Supporting Information for

Reactivity of a Lewis base supported uranium terminal imido metallocene towards small molecules

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1. Crystallographic details

Table S1. Crystal Data and Experimental Parameters for Compounds 2, 3, 5 and 7

Compound	**2**	**3**·C_6H_{14}	**5**·0.5C_6H_{14}	**7**·0.5C_6H_6
Formula	$C_{51}H_{75}NSi_6U$	$C_{55}H_{94}N_4SSi_6U$	$C_{44}H_{75}S_2Si_6U$	$C_{59}H_{85}N_2O_2Si_6U$
Fw	1108.69	1249.97	1074.73	1260.85
crystal system	triclinic	triclinic	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	11.978(1)	12.130(1)	10.880(1)	11.586(1)
b (Å)	12.258(1)	12.824(1)	10.901(1)	12.814(1)
c (Å)	21.559(1)	21.721(1)	22.508(1)	22.924(1)
α (deg)	81.13(1)	96.10(1)	77.00(1)	95.93(1)
β (deg)	80.21(1)	90.99(1)	81.20(1)	99.85(1)
γ (deg)	61.36(1)	111.07(1)	80.41(1)	110.41(1)
V (Å^3)	2727.99(10)	3129.66(13)	2546.02(17)	3093.08(11)
Z	2	2	2	2
D_{calc} (g/cm^3)	1.350	1.326	1.402	1.354
μ(Mo/Kα)$_{calc}$ (cm^{-1})	9.870	8.978	11.293	8.802
size (mm)	0.20 × 0.15 × 0.15	0.20 × 0.15 × 0.10	0.20 × 0.15 × 0.15	0.15 × 0.10 × 0.10
F(000)	1128	1288	1094	1290
2θ range (deg)	8.25 to 153.45	7.44 to 152.85	8.12 to 154.42	7.48 to 153.19
no. of reflns, collected	38415	43435	30768	41774
no of obsd reflns	10976	12555	10092	12507
no of variables	554	626	497	652
abscorr (T_{max}, T_{min})	1.00, 0.25	1.00, 0.69	1.00, 0.25	1.00, 0.89
R	0.041	0.049	0.072	0.043
R_w	0.110	0.124	0.191	0.099
R_{all}	0.042	0.054	0.093	0.049
Gof	1.09	1.06	1.21	1.11
CCDC	2277711	2277718	2277717	2277715

Table S2. Crystal Data and Experimental Parameters for Compounds 8-10

Compound	**8**	**9**	**10**
Formula	$C_{51}H_{79}N_3Si_6U$	$C_{50}H_{80}N_2Si_6U$	$C_{41}H_{72}ClNSi_7U$
Fw	1140.74	1115.73	1049.10
crystal system	triclinic	monoclinic	monoclinic
space group	$P\bar{1}$	$C2/c$	$P2_1/c$
a (Å)	15.711(1)	50.490(1)	11.067(1)
b (Å)	17.095(1)	11.775(1)	23.667(1)
c (Å)	23.342(1)	38.791(1)	19.321(2)
α (deg)	69.89(1)	90	90
β (deg)	73.79(1)	94.70(1)	93.71(1)
γ (deg)	86.00(1)	90	90
V (Å^3)	5650.68(10)	22984.1(9)	5050.0(3)
Z	4	16	4
D_{calc} (g/cm^3)	1.341	1.290	1.380
μ(Mo/Kα)$_{calc}$ (cm^{-1})	9.555	9.378	3.460
size (mm)	0.20 × 0.10 × 0.10	0.20 × 0.10 × 0.05	0.20 × 0.20 × 0.20
F(000)	2328	9120	2128
2θ range (deg)	7.43 to 152.98	7.03 to 153.43	6.57 to 59.76
no. of reflns, collected	82922	93378	28581
no of obsd reflns	22813	23043	12225
no of variables	1142	1114	486
abscorr (T_{max}, T_{min})	1.00, 0.12	1.00, 0.66	1.00, 0.51
R	0.041	0.081	0.039
R_w	0.107	0.202	0.067
R_{all}	0.044	0.116	0.055
Gof	1.04	1.04	1.03
CCDC	2277714	2277720	2277721

Table S3. Crystal Data and Experimental Parameters for Compounds 11-13

Compound	**11**	**12**	**13**
Formula	$C_{35}H_{65}INSi_6U$	$C_{41}H_{70}NSSi_6U$	$C_{42}H_{72}N_2Si_6U$
Fw	1033.35	1015.61	1011.58
crystal system	monoclinic	triclinic	triclinic
space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
a (Å)	11.242(1)	11.228(1)	12.022(1)
b (Å)	17.326(1)	19.471(1)	22.235(1)
c (Å)	24.259(1)	22.729(1)	23.189(1)
α (deg)	90	79.01(1)	92.12(1)
β (deg)	102.70(1)	86.50(1)	101.12(1)
γ (deg)	90	88.88(1)	97.78(1)
V (Å^3)	4609.43(19)	4868.61(13)	6013.1(3)
Z	4	4	4
D_{calc} (g/cm^3)	1.489	1.386	1.117
μ(Mo/Kα)$_{calc}$ (cm^{-1})	4.370	11.395	8.913
size (mm)	0.20 × 0.15 × 0.15	0.15 × 0.15 × 0.15	0.25 × 0.15 × 0.10
F(000)	2044	2060	2056
2θ range (deg)	6.46 to 59.73	6.64 to 154.15	7.58 to 155.74
no. of reflns, collected	39104	66554	24360
no of obsd reflns	11494	19740	24360
no of variables	386	939	959
abscorr (T_{max}, T_{min})	1.00, 0.66	1.00, 0.57	1.00, 0.52
R	0.054	0.053	0.108
R_w	0.077	0.148	0.289
R_{all}	0.110	0.060	0.123
Gof	1.02	1.07	1.05
CCDC	2277719	2277716	2277712

3. Spectra

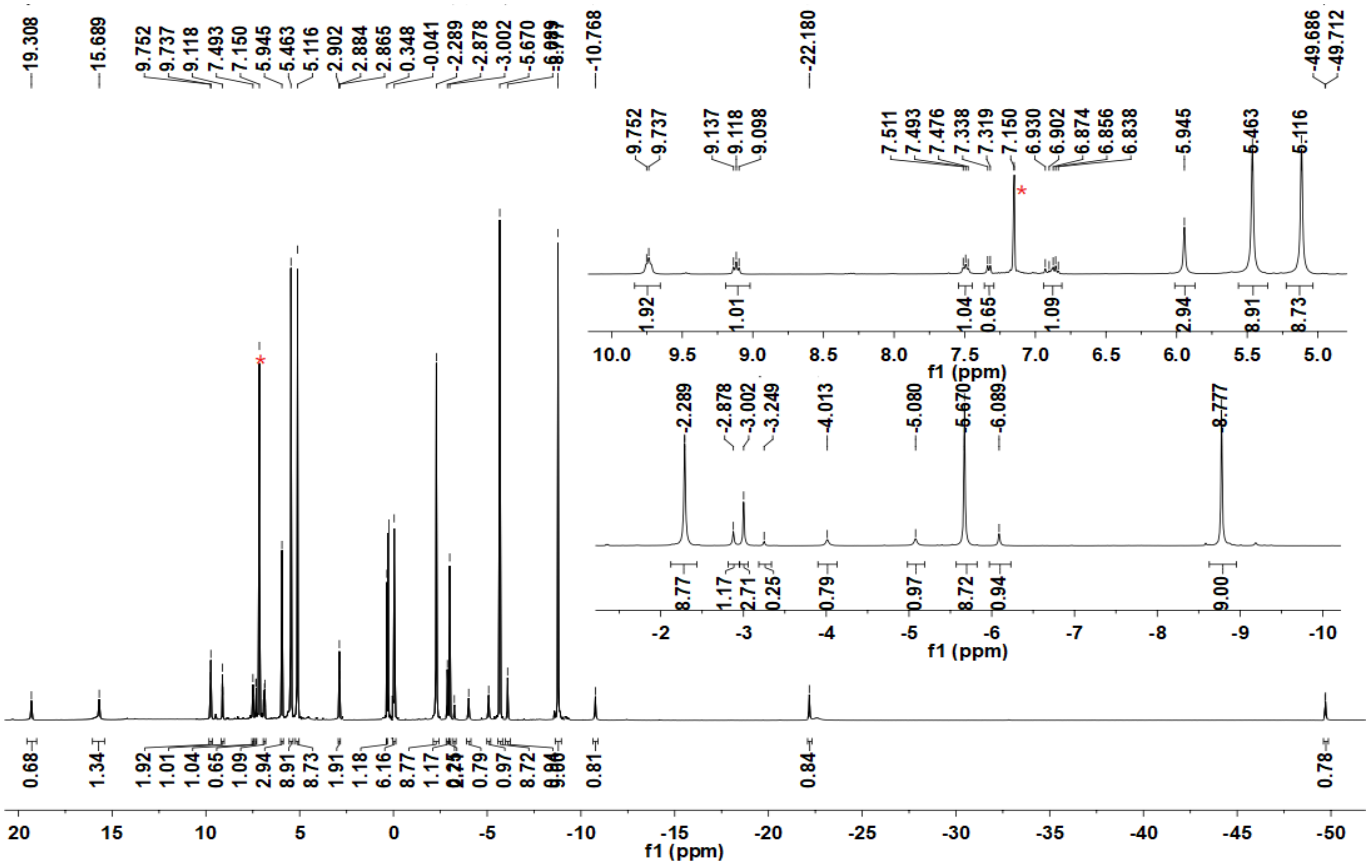

Figure S1. [1]H NMR spectrum for compound **2**.

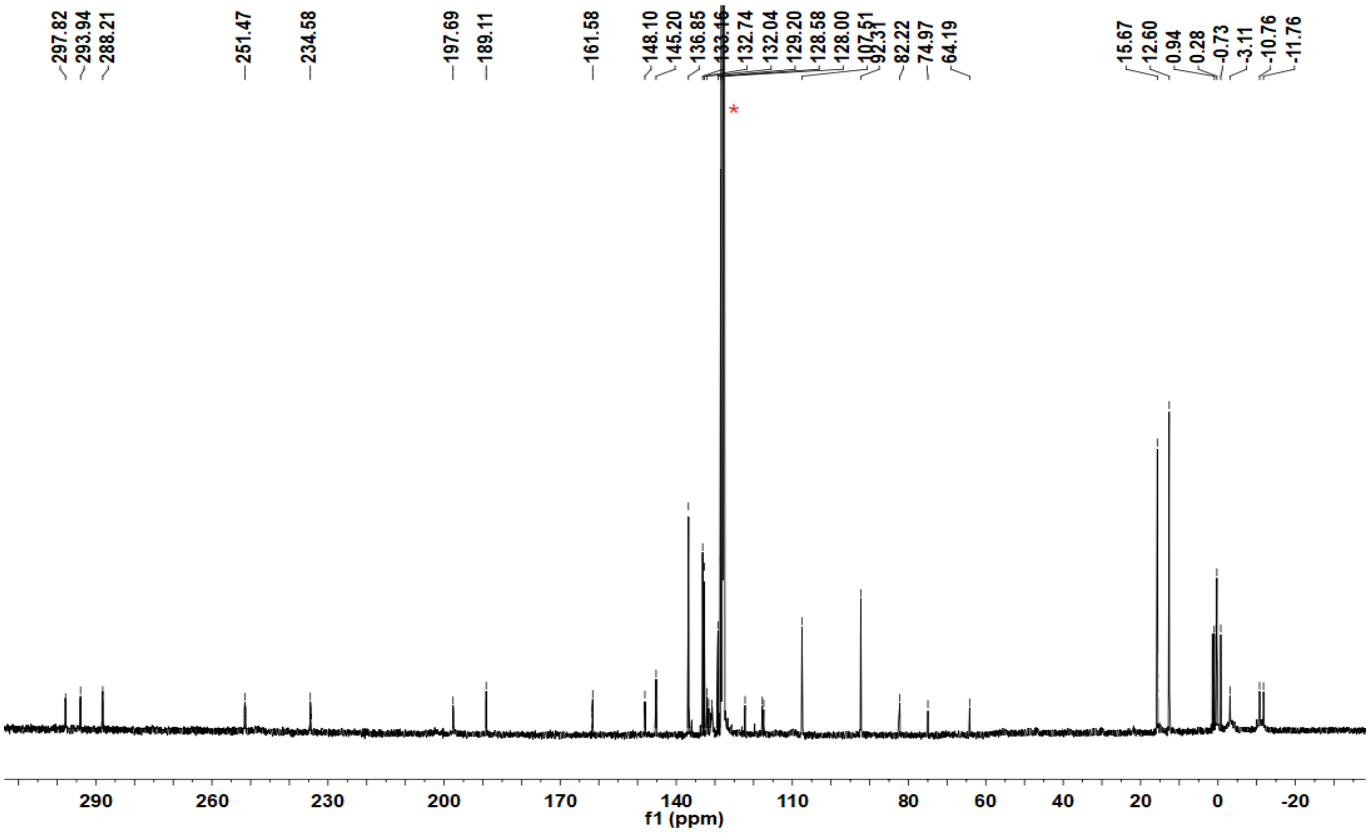

Figure S2. [13]C NMR spectrum for compound **2**.

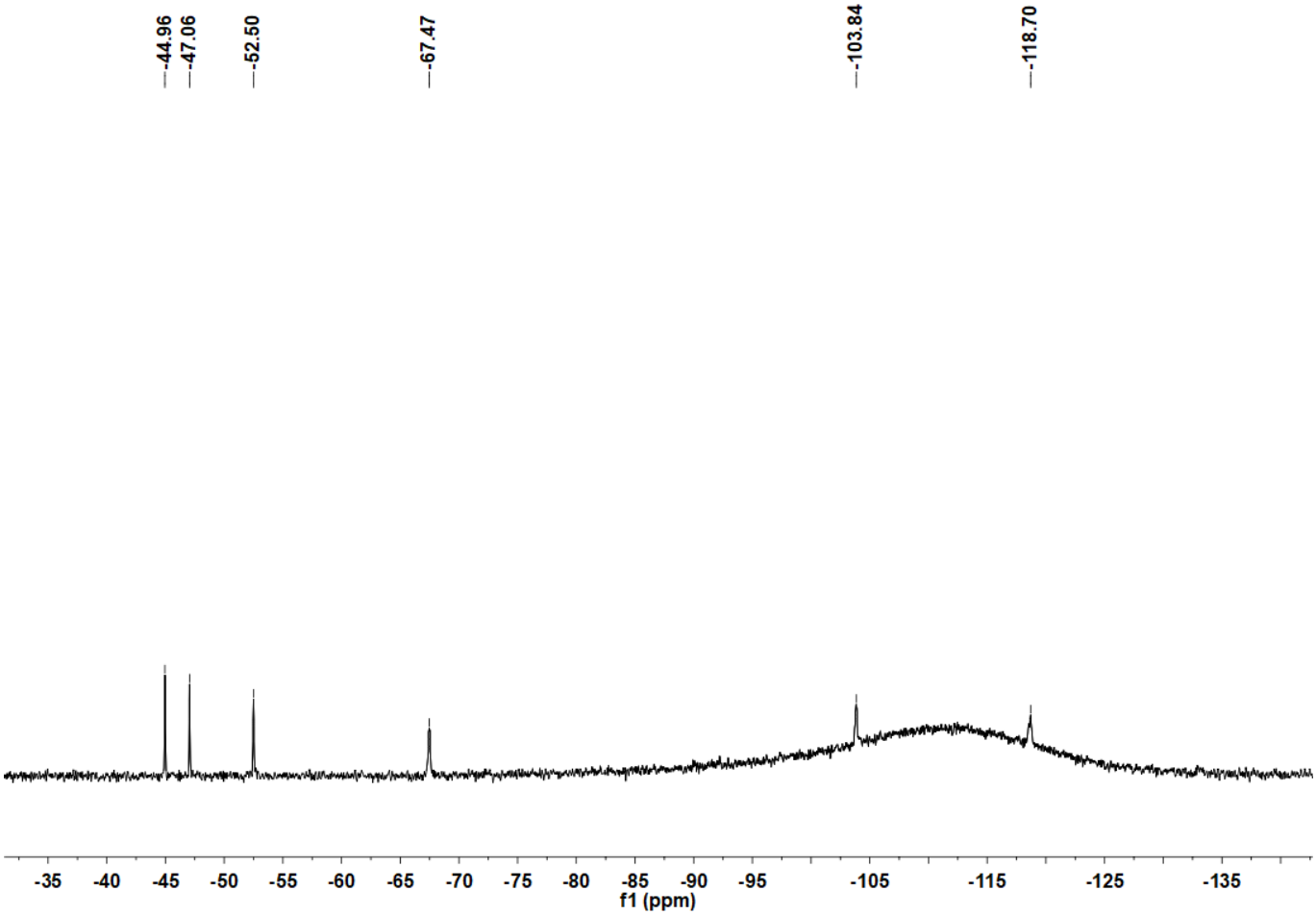

Figure S3. ^{29}Si NMR spectrum for compound **2**.

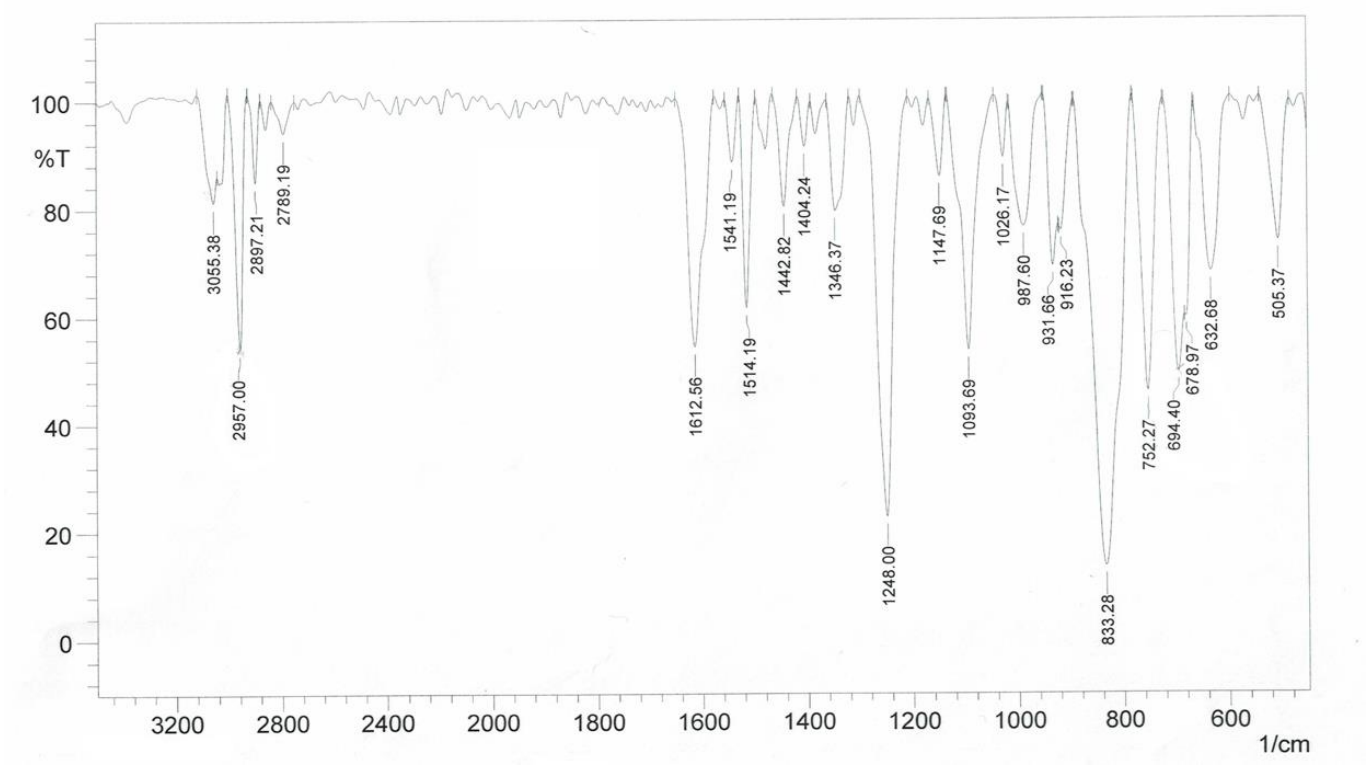

Figure S4. IR spectrum for compound **2**.

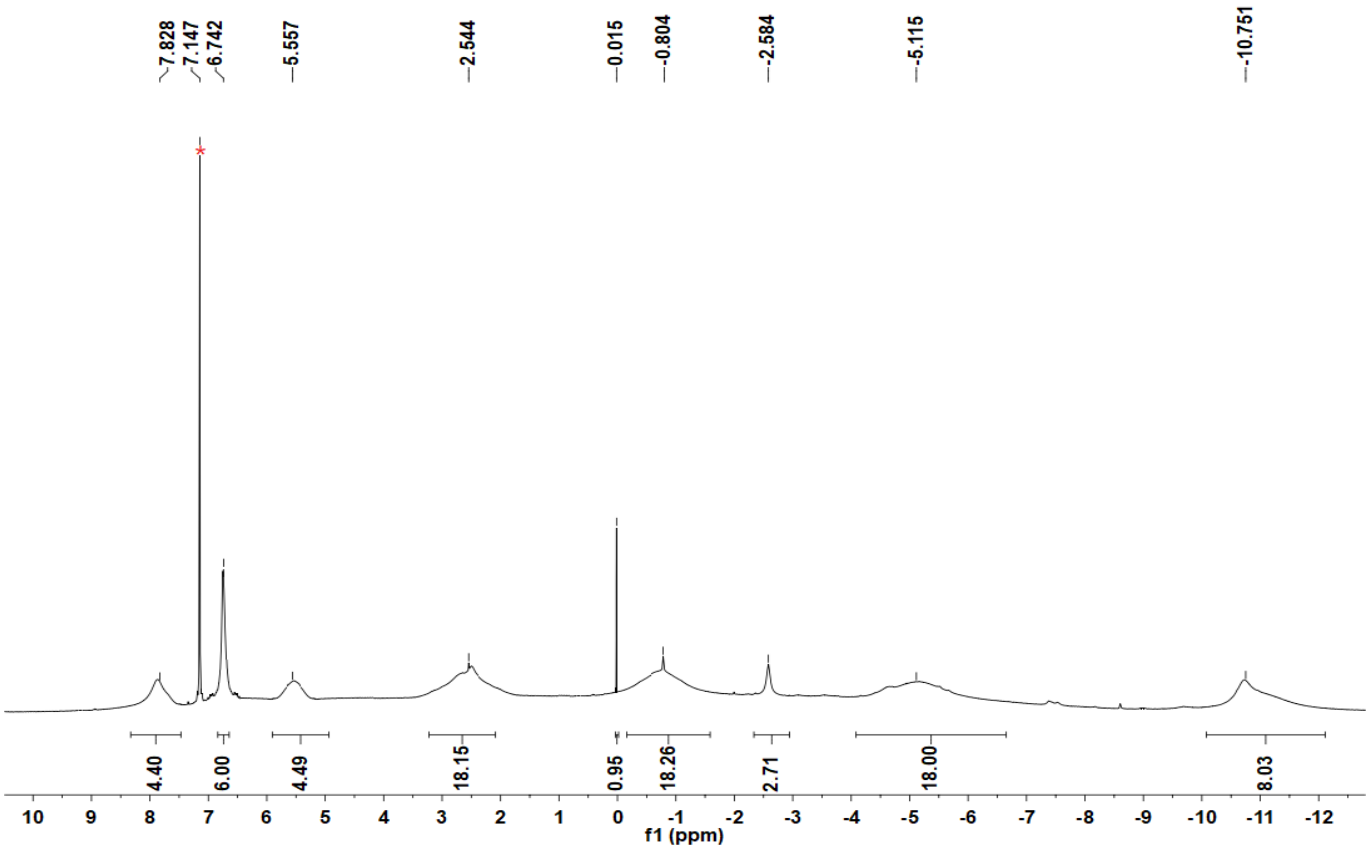

Figure S5. ^{1}H NMR spectrum for compound **3**.

