Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

LiO*t*Bu-Promoted Stereoselective Deconjugation of α,β-Unsaturated Diesters Probed by Density Functional Theory

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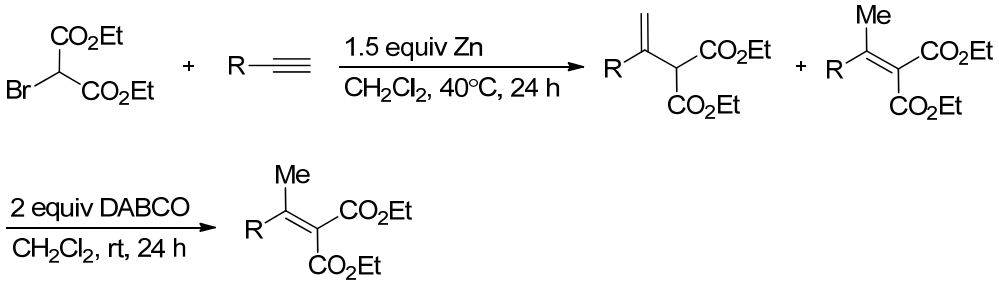
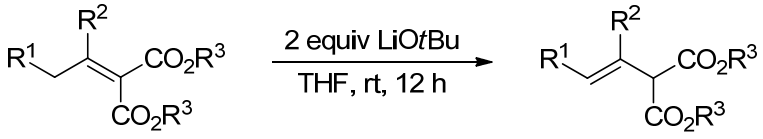
General methods: All commercial reagents were purchased from Aldrich and used as received. compounds **1a**–**1d**, and **1i**–**1k** was prepared by following literature procedures.[1] THF was purified using PureSolv solvent purification system, from Innovative Technology, Inc. Reactions with oxygen- and moisture-sensitive materials were carried out with the standard Schlenk technique. Flash chromatography was performed on silica gel from Merck (70–230 mesh). All ^{1}H NMR spectra were obtained on Bruker at 500 systems and reported in parts per million (ppm) downfield from tetramethylsilane. ^{13}C NMR spectra were reported in ppm referenced to deuteriochloroform (77.16 ppm). High resolution mass spectra (HRMS) were obtained at Korea Basic Science Institute (Cheongju, Korea) and reported in the form of *m/z* (intensity relative to peak = 100).

Preparation of tetrasubstituted α,β-unsaturated diesters (1e–1h)[2]



To an oven-dried round-bottomed flask, zinc powder (7.5 mmol, 1.5 equiv) and dichloromethane (5 mL) were charged under an atmosphere of nitrogen. Diethyl bromomalonate (5 mmol, 1 equiv), and terminal alkyne (7.5 mmol, 1.5 equiv) were added to the reaction solution. The reaction mixture was stirred at 40 °C for 24 h. The reaction mixture was filtered through a small plug of Celite, and washed with several portions of dichloromethane, and the filtrate was dried in vacuo. The crude mixture was used for the next step without further purification. The crude mixture and DABCO (10 mmol) were dissolved in dichloromethane (6 mL). The reaction mixture was stirred at room temperature for 24 h. Upon completion of the reaction, the reaction mixture was filtered through a pad of Celite and concentrated. The product was purified by silica gel chromatography.

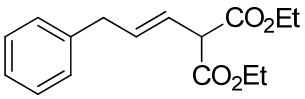
General procedure for deconjugation reaction of α,β-unsaturated diesters



1 **2**

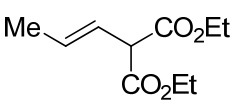
LiO*t*Bu (2 equiv, 1 mmol) was placed in an oven-dried round-bottomed flask. α,β-Unsaturated diester (**1**) dissolved in THF (1 mL) was added to the reaction mixture. The reaction mixture was stirred at room temperature for 12 h. Upon completion of the reaction, the reaction mixture was quenched with sat. NH_4Cl (5 mL). The aqueous layer was extracted with ethyl acetate (10 mL), and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The product was purified by silica gel chromatography.

Characterization of β,γ-unsaturated diesters 2 (Scheme 2)



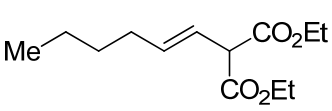
2a

(*E*)-diethyl 2-(prop-1-en-1-yl)malonate (2a) (Scheme 2): By following the general procedure, **2a** was obtained in 94% yield (colorless oil). The characterization data for **2a** was concordant with that previously reported in the literature.[3] ^{1}H NMR (500 MHz, C_6D_6) δ 7.13–7.10 (m, 2H), 7.04–7.02 (m, 3H), 6.02 (dd, *J* = 15.5, 9.0 Hz, 1H), 5.64 (dq, *J* = 15.5, 7.0 Hz, 1H), 4.05 (d, *J* = 9.0 Hz, 1H), 3.93 (q, *J* = 7.0 Hz, 4H), 3.13 (q, *J* = 7.0 Hz, 2H), 0.89 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, C_6D_6) δ 167.8, 139.5, 134.8, 128.5, 128.3, 126.1, 123.5, 61.0, 55.7, 38.7, 13.6.



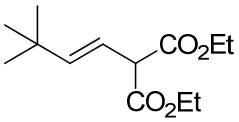
2b

(*E*)-diethyl 2-(prop-1-en-1-yl)malonate (2b) (Scheme 2): By following the general procedure, **2b** was obtained in 89% yield (colorless oil). The characterization data for **2b** was concordant with that previously reported in the literature.[4] ^{1}H NMR (500 MHz, C_6D_6) δ 6.04 (ddq, *J* = 15.0, 9.0, 2.0 Hz, 1H), 5.46 (dq, *J* = 15.0, 6.5 Hz, 1H), 4.06 (d, *J* = 9.0 Hz, 1H), 3.95 (q, *J* = 7.0 Hz, 2H), 3.94 (q, *J* = 7.0 Hz, 2H), 1.44 (dd, *J* = 6.5, 2.0 Hz, 3H), 0.90 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, C_6D_6) δ 167.9, 130.8, 123.4, 61.0, 55.9, 17.5, 13.6.



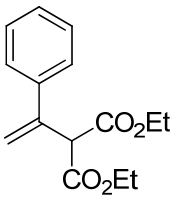
2c

(*E*)-diethyl 2-(hex-1-en-1-yl)malonate (2c) (Scheme 2): By following the general procedure, **2c** was obtained in 86% yield (colorless oil). ^{1}H NMR (500 MHz, C_6D_6) δ 6.01 (dd, *J* = 15.5, 9.0 Hz, 1H), 5.55 (dt, *J* = 15.0, 7.0 Hz, 1H), 4.11 (d, *J* = 9.0 Hz, 1H), 3.96 (q, *J* = 7.0 Hz, 4H), 1.88 (q, *J* = 7.0 Hz, 2H), 1.21–1.15 (m, 2H), 0.91 (t, *J* = 7.0 Hz, 6H), 0.78 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, C_6D_6) δ 168.0, 136.3, 122.2, 61.0, 55.9, 32.0, 30.9, 28.5, 22.0, 13.6; IR (neat) 2965, 1735, 1465, 1369, 1264, 1176, 1033 cm^{-1}; HRMS (ESI) calcd. for [$C_{13}H_{22}O_4$+Na$^+$]: 265.1416, found: 265.1417.



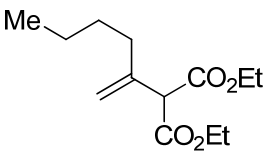
2d

(*E*)-diethyl 2-(3,3-dimethylbut-1-en-1-yl)malonate (2d) (Scheme 2): By following the general procedure, **2d** was obtained in 92% yield (colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.70 (d, *J* = 15.5 Hz, 1H), 5.59 (dd, *J* = 15.5, 8.5 Hz, 1H), 4.20 (q, *J* = 7.0 Hz, 4H), 3.94 (d, *J* = 8.5 Hz, 1H), 1.26 (t, *J* = 7.0 Hz, 6H), 1.03 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.6, 147.5, 116.7, 61.5, 55.7, 33.4, 29.3, 14.0; IR (neat) 2962, 1736, 1465, 1367, 1258, 1147, 1035 cm^{-1}; HRMS (ESI) calcd. for [$C_{13}H_{22}O_4$+Na$^+$]: 265.1416, found: 265.1416.



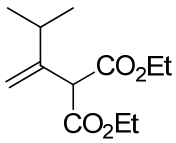
2e

Diethyl 2-(1-phenylvinyl)malonate (2e) (Scheme 2): By following the general procedure, **2e** was obtained in 98% yield (colorless oil). The characterization data for **2e** was concordant with that previously reported in the literature.[2] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42–7.39 (m, 2H), 7.35–7.27 (m, 3H), 5.64 (s, 1H), 5.42 (s, 1H), 4.62 (s, 1H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.21 (q, *J* = 7.0 Hz, 2H), 1.24 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.9, 140.7, 140.2, 128.4, 128.0, 126.3, 117.7, 61.8, 57.2, 14.0.



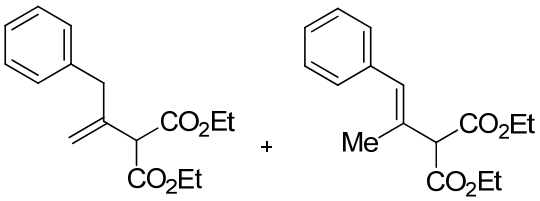
2f

Diethyl 2-(hex-1-en-2-yl)malonate (2f) (Scheme 2): By following the general procedure, **2f** was obtained in 98% yield (colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.10 (s, 1H), 5.07 (s, 1H), 4.21 (q, *J* = 7.0 Hz, 2H), 4.20 (q, *J* = 7.0 Hz, 2H), 4.06 (s, 1H), 2.15 (t, *J* = 7.0 Hz, 2H), 1.48–1.42 (m, 2H), 1.37–1.31 (m, 2H), 1.27 (t, *J* = 7.0 Hz, 6H), 0.91 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.1, 141.7, 115.0, 61.5, 58.4, 34.8, 29.6, 22.3, 14.0, 13.9; IR (neat) 2960, 1735, 1465, 1368, 1306, 1146, 1035 cm^{-1}; HRMS (ESI) calcd. for [$C_{13}H_{22}O_4$+Na$^+$]: 265.1416, found: 265.1417.



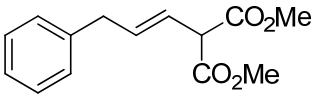
2g

Diethyl 2-(3-methylbut-1-en-2-yl)malonate (2g) (Scheme 2): By following the general procedure, **2g** was obtained in 98% yield (colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.16 (s, 1H), 5.11 (s, 1H), 4.20 (q, *J* = 7.0 Hz, 4H), 4.06 (s, 1H), 2.38–2.33 (m, 1H),1.27 (t, *J* = 7.0 Hz, 6H), 1.06 (d, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.3, 147.5, 113.2, 61.5, 56.4, 34.5, 21.7, 14.0; IR (neat) 2966, 1735, 1466, 1368, 1235, 1142, 1034 cm^{-1}; HRMS (ESI) calcd. for [$C_{12}H_{20}O_4$+Na$^+$]: 251.1259, found: 251.1260.



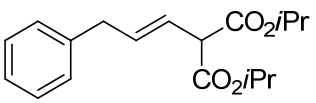
2h **2h'**

diethyl 2-(3-phenylprop-1-en-2-yl)malonate (2h) + (E)-diethyl 2-(1-phenylprop-1-en-2-yl)malonate (2h') (Scheme 2): By following the general procedure, **2h + 2h' (1:1 mixture)** were obtained in 87% yield (colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53–7.28 (m, 3H, **2h**, **2h'**), 7.23–7.19 (m, 2H, **2h**, **2h'**), 6.48 (s, 1H, **2h'**), 5.19 (s, 1H, **2h**), 5.01 (s, 1H, **2h**), 4.25 (q, *J* = 7.0 Hz, 4H, **2h'**), 4.21–4.14 (m, 5H, **2h**), 4.05 (s, 1H, **2h'**), 3.52 (s, 2H, **2h**), 2.01 (s, 3H, **2h'**), 1.30 (t, *J* = 7.0 Hz, 6H, **2h** or **2h'**), 1.30 (t, *J* = 7.0 Hz, 6H, **2h** or **2h'**); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.2 (**2h** or **2h'**), 167.9 (**2h** or **2h'**), 140.9 (**2h**), 138.2 (**2h'**), 137.0 (**2h'**), 131.5 (**2h** or **2h'**), 130.8 (**2h** or **2h'**), 129.4 (**2h** or **2h'**), 129.0 (**2h** or **2h'**), 128.4 (**2h** or **2h'**), 128.1 (**2h** or **2h'**), 126.9 (**2h** or **2h'**), 126.5 (**2h** or **2h'**), 117.7 (**2h**), 61.6 (**2h** and **2h'**) 57.7 (**2h** and **2h'**), 41.7 (**2h**), 16.5 (**2h'**), 14.1 (**2h** or **2h'**), 14.0 (**2h** or **2h'**); IR (neat) 2984, 1733, 1447, 1368, 1306, 1145, 1037 cm^{-1}; HRMS (ESI) calcd. for [$C_{16}H_{20}O_4$+Na$^+$]: 299.1259, found: 299.1260.



2i

(*E*)-dimethyl 2-(3-phenylprop-1-en-1-yl)malonate (2i) (Scheme 2): By following the general procedure, **2i** was obtained in 93% yield (colorless oil). ^{1}H NMR (500 MHz, C_6D_6) δ 7.13–7.10 (m, 2H), 7.05–7.01 (m, 3H), 5.96 (ddt, *J* = 15.0, 9.0, 1.5 Hz, 1H), 5.60 (dt, *J* = 15.0, 7.0 Hz, 1H), 4.01 (d, *J* = 9.0 Hz, 1H), 3.27 (s, 6H), 3.11 (q, *J* = 7.0 Hz, 2H); ^{13}C NMR (125 MHz, C_6D_6) δ 168.1, 139.4, 135.0, 128.5, 128.4, 126.1, 123.1, 55.2, 51.7, 38.7; IR (neat) 2966, 1735, 1466, 1368, 1235, 1142, 1034 cm^{-1}; HRMS (ESI) calcd. for [$C_{14}H_{16}O_4$+Na$^+$]: 271.0946, found: 271.0947.

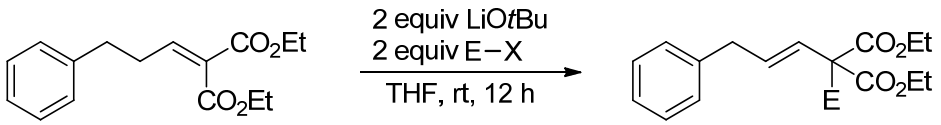


2j

(*E*)-dimethyl 2-(3-phenylprop-1-en-1-yl)malonate (2j) (Scheme 2): By following the general procedure, **2j** was obtained in 92% yield (colorless oil). ^{1}H NMR (500 MHz, C_6D_6) δ 7.13–7.10 (m, 2H), 7.04–7.01 (m, 3H), 6.05 (ddt, *J* = 15.5, 9.0, 1.5 Hz, 1H), 5.65 (dt, *J* = 15.5, 7.0 Hz, 1H), 5.05–4.97 (m, 2H), 4.04 (d, *J* = 9.0 Hz, 1H), 3.14 (d, *J* = 7.0 Hz, 1H), 1.02 (d, *J* = 6.0 Hz, 1H), 0.99 (d,

J = 6.0 Hz, 1H); ^{13}C NMR (125 MHz, C_6D_6) δ 167.4, 139.6, 134.6, 128.5, 128.3, 126.1, 123.7, 68.5, 56.0, 38.7, 21.2; IR (neat) 2966, 1735, 1466, 1368, 1235, 1142, 1034 cm^{-1}; HRMS (ESI) calcd. for [$C_{18}H_{24}O_4$+Na$^+$]: 327.1572, found: 327.1561.

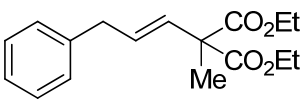
General procedure for the deconjugative alkylation of α,β-unsaturated diesters (Scheme 4)



1 **3**

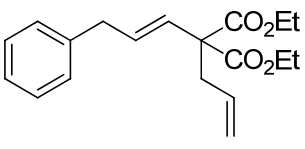
LiO*t*Bu (2 equiv, 1 mmol) was placed in an oven-dried round-bottomed flask. α,β-Unsaturated diester (**1**) and alkyl electrophile (E–X) dissolved in THF (1 mL) was added to the reaction mixture. The reaction mixture was stirred at room temperature for 12 h. Upon completion of the reaction, the reaction mixture was quenched with sat. NH_4Cl (5 mL). The aqueous layer was extracted with ethyl acetate (10 mL), and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The product was purified by silica gel chromatography.

Characterization of 3 (Scheme 4)



3a

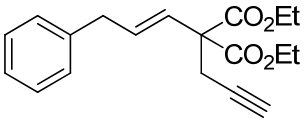
(*E*)-diethyl 2-allyl-2-(3-phenylprop-1-en-1-yl)malonate (3a) (Scheme 4): By following the general procedure, **3a** was obtained in 88% yield (colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32–7.27 (m, 2H), 7.21–7.16 (m, 3H), 6.04 (dt, J = 16.0, 1.5 Hz, 1H), 5.74 (dt, J = 16.0, 7.0 Hz, 1H), 4.20 (q, J = 7.0 Hz, 4H), 3.43 (d, J = 7.0 Hz, 2H), 1.55 (s, 3H), 1.25 (t, J = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.3, 139.9, 130.5, 129.6, 128.5, 128.4, 126.2, 61.5, 55.5, 38.9, 20.3, 14.0; IR (neat) 2973, 1731, 1454, 1375, 1252, 1193, 1032 cm^{-1}; HRMS (ESI) calcd. for [$C_{17}H_{22}O_4$+Na$^+$]: 313.1416, found: 313.1415.



3b

(*E*)-diethyl 2-allyl-2-(3-phenylprop-1-en-1-yl)malonate (3b) (Scheme 4): By following the general procedure, **3b** was obtained in 91% yield (colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29–7.26 (m, 2H), 7.21–7.15 (m, 3H), 6.04 (d, J = 16.0 Hz, 1H), 5.78–5.65 (m, 2H), 5.10–5.05 (m, 2H),

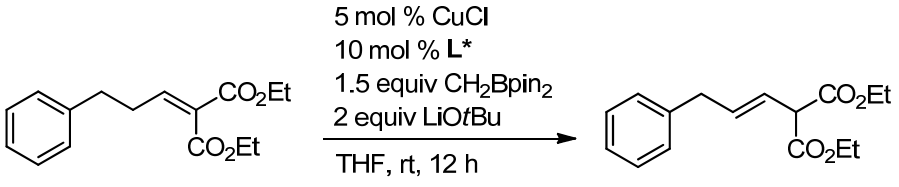
4.19 (q, *J* = 7.0 Hz, 4H), 3.43 (d, *J* = 7.0 Hz, 2H), 2.80 (d, *J* = 7.5 Hz, 2H), 1.23 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 139.8, 132.6, 131.5, 128.5, 128.4, 128.0, 126.2, 118.8, 61.5, 59.2, 39.9, 39.1, 14.1 IR (neat) 3028, 2981, 1731, 1452, 1278, 1258, 1151, 1037 cm^{-1}; HRMS (ESI) calcd. for [$C_{19}H_{24}O_4$+Na^+]: 339.1572, found: 339.1573.



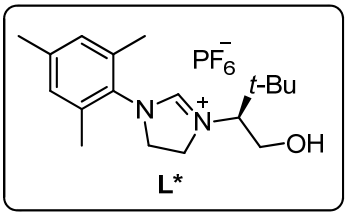
3c

(*E*)-diethyl 2-(3-phenylprop-1-en-1-yl)-2-(prop-2-yn-1-yl)malonate (3c) (Scheme 4): By following the general procedure, **3c** was obtained in 85% yield (colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29–7.26 (m, 2H), 7.21–7.18 (m, 3H), 6.13 (dt, *J* = 16.0, 1.5 Hz, 1H), 5.79 (dt, *J* = 16.0, 7.0 Hz, 1H), 4.23 (q, *J* = 7.0 Hz, 2H), 4.22 (q, *J* = 7.0 Hz, 2H), 3.47 (d, *J* = 7.0 Hz, 2H), 2.95 (d, *J* = 2.5 Hz, 2H), 1.99 (d, *J* = 2.5 Hz, 1H), 1.25 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.3, 139.6, 131.9, 128.5, 128.4, 127.1, 126.2, 126.1, 79.2, 71.2, 61.9, 68.8, 39.0, 25.3, 14.0.; IR (neat) 3289, 2981, 1733, 1454, 1368, 1276, 1190, 1033 cm^{-1}; HRMS (ESI) calcd. for [$C_{19}H_{22}O_4$+Na^+]: 337.1416, found: 337.1414.

Table S1. Optimization of reaction conditions



1a **2a**



L*

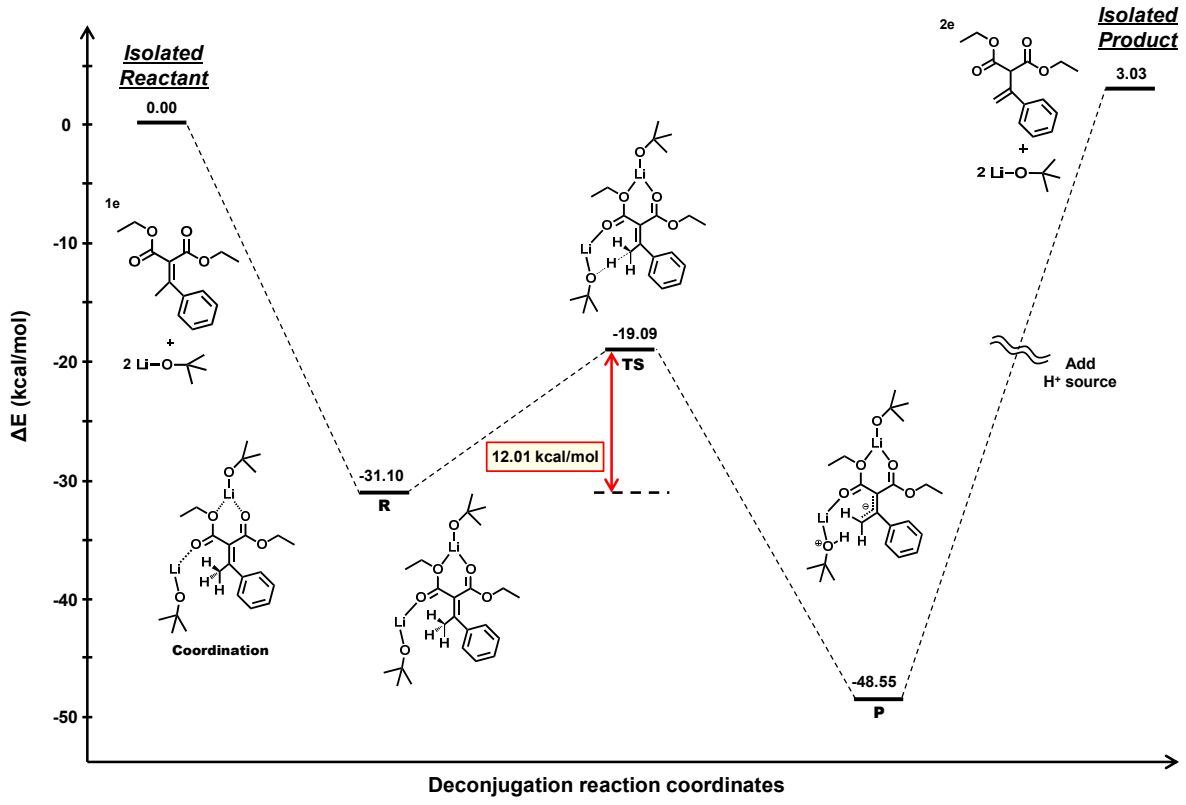
Entry	Change from standard conditions	yield[b]
1	none	22
2	without CH_2Bpin_2	55
3	without CH_2Bpin_2 & **L***	71
4	without CH_2Bpin_2 & **L*** & CuCl	91

Computational Methods

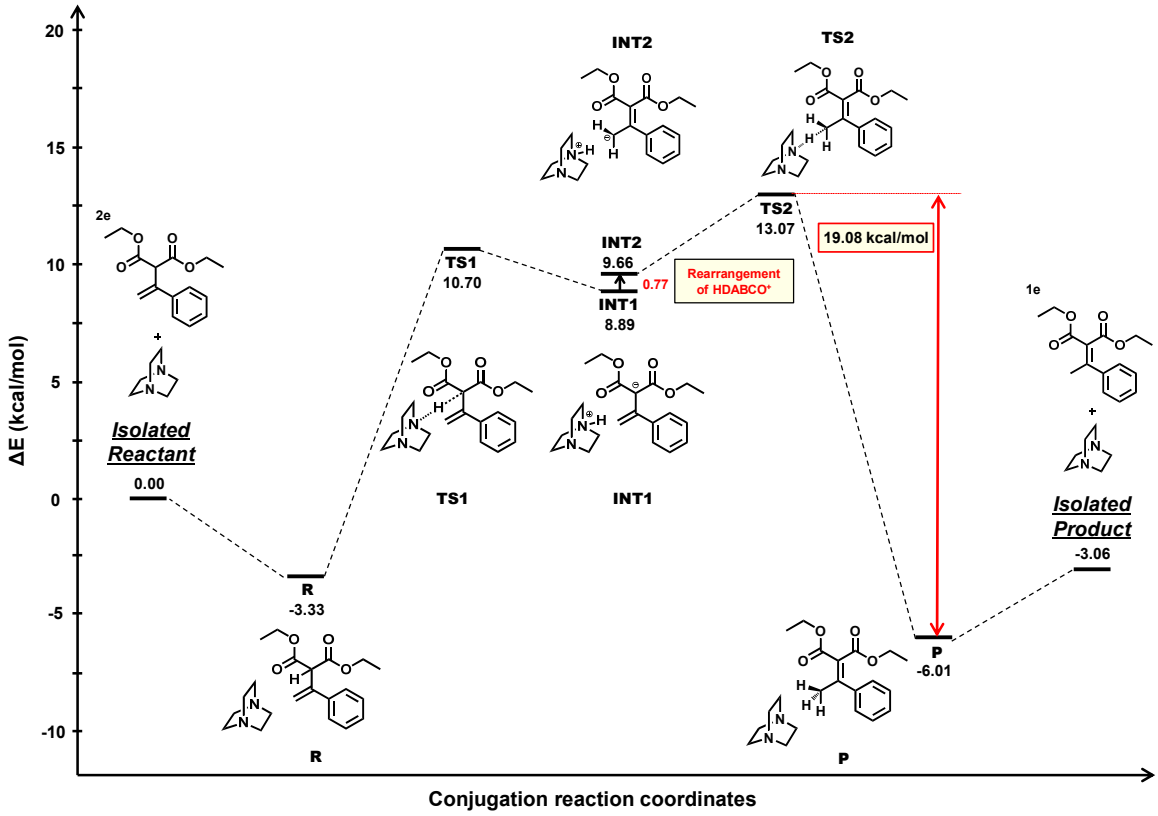
We have performed density functional theory (DFT) calculations to find the most stable structures of reactants and products using a hybrid functional B3LYP[5,6] and def2-SVP[7] basis set implemented in TUROMOLE 7.3 program[8,9] utilizing the resolution of identity (RI) method.[10] For the most reasonable reaction path and transition states (TS), *ab initio* molecular dynamics (AIMD) calculations at 298K are initially carried out. Conductor-like Screening Model (COSMO)[11] is used to consider the implicit solvent-mediated effect for the geometry optimization, AIMD, and TS calculations with dielectric constants 7.58 for THF (tetrahydrofuran) and 9.1 for DCM (dichloromethane).

Figure S1. Deconjugation of **1e** with LiO*t*Bu (**Figure S1(a)**) and conjugation of **2e** with DABCO (**Figure S1(b)**). 'INT' denotes the intermediate (**Figure S1(b)**).

(a)



(b)



This calculation shows the activation energy for deconjugation reaction with LiO*t*Bu (**12.01 kcal/mol**) is lower than that with DABCO (**19.08 kcal/mol**). The energy difference between the isolated reactant and isolated product in each reaction is caused by solvent difference used in **Figure S1(a)** (THF) and **Figure S1(b)** (DCM).

Scheme S1. Conjugation reaction of β,γ-unsaturated diesters with DABCO.

