

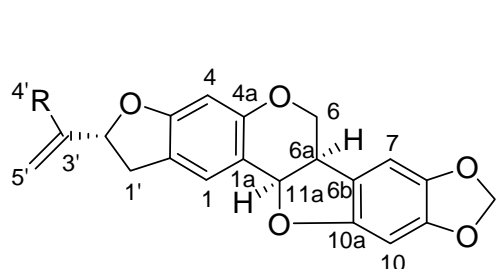
Antiproliferative Compounds from *Pongamiopsis pervilleana*

from the Madagascar Dry Forest

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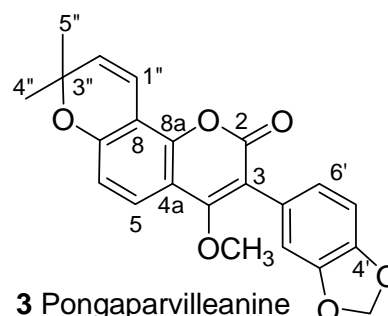
SUPPORTING INFORMATION

1. Structures and numbering of all compounds

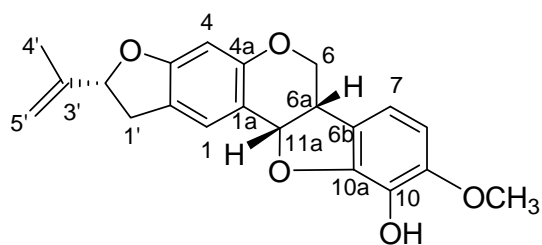


1 R = CH₂OH: 4'-hydroxy-emoroidocarpan

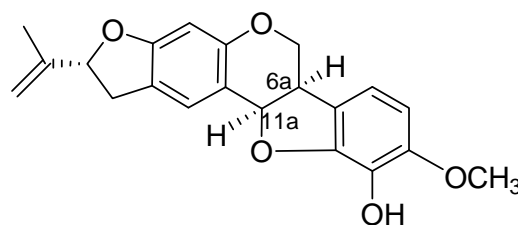
2 R = CH₃: Emoroidocarpan



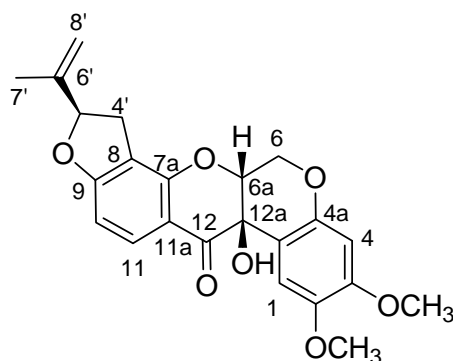
3 Pongaparvilleanine



4 Epipervilleine



6 Pervilleine



5 Rotenolone

The numbering system for rotenolone is that of Malgahaes, A. F.; Tozzi A. G. M. A.; Sales, N. L. H. B.; Malgahaes G. E. *Phytochemistry*, **1996**, *42*, 1459-1471.

2. Characterization data for rotenolone (5)

Amorphous powder, $[\alpha]_D$: -172 (*c*, 0.1, MeOH). CD (*c* 1.5, MeOH) $[\theta]_{330}$ -25,950; UV (MeOH) λ_{\max} nm (log ϵ): 293 (2.8), 245 (4.1); ^1H NMR (500 MHz, in CD_3OD , δ in ppm): ^1H -NMR (500 MHz, in CD_3OD , δ in ppm): 7.78 (1H, d, J = 8.5 Hz, H-11), 6.68 (1H, s, H-1), 6.52 (1H, s, H-4), 6.518 (1H, d, J = 8.5 Hz, H-10), 5.29 (1H, t, J = 8.8 Hz, H-2'), 5.04 (1H, brs, H-5'), 4.62 (3H, m, H-6a), 4.56 (1H, *dd*, J = 12.2, 2.5 Hz, H-6 α), 4.47 (1H, *dd*, 12.2, 1.1 Hz, H-6 β), 3.29 (overlapped with the solvent signal, H-1' α), 2.92 (1H, *dd*, J = 16.0, 9.0 Hz, H-1' β), 1.74 (3H, s, H-4'), 3.66, 3.78 (2 x 3H, 2 s, 2-OMe, 3-OMe). ^{13}C NMR (125 MHz, in CD_3OD , δ in ppm): 192.8 (C-12), 169.0 (C-9), 158.7 (C-7a), 153.0 (C-3), 150.4 (C-4a), 144.9 (C-2 and C-6'), 130.8 (C-11), 114.0 (C-8), 112.7 (C-11a), 112.6 (C-7'), 108.0 (C-1a), 105.8 (C-10), 89.3 (C-5'), 77.6 (C-6a), 68.0 (C-12a), 64.9 (C-6), 57.1 (OMe), 56.3 (OMe), 32.0 (C-4'), 17.0 (C-8'). Positive HRESIMS: m/z 433.1269 $[\text{M}+\text{Na}]^+$ (calcd for $\text{C}_{23}\text{H}_{22}\text{O}_7\text{Na}$, 433.1263).