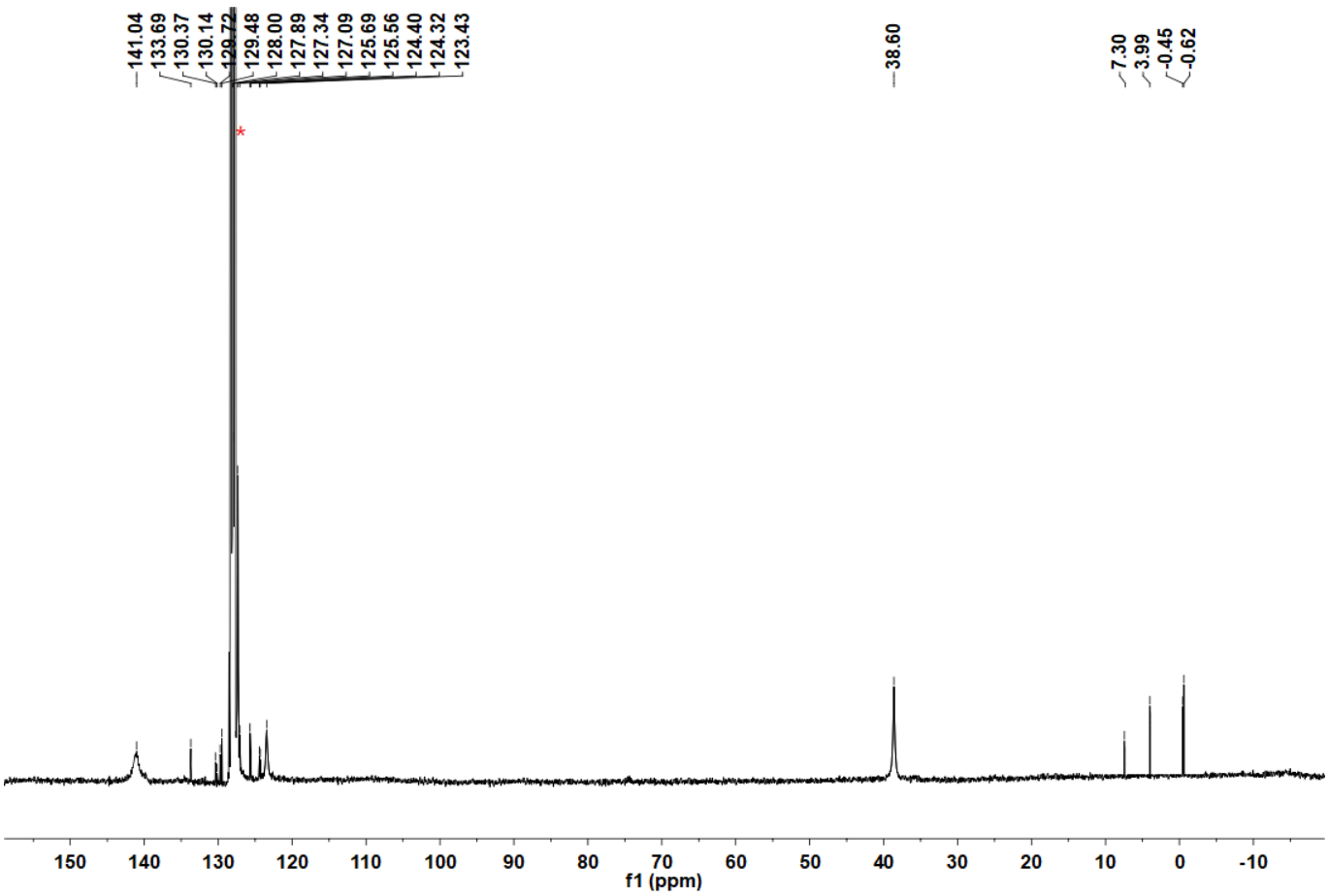

Figure S6. ^{13}C NMR spectrum for compound **3**.

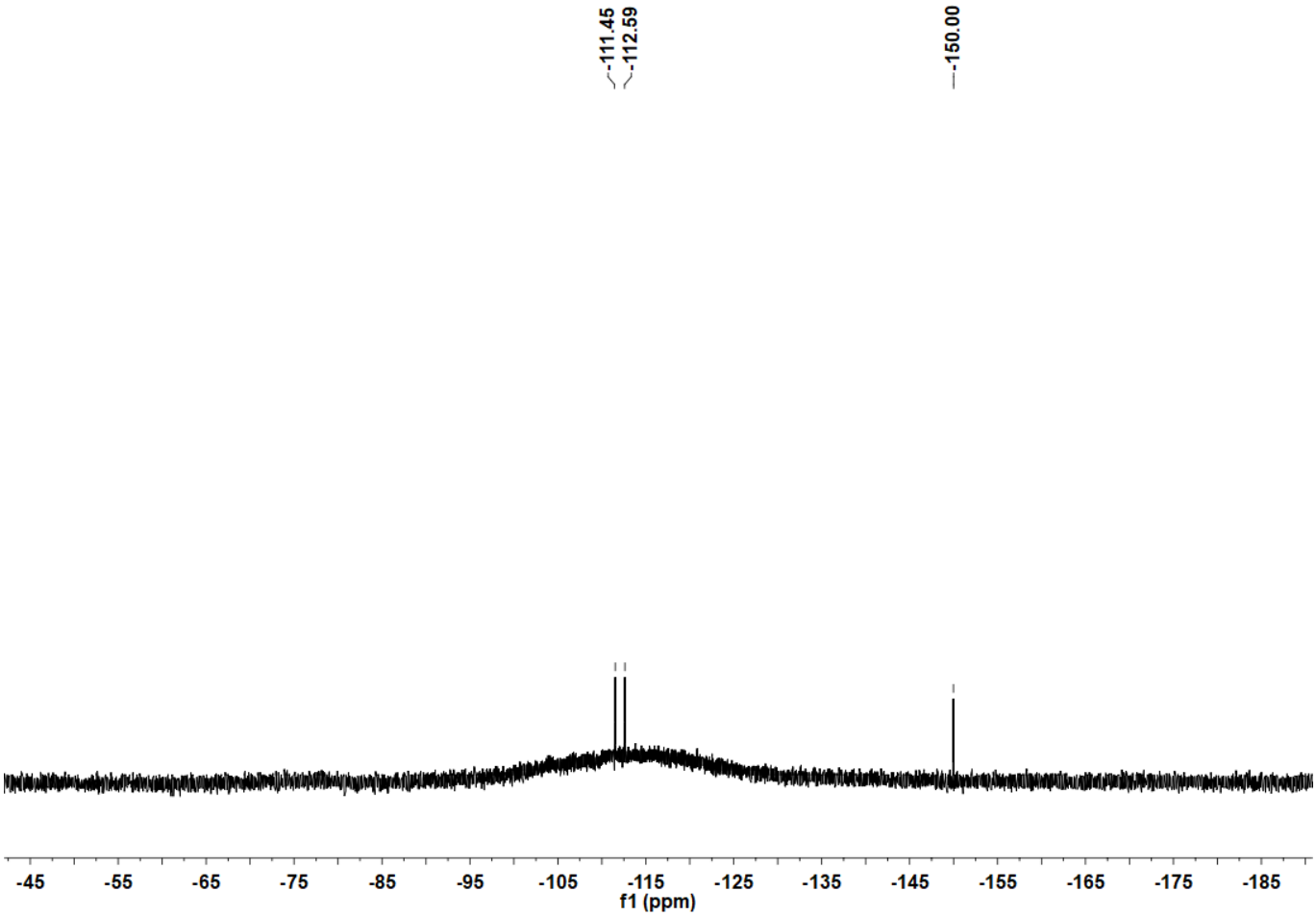

Figure S7. ^{29}Si NMR spectrum for compound **3**.

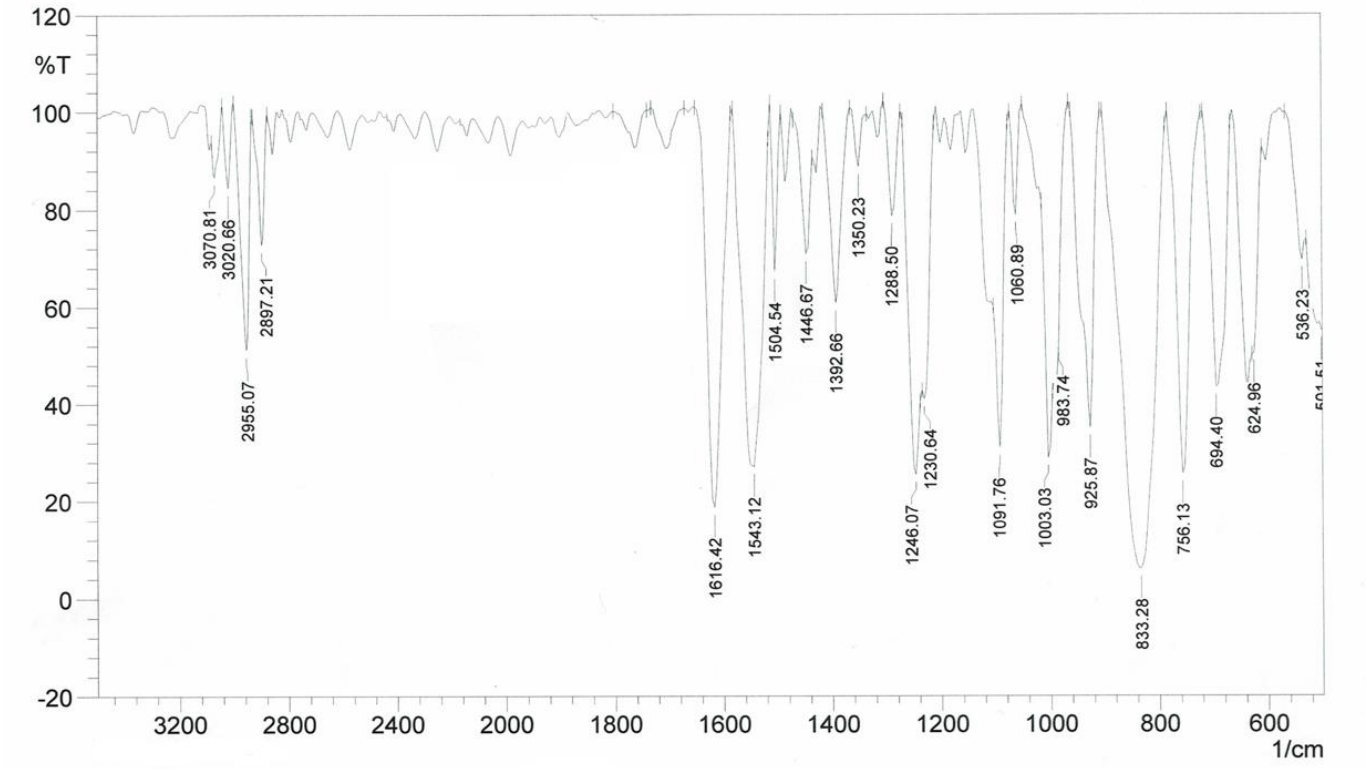

Figure S8. IR spectrum for compound **3**.

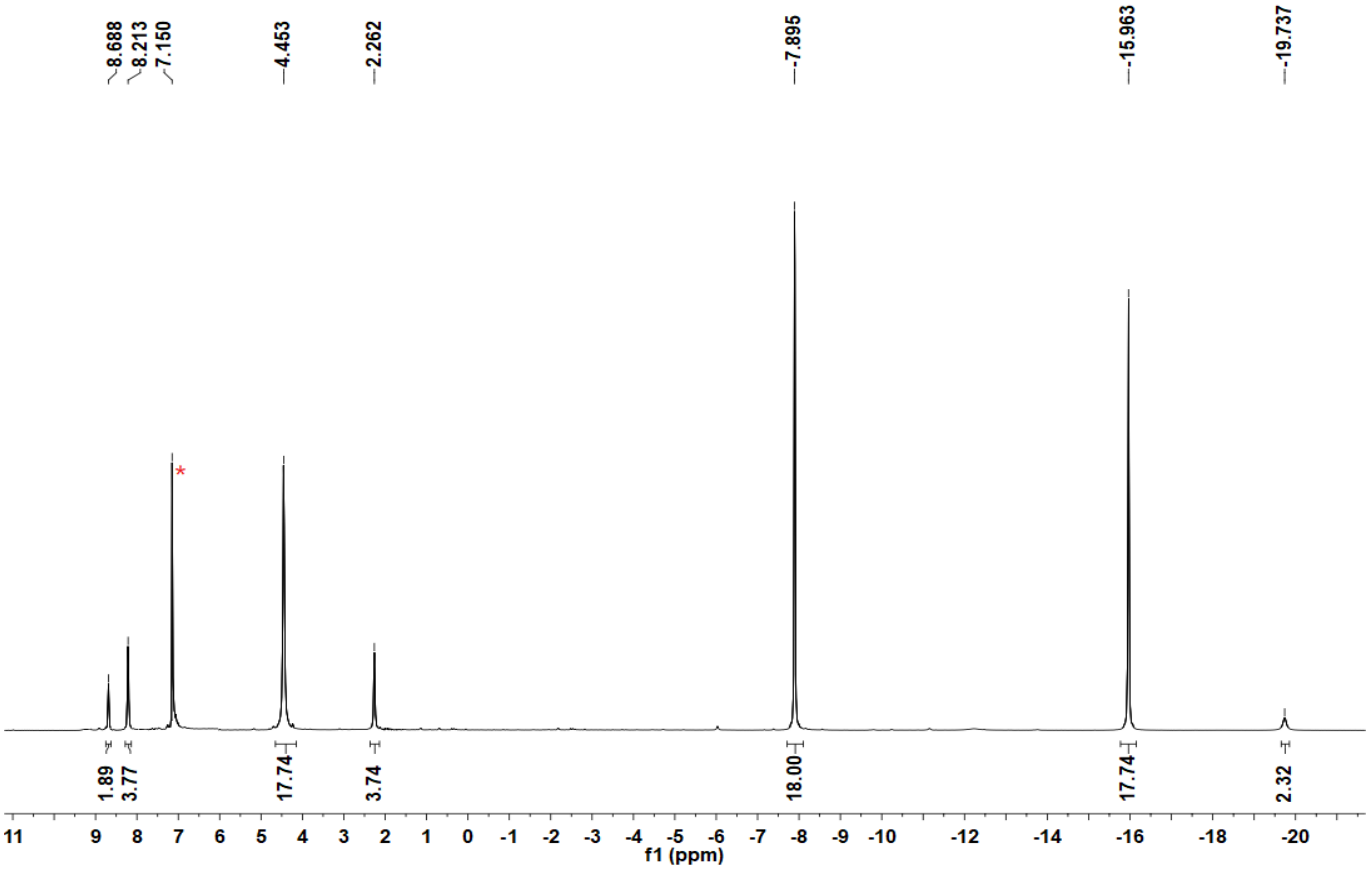

Figure S9. [1]H NMR spectrum for compound **5**.

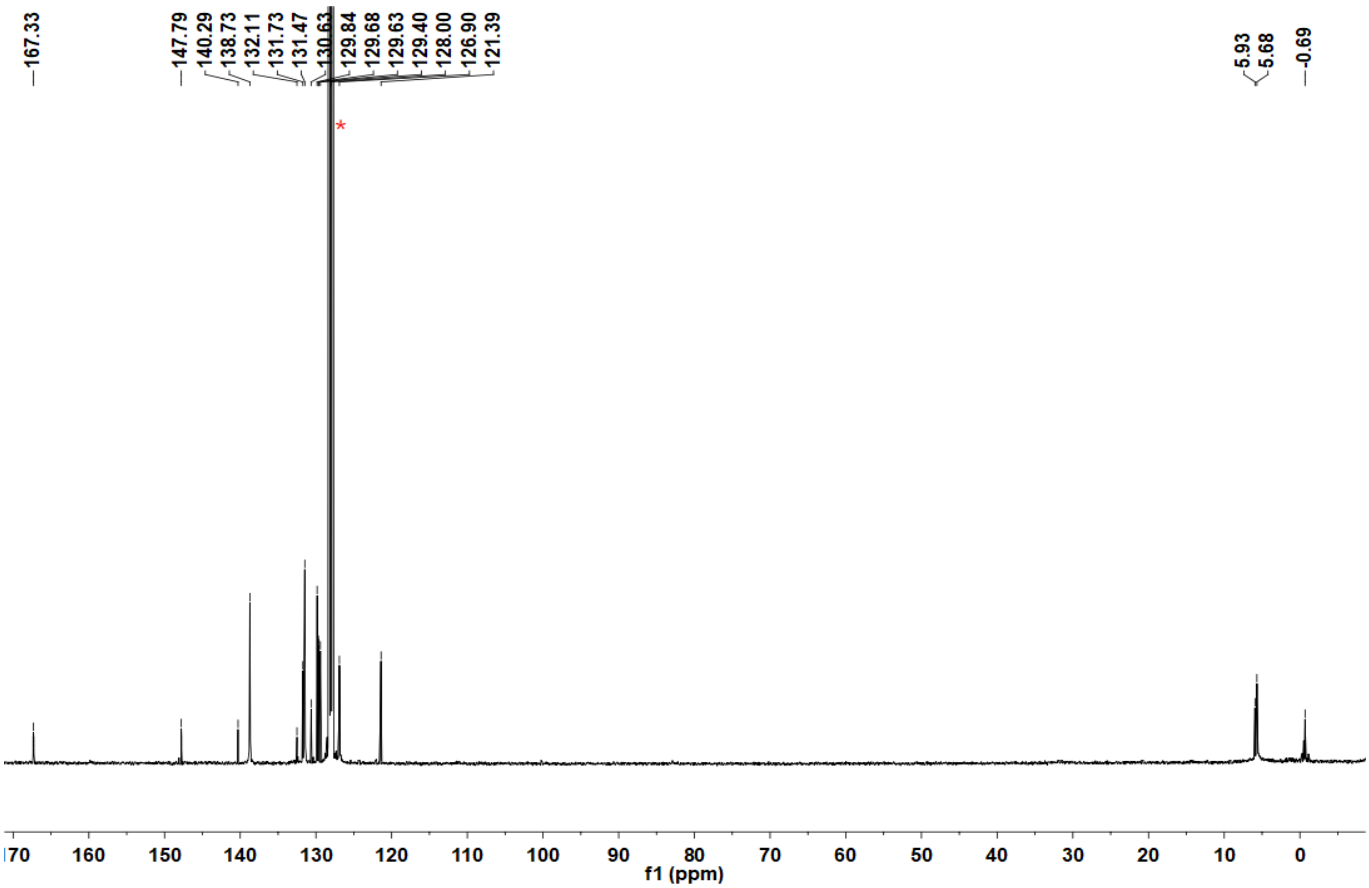

Figure S10. [13]C NMR spectrum for compound **5**.

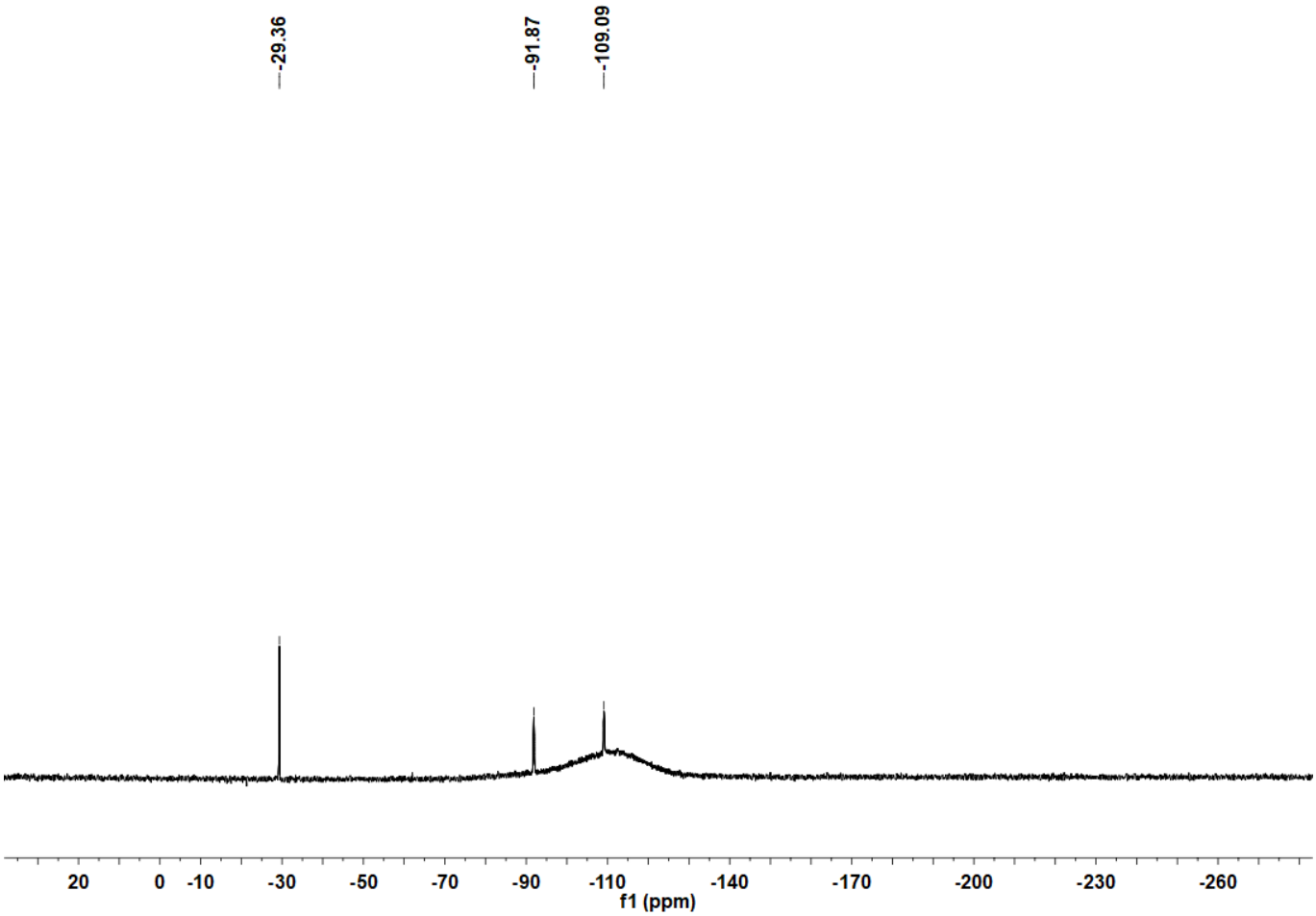

Figure S11. ^{29}Si NMR spectrum for compound **5**.

