First synthesis of pyrene functionalized silatranes for mechanistic insight into their potential anti-parasitic and anti-oxidation activities

SUPPORTING INFORMATION

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Table S1. Crystallographic detail of compound 6

Compound	**6**
Formula	$C_{52}H_{55}N_4O_6Si_2$
MW [g·mol^{-1}]	888.18
Crystal system	Orthorhombic
Space group	*Pna*2$_1$
a [Å]	27.649(3)
b [Å]	7.2495(9)
c [Å]	21.908(2)
α [deg]	90
β [deg]	90
γ [deg]	90
V [Å^3]	4391.1(8)
T [K]	170(2)
Z	4
ρ_{calc} [g·cm^{-3}]	1.343
μ [mm^{-1}]	0.139
Min/max transmission	0.987/0.989
θ_{max} [deg]	28.308
Measured reflections	33568
Unique reflections	10819
Reflections [$F_0 > 4\sigma(F_0)$]	3563
Parameter	578
R_{int}	0.1299
R_1 [$F_0 > 4\sigma(F_0)$]	0.0500

wR_2 [all data]	0.0959
GOF	0.748
$\Delta\rho_{max}/\Delta\rho_{min}$ [e·Å^{-3}]	0.365/-0.296
CCDC number	1555883

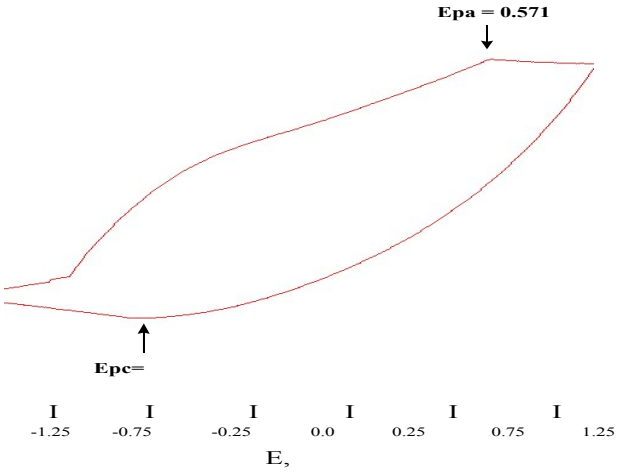

Figure S1. Cyclic voltammogram of 6 using 1mM of analyte in DCM and 0.1mM Bu_4NPF_6 with a scan rate of 50 mV s^{-1}

