

Electronic supplementary information

[Dimethylformamide-Stabilised Palladium Nanoclusters Catalysed Coupling Reactions of Aryl Halides with Hydrosilanes/Disilanes]

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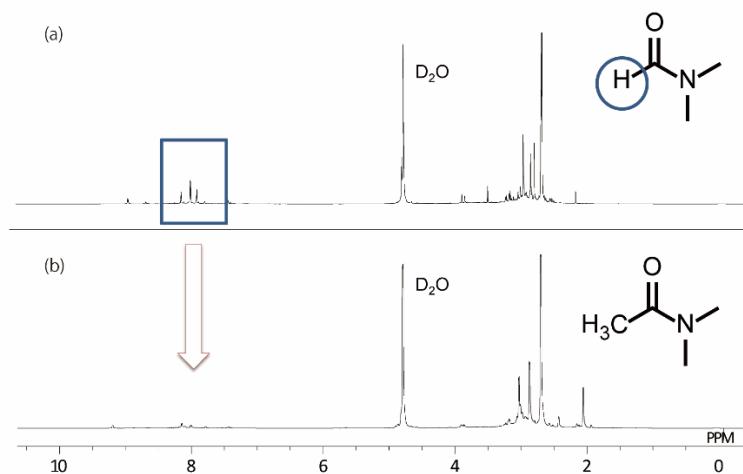


Figure S1 ^1H NMR (400 MHz, D_2O , 20 °C) spectra of (a) Pd NCs and (b) DMAc displaced Pd NCs

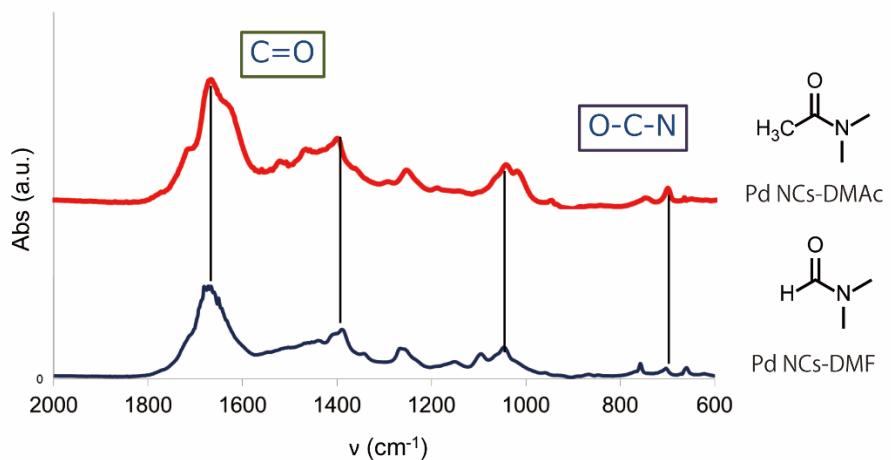


Figure S2 FT-IR measurement (red) DMAc displaced Pd NCs (blue) as prepared Pd NCs

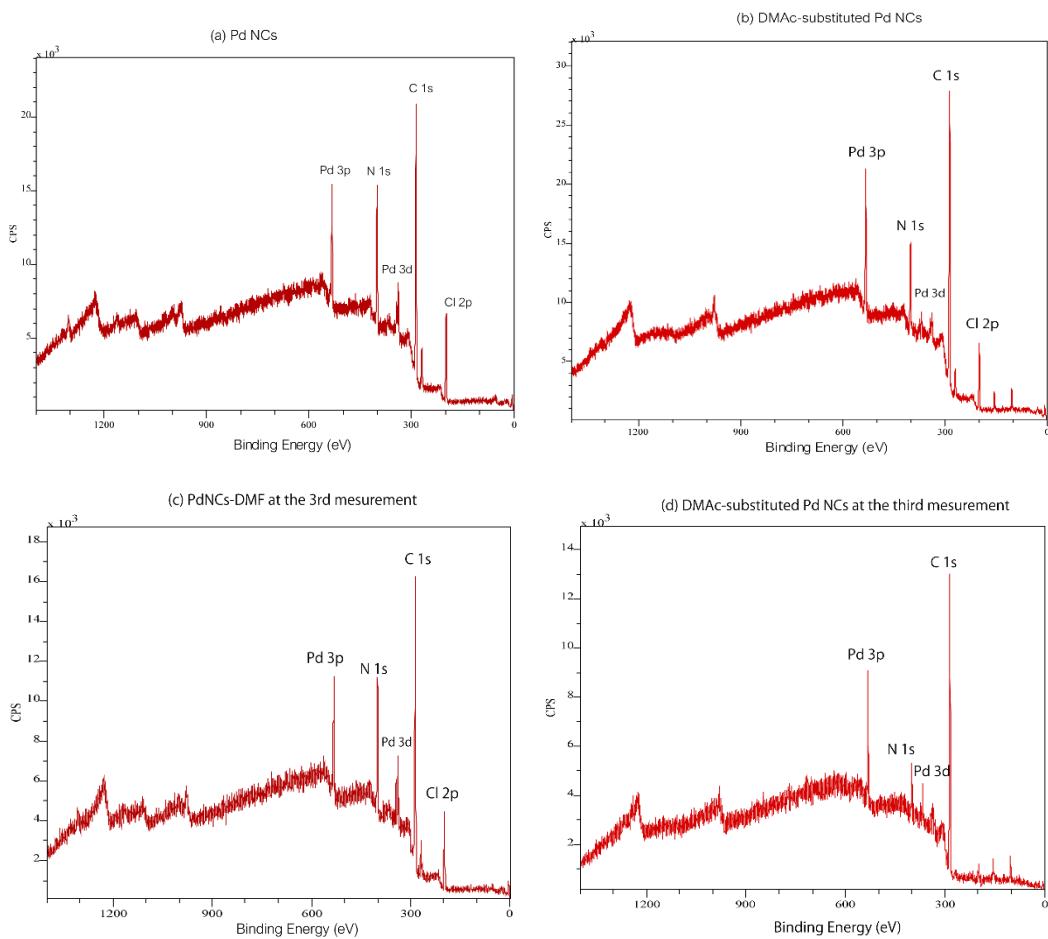
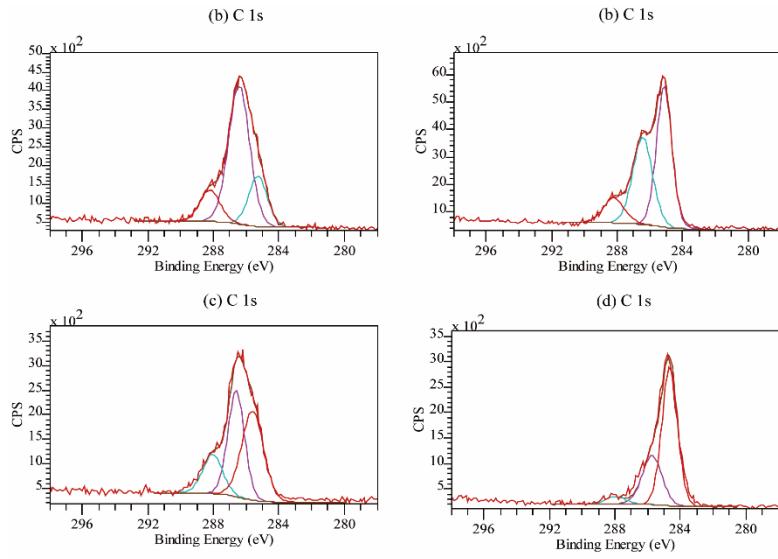


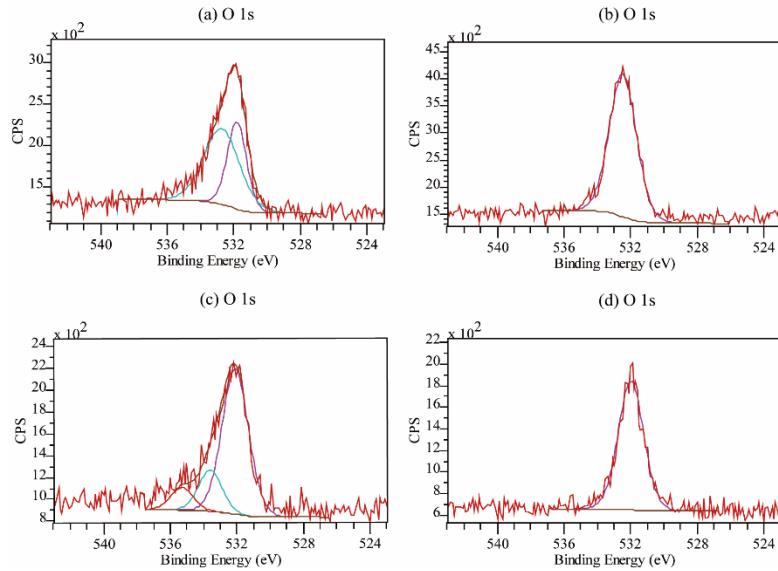
Figure S3 XPS wide scan spectra of (a) Pd NCs, (b) DMAc-substituted Pd NCs, (c) Pd NCs-DMF at the third measurement, and (d) DMAc-substituted Pd NCs at the third measurement.

Table S1 XPS peak positions, FWHMs

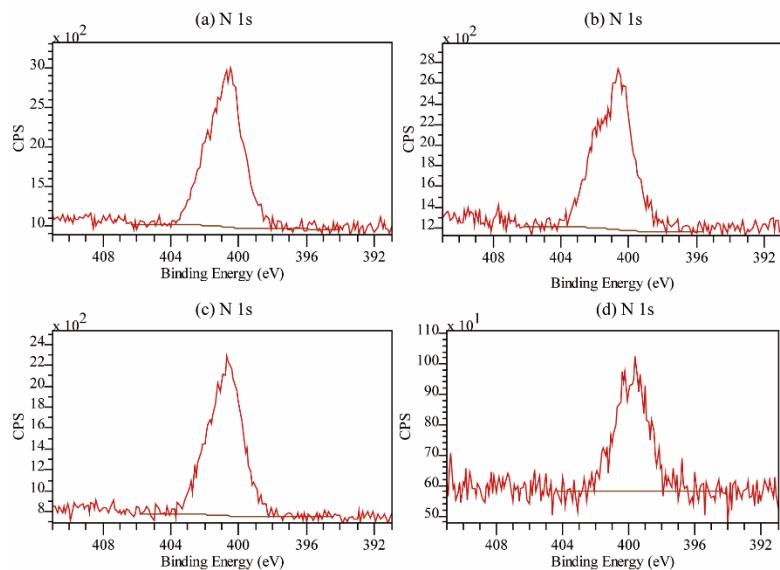
Element	Binding Energy (eV) [FWHM]				
	Pd 3d _{5/2}	Pd 3d _{3/2}	N 1s	O 1s	C 1s
(a) Pd NCs	338.8 [1.2]	344.0 [1.5]	400.8 [2.4]	532.8 [3.0]	288.2[1.5]
	337.2 [2.3]	342.1 [2.2]		531.9 [1.5]	286.4[1.4]
					285.1[1.1]
(b)DMAc-substituted Pd NCs	338.5 [1.6]	343.7 [1.9]	402.2 [1.5]	532.5 [1.9]	288.2 [1.5]
	336.6 [2.1]	341.8 [2.1]	400.5 [2.0]		286.4 [1.4]
					285.1 [1.1]
(c)Pd NCs-DMF at the third measurement	338.8 [0.9]	344.0 [1.3]	400.7 [2.4]	533.6 [2.9]	288.5 [1.2]
	338.0 [2.1]	343.3 [2.3]		532.1 [1.8]	286.3 [2.2]
(d)DMAc-substituted Pd NCs at the third measurement	335.7 [1.8]	342.1 [1.7]	399.8 [2.4]	532.0 [1.8]	288.0 [1.4]
	334.7 [1.4]	340.2 [1.6]			285.7 [1.4]
					284.6 [1.1]



