Lubricating and waxy esters. VI. Synthesis and physical properties of (E) didec-9-enyl octadec-9-enedioate and branched derivatives

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Supporting Information Available

Structure, IUPAC names and nomenclature of synthesized compounds;

^{1}H-NMR in $CDCl_3$, ^{13}C-NMR in $CDCl_3$, MS, and HPLC data of synthesized compounds;

^{1}H-NMR spectra of **H**, its epoxide and its branched derivatives;

^{13}C-NMR spectra of **H** and its branched derivatives

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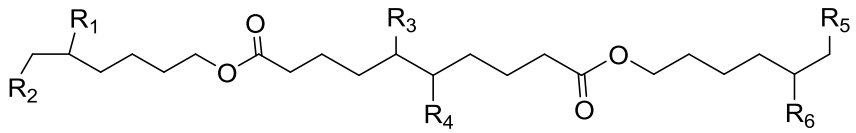
Table S1. Structure, IUPAC names and nomenclature of diester **H** and its branched derivatives. The column headed "Structure (R_1; R_2; R_3; R_4; R_5; R_6)" refers to the generalized structure shown in Scheme 1.

Compound	**IUPAC Name**	**Structure (R_1; R_2; R_3; R_4; R_5; R_6)**
H	E-didec-9-enyl octadec-9-enedioate	
EOH	bis(8-(oxiran-2-yl)octyl) 8,8'-(oxirane-2,3-diyl)dioctanoate	
H3	1-(9(10)-hydroxy-10(9)-(propionyloxy)decyl) 18-(10(9)-hydroxy-9(10)-(propionyloxy)decyl)-9(10)-hydroxy-10(9)-(propionyloxy)octadecanedioate	R_1: OH(C_2H_5COO); R_2: C_2H_5COO(OH) R_3: OH(C_2H_5COO); R_4: C_2H_5COO(OH) R_5: OH(C_2H_5COO); R_6: C_2H_5COO (OH)
H4-I	1-(9,10-bis(propionyloxy)decyl) 18-(9(10)-hydroxy-10(9)-(propionyloxy)decyl) 10(9)-hydroxy-9(10)-	R_1: C_2H_5COO; R_2: C_2H_5COO R_3: OH(C_2H_5COO); R_4: C_2H_5COO(OH) R_5: OH(C_2H_5COO); R_6: C_2H_5COO(OH)

	(propionyloxy)octadecanedioate		
H4-II	1-(9 (10)-hydroxy-10(9)-(propionyloxy)decyl) 18-(9 (10)-hydroxy-(10)9-(propionyloxy)decyl) 9,10-bis(propionyloxy)octadecanedioate	R_1: OH(C_2H_5COO); R_3: C_2H_5COO; R_5:OH(C_2H_5COO);	R_2: C_2H_5COO(OH) R_4: C_2H_5COO R_6: C_2H_5COO(OH)
H5-I	Bis (9,10-bis(propionyloxy)decyl)9(10)-hydroxy-10(9)-(propionyloxy)octadecandioate	R_1: C_2H_5COO; R_3: OH(C_2H_5COO); R_5: C_2H_5COO;	R2: C_2H_5COO R_4: C_2H_5COO(OH) R_6: C_2H_5COO
H5-II	1-(9,10-bis(propionyloxy)decyl) 18-(10(9)-(propionyloxy)-9(10)-hydroxydecyl) 9,10-bis(propionyloxy)octadecanedioate	R_1: OH(C_2H_5COO); R_3: C_2H_5COO; R_5: C_2H_5COO;	R_2: C_2H_5COO(OH) R4: C_2H_5COO R_6: C_2H_5COO
H6	Bis (9,10-bis(propionyloxy)decyl)9,10-bis (propionyloxy)octadecanedioate	R_1: C_2H_5COO; R_3:C_2H_5COO; R_5: C_2H_5COO;	R_2: C_2H_5COO R_4: C_2H_5COO R_6: C_2H_5COO