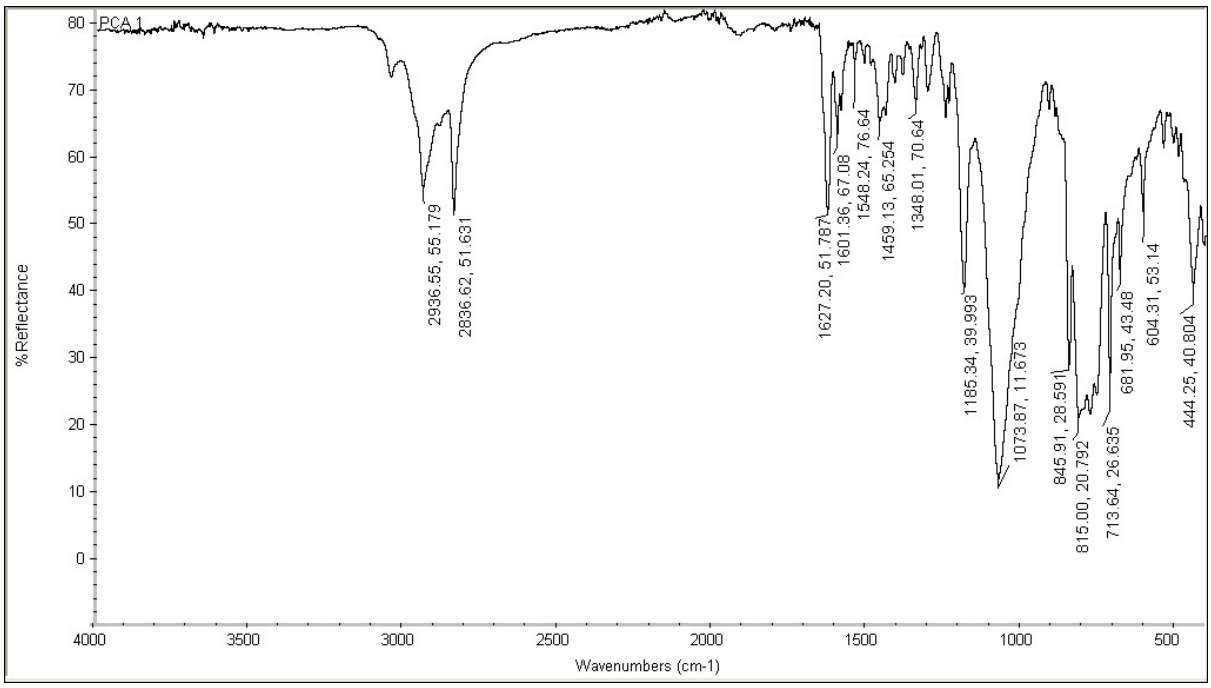

Figure S2. IR spectrum of 3

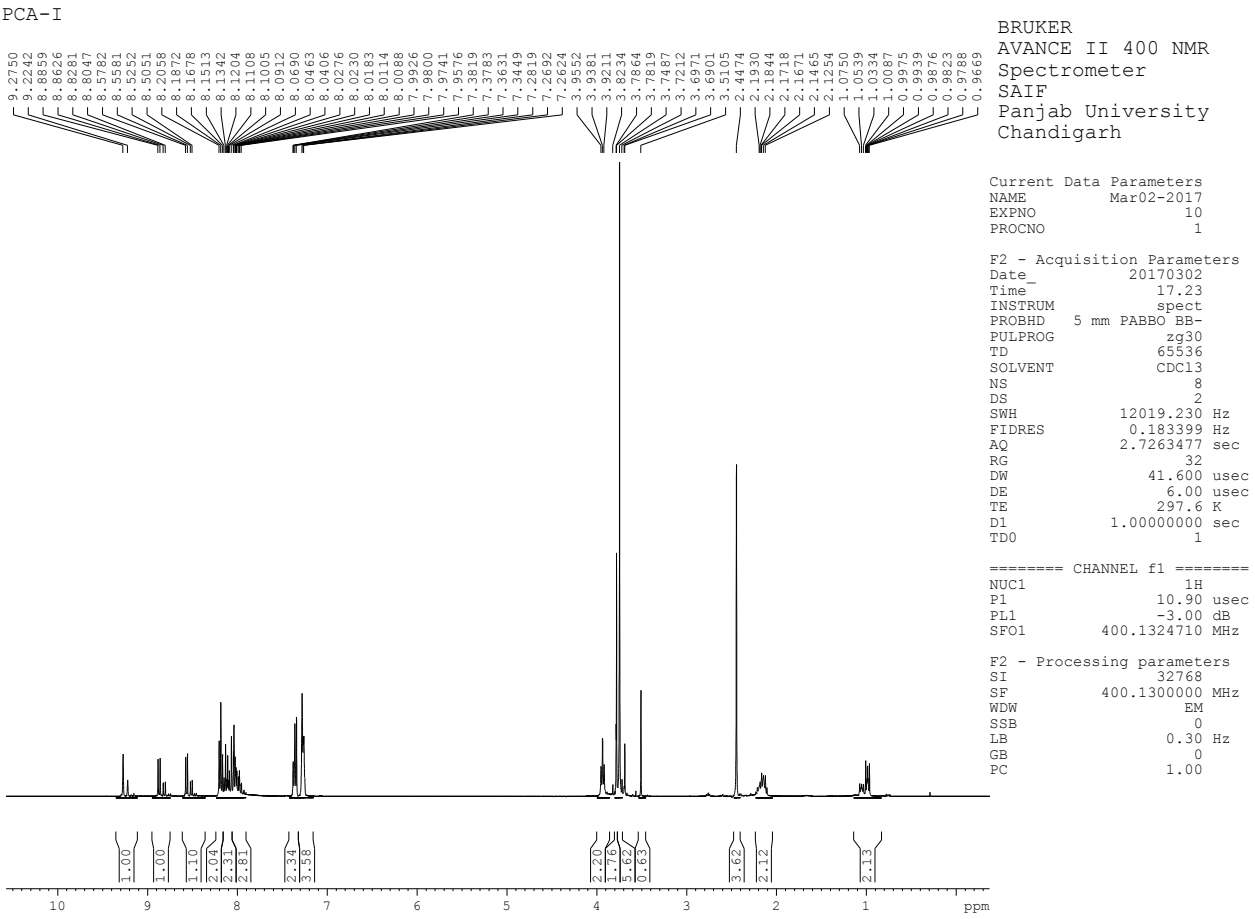

Figure S3. ^{1}H NMR spectrum of 3

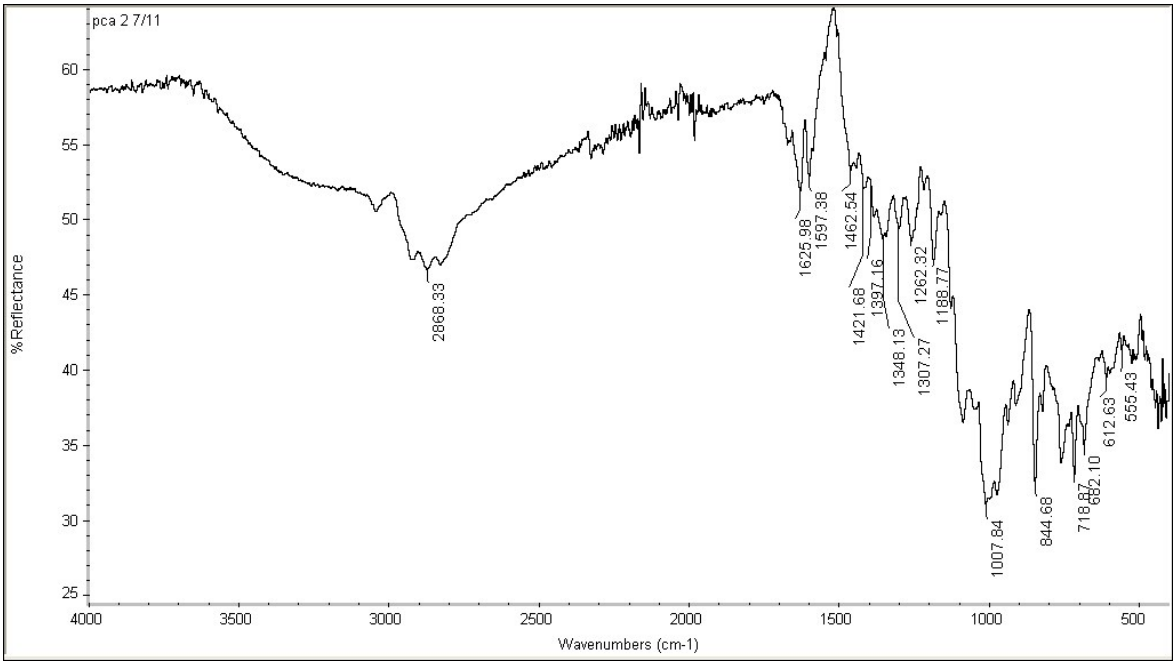