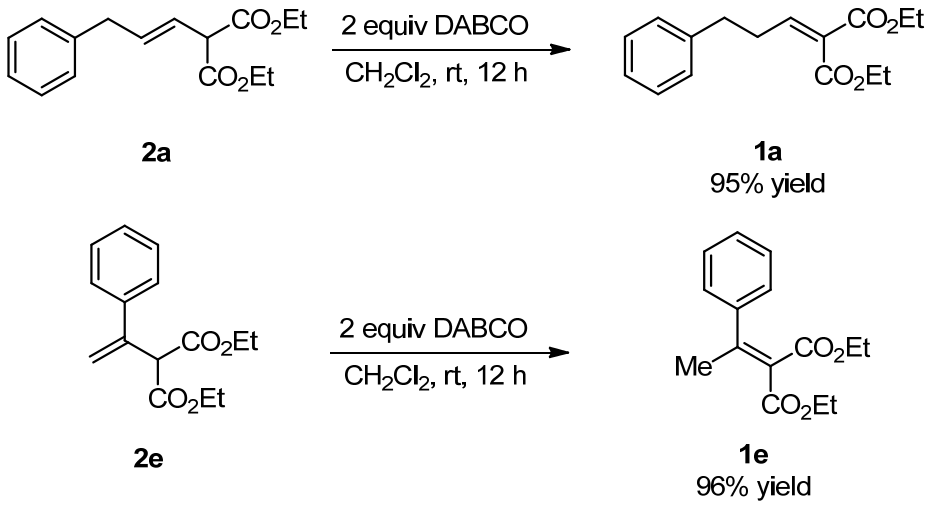
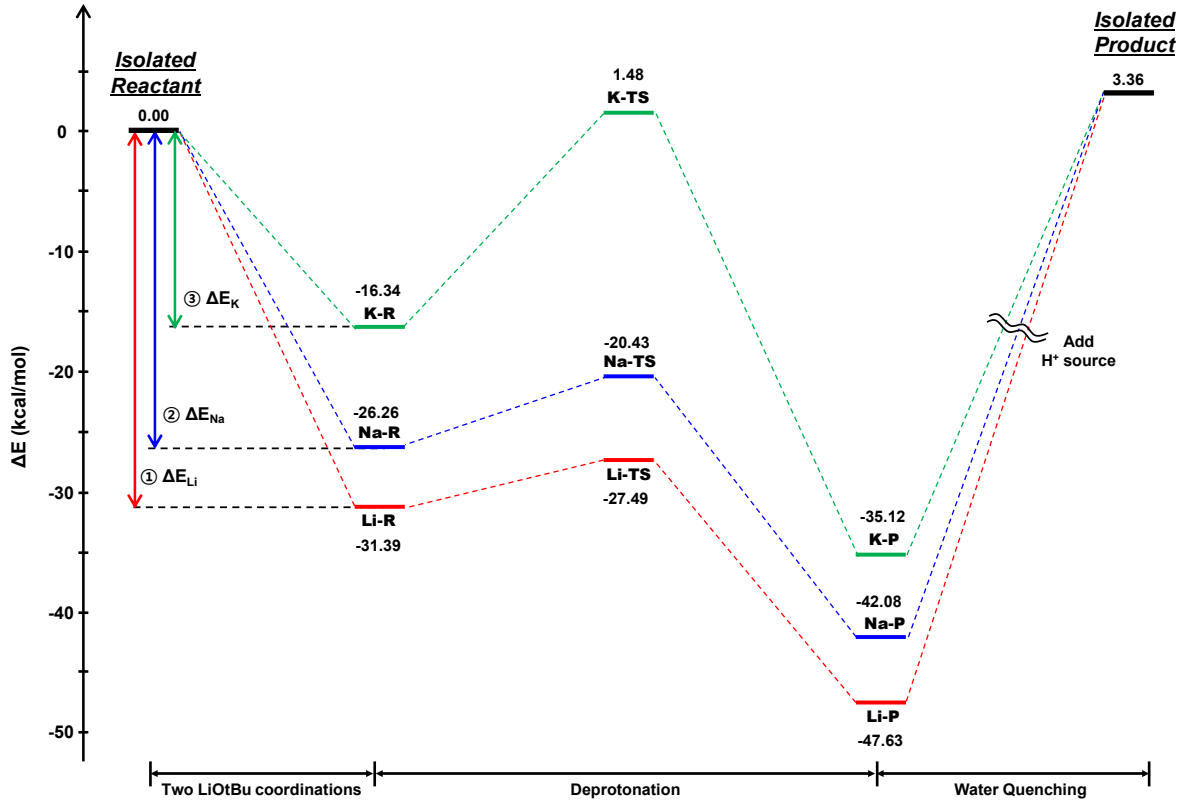
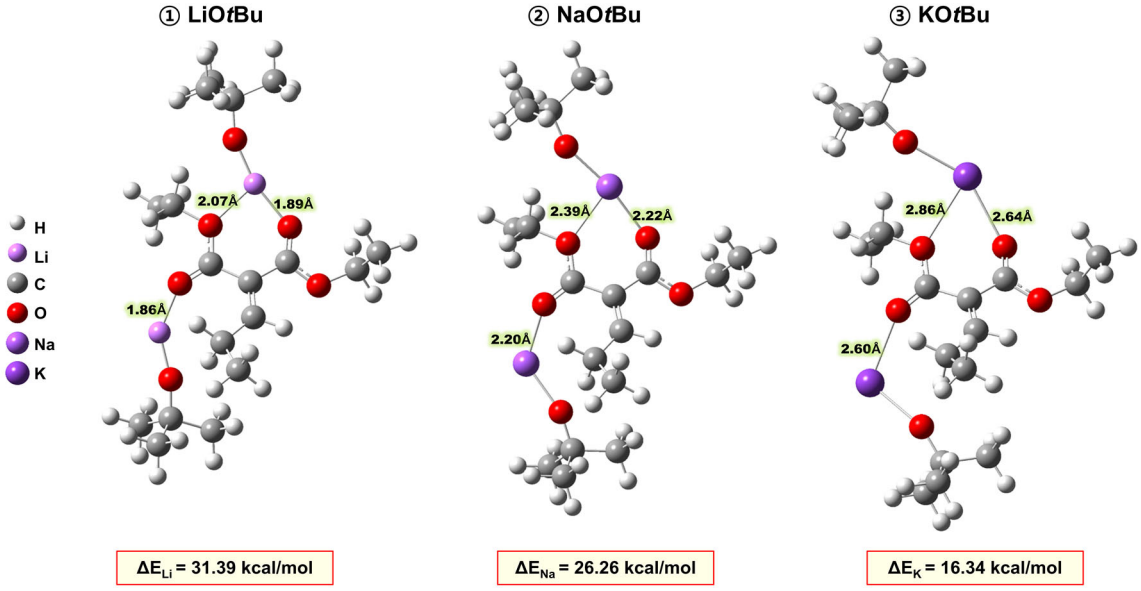


Figure S2. Different energy stability of metal-O coordination compound upon the base (LiO*t*Bu, NaO*t*Bu, and KO*t*Bu).

(a)



(b)



As shown in the energy profile calculation, the difference of stability energy for the Metal-O coordination compound is increased in the order of ΔE_K, ΔE_{Na}, and ΔE_{Li} (**Figure S2(a)**) and the coordination length is decreased in the order of K-O, Na-O, and Li-O (**Figure S2(b)**). This difference in coordination length occurs by the periodic property of the atom radius of each metal.

Figure S3. Four different possible deconjugation reaction pathways with LiO*t*Bu. Since the energy of the **R4** and the activation energy of **TS4** (3.87kcal/mol) are the lowest in other pathways, '**Path 4**' was selected as the most reasonable reaction pathway.

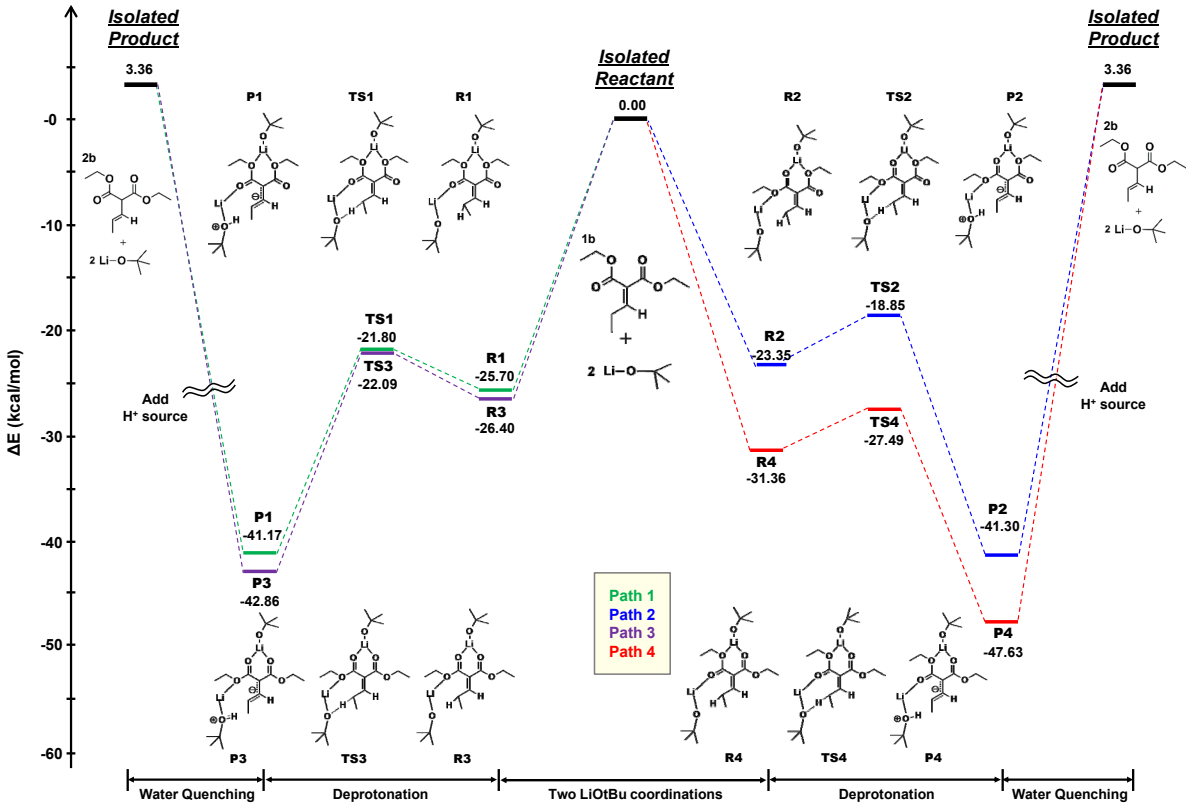
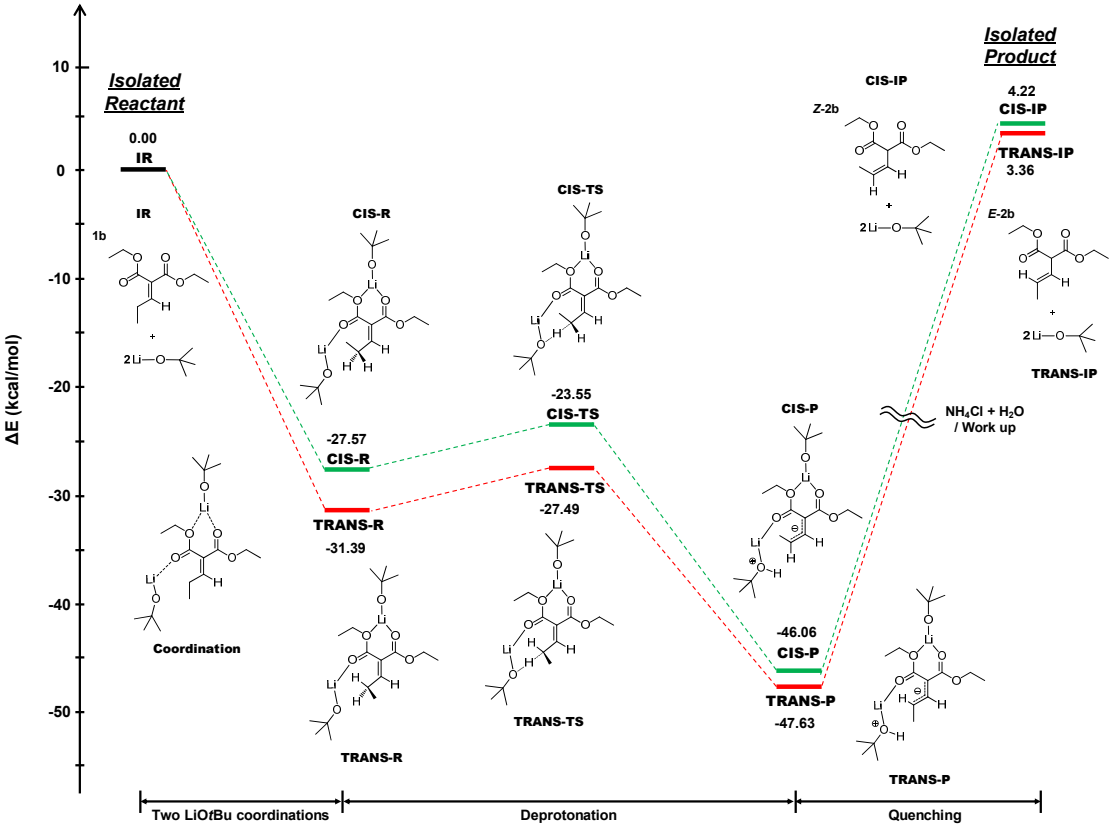
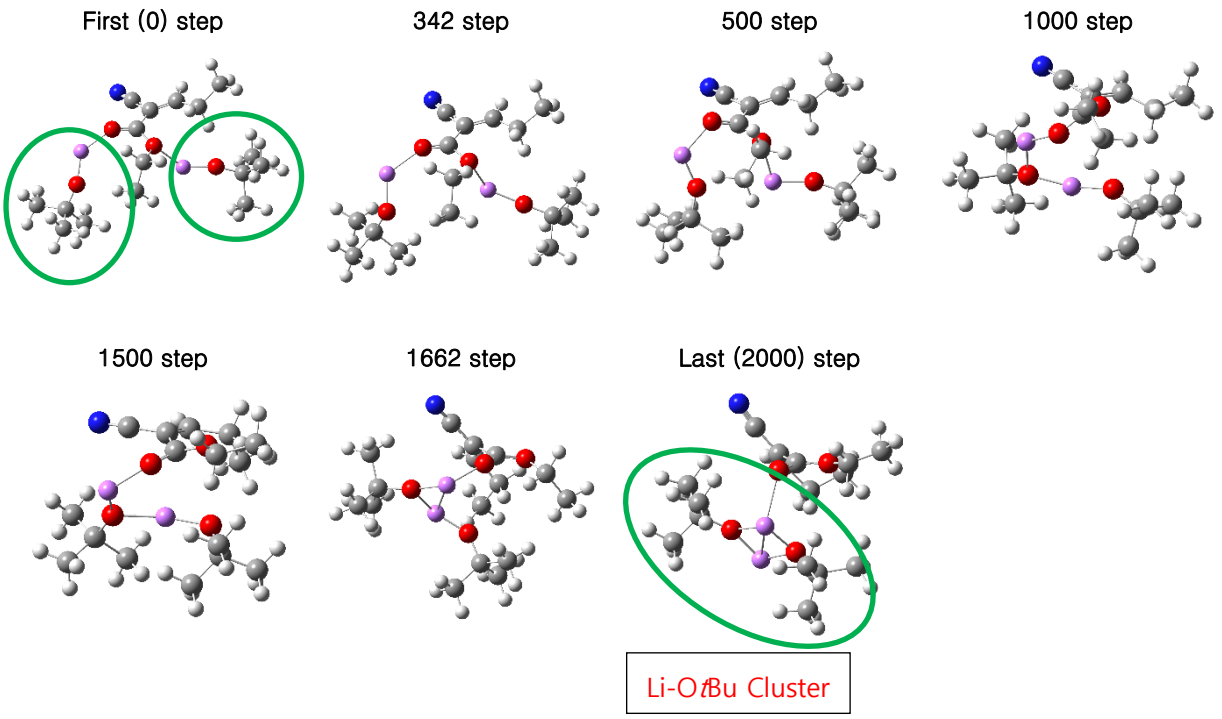


Figure S4. Deconjugation reaction pathways.



The substrate (**1b**) initially coordinates with two equivalents of LiO*t*Bu to form stable coordination compounds via ion-dipole interactions with **TRANS-R** more stable than **CIS-R** by 3.82 kcal/mol. These compounds subsequently undergo γ-deprotonation with LiO*t*Bu and form electronically delocalized anionic products **CIS-P** and **TRANS-P.** Moreover, the activation energies of both **TRANS-R** and **CIS-R** during deprotonation are similar (~4 kcal/mol). Therefore, the stability of Li^+-coordinated diesters determines the overall reaction pathway. The trans pathway is favoured due to less steric hindrance of **TRANS-R** with a low activation energy barrier of **TRANS-TS.**

Figure S5. AIMD screenshot of the conjugated molecule containing the CN group (**1k**). In the case of the conjugated molecule containing the CN group (**1k**), unlike the conjugated molecule containing the diester, the double coordinate with lithium of LiO*t*Bu is not formed. Namely, CN group is only formed the single coordination with LiO*t*Bu, which is free to move and form more stable LiO*t*Bu clusters. Therefore, deconjugation reaction of the cyano group does not occur as presented below, which is consistent with experimental result. We also performed ab initio molecular dynamics (AIMD) and confirmed the reaction mechanism of LiO*t*Bu cluster in the CN group. The following pictures are the snap shots of the cluster reaction for **1k** molecule over time.



Imaginary frequencies for all the transition states

Figure 1

TS1

---

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	RAMAN
1	a	-870.43	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	14.34	0.02350	YES	YES
9	a	16.66	0.50632	YES	YES
10	a	23.28	0.02317	YES	YES

TS2-α

---

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	RAMAN
1	a	-1171.76	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	34.11	0.19359	YES	YES
9	a	41.37	3.31799	YES	YES
10	a	43.29	1.11552	YES	YES

TS2-γ

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-1048.83	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	13.57	8.98272	YES	YES
9	a	32.19	1.34708	YES	YES
10	a	39.11	3.96145	YES	YES

Figure 2 (a)

$TS_{1f\text{-}A}$

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-499.61	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	2.55	0.50355	YES	YES
9	a	4.57	0.25960	YES	YES
10	a	8.02	0.81733	YES	YES

$TS_{1f\text{-}B}$

---

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	RAMAN
1	a	-1161.89	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	8.57	0.36393	YES	YES
9	a	12.29	0.13306	YES	YES
10	a	18.86	0.09240	YES	YES

Figure 2 (b)

$TS_{1g\text{-}A}$

---

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	RAMAN
1	a	-1165.29	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		-0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	7.14	0.31302	YES	YES
9	a	16.50	0.82126	YES	YES
10	a	20.86	0.70292	YES	YES

$TS_{1g\text{-}B}$

---

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-628.77	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	8.90	0.13491	YES	YES
9	a	16.73	0.88738	YES	YES
10	a	21.58	0.04086	YES	YES

Figure 2 (c)

$TS_{1h\text{-}A}$

---

mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-366.81	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		-0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	10.56	0.53054	YES	YES
9	a	12.24	1.64858	YES	YES
10	a	13.81	0.64612	YES	YES

$TS_{1h\text{-}B}$

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mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	RAMAN
1	a	-686.59	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	4.99	1.09839	YES	YES
9	a	9.03	0.05639	YES	YES
10	a	17.43	0.02632	YES	YES

Cartesian coordinates for all molecules

Scheme 1 (C)

1a

H	-0.7319000	2.6945000	-0.3202000
O	0.8994187	-0.7491827	3.4491132
H	3.8464382	-2.6917955	-0.6400979
C	2.7259187	-2.7277898	3.3926474
C	0.9512000	-1.5744000	-0.1574000
C	3.1159408	-2.8116662	-1.4461211
C	0.4931000	-0.9066000	1.0887000
H	-1.7263000	2.2912000	1.0797000
O	1.0266000	-1.0258000	-1.2480000
C	-1.1907000	0.6012000	-0.1510000
O	1.2617000	-2.8694000	0.0939000
H	-2.0950000	-0.0152000	-0.2357000
H	3.5958635	-3.3227419	-2.2854912
H	3.3239853	-1.8920661	3.7741825

C	1.7991025	-3.2844499	4.4587929
H	2.8231418	-1.8064051	-1.7665524
H	-0.6951000	0.5970000	1.9683000
H	3.4279202	-3.5081149	3.0802891
C	-2.8152999	2.5548000	-0.7178000
C	1.1313001	-1.2951999	2.3809000
H	-0.6386000	0.4437000	-1.0840000
H	2.3737120	-3.6503685	5.3148148
H	2.1847655	-4.6052234	-0.6655321
C	-0.4257000	0.0855000	1.0443000
H	1.0996353	-2.5229943	4.8169960
O	1.9989716	-2.3322989	2.2184941
C	-1.5772000	2.0776000	0.0128000
H	1.1798908	-3.6824463	-1.7789171
H	1.1972852	-4.1060183	4.0577971
C	1.9076001	-3.5882998	-0.9661001
C	-4.0684997	2.1685992	-0.2111460
C	-5.2515464	2.5390697	-0.8535853
H	-4.1281022	1.5708465	0.6965097
C	-2.7830562	3.3184327	-1.8917919
C	-5.2010524	3.2990899	-2.0178658
H	-6.2103332	2.2318850	-0.4445882
C	-3.9682005	3.6887603	-2.5356020
H	-1.8437811	3.6402327	-2.3317538
H	-6.1198765	3.5869811	-2.5211489
H	-3.9271296	4.2818416	-3.4456498

2a

H	0.6797363	2.7232016	-1.0777117
O	0.7984000	-0.7622000	3.3844000
H	4.3485000	-2.1895000	-0.1673000
C	2.7634000	-2.5963000	3.3160000
C	0.9590000	-1.7769000	-0.1295000

C	3.7512000	-2.4474000	-1.0478000
C	0.2114000	-1.1364000	1.0386000
H	-0.2212065	2.9119067	0.4296924
O	0.8057000	-1.5002000	-1.3138000
C	-0.1945000	0.9322000	-0.3925000
O	1.8027000	-2.7512000	0.3232000
H	4.4025000	-2.9049000	-1.7974000
H	3.1395000	-1.6474000	3.7161000
C	2.0639000	-3.4127000	4.3893000
H	3.3542000	-1.5099000	-1.4508000
H	3.6313000	-3.1536000	2.9478000
C	-1.4239441	2.9779577	-1.3201013
C	0.9783000	-1.3698000	2.3369000
H	2.7548000	-3.6466000	5.2052000
H	3.0068000	-4.3535000	-0.3514000
C	-0.0078000	0.3516000	0.8099000
H	1.2110000	-2.8724000	4.8109000
O	1.9102000	-2.3602000	2.1819000
C	-0.2395000	2.4283000	-0.5539000
H	1.9821000	-3.5683000	-1.5470000
H	1.6760000	-4.3480000	3.9744000
C	2.6183000	-3.3815000	-0.6762000
C	-1.3016402	3.2320355	-2.6962046
C	-2.3401309	3.8341046	-3.4092000
H	-0.3851769	2.9741895	-3.2231408
C	-2.6161457	3.3405868	-0.6768155
C	-3.5178518	4.1885013	-2.7570486
H	-2.2236879	4.0349046	-4.4710823
C	-3.6584312	3.9362731	-1.3935122
H	-2.7386691	3.1734938	0.3906239
H	-4.3223532	4.6662203	-3.3097540
H	-4.5771675	4.2158102	-0.8845328
H	-0.2117000	0.3221000	-1.2940000
H	0.0395000	0.9928000	1.6895000

H	-0.7616000	-1.6376000	1.1244000

Figure 1

IR (1b)

H	6.1574466	6.9238939	1.0523176
O	6.7906014	2.2988543	4.6643765
H	8.0749018	2.9296329	-0.8422258
C	5.9686332	4.0153791	6.5677029
C	6.8644761	2.8730224	1.9038837
C	7.2942008	2.2257480	-1.1667886
C	6.0606663	3.6986019	2.8723264
H	4.5242267	7.2524168	1.6773218
O	8.0642645	2.7689938	1.9521287
C	4.8678404	5.1544435	1.1315010
O	6.0916662	2.2724590	0.9771269
H	3.7947933	4.9321032	0.9744000
H	7.7400657	1.5396465	-1.9053843
H	5.7747320	2.9468645	6.7452985
C	7.3362543	4.4138554	7.0984698
H	6.4899719	2.7882370	-1.6678233
H	4.7623314	5.2530849	3.3327705
H	5.1694016	4.6088669	7.0363065
H	4.7702548	6.9799451	-0.0642036
C	6.2898300	3.3394321	4.3072822
H	5.4111709	4.5789340	0.3694495
H	7.3706257	4.2689863	8.1907271
H	7.5689901	0.8888995	0.5206975
C	5.2257651	4.6937233	2.5121514
H	8.1254681	3.7951744	6.6458918
O	5.8453902	4.2855681	5.1590233
C	5.0931033	6.6621798	0.9397043
H	5.9875852	0.7134112	-0.3044277
H	7.5487593	5.4731524	6.8841009

C	6.7575404	1.4315963	0.0135208

LiO*t*Bu

C	-0.7934059	6.3472193	-1.7858864
H	-0.2535329	6.4279923	1.6541723
H	-1.8000354	6.2464751	0.7866055
C	-0.7803157	6.6613066	0.7131805
H	1.9475512	6.3718366	0.3632363
H	1.3932892	7.7004249	-0.6986595
H	1.9366195	6.1492130	-1.4052776
H	-0.8585774	7.7589126	0.6231273
C	-0.0355700	6.0109124	-0.4781694
Li	0.1217016	3.0224671	-0.1124071
H	-1.8129738	5.9279839	-1.7440740
O	0.0294340	4.6460609	-0.3064711
H	-0.2759512	5.8884581	-2.6457417
H	-0.8724538	7.4332208	-1.9690791
C	1.3917897	6.6049177	-0.5609974

R1

C	11.6463509	-0.7550733	3.8608800
C	6.0754244	4.3238588	6.7761535
H	5.7122320	5.0182164	0.6215362
H	10.9830137	-1.1766489	4.6345580
O	2.9428359	3.2825075	0.2530579
O	7.4881191	2.9343811	4.9664982
H	1.3602487	1.9967469	-1.4681742
Li	8.9096355	1.9952935	4.1455967
H	1.1346235	2.9860890	2.1720751
C	6.6868039	2.7939880	2.0956195
H	-0.1459772	3.9724666	1.4049368
H	8.0738505	5.1787118	6.7041933

H	12.2091766	1.0610915	1.8613773
H	7.7393165	-0.6169991	2.5466825
H	12.1980898	2.3049300	5.4277111
C	11.6424430	0.7904076	3.9572446
C	7.0924773	5.3845383	7.1579059
H	1.0878096	1.3768243	0.1825515
H	11.2589695	-1.0716138	2.8776565
H	5.0979223	4.5155378	7.2405015
O	6.1178750	2.6105935	1.0213527
H	6.4175398	3.3177196	7.0560387
O	5.7969650	4.3391404	5.3541078
C	4.9731818	5.2865844	1.3950454
H	1.8090547	4.4789974	-1.8380909
H	13.2245345	0.8436566	5.5217288
C	5.4263966	4.8433218	2.7305463
H	4.0614982	4.6745944	1.1197394
H	8.2906329	1.6050564	0.4599075
H	7.2206403	5.3918511	8.2521443
H	-0.1726611	2.3555408	-0.6231401
H	12.5531798	2.4674834	2.8996630
Li	4.4617374	2.6434974	0.1854086
C	0.9160284	2.2356863	-0.4872618
C	6.2036285	3.7781715	3.1021693
H	9.3911668	1.0815236	1.8196691
H	1.8087784	5.6034527	-0.4553942
C	12.5697850	1.3655748	2.8585951
C	1.5843710	3.5003904	0.1001747
H	13.6165058	1.0294124	2.9613563
H	11.5468839	0.8045246	6.1389858
H	6.7578760	6.3862575	6.8460642
C	0.9443761	3.8162989	1.4720578
C	7.6492746	-0.1874969	1.5369236
H	6.5862395	-0.1230725	1.2593719
O	10.3613815	1.2697777	3.7913447

O	7.7816431	2.1182982	2.4171492
H	12.6525547	-1.1913399	3.9900689
C	1.3445337	4.6884841	-0.8602591
C	6.5731875	3.6281209	4.5409887
H	1.3935874	4.7283551	1.9002379
C	8.3532364	1.1521069	1.4583991
H	8.1420757	-0.8828545	0.8382088
C	12.1965710	1.2050930	5.3423291
H	0.2719827	4.8921296	-1.0223152
H	5.0981166	5.4714258	3.5654316
C	4.6157687	6.7748554	1.3264869
H	3.8403930	7.0330245	2.0664596
H	5.4894544	7.4212536	1.5122682
H	4.2174594	7.0254552	0.3317766

TS1

C	5.8406283	-1.7370874	-0.7880434
C	0.4980335	-1.1293284	3.9664289
H	-2.5114757	2.3360438	-0.1991369
H	5.7316944	-1.9770565	0.2830232
O	-3.9617173	0.0746594	-1.1448110
O	1.5173535	-0.4204792	1.6145844
H	-5.3347275	-0.9955415	-3.1502872
Li	2.7713741	-0.0301372	0.2880271
H	-4.1742534	-2.1863105	0.2416792
C	-0.1198589	0.7704997	-0.5508406
H	-5.9535119	-2.1665379	0.4085438
H	2.0077654	0.4031145	4.2730028
H	4.9563417	-0.5757775	-3.1405723
H	2.1184292	-1.2203387	-2.5359523
H	6.1216260	1.7086907	-0.3718972
C	5.4496478	-0.2581201	-1.0337164
C	1.2443332	-0.1419595	4.8477214