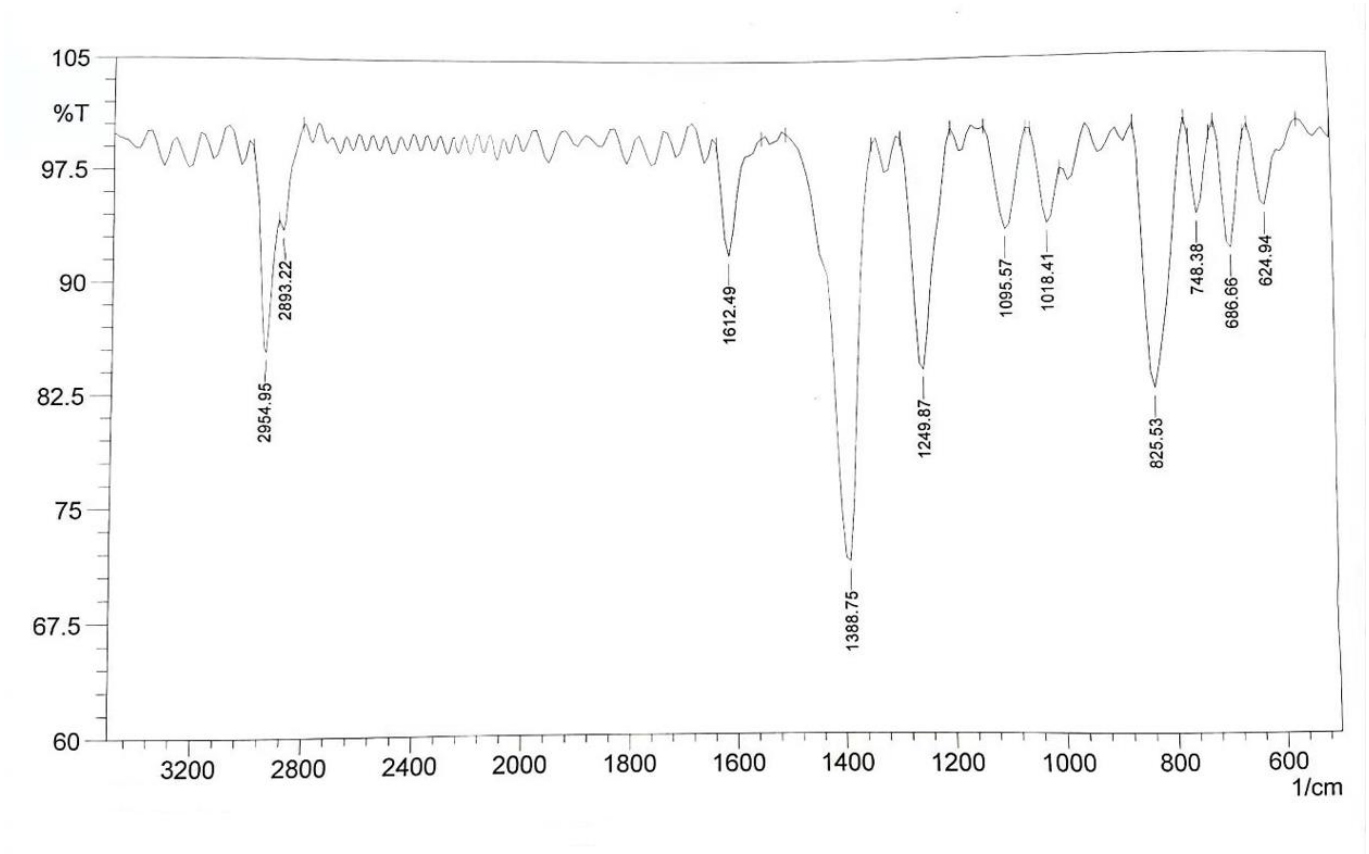

Figure S12. IR spectrum for compound **5**.

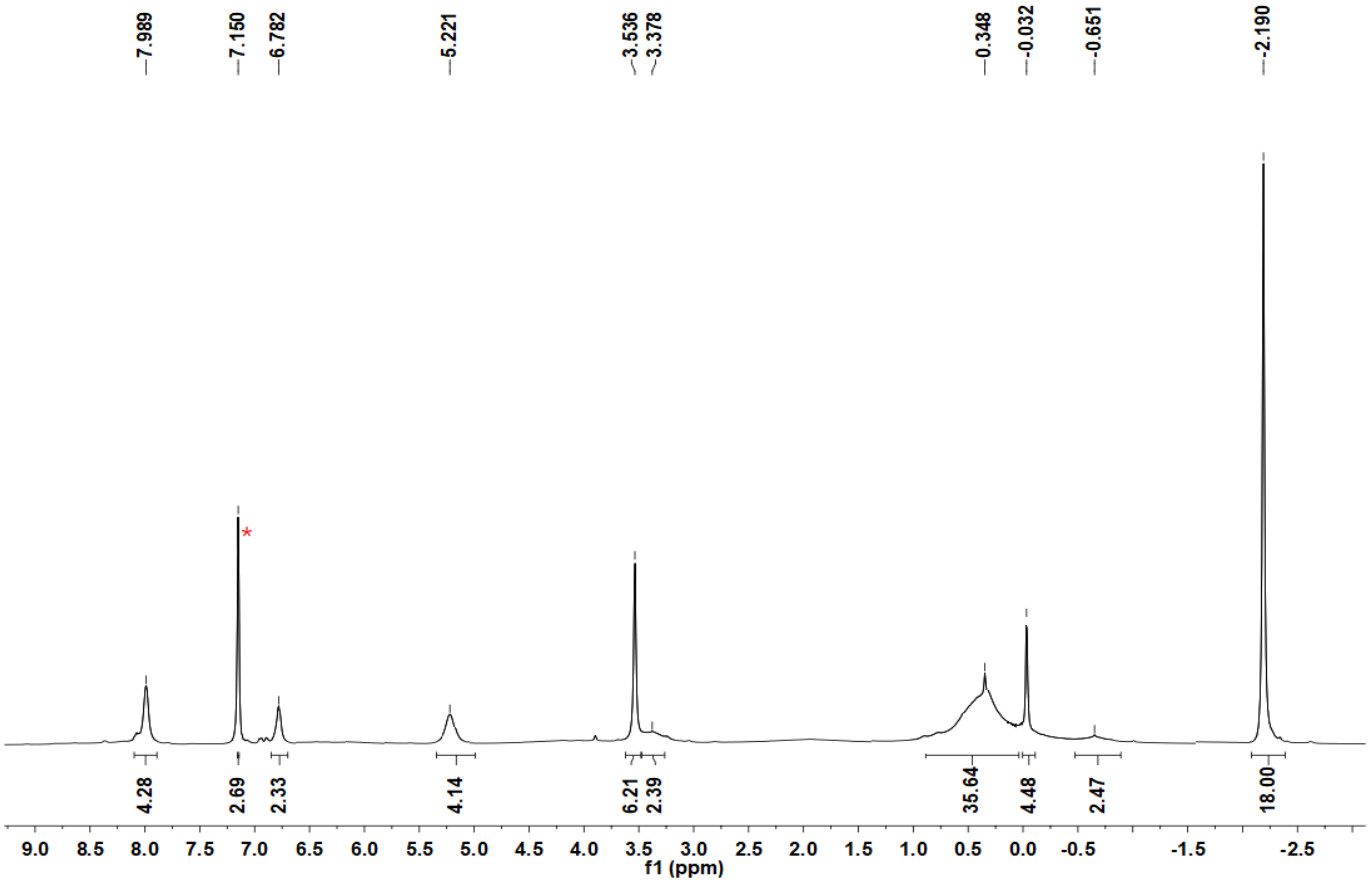

Figure S13. ^{1}H NMR spectrum for compound **7**.

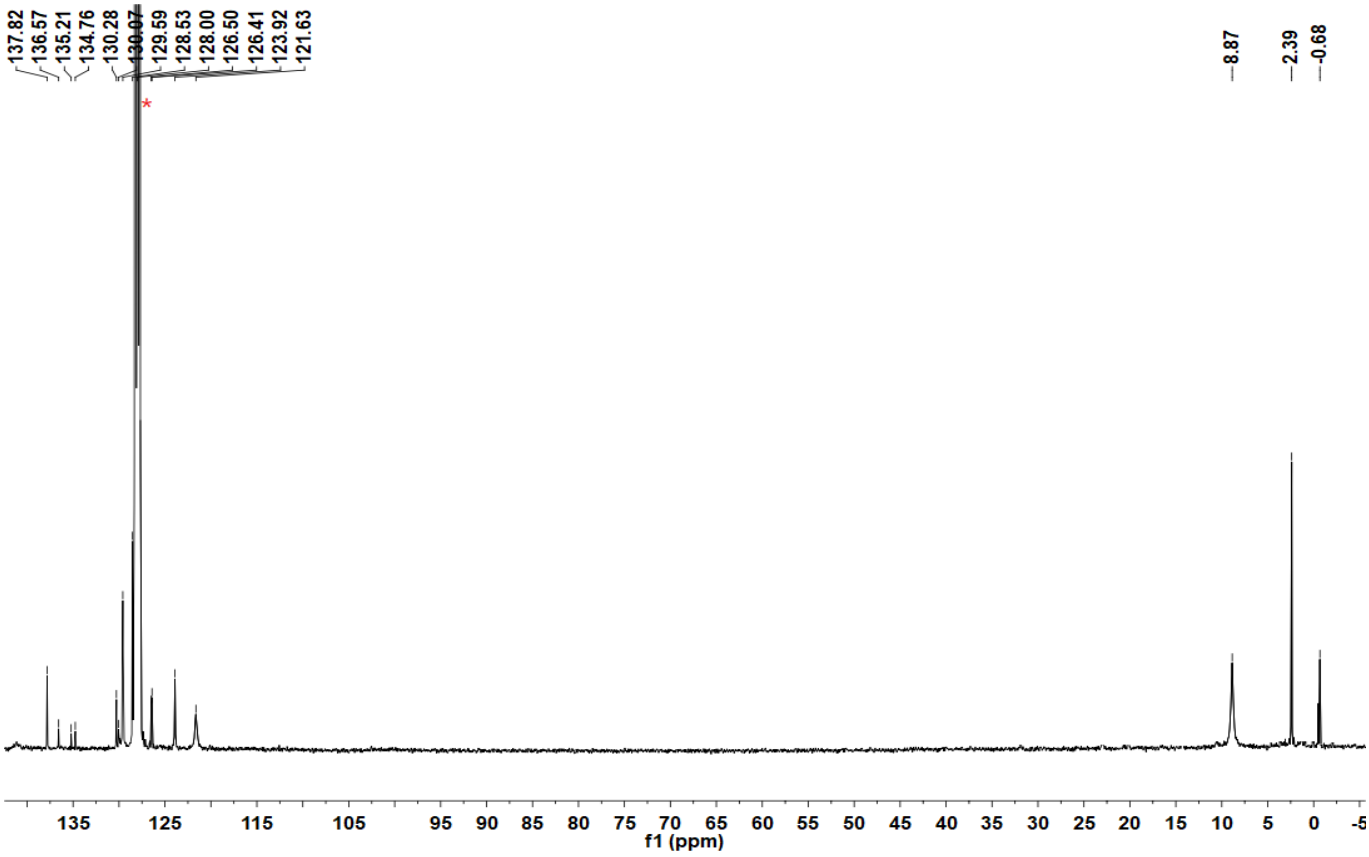

Figure S14. ^{13}C NMR spectrum for compound **7**.

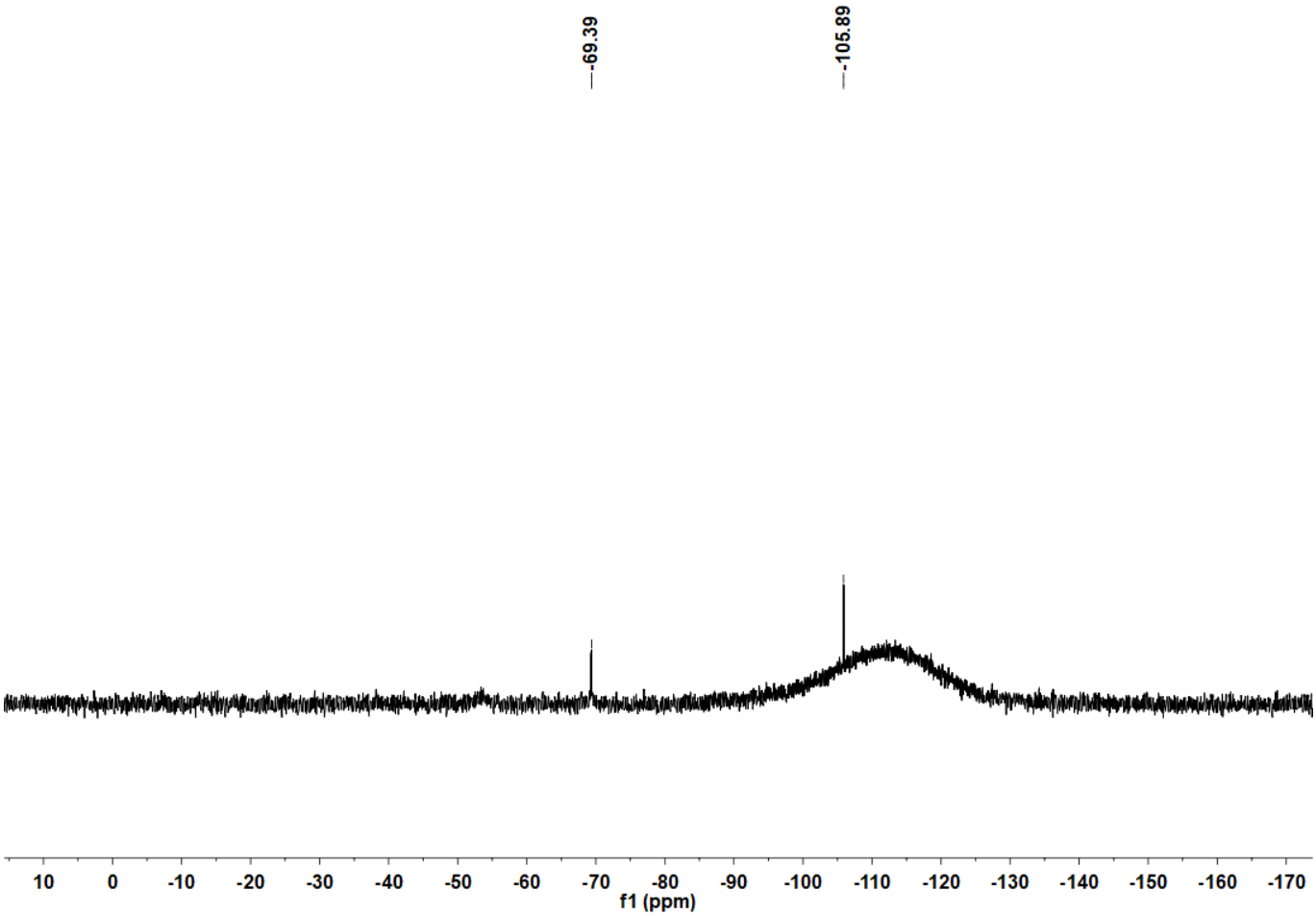

Figure S15. ^{29}Si NMR spectrum for compound **7**.

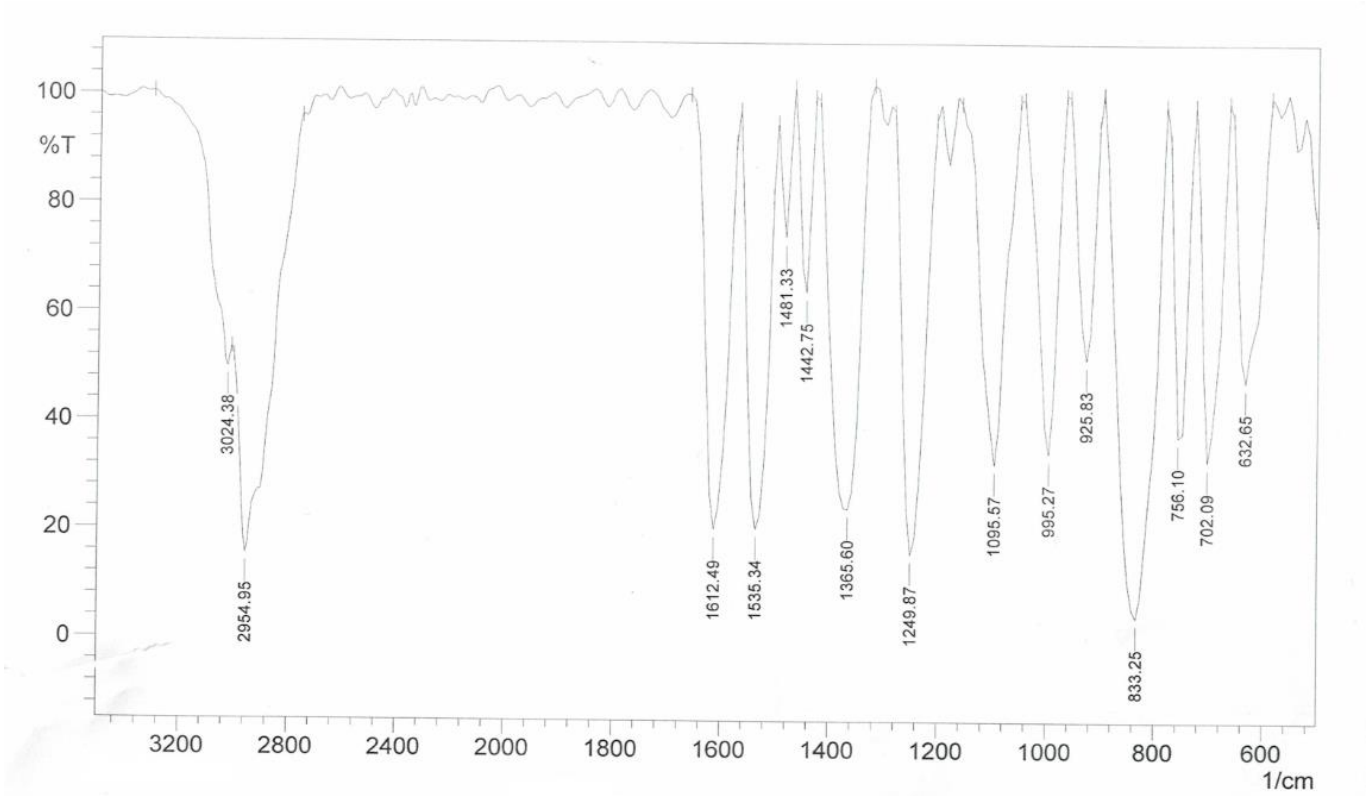

Figure S16. IR spectrum for compound **7**.

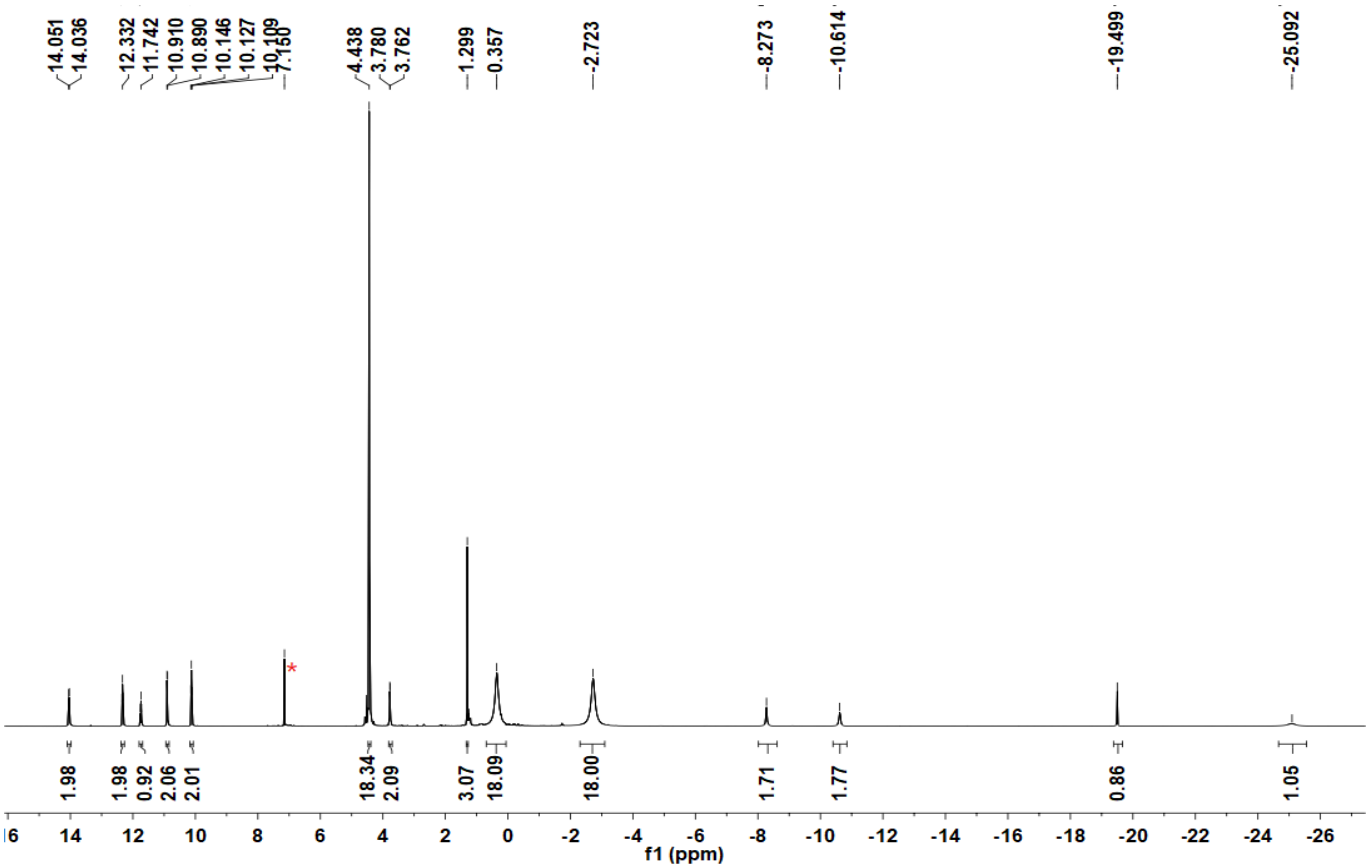

Figure S17. ^{1}H NMR spectrum for compound **8**.

