frequency doubling (640 → 320 nm, Clark MXR NOPA). For the excitation wavelength, the energy of 150-200 nJ/pulse was selected. The spectral data were evaluated using the TIMP-based GloTarAn program.[4] For every dataset, a global analysis with one to three decay-associated components was used.

Phosphorescence lifetime quenching experiments as well as TAS measurements between 230 - 880 nm were conducted using a self-constructed ns-TAS system. A Nd:YAG laser (Brilliant B, Quantel: output 1064 nm, 10 Hz, 4-8 ns pulse width) was used to excite the sample. The laser is tuned by a third harmonic generator (Quantel) to reach a 355 nm output. The emitted light passes a filter wheel (used long pass filter: 395 nm) to avoid the redirection of scattered higher harmonic wavelengths. After passing a monochromator, selecting the desired emission wavelength, the light is detected by a photomultiplier (230 – 880 nm, 10 ns time resolution). Eventually, the data are digitalized by a LeCroy digital storage oscilloscope.

The samples were prepared in Hellma cuvettes with the following characteristics: 10 x 10 mm QS cuvettes for steady-state absorption and emission spectroscopy, 8 x 10 mm QS cuvettes for phosphorescence lifetime quenching experiments, 2 x 10 mm OS cuvettes for TAS.

To record electrochemical data, a Metrohm FRA 2 µAutolab Type III potentiostat is used. A three electrode cell configuration, composed of a glassy carbon working electrode (3 mm diameter), a Ag-wire quasi-reference electrode and a platinum wire counter electrode is used to perform square wave voltammetry, differential pulse voltammetry, and cyclic voltammetry. For cyclic voltammetry, scan rates between 0.025 and 0.1 V/s with varying steps of 0.025 V/s are chosen. As conducting salt, pre-dried tetrabutylammonium hexafluorophosphate is used in a concentration of 0.1 mol/L. Potentials are referred to the ferrocene/ferrocenium ($Fc/Fc^{\bullet+}$) redox couple. To conduct spectroelectrochemical measurements, a Metrohm PGSTAT101 potentiostat is used in combination with an Agilent Cary 5000 UV/VIS/NIR spectrometer. To allow light passing the sample solution in a three-neck cell, the used working electrode is a close meshed platinum net. As reference electrode serves a silver wire, whereas the counter electrode is a platinum wire.

The samples are saturated with dry Ar gas before measurement of electrochemical/spectroelectrochemical and TAS experiments to ensure oxygen expulsion. Furthermore, the cuvettes are sealed by precision seal rubbers.

The used solvents are of spectroscopical grade and were supplied by Sigma-Aldrich. For UV/Vis absorption and emission measurements, as well as electrochemistry, and for TAS experiments, dry acetonitrile was used.

# 2 Computational details

All computational studies were carried out using the ORCA 4.1.1 software package.[5,6] Structures were visualized with Jmol.[7]

The geometries of all relevant stationary points were optimized using the B3LYP hybrid functional [8] with Grimme's D3 dispersion correction [9,10] and Ahlrichs' def2-SVP double-zeta basis set.[11] All structures were confirmed to be local minima on the potential energy surface by the absence of negative eigenvalues of the Hessian after harmonic frequency analysis at the same level. No symmetrical or internal coordinate constraints were applied. Higher energy conformers were taken into account, but not included in the final calculation. Additional single point computations on the previously optimized geometries were performed using the def2-TZVPP triple-zeta basis set [11] and the CPCM continuum solvation model with presets for the respective reaction solvent.[12,13] The reported free energy values (in kcal $mol^{-1}$) were obtained as the sum of the single point electronic energies and the respective free energy corrections (ZPVE, thermal corrections, enthalpy, entropy), as obtained from the harmonic frequency calculation.

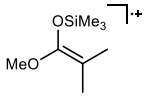
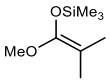
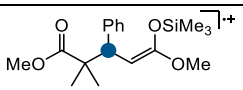
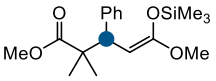
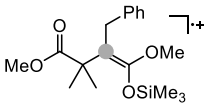
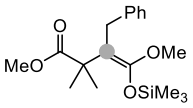
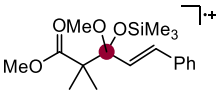
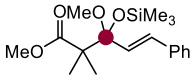
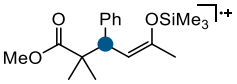
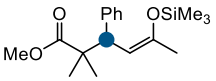
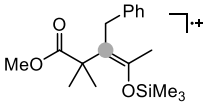
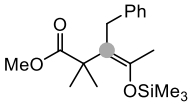
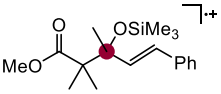
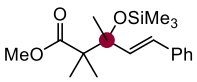
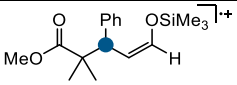
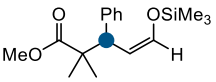
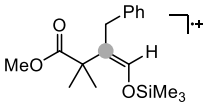
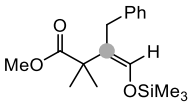
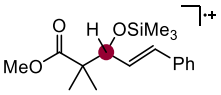
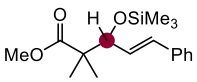
## *2.1 Computational determination of redox potentials*

Redox potentials were calculated based on a protocol reported by Nicewicz and coworkers.[14, 15] The free energy difference between reduced and oxidized species could be converted to the respective redox potential according to the following equation (1). All values are referenced to saturated calomel electrode (SCE) by subtraction of its absolute potential in acetonitrile ($E_{ref}$ = 4.442 V).[18]

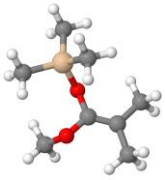
$$E = -\frac{G_{298}(\mathrm{red}) - G_{298}(\mathrm{ox})}{F} - E_{ref} \qquad (1)$$

From calculated redox potentials, it can be concluded that chain propagation is feasible for the silylated radical cations **D**. 1,4- and 1,2-addition radical cations exhibit a redox potential of more than +0.96 V and are therefore able to oxidize silyl ketene acetal **1** to its radical cation, closing the proposed "hole catalysis" chain.

**Table S1:** Calculation of redox potentials of hypothetical intermediates of the coupling of silyl ketene acetals and Michael acceptors. Free energies, given in $E_h$, were obtained as the sum of electronic energies, ZPVE, thermal corrections, enthalpy and entropy corrections.

| Oxidized Species | | Reduced Species | | Calculated |
|---|---|---|---|---|
| **Structure** | ***G*$_{298}$ / $E_h$** | **Structure** | ***G*$_{298}$ / $E_h$** | **Potential** |
|  **A** | -755.233652092 |  **1** | -755.413891662 | +0.46 V |
|  **$D_3^{Est-1,4}$** | -1292.54468226 |  **$E_3^{Est-1,4}$** | -1292.74314652 | +0.96 V |
|  **$D_3^{Est-1,3}$** | -1292.55462269 |  **$E_3^{Est-1,3}$** | -1292.72156707 | +0.10 V |
|  **$D_3^{Est-1,2}$** | -1292.51934809 |  **$E_3^{Est-1,2}$** | -1292.73343286 | +1.38 V |
|  **$D_3^{Ket-1,4}$** | -1217.32877339 |  **$E_3^{Ket-1,4}$** | -1217.53169604 | +1.08 V |
|  **$D_3^{Ket-1,3}$** | -1217.32649822 |  **$E_3^{Ket-1,3}$** | -1217.53055893 | +1.11 V |
|  **$D_3^{Ket-1,2}$** | -1217.30213460 |  **$E_3^{Ket-1,2}$** | -1217.52409113 | +1.59 V |
|  **$D_4^{Ald-1,4}$** | -1178.03780869 |  **$E_4^{Ald-1,4}$** | -1178.24566580 | +1.21 V |
|  **$D_4^{Ald-1,3}$** | -1178.039903 |  **$E_4^{Ald-1,3}$** | -1178.23212816 | +0.79 V |
|  **$D_4^{Ald-1,2}$** | -1178.03002491 |  **$E_4^{Ald-1,2}$** | -1178.25307135 | +1.63 V |

## 1



| | | | |
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| C | 1.11871951916892 | 3.40863071246837 | -0.60516420253531 |
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| C | -0.41706939422046 | 0.53037369323556 | -0.83392796614035 |
| O | -1.04859564928642 | 1.62856252109310 | -1.32646150836552 |
| O | -0.76379066680497 | 0.21023536056648 | 0.45114044300907 |
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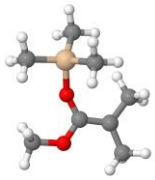
## A



| | | | |
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| H | -1.70122232520864 | 0.66065864585473 | 1.70429416025670 |
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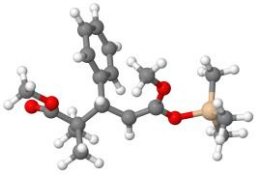
## $D_3^{Est\text{-}1,4}$



| | | | |
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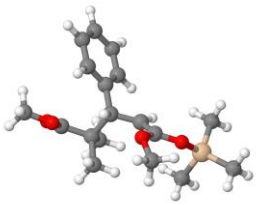
| C | -5.08127531624405 | 0.39147151407930 | -0.29342005609746 |
| C | -4.13851708623342 | -0.61678849766524 | -0.52775606341260 |
| C | -4.66846307185152 | 1.65087617084649 | 0.14246410673586 |
| C | -2.78110246698926 | -0.36091038094417 | -0.31715527263504 |
| C | -2.36675703839847 | 0.89624553612216 | 0.12768639088244 |
| C | -3.30595194596195 | 1.91750396177812 | 0.36319639798050 |
| C | -2.86332747421045 | 3.28915324145029 | 0.87378959336523 |
| C | -1.57803301456900 | 3.66199081922110 | 0.22115439597921 |
| C | -1.28835616796535 | 3.81079842591911 | -1.17272984946295 |
| O | -0.05132994753644 | 3.78135087535803 | -1.50610372684645 |
| H | -6.14424265402132 | 0.19264953634102 | -0.44805055776807 |
| H | -4.46442771389262 | -1.60223428447847 | -0.86782123972211 |
| H | -5.40700943120437 | 2.43302699081605 | 0.32982390865515 |
| H | -2.04213779549979 | -1.14703385302484 | -0.48792557870634 |
| H | -1.30533782526973 | 1.07480559563309 | 0.31509050589858 |
| Si | 0.73853035349824 | 3.89367502807824 | -3.12535126885393 |
| C | 0.25008834139425 | 5.55626836621226 | -3.81266012399160 |
| C | 0.09296857168894 | 2.43066677355851 | -4.08270378247929 |
| C | 2.52942881270451 | 3.76529419037148 | -2.64978107114449 |
| H | 0.80444241220276 | 5.73741928422907 | -4.74920067492128 |
| H | 0.50675684100440 | 6.36952809752530 | -3.11500820651380 |
| H | -0.82452606022754 | 5.60899504973224 | -4.04195471833079 |
| H | 2.82975431369479 | 4.59169675156487 | -1.98632577054028 |
| H | 2.74248442782239 | 2.81272811138038 | -2.13942716110474 |
| H | 3.16072049465291 | 3.81214820266149 | -3.55278016604938 |
| H | 0.28365460228788 | 1.48737689524428 | -3.54630158178508 |
| H | 0.61178903284798 | 2.37098311719779 | -5.05436908087152 |
| H | -0.98620864324291 | 2.51379646437961 | -4.28013141196139 |
| C | -2.78334135833853 | 3.39369308678786 | 2.43709838197031 |
| C | -1.80173944026547 | 2.39066920928210 | 3.04950393138826 |
| H | -0.77866475271398 | 2.55199651634572 | 2.67526865110822 |
| H | -1.77970208168851 | 2.50940518550025 | 4.14114843335555 |
| H | -2.09927720166594 | 1.35466884303083 | 2.84227516763610 |
| C | -2.40708359697099 | 4.83613082619028 | 2.83331445110726 |
| H | -1.38274220017251 | 5.08130571716853 | 2.51063144178432 |
| H | -2.43733685886900 | 4.94974334594251 | 3.92731875860670 |
| H | -3.10023901222935 | 5.56858512135370 | 2.39511017485863 |
| C | -4.18626338538471 | 3.10428682466816 | 2.99403601223197 |
| O | -4.43919446356195 | 2.28542429239177 | 3.83629662807451 |
| O | -5.11373777629741 | 3.90919031549350 | 2.43640565663011 |
| C | -6.45464531706399 | 3.76210822454241 | 2.92710134823503 |
| H | -6.48864758276299 | 3.94861100645888 | 4.00988391400203 |
| H | -6.82402558981538 | 2.74400979647092 | 2.73426995024960 |

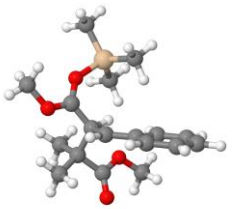
| | | | |
|---|---|---|---|
| H | -7.05878225478901 | 4.50281399774590 | 2.39011223158662 |
| H | -3.64769481129330 | 4.00344653274925 | 0.57901442460630 |
| O | -2.12833958453971 | 3.97524174296186 | -2.15936223448030 |
| H | -0.66263933834335 | 3.68591184946781 | 0.81628635142079 |
| C | -3.54197828887915 | 4.23133974396891 | -2.04119832037397 |
| H | -3.86574610415643 | 4.49971080865337 | -3.05263174575316 |
| H | -3.71839908246042 | 5.07147660160507 | -1.35650966327588 |
| H | -4.06013446821879 | 3.32531842763281 | -1.70412188126738 |

## $E_3^{Est-1,4}$



| | | | |
|---|---|---|---|
| C | -5.55851527403969 | 0.22191785705066 | 1.32658913193533 |
| C | -4.89305029540717 | -0.66771649367187 | 2.17344323062044 |
| C | -4.87831806882945 | 1.31466869753804 | 0.78285959812507 |
| C | -3.54201681604529 | -0.45655714471000 | 2.46257545865252 |
| C | -2.86677404633390 | 0.63672620070712 | 1.91481393243204 |
| C | -3.52445998320047 | 1.54726920295680 | 1.07223475662000 |
| C | -2.82844796895219 | 2.76697753022696 | 0.48425617094468 |
| C | -1.47339050336432 | 2.44147884121282 | -0.08271232999397 |
| C | -1.07180673861866 | 2.82543451148785 | -1.31001669774503 |
| O | 0.13921311357366 | 2.59484690962616 | -1.85107389789271 |
| H | -6.61227214857626 | 0.06251622813204 | 1.08243404445255 |
| H | -5.42137777169905 | -1.52350662673810 | 2.60127766741714 |
| H | -5.40223912301303 | 2.00483621346149 | 0.11787921860666 |
| H | -3.00778399223598 | -1.14953215126759 | 3.11800891398824 |
| H | -1.80969994834824 | 0.77640164195449 | 2.14865120144613 |
| Si | 1.64795317845481 | 2.33719785023401 | -1.09436522958240 |
| C | 1.70708713577092 | 0.61261145699117 | -0.35687440366387 |
| C | 1.90541035279353 | 3.66747993812117 | 0.20341026207384 |
| C | 2.86808582290389 | 2.49746772781546 | -2.50453964364405 |
| H | 2.73035818750783 | 0.37846923576441 | -0.01795439190619 |
| H | 1.41873180182608 | -0.13928448103902 | -1.10946003806497 |
| H | 1.03337807278722 | 0.50081391822307 | 0.50664225160179 |
| H | 2.66194609605842 | 1.75024505216275 | -3.28790637158283 |
| H | 2.81106344989176 | 3.49744571569444 | -2.96403785466583 |
| H | 3.90065223319499 | 2.34295228455480 | -2.15006864223341 |
| H | 1.83205733913728 | 4.67093106668583 | -0.24691493774906 |
| H | 2.90480974587715 | 3.57253745772088 | 0.65986471863492 |
| H | 1.15560469094580 | 3.60174384397180 | 1.00614254295807 |
| C | -2.77776635896733 | 3.97800423980007 | 1.50572909086961 |
| C | -1.85947966363625 | 3.70502814249480 | 2.69989621431112 |
| H | -0.83758405100889 | 3.49450571163760 | 2.35094589695985 |
| H | -1.82406202397298 | 4.58156675004282 | 3.36341670203722 |
| H | -2.21654859154823 | 2.85848405750018 | 3.30034779621257 |
| C | -2.30821377530916 | 5.24341152414177 | 0.76293191560592 |
| H | -1.27300088729473 | 5.10629786684072 | 0.41728110911796 |
| H | -2.33306944683912 | 6.11806381890522 | 1.43245009403203 |
| H | -2.94239821806308 | 5.45173482425075 | -0.10932686116513 |
| C | -4.19284114038779 | 4.21878469307964 | 2.02962964885587 |
| O | -4.53528585154782 | 4.16940816155082 | 3.18522797731872 |
| O | -5.05509320027026 | 4.50859914293795 | 1.02963100099720 |
| C | -6.41474291917868 | 4.69543976479881 | 1.41356333992702 |
| H | -6.50750856761621 | 5.51037312794315 | 2.14734762213719 |
| H | -6.81807830656377 | 3.77517958247582 | 1.86402240443831 |
| H | -6.96253343790349 | 4.94267916239492 | 0.49531111153443 |
| H | -3.45350261703241 | 3.12186310112111 | -0.34394088660623 |
| O | -1.91791484587608 | 3.47361509816022 | -2.14423875031833 |
| H | -0.78418936619374 | 1.83806847565504 | 0.50552883055493 |
| C | -1.36552300854053 | 4.36512608829459 | -3.09776058805214 |
| H | -0.79115637079727 | 5.17214183173611 | -2.60823245221607 |
| H | -2.21727164749603 | 4.80553356935107 | -3.63314736931679 |
| H | -0.70914424601581 | 3.84449878001921 | -3.81154250902034 |

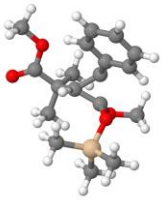
## $D_3^{Est-1,3}$



| | | | |
|---|---|---|---|
| C | -7.21028151962767 | -0.44199710414469 | 0.50273520828400 |
| C | -6.55781183520396 | -1.33583368610409 | 1.36648954402353 |
| C | -6.47947719583920 | 0.32774632761241 | -0.38979715800853 |
| C | -5.15963981084597 | -1.45194791630245 | 1.32065939270469 |
| C | -4.41674610368945 | -0.68820048976712 | 0.43073280064244 |
| C | -5.05559548760349 | 0.23256653051315 | -0.45460954298572 |
| C | -4.35892561768560 | 1.03489082605027 | -1.38842648571747 |
| C | -2.86685171434997 | 1.05505903752691 | -1.56627007494070 |
| C | -2.46520703181084 | 2.49909164033481 | -1.53510642837564 |
| O | -1.84093836343299 | 3.04524439085341 | -0.57760808446739 |
| H | -8.29852766590646 | -0.35242840706632 | 0.53205164619913 |
| H | -7.13531012313119 | -1.94189050536085 | 2.06778790448423 |
| H | -6.99215692808341 | 1.01991690044598 | -1.06239138626435 |
| H | -4.65156292046997 | -2.15378166059199 | 1.98633258886817 |
| H | -3.33452301247374 | -0.81478865882898 | 0.39732345921411 |
| Si | -1.22436318052897 | 2.55597237984894 | 1.05854185002785 |
| C | -2.76498067651118 | 2.21458554841001 | 2.04150415311345 |
| C | -0.32512251602404 | 4.10371231810098 | 1.55049905661514 |
| C | -0.09657820912022 | 1.09616345350613 | 0.79213241040916 |
| H | -3.43990492977277 | 3.08532058415406 | 2.03261984132819 |
| H | -2.48541251965163 | 2.02300482102536 | 3.09150905098649 |
| H | -3.32218859036901 | 1.33827393262642 | 1.67903131246691 |
| H | 0.35844128908006 | 0.83539163502059 | 1.76321497807301 |
| H | 0.72551610180129 | 1.35245994392221 | 0.10473434884339 |
| H | -0.60248006086997 | 0.19715360039197 | 0.40968893734340 |
| H | -1.00532933334691 | 4.96909244865395 | 1.59018090843586 |
| H | 0.49614461164733 | 4.33342389426336 | 0.85319675951229 |
| H | 0.11377337201382 | 3.97618556784950 | 2.55417139903892 |
| C | -2.31817641478918 | 0.27306640196423 | -2.82729486557902 |
| C | -3.13897642458253 | 0.52939867735571 | -4.09259396279059 |
| H | -3.11731961292725 | 1.59260482012989 | -4.36620557456779 |
| H | -4.18188872434021 | 0.21185234800168 | -3.96256985443327 |
| H | -2.72461254823744 | -0.05479145416671 | -4.92580861244069 |
| C | -0.83388408626101 | 0.62460326794761 | -3.05060544624048 |
| H | -0.72769120756260 | 1.66532540425311 | -3.39554001939654 |
| H | -0.40595350285315 | -0.01791599647377 | -3.83438492384344 |
| H | -0.23766696286309 | 0.48359758372720 | -2.13855588919620 |
| C | -2.41524150872208 | -1.22169078187409 | -2.47281578554045 |
| O | -3.02012163313182 | -2.04041688140164 | -3.10938850271239 |
| O | -1.71295951479753 | -1.51762340205793 | -1.35779534973222 |
| C | -1.71331880171905 | -2.89934417655106 | -0.96200490454816 |
| H | -2.73654731101921 | -3.22657906798617 | -0.72657671561889 |
| H | -1.07172069308992 | -2.96099277809096 | -0.07519293302340 |
| H | -1.31631361822320 | -3.52834917771821 | -1.77088734007553 |
| O | -2.81528913114354 | 3.23232708381666 | -2.53755872389041 |
| H | -4.94166462295699 | 1.67277813706477 | -2.05635587258902 |
| C | -2.52330673112480 | 4.65377477458458 | -2.54588188413108 |

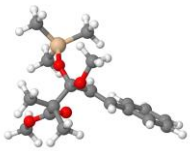
| | | | |
|---|---|---|---|
| H | -1.43735905167737 | 4.80567629824199 | -2.49077988211651 |
| H | -3.01863866188991 | 5.13431264480483 | -1.69189115824974 |
| H | -2.92587657053613 | 5.02290469418597 | -3.49425799879894 |
| H | -2.38821269374585 | 0.59981422729840 | -0.69528219033978 |

## $E_3^{Est\text{-}1,3}$



| | | | |
|---|---|---|---|
| C | -6.96667838042523 | 1.80709535212303 | -0.85207915948106 |
| C | -7.75427741930102 | 1.11261305806711 | 0.07162867139055 |
| C | -5.65072067505106 | 1.40613749847528 | -1.09473816343695 |
| C | -7.21658990859682 | 0.01579041752565 | 0.75179083004354 |
| C | -5.89952683967402 | -0.38277350034141 | 0.50845930443371 |
| C | -5.10319689570154 | 0.30554866064402 | -0.41864609070400 |
| C | -3.70171485343205 | -0.13628175157599 | -0.69189685532086 |
| C | -2.71305304195181 | -0.33673134263084 | 0.45173092892041 |
| C | -2.52581099803308 | 0.79087149770946 | -0.52181366429287 |
| O | -2.79470213350636 | 2.08697369730803 | -0.14011658431815 |
| H | -7.37851659201185 | 2.67007537573920 | -1.38219373194679 |
| H | -8.78335526281431 | 1.42781542400973 | 0.26296464958004 |
| H | -5.02936479260189 | 1.95998941541174 | -1.80157159648494 |
| H | -7.82607204793751 | -0.53125415672947 | 1.47626098061471 |
| H | -5.47050308168998 | -1.23767472296110 | 1.03511008227811 |
| Si | -1.90979646539256 | 3.03904870796084 | 0.95362065676265 |
| C | -2.17253892292569 | 2.40819972612034 | 2.70541967437112 |
| C | -2.65204734542863 | 4.74599438698521 | 0.74366824048225 |
| C | -0.08695408982481 | 3.00959231263407 | 0.50375628663898 |
| H | -3.24784060324518 | 2.30583696227422 | 2.92539022970005 |
| H | -1.74211986325305 | 3.11306101481865 | 3.43664603363286 |
| H | -1.69446596767981 | 1.42946374379686 | 2.86636127739189 |
| H | 0.48767164532607 | 3.68199468966284 | 1.16304252910952 |
| H | 0.06795064078609 | 3.33588817997693 | -0.53714854484293 |
| H | 0.32771885373702 | 1.99497975967330 | 0.60426107958390 |
| H | -3.73514990825372 | 4.72313049234556 | 0.94608803790913 |
| H | -2.50727244873844 | 5.11471769626893 | -0.28475959961677 |
| H | -2.18826251230627 | 5.46909792657662 | 1.43484759607232 |
| C | -1.76452356066023 | -1.53747968326367 | 0.60377859412337 |
| C | -1.59612365879661 | -2.36291836563696 | -0.68609024679566 |
| H | -1.17626078729239 | -1.73397486052287 | -1.48159107473335 |
| H | -2.55601497562356 | -2.77794382911383 | -1.02131232551389 |
| H | -0.90753689542867 | -3.20327740165300 | -0.50423061240850 |
| C | -0.39931226294201 | -1.04110456498968 | 1.10083177553913 |
| H | 0.05450083326211 | -0.40222617861318 | 0.33102582915464 |
| H | 0.27231173614062 | -1.88496059129674 | 1.31588978258668 |
| H | -0.50442780216805 | -0.46207725423284 | 2.03004018885530 |
| C | -2.37859672686705 | -2.44653351799975 | 1.67272604062728 |
| O | -1.87743890556380 | -2.72730204740276 | 2.73378005330609 |
| O | -3.58834597409114 | -2.91453562578398 | 1.29560214571240 |
| C | -4.24831742168077 | -3.77473338568184 | 2.22277329237214 |
| H | -5.20415497522966 | -4.04867570710853 | 1.75885548325748 |
| H | -4.42032620898615 | -3.25948804037161 | 3.18014281303583 |
| H | -3.64508897568177 | -4.67459435528227 | 2.41748248034046 |
| O | -1.46330489940240 | 0.67782697890256 | -1.40838930208167 |
| H | -3.58613118994658 | -0.83835335191337 | -1.52462660508348 |
| H | -3.09909824388460 | 0.02065872953496 | 1.41123504537171 |
| C | -1.68258249071162 | 1.31215984823642 | -2.65409820785075 |
| H | -0.79587794575207 | 1.12405907461271 | -3.27514374544723 |
| H | -1.81952196678497 | 2.39984594821313 | -2.53297322633260 |
| H | -2.57575679198113 | 0.90123765949832 | -3.16070127650580 |

## $D_3^{Est\text{-}1,2}$



| | | | |
|---|---|---|---|
| C | -4.40066737399580 | -2.45394454026630 | 1.77687352909267 |
| C | -4.83788801716650 | -1.79982088968841 | 2.94265516266346 |
| C | -3.40163638092434 | -1.88542722881367 | 1.00520811472764 |
| C | -4.26707448587372 | -0.57323068792365 | 3.33551349895912 |
| C | -3.27259344717973 | 0.00539913834460 | 2.56810956014550 |
| C | -2.81887616441052 | -0.63535927490431 | 1.37437448205264 |
| C | -1.79919211940881 | -0.08736633608382 | 0.54795404641249 |
| C | -1.21577781653899 | 1.16565814595778 | 0.71159338520484 |
| C | -0.12349800518645 | 1.68448491892113 | -0.22958415867172 |
| O | -0.10162464206550 | 3.06136372551549 | -0.25175517925982 |
| H | -4.84772903996485 | -3.40628895682491 | 1.48505178721412 |
| H | -5.62535975309843 | -2.24910709890455 | 3.55268212107814 |
| H | -3.05147894623282 | -2.38423619066917 | 0.09840213926666 |
| H | -4.60930491520468 | -0.08366092491674 | 4.24945804528315 |
| H | -2.81810355652090 | 0.94397930036325 | 2.88763194651126 |
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| C | -2.71832162480165 | 4.29845357646721 | 0.24593867121624 |
| H | 0.95094387721322 | 5.88668313103515 | -0.39117374075492 |
| H | -0.54704571501691 | 6.80940805613796 | -0.10171114262780 |
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| H | -2.98554396504369 | 4.17627541360188 | -0.81617400859163 |
| H | 0.72201106795559 | 4.48417569950968 | 2.38269362865029 |
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| C | 1.47518044398315 | -0.34996893537673 | -0.01844155147407 |
| H | 1.40020213513643 | -0.53638711833540 | -1.09755546198847 |
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| H | 0.72744197401269 | -0.96443227220730 | 0.50306276802975 |
| C | 2.40369370148357 | 1.94895858108705 | -0.44474655006637 |
| H | 2.30008012383855 | 1.83320727897406 | -1.53259953705585 |
| H | 3.38590923409550 | 1.56143205750512 | -0.14069640541929 |
| H | 2.35390023918151 | 3.01705672221750 | -0.20327870784741 |
| C | 1.27100605783291 | 1.32805646611874 | 1.75240967010078 |
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| O | 2.41719234112241 | 1.61511327707119 | 2.31504758006524 |
| C | 2.46261643211605 | 1.72094410960667 | 3.75448445827468 |
| H | 2.13602623931878 | 0.77687033204687 | 4.21177949784815 |
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| H | 3.50821024150054 | 1.93328800065595 | 4.00104209391255 |
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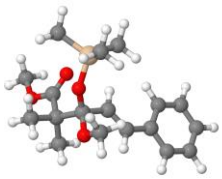

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| C | -1.21639163267023 | 1.02669913746715 | 0.70614096482306 |
| C | -0.04499873804657 | 1.62054836024370 | -0.05457854549735 |
| O | -0.10436934879639 | 3.01316533804656 | -0.08304117396725 |
| H | -5.26030392312035 | -3.24378905290607 | 0.58935472604318 |
| H | -6.14325065331545 | -2.32904792490060 | 2.73854849379407 |
| H | -3.33471305749100 | -2.14501684315323 | -0.53114711724725 |
| H | -5.08154033972677 | -0.30643263078187 | 3.74543052343468 |
| H | -3.16916357105174 | 0.78720164636227 | 2.62879138382008 |
| Si | -0.85946494007797 | 4.34281512469140 | 0.62199881325438 |
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| C | 0.47027664360584 | 5.35536741723433 | 1.47603224841040 |
| C | -2.24168864866678 | 3.92358273377095 | 1.82579506857192 |
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| H | 1.30053134789112 | 5.57166953523710 | 0.78361545051579 |
| H | 0.87155312987127 | 4.80663162894542 | 2.34128227316557 |
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| H | 0.73617729112699 | -0.86320142489730 | 1.08833432638775 |
| C | 2.47554480502043 | 1.86098494196534 | -0.24024525296510 |
| H | 2.40152722724459 | 1.56777140702637 | -1.29554337800630 |
| H | 3.45173747304486 | 1.55118016834017 | 0.15714368750621 |
| H | 2.39455886334494 | 2.95484190331800 | -0.18044036161141 |
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| O | 2.60071560317717 | 1.24736121050084 | 2.55860230338704 |
| C | 2.82164260195408 | 1.63004159272333 | 3.91514142793807 |
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| H | 2.86016898794676 | 2.72618905500807 | 4.00969413417249 |
| H | 3.78443672346298 | 1.19019744549741 | 4.20320319184365 |
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| H | -0.58978854412060 | 2.80390150059132 | -2.50531118304332 |
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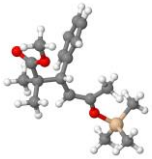
## $D_3^{Ket-1,4}$



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| C | -4.39300914707045 | 1.18572035112381 | 0.21832620585720 |
| C | -2.89196030128476 | -0.71485532699880 | 1.62799614004795 |
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| C | -3.31203650169069 | 1.60568597743010 | 1.01334832360860 |
| C | -2.95297353057389 | 3.08794987306868 | 1.09798397228610 |
| C | -1.48673949783558 | 3.16832320111029 | 0.87646194467834 |
| C | -0.84156373215515 | 2.88861680258569 | -0.34839494909632 |
| O | 0.44950376069535 | 2.95119779548995 | -0.32999306369969 |
| H | -5.58836539651076 | -0.47844368989993 | -0.45297931558873 |
| H | -4.24880304292062 | -2.17546351215531 | 0.79033260020551 |
| H | -4.98129573018810 | 1.92928198612202 | -0.32347538579613 |
| H | -2.30773797435652 | -1.45419251648927 | 2.18021305979516 |
| H | -1.71592639688095 | 0.94462901463798 | 2.33440468205329 |
| Si | 1.78958203642074 | 2.72852987571448 | -1.49350397511695 |
| C | 3.26356328463554 | 2.78951113495318 | -0.36581540369031 |
| C | 1.67693670202166 | 4.17733168627963 | -2.66445639968501 |
| C | 1.53286912282588 | 1.06246072880854 | -2.29555137320812 |
| H | 4.19158117038594 | 2.68297555238642 | -0.95168137054158 |
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| H | 3.31321971076797 | 3.74792369733806 | 0.17475775490150 |
| H | 1.37234373716038 | 0.27365930391795 | -1.54288896218676 |
| H | 0.69646596525173 | 1.04858357738798 | -3.01016124293438 |
| H | 2.44721135772066 | 0.79961546577132 | -2.85459860817837 |
| H | 0.78861503730909 | 4.14367504373234 | -3.31390323680314 |
| H | 2.56325291660411 | 4.17124278586819 | -3.32171555511941 |
| H | 1.67765549787770 | 5.13309315929351 | -2.11663008673161 |
| C | -3.45139737687367 | 3.83034137834004 | 2.37828138206682 |
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| H | -3.50616957538889 | 5.89060474844992 | 3.10275896235879 |
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| C | -4.98070398803159 | 3.68528242985709 | 2.42888567241800 |
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| O | -5.55070578613701 | 4.06399046726609 | 1.26839359355149 |
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| H | -7.26903789938324 | 4.36893938734274 | 0.22412386033956 |
| H | -3.46487783666404 | 3.57397476228806 | 0.25144836317852 |
| C | -1.55846212693072 | 2.52562959138515 | -1.60704196048454 |
| H | -0.80955801428063 | 3.38643554623380 | 1.70719224717493 |
| H | -1.46858073934170 | 1.43874316673047 | -1.77293757617758 |
| H | -1.10432609302935 | 3.03543163842303 | -2.46888014559189 |
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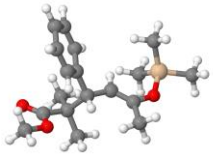
**$E_3^{Ket\text{-}1,4}$**



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| C | -2.78927318584219 | 2.82500587758338 | 0.68695937695114 |
| C | -1.41569223306554 | 2.72455375616377 | 0.08208376054308 |
| C | -1.10258150284692 | 2.77296911279780 | -1.22718867550976 |
| O | 0.17233738495841 | 2.64118969787925 | -1.68606187730696 |
| H | -5.63781545333723 | -0.56665614263215 | 2.23280151177285 |
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| H | -5.06315708843990 | 1.34929425770275 | 0.76360517697956 |
| H | -1.76060076892004 | -0.27646103632164 | 4.10006138254318 |
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| Si | 1.60005346562617 | 2.15333816800215 | -0.90408552712194 |
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| C | 1.34762717078046 | 0.46088588962673 | -0.12815277319695 |
| C | 2.11752881103769 | 3.43545307575420 | 0.37203786817413 |
| H | 3.84312431163626 | 1.76392364296040 | -1.90959762502813 |
| H | 2.97441015383388 | 3.06379888333855 | -2.76909864768935 |
| H | 2.54408374290502 | 1.35957280241870 | -3.06455862369618 |
| H | 2.13265626196752 | 4.44146022065683 | -0.07874403136282 |
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| H | 2.28576860561153 | 0.10488846400818 | 0.33006930955497 |
| H | 1.04614156841165 | -0.27159421627631 | -0.89478103149674 |
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| H | -0.59407417914456 | 2.58438191918685 | 0.78523517057462 |
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| H | -1.77651113657499 | 3.89250017476853 | -2.91927940768584 |
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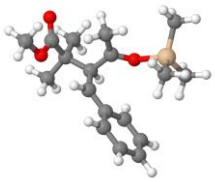
**$D_3^{Ket\text{-}1,3}$**



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| O | -2.68781300691716 | -2.00129964935892 | -2.54366074874553 |
| C | -2.39781953223859 | -2.09112756252735 | -3.94920438209556 |
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| H | -1.87059883761565 | -1.18931855734981 | -4.29430959008646 |
| C | -1.64359849285340 | 1.09395203964146 | -1.40498463454996 |
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| H | -2.11438767892233 | 0.56294380110653 | -2.23957948529476 |
| H | -0.57967487380827 | 0.79476330769639 | -1.39888411148104 |
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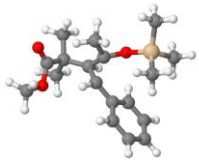
**$E_3^{Ket-1,3}$**



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| C | -6.49586472516645 | 1.13827309112839 | 1.63087507921053 |
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| C | -4.87362868818516 | 0.65285843734994 | -0.12149081457266 |
| C | -3.52014571387074 | 0.26261751591991 | -0.59306617795666 |
| C | -2.55506651022780 | -0.58182979492670 | 0.21348502557960 |
| C | -2.23150133160402 | 0.86754005706701 | -0.01015221824478 |
| O | -2.36375416833963 | 1.63926964596522 | 1.14099397922179 |
| H | -7.83246172418884 | 1.77554801525163 | -1.43691698849619 |
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| H | -6.74699475383773 | 1.17243948233447 | 2.69444709503088 |
| H | -4.50313822546350 | 0.41247943185176 | 1.99750467485132 |
| Si | -2.67032970486889 | 3.29587067059792 | 1.29674147018710 |
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| C | -3.83198738586517 | 3.92340505346256 | -0.04197060461731 |
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| O | -2.82837729897528 | -2.12763062005990 | -2.43786953686060 |
| C | -2.79483642043020 | -2.16878000669243 | -3.86378126642088 |
| H | -3.80927304795147 | -2.43494130485870 | -4.18538537911727 |
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| C | -1.14827137343884 | 1.34443622170941 | -0.95085119550796 |
| H | -3.47526287741518 | 0.10913243813120 | -1.67375820293707 |
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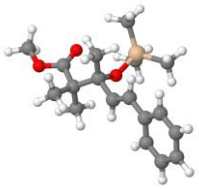
**$D_3^{Ket-1,2}$**



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| C | -4.38757593676593 | -0.58787038592708 | 0.58148186573521 |
| C | -4.05661093081451 | -1.15048161697085 | 3.31210556994560 |
| C | -3.04114348193660 | -0.50579262713516 | 2.62807732503694 |
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| C | -2.17280059107829 | 0.46081440201965 | 0.47524798653454 |
| C | -0.91823375038507 | 0.81044710136646 | 0.92683038557871 |
| C | 0.10598796787819 | 1.60332590176941 | 0.14249401457835 |
| O | -0.24459682765351 | 2.81309118764179 | 0.78794536166384 |
| H | -6.31996091726372 | -1.52091096110102 | 0.76011647829275 |
| H | -6.03528735511370 | -2.02755292656903 | 3.18610057321294 |
| H | -4.50430658293195 | -0.36278104354684 | -0.48134781370200 |
| H | -3.94518644214599 | -1.37296443499264 | 4.37520112640605 |
| H | -2.13365167753676 | -0.21921788557531 | 3.16110459292765 |
| Si | -0.91853490456175 | 4.37365548032673 | 0.40719943453445 |
| C | -0.58556551547641 | 4.89630572748531 | -1.35530543694384 |
| C | -0.05501591561774 | 5.46522631085398 | 1.64854336931161 |
| C | -2.75494479246131 | 4.18272766544270 | 0.74476549592341 |
| H | 0.48721084628960 | 4.81604338137429 | -1.58254240098397 |
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| H | -3.26809311003929 | 5.15298512578457 | 0.64100200110126 |
| H | -2.93521184047703 | 3.81044389983733 | 1.76578192426357 |
| H | -3.21900696377350 | 3.48189921631458 | 0.03119196900287 |
| H | 1.02790994651440 | 5.46468198751324 | 1.44973562195625 |
| H | -0.22475087319090 | 5.11370075557482 | 2.67833898176169 |
| H | -0.42357055183293 | 6.50165314122198 | 1.57348754483693 |
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| C | 1.83025646526024 | 1.30301767214790 | 2.03417311778629 |
| H | 1.33705691602353 | 0.47213434599835 | 2.56179021897414 |
| H | 2.90741678315423 | 1.20758845880300 | 2.23109087748324 |
| H | 1.47832964463243 | 2.25641681445816 | 2.44964513594152 |
| C | 1.90283326335184 | -0.18720593498181 | 0.00552334786186 |
| H | 1.14772507932785 | -0.90228859725892 | 0.37382727479940 |
| H | 2.88328711717288 | -0.50969701653823 | 0.37881007108202 |
| H | 1.93024092713392 | -0.24791555919221 | -1.09112082895065 |
| C | 2.50425697696801 | 2.28737564783783 | -0.10299267592385 |
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| O | 3.72667727345991 | 1.81104906785231 | -0.32244081218725 |
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| H | 4.39635822356142 | 3.14979310396189 | -1.78212821274124 |
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| H | -2.42906884201835 | 0.67488542955387 | -0.56518538381779 |
| C | -0.13977037863554 | 1.60905575098652 | -1.36363738034731 |
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| H | -0.05961600162004 | 0.59202977479283 | -1.77049568238874 |
| H | 0.58808070566721 | 2.25157078921516 | -1.87154160884301 |
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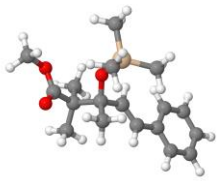
## $E_3^{Ket\text{-}1,2}$



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| C | -3.12009506991681 | -0.12220548247895 | 2.71953493974606 |
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| C | -1.01846621663066 | 1.05378586473991 | 0.85897355240171 |
| C | 0.03995059365409 | 1.68827509071733 | -0.01854993408301 |
| O | 0.30233852630219 | 2.98795671907842 | 0.50372988007089 |
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| H | -5.90002192974273 | -1.94689003334311 | 3.49528028913407 |
| H | -4.05090002450430 | -1.28067922341061 | -0.34425632793078 |
| H | -4.14384381059006 | -0.53492314043546 | 4.56972108081287 |
| H | -2.36034929686204 | 0.49117278688046 | 3.20825184373151 |
| Si | -0.54411726721572 | 4.44127282825952 | 0.44862707958266 |
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| C | 0.26166272587984 | 5.46968592191673 | 1.79479165754460 |
| C | -2.37341084831893 | 4.17798197863490 | 0.80386809307354 |
| H | 0.76788342396092 | 5.29358031417762 | -1.48694019958795 |
| H | -0.66645956578277 | 6.31454688629868 | -1.19505862891845 |
| H | -0.83637833113704 | 4.74980209805383 | -2.03016536279459 |
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| H | -2.52238808522466 | 3.68677036402066 | 1.77890970284461 |
| H | -2.85365000409381 | 3.54716491707932 | 0.03950461237930 |
| H | 1.34529737153177 | 5.55698200583606 | 1.61285112632785 |
| H | 0.12373025132729 | 5.00067390766686 | 2.78250389268554 |
| H | -0.16323746846422 | 6.48639150947749 | 1.83399497289780 |
| C | 1.42443914463858 | 0.91937805935429 | 0.15051629942125 |
| C | 1.71023371696663 | 0.65365955109006 | 1.63679547062863 |
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| H | -0.90681023501829 | 1.30617370062806 | 1.91608157001027 |
| H | -0.57206307217652 | 0.78483817950798 | -1.91689856761105 |
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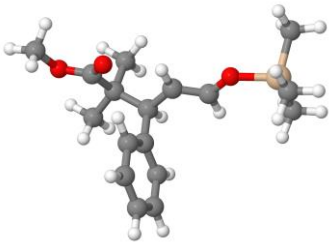

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| C | -1.79211723539999 | -1.06089895397743 | 2.62982233120507 |
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| C | -2.54367927592112 | 1.01245517984019 | 1.59936731782384 |
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| C | -1.13043601191070 | 2.78746451480784 | 1.11547333362747 |
| C | -0.69907143572824 | 2.69350900599603 | -0.20644588427193 |
| O | 0.54016467905530 | 2.85523577332659 | -0.51638522782513 |
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| H | -2.59549919351627 | -2.88512675478920 | 1.78691628021095 |
| H | -3.90330462873046 | 0.77595457014393 | -0.07613960973843 |
| H | -1.19752813574119 | -1.57799300023222 | 3.38608248037070 |
| H | -1.14443704098363 | 0.89900723776335 | 3.25805405476885 |
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| C | 2.10139436225139 | 4.51989452518730 | -2.23354227205349 |
| C | 0.06107434337399 | 2.43414795977574 | -3.36877264987148 |
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| H | 2.13912168696015 | 0.48154813081432 | -1.69413531056895 |
| H | 3.28820897796668 | 1.66977634827739 | -1.01149743508981 |
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| H | 0.53280384756651 | 2.38951805853467 | -4.36508671640996 |
| H | 1.31751839923647 | 5.29262122354986 | -2.27556437690829 |
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| H | -3.19040221182191 | 2.77603089516892 | 0.62624682576775 |
| H | -1.42060501622239 | 2.48532714510774 | -1.01267395778434 |
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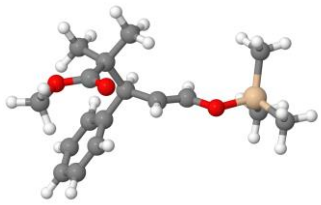
**$E_4^{Ald-1,4}$**



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| C | -3.29222620704432 | 1.43167870837845 | 1.40643788789928 |
| C | -2.56154967707918 | 2.72054859539717 | 1.04867939404548 |
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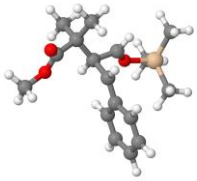
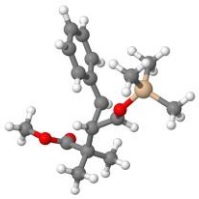
| C | -0.47672757035460 | 2.60173927863490 | -0.31166110817542 |
| O | 0.84795142178674 | 2.38500671935822 | -0.48855372227651 |
| H | -6.11345619852199 | -0.31852815049603 | 0.56730946828105 |
| H | -5.23499717731293 | -1.83707582303903 | 2.34488644747119 |
| H | -4.87718061752280 | 1.75000370863289 | -0.02369174425803 |
| H | -3.09762972782230 | -1.26583948914741 | 3.50325043844342 |
| H | -1.86578759055691 | 0.79238502931472 | 2.90309730453418 |
| Si | 1.76392693578274 | 2.80800979045853 | -1.85330499004171 |
| C | 3.48688034768099 | 2.18554373038258 | -1.47967541403024 |
| C | 1.71878806687972 | 4.67629268280298 | -2.04807541144479 |
| C | 1.03448749540514 | 1.96306556920082 | -3.36627276544202 |
| H | 4.17748613048881 | 2.41642000003482 | -2.30765560420872 |
| H | 3.48513346054779 | 1.09395261659682 | -1.32918230347452 |
| H | 3.88140951324923 | 2.65412650835545 | -0.56372544653680 |
| H | 1.01067486625541 | 0.86950998211980 | -3.23014668911387 |
| H | 0.00495227169509 | 2.30204974198353 | -3.56780394033912 |
| H | 1.63686521457061 | 2.18168576958422 | -4.26408071539836 |
| H | 0.68796037632137 | 5.03464138597753 | -2.20529691010362 |
| H | 2.32322042052454 | 5.00324566987023 | -2.91075637555892 |
| H | 2.11386337281508 | 5.17171572267401 | -1.14618843619720 |
| C | -2.91068013436770 | 3.90378646439649 | 2.04661719045850 |
| C | -2.04536985230345 | 5.12920680376483 | 1.71308846299271 |
| H | -2.16886181421221 | 5.39999072859560 | 0.65249745870640 |
| H | -2.34926198167747 | 5.99281269324997 | 2.32610043346774 |
| H | -0.98301047943020 | 4.92854111502829 | 1.89768295802350 |
| C | -4.39610644814540 | 4.26576400768305 | 1.91846327846692 |
| H | -4.60236933832542 | 4.62028679042497 | 0.89564919809149 |
| H | -4.66354816458804 | 5.07113766253835 | 2.61881857365178 |
| H | -5.04808423361268 | 3.40908439760752 | 2.12925475405753 |
| C | -2.55480673452935 | 3.43529264287708 | 3.45870307838559 |
| O | -1.42517324745329 | 3.31226663565549 | 3.87480559219626 |
| O | -3.63457919004218 | 3.12747514589114 | 4.19608408351855 |
| C | -3.38479375460443 | 2.57214385541296 | 5.48517110731655 |
| H | -2.74264391000154 | 3.23702578752371 | 6.08170513836465 |
| H | -2.88769028580977 | 1.59450936596394 | 5.39037240254779 |
| H | -4.36576265740566 | 2.45109031151762 | 5.96111371947984 |
| H | -2.96250335639663 | 3.05924553929248 | 0.07854078746228 |
| H | -1.05414183043639 | 2.85291469831711 | -1.21509847824878 |
| H | -0.47773230299402 | 2.26991618448864 | 1.75646597636982 |

**$D_4^{Ald-1,3}$**



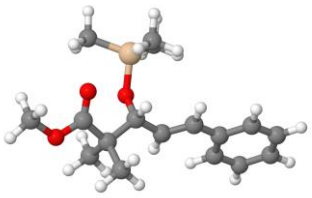
| | | | |
|---|---|---|---|
| C | -7.25166101360923 | 1.25618070595556 | -0.70117208026336 |
| C | -7.53474757498806 | 1.48865708521444 | 0.65423937379226 |
| C | -6.04845346055932 | 0.67173031151586 | -1.06590718276138 |
| C | -6.60478278411451 | 1.12730661846140 | 1.64369551445285 |
| C | -5.39812708291984 | 0.54160160049906 | 1.29104246140024 |
| C | -5.08614216845860 | 0.30033005808203 | -0.07926207994624 |
| C | -3.86802772185095 | -0.28815803522545 | -0.50568622840147 |
| C | -2.71495919167504 | -0.65062349211394 | 0.38609754002250 |
| C | -2.15917955626832 | 0.71673192282973 | 0.24632572241984 |
| O | -2.38793670796563 | 1.60328901038288 | 1.13588350539804 |
| H | -7.97947214527280 | 1.53297899869468 | -1.46674473753659 |
| H | -8.48397325670398 | 1.94680555182760 | 0.94151190375131 |
| H | -5.82492956564319 | 0.48669091792835 | -2.11955759672662 |
| H | -6.83687052007114 | 1.30219599092127 | 2.69655629542666 |
| H | -4.68801902350630 | 0.26527654698357 | 2.07040576313389 |
| Si | -2.27740198463131 | 3.39557955993063 | 1.02674934515685 |
| C | -1.79982171140894 | 3.87254777321110 | 2.75549883365883 |
| C | -4.00125230619947 | 3.88640085109345 | 0.51877251093179 |
| C | -0.98032519156654 | 3.74264789431757 | -0.26863316839654 |
| H | -2.54125441875490 | 3.51218339194770 | 3.48601872633188 |
| H | -1.74802244320734 | 4.97072276731738 | 2.84147718879156 |
| H | -0.81333434661595 | 3.46625413101360 | 3.02939789154210 |
| H | -0.81742965406331 | 4.83216380026616 | -0.32885123371113 |
| H | -1.28310227009950 | 3.40909461759618 | -1.27438546993930 |
| H | -0.01119393086266 | 3.28236950348358 | -0.01655961907294 |
| H | -4.74341624164901 | 3.57366736369195 | 1.26892928744673 |
| H | -4.27959190140351 | 3.43816169794161 | -0.44829327708270 |
| H | -4.06200488013309 | 4.98260554615915 | 0.41275957779656 |
| C | -1.82241040366384 | -1.83359515174986 | -0.07974376159745 |
| C | -1.17877366457311 | -1.61400191036885 | -1.45305037260952 |
| H | -0.44632572983194 | -0.79282798987010 | -1.42360602797236 |
| H | -1.91778328419700 | -1.41106789675873 | -2.24192868018484 |
| H | -0.64706954865483 | -2.52541158846315 | -1.75606437325623 |
| C | -0.73462601600955 | -2.06442414983367 | 0.98864749390150 |
| H | -0.08717794247513 | -1.17669882069820 | 1.07571869319068 |
| H | -0.09883914171655 | -2.91718698013950 | 0.70834887797011 |
| H | -1.17787678295697 | -2.27339432248705 | 1.97255026624944 |
| C | -2.72800919222554 | -3.07560737077820 | -0.14479377596183 |
| O | -2.79063145244992 | -3.82925416327940 | -1.08033494216148 |
| O | -3.43960912807463 | -3.21578631698591 | 0.98386234750041 |
| C | -4.30317908585779 | -4.36083415705086 | 1.05880472847356 |
| H | -4.79406881670823 | -4.30705919918829 | 2.03733119899263 |
| H | -3.71778555857707 | -5.28725976343817 | 0.97083769501855 |
| H | -5.04659317943035 | -4.33341362911146 | 0.24893645648124 |
| H | -1.61565021463101 | 0.99775870254809 | -0.66757713409807 |
| H | -3.72697929176489 | -0.43711929970220 | -1.57973102574770 |
| H | -3.04190851199918 | -0.81357868257161 | 1.41911356819572 |

**$E_4^{Ald-1,3}$**



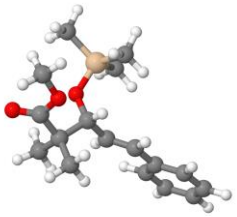
| | | | |
|---|---|---|---|
| C | -7.18500922466348 | 1.06638543921201 | -0.23986656549899 |
| C | -7.39061384609860 | 1.35085814149206 | 1.11315639246421 |
| C | -5.93353336285501 | 0.63419184151718 | -0.68335390984018 |
| C | -6.33390998636006 | 1.18654172111484 | 2.01399002449887 |
| C | -5.08382609715880 | 0.74978140756371 | 1.57034621489420 |
| C | -4.85972723519353 | 0.47372945052414 | 0.20906039456985 |
| C | -3.53440491387671 | 0.06760864811682 | -0.32572184074270 |
| C | -2.51277805259499 | -0.69030998595426 | 0.50262246434357 |
| C | -2.23211287736403 | 0.72822494620111 | 0.13636511458495 |
| O | -2.26093241665690 | 1.66394519174532 | 1.15235942236375 |
| H | -8.00275458082772 | 1.18379236618892 | -0.95583547317080 |
| H | -8.36728177870560 | 1.69375504511316 | 1.46366651306612 |
| H | -5.77893972978829 | 0.42293532946878 | -1.74499715190691 |
| H | -6.48252750543799 | 1.40152798389750 | 3.07568231701136 |
| H | -4.26826034336028 | 0.64454429942188 | 2.28545528090085 |
| Si | -2.48695020877826 | 3.33111326054657 | 0.93857812939064 |
| C | -2.99533145180946 | 3.95544868620661 | 2.62912737413464 |
| C | -3.80299924211122 | 3.67691109845003 | -0.35653932261079 |
| C | -0.84232189949629 | 4.07064809015292 | 0.39995896298551 |
| H | -3.97104972927599 | 3.53151485924661 | 2.91589583653468 |
| H | -3.08294161917873 | 5.05451781531388 | 2.63696197671551 |
| H | -2.25601302946301 | 3.66557314344496 | 3.39323541731809 |
| H | -0.91302415118427 | 5.16648573572937 | 0.29588265979388 |
| H | -0.52139780026130 | 3.66474457919634 | -0.57412205700496 |
| H | -0.05232437399277 | 3.84808502496780 | 1.13576368969064 |
| H | -4.79071518734134 | 3.31622474374629 | -0.03283633837008 |
| H | -3.56299404444261 | 3.18637328345852 | -1.31391497845226 |
| H | -3.87229067491930 | 4.76189236668615 | -0.54424716243307 |
| C | -1.76822858308410 | -1.91131044294791 | -0.06029330938421 |
| C | -1.02949215196371 | -1.61960552792790 | -1.37050601189556 |
| H | -0.20737309211332 | -0.91016905640164 | -1.19583832834736 |
| H | -1.69751307042965 | -1.21018368936235 | -2.14123812023344 |
| H | -0.60312039891714 | -2.54733311511813 | -1.77857182261036 |
| C | -0.77567281563492 | -2.42391308476080 | 0.99886215370049 |
| H | -0.03814652637180 | -1.63786037081935 | 1.22447974769818 |
| H | -0.23290890194317 | -3.31161324827029 | 0.63655502966729 |
| H | -1.29394769417773 | -2.69210636996511 | 1.92971839910291 |
| C | -2.86051527128937 | -2.95038582693485 | -0.33156894381179 |
| O | -3.20885022486267 | -3.33041994363387 | -1.42322481862879 |
| O | -3.44879792635591 | -3.35962997173746 | 0.80816455268589 |
| C | -4.56699667503816 | -4.23342412817022 | 0.66314775323943 |
| H | -4.91113807151812 | -4.46218556164147 | 1.67944209161930 |
| H | -4.27784648003126 | -5.15664049778189 | 0.13838524286257 |
| H | -5.36882449775647 | -3.74272827886343 | 0.09043792446220 |
| H | -1.49801325571862 | 0.92388567937654 | -0.65573948398998 |
| H | -3.55412741034069 | -0.18845783218087 | -1.38949868110242 |
| H | -2.80760158925663 | -0.81649324562827 | 1.54811323973507 |

**$D_4^{Ald-1,2}$**



| | | | |
|---|---|---|---|
| C | -5.43481704322734 | -1.11860745121272 | 0.76690757398093 |
| C | -5.39281540013651 | -1.60389078294253 | 2.08662713200752 |
| C | -4.35501230452985 | -0.41543193869011 | 0.26050879603971 |
| C | -4.2634875210451 | -1.37995699330024 | 2.89870999459267 |
| C | -3.1804714138173 | -0.67929831841322 | 2.40019215171484 |
| C | -3.2003075012196 | -0.17619837169713 | 1.06358449559135 |
| C | -2.11464928046163 | 0.55696599267891 | 0.49217917892109 |
| C | -0.89380675660447 | 0.80922667713175 | 1.08383227412670 |
| C | 0.15131607015623 | 1.65959653367278 | 0.43027961205239 |
| O | -0.17281789228286 | 2.85037869954335 | 1.11762959789605 |
| H | -6.31607178428603 | -1.29650637121475 | 0.14750881716331 |
| H | -6.24482358955916 | -2.15870633309557 | 2.48713193392211 |
| H | -4.37644385910607 | -0.03471924539170 | -0.76339739888225 |
| H | -4.24701026364460 | -1.75886902216046 | 3.92249379821900 |
| H | -2.31274726885653 | -0.50529592389103 | 3.03782001542177 |
| Si | -0.88892416037708 | 4.31059040555848 | 0.48497636629736 |
| C | -1.24088982906904 | 4.07762039743682 | -1.33638336424294 |
| C | 0.38324600708228 | 5.63348825437098 | 0.83212348027353 |
| C | -2.45061665251068 | 4.52683952524785 | 1.49424356517323 |
| H | -0.31380314510406 | 3.85258195429418 | -1.88493199884228 |
| H | -1.65887079896077 | 5.01263522536450 | -1.74568669637971 |
| H | -1.97954311719984 | 3.28269576226165 | -1.53104964498751 |
| H | -2.95461657223325 | 5.47091661275609 | 1.22925507095339 |
| H | -2.22441075706051 | 4.55572543266772 | 2.57207627297158 |
| H | -3.15926104010534 | 3.70225808688354 | 1.31161900060421 |
| H | 1.29266678409515 | 5.44113489522372 | 0.24434366671894 |
| H | 0.64418031408579 | 5.66163470691663 | 1.90160109999099 |
| H | -0.02322790934874 | 6.61959485132386 | 0.55096726732487 |
| C | 1.61647875016651 | 1.24398757014084 | 0.63544606783637 |
| C | 2.01333821158261 | 1.22567127535970 | 2.12065524018432 |
| H | 1.46950815391795 | 0.43583645745843 | 2.66263037920945 |
| H | 3.08615475970357 | 1.01568122710134 | 2.21918194356911 |
| H | 1.79748418460426 | 2.19070565232989 | 2.60037514242445 |
| C | 1.83441390700536 | -0.13718771137687 | -0.00963383413958 |
| H | 1.21496182857861 | -0.89910292812588 | 0.49167286826588 |
| H | 2.88602816419065 | -0.44008306859573 | 0.08619342639205 |
| H | 1.57473147212109 | -0.13165114157409 | -1.08024847781179 |
| C | 2.45986688334947 | 2.28442302504251 | -0.11583305131513 |
| O | 1.99648908716242 | 3.18106851433282 | -0.78722259763399 |
| O | 3.76243192415112 | 2.07498291934698 | 0.04139726526935 |
| C | 4.65662174339444 | 2.97650733329294 | -0.63079163694006 |
| H | 4.50509047307855 | 4.00372563731345 | -0.26898775753244 |
| H | 4.48209043631491 | 2.94955685837248 | -1.71592397077684 |
| H | 5.66839126393117 | 2.62981724204723 | -0.39267008398596 |
| H | -2.26377878393850 | 0.92950150062138 | -0.52706905796627 |
| H | -0.04019602939309 | 1.75446215219801 | -0.64898874244792 |
| H | -0.69643973686798 | 0.50405422339118 | 2.11390481877615 |

**$E_4^{Ald-1,2}$**



| | | | |
|---|---|---|---|
| C | -5.00760136290448 | -0.69905725078615 | 0.80737087933457 |
| C | -5.43614746754608 | -0.44199017004233 | 2.11183119602730 |
| C | -3.71579399186141 | -0.34528201498387 | 0.41331806340542 |
| C | -4.56062189768823 | 0.17142137641678 | 3.01649740655167 |
| C | -3.27124531731721 | 0.52236432446657 | 2.62238048413376 |
| C | -2.82258439113110 | 0.26977495293530 | 1.31034465076714 |
| C | -1.47551498076505 | 0.62712910634241 | 0.84352359447843 |
| C | -0.48631877503170 | 1.18878337080301 | 1.55731669520911 |
| C | 0.84859800468008 | 1.55591701894859 | 0.97760541436039 |
| O | 1.15349915550217 | 2.90948985509856 | 1.27133948956524 |
| H | -5.68224602126426 | -1.17667069140786 | 0.09225046246152 |
| H | -6.44666563384482 | -0.71634860391821 | 2.42452124197802 |
| H | -3.38544477237747 | -0.54759756181121 | -0.60944919333030 |
| H | -4.88833577658673 | 0.37763201230887 | 4.03869465589216 |
| H | -2.60363124958982 | 1.00123692254183 | 3.34163410424910 |
| Si | 0.47487924587242 | 4.25328978905206 | 0.50597370524339 |
| C | 1.74685361369633 | 5.61256221789937 | 0.72048300781839 |
| C | -1.14846031450258 | 4.71135441639027 | 1.33618384072640 |
| C | 0.19543217007660 | 3.84738997387163 | -1.31077876668022 |
| H | 1.97033527195087 | 5.76755041752580 | 1.78855369597624 |
| H | 1.38817327701776 | 6.56842265614632 | 0.30394094879149 |
| H | 2.69011834923949 | 5.34828436266029 | 0.21533123535988 |
| H | -0.10529518106409 | 4.74857834869153 | -1.87067426774194 |
| H | -0.59994002020815 | 3.09499411404741 | -1.43769277100466 |
| H | 1.11684860169322 | 3.45112683866961 | -1.76815037917862 |
| H | -0.99558317890834 | 4.89944333024973 | 2.41174420282086 |
| H | -1.88616856098656 | 3.89916622664561 | 1.23496481533658 |
| H | -1.58035626541124 | 5.62348225738861 | 0.89055223243934 |
| C | 2.03455611092360 | 0.70167311028486 | 1.50717389472362 |
| C | 2.11630516021299 | 0.73857647739610 | 3.03596054825498 |
| H | 1.27100200815597 | 0.19118850645148 | 3.47930351228150 |
| H | 3.05124748060632 | 0.27604417246063 | 3.38077418979473 |
| H | 2.09976535012811 | 1.77670679917632 | 3.39618918663846 |
| C | 1.91247391131333 | -0.74487634843840 | 0.99689111897190 |
| H | 0.98409903379439 | -1.20080708011219 | 1.37337948582003 |
| H | 2.76089963549792 | -1.35152224484636 | 1.34983404047340 |
| H | 1.89604972679529 | -0.78081376634814 | -0.10265815193118 |
| C | 3.31148590945199 | 1.32297936672183 | 0.93076719057948 |
| O | 4.30011668929678 | 1.60914364829145 | 1.55736079147078 |
| O | 3.22312215271494 | 1.49355274407848 | -0.40696075062348 |
| C | 4.35028981163927 | 2.09691700121891 | -1.03582897423069 |
| H | 5.25901002814751 | 1.49735463996103 | -0.87420672830316 |
| H | 4.52502988722128 | 3.10596286597754 | -0.63117838908754 |
| H | 4.11355103630011 | 2.15144858660803 | -2.10601516225749 |
| H | -1.27879425986539 | 0.40485560480201 | -0.21259362160957 |
| H | 0.81210098979555 | 1.40423410076402 | -0.11435724662536 |
| H | -0.62784319286958 | 1.44813421940186 | 2.61074442066896 |

## *2.2 Computational investigation of the radical addition step*

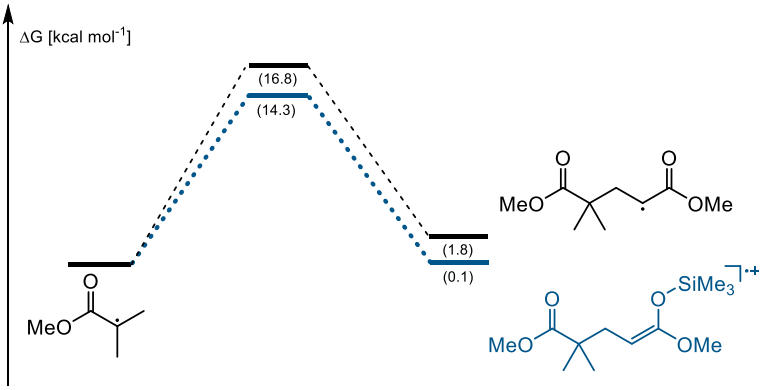
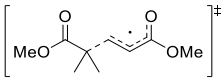
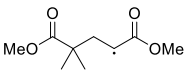
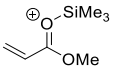
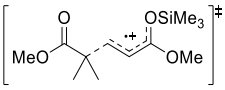
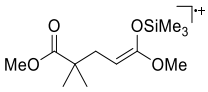



**Figure S4:** Potential energy curves for the radical addition of α-carbonyl radical **B** to methyl acrylate (black curve) or silyl-activated methyl acrylate (blue curve).

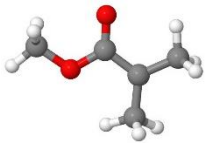
DFT studies show that radical addition to the silylated acrylate **C** is kinetically favored over addition to unactivated acrylate **2**. The difference in free activation enthalpy was calculated to be 2.5 kcal mol$^{-1}$, which would correspond to a relative reaction rate of $k_{rel}$ = 66 at 300 K. Combined with the abovementioned results concerning the feasibility of the subsequent

electron transfer event, radical addition to the activated acrylate **C** can be considered the likely operative reaction mechanism.

**Table S2:** Determination of the free enthalpy for potential reaction intermediates and the respective transition states.

