Electronic Supplementary Information (ESI) for *NJC*

Rare earth metal bisamido complexes with a NNO tridentate ligand and catalytic activity for selective polymerization of isoprene

Xiaoxia Gu,[a,b] Shaowu Wang,*[a,c] Yun Wei,[a] Xiancui Zhu,[a] Shuangliu Zhou,[a] Zeming Huang,[a] and Xiaolong Mu[a]

[a] Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, Wuhu, Anhui 241000, China. E-mail: swwang@mail.ahnu.edu.cn, Fax: +86-553-3883517; Tel: +86-553-5910015.

[b] Department of Chemistry, Wannan Medical College, Wuhu, Anhui 241002, China.

[c] State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Shanghai 200032, China.

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1. Crystallographic data of complexes 2-8

Table S1. Summary of crystal and refinement data for complexes **2-5.**

Complexes	**2**	**3**	**4**	**5**
empirical formula	$C_{24}H_{51}YN_4OSi_4$	$C_{24}H_{51}NdN_4OSi_4$	$C_{24}H_{51}SmN_4OSi_4$	$C_{24}H_{51}GdN_4OSi_4$
fw	612.96	668.29	674.40	681.30
T (K)	293(2)	293(2)	293(2)	293(2)
wavelength (Å)	0.71073	0.71073	0.71073	0.71073
cryst system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2/c$
a (Å)	10.9219(10)	12.7474(13)	12.7324(9)	16.8027(16)
b (Å)	18.9450(17	16.9894(18)	16.9061(11)	12.4348(12)
c (Å)	16.7845(15)	16.8809(18)	16.9308(12)	17.2821(16)
α(deg)	90	90	90	90
β(deg)	93.9550(10)	102.8170(10)	102.4170(10)	101.2840(10)
γ(deg)	90	90	90	90
V (Å^3)	3464.7(5)	3564.8(6)	3559.2(4)	3541.1(6)
Z	4	4	4	4
D_{calcd}(g cm^{-3})	1.175	1.245	1.259	1.278
abs coeff (mm^{-1})	1.842	2.561	1.805	2.029
F (000)	1304	1388	1396	1404
θ range for data collcn(deg)	1.62 to 27.58	1.72 to 27.58	1.72 to 27.55	1.64 to 27.68
no. of reflcnscollcd/unique	29751/8003	30310/8219	39955/8088	30173/8247
data/restns/params	8003/0/321	8219/0/321	8088/94/322	8247/66/352
goof	1.001	1.039	0.996	1.095
R_1, wR_2 [$I>2\sigma(I)$]	0.0449, 0.0859	0.0418, 0.1077	0.0569, 0.2187	0.0268, 0.0625
R_1, wR_2 (all data)	0.0989, 0.1022	0.0522, 0.1159	0.0651, 0.2503	0.0366, 0.0664
largest diff peak/hole (e Å^{-3})	0.293, -0.397	2.405, -1.364	3.569, -2.204	0.325, -1.127

Table S2. Summary of crystal and refinement data for complexes 6-8.

Complexes	**6**	**7**	**8**
empirical formula	$C_{24}H_{51}DyN_4OSi_4$	$C_{24}H_{51}ErN_4OSi_4$	$C_{24}H_{51}N_4YbOSi_4$
fw	686.55	691.31	697.09
T (K)	293(2)	293(2)	293(2)
wavelength (Å)	0.71073	0.71073	0.71073
cryst system	Orthorhombic	Orthorhombic	Orthorhombic
space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
a (Å)	9.5148(9)	9.5144(8)	9.4869(7)
b (Å)	19.1828(18)	19.1019(16)	19.0170(14)

c (Å)	19.1886(18)	19.2125(16)	19.2467(14)
α(deg)	90	90	90
β(deg)	90	90	90
γ(deg)	90	90	90
V (Å^3)	3502.3(6)	3491.7(5)	3472.3(4)
Z	4	4	4
D_{calcd}(g cm^{-3})	1.302	1.315	1.333
abs coeff (mm^{-1})	2.291	2.561	2.852
F (000)	1412	1420	1428
θ range for data collcn(deg)	1.50 to 27.45	2.12 to 27.78	1.51 to 27.76
no. of reflcnscollcd/unique	40169/7936	30315/8146	30602/8104
data/restns/params	7936/0/321	8146/0/322	8104/0/322
goof	1.079	1.023	1.027
R_1, wR_2 [$I>2\sigma(I)$]	0.0439, 0.1110	0.0259, 0.0578	0.0610, 0.1452
R_1, wR_2 (all data)	0.0471, 0.1139	0.0306, 0.0598	0.0662, 0.1511
largest diff peak/hole (e Å^{-3})	1.311, -1.374	0.860, -0.745	3.404, -1.071

2. Copies of ^{1}H NMR, ^{13}C NMR spectra of complexes 2 and 4.

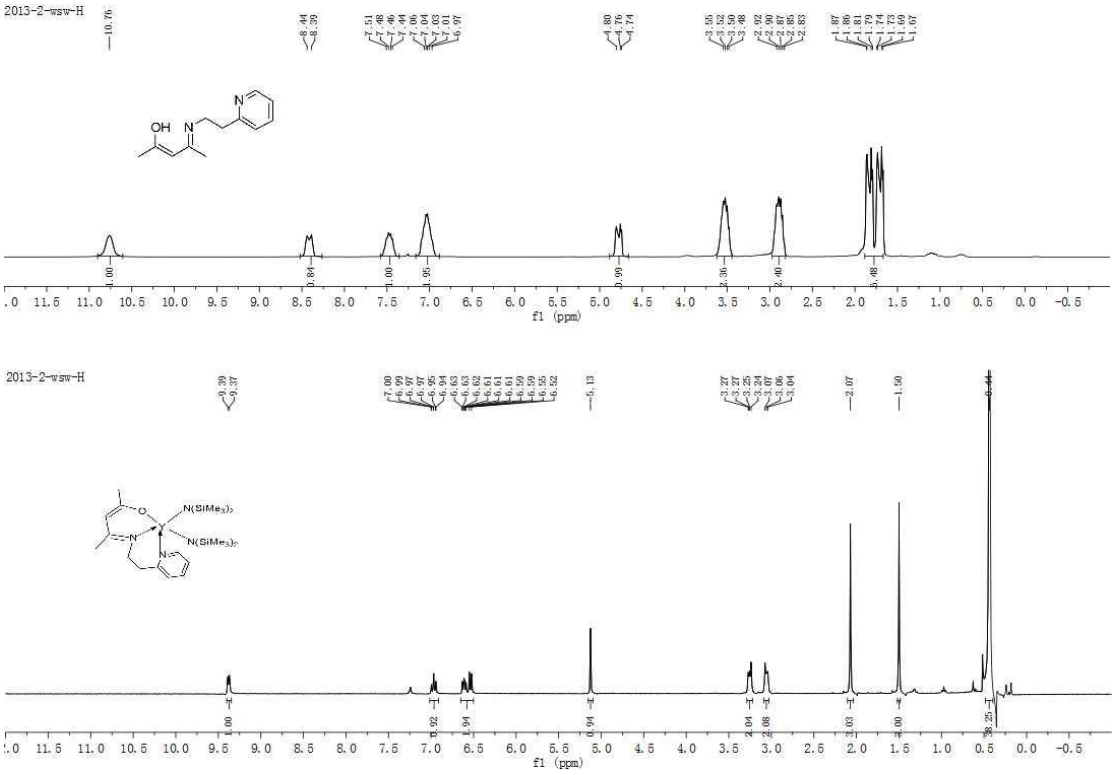

Fig. S1. ^{1}H NMR spectra (500 MHz, C_6D_6, 298 K) of complex **2** and the ligand precusor.

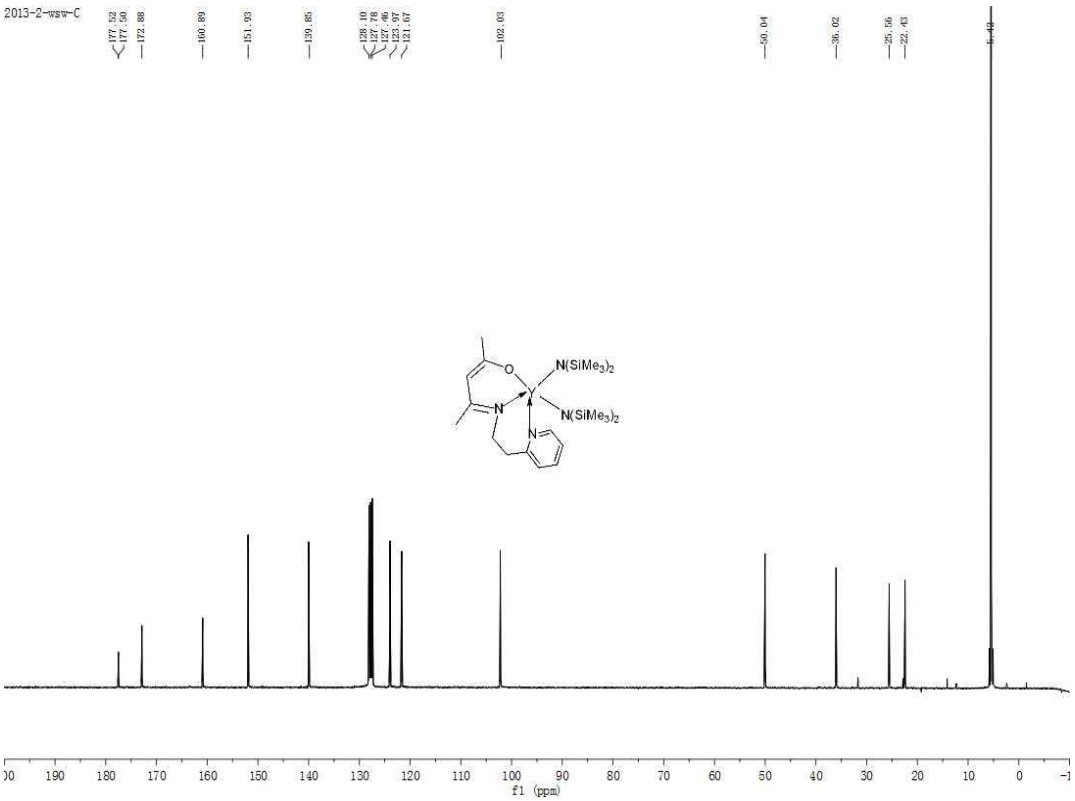

Fig. S2. ^{13}C NMR spectrum (126 MHz, C_6D_6, 298 K) of complex **2**.