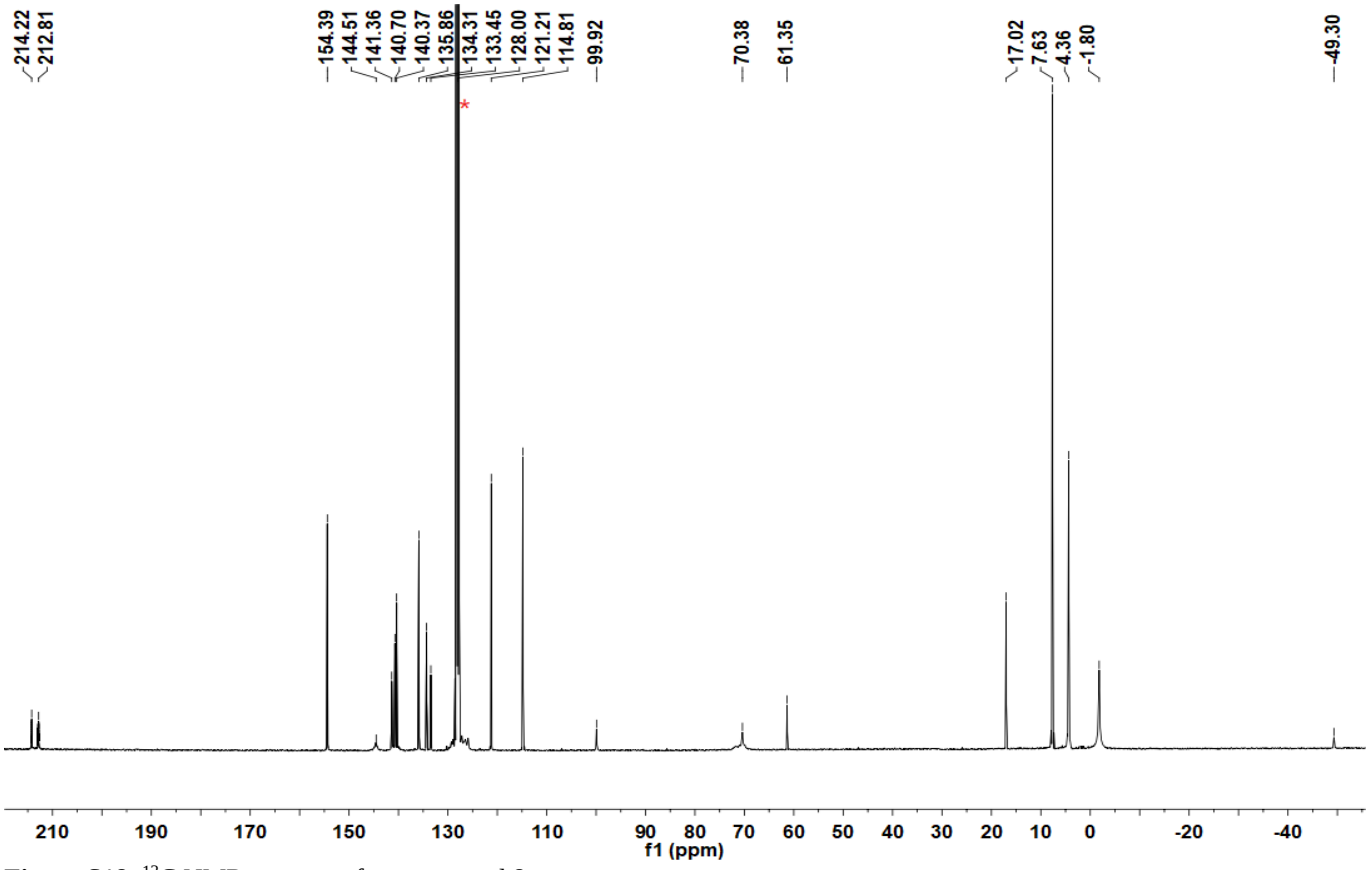

Figure S18. ^{13}C NMR spectrum for compound **8**.

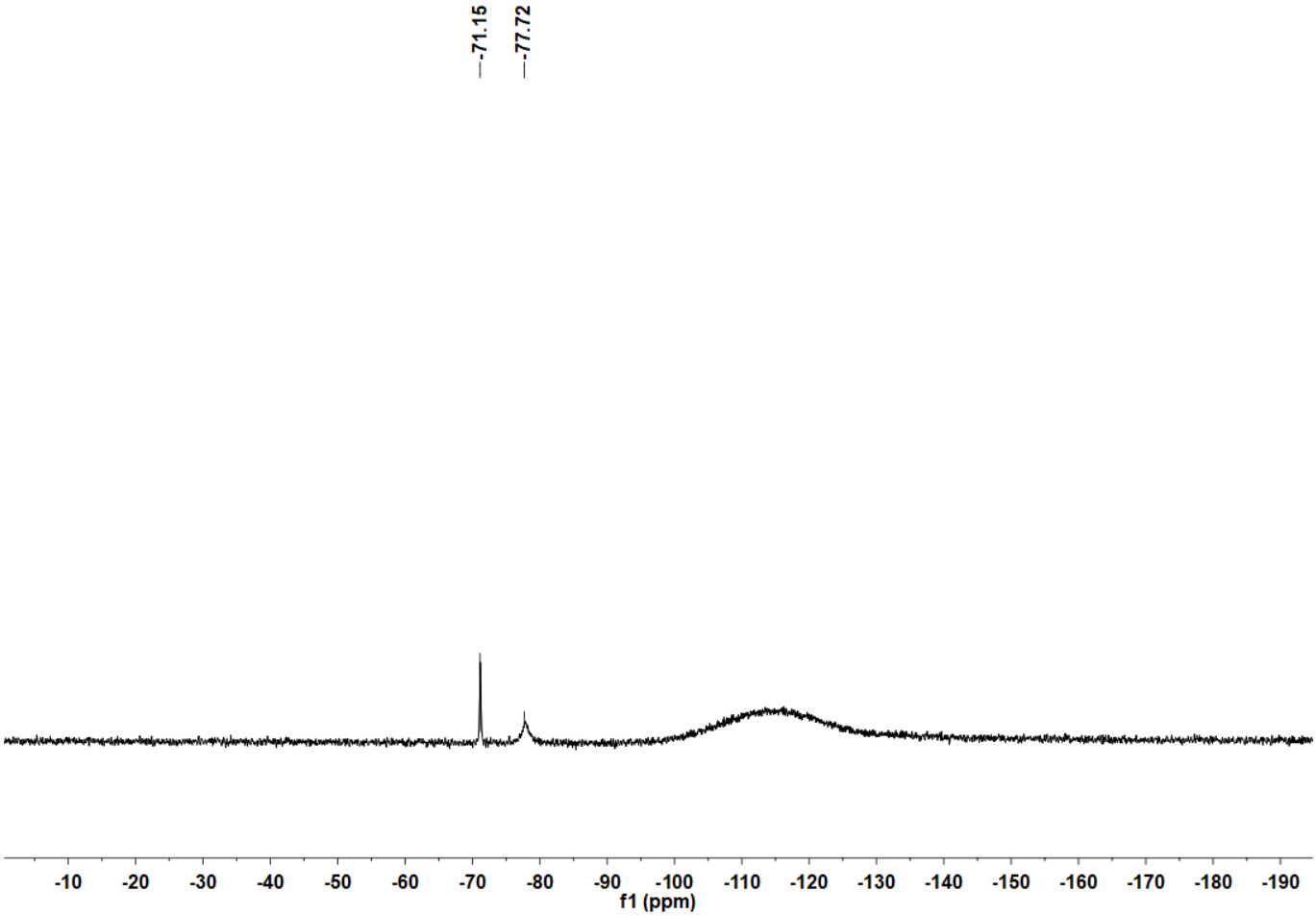

Figure S19. ^{29}Si NMR spectrum for compound **8**.

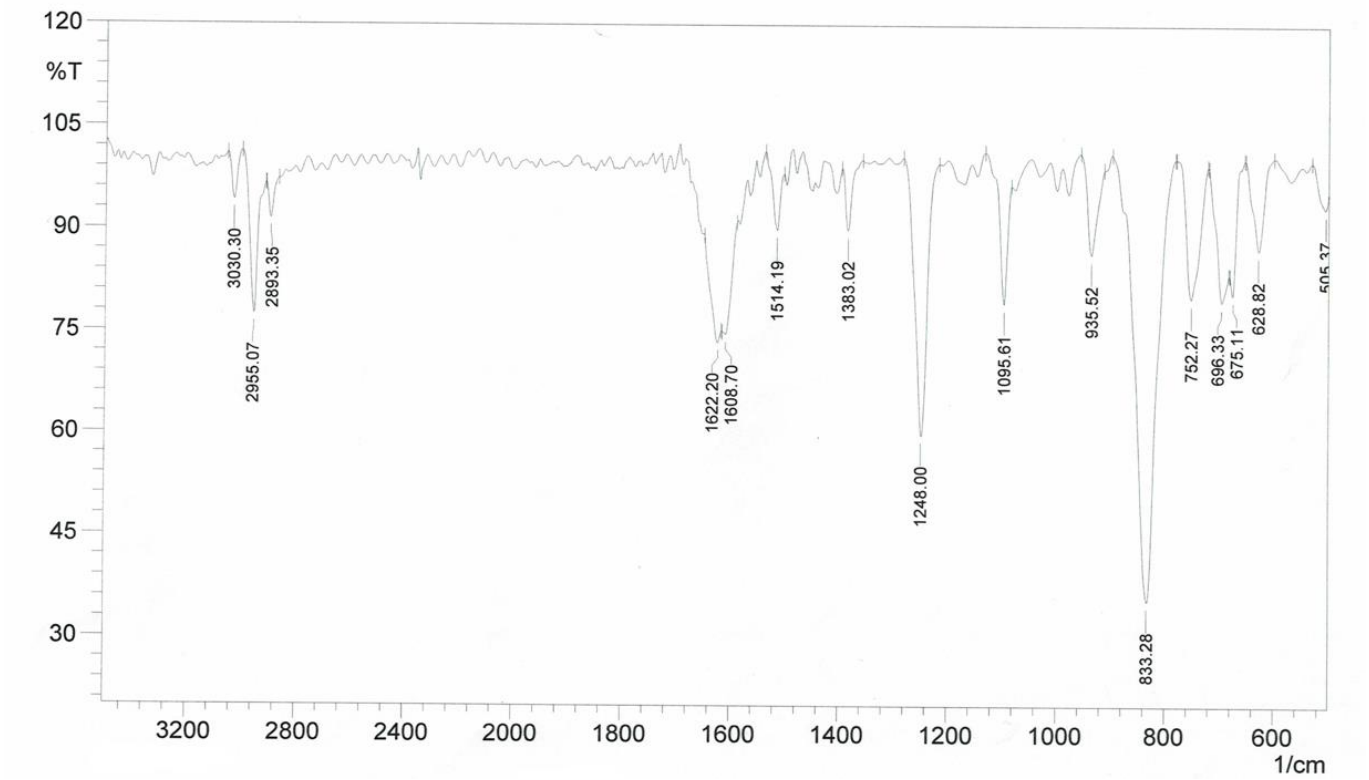

Figure S20. IR spectrum for compound **8**.

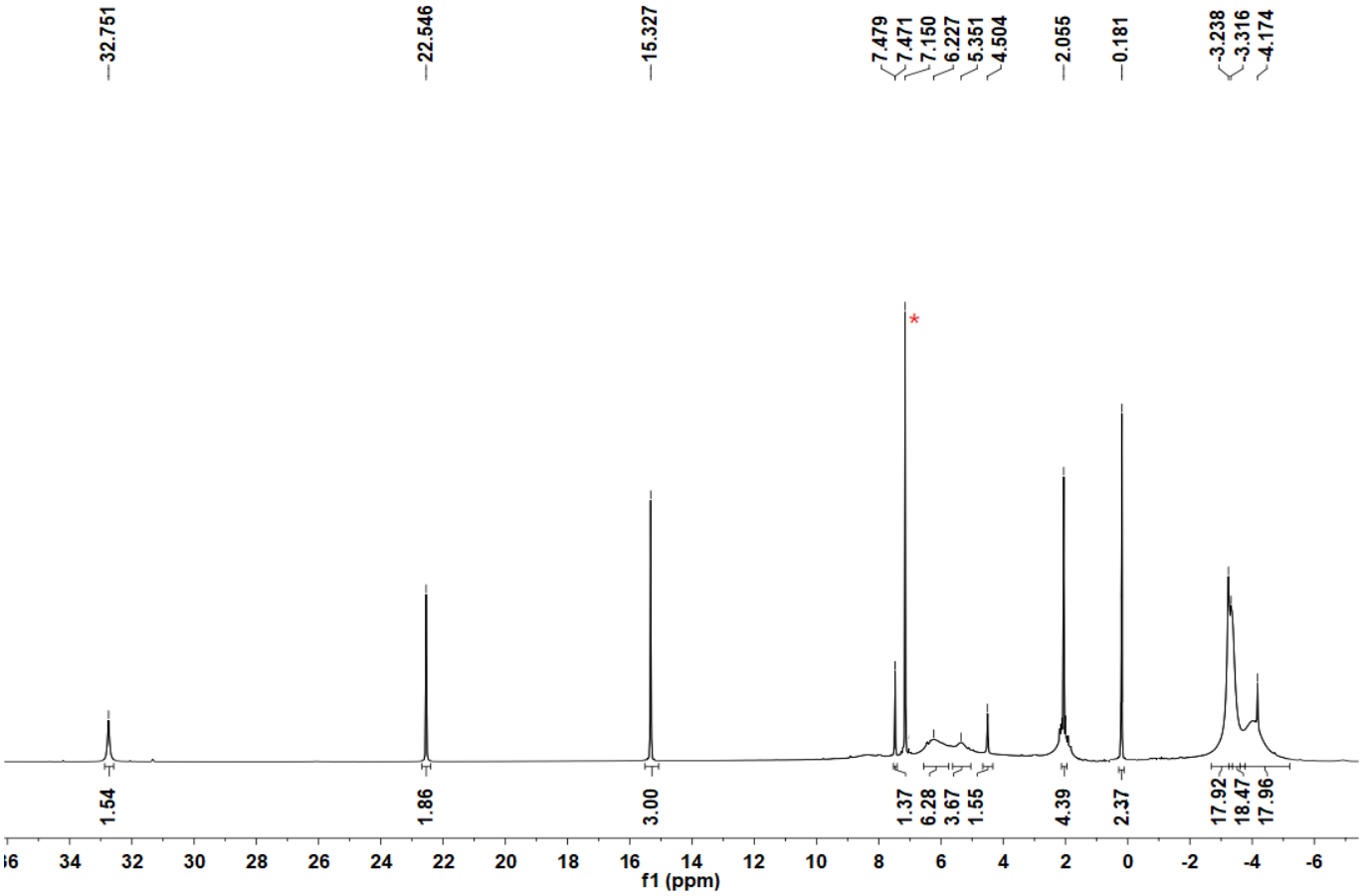

Figure S21. [1]H NMR spectrum for compound **9**.

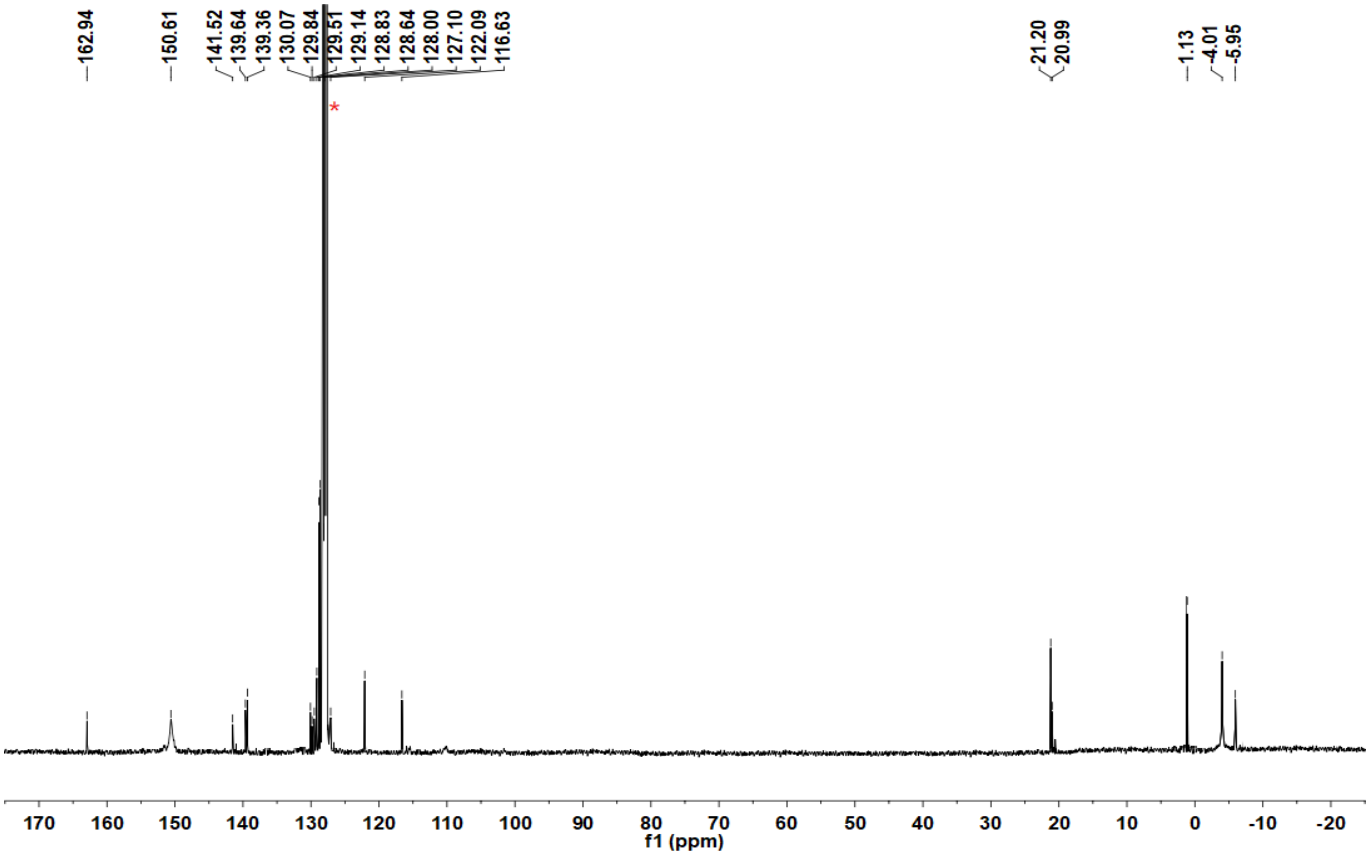

Figure S22. [13]C NMR spectrum for compound **9**.

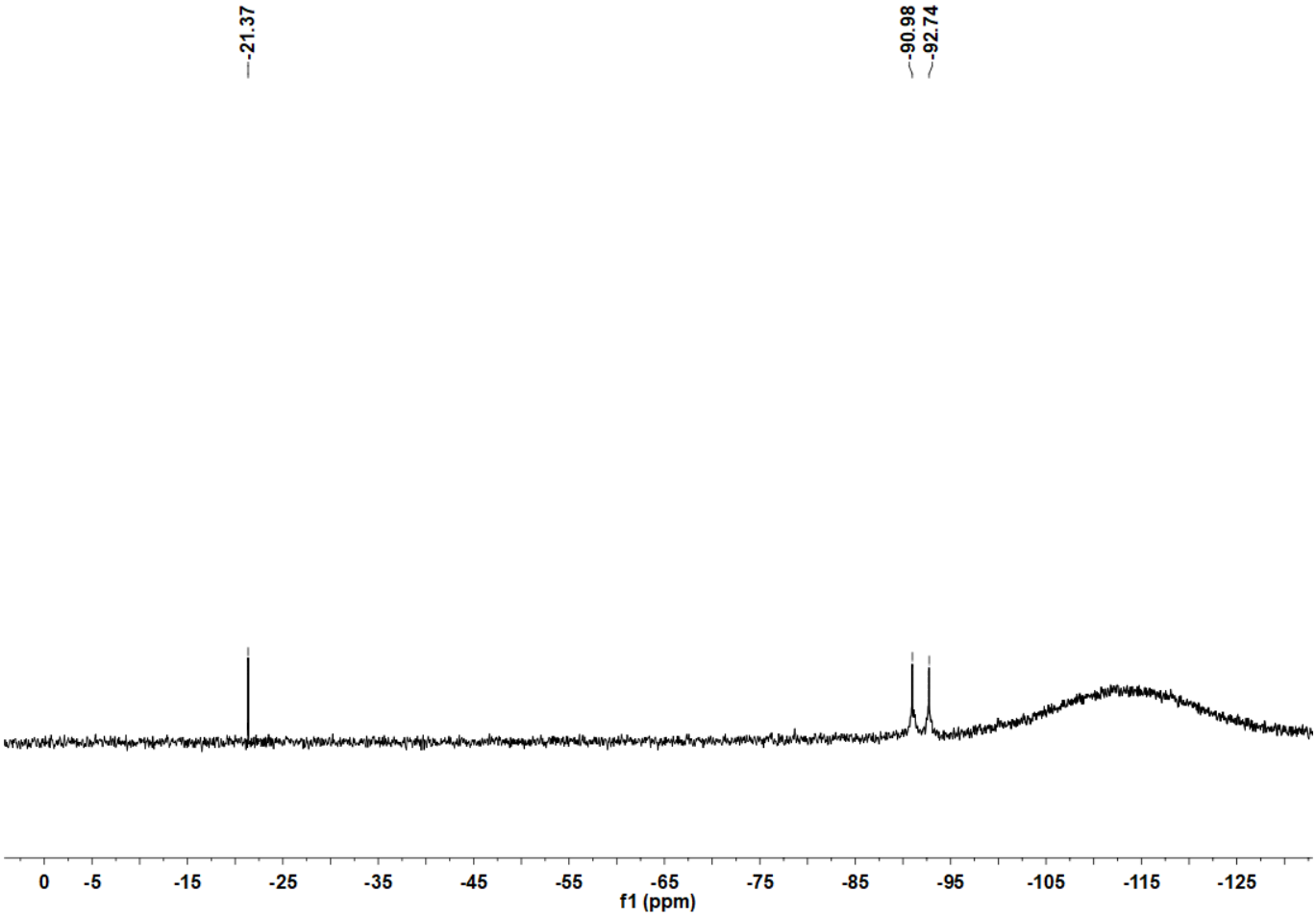

Figure S23. ^{29}Si NMR spectrum for compound **9**.