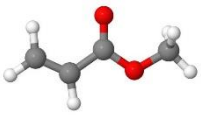
| Structure | Electronic Energy | Thermal + ZPVE | Enthalpy Corr. | Entropy Corr. | Free Enthalpy |
|---|---|---|---|---|---|
|  **B** | −346.54428007 | 0.14107205 | 0.00094421 | −0.04299135 | 346.44525586 |
|  **2** | −306.62273639 | 0.10169984 | 0.00094421 | −0.03671030 | −306.5568264 |
|  **TS 2-$D_{3x}^{Est-1,4}$** | −653.16338441 | 0.24522779 | 0.00094421 | −0.058035595 | −652.97524836 |
|  **$D_{3x}^{Est-1,4}$** | −653.19082012 | 0.24792635 | 0.00094421 | −0.05724446 | −652.99919402 |
|  **C** | −715.85786729 | 0.22284183 | 0.00094421 | −0.05479413 | −715.68887538 |
|  **TS C-$D_3^{Est-1,4}$** | −1062.404250 | 0.36659254 | 0.00094421 | −0.07454183 | −1062.1112552 |
|  **$D_3^{Est-1,4}$** | −1062.429137 | 0.36899381 | 0.00094421 | −0.07475941 | −1062.1339583 |

**B**



| | | | |
|---|---|---|---|
| C | -9.92381487032806 | 1.25118198545217 | 9.17923482959045 |
| O | -9.08522487616576 | 0.94052710992634 | 8.07400885521953 |
| C | -7.88918629060867 | 1.58472455552621 | 8.04210093237488 |
| C | -7.08214689332964 | 1.22926201454310 | 6.88100195737085 |
| O | -7.55396650299071 | 2.37481311763040 | 8.90910467802721 |
| C | -7.54303461824478 | 0.23114083204056 | 5.87349129347305 |
| C | -5.73341806522358 | 1.84604602925684 | 6.74780140379308 |
| H | -7.08539060816194 | -0.75934398488171 | 6.06934083703431 |
| H | -7.22414180768932 | 0.52076000705539 | 4.85781983916798 |
| H | -8.63194329103318 | 0.09760233744531 | 5.89235317146330 |
| H | -4.94762412758537 | 1.06811444825620 | 6.70683179808232 |
| H | -5.52292099064987 | 2.52368828604070 | 7.58479417812192 |
| H | -5.65135297085934 | 2.40922452069524 | 5.79924075653492 |
| H | -10.84224297767821 | 0.66661673481709 | 9.04403167885222 |
| H | -10.15754520738421 | 2.32679185918946 | 9.20844768964218 |
| H | -9.43909590206732 | 0.98206014700670 | 10.13080610125179 |

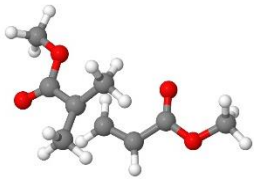
**2**



| | | | |
|---|---|---|---|
| C | -7.31608190363960 | 9.84851892627577 | 7.76823758572351 |
| C | -6.67589476976034 | 9.10550156884770 | 6.86036410154927 |
| C | -5.21036717288592 | 8.87727798507014 | 6.96238132232564 |
| O | -4.48477616460212 | 9.31787498484877 | 7.82307304818450 |
| O | -4.77441890536920 | 8.09813921167428 | 5.95192074632516 |
| C | -3.37818931046201 | 7.81180606375049 | 5.94380947051310 |
| H | -3.07904574126495 | 7.29469367027221 | 6.86855991655710 |
| H | -2.78951161234831 | 8.73837481834991 | 5.86301830984706 |
| H | -3.20085213157084 | 7.16983657709767 | 5.07208233943329 |
| H | -8.39220504476070 | 10.02777876864759 | 7.70683173767806 |

| | | | |
|---|---|---|---|
| H | -6.76118220586310 | 10.29522110786939 | 8.59803535599972 |
| H | -7.18995503747291 | 8.63996631729608 | 6.01596606586359 |

## TS 2-$D_{3x}^{Est\text{-}1,4}$



| | | | |
|---|---|---|---|
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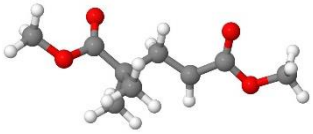
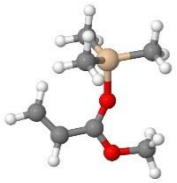
| C | -6.46042347186821 | 10.11320534617481 | 6.94951901011116 |
| C | -5.84326443130556 | 8.84915964949479 | 7.37387422140577 |
| O | -6.10630980278499 | 8.24017874810218 | 8.39110712671088 |
| O | -4.92419686394689 | 8.42201772062427 | 6.47916965825301 |
| C | -4.26013604187943 | 7.20498855675126 | 6.80320841693450 |
| H | -4.98015148967135 | 6.37664509514881 | 6.89258872970065 |
| H | -3.72088244627993 | 7.29369638257028 | 7.75897043141386 |
| H | -3.55536256480218 | 7.01073322380847 | 5.98512009474644 |
| H | -6.15235585963096 | 10.52470227748169 | 5.98638337901357 |
| H | -7.77977460230271 | 11.70961498202545 | 7.50052407591892 |
| H | -7.58478417172462 | 10.31764858393877 | 8.73053209452960 |
| C | -9.40827022521722 | 9.84428533770164 | 7.04540457064191 |
| C | -9.57809713974365 | 10.46829481365036 | 5.69471735873470 |
| C | -10.12984740394059 | 10.50879896572866 | 8.14967521218566 |
| C | -9.16975898941093 | 8.36679937342417 | 7.11158551040580 |
| H | -8.48157765834379 | 8.05054812881400 | 6.31360448896558 |
| H | -10.12324339618371 | 7.82522938550812 | 6.96238023716609 |
| H | -8.75494873202233 | 8.05509924022888 | 8.07773697560844 |
| H | -9.68943666322651 | 11.55815710092241 | 5.76842618318919 |
| H | -10.49445122486617 | 10.07423377829013 | 5.21444446826904 |
| H | -8.73330161214438 | 10.21900668569428 | 5.03464849043547 |
| O | -10.59914453356036 | 11.62874692356757 | 8.09581920594619 |
| O | -10.17433956363152 | 9.75203711155287 | 9.26945711521759 |
| C | -10.79897120485232 | 10.34941396700486 | 10.40177411927313 |
| H | -11.85250070945338 | 10.58642197945921 | 10.18932715760568 |
| H | -10.28727126165706 | 11.28204013378446 | 10.68419340891963 |
| H | -10.72872774324393 | 9.61475058956138 | 11.21361365825351 |

## $D_{3x}^{Est\text{-}1,4}$



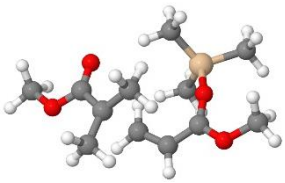
| | | | |
|---|---|---|---|
| C | -6.87627743278359 | 10.50126082477310 | 7.53589336644559 |
| C | -5.96947913467045 | 9.89339090523263 | 6.53241147818793 |
| C | -5.09490098776947 | 8.78986536889914 | 6.88865640369237 |
| O | -5.02835122139608 | 8.27766431010176 | 7.99302755753716 |
| O | -4.34815064225190 | 8.37103714360629 | 5.83820739224442 |
| C | -3.46594504950658 | 7.28597251688346 | 6.10009247488953 |
| H | -4.02202372748187 | 6.39894664128087 | 6.44192480304974 |
| H | -2.73525275666730 | 7.55121697832018 | 6.88000579606294 |
| H | -2.95214685049053 | 7.07069730026594 | 5.15496808988130 |
| H | -5.95426346847448 | 10.23520558820157 | 5.49495063688800 |
| H | -6.90106169390179 | 11.59548071995401 | 7.40578003651955 |
| H | -6.48778438052489 | 10.29685450631800 | 8.54358795414916 |
| C | -8.34498764963673 | 9.98519692653131 | 7.47180244013065 |
| C | -8.99539772179790 | 10.32942174970717 | 6.11810838149830 |
| C | -9.12422809592805 | 10.70792857210071 | 8.57496540621024 |
| C | -8.40491007263981 | 8.46619990603603 | 7.71471563778821 |
| H | -7.89842625363751 | 7.93213909908634 | 6.89671548251089 |
| H | -9.44757683534078 | 8.12307773935537 | 7.75847887172267 |
| H | -7.89851957661918 | 8.19120648619894 | 8.65162115717239 |
| H | -8.97383047612290 | 11.41450112633613 | 5.92889303718867 |
| H | -10.04241975118319 | 9.99706208766422 | 6.09617640115145 |
| H | -8.45853870295386 | 9.82818189945912 | 5.29831374903261 |
| O | -8.68599064353864 | 11.56786396115485 | 9.29899471182992 |
| O | -10.39890201084642 | 10.27825169590560 | 8.64328014387001 |
| C | -11.21979775299558 | 10.89556720277513 | 9.63305333052254 |
| H | -11.29238245452135 | 11.97996463750395 | 9.45935081464032 |
| H | -10.80561355408855 | 10.73320323923953 | 10.63967319804337 |
| H | -12.20786110223061 | 10.42774086710872 | 9.54721124714005 |

## C



| | | | |
|---|---|---|---|
| C | -5.80774904487879 | 10.72742015723054 | 7.15734047529462 |
| C | -5.96566930736320 | 9.48190897248715 | 6.68518050036548 |
| C | -4.86885761214995 | 8.52673565315850 | 6.56250090662783 |
| O | -3.71643299037498 | 8.64024980185613 | 7.06782770946216 |
| O | -5.14363925471443 | 7.48779151952458 | 5.84546276038725 |
| C | -4.14692526689660 | 6.45649660484481 | 5.63572595530395 |
| H | -4.64119893793914 | 5.70136200441812 | 5.01692843647599 |
| H | -3.84326910338352 | 6.03605007647760 | 6.60348896115286 |
| H | -3.27879586643911 | 6.88549679685464 | 5.11821003192626 |
| Si | -2.66774281747440 | 9.28571448188922 | 8.39287125434527 |
| C | -3.77886729656207 | 9.43847842651152 | 9.87747248657520 |
| C | -1.97787333273436 | 10.87547017116943 | 7.71771390455106 |
| C | -1.40861723635033 | 7.92973762556045 | 8.53676883579081 |
| H | -4.55194213300263 | 10.21415995084135 | 9.77948509450075 |
| H | -3.15358075163697 | 9.70484272706217 | 10.74686283731386 |
| H | -4.26962202832016 | 8.48059846340000 | 10.11205349204308 |
| H | -1.86927519498677 | 6.97782745263732 | 8.84361868909936 |
| H | -0.66064979242305 | 8.19787632515629 | 9.30148256596023 |
| H | -0.87303644116229 | 7.77366445485561 | 7.58729855949175 |
| H | -2.72043231598588 | 11.68269260397273 | 7.62697093835870 |
| H | -1.51204677541443 | 10.71675793503653 | 6.73237155084448 |
| H | -1.18880379637176 | 11.23355817889541 | 8.40058489398019 |
| H | -6.65548918816425 | 11.41565688584596 | 7.20231826300786 |
| H | -4.84116333844370 | 11.11072294913066 | 7.48791610873226 |
| H | -6.92689017682723 | 9.12398978118331 | 6.31052478840875 |

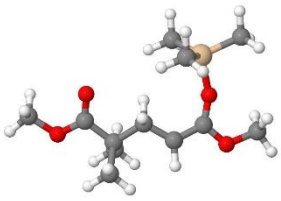
## TS C-$D_3^{Est\text{-}1,4}$



| | | | |
|---|---|---|---|
| C | -7.97958098215399 | 10.80839548191559 | 7.19901252442629 |
| C | -7.49129846138621 | 10.39301657461185 | 5.99085833544390 |
| C | -6.20998502281947 | 9.76817569249415 | 5.84305735429109 |
| O | -5.31507522819918 | 9.67225197977402 | 6.74559707705700 |
| O | -5.97535873241610 | 9.23768228310629 | 4.67480194593984 |
| C | -4.70405743326387 | 8.60746782473153 | 4.41262617559589 |
| H | -4.55664776010674 | 7.76433750138816 | 5.10054118962882 |
| H | -3.89108155437202 | 9.33617302109186 | 4.53444625873162 |
| H | -4.76074226302277 | 8.25988344559557 | 3.37658073433517 |
| H | -8.90616886286133 | 11.38079396470943 | 7.24894051512550 |
| H | -7.35223013784470 | 10.80691316822696 | 8.08876913350949 |
| C | -9.13381213499114 | 8.94883790025142 | 8.11042288384843 |
| C | -10.37821417522637 | 8.92050040854536 | 7.28898263105513 |

| | | | |
|---|---|---|---|
| C | -9.13107971886049 | 9.62329818575745 | 9.43658323835209 |
| C | -8.12441765838927 | 7.86868125934470 | 7.91896899263234 |
| H | -7.93243845777977 | 7.68173526576851 | 6.85189110464266 |
| H | -8.52715706610054 | 6.92665998990349 | 8.33856663350786 |
| H | -7.18705530324671 | 8.07934167134936 | 8.44785133810603 |
| H | -10.95439755477396 | 9.85091658990997 | 7.36456617199588 |
| H | -11.03416001812485 | 8.10801946878797 | 7.66020677727610 |
| H | -10.15684082424280 | 8.69414726710972 | 6.23526809223458 |
| O | -8.17955130877208 | 9.61653342545936 | 10.19444191513540 |
| O | -10.27087760183147 | 10.27392861890734 | 9.68253427940336 |
| C | -10.36460677644568 | 10.95934769755198 | 10.94035752760284 |
| H | -9.57786243478848 | 11.72360721563001 | 11.01978513523495 |
| H | -10.25276520317242 | 10.24819251199136 | 11.77089175101634 |
| H | -11.35759702222402 | 11.42116851275963 | 10.95838724339941 |
| H | -8.09206250072472 | 10.44654391493550 | 5.08131730417763 |
| Si | -4.38646372721960 | 10.47692572616089 | 8.04705807336643 |
| C | -4.86781346103363 | 12.27855474667543 | 8.01613717083207 |
| C | -2.63507311180184 | 10.19819715241324 | 7.48241227573346 |
| C | -4.84011353039450 | 9.54994644050557 | 9.58826374461588 |
| H | -4.82089126634742 | 12.69885875146515 | 6.99883206241989 |
| H | -4.14283346864694 | 12.83571283479536 | 8.63321557776165 |
| H | -5.86709435837926 | 12.47599488907780 | 8.42931041396976 |
| H | -5.90609805553043 | 9.63039075214055 | 9.85186771960726 |
| H | -4.25387910921965 | 9.95518174967680 | 10.43001264300814 |
| H | -4.58009916527917 | 8.48338735854258 | 9.49231316473924 |
| H | -2.42534267077292 | 10.71419522371116 | 6.53204537663580 |
| H | -2.42064892950200 | 9.12538128514387 | 7.35588621142336 |
| H | -1.93217694773145 | 10.59198224808304 | 8.23483130218140 |

**$D_3^{Est\text{-}1,4}$**



| | | | |
|---|---|---|---|
| C | -7.30363860563889 | 10.13301269371410 | 7.25326900516588 |
| C | -6.88458690348338 | 9.45919292670980 | 6.01558715563380 |
| C | -5.51709204899404 | 9.40400282926016 | 5.59933403543109 |
| O | -4.52200992945650 | 9.87818232780751 | 6.23366151575319 |
| O | -5.30798252451875 | 8.81579615667057 | 4.45292203929199 |
| C | -3.96465678690144 | 8.70646717951459 | 3.93580030705828 |
| H | -3.34410477498034 | 8.12644736205607 | 4.63288180833721 |
| H | -3.53548508852228 | 9.70850801971146 | 3.80045483574261 |
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| H | -7.31088241899253 | 11.22736753037860 | 7.05984480019569 |
| H | -6.53724998564213 | 10.01273721418657 | 8.03089399933762 |
| C | -8.67061255367946 | 9.73395719830110 | 7.84058488690272 |
| C | -9.82538373440436 | 10.09622244760800 | 6.89237357028207 |
| C | -8.79986343719328 | 10.53412913084569 | 9.14652782817448 |
| C | -8.69470633594389 | 8.23140130663349 | 8.18110487398170 |
| H | -8.58431947925889 | 7.62480188004606 | 7.26853775905625 |
| H | -9.64819446387554 | 7.96044266942139 | 8.65362955051524 |
| H | -7.88102112912879 | 7.96336963812655 | 8.87379837734239 |
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| H | -10.78948957544120 | 9.83946935391748 | 7.35021072799366 |
| H | -9.74819020969777 | 9.54017767929385 | 5.94507468056809 |
| O | -7.92841535831624 | 11.24393473547677 | 9.59882280487479 |
| O | -9.97694758582283 | 10.33892089288455 | 9.73094988731498 |
| C | -10.21160363590649 | 11.02147565348670 | 10.97283103998056 |
| H | -10.15464283728730 | 12.10939913890555 | 10.82615933950493 |
| H | -9.46316797887956 | 10.72139581464903 | 11.71974320397044 |
| H | -11.21684933152855 | 10.72645815899525 | 11.29222809602440 |
| H | -7.60001079627302 | 9.01323426437363 | 5.32102601801329 |
| Si | -3.81113297224256 | 10.61815908157879 | 7.71699864667470 |
| C | -4.70779819334173 | 12.21396851977813 | 8.05675416681540 |
| C | -2.05855570415457 | 10.85684075039846 | 7.14810021532942 |
| C | -3.99885505280680 | 9.30956568767660 | 9.03087292679416 |
| H | -4.89496742899719 | 12.78069054490513 | 7.13065133746444 |
| H | -4.04629792410989 | 12.83447430295491 | 8.68632672590464 |
| H | -5.65406190302054 | 12.07836556602074 | 8.60134876905906 |
| H | -5.04407736541143 | 9.14852980133112 | 9.33271579617188 |
| H | -3.44966119850619 | 9.63869620316129 | 9.92922297354527 |
| H | -3.56548571487786 | 8.34832827940472 | 8.71403930632379 |
| H | -2.00580396113944 | 11.53946922356413 | 6.28526129706076 |
| H | -1.58870294531496 | 9.90033546440598 | 6.87177859022316 |
| H | -1.46128684398964 | 11.30107087570977 | 7.96145751724471 |

## *2.3 Studies on reaction mechanisms*

All reaction pathways (potential energy curves) are given as relative free enthalpies (in kcal $mol^{-1}$), referenced to starting materials **1**, **A**, and **2**. To account for the entropy change in solution, $(n - m) \times 4.3$ kcal $mol^{-1}$ was subtracted for each change in the number of components (i.e., a reaction from *m* to *n* components).[16]

The electron transfer process of radical cation **D** to product **E** was analyzed computationally building on the Electron-Transfer Marcus-Hush Theory.[17, 18] $\Delta G^{\ddagger}$ is the free enthalpy barrier of the single electron transfer process and was calculated according to equation (2). $\Delta G_0$ is the standard free enthalpy for the reaction and $\lambda$ is the reorganization energy. The reorganization energy can be split into inner-sphere ($\lambda_i$) and outer-sphere ($\lambda_o$) contributions (equation (3)). The inner-sphere contribution was calculated according to the Four-Point Approach to the Electron-Transfer Marcus-Hush Theory (equation (4)).[17] The outer-sphere contribution was calculated according to equation (7), which can be derived from the solvent reorganization

energy of the Born model for the solvation of charged species in a dielectric continuum.[19] Here $r_1$ and $r_2$ are the radii of the reactants and $R$ the sum of them. The effective radius of the molecule, determined by a surfaced based volume calculator to account for the solvent effect on charged species in a dielectric continuum [20], was used to generalize the size of the molecule (using parameters: g = 0.1, p = 0.0). $\varepsilon_{op}$ and $\varepsilon_s$ are the optical and static dielectric constant of the solvent (MeCN: $\varepsilon_{op}$ = 1.344 and $\varepsilon_s$ = 36.6). $q$ is the charge transferred and $z$ the number of electrons transferred in the investigated step.

$$\Delta G^{\ddagger} = \frac{(\lambda + \Delta G_0)^2}{4\,\lambda} \tag{2}$$

$$\lambda = \lambda_i + \lambda_o \tag{3}$$

$$\lambda_i = \sqrt{\lambda_{for}\,\lambda_{back}} \tag{4}$$

$$\lambda_{for} = \lambda_{D\rightarrow D+} + \lambda_{A\rightarrow A-} \tag{5}$$

$$\lambda_{back} = \lambda_{D+\rightarrow D} + \lambda_{A-\rightarrow A} \tag{6}$$

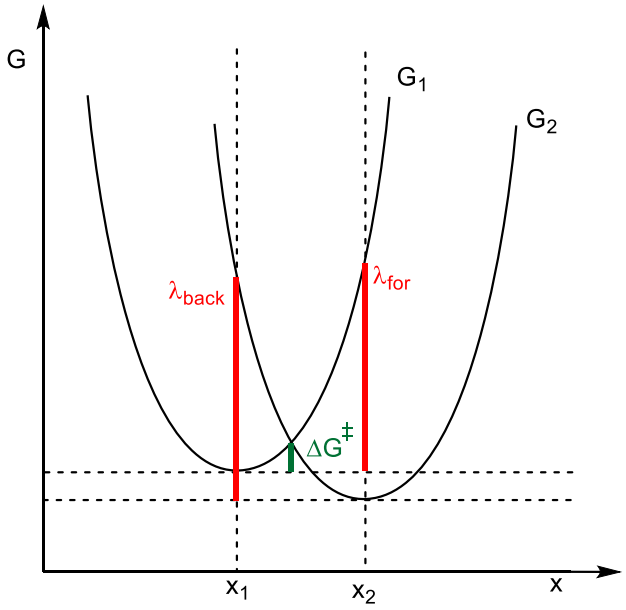



**Figure S5:** Four-Point Approach to the Electron-transfer Marcus-Hush Theory.[17]

$$\lambda_{out} = (\Delta q)^2 \left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon_s}\right)\left(\frac{1}{2r_1} + \frac{1}{2r_2} - \frac{1}{R}\right) \tag{7}$$

$$\lambda_{out} = \frac{(z\,e_0)^2}{4\,\pi\varepsilon_0}\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon_s}\right)\left(\frac{1}{2r_1} + \frac{1}{2r_2} - \frac{1}{R}\right) \tag{8}$$

$$\lambda_{out} = z^2\ 2.307\ 10^{-28}\,\frac{\mathrm{C}^2\ V\ m}{\mathrm{C}}\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon_s}\right)\left(\frac{1}{2r_1} + \frac{1}{2r_2} - \frac{1}{R}\right) \tag{9}$$

$$\lambda_{out} = z^2\ 332.2\,\frac{\mathrm{kcal\ \AA}}{\mathrm{mol}}\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon_s}\right)\left(\frac{1}{2r_1} + \frac{1}{2r_2} - \frac{1}{R}\right) \tag{10}$$

### 2.3.1 Comp. analysis of the reaction pathway of α,β-unsat. esters

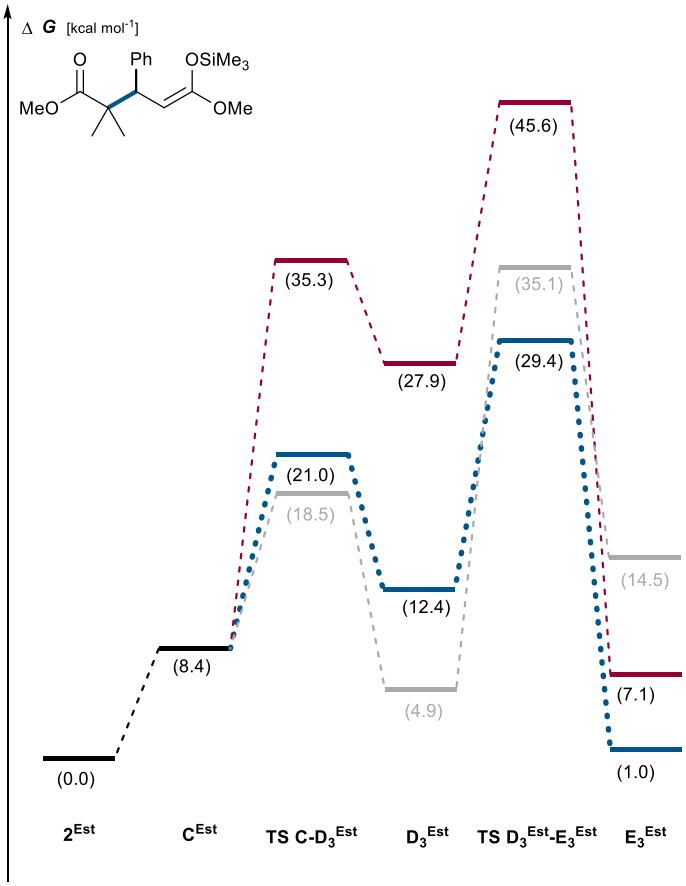
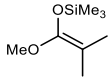
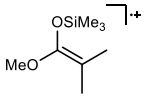
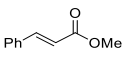
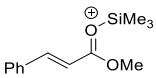



**Figure S6:** Reaction profile of radical addition of **B** to α,β-unsaturated ester $\mathbf{2}^{Est}$.

**Table S3:** Stationary point energies of relevant structures. Energy values are given in $E_h$.

| | Free energy | SP energy | ZPVE | Thermal Correction | Enthalpy Correction | Entropy Correction |
|---|---|---|---|---|---|---|
|  **1** | -755.41389166 | -755.61700281 | 0.24522497 | 0.01673055 | 0.00094421 | 0.05978858 |
|  **A** | -755.23365209 | -755.43572912 | 0.24513199 | 0.01711167 | 0.00094421 | 0.06111084 |
|  $\mathbf{2}^{Est}$ | -537.33771144 | -537.47795263 | 0.17694384 | 0.01100474 | 0.00094421 | 0.04865160 |
|  **B** | -346.23069830 | -346.32880842 | 0.13177051 | 0.00890443 | 0.00094421 | 0.04350903 |
|  $\mathbf{C}^{Est}$ | -946.32732041 | -946.57226638 | 0.29020000 | 0.01906410 | 0.00094421 | 0.06526234 |

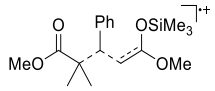
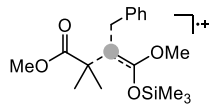
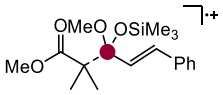
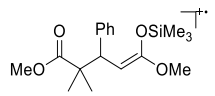
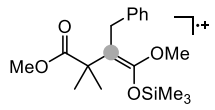
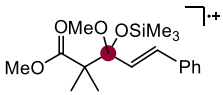
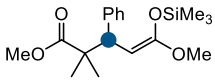
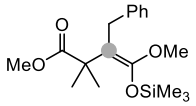
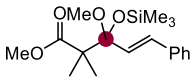
| | | | | | | |
|---|---|---|---|---|---|---|
|  **TS C-$D_3^{Est-1,4}$** | -1292.53103628 | -1292.90199372 | 0.42481833 | 0.02609686 | 0.00094421 | 0.08090196 |
|  **TS C-$D_3^{Est-1,3}$** | -1292.53496186 | -1292.90654428 | 0.42424071 | 0.02645760 | 0.00094421 | 0.08006010 |
|  **TS C-$D_3^{Est-1,2}$** | -1292.50826882 | -1292.87792480 | 0.42293277 | 0.02670399 | 0.00094421 | 0.08092499 |
|  **$D_3^{Est-1,4}$** | -1292.54468226 | -1292.91630068 | 0.42664522 | 0.02814301 | 0.00094421 | 0.08411402 |
|  **$D_3^{Est-1,3}$** | -1292.55663072 | -1292.92939753 | 0.42704033 | 0.02801632 | 0.00094421 | 0.08323405 |
|  **$D_3^{Est-1,2}$** | -1292.51998012 | -1292.89262194 | 0.42659574 | 0.02776996 | 0.00094421 | 0.08266809 |
|  **$E_3^{Est-1,4}$** | -1292.74314652 | -1293.11534120 | 0.42672979 | 0.02811614 | 0.00094421 | 0.08359546 |
|  **$E_3^{Est-1,3}$** | -1292.72239637 | -1293.09614613 | 0.42695565 | 0.02739030 | 0.00094421 | 0.08154040 |
|  **$E_3^{Est-1,2}$** | -1292.73343286 | -1293.10697133 | 0.42674789 | 0.02756341 | 0.00094421 | 0.08171704 |

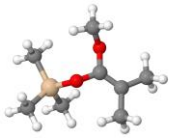
**Table S4:** Energies of relevant structures for application of Electron-transfer Marcus-Hush Theory. Energy values are given in $E_h$.

| | $G_1(x_1)$ | $G_1(x_2)$ | $G_2(x_2)$ | $G_2(x_1)$ | r |
|---|---|---|---|---|---|
| **1** | -755.41389289 | -755.38850254 | -755.23363893 | -755.20437698 | 2.27725599 |
| $D_3^{Est-1,4}$ | -1292.55297911 | -1292.53302995 | -1292.74302841 | -1292.72416572 | 2.46509668 |
| $D_3^{Est-1,3}$ | -1292.55664715 | -1292.48974375 | -1292.72198263 | -1292.67947766 | 2.48371324 |
| $D_3^{Est-1,2}$ | -1292.55086202 | -1292.53243608 | -1292.74020406 | -1292.71044074 | 2.49820693 |

**Table S5:** Data for the calculation of the activation barrier of the electron transfer via Four-Point Approach to the Electron-Transfer Marcus-Hush Theory. Energy values are given in kcal $mol^{-1}$.

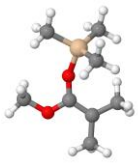
| | $\Delta G_0$ | $\lambda_i$ | $\lambda_o$ | $\lambda$ | $\Delta G^{\ddagger}$ |
|---|---|---|---|---|---|
| $D_3^{Est-1,4}$ | -6.14666213 | 29.31177400 | 50.33379065 | 79.64556465 | 16.95665257 |
| $D_3^{Est-1,3}$ | 9.36148235 | 51.07028132 | 50.16822799 | 101.23850930 | 30.20678158 |
| $D_3^{Est-1,2}$ | -5.70285011 | 31.91219965 | 50.04200499 | 81.95420464 | 17.73633547 |

**1**



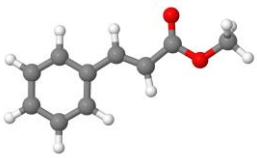
| | | | |
|---|---|---|---|
| Si | -0.73871666095863 | 3.21885893604048 | -0.78820770029077 |
| C | -1.44544649727906 | 4.31104934979919 | -2.13465632669758 |
| C | -1.60755236002462 | 3.51104399754353 | 0.85067035129574 |
| C | 1.11871951916892 | 3.40863071246837 | -0.60516420253531 |
| H | -0.93021997726184 | 4.13954079503740 | -3.09343386026655 |
| H | -1.34024280937238 | 5.37729146080419 | -1.87410349200440 |
| H | -2.51728666940907 | 4.10099876171800 | -2.28255090772136 |
| H | 1.38378104834946 | 4.42752270364781 | -0.27737871613911 |
| H | 1.63009002963274 | 3.21021702755411 | -1.56077366518442 |
| H | 1.50878526670696 | 2.69713216652683 | 0.14045148181082 |
| H | -1.42863408973314 | 4.53698945745528 | 1.21408337970046 |
| H | -1.23713834784522 | 2.80580908175176 | 1.61123636904132 |
| H | -2.69681606256839 | 3.37262123928936 | 0.75351272982760 |
| C | 0.50461437827801 | -0.17202759882952 | -1.51844908968440 |
| C | 1.13777218306104 | -1.41046239729382 | -0.94681672789735 |
| H | 0.97641935345744 | -2.27996158825015 | -1.61010877646500 |
| H | 2.23305241708492 | -1.28696942034587 | -0.85840356737089 |
| H | 0.74025967244989 | -1.64967073598220 | 0.04787650618150 |
| C | 0.96737295892894 | 0.26527104740360 | -2.88065218433752 |
| H | 0.84954931781381 | -0.55094471453929 | -3.61608599219683 |
| H | 2.04315730527112 | 0.52243815181557 | -2.87141358798934 |
| H | 0.40609159597545 | 1.13578472189716 | -3.24477775728862 |
| C | -0.41706939422046 | 0.53037369323556 | -0.83392796614035 |
| O | -1.04859564928642 | 1.62856252109310 | -1.32646150836552 |
| O | -0.76379066680497 | 0.21023536056648 | 0.45114044300907 |
| C | -2.13761418416676 | -0.08588275878652 | 0.65716108429663 |
| H | -2.43198482238290 | -0.99225959120114 | 0.09756694324851 |
| H | -2.78458081248992 | 0.74930678698811 | 0.34326957850349 |
| H | -2.27081604237493 | -0.26387916740741 | 1.73316716166021 |

**A**



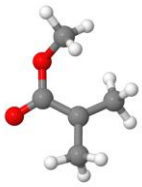
| | | | |
|---|---|---|---|
| Si | -0.70878264789662 | 3.25722568803358 | -0.73738109184549 |
| C | -1.29371802825804 | 3.83362197076937 | -2.40599297832219 |
| C | -1.78283928545257 | 3.83822310991464 | 0.66501081194277 |
| C | 1.11456888583758 | 3.46541131855299 | -0.40980592143548 |
| H | -0.66059932720196 | 3.47676381712093 | -3.23275184958438 |
| H | -1.27751063267402 | 4.93641195463975 | -2.43136810037168 |
| H | -2.33066571388435 | 3.51346947023525 | -2.59581264631445 |
| H | 1.32076207962523 | 4.53568621812779 | -0.23752103828295 |
| H | 1.74274509951240 | 3.14324509216530 | -1.25312231532837 |
| H | 1.43013884964356 | 2.92475714219474 | 0.49734141748113 |
| H | -1.73686787061097 | 4.93784434582785 | 0.73773935292486 |
| H | -1.45041009233184 | 3.42902919000993 | 1.63243673803942 |
| H | -2.83690833993505 | 3.55983350880850 | 0.50664786576070 |
| C | 0.51819727858255 | -0.17978756558232 | -1.57148649665361 |
| C | 1.04789035611243 | -1.55696724614000 | -1.38774474302179 |
| H | 0.50418687267669 | -2.25084193968286 | -2.06062180546976 |
| H | 2.10694259860173 | -1.60661588378133 | -1.68476851041209 |
| H | 0.92463983865804 | -1.93290383779040 | -0.36449885368558 |
| C | 1.02768136575134 | 0.65316166811207 | -2.69105677875109 |
| H | 1.13730478812560 | 0.03375340894833 | -3.59695889298912 |
| H | 2.04448819940404 | 1.02277111560615 | -2.45707625314276 |
| H | 0.38903492524756 | 1.51283333849414 | -2.92330418288601 |
| C | -0.51609769848514 | 0.31080379593777 | -0.70411432559681 |
| O | -1.00019758483228 | 1.49177230113770 | -0.73374783719384 |
| O | -1.01179445575363 | -0.54968692826500 | 0.14557596716584 |
| C | -2.06139907698175 | -0.14655011924233 | 1.05125795713417 |
| H | -2.93592449162593 | 0.19465423230335 | 0.48018884720484 |
| H | -1.70122232520864 | 0.66065864585473 | 1.70429416025670 |
| H | -2.30048356664596 | -1.04095781231065 | 1.63541150337705 |

## 2$^{Est}$



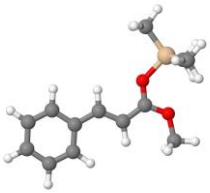
| | | | |
|---|---|---|---|
| C | -8.97187588871162 | 1.05822116873001 | -0.43049911203237 |
| C | -8.98900615144992 | -0.33887225685652 | -0.42690986621664 |
| C | -7.77082181269206 | 1.74122370901495 | -0.23436250805671 |
| C | -6.56383227256312 | 1.04457920632897 | -0.03092319186990 |
| C | -6.59895223594202 | -0.36521952135482 | -0.03023411341976 |
| C | -7.79706635548258 | -1.04712894375821 | -0.22587106629574 |
| C | -5.33328071037826 | 1.81011853085772 | 0.16961126474510 |
| C | -4.09173369723503 | 1.33050620433852 | 0.37734303786831 |
| H | -5.43312449169570 | 2.90117773936803 | 0.14829487525811 |
| H | -5.67822380461580 | -0.93112350895158 | 0.12514642257552 |
| H | -9.89723735606656 | 1.61812156754539 | -0.58660264069595 |
| H | -7.75772600716523 | 2.83440649578686 | -0.23723019261965 |
| H | -7.80544638745087 | -2.13996840025432 | -0.22221034735705 |
| H | -9.92740567158981 | -0.87758531917658 | -0.58011959181181 |
| C | -2.95699785707588 | 2.25916290814884 | 0.56120039074782 |
| H | -3.86377802184377 | 0.26361833688888 | 0.41971845209109 |
| O | -3.01556737781216 | 3.46894784771242 | 0.54639051615349 |
| O | -1.80510254721381 | 1.57932292477102 | 0.75504643300778 |
| C | -0.63841396555043 | 2.37421190737463 | 0.94494865289832 |
| H | -0.45330995109792 | 3.01542958538149 | 0.06897766797182 |
| H | 0.19310347122031 | 1.67218319809470 | 1.08588134578510 |
| H | -0.74495090758774 | 3.02318662000960 | 1.82825357127311 |

## B



| | | | |
|---|---|---|---|
| C | 0.15854831486826 | -0.26091685412808 | -1.81656301087734 |
| C | 1.09695865236965 | -1.37116260880147 | -1.46528197252030 |
| H | 0.56034294658297 | -2.25933806869162 | -1.07835753205434 |
| H | 1.63933336702863 | -1.70817674074455 | -2.36567795648130 |
| H | 1.83714335122033 | -1.07258382656553 | -0.71036856094538 |
| C | -0.54757805137152 | -0.31058875187964 | -3.12943502448994 |
| H | -1.02062585138255 | -1.29677096653879 | -3.28527018924215 |
| H | 0.16976219304299 | -0.17685725881992 | -3.96330378161707 |
| H | -1.30270398023678 | 0.48162331600071 | -3.21241222044069 |
| C | 0.05445402229010 | 0.96975897682547 | -1.02956631743780 |
| O | -0.28058519374554 | 2.02784584540263 | -1.52336752125255 |
| O | 0.41327785217069 | 0.94050692526456 | 0.28902756474136 |
| C | 0.05477733395010 | -0.15296266496769 | 1.11862197333245 |
| H | 0.92711485672229 | -0.78468153780037 | 1.35304942707963 |
| H | -0.72542184524792 | -0.78101488731380 | 0.65793653780444 |
| H | -0.34094796826169 | 0.26027910275809 | 2.05919858440099 |

## C$^{Est}$



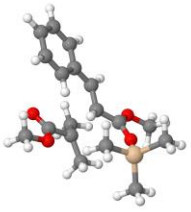
| | | | |
|---|---|---|---|
| C | -8.51246424615742 | 0.95304994468882 | 0.04675331355827 |
| C | -8.58335260476576 | -0.44375436242344 | 0.00221568779989 |
| C | -7.27053720350659 | 1.58028209270874 | 0.03472290108954 |
| C | -7.41099146209289 | -1.21485046880142 | -0.05442859689245 |
| C | -6.17019767033826 | -0.59331463588729 | -0.06664918812194 |
| C | -6.07770231501751 | 0.81982975899070 | -0.02215471714108 |
| C | -4.82359062359115 | 1.52550031759934 | -0.03198195730935 |
| C | -3.56234575457381 | 0.99024626861973 | -0.08387162163146 |
| C | -2.41475456929888 | 1.84015228283766 | -0.08661916551966 |
| O | -2.53181973576187 | 3.11186791663901 | -0.04079136937250 |
| H | -9.42689628645592 | 1.54795402455028 | 0.09072956124600 |
| H | -9.55710640094597 | -0.93929679172866 | 0.01153650653577 |
| H | -7.20793925394644 | 2.67086859162300 | 0.06931066925980 |
| H | -7.47690479052771 | -2.30423892102650 | -0.08884072624614 |
| H | -5.26642790024829 | -1.20401434745159 | -0.11081557775171 |
| Si | -1.29188050969682 | 4.41838730612075 | -0.03095944570185 |
| C | -2.37751180875207 | 5.92510435530317 | 0.04903106773677 |
| C | -0.35644404783521 | 4.24089435869614 | -1.63269708819335 |
| C | -0.27074256537890 | 4.13605193846260 | 1.50189153975523 |
| H | -3.04353633864637 | 5.98833637296533 | -0.82613168056138 |
| H | -1.75426710460318 | 6.83476231985045 | 0.06259434504283 |
| H | -2.99502461878226 | 5.92843614244887 | 0.96126091033656 |
| H | 0.44325481226730 | 4.96812946887522 | 1.62379040575740 |
| H | 0.30787167037285 | 3.20209207074502 | 1.44196867770875 |
| H | -0.90118369438159 | 4.10613657317116 | 2.40501982727997 |
| H | -1.03530403711800 | 4.27005242133255 | -2.50004667233926 |
| H | 0.22307205334402 | 3.30620277309008 | -1.66693902438852 |
| H | 0.35119784799820 | 5.08068267409775 | -1.73762008391679 |
| H | -4.89010805202523 | 2.61766708047245 | 0.00628254462354 |
| H | -3.40667850005502 | -0.08605571576567 | -0.12398585199884 |
| O | -1.18718550000261 | 1.38660639378173 | -0.13516909394903 |
| C | -0.87280590161768 | -0.01793238151920 | -0.19097865503167 |
| H | -1.24566991195028 | -0.52794418563237 | 0.70863350516148 |
| H | 0.22082512560129 | -0.07004895377706 | -0.22298169755919 |
| H | -1.29573810150997 | -0.46724268365735 | -1.10074924926561 |

## TS C-D$_3^{Est-1,4}$

| | | | |
|---|---|---|---|
| C | -6.37757 | 0.87679 | 1.56643 |
| C | -5.95458 | -0.19340 | 2.35924 |
| C | -5.44222 | 1.77517 | 1.05514 |
| C | -4.59127 | -0.36347 | 2.63074 |
| C | -3.65602 | 0.53151 | 2.11559 |
| C | -4.06858 | 1.61546 | 1.31819 |
| C | -3.12348 | 2.60255 | 0.74786 |
| C | -1.75605 | 2.27910 | 0.54393 |
| C | -0.81451 | 2.93609 | -0.28281 |
| O | 0.43453 | 2.69644 | -0.07474 |

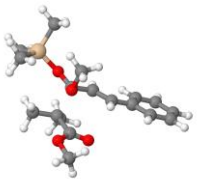
| | | | |
|---|---|---|---|
| H | -7.43878 | 1.01304 | 1.34790 |
| H | -6.68487 | -0.89623 | 2.76635 |
| H | -5.77740 | 2.60925 | 0.43398 |
| H | -4.25738 | -1.20053 | 3.24777 |
| H | -2.59956 | 0.38081 | 2.34501 |
| Si | 1.89324 | 3.30025 | -0.91664 |
| C | 3.23417 | 2.38228 | -0.01362 |
| C | 1.91230 | 5.14271 | -0.62320 |
| C | 1.71972 | 2.80505 | -2.70686 |
| H | 4.22113 | 2.66323 | -0.41715 |
| H | 3.12119 | 1.29255 | -0.12837 |
| H | 3.22943 | 2.62086 | 1.06174 |
| H | 1.52659 | 1.72461 | -2.80497 |
| H | 0.91292 | 3.35699 | -3.21143 |
| H | 2.66166 | 3.02184 | -3.23854 |
| H | 1.05887 | 5.64086 | -1.10714 |
| H | 2.83795 | 5.57494 | -1.03910 |
| H | 1.89402 | 5.37421 | 0.45402 |
| C | -3.01428 | 4.08536 | 2.13816 |
| C | -4.36564 | 4.74021 | 2.17361 |
| H | -5.14258 | 4.03383 | 2.49944 |
| H | -4.33282 | 5.56392 | 2.90847 |
| H | -4.63694 | 5.18115 | 1.20751 |
| C | -2.56626 | 3.46664 | 3.44159 |
| C | -1.95616 | 4.93247 | 1.46741 |
| O | -2.16929 | 6.02444 | 1.00765 |
| O | -0.75096 | 4.33193 | 1.45087 |
| C | 0.32614 | 5.09600 | 0.88151 |
| H | 0.47381 | 6.02613 | 1.44813 |
| H | 0.10308 | 5.35153 | -0.16465 |
| H | 1.21656 | 4.46026 | 0.94539 |
| O | -1.05021 | 3.78650 | -1.26198 |
| H | -1.29107 | 1.50847 | 1.16038 |
| C | -2.31056 | 3.97339 | -1.92831 |
| H | -2.06112 | 4.43373 | -2.89143 |
| H | -2.95564 | 4.65050 | -1.35142 |
| H | -2.80551 | 3.00629 | -2.09234 |
| H | -1.65581 | 2.86392 | 3.33959 |
| H | -3.36424 | 2.86460 | 3.89794 |
| H | -2.33050 | 4.28318 | 4.14724 |
| H | -1.52337 | 2.77789 | -0.22900 |

## TS C-$D_3^{Est-1,3}$



| | | | |
|---|---|---|---|
| C | -7.43775509961100 | -1.58326684759130 | -0.56394795464870 |
| C | -6.80649902226388 | -2.49228641119299 | 0.29546280506769 |
| C | -6.74681190069537 | -0.47214551451641 | -1.03156813966995 |
| C | -5.47529139783340 | -2.27789507900005 | 0.68576991200601 |
| C | -4.77757174711731 | -1.17367778048421 | 0.21772440325252 |
| C | -5.39531466484513 | -0.24199026342473 | -0.66009014069480 |
| C | -4.72628232469563 | 0.91405784826789 | -1.16821372470920 |
| C | -3.36183932694292 | 1.22467124185269 | -0.95376912511828 |
| C | -2.91078922727239 | 2.58392505703186 | -1.10904344679458 |
| O | -1.90807850151317 | 3.08374229501844 | -0.50060859244469 |
| H | -8.47406367016445 | -1.74738695653255 | -0.86714324034262 |
| H | -7.34976336561518 | -3.36519664564251 | 0.66408595241972 |
| H | -7.23958993084532 | 0.23572873138883 | -1.70281728318840 |
| H | -4.98691013085295 | -2.98394981682103 | 1.36139887212878 |
| H | -3.74290790228320 | -1.02627962042101 | 0.53158973220114 |
| Si | -0.83865824613827 | 2.81398648639860 | 0.91503603320476 |
| C | -1.51222459287596 | 4.04199753103785 | 2.14025269808226 |
| C | 0.83018422346953 | 3.25423586463377 | 0.22505052847299 |
| C | -0.98171841930921 | 1.04724679117081 | 1.49580099776920 |
| H | -1.47853819182320 | 5.06892633291451 | 1.74353414703769 |
| H | -0.90751182342352 | 4.01863396573567 | 3.06241508381168 |
| H | -2.55209959693575 | 3.80620404361741 | 2.41846532752674 |
| H | -0.23503845172912 | 0.90156877346877 | 2.29562308930221 |
| H | -0.77310560237668 | 0.30962768744118 | 0.70608702085382 |
| H | -1.96996236367051 | 0.83391457400839 | 1.93310939222831 |
| H | 0.82597133539534 | 4.26467750441216 | -0.21328752758218 |
| H | 1.16136140507337 | 2.54055552312089 | -0.54461317757485 |
| H | 1.57744260869457 | 3.24412001538405 | 1.03617557754693 |
| C | -2.17817979815168 | 0.43368771073246 | -2.60997562405430 |
| C | -3.02119808165931 | 0.74674319621070 | -3.80720133921209 |
| H | -3.09143895416617 | 1.82954321700197 | -3.98403961650968 |
| H | -4.02615039417618 | 0.31485378337628 | -3.71236246777661 |
| H | -2.56308541578304 | 0.28994652368960 | -4.70329256314334 |
| C | -0.80929492236941 | 1.05295249200570 | -2.55438893740854 |
| H | -0.82941557341913 | 2.12786120222254 | -2.78759311702665 |
| H | -0.17093957249700 | 0.57607198851726 | -3.32144393434009 |
| H | -0.31341857644556 | 0.89273743528410 | -1.58948150303874 |
| C | -2.29384578513196 | -0.98137159055790 | -2.14464398465099 |
| O | -3.09219006976246 | -1.77202918222430 | -2.58679901401740 |
| O | -1.42338319595639 | -1.27835278975815 | -1.15364919714412 |
| C | -1.42728615412221 | -2.64133713704151 | -0.70394649038792 |
| H | -2.42716822542781 | -2.92829443654054 | -0.34816684022197 |
| H | -0.69317379743207 | -2.69536268050313 | 0.10851366461468 |
| H | -1.14174953945520 | -3.31436755625210 | -1.52519656041760 |
| O | -3.54466899996637 | 3.34213980976740 | -1.95434432964052 |
| H | -5.30840244932020 | 1.59720937543899 | -1.79034787916331 |
| C | -3.14257886409787 | 4.71838048104650 | -2.14046382974276 |
| H | -2.11055321733015 | 4.76005800383474 | -2.51352422084601 |
| H | -3.22196975493819 | 5.26147859730480 | -1.18917194188594 |
| H | -3.84062519244817 | 5.12456899732258 | -2.87952696162826 |
| H | -2.81680753774279 | 0.67953722784500 | -0.18806253250205 |

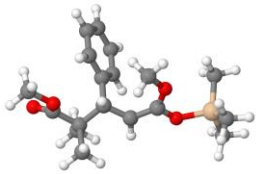
## TS C-$D_3^{Est-1,2}$



| | | | |
|---|---|---|---|
| C | -6.16161683897606 | 1.54198937357500 | -0.50224977653114 |
| C | -5.65561821646986 | 1.34719896190092 | 0.79201720028290 |
| C | -5.32557010509356 | 2.01524654756561 | -1.50350664821761 |
| C | -4.30769449136718 | 1.62563007114138 | 1.08037870812005 |
| C | -3.46783648553613 | 2.09692694860939 | 0.08416784903745 |
| C | -3.96061145676769 | 2.30215413701800 | -1.23404234368696 |
| C | -3.14133208905191 | 2.77478852754555 | -2.31217606156856 |
| C | -1.81531784909299 | 3.12602482815100 | -2.23051877322850 |
| C | -1.02025877674633 | 3.57073018626723 | -3.36678157287523 |
| O | 0.08826883163167 | 4.22456022023696 | -3.03129057349837 |
| H | -7.20812199542879 | 1.31920836717167 | -0.71960160435397 |
| H | -6.31237973044859 | 0.97444980473689 | 1.58169145082040 |
| H | -5.70807259764262 | 2.16369161939152 | -2.51594226204759 |
| H | -3.92368502253749 | 1.46738499862373 | 2.09017212764028 |
| H | -2.42282634739157 | 2.30577847378872 | 0.31809271076564 |
| Si | 1.17149558018453 | 5.49386531676131 | -3.50727947661721 |
| C | 1.19523632477733 | 5.73190034731467 | -5.36383299423076 |
| C | 2.82060696793292 | 4.92167858193151 | -2.84801140396087 |

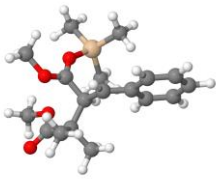
| | | | |
|---|---|---|---|
| C | 0.56291431335477 | 7.01609045850610 | -2.60353467857006 |
| H | 0.19466489354925 | 5.87084843295726 | -5.79892498544341 |
| H | 1.67946493667759 | 4.89046258408762 | -5.88062784584432 |
| H | 1.78266658481087 | 6.63892865716726 | -5.58677380989051 |
| H | 1.27532297627268 | 7.84439508257555 | -2.75516673785283 |
| H | 0.49487773994579 | 6.82682819624030 | -1.52030355104022 |
| H | -0.42252853358457 | 7.35984193685419 | -2.95432811416437 |
| H | 3.17657839024702 | 4.01095523917619 | -3.35494971585720 |
| H | 2.76421119377230 | 4.71581350563838 | -1.76719645432721 |
| H | 3.58038151629466 | 5.70580549150878 | -3.00210665872391 |
| C | 0.69843706677030 | 2.22662211005203 | -4.97165323979666 |
| C | -0.37513818212250 | 1.83695705767960 | -3.98893621872416 |
| H | 1.00728377273910 | 1.31452471785830 | -5.51142569310457 |
| H | 1.58139617976351 | 2.62302733786098 | -4.45588075622324 |
| H | 0.33468526477750 | 2.93906134833059 | -5.71988974184142 |
| C | 0.13343505299721 | 1.06281124310499 | -2.79639537559090 |
| H | 0.71552046142352 | 0.19720988207079 | -3.15796859480168 |
| H | -0.68345934900451 | 0.67980476841539 | -2.17235064950261 |
| H | 0.81535132687376 | 1.68345729832984 | -2.19594252308695 |
| C | -1.62100895838194 | 1.22700392937652 | -4.61035123328159 |
| O | -2.51385381739491 | 0.71705177033418 | -3.96917316742041 |
| O | -1.60617436724011 | 1.29385787555440 | -5.93818273625968 |
| C | -2.73273372720354 | 0.73299587808367 | -6.62627337927746 |
| H | -2.84514241883278 | -0.33146889230248 | -6.37514411887088 |
| H | -2.52679485527031 | 0.85959059308173 | -7.69501145462657 |
| H | -3.65324711234238 | 1.26527439625200 | -6.34395419247764 |
| H | -3.63120330614800 | 2.87504287091536 | -3.28199726847733 |
| H | -1.25513113850891 | 3.01342795633036 | -1.30220023544620 |
| O | -1.69566597302933 | 3.97558797984946 | -4.48671936766640 |
| C | -2.33070260526201 | 5.25684872993271 | -4.43861431484717 |
| H | -1.59555107502603 | 6.07396170319144 | -4.45454479948540 |
| H | -2.95816940041080 | 5.35147058229700 | -3.53672562920403 |
| H | -2.95847255248286 | 5.32335196695846 | -5.33565931412294 |

## $D_3^{Est\text{-}1,4}$



| | | | |
|---|---|---|---|
| C | -5.08127531624405 | 0.39147151407930 | -0.29342005609746 |
| C | -4.13851708623342 | -0.61678849766524 | -0.52775606341260 |
| C | -4.66846307185152 | 1.65087617084649 | 0.14246410673586 |
| C | -2.78110246698926 | -0.36091038094417 | -0.31715527263504 |
| C | -2.36675703839847 | 0.89624553612216 | 0.12768639088244 |
| C | -3.30595194596195 | 1.91750396177812 | 0.36319639798050 |
| C | -2.86332747421045 | 3.28915324145029 | 0.87378959336523 |
| C | -1.57803301456900 | 3.66199081922110 | 0.22115439597921 |
| C | -1.28835616796535 | 3.81079842591911 | -1.17272984946295 |
| O | -0.05132994753644 | 3.78135087535803 | -1.50610372684645 |
| H | -6.14424265402132 | 0.19264953634102 | -0.44805055776807 |
| H | -4.46442771389262 | -1.60223428447847 | -0.86782123972211 |
| H | -5.40700943120437 | 2.43302699081605 | 0.32982390865515 |
| H | -2.04213779549979 | -1.14703385302484 | -0.48792557870634 |
| H | -1.30533782526973 | 1.07480559563309 | 0.31509050589858 |
| Si | 0.73853035349824 | 3.89367502807824 | -3.12535126885393 |
| C | 0.25008834139425 | 5.55626836621226 | -3.81266012399160 |
| C | 0.09296857168894 | 2.43066677355851 | -4.08270378247929 |
| C | 2.52942881270451 | 3.76529419037148 | -2.64978107114449 |
| H | 0.80444241220276 | 5.73741928422907 | -4.74920067492128 |
| H | 0.50675684100440 | 6.36952809752530 | -3.11500820651380 |
| H | -0.82452606022754 | 5.60899504973224 | -4.04195471833079 |
| H | 2.82975431369479 | 4.59169675156487 | -1.98632577054028 |
| H | 2.74248442782239 | 2.81272811138038 | -2.13942716110474 |
| H | 3.16072049465291 | 3.81214820266149 | -3.55278016604938 |
| H | 0.28365460228788 | 1.48737689524428 | -3.54630158178508 |
| H | 0.61178903284798 | 2.37098311719779 | -5.05436908087152 |
| H | -0.98620864324291 | 2.51379646437961 | -4.28013141196139 |
| C | -2.78334135833853 | 3.39369308678786 | 2.43709838197031 |
| C | -1.80173944026547 | 2.39066920928210 | 3.04950393138826 |
| H | -0.77866475271398 | 2.55199651634572 | 2.67526865110822 |
| H | -1.77970208168851 | 2.50940518550025 | 4.14114843335555 |
| H | -2.09927720166594 | 1.35466884303083 | 2.84227516763610 |
| C | -2.40708359697099 | 4.83613082619028 | 2.83331445110726 |
| H | -1.38274220017251 | 5.08130571716853 | 2.51063144178432 |
| H | -2.43733685886900 | 4.94974334594251 | 3.92731875860670 |
| H | -3.10023901222935 | 5.56858512135370 | 2.39511017485863 |
| C | -4.18626338538471 | 3.10428682466816 | 2.99403601223197 |
| O | -4.43919446356195 | 2.28542429239177 | 3.83629662807451 |
| O | -5.11373777629741 | 3.90919031549350 | 2.43640565663011 |
| C | -6.45464531706399 | 3.76210822454241 | 2.92710134823503 |
| H | -6.48864758276299 | 3.94861100645888 | 4.00988391400203 |
| H | -6.82402558981538 | 2.74400979647092 | 2.73426995024960 |
| H | -7.05878225478901 | 4.50281399774590 | 2.39011223158662 |
| H | -3.64769481129330 | 4.00344653274925 | 0.57901442460630 |
| O | -2.12833958453971 | 3.97524174296186 | -2.15936223448030 |
| H | -0.66263933834335 | 3.68591184946781 | 0.81628635142079 |
| C | -3.54197828887915 | 4.23133974396891 | -2.04119832037397 |
| H | -3.86574610415643 | 4.49971080865337 | -3.05263174575316 |
| H | -3.71839908246042 | 5.07147660160507 | -1.35650966327588 |
| H | -4.06013446821879 | 3.32531842763281 | -1.70412188126738 |

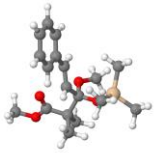
## $D_3^{Est\text{-}1,3}$



| | | | |
|---|---|---|---|
| C | -7.38669493384632 | 1.00937815044742 | -1.09151438426610 |
| C | -7.73650306834527 | 1.07794914512690 | 0.26638437119206 |
| C | -6.09345778303790 | 0.67484941456875 | -1.46526842462447 |
| C | -6.77249179706501 | 0.79858634648881 | 1.24798127188334 |
| C | -5.47461318573204 | 0.46531142072917 | 0.88576165058385 |
| C | -5.08924116366625 | 0.40002064549021 | -0.48738742494070 |
| C | -3.78052163129283 | 0.07712968534695 | -0.91837361826217 |
| C | -2.59274011334596 | -0.12066087350705 | -0.01577188186730 |
| C | -1.56612283867930 | 0.85367308217689 | -0.51379695804904 |
| O | -1.43656446468043 | 2.03830231610312 | -0.08976322232656 |
| H | -8.13599937814753 | 1.21877572233997 | -1.85823730819546 |
| H | -8.75573799961549 | 1.33964798079994 | 0.55835430317773 |
| H | -5.82638224404287 | 0.62194623699290 | -2.52373527292848 |
| H | -7.04704487036245 | 0.83507364460362 | 2.30479875537414 |
| H | -4.75179523519037 | 0.22816394475518 | 1.66763958093886 |
| Si | -2.10615274503709 | 3.12140099920456 | 1.19136423102612 |
| C | -2.31331046736308 | 2.10142084209582 | 2.74047146672539 |
| C | -3.68515400623254 | 3.76858576757324 | 0.45651834109856 |
| C | -0.73094525725211 | 4.36529049244703 | 1.31170131876959 |
| H | -3.27411895579593 | 1.56728512163834 | 2.76932649084950 |
| H | -2.28772493670964 | 2.77789027652247 | 3.61132676728680 |
| H | -1.49839229979392 | 1.37070645907224 | 2.85678044652687 |
| H | -1.00073692585452 | 5.15195755123649 | 2.03595793639579 |
| H | -0.54291275290344 | 4.85267904128590 | 0.34206671179056 |
| H | 0.20583300005175 | 3.89978791220127 | 1.65762567938986 |
| H | -4.43205890101395 | 2.97195016354009 | 0.32243549311347 |

| | | | |
|---|---|---|---|
| H | -3.50605185037021 | 4.25633868065216 | -0.51467621637162 |
| H | -4.11672566042774 | 4.52366798674133 | 1.13542911793968 |
| C | -2.08472003135252 | -1.60151495187326 | 0.10096957940799 |
| C | -3.00334400889177 | -2.32553142496083 | 1.10974226169297 |
| H | -4.04490081354415 | -2.29925393029777 | 0.75642683085058 |
| H | -2.95978662924255 | -1.85792294773095 | 2.10610769898520 |
| H | -2.69579972707603 | -3.37598497071533 | 1.20869563177557 |
| C | -2.09746116721339 | -2.36138031310699 | -1.23383543597426 |
| H | -3.12934154927114 | -2.48143812939616 | -1.59282399514043 |
| H | -1.66285416001057 | -3.35848787586342 | -1.08382920589192 |
| H | -1.51125915407975 | -1.84820740457165 | -2.00765386421245 |
| C | -0.66899384284316 | -1.64514089136783 | 0.68507737825691 |
| O | 0.05896588238274 | -2.59741076340403 | 0.64407021088085 |
| O | -0.32498024000993 | -0.48174866164378 | 1.29880924343680 |
| C | 0.97310259169059 | -0.45429176770870 | 1.91583914118092 |
| H | 1.08564266090061 | 0.54851099299283 | 2.34555215179737 |
| H | 1.75674804801312 | -0.64945667235585 | 1.16981724621326 |
| H | 1.03675654803917 | -1.21934876981049 | 2.70221520512973 |
| O | -0.83250739279485 | 0.47125973984843 | -1.50515293373934 |
| H | -3.60084333823445 | -0.01588182236867 | -1.99204563535984 |
| H | -2.84042078100450 | 0.21767651532836 | 0.99443799376365 |
| C | 0.14604778789959 | 1.37170628576540 | -2.08132996113669 |
| H | 0.62791685695433 | 0.79921399135641 | -2.88005940511112 |
| H | 0.87211620485324 | 1.66265799890725 | -1.31078210584668 |
| H | -0.36020127941218 | 2.26010761630326 | -2.48132725318938 |

## $D_3^{Est\text{-}1,2}$



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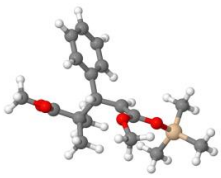
|---|---|---|---|
| C | -5.29506216447671 | -1.15735320271006 | 0.80891339796105 |
| C | -5.36606093017994 | -1.19525447495761 | 2.21191940789416 |
| C | -4.15781310203752 | -0.66271252165124 | 0.19130918399451 |
| C | -4.28985790469368 | -0.73698917936492 | 2.99526143149683 |
| C | -3.15115560509214 | -0.23862954925846 | 2.38660469768310 |
| C | -3.05710319376456 | -0.18491354754389 | 0.96318686327046 |
| C | -1.92139186037728 | 0.32743963267976 | 0.27717402963108 |
| C | -0.79372433822605 | 0.88718826685621 | 0.87533483416520 |
| C | 0.25598361401853 | 1.65144012599071 | 0.06999706830462 |
| O | 0.06046657667633 | 3.01123209259421 | 0.17176878007186 |
| H | -6.13340190397814 | -1.51845015999446 | 0.20981648524027 |
| H | -6.26233489630251 | -1.58598684497800 | 2.69968395773966 |
| H | -4.09066872531806 | -0.62998712392657 | -0.89866248134859 |
| H | -4.35486223461639 | -0.77848921704242 | 4.08441715353793 |
| H | -2.31806208146914 | 0.10242790215045 | 3.00254205855027 |
| Si | -1.26086604839419 | 4.05071007027946 | 0.52417501993851 |
| C | -2.66357173365736 | 3.76250329003039 | -0.68797038841253 |
| C | -0.50830645824470 | 5.74599495317955 | 0.34511247991523 |
| C | -1.84260415017343 | 3.72309178530678 | 2.28128208894422 |
| H | -2.36929000957574 | 3.99802573447909 | -1.72277253473766 |
| H | -3.50670000800951 | 4.42466892866315 | -0.42724232440567 |
| H | -3.03997387332603 | 2.72798076286672 | -0.66146167714874 |
| H | -2.49105387215929 | 4.55237905312371 | 2.61077799662507 |
| H | -0.99562726733307 | 3.66969870970991 | 2.98461745678278 |
| H | -2.43525096688973 | 2.79873304227050 | 2.37044633216289 |
| H | -0.10667317353020 | 5.89173890222163 | -0.67041720832175 |
| H | 0.31488303989264 | 5.89439157155879 | 1.06213271389994 |
| H | -1.26259743176332 | 6.52884772369628 | 0.52743877106732 |
| C | 1.67779968300512 | 1.29401223658073 | 0.64832112527528 |
| C | 2.80495363657919 | 1.73396564606370 | -0.28567559552457 |
| H | 2.75151703150694 | 2.82190972200273 | -0.43425017465879 |
| H | 3.78017994735030 | 1.49597204091679 | 0.16096764160922 |
| H | 2.74416930463354 | 1.23249978035451 | -1.25983254040000 |
| C | 1.88544207786442 | 1.92071681302351 | 2.04374858939297 |
| H | 1.87325694229664 | 3.01452503873156 | 1.94514550929296 |
| H | 2.86007886102548 | 1.61651896935250 | 2.45211804967011 |
| H | 1.11056048789857 | 1.62676907464415 | 2.76676278320425 |
| C | 1.61307572338399 | -0.20798934458444 | 0.82916210473168 |
| O | 0.54366599949934 | -0.76062181925478 | 1.10165014952871 |
| O | 2.73961881419209 | -0.86030854697585 | 0.72786921197154 |
| C | 2.72597435357305 | -2.29000194369640 | 0.93928332950359 |
| H | 2.04680841686360 | -2.76646413766102 | 0.21911987158990 |
| H | 2.39578496322630 | -2.51321217436462 | 1.96322088428828 |
| H | 3.75802464140602 | -2.62010767743137 | 0.78169200294287 |
| H | -1.91091193615898 | 0.27911308790013 | -0.81408992431403 |
| O | 0.16799483612162 | 1.17550699043000 | -1.25259640494649 |
| H | -0.78347031377716 | 1.06821046294156 | 1.94815186225673 |
| C | 0.27519216436324 | 2.09415393763716 | -2.33405866521201 |
| H | 0.36382281207246 | 1.47792933914613 | -3.23868136417574 |
| H | 1.15916791507523 | 2.74196421128107 | -2.25172880975170 |
| H | -0.62125565899976 | 2.72683156673260 | -2.41901523077678 |

## $E_3^{Est\text{-}1,4}$



| | | | |
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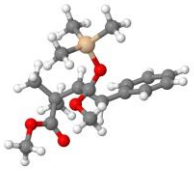
| C | -4.89305029540717 | -0.66771649367187 | 2.17344323062044 |
| C | -4.87831806882945 | 1.31466869753804 | 0.78285959812507 |
| C | -3.54201681604529 | -0.45655714471000 | 2.46257545865252 |
| C | -2.86677404633390 | 0.63672620070712 | 1.91481393243204 |
| C | -3.52445998320047 | 1.54726920295680 | 1.07223475662000 |
| C | -2.82844796895219 | 2.76697753022696 | 0.48425617094468 |
| C | -1.47339050336432 | 2.44147884121282 | -0.08271232999397 |
| C | -1.07180673861866 | 2.82543451148785 | -1.31001669774503 |
| O | 0.13921311357366 | 2.59484690962616 | -1.85107389789271 |
| H | -6.61227214857626 | 0.06251622813204 | 1.08243404445255 |
| H | -5.42137777169905 | -1.52350662673810 | 2.60127766741714 |
| H | -5.40223912301303 | 2.00483621346149 | 0.11787921860666 |
| H | -3.00778399223598 | -1.14953215126759 | 3.11800891398824 |
| H | -1.80969994834824 | 0.77640164195449 | 2.14865120144613 |
| Si | 1.64795317845481 | 2.33719785023401 | -1.09436522958240 |
| C | 1.70708713577092 | 0.61261145699117 | -0.35687440366387 |
| C | 1.90541035279353 | 3.66747993812117 | 0.20341026207384 |
| C | 2.86808582290389 | 2.49746772781546 | -2.50453964364405 |
| H | 2.73035818750783 | 0.37846923576441 | -0.01795439190619 |
| H | 1.41873180182608 | -0.13928448103902 | -1.10946003806497 |
| H | 1.03337807278722 | 0.50081391822307 | 0.50664225160179 |
| H | 2.66194609605842 | 1.75024505216275 | -3.28790637158283 |
| H | 2.81106344989176 | 3.49744571569444 | -2.96403785466583 |
| H | 3.90065223319499 | 2.34295228455480 | -2.15006864223341 |
| H | 1.83205733913728 | 4.67093106668583 | -0.24691493774906 |
| H | 2.90480974587715 | 3.57253745772088 | 0.65986471863492 |
| H | 1.15560469094580 | 3.60174384397180 | 1.00614254295807 |
| C | -2.77776635896733 | 3.97800423980007 | 1.50572909086961 |
| C | -1.85947966363625 | 3.70502814249480 | 2.69989621431112 |
| H | -0.83758405100889 | 3.49450571163760 | 2.35094589695985 |
| H | -1.82406202397298 | 4.58156675004282 | 3.36341670203722 |
| H | -2.21654859154823 | 2.85848405750018 | 3.30034779621257 |
| C | -2.30821377530916 | 5.24341152414177 | 0.76293191560592 |

| | | | |
|---|---|---|---|
| H | -1.27300088729473 | 5.10629786684072 | 0.41728110911796 |
| H | -2.33306944683912 | 6.11806381890522 | 1.43245009403203 |
| H | -2.94239821806308 | 5.45173482425075 | -0.10932686116513 |
| C | -4.19284114038779 | 4.21878469307964 | 2.02962964885587 |
| O | -4.53528585154782 | 4.16940816155082 | 3.18522797731872 |
| O | -5.05509320027026 | 4.50859914293795 | 1.02963100099720 |
| C | -6.41474291917868 | 4.69543976479881 | 1.41356333992702 |
| H | -6.50750856761621 | 5.51037312794315 | 2.14734762213719 |
| H | -6.81807830656377 | 3.77517958247582 | 1.86402240443831 |
| H | -6.96253343790349 | 4.94267916239492 | 0.49531111153443 |
| H | -3.45350261703241 | 3.12186310112111 | -0.34394088660623 |
| O | -1.91791484587608 | 3.47361509816022 | -2.14423875031833 |
| H | -0.78418936619374 | 1.83806847565504 | 0.50552883055493 |
| C | -1.36552300854053 | 4.36512608829459 | -3.09776058805214 |
| H | -0.79115637079727 | 5.17214183173611 | -2.60823245221607 |
| H | -2.21727164749603 | 4.80553356935107 | -3.63314736931679 |
| H | -0.70914424601581 | 3.84449878001921 | -3.81154250902034 |

## $E_3^{Est-1,3}$



| | | | |
|---|---|---|---|
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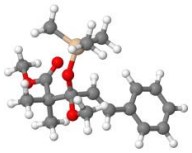
| C | -7.95452447748227 | 1.28932473036343 | 0.22279564670307 |
| C | -5.90253076929358 | 1.57192915896378 | -1.03475398738308 |
| C | -7.42449323619571 | 0.14004708932180 | 0.81614587597419 |
| C | -6.13618254789040 | -0.28824574932635 | 0.48430853639277 |
| C | -5.36111754264795 | 0.41890931503096 | -0.44615088758556 |
| C | -3.99556272383013 | -0.05603591811795 | -0.82420726275833 |
| C | -2.96750048131366 | -0.38568320356474 | 0.25396630097373 |
| C | -2.78083299047407 | 0.81207531512389 | -0.62753527427841 |
| O | -2.98088434133650 | 2.08660836636121 | -0.14332480718263 |
| H | -7.59414668265682 | 2.90780685409109 | -1.16696227356896 |
| H | -8.96062429344587 | 1.62843660338070 | 0.48290807736049 |
| H | -5.29859964651143 | 2.13918222722940 | -1.74604783098907 |
| H | -8.01631325008757 | -0.42524252814553 | 1.54108896886560 |
| H | -5.72100898783223 | -1.18587979502028 | 0.95035409568134 |
| Si | -1.94410315597776 | 2.94270618626246 | 0.89386958072951 |
| C | -1.94508349614497 | 2.14460981143616 | 2.59657385840820 |
| C | -2.70004327564787 | 4.65494267524974 | 0.95919858001417 |
| C | -0.20676240823844 | 2.97173932468506 | 0.17974644643163 |
| H | -2.97440061097416 | 2.02572890218984 | 2.97264541492057 |
| H | -1.39177732696451 | 2.77369185682038 | 3.31426346007776 |
| H | -1.46653477735475 | 1.15395693844270 | 2.58115867796503 |
| H | 0.48139884470272 | 3.53051071495544 | 0.83619011984138 |
| H | -0.19986389929120 | 3.45289058835767 | -0.81180862552599 |
| H | 0.18103988059289 | 1.94888120603237 | 0.05472841948148 |
| H | -3.73769158971030 | 4.60575693167584 | 1.32718058324680 |
| H | -2.71775252016052 | 5.11443749018814 | -0.04235930412457 |
| H | -2.12800066086809 | 5.31736596925377 | 1.62980181854224 |
| C | -2.07223767250144 | -1.63078428926109 | 0.23606147947048 |
| C | -0.89540475563178 | -1.40107553511132 | 1.19577021520130 |
| H | -1.27769733083155 | -1.21782375371447 | 2.21222565628128 |
| H | -0.29697766030145 | -0.53353133853125 | 0.88534533215938 |
| H | -0.23017422890336 | -2.27577620620446 | 1.23086753677111 |
| C | -2.91713101485052 | -2.83592437844800 | 0.69852131184025 |
| H | -3.32458699900523 | -2.64533313841912 | 1.70383587955217 |
| H | -2.30880486616856 | -3.75345922809955 | 0.74444725397384 |
| H | -3.75156223183050 | -3.00831597846366 | 0.00459974755121 |
| C | -1.59853939392665 | -1.94453297496281 | -1.18949709000614 |
| O | -2.33297295368109 | -2.26935458091369 | -2.09462179486434 |
| O | -0.26561556504116 | -1.88415532067976 | -1.32582197090477 |
| C | 0.23869615586922 | -2.11502510988897 | -2.63773832122074 |
| H | 1.33104926077701 | -2.04284323497276 | -2.56387708041288 |
| H | -0.14776717023429 | -1.35681526527067 | -3.33589178763758 |
| H | -0.05851207071188 | -3.10891553287912 | -3.00523269557702 |
| O | -1.74574093781723 | 0.71660421161839 | -1.54897712290024 |
| H | -3.94313777144905 | -0.70903346802614 | -1.70212980128825 |
| H | -3.30065589673689 | -0.13838323697085 | 1.26683814586343 |
| C | -2.02010014155400 | 1.32393116227380 | -2.79673782777522 |
| H | -1.12326627929838 | 1.20415122577765 | -3.42059490316590 |
| H | -2.23796834823373 | 2.39915053519042 | -2.67870959217205 |
| H | -2.87659406971218 | 0.83747595468781 | -3.29672877449409 |

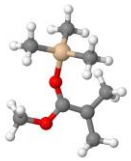
## $E_3^{Est-1,2}$



| | | | |
|---|---|---|---|
| C | -4.80070026004869 | -2.36053796030691 | 1.04046825633325 |
| C | -5.29519271256848 | -1.84985841912354 | 2.24302756801179 |
| C | -3.71830379447420 | -1.74274799379149 | 0.41067651859580 |
| C | -4.69764783724077 | -0.71579837751083 | 2.80731719257389 |
| C | -3.61686194775665 | -0.10109144473277 | 2.17871396220403 |
| C | -3.10280748950730 | -0.60600746441420 | 0.96693555829306 |
| C | -1.96405541965122 | 0.00463991007482 | 0.26538605701012 |
| C | -1.21639163267023 | 1.02669913746715 | 0.70614096482306 |
| C | -0.04499873804657 | 1.62054836024370 | -0.05457854549735 |
| O | -0.10436934879639 | 3.01316533804656 | -0.08304117396725 |
| H | -5.26030392312035 | -3.24378905290607 | 0.58935472604318 |
| H | -6.14325065331545 | -2.32904792490060 | 2.73854849379407 |
| H | -3.33471305749100 | -2.14501684315323 | -0.53114711724725 |
| H | -5.08154033972677 | -0.30643263078187 | 3.74543052343468 |
| H | -3.16916357105174 | 0.78720164636227 | 2.62879138382008 |
| Si | -0.85946494007797 | 4.34281512469140 | 0.62199881325438 |
| C | -1.57098567612804 | 5.30772353648023 | -0.82867795427593 |
| C | 0.47027664360584 | 5.35536741723433 | 1.47603224841040 |
| C | -2.24168864866678 | 3.92358273377095 | 1.82579506857192 |
| H | -0.78644674403868 | 5.54232378535096 | -1.56680990278130 |
| H | -2.01805656909551 | 6.25902345813233 | -0.49451539406572 |
| H | -2.35510048807951 | 4.72700309645120 | -1.34207326379778 |
| H | -2.71657176671919 | 4.86253815818129 | 2.15903823364784 |
| H | -1.84867836764638 | 3.40632521164566 | 2.71377200658416 |
| H | -3.02107525078801 | 3.29800691773329 | 1.36293847933593 |
| H | 1.30053134789112 | 5.57166953523710 | 0.78361545051579 |
| H | 0.87155312987127 | 4.80663162894542 | 2.34128227316557 |
| H | 0.06393315961789 | 6.31789139257773 | 1.82981697528324 |
| C | 1.33921877912292 | 1.18036443427870 | 0.55112821850683 |
| C | 1.50013898014654 | -0.34980772504141 | 0.48649436684090 |
| H | 1.39493401318858 | -0.67924146938762 | -0.55589365836871 |
| H | 2.49158138709231 | -0.64187947454685 | 0.85837283900934 |
| H | 0.73617729112699 | -0.86320142489730 | 1.08833432638775 |
| C | 2.47554480502043 | 1.86098494196534 | -0.24024525296510 |
| H | 2.40152722724459 | 1.56777140702637 | -1.29554337800630 |
| H | 3.45173747304486 | 1.55118016834017 | 0.15714368750621 |
| H | 2.39455886334494 | 2.95484190331800 | -0.18044036161141 |
| C | 1.43807841299176 | 1.63693081919532 | 2.00732361456731 |
| O | 0.61987041079407 | 2.27608654749910 | 2.63162397457540 |
| O | 2.60071560317717 | 1.24736121050084 | 2.55860230338704 |
| C | 2.82164260195408 | 1.63004159272333 | 3.91514142793807 |
| H | 2.01688942251469 | 1.25307564163930 | 4.56403395184628 |

| | | | |
|---|---|---|---|
| H | 2.86016898794676 | 2.72618905500807 | 4.00969413417249 |
| H | 3.78443672346298 | 1.19019744549741 | 4.20320319184365 |
| H | -1.71207274505986 | -0.43620128532182 | -0.70394709837246 |
| O | -0.01852614826035 | 1.13945714531010 | -1.38481577071806 |
| H | -1.39223432789761 | 1.46525278666141 | 1.68532772116049 |
| C | -0.89653058115254 | 1.76657850843867 | -2.29628434790897 |
| H | -0.85086620109864 | 1.18007355009320 | -3.22540860011773 |
| H | -0.58978854412060 | 2.80390150059132 | -2.50531118304332 |
| H | -1.93970753886430 | 1.77660444410347 | -1.93343150870335 |

## 1-$G_1(x_1)$



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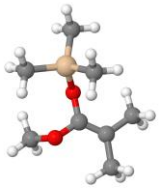
| C | -1.31718551688000 | 3.82601250536465 | -2.40330041083848 |
| C | -1.79329639530599 | 3.82622624077122 | 0.67084224010293 |
| C | 1.10270800801406 | 3.48323199518753 | -0.41817334758639 |
| H | -0.68497845941267 | 3.47331621508379 | -3.23254771913138 |
| H | -1.30949927901579 | 4.92890117745796 | -2.42968316369443 |
| H | -2.35240396245463 | 3.49759590037230 | -2.58823524841385 |
| H | 1.30024511231457 | 4.55628314564659 | -0.25331637465499 |
| H | 1.72931104785635 | 3.16116595476107 | -1.26275567226485 |
| H | 1.42731976689461 | 2.95010921764913 | 0.49020024006961 |
| H | -1.76073289979538 | 4.92645127194448 | 0.74153070390986 |
| H | -1.45043397856596 | 3.42244243619787 | 1.63687404239709 |
| H | -2.84456560286460 | 3.53402156461048 | 0.51888070660294 |
| C | 0.52912796895570 | -0.17726422891597 | -1.57429701623448 |
| C | 1.06346454646926 | -1.55294114221958 | -1.39216532376001 |
| H | 0.51019529077960 | -2.25049566309301 | -2.05340173477436 |
| H | 2.11823487941504 | -1.60282357777424 | -1.70349789867191 |
| H | 0.95451105410538 | -1.92423525726499 | -0.36550280467415 |
| C | 1.03168844104058 | 0.65896960233771 | -2.69456288325007 |
| H | 1.14306402135331 | 0.04085088708871 | -3.60107427550570 |
| H | 2.04677709399211 | 1.03405027940362 | -2.46151145157953 |
| H | 0.38807950912885 | 1.51555721442904 | -2.92455394235481 |
| C | -0.50390795705938 | 0.30976336668846 | -0.70269947162475 |
| O | -0.99281100263129 | 1.48858246629836 | -0.73259679341518 |
| O | -0.99166003196205 | -0.55174226411634 | 0.15058190006892 |
| C | -2.04153434708596 | -0.15348382332013 | 1.05750276382824 |
| H | -2.91552571533146 | 0.19202849303089 | 0.48823090265191 |
| H | -1.68142154118640 | 0.64920306744027 | 1.71619358159794 |
| H | -2.28189079514107 | -1.05094210743405 | 1.63648061415682 |

## 1-$G_2(x_2)$



| | | | |
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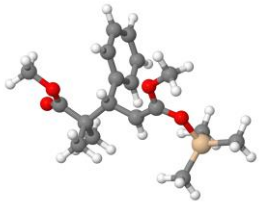
| C | -1.44544545388179 | 4.31104971911109 | -2.13465651749295 |
| C | -1.60755239174545 | 3.51104447590955 | 0.85066996427726 |
| C | 1.11871980166897 | 3.40863103751277 | -0.60516362080837 |
| H | -0.93021882677294 | 4.13954132363366 | -3.09343403368323 |
| H | -1.34024196445317 | 5.37729190486411 | -1.87410385175232 |
| H | -2.51728561504272 | 4.10099934848489 | -2.28255160001861 |
| H | 1.38378117870824 | 4.42752312289599 | -0.27737825016858 |
| H | 1.63009079807185 | 3.21021735799755 | -1.56077283140538 |
| H | 1.50878563297747 | 2.69713278542994 | 0.14045232313488 |
| H | -1.42863413578593 | 4.53698992965433 | 1.21408306816138 |
| H | -1.23713888803975 | 2.80580960490383 | 1.61123627146026 |
| H | -2.69681608855624 | 3.37262187127968 | 0.75351206100157 |
| C | 0.50461465538189 | -0.17202746258428 | -1.51844916334250 |
| C | 1.13777238139849 | -1.41046224436562 | -0.94681677095243 |
| H | 0.97641966426958 | -2.27996138219376 | -1.61010892788363 |
| H | 2.23305259741057 | -1.28696920171014 | -0.85840345094906 |
| H | 0.74025975710864 | -1.64967071911741 | 0.04787638431677 |
| C | 0.96737313180913 | 0.26527122497000 | -2.88065228643073 |
| H | 0.84954917727969 | -0.55094445302350 | -3.61608614854234 |
| H | 2.04315757623767 | 0.52243791451799 | -2.87141384331949 |
| H | 0.40609195171356 | 1.13578506645497 | -3.24477770994467 |
| C | -0.41706904669143 | 0.53037397820762 | -0.83392805062843 |
| O | -1.04859526148827 | 1.62856280153005 | -1.32646147592469 |
| O | -0.76379027205401 | 0.21023561128061 | 0.45114039271767 |
| C | -2.13761377340786 | -0.08588233917000 | 0.65716126720704 |
| H | -2.43198462540866 | -0.99225916469923 | 0.09756722713952 |
| H | -2.78458033969688 | 0.74930730943653 | 0.34326989970261 |
| H | -2.27081541534199 | -0.26387873650166 | 1.73316736369204 |

## $D_3^{Est\text{-}1,4}$-$G_1(x_1)$



| | | | |
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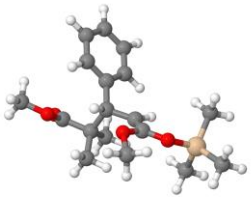
| C | -4.21286967232485 | -0.86523179592012 | 1.13372707847110 |
| C | -4.52541796812984 | 1.43889560745423 | 0.44789493384873 |
| C | -2.94845676686674 | -0.54715821205725 | 1.63489282734952 |
| C | -2.47347958473276 | 0.76335637750626 | 1.55113478543689 |
| C | -3.26634261545953 | 1.77581728336020 | 0.97300722325159 |
| C | -2.77129164595679 | 3.22192617776626 | 0.87447219210733 |
| C | -1.43920682597112 | 3.12345551979841 | 0.22865807450696 |
| C | -1.27946742400903 | 2.95258980004618 | -1.17351285601572 |
| O | -0.15486222295187 | 2.75354453714303 | -1.76064521633185 |
| H | -5.99221863512192 | -0.11421411871616 | 0.15388041960088 |
| H | -4.58825924417515 | -1.88871141682143 | 1.20281121817283 |
| H | -5.13887654024130 | 2.21628799354290 | -0.01187315511515 |
| H | -2.33071444849246 | -1.32029313024212 | 2.09710546575555 |
| H | -1.48826331159402 | 0.99919852759348 | 1.95537426708943 |
| Si | 1.53562698804480 | 2.49557163921250 | -1.22317850343489 |
| C | 1.47578183547096 | 1.00477506230397 | -0.10243950530819 |
| C | 2.04294478686907 | 4.07976166076117 | -0.38055991230644 |
| C | 2.39194493781128 | 2.19178831720982 | -2.84144986023795 |
| H | 2.50574448455574 | 0.70040579234922 | 0.14934134492067 |
| H | 0.99058164557673 | 0.15067726110663 | -0.60167040249246 |
| H | 0.95018533822107 | 1.19693144211380 | 0.84535699673756 |
| H | 1.98469219871212 | 1.30446730822841 | -3.35143084113246 |
| H | 2.29566996540038 | 3.05819167605970 | -3.51482079260725 |
| H | 3.46716690745604 | 2.01737763554541 | -2.66987210775389 |
| H | 1.90541084938226 | 4.94650193971715 | -1.04690314255769 |
| H | 3.11492410869949 | 4.02589203998845 | -0.12552056837291 |
| H | 1.49404253808749 | 4.26947242292365 | 0.55491719855910 |
| C | -2.78988160694771 | 4.04380020128955 | 2.20039860503297 |
| C | -1.86646786355373 | 3.48956569727268 | 3.28895256687088 |
| H | -0.81637617170202 | 3.46975591303166 | 2.95596130374523 |
| H | -1.91719817086698 | 4.13108690778394 | 4.17912274590350 |

| | | | |
|---|---|---|---|
| H | -2.16626675648428 | 2.48280736360719 | 3.60611381757768 |
| C | -2.41285430315428 | 5.50272626995558 | 1.87086150253473 |
| H | -1.37798482356200 | 5.55683164344276 | 1.49360218768583 |
| H | -2.46981464660105 | 6.13050595833998 | 2.77252283842025 |
| H | -3.08443431271128 | 5.92847461463363 | 1.11167521404827 |
| C | -4.23207021785098 | 4.01527431333551 | 2.73101770687695 |
| O | -4.54843947135739 | 3.69443566848918 | 3.84612996510158 |
| O | -5.11037173627292 | 4.40616518363907 | 1.78988110782201 |
| C | -6.49027194347947 | 4.42860245939936 | 2.18128041248038 |
| H | -6.63533667574407 | 5.09982177475918 | 3.03974920414746 |
| H | -6.82393851977239 | 3.41881330572088 | 2.46226886732027 |
| H | -7.04793949425282 | 4.79222192625919 | 1.31017424204239 |
| H | -3.45636757829761 | 3.72787904183390 | 0.18105588533460 |
| O | -2.35353699050575 | 3.01358721901603 | -1.91119738057382 |
| H | -0.53213333999674 | 3.08531262471161 | 0.83136171363461 |
| C | -2.26004619504861 | 2.82070955855921 | -3.33828436926008 |
| H | -1.61619918841752 | 3.59414315219741 | -3.77933592606849 |
| H | -3.28611996520241 | 2.90791381715587 | -3.70971553825186 |
| H | -1.84898365867297 | 1.82458457082045 | -3.55319871722252 |