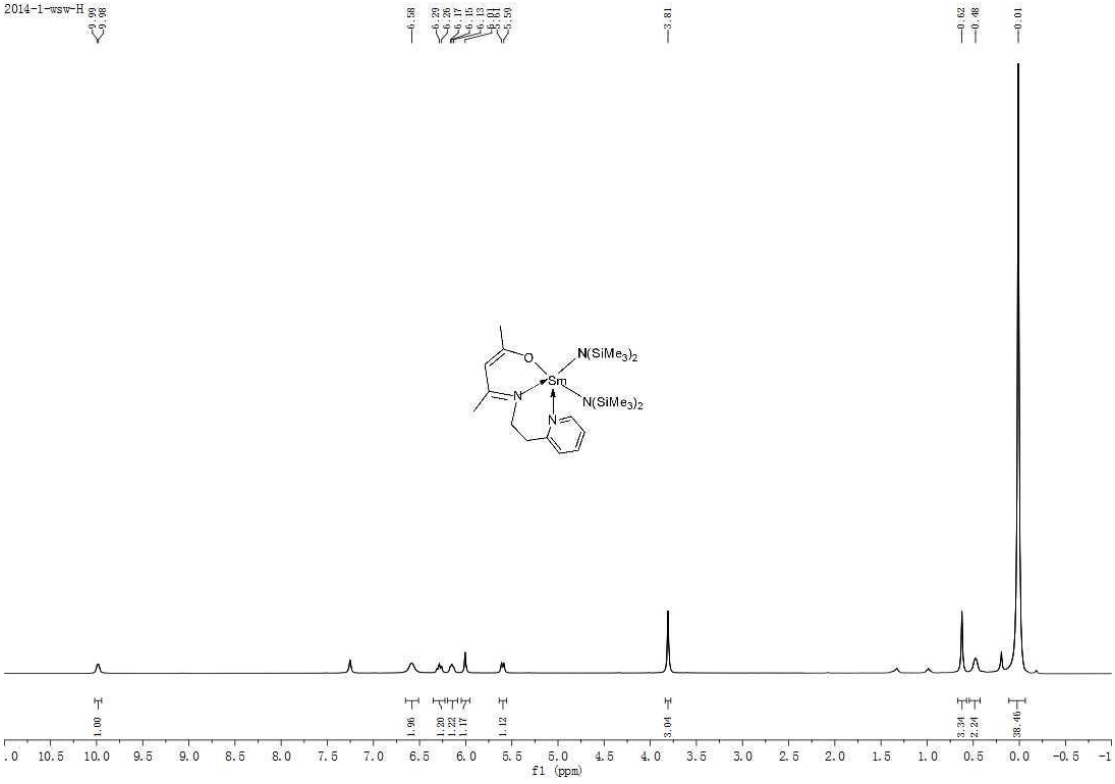

Fig. S3. ^{1}H NMR spectrum (500 MHz, C_6D_6, 298 K) of complex **4**.

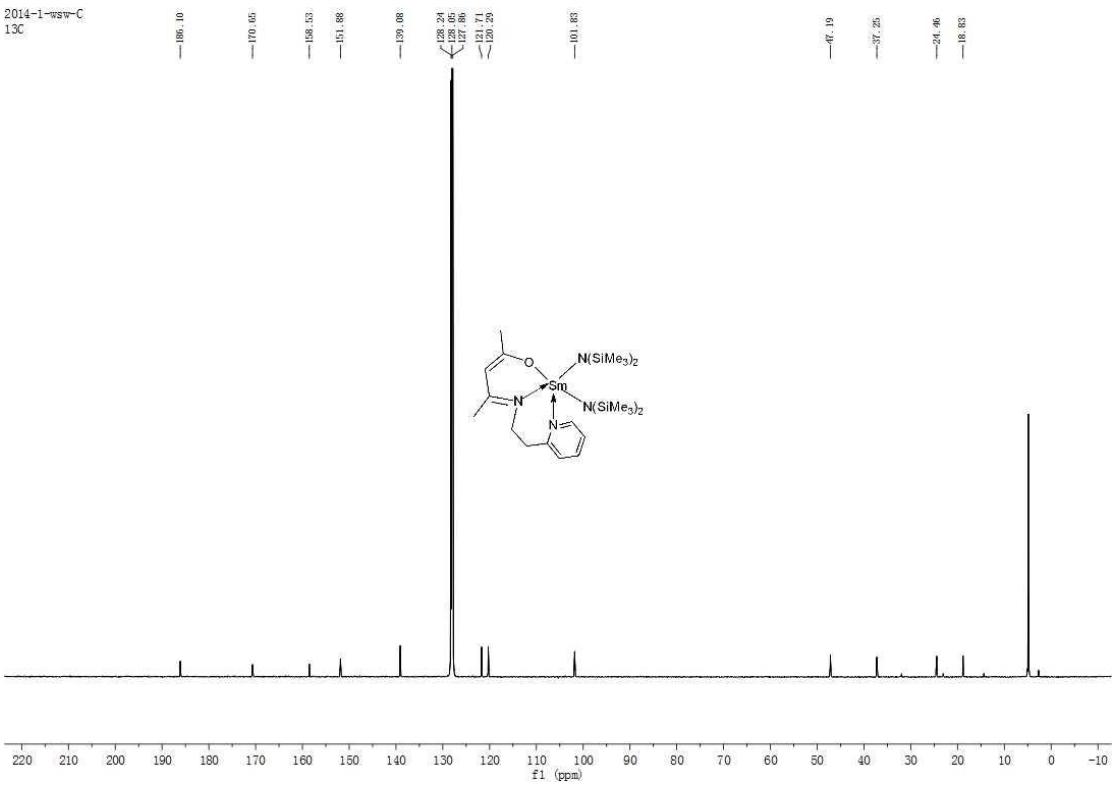

Fig. S4. ^{13}C NMR spectrum (126 MHz, C_6D_6, 298 K) of complex **4**.

3. Molecular structures of the complexes 2-8.

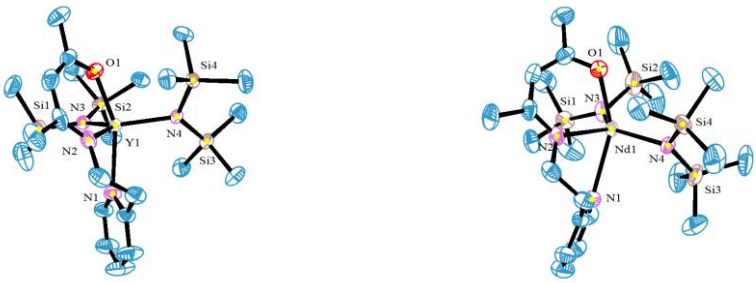

Fig. S5. Crystal structure of complexes **2-3** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity.

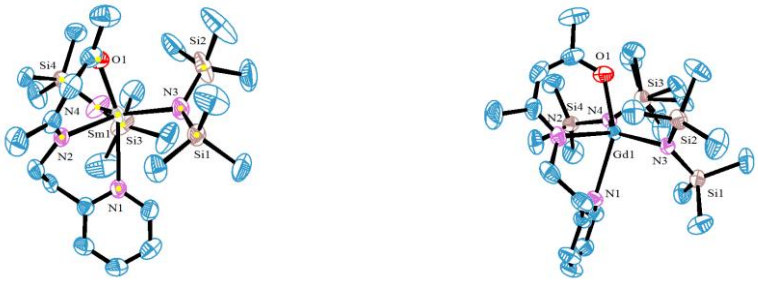

Fig. S6. Crystal structure of complexes **4-5** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity.

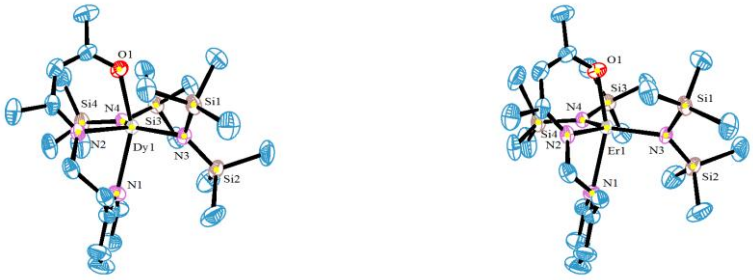

Fig. S7. Crystal structure of complexes **6-7** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity.

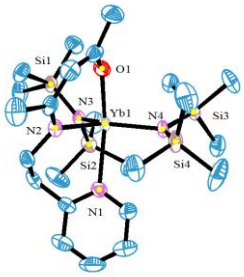

Fig. S8. Crystal structure of complex **8** (Ellipsoids at 30% probability level). Hydrogen atoms were omitted for clarity.

4. Copies of ^{1}H NMR, ^{13}C NMR and ^{13}C-int NMR spectra of PIP.

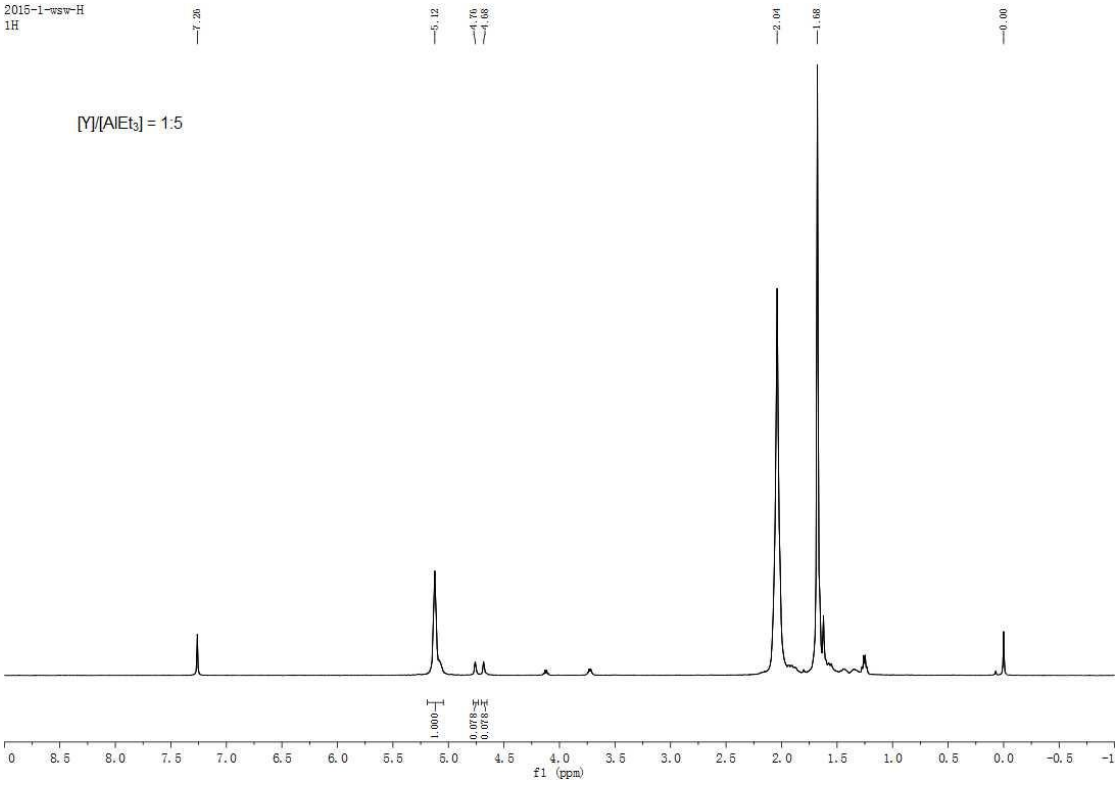

Fig. S9. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of PIP for entry 3 (Table 2)