(A) Figure S4 XPS Spectra of C 1s from (i) Pd NCs, (ii) DMA-substituted Pd NCs, (iii) Pd NCs–DMF at the third measurement, and (iv) DMAc-substituted Pd NCs at the third measurement,



(B) Figure S5 XPS Spectra of O 1s from (i) Pd NCs, (ii) DMAc-substituted Pd NCs, (iii) Pd NCs–DMF at the third measurement, and (iv) DMAc-substituted Pd NCs at the third measurement,



(C) Figure S6 XPS Spectra of N 1s from (i) Pd NCs, (ii) DMAc-substituted Pd NCs, (iii) Pd NCs–DMF at the third measurement, and (iv) DMAc-substituted Pd NCs at the third measurement,

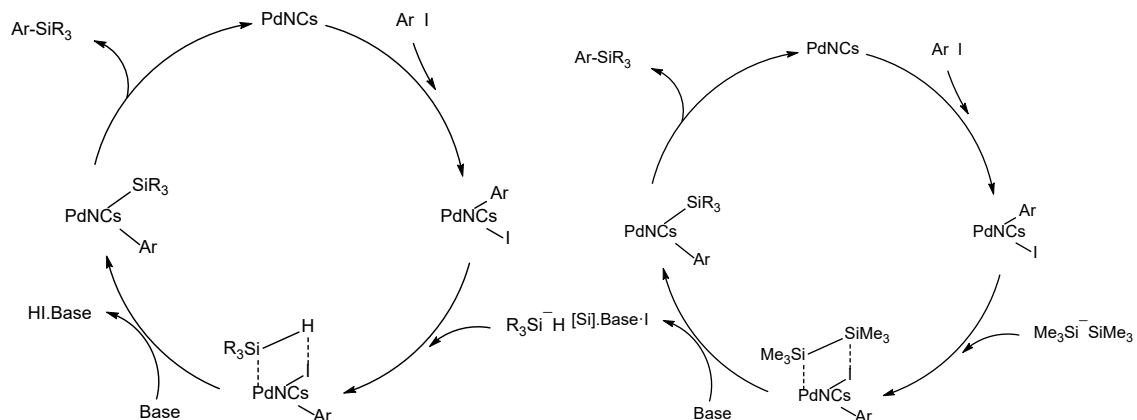


Figure S7 a plausible reaction mechanism of Pd NCs catalyzed coupling reactions of aryl halides with hydrosilanes(left)¹/disilanes(right)²

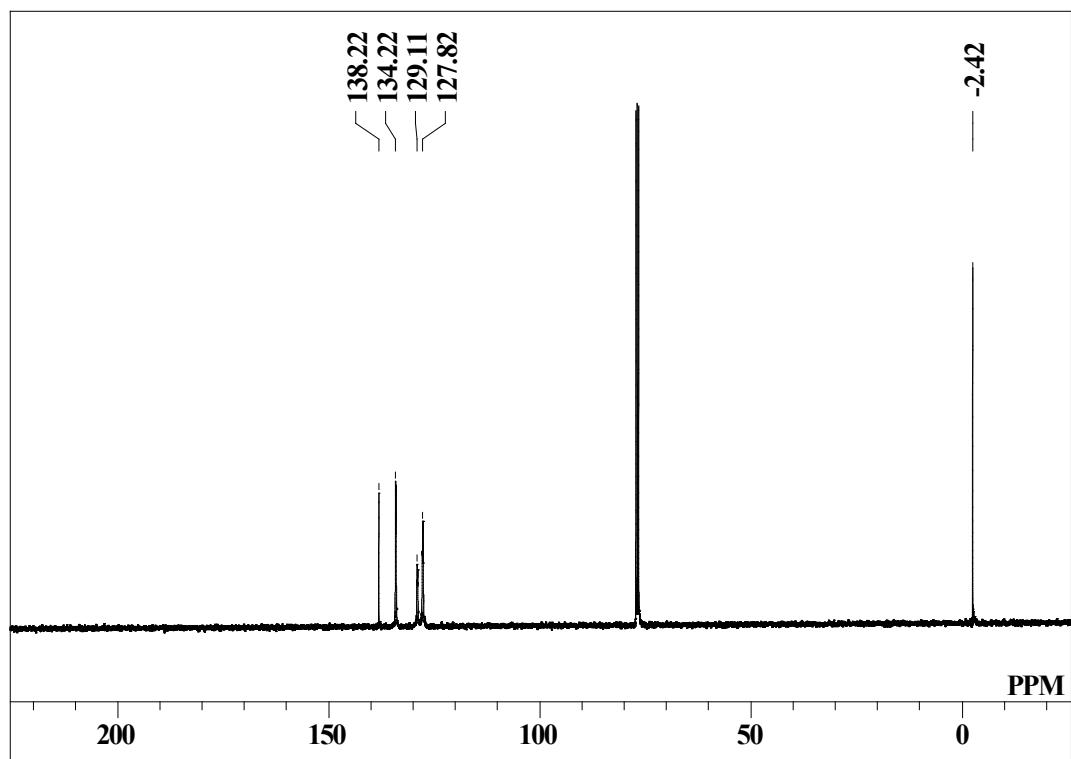
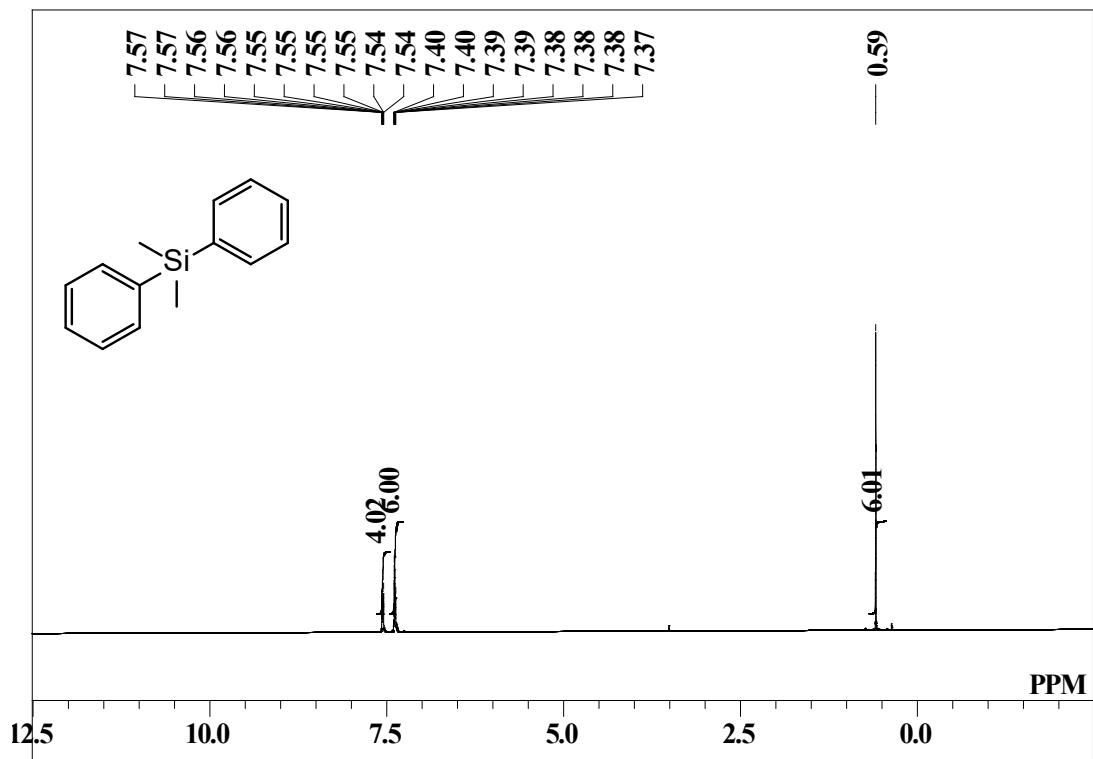
Table S2 concentration of K and Pd by ICP-AES

<intensity>			<concentration>		
element	Na	Pd	element	Na	Pd
wavelength(nm)	588.995nm	340.458nm	wavelength(nm)	588.995nm	340.458nm
Run 1	15.1392	0.627558	unit	ppm	ppm
Run 2	15.1701	0.625988	Run 1	201.354	2.3557
Run 3	15.1219	0.624458	Run 2	201.766	2.34897
			Run 3	201.123	2.34242
average	15.1438	0.626001	average	201.414	2.34903
R	0.048169	0.0031	R	0.643555	0.013282
SD	0.024401	0.00155	SD	0.326007	0.006641
RSD	0.16113	0.247599	RSD	0.161859	0.282717