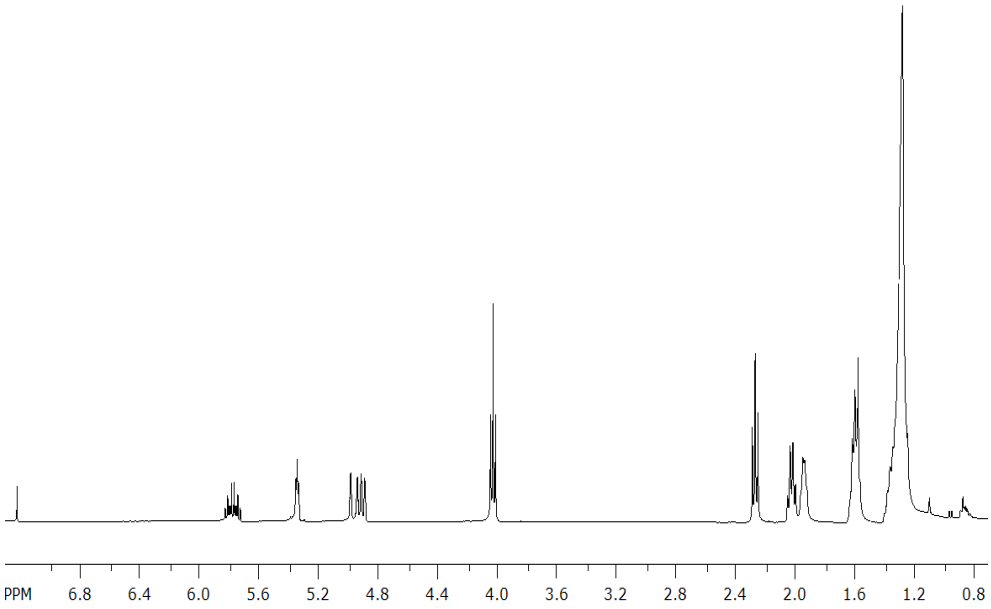
Scheme 1. Generalized structure of (E)-didec-9-enyl octadec-9-enedioate (H), and its branched derivatives. R_1-R_6 are specified in Table S1

Table S2. ^{1}H-NMR in $CDCl_3$, ^{13}C-NMR in $CDCl_3$, MS data, and HPLC retention times of synthesized compounds. **H3**, **H4**, **H5** and **H6:** 3-, 4-, 5- and 6-branched derivatives of (E)-didec-9-enyl octadec-9-enedioate (**H**), repectively

	^{1}H-NMR in DMSO-d6			HPLC Retention time (min)
1, 18-Octadec-9-enedioic acid	11.94 (2H, s), 5.36 (2H, t), 2.19-2.16 (4H, m), 1.94 (4H, m), 1.49-1.45 (4H, m), 1.31-1.26 (18H, m)			
	^{1}H-NMR in $CDCl_3$	^{13}C-NMR in $CDCl_3$	MS	
H	5.83-5.78 (2H, m), 5.36-5.34 (2H, t), 4.99-4.89 (4H, dd), 4.05-4.01 (4, t), 2.28-2.24 (4H, t), 2.04-1.99 (4H, m), 1.94-1.92 (4H, m), 1.61-1.57 (8H, m), 1.4-1.2 (36, m)			
Epoxide of H (EoH)	4.04-4.00 (4H, t), 2.88-2.84 (2H, m), 2.72-2.70 (2H, t), 2.62-2.59 (2H, t), 2.44-2.42 (2H, dd), 2.27-2.23 (4H, t), 1.65-1.22 (52H, m)			15.46
H3	δ (ppm):4.89-4.81 (~1.5H, m), 4.13-4.11(~1.5 H, dd), 4.04-3.98 (4H, t), 4.95-3.91 (~1.5 H, dd), 3.83-3.78 (~1.5 H, m), 3.70-3.56 (~2H, m), 2.38-2.24 (10H, m), 1.60-1.18 (52H, m), 1.22-1.11 (9H, t).	δ (ppm): 174.86, 174.14, 77.69, 75.64, 73.50,70.19, 68.84, 65.03, 64.56, 34.56, 33.53, 32.41, 30.69, 29.66-28.80, 28.00, 27.69, 26.10-25.16, 9.41	$C_{47}H_{86}O_{13}$ Cal. 858.61; Found: 881.5, $(M+Na)^{+}$	5.72
H4	δ (ppm):5.07-5.05 (1H, m),4.89- 4.8 (~0.25H, m) 4.83-4.81 (1H, m), 4.21-4.19 (1H, dd), 4.14-4.11 (~0.75H, dd), 4.03-3.98 (5H, m), 3.95-3.91 (~0.75, dd), 3.83-3.78 (~0.75H, m), 3.69-3.57 (~1.5 H, m), 2.38-2.14 (12H, m), 1.59 -1.18 (52H, m), 1.14-1.08 (12H, m)	δ (ppm): 174.83, 174.14, 77.65, 75.59, 73.45, 70.14, 68.80, 65.20, 64.96, 64.56, 34.53, 33.50, 32.39, 30.91, 29.63-28.80, 27.97, 27.66, 26.06-25.13, 9.39	$C_{50}H_{90}O_{14}$, Cal. 914.63, Found: 937.6 $(M + Na)^{+}$	10.72 and 11.46
H5	δ (ppm):5.08-4.80 (3H, m) (including	δ (ppm): 174.83, 174.14, 77.65,	$C_{53}H_{94}O_{15}$, Cal.	22.48 and