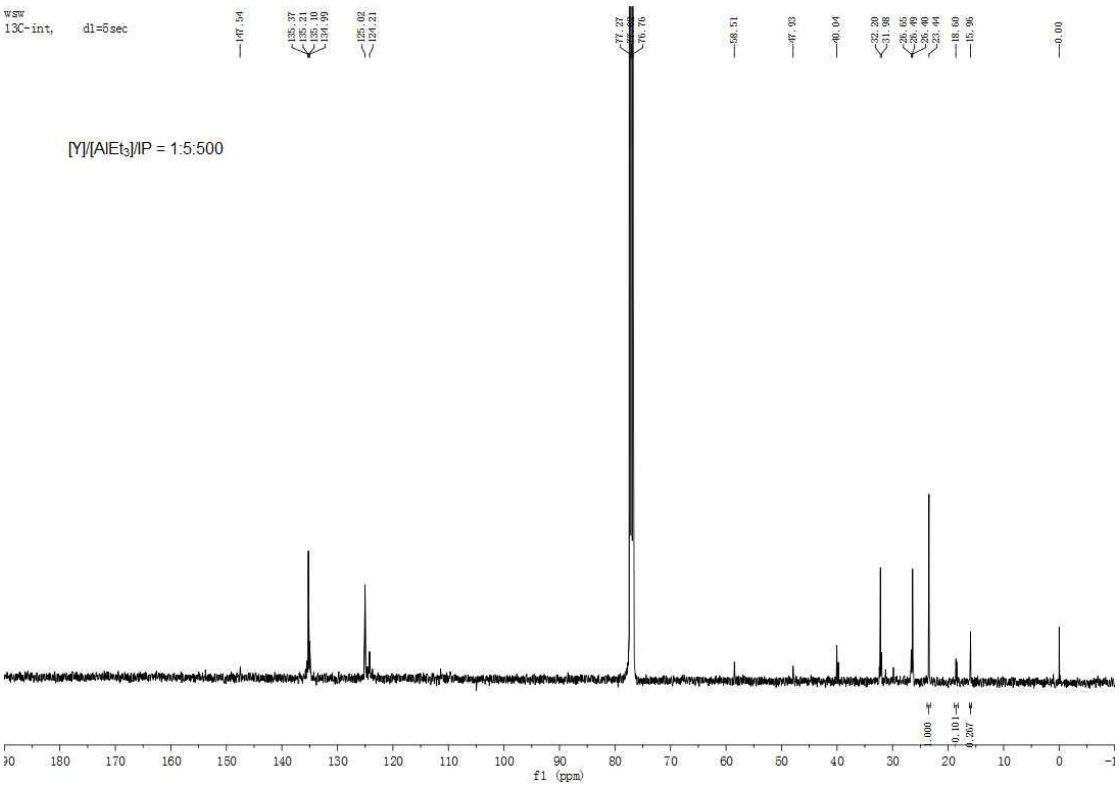

Fig. S10. ^{13}C-int NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 3 (Table 2). Scan 12288 times.

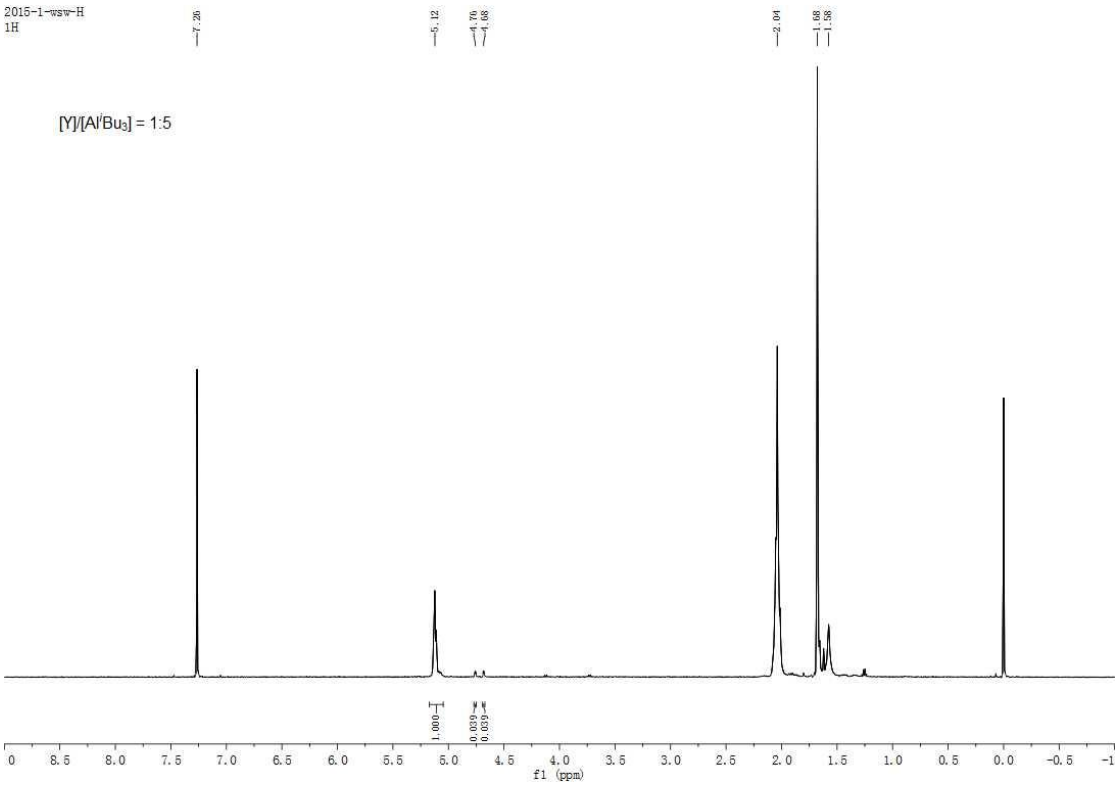

Fig. S11. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 4 (Table 2).

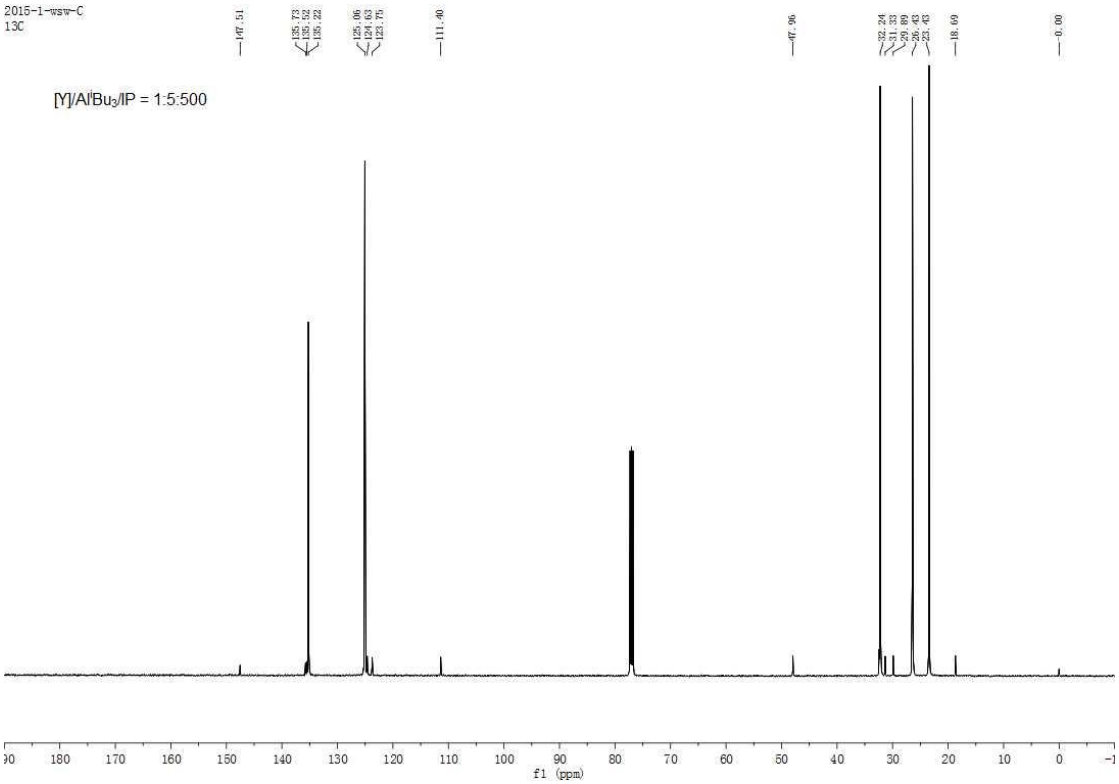

Fig. S12. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 4 (Table 2). Scan 10000 times. No 1, 4-*trans*-polymer.

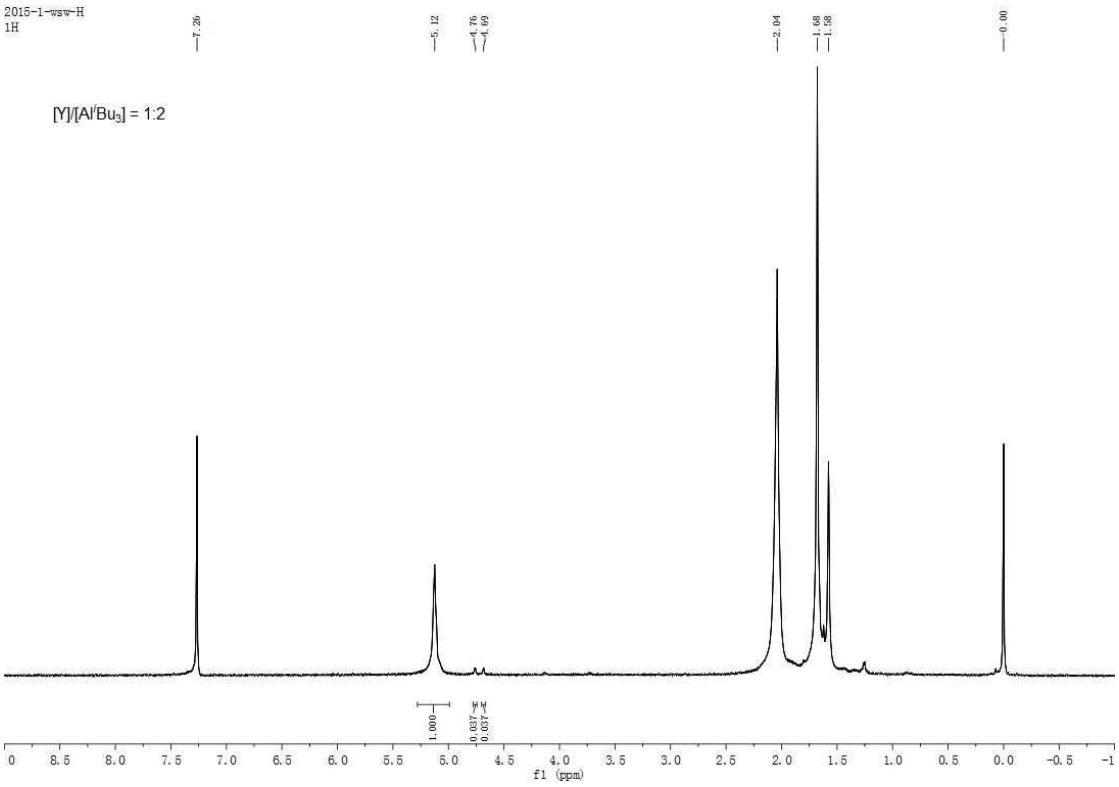

Fig. S13. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 5 (Table 2).