Figure S4. IR spectrum of 6

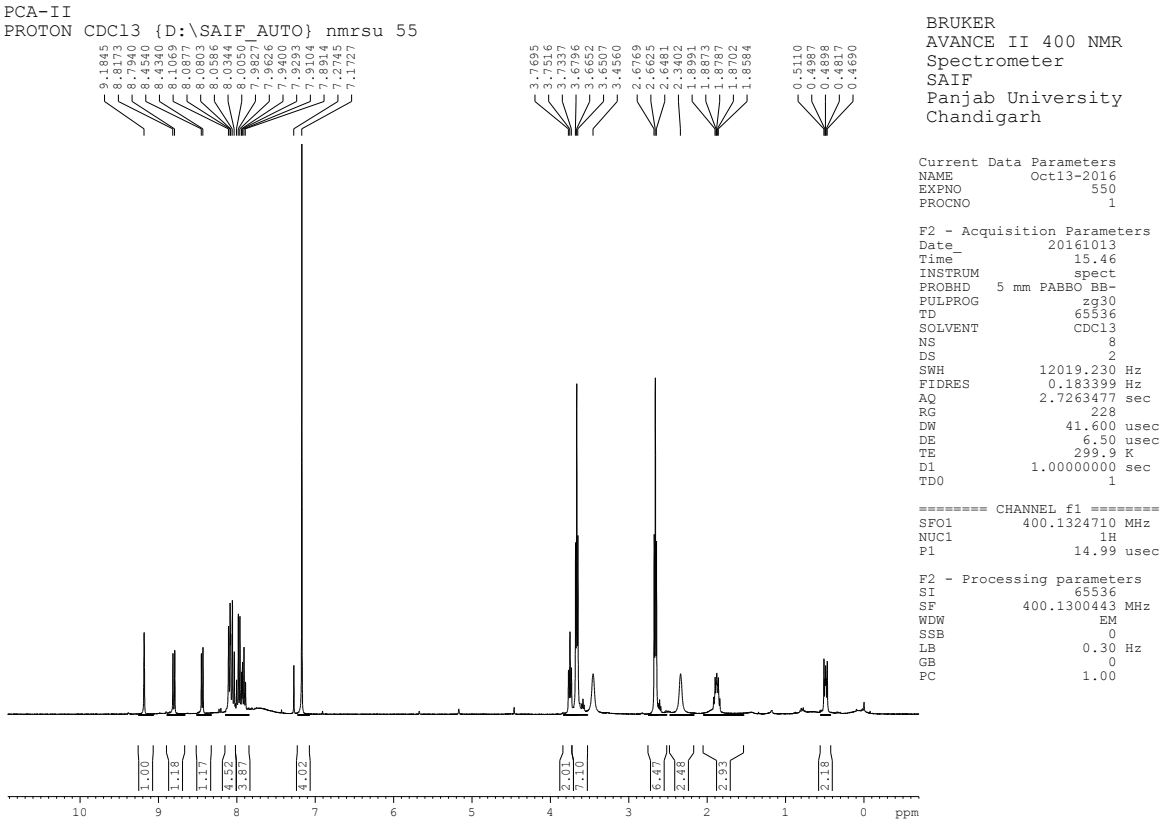

Figure S5. NMR spectrum of 6

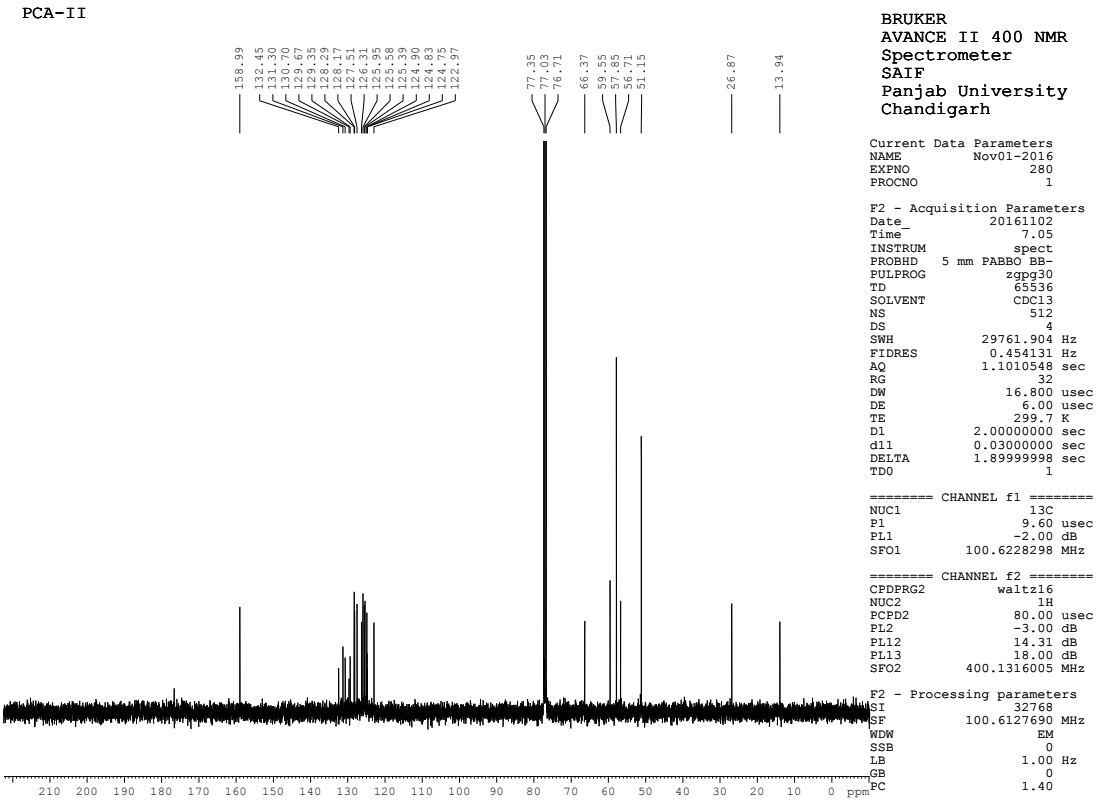

Figure S6. ^{13}C NMR spectrum of 6