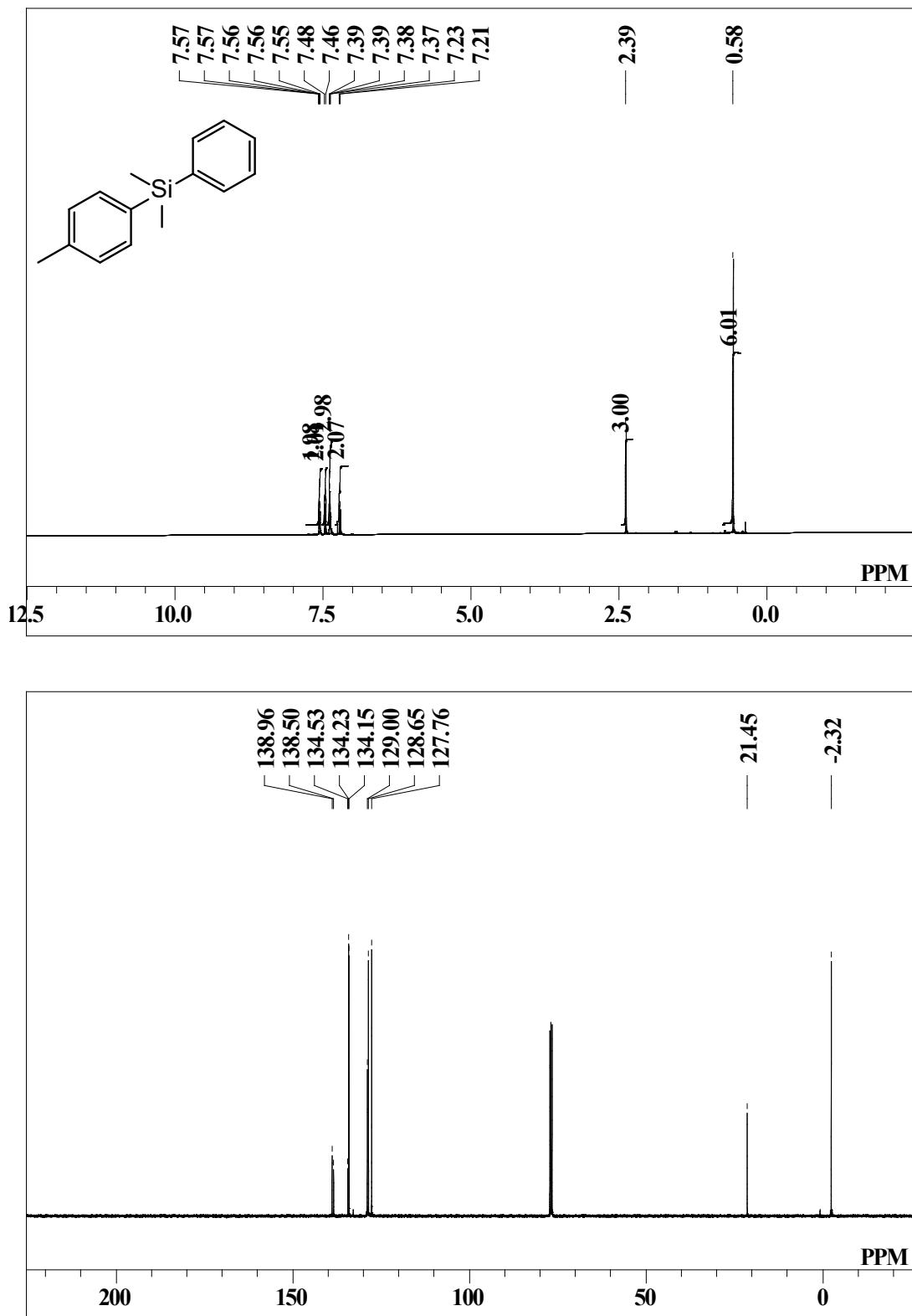
Reference

- 1 J. Cao, Y.-M. Cui, Z. Xu, J. Zhang, L.-W. Xu, Z.-J. Zheng and J.-Z. Xu, *Chem. - An Asian J.*, 2017, **12**, 1749–1757.
- 2 E. Shirakawa, T. Kurahashi, H. Yoshida and T. Hiyama, *Chem. Commun.*, 2000, **0**, 1895.

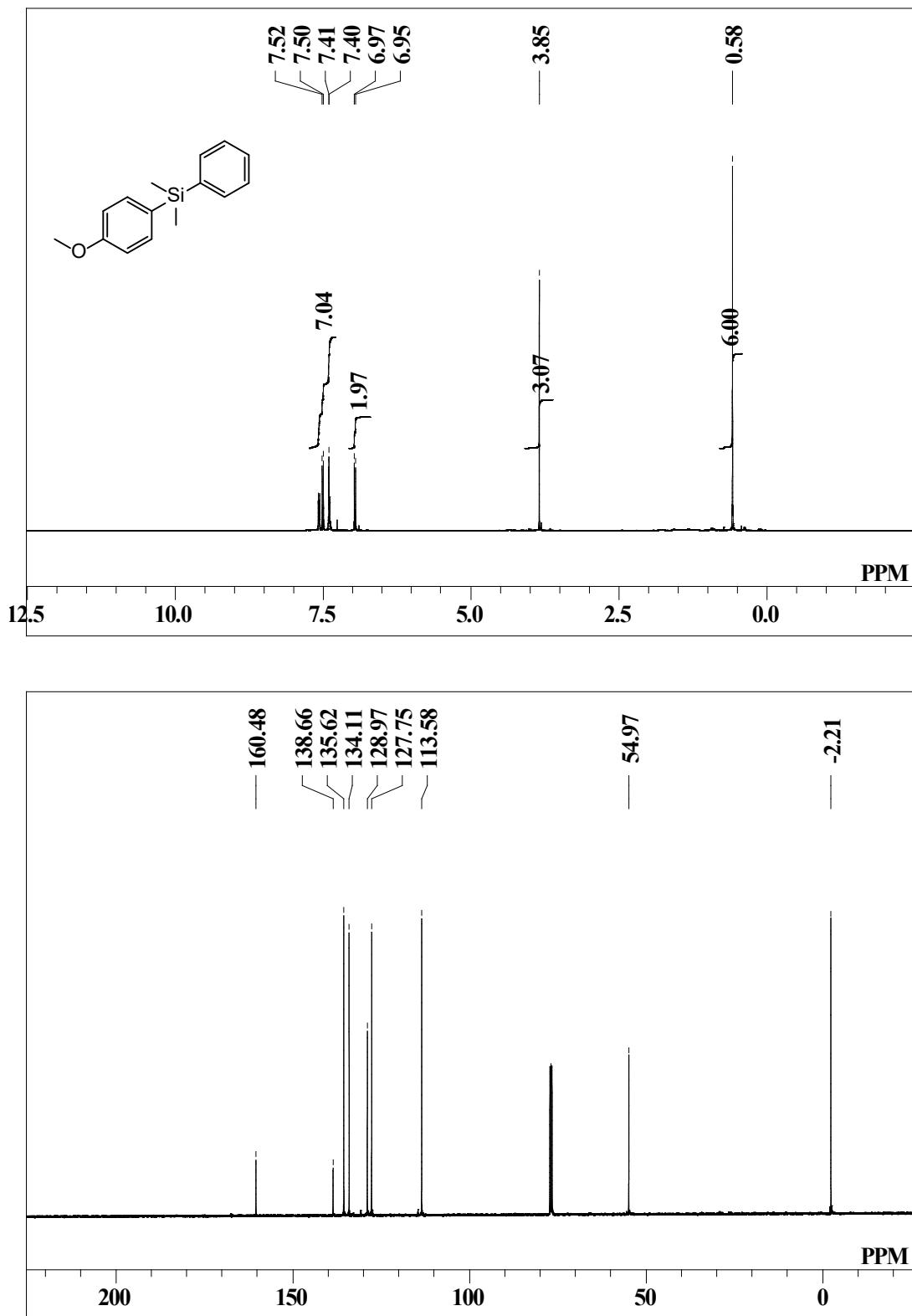
3a Dimethyldiphenylsilane



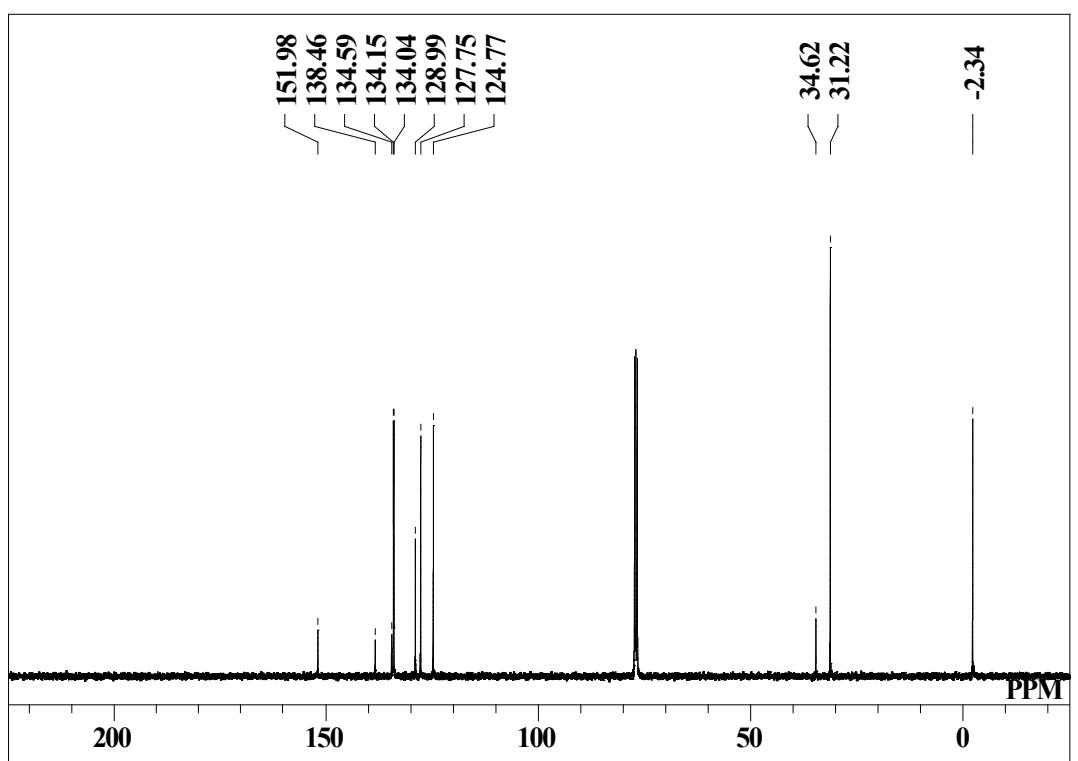
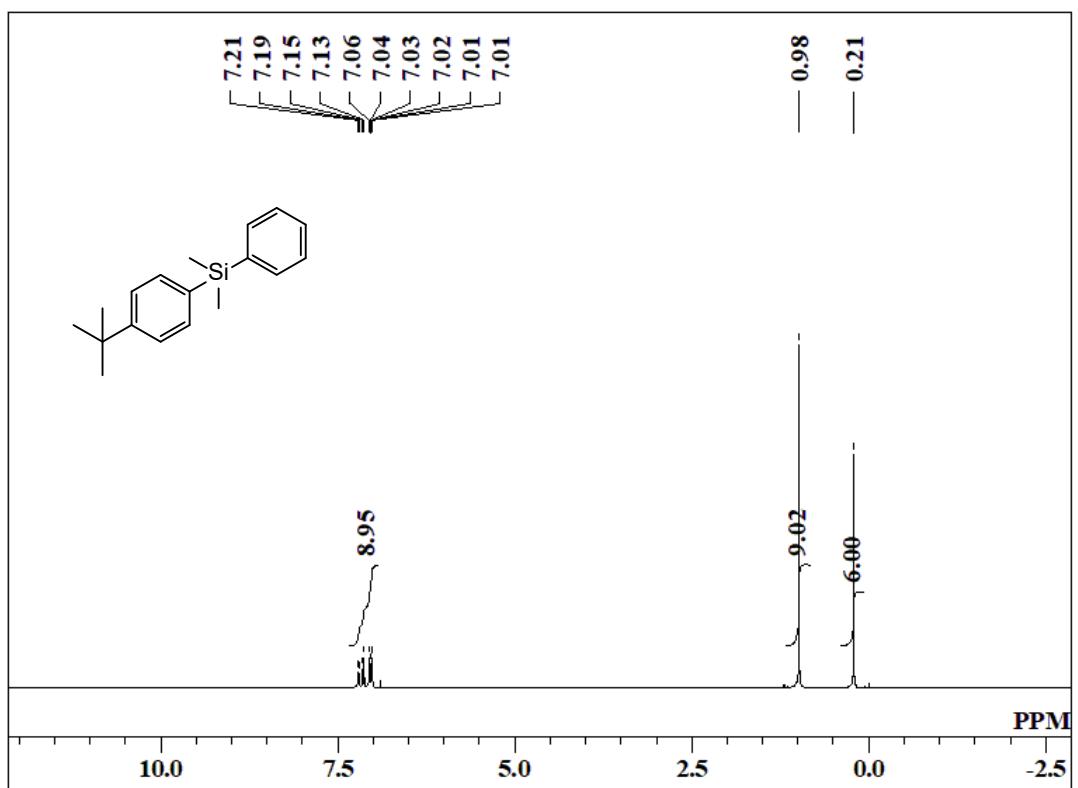
3b dimethyl(phenyl)(p-tolyl)silane