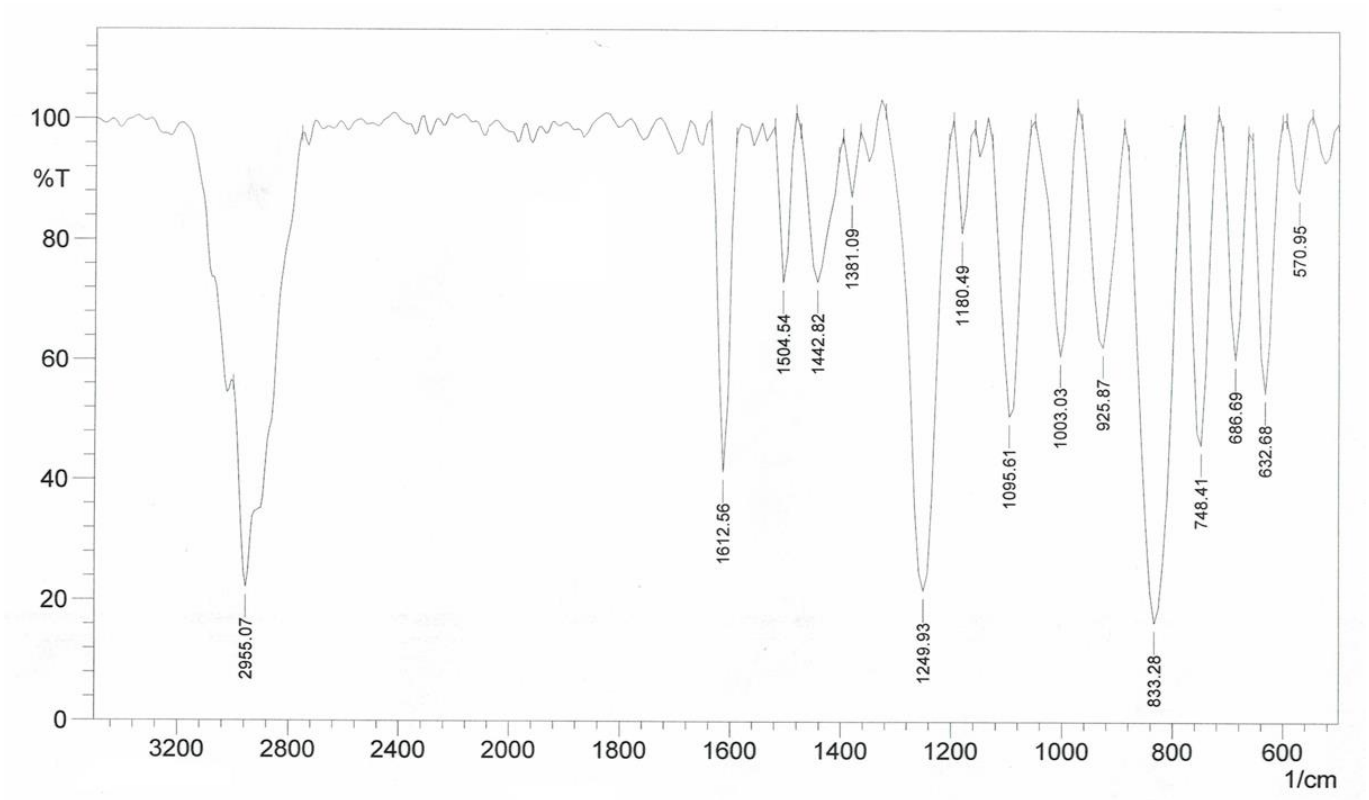

Figure S24. IR spectrum for compound **9**.

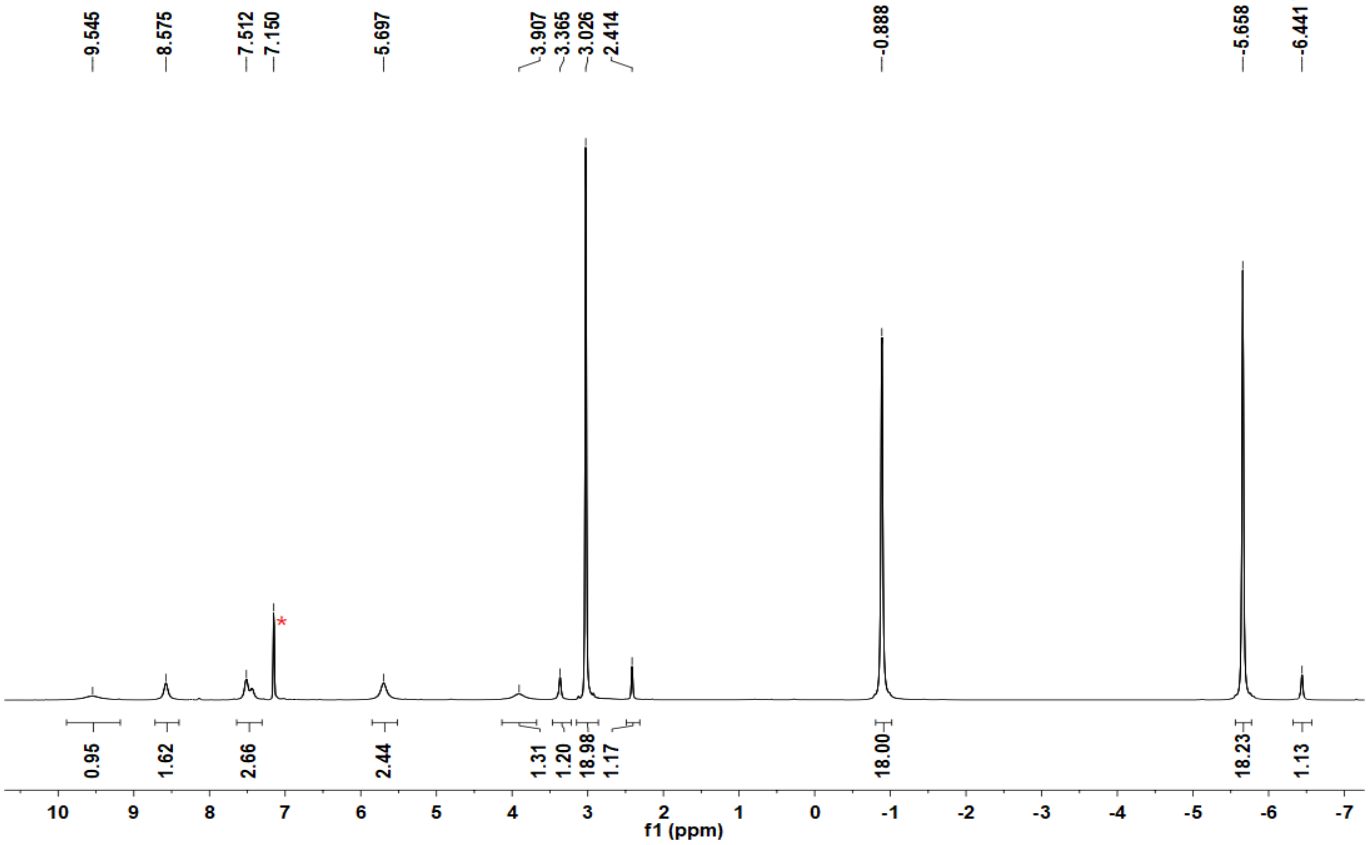

Figure S25. [1]H NMR spectrum for compound **10**.

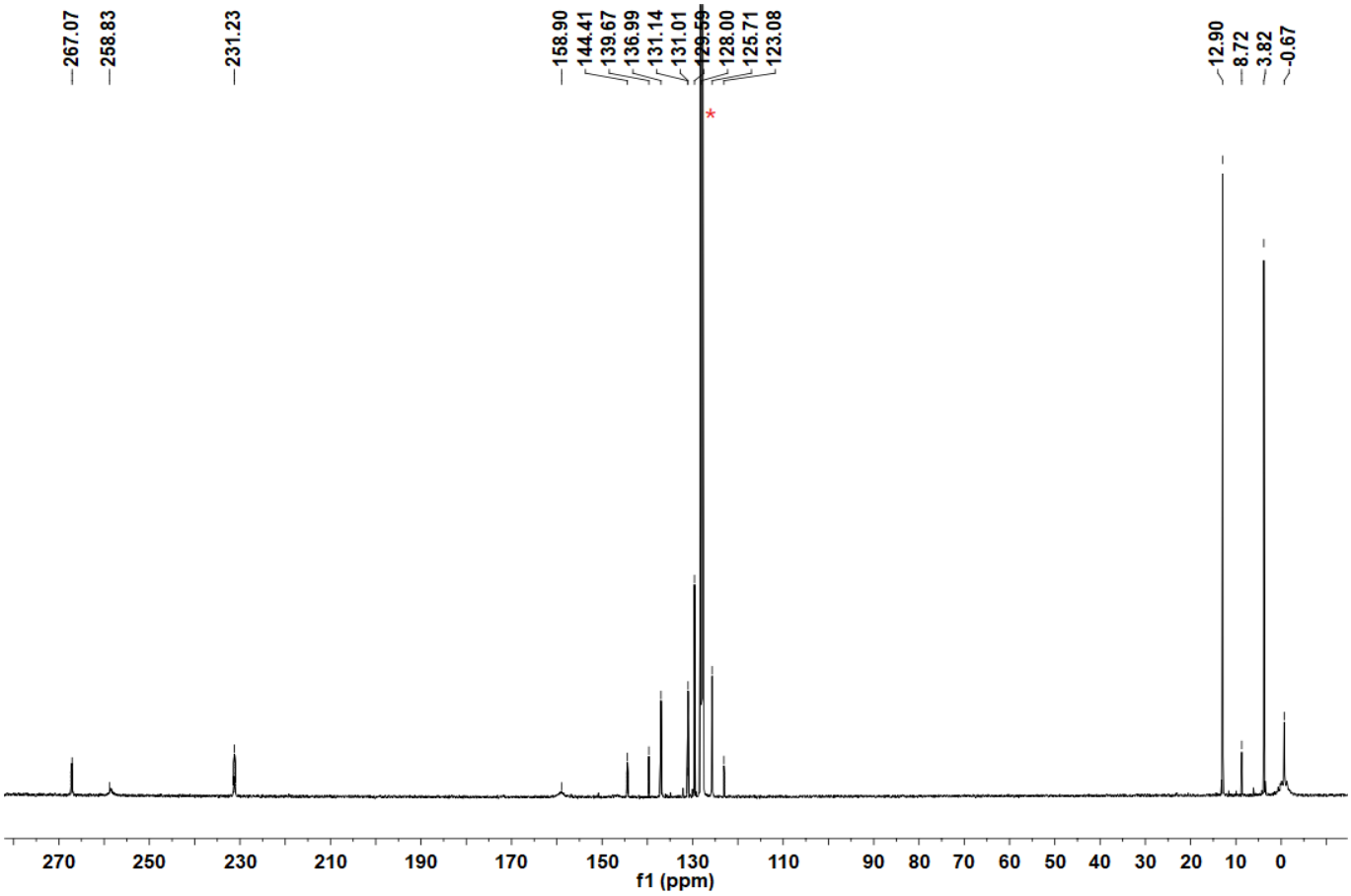

Figure S26. [13]C NMR spectrum for compound **10**.

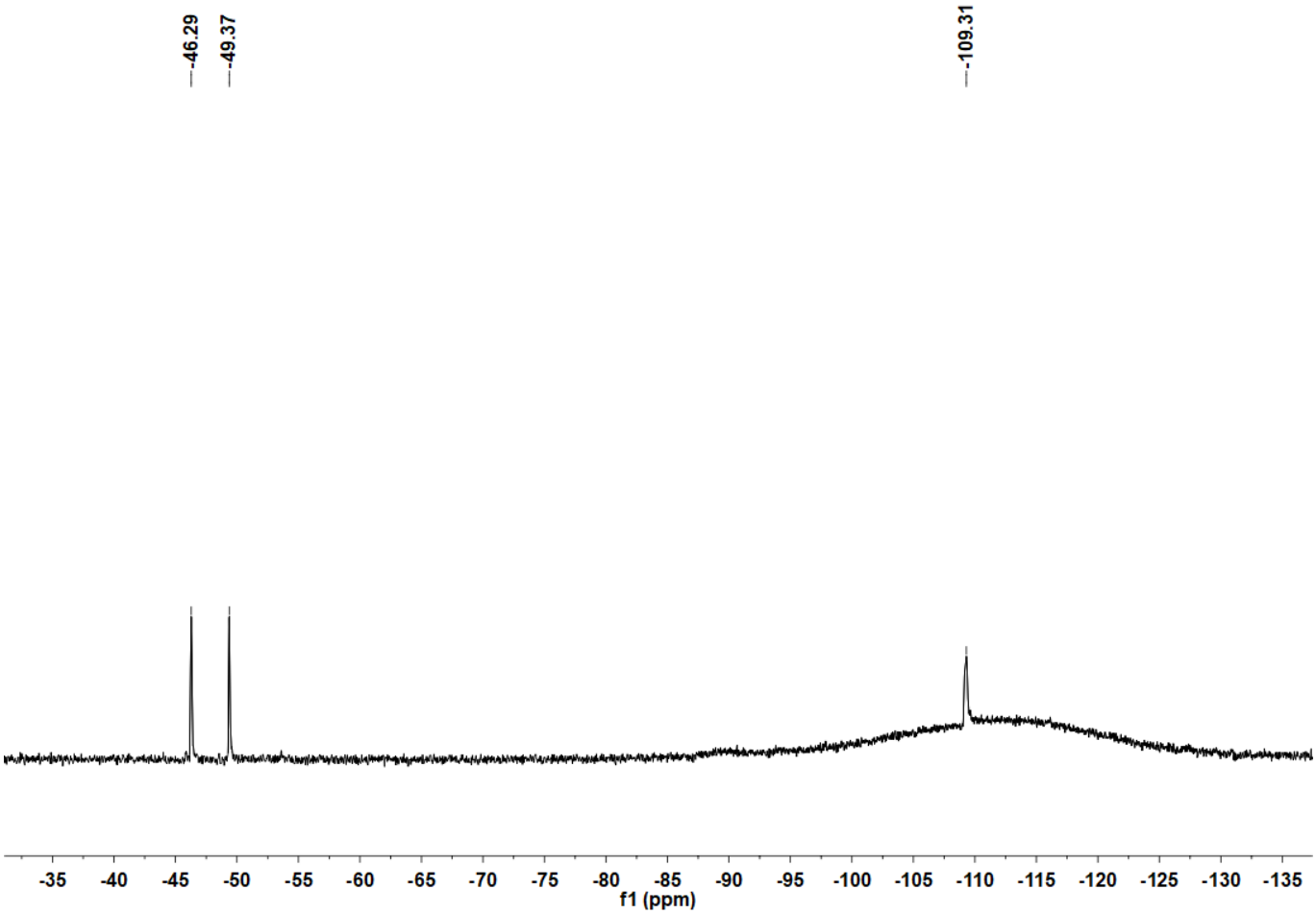

Figure S27. ^{29}Si NMR spectrum for compound **10**.

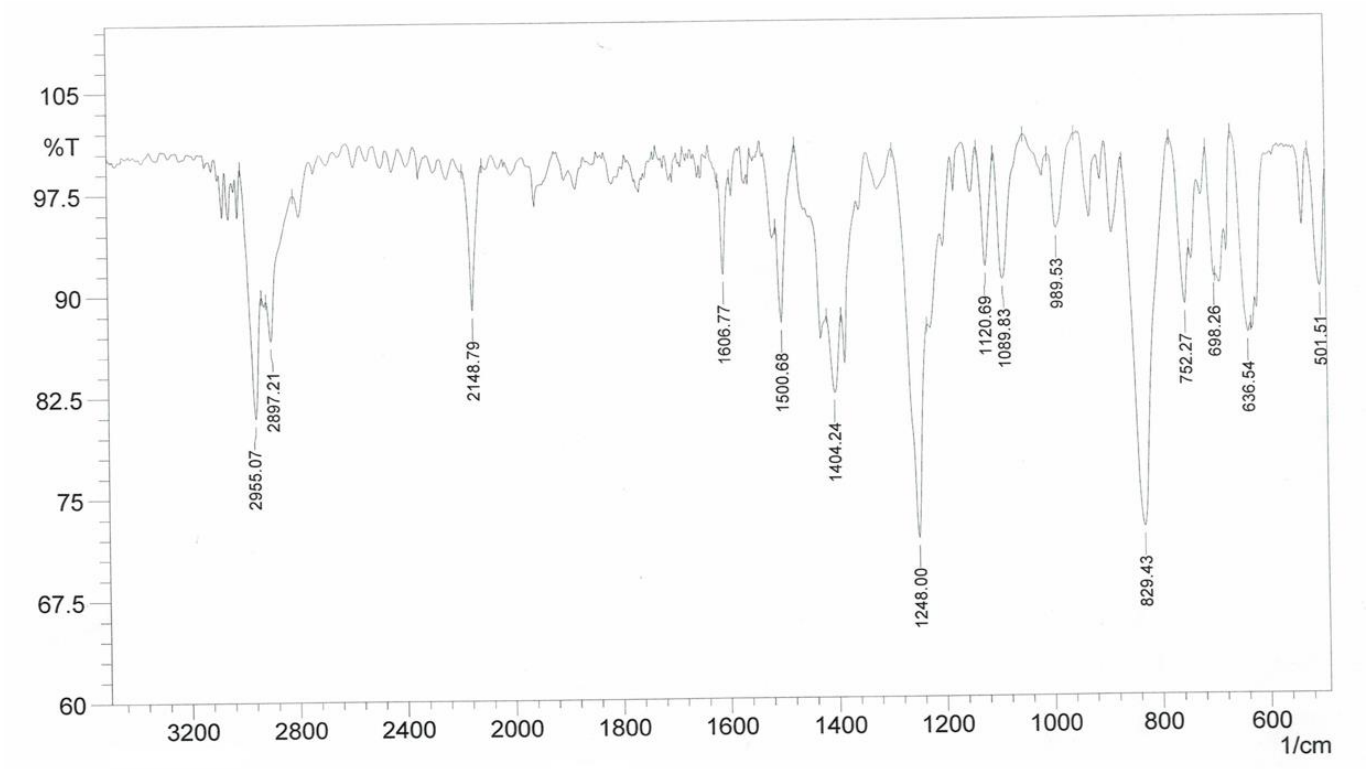

Figure S28. IR spectrum for compound **10**.

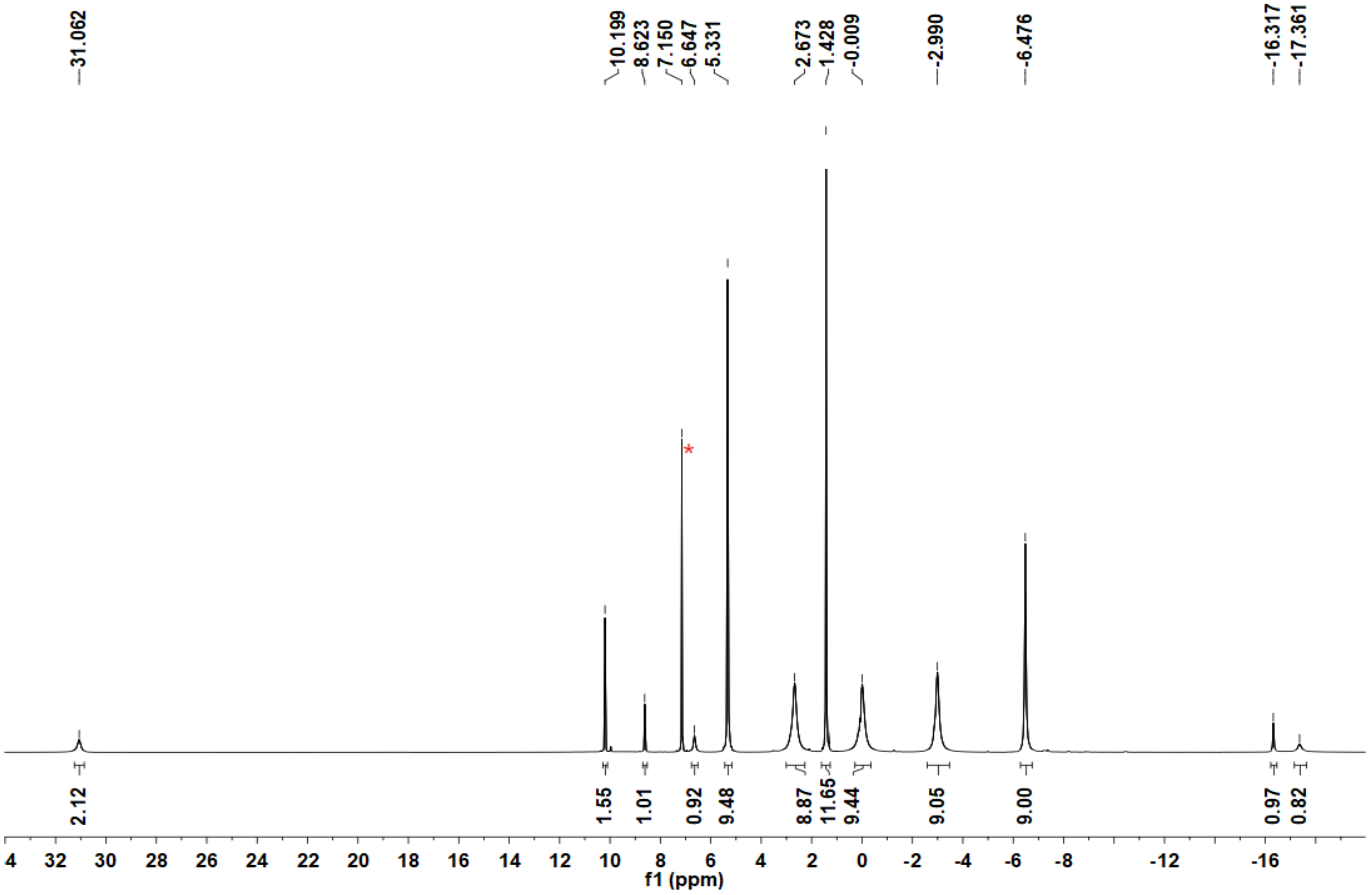

Figure S29. [1]H NMR spectrum for compound **11**.