H	-4.4144674	-2.2703190	-2.2995325
H	5.1613622	-2.3989669	-1.3512381
H	-0.2496271	-1.6934253	4.5425023
O	-0.9110690	1.0251347	-1.4727991
H	1.1897288	-1.8366874	3.4866980
O	-0.2727162	-0.4628123	2.9441447
C	-2.8522487	1.7006100	0.6338056
H	-6.4055052	0.8997855	-1.8251140
H	7.4633157	0.5305436	-0.5038099
C	-1.8083324	0.9753817	1.2768897
H	-3.4779456	0.8171518	-0.0753922
H	1.1056488	1.6974867	-2.6277928
H	1.7537894	-0.6845372	5.6603491
H	-6.1939174	-2.2154437	-2.1735893
H	5.3763010	1.1118698	-2.7389994
Li	-2.5668581	0.5501380	-2.0260639
C	-5.2835854	-1.5956545	-2.2264161
C	-0.5492244	0.5497571	0.8332411
H	2.7215824	1.0877661	-2.0412793
H	-6.2705946	0.9372862	-0.0482529
C	5.6325799	0.0569229	-2.5407082
C	-5.1452061	-0.6766126	-0.9984886
H	6.6649718	-0.1157396	-2.8923527
H	6.3041084	0.4297570	0.8551754
H	0.5531457	0.5854377	5.3020695
C	-5.0605987	-1.5326882	0.2802546
C	1.5158055	-0.4223038	-2.9945082
H	0.4684345	-0.7487873	-3.0863101
O	4.1447348	-0.0410491	-0.6551022
O	1.1854543	0.6782643	-0.8107225
H	6.8781677	-1.9663367	-1.0898619
C	-6.3570941	0.2708550	-0.9213921
C	0.3345103	-0.1392844	1.7939978
H	-4.9714945	-0.8913861	1.1722021

C	1.6586188	0.8553103	-2.1911021
H	1.9104662	-0.2486843	-4.0089654
C	6.4026431	0.6530436	-0.2205711
H	-7.3065832	-0.2826607	-0.8336809
H	-2.0249476	0.6691919	2.3057861
C	-3.8816516	2.3862225	1.5292729
H	-4.2282956	1.7129473	2.3314815
H	-3.4794756	3.2946288	2.0106417
H	-4.7676912	2.6879569	0.9486614

P

C	4.7724362	-1.8164316	-2.1634702
C	1.0322444	0.0850072	4.5786645
H	-2.5991241	2.8325362	0.5015029
H	4.2459230	-2.6334314	-1.6413112
O	-4.3592325	-0.3822427	-0.4720969
O	1.6042557	0.1407120	1.9942324
H	-4.4592678	0.5857302	-2.9412417
Li	2.5541734	0.1495556	0.3966486
H	-2.8995474	-2.4633744	-1.3469578
C	-0.3923824	0.9555155	-0.0364697
H	-4.1632323	-3.1862754	-2.3779099
H	2.5905356	1.5521650	4.2226036
H	5.0950316	0.8550087	-2.7995388
H	1.3497515	-1.5681232	-1.9554478
H	6.0214807	-0.2560133	0.6879774
C	4.9702072	-0.6226172	-1.1928570
C	1.9494585	1.2040080	5.0458209
H	-2.9095250	-0.2619851	-2.6547186
H	4.1467508	-1.5040114	-3.0167960
H	0.4094430	-0.2856552	5.4073388
O	-1.3378072	1.1150139	-0.8490052
H	1.6141836	-0.7527988	4.1673664

O	0.0905907	0.5390126	3.5943381
C	-2.7579027	2.3465421	1.4766965
H	-6.6002804	-0.2784116	-1.9175582
H	6.8499006	-1.4650921	-0.3379101
C	-1.8031974	1.5080612	1.9711508
H	-4.8113553	-0.7875798	0.2823336
H	0.4127494	1.3309570	-2.4613335
H	2.6016066	0.8411603	5.8573691
H	-4.1155230	-0.9527266	-3.7692029
H	5.8442859	1.3741416	-1.2701104
Li	-3.0088821	0.8888284	-0.1863031
C	-3.9886292	-0.4037695	-2.8243045
C	-0.5598006	1.0063428	1.3894335
H	2.0970363	0.7461698	-2.0859751
H	-6.6085641	-1.8043561	-0.9862162
C	5.7062177	0.5143125	-1.9464778
C	-4.6302008	-1.1780505	-1.6734260
H	6.6962124	0.2087738	-2.3299864
H	5.3505035	-1.9004385	0.5364280
H	1.3672047	2.0578184	5.4276970
C	-3.9866974	-2.5554254	-1.4930872
C	0.6864122	-0.8386570	-2.4438895
H	-0.3653411	-1.1027037	-2.2520771
O	3.7555316	-0.1775339	-0.7338660
O	0.8354544	0.6934016	-0.5239735
H	5.7234992	-2.2145359	-2.5606948
C	-6.1481514	-1.2792474	-1.8406368
C	0.4703601	0.5335551	2.2921368
H	-4.4110996	-3.0801728	-0.6204310
C	1.0203986	0.5621363	-1.9657349
H	0.8640042	-0.9017423	-3.5303294
C	5.8614608	-1.0921558	-0.0139386
H	-6.4018122	-1.8449058	-2.7504502
H	-1.9576004	1.1791137	3.0043334

C	-3.9336354	2.8410121	2.2801114
H	-3.9910722	2.3359638	3.2577778
H	-3.8599191	3.9274216	2.4714321
H	-4.9016985	2.6881430	1.7671698

R2

C	1.7826906	-2.3216439	2.9333526
H	-3.2431299	1.0990374	1.7863157
O	1.8604190	-0.0794174	1.5886729
C	-0.6499161	1.3819435	0.8154191
H	2.5892618	-0.7257443	4.1687395
H	-0.0229031	1.1692308	-2.6854914
C	2.2705997	-1.7744440	4.2663526
H	1.4919106	-3.3782464	3.0284034
O	-1.5833129	2.1592203	0.7489286
H	2.5632473	-2.2441413	2.1626326
O	0.5856459	-1.6729703	2.4795631
C	-3.0176258	0.2110319	2.3811312
C	-1.7579933	-0.2658548	2.4084317
H	-0.1133442	3.4330726	-0.5910990
H	3.1341571	-2.3618872	4.6194030
C	-0.5510046	0.2345640	1.7263334
H	1.3877015	2.7472145	-1.3002991
H	1.4789828	-1.8331017	5.0299733
C	-0.4447988	2.0939926	-2.2614054
H	-1.4983803	1.9160907	-2.0004814
O	0.4144257	1.4994747	-0.0458021
C	0.6414106	-0.4627451	1.9043575
C	0.3396765	2.5319318	-1.0335659
H	-0.4087484	2.8789654	-3.0350343
H	-1.5735022	-1.1521990	3.0230213
C	-4.1543509	-0.4122169	3.1391693
H	-3.8328238	-1.2967065	3.7136558

H	-4.6121324	0.3029730	3.8482889
H	-4.9685145	-0.7287552	2.4605335
H	3.1612928	2.6925799	2.5495148
H	1.9713712	0.9262083	1.5574488
H	1.5448547	2.9628351	2.4333956
H	2.4910972	3.1061920	1.1060716
N	2.3459599	2.5498194	1.9502043
H	-1.9313982	-1.8552412	-0.9546109
H	-0.4441509	-1.2337449	-1.6646647
H	-0.8070762	-1.0794198	0.0469413
H	-0.4966935	-2.6280830	-0.5809227
N	-0.9325480	-1.7232549	-0.7759396

TS2-α

C	2.0461396	-2.3288859	2.9174317
H	-3.0249100	1.0018978	1.4545801
O	1.9729592	0.0838289	1.7428364
C	-0.3820732	1.2877887	0.7092261
H	2.3547399	-0.8493938	4.4821478
H	-0.8771274	1.4971393	-2.9686888
C	2.1947870	-1.9332537	4.3749981
H	1.9083742	-3.4142155	2.8124733
O	-0.8128659	2.3658362	1.0664749
H	2.9150045	-2.0193144	2.3205437
O	0.8457486	-1.7664872	2.3241484
C	-2.8528412	0.1744074	2.1537639
C	-1.6204951	-0.3572995	2.2582429
H	0.4545724	3.1660285	-0.7376571
H	3.0684921	-2.4462426	4.8075130
C	-0.4147961	0.0080248	1.4742557
H	1.3303891	2.0954893	-1.8820991
H	1.3069084	-2.2203466	4.9591659
C	-0.7759624	2.3994126	-2.3441732

H	-1.7245173	2.5803102	-1.8161605
O	0.2054110	1.1112437	-0.5047232
C	0.8580486	-0.5160843	1.8540559
C	0.3749410	2.2651780	-1.3633728
H	-0.5950248	3.2526823	-3.0166913
H	-1.4602024	-1.1664456	2.9791999
C	-4.0271281	-0.2349958	2.9932869
H	-3.7794250	-1.0654457	3.6728196
H	-4.3876862	0.6092417	3.6075934
H	-4.8846153	-0.5448568	2.3695718
H	2.3505857	2.7299930	3.1140933
H	1.9843190	1.3270429	1.9162156
H	1.0211391	2.9050465	2.1164635
H	2.5615444	3.0724168	1.5077136
N	1.9865252	2.5495457	2.1745258
H	-2.0352818	-1.8099035	-0.5889738
H	-0.6167656	-1.4850968	-1.4266625
H	-0.6925818	-1.0510195	0.2971982
H	-0.6712747	-2.7341641	-0.3057285
N	-1.0120970	-1.7953366	-0.5341163

TS2-γ

C	1.7826906	-2.3216439	2.9333526
H	-3.2431299	1.0990374	1.7863157
O	1.8604190	-0.0794174	1.5886729
C	-0.6499161	1.3819435	0.8154191
H	2.5892618	-0.7257443	4.1687395
H	-0.0229031	1.1692308	-2.6854914
C	2.2705997	-1.7744440	4.2663526
H	1.4919106	-3.3782464	3.0284034
O	-1.5833129	2.1592203	0.7489286
H	2.5632473	-2.2441413	2.1626326
O	0.5856459	-1.6729703	2.4795631

C	-3.0176258	0.2110319	2.3811312
C	-1.7579933	-0.2658548	2.4084317
H	-0.1133442	3.4330726	-0.5910990
H	3.1341571	-2.3618872	4.6194030
C	-0.5510046	0.2345640	1.7263334
H	1.3877015	2.7472145	-1.3002991
H	1.4789828	-1.8331017	5.0299733
C	-0.4447988	2.0939926	-2.2614054
H	-1.4983803	1.9160907	-2.0004814
O	0.4144257	1.4994747	-0.0458021
C	0.6414106	-0.4627451	1.9043575
C	0.3396765	2.5319318	-1.0335659
H	-0.4087484	2.8789654	-3.0350343
H	-1.5735022	-1.1521990	3.0230213
C	-4.1543509	-0.4122169	3.1391693
H	-3.8328238	-1.2967065	3.7136558
H	-4.6121324	0.3029730	3.8482889
H	-4.9685145	-0.7287552	2.4605335
H	3.1612928	2.6925799	2.5495148
H	1.9713712	0.9262083	1.5574488
H	1.5448547	2.9628351	2.4333956
H	2.4910972	3.1061920	1.1060716
N	2.3459599	2.5498194	1.9502043
H	-3.2655555	-2.8033134	0.7875447
H	-3.4379699	-1.6235264	-0.5088797
H	-2.9360008	-0.8704003	1.3887896
H	-1.8769835	-2.1255335	0.1489597
N	-2.8543754	-1.9518322	0.3964477

IP (*E*-2b)

C	0.9584703	0.4007858	4.4700085
H	-3.2769208	0.9418645	0.5752475
O	0.2253282	-0.4778261	2.0145609

C	-0.5797246	1.1999721	-0.0495324
H	2.7250364	-0.1643577	3.3435958
H	2.1815362	-0.8525901	-0.9447377
C	2.4659683	0.3313487	4.2912410
H	0.6892755	0.8675390	5.4289114
O	-1.4605498	0.7487547	-0.7371292
H	0.5071282	-0.6011767	4.4176095
O	0.3436657	1.2411395	3.4714067
C	-3.2562613	1.5524482	1.4820671
C	-2.0757528	1.9816615	1.9457650
H	0.2096094	0.9922048	-2.4502309
H	2.9137771	-0.2487181	5.1145170
C	-0.6925786	1.6925808	1.3915510
H	1.9124623	1.4019758	-2.0727605
H	2.9109995	1.3388708	4.2983683
C	1.3753957	-0.6706090	-1.6721593
H	0.4943212	-1.2540896	-1.3663025
O	0.6932433	1.3423868	-0.4606604
C	0.0163752	0.6749256	2.2985432
C	1.0418356	0.8099448	-1.7539314
H	1.7064960	-1.0343294	-2.6586362
H	-2.0503145	2.5858872	2.8610752
C	-4.5746770	1.8725290	2.1217120
H	-4.4599918	2.4894659	3.0272205
H	-5.2353798	2.4116184	1.4193946
H	-5.1113678	0.9481592	2.4009404
H	-0.0914054	2.6145336	1.4575451

Figure 2 (a)

1f

H	6.3044168	6.6682018	0.4928378
O	7.8845904	3.9395231	4.1627204
H	5.9124640	1.3551822	-0.5562027

C	6.3486989	2.6366273	5.9516024
C	6.5657614	3.6105720	1.3889444
C	6.6944715	0.7628595	-0.0579582
C	6.0699685	4.2772776	2.6282498
H	5.4408392	7.7998067	1.5479966
O	6.4734148	4.0354666	0.2571455
C	4.5147742	5.8325089	1.3625158
O	7.1376880	2.4254218	1.6843756
H	3.4933917	6.1694742	1.6151034
H	7.1881043	0.1374754	-0.8196362
H	7.3529125	2.2253448	5.7693840
C	6.3845431	3.6770018	7.0597722
H	6.2191562	0.0966898	0.6794466
C	4.6699500	5.9292623	3.8892489
H	5.6620095	1.8138009	6.1998752
C	4.6148874	7.6425099	-0.4483950
C	6.7154098	3.7939183	3.9028636
H	4.4308693	5.0579880	0.5886712
H	6.7148101	3.2092835	8.0016752
H	8.1574743	2.3670720	-0.1209178
C	5.1447780	5.2718229	2.6188669
H	7.0912822	4.4838587	6.8150189
O	5.8366282	3.1770351	4.7178644
C	5.2997033	7.0228467	0.7739538
H	8.5224513	1.0866032	1.0784290
H	5.3867985	4.1132359	7.2275822
C	7.7173111	1.6694907	0.6072957
H	4.6656055	7.0250993	3.7650032
H	5.2678676	5.6801048	4.7736868
H	3.6251666	5.6332635	4.0910634
H	4.4792547	6.8606687	-1.2172598
C	5.3915767	8.8180427	-1.0446413
H	3.5968494	7.9737719	-0.1708565
H	6.4011449	8.5088946	-1.3636712

H	5.5133716	9.6332718	-0.3109791
H	4.8778416	9.2372764	-1.9249320

$R_{1f\text{-}A}$

H	3.2742007	6.7091395	4.2412324
O	8.5531601	3.3309801	4.6743885
H	8.6907264	1.2555600	0.8904355
C	9.4847208	5.7480627	5.3732750
C	6.3713030	3.1733919	2.6807465
C	7.6027150	1.2164214	0.7187915
C	6.5013068	4.2008417	3.7667850
H	2.9400599	5.3401683	5.3072191
O	5.5134077	3.1552973	1.8089074
C	4.0611035	4.8285495	3.5014476
O	6.8994153	1.9901148	2.9578402
H	3.7896767	3.7639274	3.5553687
H	7.4119427	0.4268026	-0.0261677
H	9.6603827	4.9282570	6.0837219
C	10.6085182	5.8562181	4.3588036
H	7.2646427	2.1693131	0.2827857
C	5.5079412	6.0480598	5.1834136
H	9.3477968	6.6875259	5.9271994
C	1.5935457	5.4899181	3.6071112
C	7.8371679	4.2927228	4.4312921
H	4.0437921	5.1049357	2.4368750
H	11.5480482	6.1016705	4.8793085
H	7.1597828	-0.0266815	2.4654878
C	5.4301417	4.9776363	4.1204824
H	10.7558627	4.9054904	3.8250128
O	8.2027407	5.5346761	4.7230683
C	2.9787481	5.6446967	4.2456431
H	5.7224003	0.8476349	1.7897781
H	10.4044215	6.6517670	3.6256382

C	6.8106754	0.8888249	1.9676762
H	4.5045917	6.2819332	5.5658381
H	5.9294521	6.9715204	4.7531125
H	6.1541838	5.7744535	6.0269141
H	1.6498239	5.8108082	2.5514436
C	0.5077687	6.2833154	4.3356984
H	1.3221847	4.4181721	3.5908255
H	0.7363602	7.3627222	4.3420132
H	0.4000984	5.9609457	5.3858886
H	-0.4710482	6.1586158	3.8459825
C	11.0579347	-0.7670566	2.4345755
H	10.3563138	-1.0871358	5.8301526
H	11.5288348	0.0037071	5.0437796
C	11.0003858	-0.9596635	4.9435583
H	8.7273414	-2.4437054	4.4075729
H	10.0948118	-3.1674056	3.5081767
H	8.7833088	-2.3281349	2.6309554
H	11.7538499	-1.7672107	4.9470354
C	10.1317900	-0.9501056	3.6618111
Li	8.5097688	1.4977977	4.2104986
H	11.5689697	0.2082906	2.4980993
O	9.2127736	0.0770284	3.7147415
H	10.4617054	-0.7746300	1.5065692
H	11.8257165	-1.5567857	2.3547833
C	9.4007497	-2.3092796	3.5448247
C	2.8583474	0.1234476	4.3138450
H	2.3148233	3.3311704	5.5596043
H	3.7163227	2.2666427	5.8394610
C	2.6402279	2.2782618	5.5980095
H	0.5351282	2.6771031	3.8499494
H	0.2789479	1.1072357	4.6641331
H	0.7029828	1.1622522	2.9274830
H	2.0974251	1.7807817	6.4207339
C	2.4003394	1.5991891	4.2279090

Li	3.9419764	3.0325095	2.0837360
H	3.9357149	0.0763684	4.5448168
O	3.1080067	2.2571353	3.2436553
H	2.6994944	-0.3741661	3.3423897
H	2.3155039	-0.4477942	5.0870913
C	0.8866304	1.6333842	3.9074229

$TS_{1f\text{-}A}$

H	-3.5314932	2.4932814	-1.6180822
O	1.9362369	1.3123982	1.0022335
H	2.5937118	-0.7338082	-3.3207023
C	1.4976954	3.9250668	1.1619980
C	0.2399935	-0.4160958	-0.6380951
C	2.0090203	-1.6115582	-3.0037066
C	-0.1908190	0.8441825	-0.0374239
H	-4.4967561	1.6179196	-0.4355928
O	-0.5222234	-1.3352635	-0.9836498
C	-2.5742427	0.6615409	-0.8891632
O	1.5621281	-0.5760693	-0.8187660
H	-3.0739376	-0.3466147	-0.1772468
H	2.4563935	-2.5007343	-3.4772152
H	1.9771857	3.4387398	2.0235727
C	2.5305910	4.4050940	0.1566862
H	0.9777256	-1.5084632	-3.3762235
C	-2.0435988	2.3654532	0.8320631
H	0.8731027	4.7576750	1.5188608
C	-4.5927745	0.7940608	-2.4264145
C	0.8557689	1.6989631	0.5589953
H	-2.1671579	0.1018666	-1.7429830
H	3.1766478	5.1660799	0.6236765
H	3.0893496	-1.8538407	-1.1116145
C	-1.5588988	1.2570752	-0.0756899
H	3.1700734	3.5752401	-0.1785922

O	0.5604883	3.0061578	0.5616892
C	-3.8148340	1.4737923	-1.2931592
H	1.4598060	-2.6350615	-1.1588616
H	2.0452449	4.8580335	-0.7220769
C	2.0580627	-1.7782886	-1.4974878
H	-3.0767315	2.1558084	1.1413532
H	-2.0566644	3.3271513	0.2935709
H	-1.4276533	2.4965224	1.7275006
H	-3.9327639	0.7008242	-3.3084020
C	-5.8696398	1.5367675	-2.8213476
H	-4.8380428	-0.2382285	-2.1217454
H	-5.6510341	2.5671325	-3.1501371
H	-6.5743386	1.6049504	-1.9748982
H	-6.3924998	1.0286913	-3.6474980
C	6.5186203	-1.3697413	-0.9589192
H	6.0172089	-0.5957299	2.3989089
H	6.5663973	0.4825562	1.0895961
C	6.5384482	-0.5673027	1.4270102
H	5.1931505	-2.9490097	1.8486160
H	6.7486225	-3.3173738	1.0418106
H	5.2053006	-3.5280850	0.1643165
H	7.5776108	-0.9082011	1.5825138
C	5.7673119	-1.4271388	0.3946628
Li	3.1129464	-0.0330698	0.4762278
H	6.5267658	-0.3323746	-1.3332431
O	4.4832213	-0.9558999	0.2412657
H	5.9962966	-1.9911221	-1.7061878
H	7.5624848	-1.7229631	-0.8867083
C	5.7394435	-2.8939974	0.8922760
C	-4.2923769	-3.1127402	1.8639719
H	-4.5114283	0.3631359	1.8960764
H	-3.3594407	-0.6668102	2.7890275
C	-4.3574851	-0.6412153	2.3229863
H	-5.9791757	-0.6439596	0.0761873

H	-6.6654423	-1.7956917	1.2512284
H	-5.9147073	-2.3936944	-0.2555227
H	-5.1122600	-0.7881462	3.1124708
C	-4.4662764	-1.7203619	1.2297113
Li	-2.0342291	-2.1771586	-0.5177336
H	-3.3102355	-3.1879472	2.3592700
O	-3.4357118	-1.5487585	0.2778921
H	-4.3530961	-3.8965043	1.0902304
H	-5.0709378	-3.3198090	2.6162960
C	-5.8396474	-1.6338231	0.5389844

$P_{1f\text{-}A}$

H	-3.5314932	2.4932814	-1.6180822
O	1.9362369	1.3123982	1.0022335
H	2.5937118	-0.7338082	-3.3207023
C	1.4976954	3.9250668	1.1619980
C	0.2399935	-0.4160958	-0.6380951
C	2.0090203	-1.6115582	-3.0037066
C	-0.1908190	0.8441825	-0.0374239
H	-4.4967561	1.6179196	-0.4355928
O	-0.5222234	-1.3352635	-0.9836498
C	-2.5742427	0.6615409	-0.8891632
O	1.5621281	-0.5760693	-0.8187660
H	-3.1377007	-0.5584938	-0.0970281
H	2.4563935	-2.5007343	-3.4772152
H	1.9771857	3.4387398	2.0235727
C	2.5305910	4.4050940	0.1566862
H	0.9777256	-1.5084632	-3.3762235
C	-2.0435988	2.3654532	0.8320631
H	0.8731027	4.7576750	1.5188608
C	-4.5927745	0.7940608	-2.4264145
C	0.8557689	1.6989631	0.5589953
H	-2.1671579	0.1018666	-1.7429830

H	3.1766478	5.1660799	0.6236765
H	3.0893496	-1.8538407	-1.1116145
C	-1.5588988	1.2570752	-0.0756899
H	3.1700734	3.5752401	-0.1785922
O	0.5604883	3.0061578	0.5616892
C	-3.8148340	1.4737923	-1.2931592
H	1.4598060	-2.6350615	-1.1588616
H	2.0452449	4.8580335	-0.7220769
C	2.0580627	-1.7782886	-1.4974878
H	-3.0767315	2.1558084	1.1413532
H	-2.0566644	3.3271513	0.2935709
H	-1.4276533	2.4965224	1.7275006
H	-3.9327639	0.7008242	-3.3084020
C	-5.8696398	1.5367675	-2.8213476
H	-4.8380428	-0.2382285	-2.1217454
H	-5.6510341	2.5671325	-3.1501371
H	-6.5743386	1.6049504	-1.9748982
H	-6.3924998	1.0286913	-3.6474980
C	6.8120433	-0.7020603	-0.4023497
H	6.1279678	0.0704669	2.9234250
H	6.6220970	1.1756130	1.6145714
C	6.6775206	0.1324174	1.9688356
H	5.5391433	-2.3554572	2.3867765
H	7.1482664	-2.5923497	1.6379585
H	5.6612707	-2.9547214	0.7139608
H	7.7372789	-0.1104568	2.1642276
C	6.0230288	-0.8083750	0.9265969
Li	3.1129464	-0.0330698	0.4762278
H	6.7393021	0.3263770	-0.7939350
O	4.7076448	-0.4579298	0.7230261
H	6.3738938	-1.3787882	-1.1556168
H	7.8804498	-0.9579528	-0.2898274
C	6.1106986	-2.2645391	1.4481026
C	-4.2923769	-3.1127402	1.8639719

H	-4.5114283	0.3631359	1.8960764
H	-3.3594407	-0.6668102	2.7890275
C	-4.3574851	-0.6412153	2.3229863
H	-5.9791757	-0.6439596	0.0761873
H	-6.6654423	-1.7956917	1.2512284
H	-5.9147073	-2.3936944	-0.2555227
H	-5.1122600	-0.7881462	3.1124708
C	-4.4662764	-1.7203619	1.2297113
Li	-2.0342291	-2.1771586	-0.5177336
H	-3.3102355	-3.1879472	2.3592700
O	-3.4357118	-1.5487585	0.2778921
H	-4.3530961	-3.8965043	1.0902304
H	-5.0709378	-3.3198090	2.6162960
C	-5.8396474	-1.6338231	0.5389844

2f'

O	5.5800600	2.8903350	5.1857480
H	7.4856600	2.4775480	-0.6609840
C	7.0640490	5.1117720	5.6055740
C	6.2372500	2.5697790	2.1029810
C	6.8604710	1.5943690	-0.8613360
C	5.1972560	3.3944590	2.8588630
O	7.4332690	2.6750200	2.2344890
C	4.6777880	5.8395810	2.6749280
O	5.6407940	1.7128880	1.2597940
H	7.4342620	0.9101740	-1.5074820
H	6.4368200	4.7544660	6.4361250
C	8.4478730	4.4857770	5.6519330
H	5.9608660	1.9148270	-1.4099660
C	4.4054870	4.3478660	0.6422260
H	7.1181530	6.2098580	5.6398220
C	5.7348080	3.6633570	4.2716470
H	8.9671300	4.7911810	6.5751640

H	7.3837530	0.6115070	1.0057790
C	4.7580790	4.6373550	2.0790830
H	8.3798710	3.3879900	5.6410080
O	6.4016530	4.8186300	4.3598190
C	4.2315900	7.1457040	2.0794220
H	5.8898920	-0.0134550	0.2375840
H	9.0512640	4.8052380	4.7883320
C	6.4870510	0.8895120	0.4319690
H	4.3272980	2.7379520	3.0037190
H	4.0236130	5.2276200	0.1077270
H	3.6349770	3.5580680	0.5833570
H	5.2839480	3.9681900	0.0905700
C	2.5354080	9.0644680	2.1875280
C	2.9572060	7.7026910	2.7414400
H	4.9301250	5.8902760	3.7409490
H	3.3248880	9.8208460	2.3365760
H	1.6222880	9.4354390	2.6806110
H	2.3304350	9.0125620	1.1045660
H	2.1390940	6.9724050	2.6113400
H	3.1197740	7.7782610	3.8319520
H	4.0704640	7.0603040	0.9924020
H	5.0423290	7.8889680	2.2084030

$R_{1f\text{-}B}$

H	-2.4925865	-0.9955323	2.2025965
O	1.8485633	0.0410669	1.8274544
H	1.3590237	-2.3067874	-2.3734453
C	0.5843512	-0.9095092	3.9512431
C	0.4575899	0.1052795	-0.7708405
C	2.3905798	-1.9359169	-2.2673129
C	-0.1559523	0.3733320	0.5335400
H	-3.7937836	-0.1916120	1.3184206
O	-0.1855565	-0.0321789	-1.8250005

C	-2.1825058	1.1335153	1.9224519
O	1.7864576	-0.0478336	-0.8034714
H	-2.8043576	2.0415674	1.8825021
H	2.9396897	-2.1864062	-3.1896965
H	1.5396186	-1.3832386	3.6846540
C	0.7992278	0.2692659	4.8859351
H	2.8816634	-2.4634508	-1.4353323
C	-2.0734666	1.6530413	-0.4959084
H	-0.0769922	-1.6628247	4.4030976
C	-3.9088286	0.0442736	3.4692908
C	0.6256921	-0.0299811	1.7258401
H	-1.5052356	1.2476930	2.7777220
H	1.2729893	-0.0817264	5.8169007
H	1.9750048	0.1222140	-2.8740068
C	-1.4151601	1.0320771	0.6132723
H	1.4624199	1.0200396	4.4309773
O	-0.1003091	-0.5265316	2.7367235
C	-3.1035563	-0.0795642	2.1717633
H	3.4818768	-0.1002554	-1.8741891
H	-0.1560373	0.7495675	5.1511409
C	2.4479399	-0.4356558	-2.0547453
H	-2.7672299	2.4499636	-0.1998340
H	-2.7444728	0.9638367	-1.0295259
H	-1.4412902	1.9523087	-1.3410457
H	-3.2113986	0.1584045	4.3197833
C	-4.8336986	-1.1483218	3.7216954
H	-4.5043518	0.9755074	3.4442895
H	-4.2640884	-2.0909018	3.7867343
H	-5.5688291	-1.2644328	2.9074892
H	-5.3953402	-1.0327052	4.6627982
C	6.5870979	1.6399305	-0.7394941
H	6.4322651	-0.9360065	1.5982101
H	6.4201040	0.8225291	1.8926921
C	6.7597549	0.0374147	1.1955285