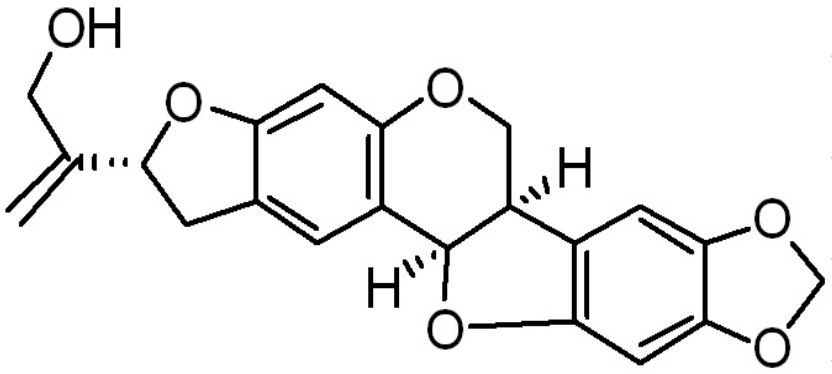
3. NMR spectra of compounds.

a) ^1H and ^{13}C NMR spectra of compounds 1–5

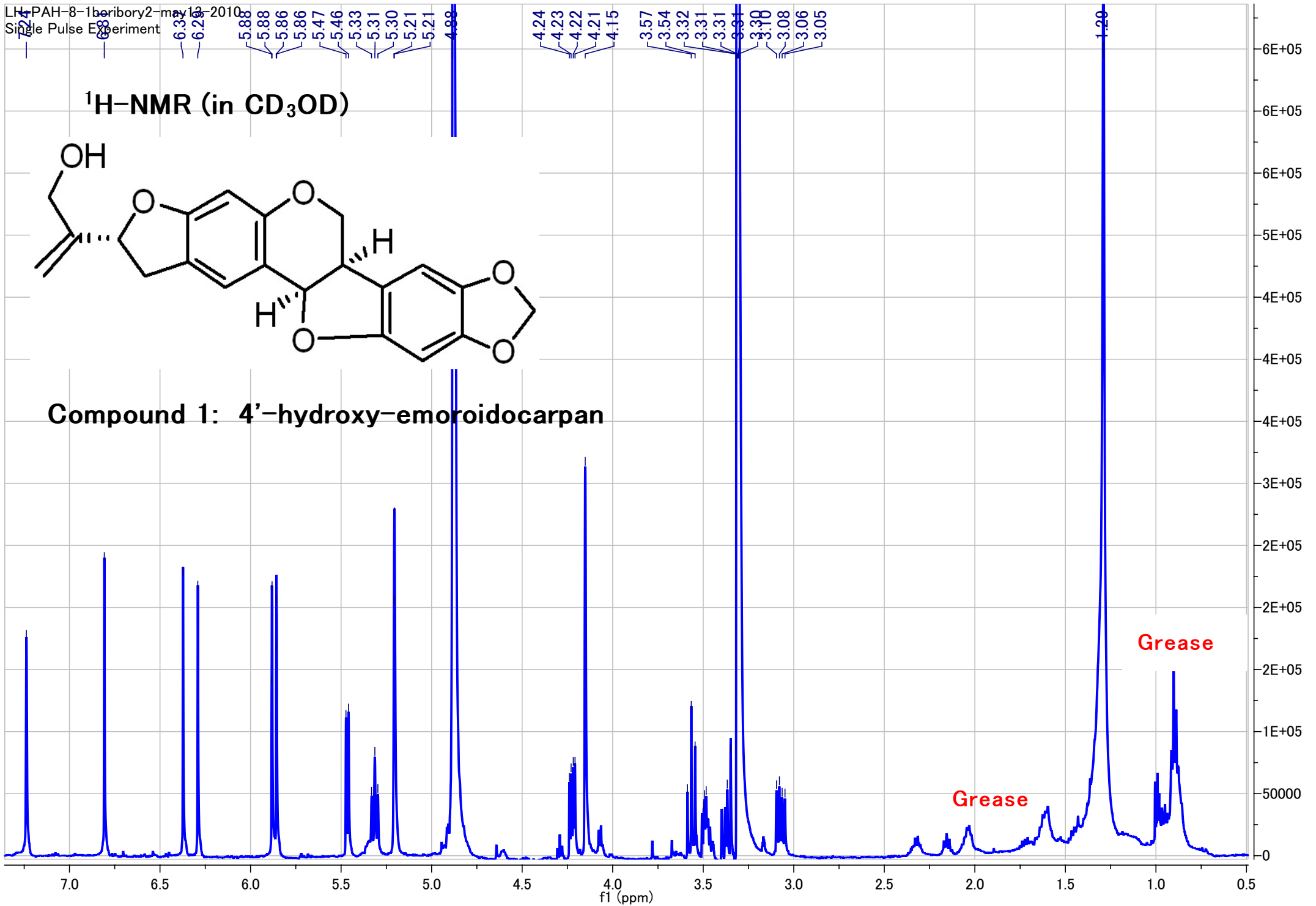
b) HMBC spectra of compounds 1, 3 and 4.

6.38, 6.29, 5.88, 5.88, 5.86, 5.86, 5.47, 5.46, 5.33, 5.31, 5.30, 5.21, 5.21, 4.88, 4.24, 4.23, 4.22, 4.21, 4.15, 3.57, 3.54, 3.32, 3.31, 3.31, 3.31, 3.31, 3.30, 3.08, 3.06, 3.05, 1.20

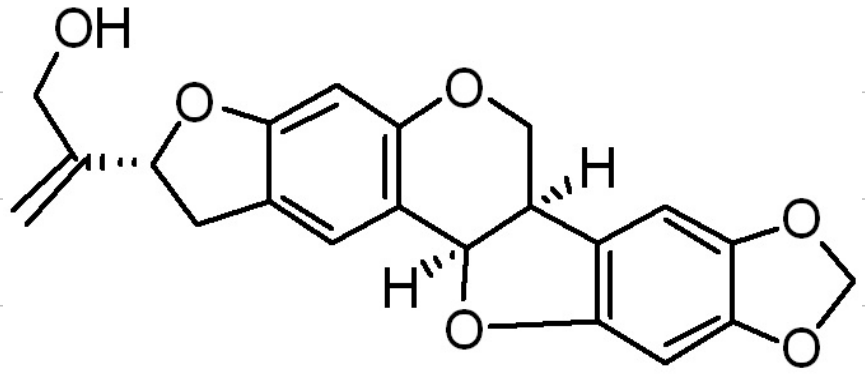
¹H-NMR (in CD₃OD)