## $D_3^{Est\text{-}1,4}$-$G_2(x_2)$



| | | | |
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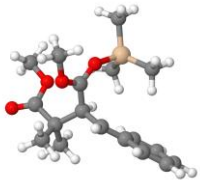
| C | -4.50258978489509 | -0.92482840918359 | 2.33210380259240 |
| C | -4.73284128546051 | 1.05358852949845 | 0.95479435876332 |
| C | -3.17360815606421 | -0.57464433005408 | 2.58642139961848 |
| C | -2.63137869545754 | 0.58521418086778 | 2.02785537633402 |
| C | -3.40319674115199 | 1.42526829384673 | 1.20896729054434 |
| C | -2.85365125749311 | 2.71221432043647 | 0.60901110134797 |
| C | -1.49104332521428 | 2.52466040970236 | -0.00019659464372 |
| C | -1.16612824969016 | 2.94700110063262 | -1.23815099454920 |
| O | 0.03854547374866 | 2.82741630716503 | -1.82503497963878 |
| H | -6.31784757999930 | -0.37402086233381 | 1.29264742737848 |
| H | -4.92685741830785 | -1.83275354192438 | 2.76823960672299 |
| H | -5.34401936572442 | 1.68802674722728 | 0.30906564407859 |
| H | -2.55241969166553 | -1.21021298209107 | 3.22312772097841 |
| H | -1.58887330076502 | 0.83409307520706 | 2.23487852770537 |
| Si | 1.55668378687276 | 2.39455125544372 | -1.17380525120469 |
| C | 1.53204565385249 | 0.58551283926510 | -0.67701998416082 |
| C | 1.94748210786387 | 3.52482860805410 | 0.27223999795476 |
| C | 2.73174032974466 | 2.68096644081383 | -2.60185643513738 |
| H | 2.53808073755771 | 0.26184206648299 | -0.36105159369989 |
| H | 1.22642573126875 | -0.04190648149044 | -1.53020868350128 |
| H | 0.83585797711605 | 0.38579970354730 | 0.15174641004355 |
| H | 2.45772025179595 | 2.05569060985884 | -3.46691534857442 |
| H | 2.71322562192711 | 3.73494731839118 | -2.92299936895265 |
| H | 3.76625178036824 | 2.43013004896204 | -2.31441526433831 |
| H | 1.90796945641196 | 4.58125566611678 | -0.03999132930445 |
| H | 2.96220318647481 | 3.32209722582310 | 0.65383853465555 |
| H | 1.23828592880719 | 3.39200509009316 | 1.10294803323289 |
| C | -2.89413691393227 | 3.91848797593755 | 1.63655652165586 |
| C | -1.90462599635485 | 3.74355548753538 | 2.79145037749217 |
| H | -0.88038365691253 | 3.65074697499703 | 2.40053266973718 |
| H | -1.94032593891824 | 4.61573388260036 | 3.46071814332979 |
| H | -2.14156867068334 | 2.86024671322436 | 3.39844369139913 |
| C | -2.59287156605698 | 5.22869212246364 | 0.88452652870584 |
| H | -1.56508282308282 | 5.20118951586160 | 0.49333161836672 |
| H | -2.67956094093652 | 6.09346254184055 | 1.56172274744197 |
| H | -3.28264794121793 | 5.37285656717020 | 0.04204426632630 |
| C | -4.30515731154375 | 4.00223592103878 | 2.21662708519134 |
| O | -4.59494091615857 | 3.90961464237551 | 3.38397284036509 |
| O | -5.23229600603590 | 4.20167447011125 | 1.25322696952456 |
| C | -6.58806501869935 | 4.23677739066051 | 1.69060885212864 |
| H | -6.74013361448301 | 5.03191548500499 | 2.43612452105145 |
| H | -6.87126722546216 | 3.27509793776661 | 2.14609358719421 |
| H | -7.19491551041874 | 4.42891517932683 | 0.79660430658663 |
| H | -3.53676946071048 | 3.00494514240015 | -0.19742995554934 |
| O | -2.09341174602017 | 3.52670574197722 | -2.03516768354961 |
| H | -0.73024315946085 | 1.99218250091288 | 0.56724148612149 |
| C | -1.65209994480134 | 4.43411128308509 | -3.03055587756777 |
| H | -1.10186800956928 | 5.28271351599219 | -2.58643939695636 |
| H | -2.55887743662172 | 4.81120664902609 | -3.52214699701948 |
| H | -1.00543409731409 | 3.94297818455193 | -3.77358230441132 |

## $D_3^{Est\text{-}1,3}$-$G_1(x_1)$



| | | | |
|---|---|---|---|
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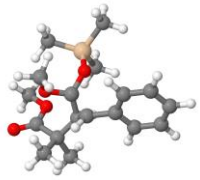
| C | -7.73500528669961 | 1.07112243796155 | 0.18025364614252 |
| C | -6.06026367984710 | 0.69183782765612 | -1.52630540155567 |
| C | -6.78868932523581 | 0.78046631661624 | 1.17564143518385 |
| C | -5.48394482166397 | 0.45328468016773 | 0.83290319192267 |
| C | -5.07362200054155 | 0.40589199417707 | -0.53374662425376 |
| C | -3.75682523736801 | 0.09001016956262 | -0.94483461550881 |
| C | -2.58504548853046 | -0.11642833085337 | -0.02350561642816 |
| C | -1.55146573004957 | 0.86535373312342 | -0.49154378291564 |
| O | -1.43139077453986 | 2.04525513801679 | -0.05171481892114 |
| H | -8.09611721106520 | 1.23832327598646 | -1.94929500902498 |
| H | -8.75975490111119 | 1.32792385284397 | 0.45689526831907 |
| H | -5.77400221943345 | 0.65262262762809 | -2.58033743288408 |
| H | -7.08252606125437 | 0.80321203385310 | 2.22764358281179 |
| H | -4.77514063919319 | 0.20689344404805 | 1.62466832924453 |
| Si | -2.12633583196093 | 3.11233333747044 | 1.22933562611433 |
| C | -2.36462684077932 | 2.07353775459659 | 2.76128295590418 |
| C | -3.69038816760657 | 3.76834536514721 | 0.47086794714162 |
| C | -0.75413982131457 | 4.35498198403373 | 1.39258802568061 |
| H | -3.32516204616077 | 1.53819512267248 | 2.76307444227318 |
| H | -2.35814673521127 | 2.73929275432326 | 3.64067751912914 |
| H | -1.55146799083656 | 1.34223893806365 | 2.88597554444356 |
| H | -1.03907171564928 | 5.13254310678866 | 2.12090538170241 |
| H | -0.54714007085311 | 4.85467454349510 | 0.43313078404031 |
| H | 0.17581086171084 | 3.88569860468440 | 1.75151238534620 |
| H | -4.43368126242227 | 2.97308971318919 | 0.31093323358582 |
| H | -3.49142602779049 | 4.26880376077832 | -0.48991155193324 |
| H | -4.13642352875187 | 4.51435705701697 | 1.15047247191222 |
| C | -2.07627117044209 | -1.59768474398750 | 0.08452233009040 |
| C | -3.01128833066725 | -2.33511436168584 | 1.06820471661727 |
| H | -4.04660145086040 | -2.30566840608992 | 0.69717724024389 |
| H | -2.98567354225583 | -1.87964409954357 | 2.07079632168416 |
| H | -2.70421670327920 | -3.38639434252945 | 1.15964881788940 |
| C | -2.06405010483274 | -2.34147677876496 | -1.25922544160741 |
| H | -3.08935679222636 | -2.46010828461926 | -1.63704419640609 |
| H | -1.62904395779232 | -3.33906861091160 | -1.11365175920717 |
| H | -1.46625320138627 | -1.81772512603424 | -2.01693544831567 |
| C | -0.67112453094304 | -1.64580154620666 | 0.69329172912612 |
| O | 0.06052374600311 | -2.59524069556736 | 0.65179471162311 |
| O | -0.34191393001112 | -0.49032176224966 | 1.32971986035909 |

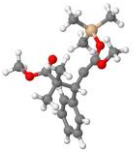
| | | | |
|---|---|---|---|
| C | 0.94466001192067 | -0.46812118848180 | 1.97074227228222 |
| H | 1.04571733810404 | 0.52833410812094 | 2.41766419170297 |
| H | 1.74248882396233 | -0.64942009989338 | 1.23637243468553 |
| H | 0.99652959698778 | -1.24495909676420 | 2.74635413131538 |
| O | -0.79879049663796 | 0.49511356196606 | -1.47317709628407 |
| H | -3.55789577509368 | 0.00993185934448 | -2.01616592366971 |
| H | -2.85143524469549 | 0.20938581469779 | 0.98603320235260 |
| C | 0.18930134680662 | 1.40324460800149 | -2.02046459417162 |
| H | 0.68780694762600 | 0.84001470514500 | -2.81555616226364 |
| H | 0.89958142933494 | 1.68699066673840 | -1.23268281903866 |
| H | -0.31068901837806 | 2.29498605396018 | -2.42084936527548 |

## $D_3^{Est\text{-}1,3}$-$G_2(x_2)$



| | | | |
|---|---|---|---|
| C | -6.87068141512345 | 1.83512462388675 | -1.36317764687702 |
| C | -7.72325803836526 | 1.20892772918094 | -0.44756362226308 |
| C | -5.54838926544328 | 1.40771023337361 | -1.49586378429900 |
| C | -7.24249106733527 | 0.15453091151933 | 0.33328742027062 |
| C | -5.91715326313581 | -0.26944934490462 | 0.19832155576818 |
| C | -5.05555045274761 | 0.34791861135220 | -0.71868365480179 |
| C | -3.64164800014777 | -0.10578574270458 | -0.88572065482990 |
| C | -2.77584235771119 | -0.43390744265234 | 0.33239758020566 |
| C | -2.49197488175755 | 0.78432592008263 | -0.48916058218568 |
| O | -2.81882776416764 | 2.04144847774274 | -0.03631629151768 |
| H | -7.23759576880373 | 2.66552530548480 | -1.97233107944960 |
| H | -8.75807236638055 | 1.54459263884694 | -0.34148946981798 |
| H | -4.87804778450172 | 1.90805958364300 | -2.19871158060311 |
| H | -7.90148076074870 | -0.34028288617663 | 1.05170955850967 |
| H | -5.54238580338188 | -1.09209759794776 | 0.81303569474291 |
| Si | -2.09548922539615 | 2.95432995857667 | 1.19803786709164 |
| C | -2.41633044359303 | 2.15006805370144 | 2.86458346261131 |
| C | -2.97234360812133 | 4.60694994039109 | 1.08594972309745 |
| C | -0.25939245311337 | 3.13011506191356 | 0.83697290570723 |
| H | -3.50024768827477 | 2.03372058810107 | 3.02942589989809 |
| H | -2.01541407210886 | 2.77468963790869 | 3.68085034666706 |
| H | -1.94669524353048 | 1.15762840271170 | 2.92071658137543 |
| H | 0.28059052873878 | 3.59341921840002 | 1.67942924149377 |
| H | -0.10279428873390 | 3.75966995254224 | -0.05428680025202 |
| H | 0.18344107053471 | 2.14550526835509 | 0.63053045634765 |
| H | -4.05721207772208 | 4.48012380903078 | 1.23295032291174 |
| H | -2.81620053669070 | 5.07000574492620 | 0.09814390473122 |
| H | -2.60116212919510 | 5.30616993470661 | 1.85379568010054 |
| C | -1.85154129465197 | -1.66108417613274 | 0.39329428266579 |
| C | -2.39695739848225 | -2.61021594964978 | 1.48621734922431 |
| H | -3.41740643549401 | -2.92978666899960 | 1.22188936953452 |
| H | -2.43384558043849 | -2.10843379837889 | 2.46470935332421 |
| H | -1.76727411593939 | -3.50892053653660 | 1.57717857151944 |
| C | -1.74735845592116 | -2.42670130955790 | -0.93069970758437 |
| H | -2.73168707303538 | -2.82438400233520 | -1.21793435288351 |
| H | -1.04577452614617 | -3.26487300748202 | -0.82314030656897 |
| H | -1.37177048686805 | -1.77877891480205 | -1.73355354486524 |
| C | -0.43759873662044 | -1.25698929919058 | 0.82521115446901 |
| O | 0.58615275083959 | -1.73141957105328 | 0.40236651822792 |
| O | -0.45429240575422 | -0.34076193584205 | 1.81914138758796 |
| C | 0.81597698046008 | 0.02057679027586 | 2.35920107076329 |
| H | 0.62157896105305 | 0.81204270486655 | 3.09354042702698 |
| H | 1.48588634573551 | 0.38810583998828 | 1.56870266499092 |
| H | 1.29087758931119 | -0.84589888541430 | 2.84460833797012 |
| O | -1.32010349704535 | 0.72736836751050 | -1.22936639960036 |
| H | -3.44964228384483 | -0.71093319171131 | -1.77690505537697 |
| H | -3.25555763570793 | -0.19541073360949 | 1.28456936836484 |
| C | -1.35001440295700 | 1.46556394739085 | -2.43549043248236 |
| H | -0.37943179448019 | 1.32008961129175 | -2.92916114471450 |
| H | -1.50688415020236 | 2.54058016318542 | -2.24537158677508 |
| H | -2.15516319685250 | 1.10646796419435 | -3.10352035945127 |

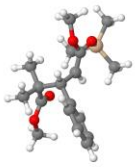
## $D_3^{Est\text{-}1,2}$-$G_1(x_1)$



| | | | |
|---|---|---|---|
| C | -3.65432618927502 | -1.68405164550726 | 2.33052696603725 |
| C | -3.63426624366910 | -1.03069429002809 | 3.56518008352872 |
| C | -2.83700888533237 | -1.23769977275807 | 1.28848985179013 |
| C | -2.79669858572980 | 0.07362995609795 | 3.75065897002540 |
| C | -1.98142647531072 | 0.51910547123903 | 2.70811429053660 |
| C | -1.98677428414701 | -0.13888867528850 | 1.46748733263071 |
| C | -1.07598561460827 | 0.29820933022780 | 0.32987984057416 |
| C | -1.29405219410329 | 1.73565410000793 | 0.01886050792989 |
| C | -1.19261738121190 | 2.30957522457578 | -1.27641259105437 |
| O | -1.16595948492726 | 3.57087487141662 | -1.50223822358904 |
| H | -4.30934322315396 | -2.54443113826178 | 2.17541005015638 |
| H | -4.27328144539800 | -1.37731217383207 | 4.38042177069550 |
| H | -2.85569485712617 | -1.75600737538066 | 0.32586451285948 |
| H | -2.78064200408284 | 0.59284829017953 | 4.71178299283392 |
| H | -1.34051016120482 | 1.38896435034523 | 2.87206371484757 |
| Si | -0.65802469284635 | 5.04606623037941 | -0.60648163208097 |
| C | -1.39540684788869 | 6.37067350146920 | -1.68062293770800 |
| C | 1.19920331485634 | 4.93198044323563 | -0.63597379103477 |
| C | -1.37167062600179 | 4.98348574352720 | 1.11532924143071 |
| H | -1.01999442423508 | 6.30615536179042 | -2.71404624046637 |
| H | -1.12656609250692 | 7.36479045871185 | -1.28626640273054 |
| H | -2.49494674822939 | 6.30539461361654 | -1.70346370972336 |
| H | -1.24776071246504 | 5.97860490943073 | 1.57594112330384 |
| H | -0.83563640934810 | 4.25777906685163 | 1.74529725666505 |
| H | -2.44969703415861 | 4.75589994132169 | 1.11923521063493 |
| H | 1.58952845705562 | 4.86398899224804 | -1.66363740471216 |
| H | 1.53288891678328 | 4.05796993047149 | -0.05516353921543 |
| H | 1.63343997146161 | 5.83317854164908 | -0.17099442847383 |
| C | 0.45837017778363 | -0.03044322172849 | 0.60349755632153 |
| C | 0.60048962224904 | -1.46672234019902 | 1.11142305669642 |
| H | 0.16676333760901 | -2.16579962488490 | 0.38013095377585 |
| H | 1.66158308125633 | -1.72051914388567 | 1.24179551953521 |
| H | 0.09386634326916 | -1.61557308158419 | 2.07291794700450 |
| C | 1.28765201216837 | 0.14806496240580 | -0.68562121580782 |
| H | 0.91061768773759 | -0.51967694970349 | -1.47435335752787 |
| H | 2.33928180804187 | -0.11304166167112 | -0.49371793157067 |
| H | 1.26441165298731 | 1.18239764085040 | -1.05560124134316 |
| C | 0.98337427647276 | 1.01419945465092 | 1.59000687427025 |
| O | 0.79917877922280 | 2.21137395445959 | 1.43555310433256 |
| O | 1.68250419375427 | 0.51119778571641 | 2.58961080324491 |
| C | 2.25089565179646 | 1.43247485731303 | 3.53657539784871 |
| H | 1.45266264583952 | 1.99656065595437 | 4.04018278519941 |
| H | 2.92544355230095 | 2.13477519447763 | 3.02684033033407 |
| H | 2.80172591541773 | 0.81806044124712 | 4.25701178818009 |
| H | -1.32200097364613 | -0.29139019257212 | -0.56662155256379 |
| O | -1.14229902304610 | 1.49606492779048 | -2.29908653847156 |
| H | -1.57964345110310 | 2.41740474376381 | 0.81440585756240 |
| C | -1.01011483680639 | 2.03085638614606 | -3.63271110753238 |

| | | | |
|---|---|---|---|
| H | -0.98963936167004 | 1.15892285625850 | -4.29444426677885 |
| H | -0.07689042172292 | 2.60565612046574 | -3.71335677241765 |
| H | -1.86785271310859 | 2.67742197699285 | -3.86334080598358 |

## $D_3^{Est\text{-}1,2}$-$G_2(x_2)$



| | | | |
|---|---|---|---|
| C | -3.20852438709441 | -1.67344675564338 | 2.58573554736588 |
| C | -3.21381404416665 | -0.94463128157387 | 3.77741346769907 |
| C | -2.47295885497073 | -1.21723387998979 | 1.48803232625569 |
| C | -2.48317037022374 | 0.24502021395085 | 3.85630265259211 |
| C | -1.75309996536679 | 0.69714119845797 | 2.75537275953939 |
| C | -1.72954781942304 | -0.03031228871985 | 1.55381151714422 |
| C | -0.91670919074908 | 0.43524706049658 | 0.35449643009799 |
| C | -1.16379617041867 | 1.88224980428574 | 0.03686580989637 |
| C | -1.44883681814671 | 2.34231182678641 | -1.19469336667866 |
| O | -1.58566809264078 | 3.63744081756076 | -1.53246219029565 |
| H | -3.78181479965954 | -2.60104500770533 | 2.50746915709945 |
| H | -3.78851456340133 | -1.29720778854948 | 4.63766336894372 |
| H | -2.47433781902534 | -1.79280270881716 | 0.55836112823353 |
| H | -2.48636025174417 | 0.82887017351775 | 4.78079685723276 |
| H | -1.19778431588974 | 1.63413536022195 | 2.83305266236826 |
| Si | -0.88879342054646 | 5.01511791755870 | -0.79128718086640 |
| C | -1.16060891931292 | 6.35783333132333 | -2.06937961785649 |
| C | 0.92961170630911 | 4.69607252969097 | -0.47782891708029 |
| C | -1.82097000771562 | 5.41419723674936 | 0.78875781420836 |
| H | -0.64513524734287 | 6.11458552381797 | -3.01264051829221 |
| H | -0.77374210982616 | 7.32574966625409 | -1.70975115951304 |
| H | -2.23357720063648 | 6.48058347068792 | -2.28910876205137 |
| H | -1.49532302734816 | 6.39031587498616 | 1.18630483910419 |
| H | -1.65217532257602 | 4.65998907324191 | 1.57264841121295 |
| H | -2.90499275418714 | 5.46973818058537 | 0.59708966146975 |
| H | 1.43868982321546 | 4.40534892328010 | -1.41179846587025 |
| H | 1.08822035370028 | 3.89905391832408 | 0.26531549641298 |
| H | 1.41195571466057 | 5.61611084374802 | -0.10585728904463 |
| C | 0.62767651065359 | 0.07776803614342 | 0.50261959977190 |
| C | 0.79416423656671 | -1.44224056073436 | 0.62674168785177 |
| H | 0.40175899376267 | -1.92844934655546 | -0.28071299835982 |
| H | 1.85583321284212 | -1.71380265655091 | 0.72786891745327 |
| H | 0.25950473247340 | -1.84585593183818 | 1.49532208638910 |
| C | 1.38838848899184 | 0.58119037422595 | -0.73501356396474 |
| H | 0.94371568866808 | 0.15245694801072 | -1.64600154401748 |
| H | 2.44573057454359 | 0.27485953051639 | -0.68890989741604 |
| H | 1.34701842563929 | 1.67409407229088 | -0.80858593579116 |
| C | 1.16277603714166 | 0.81783198245286 | 1.72533553266547 |
| O | 1.34308129824919 | 2.01535420747338 | 1.78278564165654 |
| O | 1.38748863657007 | 0.01036066805187 | 2.77491174192939 |
| C | 1.79193981319200 | 0.63972667987749 | 3.98786954623059 |
| H | 0.98431631018922 | 1.27938971887790 | 4.37639536082191 |
| H | 2.68584048142054 | 1.26105930541894 | 3.82932718717805 |
| H | 2.00330748892080 | -0.17016201817093 | 4.69700821468994 |
| H | -1.24144951962768 | -0.15510446423257 | -0.51402079647904 |
| O | -1.65468973420889 | 1.48837473270097 | -2.22837561464565 |
| H | -1.07537508350425 | 2.61071720594663 | 0.83923193137265 |
| C | -1.35206624691931 | 1.94235736703746 | -3.53651670592577 |
| H | -1.55929571867116 | 1.09863933420345 | -4.20869276053453 |
| H | -0.28771833962572 | 2.22456678972081 | -3.62925118697130 |
| H | -1.97301841274074 | 2.80444479060619 | -3.82367888323275 |

## 2.3.2 Comp. analysis of the reaction pathway of α,β-unsat. ketones

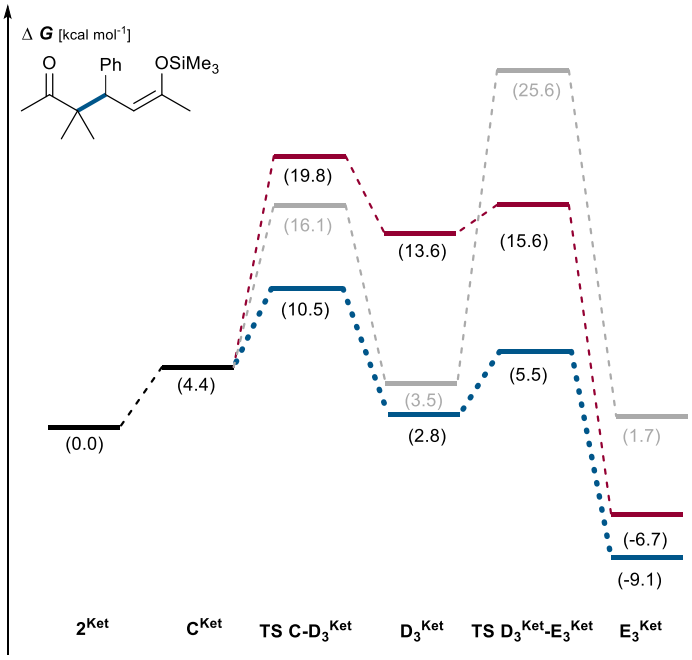
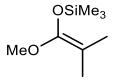
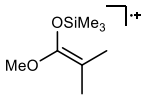
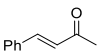
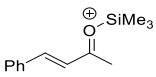
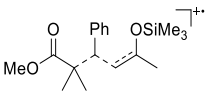



**Figure S7:** Reaction profile of radical addition of **B** to α,β-unsaturated ketones **2.**

**Table S6:** Energies of relevant structures for application of Electron-transfer Marcus-Hush Theory. Energy values are given in $E_h$.

| | Free energy | SP energy | ZPVE | Thermal Correction | Enthalpy Correction | Entropy Correction |
|---|---|---|---|---|---|---|
|  **1** | -755.41389166 | -755.61700281 | 0.24522497 | 0.01673055 | 0.00094421 | 0.05978858 |
|  **A** | -755.23365209 | -755.43572912 | 0.24513199 | 0.01711167 | 0.00094421 | 0.06111084 |
|  **2$^{Ket}$** | -462.10639437 | -462.24183131 | 0.17098266 | 0.01013238 | 0.00094421 | 0.04662231 |
|  **B** | -346.23069830 | -346.32880842 | 0.13177051 | 0.00890443 | 0.00094421 | 0.04350903 |
|  **C$^{Ket}$** | -871.10227080 | -871.34241616 | 0.28446110 | 0.01815190 | 0.00094421 | 0.06341185 |
|  **TS C-D$_3$$^{Ket-1,4}$** | -1217.31650356 | -1217.68048486 | 0.41906153 | 0.02721624 | 0.00094421 | 0.08324068 |

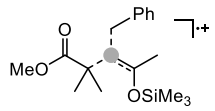
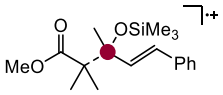
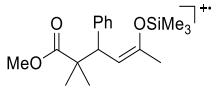
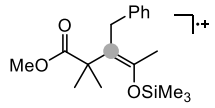
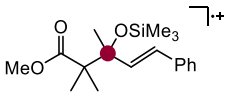
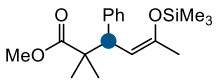
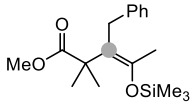
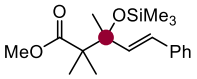
| | | | | | | |
|---|---|---|---|---|---|---|
|  **TS C-$D_3^{Ket-1,3}$** | -1217.30753364 | -1217.67397695 | 0.41933191 | 0.02680490 | 0.00094421 | 0.08063771 |
|  **TS C-$D_3^{Ket-1,2}$** | -1217.30163985 | -1217.66803118 | 0.41964825 | 0.02678603 | 0.00094421 | 0.08098716 |
|  **$D_3^{Ket-1,4}$** | -1217.32877339 | -1217.69589621 | 0.42109946 | 0.02721522 | 0.00094421 | 0.08213607 |
|  **$D_3^{Ket-1,3}$** | -1217.32768925 | -1217.69566741 | 0.42127569 | 0.02705826 | 0.00094421 | 0.08130000 |
|  **$D_3^{Ket-1,2}$** | -1217.31150565 | -1217.68092276 | 0.42203383 | 0.02649600 | 0.00094421 | 0.08005693 |
|  **$E_3^{Ket-1,4}$** | -1217.53169604 | -1217.90063431 | 0.42193619 | 0.02692781 | 0.00094421 | 0.08086994 |
|  **$E_3^{Ket-1,3}$** | -1217.53055893 | -1217.89935219 | 0.42188401 | 0.02683247 | 0.00094421 | 0.08086743 |
|  **$E_3^{Ket-1,2}$** | -1217.52409113 | -1217.89417027 | 0.42228696 | 0.02643488 | 0.00094421 | 0.07958691 |

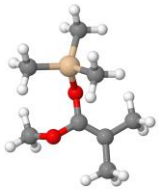
**Table S7:** Stationary point energies of relevant structures. Energy values are given in $E_h$.

| | $G_1(x_1)$ | $G_1(x_2)$ | $G_2(x_2)$ | $G_2(x_1)$ | r |
|---|---|---|---|---|---|
| **1** | -755.41389289 | -755.38850254 | -755.23363893 | -755.20437698 | 2.27725599 |
| **$D_3^{Ket-1,4}$** | -1217.284876 | -1217.301964 | -1217.530187 | -1217.482616 | 2.50273398 |
| **$D_3^{Ket-1,3}$** | -1217.32772468 | -1217.28826138 | -1217.51067701 | -1217.47028128 | 2.48696500 |
| **$D_3^{Ket-1,2}$** | -1217.28271092 | -1217.30370474 | -1217.52426806 | -1217.48629544 | 2.51339530 |

**Table S8:** Data for the calculation of the activation barrier of the electron transfer via Four-Point Approach to the Electron-Transfer Marcus-Hush Theory. Energy values are given in kcal $mol^{-1}$.

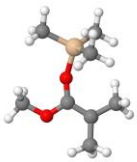
| | $\Delta G_0$ | $\lambda_i$ | $\lambda_o$ | $\lambda$ | $\Delta G^{\ddagger}$ |
|---|---|---|---|---|---|
| **$D_3^{Ket-1,4}$** | -40.82382603 | 15.84879979 | 50.00305086 | 65.85185065 | 2.37807294 |
| **$D_3^{Ket-1,3}$** | -1.69324958 | 42.17660947 | 50.13970740 | 92.31631687 | 22.24021875 |
| **$D_3^{Ket-1,2}$** | -38.46829530 | 10.78875388 | 49.91218664 | 60.70094052 | 2.03576135 |

## 1



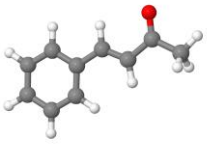
| | | | |
|---|---|---|---|
| Si | -0.73871666095863 | 3.21885893604048 | -0.78820770029077 |
| C | -1.44544649727906 | 4.31104934979919 | -2.13465632669758 |
| C | -1.60755236002462 | 3.51104399754353 | 0.85067035129574 |
| C | 1.11871951916892 | 3.40863071246837 | -0.60516420253531 |
| H | -0.93021997726184 | 4.13954079503740 | -3.09343386026655 |
| H | -1.34024280937238 | 5.37729146080419 | -1.87410349200440 |
| H | -2.51728666940907 | 4.10099876171800 | -2.28255090772136 |
| H | 1.38378104834946 | 4.42752270364781 | -0.27737871613911 |
| H | 1.63009002963274 | 3.21021702755411 | -1.56077366518442 |
| H | 1.50878526670696 | 2.69713216652683 | 0.14045148181082 |
| H | -1.42863408973314 | 4.53698945745528 | 1.21408337970046 |
| H | -1.23713834784522 | 2.80580908175176 | 1.61123636904132 |
| H | -2.69681606256839 | 3.37262123928936 | 0.75351272982760 |
| C | 0.50461437827801 | -0.17202759882952 | -1.51844908968440 |
| C | 1.13777218306104 | -1.41046239729382 | -0.94681672789735 |
| H | 0.97641935345744 | -2.27996158825015 | -1.61010877646500 |
| H | 2.23305241708492 | -1.28696942034587 | -0.85840356737089 |
| H | 0.74025967244989 | -1.64967073598220 | 0.04787650618150 |
| C | 0.96737295892894 | 0.26527104740360 | -2.88065218433752 |
| H | 0.84954931781381 | -0.55094471453929 | -3.61608599219683 |
| H | 2.04315730527112 | 0.52243815181557 | -2.87141358798934 |
| H | 0.40609159597545 | 1.13578472189716 | -3.24477775728862 |
| C | -0.41706939422046 | 0.53037369323556 | -0.83392796614035 |
| O | -1.04859564928642 | 1.62856252109310 | -1.32646150836552 |
| O | -0.76379066680497 | 0.21023536056648 | 0.45114044300907 |
| C | -2.13761418416676 | -0.08588275878652 | 0.65716108429663 |
| H | -2.43198482238290 | -0.99225959120114 | 0.09756694324851 |
| H | -2.78458081248992 | 0.74930678698811 | 0.34326957850349 |
| H | -2.27081604237493 | -0.26387916740741 | 1.73316716166021 |

## A



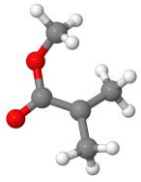
| | | | |
|---|---|---|---|
| Si | -0.70878264789662 | 3.25722568803358 | -0.73738109184549 |
| C | -1.29371802825804 | 3.83362197076937 | -2.40599297832219 |
| C | -1.78283928545257 | 3.83822310991464 | 0.66501081194277 |
| C | 1.11456888583758 | 3.46541131855299 | -0.40980592143548 |
| H | -0.66059932720196 | 3.47676381712093 | -3.23275184958438 |
| H | -1.27751063267402 | 4.93641195463975 | -2.43136810037168 |
| H | -2.33066571388435 | 3.51346947023525 | -2.59581264631445 |
| H | 1.32076207962523 | 4.53568621812779 | -0.23752103828295 |
| H | 1.74274509951240 | 3.14324509216530 | -1.25312231532837 |
| H | 1.43013884964356 | 2.92475714219474 | 0.49734141748113 |
| H | -1.73686787061097 | 4.93784434582785 | 0.73773935292486 |
| H | -1.45041009233184 | 3.42902919000993 | 1.63243673803942 |
| H | -2.83690833993505 | 3.55983350880850 | 0.50664786576070 |
| C | 0.51819727858255 | -0.17978756558232 | -1.57148649665361 |
| C | 1.04789035611243 | -1.55696724614000 | -1.38774474302179 |
| H | 0.50418687267669 | -2.25084193968286 | -2.06062180546976 |
| H | 2.10694259860173 | -1.60661588378133 | -1.68476851041209 |
| H | 0.92463983865804 | -1.93290383779040 | -0.36449885368558 |
| C | 1.02768136575134 | 0.65316166811207 | -2.69105677875109 |
| H | 1.13730478812560 | 0.03375340894833 | -3.59695889298912 |
| H | 2.04448819940404 | 1.02277111560615 | -2.45707625314276 |
| H | 0.38903492524756 | 1.51283333849414 | -2.92330418288601 |
| C | -0.51609769848514 | 0.31080379593777 | -0.70411432559681 |
| O | -1.00019758483228 | 1.49177230113770 | -0.73374783719384 |
| O | -1.01179445575363 | -0.54968692826500 | 0.14557596716584 |
| C | -2.06139907698175 | -0.14655011924233 | 1.05125795713417 |
| H | -2.93592449162593 | 0.19465423230335 | 0.48018884720484 |
| H | -1.70122232520864 | 0.66065864585473 | 1.70429416025670 |
| H | -2.30048356664596 | -1.04095781231065 | 1.63541150337705 |

## 2$^{Ket}$



| | | | |
|---|---|---|---|
| C | -8.30805260886242 | 2.04141879523285 | -0.34977849867533 |
| C | -9.67877738826299 | 1.77829401236564 | -0.28196100367391 |
| C | -7.40145151709364 | 0.98799127111343 | -0.47530149738835 |
| C | -7.84340164122305 | -0.34846275633956 | -0.53577363845923 |
| C | -9.23049899315288 | -0.59569497006786 | -0.46584716522861 |
| C | -10.13559759706156 | 0.45498443489040 | -0.34055695842366 |
| C | -6.84913502199967 | -1.41226127719080 | -0.66755460911707 |
| C | -7.05797455959819 | -2.74276626684329 | -0.74328133737282 |
| H | -5.80080281306374 | -1.09436158677083 | -0.71072489081219 |
| H | -9.60205517785505 | -1.62150597767826 | -0.51009080262894 |
| H | -7.94391421814259 | 3.07072801625385 | -0.30471971305661 |
| H | -6.32907328051876 | 1.19360045779651 | -0.52834955864005 |
| H | -11.20677085716416 | 0.24479481373405 | -0.28779202713750 |
| H | -10.39216434965119 | 2.60028559482596 | -0.18361437261919 |
| C | -5.91062146313977 | -3.68230656508935 | -0.87601338169578 |
| H | -8.06402818599754 | -3.17136240745999 | -0.71024711058197 |
| O | -4.75686720105815 | -3.29604206799769 | -0.92246759336991 |
| C | -6.26297474844187 | -5.15535063599444 | -0.95450017082636 |
| H | -5.34835914078770 | -5.75429889318107 | -1.05159486260886 |
| H | -6.92602284767364 | -5.34340929701013 | -1.81614771206102 |
| H | -6.81726638925142 | -5.46337469458942 | -0.05156309562269 |

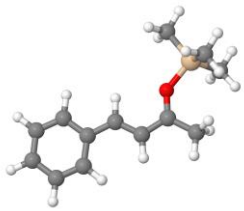
## B



| | | | |
|---|---|---|---|
| C | 0.15854831486826 | -0.26091685412808 | -1.81656301087734 |
| C | 1.09695865236965 | -1.37116260880147 | -1.46528197252030 |
| H | 0.56034294658297 | -2.25933806869162 | -1.07835753205434 |
| H | 1.63933336702863 | -1.70817674074455 | -2.36567795648130 |
| H | 1.83714335122033 | -1.07258382656553 | -0.71036856094538 |
| C | -0.54757805137152 | -0.31058875187964 | -3.12943502448994 |
| H | -1.02062585138255 | -1.29677096653879 | -3.28527018924215 |
| H | 0.16976219304299 | -0.17685725881992 | -3.96330378161707 |
| H | -1.30270398023678 | 0.48162331600071 | -3.21241222044069 |
| C | 0.05445402229010 | 0.96975897682547 | -1.02956631743780 |

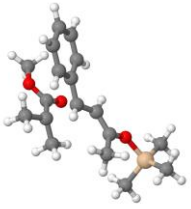
| | | | |
|---|---|---|---|
| O | -0.28058519374554 | 2.02784584540263 | -1.52336752125255 |
| O | 0.41327785217069 | 0.94050692526456 | 0.28902756474136 |
| C | 0.05477733395010 | -0.15296266496769 | 1.11862197333245 |
| H | 0.92711485672229 | -0.78468153780037 | 1.35304942707963 |
| H | -0.72542184524792 | -0.78101488731380 | 0.65793653780444 |
| H | -0.34094796826169 | 0.26027910275809 | 2.05919858440099 |

### $C^{Ket}$



| | | | |
|---|---|---|---|
| C | -8.52993266834962 | 1.12540575788512 | -0.54959813260257 |
| C | -8.69024896343651 | -0.24791783408471 | -0.32677204550346 |
| C | -7.26458145708278 | 1.69308232200605 | -0.45711664961485 |
| C | -7.58458859853994 | -1.05530406434897 | -0.01108064108498 |
| C | -6.31965940411726 | -0.49433296849504 | 0.08246063908674 |
| C | -6.13540078693611 | 0.89548673342673 | -0.13964027578953 |
| C | -4.85553482371455 | 1.53476472042495 | -0.05819495834729 |
| C | -3.63894483842949 | 0.95397201681508 | 0.23287462700155 |
| C | -2.44358070042719 | 1.71188991825166 | 0.27791508411032 |
| O | -2.48814109816324 | 2.97806191462542 | 0.04349414930373 |
| H | -9.39414458618258 | 1.74596638358263 | -0.79447965622143 |
| H | -9.68390527319191 | -0.69680651055951 | -0.39881326335668 |
| H | -7.12978134029478 | 2.76384754687529 | -0.62939415122871 |
| H | -7.72272596918682 | -2.12472232737413 | 0.16040230294274 |
| H | -5.46718943869997 | -1.12976357464306 | 0.32815032609339 |
| Si | -1.35227449270640 | 4.35303903529206 | 0.02171554970387 |
| C | -0.81786665733654 | 4.59766105673397 | 1.79266330139918 |
| C | -2.44911716136378 | 5.70902648971027 | -0.62113015123665 |
| C | 0.03593105833736 | 3.91021973546685 | -1.14391620919126 |
| H | -1.68604445603243 | 4.69526255375663 | 2.46381720919018 |
| H | -0.23657043055108 | 5.53275450012520 | 1.86468907952528 |
| H | -0.17361966411354 | 3.78646209248055 | 2.16580333774292 |
| H | 0.73142572906854 | 3.16644161192250 | -0.72643480767696 |
| H | 0.62062429474349 | 4.82231912959886 | -1.35335182599450 |
| H | -0.34551231479262 | 3.53849476372913 | -2.10868569170894 |
| H | -3.30900469324996 | 5.87756460187852 | 0.04656954663943 |
| H | -2.82848468728793 | 5.47380908761111 | -1.62834367546104 |
| H | -1.88463811869085 | 6.65384220286576 | -0.68713326255577 |
| H | -4.84331934822009 | 2.61290525507899 | -0.25024846987639 |
| H | -3.55388277762941 | -0.11336223036719 | 0.43799742395423 |
| C | -1.13440297505747 | 1.05933183287794 | 0.57782981885925 |
| H | -1.25317464805460 | 0.00495492551176 | 0.85350607843580 |
| H | -0.62056797084187 | 1.59392519519257 | 1.39237016132010 |
| H | -0.48417073946805 | 1.12267812614702 | -0.31107476785771 |

### TS C-$D_3^{Ket-1,4}$



| | | | |
|---|---|---|---|
| C | -6.07970937695149 | 0.19691519210460 | 1.42553257014235 |
| C | -5.56044276638251 | -0.63241273646683 | 2.42419095166179 |
| C | -5.26896787121363 | 1.16427631468944 | 0.83287390157129 |
| C | -4.22359449598694 | -0.49526202297684 | 2.81873708923288 |
| C | -3.41066198970142 | 0.46653366536206 | 2.22408098563609 |
| C | -3.92336981559164 | 1.31406258414866 | 1.22159999456628 |
| C | -3.10261199813499 | 2.34895346533821 | 0.55885802578264 |
| C | -1.69287690858760 | 2.22468729943238 | 0.46610433121113 |
| C | -0.87101581450709 | 2.81267961964813 | -0.50699991230222 |
| O | 0.40600950586428 | 2.61924039162023 | -0.36322591893157 |
| H | -7.11813425664517 | 0.08721322005673 | 1.10552228824356 |
| H | -6.19409837324077 | -1.38940091073682 | 2.89179162554047 |
| H | -5.67789783717879 | 1.80526807769113 | 0.04764993336281 |
| H | -3.81309175773997 | -1.14752615522036 | 3.59291998481681 |
| H | -2.37469908722498 | 0.56433547645126 | 2.55194110947744 |
| Si | 1.91082288682222 | 3.13814854411728 | -1.13500296599423 |
| C | 3.17554588262652 | 2.15431867299135 | -0.19436952622784 |
| C | 2.01943073526061 | 4.97842425037337 | -0.82752040770127 |
| C | 1.81832668481841 | 2.68229269432810 | -2.94475950628736 |
| H | 4.19003182106769 | 2.39838923775109 | -0.55050441663169 |
| H | 3.02066097684886 | 1.07217578410274 | -0.33060638040339 |
| H | 3.13028788259800 | 2.37763603978703 | 0.88327333845950 |
| H | 1.51207605761216 | 1.63247475238392 | -3.08131294228004 |
| H | 1.13809580384476 | 3.32863738604034 | -3.51991755054500 |
| H | 2.82338686382693 | 2.78979569622889 | -3.38721119926297 |
| H | 1.26208574622800 | 5.55303486930504 | -1.38339321087897 |
| H | 3.00877085296605 | 5.34206936267174 | -1.15319389782616 |
| H | 1.91855911018821 | 5.20723253375755 | 0.24557678118766 |
| C | -3.32203962558483 | 4.03316584091641 | 1.76844462215032 |
| C | -2.38017624525386 | 5.07919777457430 | 1.23845194977006 |
| H | -2.59496274586287 | 5.32863476467403 | 0.18981083359540 |
| H | -2.53625129413322 | 6.00388450633988 | 1.82372505104668 |
| H | -1.33008621960912 | 4.78745274059796 | 1.36134363270762 |
| C | -4.78185800822939 | 4.35665311716898 | 1.64556282726140 |
| H | -5.04024503987505 | 4.66544075149408 | 0.62133858611612 |
| H | -4.99943783365672 | 5.21214549970856 | 2.31131324872532 |
| H | -5.42599160493307 | 3.53001014990740 | 1.96464892030796 |
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| H | -2.80791045038887 | 3.22034809723423 | 5.70536695694906 |
| H | -3.11584078961161 | 1.59224797552992 | 5.02283816493948 |
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| H | -0.87124177313347 | 4.56870632580365 | -1.73216441731062 |
| H | -2.44148287740007 | 3.71678972699509 | -1.70445207214167 |
| H | -1.06786444267622 | 3.04371489582658 | -2.61432866671263 |
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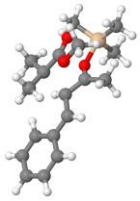

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| C | -7.25868579200548 | -0.64408133978623 | -1.18825142940227 |
| C | -6.33112977041765 | -2.58146289543904 | 0.60437122647951 |
| C | -5.48149996933554 | -1.55808903772077 | 0.20719411097245 |
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| C | -5.09590675361266 | 0.51415052234470 | -1.15370878732334 |
| C | -3.72416290410601 | 0.71011728395705 | -0.78149389855008 |
| C | -3.14033762036352 | 2.03359890716292 | -0.84072123166750 |

| | | | |
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| O | -2.13226071481908 | 2.25618076557866 | -0.10531198901776 |
| H | -9.12288522211778 | -1.71917034173980 | -1.17034844056970 |
| H | -8.30688421399738 | -3.45521629432599 | 0.42768933537531 |
| H | -7.61827345471749 | 0.11437581491657 | -1.88852043100283 |
| H | -5.97579734713821 | -3.33917658262004 | 1.30640288709482 |
| H | -4.46658473562181 | -1.52793099763104 | 0.60806583275815 |
| Si | -0.77921180470138 | 3.42525320421770 | 0.14250071207495 |
| C | -1.30314328696819 | 4.25932991694233 | 1.72255558588438 |
| C | -0.62696849047339 | 4.57676814180990 | -1.31559859331492 |
| C | 0.67323525806732 | 2.27857590221895 | 0.30326805095864 |
| H | -0.51545348717147 | 4.95943742988185 | 2.04829070599195 |
| H | -1.45980858785619 | 3.52917031560605 | 2.53202137489834 |
| H | -2.22998448530829 | 4.84027869870230 | 1.59004549830061 |
| H | 1.57648798961535 | 2.85912212718900 | 0.55477746212881 |
| H | 0.85248232522378 | 1.75991547654572 | -0.65074721544277 |
| H | 0.51839699706291 | 1.53295994785604 | 1.09847211826622 |
| H | -1.42995471823773 | 5.32732763738108 | -1.37437142261829 |
| H | -0.56877576472719 | 4.00835593870712 | -2.25601436328467 |
| H | 0.32283529404067 | 5.12740475512409 | -1.19962768840692 |
| C | -2.43558276235627 | -0.22006248161991 | -2.08654938693167 |
| C | -1.36233063163367 | -0.73140178363161 | -1.16056745572399 |
| H | -0.56684388725540 | -1.21116079268310 | -1.75815867885367 |
| H | -1.76313244337212 | -1.48591624260272 | -0.46887148872283 |
| H | -0.88929450500669 | 0.07673817717094 | -0.59011036280408 |
| C | -3.31342700104465 | -1.26200035989008 | -2.72549114141446 |
| H | -3.68953752765039 | -1.97800625069663 | -1.98313331380092 |
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| O | -2.68119140101176 | 0.99132840627349 | -4.10828624167523 |
| C | -2.24716283423872 | 1.95944423007227 | -5.07616384323095 |
| H | -2.31166155821279 | 2.97643796508027 | -4.66157178216912 |
| H | -2.92213290100152 | 1.85201610963780 | -5.93268763270561 |
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| H | -4.53633509140132 | 3.57312485702541 | -1.18335442337350 |
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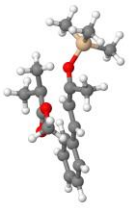
## TS C-$D_3^{Ket-1,2}$



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| C | -5.19548529717518 | 2.26407656381243 | -1.42254896795577 |
| C | -3.95078470837518 | 1.64048527303216 | 1.01274820896578 |
| C | -3.19505600674576 | 2.17814869018465 | -0.01576286740138 |
| C | -3.80234297862615 | 2.50255890627890 | -1.26227375593366 |
| C | -3.07681241302245 | 3.04874135638813 | -2.37062855453807 |
| C | -1.73377635256513 | 3.35775244660024 | -2.38075724971833 |
| C | -0.97692523524668 | 3.88220528096420 | -3.50385496692425 |
| O | 0.23624690407449 | 4.33919331253521 | -3.13347944407757 |
| H | -7.01433106237585 | 1.54111786603685 | -0.52302112820149 |
| H | -5.91726286116966 | 0.98718596102603 | 1.64704563887861 |
| H | -5.66720094458225 | 2.50493537596414 | -2.37800376802157 |
| H | -3.47928566516902 | 1.39155132415402 | 1.96557202650078 |
| H | -2.12818656165754 | 2.34790622519144 | 0.13573163446159 |
| Si | 1.13251611870390 | 5.81360203994405 | -3.25304241225037 |
| C | 1.33000654455347 | 6.33402152809902 | -5.04198718030693 |
| C | 2.76474838367511 | 5.34847149402526 | -2.48183474959208 |
| C | 0.19620731155635 | 7.09336689043369 | -2.25565581700308 |
| H | 2.04081451543293 | 7.17668066027277 | -5.08725149415431 |
| H | 0.38830868783579 | 6.67827439363756 | -5.49615141048090 |
| H | 1.74370690842179 | 5.52343279515246 | -5.66207623840158 |
| H | 0.03415987116956 | 6.75211371669989 | -1.22056156654179 |
| H | -0.78345907932226 | 7.33630751028532 | -2.69771824048617 |
| H | 0.77653519446563 | 8.03042701930429 | -2.21171489201033 |
| H | 3.27089630187610 | 4.55990646401594 | -3.06174693477005 |
| H | 2.62863874238370 | 4.98354823250262 | -1.45141459862149 |
| H | 3.43670870124915 | 6.22167120627148 | -2.44644419467208 |
| C | 0.62080963636114 | 2.58392250840287 | -5.29952493621218 |
| C | -0.49230646603202 | 2.19268800234195 | -4.35813914512145 |
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| H | 0.33597335343362 | 3.36425684929454 | -6.01441540137999 |
| H | 0.88746121428208 | 1.69180846226914 | -5.89285847698482 |
| C | -0.03594639322337 | 1.24108975949131 | -3.27305168439269 |
| H | 0.45765047881816 | 0.37598760270582 | -3.74822061866486 |
| H | -0.87285596234759 | 0.86039117743216 | -2.67541922065090 |
| H | 0.70806358930537 | 1.72689147000320 | -2.62545282947955 |
| C | -1.78340695269677 | 1.75223606766108 | -5.01805585176089 |
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| O | -1.81745210812071 | 2.05662269163184 | -6.31680713543963 |
| C | -2.99188765275112 | 1.66409269056605 | -7.04357370416782 |
| H | -3.13274021061973 | 0.57563898020889 | -6.98240268887013 |
| H | -2.82303517215878 | 1.97566674075987 | -8.08035092344553 |
| H | -3.88165205762510 | 2.16138816538002 | -6.62917275470851 |
| H | -3.66398782245046 | 3.23373211237859 | -3.27059080921442 |
| H | -1.12548179604969 | 3.16603820201074 | -1.49486349577553 |
| C | -1.70871236167273 | 4.69201055445851 | -4.55997220163827 |
| H | -2.66861992171702 | 4.24378745537196 | -4.84175646682958 |
| H | -1.10334311475415 | 4.80212296145919 | -5.46599087675316 |
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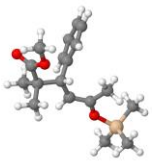
## $D_3^{Ket-1,4}$



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| C | -4.39300914707045 | 1.18572035112381 | 0.21832620585720 |
| C | -2.89196030128476 | -0.71485532699880 | 1.62799614004795 |
| C | -2.55629517714007 | 0.63763913278198 | 1.70954943087297 |
| C | -3.31203650169069 | 1.60568597743010 | 1.01334832360860 |
| C | -2.95297353057389 | 3.08794987306868 | 1.09798397228610 |
| C | -1.48673949783558 | 3.16832320111029 | 0.87646194467834 |
| C | -0.84156373215515 | 2.88861680258569 | -0.34839494909632 |
| O | 0.44950376069535 | 2.95119779548995 | -0.32999306369969 |
| H | -5.58836539651076 | -0.47844368989993 | -0.45297931558873 |
| H | -4.24880304292062 | -2.17546351215531 | 0.79033260020551 |
| H | -4.98129573018810 | 1.92928198612202 | -0.32347538579613 |
| H | -2.30773797435652 | -1.45419251648927 | 2.18021305979516 |
| H | -1.71592639688095 | 0.94462901463798 | 2.33440468205329 |
| Si | 1.78958203642074 | 2.72852987571448 | -1.49350397511695 |
| C | 3.26356328463554 | 2.78951113495318 | -0.36581540369031 |
| C | 1.67693670202166 | 4.17733168627963 | -2.66445639968501 |
| C | 1.53286912282588 | 1.06246072880854 | -2.29555137320812 |

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| H | 3.23639403311643 | 1.97359653712630 | 0.37376883084792 |
| H | 3.31321971076797 | 3.74792369733806 | 0.17475775490150 |
| H | 1.37234373716038 | 0.27365930391795 | -1.54288896218676 |
| H | 0.69646596525173 | 1.04858357738798 | -3.01016124293438 |
| H | 2.44721135772066 | 0.79961546577132 | -2.85459860817837 |
| H | 0.78861503730909 | 4.14367504373234 | -3.31390323680314 |
| H | 2.56325291660411 | 4.17124278586819 | -3.32171555511941 |
| H | 1.67765549787770 | 5.13309315929351 | -2.11663008673161 |
| C | -3.45139737687367 | 3.83034137834004 | 2.37828138206682 |
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| H | -2.01943891024128 | 5.48063091226403 | 2.22626538073711 |
| H | -3.50616957538889 | 5.89060474844992 | 3.10275896235879 |
| H | -3.54007118310421 | 5.75742253352683 | 1.32623922443608 |
| C | -4.98070398803159 | 3.68528242985709 | 2.42888567241800 |
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| O | -5.55070578613701 | 4.06399046726609 | 1.26839359355149 |
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| H | -7.32914158196810 | 2.97076287999764 | 1.36761513561977 |
| H | -7.26903789938324 | 4.36893938734274 | 0.22412386033956 |
| H | -3.46487783666404 | 3.57397476228806 | 0.25144836317852 |
| C | -1.55846212693072 | 2.52562959138515 | -1.60704196048454 |
| H | -0.80955801428063 | 3.38643554623380 | 1.70719224717493 |
| H | -1.46858073934170 | 1.43874316673047 | -1.77293757617758 |
| H | -1.10432609302935 | 3.03543163842303 | -2.46888014559189 |
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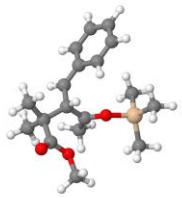
## $D_3^{Ket\text{-}1,3}$



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| C | -6.47431084999797 | 1.26072525271703 | 1.58630823589569 |
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| C | -3.91487914833697 | -0.31200590737770 | -0.67596961264557 |
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| C | -2.10784931125725 | 0.76210217073720 | -0.00928800646686 |
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| H | -8.01959135723130 | 1.61564072648189 | -1.44598492809054 |
| H | -8.35911852752453 | 2.13744123969847 | 0.97163248984395 |
| H | -5.95492195370434 | 0.46138093816413 | -2.18912644971347 |
| H | -6.63389379430805 | 1.47608706560905 | 2.64537800631383 |
| H | -4.57553751173212 | 0.32906815290466 | 1.93070634013783 |
| Si | -2.40775234858990 | 3.31313214554558 | 1.25566728619398 |
| C | -2.95427148501664 | 3.36593121516364 | 3.03038908476752 |
| C | -3.69734530291596 | 3.93617950623846 | 0.05893028136748 |
| C | -0.68697679352068 | 3.97586964073496 | 0.97784617252887 |
| H | -3.94477576708823 | 2.90037415525035 | 3.15130493787611 |
| H | -3.02701838919948 | 4.41098001535163 | 3.37417168940670 |
| H | -2.23921451524727 | 2.84455244466872 | 3.68629297565161 |
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| H | -3.38032103973820 | 3.87687530338562 | -0.99352106345558 |
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| C | -2.78489887435705 | -3.09522794362836 | 0.09937859001845 |
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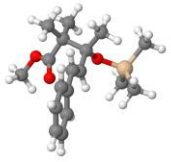
| H | -2.21065957056935 | -1.87728335583051 | -2.38632088235824 |
| H | -0.94626283604460 | -2.98167629378306 | -1.82646105532427 |
| H | -0.60600091401921 | -1.24731976339014 | -1.89817406249593 |
| C | -0.65273869502723 | -1.93131390480637 | 0.69923629353584 |
| O | -0.25270617342126 | -2.89917840987428 | 1.28544049643251 |
| O | -0.03388445394598 | -0.72821930134295 | 0.74139876746377 |
| C | 1.15987025521785 | -0.65409334508437 | 1.53799587540646 |
| H | 1.51113721340781 | 0.38227754767940 | 1.46558209151679 |
| H | 1.92075006464451 | -1.34613865034019 | 1.15004170466388 |
| H | 0.94042090164526 | -0.91743932090172 | 2.58248701325137 |
| C | -1.42928695393650 | 1.26887112879011 | -1.23497110929697 |
| H | -3.84807504460670 | -0.49794739787788 | -1.75121603831519 |
| H | -2.96864068540080 | -0.69170842454592 | 1.20561737244829 |
| H | -1.57819400892939 | 0.61536642321956 | -2.09837191873458 |
| H | -0.34783569433956 | 1.31491981459579 | -1.02064245009757 |
| H | -1.76934128323156 | 2.28449900661762 | -1.48106097197390 |

## $D_3^{Ket\text{-}1,2}$



| | | | |
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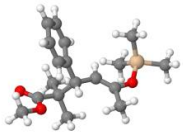
| C | -4.89151666833339 | -1.56786721361485 | 2.94939687916491 |
| C | -3.52653381443090 | -1.56027990655543 | 0.95885571196751 |
| C | -4.20228631443370 | -0.44517782201021 | 3.44647800194085 |
| C | -3.18351968734546 | 0.12833662708249 | 2.70652290129649 |
| C | -2.82355312493826 | -0.41267554181782 | 1.43474362429203 |
| C | -1.78440553374092 | 0.13525393997554 | 0.63065808059257 |
| C | -1.08601771542721 | 1.30867245361020 | 0.91934488813086 |
| C | -0.00330158615224 | 1.93908374936639 | 0.06389398330158 |
| O | 0.20223222030219 | 3.24415081435014 | 0.53128479727068 |
| H | -5.08609871923032 | -2.99686225240539 | 1.32925419356435 |
| H | -5.69698227120471 | -2.01294754807386 | 3.53851658110463 |
| H | -3.25150105057529 | -1.98579680932471 | -0.00930958683789 |
| H | -4.47133632430258 | -0.03051301757621 | 4.42005520878366 |
| H | -2.63946313488675 | 0.98401053601393 | 3.10771061405752 |
| Si | -0.65392750332073 | 4.70919645789679 | 0.33789611824517 |
| C | -0.36106815199917 | 5.40320080527647 | -1.37882076161964 |
| C | 0.07571181073152 | 5.81040194650176 | 1.65718193851334 |
| C | -2.48751022750250 | 4.39682759451694 | 0.63569217959400 |
| H | 0.71656573996308 | 5.43816952674335 | -1.60788986443027 |
| H | -0.74580917501705 | 6.43532594802819 | -1.43545022043287 |
| H | -0.86125138086223 | 4.82085462987638 | -2.16788900099645 |
| H | -3.05041702716717 | 5.33289630798878 | 0.48247006414189 |
| H | -2.68485457262135 | 4.06636064729377 | 1.66915483775438 |
| H | -2.91362987198387 | 3.64973085712895 | -0.05414020559875 |
| H | 1.15545727837152 | 5.95831405921455 | 1.49413185389171 |
| H | -0.06179454507997 | 5.37451432651214 | 2.65974539536588 |
| H | -0.40494174959226 | 6.80241665344230 | 1.64794902058636 |
| C | 1.36848343961432 | 1.18841843011741 | 0.32337958045079 |

| | | | |
|---|---|---|---|
| C | 1.41763617080712 | -0.25505565682570 | -0.22101103537858 |
| H | 1.36879810554820 | -0.25296758452543 | -1.31909839465168 |
| H | 2.37291246303930 | -0.71958873403626 | 0.06410786239944 |
| H | 0.61103968706116 | -0.88874546182675 | 0.17275388195449 |
| C | 2.55072034596461 | 1.98601671050444 | -0.23240383231474 |
| H | 2.49296457326475 | 2.03561274292116 | -1.32948747265467 |
| H | 3.49421978237324 | 1.48876010497587 | 0.03125274245063 |
| H | 2.56411466535942 | 3.00643533683588 | 0.16683467031077 |
| C | 1.41293016033043 | 1.06473317554358 | 1.84245584140409 |
| O | 0.38734871317871 | 0.88275764155689 | 2.49451817562308 |
| O | 2.60456985473869 | 1.09699805661765 | 2.38215921267731 |
| C | 2.70941020017383 | 0.92264412133722 | 3.81155607441002 |
| H | 2.31696432177297 | -0.06273429984567 | 4.09890015050312 |
| H | 2.14193221162310 | 1.71047314457543 | 4.32585555893055 |
| H | 3.77761644503332 | 0.99879662333959 | 4.04027668665170 |
| H | -1.53032435259503 | -0.41672580993483 | -0.27719931745843 |
| C | -0.39813890297711 | 1.91442671450930 | -1.42364258129321 |
| H | -1.48381171286127 | 1.97207301865791 | 1.68397560758313 |
| H | -0.50471117915775 | 0.89314822609552 | -1.81108418194703 |
| H | 0.37018045406316 | 2.43265754416246 | -2.01237893189454 |
| H | -1.35433211949726 | 2.43436670206376 | -1.57408907252437 |

## $E_3^{Ket\text{-}1,4}$



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| C | -3.74071269408765 | -0.54373124993747 | 3.27178021985843 |
| C | -4.33877843403128 | 0.99547452067518 | 1.50072043464517 |
| C | -2.49347671054329 | 0.07891321651536 | 3.37098537054115 |
| C | -2.17438596680149 | 1.15498235690805 | 2.53923500389238 |
| C | -3.09446441349901 | 1.63843917625176 | 1.59459879942210 |
| C | -2.78927318584219 | 2.82500587758338 | 0.68695937695114 |
| C | -1.41569223306554 | 2.72455375616377 | 0.08208376054308 |
| C | -1.10258150284692 | 2.77296911279780 | -1.22718867550976 |
| O | 0.17233738495841 | 2.64118969787925 | -1.68606187730696 |
| H | -5.63781545333723 | -0.56665614263215 | 2.23280151177285 |
| H | -3.98972927132062 | -1.38639859337528 | 3.92157630783647 |
| H | -5.06315708843990 | 1.34929425770275 | 0.76360517697956 |
| H | -1.76060076892004 | -0.27646103632164 | 4.10006138254318 |
| H | -1.19089459366394 | 1.61893183025940 | 2.63111000017533 |
| Si | 1.60005346562617 | 2.15333816800215 | -0.90408552712194 |
| C | 2.85705642493387 | 2.07827446149313 | -2.29011565431773 |
| C | 1.34762717078046 | 0.46088588962673 | -0.12815277319695 |
| C | 2.11752881103769 | 3.43545307575420 | 0.37203786817413 |
| H | 3.84312431163626 | 1.76392364296040 | -1.90959762502813 |
| H | 2.97441015383388 | 3.06379888333855 | -2.76909864768935 |
| H | 2.54408374290502 | 1.35957280241870 | -3.06455862369618 |
| H | 2.13265626196752 | 4.44146022065683 | -0.07874403136282 |
| H | 1.44511775941655 | 3.46719682901487 | 1.24318540356628 |
| H | 3.13376104451195 | 3.21577996949406 | 0.74069729998161 |
| H | 0.56928039057442 | 0.46912562323084 | 0.65014877652351 |
| H | 2.28576860561153 | 0.10488846400818 | 0.33006930955497 |
| H | 1.04614156841165 | -0.27159421627631 | -0.89478103149674 |
| C | -3.02629411744546 | 4.21536450046083 | 1.40795740009764 |
| C | -1.99900474782164 | 4.49554702846543 | 2.50842753356038 |
| H | -0.98352894533794 | 4.51896769128323 | 2.08626125063836 |
| H | -2.20015827373594 | 5.47097660075997 | 2.97468434925556 |
| H | -2.04311241680444 | 3.74222350222371 | 3.30568895908758 |
| C | -2.98287539137265 | 5.33772321743824 | 0.35387693989866 |
| H | -1.98709128855080 | 5.37170045957954 | -0.11199427482887 |
| H | -3.18023356980947 | 6.31605949515589 | 0.81998187431121 |
| H | -3.73209298759789 | 5.17494503746954 | -0.43369384924503 |
| C | -4.41772413587082 | 4.19057962237825 | 2.04083670775077 |
| O | -4.66216641470907 | 4.33219730905309 | 3.21300971415756 |
| O | -5.38413380288798 | 3.98914307251597 | 1.11686041437199 |
| C | -6.71590292051616 | 3.89525346126062 | 1.61724549665993 |
| H | -6.99434569560045 | 4.80802684495714 | 2.16507539749073 |
| H | -6.81084489285233 | 3.03692526518951 | 2.30029373882487 |
| H | -7.36446931079589 | 3.76080665502142 | 0.74228079013553 |
| H | -3.53504652072026 | 2.79721127514007 | -0.11666824390332 |
| C | -2.05495985680376 | 2.97899643124000 | -2.36778132142161 |
| H | -0.59407417914456 | 2.58438191918685 | 0.78523517057462 |
| H | -1.97035755313451 | 2.13917439985008 | -3.07697903319137 |
| H | -1.77651113657499 | 3.89250017476853 | -2.91927940768584 |
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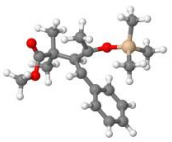
## $E_3^{Ket\text{-}1,3}$



| | | | |
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| C | -7.43903451553572 | 1.53291170944150 | 0.67737958529156 |
| C | -5.83633585513117 | 1.04123952305435 | -1.06934003503882 |
| C | -6.49586472516645 | 1.13827309112839 | 1.63087507921053 |
| C | -5.22936129362089 | 0.70020737262490 | 1.23744828462900 |
| C | -4.87362868818516 | 0.65285843734994 | -0.12149081457266 |
| C | -3.52014571387074 | 0.26261751591991 | -0.59306617795666 |
| C | -2.55506651022780 | -0.58182979492670 | 0.21348502557960 |
| C | -2.23150133160402 | 0.86754005706701 | -0.01015221824478 |
| O | -2.36375416833963 | 1.63926964596522 | 1.14099397922179 |
| H | -7.83246172418884 | 1.77554801525163 | -1.43691698849619 |
| H | -8.42865327610591 | 1.87666817498940 | 0.98837285698698 |
| H | -5.57849386908783 | 1.00994671023297 | -2.13162788173102 |
| H | -6.74699475383773 | 1.17243948233447 | 2.69444709503088 |
| H | -4.50313822546350 | 0.41247943185176 | 1.99750467485132 |
| Si | -2.67032970486889 | 3.29587067059792 | 1.29674147018710 |
| C | -3.43315900010930 | 3.47955866682954 | 2.99951049724685 |
| C | -3.83198738586517 | 3.92340505346256 | -0.04197060461731 |
| C | -1.03389962696550 | 4.22530173416574 | 1.22523215414926 |
| H | -4.42426550362287 | 3.00133742959205 | 3.03559207741843 |
| H | -3.55488662928354 | 4.54329819995275 | 3.26341008918149 |
| H | -2.79447406883544 | 3.00941816475849 | 3.76493029171798 |
| H | -1.17978824684597 | 5.29197429434442 | 1.46610484629229 |
| H | -0.57096212750857 | 4.16614413904949 | 0.22737632264972 |
| H | -0.31968542949790 | 3.80806448884950 | 1.95408447012640 |
| H | -4.83805618921833 | 3.49180640379761 | 0.06521877346047 |
| H | -3.46556366836804 | 3.67705478447377 | -1.05147777412128 |
| H | -3.91656276352260 | 5.02161110367361 | 0.02336884163305 |
| C | -1.80433375574717 | -1.82481686959030 | -0.29660218321734 |
| C | -0.40229165688146 | -1.85969353473512 | 0.32851148117594 |
| H | -0.48350336829619 | -1.80466019412474 | 1.42481574533461 |
| H | 0.20896411110032 | -1.01701682017253 | -0.01904089676634 |
| H | 0.12537259527430 | -2.78879543627044 | 0.06337577427098 |
| C | -2.61451571351232 | -3.06529002938467 | 0.13810969812527 |
| H | -2.65107550602819 | -3.11291696195261 | 1.23753261065392 |
| H | -2.14887921078951 | -3.99412404691605 | -0.22787760779568 |
| H | -3.64282620094347 | -3.01709191747546 | -0.24419962421384 |
| C | -1.66496057779583 | -1.84456254250486 | -1.82131473635578 |
| O | -0.64293653869632 | -1.64358245880432 | -2.43456434628636 |

| | | | |
|---|---|---|---|
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| C | -2.79483642043020 | -2.16878000669243 | -3.86378126642088 |
| H | -3.80927304795147 | -2.43494130485870 | -4.18538537911727 |
| H | -2.06962435795269 | -2.91773505427720 | -4.21562053846572 |
| H | -2.50734327665344 | -1.18909213520709 | -4.27586894477687 |
| C | -1.14827137343884 | 1.34443622170941 | -0.95085119550796 |
| H | -3.47526287741518 | 0.10913243813120 | -1.67375820293707 |
| H | -2.88039686393220 | -0.73865683573566 | 1.24673621347144 |
| H | -0.99177889549811 | 0.66016748589245 | -1.79297588633942 |
| H | -0.19468430298240 | 1.43824759657719 | -0.40759468465130 |
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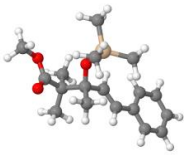
## $E_3^{Ket\text{-}1,2}$



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| C | -4.07089546795968 | -1.11710905995882 | 0.73696786518630 |
| C | -4.12647441674305 | -0.70139551484859 | 3.48947788616514 |
| C | -3.12009506991681 | -0.12220548247895 | 2.71953493974606 |
| C | -3.07213273807574 | -0.31854558369926 | 1.32474153583452 |
| C | -2.03677083834148 | 0.27451317165120 | 0.46396585866172 |
| C | -1.01846621663066 | 1.05378586473991 | 0.85897355240171 |
| C | 0.03995059365409 | 1.68827509071733 | -0.01854993408301 |
| O | 0.30233852630219 | 2.98795671907842 | 0.50372988007089 |
| H | -5.84336337964333 | -2.31546213549402 | 1.02569491718161 |
| H | -5.90002192974273 | -1.94689003334311 | 3.49528028913407 |
| H | -4.05090002450430 | -1.28067922341061 | -0.34425632793078 |
| H | -4.14384381059006 | -0.53492314043546 | 4.56972108081287 |
| H | -2.36034929686204 | 0.49117278688046 | 3.20825184373151 |
| Si | -0.54411726721572 | 4.44127282825952 | 0.44862707958266 |
| C | -0.30225714812469 | 5.27353615646081 | -1.22240453137417 |
| C | 0.26166272587984 | 5.46968592191673 | 1.79479165754460 |
| C | -2.37341084831893 | 4.17798197863490 | 0.80386809307354 |
| H | 0.76788342396092 | 5.29358031417762 | -1.48694019958795 |
| H | -0.66645956578277 | 6.31454688629868 | -1.19505862891845 |
| H | -0.83637833113704 | 4.74980209805383 | -2.03016536279459 |
| H | -2.90288661514439 | 5.14577615027461 | 0.82571840429037 |
| H | -2.52238808522466 | 3.68677036402066 | 1.77890970284461 |
| H | -2.85365000409381 | 3.54716491707932 | 0.03950461237930 |
| H | 1.34529737153177 | 5.55698200583606 | 1.61285112632785 |
| H | 0.12373025132729 | 5.00067390766686 | 2.78250389268554 |
| H | -0.16323746846422 | 6.48639150947749 | 1.83399497289780 |
| C | 1.42443914463858 | 0.91937805935429 | 0.15051629942125 |
| C | 1.71023371696663 | 0.65365955109006 | 1.63679547062863 |
| H | 1.03381486962833 | -0.12361070761454 | 2.02149445199833 |
| H | 2.74270665340418 | 0.29993317526163 | 1.76892770117326 |
| H | 1.58743845004325 | 1.56698063470284 | 2.23277774547532 |
| C | 1.43291349338460 | -0.40668236523240 | -0.62349780776096 |
| H | 0.55363403880109 | -1.01073794557368 | -0.35166407806710 |
| H | 2.33289088406571 | -0.98757920388383 | -0.36749675558421 |
| H | 1.43875538791820 | -0.24209649136415 | -1.70845828062220 |
| C | 2.48313216444725 | 1.84972783245073 | -0.45701668447002 |
| O | 2.63847523158726 | 2.02548662587671 | -1.64447862168704 |
| O | 3.23700660617626 | 2.46839081770038 | 0.46471652361061 |
| C | 4.17939498103521 | 3.41527511658285 | -0.02980779235482 |
| H | 3.66293643899951 | 4.23728110094352 | -0.54978346614198 |
| H | 4.87889797094276 | 2.94402082702365 | -0.73675249816522 |
| H | 4.71761140830014 | 3.79868021131240 | 0.84614354964806 |
| H | -2.14234256096455 | 0.03882694741185 | -0.59921992614718 |
| C | -0.40197971074230 | 1.77831329831289 | -1.48257164855577 |
| H | -0.90681023501829 | 1.30617370062806 | 1.91608157001027 |
| H | -0.57206307217652 | 0.78483817950798 | -1.91689856761105 |
| H | 0.36446710276590 | 2.28256442746951 | -2.08203177736328 |
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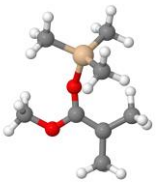
## $1\text{-}G_1(x_1)$



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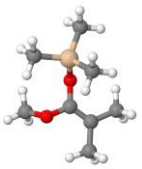
| C | -1.79329639530599 | 3.82622624077122 | 0.67084224010293 |
| C | 1.10270800801406 | 3.48323199518753 | -0.41817334758639 |
| H | -0.68497845941267 | 3.47331621508379 | -3.23254771913138 |
| H | -1.30949927901579 | 4.92890117745796 | -2.42968316369443 |
| H | -2.35240396245463 | 3.49759590037230 | -2.58823524841385 |
| H | 1.30024511231457 | 4.55628314564659 | -0.25331637465499 |
| H | 1.72931104785635 | 3.16116595476107 | -1.26275567226485 |
| H | 1.42731976689461 | 2.95010921764913 | 0.49020024006961 |
| H | -1.76073289979538 | 4.92645127194448 | 0.74153070390986 |
| H | -1.45043397856596 | 3.42244243619787 | 1.63687404239709 |
| H | -2.84456560286460 | 3.53402156461048 | 0.51888070660294 |
| C | 0.52912796895570 | -0.17726422891597 | -1.57429701623448 |
| C | 1.06346454646926 | -1.55294114221958 | -1.39216532376001 |
| H | 0.51019529077960 | -2.25049566309301 | -2.05340173477436 |
| H | 2.11823487941504 | -1.60282357777424 | -1.70349789867191 |
| H | 0.95451105410538 | -1.92423525726499 | -0.36550280467415 |
| C | 1.03168844104058 | 0.65896960233771 | -2.69456288325007 |
| H | 1.14306402135331 | 0.04085088708871 | -3.60107427550570 |
| H | 2.04677709399211 | 1.03405027940362 | -2.46151145157953 |
| H | 0.38807950912885 | 1.51555721442904 | -2.92455394235481 |
| C | -0.50390795705938 | 0.30976336668846 | -0.70269947162475 |
| O | -0.99281100263129 | 1.48858246629836 | -0.73259679341518 |
| O | -0.99166003196205 | -0.55174226411634 | 0.15058190006892 |
| C | -2.04153434708596 | -0.15348382332013 | 1.05750276382824 |
| H | -2.91552571533146 | 0.19202849303089 | 0.48823090265191 |
| H | -1.68142154118640 | 0.64920306744027 | 1.71619358159794 |
| H | -2.28189079514107 | -1.05094210743405 | 1.63648061415682 |