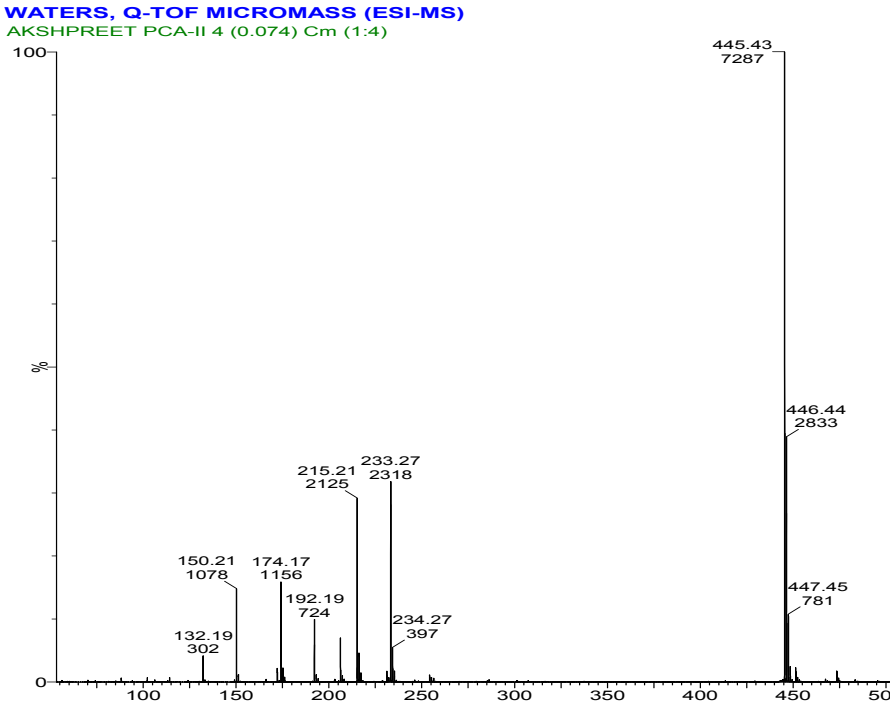

Figure S7. Mass spectrum of 6

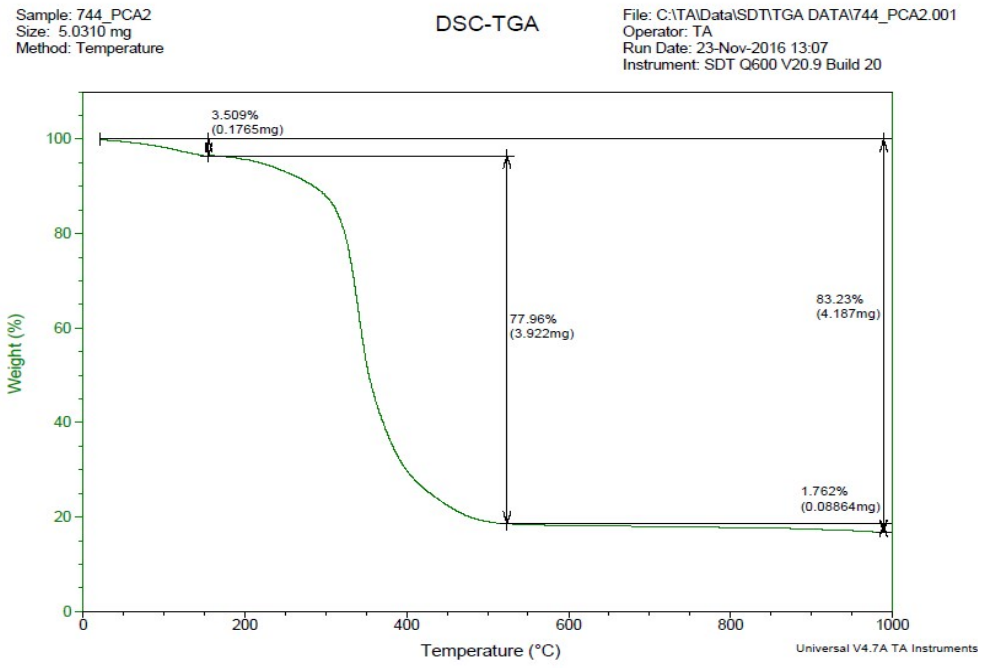

Figure S8. TGA curve of 6

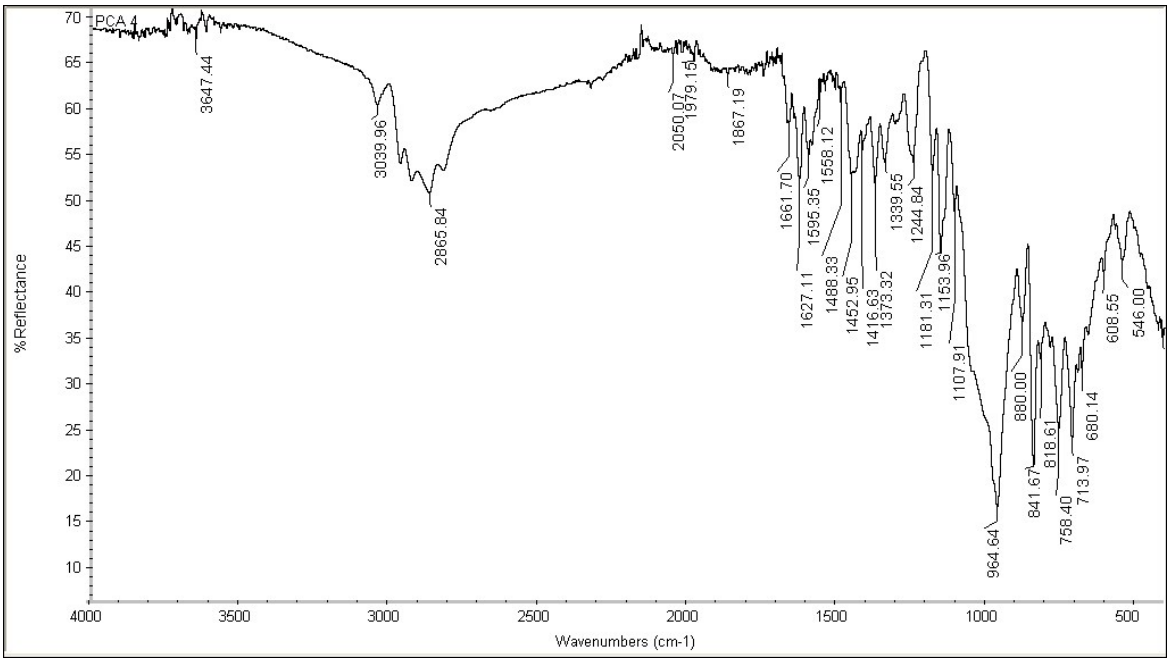