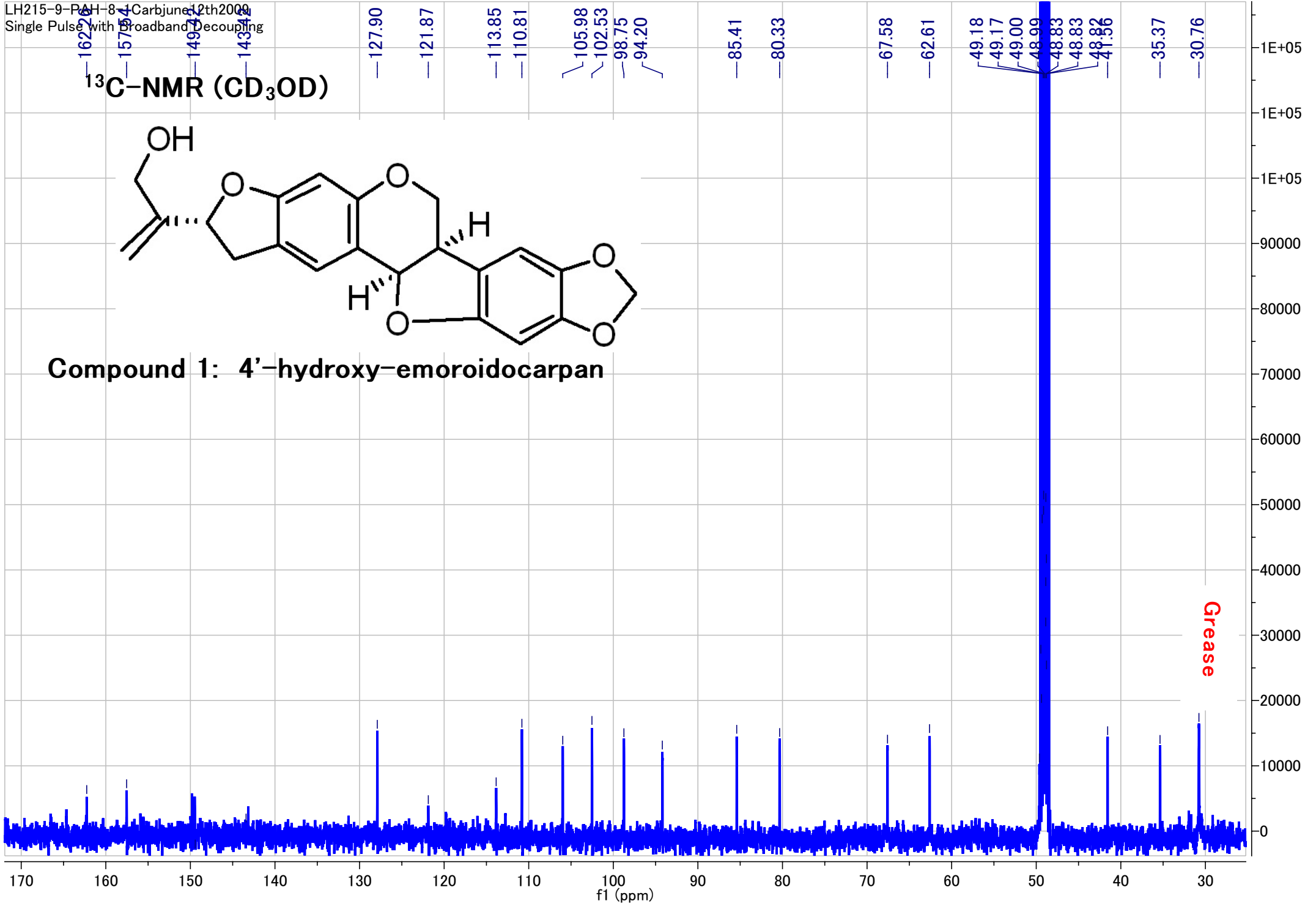
Compound 1: 4'-hydroxy-emoroidocarpan



¹³C-NMR (CD₃OD)