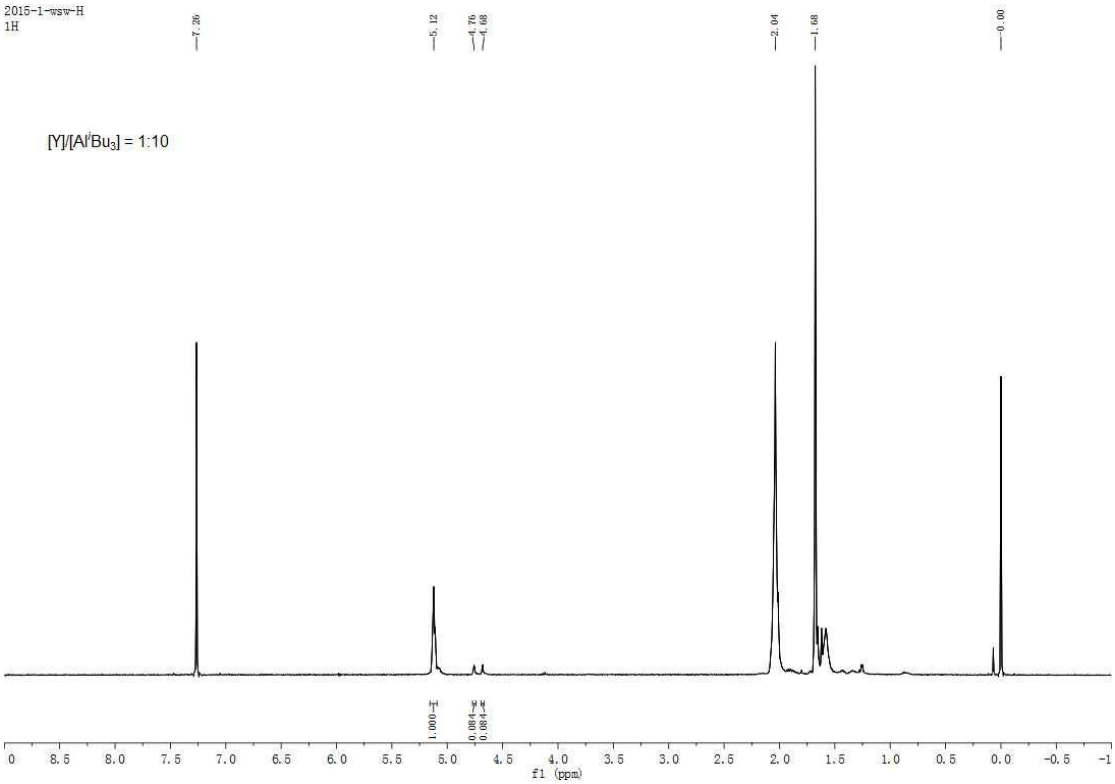

Fig. S14. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 6 (Table 2).

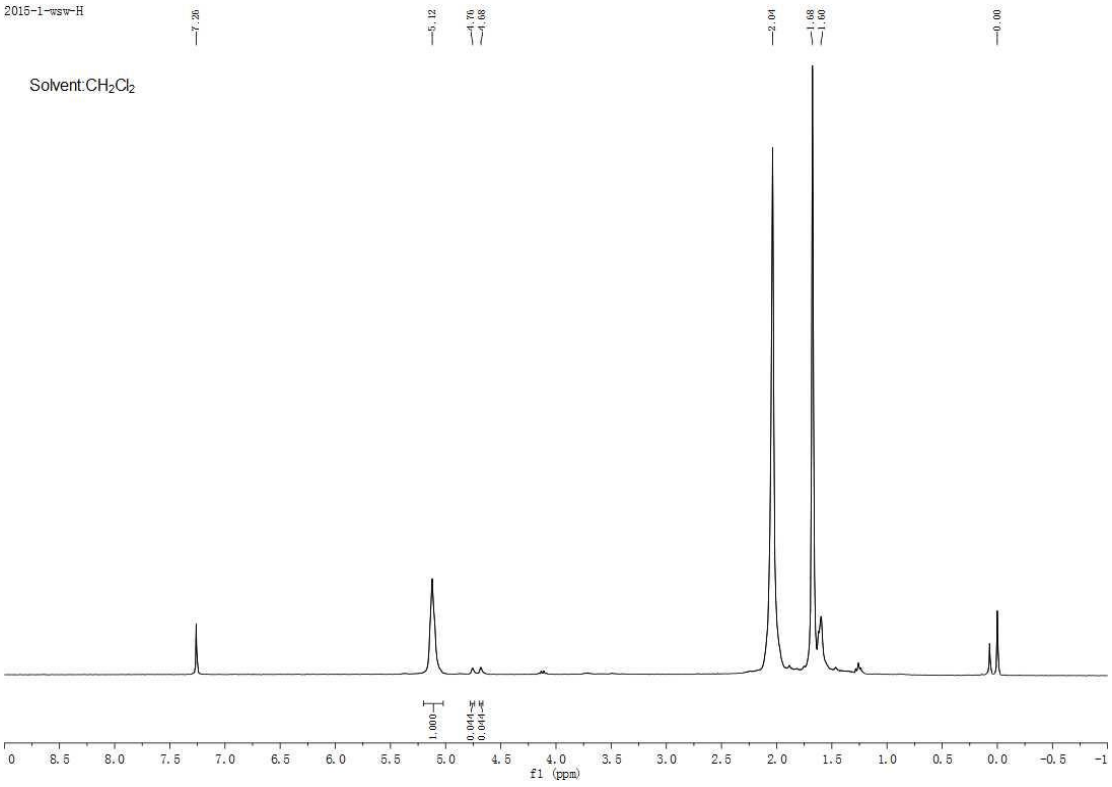

Fig. S15. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 7 (Table 2).

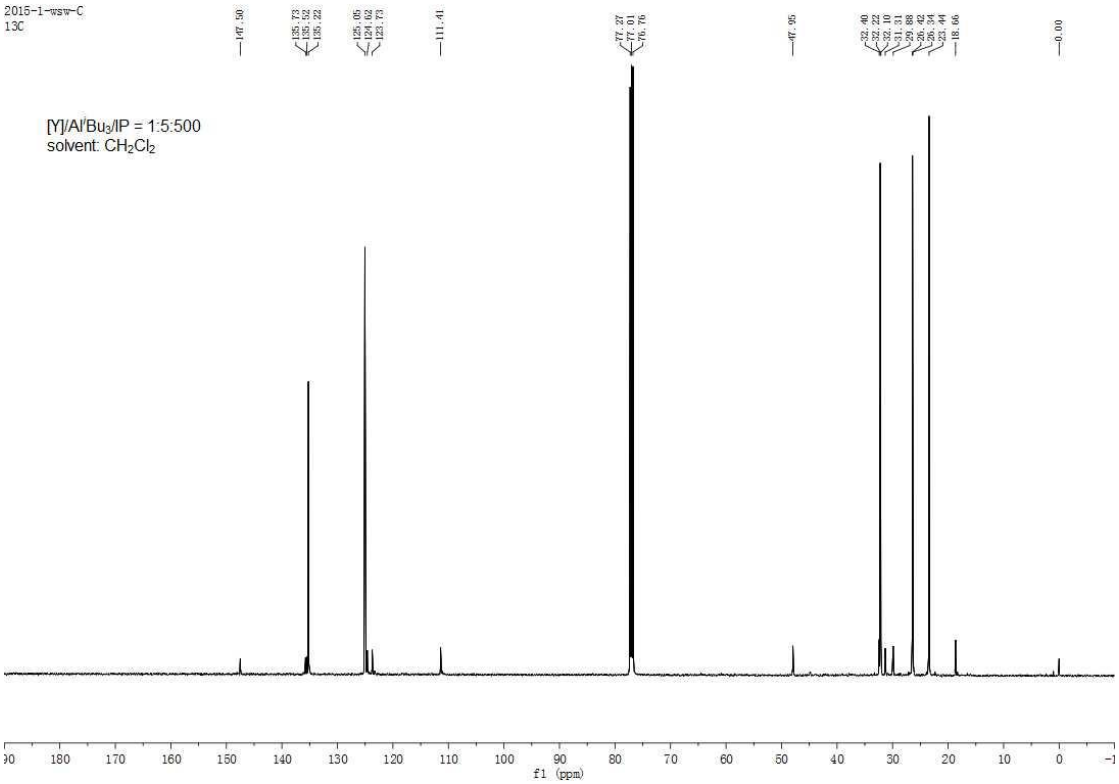

Fig. S16. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 7 (Table 2). Scan 10000 times. No 1, 4-*trans*-polymer.

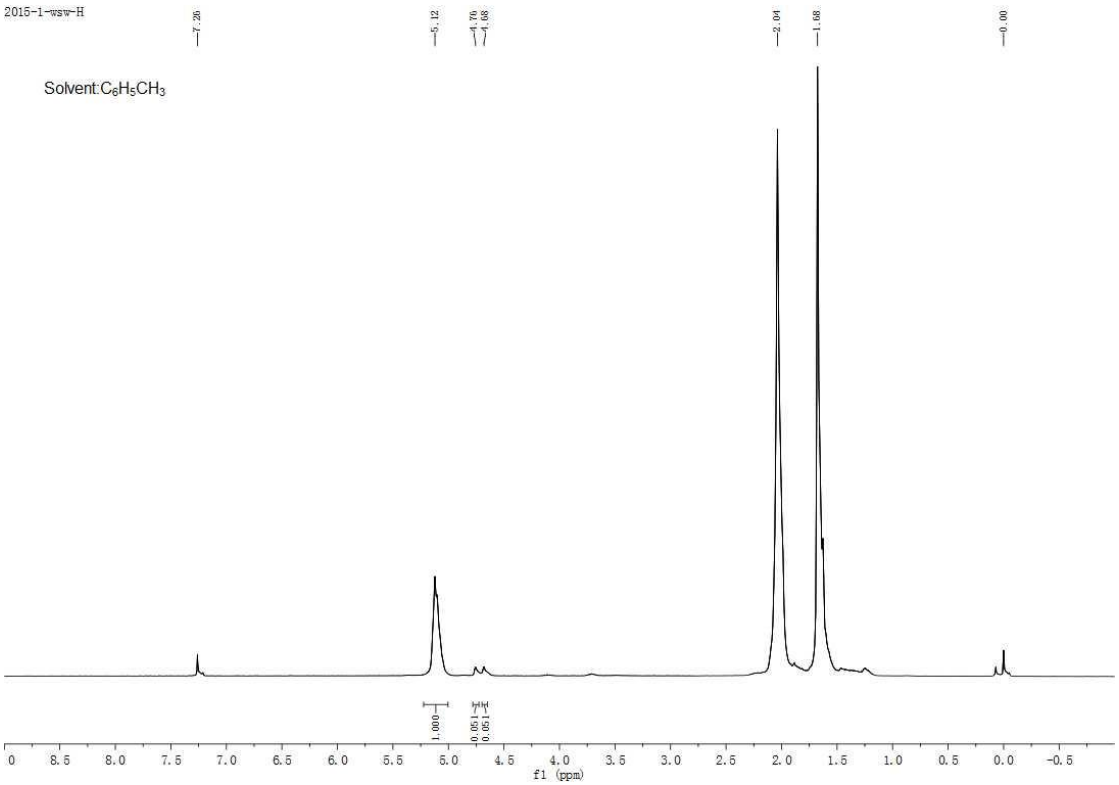

Fig. S17. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 8 (Table 2).