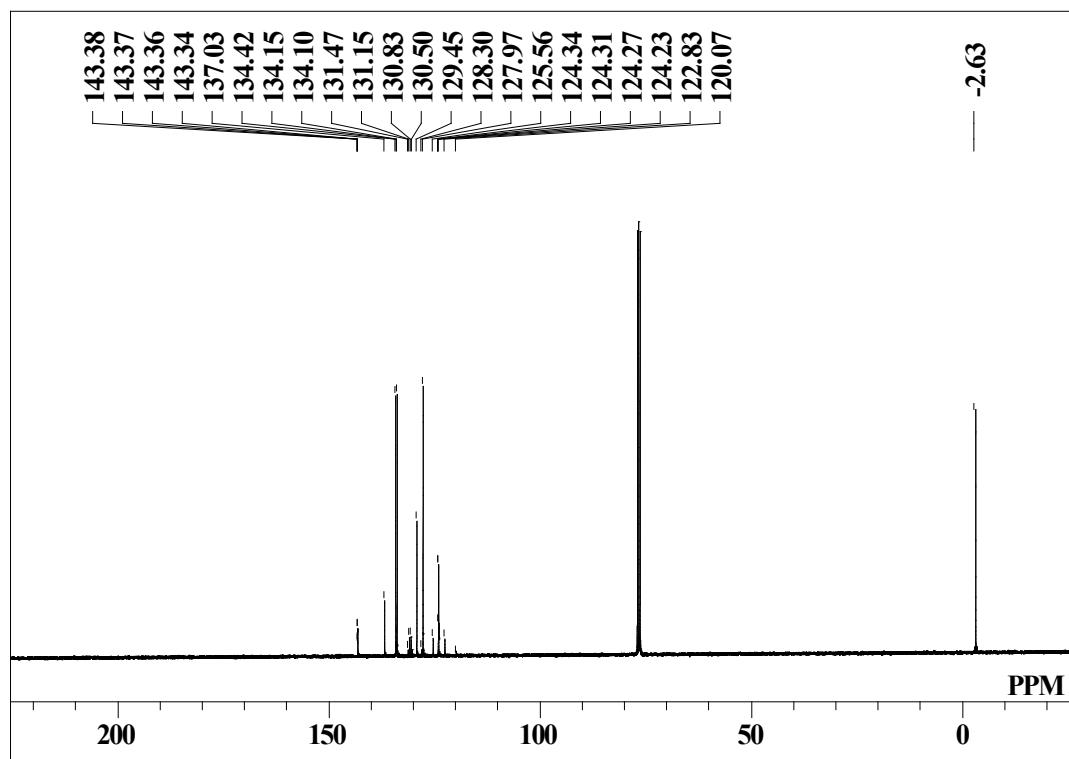
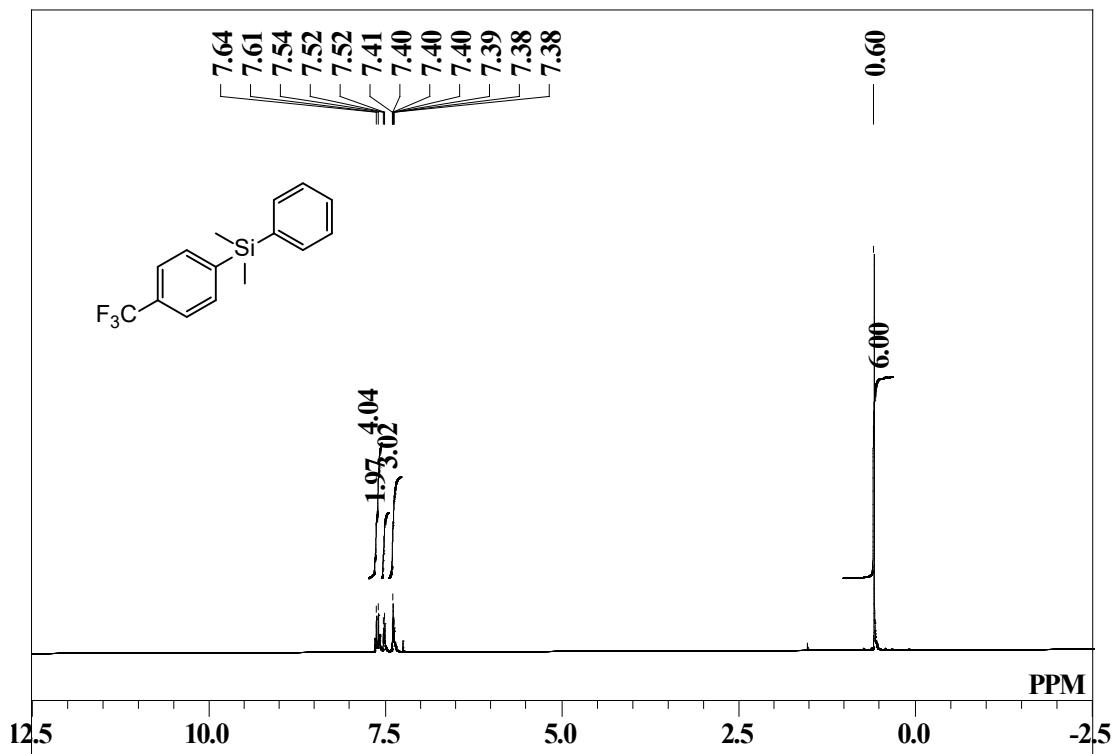
3c (4-methoxyphenyl)dimethyl(phenyl)silane



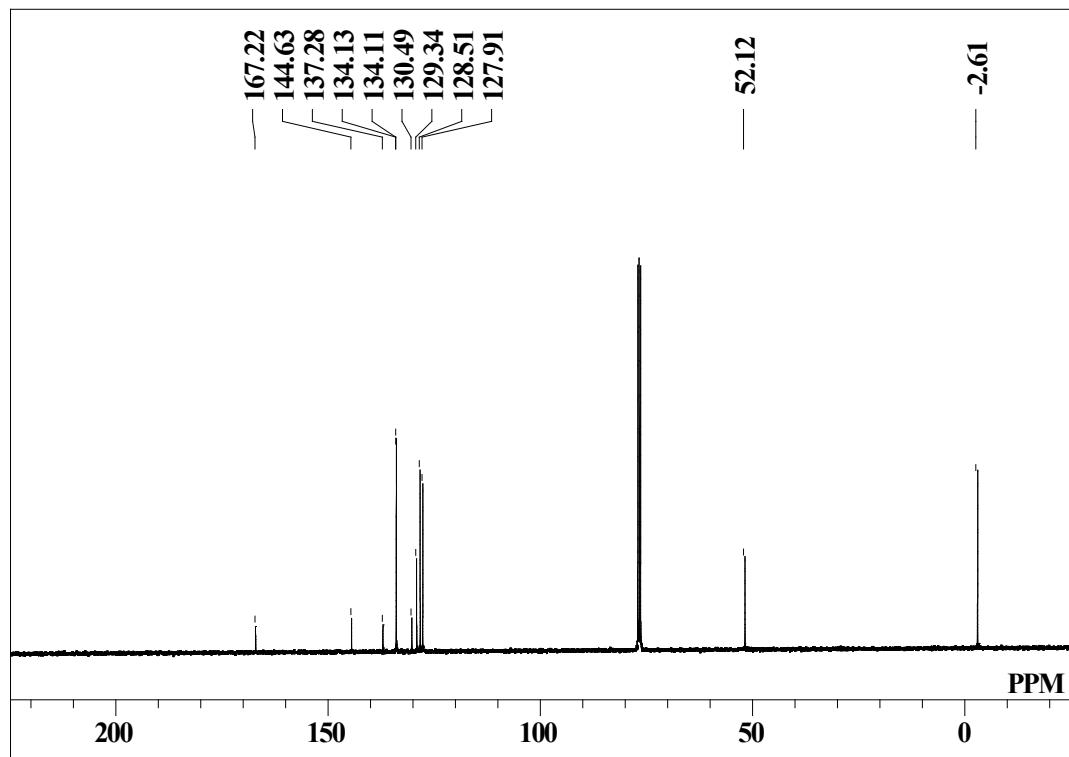
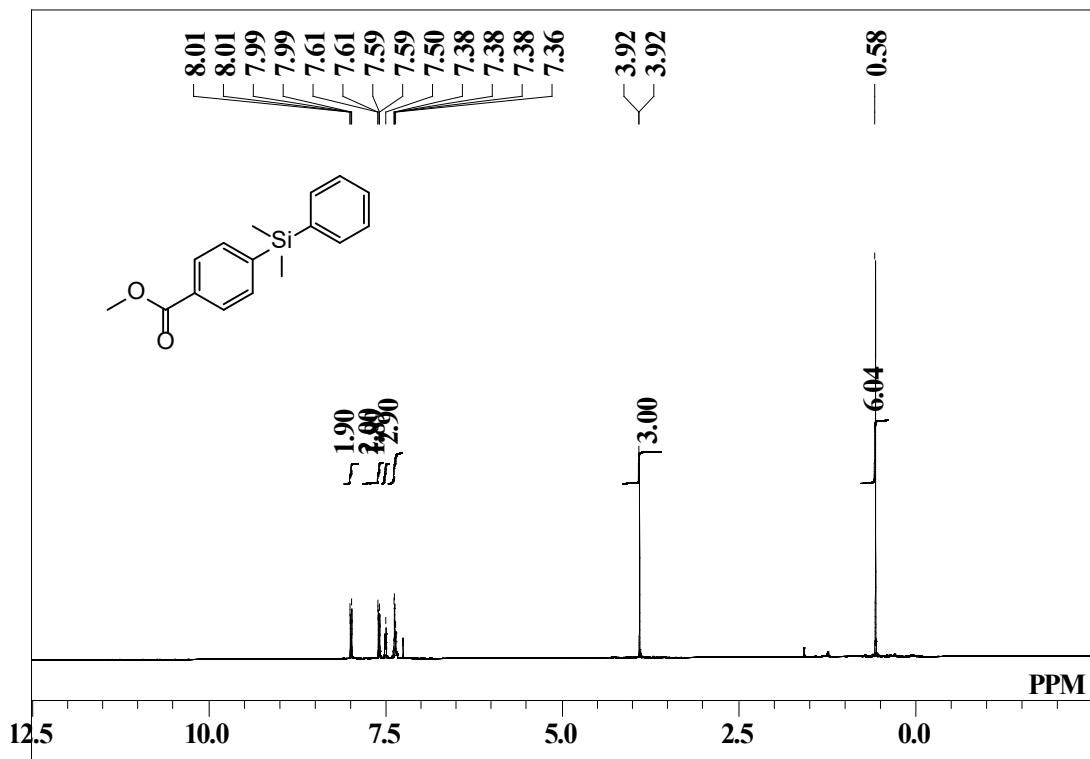
3d (4-(tert-butyl)phenyl)dimethyl(phenyl)silane