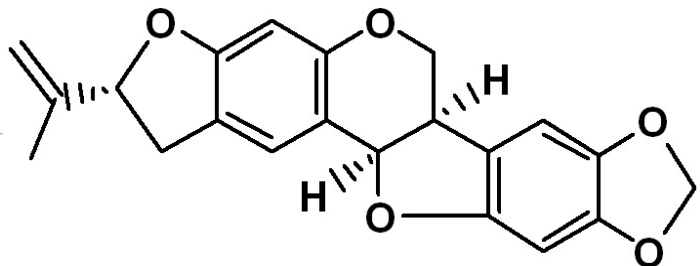
Compound 1: 4'-hydroxy-emoroidocarpan



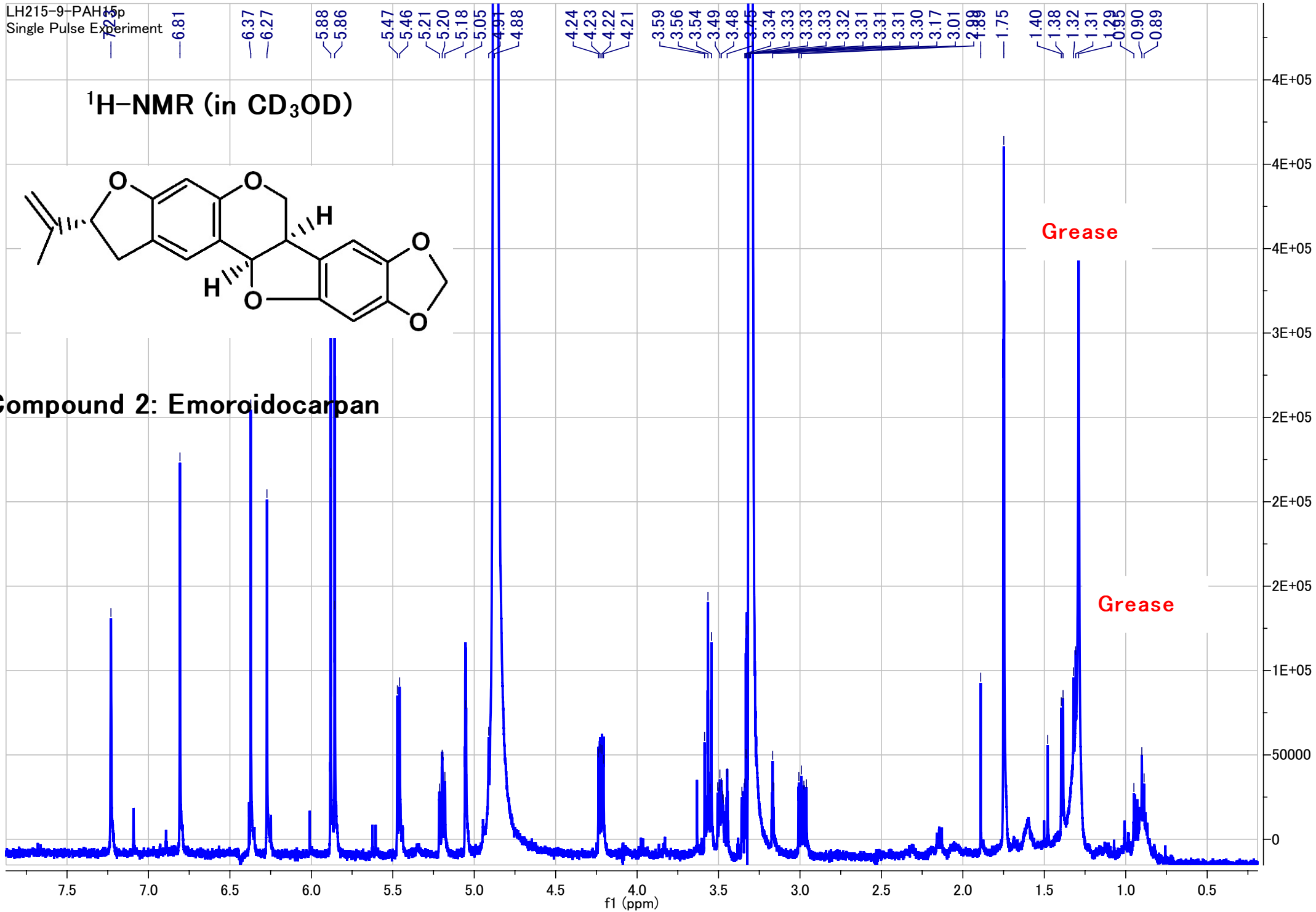
Grease

LH215-9-PAH15p
Single Pulse Experiment

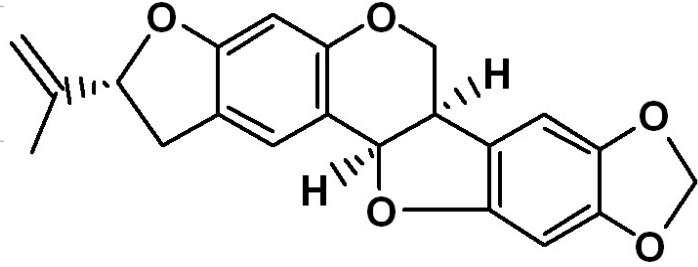
¹H-NMR (in CD₃OD)