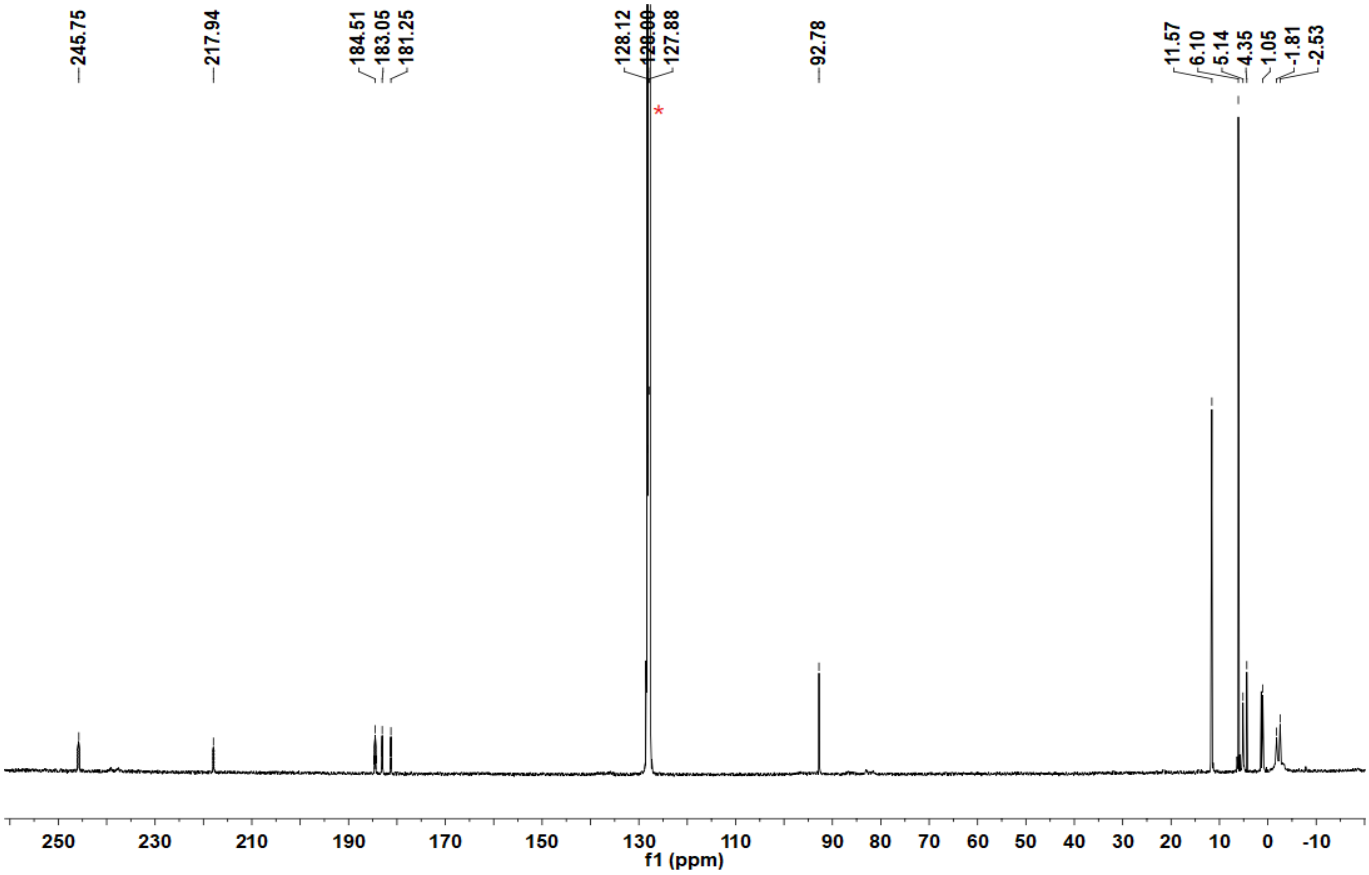

Figure S30. [13]C NMR spectrum for compound **11**.

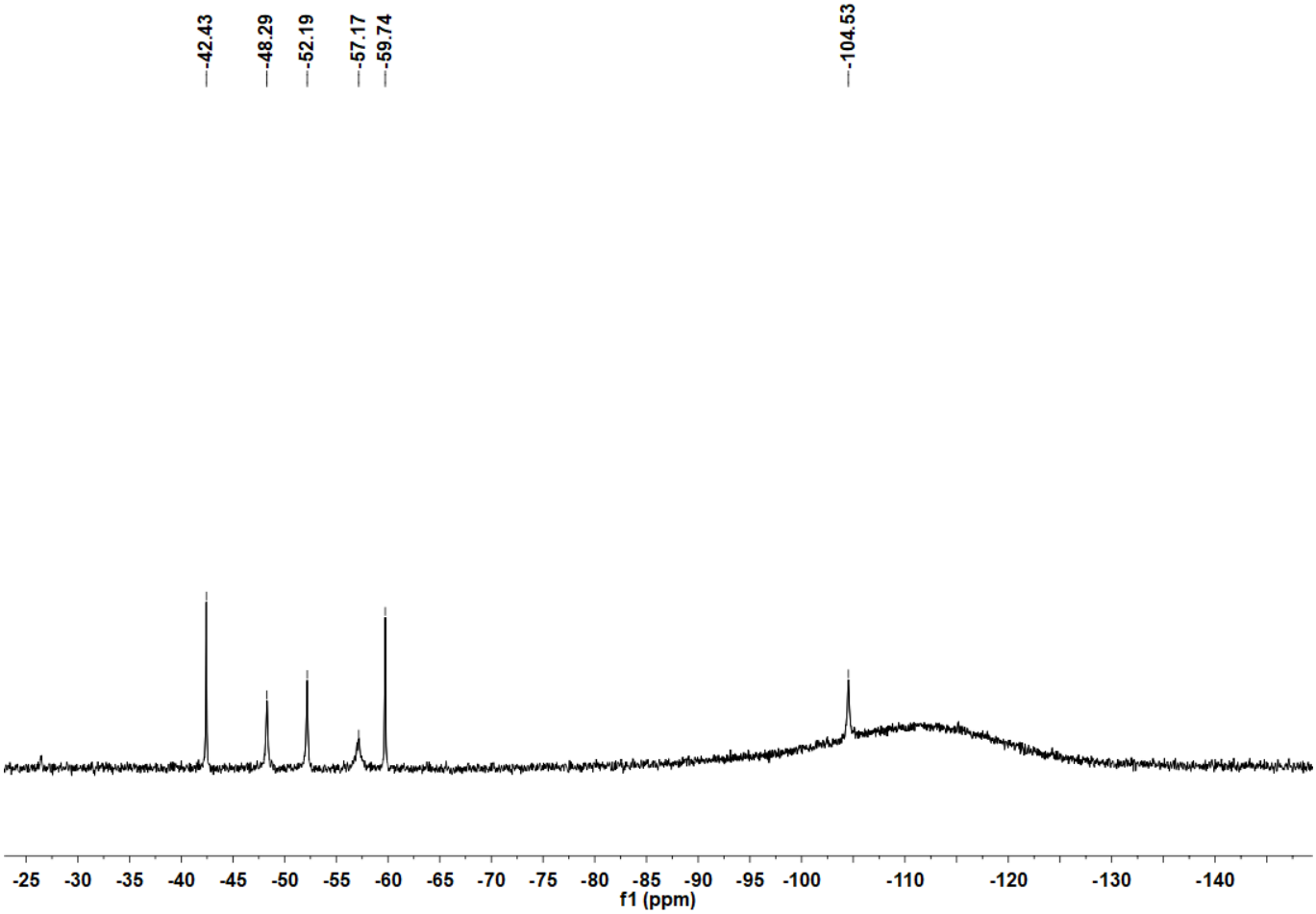

Figure S31. ^{29}Si NMR spectrum for compound **11**.

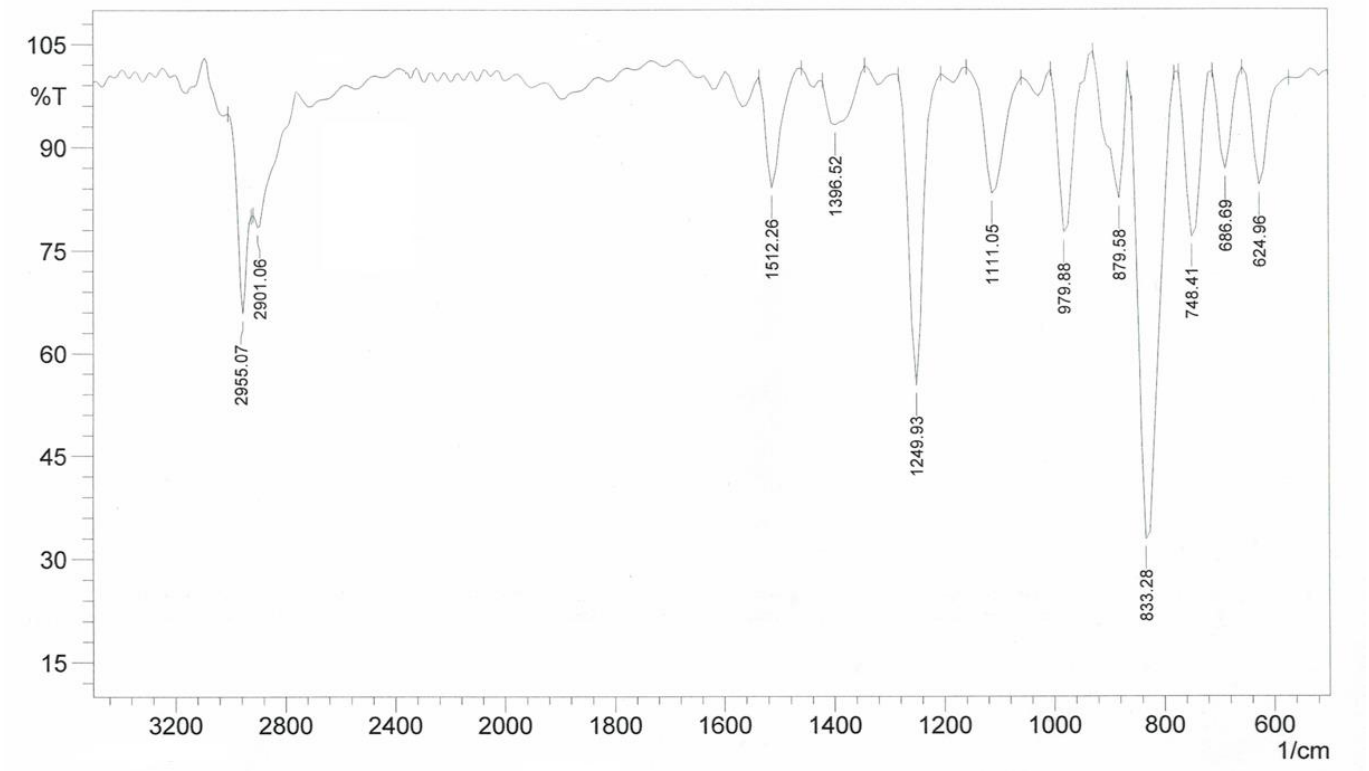

Figure S32. IR spectrum for compound **11**.

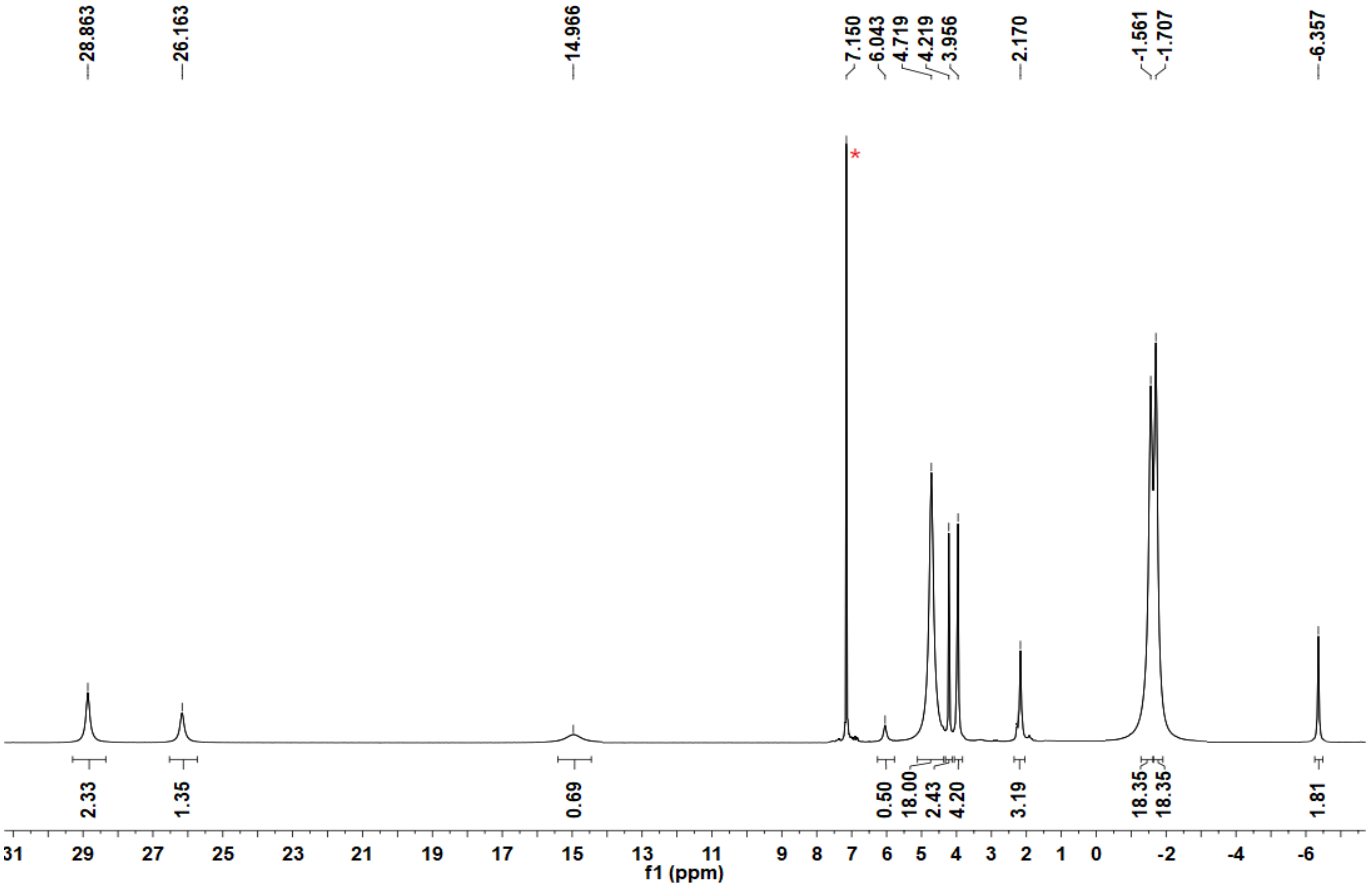

Figure S33. [1]H NMR spectrum for compound **12**.

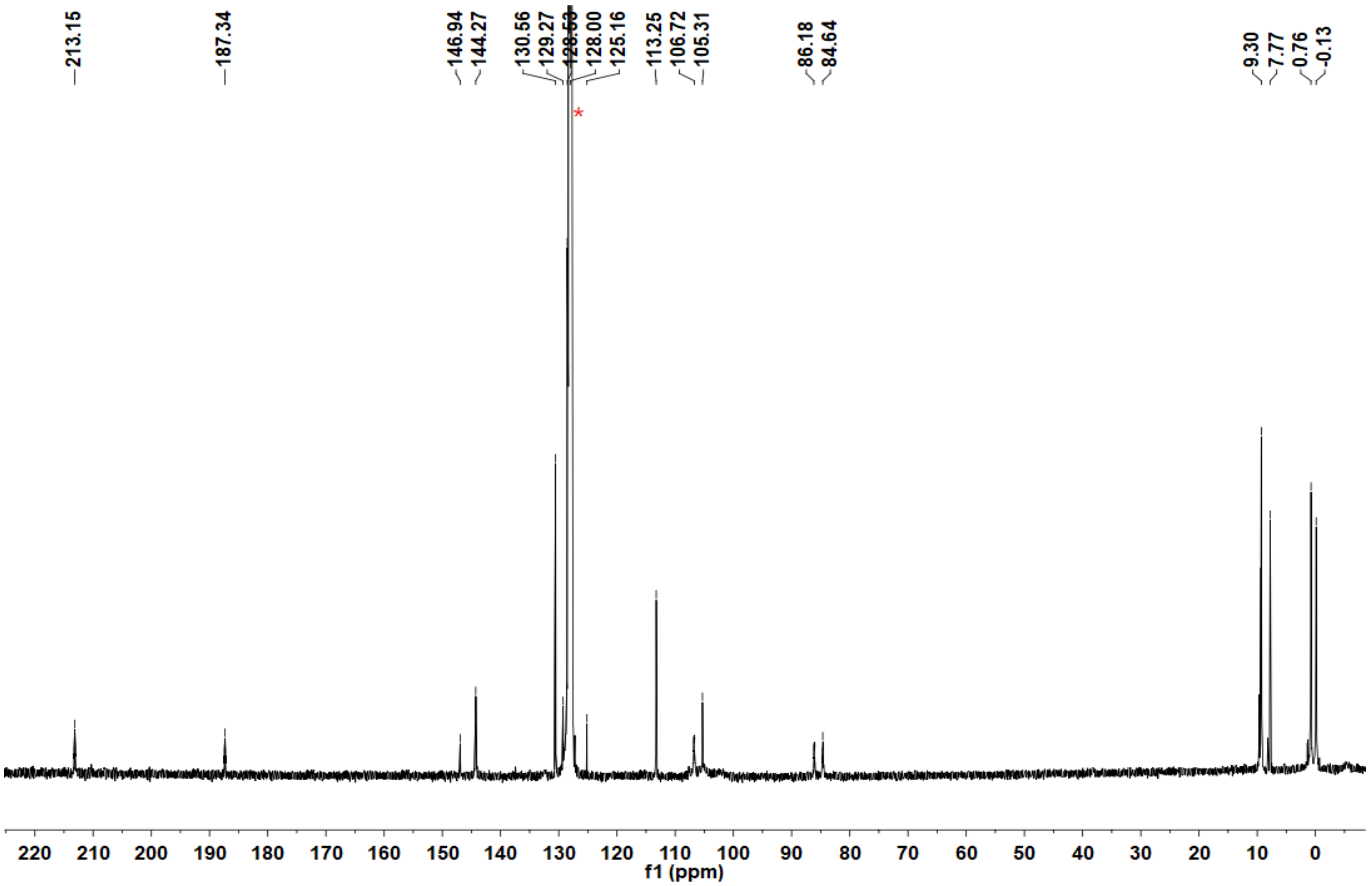

Figure S34. [13]C NMR spectrum for compound **12**.

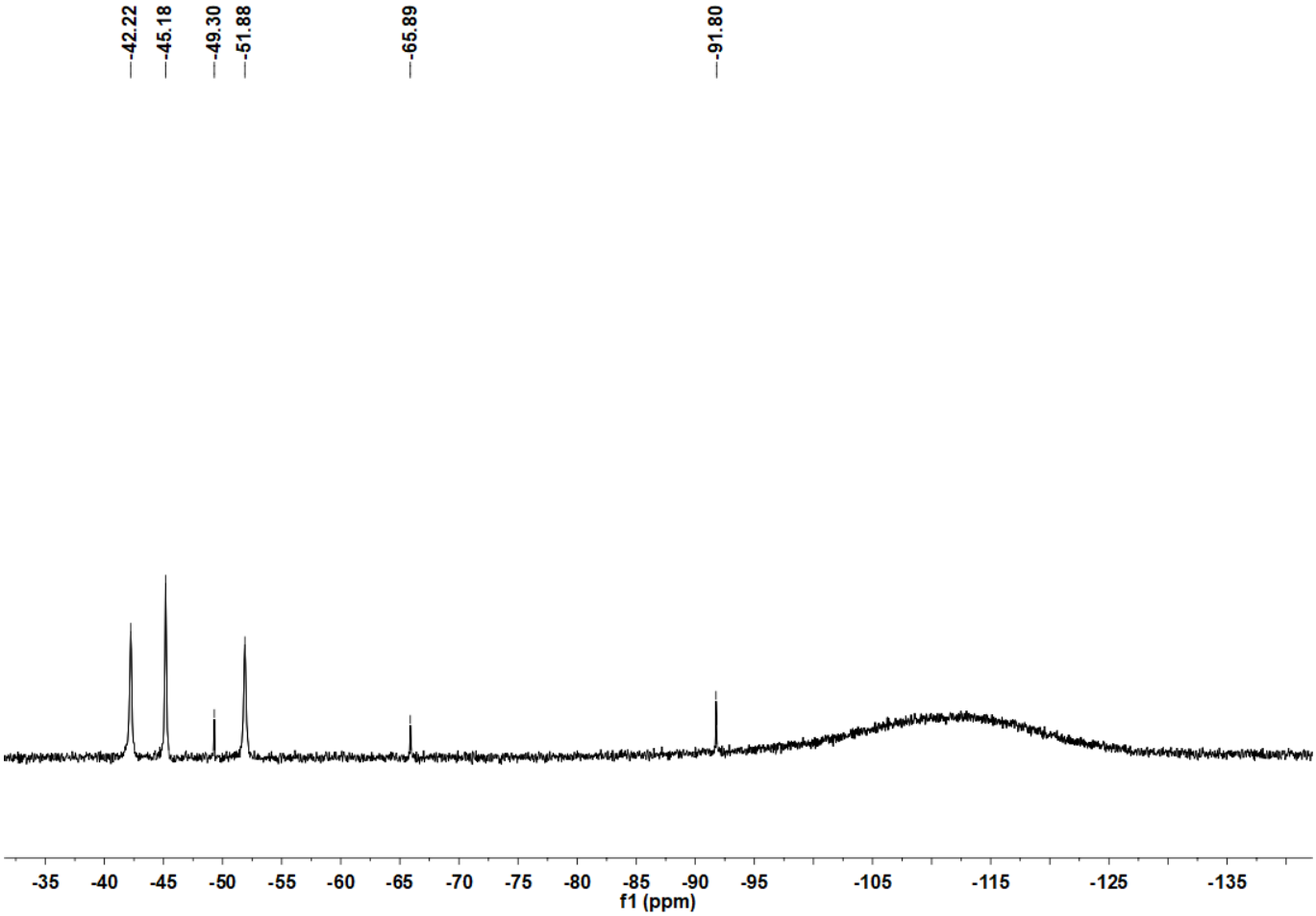

Figure S35. ^{29}Si NMR spectrum for compound **12**.

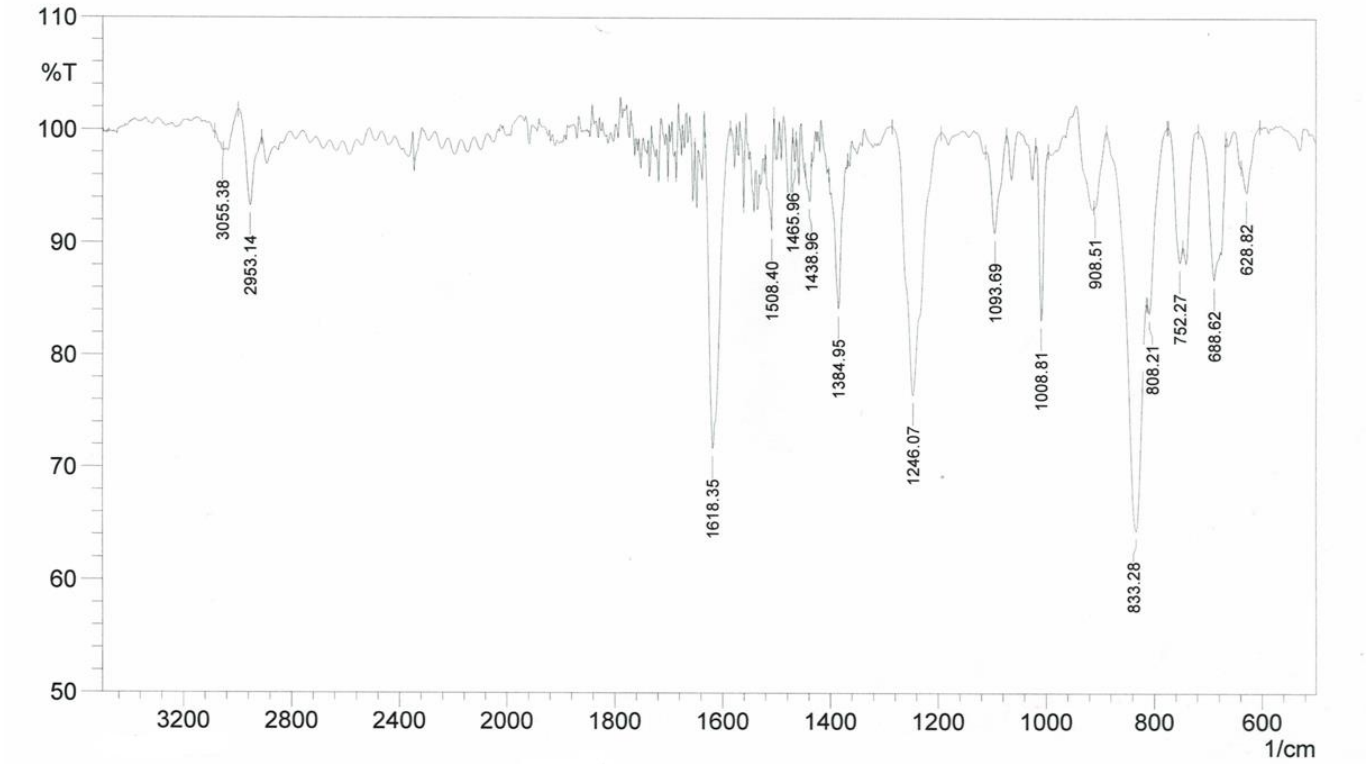

Figure S36. IR spectrum for compound **12**.