	5.08-5.08 (~1.87H,m), 4.96-4.94 (~0.26 H, m), 4.84-4.80 (~0.87H, m)), 4.22-4.11 (2H, dd) (including 4.14-4.11(~0.13H, dd)), 4.03-3.91(6H, m) (including 3.95-3.91 (~0.13H, dd)), 3.83-3.78 (~0.13H, m), 3.69-3.57 (~0.87H, m), 2.36-2.24 (14H, m), 1.76-1.50 (16, m), 1.40--1.27 (36H, m), 1.17-1.09 (15H, m)	74.17, 73.46, 71.53, 70.15, 68.80, 65.20, 64.54, 34.51, 33.89, 33.50, 32.39, 30.92, 29.58-28.80, 27.97, 27.63, 26.05-24.83, 9.39	970.66, Found: 993.9 $(M + Na)^+$	23.69
H6	5.07-5.05 (2H, m), 4.96-4.94 (2H, m), 4.23-4.19 (2H, dd), 4.06-4.00(6H, q), 2.34-2.24 (18H, m), 1.65-1.49 (16H, m), 1.27(36H, m), 1.14-1.10 (18H, m)	174.10, 74.18, 71.53, 65.21, 64.55, 34.52, 30.92, 29.49-28.82, 27.91, 27.64, 26.07-25.13, 9.40	$C_{56}H_{98}O_{16}$, Cal. 1026.69; Found: 1049.9 $(M + Na)^+$	40.89