H	6.2728479	-1.8272001	-0.7991749
H	7.7241936	-0.8769449	-1.2419522
H	6.2083513	-0.6860560	-2.1675741
H	7.8640794	0.0503415	1.1742166
C	6.1231689	0.2645900	-0.1983380
Li	3.2354300	0.2931106	0.5926655
H	6.2411963	2.4404527	-0.0642741
O	4.7505160	0.2278084	-0.1102759
H	6.1392340	1.8221979	-1.7309672
H	7.6848168	1.7169146	-0.8354227
C	6.6236034	-0.8448583	-1.1573720
C	-5.1111782	-0.9061862	-3.4470872
H	-5.4381508	0.5829580	-0.3158573
H	-5.4206995	-1.1565569	-0.7081936
C	-5.6484625	-0.1549986	-1.1065580
H	-4.8419598	2.3014811	-2.1086133
H	-6.1279248	1.6731452	-3.1701136
H	-4.4447715	1.7607379	-3.7598742
H	-6.7259995	-0.1082814	-1.3343236
C	-4.7912508	0.1271293	-2.3534385
Li	-1.8027565	-0.4065481	-2.5017025
H	-4.8902464	-1.9241950	-3.0868470
O	-3.4198401	-0.0002093	-2.0289654
H	-4.5015249	-0.7168819	-4.3468417
H	-6.1721180	-0.8697418	-3.7441293
C	-5.0719947	1.5477702	-2.8788990

$TS_{1f\text{-}B}$

H	-2.4925865	-0.9955323	2.2025965
O	1.8485633	0.0410669	1.8274544
H	1.3590237	-2.3067874	-2.3734453
C	0.5843512	-0.9095092	3.9512431
C	0.4575899	0.1052795	-0.7708405

C	2.3905798	-1.9359169	-2.2673129
C	-0.1559523	0.3733320	0.5335400
H	-3.7937836	-0.1916120	1.3184206
O	-0.1855565	-0.0321789	-1.8250005
C	-2.1825058	1.1335153	1.9224519
O	1.7864576	-0.0478336	-0.8034714
H	-2.8043576	2.0415674	1.8825021
H	2.9396897	-2.1864062	-3.1896965
H	1.5396186	-1.3832386	3.6846540
C	0.7992278	0.2692659	4.8859351
H	2.8816634	-2.4634508	-1.4353323
C	-2.0734666	1.6530413	-0.4959084
H	-0.0769922	-1.6628247	4.4030976
C	-3.9088286	0.0442736	3.4692908
C	0.6256921	-0.0299811	1.7258401
H	-1.5052356	1.2476930	2.7777220
H	1.2729893	-0.0817264	5.8169007
H	1.9750048	0.1222140	-2.8740068
C	-1.4151601	1.0320771	0.6132723
H	1.4624199	1.0200396	4.4309773
O	-0.1003091	-0.5265316	2.7367235
C	-3.1035563	-0.0795642	2.1717633
H	3.4818768	-0.1002554	-1.8741891
H	-0.1560373	0.7495675	5.1511409
C	2.4479399	-0.4356558	-2.0547453
H	-2.7672299	2.4499636	-0.1998340
H	-2.8980309	0.8061140	-1.1516429
H	-1.4412902	1.9523087	-1.3410457
H	-3.2113986	0.1584045	4.3197833
C	-4.8336986	-1.1483218	3.7216954
H	-4.5043518	0.9755074	3.4442895
H	-4.2640884	-2.0909018	3.7867343
H	-5.5688291	-1.2644328	2.9074892
H	-5.3953402	-1.0327052	4.6627982

C	6.5870979	1.6399305	-0.7394941
H	6.4322651	-0.9360065	1.5982101
H	6.4201040	0.8225291	1.8926921
C	6.7597549	0.0374147	1.1955285
H	6.2728479	-1.8272001	-0.7991749
H	7.7241936	-0.8769449	-1.2419522
H	6.2083513	-0.6860560	-2.1675741
H	7.8640794	0.0503415	1.1742166
C	6.1231689	0.2645900	-0.1983380
Li	3.2354300	0.2931106	0.5926655
H	6.2411963	2.4404527	-0.0642741
O	4.7505160	0.2278084	-0.1102759
H	6.1392340	1.8221979	-1.7309672
H	7.6848168	1.7169146	-0.8354227
C	6.6236034	-0.8448583	-1.1573720
C	-5.1111782	-0.9061862	-3.4470872
H	-5.4381508	0.5829580	-0.3158573
H	-5.4206995	-1.1565569	-0.7081936
C	-5.6484625	-0.1549986	-1.1065580
H	-4.8419598	2.3014811	-2.1086133
H	-6.1279248	1.6731452	-3.1701136
H	-4.4447715	1.7607379	-3.7598742
H	-6.7259995	-0.1082814	-1.3343236
C	-4.7912508	0.1271293	-2.3534385
Li	-1.8027565	-0.4065481	-2.5017025
H	-4.8902464	-1.9241950	-3.0868470
O	-3.4198401	-0.0002093	-2.0289654
H	-4.5015249	-0.7168819	-4.3468417
H	-6.1721180	-0.8697418	-3.7441293
C	-5.0719947	1.5477702	-2.8788990

$P_{1f\text{-}B}$

H	-2.1131709	-1.3444615	1.5737156

O	1.9964959	0.4506585	2.3390752
H	0.1324085	-2.1509147	-1.7109091
C	1.2315042	1.4556288	4.6751088
C	0.1014870	0.3390967	0.0367404
C	1.2266961	-2.0448223	-1.7688424
C	-0.1680894	0.8089617	1.3500833
H	-3.6016314	-0.5158116	1.0903160
O	-0.7488284	0.3222290	-0.8974023
C	-2.4316058	0.5522546	2.5810488
O	1.3404446	-0.1340111	-0.2228901
H	-3.2817324	1.1763280	2.9084220
H	1.5548211	-2.3838199	-2.7654341
H	1.9025614	0.5842337	4.6924032
C	2.0281133	2.7504133	4.6373588
H	1.6932614	-2.7062435	-1.0217616
C	-2.0048066	2.4756948	1.0586975
H	0.5780084	1.4206032	5.5606080
C	-3.7682286	-1.6084325	2.9480183
C	0.8192062	0.8269386	2.3958743
H	-1.8462843	0.3111189	3.4818272
H	2.6414387	2.8422343	5.5488440
H	1.1956228	0.0692720	-2.2900405
C	-1.5393426	1.3456567	1.6411737
H	2.7026723	2.7678812	3.7683097
O	0.3365030	1.3448876	3.5589234
C	-2.9617146	-0.7544543	1.9634611
H	2.7619754	-0.5094474	-1.5814120
H	1.3577115	3.6231735	4.5832957
C	1.6645747	-0.6062920	-1.5613144
H	-3.0016879	2.8671074	1.2946032
H	-4.7640457	1.6349813	-1.2445570
H	-1.3608697	3.0920926	0.4206946
H	-3.1280546	-1.8541239	3.8143828
C	-4.3150490	-2.8977798	2.3328723

H	-4.6033718	-1.0077739	3.3537257
H	-3.5008795	-3.5385884	1.9543955
H	-4.9885394	-2.6847844	1.4845310
H	-4.8867711	-3.4862391	3.0684314
C	6.6809467	0.1975236	-0.3831399
H	6.1650138	-1.7940620	2.4276186
H	6.6308113	-0.0754950	2.3668555
C	6.6751943	-1.0304326	1.8161465
H	5.4783957	-3.0034218	0.2765486
H	7.0600173	-2.5846998	-0.4528946
H	5.5386116	-2.1451660	-1.2831126
H	7.7362741	-1.3210484	1.7120620
C	5.9467653	-0.8804892	0.4555521
Li	3.0314192	-0.0750190	0.8820333
H	6.6366749	1.1664792	0.1419804
O	4.6374666	-0.5187478	0.6470872
H	6.1726064	0.3210718	-1.3543367
H	7.7413503	-0.0479190	-0.5743113
C	6.0238699	-2.2347305	-0.2960273
C	-3.4235241	-0.6013783	-3.1652168
H	-6.5842054	0.1420770	-1.8794507
H	-5.4870052	-1.1941353	-1.4246790
C	-5.7761106	-0.5160557	-2.2420763
H	-5.7587906	1.9774963	-3.4721769
H	-5.3504716	0.7635692	-4.7043228
H	-4.0978246	1.8962016	-4.1272443
H	-6.1875433	-1.1213588	-3.0643541
C	-4.5734551	0.3008958	-2.7214141
Li	-2.3564511	1.0603007	-0.7743211
H	-3.1248362	-1.2883755	-2.3586395
O	-4.0583237	1.0635126	-1.5806358
H	-2.5421990	-0.0091941	-3.4583453
H	-3.7297162	-1.2060564	-4.0318484
C	-4.9656531	1.2933948	-3.8191681

2f

O	6.7767700	2.2136100	4.5564100
H	8.0677000	2.9409000	-0.8785000
C	6.0529800	3.9650900	6.5156100
C	6.6985300	3.0100200	1.7964300
C	7.3269400	2.2011300	-1.1950100
C	5.6554900	3.5100200	2.8144800
O	7.8992800	3.1656600	1.8362000
C	4.7481500	5.3654300	1.1472800
O	6.0255500	2.2774900	0.8508100
H	7.7930900	1.5254100	-1.9176900
H	5.8458000	2.9047400	6.6937800
C	7.3800300	4.3873500	7.1013500
H	6.5173100	2.7466000	-1.6899200
C	4.3849442	5.4404725	3.4757966
H	5.2445000	4.5292800	6.9976700
C	6.2514400	3.2778300	4.2269800
H	7.3897300	4.2351700	8.1842300
H	7.5896300	0.9102400	0.5408600
C	4.9795500	4.8459500	2.5495200
H	8.1956800	3.8119900	6.6550500
O	6.0129800	4.2794900	5.1157100
H	6.0971300	0.6598100	-0.3621400
H	7.5747500	5.4442500	6.8916300
C	6.7946500	1.4275100	-0.0090700
H	4.8222200	2.8041600	2.7621000
C	4.7022000	6.8649600	1.2396200
C	5.3560500	7.4839700	0.0594000
H	5.2984000	7.2092300	2.0949400
H	3.6762400	7.2437300	1.3761700
H	4.2859142	6.5215225	3.5208866
H	4.0585342	4.9321825	4.3672566
H	3.7685300	5.0267400	0.7730500

H	5.4763100	5.0350400	0.3979600
H	6.3613700	7.0633700	-0.0561900
C	5.4376100	8.9308100	0.4425600
H	4.7595900	7.3181700	-0.8395600
H	5.9997200	9.0338100	1.3823300
H	4.4234000	9.3085700	0.6166000
H	5.9399500	9.4636500	-0.3526700

Figure 2 (b)

1g

O	7.8730150	3.3466650	4.1955010
H	6.8626130	2.0707950	-1.1646670
C	6.1086030	2.8604780	6.1546570
C	7.0199440	3.5761870	1.5335910
C	7.0888810	1.1581750	-0.5931100
C	6.2422050	4.1826370	2.6723340
O	7.6130850	4.1863100	0.6746380
C	4.1869470	5.4785520	3.5074330
O	6.9926970	2.2342090	1.6073910
H	4.6037810	5.2138730	4.4956630
H	7.7171560	0.5079470	-1.2236020
H	6.8800860	2.0950890	5.9834910
C	6.6032490	3.9145130	7.1324340
H	6.1459240	0.6279770	-0.3853820
C	5.2946340	6.0842350	1.3239930
H	5.1928140	2.3738000	6.5213280
C	6.7146630	3.6263150	3.9848300
C	2.9054870	4.6419710	3.3553580
H	6.8252480	3.4455980	8.1050570
H	8.7356070	2.0690360	0.4933670
C	5.3201770	5.1679230	2.5233970
H	7.5261430	4.3862090	6.7637240
O	5.7314030	3.4283370	4.8850290

C	3.8858840	6.9919020	3.5486710
H	8.0916580	0.5770370	1.2473610
H	5.8430260	4.6948270	7.2966340
C	7.8222600	1.4900910	0.6958650
H	4.2522320	6.2138190	0.9874490
H	5.9001650	5.7385400	0.4809620
H	5.6581660	7.0873050	1.6103790
H	2.2887600	4.7527740	4.2623100
H	3.1342290	3.5708660	3.2344650
H	2.2918540	4.9663780	2.5047290
H	3.1725420	7.2138240	4.3593900
H	3.4522930	7.3202490	2.5935730
H	4.7985470	7.5808370	3.7360120

$R_{1g\text{-}A}$

O	7.5386401	3.3620219	5.5172279
H	8.8652752	2.2886139	0.8389591
C	5.1192436	2.2073939	5.7491081
C	7.9550890	4.4781010	2.7131623
C	9.6966885	2.0989273	1.5350023
C	6.8675841	4.7850854	3.6910110
O	7.9390147	4.8432418	1.5465053
C	6.3683571	7.0511043	2.6253977
O	8.9460014	3.7451934	3.2134533
H	5.8134509	6.8675523	1.8139859
H	10.5746321	1.7951626	0.9422144
H	5.9991382	1.5592003	5.8654493
C	4.6842943	2.7964996	7.0790164
H	9.4376201	1.2585588	2.1969366
C	5.0928668	6.2534734	4.6873249
H	4.3086137	1.6375660	5.2743299
C	6.6606889	3.7437900	4.7580942
C	7.8234643	7.1611114	2.1382270

H	4.4090096	1.9801629	7.7656930
H	10.3430742	4.1827981	1.7243626
C	6.1490881	5.9508528	3.6574104
H	5.4988309	3.3691349	7.5474337
O	5.4333312	3.2411298	4.7757373
C	5.8760854	8.3999641	3.1967884
H	10.8403744	3.0902850	3.0964444
H	3.8056548	3.4498325	6.9603988
C	10.0652695	3.3223450	2.3485551
H	5.2583515	7.2620897	5.1005580
H	5.0564894	5.5382032	5.5130908
H	4.1007712	6.2784059	4.2083378
H	7.8609075	7.8759665	1.3024267
H	8.2042760	6.1974324	1.7626255
H	8.5113282	7.5258029	2.9173741
H	5.9640734	9.1713979	2.4170549
H	6.4692694	8.7186445	4.0701962
H	4.8201698	8.3432825	3.5017408
C	12.7491821	2.6744275	7.0949581
H	9.9160060	0.7183767	7.6162809
H	10.3437162	2.2688047	8.3881014
C	10.7597891	1.3654838	7.9105527
H	11.3192618	-0.1650108	5.6727210
H	12.7861397	-0.1011899	6.6960154
H	12.7522857	0.7410504	5.1217491
H	11.3616533	0.8257015	8.6627504
C	11.5762444	1.7647731	6.6571119
Li	9.4128896	3.1961363	5.1868489
H	12.3544235	3.5966248	7.5528556
O	10.7733949	2.4302591	5.7544035
H	13.3476694	2.9670371	6.2159831
H	13.4210954	2.1860579	7.8224573
C	12.1483112	0.4807065	6.0077726
C	3.1468134	6.8314131	-0.1678758

H	6.0265931	7.5271456	-2.0012524
H	5.3190872	8.4692084	-0.6649401
C	5.0835496	7.7663407	-1.4820595
H	5.0660671	5.2404009	-2.5982148
H	3.4327135	5.9416297	-2.7990276
H	3.6950812	4.5789098	-1.6701724
H	4.4147708	8.2790240	-2.1952358
C	4.4622581	6.4722624	-0.9011843
Li	6.5441970	4.8522859	0.3307100
H	3.3573810	7.5260139	0.6636253
O	5.3438784	5.8774478	-0.0275041
H	2.6993652	5.9193472	0.2607104
H	2.4026525	7.3059991	-0.8310728
C	4.1370163	5.5078212	-2.0676060

$TS_{1g\text{-}A}$

O	-2.2150897	0.0579255	-1.7882790
H	1.8000777	2.5425416	-1.1875953
C	-4.2036851	1.5672176	-0.8961983
C	0.2714591	0.1337303	-0.1963428
C	1.8021970	2.0808188	-2.1872472
C	-1.0782038	-0.0955977	0.3214902
O	1.2533879	0.3972845	0.5174524
C	-0.4008314	-1.5579195	2.2952341
O	0.4161059	0.1527818	-1.5294926
H	0.2214775	-0.6591735	3.0897744
H	2.7496313	2.3477322	-2.6836054
H	-3.8136716	1.8062119	-1.8955372
C	-5.3089287	0.5274897	-0.9709868
H	0.9818776	2.5070268	-2.7851760
C	-2.6810661	-0.5372495	2.2447764
H	-4.5548567	2.4919115	-0.4165669
C	-2.1669169	0.3464954	-0.5957643

C	0.7109311	-2.2692380	1.5066781
H	-6.1469931	0.9248389	-1.5662989
H	2.5003577	0.1128803	-1.5437598
C	-1.3310275	-0.7072285	1.5807340
H	-4.9539430	-0.3926145	-1.4583027
O	-3.1039482	1.1371455	-0.0585147
C	-1.0053229	-2.5047552	3.3482546
H	1.6151113	0.1336976	-3.1336766
H	-5.6918913	0.2767849	0.0308724
C	1.6879128	0.5696549	-2.1249438
H	-3.2374963	-1.4896511	2.2465110
H	-3.2970895	0.2376299	1.7900231
H	-2.5248735	-0.2704103	3.3012383
H	0.8700541	-3.2807629	1.9099751
H	1.6888248	-1.7628985	1.5389761
H	0.4538384	-2.3838267	0.4393559
H	-0.1950963	-3.0100816	3.8958268
H	-1.6252588	-3.2963363	2.8865505
H	-1.6276598	-2.0009990	4.1006806
C	-0.9115903	-1.4916781	-6.4751032
H	0.7144929	1.5545868	-6.0188755
H	-1.0262072	1.2590928	-6.2535072
C	-0.0189250	0.8633789	-6.4678654
H	2.3158028	-0.4080328	-5.7370442
H	1.7387489	-1.1814358	-7.2406141
H	1.6831137	-2.0732216	-5.6892903
H	0.1289655	0.8646916	-7.5625395
C	0.1341933	-0.5435420	-5.8365165
Li	-0.8596617	-0.4244003	-3.0154682
H	-1.9289350	-1.1227641	-6.2598198
O	-0.0495195	-0.4721956	-4.4752239
H	-0.8178922	-2.4982265	-6.0340214
H	-0.8019451	-1.5813220	-7.5705794
C	1.5506931	-1.0832358	-6.1568646

C	-0.3319338	0.5644786	5.6849523
H	2.7063280	-1.0971331	5.2576220
H	1.0884814	-1.8140967	5.4690651
C	1.7065666	-0.9304213	5.6908206
H	2.9714775	1.4172337	4.9956668
H	2.0639818	1.7171684	6.4984230
H	1.5252259	2.4717153	4.9745457
H	1.8134856	-0.8574882	6.7856203
C	1.0724446	0.3395432	5.0948703
Li	1.7231820	0.7362291	2.2032417
H	-0.9815684	-0.3029206	5.4884825
O	0.9918900	0.2275237	3.6871744
H	-0.7970674	1.4520582	5.2268217
H	-0.2950648	0.7155719	6.7761250
C	1.9595271	1.5579071	5.4126577

$P_{1g\text{-}A}$

O	-2.2150897	0.0579255	-1.7882790
H	1.8000777	2.5425416	-1.1875953
C	-4.2036851	1.5672176	-0.8961983
C	0.2714591	0.1337303	-0.1963428
C	1.8021970	2.0808188	-2.1872472
C	-1.0782038	-0.0955977	0.3214902
O	1.2533879	0.3972845	0.5174524
C	-0.4008314	-1.5579195	2.2952341
O	0.4161059	0.1527818	-1.5294926
H	0.2823381	-0.5511813	3.3707018
H	2.7496313	2.3477322	-2.6836054
H	-3.8136716	1.8062119	-1.8955372
C	-5.3089287	0.5274897	-0.9709868
H	0.9818776	2.5070268	-2.7851760
C	-2.6810661	-0.5372495	2.2447764
H	-4.5548567	2.4919115	-0.4165669

C	-2.1669169	0.3464954	-0.5957643
C	0.7109311	-2.2692380	1.5066781
H	-6.1469931	0.9248389	-1.5662989
H	2.5003577	0.1128803	-1.5437598
C	-1.3310275	-0.7072285	1.5807340
H	-4.9539430	-0.3926145	-1.4583027
O	-3.1039482	1.1371455	-0.0585147
C	-1.0053229	-2.5047552	3.3482546
H	1.6151113	0.1336976	-3.1336766
H	-5.6918913	0.2767849	0.0308724
C	1.6879128	0.5696549	-2.1249438
H	-3.2374963	-1.4896511	2.2465110
H	-3.2970895	0.2376299	1.7900231
H	-2.5248735	-0.2704103	3.3012383
H	0.8700541	-3.2807629	1.9099751
H	1.6888248	-1.7628985	1.5389761
H	0.4538384	-2.3838267	0.4393559
H	-0.1950963	-3.0100816	3.8958268
H	-1.6252588	-3.2963363	2.8865505
H	-1.6276598	-2.0009990	4.1006806
C	-0.9115903	-1.4916781	-6.4751032
H	0.7144929	1.5545868	-6.0188755
H	-1.0262072	1.2590928	-6.2535072
C	-0.0189250	0.8633789	-6.4678654
H	2.3158028	-0.4080328	-5.7370442
H	1.7387489	-1.1814358	-7.2406141
H	1.6831137	-2.0732216	-5.6892903
H	0.1289655	0.8646916	-7.5625395
C	0.1341933	-0.5435420	-5.8365165
Li	-0.8596617	-0.4244003	-3.0154682
H	-1.9289350	-1.1227641	-6.2598198
O	-0.0495195	-0.4721956	-4.4752239
H	-0.8178922	-2.4982265	-6.0340214
H	-0.8019451	-1.5813220	-7.5705794

C	1.5506931	-1.0832358	-6.1568646
C	-0.3319338	0.5644786	5.6849523
H	2.7063280	-1.0971331	5.2576220
H	1.0884814	-1.8140967	5.4690651
C	1.7065666	-0.9304213	5.6908206
H	2.9714775	1.4172337	4.9956668
H	2.0639818	1.7171684	6.4984230
H	1.5252259	2.4717153	4.9745457
H	1.8134856	-0.8574882	6.7856203
C	1.0724446	0.3395432	5.0948703
Li	1.7231820	0.7362291	2.2032417
H	-0.9815684	-0.3029206	5.4884825
O	0.9918900	0.2275237	3.6871744
H	-0.7970674	1.4520582	5.2268217
H	-0.2950648	0.7155719	6.7761250
C	1.9595271	1.5579071	5.4126577

2g

O	7.0634960	2.5428040	4.0062660
H	7.0732760	-0.0837380	-0.1176870
C	6.2034220	4.1266450	6.0221090
C	7.0149310	3.3861670	1.3287710
C	7.9725070	-0.0022120	0.5112090
C	5.9594730	3.8994430	2.3140480
O	7.5286240	4.0233730	0.4448390
C	4.6014700	5.9217680	1.6703320
O	7.2809590	2.0917910	1.5803050
H	8.8087850	-0.4805740	-0.0243960
H	7.0553560	4.7703610	6.2876230
C	5.0182320	4.3862590	6.9370380
H	7.8033750	-0.5560810	1.4482920
C	6.8573290	6.2382390	2.7847390
H	6.5199190	3.0741010	6.0657540

C	6.3681130	3.4897310	3.7325360
H	5.2835340	4.1290030	7.9754150
H	8.4324990	2.0174320	-0.1448440
C	5.7271270	5.4059680	2.2177440
H	4.7295340	5.4480340	6.9127850
O	5.8667080	4.3473440	4.6376610
C	4.3262290	7.4063510	1.5878590
H	9.2196320	1.5477800	1.3946550
H	4.1509780	3.7752060	6.6412530
C	8.3044450	1.4543080	0.7914660
H	5.0356580	3.3493060	2.1004800
H	6.8595600	7.2678970	2.4070540
H	7.8266020	5.7886630	2.5268680
H	6.8087520	6.2881840	3.8878890
C	3.4782540	5.1091420	1.0663200
H	3.2722470	5.4569930	0.0383340
H	2.5419870	5.2575580	1.6343610
H	3.6670600	4.0297970	1.0125910
H	5.0711870	8.0294010	2.0963970
H	3.3409770	7.6344940	2.0327910
H	4.2697400	7.7338410	0.5336980

$R_{1g\text{-}B}$

O	-0.7656275	-1.7955429	-1.5145818
H	3.1927305	-1.1724042	1.5354294
C	-1.3609037	-1.2506187	-4.0397929
C	0.6352267	-0.1000995	0.2749155
C	2.6949591	-2.1535771	1.5845045
C	0.1872735	0.3704864	-1.0642463
O	0.9553720	0.6321244	1.2072329
C	-0.2745257	2.1986427	-2.7650126
O	0.6645153	-1.4279849	0.4033071
H	-0.9851511	1.4504264	-3.1370904

H	3.0441777	-2.6651721	2.4960328
H	-2.3445420	-1.5098833	-3.6170407
C	-1.4695662	-0.6223157	-5.4118790
H	3.0058583	-2.7599781	0.7197125
C	1.1627689	2.6817178	-0.7234932
H	-0.7541953	-2.1691397	-4.0483910
C	-0.4854338	-0.6704659	-1.9064407
C	0.7706230	2.4214876	-3.8760761
H	-1.9433029	-1.3348846	-6.1049025
H	0.8554242	-1.4020452	2.4841850
C	0.3690470	1.6713648	-1.4858950
H	-2.0824841	0.2920667	-5.3880372
O	-0.7221026	-0.2927162	-3.1566021
C	-1.0859693	3.4801983	-2.4852667
H	0.6710098	-3.0032568	1.6594097
H	-0.4755650	-0.3661016	-5.8098325
C	1.1861375	-2.0274689	1.6437821
H	2.0245956	2.2364172	-0.2097620
H	0.5449911	3.1913192	0.0618882
H	1.5225547	3.4726418	-1.3956697
H	0.2672223	2.7663552	-4.7935748
H	1.3073453	1.4902422	-4.1094175
H	1.5091249	3.1894427	-3.5972944
H	-1.6366539	3.7659565	-3.3957566
H	-0.4478916	4.3308564	-2.2027829
H	-1.8195625	3.3271024	-1.6789589
C	-1.0931075	-6.3153461	1.7834717
H	-2.3332006	-6.3626908	-1.4696428
H	-3.1854867	-5.9073449	0.0291084
C	-2.3660090	-6.5228268	-0.3786831
H	0.1901118	-6.7947924	-1.4193874
H	-0.0528285	-8.0469338	-0.1634613
H	1.0780518	-6.6943230	0.1220813
H	-2.6064109	-7.5844326	-0.1925457

C	-1.0211968	-6.0897552	0.2538282
Li	-0.4743669	-3.1665113	-0.3425976
H	-1.8903682	-5.6873711	2.2143828
O	-0.7725630	-4.7606079	-0.0173564
H	-0.1408689	-6.0173241	2.2539893
H	-1.2949430	-7.3671462	2.0521974
C	0.1108798	-6.9684321	-0.3330353
C	-0.6780442	5.2407684	3.6973366
H	-0.2284835	5.7666176	0.2825421
H	0.8986923	6.1397726	1.6113628
C	-0.1668924	6.0196062	1.3539613
H	-2.3819879	4.4816576	0.7581352
H	-2.8546602	5.6721259	2.0046979
H	-2.7459053	3.9355726	2.4164247
H	-0.6686623	6.9901078	1.5111461
C	-0.7896780	4.8817958	2.1968141
Li	0.5692207	2.2136328	2.0924748
H	0.3806738	5.3662166	3.9810132
O	-0.1292209	3.6935440	1.9447124
H	-1.0957345	4.4233749	4.3079592
H	-1.2122785	6.1726236	3.9511052
C	-2.2846553	4.7440423	1.8248849

$TS_{1g\text{-}B}$

O	-0.8345754	-1.7547639	-1.7348277
H	3.2582827	-1.1939842	1.5495478
C	-0.2561802	-1.4634478	-4.2766343
C	0.6867166	-0.1853758	0.2550587
C	2.7839102	-2.1865316	1.6040687
C	0.2442745	0.2960454	-1.0485520
O	0.9931742	0.5345179	1.2192111
C	-0.5399532	2.1763631	-2.5911920
O	0.7476143	-1.5227411	0.3986391