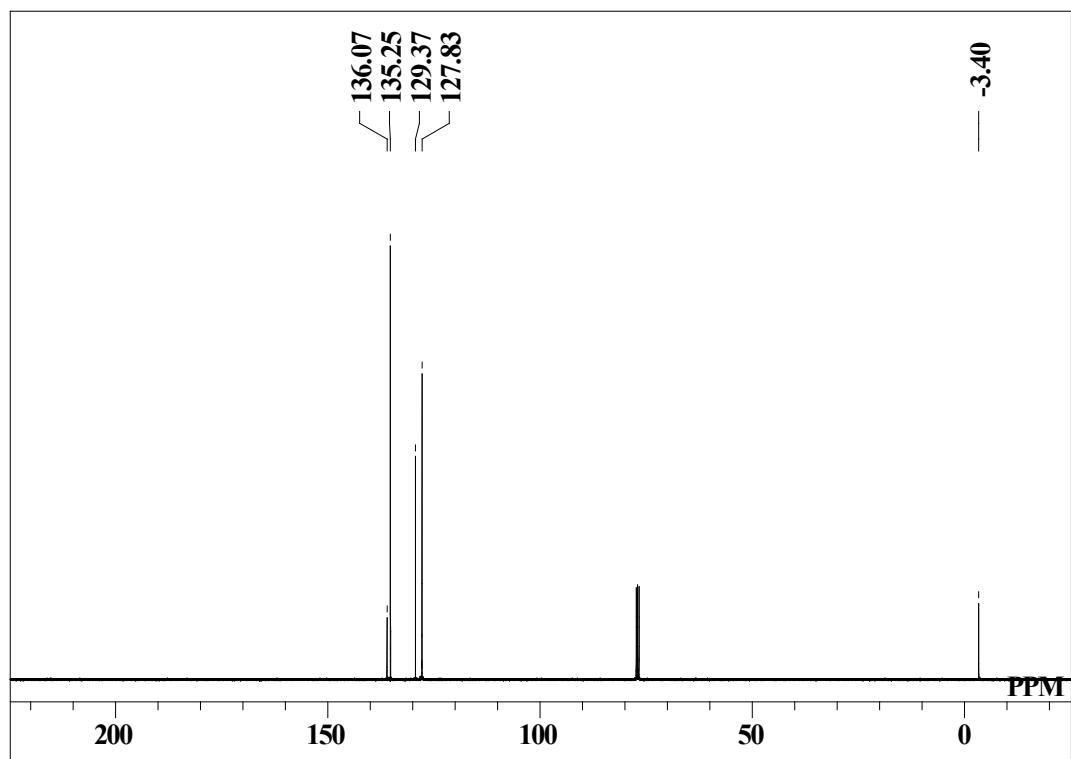
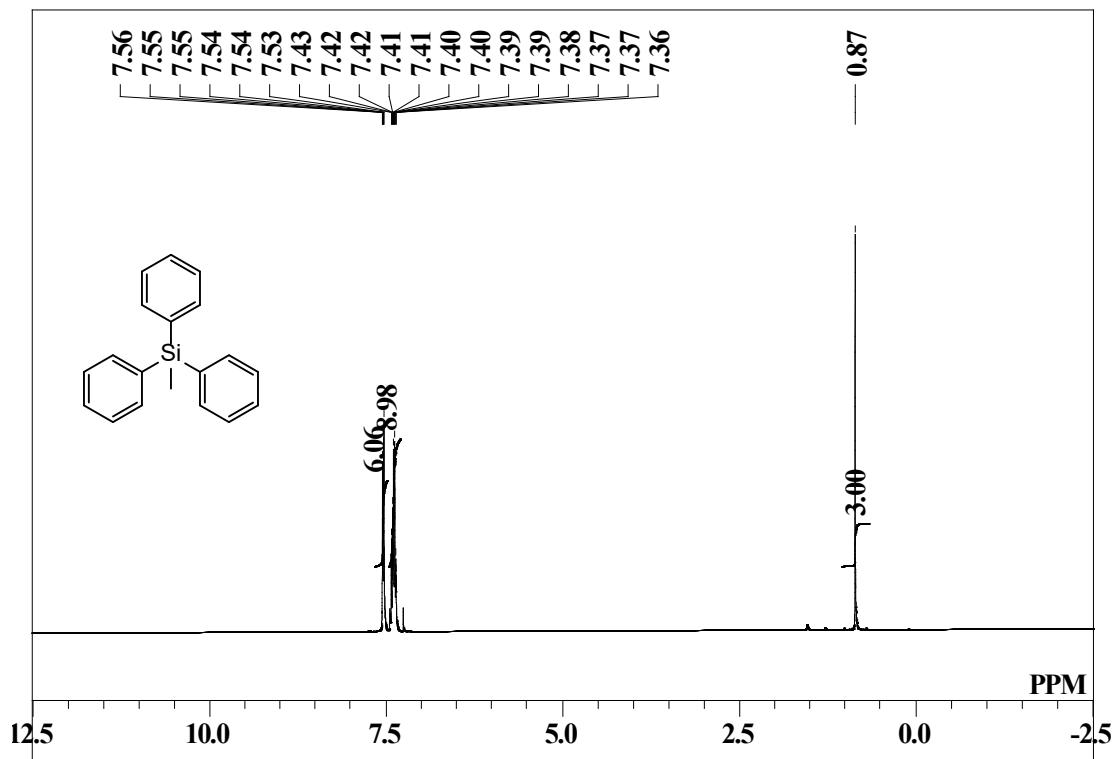
3e dimethyl(phenyl)(4-(trifluoromethyl)phenyl)silane



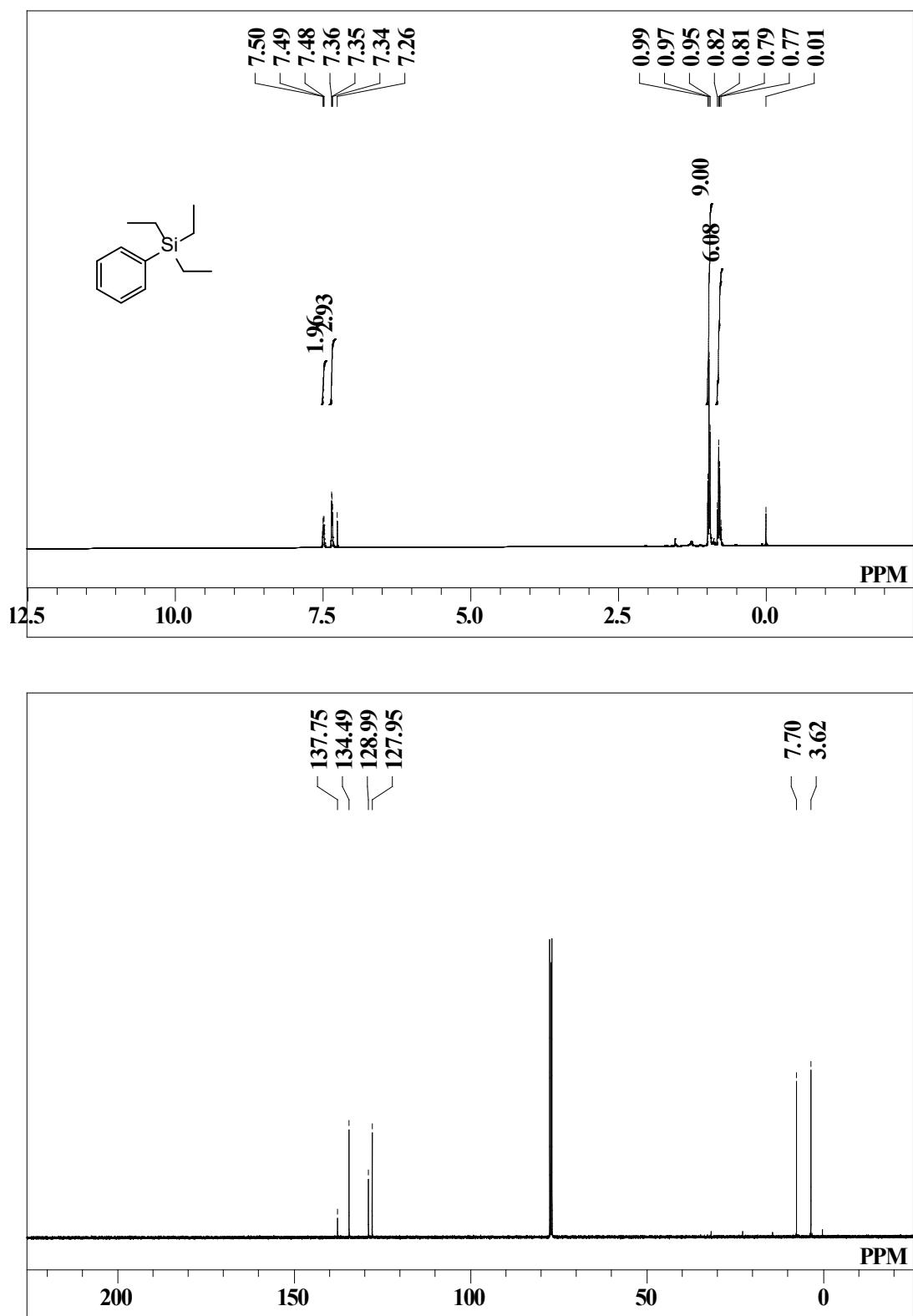
3f methyl 4-(dimethyl(phenyl)silyl)benzoate