(a)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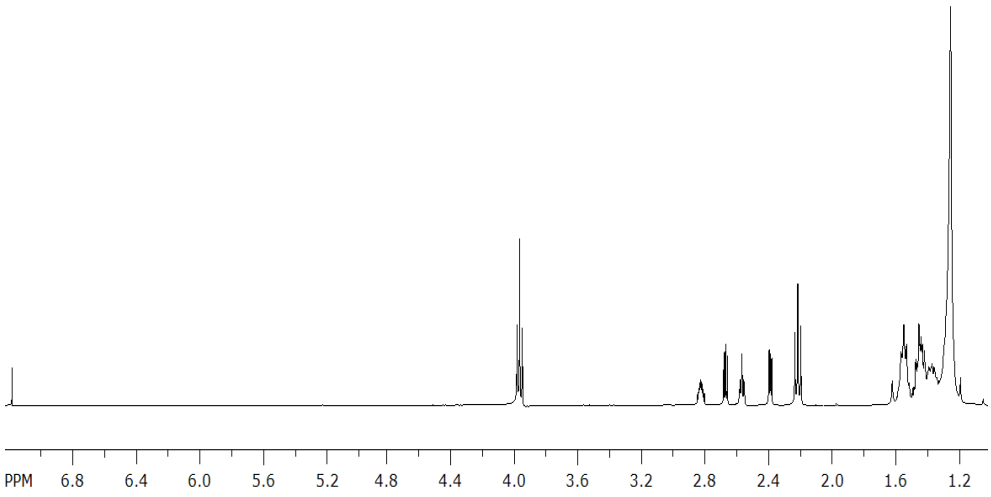
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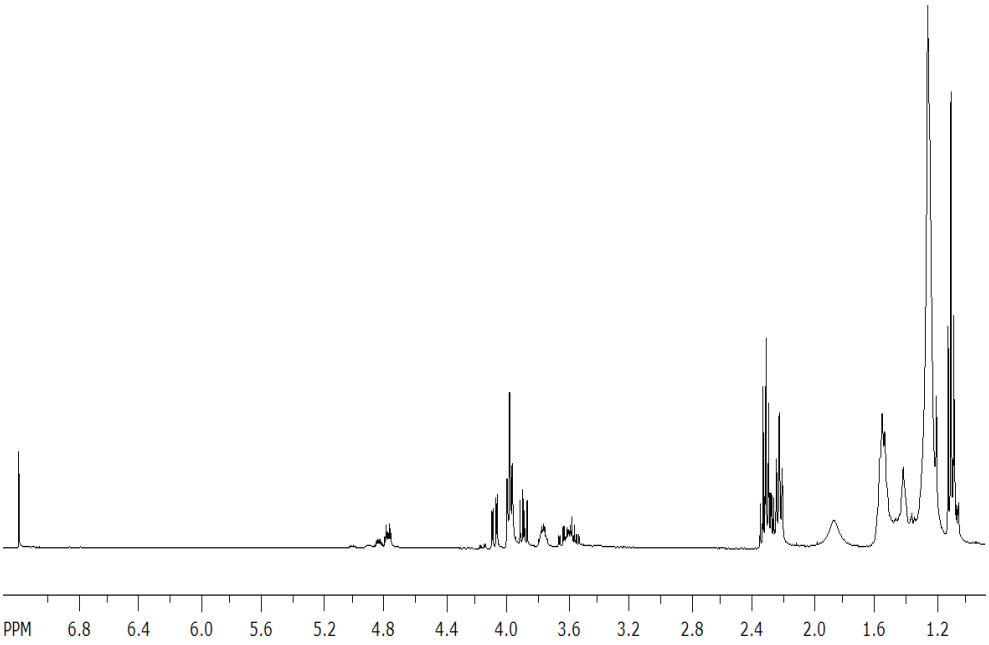
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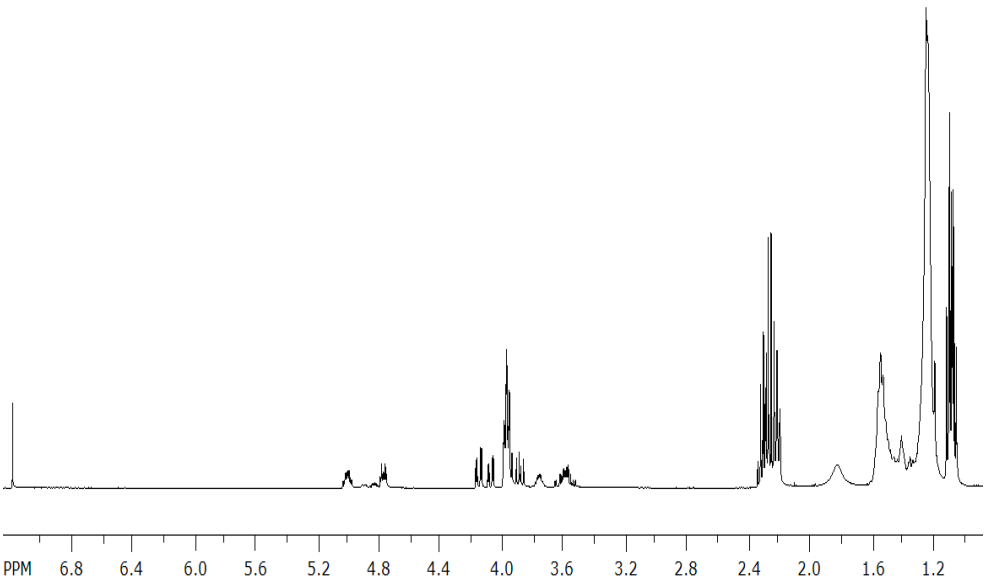
(d)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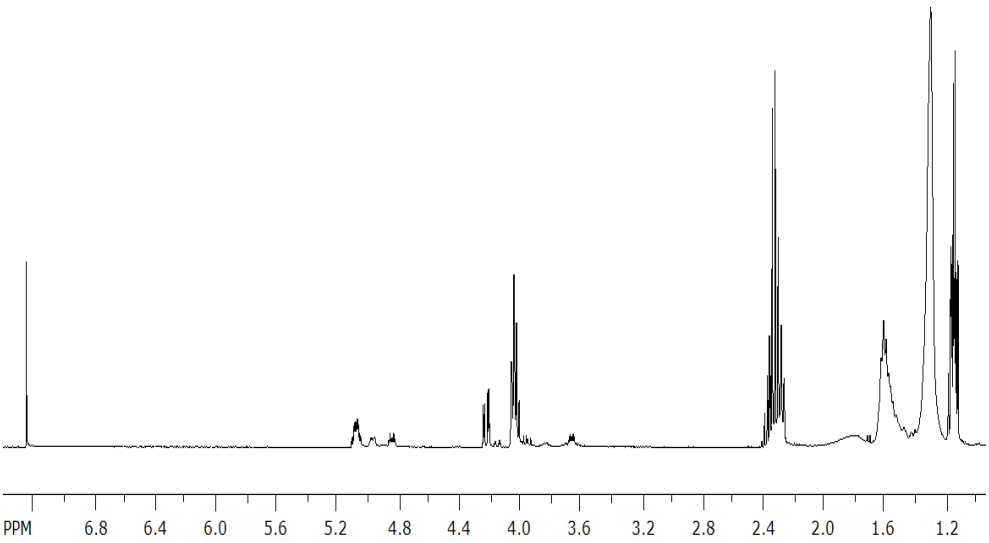
(e)