H	-1.1399898	1.3447714	-2.9801142
H	3.1370398	-2.6834478	2.5225119
H	-1.3580630	-1.4880813	-4.2985030
C	0.3331844	-1.0468849	-5.6078920
H	3.1193648	-2.7905271	0.7464527
C	0.9336960	2.6922304	-0.6295493
H	0.0831587	-2.4649502	-3.9705015
C	-0.2081141	-0.7363460	-2.0138180
C	0.3733783	2.6543272	-3.7348210
H	0.0340012	-1.7672348	-6.3854317
H	0.9187696	-1.4758161	2.4798455
C	0.2660727	1.6781972	-1.3830082
H	-0.0204332	-0.0489369	-5.9095659
O	0.1667686	-0.5090409	-3.2782422
C	-1.5407541	3.2741470	-2.1825372
H	0.7782757	-3.0813062	1.6696992
H	1.4332227	-1.0262027	-5.5635929
C	1.2707909	-2.0942310	1.6429978
H	1.8338851	2.3646437	-0.0952322
H	0.2356404	3.1677067	0.4097817
H	1.1058118	3.6173908	-1.1938342
H	-0.2358480	2.9364428	-4.6093634
H	1.0687107	1.8609879	-4.0433183
H	0.9635690	3.5371899	-3.4418839
H	-2.1776912	3.5297544	-3.0448586
H	-1.0378803	4.1974247	-1.8566293
H	-2.1969064	2.9377782	-1.3649177
C	-1.7809691	-5.3173240	2.5660189
H	-1.5780752	-6.3371209	-0.7571135
H	-2.9562168	-5.5780172	0.0809167
C	-2.0595574	-6.2036992	0.2264223
H	0.6910374	-6.5032474	0.4191411
H	-0.0794171	-7.3992754	1.7642472
H	0.8690717	-5.9211145	2.0933830

H	-2.3849181	-7.1945481	0.5899850
C	-1.0809192	-5.4951627	1.1953811
Li	-0.6727967	-2.9172428	-0.2792090
H	-2.6687140	-4.6732725	2.4491948
O	-0.7097477	-4.2693335	0.6908289
H	-1.0977833	-4.8201589	3.2755223
H	-2.1033904	-6.2751176	3.0116906
C	0.1678712	-6.3923795	1.3834711
C	0.1063408	5.8433583	1.2149375
H	-2.7280431	3.9894946	2.0414986
H	-2.2737974	4.6435965	0.4484568
C	-2.1685512	4.7916811	1.5342066
H	-1.1120036	4.1523446	4.0038279
H	-0.9780259	5.9162320	3.7861149
H	0.4936487	4.9079316	3.7759369
H	-2.6342785	5.7568424	1.7940170
C	-0.6857597	4.7436074	1.9459690
Li	0.5487794	1.9842072	2.1615926
H	0.0216626	5.7264812	0.1225790
O	-0.1469387	3.4744005	1.6335983
H	1.1739084	5.7873446	1.4822449
H	-0.2631020	6.8484189	1.4755790
C	-0.5643864	4.9453609	3.4673063

$P_{1g\text{-}B}$

O	-0.8345754	-1.7547639	-1.7348277
H	3.2582827	-1.1939842	1.5495478
C	-0.2561802	-1.4634478	-4.2766343
C	0.6867166	-0.1853758	0.2550587
C	2.7839102	-2.1865316	1.6040687
C	0.2442745	0.2960454	-1.0485520
O	0.9931742	0.5345179	1.2192111
C	-0.5399532	2.1763631	-2.5911920

O	0.7476143	-1.5227411	0.3986391
H	-1.1399898	1.3447714	-2.9801142
H	3.1370398	-2.6834478	2.5225119
H	-1.3580630	-1.4880813	-4.2985030
C	0.3331844	-1.0468849	-5.6078920
H	3.1193648	-2.7905271	0.7464527
C	0.9336960	2.6922304	-0.6295493
H	0.0831587	-2.4649502	-3.9705015
C	-0.2081141	-0.7363460	-2.0138180
C	0.3733783	2.6543272	-3.7348210
H	0.0340012	-1.7672348	-6.3854317
H	0.9187696	-1.4758161	2.4798455
C	0.2660727	1.6781972	-1.3830082
H	-0.0204332	-0.0489369	-5.9095659
O	0.1667686	-0.5090409	-3.2782422
C	-1.5407541	3.2741470	-2.1825372
H	0.7782757	-3.0813062	1.6696992
H	1.4332227	-1.0262027	-5.5635929
C	1.2707909	-2.0942310	1.6429978
H	1.8338851	2.3646437	-0.0952322
H	0.1722663	3.2185104	0.6125064
H	1.1058118	3.6173908	-1.1938342
H	-0.2358480	2.9364428	-4.6093634
H	1.0687107	1.8609879	-4.0433183
H	0.9635690	3.5371899	-3.4418839
H	-2.1776912	3.5297544	-3.0448586
H	-1.0378803	4.1974247	-1.8566293
H	-2.1969064	2.9377782	-1.3649177
C	-1.7809691	-5.3173240	2.5660189
H	-1.5780752	-6.3371209	-0.7571135
H	-2.9562168	-5.5780172	0.0809167
C	-2.0595574	-6.2036992	0.2264223
H	0.6910374	-6.5032474	0.4191411
H	-0.0794171	-7.3992754	1.7642472

H	0.8690717	-5.9211145	2.0933830
H	-2.3849181	-7.1945481	0.5899850
C	-1.0809192	-5.4951627	1.1953811
Li	-0.6727967	-2.9172428	-0.2792090
H	-2.6687140	-4.6732725	2.4491948
O	-0.7097477	-4.2693335	0.6908289
H	-1.0977833	-4.8201589	3.2755223
H	-2.1033904	-6.2751176	3.0116906
C	0.1678712	-6.3923795	1.3834711
C	0.1063408	5.8433583	1.2149375
H	-2.7280431	3.9894946	2.0414986
H	-2.2737974	4.6435965	0.4484568
C	-2.1685512	4.7916811	1.5342066
H	-1.1120036	4.1523446	4.0038279
H	-0.9780259	5.9162320	3.7861149
H	0.4936487	4.9079316	3.7759369
H	-2.6342785	5.7568424	1.7940170
C	-0.6857597	4.7436074	1.9459690
Li	0.5487794	1.9842072	2.1615926
H	0.0216626	5.7264812	0.1225790
O	-0.1469387	3.4744005	1.6335983
H	1.1739084	5.7873446	1.4822449
H	-0.2631020	6.8484189	1.4755790
C	-0.5643864	4.9453609	3.4673063

2g'

O	4.3293240	3.3002110	3.9698650
H	8.7940990	2.7194230	-0.5372370
C	6.2984940	3.5821810	5.8134650
C	7.1551890	3.7953030	1.7816850
C	8.8031230	1.7465130	-0.0235480
C	5.7130640	4.1336210	2.1677710
O	8.0373460	4.5675290	1.5109920

C	6.4372780	6.5817650	1.9030500
O	7.3003360	2.4544650	1.7770600
H	9.7757890	1.2658090	-0.2182200
H	5.2851380	3.8794090	6.1215680
C	6.5487030	2.1115560	6.1026230
H	8.0133310	1.1101460	-0.4532460
C	3.9884090	5.9220300	1.8965130
H	7.0329130	4.2228190	6.3230540
C	5.4059170	3.7020830	3.6052760
H	6.4949270	1.9299150	7.1884150
H	9.3683600	2.5938560	1.8954220
C	5.2820780	5.5918620	2.0003880
H	5.7912050	1.4821900	5.6121020
O	6.4634640	3.8845570	4.4130090
C	6.3117710	7.6830930	2.9755600
H	8.6421240	0.9581700	1.9981120
H	7.5465000	1.8053580	5.7511510
C	8.6045180	1.9239590	1.4728430
H	5.0734820	3.4869430	1.5508080
C	6.6161640	7.2022180	0.5144840
H	7.5170700	7.8359600	0.4936810
H	5.7603790	7.8421470	0.2418380
H	6.7259700	6.4313020	-0.2644250
H	6.2160540	7.2701800	3.9928210
H	5.4245270	8.3093560	2.7854200
H	7.1995700	8.3363140	2.9699550
H	3.6744120	6.9570210	1.7444430
H	3.2005850	5.1722100	1.9817850
H	7.3531450	6.0021260	2.1280470

Figure 2 (c)

1h

O	7.9199630	3.9902890	3.7116400

H	5.8438150	1.3789020	-0.9216100
C	6.3814260	3.1330230	5.7485180
C	6.5726770	3.5829280	1.0641200
C	6.4828620	0.7057200	-0.3305700
C	6.0605670	4.3465840	2.2457410
O	6.6494610	3.9860590	-0.0770140
C	3.9672340	5.4865240	3.1263150
O	6.9460690	2.3435710	1.4310510
H	6.9713540	0.0016910	-1.0238040
H	7.3178380	2.5834750	5.5700370
C	6.6122950	4.3008400	6.6945560
H	5.8476780	0.1256890	0.3575500
C	5.1763080	6.3965380	1.0938220
H	5.6270550	2.4389570	6.1477380
C	6.7251730	3.9590620	3.5421600
H	6.9617310	3.9264550	7.6705660
H	8.1401790	2.1085470	-0.2491420
C	5.1299660	5.3310570	2.1582090
H	7.3803500	4.9809470	6.2967180
O	5.8450250	3.5599120	4.4805260
H	8.2028800	0.8233210	0.9984910
H	5.6829330	4.8687560	6.8602930
C	7.5368260	1.4912300	0.4327960
H	4.1681260	6.5494460	0.6765190
H	5.8676600	6.1741750	0.2737980
H	5.4850650	7.3572430	1.5431000
C	2.6153380	5.1631980	2.5031750
H	3.9580810	6.5407930	3.4527090
H	4.1153150	4.8578610	4.0116570
C	2.2658210	3.8310120	2.2221120
C	1.6947050	6.1774790	2.1984990
C	0.4551390	5.8741190	1.6241430
C	1.0289690	3.5273520	1.6479220
C	0.1194440	4.5469870	1.3450020

H	1.9458440	7.2194300	2.4206560
H	-0.2499620	6.6787900	1.3976030
H	-0.8484740	4.3067630	0.8966990
H	2.9709980	3.0353580	2.4734350
H	0.7715860	2.4851120	1.4391310

$R_{1h\text{-}A}$

O	6.4813000	2.7197000	4.6146000
H	10.1922000	2.2124000	1.2010000
C	4.0164000	3.0337000	5.6353000
C	6.6383000	2.4473000	1.6589000
C	9.5255000	1.5055000	0.6832000
C	5.8529000	3.4711000	2.4178000
O	6.3139000	2.0447000	0.5447000
C	5.6833000	4.9327000	0.3554000
O	7.7080000	1.9744000	2.2822000
H	10.1509000	0.6902000	0.2849000
H	3.1624000	3.6953000	5.8376000
C	3.6462000	1.5734000	5.8197000
H	9.0460000	2.0121000	-0.1686000
C	4.5447000	5.6336000	2.5115000
H	4.8609000	3.3208000	6.2777000
C	5.6158000	3.1450000	3.8602000
H	3.3075000	1.4106000	6.8554000
H	8.9979000	0.4506000	2.5251000
C	5.3936000	4.6121000	1.8087000
H	2.8285000	1.2845000	5.1414000
O	4.3622000	3.3205000	4.2532000
H	7.8214000	0.2225000	1.1501000
H	4.5110000	0.9175000	5.6396000
C	8.5181000	0.9125000	1.6453000
H	4.9151000	6.6466000	2.3017000
H	4.4622000	5.4882000	3.5913000

H	3.5278000	5.5772000	2.0820000
C	5.9741000	6.3893000	0.0415000
H	4.7841000	4.5861000	-0.2093000
H	6.5182000	4.3227000	-0.0162000
C	7.1808000	6.9799000	0.4547000
C	5.0642000	7.1675000	-0.6897000
C	5.3475000	8.5038000	-0.9931000
C	7.4656000	8.3145000	0.1555000
C	6.5473000	9.0819000	-0.5698000
H	4.1271000	6.7188000	-1.0304000
H	4.6268000	9.0934000	-1.5661000
H	6.7699000	10.1255000	-0.8074000
H	7.9089000	6.3857000	1.0164000
H	8.4101000	8.7560000	0.4851000
C	11.5829000	-0.0656000	4.6357000
H	9.3440000	0.5005000	7.2414000
H	10.7371000	1.4992000	6.7473000
C	10.3325000	0.4730000	6.7523000
H	8.6126000	-1.4692000	5.7934000
H	10.2521000	-2.1776000	5.9007000
H	9.5086000	-1.8663000	4.3055000
H	11.0014000	-0.1582000	7.3636000
C	10.1840000	-0.0380000	5.2985000
Li	8.1834000	1.9520000	4.3267000
H	11.9908000	0.9578000	4.5876000
O	9.3389000	0.7856000	4.5840000
H	11.5041000	-0.4457000	3.6030000
H	12.3023000	-0.7017000	5.1805000
C	9.6144000	-1.4776000	5.3326000
C	2.5885981	4.0700074	-2.9328111
H	2.5253933	0.7599331	-1.8466564
H	3.6024626	1.4887627	-3.0602792
C	2.6095074	1.5721834	-2.5871343
H	0.9753516	2.2280034	-0.4592267

H	0.2509828	2.9220636	-1.9378258
H	0.9685763	3.9954524	-0.7005931
H	1.8416443	1.4158119	-3.3644515
C	2.4728455	2.9406336	-1.8794825
Li	4.8195000	2.2257000	-0.5689000
H	3.5630226	4.0113759	-3.4476612
O	3.4609995	3.0806999	-0.9249997
H	2.5253361	5.0517554	-2.4338042
H	1.7977083	4.0198267	-3.7010121
C	1.0782461	3.0255828	-1.2140610

$TS_{1h\text{-}A}$

O	-0.6267925	2.1052197	-2.0042953
H	2.5249666	2.9911620	1.7406271
C	-2.1806607	0.8526559	-3.7634289
C	0.0292685	0.7366024	0.5182286
C	1.7358687	2.6345735	2.4205979
C	-0.0903923	0.0820218	-0.7959557
O	-0.1134191	0.1543589	1.6049137
C	0.8768997	-2.0994288	0.0331733
O	0.2953366	2.0438367	0.5091004
H	1.7708870	3.2597990	3.3275693
H	-2.3085150	0.0724379	-4.5281582
C	-3.5188584	1.4296307	-3.3351036
H	1.9499569	1.5949716	2.7122670
C	0.3543820	-1.8075331	-2.4173676
H	-1.5165566	1.6370658	-4.1543011
C	-0.7294743	0.8890930	-1.8602650
H	-4.0333196	1.8604163	-4.2092956
H	0.1838904	3.8183359	1.4470946
C	0.3655294	-1.2391646	-1.0162526
H	-4.1658396	0.6483336	-2.9060914
O	-1.5208478	0.1758495	-2.6701151

H	-0.4365039	2.4171687	2.4300842
H	-3.3830193	2.2290235	-2.5916687
C	0.3703075	2.7832046	1.7803561
H	1.1912568	-2.5037819	-2.5515567
H	0.4126756	-1.0345854	-3.1902413
H	-0.5782649	-2.3691323	-2.5932411
C	1.8404930	-3.2253735	-0.2270051
H	-0.2140479	-2.6179432	0.5793686
H	1.2111087	-1.5265225	0.9083849
C	3.1374105	-3.1605635	0.3194796
C	1.4955395	-4.3923143	-0.9367560
C	2.4114107	-5.4343028	-1.1126646
C	4.0542480	-4.2012130	0.1505565
C	3.6968991	-5.3441280	-0.5714611
H	0.4896872	-4.4965761	-1.3496306
H	2.1121784	-6.3271319	-1.6686790
H	4.4116184	-6.1602923	-0.7056027
H	3.4328986	-2.2716198	0.8850349
H	5.0546581	-4.1167558	0.5842688
C	1.3750858	6.9558374	0.4019414
H	-0.9546735	6.6031278	-2.1620240
H	0.8212976	6.6950778	-2.2932144
C	-0.0438567	6.9940250	-1.6773320
H	-2.0543902	6.4083423	0.1375447
H	-1.2469388	7.9214438	0.6501525
H	-1.0505014	6.4263482	1.6091271
H	-0.1005140	8.0970299	-1.6745649
C	0.0917208	6.3921591	-0.2566871
Li	0.1126916	3.4822996	-0.9758180
H	2.2576543	6.6466125	-0.1824070
O	0.1578873	5.0183868	-0.3214279
H	1.4864451	6.5451443	1.4198194
H	1.3731930	8.0578446	0.4737869
C	-1.1358060	6.8246301	0.5837357

C	-1.2337544	-5.2507467	1.7195038
H	-3.8155585	-2.9338667	2.0353639
H	-2.8673725	-3.7222178	3.3326444
C	-3.2308095	-3.8316815	2.2969315
H	-3.1231494	-3.2232508	-0.4003604
H	-3.2580630	-4.9964396	-0.2160696
H	-1.7480112	-4.2764058	-0.8223547
H	-3.9094580	-4.6999643	2.2684183
C	-2.0450409	-4.0019528	1.3290693
Li	-0.9414965	-1.3416042	2.2079009
H	-0.8540491	-5.1489619	2.7491085
O	-1.2333551	-2.8509642	1.4318887
H	-0.3667224	-5.3744825	1.0525005
H	-1.8442377	-6.1675331	1.6655152
C	-2.5774099	-4.1357968	-0.1107120

$P_{1h\text{-}A}$

O	0.1146832	2.5106798	-2.2166149
H	2.3080360	3.0210363	1.8809766
C	0.1864796	1.5087826	-4.6682997
C	0.1176151	0.7244637	0.1699563
C	1.5839741	2.4210809	2.4547494
C	0.0587142	0.3272468	-1.1980835
O	0.0524122	-0.0712167	1.1460229
C	0.9157757	-1.9937472	-1.0900522
O	0.2216558	2.0438042	0.4397459
H	1.5396464	2.8382619	3.4744933
H	0.6660483	0.8832826	-5.4366841
C	-1.1971417	1.9567757	-5.1144685
H	1.9497381	1.3847313	2.5229859
C	-1.2990912	-1.5739431	-2.2505884
H	0.8294023	2.3777402	-4.4649015
C	0.0941480	1.2761749	-2.2837499

H	-1.1194808	2.5410875	-6.0461317
H	-0.1431443	3.5358446	1.7255782
C	-0.0580238	-1.1276697	-1.5082941
H	-1.8525920	1.0922769	-5.3082134
O	0.1407633	0.6733085	-3.5017229
H	-0.5258971	1.8868754	2.3777263
H	-1.6662583	2.5951762	-4.3510115
C	0.2042237	2.4947228	1.8263823
H	-1.1175759	-2.4429505	-2.9000524
H	-1.6868314	-0.7548718	-2.8665438
H	-2.0990344	-1.8414250	-1.5356498
C	1.0202565	-3.4626518	-1.1802640
H	-0.4585308	-4.1618585	1.2171653
H	1.8191880	-1.5176798	-0.6853090
C	2.3108594	-4.0392189	-1.1056379
C	-0.0762841	-4.3545461	-1.2758706
C	0.1179168	-5.7398736	-1.3157189
C	2.5026485	-5.4197068	-1.1518871
C	1.4057380	-6.2826700	-1.2593646
H	-1.0946932	-3.9684482	-1.3080935
H	-0.7505058	-6.3999199	-1.3959054
H	1.5529545	-7.3649597	-1.2971757
H	3.1783170	-3.3783909	-1.0199655
H	3.5165823	-5.8260788	-1.1034239
C	0.0851654	6.9780101	1.4241897
H	-1.4900068	6.6861232	-1.6674620
H	0.1861828	7.1866430	-1.3271888
C	-0.8355250	7.1539880	-0.9124674
H	-2.9585271	5.7857130	0.2216215
H	-2.6875996	7.2834899	1.1659704
H	-2.3151749	5.6848422	1.8786414
H	-1.1784621	8.1922895	-0.7526654
C	-0.8446500	6.3024775	0.3832898
Li	-0.0067727	3.6536532	-0.7566644

H	1.1201268	6.9857343	1.0433266
O	-0.4166874	5.0244947	0.1235092
H	0.0781793	6.4002401	2.3641933
H	-0.2091254	8.0172882	1.6571454
C	-2.2888283	6.2763016	0.9478328
C	-0.4894605	-5.5901459	3.0658266
H	1.9711177	-3.1454407	3.4637112
H	2.1124821	-4.7403094	2.6665002
C	1.5701462	-4.1712316	3.4383831
H	-0.3043749	-2.3010188	4.2221952
H	-0.5880285	-3.7665651	5.2003562
H	-1.7677265	-3.2913923	3.9566338
H	1.7769774	-4.6399916	4.4120179
C	0.0678180	-4.1666429	3.1590291
Li	0.1670705	-1.8284306	1.1295492
H	0.0439509	-6.1670922	2.2946558
O	-0.0858986	-3.5294517	1.8558876
H	-1.5614133	-5.5775912	2.8076733
H	-0.3824989	-6.1158447	4.0275197
C	-0.6914655	-3.3313272	4.1942639

2h

O	5.4791240	2.7794290	5.2097930
H	7.4562090	2.9508460	-0.6524210
C	7.0120420	4.9014370	5.8990140
C	6.2074660	2.7890990	2.1176110
C	6.8325890	2.0874460	-0.9293240
C	5.1671820	3.5452050	2.9430820
O	7.4029360	2.8736470	2.2683030
C	5.4737350	6.0000340	2.5621470
O	5.6116670	2.0216280	1.1932720
H	7.4083860	1.4625440	-1.6312810
H	6.3488950	4.4866800	6.6730700

C	8.3717260	4.2232660	5.9175600
H	5.9339270	2.4537210	-1.4499020
C	3.5135230	4.7939320	1.4757330
H	7.1017450	5.9879410	6.0442760
C	5.6784270	3.6414000	4.3889640
H	8.8744310	4.4177130	6.8791800
H	7.3534070	0.9438470	0.8451100
C	4.7670220	4.8786500	2.3079160
H	8.2666070	3.1350780	5.7970180
O	6.3754610	4.7587810	4.6133170
C	5.2637410	7.3708490	2.0576580
H	5.8593530	0.3904880	0.0237780
H	9.0102690	4.6035170	5.1054180
C	6.4580260	1.2719100	0.2965390
H	4.2800350	2.8981740	2.9938940
H	3.0679720	5.7782880	1.2811100
H	2.7592420	4.1737580	1.9905640
H	3.7067100	4.3044920	0.5037340
C	5.3883230	9.7747150	2.4921940
C	5.5582110	8.4548490	2.9114000
H	5.9169260	8.2493020	3.9241000
C	4.8316210	7.6661620	0.7483070
C	4.6672290	8.9879260	0.3259020
H	4.6531700	6.8546910	0.0405340
C	4.9365760	10.0482420	1.1965110
H	4.3363910	9.1903690	-0.6965890
H	5.6142040	10.5952520	3.1788250
H	4.8077820	11.0816310	0.8636990
H	6.2933210	5.9121040	3.2834360

$R_{1h\text{-}B}$

O	0.6318657	-0.4667067	1.9418828
H	-4.1693922	0.7740931	-2.6129510

C	1.5638248	-2.8893056	1.1418707
C	-1.1809572	-0.5462636	-1.1487517
C	-3.9103615	-0.2875757	-2.7484175
C	-0.2323554	0.1332489	-0.2246135
O	-1.5851321	-1.6916707	-0.9715972
C	-0.6737736	2.5378194	-1.0033192
O	-1.5467272	0.1529281	-2.2180020
H	-4.5657088	-0.7011341	-3.5317612
H	1.2583329	-3.8724261	0.7442313
C	3.0474707	-2.6218721	0.9953120
H	-4.1166547	-0.8293219	-1.8135396
C	1.1133294	2.0727879	0.6785894
H	1.2187926	-2.7659560	2.1769657
C	0.4263287	-0.7768823	0.7732190
H	3.6027229	-3.3728070	1.5802349
H	-2.2498324	0.0828337	-4.1069369
C	0.0617106	1.4811679	-0.2023335
H	3.3628697	-2.7135860	-0.0554746
O	0.7903548	-1.9607310	0.2943325
H	-2.1933169	-1.5102544	-3.2890037
H	3.3304853	-1.6252625	1.3699925
C	-2.4614904	-0.4511316	-3.1701887
H	1.5278859	2.9744460	0.2050370
H	1.9348255	1.3850805	0.9171139
H	0.6517199	2.3958868	1.6494911
C	0.1555247	3.1672565	-2.1169522
H	-0.9284408	3.3265940	-0.2755105
H	-1.6137309	2.1548355	-1.4119964
C	0.7620283	2.3773676	-3.1081765
C	0.3074027	4.5607815	-2.1861988
C	1.0384635	5.1529727	-3.2212429
C	1.4970999	2.9668795	-4.1402040
C	1.6367288	4.3573061	-4.2017952
H	-0.1544276	5.1923187	-1.4214600

H	1.1428274	6.2406911	-3.2570725
H	2.2117672	4.8176439	-5.0095478
H	0.6541882	1.2909078	-3.0733550
H	1.9641534	2.3356279	-4.9012308
C	1.3800016	-6.4526928	-1.5113537
H	-0.9310979	-6.8118861	1.0707607
H	0.8387995	-6.6471968	1.1906248
C	0.0180961	-6.9944720	0.5400405
H	-2.0859258	-6.5680163	-1.1976871
H	-1.0241128	-7.8142617	-1.9169999
H	-1.1216232	-6.1856771	-2.6487801
H	0.1327695	-8.0829793	0.3961006
C	0.0293210	-6.2091212	-0.7940705
Li	-0.7021604	-3.3102558	-0.5960081
H	2.2125188	-6.0962374	-0.8810480
O	-0.1376113	-4.8623111	-0.5512131
H	1.4062575	-5.8830176	-2.4550740
H	1.5573260	-7.5179460	-1.7420763
C	-1.1149354	-6.7367433	-1.6931102
C	-1.4901446	4.2844579	3.0581645
H	-0.6620720	2.8350506	6.1123609
H	-2.1862537	2.6858624	5.1992697
C	-1.3178965	3.3401010	5.3837557
H	1.3507541	3.9894985	5.0537977
H	0.3799292	5.4643507	4.7674372
H	1.2298069	4.6682318	3.4118117
H	-1.6815191	4.2779529	5.8383793
C	-0.5490713	3.5765599	4.0630689
Li	0.2509189	0.7956807	3.2565045
H	-2.3436739	3.6274772	2.8220116
O	-0.1262531	2.3681103	3.5432233
H	-0.9523825	4.4964508	2.1175724
H	-1.8832588	5.2404593	3.4443552
C	0.6691783	4.4868065	4.3441218

$TS_{1h\text{-}B}$

O	1.0048846	-0.2970783	2.0552573
H	-3.1369456	0.5817399	-3.4246500
C	1.5747710	-2.8780002	1.6712561
C	-0.6270267	-0.6955501	-1.1990486
C	-2.8713867	-0.4871430	-3.4343008
C	0.0517813	0.0502744	-0.1191482
O	-1.0732849	-1.8374835	-1.1057286
C	-0.7973339	2.3372782	-0.9362027
O	-0.6994752	-0.0413989	-2.3658086
H	-3.3264630	-0.9421038	-4.3289197
H	1.2030371	-3.8877193	1.4254341
C	3.0770549	-2.7528201	1.5126653
H	-3.3064264	-0.9738798	-2.5486876
C	0.9798413	2.2340054	0.7671736
H	1.2398180	-2.5785037	2.6733901
C	0.6686710	-0.7453171	0.9480183
H	3.5694129	-3.4423208	2.2177392
H	-0.9259735	-0.1930643	-4.3619126
C	0.1360654	1.4705572	-0.0947423
H	3.3890425	-3.0354863	0.4952959
O	0.8724192	-2.0446348	0.6866426
H	-1.0998385	-1.7460572	-3.4854021
H	3.4341035	-1.7333355	1.7276193
C	-1.3646688	-0.6791639	-3.4789512
H	1.1549403	3.2558692	0.4050327
H	1.8991933	1.7498188	1.1176513
H	0.3592716	2.4742861	1.9202428
C	-0.1292823	3.1713986	-2.0199524
H	-1.2750482	3.0288774	-0.2219497
H	-1.6080001	1.7463434	-1.3776961
C	0.8995393	2.6553174	-2.8251111
C	-0.5626077	4.4860477	-2.2558841

C	0.0053411	5.2618002	-3.2713713
C	1.4732773	3.4304979	-3.8366015
C	1.0272593	4.7359892	-4.0664358
H	-1.3578884	4.9104292	-1.6351625
H	-0.3490794	6.2829823	-3.4367136
H	1.4771809	5.3407762	-4.8583209
H	1.2513331	1.6351880	-2.6595588
H	2.2756393	3.0103406	-4.4496201
C	-1.1384707	-6.8627385	-0.9026221
H	1.9211070	-6.5715158	0.7395107
H	1.6139294	-6.5637427	-1.0154934
C	1.2274112	-6.9185793	-0.0456102
H	-0.0273704	-6.4502981	2.3734479
H	-0.7666124	-7.9088408	1.6511860
H	-1.7005890	-6.3863061	1.7661717
H	1.2388044	-8.0229677	-0.0481819
C	-0.1852012	-6.3297162	0.1953347
Li	-0.4535023	-3.3748074	-0.2566493
H	-0.7914688	-6.5225280	-1.8928962
O	-0.1346223	-4.9546536	0.1603208
H	-2.1528849	-6.4592379	-0.7433934
H	-1.2042554	-7.9650959	-0.9186206
C	-0.6998418	-6.8090037	1.5757907
C	-1.6470233	4.2688983	2.7705442
H	-0.3451560	3.0389815	5.7573657
H	-1.9378899	2.6977733	5.0214380
C	-1.1251099	3.4392739	5.0881095
H	1.4122435	4.3320413	4.4441662
H	0.2760350	5.6922713	4.2212035
H	1.0477124	4.9311859	2.8055861
H	-1.5311645	4.3541533	5.5500565
C	-0.5419467	3.7180384	3.6917045
Li	0.5634973	0.8959401	3.3221608
H	-2.4527139	3.5258878	2.6582175