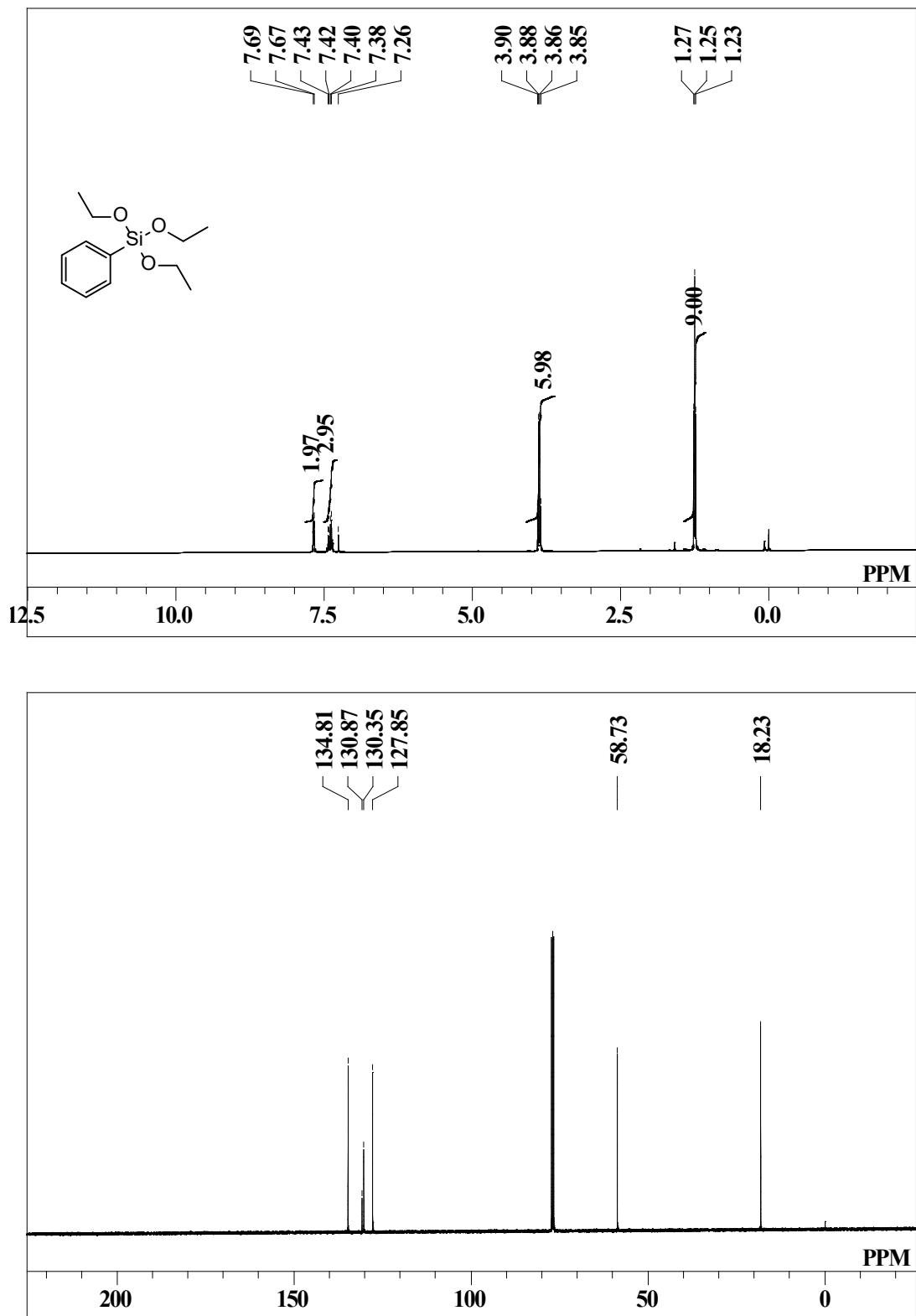
3g methyltriphenylsilane



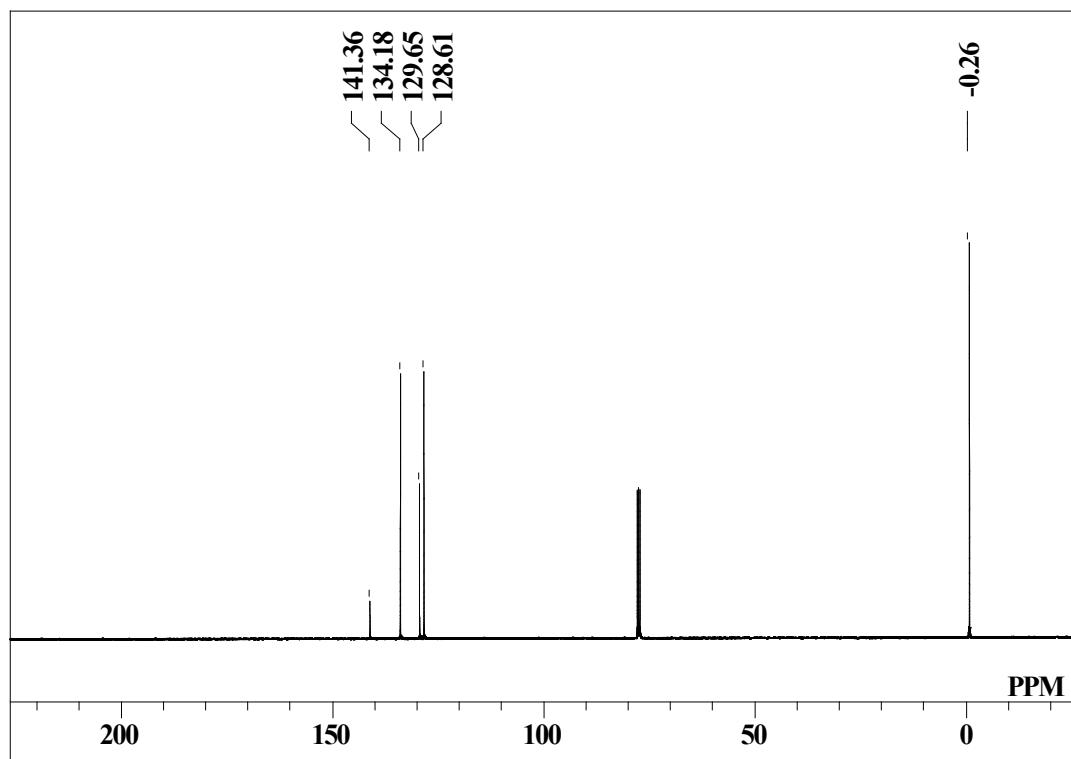
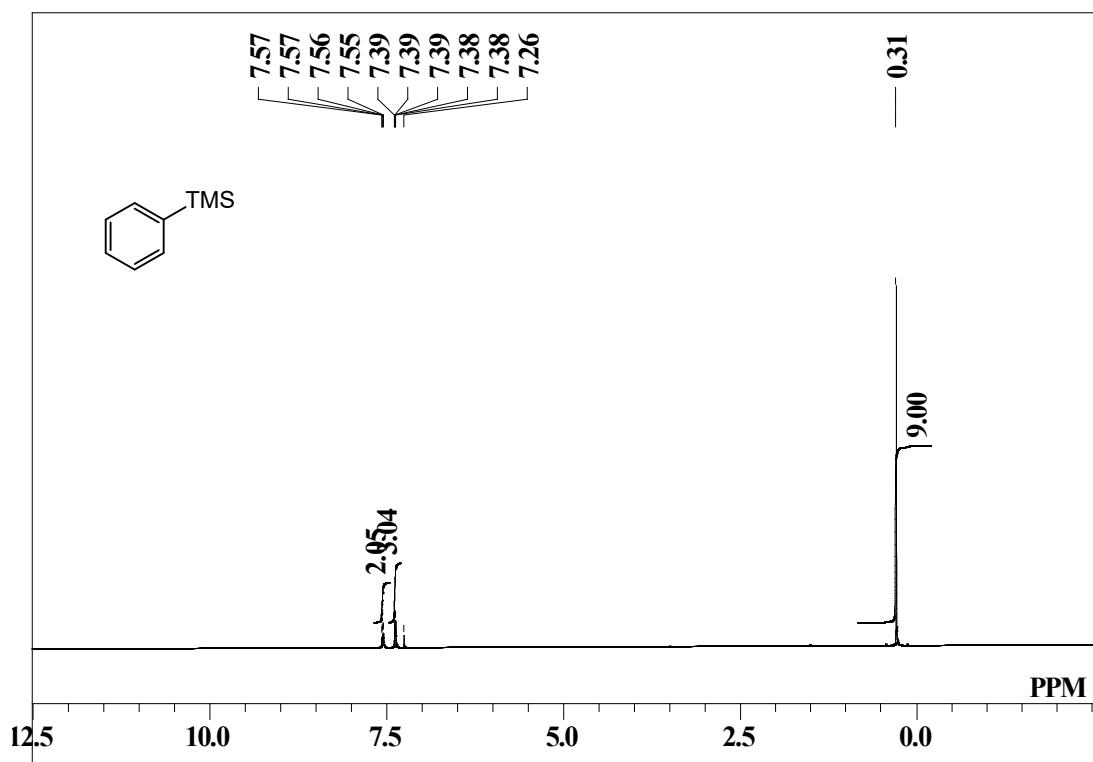
3h triethyl(phenyl)silane