(f)

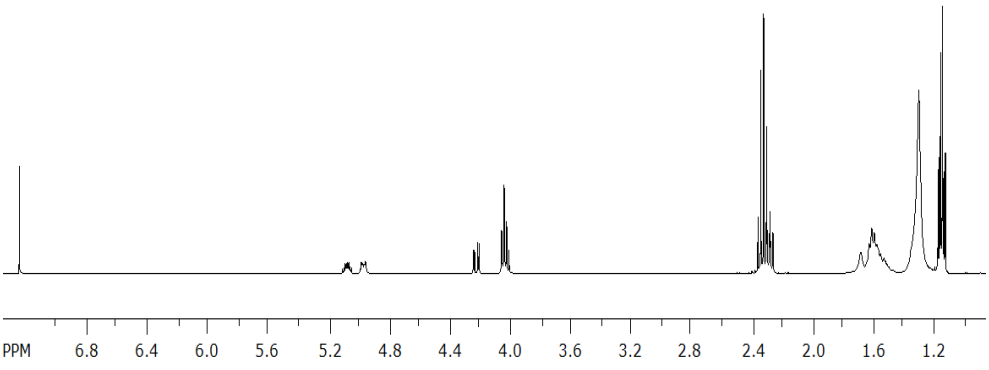
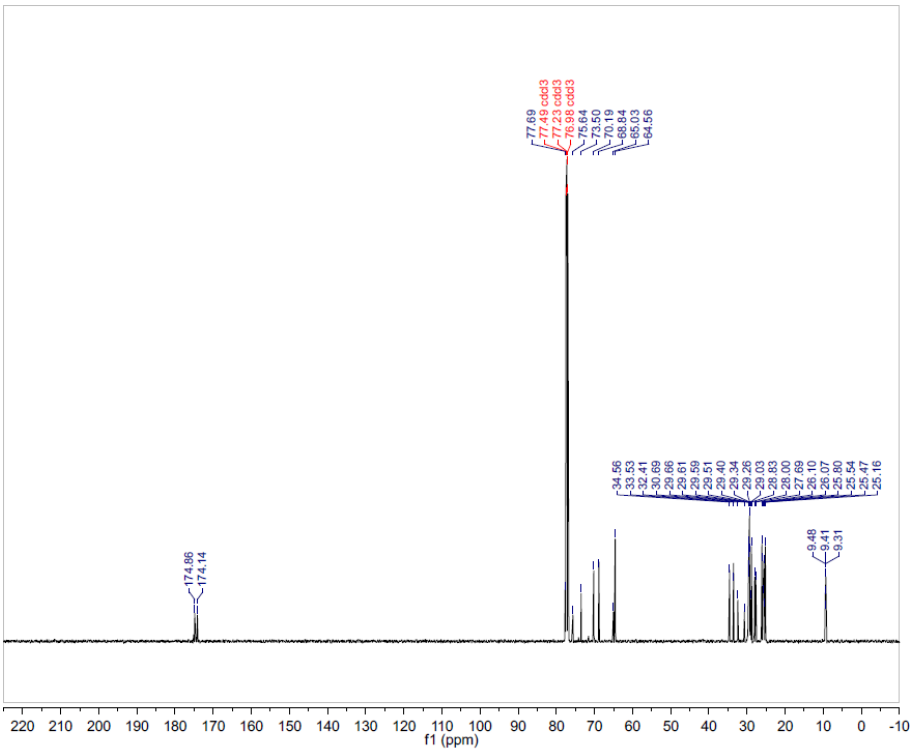