O	-0.0571724	2.4969047	3.1733722
H	-1.2432282	4.4926333	1.7693400
H	-2.0837727	5.1984116	3.1703781
C	0.6132901	4.7315553	3.7985500

$P_{1h\text{-}B}$

O	0.7031883	0.0530765	1.0390991
H	-2.2988964	-0.4519128	-5.0259917
C	0.6026173	-2.5648082	1.5756543
C	0.1280413	-1.0506024	-2.4245925
C	-1.7011804	-1.3778055	-5.0199704
C	0.3723534	-0.2050948	-1.2910397
O	0.0385577	-2.2842303	-2.4491502
C	-0.9380243	1.9492954	-1.7711060
O	0.0035312	-0.3449912	-3.5850654
H	-1.8396431	-1.8800273	-5.9916462
H	0.1260730	-3.5523277	1.4712237
C	2.0516809	-2.6964322	2.0078676
H	-2.0863791	-2.0441787	-4.2340459
C	1.5536730	1.9871314	-1.3401960
H	0.0321158	-1.9153147	2.2539190
C	0.5350721	-0.6923259	0.0326894
H	2.0913833	-3.1696018	3.0031140
H	0.1700857	-0.4303882	-5.5938843
C	0.4078865	1.2836492	-1.4695990
H	2.6076032	-3.3425531	1.3103272
O	0.4916218	-2.0281090	0.2256735
H	0.3584939	-2.0094794	-4.7722008
H	2.5515100	-1.7176604	2.0710742
C	-0.2265703	-1.0787547	-4.7972732
H	1.5894926	3.0744555	-1.4564922
H	2.5057495	1.4646217	-1.1947309
H	1.4548466	4.0361190	2.0385354

C	-1.0105190	3.4541782	-1.6594908
H	-1.6883431	1.4910186	-1.1054229
H	-1.2122349	1.6241125	-2.7884343
C	-0.4821425	4.2914587	-2.6573391
C	-1.6129183	4.0593657	-0.5410638
C	-1.6687771	5.4533892	-0.4130491
C	-0.5328186	5.6833119	-2.5321446
C	-1.1208884	6.2710441	-1.4072131
H	-2.0709759	3.4262018	0.2257832
H	-2.1643220	5.9019400	0.4532809
H	-1.1683407	7.3591920	-1.3148252
H	-0.0276756	3.8438359	-3.5458005
H	-0.1168568	6.3140200	-3.3225864
C	-0.6614335	-7.0481203	-1.3431064
H	0.3886103	-6.3997184	1.9151040
H	1.3880287	-6.8565522	0.5124784
C	0.3768385	-6.9290754	0.9469903
H	-2.0632443	-5.7947791	1.5892998
H	-2.3821187	-7.3824415	0.8264261
H	-2.7917345	-5.8653878	-0.0333798
H	0.1562255	-7.9944058	1.1406362
C	-0.6458187	-6.2597814	-0.0077946
Li	0.0285744	-3.5240496	-1.0528518
H	0.3351960	-6.9999407	-1.8138513
O	-0.3040584	-4.9488706	-0.2248991
H	-1.3837564	-6.5861093	-2.0373533
H	-0.9344707	-8.1114014	-1.2165958
C	-2.0552486	-6.3447204	0.6331457
C	-0.0220778	4.5517524	4.1395160
H	2.0504403	1.8049423	4.7199404
H	0.2689364	1.8229594	4.5275847
C	1.1429776	2.4197831	4.8354743
H	3.4049457	3.8956176	4.2551044
H	2.4528893	4.8402072	5.4338743

H	2.5940051	5.4053234	3.7528570
H	1.0303739	2.6550528	5.9042084
C	1.2482983	3.7050693	4.0140781
Li	1.0328297	1.6169931	1.8126464
H	-0.9085557	3.9741051	3.8350523
O	1.3805348	3.2666128	2.6285816
H	0.0401277	5.4528556	3.5071979
H	-0.1678143	4.8842455	5.1790423
C	2.4988429	4.5068248	4.3854603

2h'

O	4.2943420	1.3354070	3.0648430
H	8.1733330	4.6702380	6.3932660
C	2.5533700	1.5714470	1.0081540
C	5.0196160	3.7471070	4.4217090
C	7.2618890	4.2210980	6.8155060
C	5.0473220	3.6207420	2.8957010
O	4.3378940	3.0776520	5.1586590
C	5.7550860	5.5649590	1.3287640
O	5.8854990	4.6855240	4.8357760
H	7.2950650	4.3492110	7.9097630
H	1.6031990	1.6749680	1.5525450
C	2.3331970	1.5976340	-0.4949470
H	7.2616860	3.1412400	6.5981200
C	3.4208410	5.3873150	2.2806970
H	3.0524250	0.6445710	1.3268210
C	4.2288450	2.3915080	2.4883820