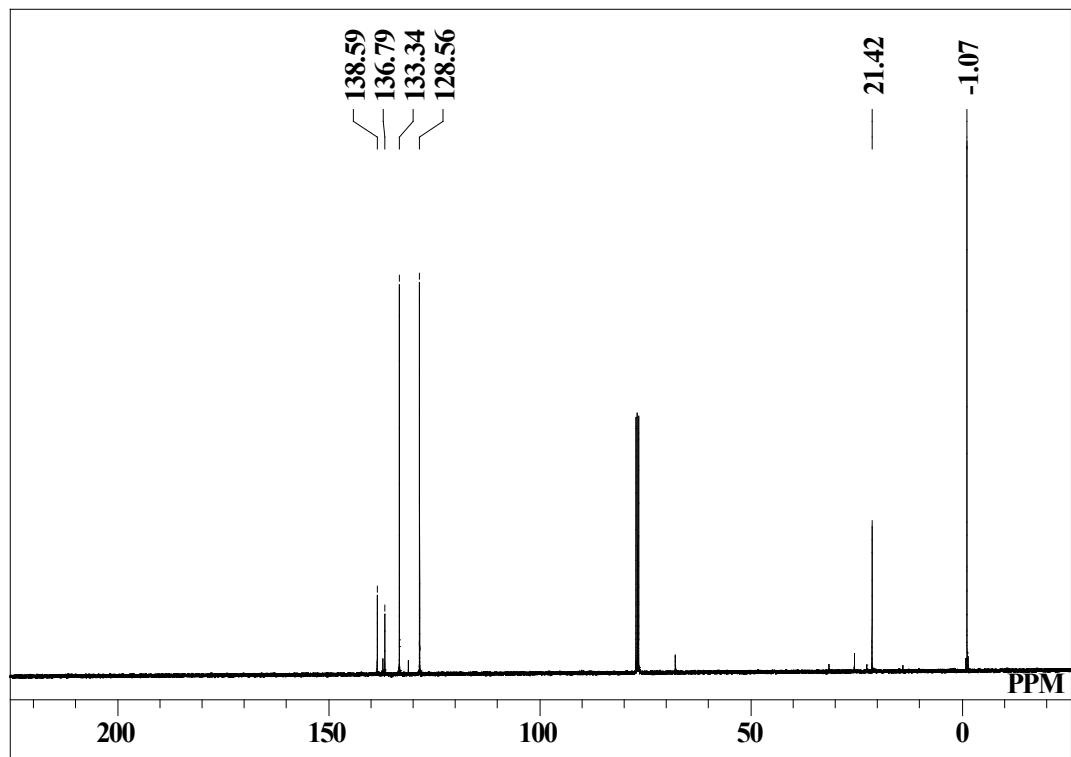
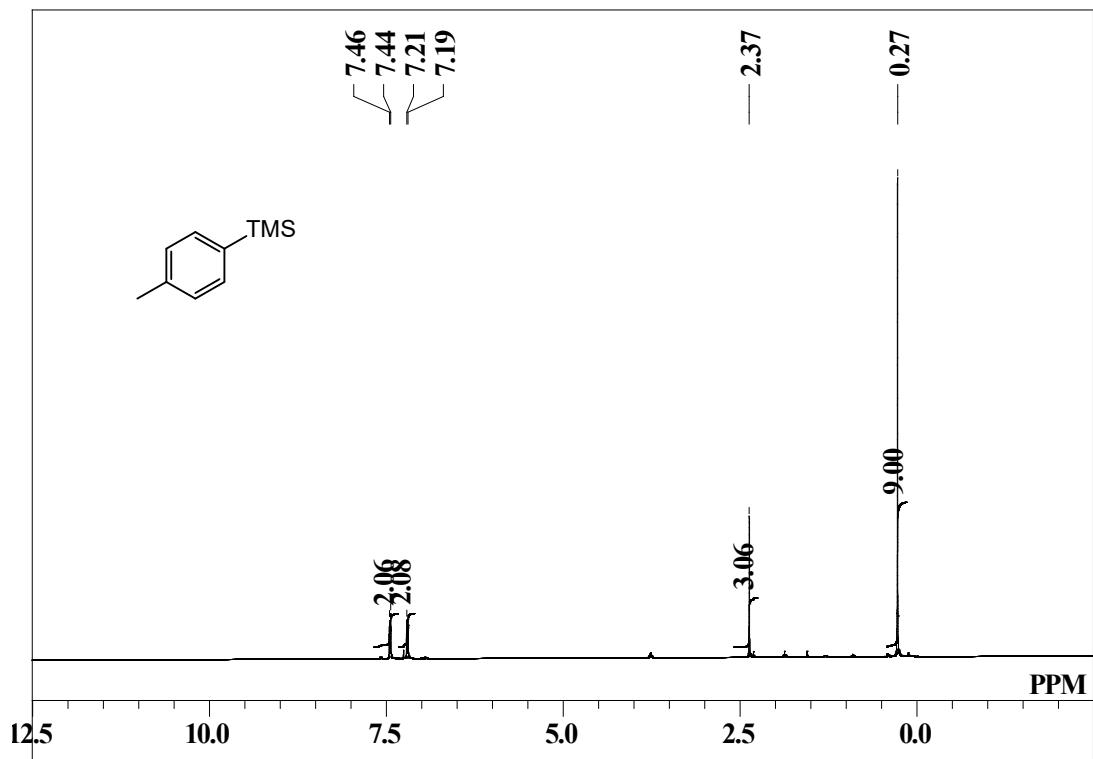
3i triethoxy(phenyl)silane