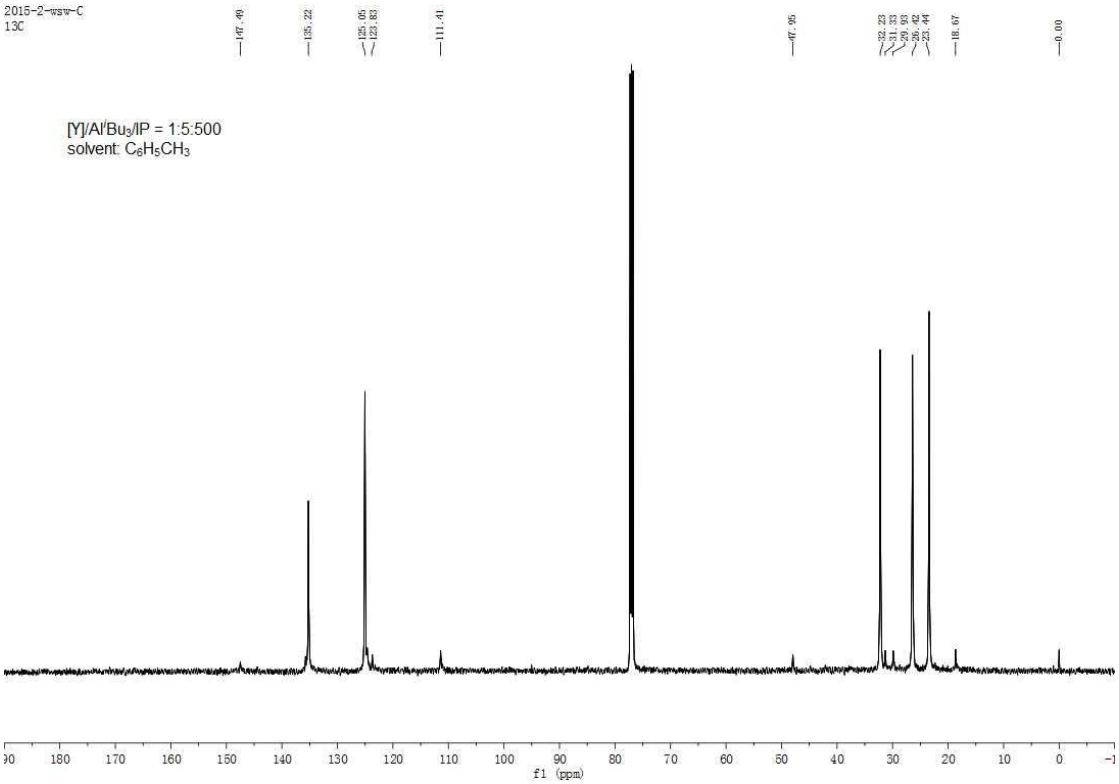

Fig. S18. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 8 (Table 2). Scan 10000 times. No 1, 4-*trans*-polymer.

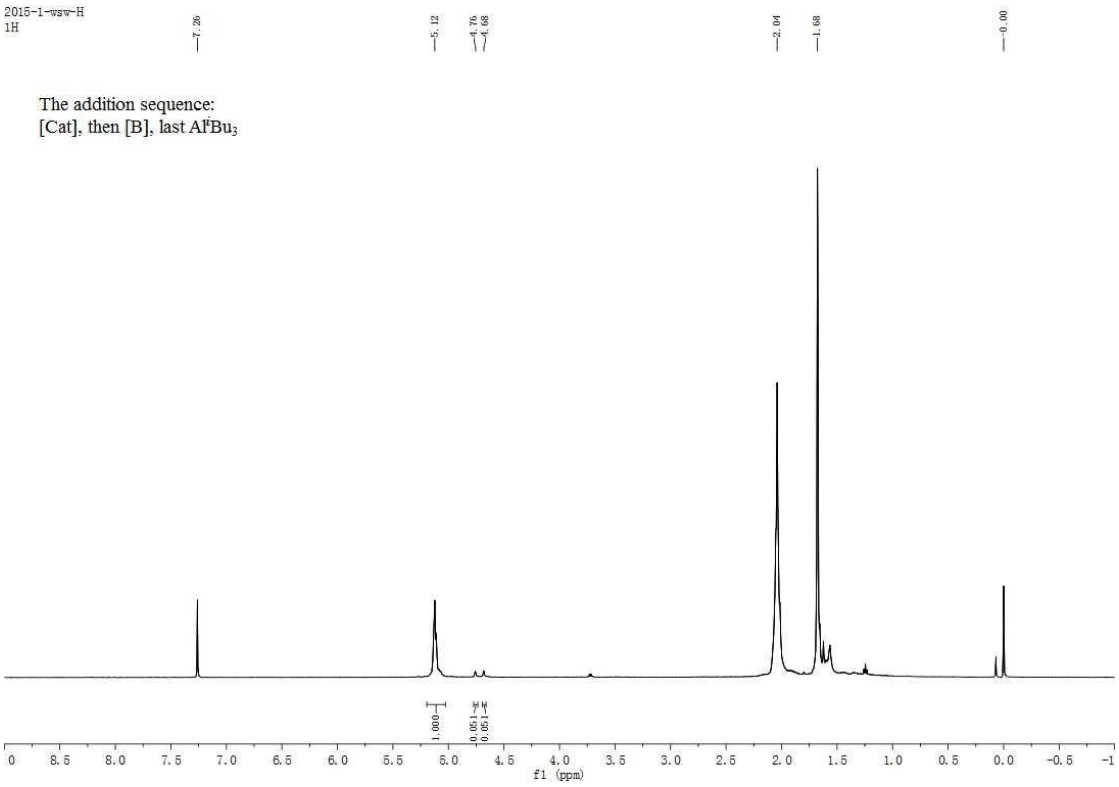

Fig. S19. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 9 (Table 2).

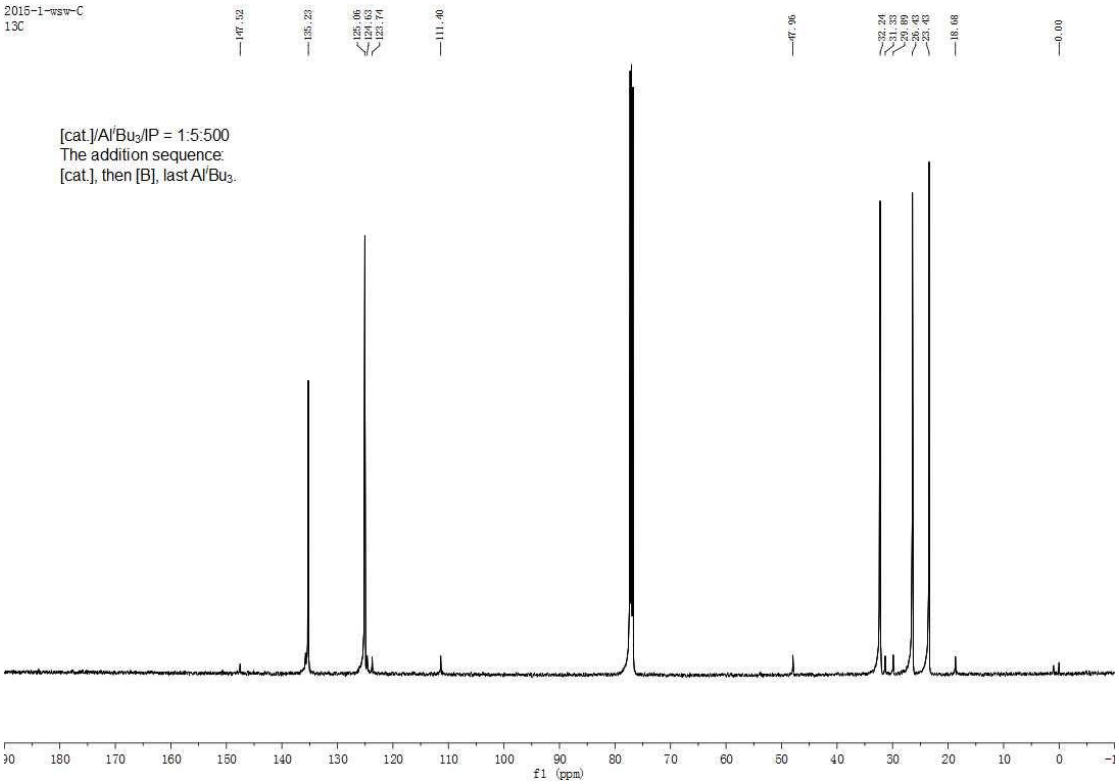

Fig. S20. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 9 (Table 2). Scan 10000 times. No 1, 4-*trans*-polymer.

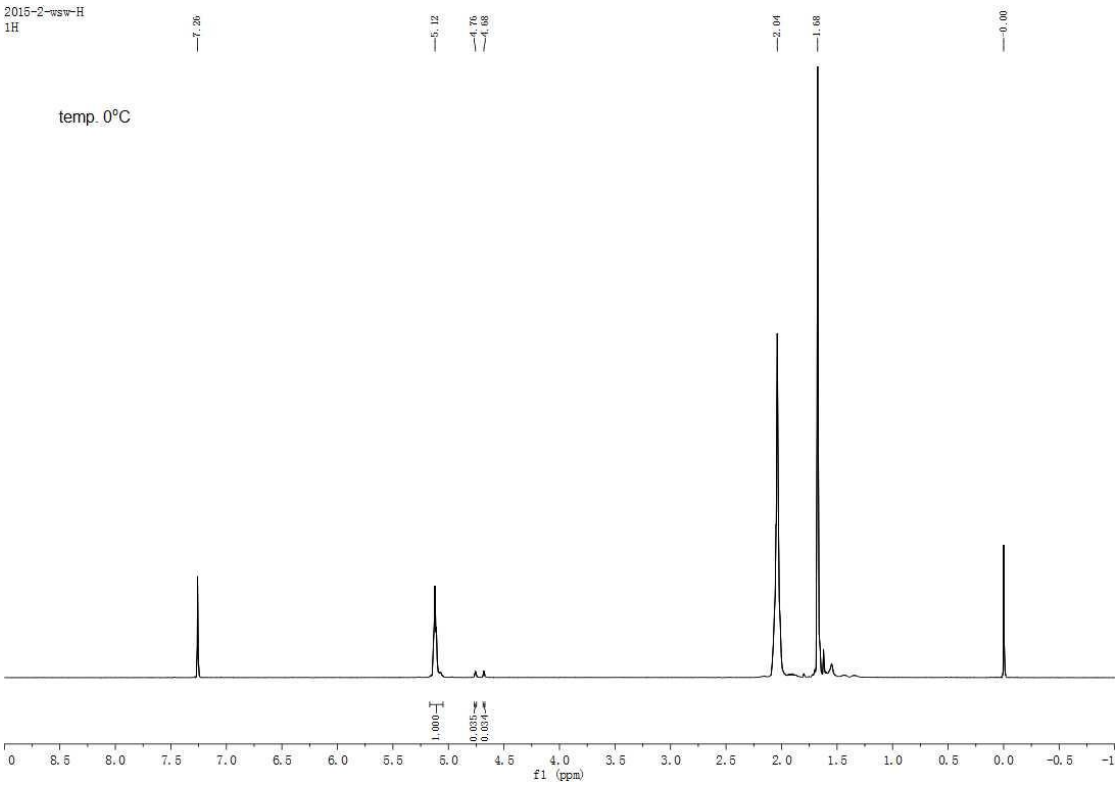

Fig. S21. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 10 (Table 2).