## $1\text{-}G_2(x_2)$



| | | | |
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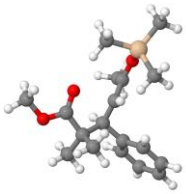
| Si | -0.73871620566867 | 3.21885931529044 | -0.78820768956357 |
| C | -1.44544545388179 | 4.31104971911109 | -2.13465651749295 |
| C | -1.60755239174545 | 3.51104447590955 | 0.85066996427726 |
| C | 1.11871980166897 | 3.40863103751277 | -0.60516362080837 |
| H | -0.93021882677294 | 4.13954132363366 | -3.09343403368323 |
| H | -1.34024196445317 | 5.37729190486411 | -1.87410385175232 |
| H | -2.51728561504272 | 4.10099934848489 | -2.28255160001861 |
| H | 1.38378117870824 | 4.42752312289599 | -0.27737825016858 |
| H | 1.63009079807185 | 3.21021735799755 | -1.56077283140538 |

| | | | |
|---|---|---|---|
| H | 1.50878563297747 | 2.69713278542994 | 0.14045232313488 |
| H | -1.42863413578593 | 4.53698992965433 | 1.21408306816138 |
| H | -1.23713888803975 | 2.80580960490383 | 1.61123627146026 |
| H | -2.69681608855624 | 3.37262187127968 | 0.75351206100157 |
| C | 0.50461465538189 | -0.17202746258428 | -1.51844916334250 |
| C | 1.13777238139849 | -1.41046224436562 | -0.94681677095243 |
| H | 0.97641966426958 | -2.27996138219376 | -1.61010892788363 |
| H | 2.23305259741057 | -1.28696920171014 | -0.85840345094906 |
| H | 0.74025975710864 | -1.64967071911741 | 0.04787638431677 |
| C | 0.96737313180913 | 0.26527122497000 | -2.88065228643073 |
| H | 0.84954917727969 | -0.55094445302350 | -3.61608614854234 |
| H | 2.04315757623767 | 0.52243791451799 | -2.87141384331949 |
| H | 0.40609195171356 | 1.13578506645497 | -3.24477770994467 |
| C | -0.41706904669143 | 0.53037397820762 | -0.83392805062843 |
| O | -1.04859526148827 | 1.62856280153005 | -1.32646147592469 |
| O | -0.76379027205401 | 0.21023561128061 | 0.45114039271767 |
| C | -2.13761377340786 | -0.08588233917000 | 0.65716126720704 |
| H | -2.43198462540866 | -0.99225916469923 | 0.09756722713952 |
| H | -2.78458033969688 | 0.74930730943653 | 0.34326989970261 |
| H | -2.27081541534199 | -0.26387873650166 | 1.73316736369204 |

## $D_3^{Ket\text{-}1,4}$-$G_1(x_1)$



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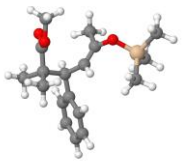
| C | -5.51946859320553 | -0.58428014890620 | -0.44242432423405 |
| C | -5.10604740840507 | 1.80028059714812 | -0.34588093682005 |
| C | -4.21852460741709 | -0.82416015091638 | 0.00756938845985 |
| C | -3.36334092221074 | 0.24499642098175 | 0.28524595246725 |
| C | -3.80302564137901 | 1.57091105511223 | 0.12232645266425 |
| C | -2.89067550220458 | 2.75968431923659 | 0.41785782082381 |
| C | -1.56478815663648 | 2.50944908135894 | -0.21183794782522 |
| C | -1.23796031894680 | 2.86618117951519 | -1.53827237765813 |
| O | -0.06764041326589 | 2.62532791530278 | -2.02866361548608 |
| H | -6.97734769895616 | 0.92558738658441 | -0.97078862539337 |
| H | -6.18762409561664 | -1.42064056559924 | -0.65934987992941 |
| H | -5.45791408465786 | 2.82577846053401 | -0.48625620224685 |
| H | -3.86560905339328 | -1.84912979926723 | 0.14230111325180 |
| H | -2.35042156729590 | 0.03666031005479 | 0.63417966105189 |
| Si | 1.51374216749219 | 2.06916320544815 | -1.42023364818794 |
| C | 2.43125861148855 | 1.76182655639657 | -3.00558148653613 |
| C | 1.23647879379172 | 0.50134091001463 | -0.43263458069914 |
| C | 2.13991643077287 | 3.50209201232690 | -0.40822501910046 |
| H | 3.46942160052199 | 1.46010372716543 | -2.78845025015290 |
| H | 2.46544675033601 | 2.67098656283061 | -3.62626679538598 |
| H | 1.96170762066992 | 0.95725691803611 | -3.59360796993448 |
| H | 2.32479908376595 | 4.38108788057936 | -1.04589277326936 |
| H | 1.41670988612349 | 3.78886117955098 | 0.37068750889746 |
| H | 3.09205524339592 | 3.23055650453870 | 0.07761961296404 |
| H | 0.90081677496225 | 0.68834926160640 | 0.59944750366678 |
| H | 2.19316994979988 | -0.04379197132290 | -0.36571876163801 |
| H | 0.51387745378880 | -0.16850199944821 | -0.92671583173875 |
| C | -2.76374337129180 | 3.14506641894907 | 1.92672529676900 |
| C | -4.11150127550768 | 3.65486914172480 | 2.45322963442535 |
| H | -4.86446189810076 | 2.85668118604783 | 2.38160835425083 |
| H | -4.02739032519270 | 3.96006252597210 | 3.50451617161903 |
| H | -4.47025880617409 | 4.52008533359019 | 1.87432874247029 |
| C | -2.26486552346564 | 1.98834964986422 | 2.81728127682700 |
| H | -3.00835374137547 | 1.17924708463797 | 2.83135207005309 |
| H | -2.12781641200918 | 2.34412596752226 | 3.84842695350322 |
| H | -1.30384117794166 | 1.57331270496027 | 2.47606334971995 |
| C | -1.69204988832344 | 4.23625269983015 | 1.97708030148203 |
| O | -0.83413242812876 | 4.36411746411280 | 1.11365049644888 |
| O | -1.74752442288277 | 4.99368035689168 | 3.05278457731760 |
| C | -0.73842252972795 | 6.00941414427714 | 3.21648618003207 |
| H | -0.75473821926458 | 6.70014679537257 | 2.36205214607876 |
| H | 0.25512173950745 | 5.54506651211237 | 3.29221530312161 |
| H | -0.99228006824499 | 6.53263693994837 | 4.14461539056205 |
| H | -3.34379373317714 | 3.63178941306913 | -0.07575157805169 |
| C | -2.20047076633887 | 3.56154002670617 | -2.44265475705339 |
| H | -0.83489557513959 | 1.91320212275757 | 0.33273235312264 |
| H | -2.31894549571472 | 4.60884564056070 | -2.11192093687646 |
| H | -3.19352145062392 | 3.08904448735881 | -2.40914059946814 |
| H | -1.81666710549283 | 3.56023606936997 | -3.47007012018152 |

## $D_3^{Ket\text{-}1,4}$-$G_2(x_2)$



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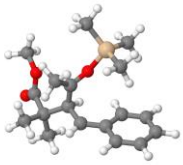
| C | -4.65097625314792 | -1.22292071181974 | 0.64057833135575 |
| C | -4.72847155579793 | 1.10835015083257 | -0.00889497881279 |
| C | -3.40213872077489 | -1.00243340366274 | 1.22866271270635 |
| C | -2.82239502457668 | 0.26831930558626 | 1.19694192565680 |
| C | -3.47784195166635 | 1.34760833409350 | 0.58138391902507 |
| C | -2.87765937071452 | 2.74462496400044 | 0.53612828453543 |
| C | -1.41195867630003 | 2.72038922140517 | 0.19022589230628 |
| C | -0.82342611130615 | 3.35002378652605 | -0.84268421096067 |
| O | 0.52682919430229 | 3.22771645251914 | -1.05395893439746 |
| H | -6.28640002789030 | -0.32052151568423 | -0.45129346523611 |
| H | -5.10291278779535 | -2.21775860319461 | 0.66253550921061 |
| H | -5.25005932927649 | 1.93326287564971 | -0.50159066749345 |
| H | -2.87211481711258 | -1.82645947098999 | 1.71358682473792 |
| H | -1.84408149004832 | 0.41618574994026 | 1.65684150908753 |
| Si | 1.31049160109210 | 1.80675459988064 | -1.55216549324167 |
| C | 3.04206027795894 | 2.36213186729479 | -1.99845692287524 |
| C | 0.37909502508186 | 1.11301105829815 | -3.02915873304518 |
| C | 1.35059109451700 | 0.53809387816587 | -0.16418358975362 |
| H | 3.65017492786685 | 1.51231207117096 | -2.35042500327255 |
| H | 3.54920997860659 | 2.80478077797559 | -1.12570303480377 |
| H | 3.01736815050659 | 3.12073383382132 | -2.79728664005215 |
| H | 1.76412961516799 | 0.97309828599807 | 0.76043042153481 |
| H | 0.34170253614314 | 0.15414518044175 | 0.05483133543651 |
| H | 1.98308797136383 | -0.32031728380144 | -0.44771310517468 |
| H | -0.66792242094984 | 0.90132683696993 | -2.75588891110156 |
| H | 0.83175284560504 | 0.17053840257830 | -3.37970467252444 |
| H | 0.37729482965528 | 1.82438827587833 | -3.87093693741323 |
| C | -3.15793406394193 | 3.58070793720954 | 1.85238833234979 |
| C | -4.67048782715175 | 3.77568008983579 | 2.04414512117437 |
| H | -5.16661434867690 | 2.80569203489131 | 2.19186584473113 |
| H | -4.87020663140429 | 4.40039909226489 | 2.92938840057108 |
| H | -5.11373667383297 | 4.27380872381827 | 1.17017276514059 |
| C | -2.55099560796660 | 2.93640117889611 | 3.10269473395336 |
| H | -3.05237126838871 | 1.98147127452320 | 3.31605083455274 |
| H | -2.68341729914588 | 3.59352599322311 | 3.97495537311718 |
| H | -1.47379461819300 | 2.75334904956108 | 2.99154108311254 |
| C | -2.54431112482663 | 4.94926559388552 | 1.54278580483301 |
| O | -2.97232755903172 | 5.70109419662453 | 0.69695808775130 |
| O | -1.45225337724142 | 5.22234381743191 | 2.27297812557623 |

| | | | |
|---|---|---|---|
| C | -0.75192645310644 | 6.41841686964115 | 1.93367078791345 |
| H | -1.41559357825426 | 7.29350946915110 | 1.99681959838698 |
| H | -0.35570531898890 | 6.34974155953734 | 0.90884217568610 |
| H | 0.07164735617556 | 6.50531538612414 | 2.65321731126950 |
| H | -3.41116610612712 | 3.28947740847414 | -0.25317276204814 |
| C | -1.47679475222277 | 4.24061271645691 | -1.85745456213280 |
| H | -0.75294222748865 | 2.14909231908316 | 0.84680435213949 |
| H | -0.90147761828975 | 5.17726793609244 | -1.93186916975058 |
| H | -2.51144927720764 | 4.49625829483077 | -1.60350931853366 |
| H | -1.44627640005007 | 3.76488158823636 | -2.85305153357015 |

## $D_3^{Ket\text{-}1,3}$-$G_1(x_1)$



| | | | |
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| C | -7.44816668795177 | 1.62492556254571 | 0.64960530142637 |
| C | -6.10438382525337 | 0.68299631036075 | -1.12603624673935 |
| C | -6.47188283673982 | 1.25825547659438 | 1.59038083744598 |
| C | -5.31266449750121 | 0.61123562940967 | 1.18600790674411 |
| C | -5.09133618843959 | 0.31092208185354 | -0.19133235672102 |
| C | -3.91318749852940 | -0.31379495788984 | -0.67312980749513 |
| C | -2.69076424316093 | -0.60741599858557 | 0.14760555468947 |
| C | -2.10641676998612 | 0.76398133396068 | -0.01049883835384 |
| O | -2.32822564442738 | 1.55244682920538 | 0.96963159888635 |
| H | -8.02165425304726 | 1.60671351837463 | -1.44032494220919 |
| H | -8.35877699179178 | 2.13151912700248 | 0.97707737298809 |
| H | -5.95660219544322 | 0.45449413531875 | -2.18452374845305 |
| H | -6.63018096243855 | 1.47464938590131 | 2.64944165885108 |
| H | -4.57145351891203 | 0.32994596758234 | 1.93381076691912 |
| Si | -2.41433694849606 | 3.31688590655499 | 1.25015850246466 |
| C | -2.96813951873955 | 3.37127070693653 | 3.02258864352473 |
| C | -3.70050532687165 | 3.93436244282714 | 0.04713067571419 |
| C | -0.69309560940119 | 3.98129574464390 | 0.97958212169082 |
| H | -3.95931402836089 | 2.90623703738146 | 3.13979506216566 |
| H | -3.04204261066932 | 4.41673851936317 | 3.36489740605746 |
| H | -2.25600210778654 | 2.85049554572532 | 3.68212079748256 |
| H | -0.65950234542258 | 5.03959199378824 | 1.28926944109813 |
| H | -0.37621979727314 | 3.93592515568113 | -0.07335227259087 |
| H | 0.04279477146030 | 3.43634039392982 | 1.59281854802228 |
| H | -4.64207426043749 | 3.37483689904183 | 0.16265131375408 |
| H | -3.38035866985208 | 3.87051635538273 | -1.00409334923843 |
| H | -3.91143446897395 | 4.99598030369447 | 0.26084843493872 |
| C | -1.88253126155983 | -1.88781461166926 | -0.21190661127052 |
| C | -2.78011475310442 | -3.09434260510765 | 0.09837066312348 |
| H | -3.64786642427404 | -3.10880295037585 | -0.57829852322900 |
| H | -3.14767397621401 | -3.06671266175545 | 1.13507464445247 |
| H | -2.21671050617773 | -4.02783010263955 | -0.02871173504108 |
| C | -1.38035535806435 | -1.98298505234305 | -1.66732124972782 |
| H | -2.20717502171862 | -1.87800799761295 | -2.38637115302916 |
| H | -0.93910673122581 | -2.97778183415716 | -1.82550424059114 |
| H | -0.60438709212762 | -1.24247942618923 | -1.89929844287760 |
| C | -0.64783824853042 | -1.93097412313932 | 0.69831591751911 |
| O | -0.24340684269932 | -2.90186024528496 | 1.27644515882337 |
| O | -0.03357808065852 | -0.72589342636341 | 0.74934592551328 |
| C | 1.16015356417547 | -0.65328678659746 | 1.54605668085868 |
| H | 1.50672080738785 | 0.38525893301029 | 1.48276266796199 |
| H | 1.92408365772236 | -1.33842873518799 | 1.15184360686906 |
| H | 0.94257203410634 | -0.92679253978144 | 2.58832090814993 |
| C | -1.42444630950125 | 1.26788113094872 | -1.23544668668155 |
| H | -3.84749311794094 | -0.50240871875896 | -1.74798159821871 |
| H | -2.96275547249745 | -0.69014629675721 | 1.20754535124894 |
| H | -1.58784720799942 | 0.62294130282005 | -2.10283055946729 |
| H | -0.34137385177517 | 1.29153197827426 | -1.02508825586841 |
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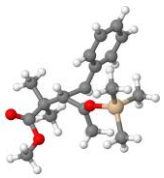
## $D_3^{Ket\text{-}1,3}$-$G_2(x_2)$



| | | | |
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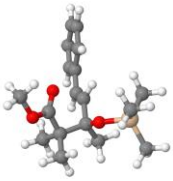
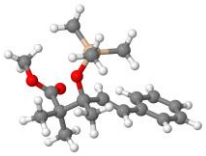
| C | -7.42100038371359 | 1.49276772519928 | 0.76520945710209 |
| C | -5.86835153204330 | 0.92528785052068 | -1.00363125957908 |
| C | -6.45187243884621 | 1.13687857155534 | 1.70778886717490 |
| C | -5.19734042897016 | 0.67987651856767 | 1.29794285668037 |
| C | -4.87999457579313 | 0.57505849379744 | -0.06717413910993 |
| C | -3.53841573393617 | 0.16610129451318 | -0.55644106847955 |
| C | -2.53909649883951 | -0.61932167874341 | 0.26798803650127 |
| C | -2.23298992465493 | 0.81344660417845 | -0.05414972002836 |
| O | -2.32759328927283 | 1.63780862024378 | 1.06375486957786 |
| H | -7.87364618708384 | 1.64659456591186 | -1.34565944408607 |
| H | -8.40143402687715 | 1.85064026543626 | 1.08904160792488 |
| H | -5.64092837807439 | 0.84959000966386 | -2.07069433849061 |
| H | -6.67323959494918 | 1.21527208595900 | 2.77557785763631 |
| H | -4.45144935474670 | 0.42042367659008 | 2.04906559176743 |
| Si | -2.64905821952543 | 3.29466937105591 | 1.17493912006649 |
| C | -3.37872773001099 | 3.52614182781744 | 2.88608003042587 |
| C | -3.84329446603795 | 3.87009120364087 | -0.15847132478447 |
| C | -1.02144165227691 | 4.23446981097032 | 1.04650063296312 |
| H | -4.36663636255405 | 3.04539894772135 | 2.95661613971753 |
| H | -3.49947780797950 | 4.59684568083433 | 3.12065506995796 |
| H | -2.72262906578128 | 3.08118973300677 | 3.65181861289809 |
| H | -1.17206908699012 | 5.30780577009001 | 1.25224503761421 |
| H | -0.56954441213111 | 4.14396345103684 | 0.04590916666665 |
| H | -0.29532263959569 | 3.84794754725874 | 1.78061684369476 |
| H | -4.83867528627601 | 3.42148650812802 | -0.02410776123513 |
| H | -3.48979203748346 | 3.60961720959061 | -1.16902729925572 |
| H | -3.94908345873496 | 4.96754283055798 | -0.11493572537449 |
| C | -1.87460262685570 | -1.93224889489138 | -0.18102918126695 |
| C | -2.86011378628840 | -3.06919348957352 | 0.13012546328113 |
| H | -3.77754335645674 | -2.93402023252992 | -0.46273540435713 |
| H | -3.13108874746402 | -3.07834185957488 | 1.19491187276977 |
| H | -2.42264439180154 | -4.04940916654801 | -0.11109494010432 |
| C | -1.47104577059813 | -2.00468960844142 | -1.66355647948151 |
| H | -2.33764082427906 | -1.80409430207357 | -2.31172791376135 |
| H | -1.11353076292278 | -3.01958106995325 | -1.89793455345703 |
| H | -0.66703154839432 | -1.30338493364121 | -1.91244824857830 |
| C | -0.63057856815993 | -2.09697827577664 | 0.69861925325462 |
| O | -0.50430824534188 | -2.89409006668840 | 1.59558672846999 |
| O | 0.32820844221064 | -1.20512452272933 | 0.37669908962819 |
| C | 1.50429830020774 | -1.22530259350385 | 1.18307560264000 |
| H | 2.16300479207506 | -0.44367274725312 | 0.78432797311147 |
| H | 1.99872355716091 | -2.20726898518776 | 1.13042040997957 |
| H | 1.25775434376777 | -1.01673948797431 | 2.23535016955861 |
| C | -1.20381781753663 | 1.27194209337459 | -1.06082703973504 |
| H | -3.51724143178563 | -0.04208182575977 | -1.63055364855184 |
| H | -2.83398206744886 | -0.69585347574727 | 1.31921889154071 |
| H | -1.19401177269099 | 0.64081094180504 | -1.95650063710851 |
| H | -0.19934198694443 | 1.25530539697193 | -0.61275727467302 |
| H | -1.42821519397887 | 2.30060782137815 | -1.38415900387261 |

## $D_3^{Ket\text{-}1,2}$-$G_1(x_1)$



| | | | |
|---|---|---|---|
| C | -4.56671066098728 | -1.33494487134776 | 1.98904174602479 |
| C | -4.91964119393992 | -0.59964863329443 | 3.13449727556921 |
| C | -3.41461740226104 | -1.01055553224838 | 1.29279410059567 |
| C | -4.10947299580275 | 0.46144313332348 | 3.58195664482938 |
| C | -2.95941323579616 | 0.79707397225437 | 2.88978925258084 |
| C | -2.58571376640521 | 0.07117744235663 | 1.71785754301366 |
| C | -1.41436050612342 | 0.37228952622759 | 0.96691906600210 |
| C | -0.57374218528596 | 1.46147461152704 | 1.20227729229950 |
| C | 0.65912467074638 | 1.83158037233485 | 0.39952009471297 |
| O | 1.01894079122545 | 3.13964159344640 | 0.75071019910544 |
| H | -5.19949766994288 | -2.15862496644768 | 1.65260939376821 |
| H | -5.82800417778506 | -0.85621196860333 | 3.68494344101038 |
| H | -3.13089397394702 | -1.57675847296798 | 0.40233128819449 |
| H | -4.38916199765622 | 1.01640145398787 | 4.47972477467693 |
| H | -2.32478326629619 | 1.60526759496217 | 3.25480564547340 |
| Si | 0.41430982821094 | 4.67917339816535 | 0.32532253410336 |
| C | 1.19063294286922 | 5.81053272324527 | 1.59134340600340 |
| C | -1.46359523183847 | 4.66590364569092 | 0.46993472533821 |
| C | 0.95237825999916 | 5.12267186973446 | -1.41489865488415 |
| H | 0.90553271555380 | 5.51805178620153 | 2.61467052163636 |
| H | 0.86982900356978 | 6.85321696671173 | 1.43294897578404 |
| H | 2.29006869496685 | 5.78275916169231 | 1.52186057039359 |
| H | 0.73497482440906 | 6.18560373563489 | -1.61360791799773 |
| H | 0.43813754477105 | 4.53079687421722 | -2.18768302309513 |
| H | 2.03833355188859 | 4.97833970050214 | -1.53687638100949 |
| H | -1.79388861741183 | 4.48609443129313 | 1.50664013102894 |
| H | -1.93948199582644 | 3.91362146157306 | -0.18059669492813 |
| H | -1.86325354770011 | 5.64899753421710 | 0.16925336382141 |
| C | 1.87596191210900 | 0.93091674149631 | 0.86853337696501 |
| C | 1.75478229822431 | -0.55759438623335 | 0.47854844130460 |
| H | 1.80376570635162 | -0.67326344484207 | -0.61349169525726 |
| H | 2.60035428601632 | -1.11635607592548 | 0.90568978469957 |
| H | 0.83053032049917 | -1.02324756968657 | 0.84750410967622 |
| C | 3.20687449602874 | 1.48737470111727 | 0.35682165280234 |
| H | 3.24776100199862 | 1.42428614737505 | -0.74032991035731 |
| H | 4.03975316228695 | 0.89377150088960 | 0.75795249685792 |
| H | 3.34128513292542 | 2.53324242099831 | 0.65515677252106 |
| C | 1.77337592610034 | 0.97524651734346 | 2.38928191758044 |
| O | 0.68105919525292 | 1.01430427965655 | 2.95092928011813 |
| O | 2.90683555616715 | 0.90139239392324 | 3.03905982455211 |
| C | 2.86369653639022 | 0.87776208283804 | 4.48206685319910 |
| H | 2.30544027620812 | -0.00397367051766 | 4.82621450077665 |
| H | 2.37928010816650 | 1.79051178349206 | 4.85545860595935 |
| H | 3.90821352898321 | 0.82943380078167 | 4.80738816220737 |
| H | -1.17334993872039 | -0.30961598964783 | 0.14811363595776 |
| C | 0.39068312873731 | 1.69268888255352 | -1.10970700586112 |
| H | -0.93002933246747 | 2.25725302678405 | 1.85251938069739 |
| H | 1.27421508960383 | 2.02903438579222 | -1.66804841210760 |
| H | -0.46154872186228 | 2.32003986460610 | -1.40545941518565 |
| H | 0.16619992779603 | 0.65875386281557 | -1.40138167115773 |

## $D_3^{Ket\text{-}1,2}$-$G_2(x_2)$



| | | | |
|---|---|---|---|
| C | -5.16744599186563 | -0.49688390692656 | 1.29609320457549 |
| C | -5.24246097860370 | -0.46128224706722 | 2.69068903400748 |
| C | -3.97395871741099 | -0.16602151918056 | 0.65136848267280 |
| C | -4.11152543644418 | -0.09725669520331 | 3.43192278038607 |
| C | -2.92075436405922 | 0.23308481249725 | 2.78778778895337 |
| C | -2.83196964201136 | 0.21315217696228 | 1.38109171386009 |
| C | -1.60279042694721 | 0.57247991693074 | 0.65704676100628 |
| C | -0.51734030313535 | 1.14566509424390 | 1.19677158928994 |
| C | 0.75967175630226 | 1.53156578830371 | 0.48363011752459 |
| O | 1.08473451712577 | 2.87122999025733 | 0.84506796000448 |
| H | -6.04192858585475 | -0.78479742804778 | 0.70674089931998 |
| H | -6.17373945973668 | -0.72196164775630 | 3.19976508560452 |
| H | -3.92085854227107 | -0.19483407351763 | -0.44083686430520 |
| H | -4.15764936881804 | -0.07846415275816 | 4.52396865530609 |
| H | -2.04208389262637 | 0.49291643441596 | 3.38187603289126 |
| Si | 0.32760441901963 | 4.35824734224586 | 0.62708736518869 |
| C | 1.10650735800674 | 5.43595062740660 | 1.95116226411935 |
| C | -1.53603956051768 | 4.25441841295013 | 0.85407692042233 |
| C | 0.73277384442925 | 5.03085824080250 | -1.08459824829324 |
| H | 0.84470763294655 | 5.06284559188462 | 2.95494845444677 |
| H | 0.76839048465593 | 6.48261043945656 | 1.87536520798034 |
| H | 2.20483218180615 | 5.42090486493223 | 1.86035346512401 |
| H | 0.36734666540583 | 6.06602825904410 | -1.19403564051132 |
| H | 0.27087199985032 | 4.42659182658962 | -1.88176291267600 |
| H | 1.82242436197175 | 5.03666556119929 | -1.25203401019519 |
| H | -1.79914535806296 | 3.82992076662893 | 1.83567274943135 |
| H | -2.01004695224541 | 3.62465606115533 | 0.08555621904803 |
| H | -1.97685673552989 | 5.26406325578705 | 0.78783660863219 |
| C | 1.98060870147565 | 0.67403261398353 | 1.04051680204362 |
| C | 1.63885396004613 | -0.82274430438639 | 1.09568309599884 |
| H | 1.31966171700406 | -1.18532785023796 | 0.10671492655325 |
| H | 2.52606497288461 | -1.40244160200088 | 1.39582897792134 |
| H | 0.83681685869927 | -1.02423687698012 | 1.81636736086815 |
| C | 3.23802583015602 | 0.89997368953336 | 0.18892485706035 |
| H | 3.13625214681144 | 0.40850070148425 | -0.78949997515090 |
| H | 4.11829377128031 | 0.47158251712558 | 0.68930518864235 |
| H | 3.42623565173619 | 1.97066911064188 | 0.03678977585984 |
| C | 2.19487184630678 | 1.17178273604317 | 2.47827419804376 |
| O | 1.47034919383593 | 0.90226431396869 | 3.40977903227836 |
| O | 3.27847404558731 | 1.95051504380678 | 2.61267966457122 |
| C | 3.47493794759147 | 2.53484832688173 | 3.89724536315781 |
| H | 3.53759620379413 | 1.76161198866560 | 4.67761876733206 |
| H | 2.64099308565710 | 3.21108594815055 | 4.14132798809573 |
| H | 4.41429142779261 | 3.09871642435792 | 3.83714463401264 |
| H | -1.62193090082889 | 0.34899117685836 | -0.41420254710174 |
| C | 0.63881455918839 | 1.42041428298472 | -1.03830619023678 |
| H | -0.49946929346145 | 1.37861613011678 | 2.26260194478660 |
| H | 1.50911649779690 | 1.87757186601905 | -1.52412491187109 |
| H | -0.25966093324312 | 1.95317921660998 | -1.38213382183625 |
| H | 0.55870180450949 | 0.37537075313695 | -1.37023681484368 |

### 2.3.3 Comp. analysis of the reaction pathway of α,β-unsat. aldehydes

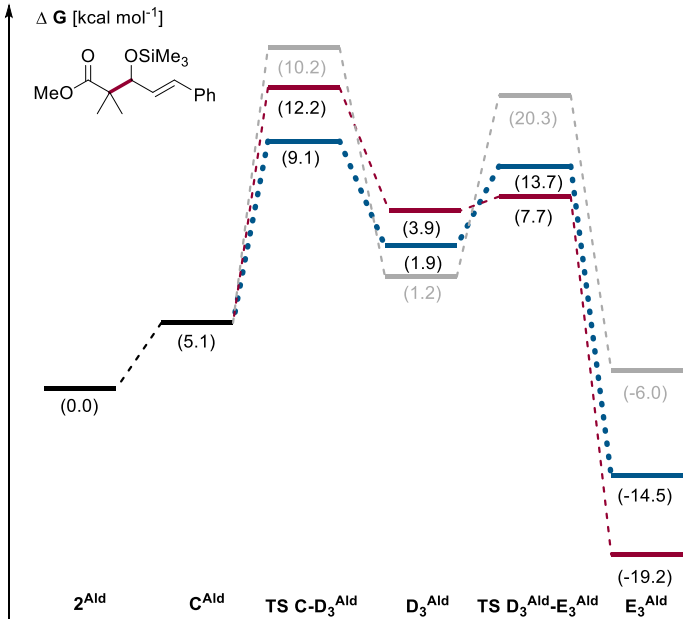
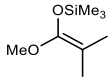
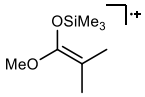
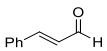
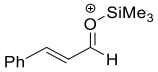
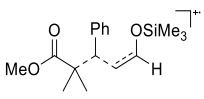



**Figure S8:** Reaction profile of radical addition of **B** to α,β-unsaturated ketones **2$^{Ald}$.**

**Table S9:** Stationary point energies of relevant structures. Energy values are given in $E_h$.

| | Free energy | SP energy | ZPVE | Thermal Correction | Enthalpy Correction | Entropy Correction |
|---|---|---|---|---|---|---|
|  **1** | -755.41389166 | -755.61700281 | 0.24522497 | 0.01673055 | 0.00094421 | 0.05978858 |
|  **A** | -755.23365209 | -755.43572912 | 0.24513199 | 0.01711167 | 0.00094421 | 0.06111084 |
|  **2$^{Ald}$** | -422.81549233 | -422.92544579 | 0.14349693 | 0.00849254 | 0.00094421 | 0.04298022 |
|  **B** | -346.23069830 | -346.32880842 | 0.13177051 | 0.00890443 | 0.00094421 | 0.04350903 |
|  **C $^{Ald}$** | -831.81035984 | -832.02446979 | 0.25698873 | 0.01661160 | 0.00094421 | 0.06043459 |
|  **TS C-D$_4^{Ald-1,4}$** | -1178.02782643 | -1178.36704863 | 0.39167532 | 0.02545945 | 0.00094421 | 0.07885678 |

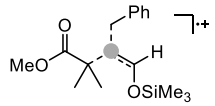
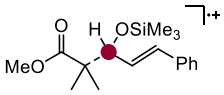
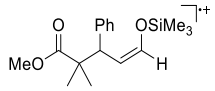
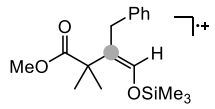
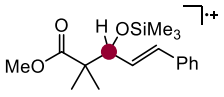
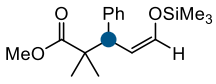
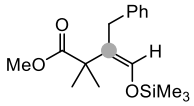
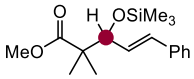
| | | | | | | |
|---|---|---|---|---|---|---|
|  **TS C-D$_4^{Ald-1,3}$** | -1178.02609653 | -1178.35853130 | 0.38478919 | 0.02538080 | 0.00094421 | 0.07867943 |
|  **TS C-D$_4^{Ald, 1,2}$** | -1178.02284071 | -1178.36195552 | 0.38952468 | 0.02393605 | 0.00094421 | 0.07529013 |
|  **D$_4^{Ald-1,4}$** | -1178.03926849 | -1178.37993005 | 0.39365269 | 0.02575047 | 0.00094421 | 0.07968581 |
|  **D$_4^{Ald-1,3}$** | -1178.04025220 | -1178.38123843 | 0.39333049 | 0.02562002 | 0.00094421 | 0.07890849 |
|  **D$_4^{Ald-1,2}$** | -1178.03612540 | -1178.37770151 | 0.39399608 | 0.02533366 | 0.00094421 | 0.07869784 |
|  **E$_4^{Ald-1,4}$** | -1178.24566580 | -1178.58762688 | 0.39393967 | 0.02539178 | 0.00094421 | 0.07831458 |
|  **E$_4^{Ald-1,3}$** | -1178.23212816 | -1178.57599017 | 0.39480232 | 0.02488190 | 0.00094421 | 0.07676642 |
|  **E$_4^{Ald-1,2}$** | -1178.25307135 | -1178.59534541 | 0.39411853 | 0.02545722 | 0.00094421 | 0.07824590 |

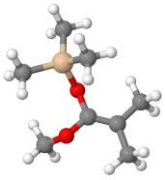
**Table S10:** Energies of relevant structures for application of Electron-transfer Marcus-Hush Theory. Energy values are given in $E_h$.

| | $G_1(x_1)$ | $G_1(x_2)$ | $G_2(x_2)$ | $G_2(x_1)$ | r |
|---|---|---|---|---|---|
| **1** | -755.41389289 | -755.38850254 | -755.23363893 | -755.20437698 | 2.27725599 |
| **D$_4^{Ald-1,4}$** | -1178.03778642 | -1178.02280298 | -1178.24692291 | -1178.22399604 | 2.47121850 |
| **D$_4^{Ald-1,3}$** | -1178.03912481 | -1178.00691172 | -1178.23215119 | -1178.19055620 | 2.46693117 |
| **D$_4^{Ald-1,2}$** | -1178.03022252 | -1178.02953435 | -1178.25276279 | -1178.23264759 | 2.45103060 |

**Table S11:** Data for the calculation of the activation barrier of the electron transfer via Four-Point Approach to the Electron-Transfer Marcus-Hush Theory. Energy values are given in kcal mol$^{-1}$.

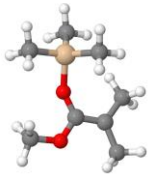
| | $\Delta G_0$ | $\lambda_i$ | $\lambda_o$ | $\lambda$ | $\Delta G^{\ddagger}$ |
|---|---|---|---|---|---|
| **D$_4^{Ald-1,4}$** | -18.12404564 | 28.80437426 | 50.27891572 | 79.08328998 | 11.74720182 |
| **D$_4^{Ald-1,3}$** | -8.01480662 | 40.08993538 | 50.31730179 | 90.40723717 | 18.77203868 |
| **D$_4^{Ald-1,2}$** | -26.53503822 | 22.51772059 | 50.46150452 | 72.97922511 | 7.38930323 |

## 1



| | | | |
|---|---|---|---|
| Si | -0.73871666095863 | 3.21885893604048 | -0.78820770029077 |
| C | -1.44544649727906 | 4.31104934979919 | -2.13465632669758 |
| C | -1.60755236002462 | 3.51104399754353 | 0.85067035129574 |
| C | 1.11871951916892 | 3.40863071246837 | -0.60516420253531 |
| H | -0.93021997726184 | 4.13954079503740 | -3.09343386026655 |
| H | -1.34024280937238 | 5.37729146080419 | -1.87410349200440 |
| H | -2.51728666940907 | 4.10099876171800 | -2.28255090772136 |
| H | 1.38378104834946 | 4.42752270364781 | -0.27737871613911 |
| H | 1.63009002963274 | 3.21021702755411 | -1.56077366518442 |
| H | 1.50878526670696 | 2.69713216652683 | 0.14045148181082 |
| H | -1.42863408973314 | 4.53698945745528 | 1.21408337970046 |
| H | -1.23713834784522 | 2.80580908175176 | 1.61123636904132 |
| H | -2.69681606256839 | 3.37262123928936 | 0.75351272982760 |
| C | 0.50461437827801 | -0.17202759882952 | -1.51844908968440 |
| C | 1.13777218306104 | -1.41046239729382 | -0.94681672789735 |
| H | 0.97641935345744 | -2.27996158825015 | -1.61010877646500 |
| H | 2.23305241708492 | -1.28696942034587 | -0.85840356737089 |
| H | 0.74025967244989 | -1.64967073598220 | 0.04787650618150 |
| C | 0.96737295892894 | 0.26527104740360 | -2.88065218433752 |
| H | 0.84954931781381 | -0.55094471453929 | -3.61608599219683 |
| H | 2.04315730527112 | 0.52243815181557 | -2.87141358798934 |
| H | 0.40609159597545 | 1.13578472189716 | -3.24477775728862 |
| C | -0.41706939422046 | 0.53037369323556 | -0.83392796614035 |
| O | -1.04859564928642 | 1.62856252109310 | -1.32646150836552 |
| O | -0.76379066680497 | 0.21023536056648 | 0.45114044300907 |
| C | -2.13761418416676 | -0.08588275878652 | 0.65716108429663 |
| H | -2.43198482238290 | -0.99225959120114 | 0.09756694324851 |
| H | -2.78458081248992 | 0.74930678698811 | 0.34326957850349 |
| H | -2.27081604237493 | -0.26387916740741 | 1.73316716166021 |

## A



| | | | |
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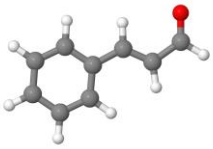
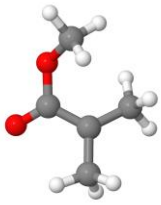
| Si | -0.70878264789662 | 3.25722568803358 | -0.73738109184549 |
| C | -1.29371802825804 | 3.83362197076937 | -2.40599297832219 |
| C | -1.78283928545257 | 3.83822310991464 | 0.66501081194277 |
| C | 1.11456888583758 | 3.46541131855299 | -0.40980592143548 |
| H | -0.66059932720196 | 3.47676381712093 | -3.23275184958438 |
| H | -1.27751063267402 | 4.93641195463975 | -2.43136810037168 |
| H | -2.33066571388435 | 3.51346947023525 | -2.59581264631445 |
| H | 1.32076207962523 | 4.53568621812779 | -0.23752103828295 |
| H | 1.74274509951240 | 3.14324509216530 | -1.25312231532837 |
| H | 1.43013884964356 | 2.92475714219474 | 0.49734141748113 |
| H | -1.73686787061097 | 4.93784434582785 | 0.73773935292486 |
| H | -1.45041009233184 | 3.42902919000993 | 1.63243673803942 |
| H | -2.83690833993505 | 3.55983350880850 | 0.50664786576070 |
| C | 0.51819727858255 | -0.17978756558232 | -1.57148649665361 |
| C | 1.04789035611243 | -1.55696724614000 | -1.38774474302179 |
| H | 0.50418687267669 | -2.25084193968286 | -2.06062180546976 |
| H | 2.10694259860173 | -1.60661588378133 | -1.68476851041209 |
| H | 0.92463983865804 | -1.93290383779040 | -0.36449885368558 |
| C | 1.02768136575134 | 0.65316166811207 | -2.69105677875109 |
| H | 1.13730478812560 | 0.03375340894833 | -3.59695889298912 |
| H | 2.04448819940404 | 1.02277111560615 | -2.45707625314276 |
| H | 0.38903492524756 | 1.51283333849414 | -2.92330418288601 |
| C | -0.51609769848514 | 0.31080379593777 | -0.70411432559681 |
| O | -1.00019758483228 | 1.49177230113770 | -0.73374783719384 |
| O | -1.01179445575363 | -0.54968692826500 | 0.14557596716584 |
| C | -2.06139907698175 | -0.14655011924233 | 1.05125795713417 |
| H | -2.93592449162593 | 0.19465423230335 | 0.48018884720484 |
| H | -1.70122232520864 | 0.66065864585473 | 1.70429416025670 |
| H | -2.30048356664596 | -1.04095781231065 | 1.63541150337705 |

## 2 Ald



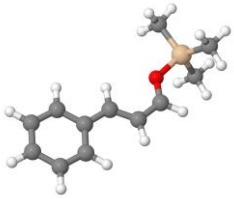
| | | | |
|---|---|---|---|
| C | -8.61619121366215 | 0.87763504317281 | 0.01270958621316 |
| C | -8.65073988895798 | -0.51932121896510 | 0.00696965858805 |
| C | -7.39046217235532 | 1.54393277794249 | 0.01113713634749 |
| C | -7.45199902440543 | -1.24481194517313 | -0.00034468176641 |
| C | -6.22902761697512 | -0.57984987816077 | -0.00191327519476 |
| C | -6.17545624552648 | 0.83006031457290 | 0.00380981916961 |
| C | -4.92148057343277 | 1.57848696057384 | 0.00246630629885 |
| C | -3.65987105510918 | 1.09341207502670 | -0.00410124391844 |
| C | -2.50038973016060 | 2.00706834454522 | -0.00443734233753 |
| O | -2.57154394424841 | 3.21856970151204 | 0.00095159254532 |
| H | -9.54715950389627 | 1.44968709945916 | 0.01842804351364 |
| H | -9.60878862205387 | -1.04505140986422 | 0.00817700498719 |
| H | -7.36250101355940 | 2.63676642665146 | 0.01562265694059 |
| H | -7.47539759245841 | -2.33735742325405 | -0.00484540838285 |
| H | -5.30318580494695 | -1.15857074707008 | -0.00764101370974 |
| H | -3.44718435513968 | 0.02023653772670 | -0.00937718227425 |
| H | -5.01098518888765 | 2.67122565704551 | 0.00737724648903 |
| H | -1.50243645422431 | 1.49689168425854 | -0.01011890350895 |

## B



| | | | |
|---|---|---|---|
| C | 0.15854831486826 | -0.26091685412808 | -1.81656301087734 |
| C | 1.09695865236965 | -1.37116260880147 | -1.46528197252030 |
| H | 0.56034294658297 | -2.25933806869162 | -1.07835753205434 |
| H | 1.63933336702863 | -1.70817674074455 | -2.36567795648130 |
| H | 1.83714335122033 | -1.07258382656553 | -0.71036856094538 |
| C | -0.54757805137152 | -0.31058875187964 | -3.12943502448994 |
| H | -1.02062585138255 | -1.29677096653879 | -3.28527018924215 |
| H | 0.16976219304299 | -0.17685725881992 | -3.96330378161707 |
| H | -1.30270398023678 | 0.48162331600071 | -3.21241222044069 |
| C | 0.05445402229010 | 0.96975897682547 | -1.02956631743780 |
| O | -0.28058519374554 | 2.02784584540263 | -1.52336752125255 |
| O | 0.41327785217069 | 0.94050692526456 | 0.28902756474136 |
| C | 0.05477733395010 | -0.15296266496769 | 1.11862197333245 |
| H | 0.92711485672229 | -0.78468153780037 | 1.35304942707963 |
| H | -0.72542184524792 | -0.78101488731380 | 0.65793653780444 |
| H | -0.34094796826169 | 0.26027910275809 | 2.05919858440099 |

## C Ald



| | | | |
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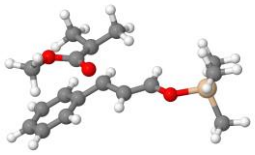
| C | -8.59924837816182 | 0.89613170554694 | 0.01272149326708 |

| | | | |
|---|---|---|---|
| C | -8.61939346099966 | -0.50491058524258 | 0.00691365298781 |
| C | -7.38160725467007 | 1.56442777541601 | 0.01119201985561 |
| C | -7.42148354919957 | -1.24032402848401 | -0.00043522888486 |
| C | -6.20291534539310 | -0.57981667469236 | -0.00200434880984 |
| C | -6.15951988500233 | 0.84077100176912 | 0.00380101513059 |
| C | -4.93677356136045 | 1.57930214844690 | 0.00253277890497 |
| C | -3.64466644679395 | 1.08000011958675 | -0.00420381382129 |
| C | -2.53015612072128 | 1.93112016701997 | -0.00463297297709 |
| O | -2.61674462409546 | 3.20902932787608 | 0.00105856564452 |
| H | -9.53518144040729 | 1.45809927868935 | 0.01841142272531 |
| H | -9.57621326394874 | -1.03281678742412 | 0.00810419668729 |
| H | -7.35462722264603 | 2.65692776908189 | 0.01568104231715 |
| H | -7.45283287888294 | -2.33165728975059 | -0.00490116958184 |
| H | -5.27760587962219 | -1.15816124123160 | -0.00772523180555 |
| Si | -1.29337053424132 | 4.43044017877671 | 0.00155778513081 |
| C | -2.24201361925543 | 6.02544605052223 | 0.01007118843663 |
| C | -0.34277823862685 | 4.09298471719954 | -1.56583296486406 |
| C | -0.33370137009908 | 4.08171656406888 | 1.56092371463761 |
| H | -2.88092776238456 | 6.11749717498505 | -0.88248885948717 |
| H | -1.54141338371831 | 6.87706179464758 | 0.01110553857261 |
| H | -2.87569746483599 | 6.11102561384619 | 0.90699346848462 |
| H | 0.48135936983363 | 4.81806350944565 | 1.66325053190947 |
| H | 0.13038398053641 | 3.08216202370253 | 1.55105121539282 |
| H | -0.97158800570339 | 4.16482199020177 | 2.45531066574131 |
| H | -0.98586022287169 | 4.18240818135738 | -2.45588039155406 |
| H | 0.12148903146941 | 3.09346522859220 | -1.56582770318668 |
| H | 0.47159875584774 | 4.83016241723680 | -1.66762244289184 |
| H | -5.03258719383099 | 2.67077259734799 | 0.00746603085561 |
| H | -3.44048859856520 | 0.00834524225457 | -0.00945398516569 |
| H | -1.52468543164950 | 1.47796402920716 | -0.01017721365183 |

## TS C-$D_4$$^{Ald-1,4}$



| | | | |
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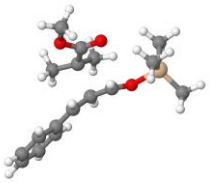
| C | -3.88070388818471 | -1.41909254054611 | 3.81879595266842 |
| C | -4.20647540785258 | 0.07616579009656 | 1.94685965228398 |
| C | -2.60692493733115 | -0.87534614023792 | 4.02936722190470 |
| C | -2.13177201695100 | 0.13878327247746 | 3.20201350752096 |
| C | -2.92666977753092 | 0.63034882879308 | 2.14665906969113 |
| C | -2.46271044202718 | 1.70368580099371 | 1.24519460066009 |
| C | -1.07815483793625 | 1.89614704075391 | 0.97537219108382 |
| C | -0.63263683864896 | 2.51724489458889 | -0.18464128881357 |
| O | 0.62416353404477 | 2.69519841413648 | -0.41424534925707 |
| H | -5.66687537382233 | -1.37188730886841 | 2.59752677396173 |
| H | -4.24937117320972 | -2.21578064319730 | 4.46886348034031 |
| H | -4.83030719067455 | 0.44113308751841 | 1.12700672678757 |
| H | -1.98088241910597 | -1.24970981581838 | 4.84244843992606 |
| H | -1.14099319865237 | 0.55761960793369 | 3.38603004642076 |
| Si | 1.47206133853558 | 3.44324263134795 | -1.78833029831554 |
| C | 2.52241221280572 | 2.06053428602699 | -2.45566630728698 |
| C | 2.43121286471414 | 4.82288507551783 | -0.98906901578935 |
| C | 0.14463354463699 | 4.02777738061266 | -2.96694687742497 |
| H | 3.14502350369745 | 2.43015791932526 | -3.28759486381415 |
| H | 1.90613584753435 | 1.23113919122464 | -2.83744645022137 |
| H | 3.19649145415127 | 1.66593887347027 | -1.67905393146243 |
| H | -0.46760478800152 | 3.19844267453943 | -3.35705840715309 |
| H | -0.52049237895877 | 4.77898426937105 | -2.51056444944209 |
| H | 0.62587065299259 | 4.50891861226572 | -3.83522863709986 |
| H | 1.76273803030426 | 5.57277840593021 | -0.53706798229969 |
| H | 3.05291571695410 | 5.33437898758570 | -1.74286929645788 |
| H | 3.10078177894312 | 4.43572234486613 | -0.20487760054191 |
| C | -3.01351164788278 | 3.44716141671159 | 2.17794658450157 |
| C | -2.47476823335253 | 4.57400683977847 | 1.33780263170456 |
| H | -2.83498697849608 | 4.51589316924512 | 0.29943529139212 |
| H | -2.85838802142215 | 5.52281040017478 | 1.75459968785020 |
| H | -1.37944472953225 | 4.62018435990633 | 1.36492109069124 |
| C | -4.51082402735420 | 3.36126518868047 | 2.24601374040699 |
| H | -4.96010470240427 | 3.37936556553785 | 1.24162234677668 |
| H | -4.87720317793906 | 4.25332657278999 | 2.78621353263284 |
| H | -4.86050728816800 | 2.48334450406731 | 2.79968680411323 |
| C | -2.24828862195676 | 3.25767141708708 | 3.47396272053031 |
| O | -1.04560380747092 | 3.35788557315657 | 3.55602477650783 |
| O | -3.05604310762967 | 2.96759491315732 | 4.48927249933018 |
| C | -2.44112224399958 | 2.75671367095473 | 5.77012003505109 |
| H | -1.84355011318179 | 3.63355504758312 | 6.05616135938722 |
| H | -1.78963417335233 | 1.87185953880576 | 5.73230879110975 |
| H | -3.26422166714370 | 2.59739684849597 | 6.47531457443029 |
| H | -3.12835390152083 | 1.88954205487225 | 0.39368737627118 |
| H | -1.35469600187092 | 2.86117730645963 | -0.94133165695358 |
| H | -0.31589720017563 | 1.57652935487966 | 1.68753018545999 |

## TS C-$D_4$$^{Ald-1,3}$



| | | | |
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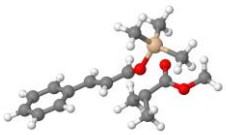
| C | -8.051927 | -1.154691 | -1.677402 |
| C | -6.696432 | 0.763233 | -2.251269 |
| C | -7.011076 | -1.656951 | -0.880051 |
| C | -5.815885 | -0.961106 | -0.767038 |
| C | -5.624208 | 0.270790 | -1.454685 |
| C | -4.420311 | 1.026418 | -1.376729 |
| C | -3.234481 | 0.662263 | -0.654674 |
| C | -2.424329 | 1.764739 | -0.234297 |
| O | -1.640000 | 1.700919 | 0.751443 |
| H | -8.697868 | 0.451283 | -2.979205 |
| H | -8.989554 | -1.708353 | -1.762916 |
| H | -6.569932 | 1.709528 | -2.783540 |
| H | -7.142906 | -2.599851 | -0.344699 |
| H | -5.021425 | -1.368109 | -0.138902 |
| Si | -0.327931 | 2.868520 | 1.231750 |
| C | -0.745838 | 3.208798 | 3.010134 |
| C | -0.511483 | 4.320818 | 0.079866 |
| C | 1.209966 | 1.865430 | 0.952392 |
| H | -1.720911 | 3.711078 | 3.111691 |
| H | 0.019805 | 3.868884 | 3.451331 |
| H | -0.766846 | 2.278766 | 3.599975 |
| H | 2.095911 | 2.458348 | 1.235273 |
| H | 1.297271 | 1.597391 | -0.111363 |
| H | 1.211045 | 0.947749 | 1.561168 |
| H | -1.480818 | 4.834003 | 0.187664 |
| H | -0.371043 | 4.008525 | -0.966873 |
| H | 0.272765 | 5.060154 | 0.315298 |
| C | -1.879047 | -0.323625 | -1.855008 |
| C | -0.939403 | -0.974308 | -0.874496 |
| H | -1.466813 | -1.704982 | -0.243644 |
| H | -0.425243 | -0.245097 | -0.237291 |
| H | -0.159614 | -1.524082 | -1.432678 |
| C | -2.757435 | -1.250809 | -2.647837 |
| H | -3.232329 | -2.000123 | -1.999137 |
| H | -2.134471 | -1.787875 | -3.385269 |
| H | -3.532836 | -0.715749 | -3.210291 |
| C | -1.267562 | 0.829872 | -2.599723 |
| O | -0.494574 | 1.625486 | -2.092027 |
| O | -1.702641 | 0.928285 | -3.852015 |
| C | -1.182445 | 2.006062 | -4.647326 |
| H | -1.456299 | 2.974871 | -4.204261 |
| H | -1.635478 | 1.893425 | -5.638451 |
| H | -0.087222 | 1.938790 | -4.710605 |
| H | -2.478898 | 2.705425 | -0.804262 |
| H | -4.389000 | 1.962265 | -1.944641 |
| H | -3.292761 | -0.151742 | 0.072840 |

## TS C-$D_4^{Ald-1,2}$



| | | | |
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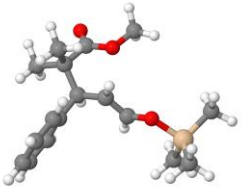
| C | -6.583372 | 2.018877 | -1.673841 |
| C | -6.406638 | 1.586485 | -0.350757 |
| C | -5.500546 | 2.515159 | -2.386218 |
| C | -5.140363 | 1.651683 | 0.257471 |
| C | -4.055155 | 2.146054 | -0.448231 |
| C | -4.211794 | 2.588306 | -1.791377 |
| C | -3.125778 | 3.105773 | -2.574093 |
| C | -1.827453 | 3.296093 | -2.160192 |
| C | -0.809765 | 3.833491 | -3.021454 |
| O | 0.281819 | 4.309658 | -2.429297 |
| H | -7.569220 | 1.965242 | -2.140000 |
| H | -7.258244 | 1.196424 | 0.211760 |
| H | -5.630997 | 2.855330 | -3.416525 |
| H | -5.013665 | 1.312095 | 1.287452 |
| H | -3.077374 | 2.191879 | 0.033913 |
| Si | 1.159531 | 5.811261 | -2.587055 |
| C | 0.600832 | 6.840465 | -1.130933 |
| C | 0.693826 | 6.594233 | -4.218751 |
| C | 2.946488 | 5.297060 | -2.450977 |
| H | 1.144394 | 7.800191 | -1.115159 |
| H | 0.799644 | 6.324901 | -0.177929 |
| H | -0.476153 | 7.067387 | -1.186340 |
| H | 3.608113 | 6.174341 | -2.539332 |
| H | 3.223375 | 4.575527 | -3.232999 |
| H | 3.139363 | 4.828160 | -1.472711 |
| H | -0.367700 | 6.892107 | -4.233533 |
| H | 0.873840 | 5.936391 | -5.081820 |
| H | 1.287282 | 7.513682 | -4.357613 |
| C | 0.489408 | 1.376600 | -2.915384 |
| C | -0.188562 | 2.217545 | -3.961819 |
| H | 1.076731 | 0.591563 | -3.421981 |
| H | -0.244846 | 0.882612 | -2.263370 |
| H | 1.189247 | 1.968084 | -2.311188 |
| C | -1.345587 | 1.582611 | -4.688579 |
| H | -0.941873 | 0.788274 | -5.342731 |
| H | -1.858664 | 2.299902 | -5.344618 |
| H | -2.058343 | 1.110992 | -3.999212 |
| C | 0.719415 | 2.945850 | -4.945599 |
| O | 0.299017 | 3.682894 | -5.806843 |
| O | 2.004332 | 2.654509 | -4.762269 |
| C | 2.933382 | 3.206916 | -5.713139 |
| H | 2.662301 | 2.896149 | -6.731864 |
| H | 3.916425 | 2.812495 | -5.433468 |
| H | 2.926081 | 4.304685 | -5.659250 |
| H | -3.374227 | 3.397020 | -3.599928 |
| H | -1.506570 | 3.038008 | -1.147647 |
| H | -1.144538 | 4.341498 | -3.940449 |

## $D_4^{Ald-1,4}$



| | | | |
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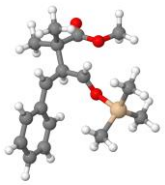
| C | -4.48890339258809 | -0.36797541835169 | 0.19382007888667 |
| C | -4.06401883351565 | -1.16659504887940 | 1.26626990623535 |
| C | -4.08258785188618 | 0.96097225832552 | 0.10851476367787 |
| C | -3.23215976395429 | -0.62687196647694 | 2.25189432315367 |
| C | -2.82879212078700 | 0.70612906766533 | 2.17388182536823 |
| C | -3.27046951677078 | 1.52535434996559 | 1.11099290819004 |
| C | -2.85710813460122 | 2.99324159501798 | 1.00323987833160 |
| C | -1.37415170908776 | 2.92192458950713 | 1.01956036272409 |
| C | -0.62471262511532 | 2.79587930983499 | -0.15042818687040 |
| O | 0.65815516039528 | 2.69787979000796 | -0.10974219209931 |
| H | -5.14412291775036 | -0.78645829799771 | -0.57347531561633 |
| H | -4.38066471458312 | -2.21019030417529 | 1.32833142912171 |
| H | -4.42101312955133 | 1.58197168450749 | -0.72457837922872 |
| H | -2.89471952606756 | -1.24739117869459 | 3.08485395603007 |
| H | -2.17752057376036 | 1.11010856143196 | 2.94915980604363 |
| Si | 1.87015696708039 | 2.57190753186817 | -1.42458683987925 |
| C | 2.77933985247255 | 1.00838644580776 | -0.99430376318806 |
| C | 2.86395264522596 | 4.13133733089351 | -1.21760564500318 |
| C | 0.90003734442397 | 2.48695207767944 | -3.01667470507028 |
| H | 3.60191212085795 | 0.84887373925397 | -1.71165338088652 |
| H | 2.11777861665023 | 0.12883798257746 | -1.03848798137370 |
| H | 3.21791674647088 | 1.06771948374212 | 0.01421333079957 |
| H | 0.23471635551361 | 1.60917723416032 | -3.05638770492576 |
| H | 0.30436084228174 | 3.39631892646312 | -3.19809174584067 |
| H | 1.60771707917019 | 2.39360443649607 | -3.85797166839641 |
| H | 2.25045459767143 | 5.02964112934626 | -1.39135125419314 |
| H | 3.69197591618227 | 4.14339859452005 | -1.94622274844738 |
| H | 3.30202119533530 | 4.19332605316819 | -0.20898333614186 |
| C | -3.51666196869380 | 3.97809516030584 | 2.02057489756890 |
| C | -5.03771398221241 | 3.93469129408421 | 1.84425123514074 |
| H | -5.42643089433326 | 2.94208027702393 | 2.11404388199525 |
| H | -5.51561200139834 | 4.68665467168727 | 2.48617134933221 |
| H | -5.32940885558160 | 4.15645076465096 | 0.80655001802390 |
| C | -3.15100116772209 | 3.69275577467736 | 3.49021522104073 |
| H | -3.58184347181610 | 2.73591932103683 | 3.81710671258242 |
| H | -3.57494711539571 | 4.47919200417208 | 4.13233608590963 |
| H | -2.06491575722471 | 3.67729602103285 | 3.66315538097891 |
| C | -3.01494806428892 | 5.38867914661518 | 1.68534592206261 |
| O | -3.69921138713099 | 6.36595917105800 | 1.55139475043511 |
| O | -1.66437119062660 | 5.41315751096141 | 1.57738317327020 |
| C | -1.06179943514073 | 6.68904660275711 | 1.31211537173863 |
| H | -1.27325572607790 | 7.38666361640369 | 2.13516720733364 |
| H | -1.45524820818348 | 7.11509463893791 | 0.37791588253613 |
| H | 0.01673045931826 | 6.50595789720712 | 1.23469321122646 |
| H | -3.17475067832228 | 3.32606018918126 | 0.00173214906681 |
| H | -1.12714970059708 | 2.79230772888805 | -1.13029034975219 |
| H | -0.82783148428504 | 2.88706825165420 | 1.96445017810837 |

## $D_4^{Ald-1,3}$



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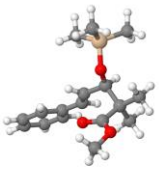
| C | -7.59393041439684 | 1.59757279619800 | 0.28269646241110 |
| C | -6.01232758659193 | 0.80913117503494 | -1.36556455888397 |
| C | -6.74686230513627 | 1.16254213877926 | 1.31527370301722 |
| C | -5.53522066842458 | 0.55463024907435 | 1.02052553067368 |
| C | -5.13193399658382 | 0.36238152599946 | -0.33403847725258 |
| C | -3.90275576597173 | -0.24174038612866 | -0.70252283984505 |
| C | -2.81715890344677 | -0.65678170246342 | 0.25013724335765 |
| C | -2.20923403097919 | 0.69255188067695 | 0.26313398852196 |
| O | -2.50015251537303 | 1.52171459941360 | 1.18157167314037 |
| H | -7.88326291294913 | 1.74949779976992 | -1.85994299055777 |
| H | -8.54757136931076 | 2.07250727451326 | 0.52404383648790 |
| H | -5.72111368789372 | 0.66451469748152 | -2.40902345565036 |
| H | -7.04719314518094 | 1.29712179684056 | 2.35681296925375 |
| H | -4.89207525618457 | 0.22356538304153 | 1.83603483046247 |
| Si | -2.28339554050057 | 3.30588384195840 | 1.23452596633042 |
| C | -1.81596053915549 | 3.59885919191768 | 3.00719508859963 |
| C | -3.96506922310474 | 3.93415824835614 | 0.74183069951198 |
| C | -0.93455970272173 | 3.68014325967213 | 0.00067067201337 |
| H | -2.59190338841108 | 3.21843565087792 | 3.69016668200366 |
| H | -1.70318935378876 | 4.67978821251411 | 3.19394950161700 |
| H | -0.86043983890630 | 3.11198814468882 | 3.25871815869446 |
| H | -0.69052211288825 | 4.75489149200637 | 0.04837566773084 |
| H | -1.23807984761344 | 3.46612944848063 | -1.03683760303198 |
| H | -0.00834615349048 | 3.12528916841290 | 0.22221363420721 |
| H | -4.73840712654433 | 3.59547318319931 | 1.44813851435369 |
| H | -4.24395581327942 | 3.58421692483463 | -0.26497804457285 |

| | | | |
|---|---|---|---|
| H | -3.96933555451395 | 5.03696741551016 | 0.73104045809208 |
| C | -1.90477017349919 | -1.83187541961344 | -0.19812558136732 |
| C | -2.72130667772259 | -3.12774083141159 | -0.16956931587259 |
| H | -3.54620339024796 | -3.07620117463332 | -0.89637354867702 |
| H | -3.14564993391077 | -3.31144425151913 | 0.82867235690883 |
| H | -2.08349535682538 | -3.98564526556897 | -0.42076814488846 |
| C | -1.27628703891235 | -1.62608726482174 | -1.59244272272640 |
| H | -2.04571559710001 | -1.61416217061277 | -2.37864593084441 |
| H | -0.60286303962124 | -2.46695947435813 | -1.81425621413488 |
| H | -0.68018593303150 | -0.70395179178558 | -1.65900903265212 |
| C | -0.75206089567395 | -1.92938019166325 | 0.81028866624193 |
| O | -0.34344766603672 | -2.94094138803480 | 1.30914719605414 |
| O | -0.21465285796068 | -0.70959513002044 | 1.05069393042869 |
| C | 0.90465153992562 | -0.66782380866147 | 1.95165276399061 |
| H | 1.18929840888892 | 0.38777772413285 | 2.03566978083608 |
| H | 1.73835143753734 | -1.26021505802922 | 1.54874579769753 |
| H | 0.62108048302610 | -1.07353516500516 | 2.93314461765359 |
| H | -1.58999646230534 | 1.01768093842133 | -0.58390762212015 |
| H | -3.68703460814499 | -0.33577276055750 | -1.76959930388339 |
| H | -3.22040705484596 | -0.86836147211752 | 1.25009922701484 |

## $D_4^{Ald-1,2}$



| | | | |
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| C | -3.89136681087724 | -1.24772195648385 | 0.20038547146474 |
| C | -4.31539855421178 | -1.11717708803168 | 2.97557289929178 |
| C | -3.27336109948879 | -0.39680920043179 | 2.42051883752684 |
| C | -3.03940450510128 | -0.43812140803600 | 1.01146980786432 |
| C | -1.98143026911527 | 0.28131648548621 | 0.38873189033731 |
| C | -1.14183417826295 | 1.18976653269255 | 1.02828517309160 |
| C | -0.02031746285024 | 1.93652018886021 | 0.36455797894383 |
| O | 0.26100683114300 | 3.08859046754000 | 1.09108712313732 |
| H | -5.58773642473714 | -2.57104429815245 | 0.13777207309532 |
| H | -5.97549361218682 | -2.46012978811826 | 2.59909728285237 |
| H | -3.71265388779007 | -1.29111493095570 | -0.87670222578968 |
| H | -4.48893290374644 | -1.08691835099901 | 4.05309868581534 |
| H | -2.61412184464186 | 0.18684655221822 | 3.06391578175792 |
| Si | -0.42458790174044 | 4.63138780475349 | 0.79260550941890 |
| C | 0.00441018990615 | 5.12258353956358 | -0.96601877272815 |
| C | 0.35715439910078 | 5.74187470499542 | 2.06813031080161 |
| C | -2.28502936087039 | 4.47259228956051 | 1.01246974056892 |
| H | 1.09633572161597 | 5.15269248223755 | -1.11266385802903 |
| H | -0.39132956327274 | 6.12681849232616 | -1.19165566881514 |
| H | -0.42337382313698 | 4.43270048219386 | -1.71251031736339 |
| H | -2.78297909798491 | 5.43901544063911 | 0.82751999132695 |
| H | -2.54168058438724 | 4.15976838239663 | 2.03815494607468 |
| H | -2.72350255095443 | 3.74439791780511 | 0.30896977967954 |
| H | 1.45082331757283 | 5.78084832038593 | 1.94046505737093 |
| H | 0.14360361679015 | 5.38671331240324 | 3.08894438352765 |
| H | -0.03059037319954 | 6.76984804612227 | 1.97807633386114 |
| C | 1.27433215302196 | 1.05690124235763 | 0.26362682121650 |
| C | 1.11954689020059 | -0.07925169712867 | -0.76992266745271 |
| H | 0.92382390044441 | 0.34355698874368 | -1.76742432553857 |
| H | 2.05210043756241 | -0.65888439356383 | -0.82819434691763 |
| H | 0.30901078921815 | -0.77649732963966 | -0.51450069907185 |
| C | 2.48022257918824 | 1.92858917846398 | -0.09100095936565 |
| H | 2.31478047418299 | 2.41166115031438 | -1.06629428601196 |
| H | 3.38592756726107 | 1.31070296520236 | -0.16181492066793 |
| H | 2.64072543919340 | 2.70994036492986 | 0.66106400701399 |
| C | 1.39690239131337 | 0.38780171612368 | 1.62967323820365 |
| O | 0.40462835294073 | 0.06269162861601 | 2.27170130282074 |
| O | 2.62369590228008 | 0.13863288569585 | 2.02042260794961 |
| C | 2.80730870629334 | -0.54843476771639 | 3.27633676813908 |
| H | 2.33651896464073 | -1.54056504077094 | 3.23378246067787 |
| H | 2.36005146697723 | 0.03682530123132 | 4.09170631159636 |
| H | 3.89078173871929 | -0.63679657089912 | 3.40897084598244 |
| H | -1.82809873908614 | 0.10105561134112 | -0.67946264040686 |
| H | -0.31673559875170 | 2.15988015627208 | -0.68177757039192 |
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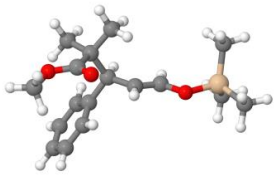
## $E_4^{Ald-1,4}$



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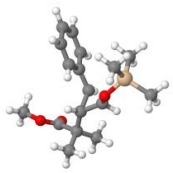
| C | -4.48703196826612 | 1.09082955306557 | 0.75683444220504 |
| C | -3.49755650917374 | -0.60233857748984 | 2.73170913680844 |
| C | -2.80281660691706 | 0.56087665142075 | 2.39390248489044 |
| C | -3.29222620704432 | 1.43167870837845 | 1.40643788789928 |
| C | -2.56154967707918 | 2.72054859539717 | 1.04867939404548 |
| C | -1.08180991692403 | 2.50514367805606 | 0.87718315866558 |
| C | -0.47672757035460 | 2.60173927863490 | -0.31166110817542 |
| O | 0.84795142178674 | 2.38500671935822 | -0.48855372227651 |
| H | -6.11345619852199 | -0.31852815049603 | 0.56730946828105 |
| H | -5.23499717731293 | -1.83707582303903 | 2.34488644747119 |
| H | -4.87718061752280 | 1.75000370863289 | -0.02369174425803 |
| H | -3.09762972782230 | -1.26583948914741 | 3.50325043844342 |
| H | -1.86578759055691 | 0.79238502931472 | 2.90309730453418 |
| Si | 1.76392693578274 | 2.80800979045853 | -1.85330499004171 |
| C | 3.48688034768099 | 2.18554373038258 | -1.47967541403024 |
| C | 1.71878806687972 | 4.67629268280298 | -2.04807541144479 |
| C | 1.03448749540514 | 1.96306556920082 | -3.36627276544202 |
| H | 4.17748613048881 | 2.41642000003482 | -2.30765560420872 |
| H | 3.48513346054779 | 1.09395261659682 | -1.32918230347452 |
| H | 3.88140951324923 | 2.65412650835545 | -0.56372544653680 |
| H | 1.01067486625541 | 0.86950998211980 | -3.23014668911387 |
| H | 0.00495227169509 | 2.30204974198353 | -3.56780394033912 |
| H | 1.63686521457061 | 2.18168576958422 | -4.26408071539836 |
| H | 0.68796037632137 | 5.03464138597753 | -2.20529691010362 |
| H | 2.32322042052454 | 5.00324566987023 | -2.91075637555892 |
| H | 2.11386337281508 | 5.17171572267401 | -1.14618843619720 |
| C | -2.91068013436770 | 3.90378646439649 | 2.04661719045850 |
| C | -2.04536985230345 | 5.12920680376483 | 1.71308846299271 |
| H | -2.16886181421221 | 5.39999072859560 | 0.65249745870640 |
| H | -2.34926198167747 | 5.99281269324997 | 2.32610043346774 |
| H | -0.98301047943020 | 4.92854111502829 | 1.89768295802350 |
| C | -4.39610644814540 | 4.26576400768305 | 1.91846327846692 |
| H | -4.60236933832542 | 4.62028679042497 | 0.89564919809149 |
| H | -4.66354816458804 | 5.07113766253835 | 2.61881857365178 |
| H | -5.04808423361268 | 3.40908439760752 | 2.12925475405753 |
| C | -2.55480673452935 | 3.43529264287708 | 3.45870307838559 |
| O | -1.42517324745329 | 3.31226663565549 | 3.87480559219626 |
| O | -3.63457919004218 | 3.12747514589114 | 4.19608408351855 |
| C | -3.38479375460443 | 2.57214385541296 | 5.48517110731655 |
| H | -2.74264391000154 | 3.23702578752371 | 6.08170513836465 |
| H | -2.88769028580977 | 1.59450936596394 | 5.39037240254779 |
| H | -4.36576265740566 | 2.45109031151762 | 5.96111371947984 |
| H | -2.96250335639663 | 3.05924553929248 | 0.07854078746228 |
| H | -1.05414183043639 | 2.85291469831711 | -1.21509847824878 |
| H | -0.47773230299402 | 2.26991618448864 | 1.75646597636982 |

## $E_4^{Ald-1,3}$



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| C | -5.93353336285501 | 0.63419184151718 | -0.68335390984018 |
| C | -6.33390998636006 | 1.18654172111484 | 2.01399002449887 |
| C | -5.08382609715880 | 0.74978140756371 | 1.57034621489420 |
| C | -4.85972723519353 | 0.47372945052414 | 0.20906039456985 |

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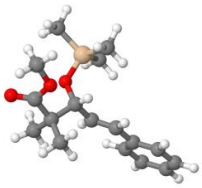
| C | -3.53440491387671 | 0.06760864811682 | -0.32572184074270 |
| C | -2.51277805259499 | -0.69030998595426 | 0.50262246434357 |
| C | -2.23211287736403 | 0.72822494620111 | 0.13636511458495 |
| O | -2.26093241665690 | 1.66394519174532 | 1.15235942236375 |
| H | -8.00275458082772 | 1.18379236618892 | -0.95583547317080 |
| H | -8.36728177870560 | 1.69375504511316 | 1.46366651306612 |
| H | -5.77893972978829 | 0.42293532946878 | -1.74499715190691 |
| H | -6.48252750543799 | 1.40152798389750 | 3.07568231701136 |
| H | -4.26826034336028 | 0.64454429942188 | 2.28545528090085 |
| Si | -2.48695020877826 | 3.33111326054657 | 0.93857812939064 |
| C | -2.99533145180946 | 3.95544868620661 | 2.62912737413464 |
| C | -3.80299924211122 | 3.67691109845003 | -0.35653932261079 |
| C | -0.84232189949629 | 4.07064809015292 | 0.39995896298551 |
| H | -3.97104972927599 | 3.53151485924661 | 2.91589583653468 |
| H | -3.08294161917873 | 5.05451781531388 | 2.63696197671551 |
| H | -2.25601302946301 | 3.66557314344496 | 3.39323541731809 |
| H | -0.91302415118427 | 5.16648573572937 | 0.29588265979388 |
| H | -0.52139780026130 | 3.66474457919634 | -0.57412205700496 |
| H | -0.05232437399277 | 3.84808502496780 | 1.13576368969064 |
| H | -4.79071518734134 | 3.31622474374629 | -0.03283633837008 |
| H | -3.56299404444261 | 3.18637328345852 | -1.31391497845226 |
| H | -3.87229067491930 | 4.76189236668615 | -0.54424716243307 |
| C | -1.76822858308410 | -1.91131044294791 | -0.06029330938421 |
| C | -1.02949215196371 | -1.61960552792790 | -1.37050601189556 |
| H | -0.20737309211332 | -0.91016905640164 | -1.19583832834736 |
| H | -1.69751307042965 | -1.21018368936235 | -2.14123812023344 |
| H | -0.60312039891714 | -2.54733311511813 | -1.77857182261036 |
| C | -0.77567281563492 | -2.42391308476080 | 0.99886215370049 |
| H | -0.03814652637180 | -1.63786037081935 | 1.22447974769818 |
| H | -0.23290890194317 | -3.31161324827029 | 0.63655502966729 |
| H | -1.29394769417773 | -2.69210636996511 | 1.92971839910291 |
| C | -2.86051527128937 | -2.95038582693485 | -0.33156894381179 |
| O | -3.20885022486267 | -3.33041994363387 | -1.42322481862879 |
| O | -3.44879792635591 | -3.35962997173746 | 0.80816455268589 |
| C | -4.56699667503816 | -4.23342412817022 | 0.66314775323943 |
| H | -4.91113807151812 | -4.46218556164147 | 1.67944209161930 |
| H | -4.27784648003126 | -5.15664049778189 | 0.13838524286257 |
| H | -5.36882449775647 | -3.74272827886343 | 0.09043792446220 |
| H | -1.49801325571862 | 0.92388567937654 | -0.65573948398998 |
| H | -3.55412741034069 | -0.18845783218087 | -1.38949868110242 |
| H | -2.80760158925663 | -0.81649324562827 | 1.54811323973507 |