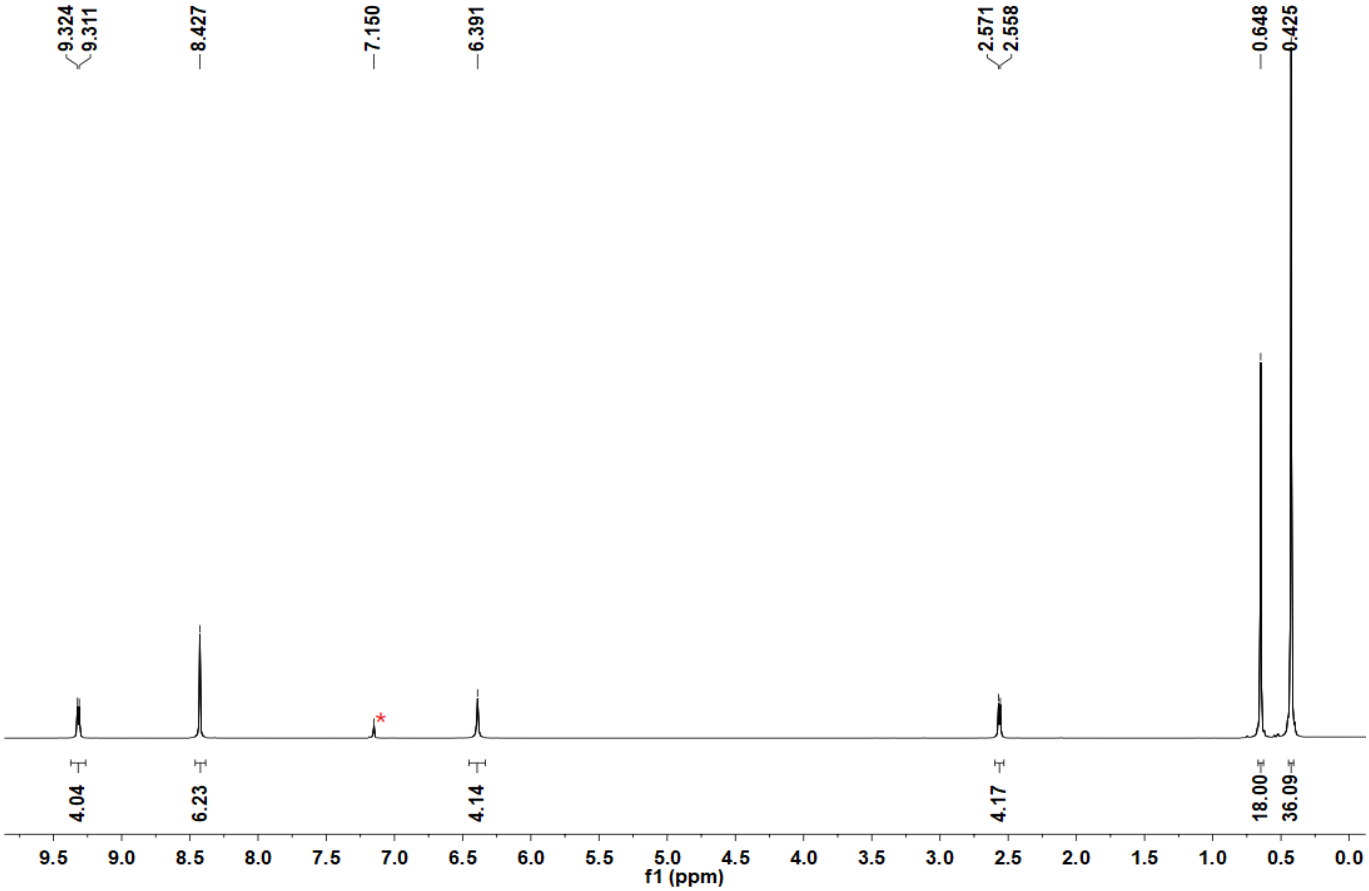

Figure S37. [1]H NMR spectrum for compound **13**.

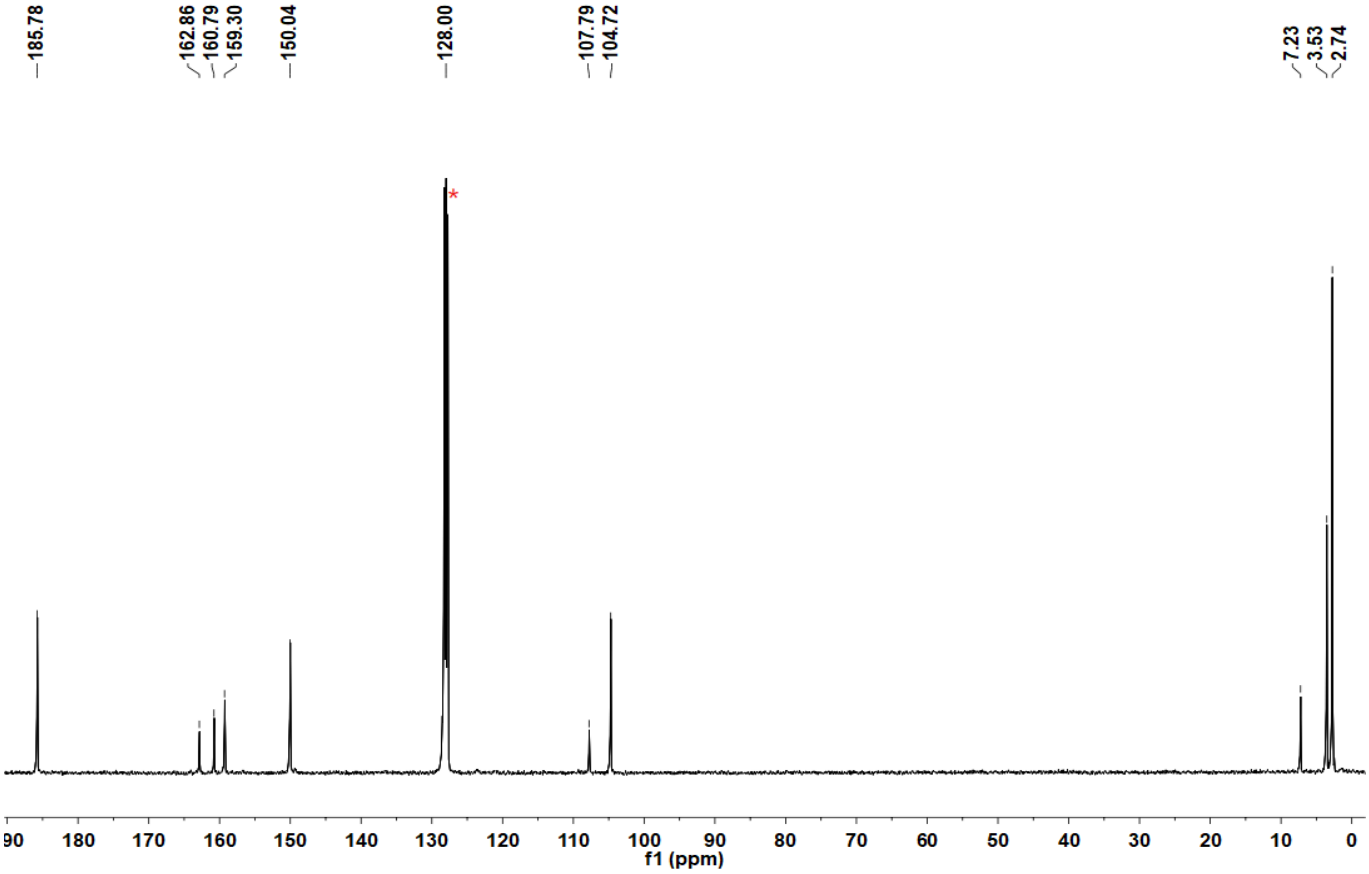

Figure S38. [13]C NMR spectrum for compound **13**.

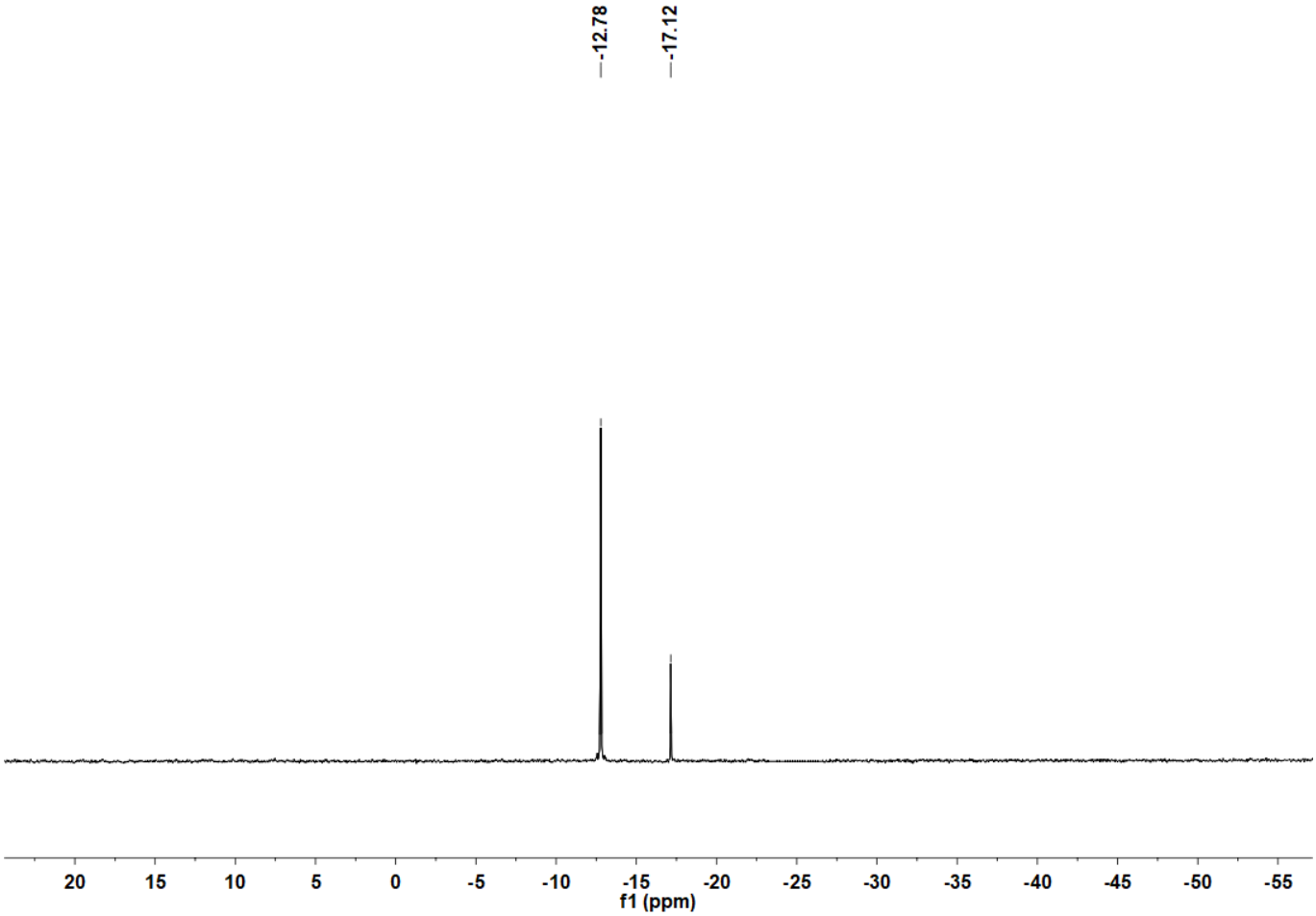

Figure S39. ^{29}Si NMR spectrum for compound **13**.

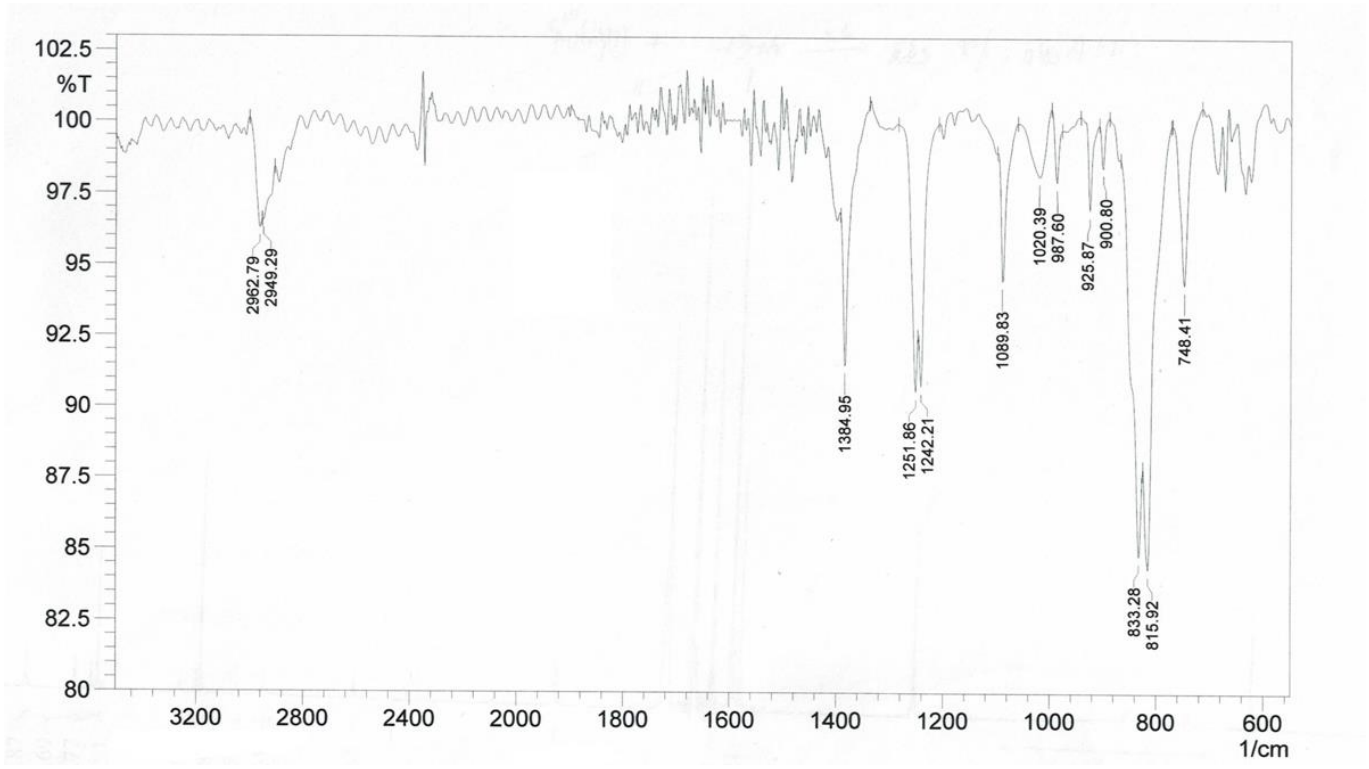

Figure S40. IR spectrum for compound **13**.

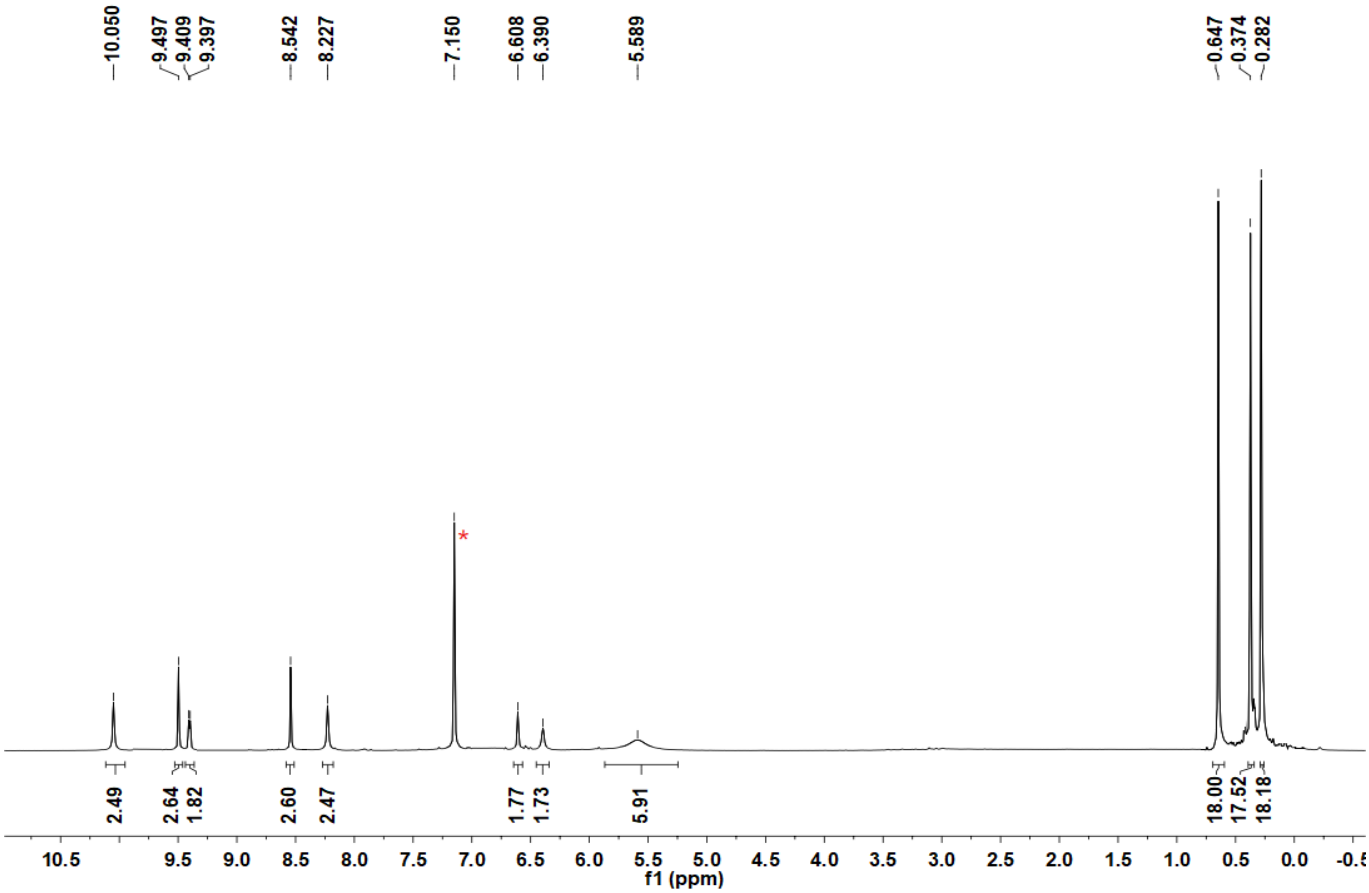

Figure S41. [1]H NMR spectrum for compound **14**.

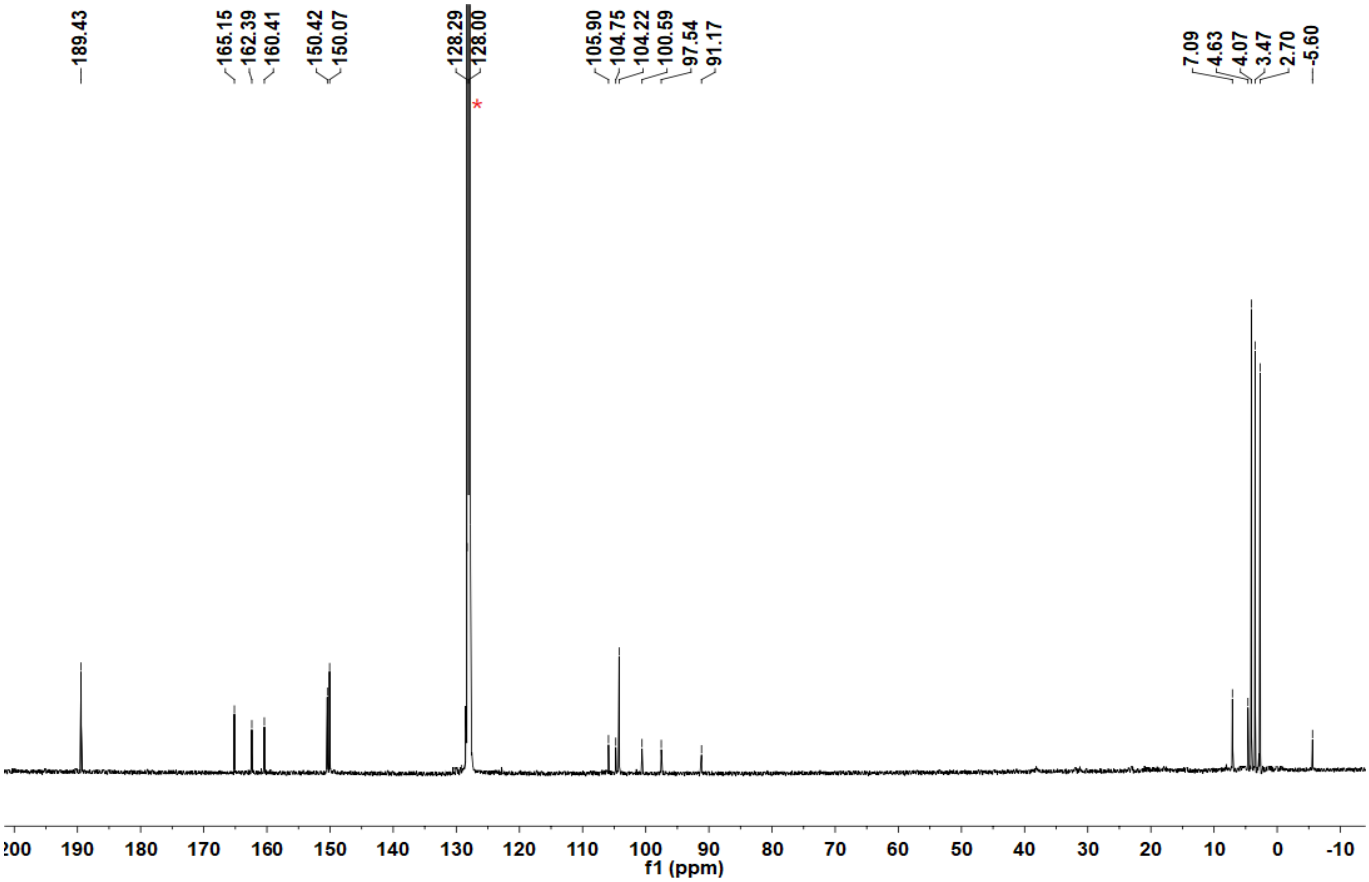

Figure S42. [13]C NMR spectrum for compound **14**.