H	1.7110480	0.7390620	-0.7962780
H	6.0309770	5.9736390	6.4577660
C	4.6639350	4.9046550	2.1580960
H	1.8182010	2.5210130	-0.7983610
O	3.4445970	2.6268990	1.4255730
C	5.4355510	6.9382990	0.7827130

H	5.1026570	4.4571980	6.6859520
H	3.2916260	1.5410910	-1.0334880
C	6.0177900	4.8918350	6.2580220
H	5.9932310	4.8875390	0.4891370
H	6.6663140	5.6111610	1.9455340
C	5.6731620	8.0871050	1.5555360
C	4.8891390	7.1006850	-0.5000920
C	4.5893360	8.3724300	-0.9992400
C	5.3754030	9.3598390	1.0612640
C	4.8320380	9.5070110	-0.2194630
H	4.6977340	6.2176450	-1.1175300
H	4.1674040	8.4766350	-2.0027710
H	4.6016670	10.5024130	-0.6087010
H	6.0980380	7.9785210	2.5579610
H	5.5712070	10.2417710	1.6775710
H	3.1191730	6.3191700	1.7970500
H	2.6652640	4.8645000	2.8741450
H	6.0856240	3.3695760	2.6328980

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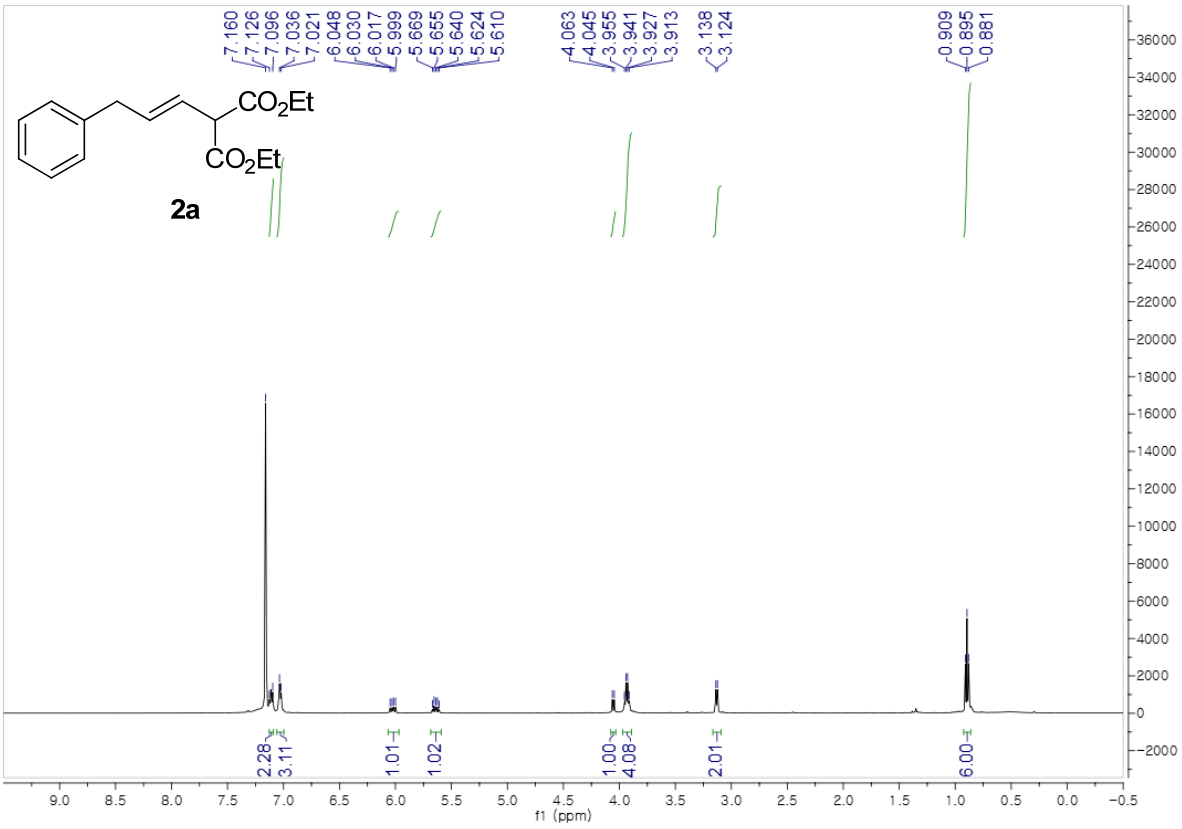
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5.624
5.610
4.063
4.045
3.955
3.941
3.927
3.913
3.138
3.124
0.909
0.895
0.881
CO2Et
CO2Et
2a
2.28
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1.01
1.02
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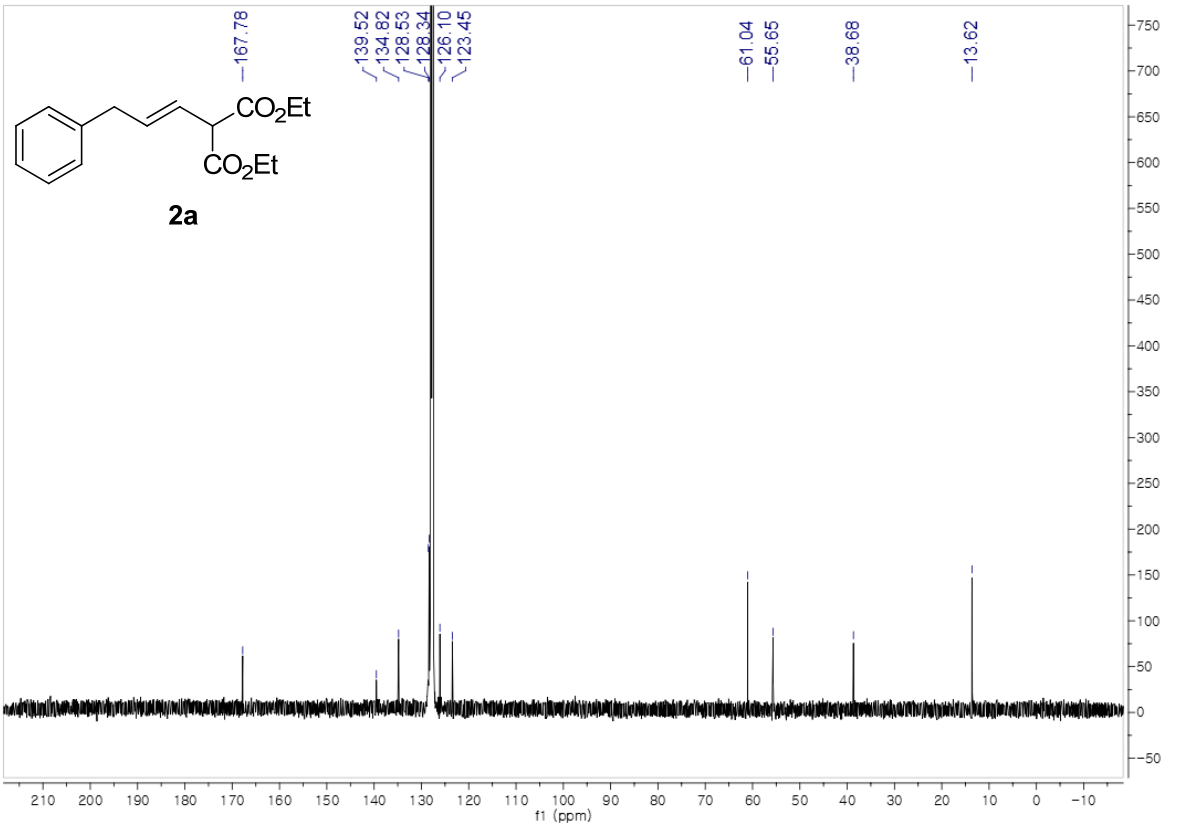
6.00
f1 (ppm)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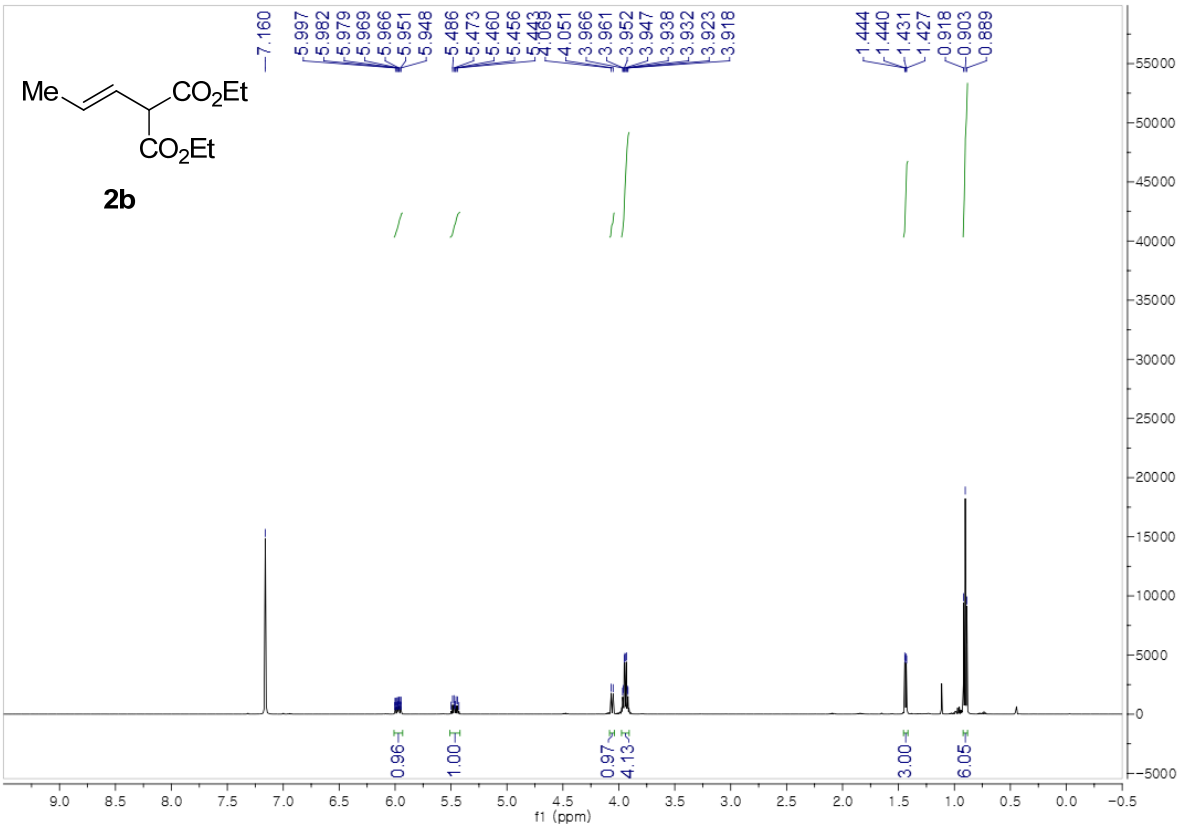
CO2Et
2a
f1 (ppm)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CO2Et
2b
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5.460
5.456
4.069
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3.947
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3.923
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1.444
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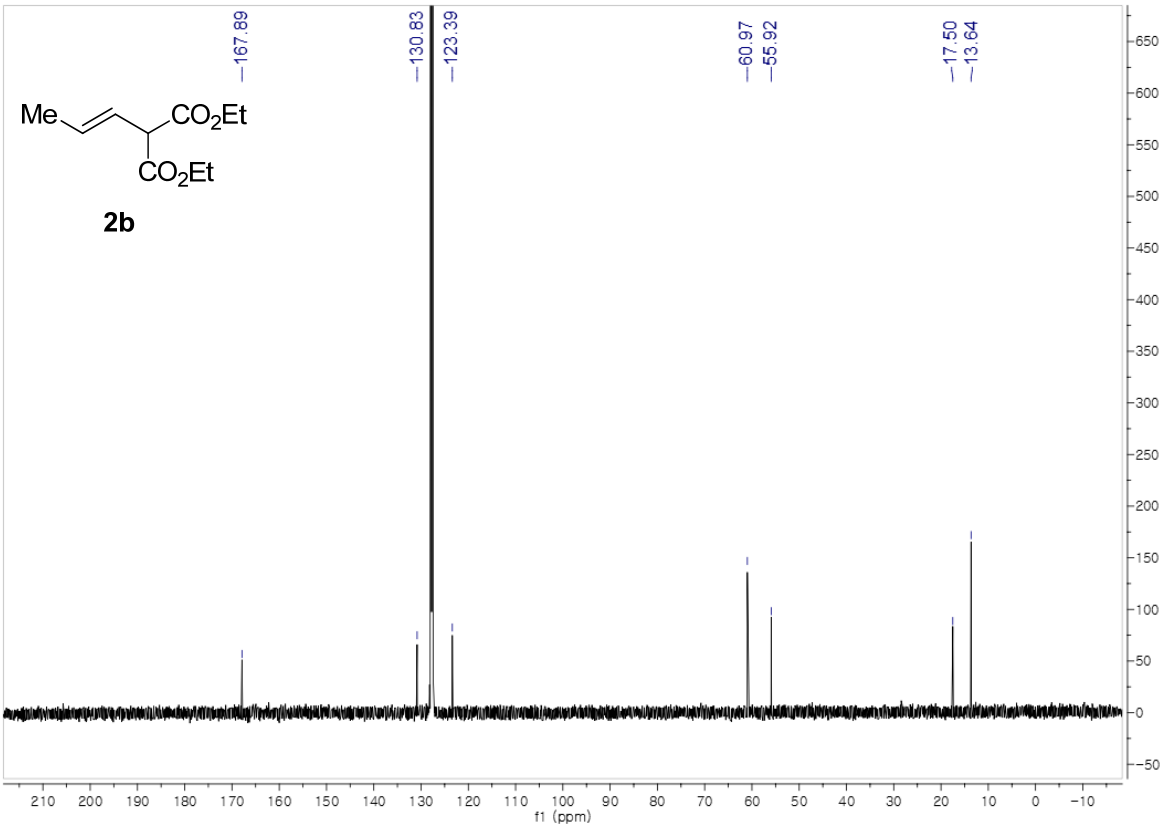
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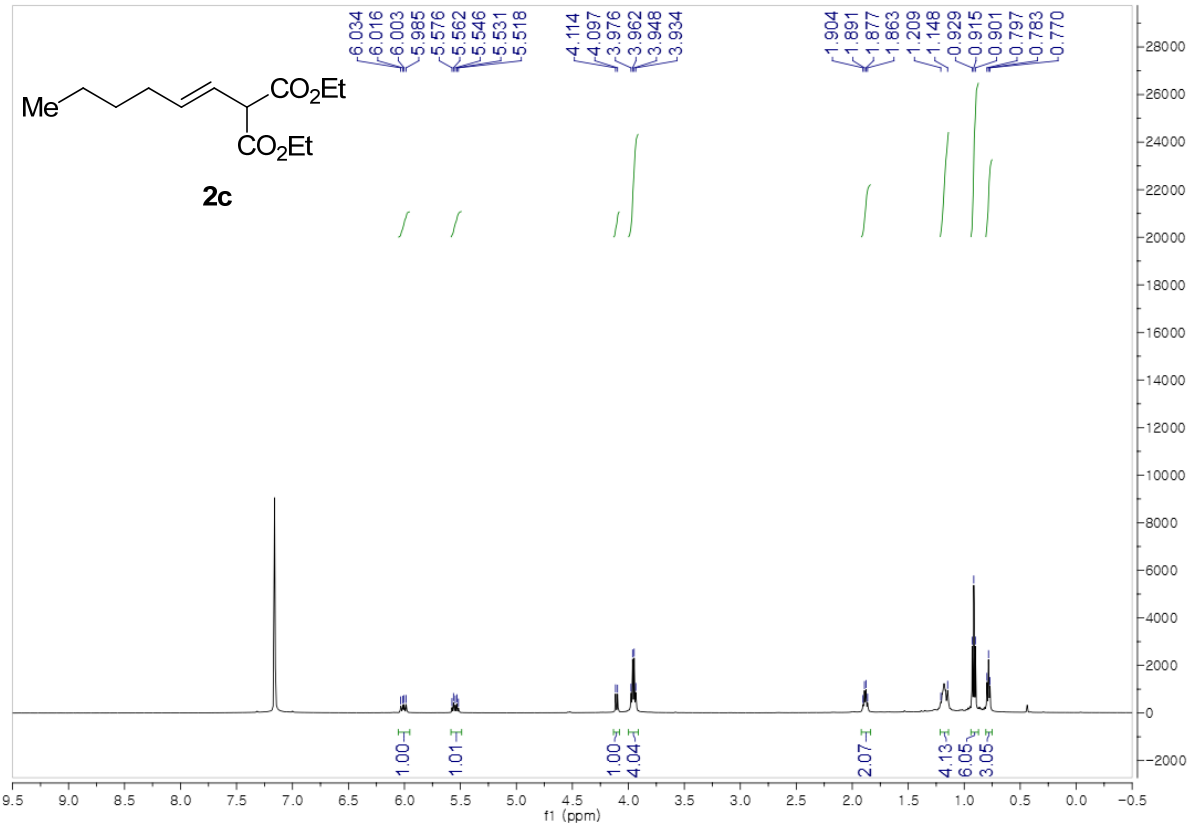
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4.097
3.976
3.962
3.948
3.934
1.904
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1.877
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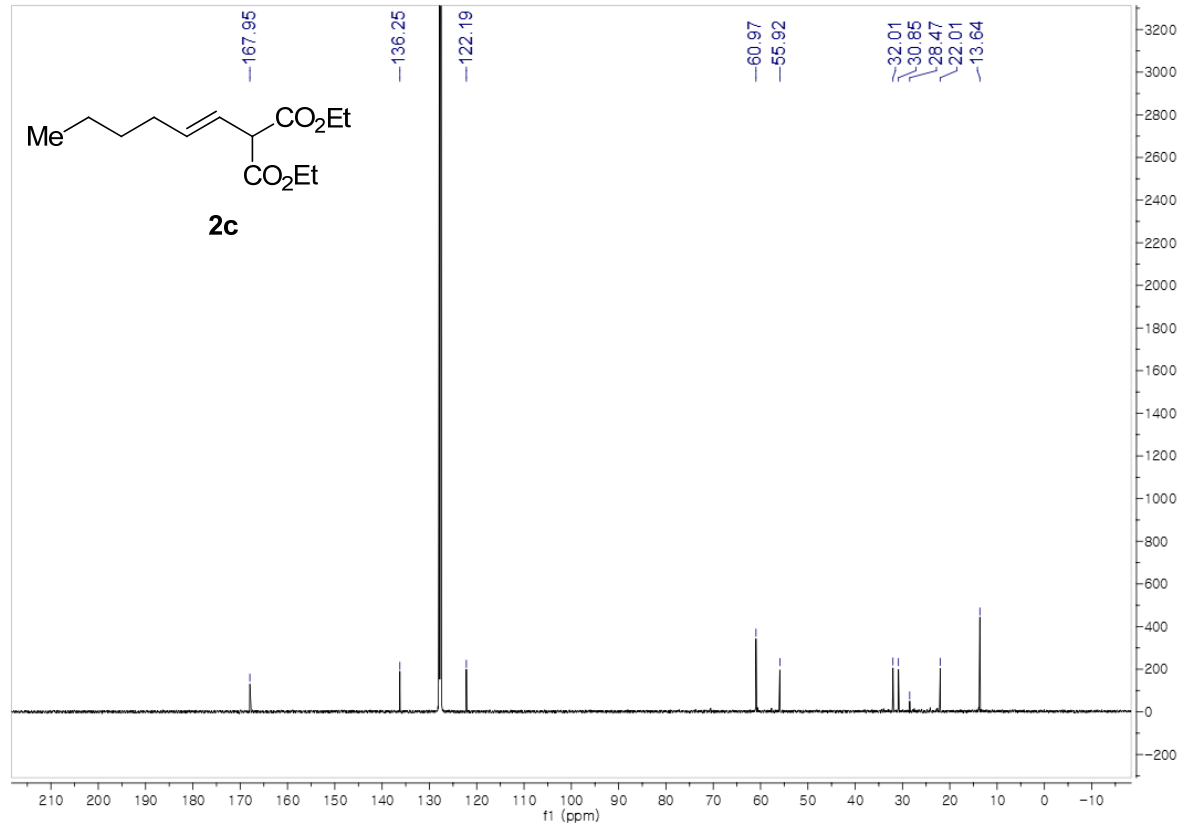
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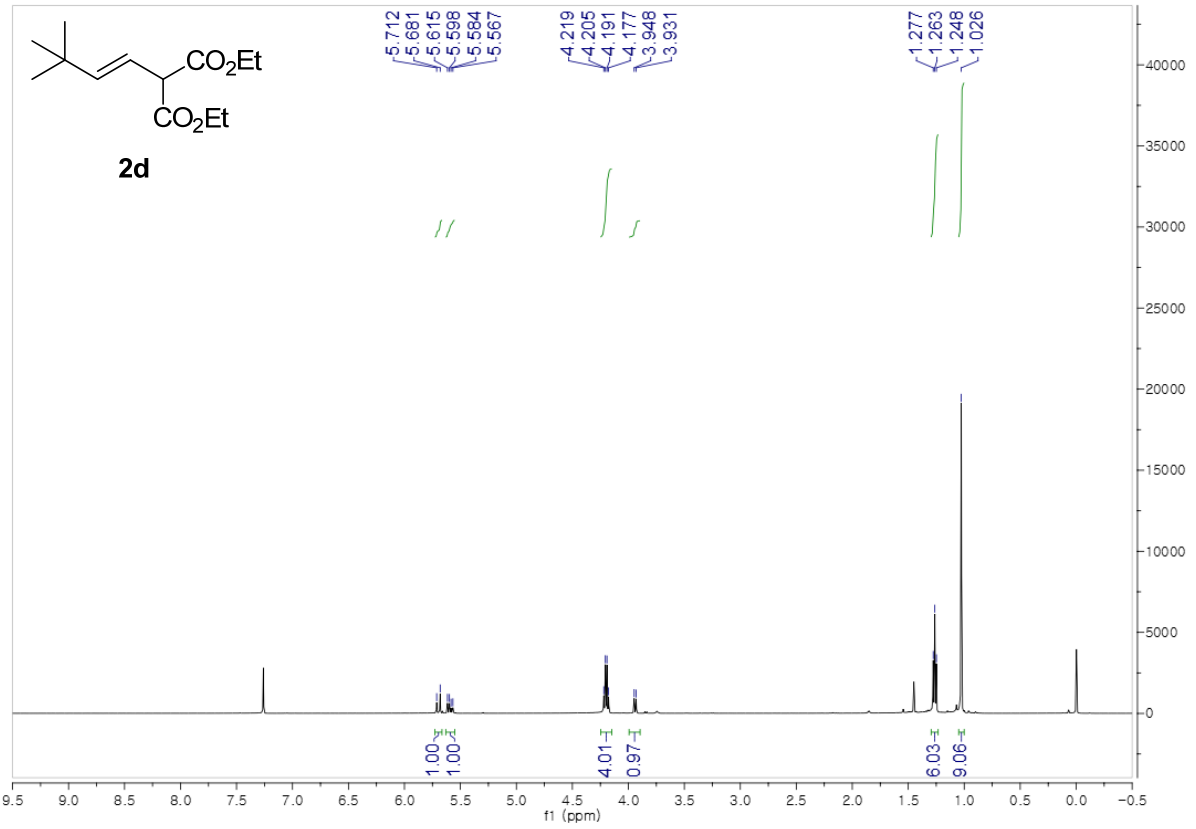
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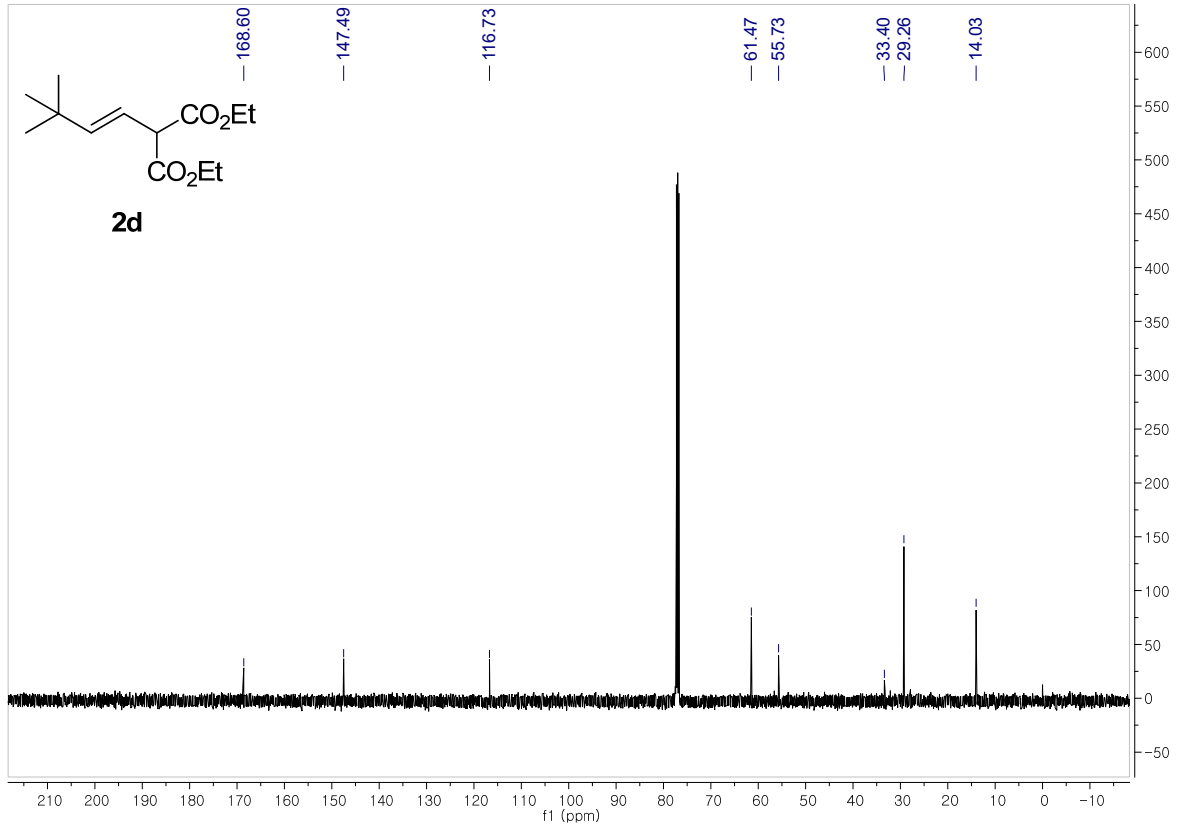
f1 (ppm)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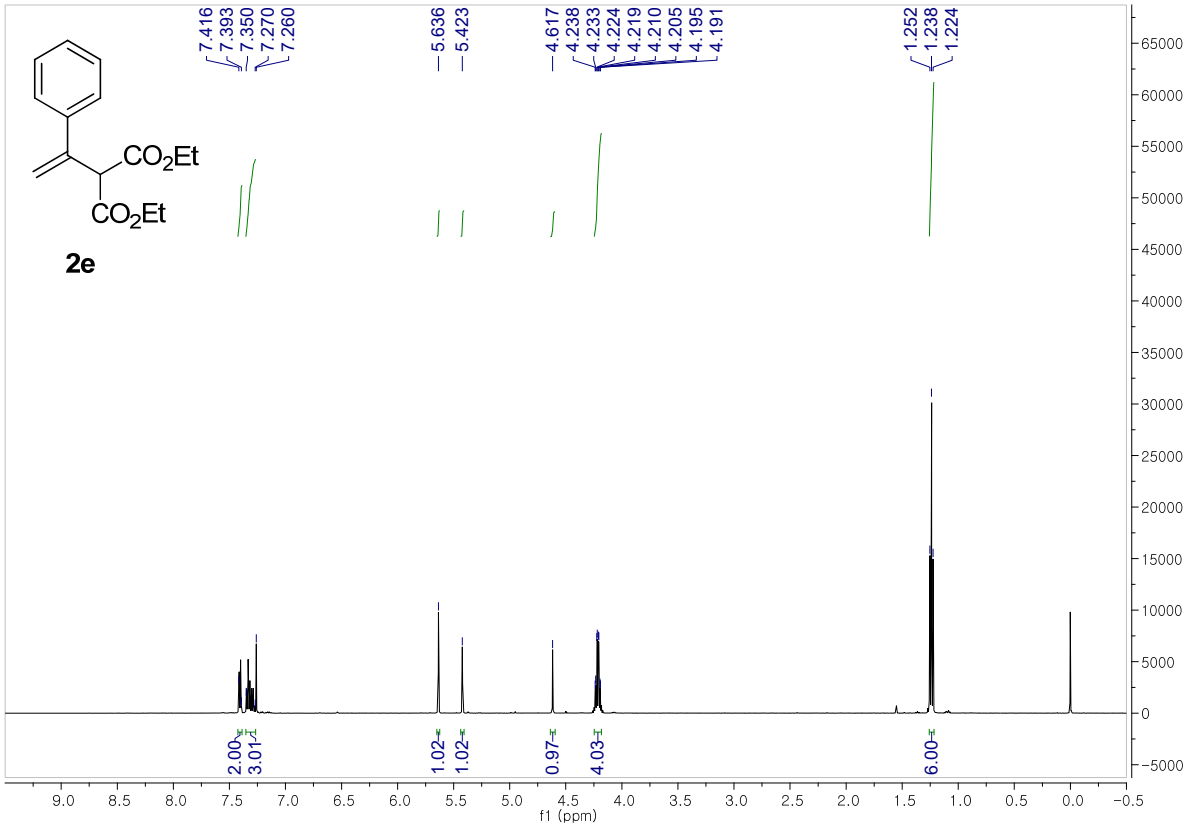
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4.205
4.195
4.191
1.252
1.238
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CO2Et
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2e
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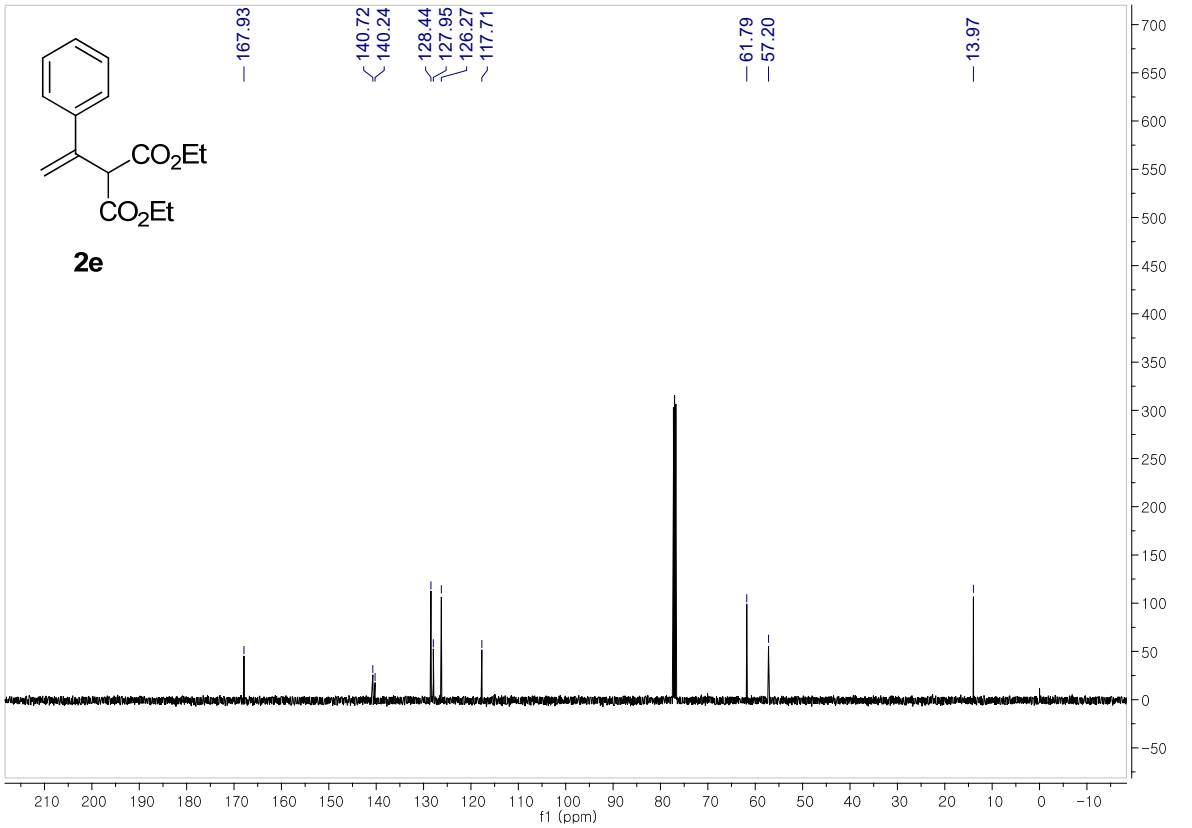
f1 (ppm)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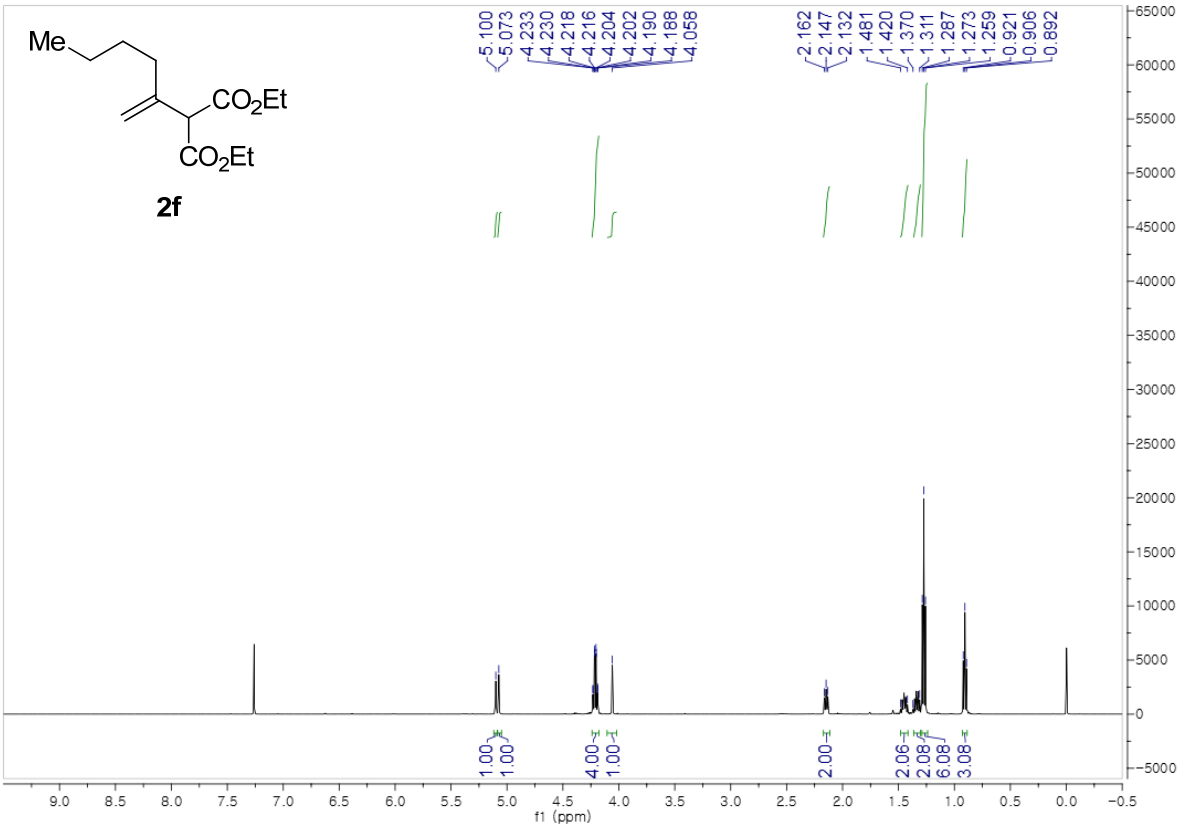
f1 (ppm)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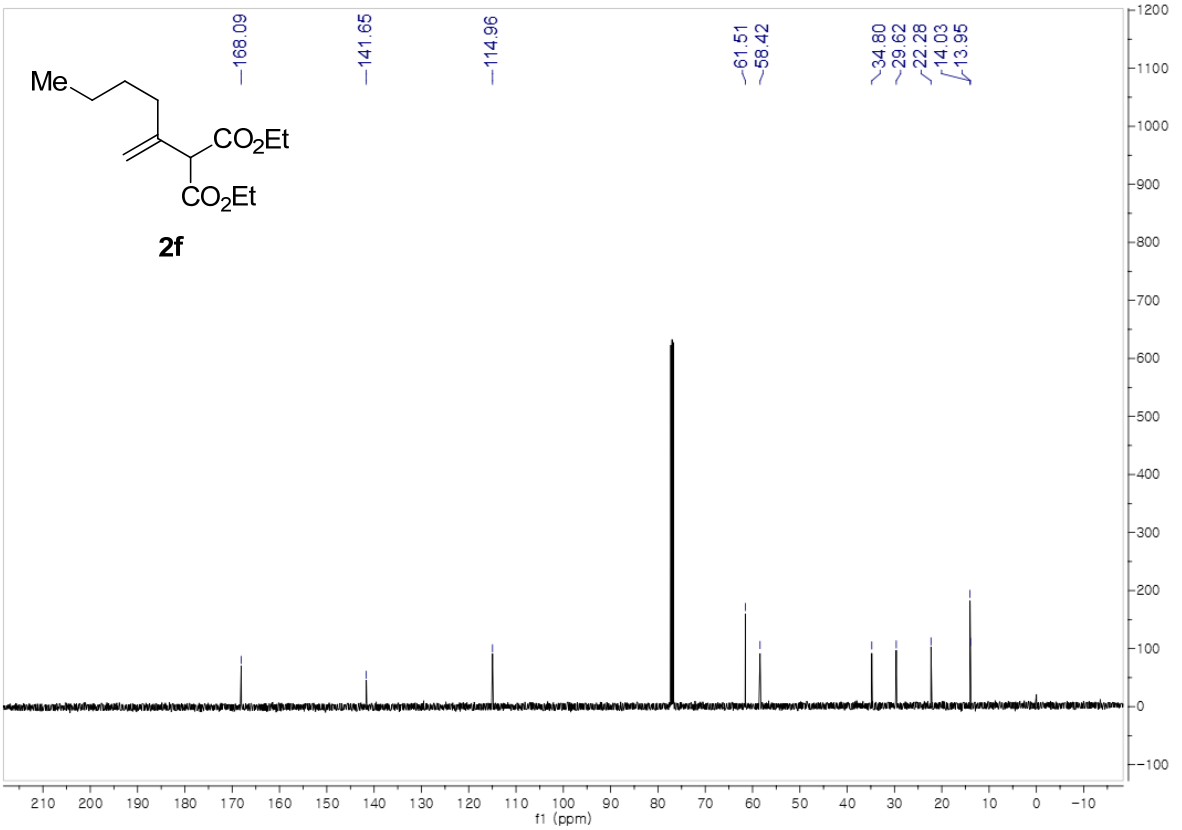
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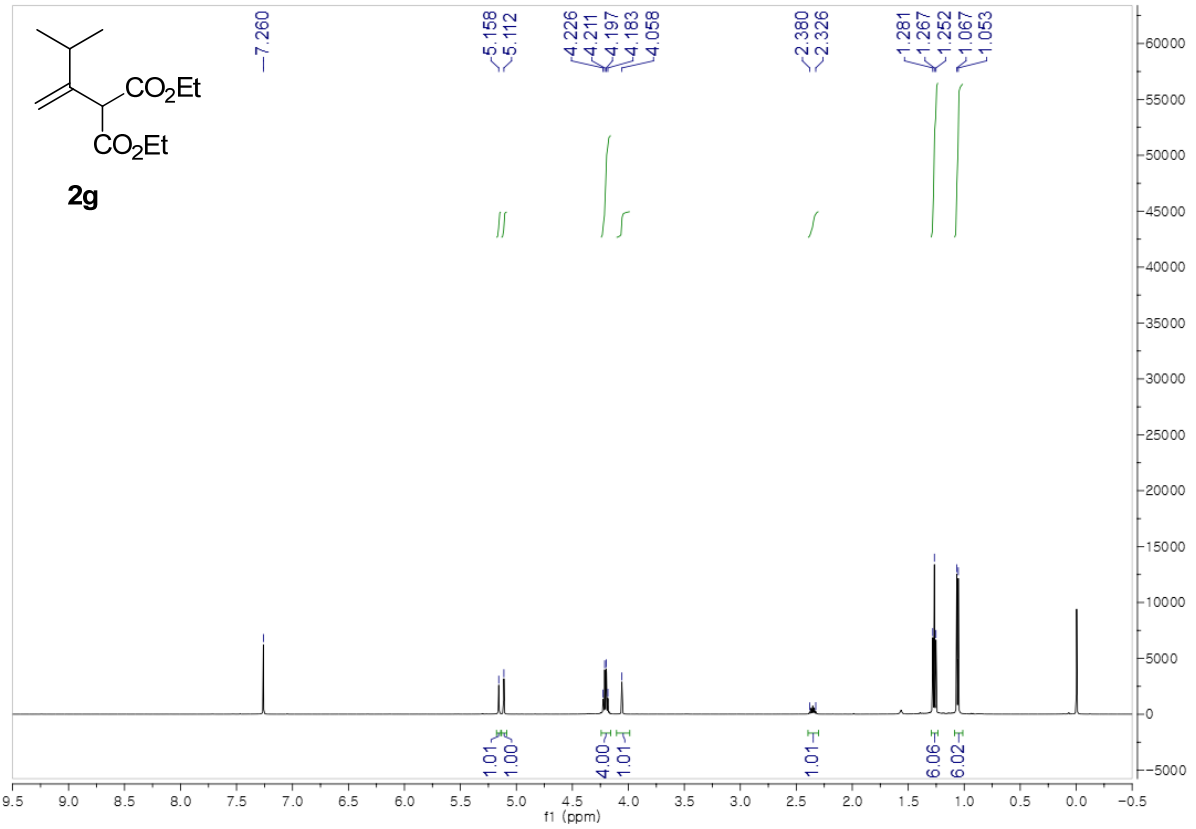
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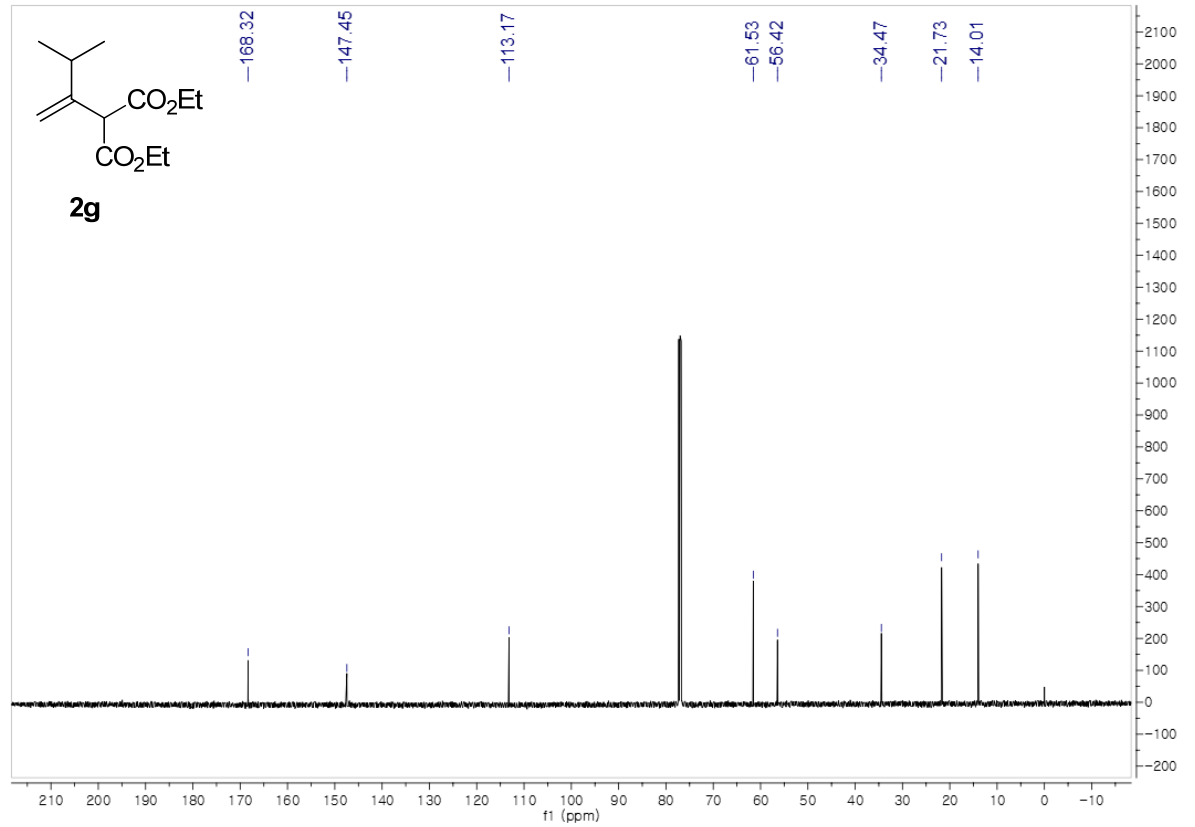
f1 (ppm)