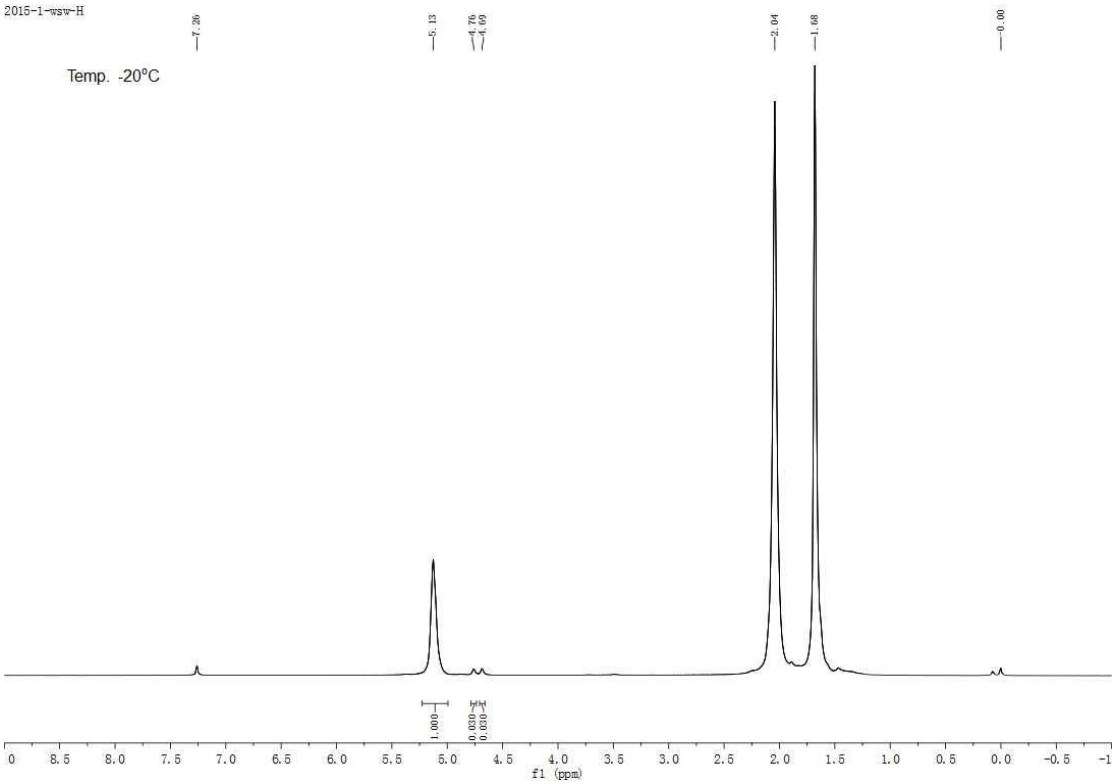

Fig. S22. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 11 (Table 2).

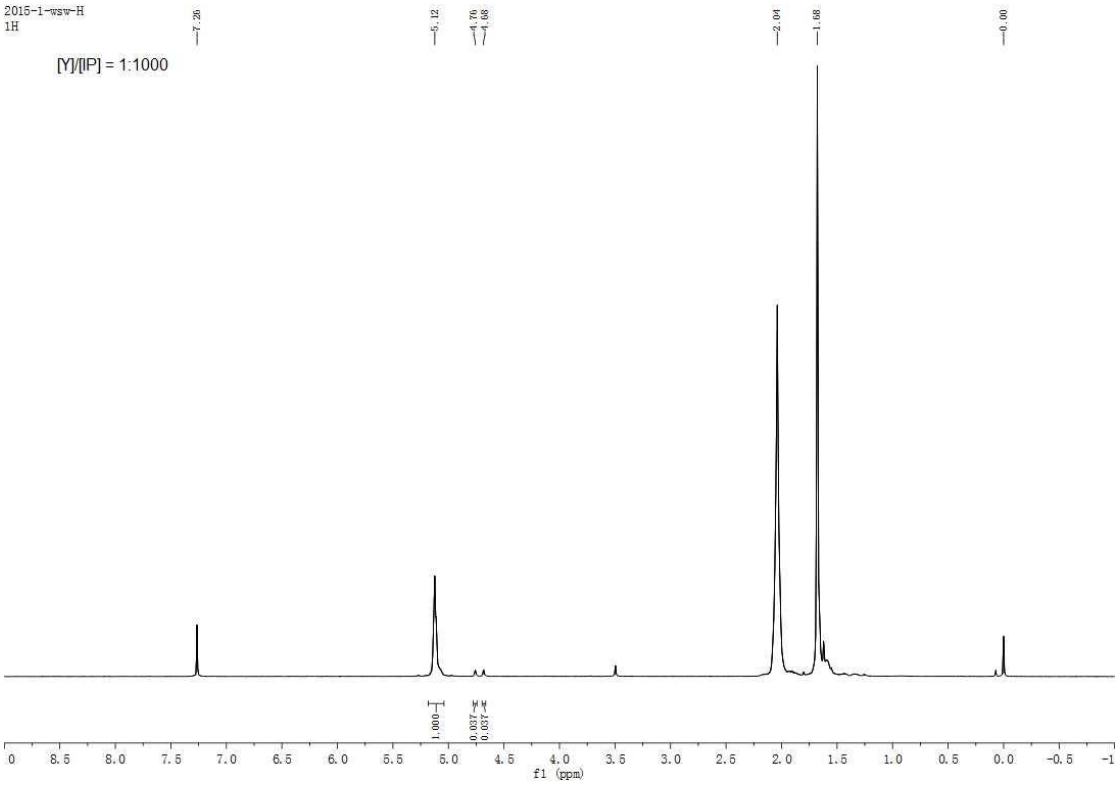

Fig. S23. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 12 (Table 2).

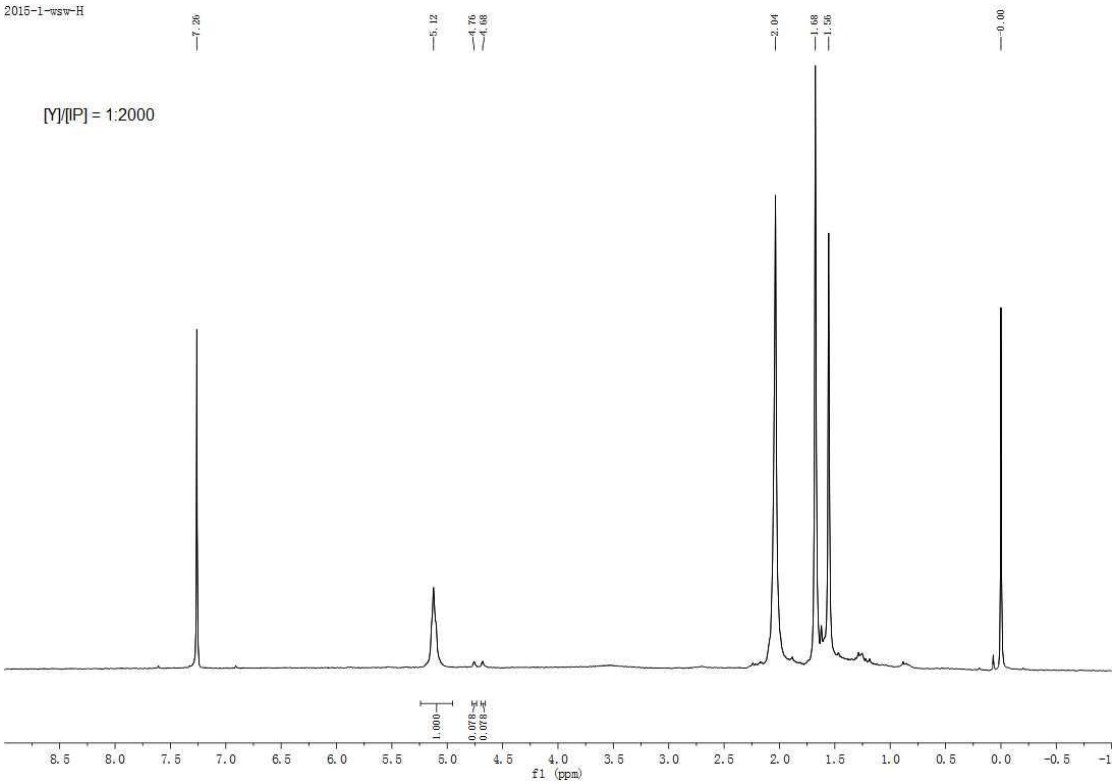

Fig. S24. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 13 (Table 2).

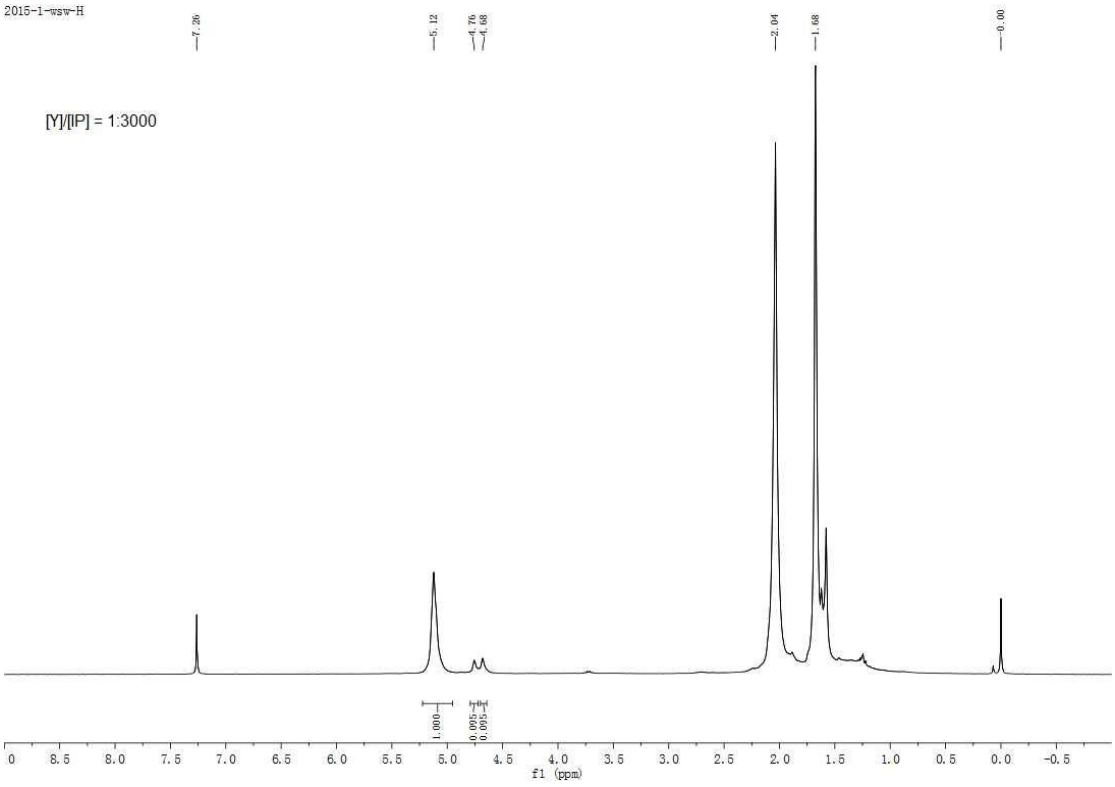

Fig. S25. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 14 (Table 2).