## $D_4^{Ald-1,2}$



| | | | |
|---|---|---|---|
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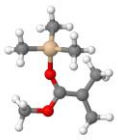
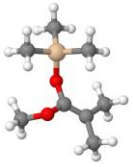
| C | -5.43614746754608 | -0.44199017004233 | 2.11183119602730 |
| C | -3.71579399186141 | -0.34528201498387 | 0.41331806340542 |
| C | -4.56062189768823 | 0.17142137641678 | 3.01649740655167 |
| C | -3.27124531731721 | 0.52236432446657 | 2.62238048413376 |
| C | -2.82258439113110 | 0.26977495293530 | 1.31034465076714 |
| C | -1.47551498076505 | 0.62712910634241 | 0.84352359447843 |
| C | -0.48631877503170 | 1.18878337080301 | 1.55731669520911 |
| C | 0.84859800468008 | 1.55591701894859 | 0.97760541436039 |
| O | 1.15349915550217 | 2.90948985509856 | 1.27133948956524 |
| H | -5.68224602126426 | -1.17667069140786 | 0.09225046246152 |
| H | -6.44666563384482 | -0.71634860391821 | 2.42452124197802 |
| H | -3.38544477237747 | -0.54759756181121 | -0.60944919333030 |
| H | -4.88833577658673 | 0.37763201230887 | 4.03869465589216 |
| H | -2.60363124958982 | 1.00123692254183 | 3.34163410424910 |
| Si | 0.47487924587242 | 4.25328978905206 | 0.50597370524339 |
| C | 1.74685361369633 | 5.61256221789937 | 0.72048300781839 |
| C | -1.14846031450258 | 4.71135441639027 | 1.33618384072640 |
| C | 0.19543217007660 | 3.84738997387163 | -1.31077876668022 |
| H | 1.97033527195087 | 5.76755041752580 | 1.78855369597624 |
| H | 1.38817327701776 | 6.56842265614632 | 0.30394094879149 |
| H | 2.69011834923949 | 5.34828436266029 | 0.21533123535988 |
| H | -0.10529518106409 | 4.74857834869153 | -1.87067426774194 |
| H | -0.59994002020815 | 3.09499411404741 | -1.43769277100466 |
| H | 1.11684860169322 | 3.45112683866961 | -1.76815037917862 |
| H | -0.99558317890834 | 4.89944333024973 | 2.41174420282086 |
| H | -1.88616856098656 | 3.89916622664561 | 1.23496481533658 |
| H | -1.58035626541124 | 5.62348225738861 | 0.89055223243934 |
| C | 2.03455611092360 | 0.70167311028486 | 1.50717389472362 |
| C | 2.11630516021299 | 0.73857647739610 | 3.03596054825498 |
| H | 1.27100200815597 | 0.19118850645148 | 3.47930351228150 |
| H | 3.05124748060632 | 0.27604417246063 | 3.38077418979473 |
| H | 2.09976535012811 | 1.77670679917632 | 3.39618918663846 |
| C | 1.91247391131333 | -0.74487634843840 | 0.99689111897190 |
| H | 0.98409903379439 | -1.20080708011219 | 1.37337948582003 |
| H | 2.76089963549792 | -1.35152224484636 | 1.34983404047340 |
| H | 1.89604972679529 | -0.78081376634814 | -0.10265815193118 |
| C | 3.31148590945199 | 1.32297936672183 | 0.93076719057948 |
| O | 4.30011668929678 | 1.60914364829145 | 1.55736079147078 |
| O | 3.22312215271494 | 1.49355274407848 | -0.40696075062348 |
| C | 4.35028981163927 | 2.09691700121891 | -1.03582897423069 |
| H | 5.25901002814751 | 1.49735463996103 | -0.87420672830316 |
| H | 4.52502988722128 | 3.10596286597754 | -0.63117838908754 |
| H | 4.11355103630011 | 2.15144858660803 | -2.10601516225749 |
| H | -1.27879425986539 | 0.40485560480201 | -0.21259362160957 |
| H | 0.81210098979555 | 1.40423410076402 | -0.11435724662536 |
| H | -0.62784319286958 | 1.44813421940186 | 2.61074442066896 |

## $1\text{-}G_1(x_1)$



| | | | |
|---|---|---|---|
| Si | -0.71970925562678 | 3.25679506237416 | -0.73667216295693 |
| C | -1.31718551688000 | 3.82601250536465 | -2.40330041083848 |
| C | -1.79329639530599 | 3.82622624077122 | 0.67084224010293 |
| C | 1.10270800801406 | 3.48323199518753 | -0.41817334758639 |
| H | -0.68497845941267 | 3.47331621508379 | -3.23254771913138 |
| H | -1.30949927901579 | 4.92890117745796 | -2.42968316369443 |
| H | -2.35240396245463 | 3.49759590037230 | -2.58823524841385 |
| H | 1.30024511231457 | 4.55628314564659 | -0.25331637465499 |
| H | 1.72931104785635 | 3.16116595476107 | -1.26275567226485 |
| H | 1.42731976689461 | 2.95010921764913 | 0.49020024006961 |
| H | -1.76073289979538 | 4.92645127194448 | 0.74153070390986 |
| H | -1.45043397856596 | 3.42244243619787 | 1.63687404239709 |
| H | -2.84456560286460 | 3.53402156461048 | 0.51888070660294 |
| C | 0.52912796895570 | -0.17726422891597 | -1.57429701623448 |
| C | 1.06346454646926 | -1.55294114221958 | -1.39216532376001 |
| H | 0.51019529077960 | -2.25049566309301 | -2.05340173477436 |
| H | 2.11823487941504 | -1.60282357777424 | -1.70349789867191 |
| H | 0.95451105410538 | -1.92423525726499 | -0.36550280467415 |
| C | 1.03168844104058 | 0.65896960233771 | -2.69456288325007 |
| H | 1.14306402135331 | 0.04085088708871 | -3.60107427550570 |
| H | 2.04677709399211 | 1.03405027940362 | -2.46151145157953 |
| H | 0.38807950912885 | 1.51555721442904 | -2.92455394235481 |
| C | -0.50390795705938 | 0.30976336668846 | -0.70269947162475 |
| O | -0.99281100263129 | 1.48858246629836 | -0.73259679341518 |
| O | -0.99166003196205 | -0.55174226411634 | 0.15058190006892 |
| C | -2.04153434708596 | -0.15348382332013 | 1.05750276382824 |
| H | -2.91552571533146 | 0.19202849303089 | 0.48823090265191 |
| H | -1.68142154118640 | 0.64920306744027 | 1.71619358159794 |
| H | -2.28189079514107 | -1.05094210743405 | 1.63648061415682 |

## $1\text{-}G_2(x_2)$



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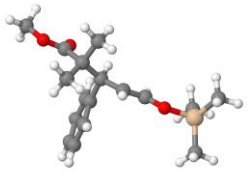
| C | -1.44544545388179 | 4.31104971911109 | -2.13465651749295 |
| C | -1.60755239174545 | 3.51104447590955 | 0.85066996427726 |

| | | | |
|---|---|---|---|
| C | 1.11871980166897 | 3.40863103751277 | -0.60516362080837 |
| H | -0.93021882677294 | 4.13954132363366 | -3.09343403368323 |
| H | -1.34024196445317 | 5.37729190486411 | -1.87410385175232 |
| H | -2.51728561504272 | 4.10099934848489 | -2.28255160001861 |
| H | 1.38378117870824 | 4.42752312289599 | -0.27737825016858 |
| H | 1.63009079807185 | 3.21021735799755 | -1.56077283140538 |
| H | 1.50878563297747 | 2.69713278542994 | 0.14045232313488 |
| H | -1.42863413578593 | 4.53698992965433 | 1.21408306816138 |
| H | -1.23713888803975 | 2.80580960490383 | 1.61123627146026 |
| H | -2.69681608855624 | 3.37262187127968 | 0.75351206100157 |
| C | 0.50461465538189 | -0.17202746258428 | -1.51844916334250 |
| C | 1.13777238139849 | -1.41046224436562 | -0.94681677095243 |
| H | 0.97641966426958 | -2.27996138219376 | -1.61010892788363 |
| H | 2.23305259741057 | -1.28696920171014 | -0.85840345094906 |
| H | 0.74025975710864 | -1.64967071911741 | 0.04787638431677 |
| C | 0.96737313180913 | 0.26527122497000 | -2.88065228643073 |
| H | 0.84954917727969 | -0.55094445302350 | -3.61608614854234 |
| H | 2.04315757623767 | 0.52243791451799 | -2.87141384331949 |
| H | 0.40609195171356 | 1.13578506645497 | -3.24477770994467 |
| C | -0.41706904669143 | 0.53037397820762 | -0.83392805062843 |
| O | -1.04859526148827 | 1.62856280153005 | -1.32646147592469 |
| O | -0.76379027205401 | 0.21023561128061 | 0.45114039271767 |
| C | -2.13761377340786 | -0.08588233917000 | 0.65716126720704 |
| H | -2.43198462540866 | -0.99225916469923 | 0.09756722713952 |
| H | -2.78458033969688 | 0.74930730943653 | 0.34326989970261 |
| H | -2.27081541534199 | -0.26387873650166 | 1.73316736369204 |

## $D_4^{Ald\text{-}1,4}$-$G_1(x_1)$



| | | | |
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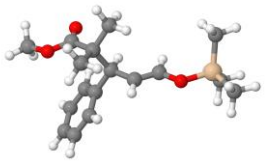
| C | -3.67528343850172 | -1.23574884494346 | 0.74034784357067 |
| C | -4.02048804804517 | 0.99048114198336 | -0.15885790089494 |
| C | -2.82060784498754 | -0.71944129684716 | 1.71972192293734 |
| C | -2.56607233026620 | 0.64978664989372 | 1.76685028649170 |
| C | -3.17963809066176 | 1.52721554954586 | 0.83811100727932 |
| C | -2.90288806317113 | 3.02776692819761 | 0.87424915763268 |
| C | -1.41693571386862 | 3.09714132319012 | 0.87878905111628 |
| C | -0.68431903954693 | 2.83161714332020 | -0.27520888954796 |
| O | 0.60297719078404 | 2.84345414733158 | -0.27377179204920 |
| H | -4.95424068768407 | -0.78128459740594 | -0.95031085873493 |
| H | -3.87860724444744 | -2.30850748745344 | 0.70262720550710 |
| H | -4.50616229831078 | 1.66573815835880 | -0.86485174437848 |
| H | -2.35469297369323 | -1.38560018763787 | 2.44895709641482 |
| H | -1.90442673776705 | 1.04434066791779 | 2.53882019363419 |
| Si | 1.77701720374111 | 2.57415863795916 | -1.59875440415944 |
| C | 2.77226042523621 | 1.13065174307146 | -0.97726237903185 |
| C | 2.70723091484093 | 4.18342262743691 | -1.66674298786977 |
| C | 0.76403461090298 | 2.20690189144395 | -3.12310422229820 |
| H | 3.57849401006477 | 0.89965903888862 | -1.69366223848568 |
| H | 2.15158027698445 | 0.22763830530765 | -0.86492175827740 |
| H | 3.23924901996527 | 1.35890062649533 | -0.00623643262484 |
| H | 0.14458967847225 | 1.30248076476785 | -3.00888883461284 |
| H | 0.11610961808258 | 3.05022205540076 | -3.41244072372561 |
| H | 1.44967530511600 | 2.02401321977093 | -3.96791409205991 |
| H | 2.04966655111534 | 5.02088582185607 | -1.94891459532150 |
| H | 3.51085534940444 | 4.11695136892329 | -2.41931249472409 |
| H | 3.17286855500970 | 4.41463985137821 | -0.69577399528552 |
| C | -3.61900830733399 | 3.85972576413971 | 1.97377189641044 |
| C | -3.38787626562805 | 3.33250804354319 | 3.39592309197111 |
| H | -2.31269291546946 | 3.30220879528931 | 3.63506251778063 |
| H | -3.87106879595812 | 3.99559660812343 | 4.12481348939693 |
| H | -3.80542632360611 | 2.32549253981460 | 3.53464784950602 |
| C | -3.14655615146338 | 5.32658988907216 | 1.86997554269957 |
| H | -2.07572647126016 | 5.40955605801624 | 2.11681613809088 |
| H | -3.70155478537378 | 5.95707800380600 | 2.57917375069958 |
| H | -3.30208333588350 | 5.72710511069429 | 0.85621196035415 |
| C | -5.11246782200963 | 3.85596499601929 | 1.60913080492386 |
| O | -5.53408955565337 | 3.62689189476657 | 0.49778759926223 |
| O | -5.88247169653004 | 4.18850725034920 | 2.64118522344007 |
| C | -7.29404041483829 | 4.28714317307777 | 2.39313681366546 |
| H | -7.68932594299787 | 3.31977812944412 | 2.05138441628727 |
| H | -7.49428652486097 | 5.04632301451869 | 1.62338841352364 |
| H | -7.74809411088401 | 4.57460073931584 | 3.34809605539709 |
| H | -3.27713870522479 | 3.41987470107513 | -0.08514027484726 |
| H | -1.21079964818532 | 2.61514896366211 | -1.21805859576586 |
| H | -0.85104913318552 | 3.28270294166125 | 1.79718877520815 |

## $D_4^{Ald\text{-}1,4}$-$G_2(x_2)$



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| C | -5.30294740481494 | -0.89503632313038 | 1.24920781982847 |
| C | -4.78805399455566 | 1.18018370168275 | 0.11092232747670 |
| C | -4.15536634737557 | -0.73468391439151 | 2.03060646786939 |
| C | -3.33131225523077 | 0.37961338076037 | 1.85305328817833 |
| C | -3.63834439835932 | 1.36030303776246 | 0.89708608538912 |
| C | -2.78777419869757 | 2.61130246832227 | 0.71050813101893 |
| C | -1.31181838125574 | 2.33596971084094 | 0.78429594960583 |
| C | -0.47819534505588 | 2.60395851453564 | -0.22840240116677 |
| O | 0.84960295573416 | 2.35404733912738 | -0.18149029174278 |
| H | -6.50219559105322 | -0.05183852145074 | -0.34238678342229 |
| H | -5.94576745289294 | -1.76832303189319 | 1.38625530464298 |
| H | -5.04157864102742 | 1.93193188262467 | -0.64013818712879 |
| H | -3.89601654844848 | -1.48469166796123 | 2.78251914445707 |
| H | -2.43484957543685 | 0.48041978197148 | 2.46716106569959 |
| Si | 1.98742822419237 | 2.75657140123643 | -1.37982066490174 |
| C | 3.61753638983807 | 2.13395634018244 | -0.70868016422381 |
| C | 1.98679810437498 | 4.62222420154576 | -1.60079630056003 |
| C | 1.51411827749489 | 1.89085947969814 | -2.97848195919781 |
| H | 4.43873820814736 | 2.34440326626615 | -1.41374044804021 |
| H | 3.58177046269269 | 1.04556648781767 | -0.54029702072348 |
| H | 3.85791570041424 | 2.61915138023221 | 0.25100438251405 |
| H | 1.47140373870412 | 0.79904677738555 | -2.83350350268742 |
| H | 0.52804583608761 | 2.22254311690929 | -3.34318928961087 |
| H | 2.25048464901620 | 2.10122568898074 | -3.77226677399868 |
| H | 1.00285202134670 | 4.98710657496520 | -1.93873910779131 |
| H | 2.73357377937923 | 4.93237268523722 | -2.35088097331744 |
| H | 2.22694488480456 | 5.12798602764400 | -0.65130087284403 |
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| C | -2.94500940410671 | 3.46062965310716 | 3.15269287231920 |
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| H | -3.44558904222233 | 2.53975856631986 | 3.47734348910309 |
| C | -2.52052803620935 | 5.08038769671149 | 1.27327071892641 |
| H | -1.43270040297442 | 4.96314776784910 | 1.37785808428280 |
| H | -2.84363836089133 | 5.91915380727463 | 1.91027279887225 |
| H | -2.75111594071690 | 5.33869945647143 | 0.22988262734087 |
| C | -4.73065150402852 | 3.97639460668346 | 1.41529573554203 |
| O | -5.17837070865194 | 4.42701540126900 | 0.38544293876385 |
| O | -5.50986456180861 | 3.54968624862869 | 2.42127586266750 |
| C | -6.91604259292453 | 3.57114639308678 | 2.18362439524679 |
| H | -7.17226578558249 | 2.89362730437987 | 1.35487750650711 |
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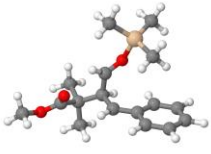
| H | -3.00616131911856 | 2.99531347179617 | -0.29810412320020 |
| H | -0.86244743340624 | 3.04529183404807 | -1.16077175627182 |
| H | -0.88607116607011 | 1.89658631747577 | 1.69030983545708 |

## $D_4^{Ald\text{-}1,3}$-$G_1(x_1)$



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| C | -6.19110539724836 | 1.24010866416030 | -1.16465191107081 |
| C | -6.82102317413735 | 1.30410091391233 | 1.56544255151334 |
| C | -5.64474383829846 | 0.69248187378281 | 1.15674067284081 |
| C | -5.29583177289537 | 0.64726869149954 | -0.22476013657205 |
| C | -4.09951054828819 | 0.05822573973349 | -0.71053454394283 |
| C | -2.99177732692917 | -0.49464924636178 | 0.14121932452870 |
| C | -2.37086661734789 | 0.85348157157314 | 0.23623225298596 |
| O | -2.60036040900691 | 1.58656454959006 | 1.25726840661372 |
| H | -8.04028449807937 | 2.29584432150086 | -1.47652789779441 |
| H | -8.61013323999360 | 2.36169466166925 | 0.95197774958637 |
| H | -5.93653086074724 | 1.21102666521964 | -2.22698196690255 |
| H | -7.08061628083528 | 1.32854866210899 | 2.62609771354932 |
| H | -4.98664825498081 | 0.24777841936012 | 1.90335835705368 |
| Si | -2.43312167277103 | 3.37119340223115 | 1.40260550979597 |
| C | -2.36652333216405 | 3.60967218329122 | 3.24231120593266 |
| C | -3.97955535121701 | 4.00957040321239 | 0.58076729095208 |
| C | -0.86216901466836 | 3.80426834653245 | 0.49601239942327 |
| H | -3.27371387655846 | 3.21422364843146 | 3.72592570011326 |
| H | -2.29697792206665 | 4.68368688672517 | 3.48201567291350 |
| H | -1.48948893626281 | 3.10895512901219 | 3.68210559941389 |
| H | -0.67296885085928 | 4.88684753539022 | 0.59158221819177 |
| H | -0.92156173266472 | 3.58108549654391 | -0.58147995212765 |
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| H | -4.02210164493862 | 3.71236128206547 | -0.47912574909328 |
| H | -3.99803094509725 | 5.11157759787851 | 0.62163249012170 |
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| C | -0.98798882506274 | -1.95966950610596 | 0.52253581752701 |
| H | -1.37118101799332 | -2.21425544043454 | 1.52291988547751 |
| H | -0.31825377660545 | -1.08986792902954 | 0.62088483245105 |
| H | -0.39524549383995 | -2.80777993725866 | 0.15393202864954 |
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| H | -3.49224517687224 | -3.15403174778566 | 0.43124977101687 |
| H | -2.51426944501430 | -3.76002555155503 | -0.93190247125494 |
| H | -3.91804417114042 | -2.70849121099145 | -1.24176017641257 |
| C | -1.56921016021547 | -1.31041718685883 | -1.80777818008531 |
| O | -1.57298740600672 | -0.19897907018825 | -2.29799979243345 |
| O | -1.01720253749063 | -2.36589023828203 | -2.39153790892344 |
| C | -0.38670639946031 | -2.15903508628053 | -3.66725247869477 |
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| H | 0.42883634130733 | -1.42765944080485 | -3.57465358717757 |
| H | -1.11953541228706 | -1.78893694382908 | -4.39826990709076 |
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| H | -3.90968847592457 | 0.09322710206164 | -1.78536507197373 |
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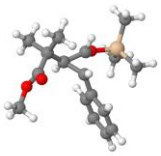
## $D_4^{Ald\text{-}1,3}$-$G_2(x_2)$



| | | | |
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| C | -5.81838974916371 | 0.38123819640927 | -0.54616009968351 |
| C | -6.22629088417213 | 1.17518228060036 | 2.08908040198993 |
| C | -4.95408349392638 | 0.78087789579934 | 1.66925639136249 |
| C | -4.72647264025681 | 0.38435106779198 | 0.33864586045685 |
| C | -3.38230106329291 | 0.01623101087309 | -0.17613833288504 |
| C | -2.30149645489586 | -0.58134804220574 | 0.70640844116953 |
| C | -2.12398134393437 | 0.80785046293046 | 0.19264273984095 |
| O | -2.20633125447494 | 1.83896425266419 | 1.10831908481278 |
| H | -7.92336253919658 | 0.76010606783256 | -0.83542176497970 |
| H | -8.29558884092500 | 1.48627689983505 | 1.52693907244666 |
| H | -5.66119673997103 | 0.07472156584033 | -1.58392410102092 |
| H | -6.37774319257387 | 1.48588587318167 | 3.12639434374771 |
| H | -4.12547218971122 | 0.80322865102258 | 2.37674251004656 |
| Si | -2.55064332587472 | 3.45620807371211 | 0.73163627769950 |
| C | -3.07423643032501 | 4.21459707719157 | 2.36163890034442 |
| C | -3.90737533976126 | 3.57902275291482 | -0.56176170893365 |
| C | -0.96972780468438 | 4.24569509223951 | 0.08413954359172 |
| H | -4.01295458546605 | 3.75703100878937 | 2.71297259878632 |
| H | -3.23871613024496 | 5.30012752403618 | 2.26020762257187 |
| H | -2.30392416529282 | 4.05580264615099 | 3.13357741353327 |
| H | -1.11739303540480 | 5.31790074290408 | -0.12854567919889 |
| H | -0.63679116273475 | 3.76472088945457 | -0.85096888314753 |
| H | -0.15490868057916 | 4.15309392554419 | 0.82071076991675 |
| H | -4.86355461070742 | 3.19107857776596 | -0.18015391495834 |
| H | -3.65051979695897 | 3.00781564960771 | -1.46868615699431 |
| H | -4.05193911555420 | 4.63172742074044 | -0.85865279102850 |
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| C | -0.77676555848184 | -1.59441428994593 | -1.08848825139982 |
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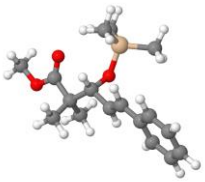
| H | -1.47967228461691 | -1.31227357381562 | -1.88489907821459 |
| H | -0.29119011127179 | -2.52781631066081 | -1.40775235117421 |
| C | -0.44304619950726 | -2.13250926208752 | 1.34559858924256 |
| H | 0.24057158741210 | -1.27927595069151 | 1.47741427863328 |
| H | 0.15627151349060 | -3.01364992395652 | 1.06571876936741 |
| H | -0.93169693332218 | -2.33856921805122 | 2.30776022244362 |
| C | -2.49986293109781 | -2.93348938034599 | 0.11200850823135 |
| O | -2.83148627257361 | -3.44703312428948 | -0.92901104530022 |
| O | -3.04734305171659 | -3.26177943114209 | 1.29735173948570 |
| C | -4.10394423815140 | -4.21949894216353 | 1.26132611906642 |
| H | -4.42073386635362 | -4.36575955834410 | 2.30145248565321 |
| H | -3.75726778151285 | -5.16985259851996 | 0.82781001371226 |
| H | -4.94374284824876 | -3.84525468824855 | 0.65600517366744 |
| H | -1.41375918810780 | 0.97029372274548 | -0.62821918467369 |
| H | -3.39576568197591 | -0.34869348823159 | -1.20776752180150 |
| H | -2.57469560521996 | -0.61970222557176 | 1.76458547900798 |

## $D_4^{Ald\text{-}1,2}$-$G_1(x_1)$



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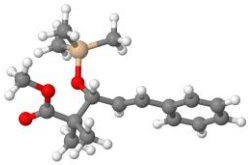
| C | -4.38518145336098 | 0.38246957224005 | 1.04714105709269 |
| C | -4.33307972197110 | 0.01656448362396 | 3.83328855399645 |
| C | -3.15273829548987 | 0.29537165811993 | 3.16883348994946 |
| C | -3.15006030817508 | 0.48762004249903 | 1.75351390434224 |
| C | -1.96477945288378 | 0.78100482742061 | 1.01076708411909 |
| C | -0.67840561139690 | 0.83706376711248 | 1.50715541519986 |
| C | 0.48953510926653 | 1.23512820814218 | 0.65862597299469 |
| O | 0.51421319658690 | 2.58824004292599 | 1.06367510492662 |
| H | -6.50444532827855 | 0.02499150616890 | 1.17362511493793 |
| H | -6.46935639875026 | -0.30338287385830 | 3.64597710751902 |
| H | -4.39004364643354 | 0.52691866723968 | -0.03585588206770 |
| H | -4.33251937725023 | -0.12499271897463 | 4.91585543157520 |
| H | -2.22335438193184 | 0.37628087882090 | 3.73404518676673 |
| Si | 0.12757271929245 | 4.01079596642301 | 0.13068976268819 |
| C | 1.70467536778208 | 5.01167665729018 | 0.14462389860080 |
| C | -1.25423781482394 | 4.82622048338195 | 1.09478935730531 |
| C | -0.40607308701559 | 3.48863496459662 | -1.58326113272032 |
| H | 2.04419682028272 | 5.20121361184759 | 1.17490788613752 |
| H | 1.52975268213683 | 5.98466842206227 | -0.34457990464922 |
| H | 2.49336809415770 | 4.47373413610958 | -0.40139157950557 |
| H | -0.61526628043169 | 4.38813781821038 | -2.18630661143686 |
| H | -1.32736099338068 | 2.88315815296332 | -1.57869713232470 |
| H | 0.39536074643757 | 2.92475353783486 | -2.08411176695505 |
| H | -0.94655649648593 | 5.02698611514732 | 2.13342626372414 |
| H | -2.15320286211938 | 4.18839548426021 | 1.11755031638248 |
| H | -1.53333888915420 | 5.78773674643602 | 0.63317442221783 |
| C | 1.82209185116967 | 0.51824020431593 | 0.92568016378252 |
| C | 2.31374926047588 | 0.72206468238088 | 2.36812350224421 |
| H | 1.63769395238796 | 0.23176851101113 | 3.08635192631062 |
| H | 3.30831631070966 | 0.27444681971422 | 2.49146204532013 |
| H | 2.37437014855751 | 1.79043064191405 | 2.61901882624729 |
| C | 1.65072440204069 | -0.97905766174370 | 0.60909562317435 |
| H | 0.90585709140019 | -1.43302703011602 | 1.28332712326244 |
| H | 2.60249424935101 | -1.50902119978116 | 0.75072072801212 |
| H | 1.31915635172080 | -1.13984492636042 | -0.42913678732068 |
| C | 2.83274936571693 | 1.12435586706819 | -0.05885150276869 |
| O | 2.55066424618173 | 1.94286306121072 | -0.90742802532751 |

| | | | |
|---|---|---|---|
| O | 4.05383827621487 | 0.63121636494133 | 0.11658137515563 |
| C | 5.08607193141659 | 1.11038654068464 | -0.76059446478682 |
| H | 5.22181714844772 | 2.19399420371039 | -0.63232790342835 |
| H | 4.82401792137068 | 0.90351740663011 | -1.80802787902981 |
| H | 5.99679119926016 | 0.57204093445119 | -0.47539928804745 |
| H | -2.09489988288276 | 0.95114120932433 | -0.06347237000609 |
| H | 0.24691813467784 | 1.14079682536674 | -0.41034508244433 |
| H | -0.48409010806151 | 0.72066923576094 | 2.57568965092991 |

**$D_4^{Ald\text{-}1,2}$-$G_2(x_2)$**



| | | | |
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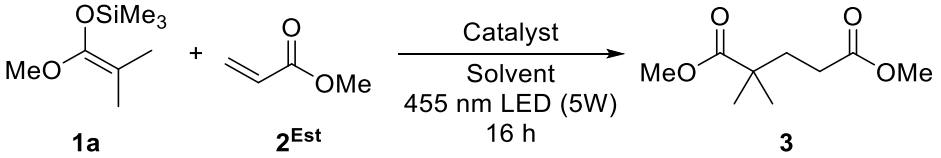
| C | -4.07030708496451 | -0.29387687375235 | 1.22656106699362 |
| C | -4.39252309121918 | 0.39049540291659 | 3.90684183633790 |
| C | -3.18405270164278 | 0.65025571151569 | 3.26421010080223 |
| C | -2.99962428122256 | 0.31456835534685 | 1.90786959699200 |
| C | -1.74851528664732 | 0.57584372124119 | 1.18243319174188 |
| C | -0.64532882720877 | 1.18131269695998 | 1.64973018831771 |
| C | 0.59106988867462 | 1.41127495378525 | 0.82925970490328 |
| O | 1.02636998203115 | 2.75316947670062 | 0.97547761469619 |
| H | -6.09821812348148 | -1.02910433480655 | 1.31817542156841 |
| H | -6.39469345556488 | -0.41756029339176 | 3.72110562356902 |
| H | -3.94504218944732 | -0.56286050163460 | 0.17389551285435 |
| H | -4.51374583053687 | 0.65932216465408 | 4.95941008514745 |
| H | -2.37073862529681 | 1.11803915191680 | 3.82286601331472 |
| Si | 0.50105245232284 | 4.06438804130321 | 0.05078196358251 |
| C | 1.35431238277851 | 5.54672306211422 | 0.81297335846373 |
| C | -1.37063111720065 | 4.22383814037849 | 0.14707988258247 |
| C | 1.03564969693722 | 3.82120178187217 | -1.73776953540463 |
| H | 1.03991997842541 | 5.68469072319124 | 1.86016059438529 |
| H | 1.11677915010742 | 6.47048700964114 | 0.25966008781655 |
| H | 2.44800816182414 | 5.41155330670785 | 0.80305876251753 |
| H | 0.64992182013856 | 4.63377373456811 | -2.37611831550960 |
| H | 0.66418276929764 | 2.86682863934349 | -2.14442575625198 |
| H | 2.13393522160274 | 3.81606752564797 | -1.81903204075456 |
| H | -1.70710597425618 | 4.29902803942832 | 1.19378659901454 |
| H | -1.87493739524650 | 3.35277984437677 | -0.30050942654277 |
| H | -1.71166562189392 | 5.12655250629129 | -0.38784605676798 |
| C | 1.78456559703054 | 0.49428230518188 | 1.23123335073221 |
| C | 2.14199452388233 | 0.66303902374089 | 2.71079807622802 |
| H | 1.34371216806002 | 0.25363108921505 | 3.34773427067187 |
| H | 3.07753175854167 | 0.13514305796637 | 2.94164624617898 |
| H | 2.28404071591944 | 1.72534474334068 | 2.95255642537334 |
| C | 1.45874258745740 | -0.97462318315121 | 0.90783612529166 |
| H | 0.59458491404803 | -1.31024470777662 | 1.50044189945551 |
| H | 2.31526753499228 | -1.62171270384518 | 1.15324331261927 |
| H | 1.22200252945825 | -1.10630735325349 | -0.15843336435901 |
| C | 2.98425938270411 | 0.92537135837214 | 0.38223039823819 |
| O | 4.08079008508360 | 1.20126465177383 | 0.79891080645687 |
| O | 2.68425069916170 | 0.93039557635356 | -0.93545840731857 |
| C | 3.73977756417815 | 1.30471364647793 | -1.81637563211648 |
| H | 4.57156145323180 | 0.58587574734401 | -1.75718924557373 |
| H | 4.12693093909030 | 2.30205708615094 | -1.55897448960525 |
| H | 3.31086298179977 | 1.31093841358675 | -2.82609033243612 |
| H | -1.74038505216902 | 0.23451560047189 | 0.13983554024021 |
| H | 0.36175148991420 | 1.18866517122878 | -0.22786795313044 |
| H | -0.60203773109678 | 1.56486344341860 | 2.67337785868142 |

# 3 Experimental

## *3.1 Reaction optimization*

All optimization reactions were carried out on a 0.10 mmol scale: In an oven-dried Schlenk tube, 2-methyl-1-methoxy-1-(trimethylsiloxy)propene **1a**, methyl acrylate **$2^{Est}$** and the photocatalyst were dissolved in the indicated amount of solvent. The mixture was degassed using three freeze-pump-thaw cycles, backfilled with argon and stirred under irradiation in the custom-made “light box”. After 16 h, mesitylene (14 µL, 0.10 mmol, 1.0 equiv) was added as an internal standard and the mixture was filtered through a short plug of silica gel. The eluate was analyzed and quantified by GC-FID.

**Table S12:** Optimization table for the coupling of silyl ketene acetal (**1a)** and acrylate (**$2^{Est}$**).




**1a** **$2^{Est}$** **3**

| Entry | Catalyst (mol%) | | Equivalents | | Solvent | Conc. | Yield[a] |
|---|---|---|---|---|---|---|---|
| | | | **1** | **2$^{Est}$** | | | |
| 1 | $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ | (2.5) | 1.0 | 3.0 | MeCN | 0.2 M | 24% |
| 2 | $[Ru(bpy)_3](BF_4)_2$ | (2.5) | 1.0 | 3.0 | MeCN | 0.2 M | 38% |
| 3 | $MesAcrClO_4$ | (5.0) | 1.0 | 3.0 | MeCN | 0.2 M | 16% |
| 4 | $[Ru(bpy)_3](PF_6)_2$ | (2.5) | 1.0 | 5.0 | MeCN | 0.2 M | 29% |
| 5 | $[Ru(bpy)_3](PF_6)_2$ | (2.5) | 1.0 | 1.0 | MeCN | 0.2 M | 49% |
| 6 | $[Ru(bpy)_3](PF_6)_2$ | (2.5) | 3.0 | 1.0 | MeCN | 0.2 M | 69% |
| 7 | $[Ru(bpy)_3](PF_6)_2$ | (1.0) | 1.0 | 3.0 | MeCN | 0.2 M | 31% |
| 8 | $[Ru(bpy)_3](PF_6)_2$ | (2.5) | 1.0 | 3.0 | MeCN | 0.1 M | 5% |
| 9 | $[Ru(bpy)_3](PF_6)_2$ | (2.5) | 1.0 | 3.0 | MeCN | 1.0 M | 15% |
| 10 | $[Ru(bpy)_3](PF_6)_2$ | (2.5) | 1.0 | 3.0 | DMA | 0.2 M | 21% |
| 11 | $[Ru(bpy)_3](PF_6)_2$ | (2.5) | 1.0 | 3.0 | DMSO | 0.2 M | 11% |
| 12 | $[Ru(bpy)_3](BF_4)_2$ | (2.5) | 2.0 | 1.0 | MeCN | 0.2 M | 49% |
| 13 | $[Ru(bpy)_3](BF_4)_2$ | (2.5) | 3.0 | 1.0 | MeCN | 0.2 M | 54% |
| 14 | $[Ru(bpy)_3](BF_4)_2$ | (2.5) | 4.0 | 1.0 | MeCN | 0.2 M | 59% |
| 15 | $[Ru(bpy)_3](BF_4)_2$ | (2.5) | 3.0 | 1.0 | MeCN | 0.5 M | 48% |
| 16 | $[Ru(bpy)_3](BF_4)_2$ | (2.5) | 3.0 | 1.0 | MeCN | 0.1 M | 68% |
| 17 | $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ | (2.5) | 1.0 | 3.0 | DCE | 0.2 M | 22% |
| 18 | $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ | (2.5) | 1.0 | 3.0 | $CH_2Cl_2$ | 0.2 M | 16% |
| 19 | $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ | (2.5) | 1.0 | 3.0 | EtOAc | 0.2 M | 15% |
| 20 | $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ | (2.5) | 3.0 | 1.0 | MeCN | 0.2 M | 65% |
| 21 | $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ | (2.5) | 3.0 | 1.0 | MeCN | 0.1 M | 96% |
| 22 | $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ | (2.5) | 3.0 | 1.0 | MeCN | 0.05 M | 81% |

| Entry | Catalyst (mol%) | | Equivalents | | Solvent | Conc. | Yield[a] |
|---|---|---|---|---|---|---|---|
| | | | **1** | **2$^{Est}$** | | | |
| 23 | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (2.5) | 1.0 | 1.0 | MeCN | 0.1 M | 77% |
| 24 | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (2.5) | 2.0 | 1.0 | MeCN | 0.1 M | 88% |
| 25 | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (2.5) | 5.0 | 1.0 | MeCN | 0.1 M | 94% |
| 26[b] | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (2.5) | 3.0 | 1.0 | MeCN | 0.1 M | 96% |
| 27[c] | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (2.5) | 3.0 | 1.0 | MeCN | 0.1 M | 40% |
| 28[b] | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (5.0) | 3.0 | 1.0 | MeCN | 0.1 M | 98% |
| **29[b]** | **[Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$** | **(1.0)** | **3.0** | **1.0** | **MeCN** | **0.1 M** | **93%** |
| 30[b] | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (0.5) | 3.0 | 1.0 | MeCN | 0.1 M | 81% |
| 31[b] | - | | 3.0 | 3.0 | MeCN | 0.1 M | 0% |
| 32[b,d] | [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ | (1.0) | 1.0 | 1.0 | MeCN | 0.1 M | 0% |

[a] Yield was determined via calibrated GC-FID (1.0 equiv mesitylene as an internal standard).

[b] Reaction was carried out without freeze-pump-thaw degassing.

[c] Reaction was carried out under air.

[d] Reaction was carried out without irradiation.

## *3.2 Preparation and characterization of products*

**P1: Coupling of commercially available silyl ketene acetals**

In an oven-dried Schlenk tube, $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ (5.6 mg, 0.005 mmol, 1.0 mol%), the silyl ketene acetal (1.5 mmol, 3.0 equiv) and the respective olefin (0.50 mmol, 1.0 equiv) were dissolved in anhydrous acetonitrile (5.0 mL) under an argon atmosphere. The reaction mixture was stirred at room temperature and 455 nm irradiation in the described custom-made "light box" for 16 h. After the indicated reaction time, the mixture was quenched with aqueous HCl (2 M, 5 mL), followed by extraction with dichloromethane (3 × 10 mL). The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel.

**P2: Coupling of commercially available silyl Ketene acetals with $Bu_4NF$ workup**

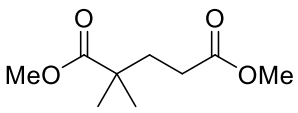
Reaction setup and performance was carried out as described in procedure **P1** on a 0.4 mmol scale. After 16 h, a solution of $Bu_4NF$ (1 M in THF, 0.5 mL) was added and the mixture was stirred for another hour. Subsequently, aqueous workup and purification were performed as described in procedure **P1**.

**P3: Pre-formation of silyl ketene acetals and subsequent coupling**

In a dried Schlenk tube, lithium diisopropyl amide (353 mg, 3.3 mmol, 6.6 equiv) was dissolved in anhydrous THF (10 mL) and cooled to −78 °C. A solution of the respective ester (3.0 mmol, 6.0 equiv) in THF (5.0 mL) was added dropwise and the reaction was stirred at −78 °C for 30 min. Trimethylchlorosilane (455 µL, 3.6 mmol, 7.2 equiv) was added dropwise and the mixture was allowed to reach room temperature. After concentration under reduced pressure, the residue was dissolved in pentane and filtered through a short plug of celite. The crude silyl ketene acetal was used for performing the reaction as described in procedure **P1.**

### 3.2.1 Reaction with esters

#### 3.2.1.1 Dimethyl 2,2-dimethylpentanedioate (3a)




Product **3a** was prepared according to general procedure **P1** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (305 µL, 1.5 mmol, 3.0 equiv), methyl acrylate (45 µL, 0.5 mmol, 1.0 equiv). Purification by column chromatography on silica gel (5% EtOAc in pentane) afforded **3a** as a colorless liquid (73 mg, 0.39 mmol, 77%).

**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 3.65 (s, 6H), 2.33 – 2.22 (m, 2H), 1.92 – 1.81 (m, 2H), 1.18 (s, 6H).

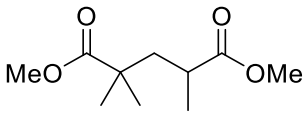
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 177.8, 174.0, 52.0, 51.8, 41.8, 35.3, 30.1, 25.1.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_9H_{16}NaO_4^+$): 211.0941, found: 211.0940.

**EI-MS:** *m*/*z* (%): 157 (11), 129 (85), 102 (33), 97 (78), 87 (19), 69 (100), 59 (17), 55 (20), 41 (24).

**$R_f$** (5% EtOAc in pentane)**:** 0.22.

### 3.2.1.2 Dimethyl 2,2,4-trimethylpentanedioate (3b)




Product **3b** was prepared according to general procedure **P1** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (305 µL, 1.5 mmol, 3.0 equiv) and methyl methacrylate (53 µL, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (5% EtOAc in pentane) afforded **3b** as a colorless liquid (93 mg, 0.46 mmol, 92%).

**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 3.64 (s, 3H), 3.64 (s, 3H), 2.58 – 2.38 (m, 1H), 2.08 (dd, *J* = 14.2, 8.8 Hz, 1H), 1.61 (dd, *J* = 14.1, 4.0 Hz, 1H), 1.35 – 0.96 (m, 9H).

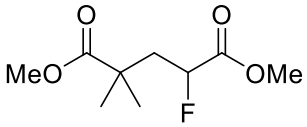
**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 178.1, 177.5, 51.9, 51.8, 44.1, 42.0, 36.6, 26.0, 24.9, 19.5.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{10}H_{18}NaO_4^+$): 225.1097, found: 225.1098.

**EI-MS:** *miz* (%): 171 (13), 143 (53), 111 (33), 102 (40), 87 (15), 83 (100), 70 (12), 69 (20), 59 (17), 55 (27), 41 (21).

**$R_f$** (10% EtOAc in pentane)**:** 0.79.

### 3.2.1.3 Dimethyl 4-fluoro-2,2-dimethylpentanedioate (3c)




Product **3c** was prepared according to general procedure **P1** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (305 µL, 1.5 mmol, 3.0 equiv) and methyl 2-fluoroacrylate (47 µL, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (5% EtOAc in pentane) afforded **3c** as a colorless liquid (93 mg, 0.45 mmol, 90%).

**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 5.02 (ddd, *J* = 49.8, 9.1, 3.5 Hz, 1H), 3.79 (s, 3H), 3.68 (s, 3H), 2.31 – 1.95 (m, 2H), 1.34 – 1.24 (m, 6H).

**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 177.4, 170.4 (d, *J* = 24 Hz), 87.1 (d, *J* = 185 Hz), 52.6, 52.2, 42.4 (d, *J* = 20 Hz), 40.8, 25.8 (d, *J* = 1 Hz), 25.1.

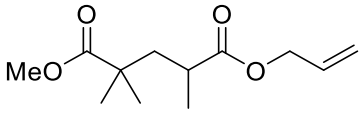
**$^{19}$F NMR (282 MHz, $CDCl_3$):** δ (ppm): -190.0.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_9H_{15}FNaO_4^+$): 229.0847, found: 229.0853.

**EI-MS:** *m*/*z* (%): 175 (15), 127 (100), 102 (31), 99 (14), 95 (45), 87 (17), 70 (11), 67 (22), 59 (23), 41 (15).

**$R_f$** (10% EtOAc in pentane)**:** 0.63.

**5-Allyl 1-methyl 2,2-dimethylpentanedioate (3d)**




Product **3d** was prepared according to general procedure **P1** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (305 µL, 1.5 mmol, 3.0 equiv) and allyl methacrylate (66 µL, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (15% EtOAc in pentane) afforded **3d** as a colorless liquid (55 mg, 0.21 mmol, 41%). The product contains residual methyl isobutyrate, the yield was calculated accordingly.

**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 5.91 (ddt, J = 17.2, 10.4, 5.7 Hz, 1H), 5.35 – 5.20 (m, 2H), 4.55 (d, J = 5.8 Hz, 2H), 3.64 (s, 3H), 2.56 – 2.43 (m, 1H), 2.10 (dd, J = 14.2, 8.5 Hz, 1H), 1.64 (dd, J = 14.2, 4.1 Hz, 1H), 1.20 – 1.11 (m, 9H).

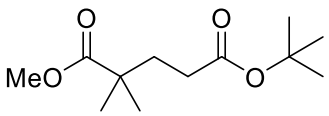
**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 178.1, 176.7, 132.4, 118.3, 65.2, 51.9, 43.9, 42.1, 36.7, 26.2, 24.8, 19.5.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{12}H_{20}NaO_4^+$): 251.1254, found: 251.1257.

**EI-MS:** *m*/*z* (%): 228 (2), 197 (7), 171 (14), 169 (25), 143 (43), 127 (12), 115 (10), 111 (14), 102 (22), 83 (100), 69 (27), 59 (39), 57 (10).

**$R_f$** (20% EtOAc in Pentane)**:** 0.39.

### 3.2.1.4 5-(*tert*-Butyl) 1-methyl 2,2-dimethylpentanedioate (3e)




Product **3e** was prepared according to general procedure **P1** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (305 µL, 1.5 mmol, 3.0 equiv) and *tert*-butyl acrylate (73 µL, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (5% EtOAc in pentane) afforded **3e** as a colorless liquid (107 mg, 0.46 mmol, 93%).

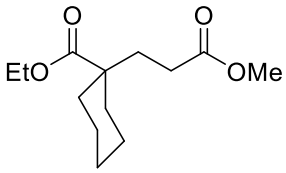
**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 3.66 (s, 3H), 2.26 – 2.10 (m, 2H), 1.89 – 1.75 (m, 2H), 1.43 (s, 9H), 1.17 (s, 6H).

**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 178.0, 172.9, 80.4, 52.0, 41.8, 35.3, 31.5, 28.2, 25.1.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{12}H_{22}NaO_4^+$): 253.1410, found: 253.1419.

**EI-MS:** *m*/*z* (%): 157 (37), 143 (29), 129 (54), 115 (34), 102 (27), 97 (42), 69 (27), 57 (100), 41 (30). **$R_f$** (10% EtOAc in pentane): 0.32.

### 3.2.1.5 Ethyl 1-(3-methoxy-3-oxopropyl)cyclohexane-1-carboxylate (3f)




Product **3f** was prepared according to general procedure **P3** using ethyl cyclohexanecarboxylate (499 µL, 3.0 mmol, 6.0 equiv) and methyl acrylate (45 µL, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded **3f** as a colorless oil (91 mg, 0.38 mmol, 75%).

**$^1$H NMR (400 MHz, $CDCl_3$)**: δ (ppm): 4.13 (q, *J* = 7.1 Hz, 2H), 3.65 (s, 3H), 2.28 – 2.20 (m, 2H), 2.05 (ddt, *J* = 14.3, 4.8, 2.0 Hz, 2H), 1.86 – 1.76 (m, 2H), 1.62 – 1.50 (m, 3H), 1.40 – 1.13 (m, 5H) 1.25 (t, *J* = 7.1 Hz, 3H).

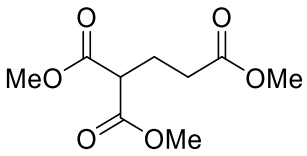
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 176.0, 173.9, 60.3, 51.6, 46.2, 34.9, 33.9, 29.1, 25.8, 23.1, 14.3.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{13}H_{22}NaO_4^+$): 265.1410, found: 265.1422.

**EI-MS:** *m*/*z* (%): 211 (11), 183 (21), 169 (83), 156 (65), 137 (100), 119 (51), 95 (87), 81 (31), 67 (36), 55 (19), 41 (15).

**$R_f$** (10% EtOAc in pentane): 0.22.

### 3.2.1.6 Trimethyl propane-1,1,3-tricarboxylate (3g)




Product **3g** was prepared according to general procedure **P3** using dimethyl malonate (345 µL, 3.0 mmol, 6.0 equiv) and methyl acrylate (45 µL, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded **3g** as a colorless liquid (93 mg, 0.43 mmol, 85%).

**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 3.74 (s, 6H), 3.67 (s, 3H), 3.48 (t, *J* = 7.4 Hz, 1H), 2.41 (t, *J* = 7.2 Hz, 2H), 2.22 (qd, *J* = 7.4, 0.8 Hz, 2H).

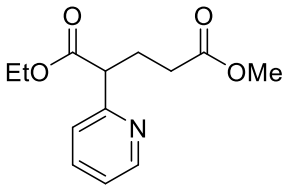
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 172.8, 169.3, 52.6, 51.7, 50.5, 31.2, 23.8.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_9H_{14}NaO_6^+$): 241.0683, found: 241.0686.

**EI-MS:** *m*/*z* (%): 187 (29), 158 (50), 155 (100), 145 (23), 132 (42), 126 (28), 113 (83), 100 (21), 69 (17), 59 (32), 55 (31).

**$R_f$** (15% EtOAc in pentane): 0.19.

### 3.2.1.7 1-Ethyl 5-methyl 2-(pyridin-2-yl)pentanedioate (3h)




Product **3h** was prepared according to general procedure **P3** using ethyl (2-pyridine)acetate (466 µL, 3.0 mmol, 6.0 equiv) and methyl acrylate (45 µL, 0.50 mmol, 1.0 equiv). No aqueous workup was performed. Purification by column chromatography on silica gel (1% $NEt_3$ , 10% EtOAc in pentane) afforded **3h** as a yellow oil (94 mg, 0.37 mmol, 75%).

**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 8.44 (ddd, *J* = 4.9, 1.9, 0.9 Hz, 1H), 7.54 (td, *J* = 7.7, 1.9 Hz, 1H), 7.17 (dt, *J* = 7.8, 1.1 Hz, 1H), 7.06 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 4.12 – 3.96 (m, 2H), 3.78 – 3.69 (m, 1H), 3.53 (s, 3H), 2.39 – 2.24 (m, 1H), 2.24 – 2.08 (m, 3H), 1.08 (t, *J* = 7.1 Hz, 3H).

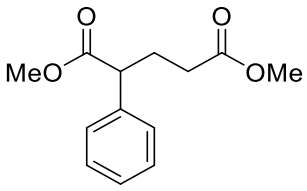
**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 173.3, 172.4, 158.1, 149.6, 136.8, 122.8, 122.3, 61.0, 52.8, 51.6, 31.6, 27.1, 14.1.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{13}H_{17}NNaO_4^+$): 274.1050, found: 274.1060.

**EI-MS:** *m*/*z* (%): 220 (21), 206 (21), 178 (86), 165 (100), 146 (21), 132 (24), 118 (99), 106 (16), 104 (14), 93 (40), 78 (10).

**$R_f$** (1% $NEt_3$, 20% EtOAc in pentane)**:** 0.36.

### 3.2.1.8 Dimethyl 2-phenylpentanedioate (3i)




Product **3i** was prepared according to general procedure **P3** using methyl phenylacetate (421 µL, 3.0 mmol, 6.0 equiv) and methyl acrylate (45 µL, 0.50 mmol, 1.0 equiv). Purification

by column chromatography on silica gel (10% EtOAc in pentane) afforded **3i** as a colorless oil (57 mg, 0.24 mmol, 48%).

**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.35 – 7.26 (m, 5H), 3.66 (s, 3H), 3.65 (s, 3H), 3.66 – 3.58 (m, 1H), 2.45 – 2.31 (m, 1H), 2.30 – 2.24 (m, 2H), 2.18 – 2.05 (m, 1H).

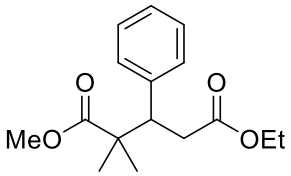
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 174.0, 173.4, 138.3, 128.9, 128.1, 127.7, 52.3, 51.8, 50.6, 31.8, 28.5.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{13}H_{16}NaO_4$): 259.0941, found: 259.0952.

**EI-MS:** *m*/*z* (%): 205 (74), 176 (25), 162 (49), 145 (10), 121 (14), 117 (100), 103 (27), 91 (35), 89 (11), 77 (17), 59 (20).

**$R_f$** (10% EtOAc in pentane): 0.34.

### 3.2.1.9 5-Ethyl 1-methyl 2,2-dimethyl-3-phenylpentanedioate (3k)




Product **3k** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and ethyl cinnamate (70.5 mg, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded **3i** as a colorless oil (63 mg, 0.23 mmol, 57%).

**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.24 – 7.06 (m, 5H), 3.94 – 3.76 (m, 2H), 3.58 (s, 3H), 3.45 (dd, J = 11.4, 4.3 Hz, 1H), 2.74 (d, J = 11.4 Hz, 1H), 2.58 (dd, J = 15.5, 4.3 Hz, 1H), 1.09 (s, 3H), 1.03 (s, 3H), 0.94 (t, J = 7.1 Hz, 3H).

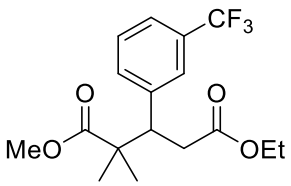
**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 177.5, 172.2, 139.4, 129.4, 128.0, 127.1, 60.4, 52.0, 49.1, 46.2, 36.0, 24.3, 21.7, 14.1.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{16}H_{22}O_4Na$): 301.1416, found: 301.1410.

**EI-MS:** *m*/*z* (%): 278 (5), 249 (5), 177 (34), 135 (100), 91 (39), 87 (5).

**$R_f$** (10% EtOAc in pentane): 0.25.

### 3.2.1.10 5-Ethyl 1-methyl 2,2-dimethyl-3-(3-(trifluoromethyl)phenyl)pentanedioate (3l)



Product **3l** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and ethyl 2-(trifluoromethyl)cinnamate (98 mg, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (gradient 5%,10% EtOAc in pentane) afforded **3l** as a colorless oil (80 mg, 0.23 mmol, 58%).

**$^{1}$H NMR (300 MHz, $CDCl_3$)**: δ(ppm): 7.52 – 7.47 (m, 1H), 7.44 – 7.36 (m, 3H), 3.99 – 3.86 (m, 2H), 3.65 (s, 3H), 3.58 (dd, *J* = 11.4, 4.4 Hz, 1H), 2.85 (dd, *J* = 15.7, 11.4 Hz, 1H), 2.71 (dd, *J* = 15.7, 4.4 Hz, 1H), 1.16 (s, 3H), 1.11 (s, 3H), 1.00 (t, *J* = 7.1 Hz, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)**: δ(ppm): 177.0, 171.8, 140.7, 132.8, 130.4 (d, *J* = 32.2 Hz), 128.5, 126.1 (d, *J* = 3.9 Hz), 124.1 (d, *J* = 3.8 Hz), 60.6, 52.1, 49.1, 46.1, 35.7, 23.9, 22.2, 14.0. (1 signal not detected)

**$^{19}$F NMR (282 MHz, $CDCl_3$)**: δ(ppm): -62.6.

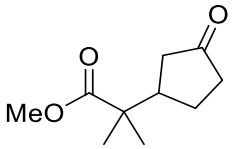
**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{17}H_{21}O_4F_3Na$): 369.1290, found: 369.1302.

**EI-MS:** *m*/*z* (%): 346 (9), 327 (16), 245 (31), 203 (100), 145 (5), 87 (10).

**$R_f$** (10% EtOAc in pentane)**:** 0.19.

### 3.2.2 Reaction with ketones

#### 3.2.2.1 Methyl 2-methyl-2-(3-oxocyclopentyl)propanoate (3m)




Product **3m** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (305 µL, 1.5 mmol, 3.0 equiv) and cyclopenten-2-one (42 µL, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (15% EtOAc in pentane) afforded **3m** as a colorless liquid (90 mg, 0.49 mmol, 98%).

**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 3.67 (s, 3H), 2.52 – 1.93 (m, 6H), 1.62 (qd, *J* = 11.8, 8.5 Hz, 1H), 1.19 (s, 3H), 1.18 (s, 3H).

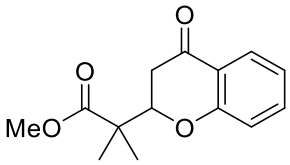
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 218.4, 177.4, 52.0, 45.2, 43.9, 40.6, 39.0, 24.6, 22.8, 22.7.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{10}H_{16}NaO_3^+$): 207.0992, found: 207.0993.

**EI-MS:** *m*/*z* (%): 184 (10), 169 (11), 125 (19), 102 (100), 87 (16), 83 (55), 69 (30), 55 (54), 41 (21).

**$R_f$** (15% EtOAc in pentane): 0.27.

### 3.2.2.2 Methyl 2-methyl-2-(4-oxochroman-2-yl)propanoate (3n)



Product **5n** was prepared according to general procedure **P1** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (305 µL, 1.5 mmol, 3.0 equiv) and 4-chromanone (73 mg, 0.50 mmol, 1.0 equiv). Purification by column chromatography on silica gel (5% EtOAc in pentane) afforded **5n** as a colorless liquid (116 mg, 0.47 mmol, 93%).

**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.87 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.46 (ddd, *J* = 8.4, 7.2, 1.8 Hz, 1H), 7.01 (ddd, *J* = 8.1, 7.2, 1.1 Hz, 1H), 6.96 (dd, *J* = 8.3, 1.0 Hz, 1H), 4.65 (dd, *J* = 14.2, 2.5 Hz, 1H), 3.73 (s, 3H), 2.79 (dd, *J* = 16.5, 14.2 Hz, 1H), 2.60 (dd, *J* = 16.5, 2.5 Hz, 1H), 1.37 (s, 3H), 1.28 (s, 3H).

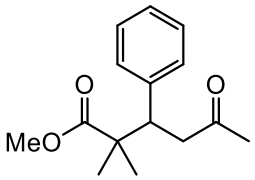
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 192.4, 175.7, 161.7, 136.2, 127.1, 121.6, 120.9, 118.0, 81.8, 52.4, 46.3, 38.5, 20.9, 20.7.

**HRMS (ESI):** *m*/*z* calculated for $[M+Na]^+$ ($C_{14}H_{16}NaO_4^+$): 271.0941, found: 271.0948.

**EI-MS:** *m*/*z* (%): 219 (100), 73 (26).

**$R_f$** (10% EtOAc in pentane): 0.24.

### 3.2.2.3 Methyl 2,2-dimethyl-5-oxo-3-phenylhexanoate (3o)



Product **3o** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and 4-phenylbut-3-en-2-one (58 mg, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded **3o** as a colorless oil (80 mg, 0.23 mmol, 58%).

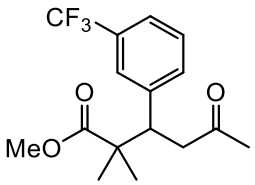
**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.23 – 7.06 (m, 5H), 3.57 (s, 3H), 3.49 (dd, *J* = 10.6, 4.0 Hz, 1H), 2.95 (dd, *J* = 16.5, 10.5 Hz, 1H), 2.64 (dd, *J* = 16.5, 4.0 Hz, 1H), 1.93 (s, 3H), 1.07 (s, 3H), 1.01 (s, 3H).

**$^{13}$C NMR (75 MHz, $CDCl_3$)**: δ (ppm): 207.0, 177.6, 139.8, 129.3, 128.0, 127.0, 51.9, 47.9, 46.0, 45.0, 30.4, 24.5, 21.5.

**EI-MS:** *m*/*z* (%): 147 (28), 102 (23) ,43 (100).

**$R_f$** (10% EtOAc in pentane): 0.19.

### 3.2.2.4 Methyl 2,2-dimethyl-5-oxo-3-(3-(trifluoromethyl)phenyl)hexanoate (3p)




Product **3p** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and 4-(3-trifluoromethyl)phenyl)but-3-en-2-one (86 mg, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (gradient: 5%, 10% EtOAc in pentane) afforded **3p** as a colorless oil (56.3 mg, 0.18 mmol, 44%).

**$^{1}$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.50 – 7.45 (m, 1H), 7.42 – 7.34 (m, 3H), 3.63 (m, 4H), 3.03 (dd, *J* = 17.2, 10.4 Hz, 1H), 2.81 (dd, *J* = 17.2, 3.9 Hz, 1H), 2.03 (s, 3H), 1.13 (s, 3H), 1.09 (s, 3H).

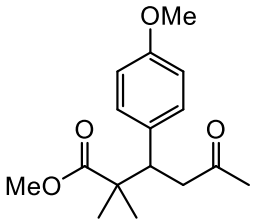
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 206.4, 177.2, 141.4, 132.9 (d, *J* = 1.5 Hz), 130.5 (q, *J* = 32.1 Hz), 128.6, 125.8 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 273.0 Hz), 52.0, 47.7, 46.0, 44.8, 30.6, 24.3, 22.2.

**$^{19}$F NMR (282 MHz, $CDCl_3$):** δ(ppm): -62.54.

**EI-MS:** m/z (%): 215 (13), 102 (40) ,43 (100).

**$R_f$** (10% EtOAc in pentane): 0.31.

### 3.2.2.5 Methyl 3-(4-methoxyphenyl)-2,2-dimethyl-5-oxohexanoate (3q)




Product **3q** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and 4-(4-methoxy)phenyl)but-3-en-2-one (71 mg, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (gradient: 5%, 10% EtOAc in pentane) afforded **3q** as a colorless oil (47.4 mg, 0.17 mmol, 43%).

**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.10 – 7.03 (m, 2H), 6.82 – 6.77 (m, 2H), 3.77 (s, 3H), 3.64 (s, 3H), 3.50 (dd, *J* = 10.8, 3.9 Hz, 1H), 2.96 (dd, *J* = 16.3, 10.8 Hz, 1H), 2.66 (dd, *J* = 16.3, 3.9 Hz, 1H), 1.99 (s, 3H), 1.11 (s, 3H), 1.07 (s, 3H).

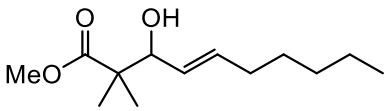
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 207.2, 177.7, 158.5, 131.6, 130.3, 113.4, 55.2, 51.8, 47.2, 46.1, 45.1, 30.4, 24.4, 21.5.

**EI-MS:** m/z (%): 278 (6), 177 (31),43 (100).

**$R_f$** (10% EtOAc in pentane): 0.18.

### 3.2.3 Reaction with aldehydes

#### 3.2.3.1 Methyl 3-hydroxy-2,2-dimethyldec-4-enoate (4a)




Product **4a** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and oct-2-enal (30 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4a** (colorless liquid, 84 mg, 0.37 mmol, 92%).

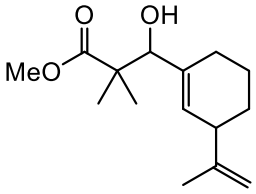
**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 5.69 (dd, *J* = 15.3, 1.0 Hz, 1H), 5.43 (ddt, *J* = 15.3, 7.5, 1.5 Hz, 1H), 4.10 (d, *J* = 7.5 Hz, 1H), 3.69 (s, 3H), 2.56 (d, *J* = 20.2 Hz, 1H), 2.07 – 1.99 (m, 2H), 1.43 – 1.20 (m, 6H), 1.16 (s, 6H), 0.88 (t, *J* = 6.9 Hz, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.0, 135.1, 127.7, 78.0, 51.9, 46.9, 32.3, 31.3, 28.8, 22.7, 22.5, 19.9, 14.0.

**EI-MS:** m/z (%): 131 (9), 128 (5), 102 (21).

**$R_f$** (10% EtOAc in pentanes): 0.13.

#### 3.2.3.1 Methyl 3-hydroxy-2,2-dimethyl-3-(3-(prop-1-en-2-yl)cyclohex-1-en-1-yl)propanoate (4b)




Product **4b** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and perillaldehyde (62 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4b** as a mixture of diastereomers (1:1, colorless liquid, 90.6 mg, 0.36 mmol, 90%).

**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 5.66 (s, 1H), 4.76 – 4.65 (m, 2H), 4.02 (dd, *J* = 22.8, 6.4 Hz, 1H), 3.71 (m, 3H), 3.13 (m, 1H), 2.15 (q, *J* = 14.0 Hz, 2H), 2.00 – 1.77 (m, 2H), 1.73 (d, *J* = 1.6 Hz, 3H), 1.53 – 1.35 (m, 2H), 1.22 – 1.13 (m, 6H).

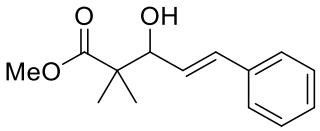
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.5, 178.4, 149.7, 149.4, 136.8, 136.8, 126.3, 125.2, 108.7, 108.7, 81.9, 81.3, 52.1, 52.0, 46.5, 46.1, 41.3, 40.6, 30.7, 30.4, 27.7, 27.4, 25.9, 25.1, 24.3, 23.5, 21.3, 21.1, 20.8, 20.6.

**EI-MS:** m/z (%): 151 (5), 121 (5), 102 (100).

**$R_f$** (10% EtOAc in pentanes): 0.20.

### 3.2.3.2 Methyl 3-hydroxy-2,2-dimethyl-5-phenylpent-4-enoate (4c)

Product **4c** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and *trans*-cinnamaldehyde (50 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded **4c** as two isomers (*Z*: colorless oil, 13.8 mg; *E*: colorless oil, 47.1 mg; in total: 60.9 mg, 65%, 3.4:1 *E:Z*).

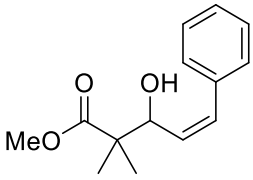



**$^{1}$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.42 – 7.21 (m, 5H), 6.64 (dd, *J* = 15.9, 1.1 Hz, 1H), 6.21 (dd, *J* = 15.9, 7.1 Hz, 1H), 4.35 (d, *J* = 7.1 Hz, 1H), 3.73 (s, 3H), 1.25 (s, 3H), 1.23 (s, 3H).

**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 178.1, 136.7, 133.1, 128.7, 127.9, 127.5, 126.7, 78.1, 52.2, 47.3, 23.0, 20.1.

**HR-MS (ESI)**: m/z calculated for $[C_{14}H_{18}O_3Na]^+$ ($[M+Na]^+$): 257.1148 measured: 257.1153.

**$R_f$** (5% EtOAc in pentane): 0.13.




**$^{1}$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.41 – 7.27 (m, 4H), 7.18 – 7.12 (m, 1H), 6.70 (d, *J* = 11.7 Hz, 1H), 5.70 (dd, *J* = 11.7, 9.9 Hz, 1H), 4.51 (d, *J* = 9.9 Hz, 1H), 3.69 (s, 3H), 3.00 – 2.90 (m, 1H), 1.19 (s, 3H), 1.16 (s, 3H).

**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 178.0, 136.7, 133.1, 128.7, 128.0, 127.5, 126.7, 78.0, 52.2, 47.3, 23.0, 20.1.

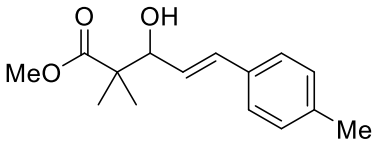
**HR-MS (ESI)**: m/z calculated for $[C_{14}H_{18}O_3Na]^+$ ($[M+Na]^+$): 257.1148 measured: 257.1155.

**$R_f$** (5% EtOAc in pentane): 0.07.

### 3.2.3.3 Methyl 3-hydroxy-2,2-dimethyl-5-(p-tolyl)pent-4-enoate (4d)

Product **4d** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and 3-(p-tolyl)acrylaldehyde (58.5 mg,

0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded **4d** as two isomers (*Z*: colorless oil, 20.8 mg; *E*: colorless oil, 40.1 mg; in total: 60.9 mg, 65%, 1.9:1 *E:Z*).

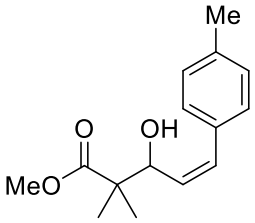



**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.28 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 6.60 (d, *J* = 15.8 Hz, 1H), 6.16 (ddd, *J* = 15.9 Hz, 7.1, 1.3, 1H), 4.34 (d, *J* = 7.2 Hz, 1H), 3.72 (s, *J* = 1.4 Hz, 3H), 2.74 (s, 1H), 2.34 (s, 3H), 1.24 (s, 3H), 1.23 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.0, 137.8, 133.9, 133.0, 129.4, 126.6, 126.5, 78.1, 52.2, 47.4, 23.0, 21.3, 20.1.

**HR-MS (ESI)**: m/z calculated for $[C_{15}H_{20}NaO_3]^+$ ([M+Na]$^+$): 271.1305, measured: 271.1314.

**$R_f$** (20% EtOAc in pentane): 0.42.




**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.28 (d, *J* = 7.9 Hz, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 6.66 (d, *J* = 11.7 Hz, 1H), 5.65 (ddd, *J* = 11.5, 9.8, 1.2 Hz, 1H), 4.53 (d, *J* = 9.8 Hz, 1H), 3.70 (s, 3H), 2.94 (s, 1H), 2.35 (s, 3H), 1.19 (s, 3H), 1.16 (s, 3H).

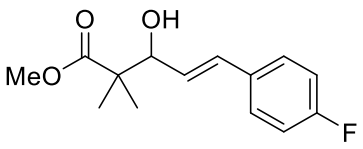
**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.2, 137.3, 134.2, 133.7, 129.2, 128.9, 128.7, 72.6, 52.2, 47.0, 23.1, 21.4, 20.4.

**HR-MS (ESI)**: m/z calculated for $[C_{15}H_{20}NaO_3]^+$ ([M+Na]$^+$): 271.1305, measured: 271.1318;

**$R_f$** (20% EtOAc in pentane): 0.50;

### 3.2.3.4 Methyl 5-(4-fluorophenyl)-3-hydroxy-2,2-dimethylpent-4-enoate (4e)

Product **4e** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and *trans*-4-fluorocinnamaldehyde (53 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded **4e** as two isomers (*Z*: colorless liquid, 58.3 mg; *E*: colorless oil, 11.9 mg; in total: 70.2 mg, 70%, 4.9:1 *E:Z*).



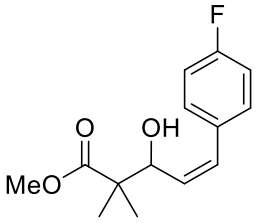
**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.34 (ddd, *J* = 9.3, 5.1, 2.4 Hz, 2H), 7.06 – 6.96 (m, 2H), 6.60 (d, *J* = 15.9 Hz, 1H), 6.13 (ddd, *J* = 15.9, 7.1, 2.4 Hz, 1H), 4.37 – 4.28 (m, 1H), 3.73 (s, 3H), 2.80 (s, 1H), 1.24 (s, 3H), 1.22 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.0, 162.6 (d, J = 247.1 Hz), 132.9 (d, J = 3.2 Hz), 131.9, 128.2 (d, *J* = 8.0 Hz), 127.3 (d, J = 2.2 Hz), 115.64 (d, *J* = 21.6 Hz), 77.9, 52.2, 47.3, 23.0, 20.2.

**$^{19}$F NMR (282 MHz, $CDCl_3$):** δ (ppm): -114.2.

**HR-MS (ESI)**: m/z calculated for $[C_{14}H_{17}FO_3Na]^+$ ([M+Na]$^+$): 275.1059 measured: 275.1054.

**$R_f$** (5% EtOAc in pentane): 0.05.




**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.40 – 7.33 (m, 2H), 7.06 – 7.00 (m, 2H), 6.65 (d, *J* = 11.6 Hz, 1H), 5.73 – 5.64 (m, 1H), 4.42 (d, *J* = 9.9 Hz, 1H), 3.70 (s, 3H), 3.00 (s, 1H), 1.19 (d, *J* = 1.4 Hz, 3H), 1.16 (d, *J* = 1.5 Hz, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 180.6, 175.2, 133.2, 130.7 (d, *J* = 8.1 Hz), 129.4, 124.8, 115.4 (d, *J* = 21.4 Hz), 72.6, 52.2, 50.6, 23.1, 20.5.

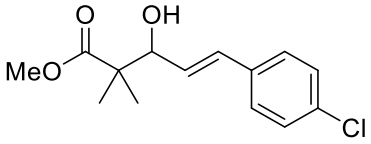
**$^{19}$F NMR (282 MHz, $CDCl_3$):** δ (ppm): -114.6.

**HR-MS (ESI)**: m/z calculated for $[C_{14}H_{17}FO_3Na]^+$ ([M+Na]$^+$): 275.1059 measured: 275.1058.

**$R_f$**(5% EtOAc in pentane): 0.11.

### 3.2.3.5 Methyl 5-(4-chlorophenyl)-3-hydroxy-2,2-dimethylpent-4-enoate (4f)

Product **4f** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and *trans*-4-chlorocinnamaldehyde (56 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4f** as two isomers (*Z*: colorless liquid, 36.6 mg; *E*: colorless oil, 11.4 mg; in total: 48 mg, 45%, 1:3.2 *E:Z*).

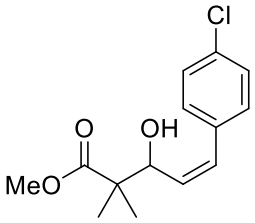



**$^{1}$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.32 – 7.24 (m, 4H), 6.58 (dd, *J* = 15.9, 1.2 Hz, 1H), 6.17 (dd, *J* = 15.9, 6.9 Hz, 1H), 4.36 – 4.28 (m, 1H), 3.71 (s, 3H), 2.82 (d, *J* = 5.7 Hz, 1H), 1.23 (s, 3H), 1.21 (s, 3H).

**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 171.2, 135.2, 131.8, 128.9, 128.7, 128.2, 127.9, 77.8, 52.3, 47.3, 23.0, 20.3.

**HR-MS (ESI)**: m/z calculated for $[C_{14}H_{17}ClO_3Na]^+$ ([M+Na]$^+$): 291.0764 measured: 291.07659.

**$R_f$** (20% EtOAc in pentane): 0.29.




**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.35 – 7.27 (m, 4H), 6.64 (dd, *J* = 11.7, 0.9 Hz, 1H), 5.71 (dd, *J* = 11.7, 9.9 Hz, 1H), 4.40 (dd, *J* = 10.0, 5.9 Hz, 1H), 3.70 (s, 3H), 3.05 (d, *J* = 7.0 Hz, 1H), 1.18 (s, 3H), 1.15 (s, 3H), .

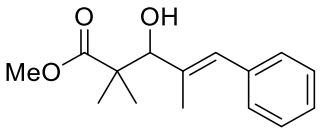
**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 178.2, 135.0, 133.4, 133.1, 130.4, 130.1, 128.6, 72.6, 52.3, 46.9, 23.1, 20.4.

**HR-MS (ESI)**: m/z calculated for $[C_{14}H_{17}ClO_3Na]^+$ ([M+Na]$^+$): 291.0764 measured: 291.0761.

**$R_f$** (20% EtOAc in pentane): 0.32.

### 3.2.3.6 Methyl 3-hydroxy-2,2,4-trimethyl-5-phenylpent-4-enoate (4g)

Product **4g** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and α-methyl-cinnamaldehyde (56 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4g** as two isomers (*Z*: colorless liquid, 10.6 mg; *E*: colorless oil, 36.7 mg; in total: 47.3 mg, 48%, 4.9:1 *E:Z*).

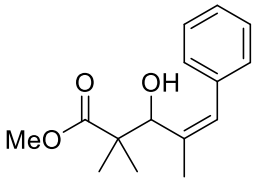



**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.31 (t, *J* = 7.6 Hz, 2H), 7.28 – 7.19 (m, 3H), 6.51 (s, 1H), 4.50 (s, 1H), 4.03 (s, 1H), 3.71 (s, 3H), 1.76 (s, 3H), 1.21 (s, 3H), 1.00 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 179.0, 137.6, 137.2, 131.1, 128.8, 128.3, 126.5, 75.6, 52.2, 44.9, 25.5, 21.2, 18.5.

**EI-MS:** m/z (%): 177 (5), 147 (100), 102 (43), 91 (53).

**$R_f$** (10% EtOAc in pentane): 0.20.



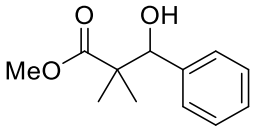

**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.38 – 7.18 (m, 5H), 6.47 (s, 1H), 4.27 (d, *J* = 4.8 Hz, 1H), 3.73 (s, 3H), 3.21 (d, *J* = 4.8 Hz, 1H), 1.83 (s, 3H), 1.30 (s, 3H), 1.24 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.3, 137.3, 137.1, 129.2, 129.1, 128.1, 126.6, 83.0, 52.2, 46.9, 24.0, 21.1, 14.8.

**HR-MS (ESI)**: m/z calculated for $[C_{15}H_{20}O_3Na]^+$ ([M+Na]$^+$): 271.1210 measured: 271.1310

**$R_f$** (10% EtOAc in pentane): 0.16.

### 3.2.3.7 Methyl 3-hydroxy-2,2-dimethyl-3-phenylpropanoate (4h)




Product **4h** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and benzaldehyde (41 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4h** (colorless liquid, 65.4 mg, 0.30 mmol, 79%).

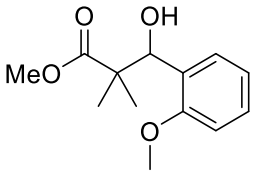
**$^{1}$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.23 – 7.12 (m, 5H), 4.76 (d, *J* = 3.9 Hz, 1H), 3.59 (s, 3H), 2.97 (d, *J* = 3.9 Hz, 1H), 1.02 (d, *J* = 1.4 Hz, 3H), 0.98 (d, *J* = 1.3 Hz, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.2, 134.0, 127.8, 127.8, 127.7, 78.7, 52.1, 47.7, 23.0, 19.1.

**HR-MS (ESI)**: m/z calculated for $[C_{12}H_{16}O_3Na]^+$ ([M+Na]$^+$): 231.0997 measured : 231.0983.

**$R_f$**(10% EtOAc in pentane): 0.55.

### 3.2.3.8 Methyl 3-hydroxy-3-(2-methoxyphenyl)-2,2-dimethylpropanoate (4i)




Product **4i** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and 2-methoxy-benzaldehyde (48 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4i** (colorless liquid, 88.7 mg, 0.37 mmol, 93%).

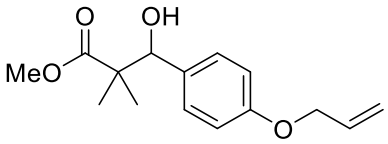
**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.23 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.20 – 7.14 (m, 1H), 6.92 – 6.84 (m, 1H), 6.79 (d, *J* = 8.3 Hz, 1H), 5.20 (d, *J* = 5.5 Hz, 1H), 3.73 (s, 3H), 3.64 (s, 3H), 3.45 (d, *J* = 6.3 Hz, 1H), 1.08 (s, 3H), 1.04 (s, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ (ppm): 178.2, 157.0, 129.1, 128.7, 128.1, 120.4, 110.6, 74.1, 55.2, 52.0, 48.6, 23.0, 19.2.