Figure S1. ^{1}H-NMR of (a) **H**, (b) epoxide of **H** (**EoH**), and branched derivatives of **H**, (c) **H3**, (d) **H4**, (e) **H5** and (f) **H6**

(a)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33.53
32.41
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29.26
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28.83
28.00
27.69
26.10
26.07
25.80
25.54
25.47
25.16
174.86
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9.31
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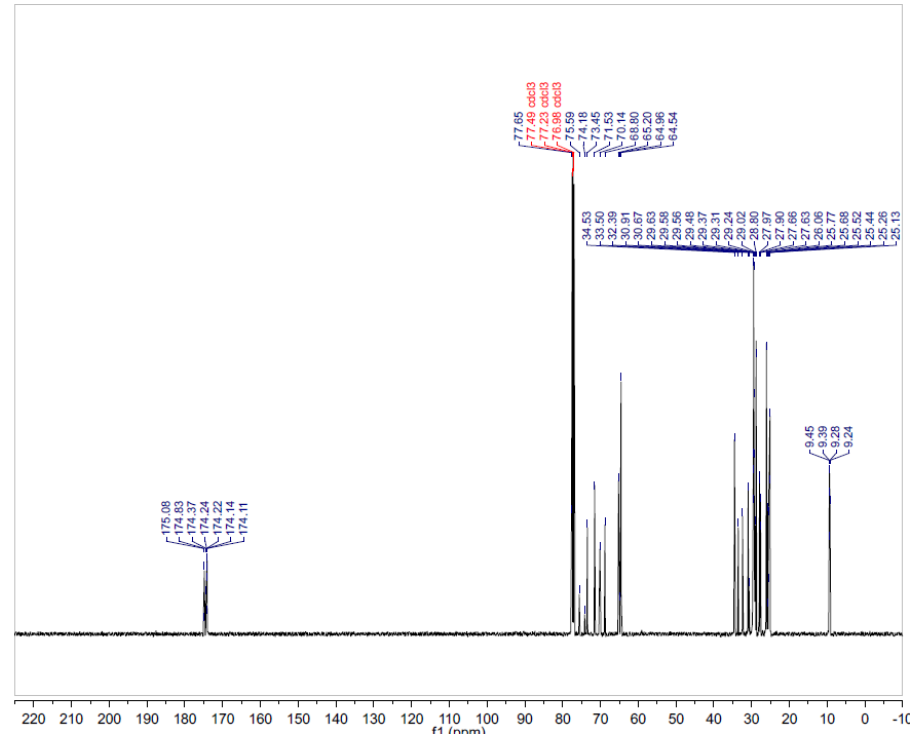
f1 (ppm)