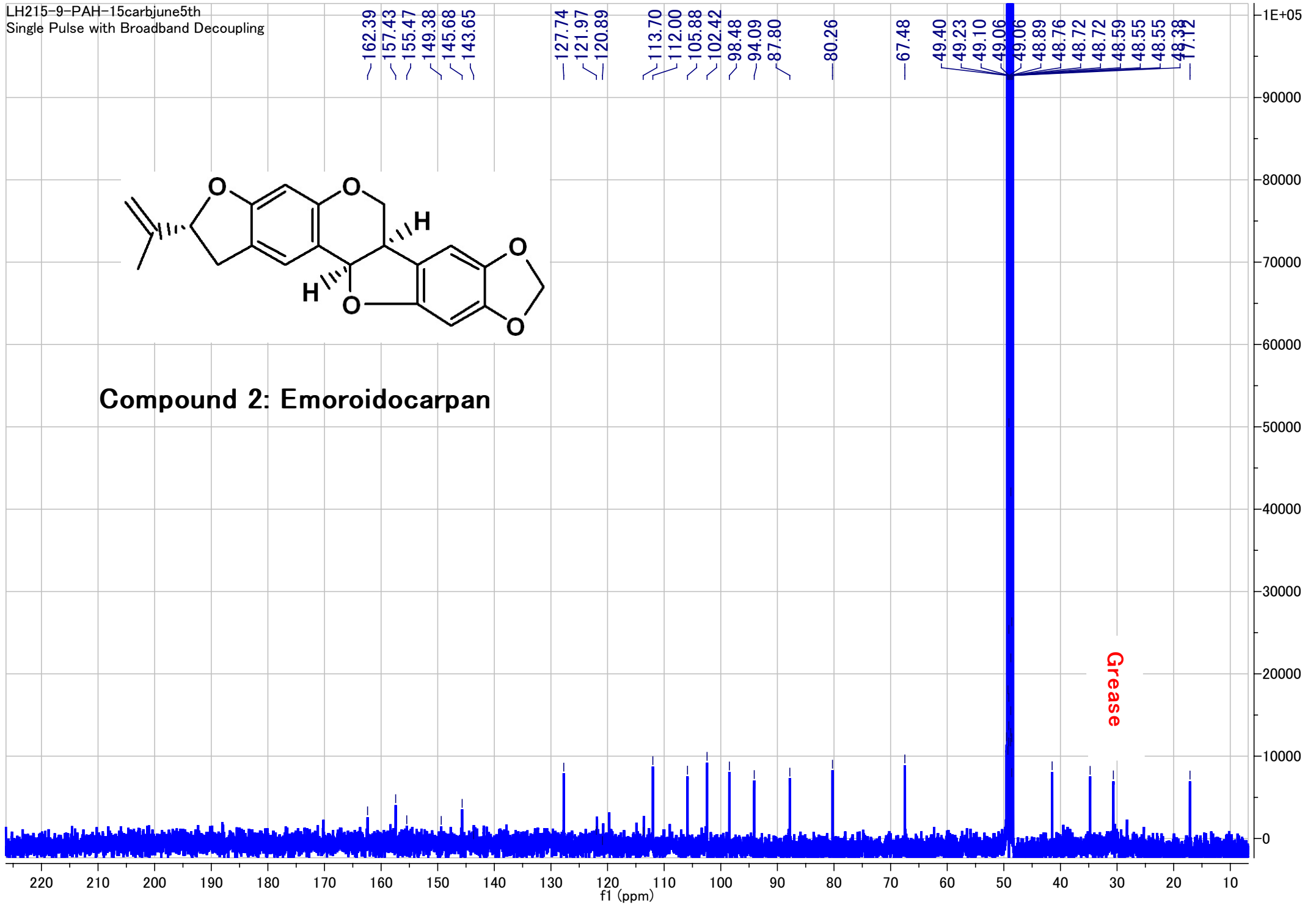
Compound 2: Emoroidocarpan



LH215-9-PAH-15carbJune5th
Single Pulse with Broadband Decoupling

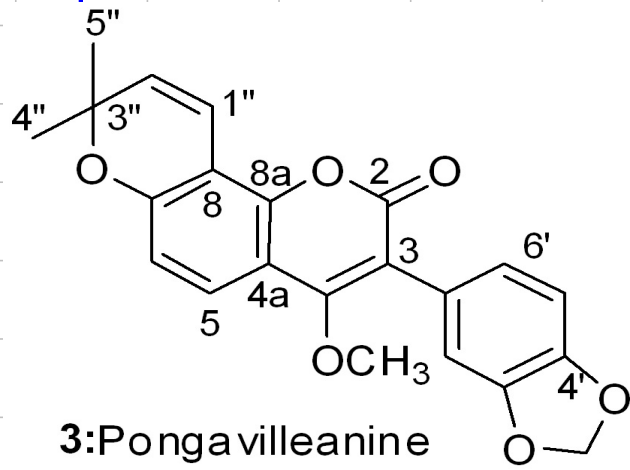