**HR-MS (ESI):** m/z calculated for $[C_{13}H_{18}O_4Na]^+$ ([M+Na]$^+$): 261.1097 measured: 261.1111.

**$R_f$**(10% EtOAc in pentane): 0.54.

### 3.2.3.9 Methyl 3-(4-(allyloxy)phenyl)-3-hydroxy-2,2-dimethylpropanoate (4k)




Product **4k** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and 4-(allyloxy)benzaldehyde (61 µL, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4k** (colorless liquid, 95.7 mg, 0.36 mmol, 91%).

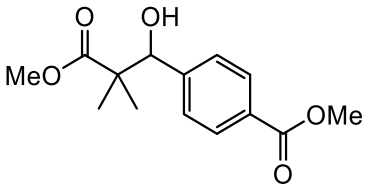
**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.24 – 7.15 (m, 2H), 6.93 – 6.81 (m, 2H), 6.05 (ddt, *J* = 17.3, 10.5, 5.3 Hz, 1H), 5.40 (dq, *J* = 17.3, 1.6 Hz, 1H), 5.28 (dq, *J* = 10.5, 1.6 Hz, 1H), 4.83 (d, *J* = 3.6 Hz, 1H), 4.52 (dt, *J* = 5.3, 1.6 Hz, 2H), 3.70 (s, 3H), 3.04 (d, *J* = 3.6 Hz, 1H), 1.12 (s, 3H), 1.08 (s, 3H).

**$^{13}$C NMR (75 MHz, $CDCl_3$):** δ (ppm): 178.4, 158.4, 133.4, 132.4, 128.8, 117.8, 114.1, 78.4, 68.9, 52.2, 47.9, 23.1, 19.1.

**HR-MS (ESI)**: m/z calculated for $[C_{15}H_{20}O_4Na]^+$ ([M+Na]$^+$): 287.1254 measured: 287.1264.

**$R_f$** (10% EtOAc in pentane): 0.36.

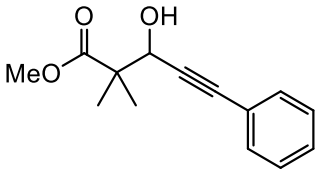
### 3.2.3.10 Methyl 4-(1-hydroxy-3-methoxy-2,2-dimethyl-3-oxopropyl)benzoate (4l)




Product **4l** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and methyl benzaldehyde 4-carboxylate (66 mg, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4l** (white solid, 49.5 mg, 0.19 mmol, 46%).

**$^1$H NMR (300 MHz, $CDCl_3$):** δ (ppm): 7.98 (d, *J* = 8.3 Hz, 2H), 7.41 – 7.33 (m, 2H), 4.94 (d, *J* = 3.9 Hz, 1H), 3.91 (s, 3H), 3.72 (s, 3H), 3.28 (d, *J* = 4.3 Hz, 1H), 1.13 (s, 3H), 1.11 (s, 3H).
**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ (ppm): 178.1, 167.0, 145.2, 129.7, 129.1, 127.8, 78.4, 52.3, 52.2, 47.8, 23.0, 19.3.
**EI-MS:** m/z (%): 179 (2), 101 (6), 73 (26).
**$R_f$** (10% EtOAc in pentane): 0.16.

#### 3.2.3.11 Methyl 3-hydroxy-2,2-dimethyl-5-phenylpent-4-ynoate (4m)




Product **4m** was prepared according to general procedure **P2** using 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (122 µL, 0.6 mmol, 1.5 equiv) and phenylpropiolaldehyde (52 mg, 0.4 mmol, 1.0 equiv). Purification by column chromatography on silica gel (10% EtOAc in pentane) afforded the product **4m** (colorless liquid, 60.4 mg, 0.26 mmol, 65%).
**$^1$H NMR (400 MHz, $CDCl_3$):** δ (ppm): 7.40 – 7.35 (m, 2H), 7.28 – 7.23 (m, 3H), 4.66 (s, 1H), 3.69 (s, 3H), 2.86 (s, 1H), 1.33 (s, 3H), 1.29 (s, 3H).
**$^{13}$C NMR (101 MHz, $CDCl_3$);** δ (ppm): 177.2, 131.9, 128.6, 128.4, 122.5, 87.2, 86.2, 69.0, 52.3, 48.0, 22.8, 20.0.
**HR-MS (ESI)**: m/z calculated for $[C_{14}H_{16}NaO_3]^+$ ($[M+Na]^+$): 255.0997 measured: 255.0996.
**$R_f$** (10% EtOAc in pentanes): 0.32.

## *3.3 Mechanistic experiments*

### 3.3.1 Stern-Volmer luminescence quenching analysis

All studies were carried out in an argon-filled glove-box using a 10 µM solution of the respective photocatalyst in the dry degassed solvent at room temperature. Varying amounts of the respective substrate were added to this solution in a quartz cuvette. The cuvette was capped with a PTFE stopper and sealed with parafilm before being removed from the glove-box. Fluorescence spectra of the mixtures were measured and the emission intensity at a certain wavelength was recorded as a function of the quencher concentration.

Stern-Volmer Analysis was performed according to the abovementioned procedure with $\lambda_{ex}$ = 420 nm, $\lambda_{em}$ = 472 nm.

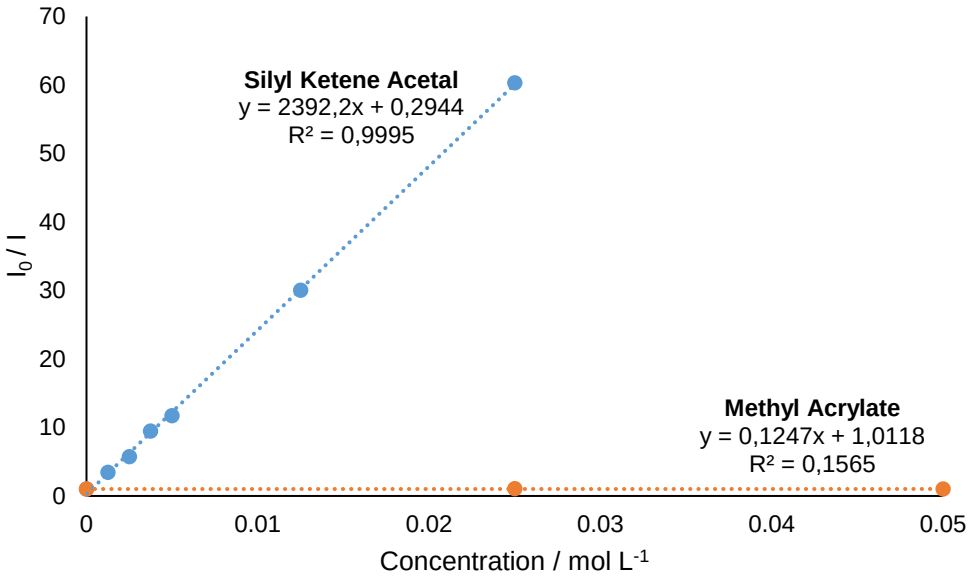



**Figure S9:** Stern-Volmer Luminescence Quenching Studies on $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$, using 1-methoxy-2-methyl-1-(trimethylsiloxy)propene **1a** and methyl acrylate $\mathbf{2^{Est}}$ as potential quenchers.

### 3.3.2 Quantum yield determination

Reaction quantum yields were determined following a procedure by Yoon and coworkers.[21] The reaction was performed in a pre-calibrated apparatus using a 420 nm LED (for an emission spectrum see Figure S2). The reaction yield can then be converted to its quantum yield using the pre-determined photon flux of the system.

The effective photon flux of the used apparatus was determined using standard ferrioxalate actinometry.[22,23] A 0.15 m ferrioxalate solution was prepared by dissolving potassium ferrioxalate hydrate (737 mg, 1.50 mmol) in 0.05 M $H_2SO_4$ (10 mL). A buffered solution of 1,10-phenanthroline was prepared by dissolving 1,10-phenanthroline (25 mg, 0.14 mmol) and sodium acetate (5.63 g, 68.6 mmol) in 0.5 M $H_2SO_4$ (25 mL). The ferrioxalate solution (1.0 mL) was added to the cuvette and was irradiated for 90 s in the apparatus. After irradiation, the phenanthroline solution (175 µL) was added to the cuvette and the mixture was stirred in the absence of light for 90 min to achieve full phenanthroline coordination to the ferrous ions. In addition, a non-irradiated sample was prepared similarly.

The absorbance of both samples was measured at 510 nm. From these values, conversion could be determined using Lambert-Beer's law:

$$n(\mathrm{Fe}^{2+}) = \frac{V \cdot \Delta A(510\ \mathrm{nm})}{l \cdot \varepsilon_F} \qquad (11)$$

where $V$ is the total volume (1.175 mL), $l$ is the optical path length of the cuvette (1.00 cm), $\varepsilon_F$ is the molar absorptivity of the ferrioxalate actinometer ($1.11 \cdot 10^4$ L mol$^{-1}$ cm$^{-1}$)[22,23] and $\Delta A$(510 nm) is the absorbance difference between the irradiated and non-irradiated sample.

From this value, the photon flux $\Phi_q$ in the system can be calculated as

$$\Phi_q = \frac{n(\mathrm{Fe}^{2+})}{\Phi_F \cdot t \cdot f} \tag{12}$$

where $\Phi_F$ is the quantum yield of the ferrioxalate system (1.12 at $\lambda_{ex}$ = 415 nm)[22,23], $t$ is the irradiation time and $f$ is the fraction of light absorbed at $\lambda_{ex}$ = 415 nm. The absorption fraction is calculated as

$$f = 1 - 10^{-A(415\ \mathrm{nm})} \tag{13}$$

Combining these equations, the effective photon flux can be determined as:

$$\Phi_q = \frac{V \cdot \Delta A(510\ \mathrm{nm})}{l \cdot \varepsilon_F \cdot \Phi_F \cdot t \cdot (1 - 10^{-A(415\ \mathrm{nm})})} \tag{14}$$

The respective transformation was set up under standard conditions and run in the pre-calibrated actinometer. After the indicated reaction time, the amount of product formed was determined by GC-FID. From this value, the quantum yield of the reaction $\Phi_R$ could be calculated as

$$\Phi_\mathrm{R} = \frac{\mathrm{n(Prod)}}{\Phi_\mathrm{q} \cdot \mathrm{t} \cdot \mathrm{f}} \tag{15}$$

The effective photon flux of the actinometer was determinded to be 5.2 $10^{-10}$ einstein s$^{-1}$.

**Table S13:** Calibration of the ferrioxalate actinometer by determination of the effective photon flux.

| | **Experiment 1** | **Experiment 2** | **Experiment 3[a]** |
|---|---|---|---|
| $A$ (510 nm) | 0.667 | 0.643 | 0.734 |
| $A_0$ (510 nm) | 0.156 | 0.162 | 0.158 |
| $t$ | 90 s | 90 s | 90 s |

| | | | |
|---|---|---|---|
| *A* (415 nm) | 3.93 | 3.93 | 3.93 |
| $\Phi_Q$ | 5.37 $\cdot 10^{-10}$ einstein $s^{-1}$ | 5.10 $\cdot 10^{-10}$ einstein $s^{-1}$ | 6.05 $10^{-10}$ einstein $s^{-1}$ |

[a] This experiment was regarded as a statistical outlier and was therefore not included in any further calculations.

For the determination of the reaction's quantum yield, the reaction was performed in the apparatus described in section 1.2: $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ (1.1 mg, 0.001 mmol, 1.0 mol%), 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (61 µL, 0.30 mmol, 3.0 equiv) and methyl acrylate (9 µL, 0.10 mmol, 1.0 equiv) were dissolved in anhydrous acetonitrile (1.0 mL). The mixture was degassed using three freeze-pump-thaw cycles and the tube was backfilled with argon. The mixture was transferred into a cuvette under an argon atmosphere. The sealed cuvette was stirred under irradiation in the abovementioned apparatus for 30 min. After the indicated time, mesitylene (14 µL, 0.10 mmol, 1.0 equiv) was added as an internal standard, the mixture was filtered through a short plug of silica gel and the product yield *n*(Prod) was determined via calibrated GC-FID.

**Table S14:** Quantum Yield Determination for the Mukaiyama-Michael-type coupling of silyl ketene acetal **1** and methyl acrylate (**2$^{Est}$**).

| | **Result** |
|---|---|
| *n*(Prod) | 0.0155 mmol |
| *t* | 30 min |
| *A*(415 nm) | >3 |
| $\Phi_R$ | 15.6 |

The reaction quantum yield was thus determined to be 15.6.

The quenching fraction was determined by performing a simple luminescence quenching study of the reaction mixture. The reaction was set up in a cuvette as described above, another sample was prepared without silyl ketene acetal **1**. Fluorescence spectra ($\lambda_{ex}$ = 420 nm) of both samples were recorded, and the quenching fraction was determined from the luminescence intensity at $\lambda_{em}$ = 472 nm.

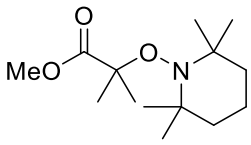
$$Q = \frac{I_0 - I}{I_0} \tag{16}$$

A quenching fraction of 0.991 was determined for the reaction mixture, which corresponds to a chain length of $I_C$ = 15.7.

### 3.3.3 TEMPO trapping experiments

In a dried Schlenk tube, [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ (1.1 mg, 0.001 mmol, 1.0 mol%), the respective substrates (1.0 – 3.0 equiv) and TEMPO (31.3 mg, 0.20 mmol, 2.0 equiv) were dissolved in anhydrous acetonitrile (1.0 mL) under an argon atmosphere. The reaction mixture was stirred at room temperature under visible light irradiation (six 5 W blue LEDs, $\lambda_{max}$ = 455 nm) for 16 h. After the indicated reaction time, the mixture was filtered through a short plug of silica gel. The crude eluate was analyzed via ESI-MS.

*a)*

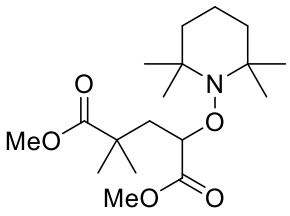



**B'**

From 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (**1a**, 21 µL, 0.10 mmol, 1.0 equiv).

**ESI-MS:** *m*/*z* calculated for $[M+Na]^+$ ($C_{14}H_{27}NNaO_3^+$): 280.1883, found: 280.1876.

*b)*



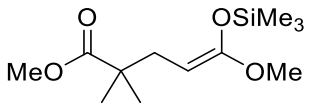

**D$^{Est}$**

From 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (**1a**, 64 µL, 0.30 mmol, 3.0 equiv) and methyl acrylate (**2$^{Est}$**, 9.0 µL, 0.10 mmol, 1.0 equiv).

**ESI-MS:** *m*/*z* calculated for $[M+Na]^+$ ($C_{18}H_{33}NNaO_5^+$): 366.2251, found: 366.2242.

### 3.3.4 Detection of intermediate E

In a dried Schlenk tube, [Ir(dF-$CF_3$-ppy)$_2$(dtbpy)]$PF_6$ (1.1 mg, 0.001 mmol, 1.0 mol%), 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (61 µL, 0.30 mmol, 3.0 equiv) and methyl acrylate (9.1 µL, 0.10 mmol, 1.0 equiv) were dissolved in anhydrous acetonitrile (1.0 mL) under an argon atmosphere. The reaction mixture was stirred at room temperature under visible light irradiation (six 5 W blue LED, $\lambda_{max}$ = 455 nm) for 16 h. After the indicated reaction time, the reaction mixture was analyzed via ESI-MS.




**E**$^{\mathbf{Est}}$

**ESI-MS**: *m/z* calculated for $[M+Na]^+$ ($C_{12}H_{24}NaO_4Si^+$): 283.1336, found: 283.1337.

### 3.3.5 Addition of Lewis acids

In order to investigate a possible competing Lewis acid catalysis cycle, the reaction was carried out in the absence of light and in the presence of $Me_3SiOTf$ as Lewis acid: In a dried Schlenk tube, $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ (1.1 mg, 0.001 mmol, 1.0 mol%), 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (30 µL, 0.15 mmol, 1.5 equiv) and a) ethyl cinnamate (16.7 µL, 0.10 mmol, 1.0 equiv) b) 4-phenylbut-3-en-2-one (14.6 mg, 0.10 mmol, 1.0 equiv) c) 2-methoxycinnamaldehyde (16.2 mg, .10 mmol, 1.0 equiv) were dissolved in anhydrous acetonitrile (1.0 mL). To this reaction mixture, the Lewis acid catalyst TMSOTf (9 µL, 0.05 mmol, 0.5 equiv) was added. After stirring for 16 h in the dark, the mixture was filtered through a short plug of silica and analyzed by GC-MS.

To investigate the influence of the triflate anion, *tert*-butyl ammonium triflate (19.6 mg, 0.05 mmol, 0.5 equiv) were added under otherwise identical reaction conditions instead of TMSOTf. Without irradiation, no product formation and only starting material was detected. Under irradiation, similar reaction a similar reaction outcome to the standard reaction conditions was observed.

**Table S15:** Determination of product formation under Lewis-acid catalysis conditions.

| Michael acceptor | Result |
|---|---|
| ethyl cinnamate | starting material |
| 4-phenylbut-3-en-2-one | 1,4-addition product |
| 2-methoxycinnamaldehyde | 1,4-addition product |

### 3.3.6 Addition of CAN

In a dried Schlenk tube, cerium ammonium nitrate (5.5 mg, 0.01 mmol, 10 mol%), 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (30 µL, 0.15 mmol, 1.5 equiv) and a) ethyl cinnamate (16.7 µL, 0.10 mmol, 1.0 equiv) b) 4-phenylbut-3-en-2-one (14.6 mg, 0.10 mmol, 1.0 equiv) c) 2-methoxycinnamaldehyde (16.2 mg, .10 mmol, 1.0 equiv) were dissolved in anhydrous

acetonitrile (1.0 mL). After stirring for 16 h in the dark, the mixture was filtered through a short plug of silica and analyzed by GC-MS.

**Table S16:** Determination of product formation after addition of CAN.

| Michael acceptor | Result |
|---|---|
| ethyl cinnamate | Starting material; 1,4-addition product |
| 4-phenylbut-3-en-2-one | 1,4-addition product |
| 2-methoxycinnamaldehyde | 1,2-addition product; 1,4-addition product |

## 3.3.7 Deuteration experiments

*a) Reaction in acetonitrile-$d_3$*

Acetonitrile-$d_3$ was degassed by sparging with argon prior to use. In a dried Schlenk tube, $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ (1.1 mg, 0.001 mmol, 1.0 mol%), 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (61 µL, 0.30 mmol, 3.0 equiv) and methyl acrylate (9.0 µL, 0.10 mmol, 1.0 equiv) were dissolved in acetonitrile-$d_3$ (1.0 mL) under an argon atmosphere. The reaction mixture was stirred at room temperature under visible light irradiation (5 W blue LED, $\lambda_{max}$ = 455 nm) for 16 h. After the indicated reaction time, the mixture was filtered through a short plug of silica. The eluate was analyzed for isotope distribution via ESI-MS.

**ESI-MS:** *m/z* calculated for $[M_H+Na]^+$ ($C_9H_{16}NaO_4^+$): 211.0941, found: 211.0944
calculated for $[M_D+Na]^+$ ($C_9H_{15}DNaO_4^+$): 212.1004, not found.

distribution: $C_9H_{16}NaO_4^+$ (100.0%)
$C_9H_{15}DNaO_4^+$ (0.00%)
$C_9H_{14}D_2NaO_4^+$ (0.00%)
$C_9H_{13}D_3NaO_4^+$ (0.00%)

*b) Workup with $D_2O$*

In a dried Schlenk tube, $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ (1.1 mg, 0.001 mmol, 1.0 mol%), 2-methyl-1-methoxy-1-(trimethylsiloxy)propene (61 µL, 0.30 mmol, 3.0 equiv) and methyl acrylate (9.0 µL, 0.10 mmol, 1.0 equiv) were dissolved in anhydrous acetonitrile (1.0 mL) under argon atmosphere. The reaction mixture was stirred at room temperature under visible light irradiation (six 5 W blue LEDs, $\lambda_{max}$ = 455 nm) for 16 h. After the indicated reaction time, $D_2O$ (5 mL) was added, followed by extraction with $CH_2Cl_2$ (3 × 10 mL). The combined organic layers were concentrated in vacuo and analyzed for isotope distribution via ESI-MS.

**ESI-MS:** *m/z* calculated for $[M_H+Na]^+$ ($C_9H_{16}NaO_4^+$): 211.0941, found: 211.0940
calculated for $[M_D+Na]^+$ ($C_9H_{15}DNaO_4^+$): 212.1004, found: 212.1001

distribution: $C_9H_{16}NaO_4^+$ (37.15%)
$C_9H_{15}DNaO_4^+$ (62.85%)
$C_9H_{14}D_2NaO_4^+$ (0.00%)
$C_9H_{13}D_3NaO_4^+$ (0.00%)

### 3.3.8 Steady-State absorption spectroscopy

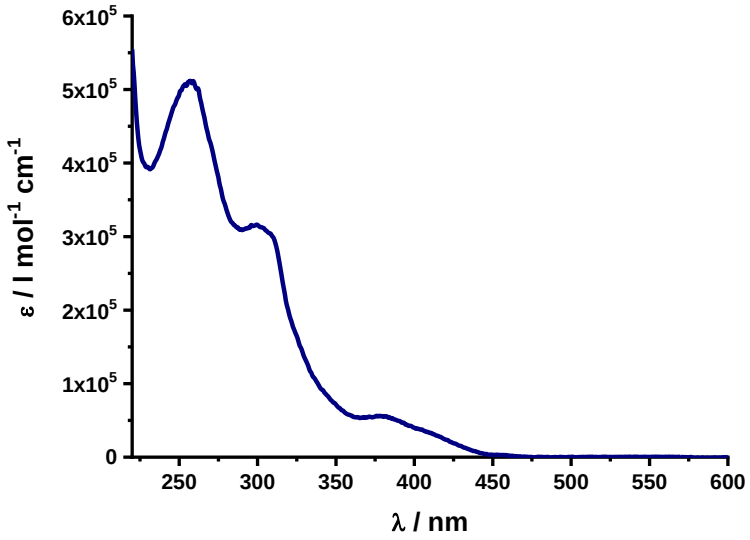



**Figure S10:** Absorption spectrum and corresponding extinction coefficients of **PC-1** in acetonitrile.

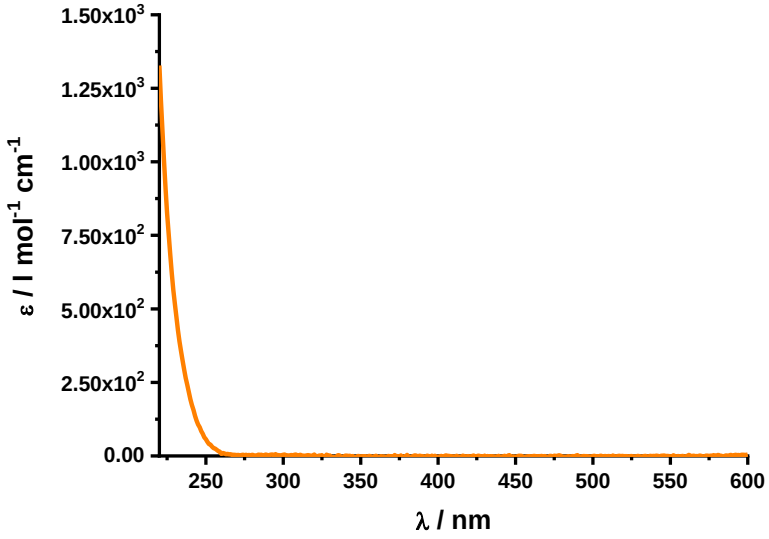



**Figure S11:** Absorption spectrum and corresponding extinction coefficients of **1a** in acetonitrile.

### 3.3.9 Steady-State emission spectroscopy

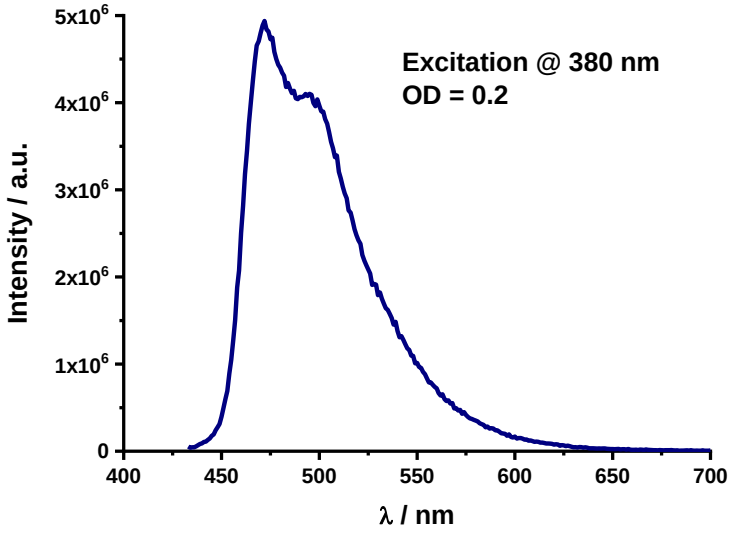



**Figure S12:** Steady-State emission spectrum of **PC-1** (c = 3.60 x $10^{-6}$ M) in acetonitrile excited at 380 nm.

### 3.3.10 Transient absorption spectroscopy

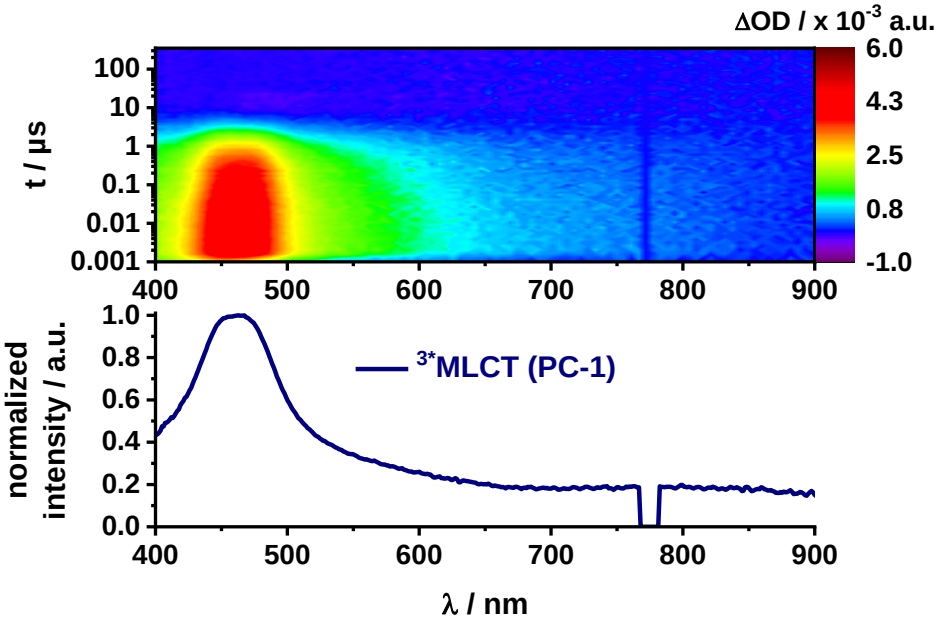



**Figure S13:** Top: Differential absorption spectra (visible) registered upon nanosecond transient absorption spectroscopy (387 nm, 150 nJ) of $[Ir(dF\text{-}CF_3\text{-}ppy)_2(dtbpy)]PF_6$ (**PC-1**, 2 x $10^{-4}$ M) in Ar-saturated acetonitrile with time delays between 0 and 355 µs at room temperature. Bottom: Corresponding global analysis results showing the normalized spectral fingerprint of $^{3*}$MLCT (**PC-1**).

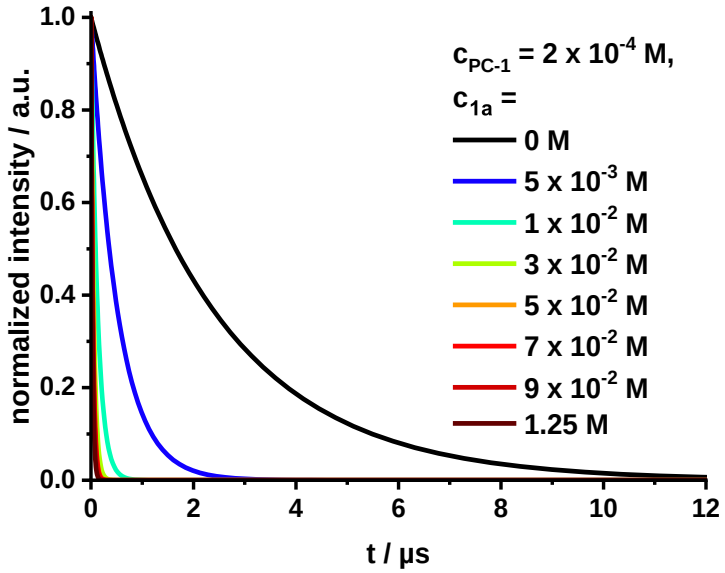



**Figure S14:** The lifetime of the $^{3*}$MLCT (**PC-1**) (c = 2 x 10$^{-4}$ M) is subsequently quenched upon addition of different amounts of **1a** (c = 0 – 1.25 M). The kinetics were determied by global analysis using the GloTarAn software[4].

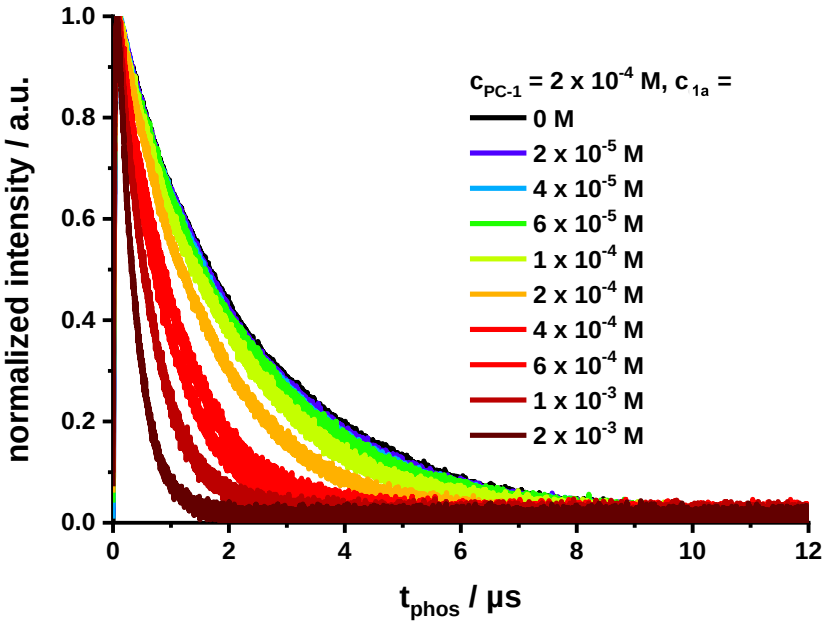



**Figure S15:** The luminescence lifetime of **PC-1** (c = 2 x10$^{-4}$ M) is subsequently quenched upon addition of different amounts of **1a** (0 M – 2 x 10$^{-3}$ M). The measurment is conducted in Ar-saturated acetonitrile. **PC-1** is excited at 355 nm. The luminescence is detected at 470 nm.

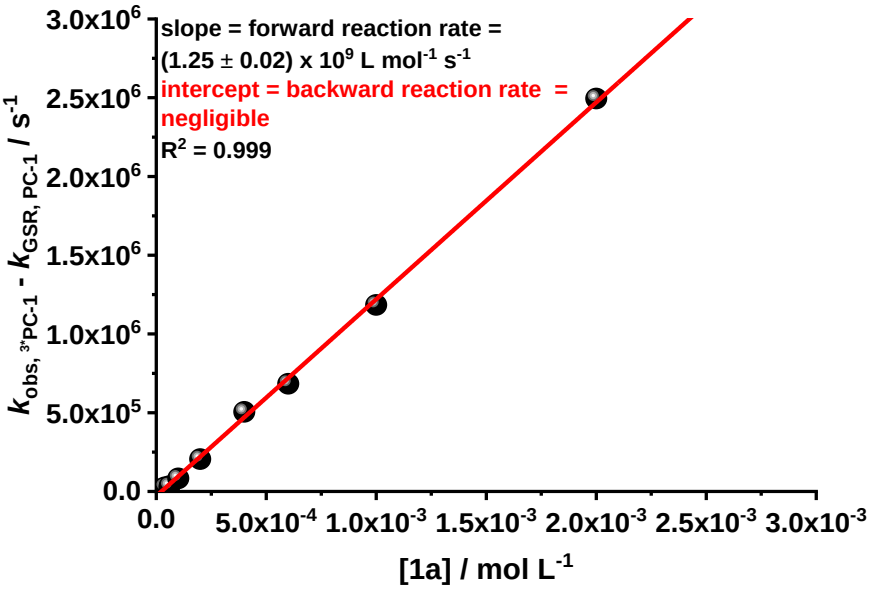



**Figure S16:** Plot of the observed rate ($k_{obs}$) constant of $^{3*}$MLCT (**PC-1**) deactivation corrected by the intrinsic GSR rate ($k_{GSR,\ \mathbf{PC\text{-}1}}$) of **PC-1** *vs.* [**1a**]. Data were recorded by the use of luminescence lifetime measurements upon addition of **1a**.

## 3.3.11 Electrochemical Studies

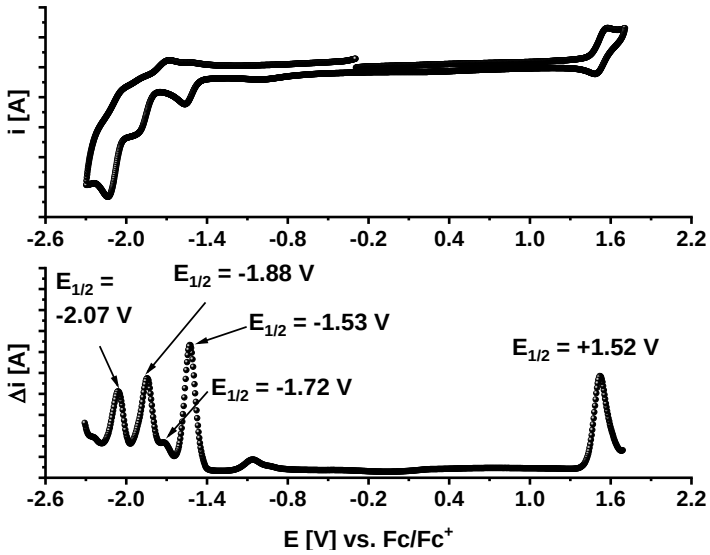



**Figure S17:** Overview of the oxidation and reduction potentials recorded by cyclic voltammetry (top) and differential pulse voltammetry (bottom) of **PC-1** measured in dry Ar-saturated acetonitrile with 0.1 M $TBAPF_6$ as supporting electrolyte.

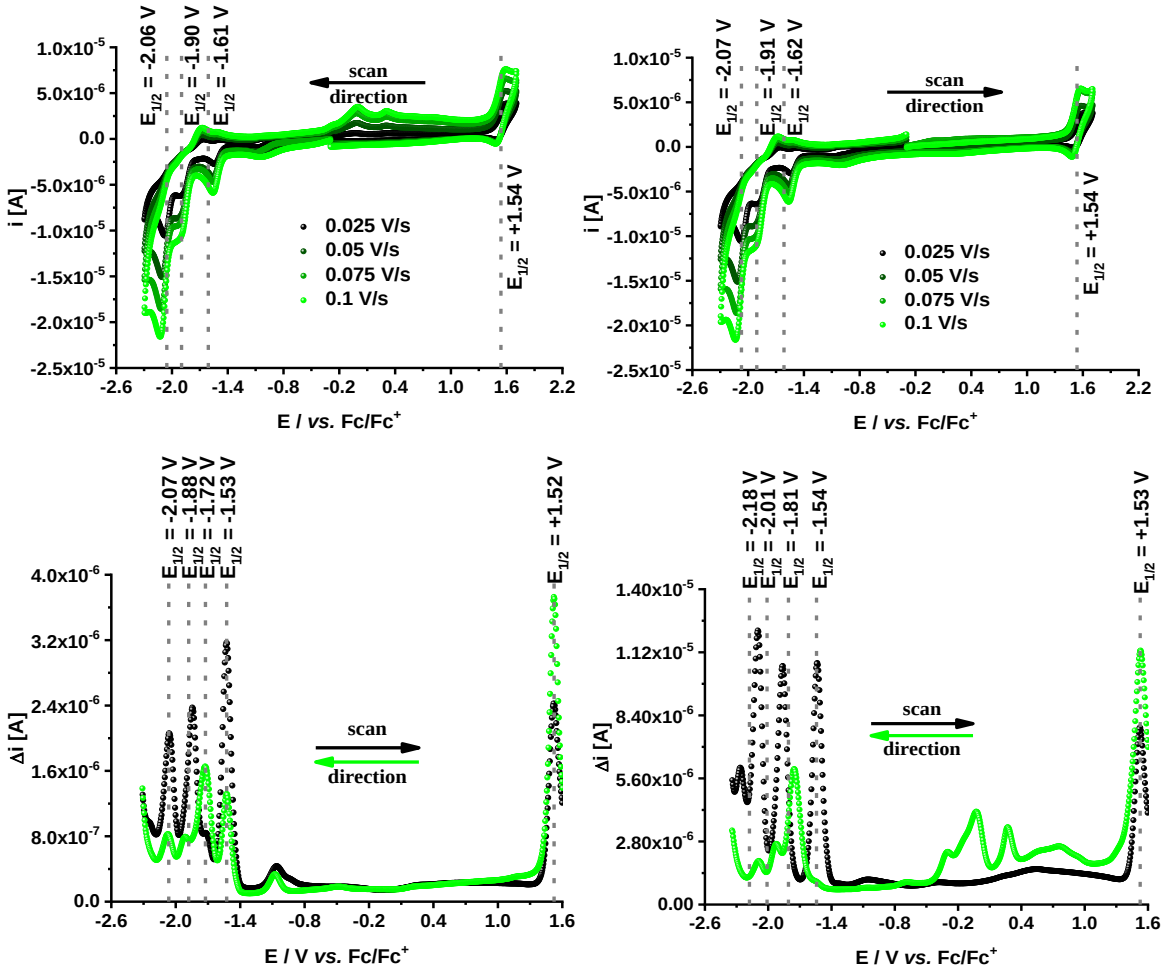



**Figure S18:** Cyclic voltammograms (top), differential pulse voltammograms (bottom left) and square wave voltammograms (bottom right) of **PC-1** measured in dry Ar-saturated acetonitrile with 0.1 M $TBAPF_6$ as supporting electrolyte.

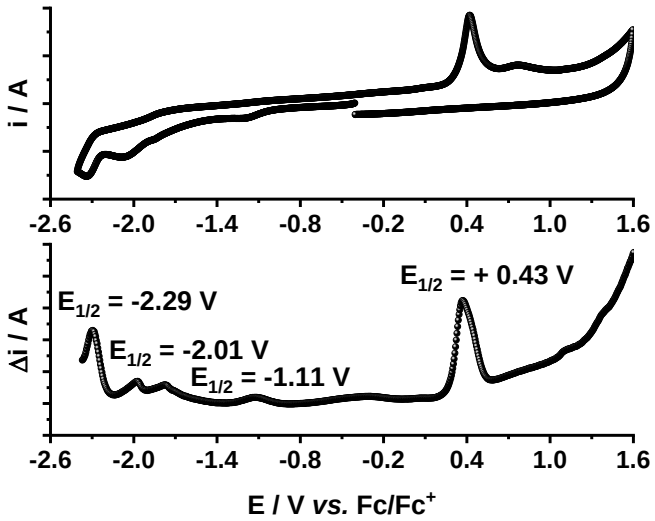



**Figure S19:** Overview of the oxidation and reduction potentials recorded by cyclic voltammetry (top) and differential pulse voltammetry (bottom) of **1a** measured in dry Ar-saturated acetonitrile with 0.1 M $TBAPF_6$ as supporting electrolyte.

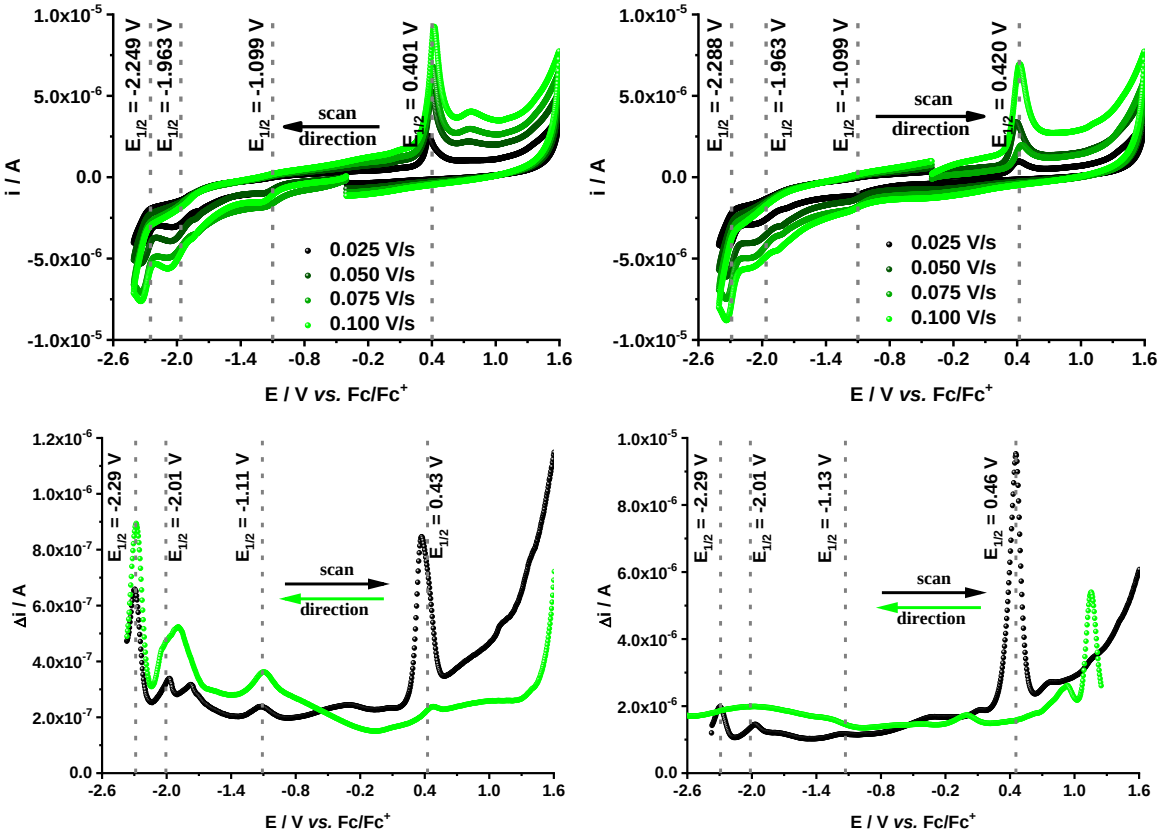



**Figure S20:** Cyclic voltammograms (top), differential pulse voltammograms (bottom left) and square wave voltammograms (bottom right) of **1a** measured in dry Ar-saturated acetonitrile with 0.1 M $TBAPF_6$ as supporting electrolyte.

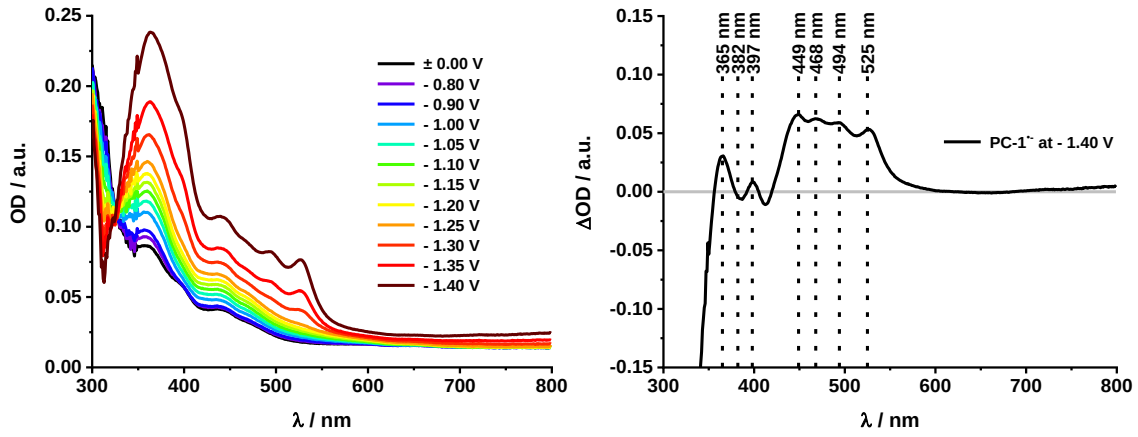



**Figure S21:** Left: Differential absorption spectra (visible) registered upon spectroelectrochemical reduction (0.00 to -1.40 V *vs.* $Ag/Ag^+$) of **PC-1** in Ar-saturated acetonitrile with 0.1 M $TBAPF_6$ as supporting electrolyte at room temperature. Right: Spectroscopic fingerprints of **PC-1**$^{\bullet-}$ after baseline correction and subtraction of the steady-state absorption spectrum of **PC-1** in the absence of any applied bias.

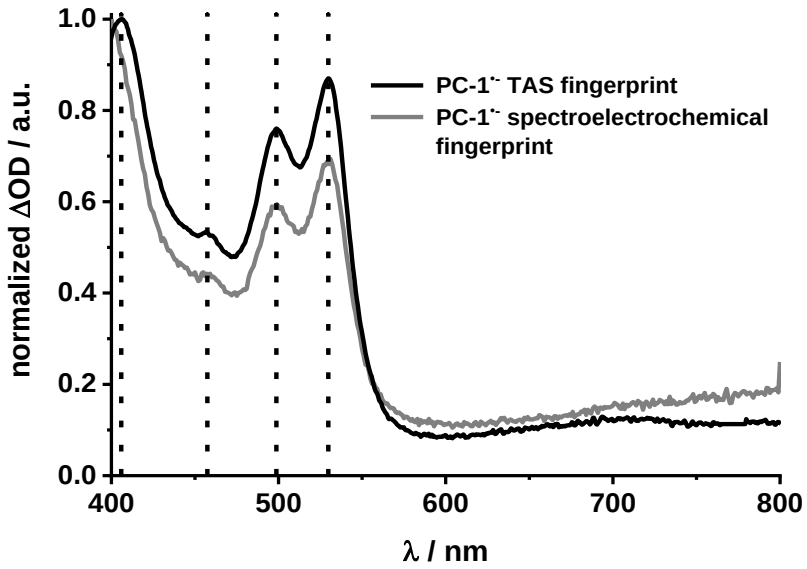



**Figure S22:** Spectroscopic fingerprint of **PC-1**$^{\bullet-}$ determined by spectroelectrochemistry in comparison to the **PC-1**$^{\bullet-}$ features obtained by target analysis using GloTarAn[4]. The target analysis is based on ns-TAS of **PC-1** (c = 2 x $10^{-4}$ M) mixed with **1a** (c = 2.5 M) (excitation: 387 nm) both in Ar-saturated acetonitrile.

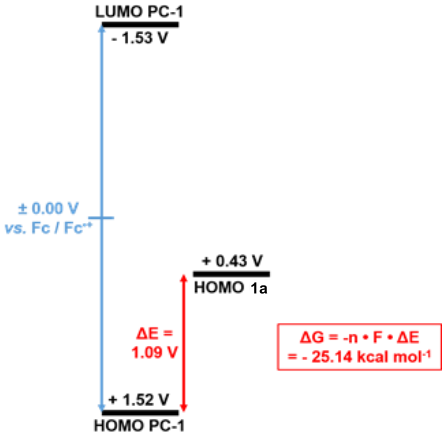



**Figure S23:** Calculation of the driving force of electron transfer from **1a** to **PC-1** based on a model supplied by electrochemical studies of the corresponding substances.

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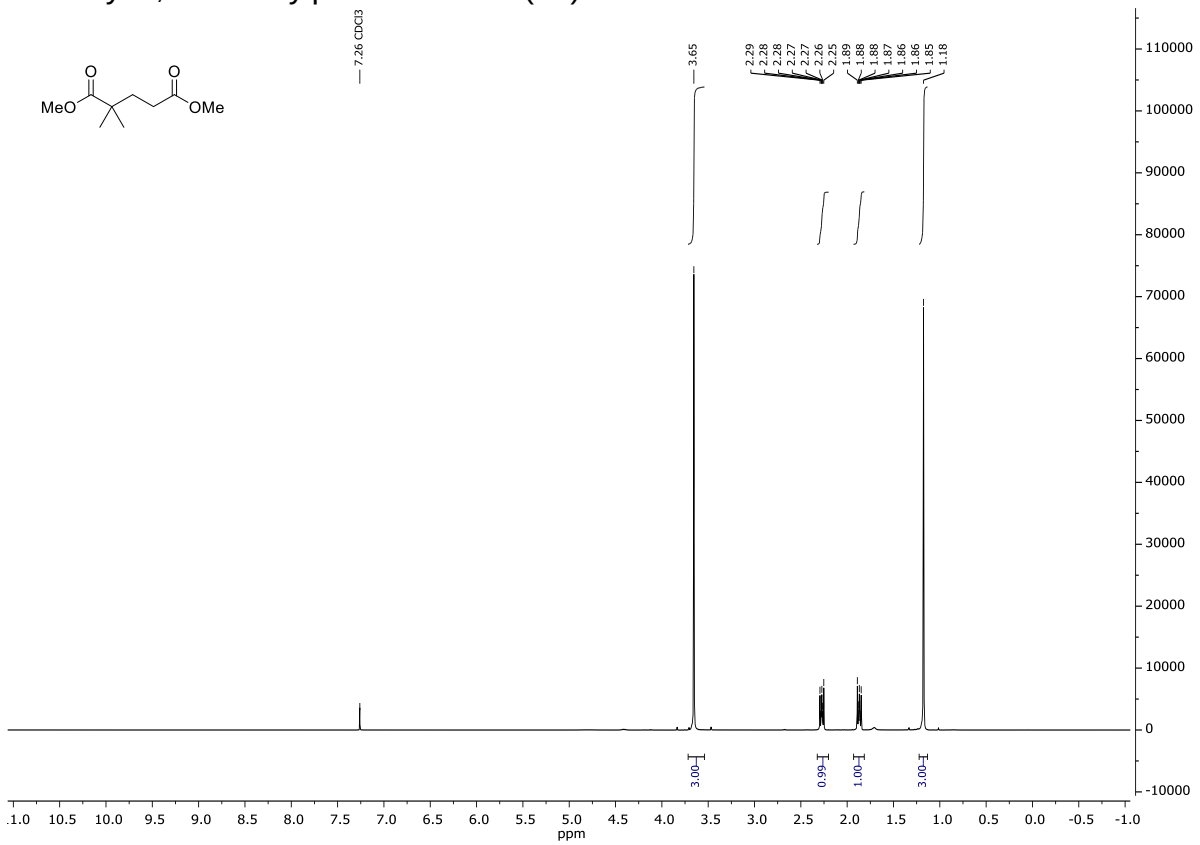
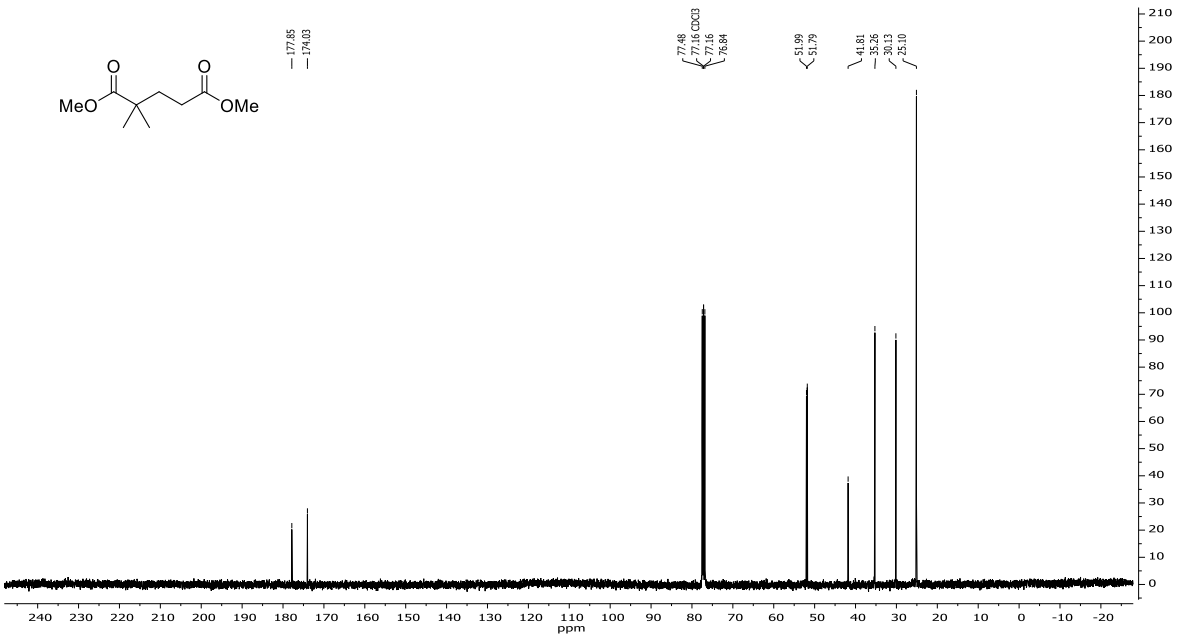
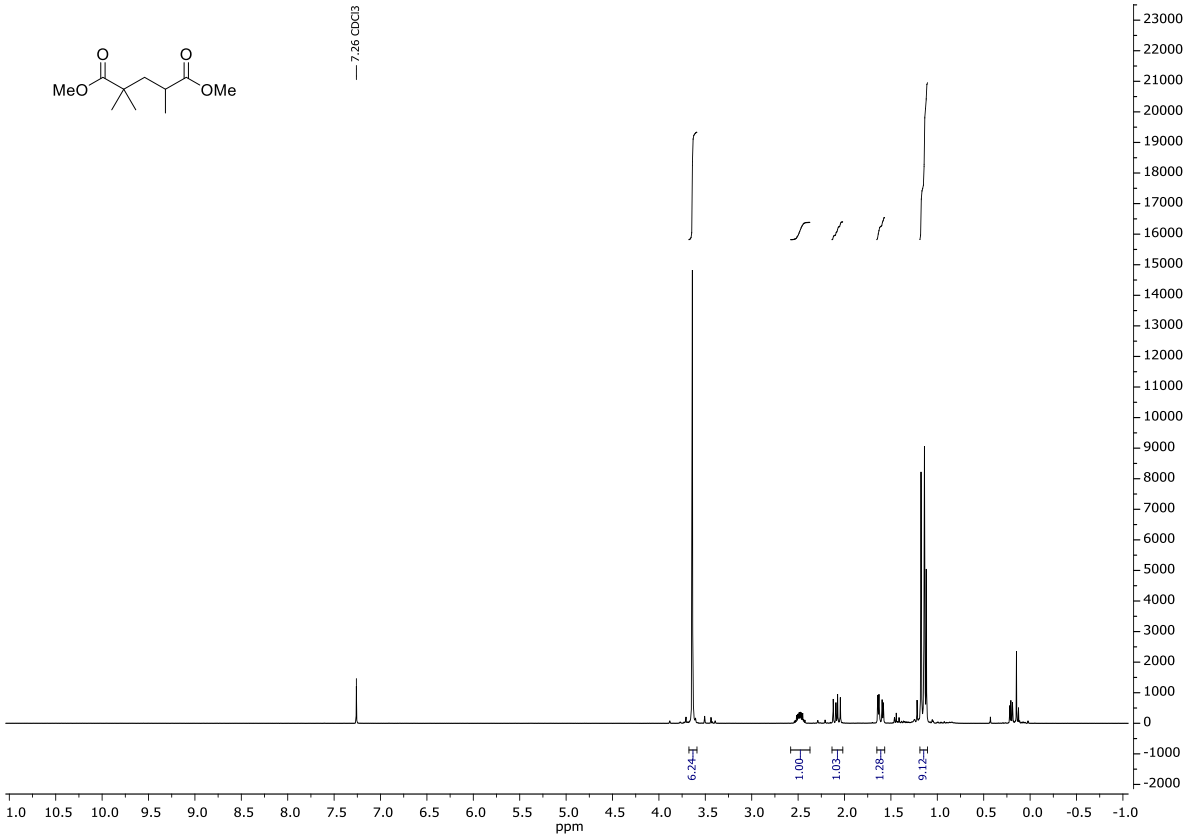
# 5 Product spectra

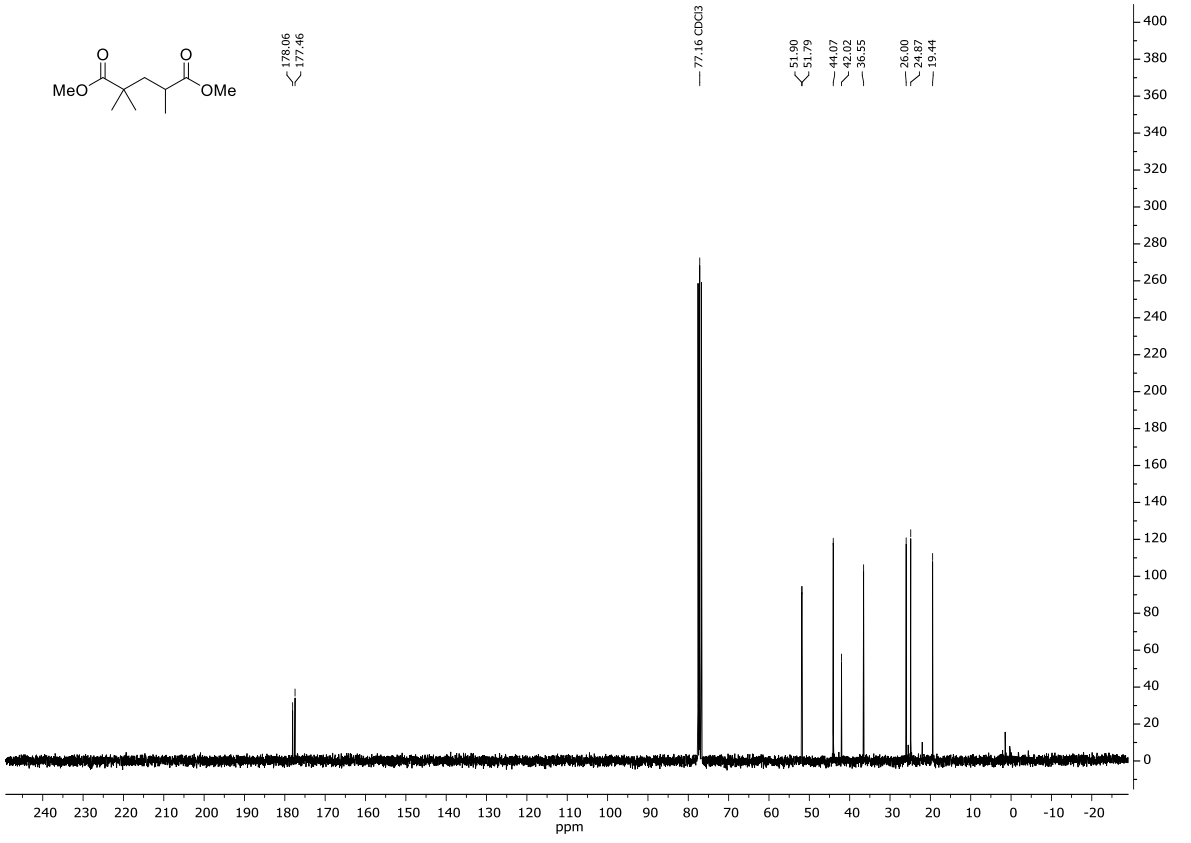
Dimethyl 2,2-dimethylpentanedioate (**3a**)



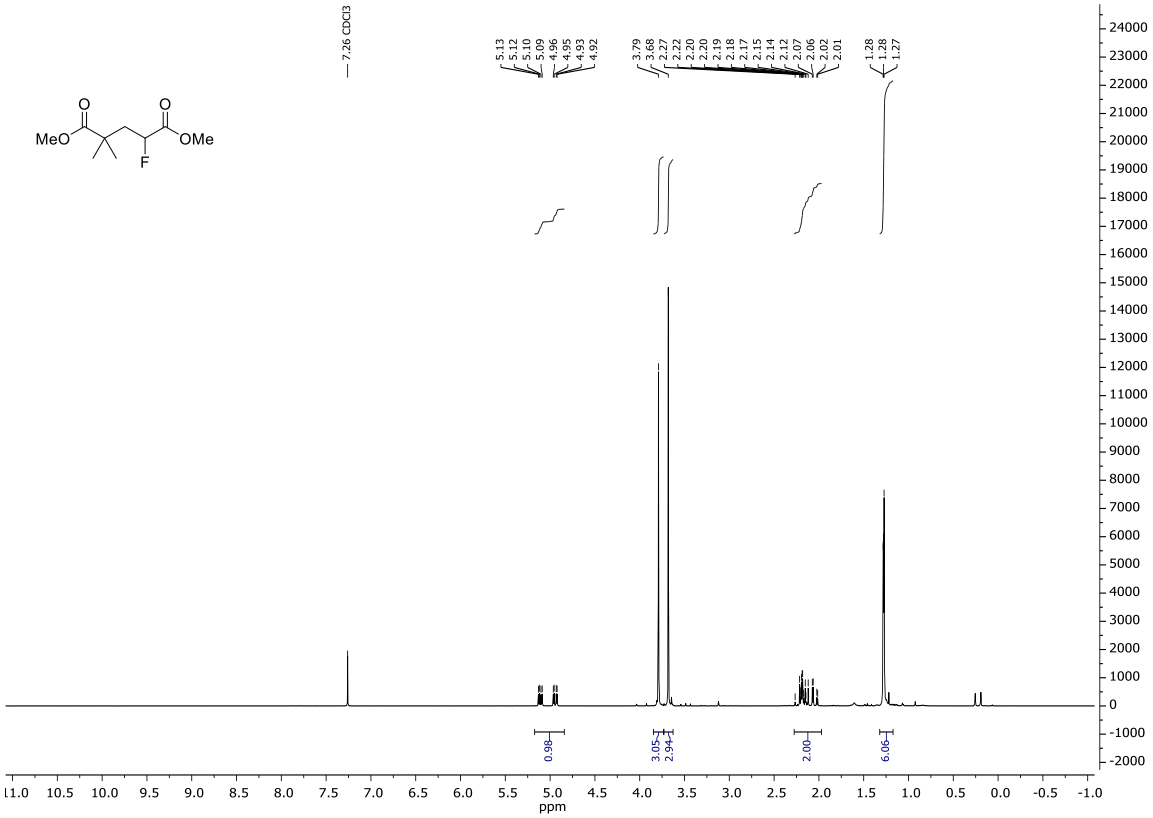



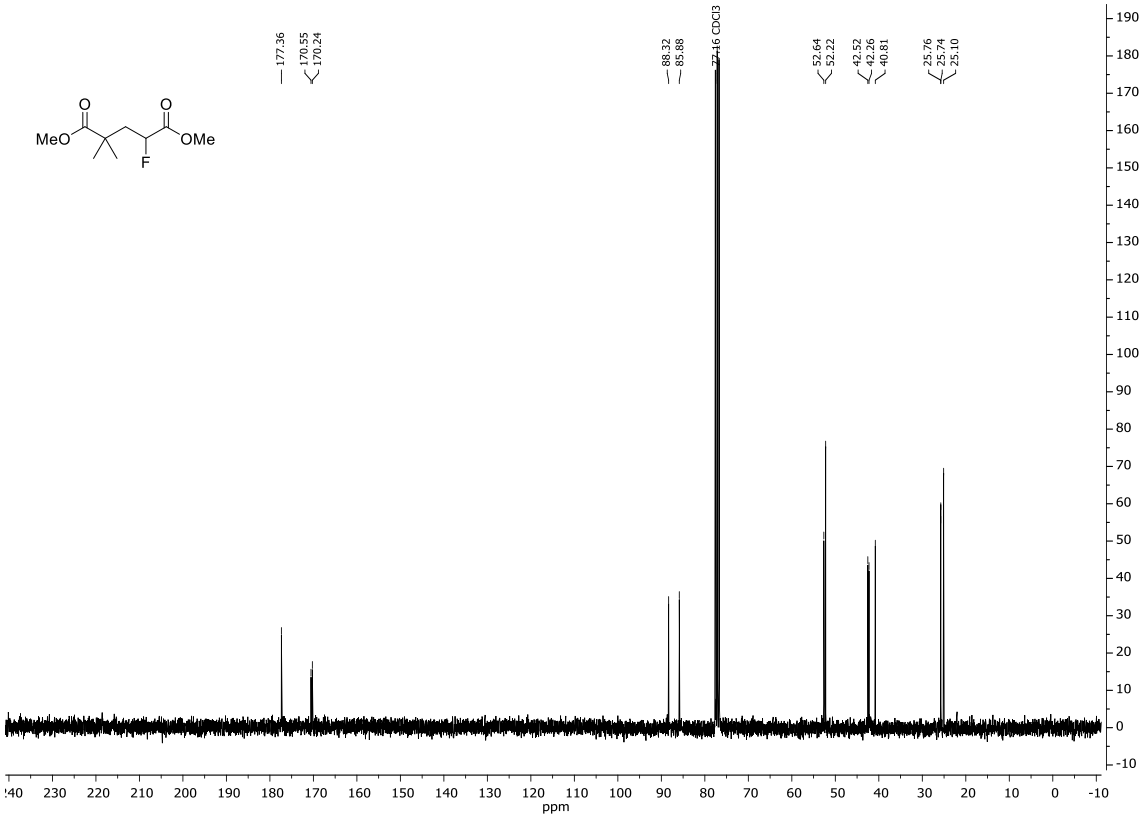
Dimethyl 2,2,4-trimethylpentanedioate (**3b**)

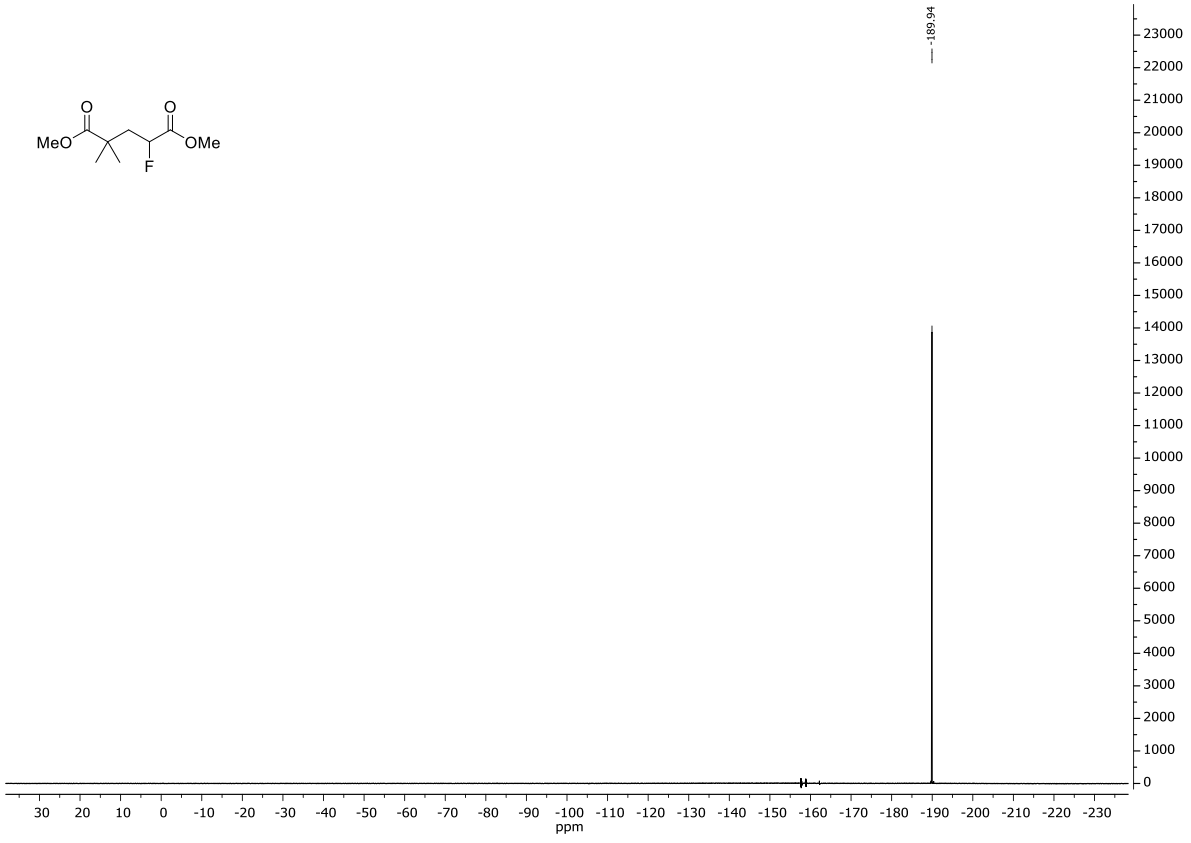


Dimethyl 4-fluoro-2,2-dimethylpentanedioate (**3c**)




MeO
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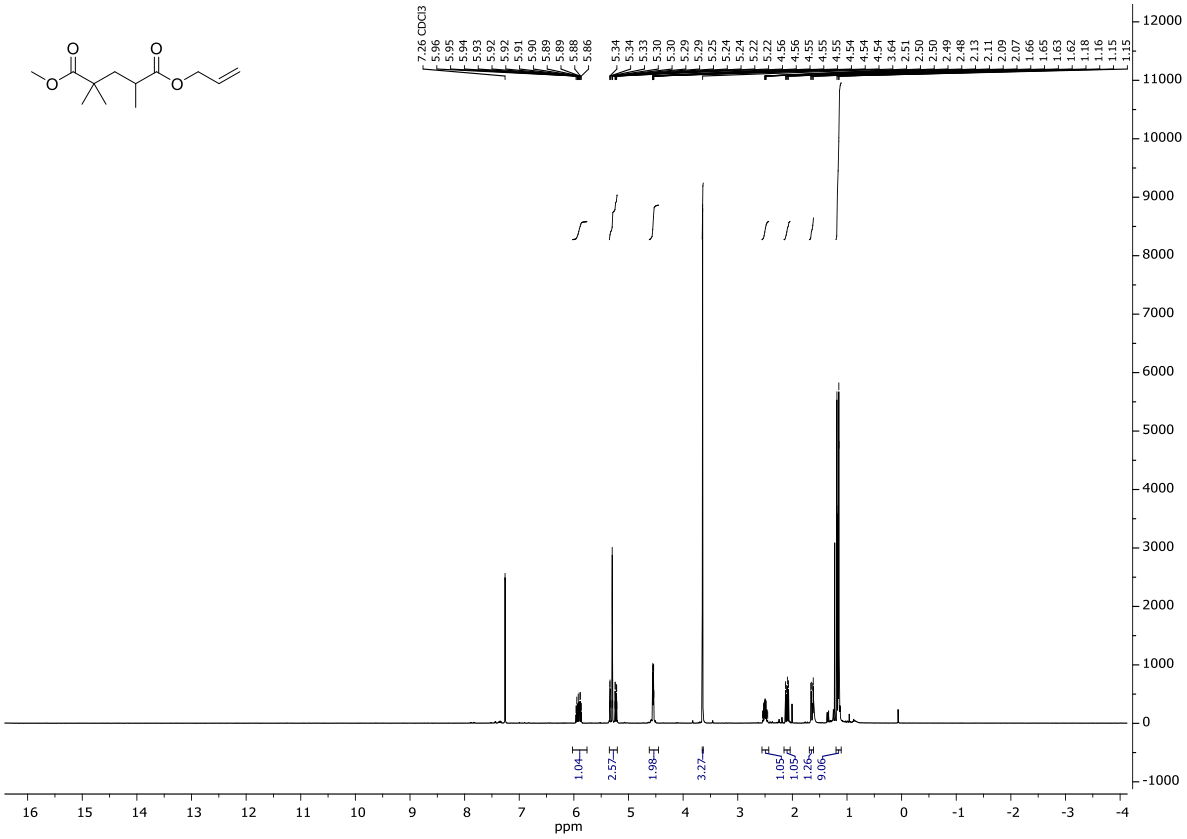
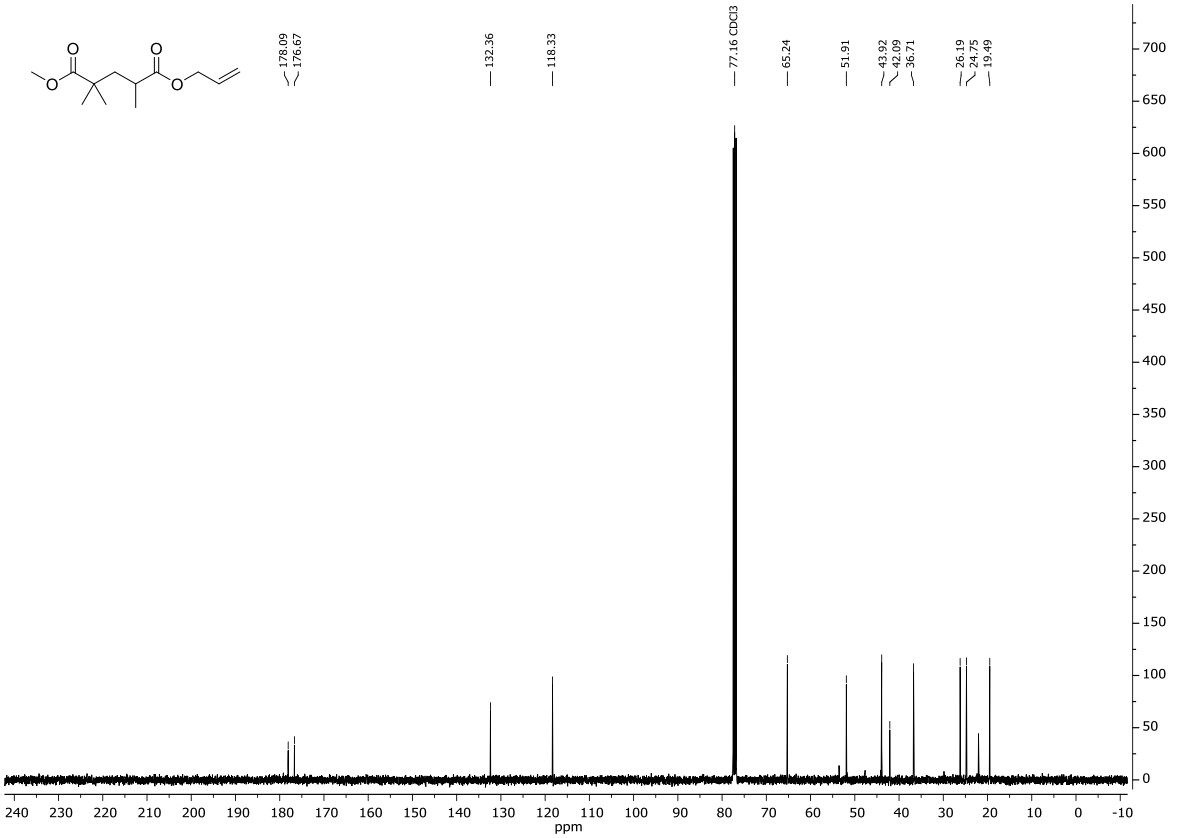
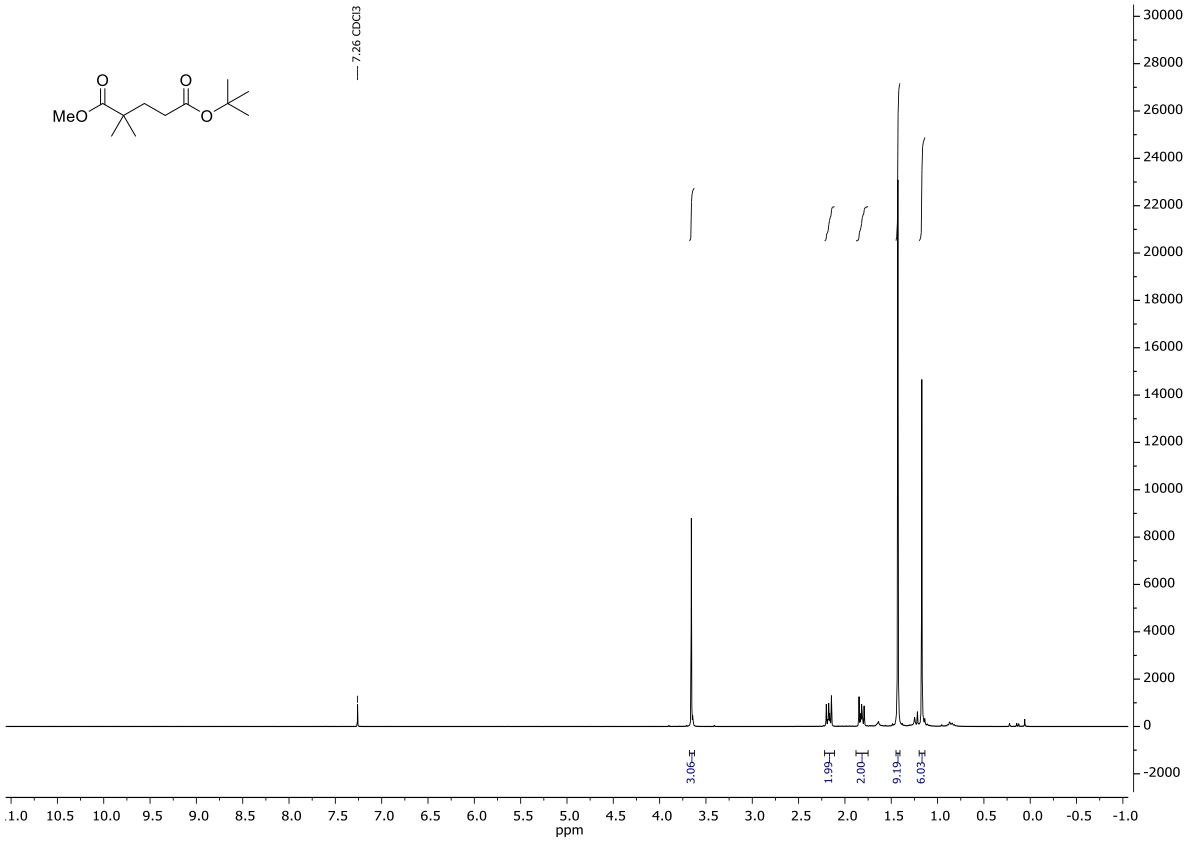
1000
0
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
ppm