2g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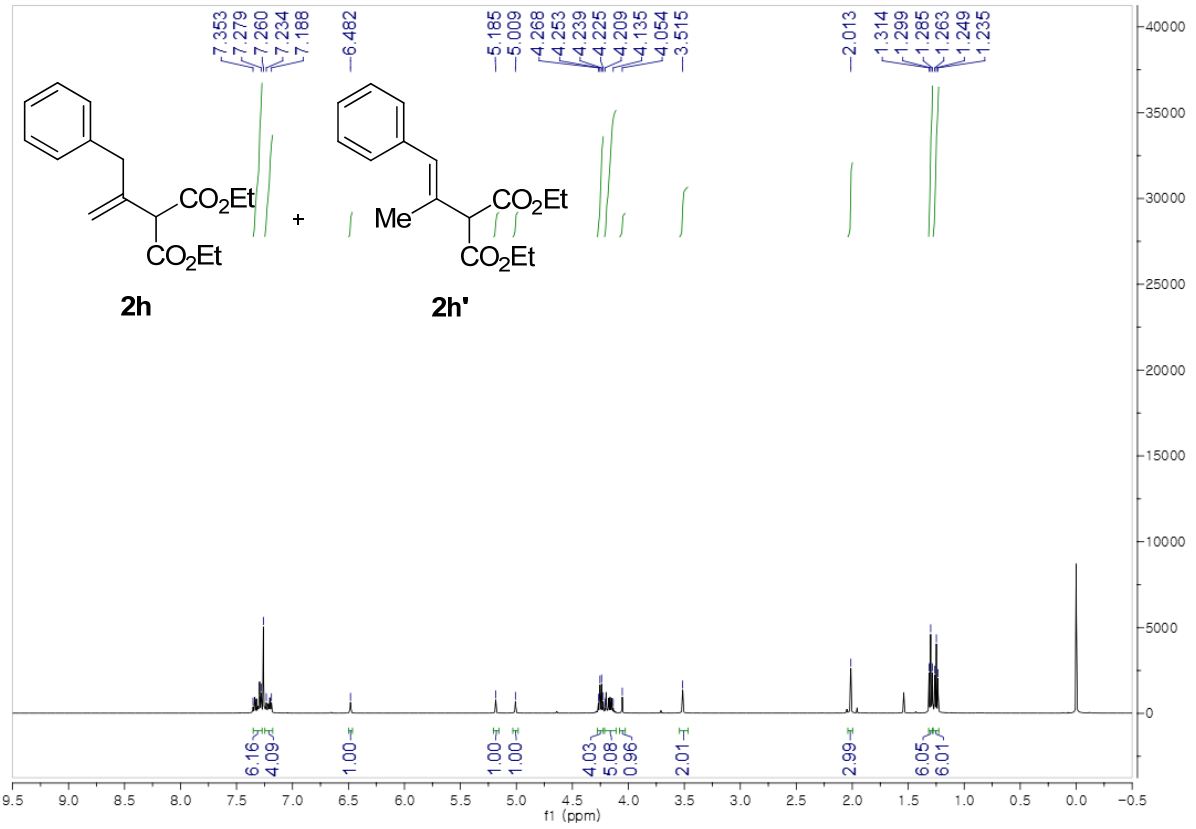
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CO2Et
+
Me
CO2Et
CO2Et
2h
2h'
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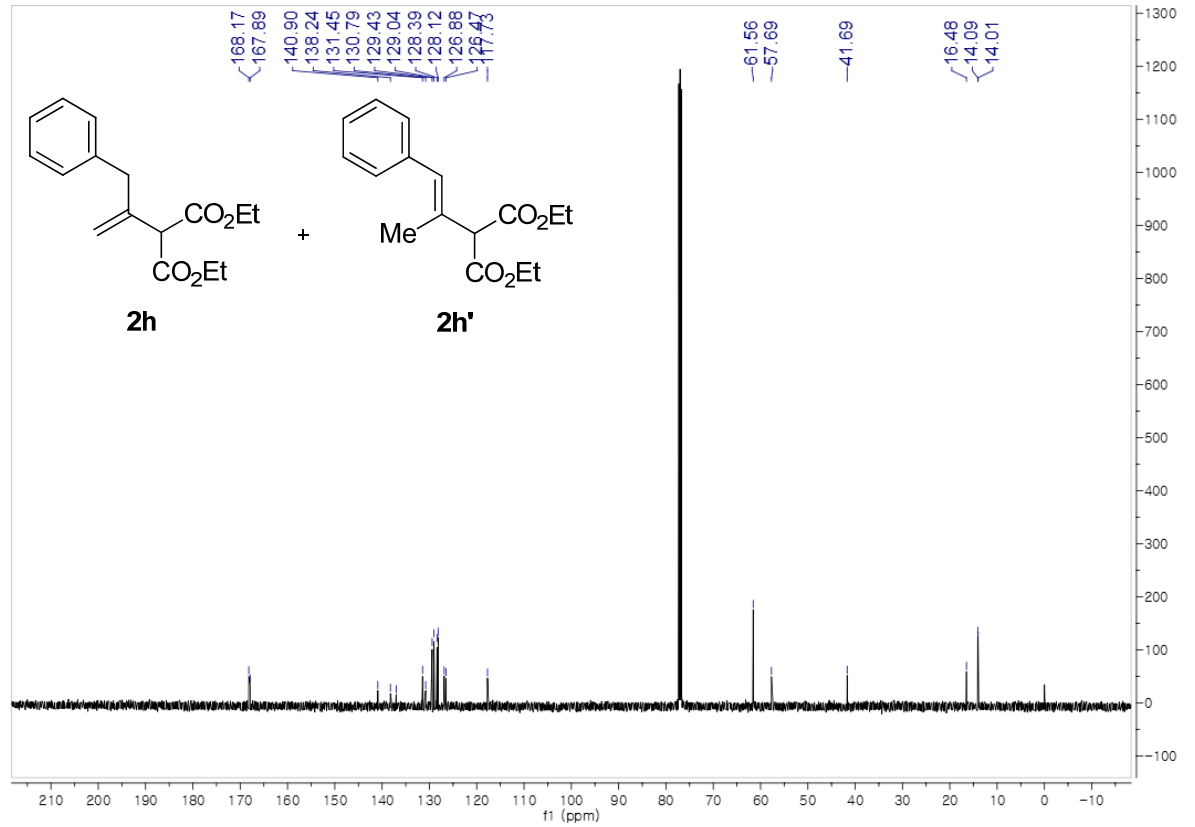
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+
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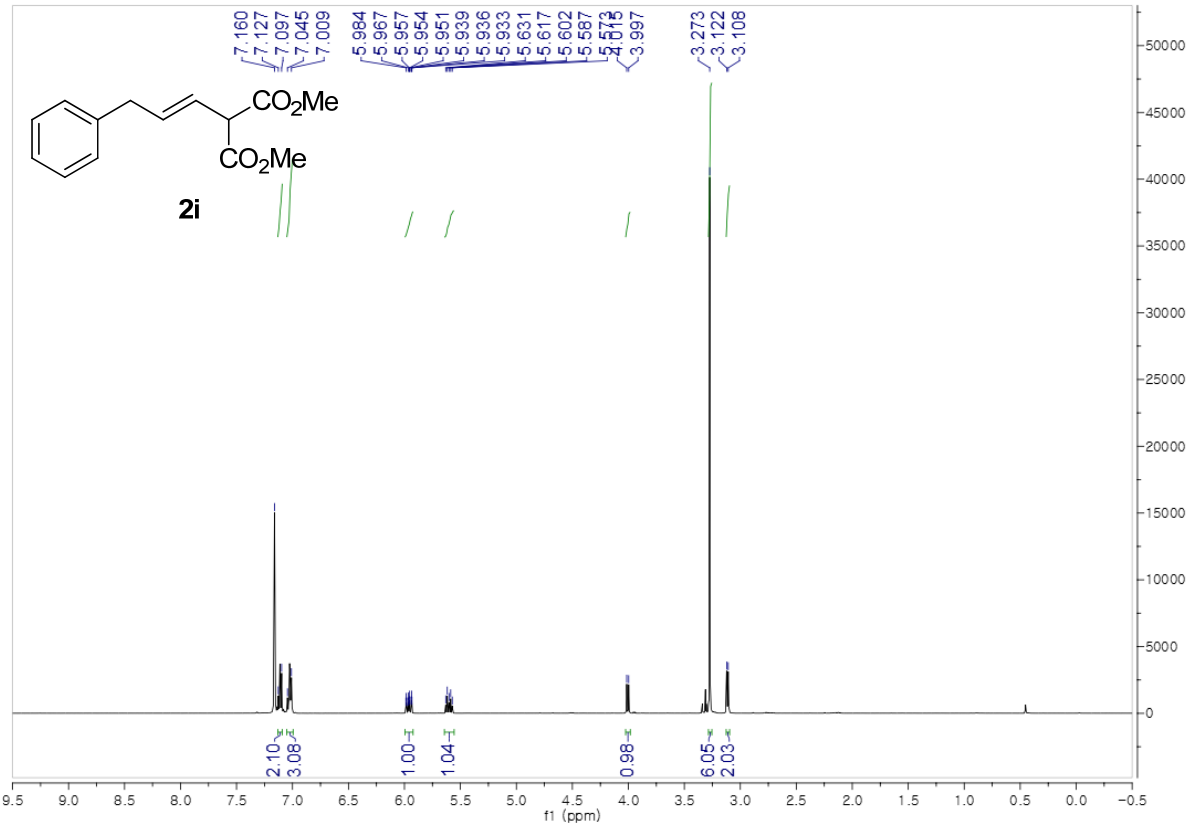
2h
2h'
f1 (ppm)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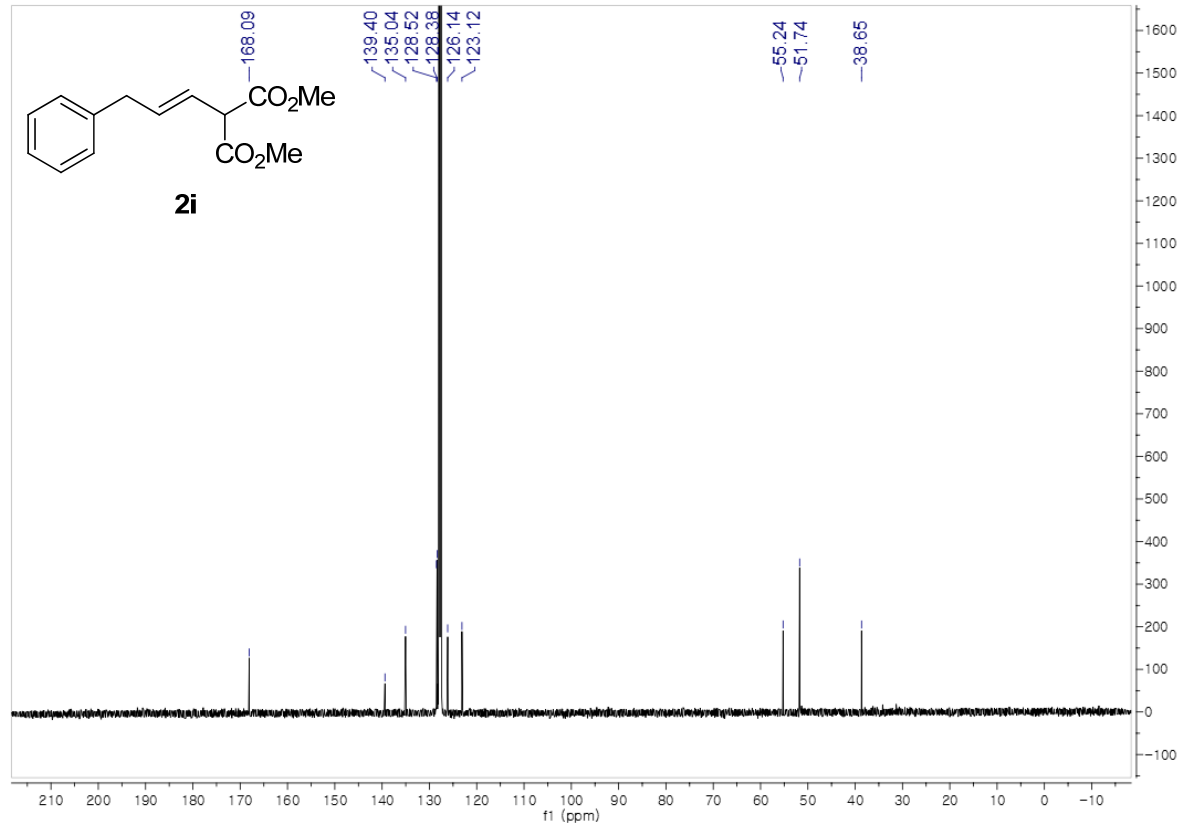
f1 (ppm)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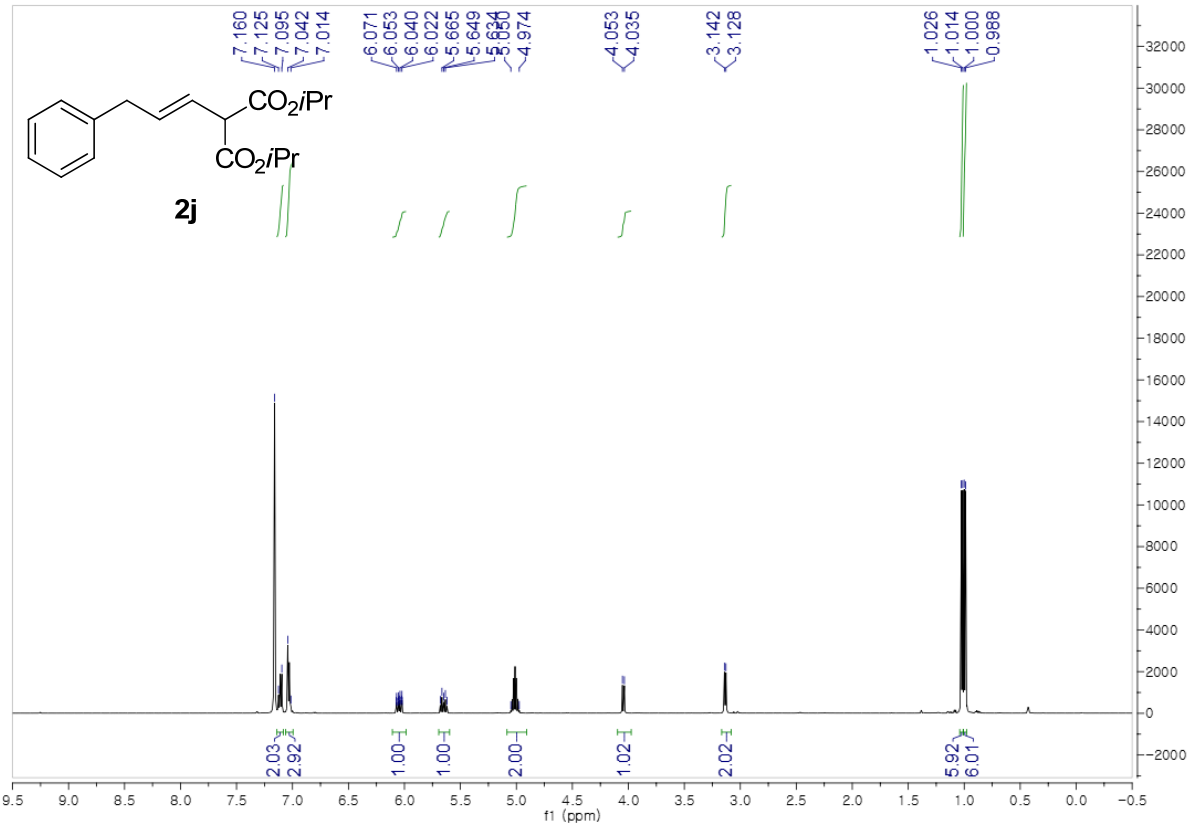
CO2Me
2i
f1 (ppm)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CO2iPr
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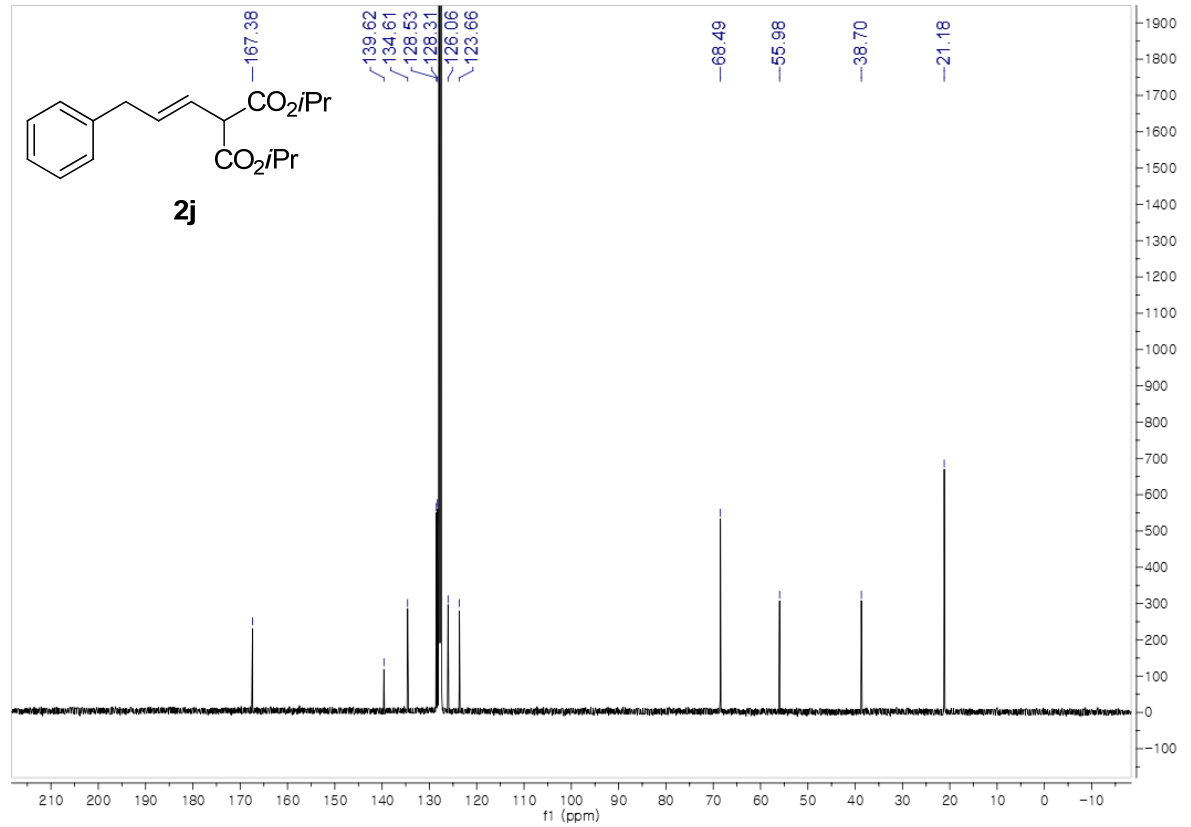
f1 (ppm)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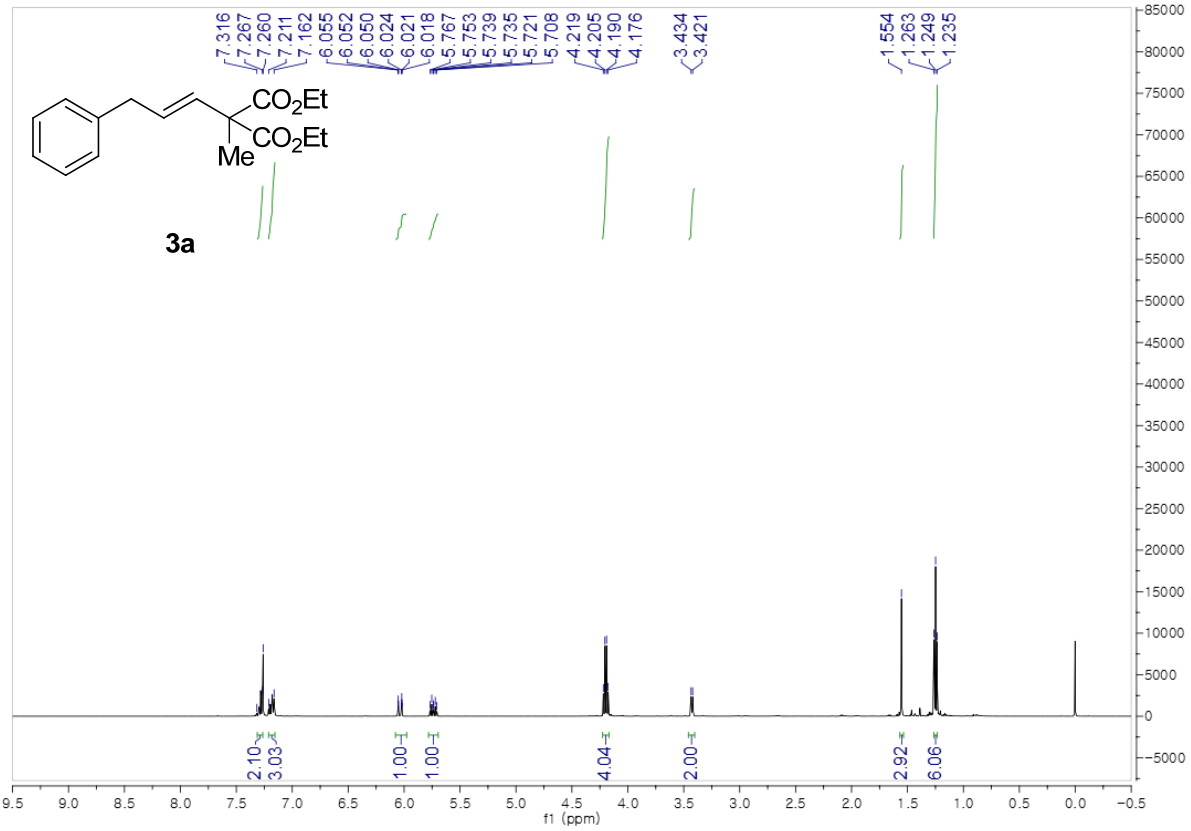
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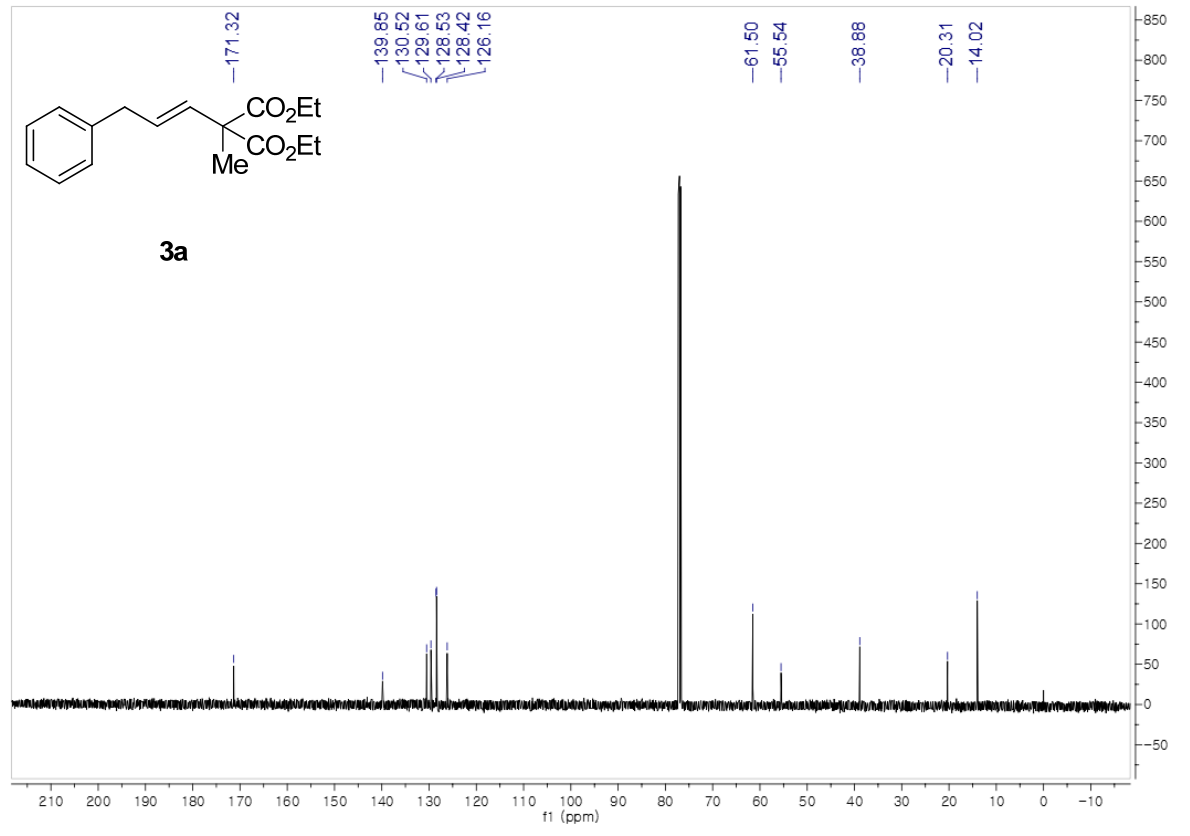
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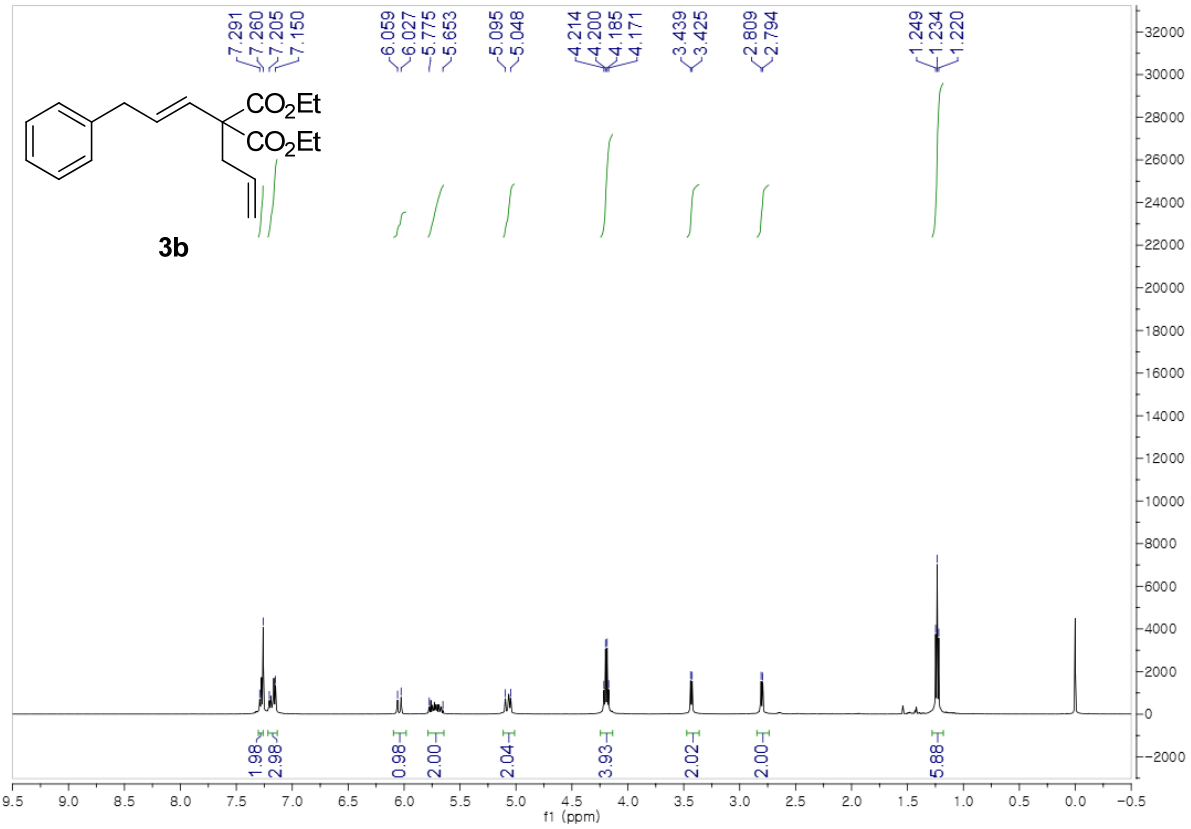
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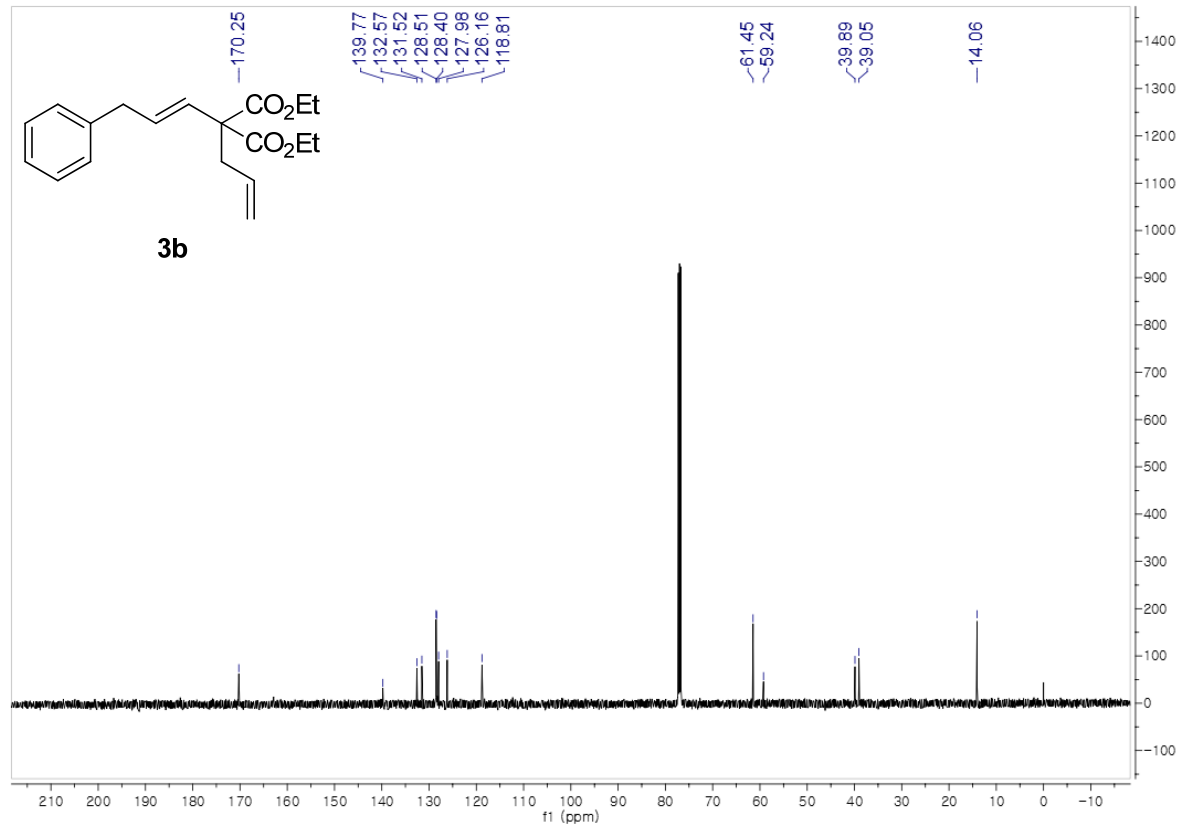
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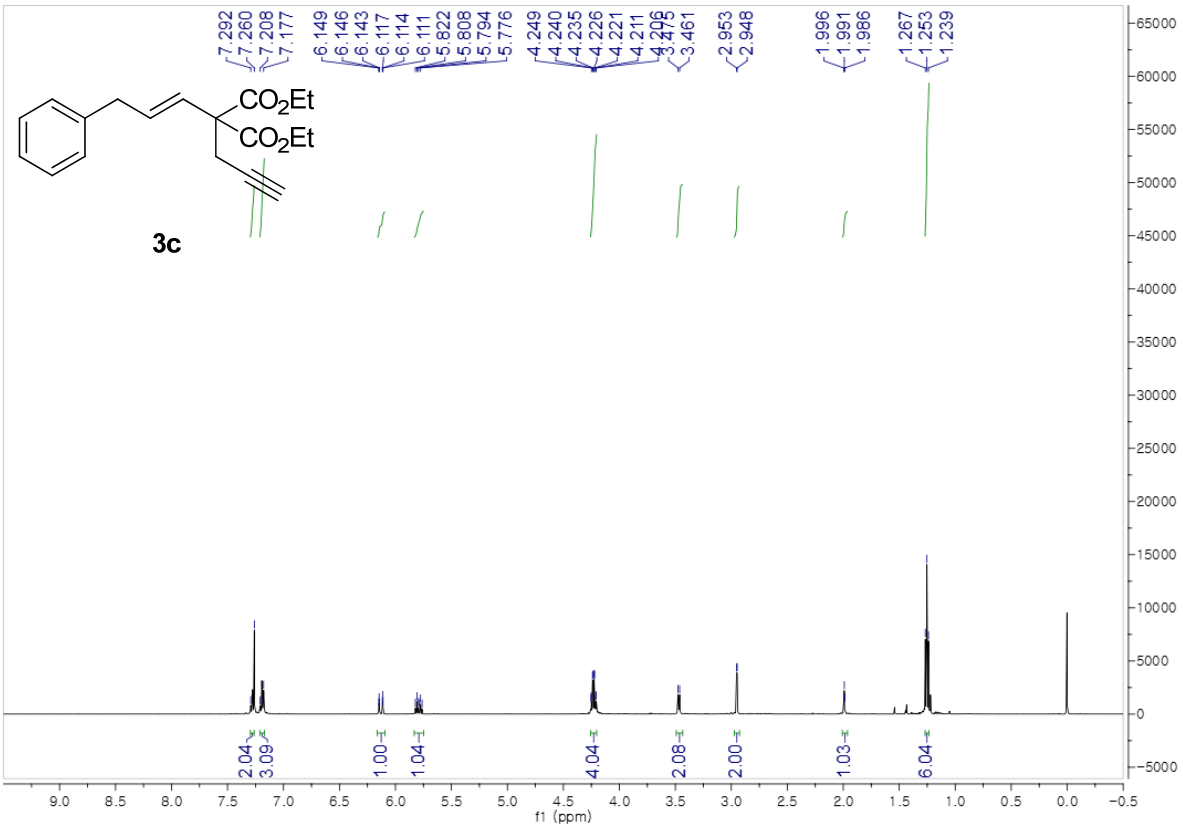
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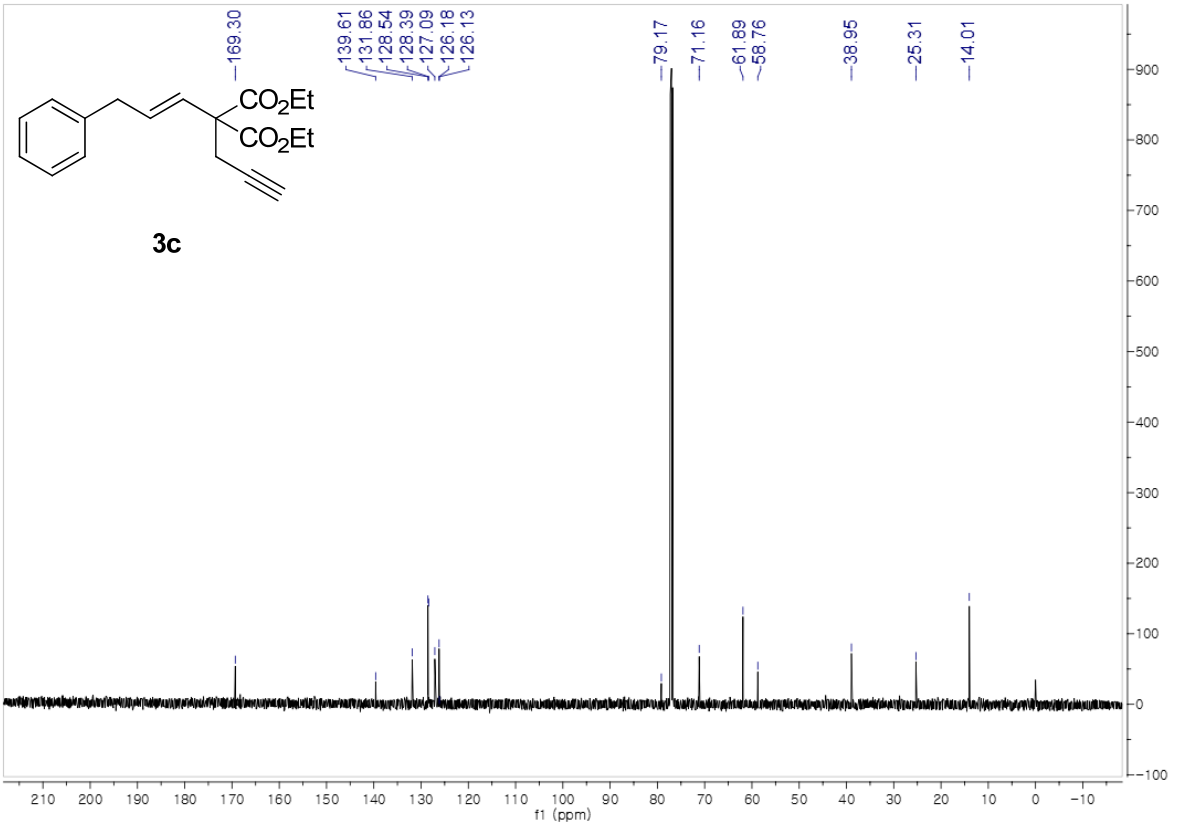
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CO2Et
3c
f1 (ppm)