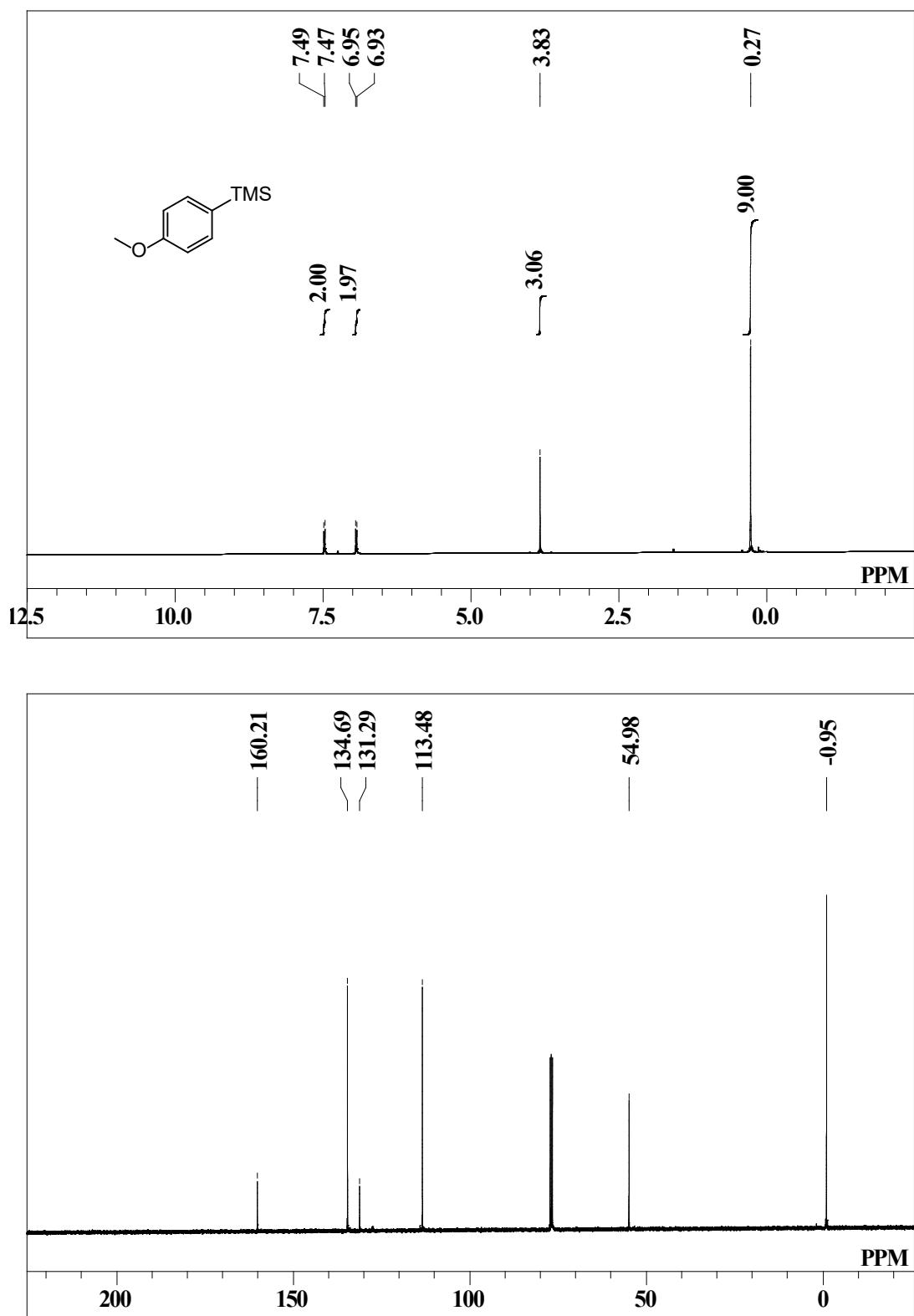
5a trimethyl(phenyl)silane



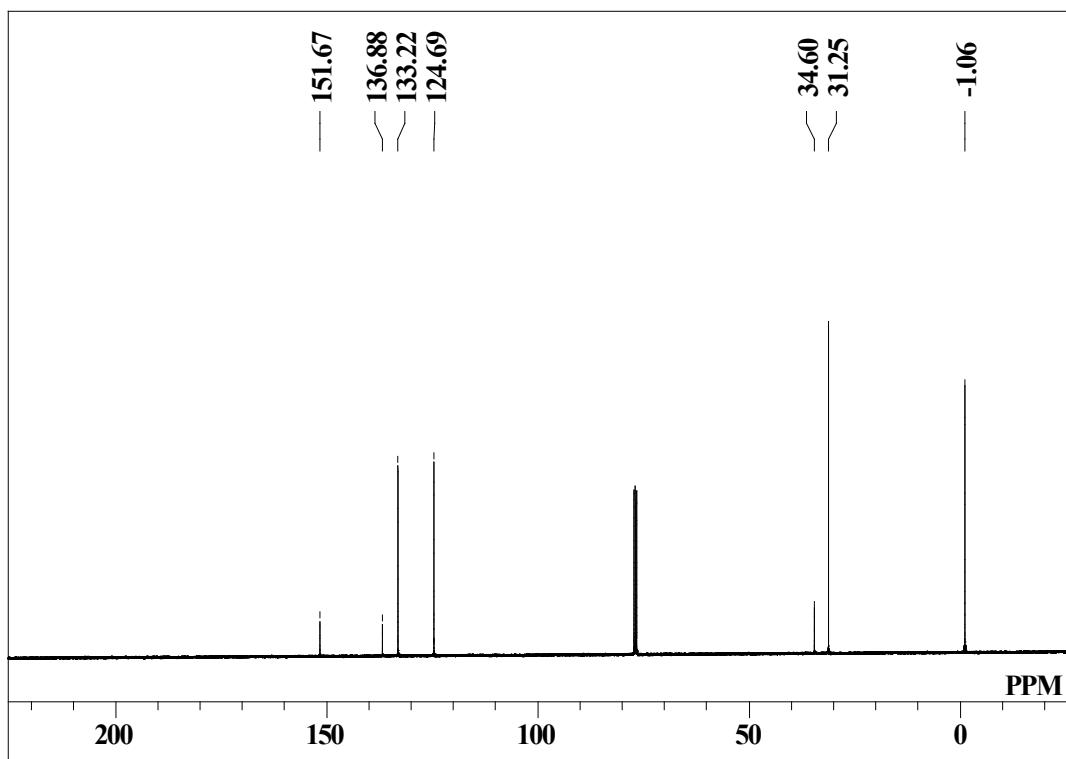
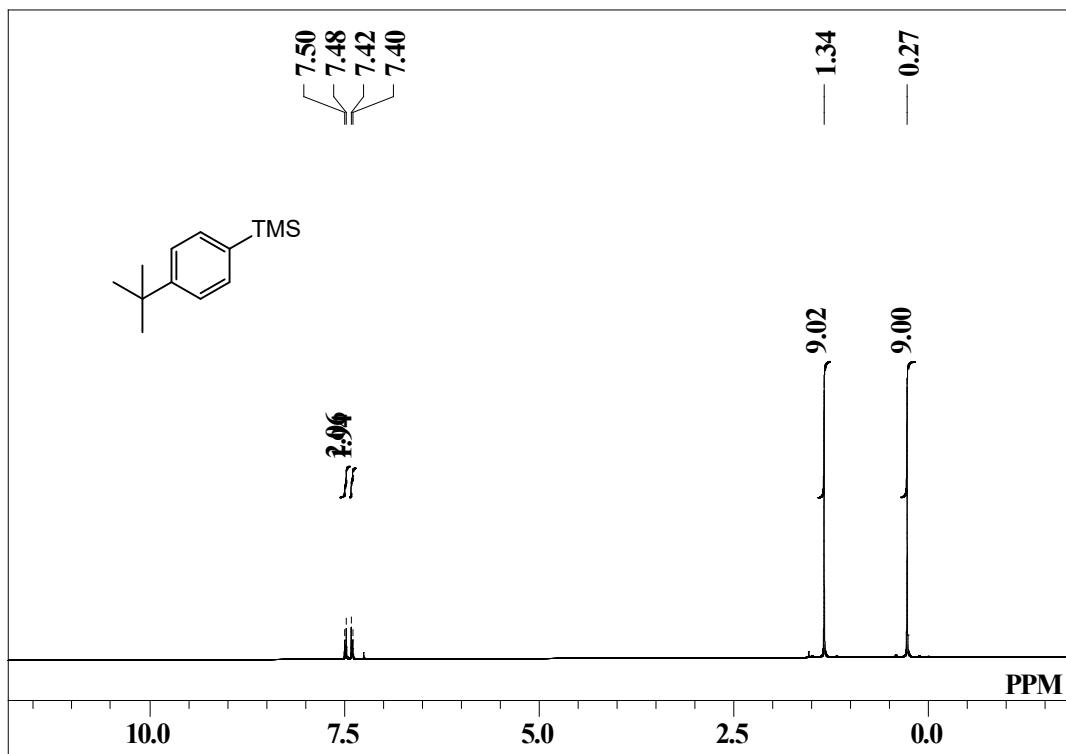
5b trimethyl(p-tolyl)silane



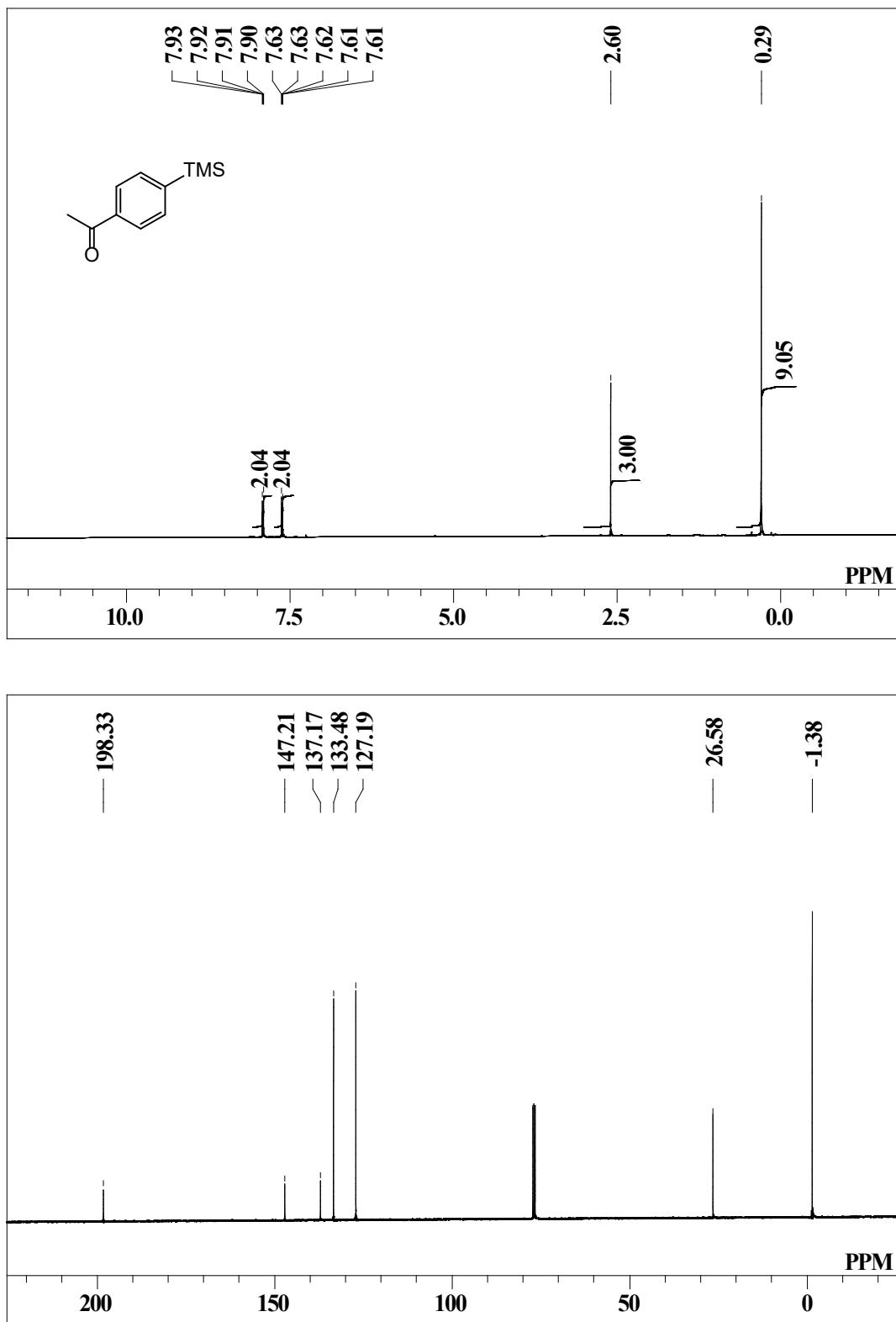
5c (4-methoxyphenyl)trimethylsilane



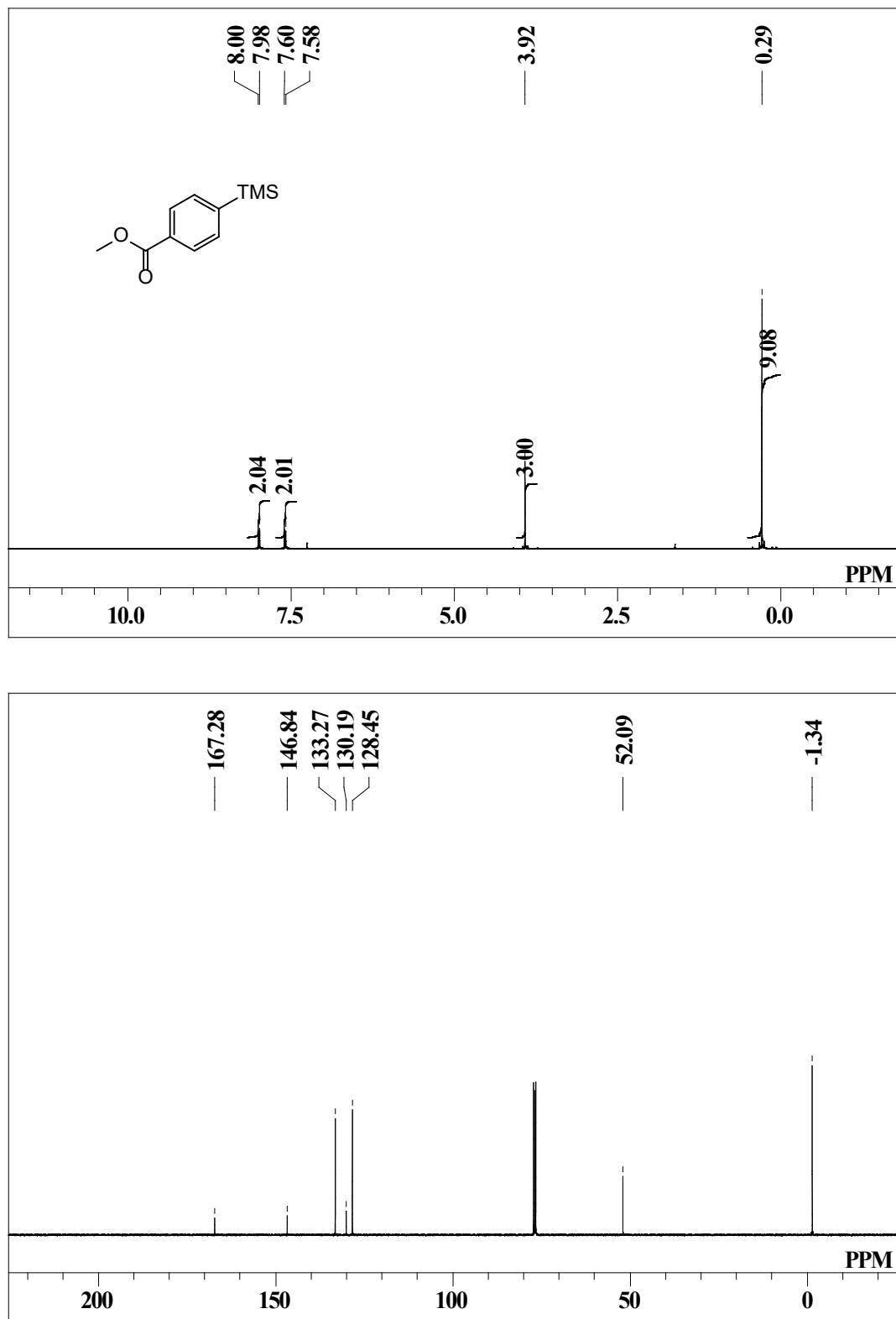
5d (4-(tert-butyl)phenyl)trimethylsilane



5e 1-(4-(trimethylsilyl)phenyl)ethan-1-one



5f methyl 4-(trimethylsilyl)benzoate



5g trimethyl(4-(trifluoromethyl)phenyl)silane