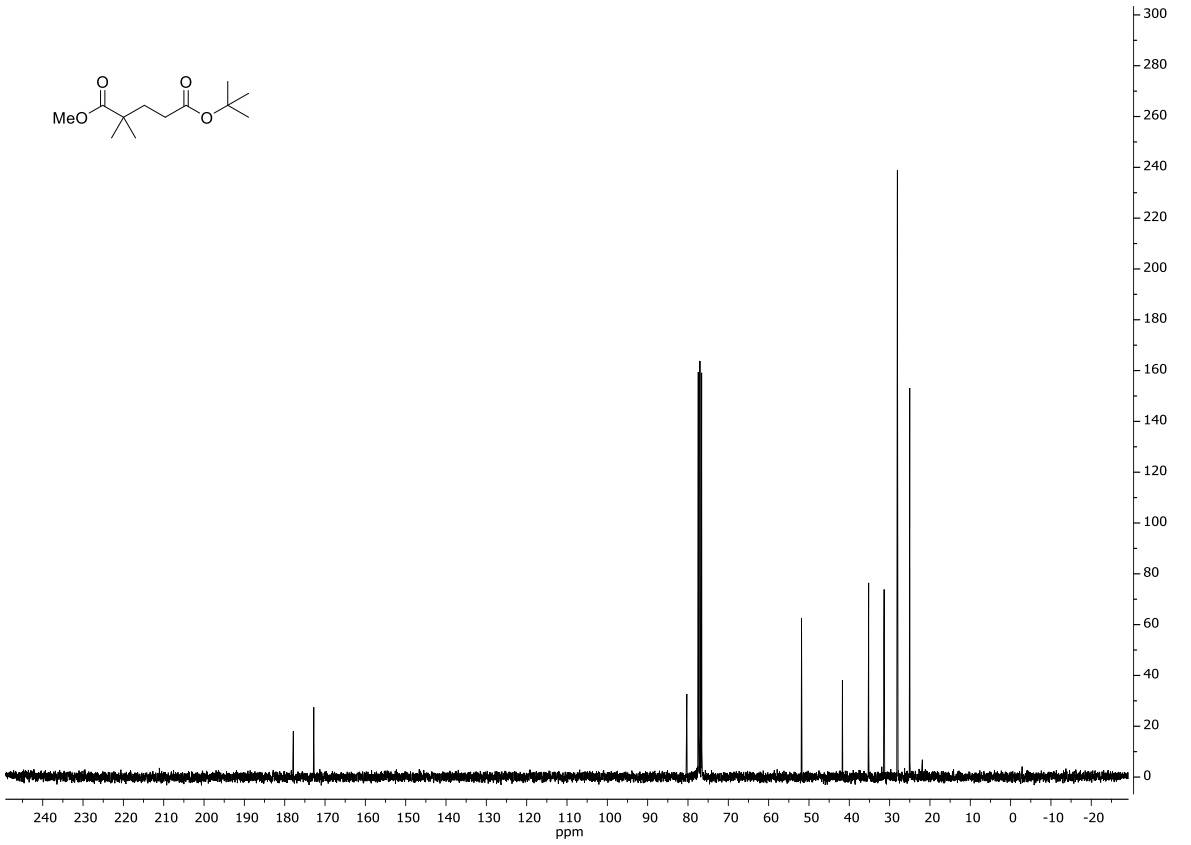
5-Allyl 1-methyl 2,2-dimethylpentanedioate (**3d**):



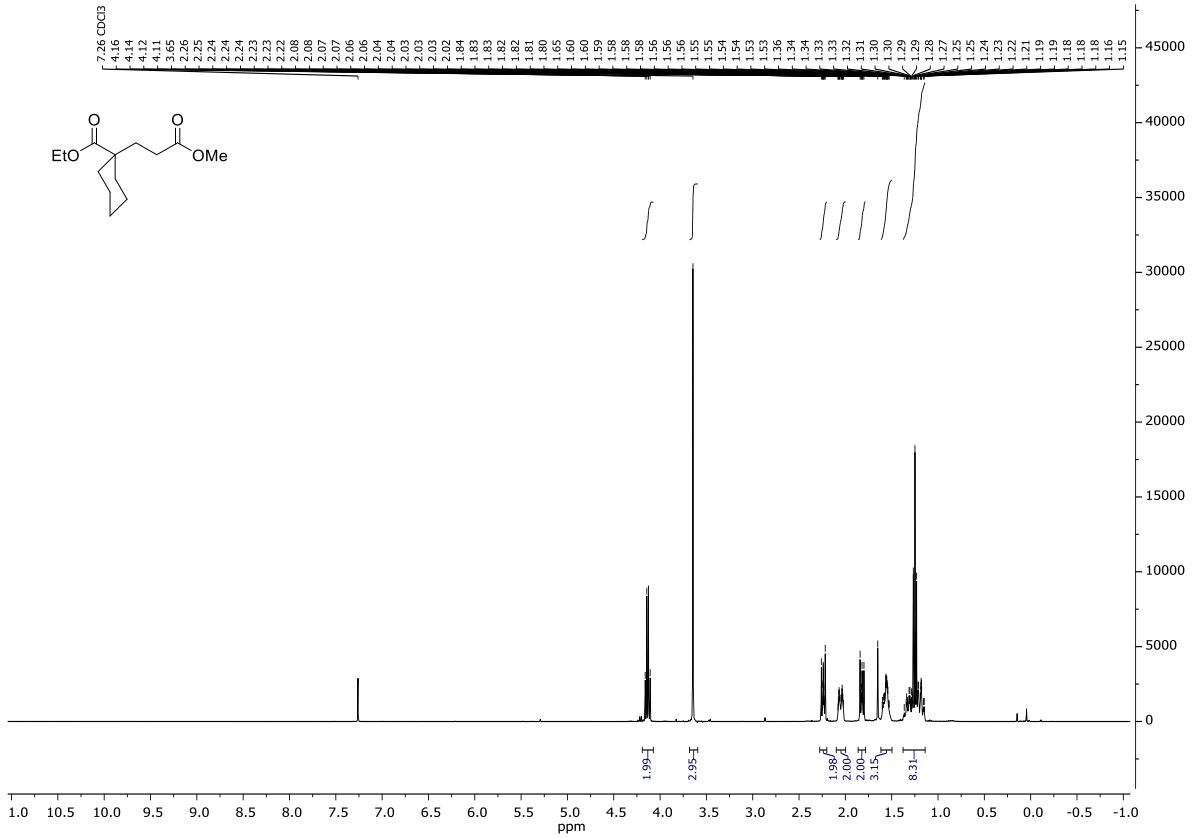



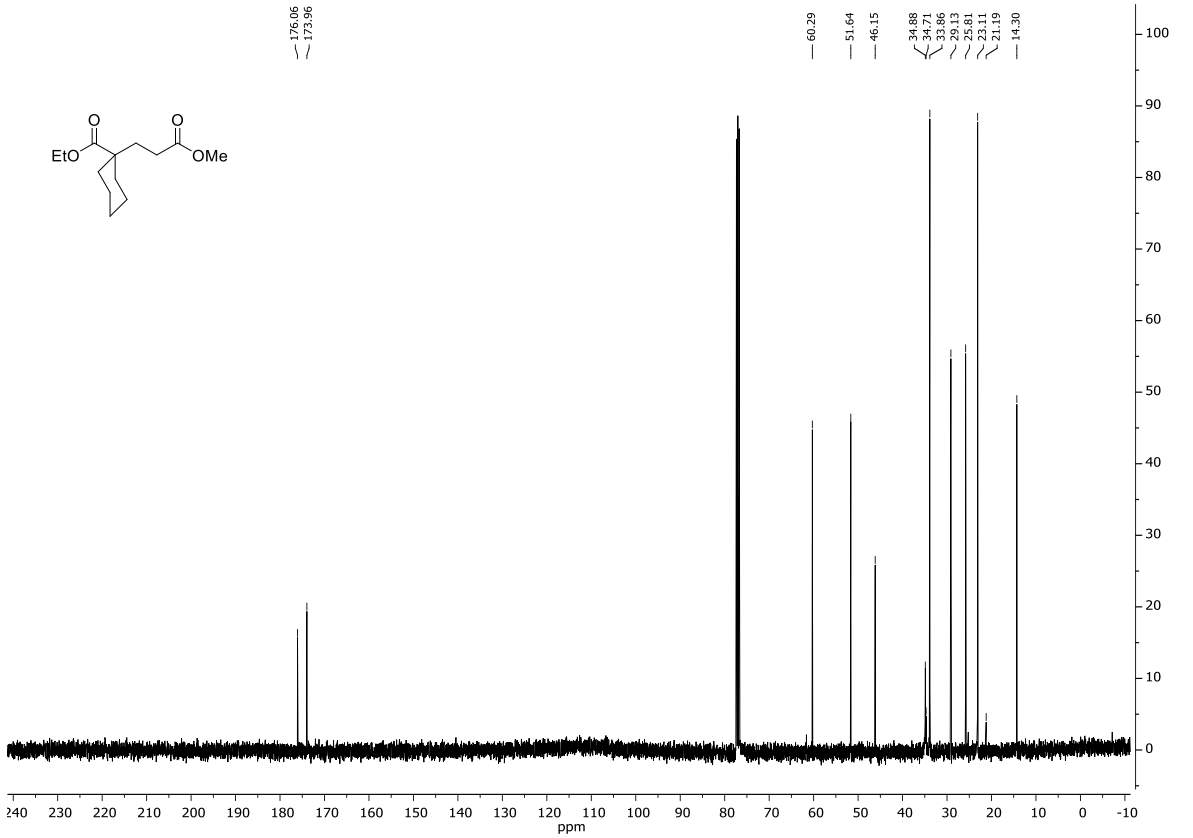
5-(*tert*-Butyl) 1-methyl 2,2-dimethylpentanedioate (**3e**):



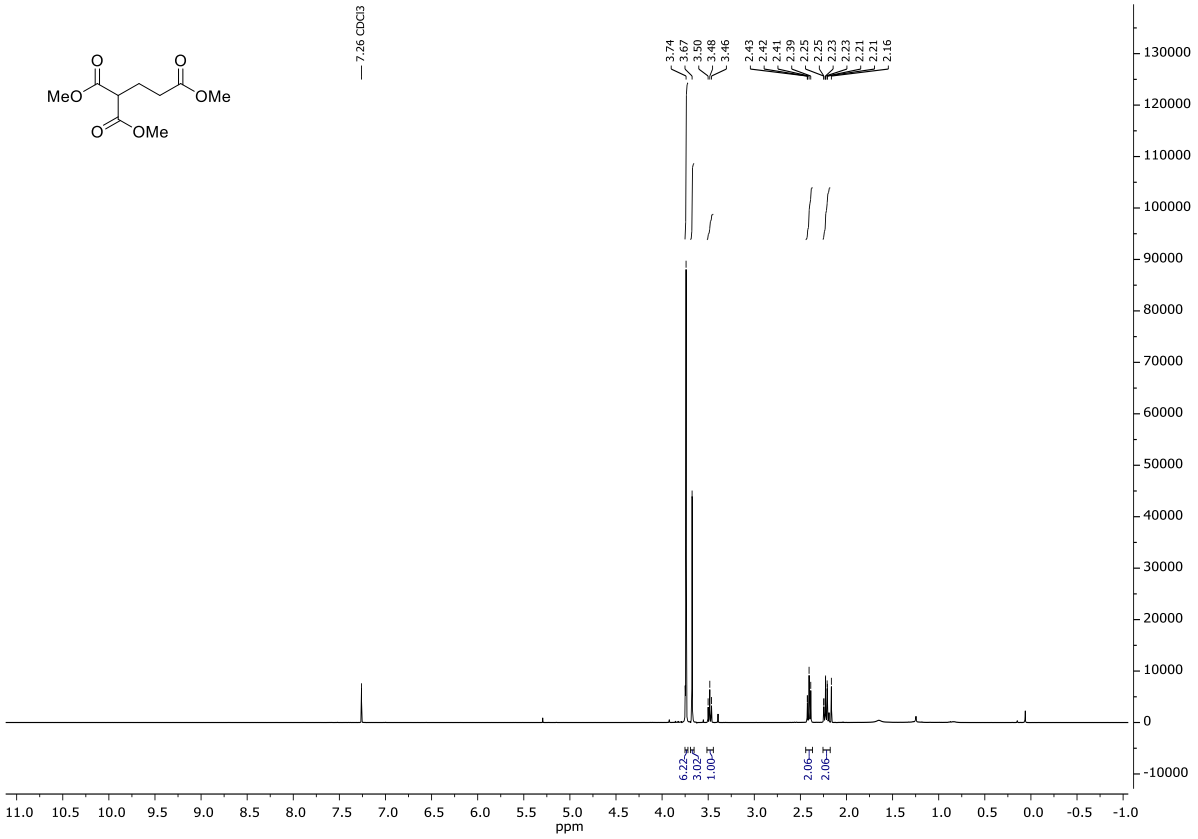



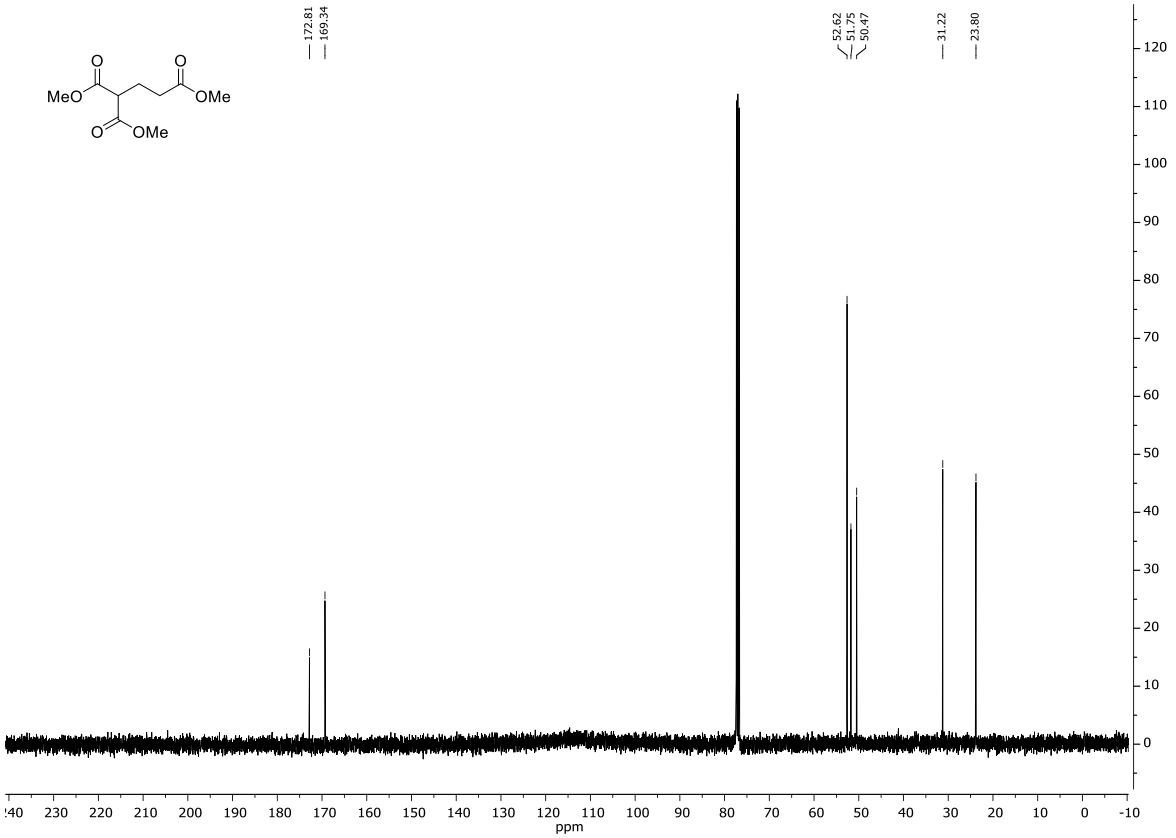
Ethyl 1-(3-methoxy-3-oxopropyl)cyclohexane-1-carboxylate (**3f**)



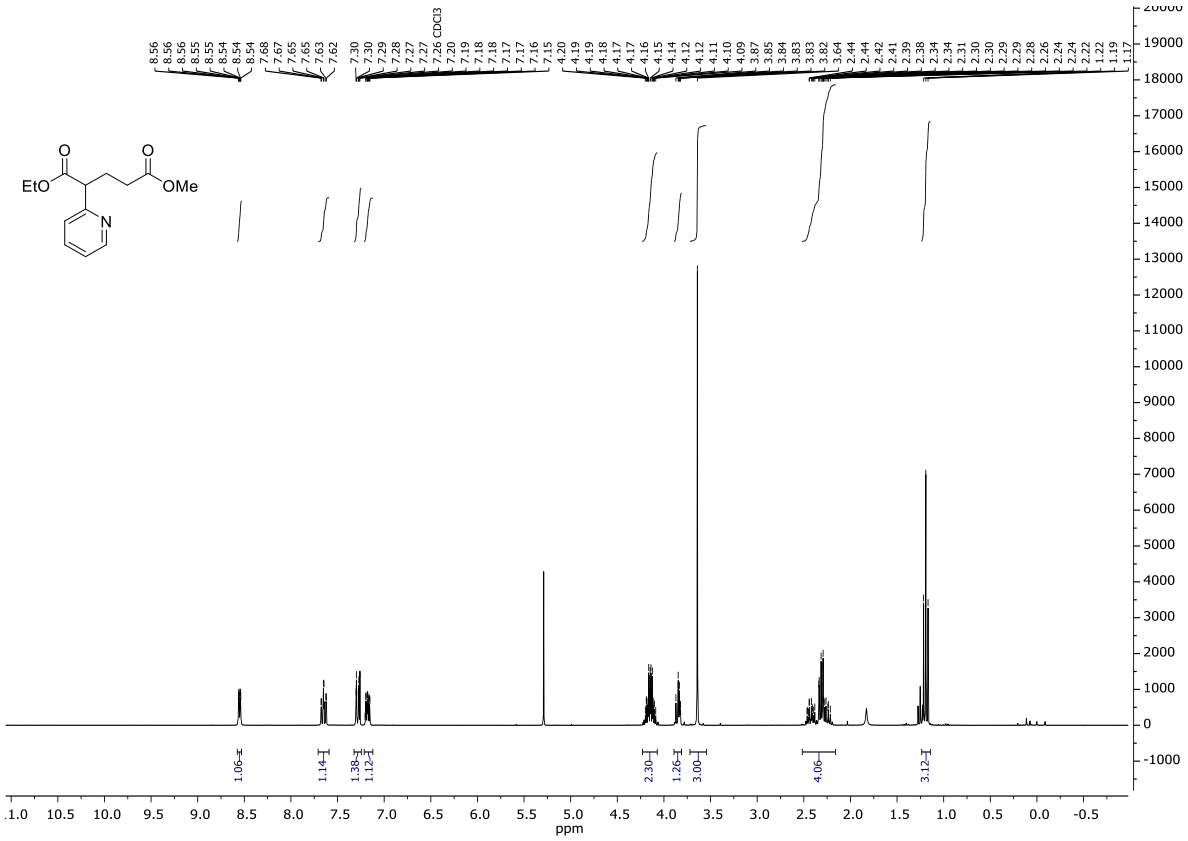



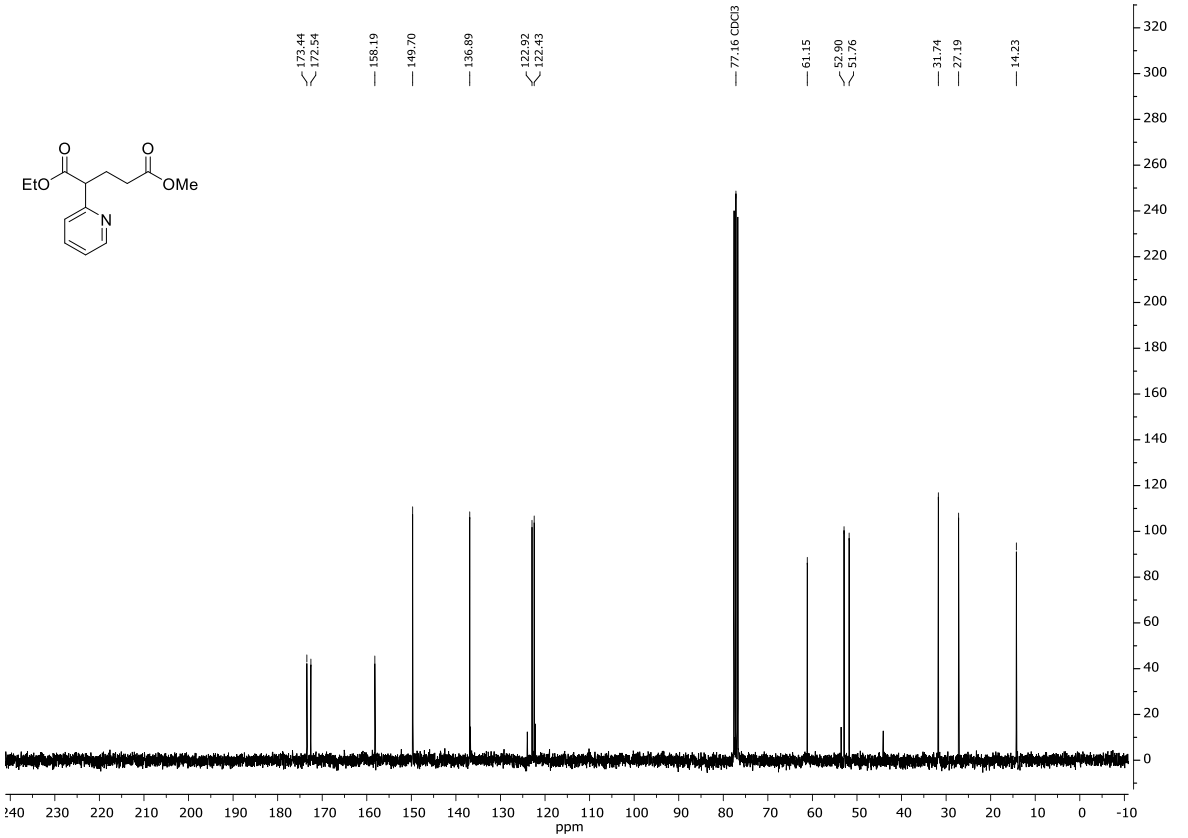
Trimethyl propane-1,1,3-tricarboxylate (**3g**)



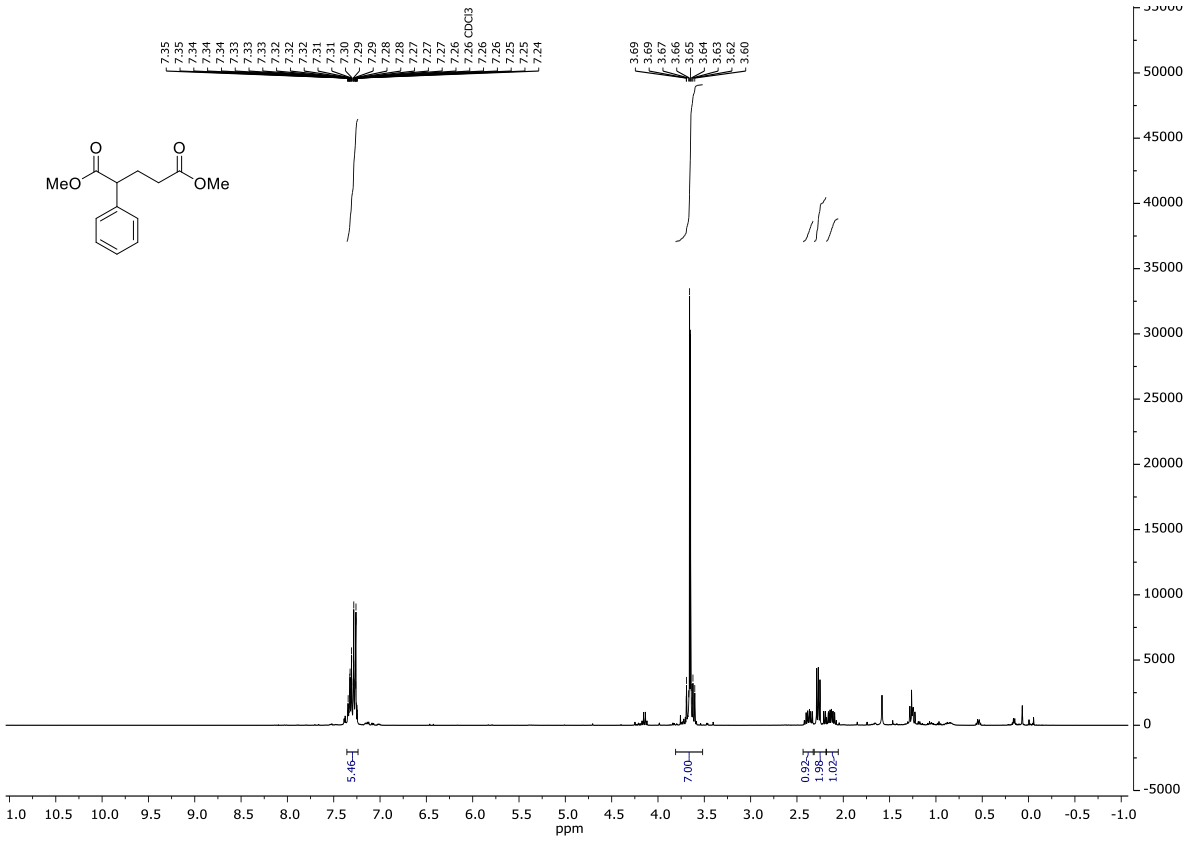



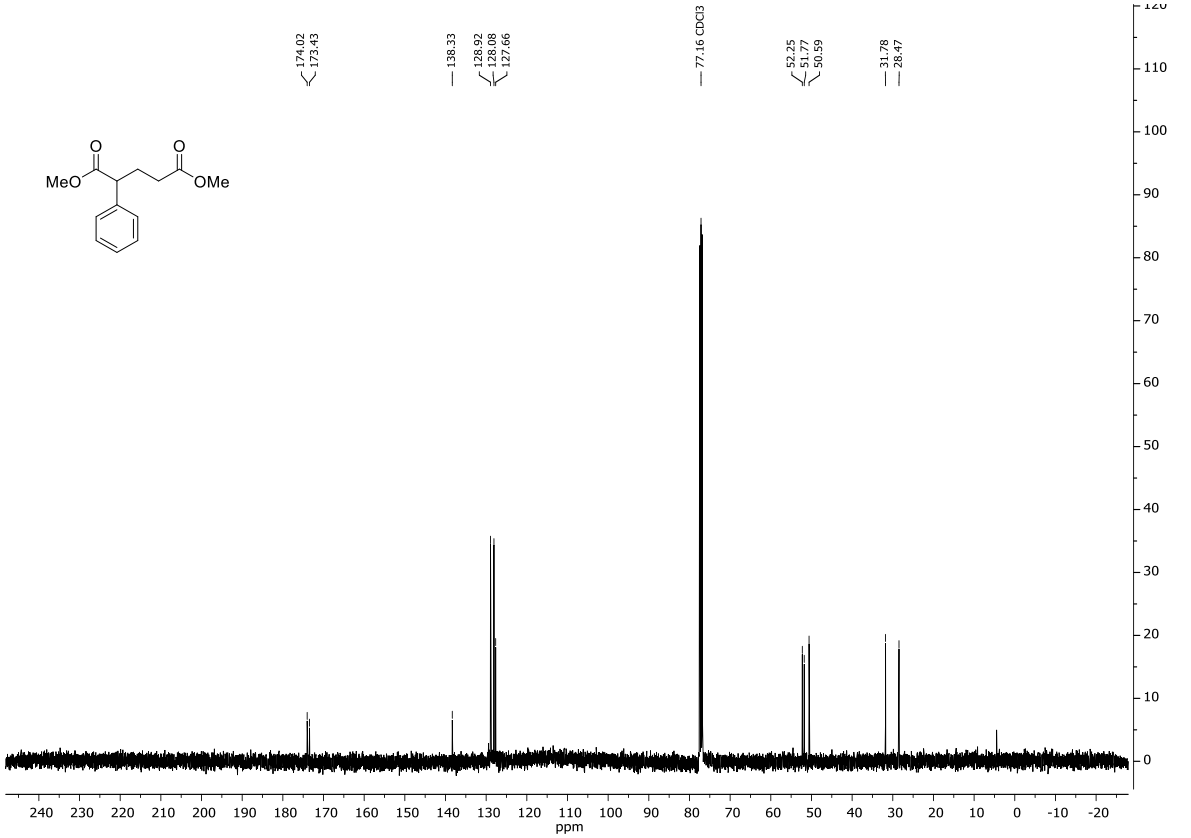
1-Ethyl 5-methyl 2-(pyridin-2-yl)pentanedioate (**3h**)



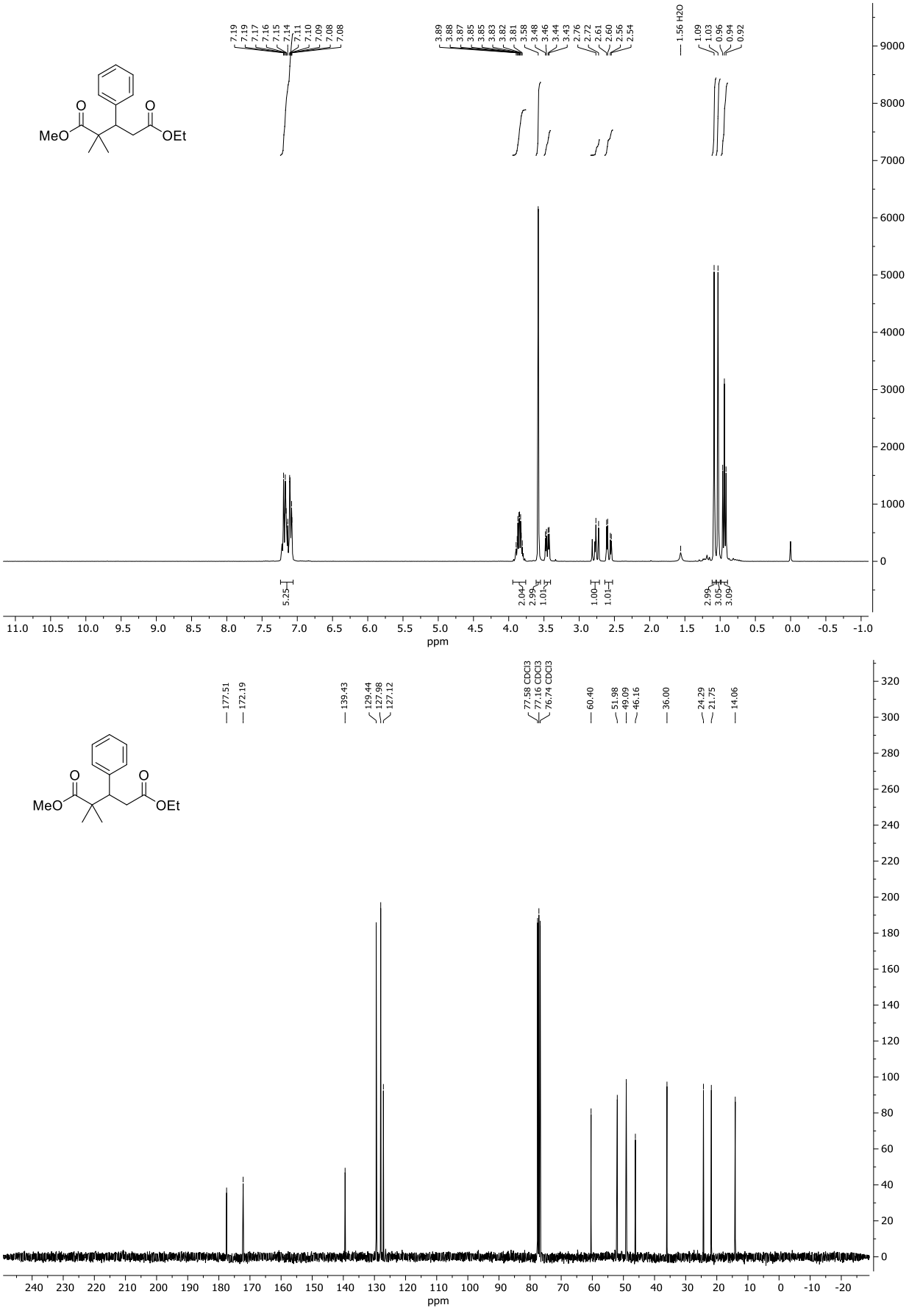



Dimethyl 2-phenylpentanedioate (**3i**):

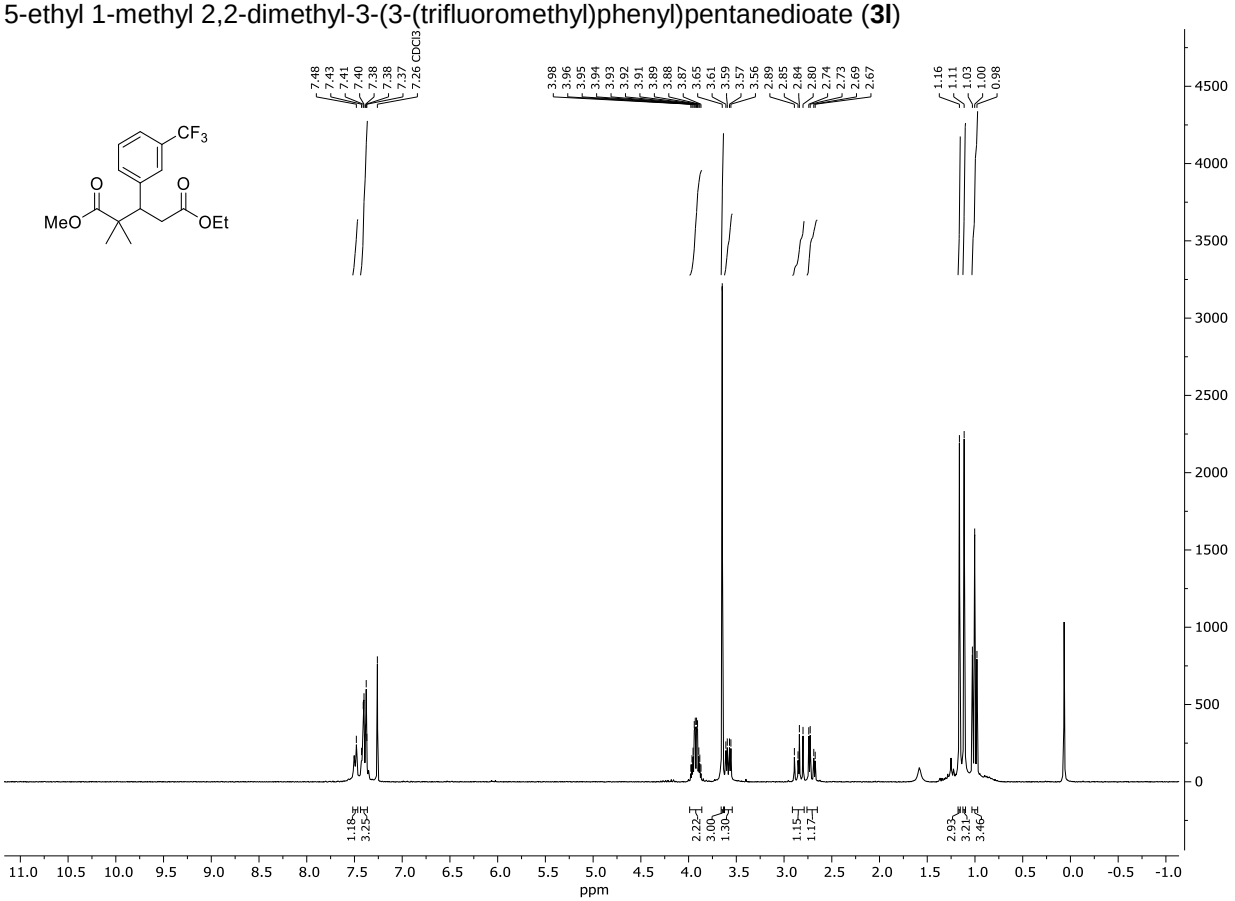


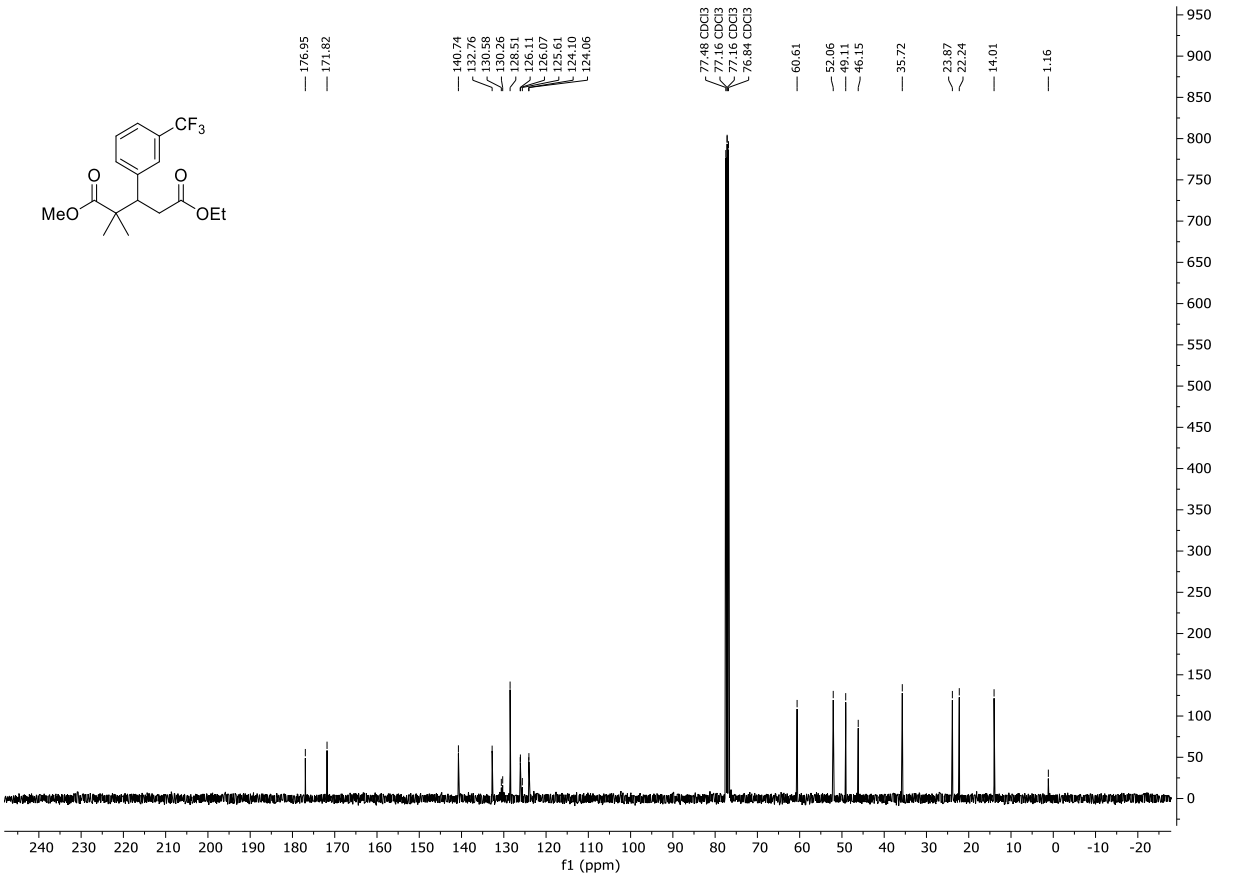



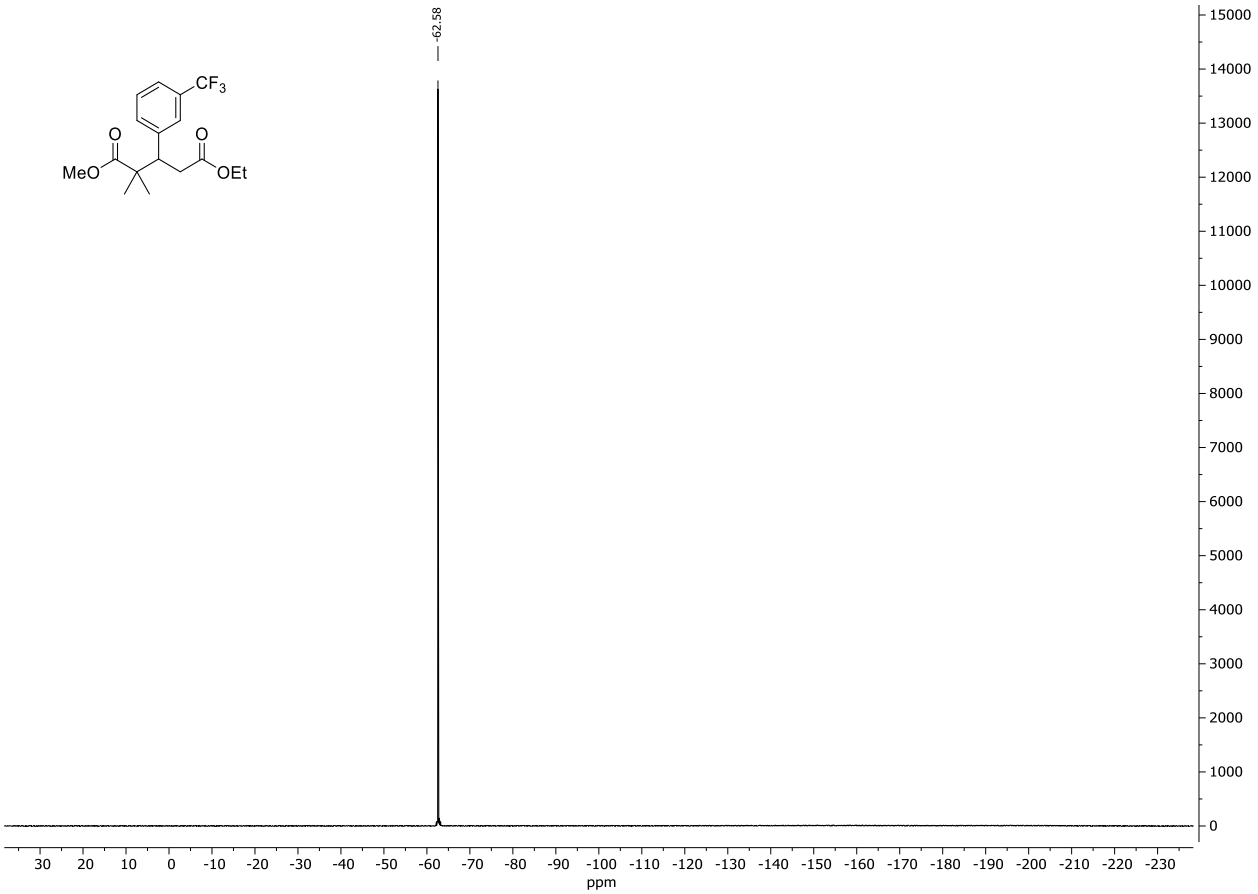
5-Ethyl 1-methyl 2,2-dimethyl-3-phenylpentanedioate (**3k**)



5-ethyl 1-methyl 2,2-dimethyl-3-(3-(trifluoromethyl)phenyl)pentanedioate (**3l**)

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4000
3000
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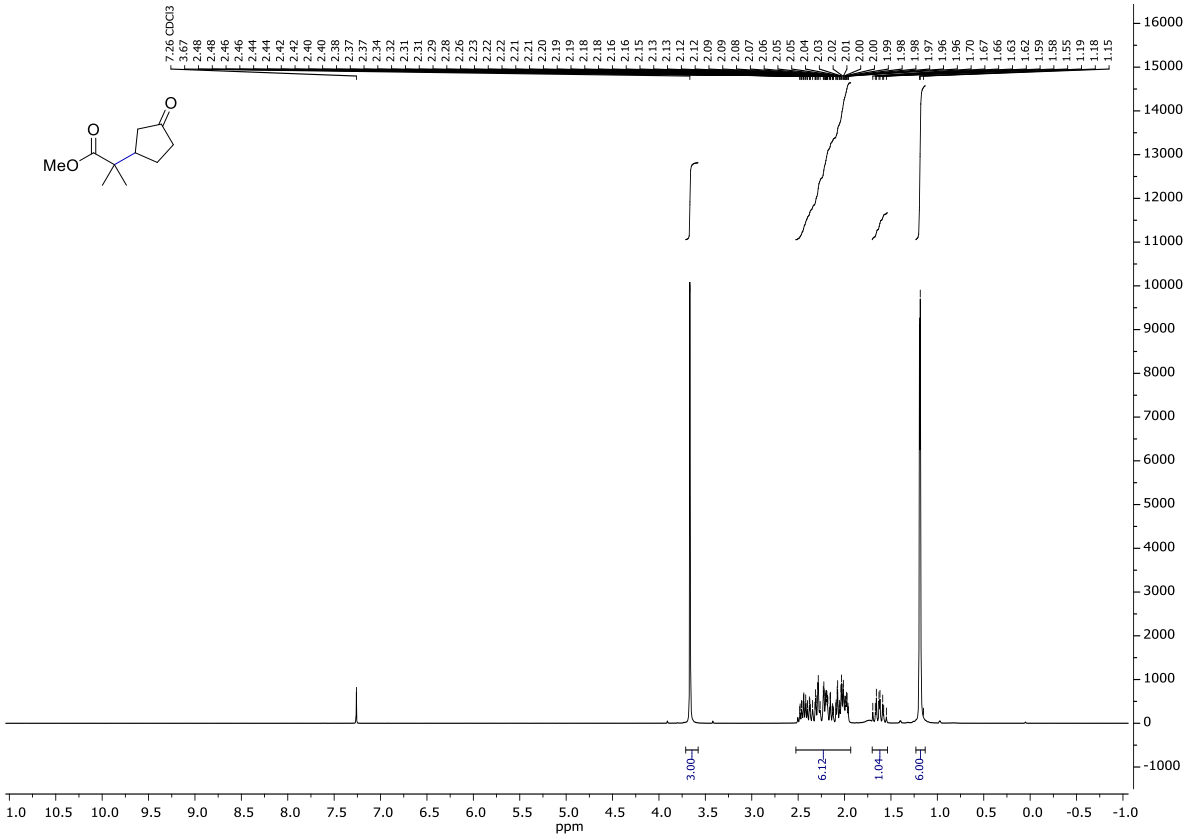
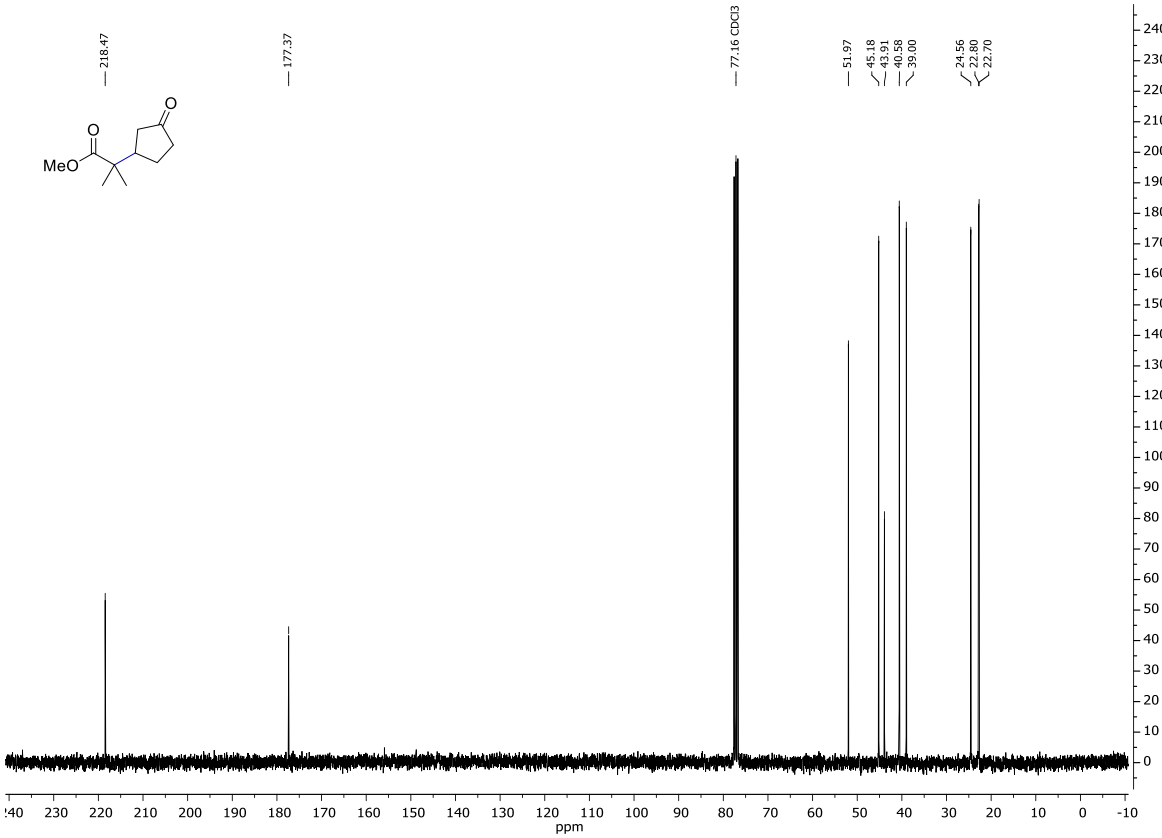
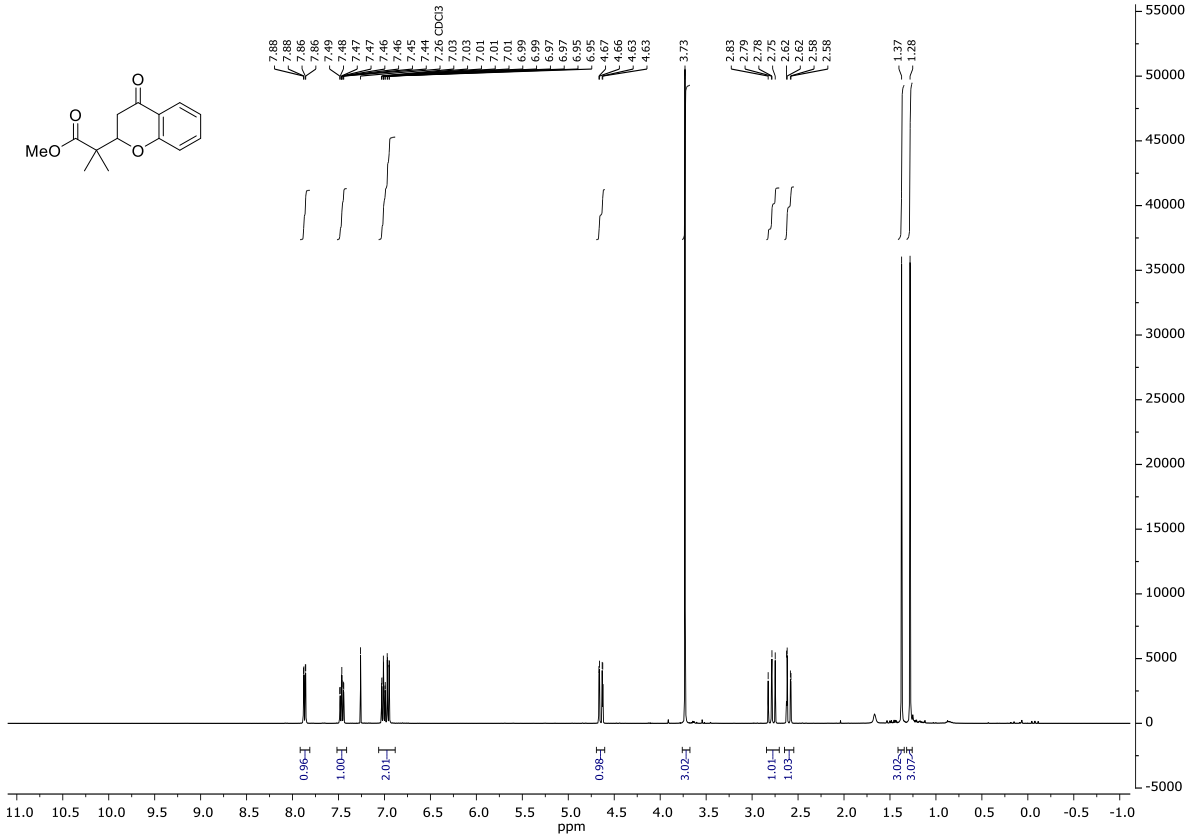
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
ppm

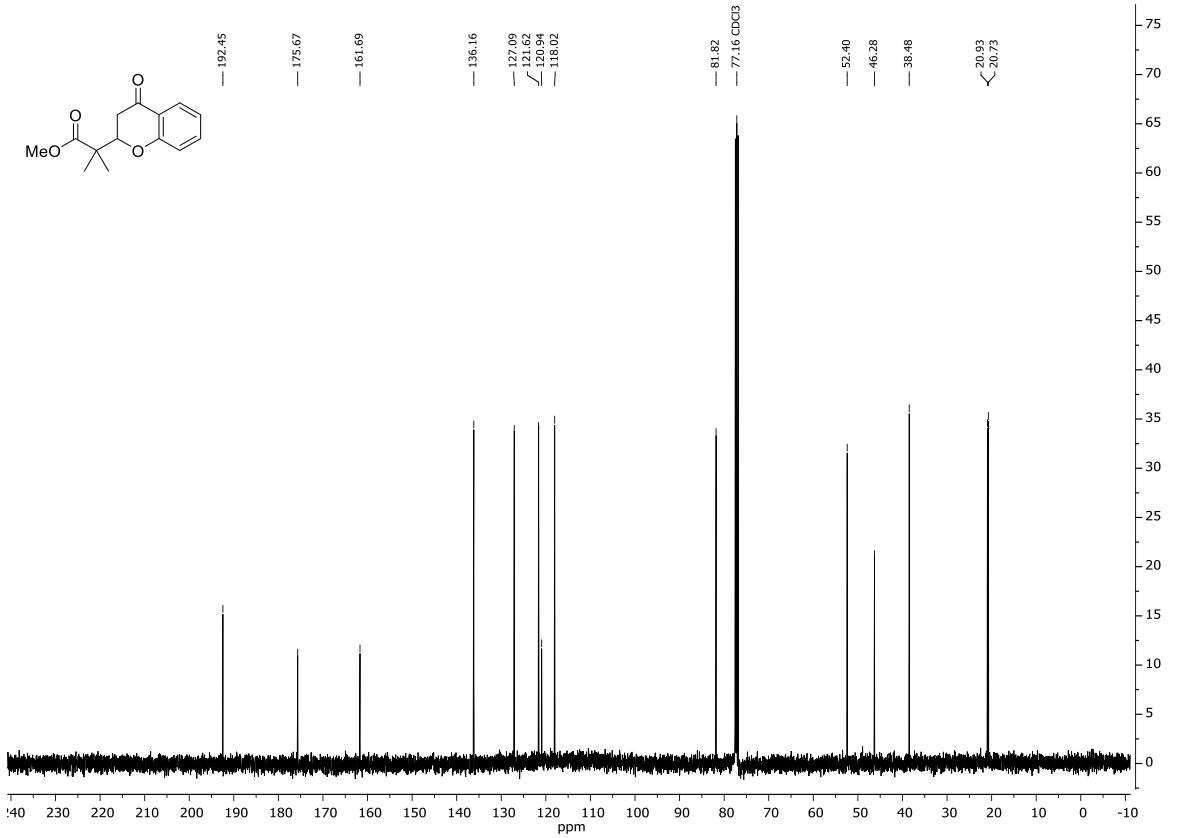
Methyl 2-methyl-2-(3-oxocyclopentyl)propanoate (**3m**)



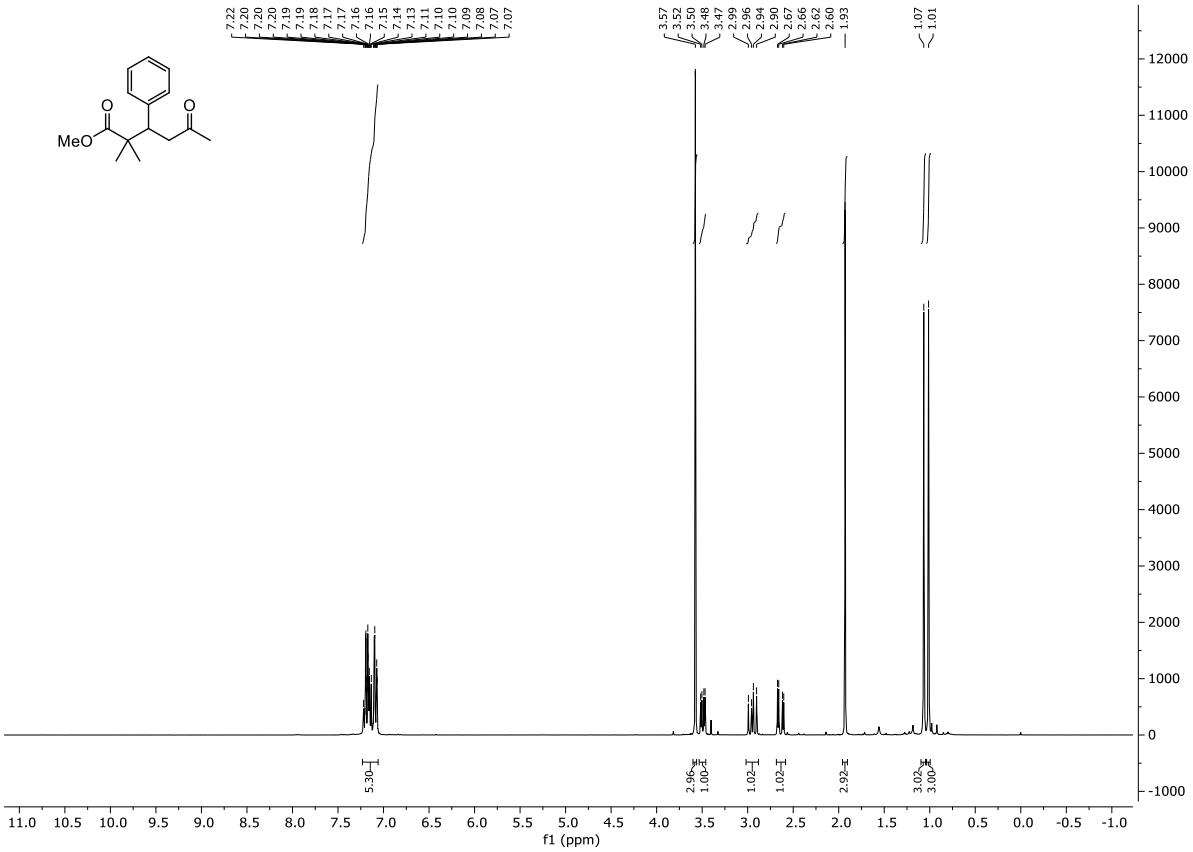



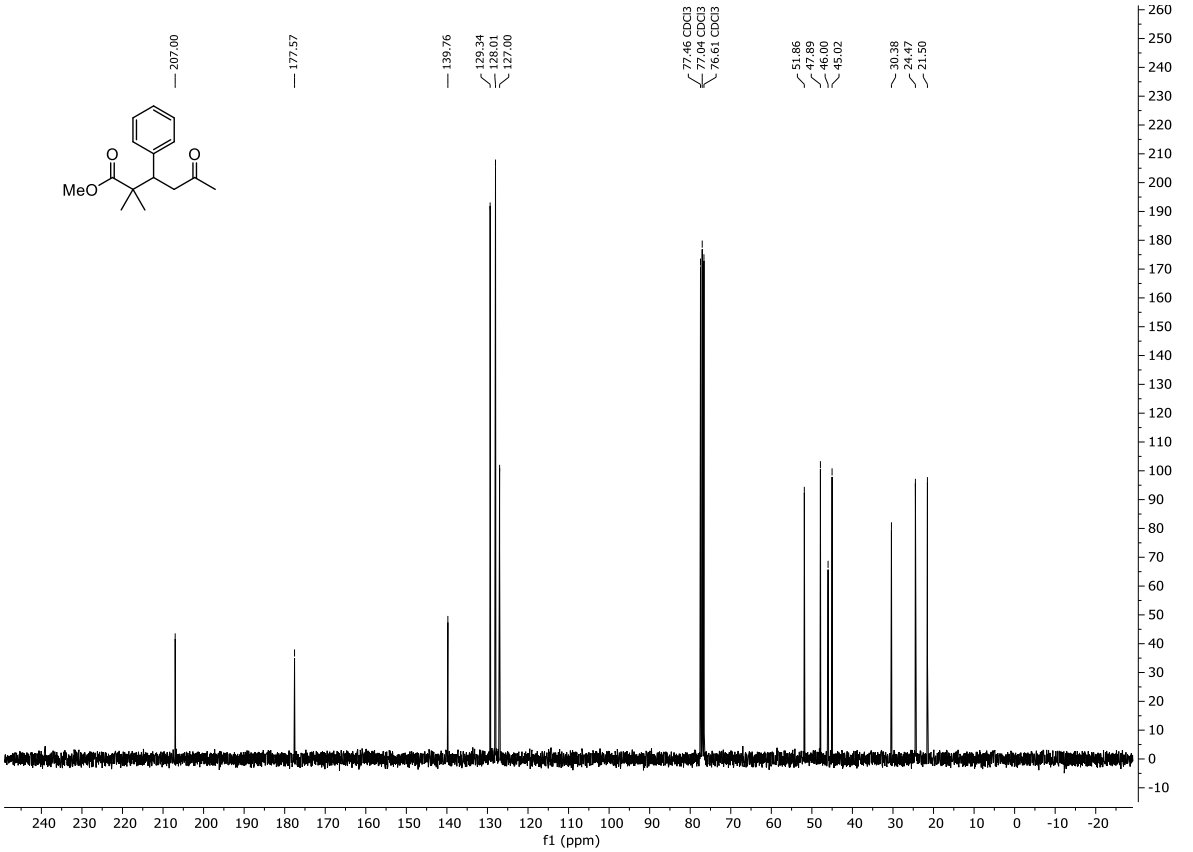
Methyl 2-methyl-2-(4-oxochroman-2-yl)propanoate (**3n**)



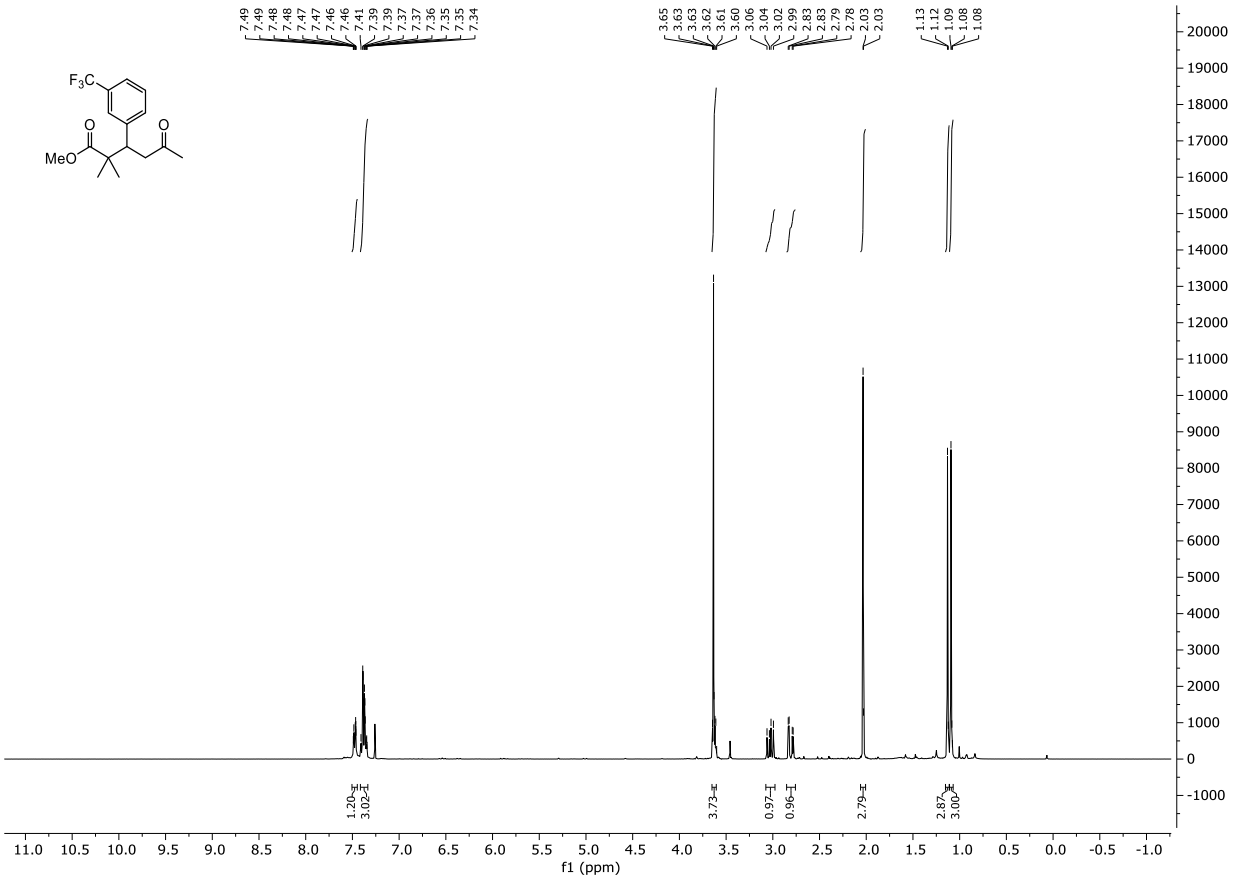



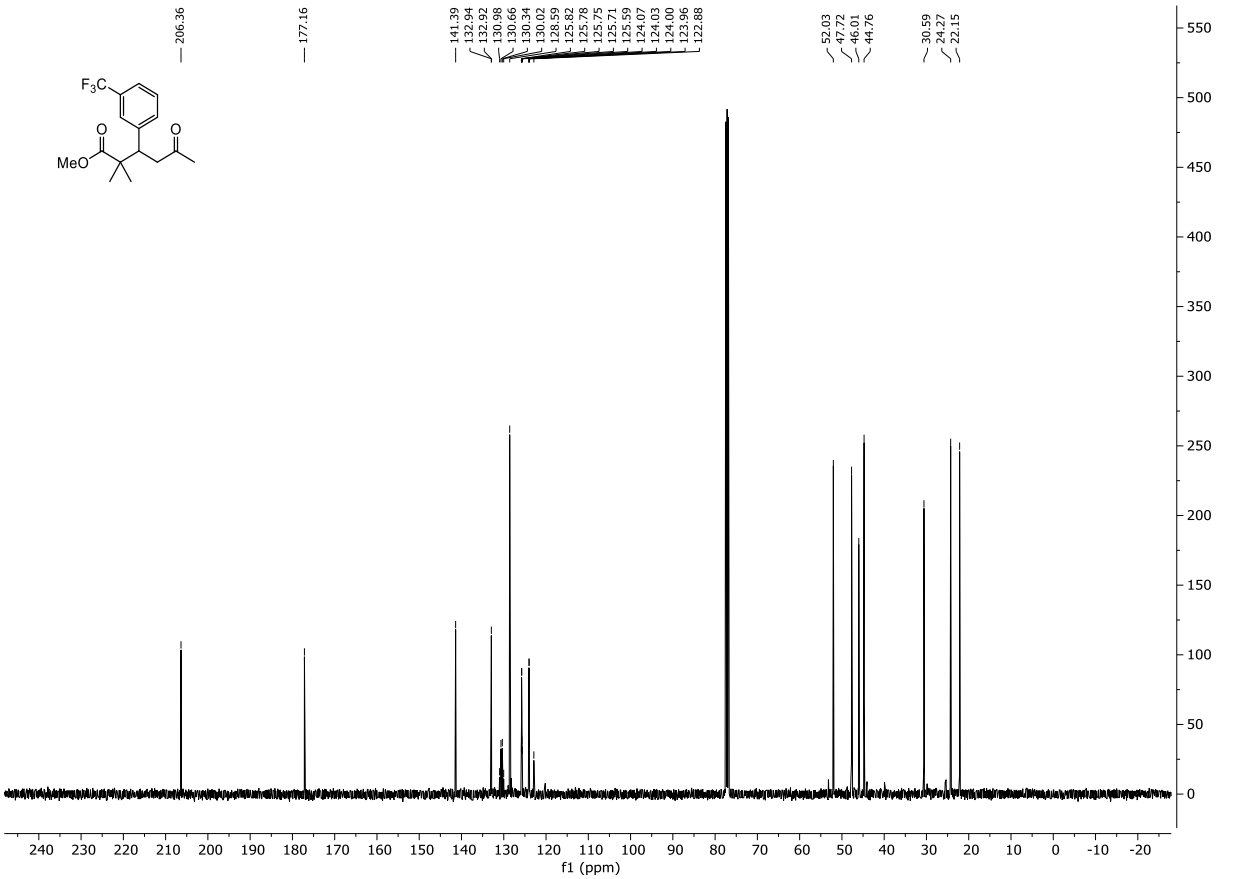
Methyl 2,2-dimethyl-5-oxo-3-phenylhexanoate (**3o**)

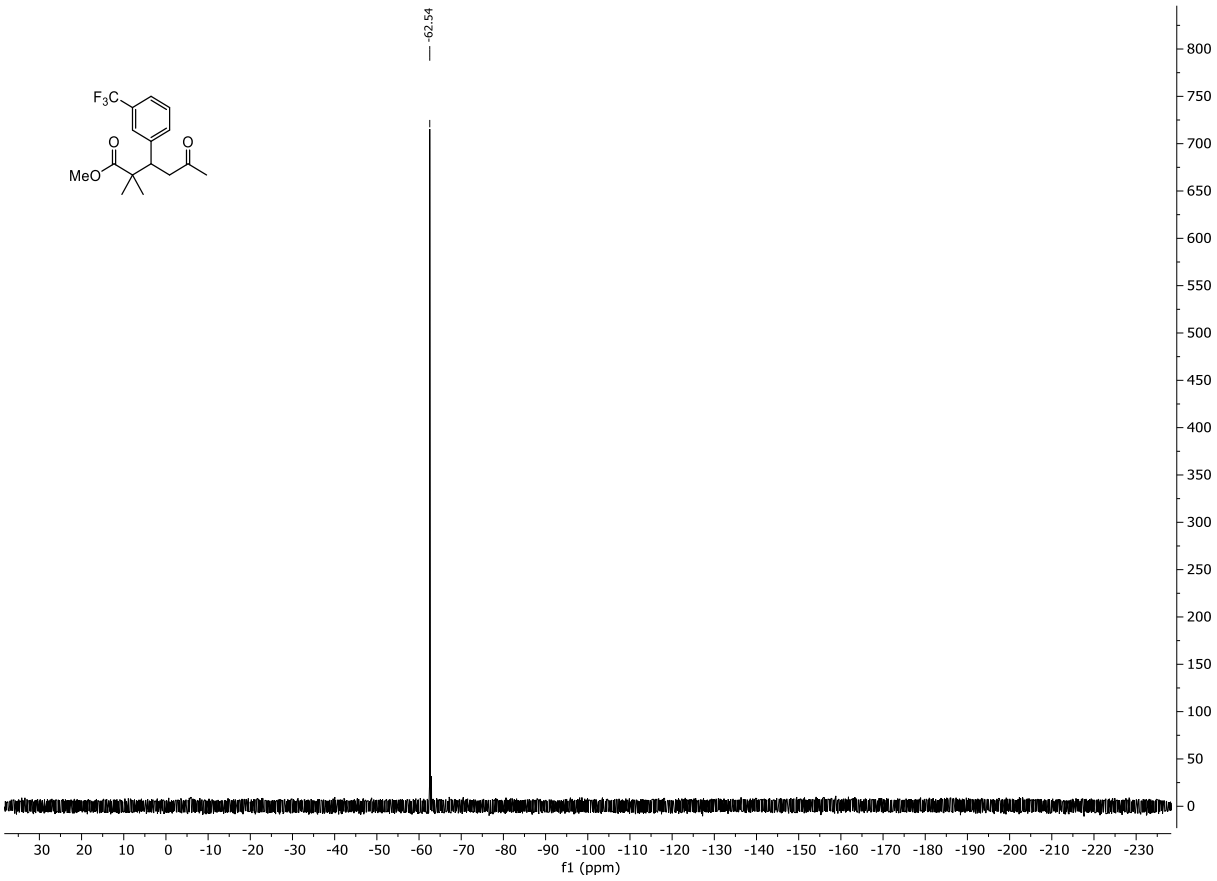


Methyl 2,2-dimethyl-5-oxo-3-(3-(trifluoromethyl)phenyl)hexanoate (**3p**)