Compound 2: Emoroidocarpan

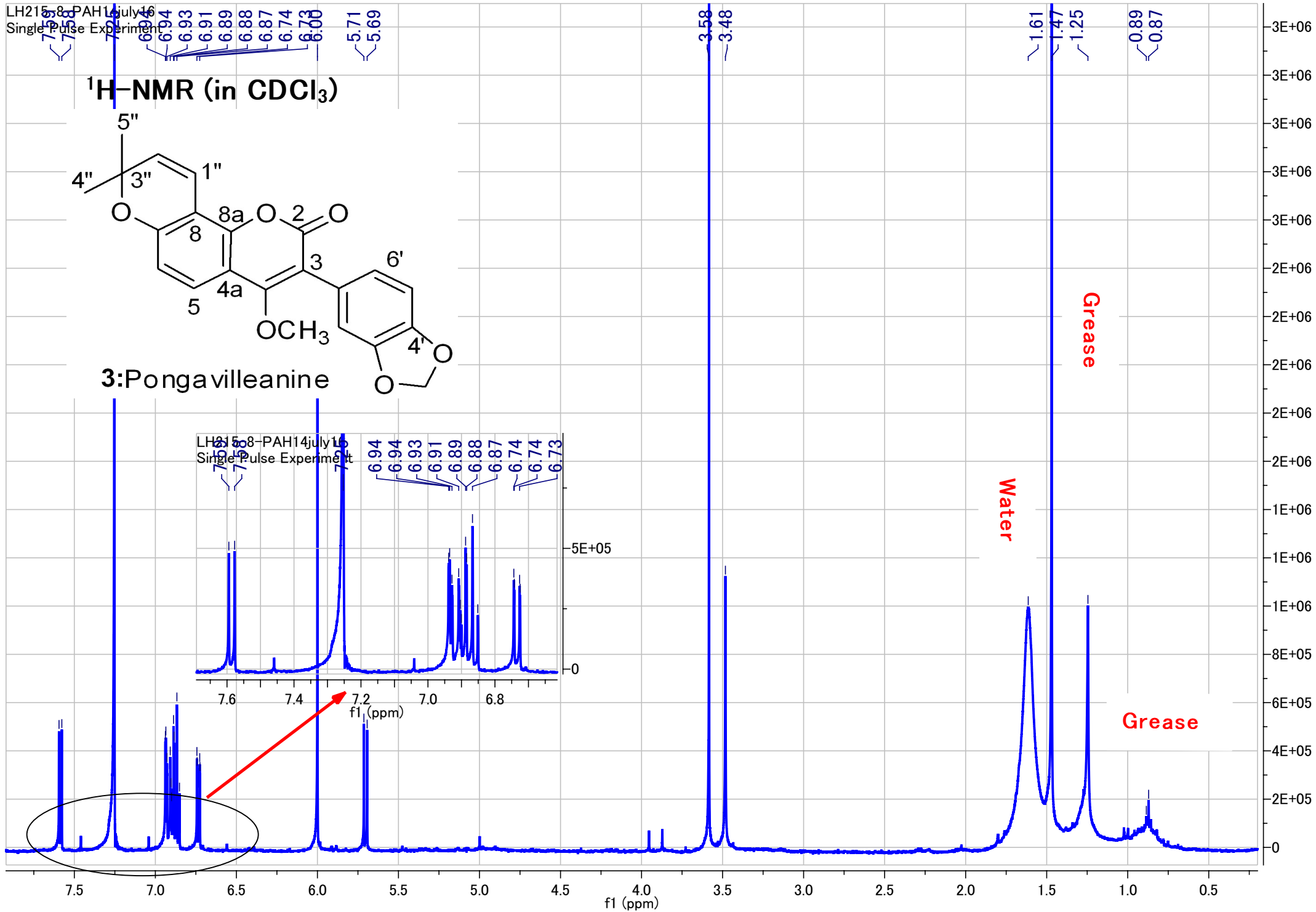


LH2158-PAH14july16
Single Pulse Experiment

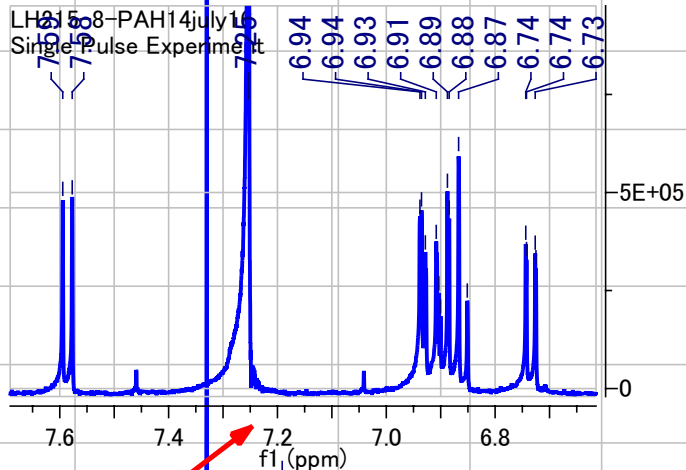
¹H-NMR (in CDCl₃)