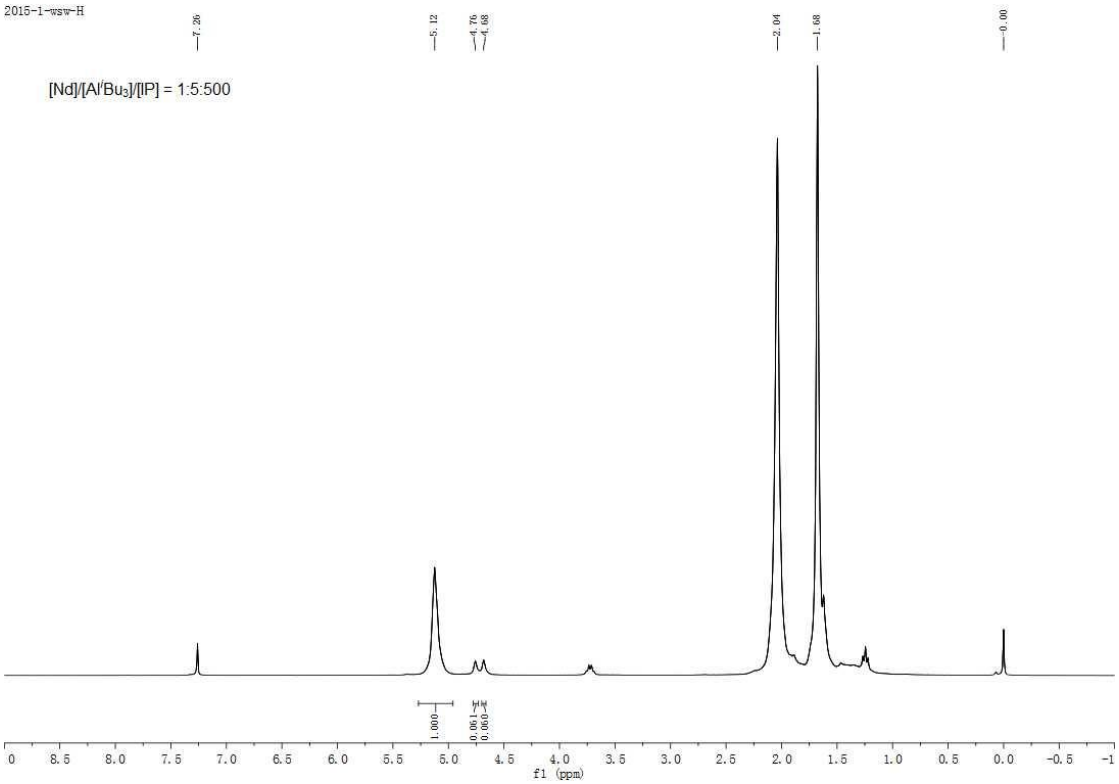

Fig. S26. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 2 (Table 3).

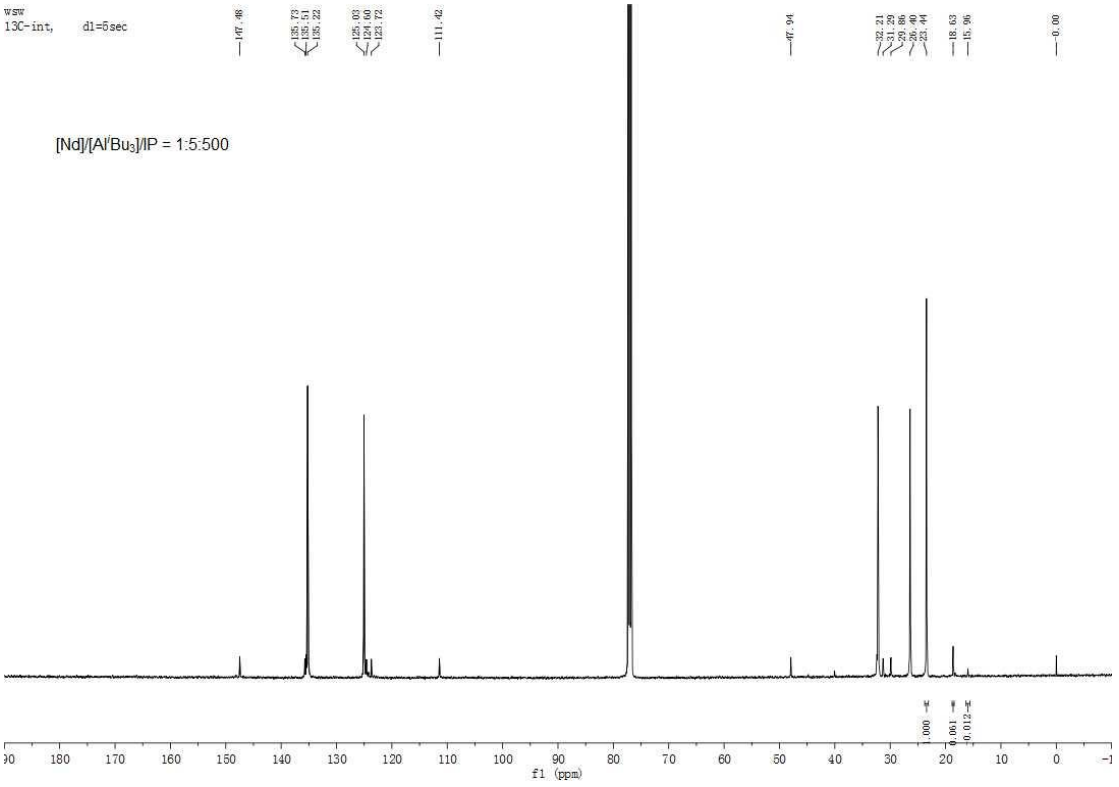

Fig. S27. ^{13}C-int NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 2 (Table 3). Scan 12288 times.

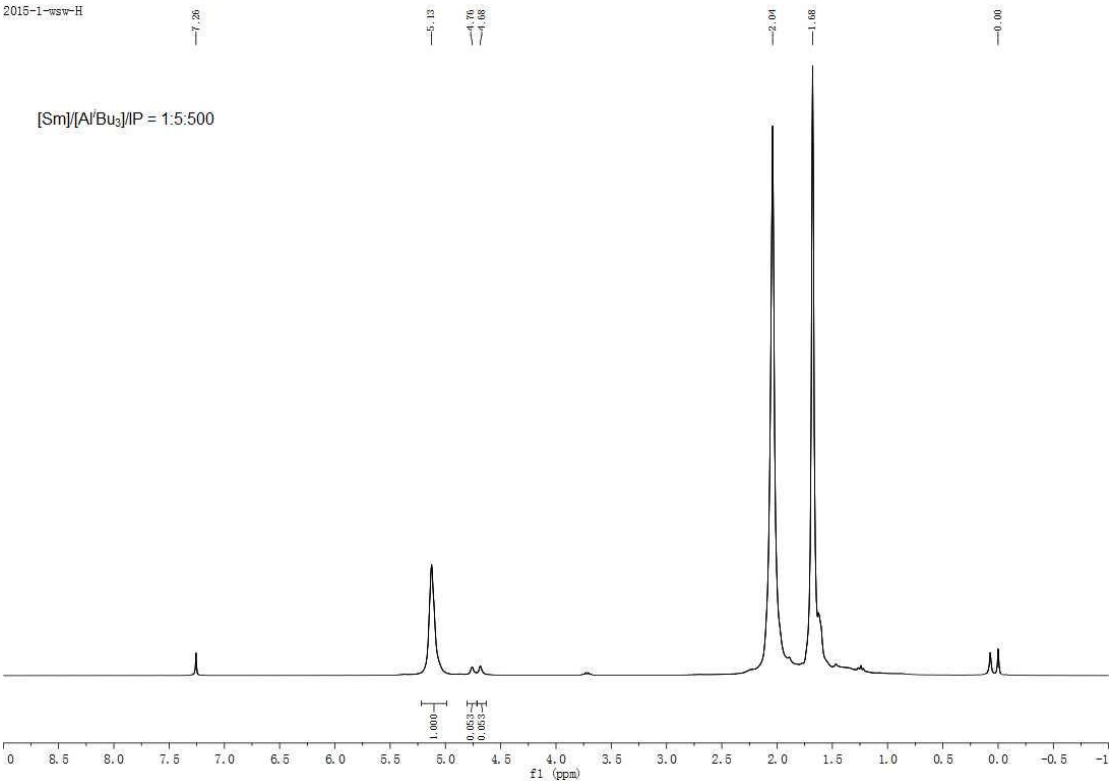

Fig. S28. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 3 (Table 3).

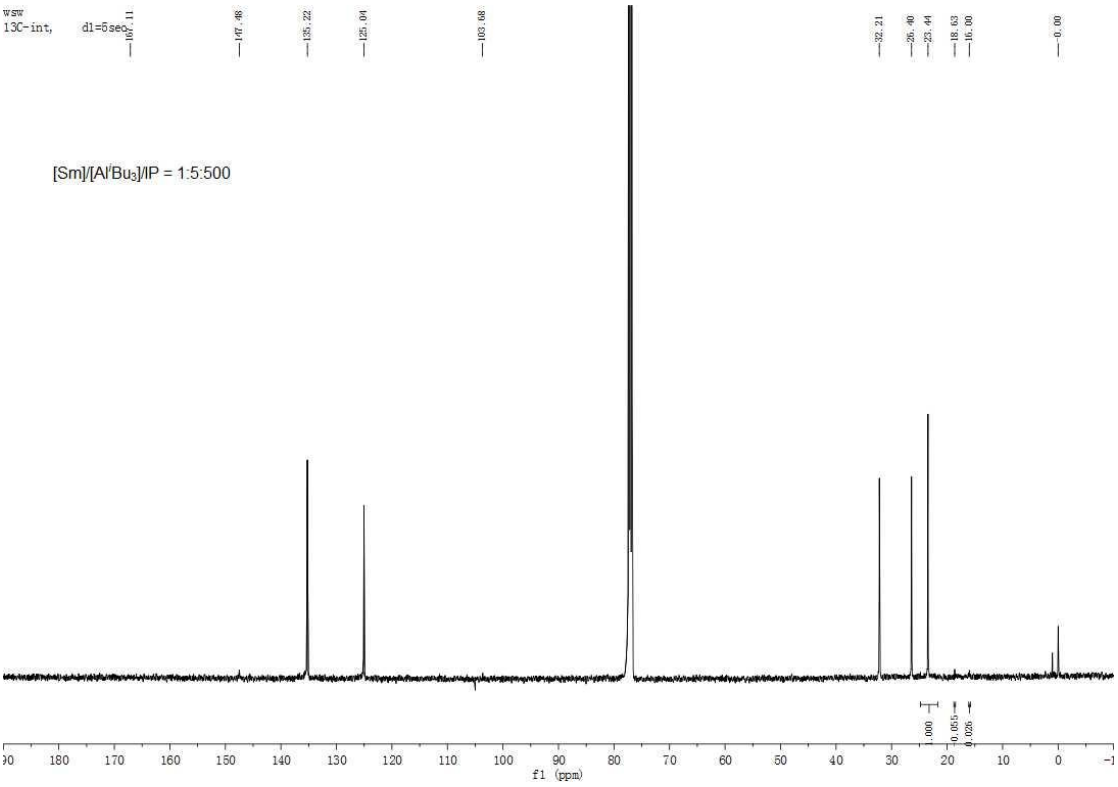

Fig. S29. ^{13}C-int NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 3 (Table 3). Scan 5570 times.