Figure S9. IR spectrum of 7

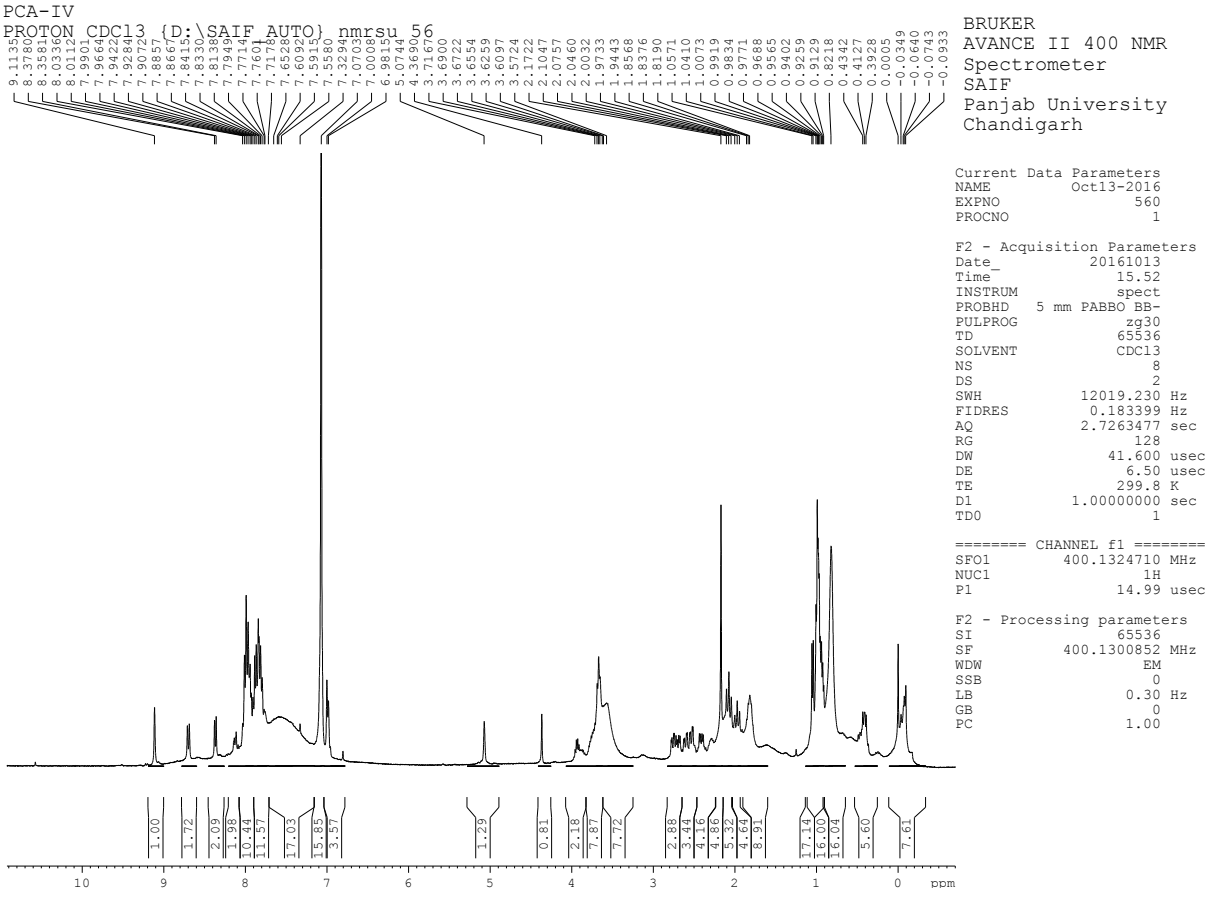

Figure S10. ^{1}H NMR spectrum of 7

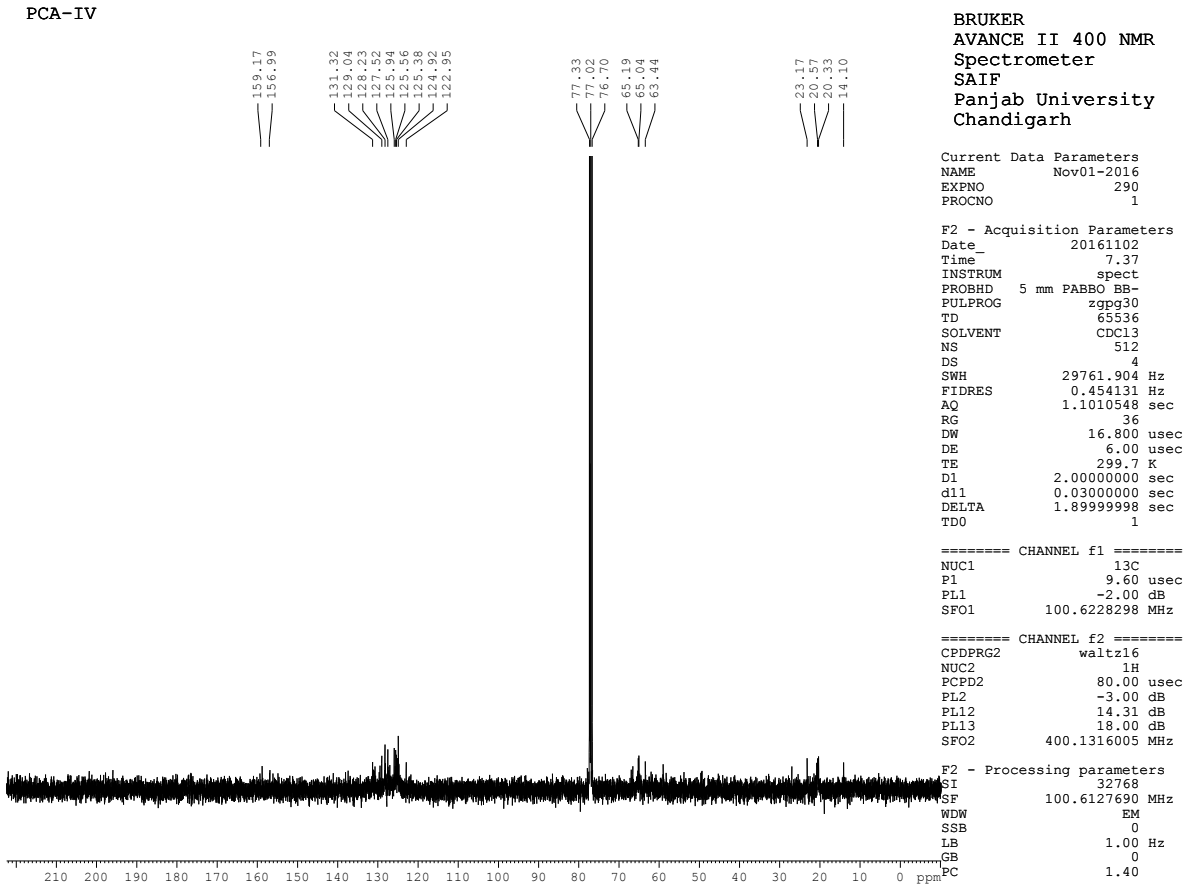

Figure S11. ^{13}C NMR spectrum of 7