3:Pongavilleanine



LH2158-PAH14july16
Single Pulse Experiment

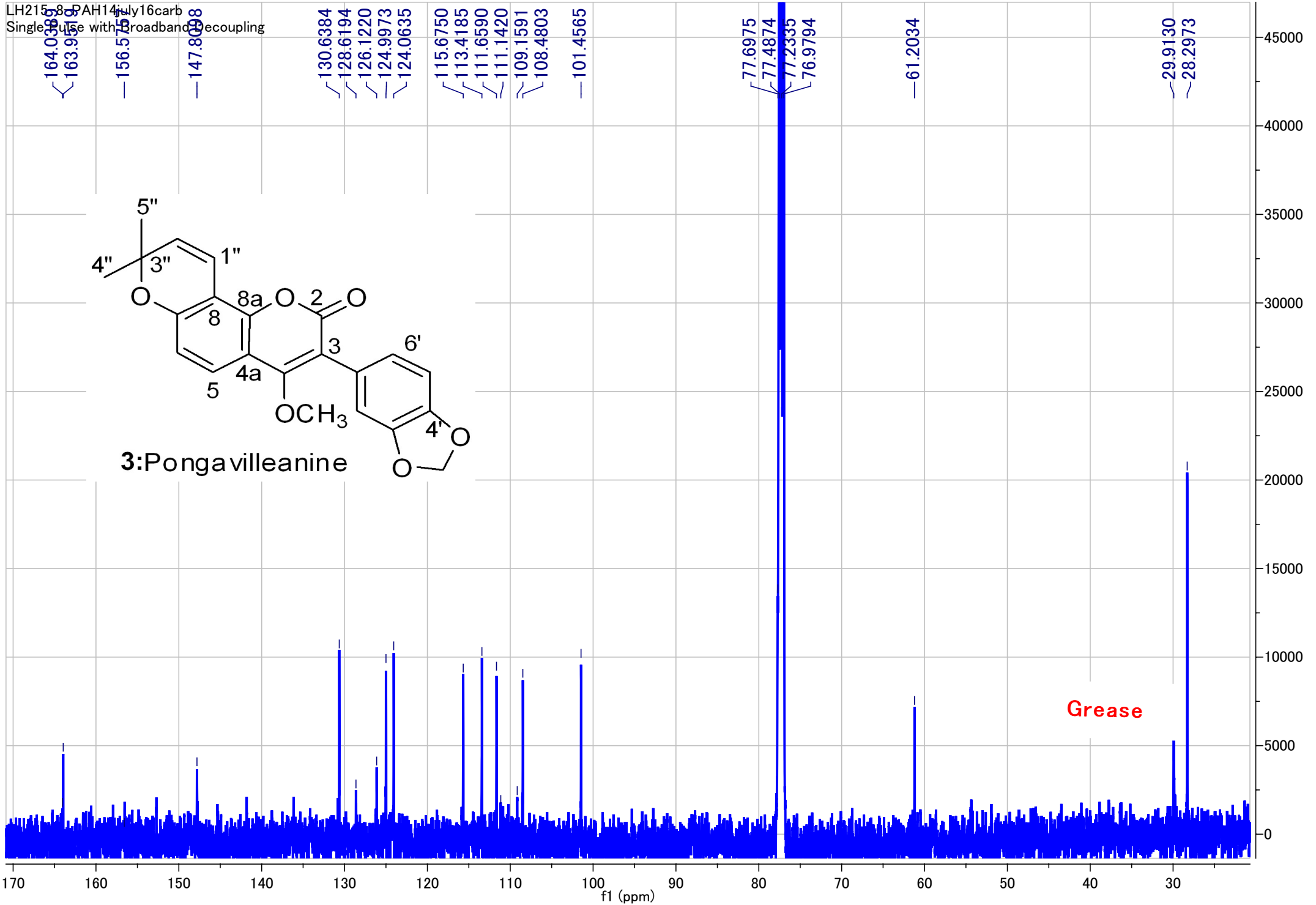


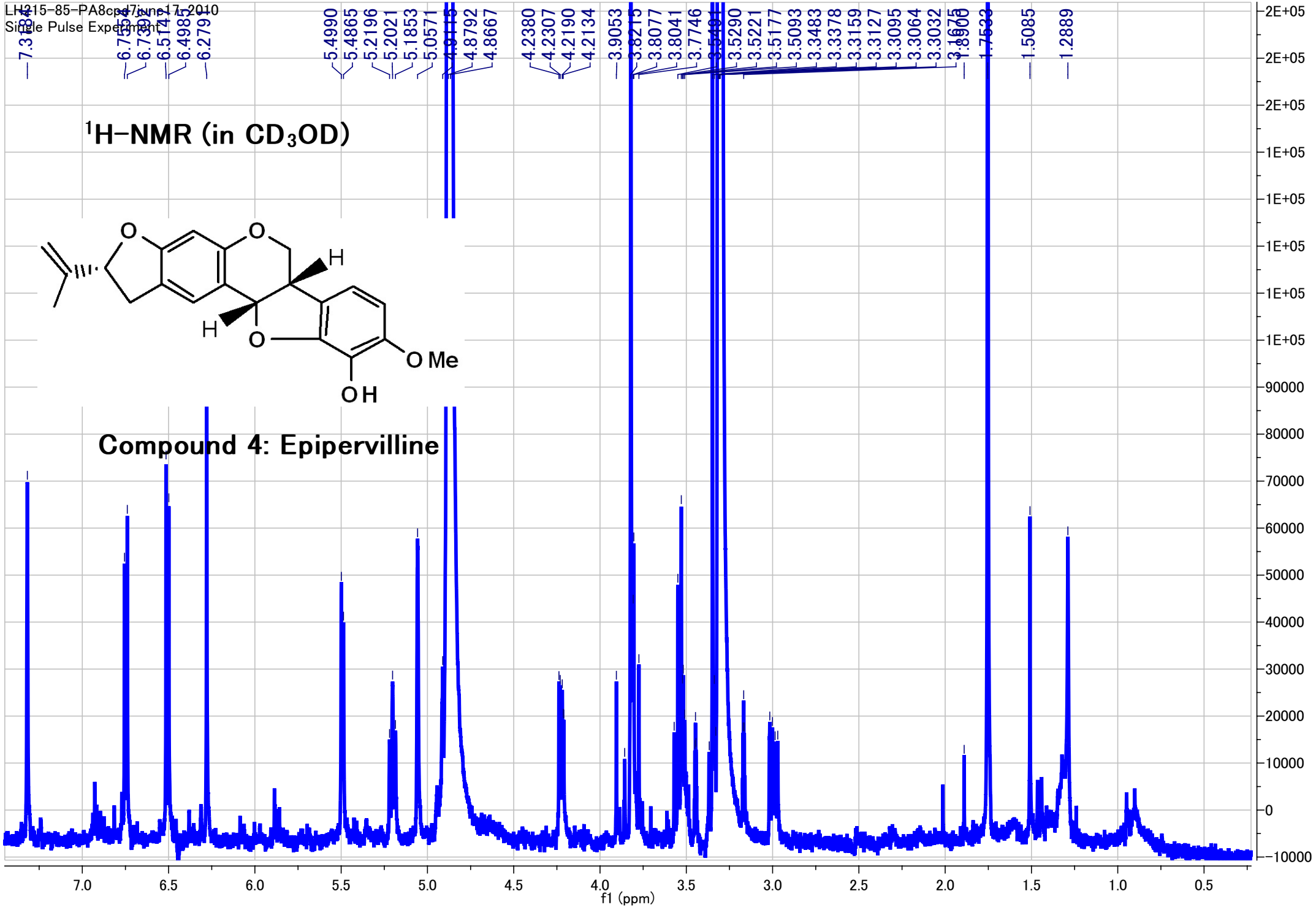
Grease

Water

Grease

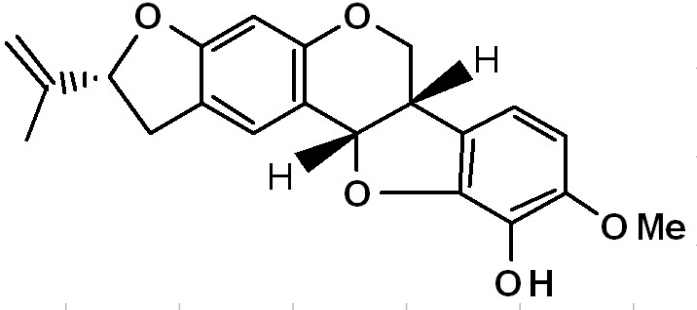
LH215-8-PAH14 July 16 carb
Single pulse with broadband decoupling