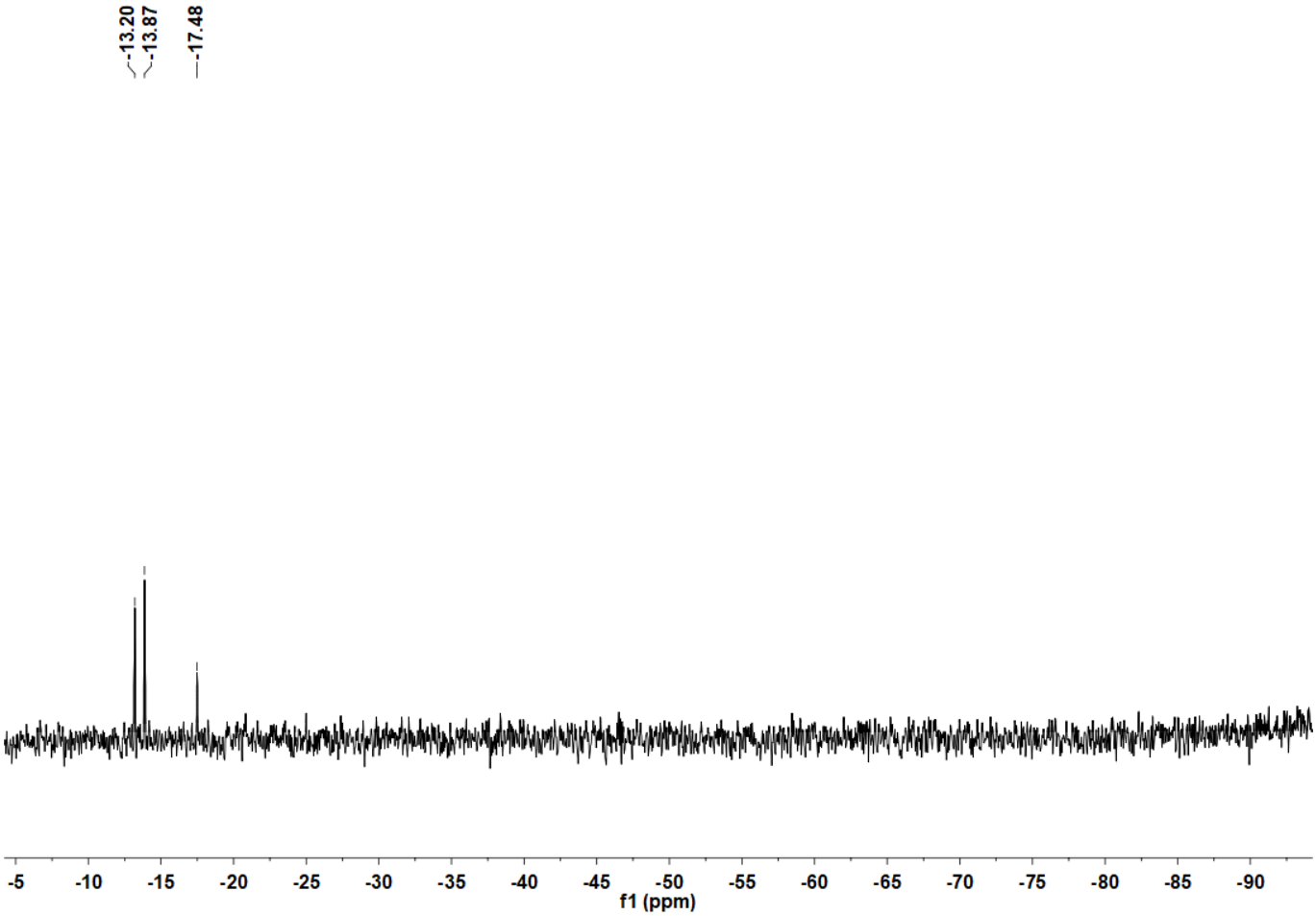

Figure S43. ^{29}Si NMR spectrum for compound **14**.

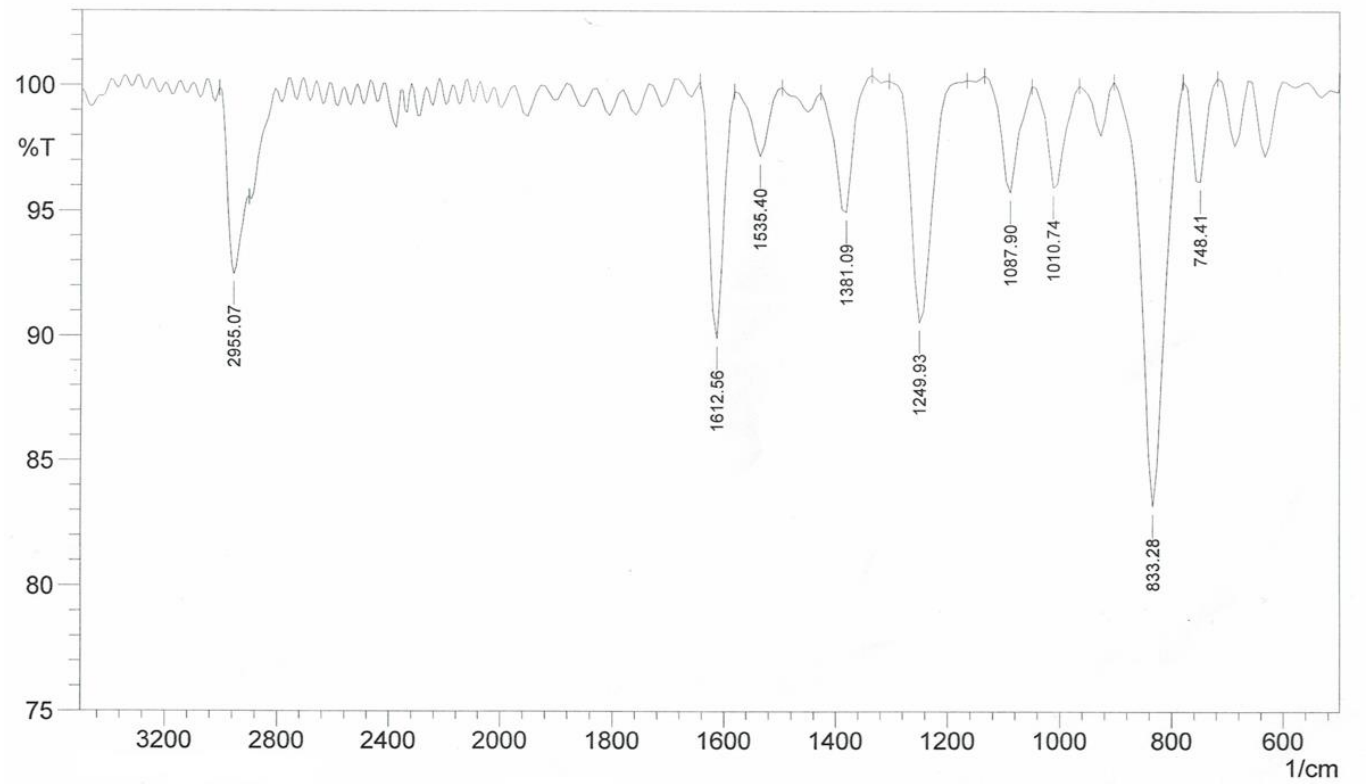

Figure S44. IR spectrum for compound **14**.

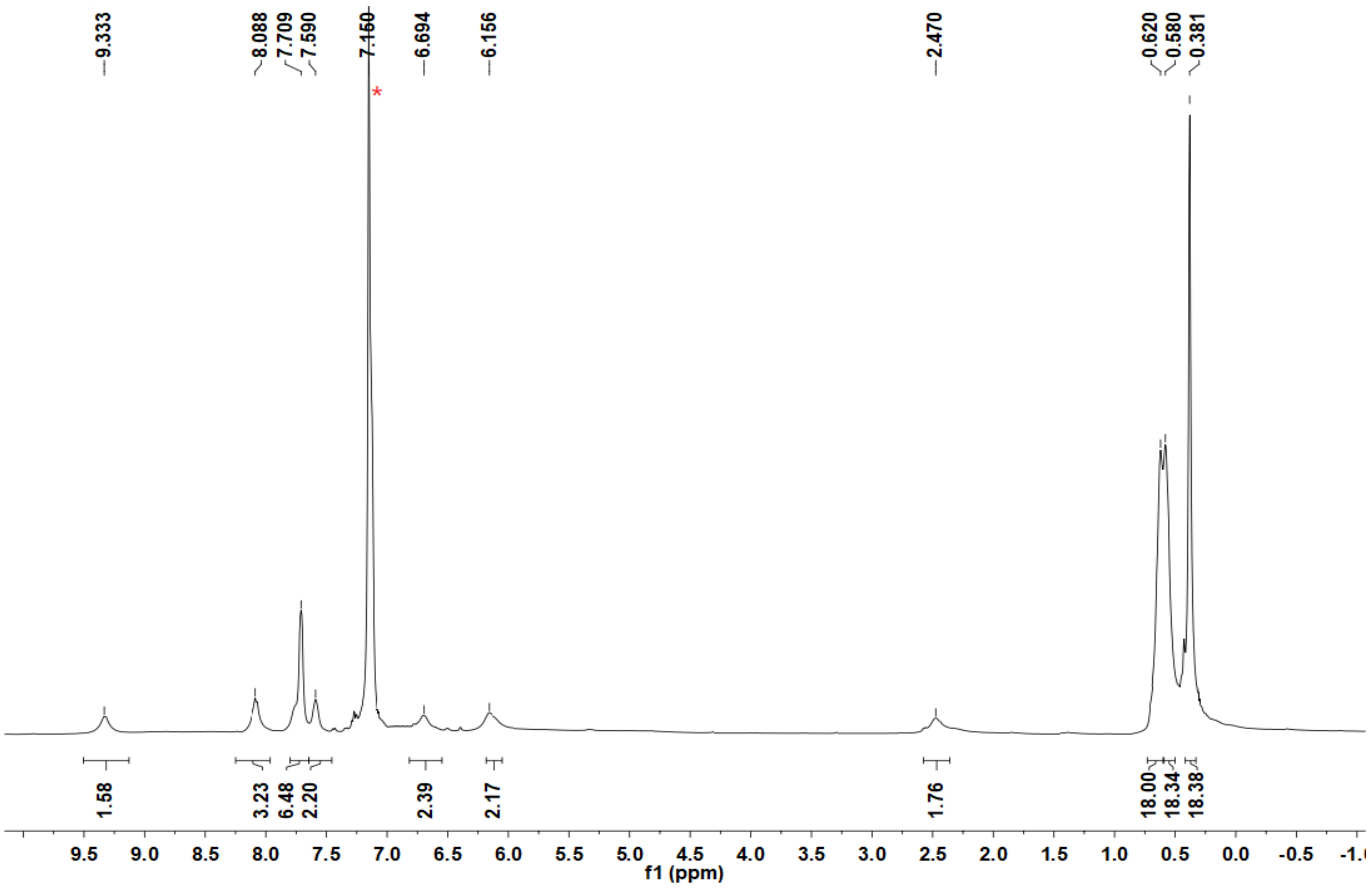

Figure S45. [1]H NMR spectrum for compound **15**.

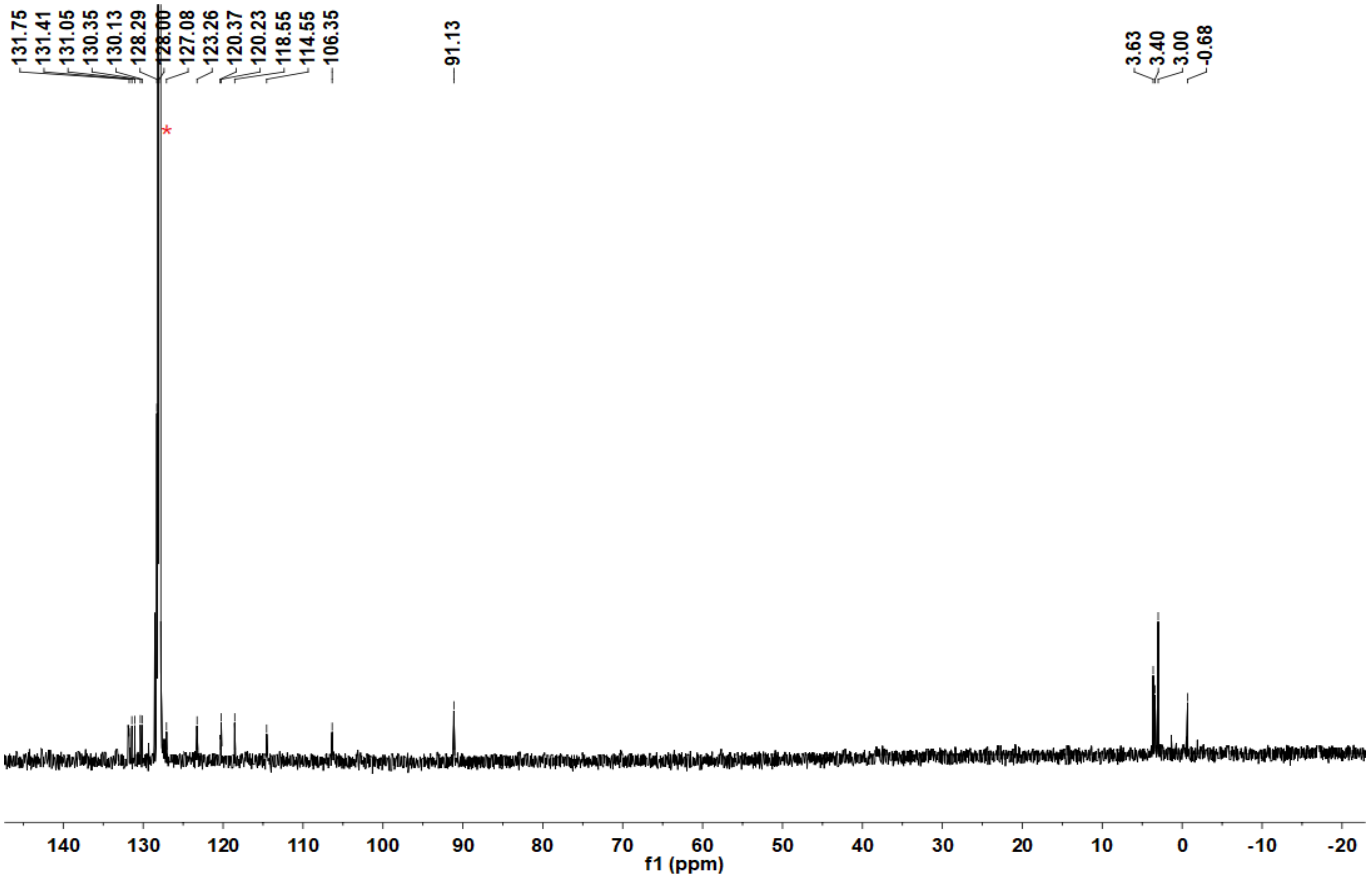

Figure S46. [13]C NMR spectrum for compound **15**.

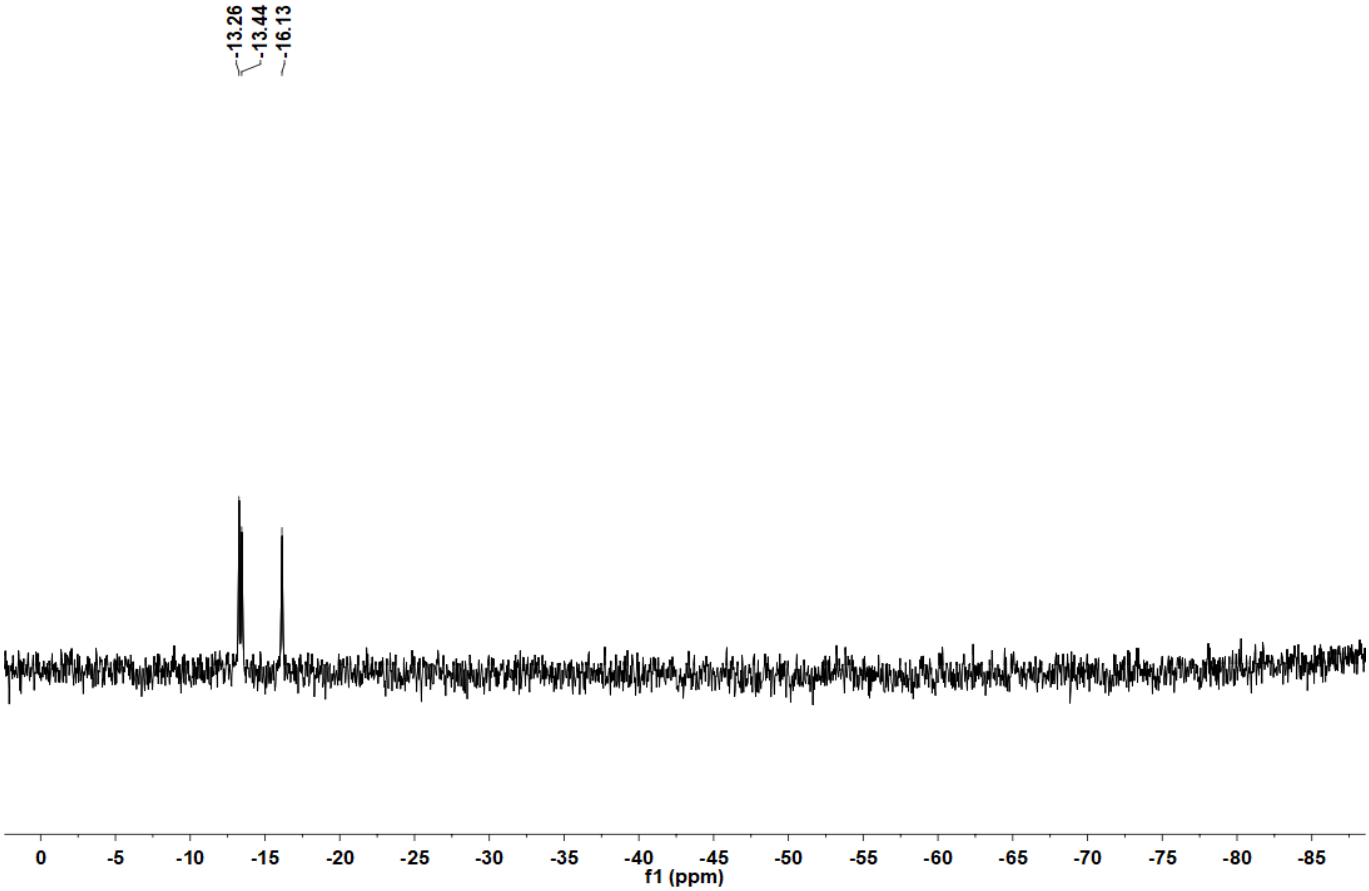

Figure S47. ^{29}Si NMR spectrum for compound **15**.

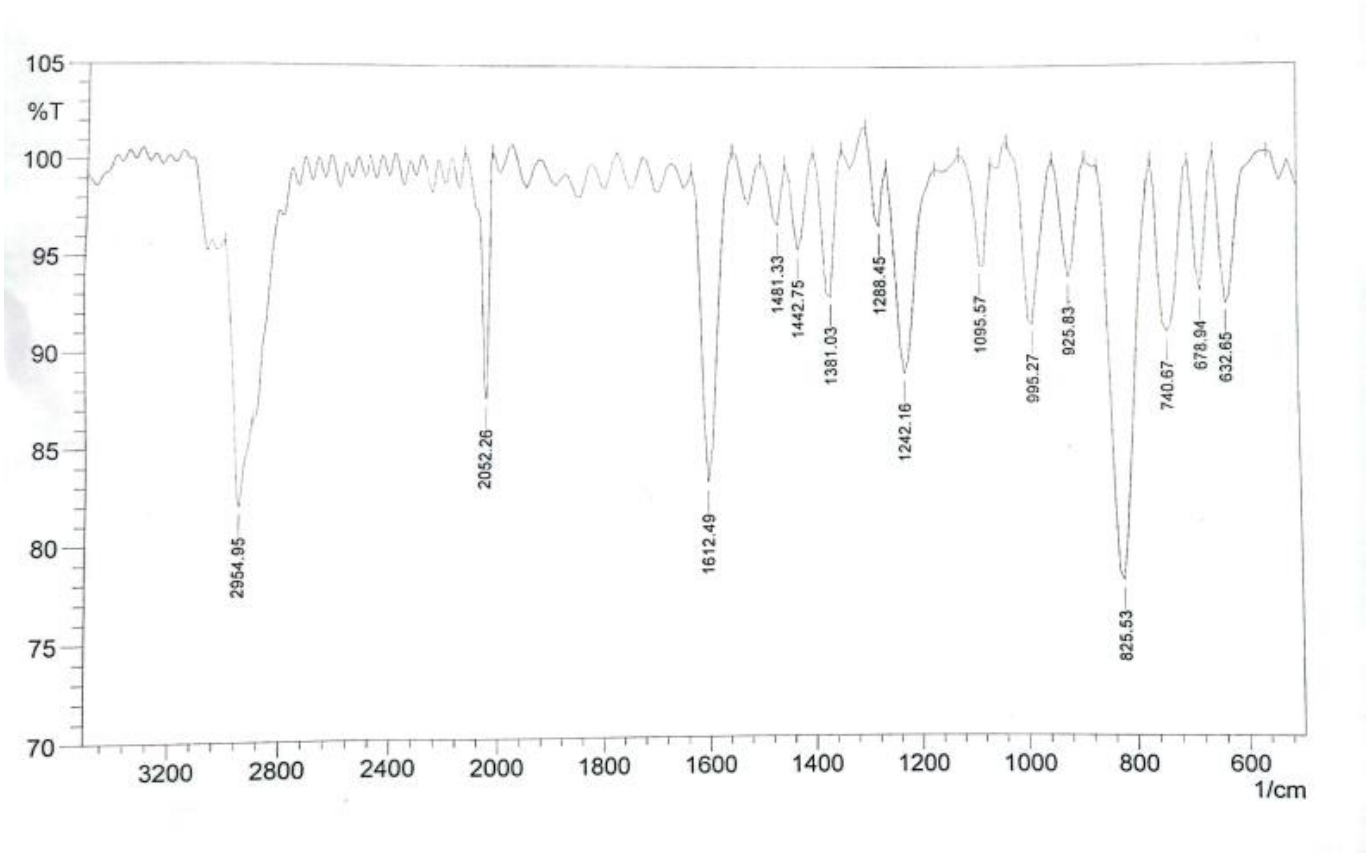

Figure S48. IR spectrum for compound **15**.