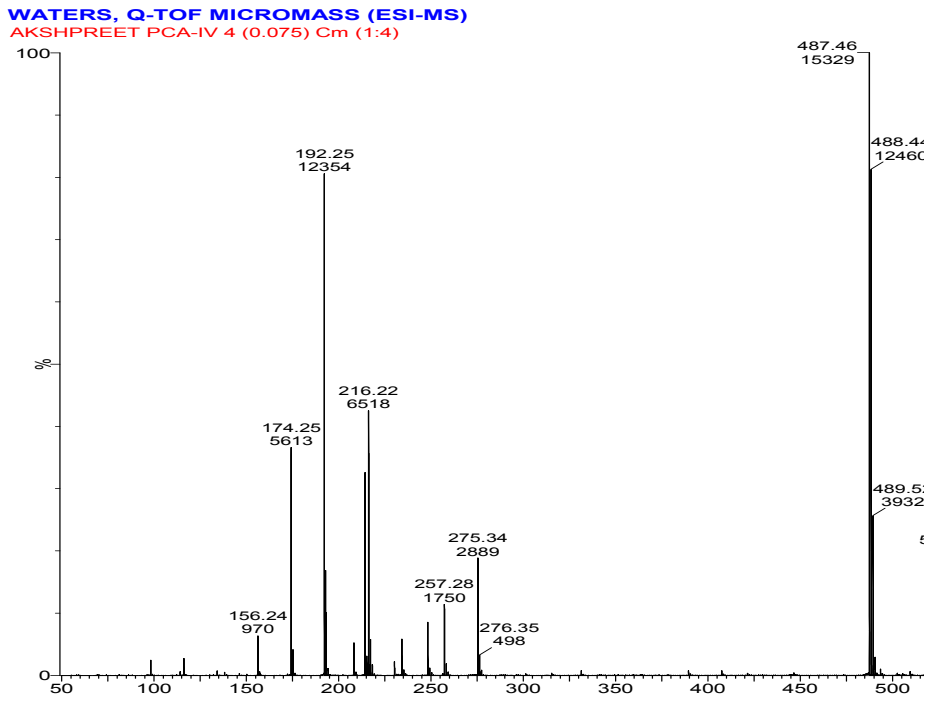

Figure S12. Mass spectrum of 7

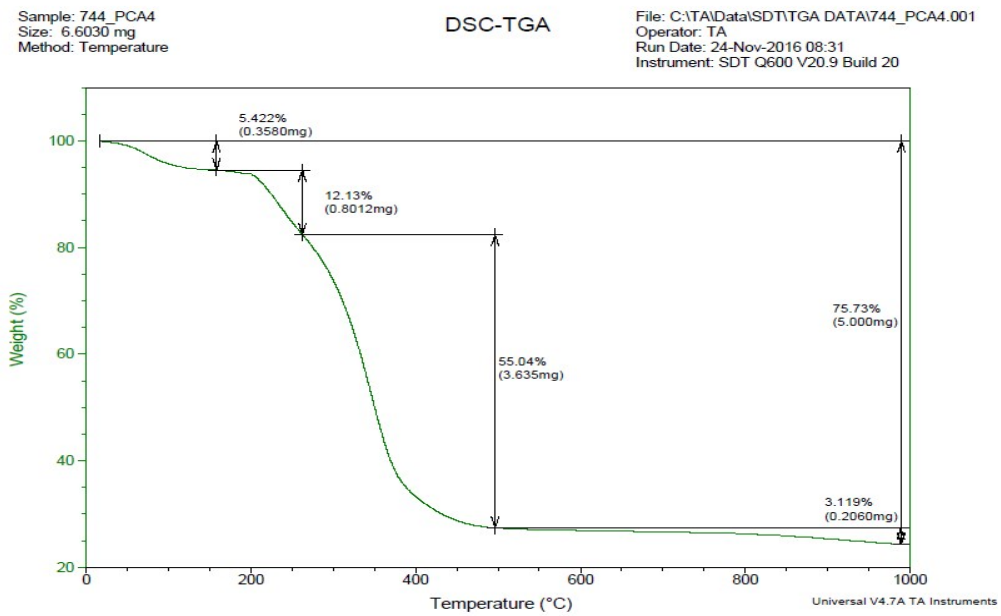

Figure S13. TGA curve of 7

Table S2. Global reactivity descriptors for 6 and 7 calculated at the B3LYP/6-31+G(d) level of theory.

Molecule	Ionization potential, IP (eV)	Electron affinity, EA (eV)	Electronegativity, χ (eV)	Chemical potential, μ (eV)	Chemical hardness, η (eV)	Chemical softness, s (eV)	Dipole Moment (Debye)
6	5.462	2.048	3.755	-3.755	1.707	0.854	4.034
7	5.446	2.029	3.738	-3.738	1.708	0.854	4.257