(b)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75.59
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64.96
64.54
34.53
33.50
32.39
30.91
30.67
29.63
29.58
29.56
29.48
29.37
29.31
29.24
29.02
28.80
27.97
27.90
27.66
27.63
26.06
25.77
25.68
25.52
25.44
25.26
25.13
175.08
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174.37
174.24
174.22
174.14
174.11
9.45
9.39
9.28
9.24
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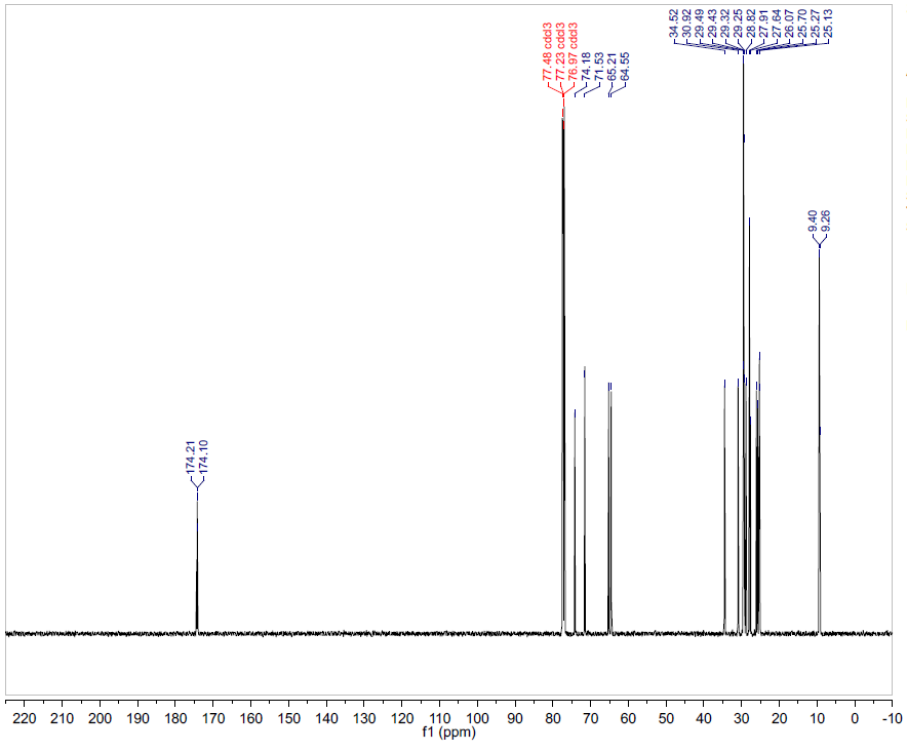
f1 (ppm)

(c)



(d)

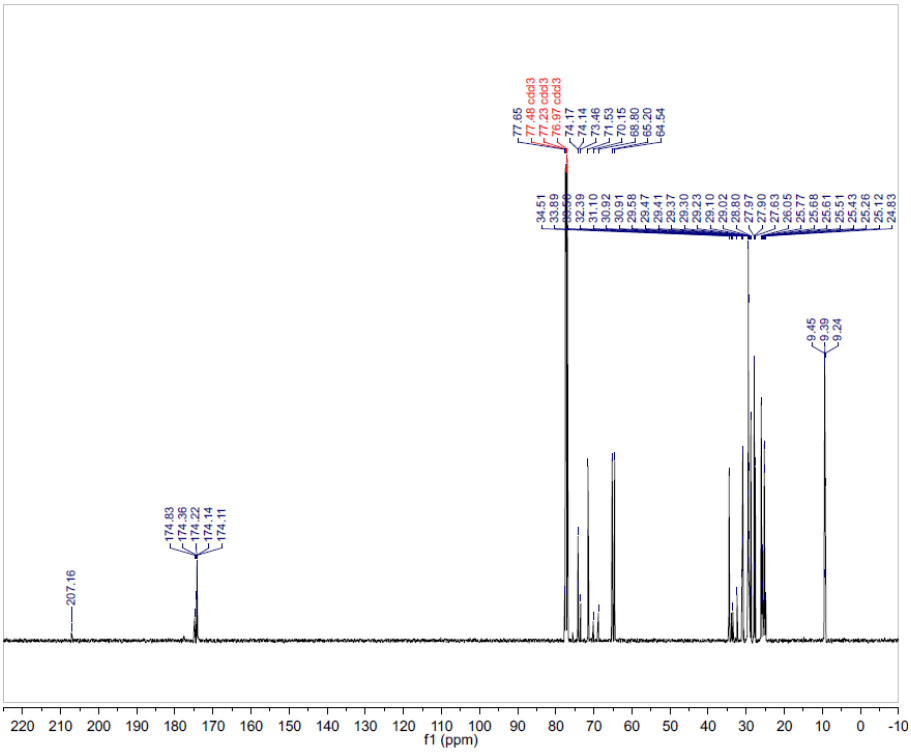


Figure S2. ^{13}C-NMR of the branched derivatives of **H.** (a) **H3**, (b) **H4**, (c) **H5**, and (d) **H6**