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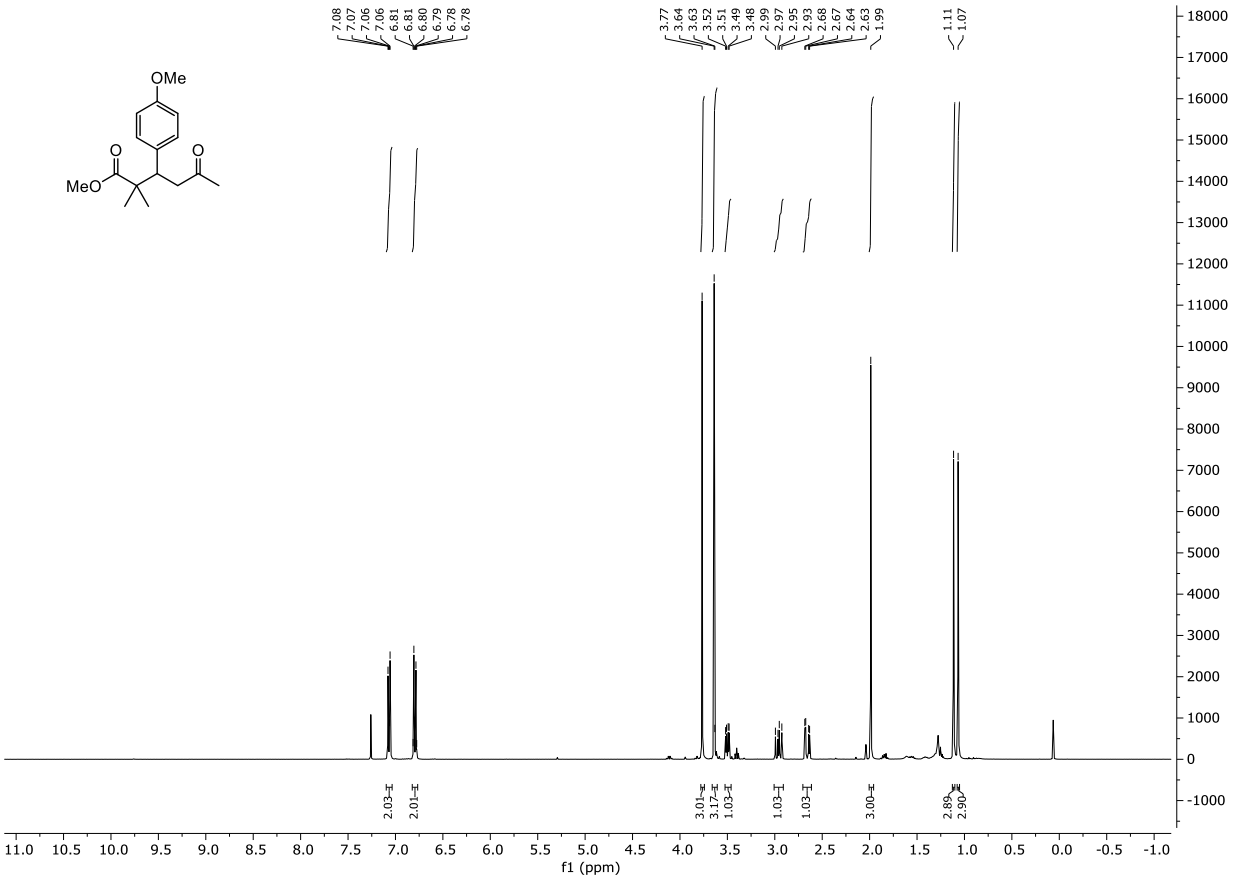
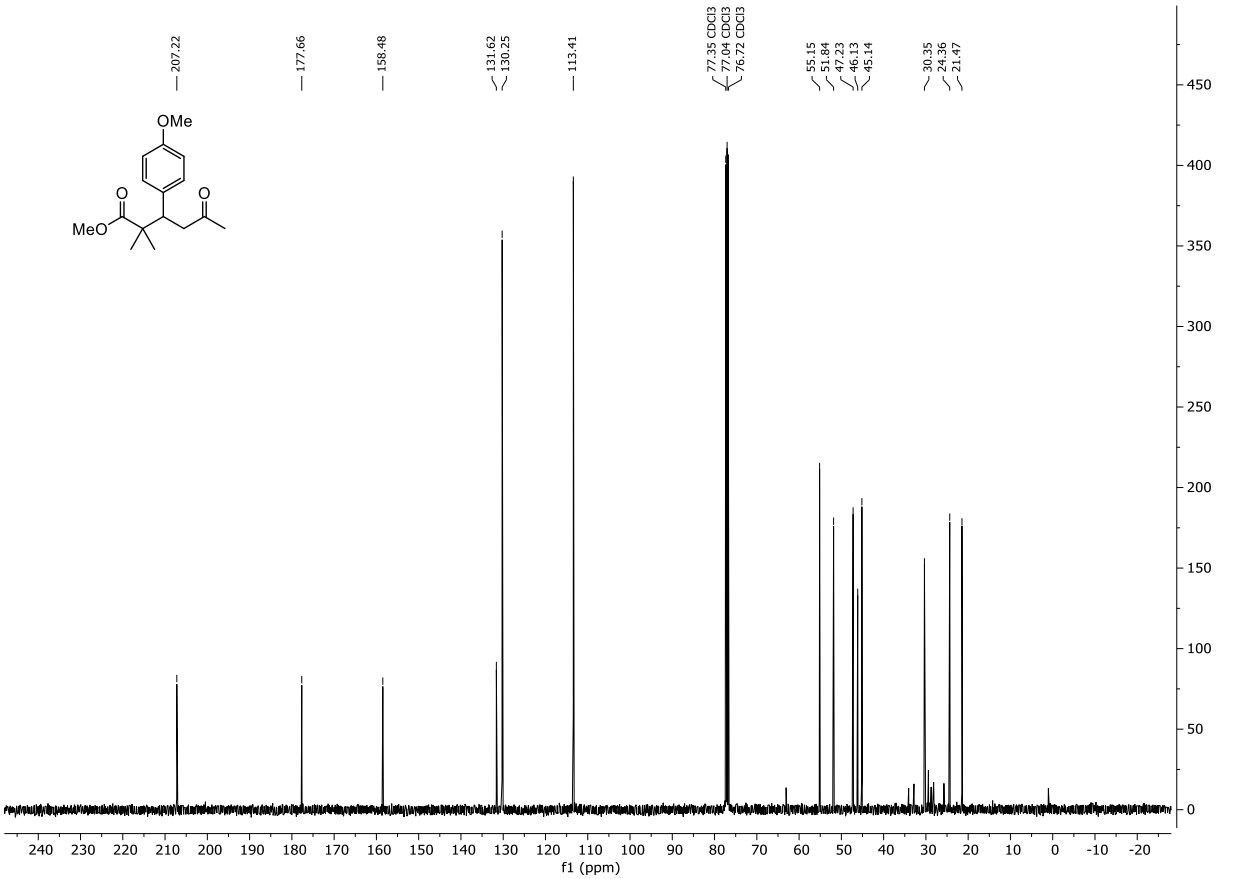
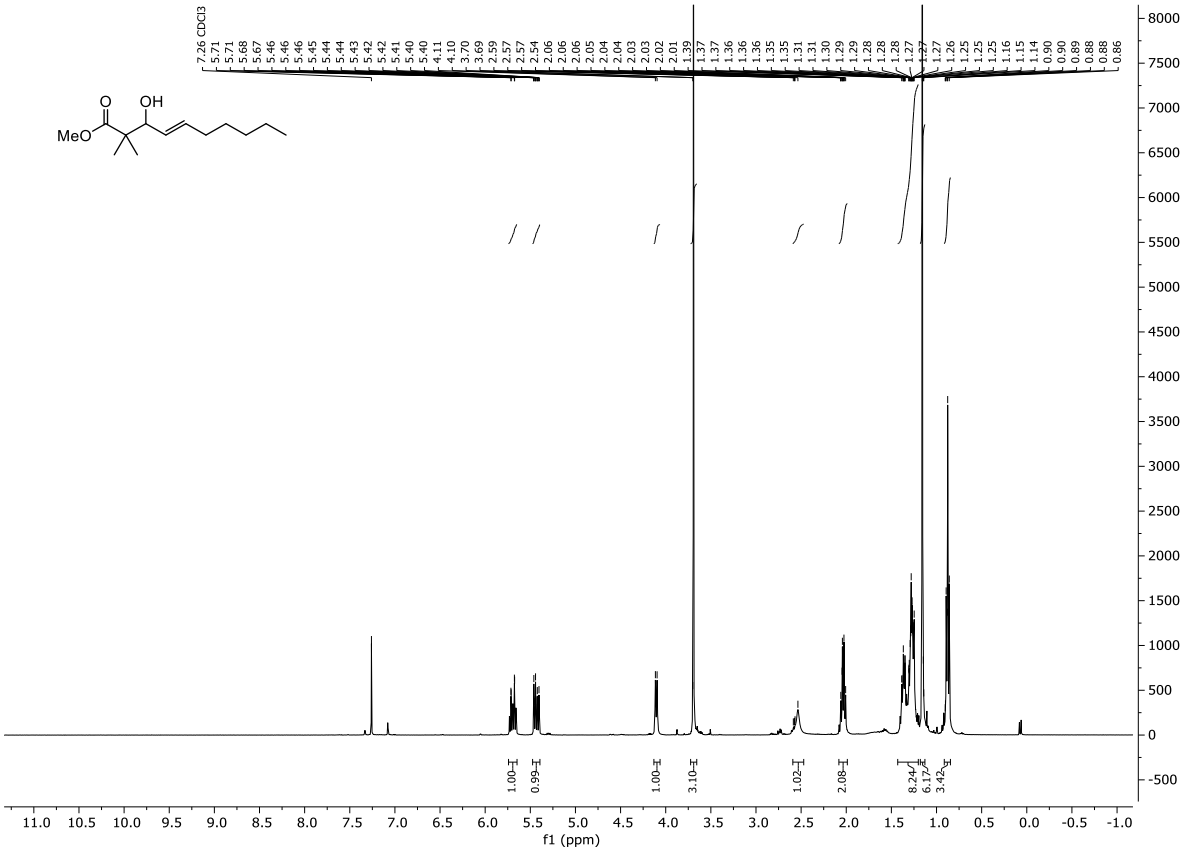
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
f1 (ppm)

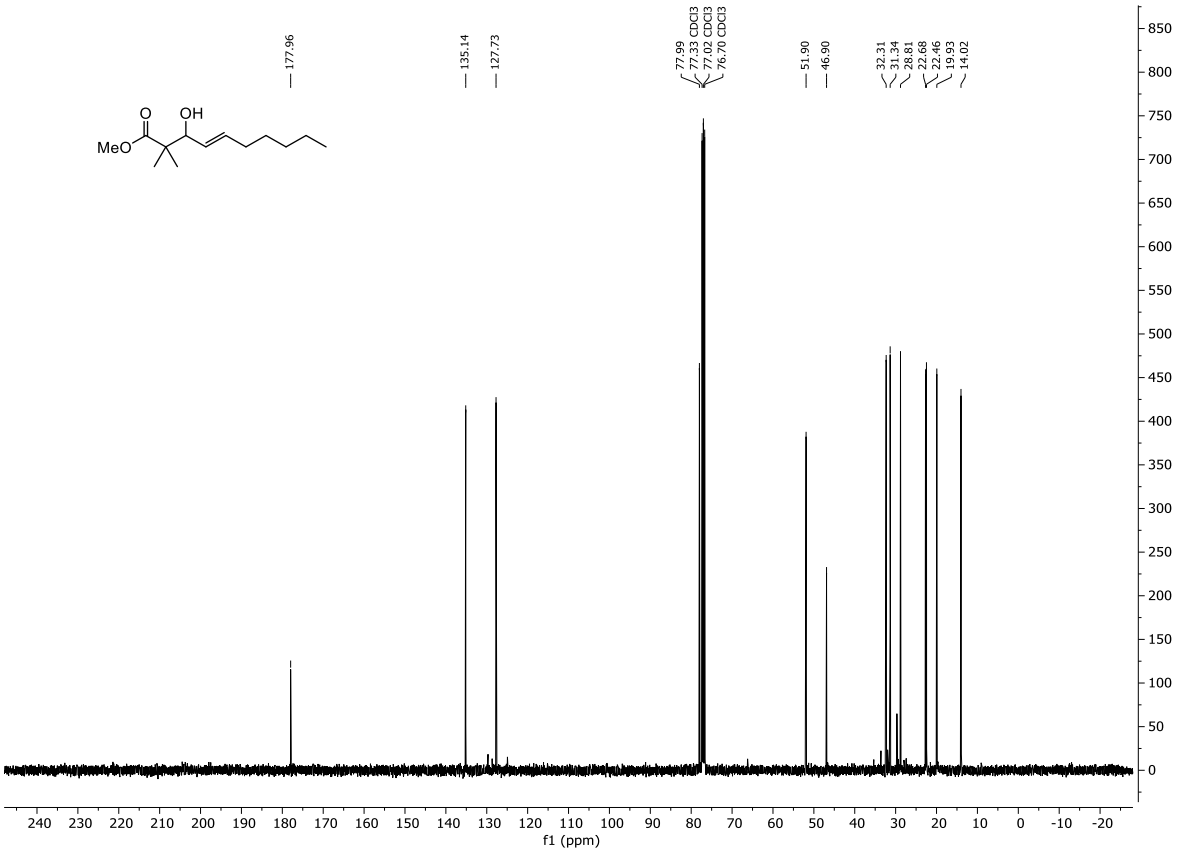
Methyl 3-(4-methoxyphenyl)-2,2-dimethyl-5-oxohexanoate (**3q**)



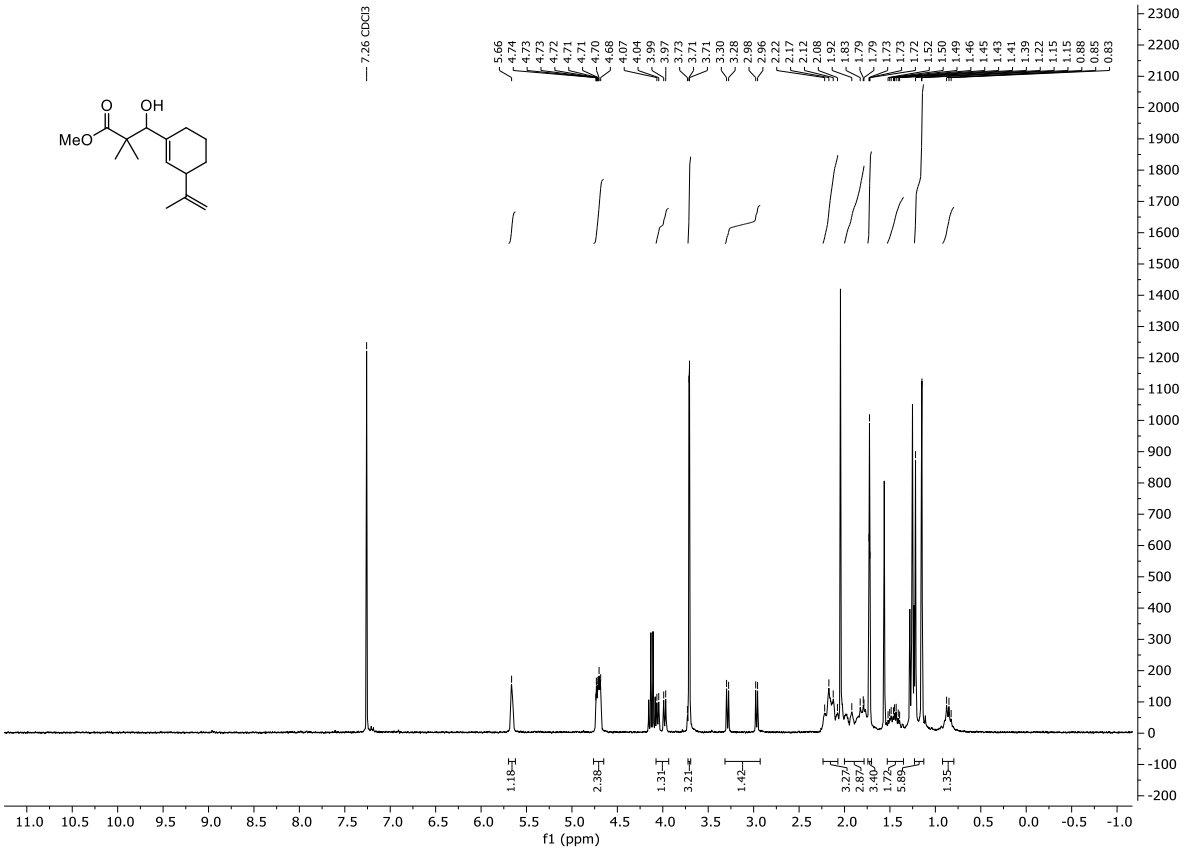



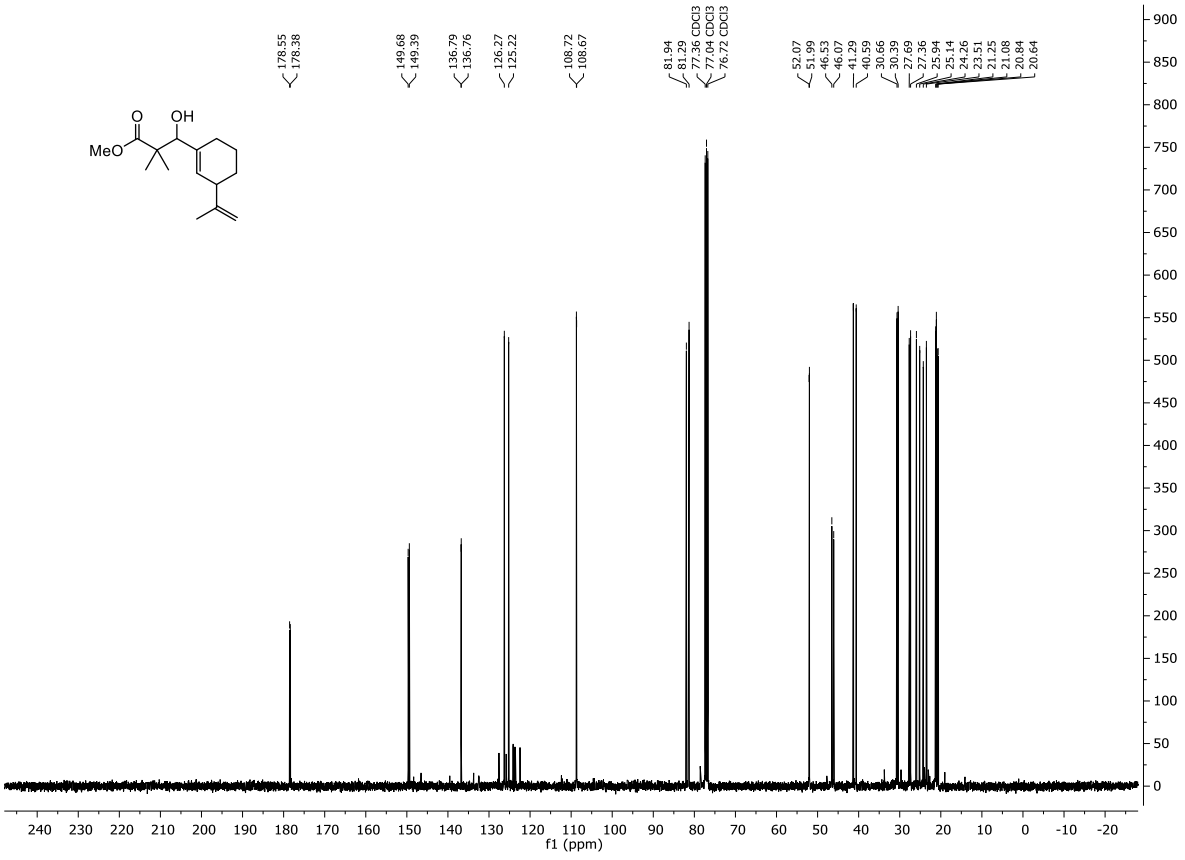
Methyl 3-hydroxy-2,2-dimethyldec-4-enoate (**4a**)



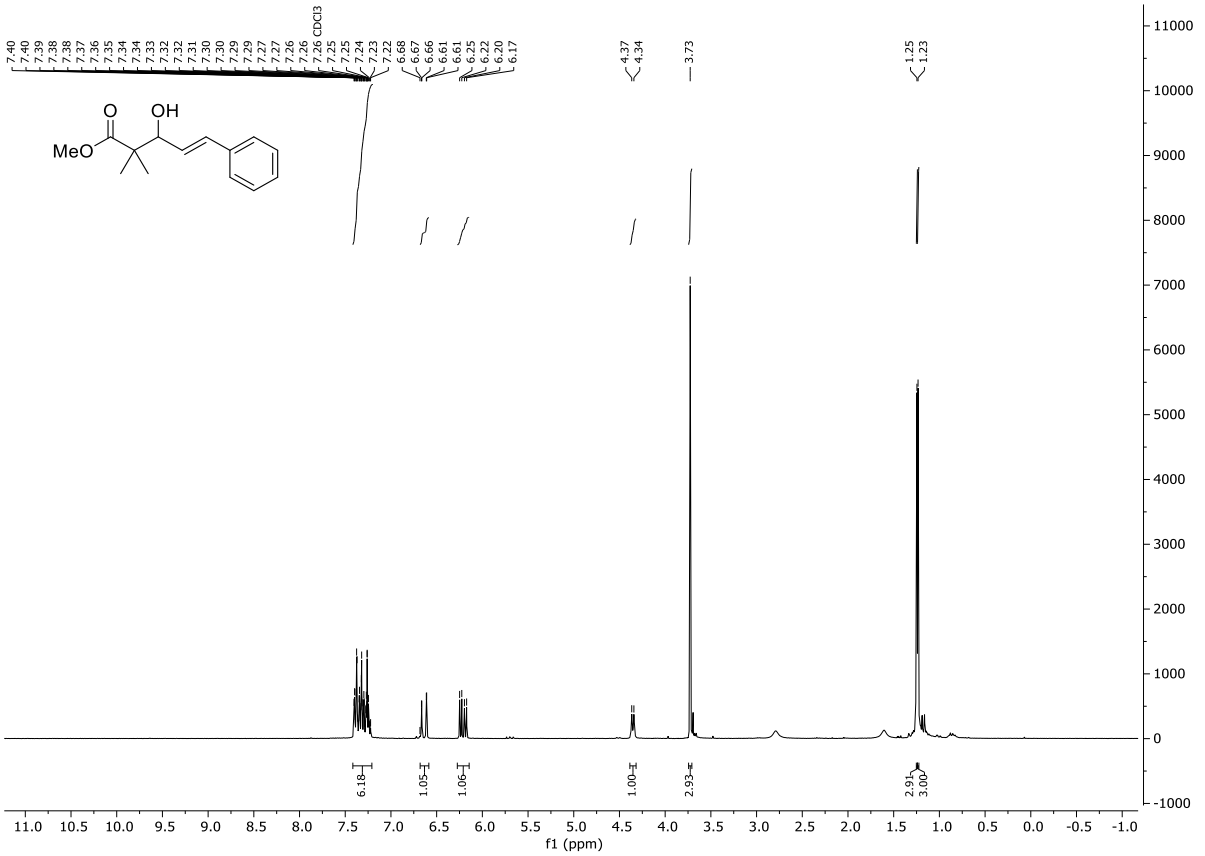



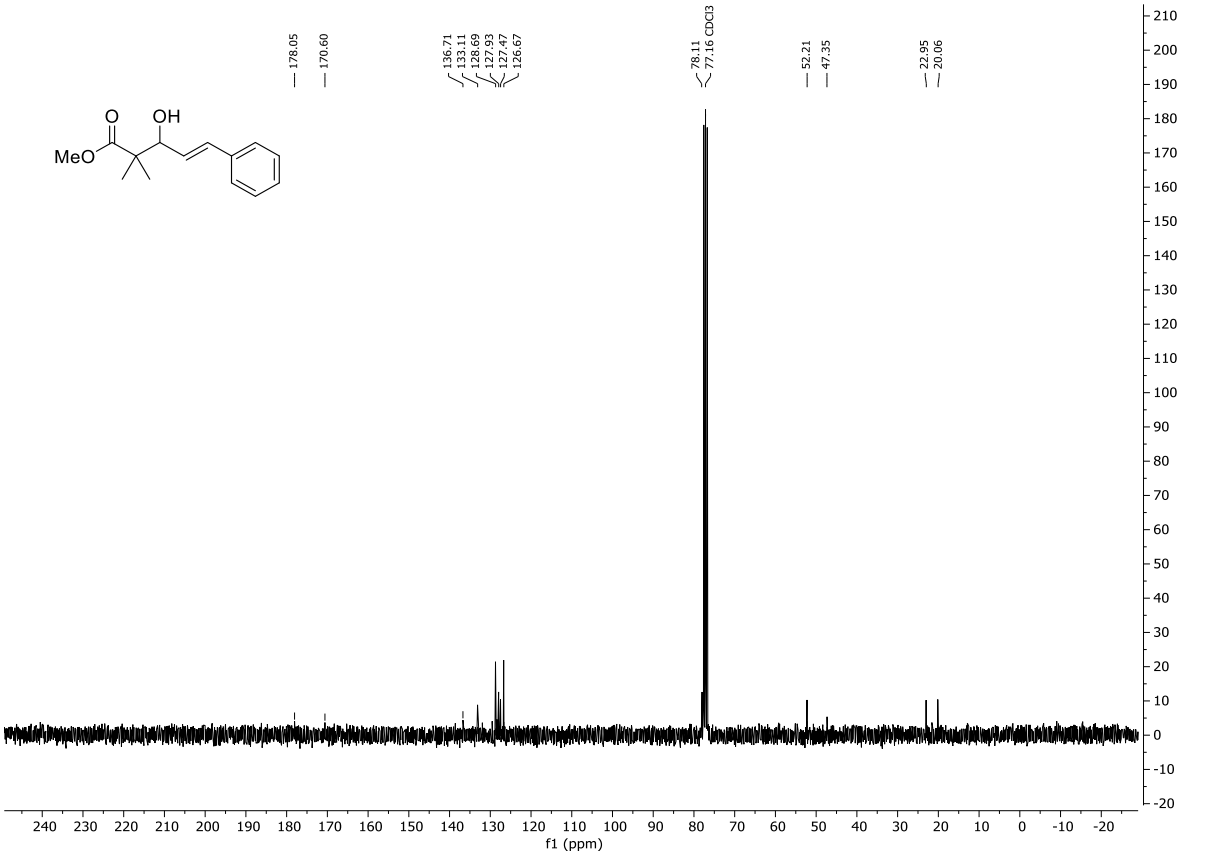
Methyl 3-hydroxy-2,2-dimethyl-3-(3-(prop-1-en-2-yl)cyclohex-1-en-1-yl)propanoate (**4b**)



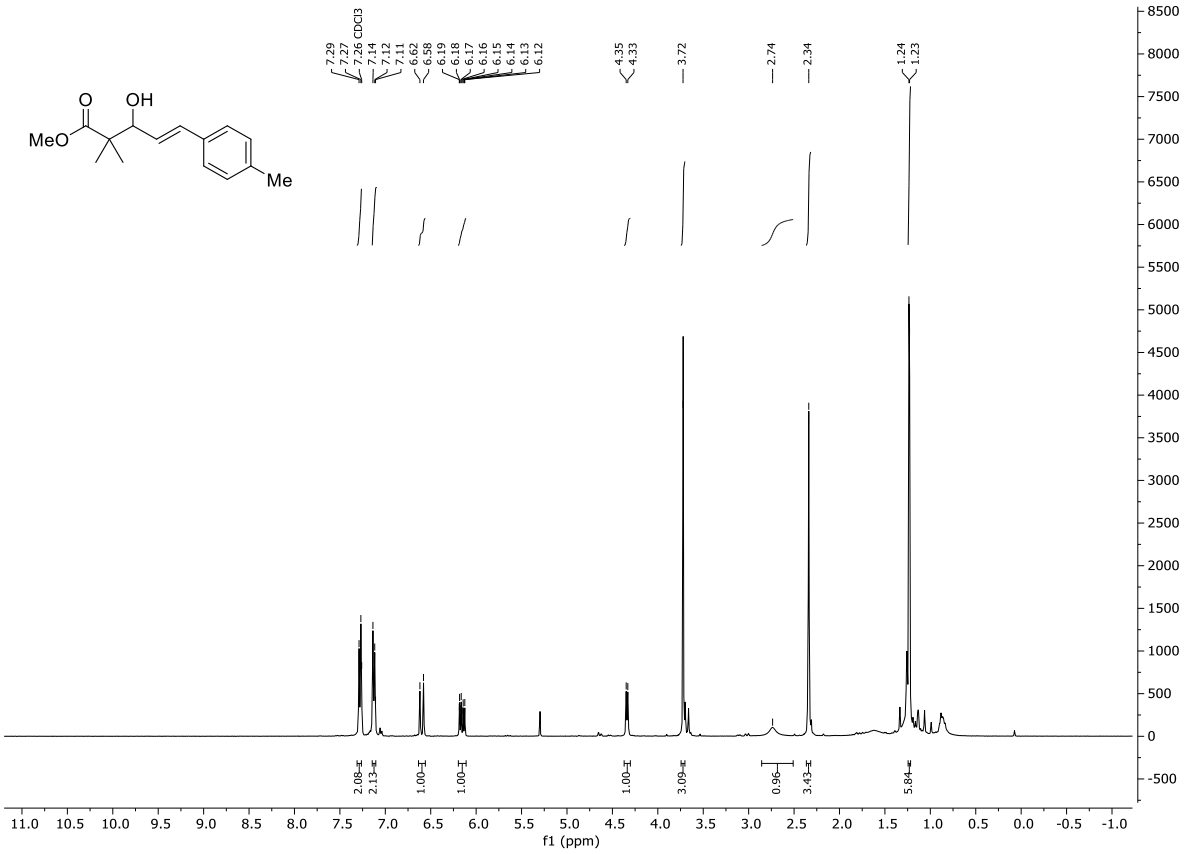



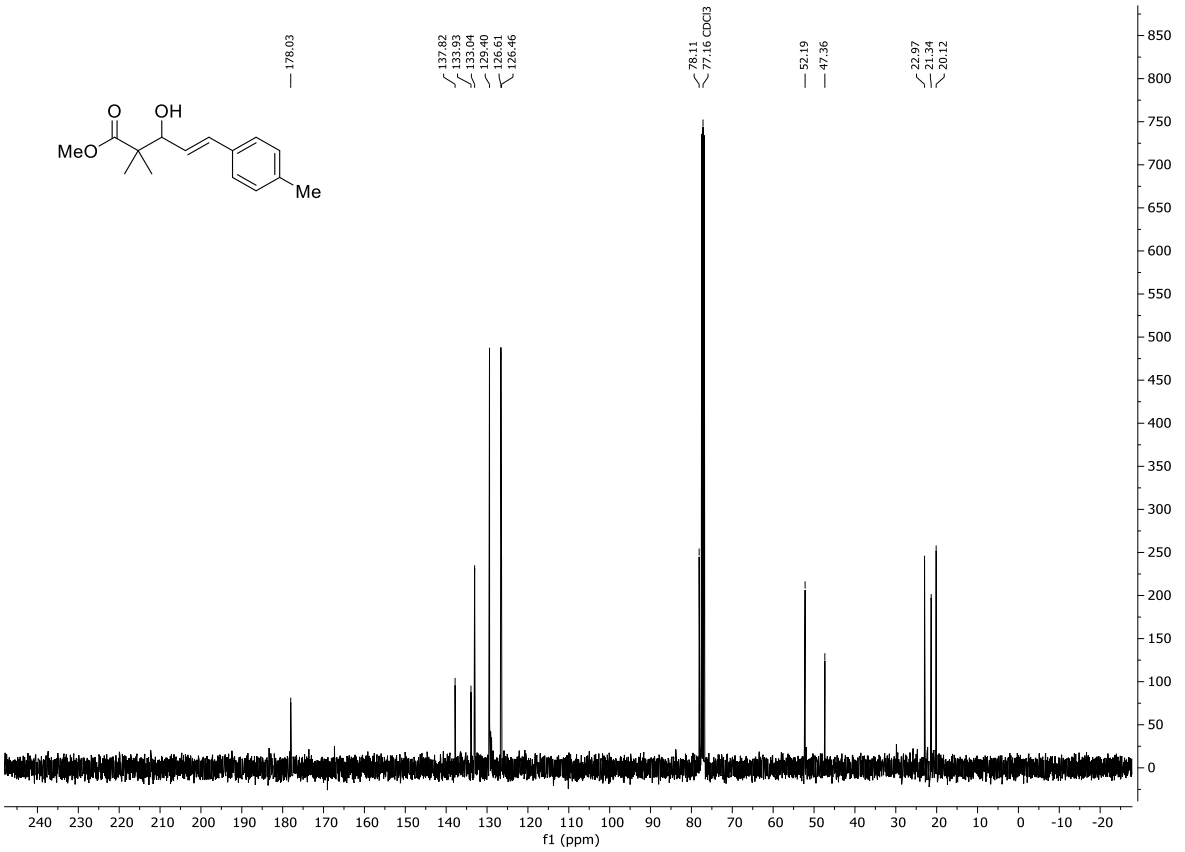
Methyl 3-hydroxy-2,2-dimethyl-5-phenylpent-4-enoate (**4c**)



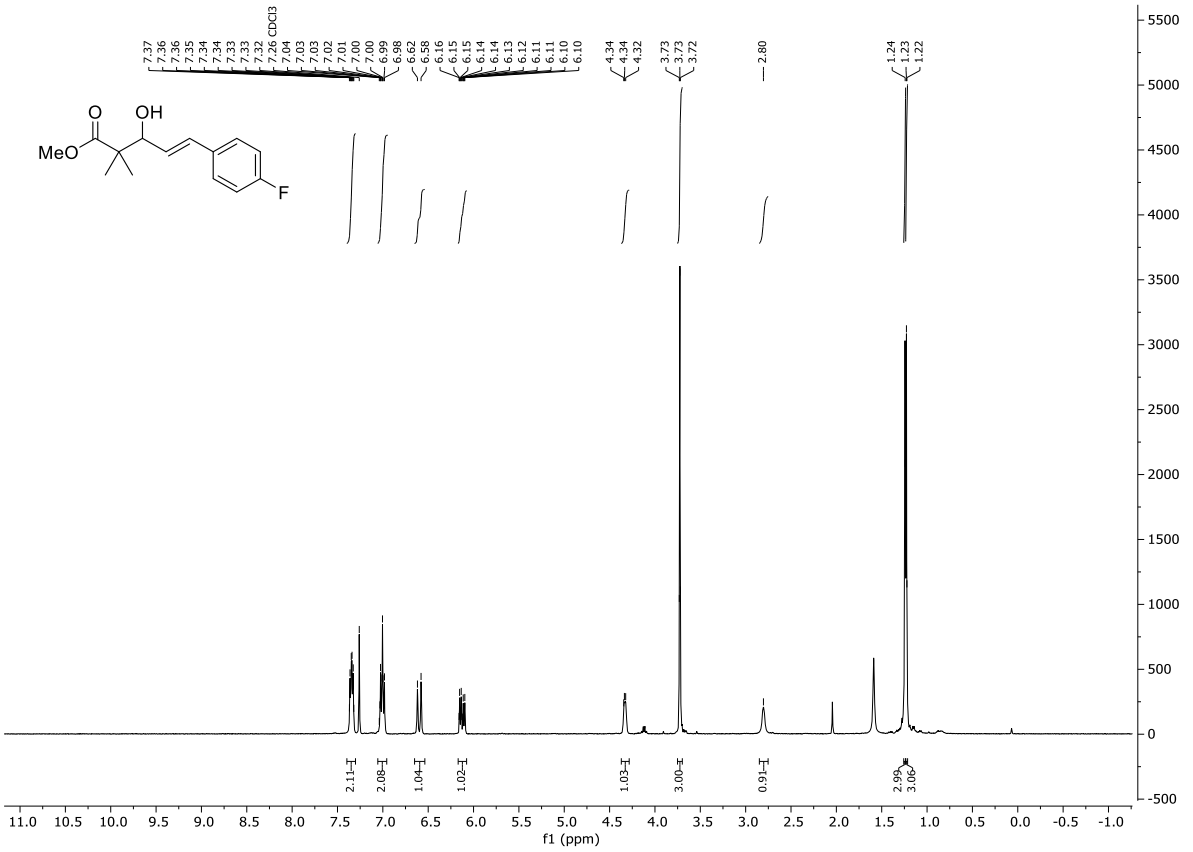



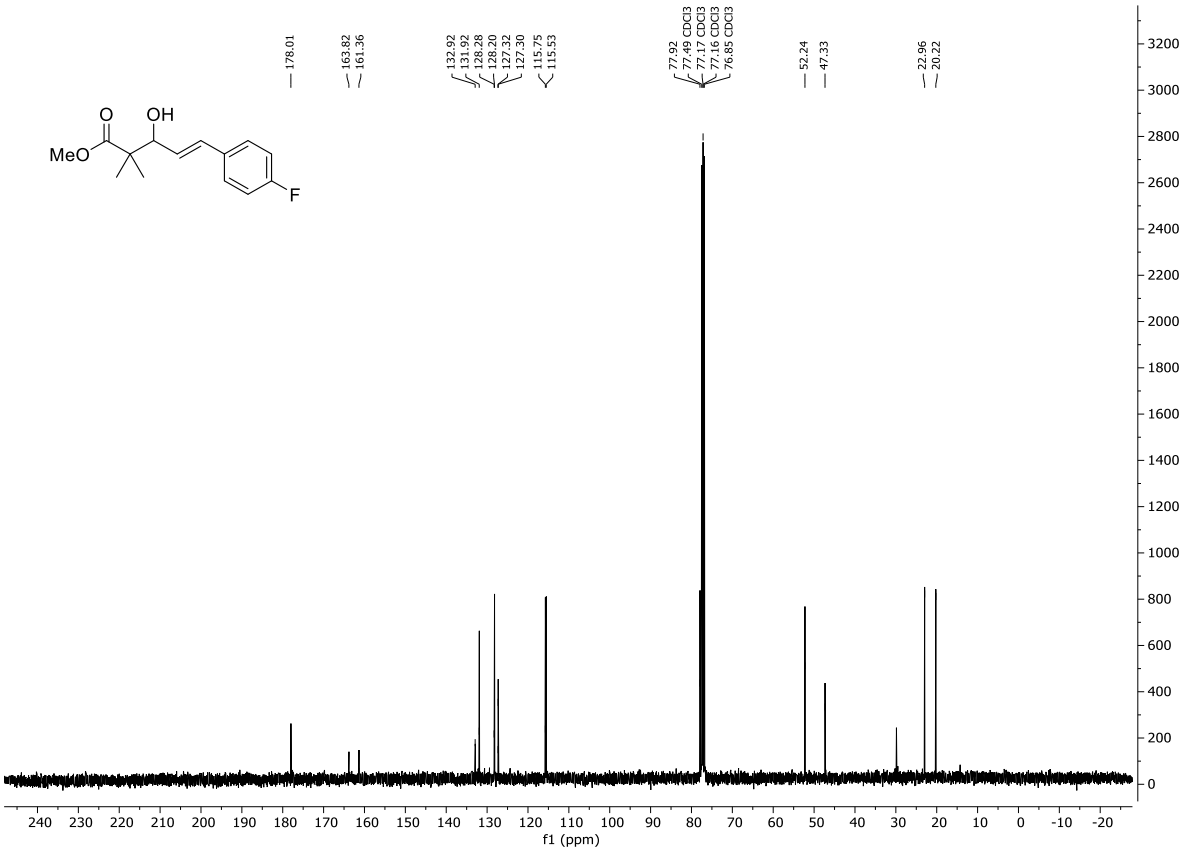
Methyl 3-hydroxy-2,2-dimethyl-5-(p-tolyl)pent-4-enoate (**4d**)



Methyl 5-(4-fluorophenyl)-3-hydroxy-2,2-dimethylpent-4-enoate (**4e**)

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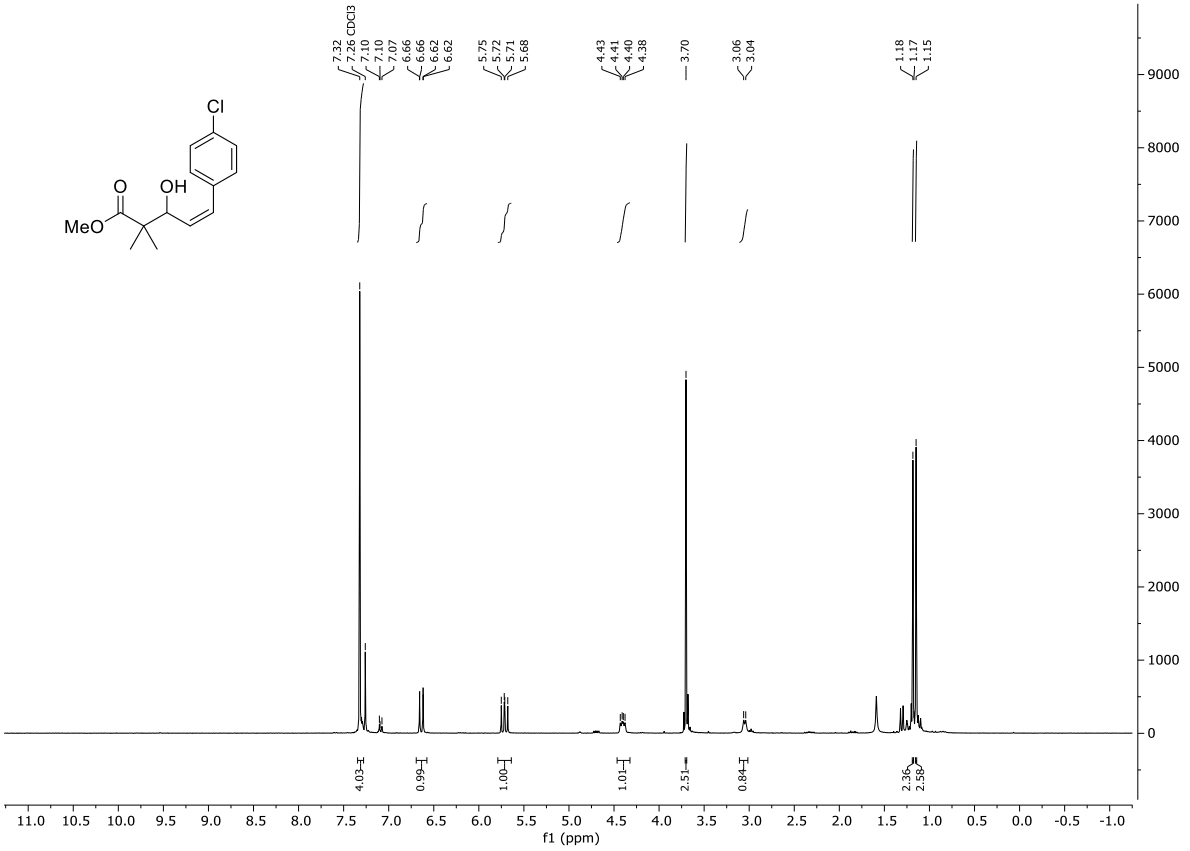
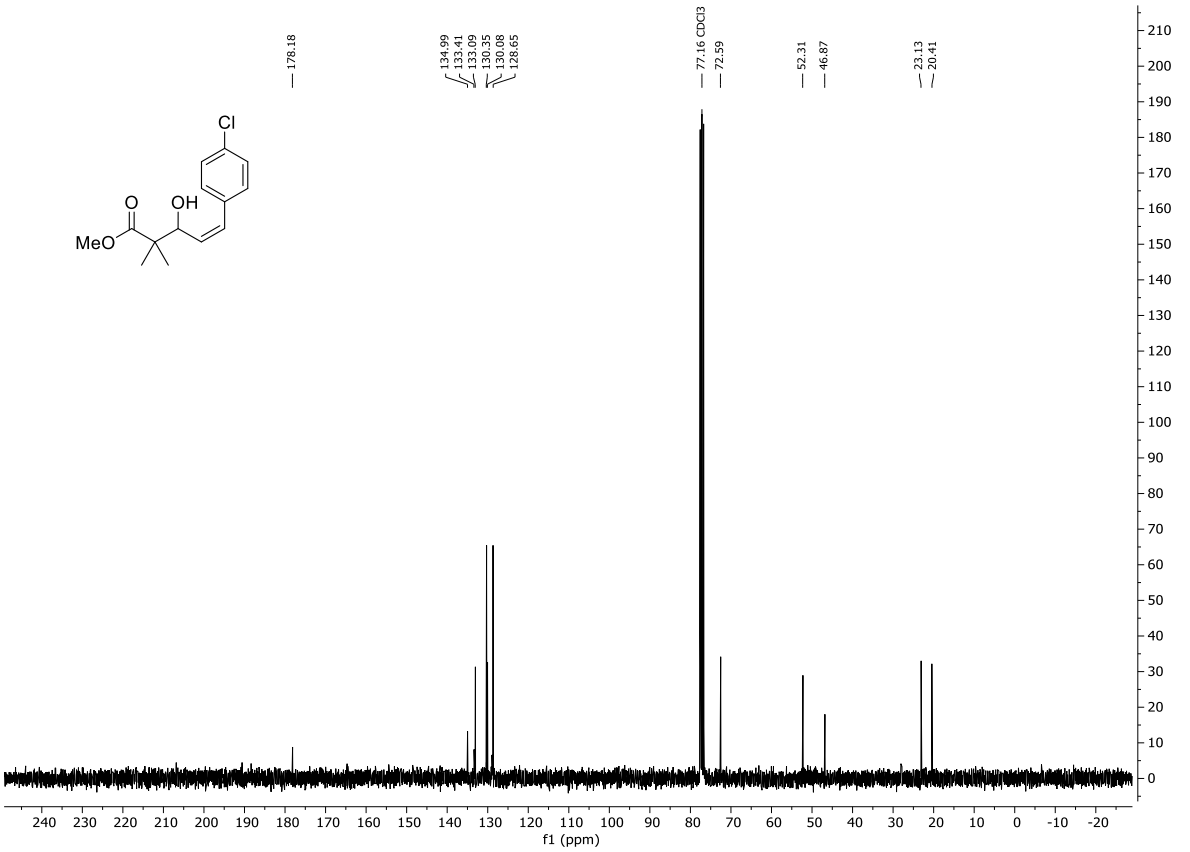
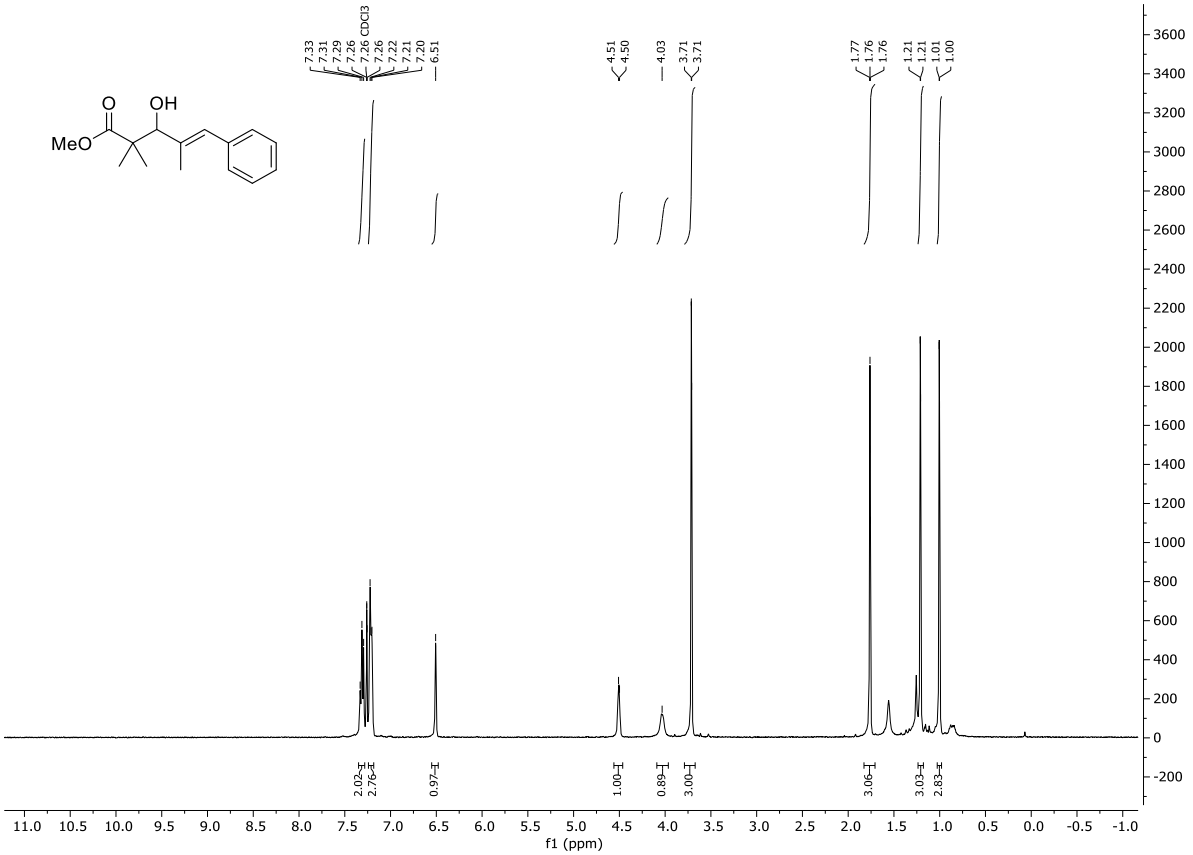
-500
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
f1 (ppm)

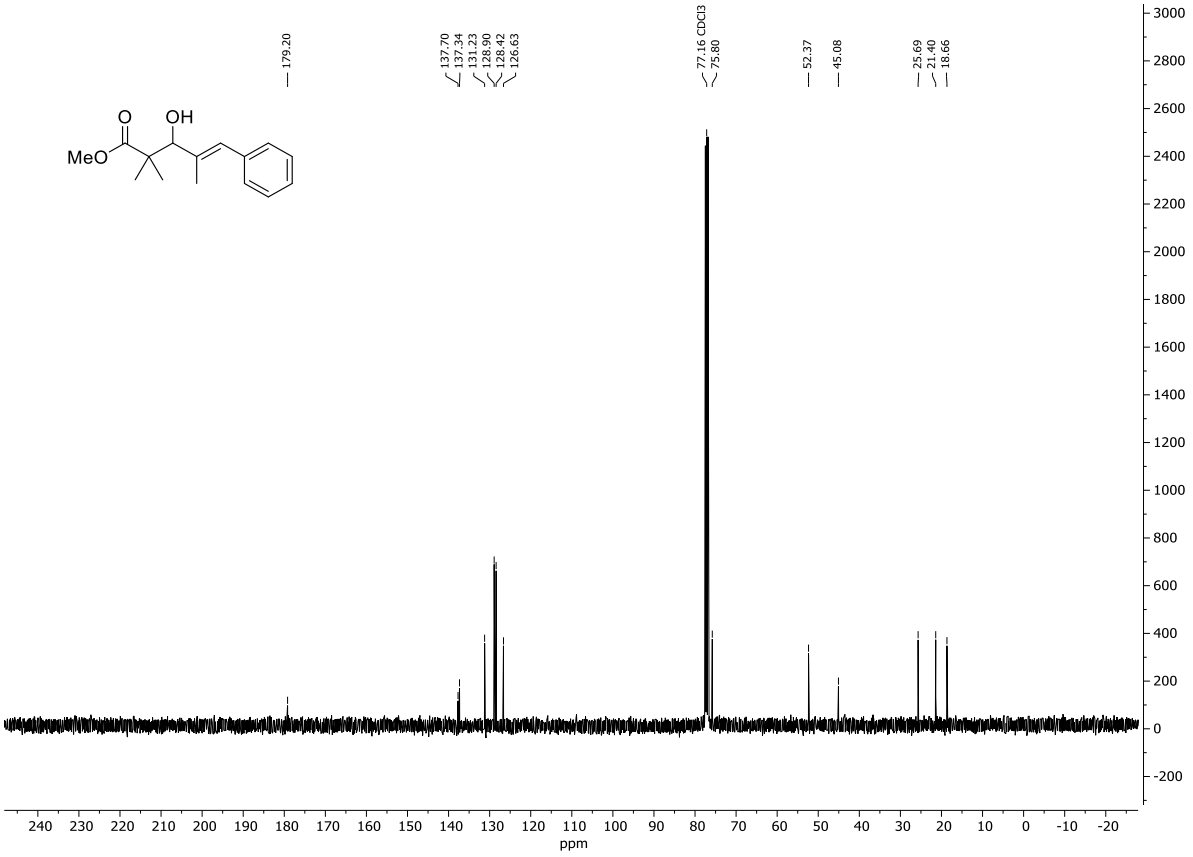
Methyl 5-(4-chlorophenyl)-3-hydroxy-2,2-dimethylpent-4-enoate (**4f**)



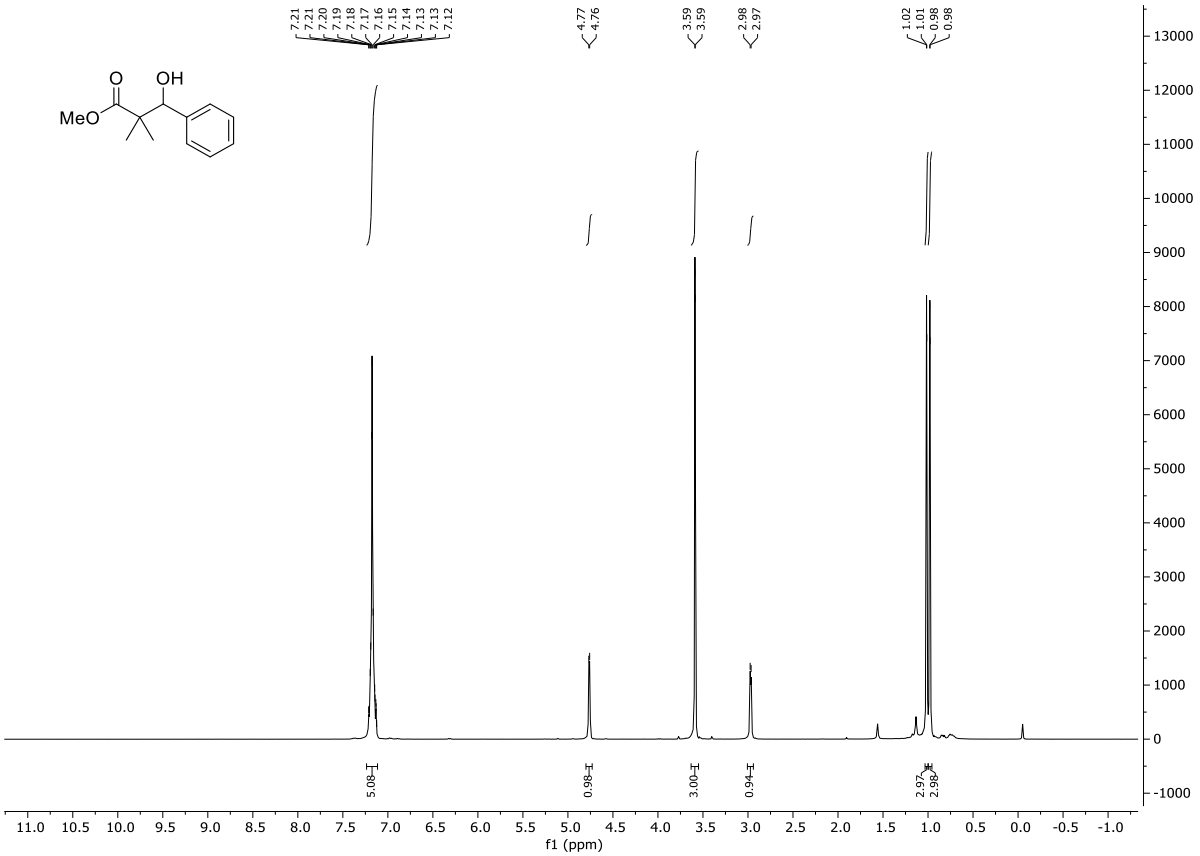



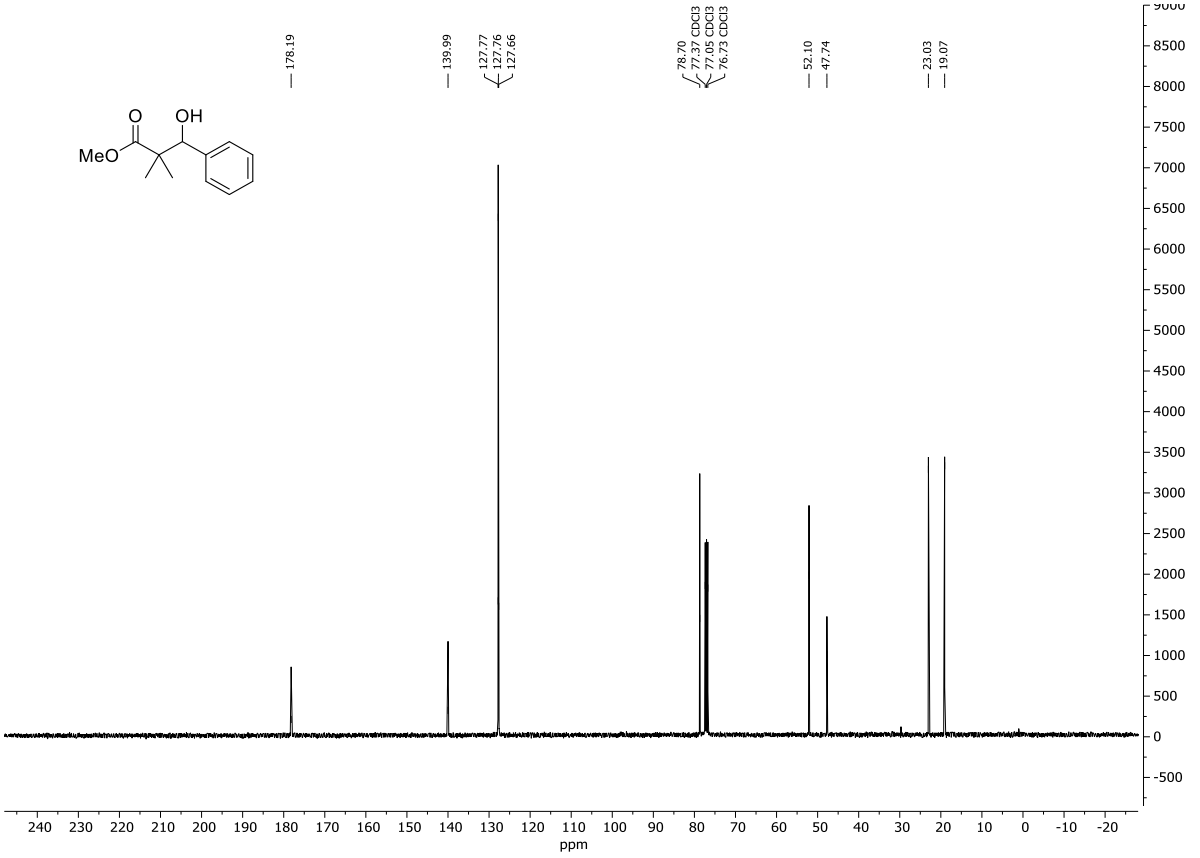
Methyl 3-hydroxy-2,2,4-trimethyl-5-phenylpent-4-enoate (**4g**)



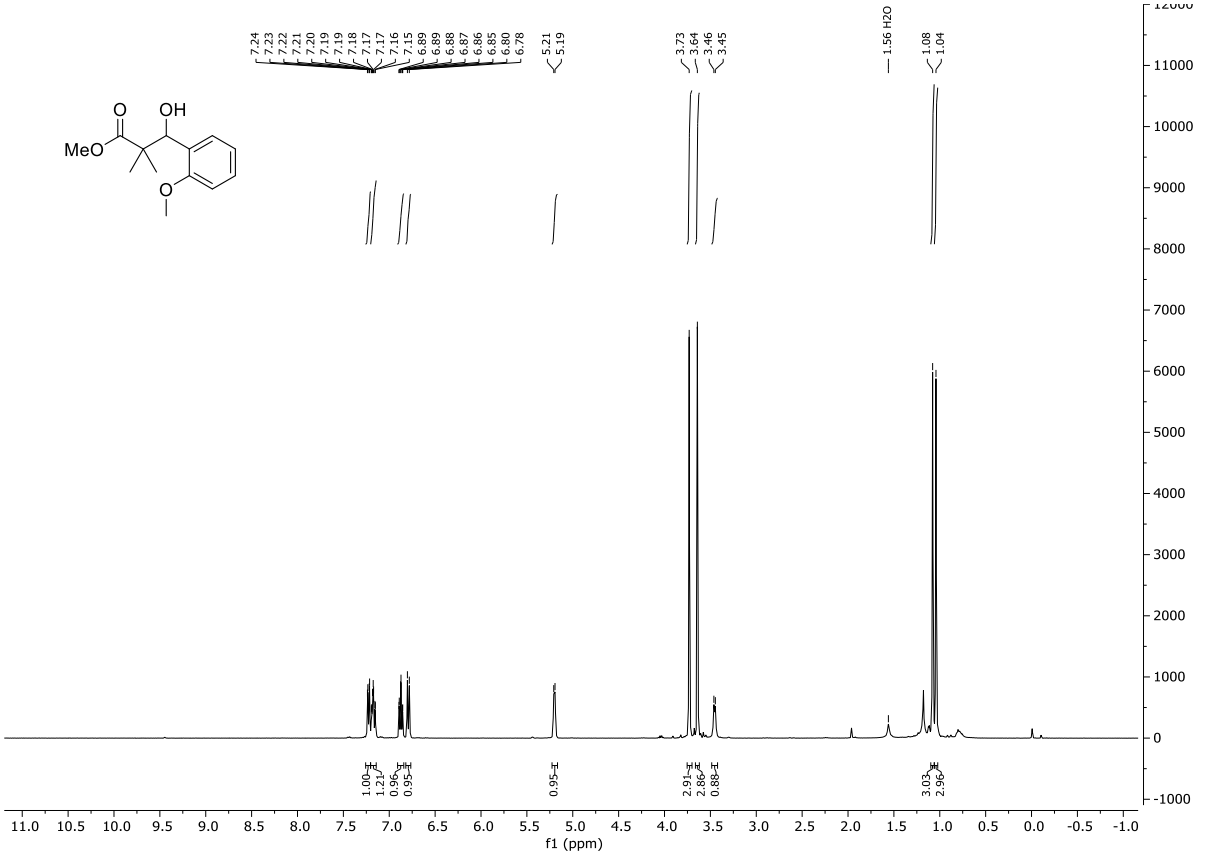



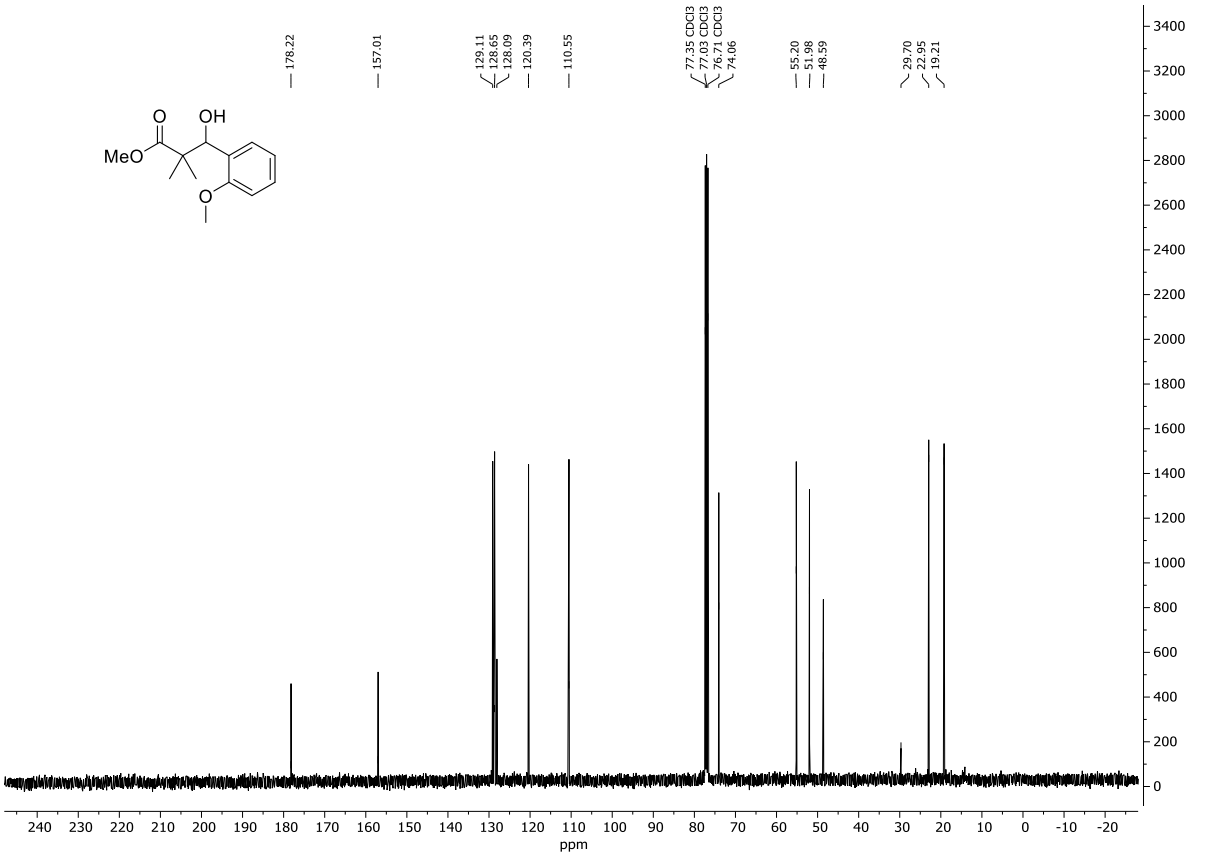
Methyl 3-hydroxy-2,2-dimethyl-3-phenylpropanoate (**4h**)



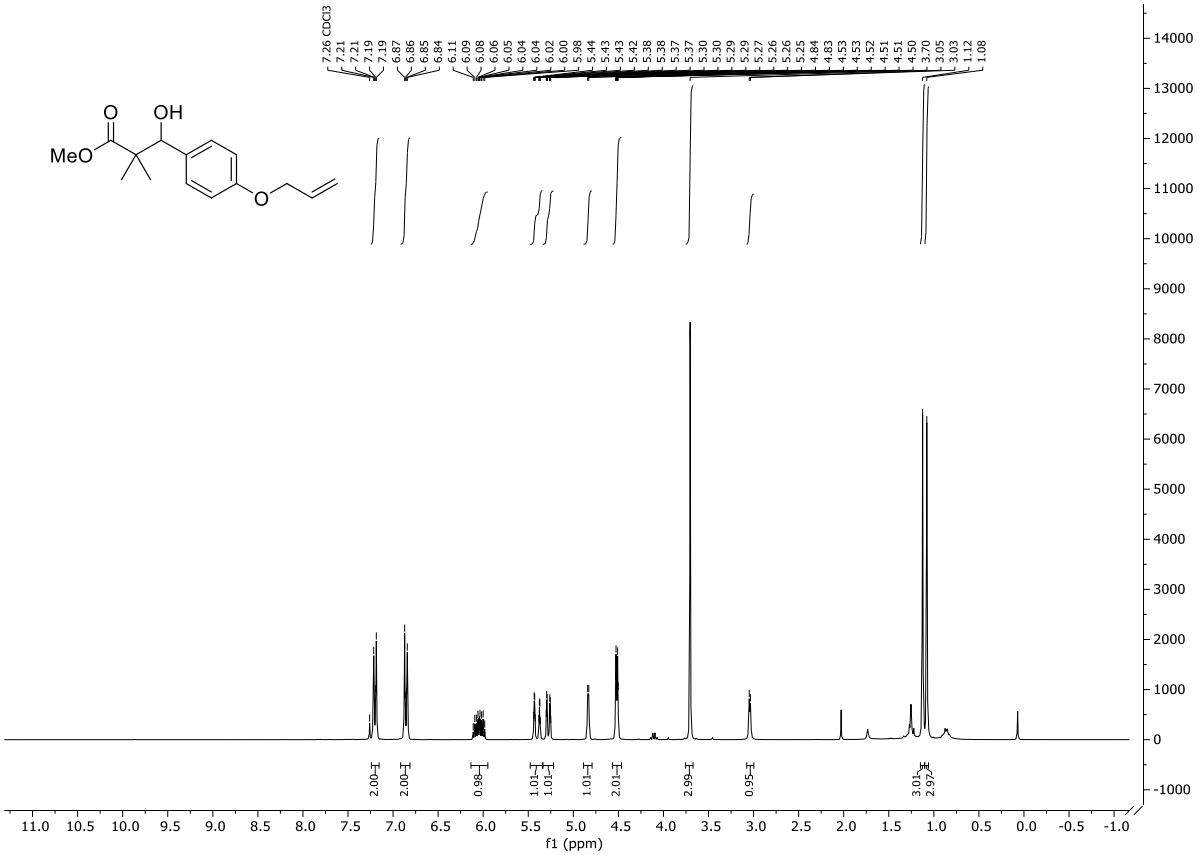



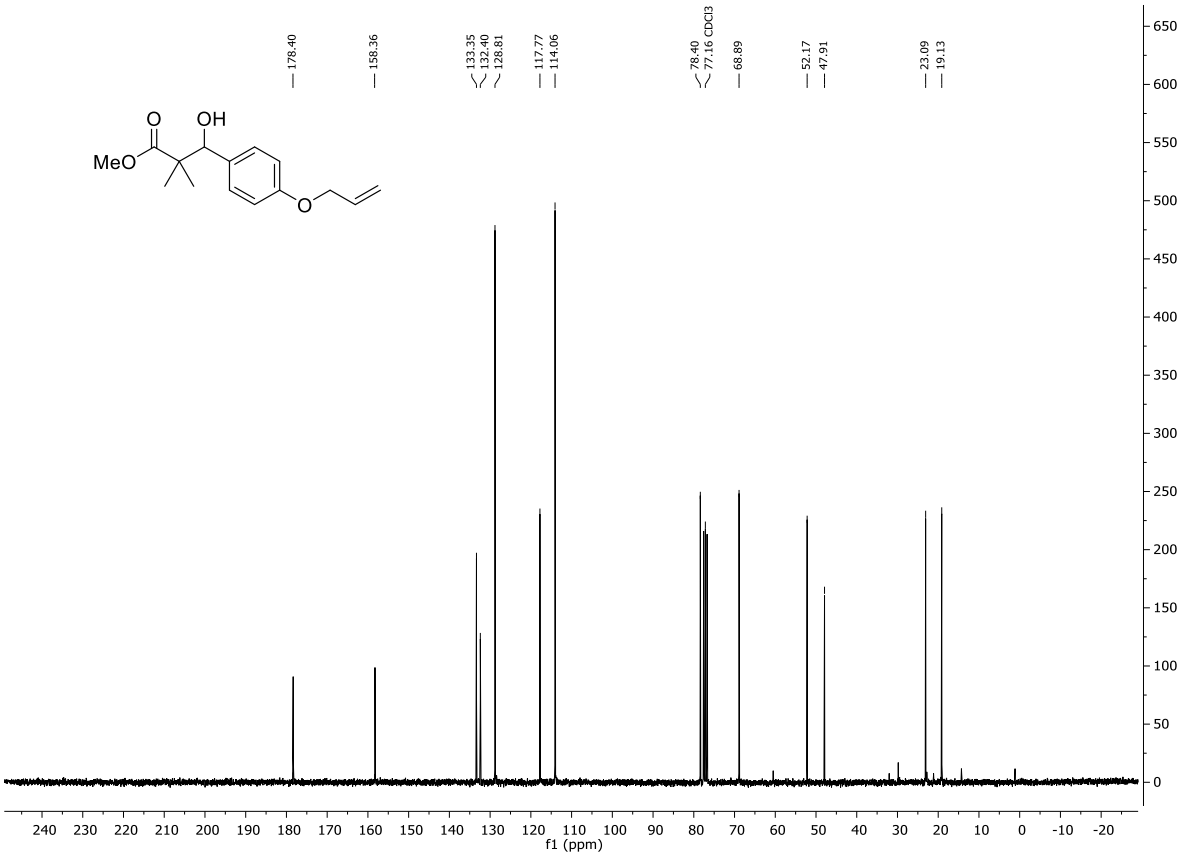
Methyl 3-hydroxy-3-(2-methoxyphenyl)-2,2-dimethylpropanoate (**4i**)



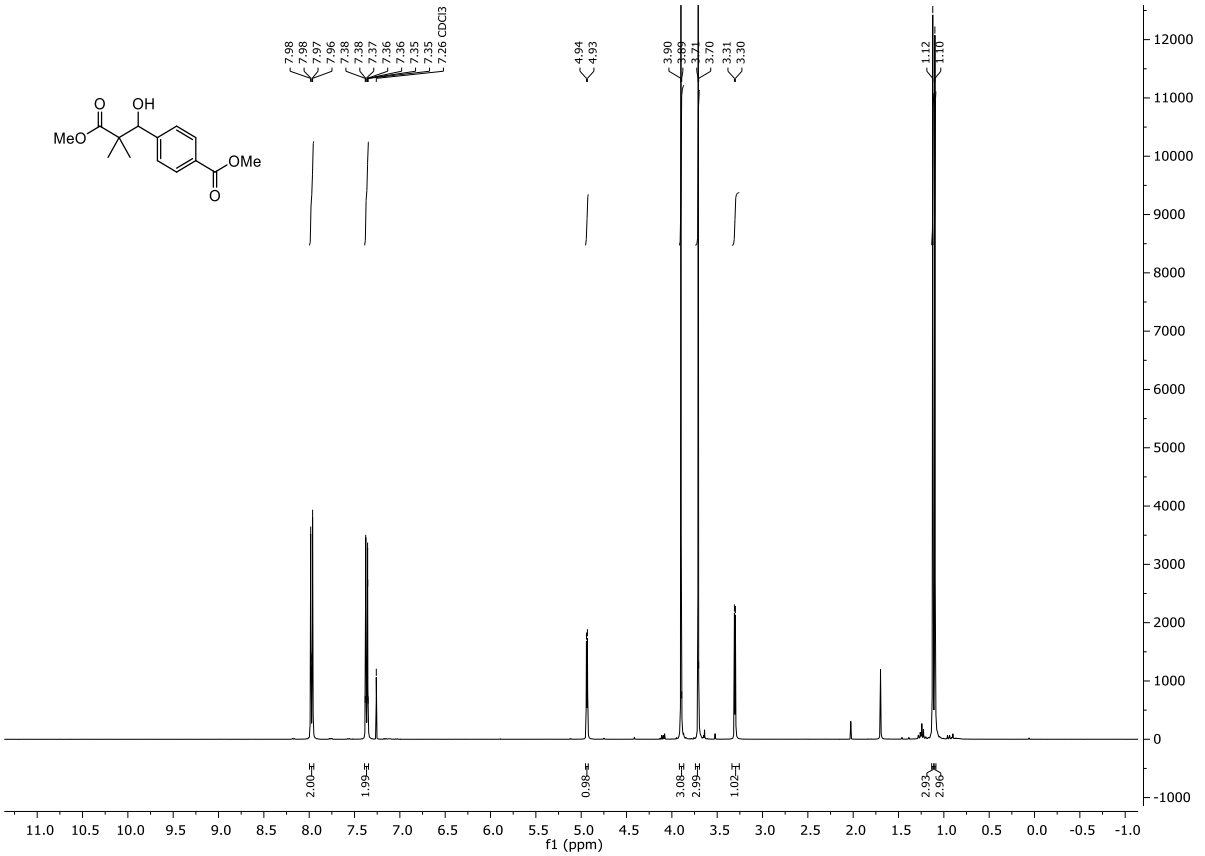



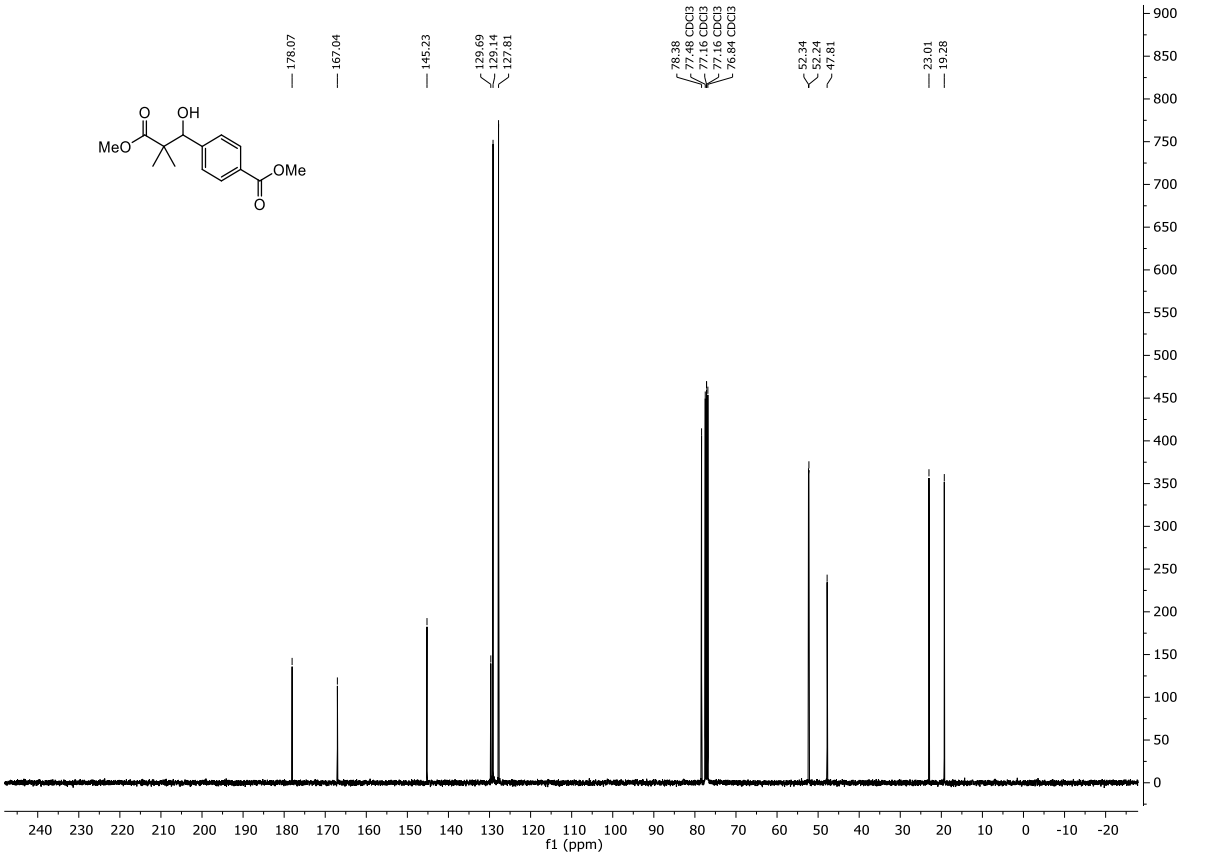
Methyl 3-(4-(allyloxy)phenyl)-3-hydroxy-2,2-dimethylpropanoate (**4k**)



Methyl 4-(1-hydroxy-3-methoxy-2,2-dimethyl-3-oxopropyl)benzoate (**4l**)



Methyl 3-hydroxy-2,2-dimethyl-5-phenylpent-4-ynoate (**4m**)