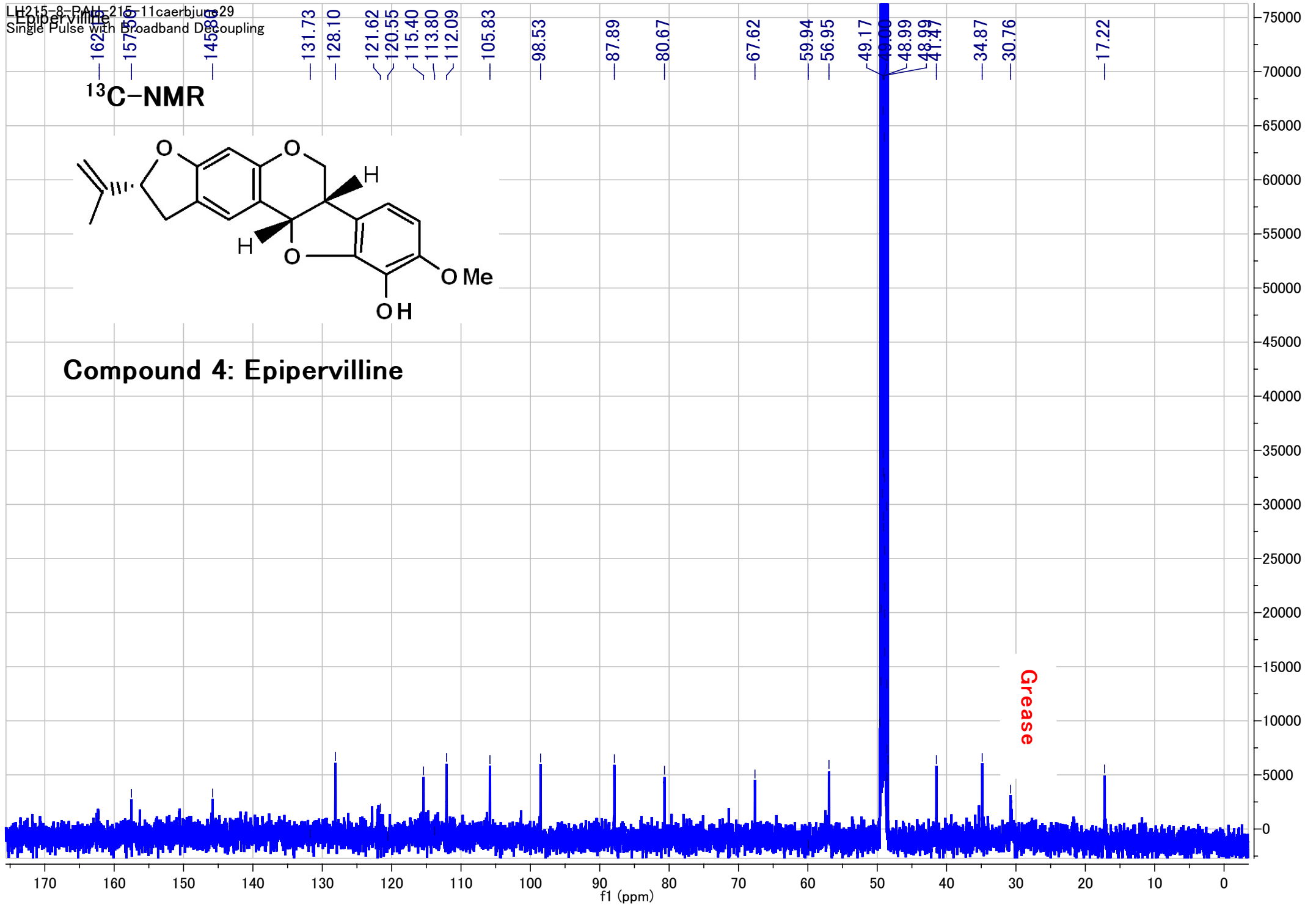


LH215-8-PAH-215-11caerbjun29
Epipervilline
Single Pulse with Broadband Decoupling

¹³C-NMR

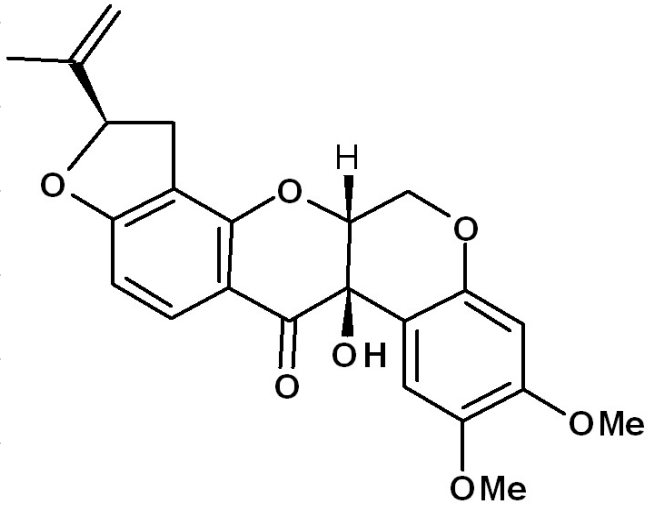


Compound 4: Epipervilline



LH215 Epirotenolone
Single Pulse Experiment

¹H-NMR (in CD₃OD)



Compound 5: Rotenolone