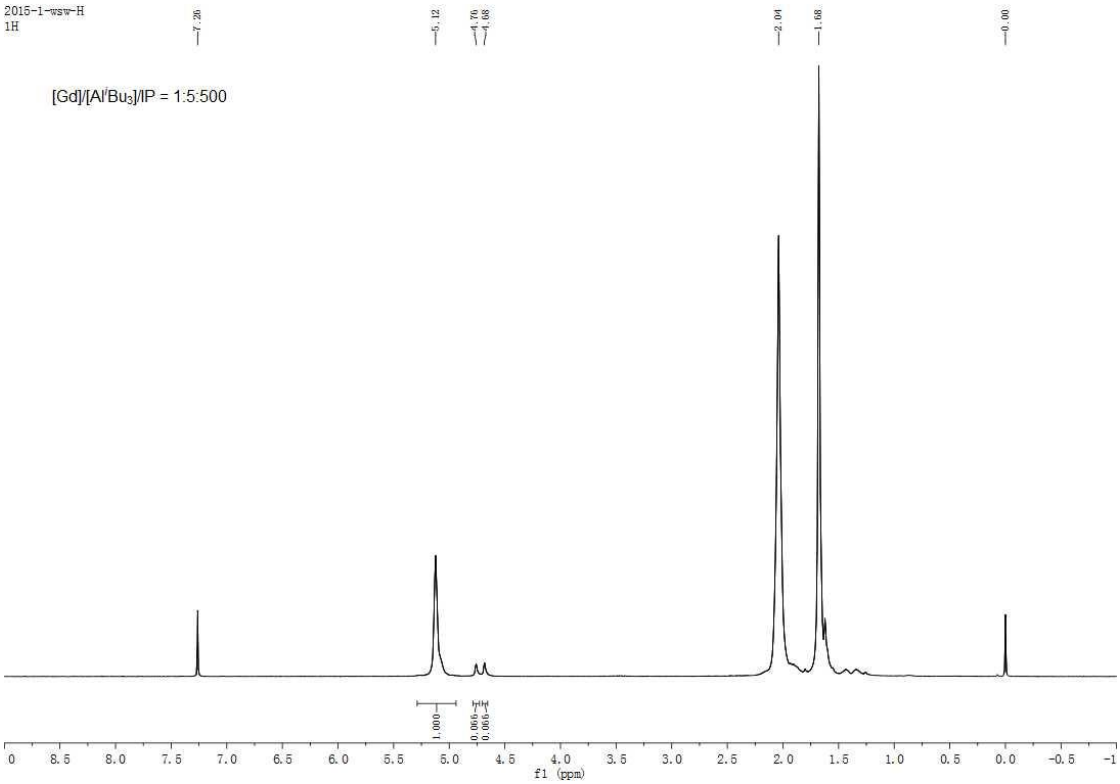

Fig. S30. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 4 (Table 3).

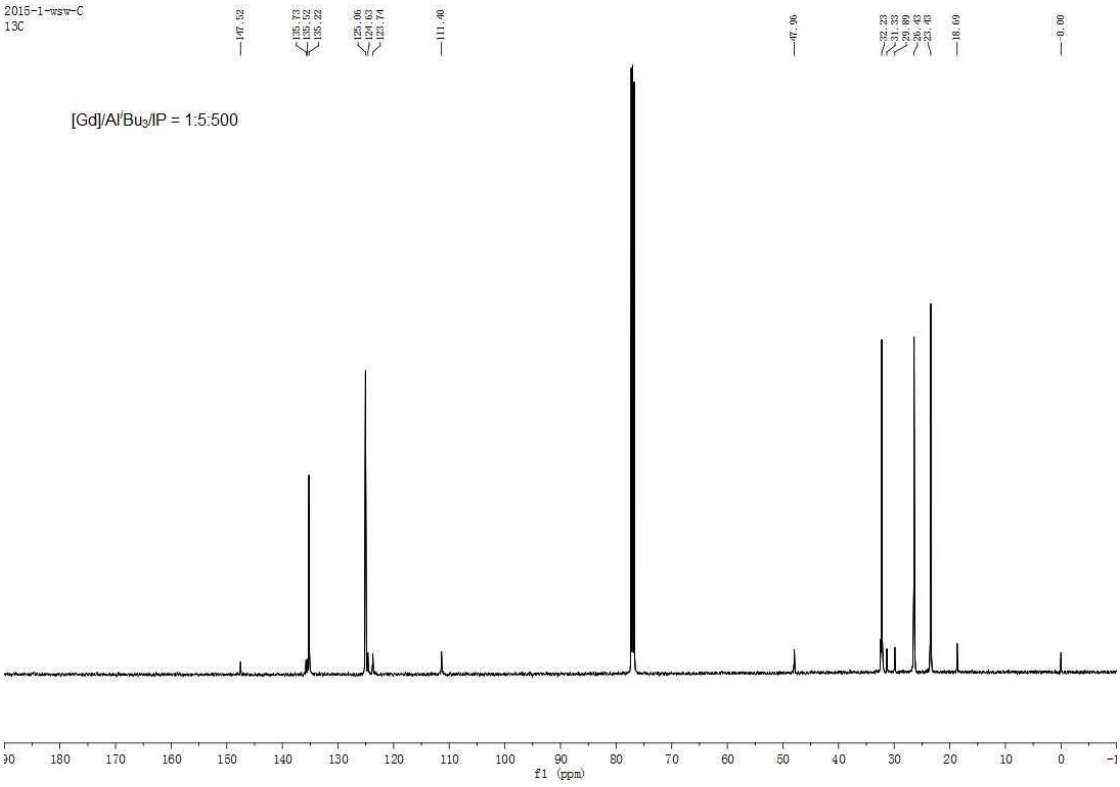

Fig. S31. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 4 (Table 3). Scan 3000 times. No 1, 4-*trans*-polymer.

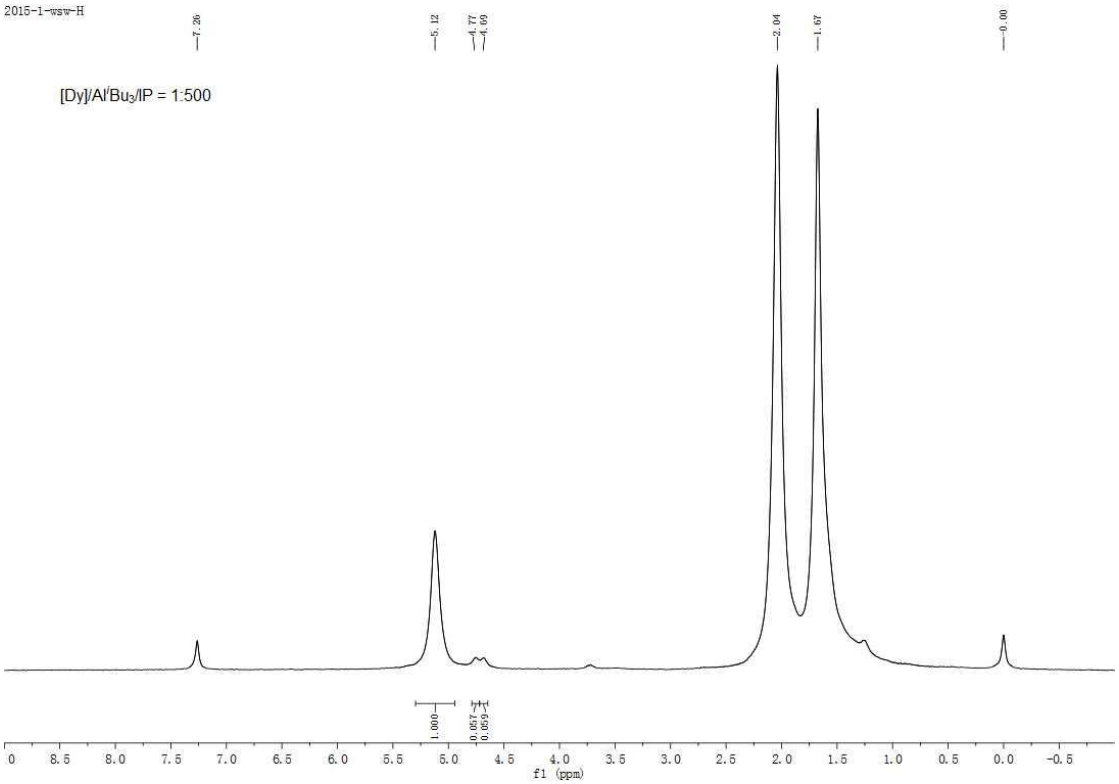

Fig. S32. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 5 (Table 3).

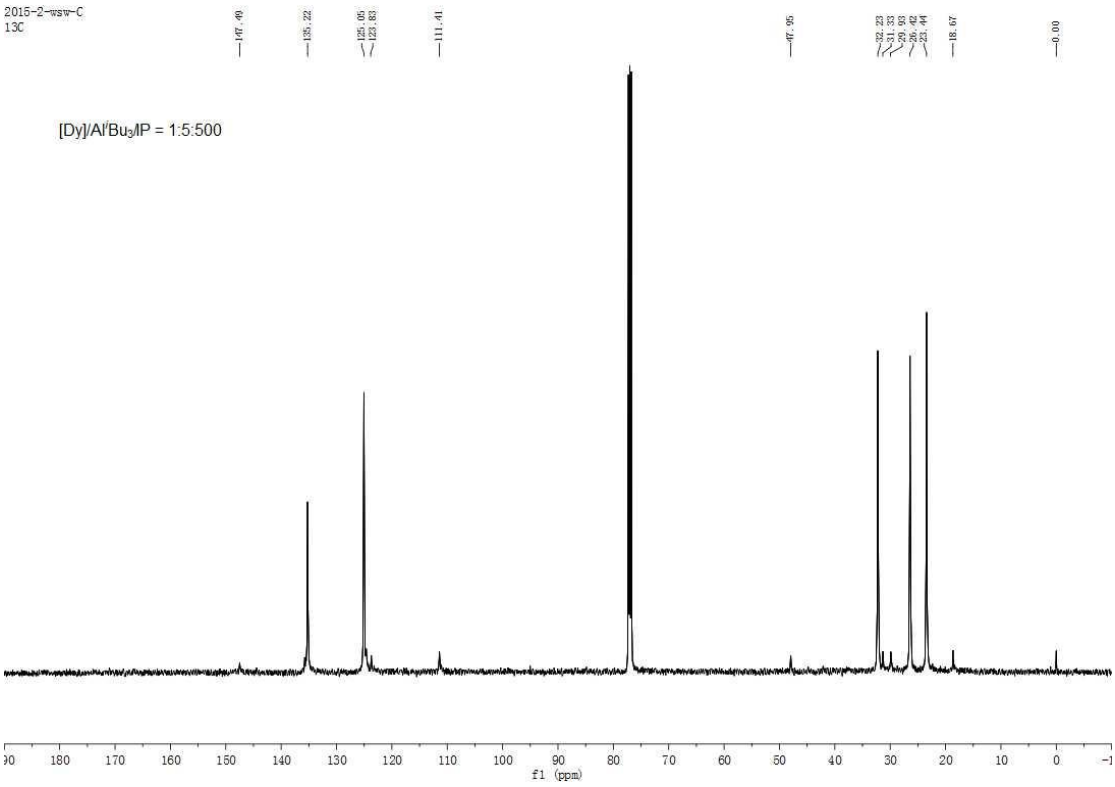

Fig. S33. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 5 (Table 3). Scan 10240 times. No 1, 4-*trans*-polymer.

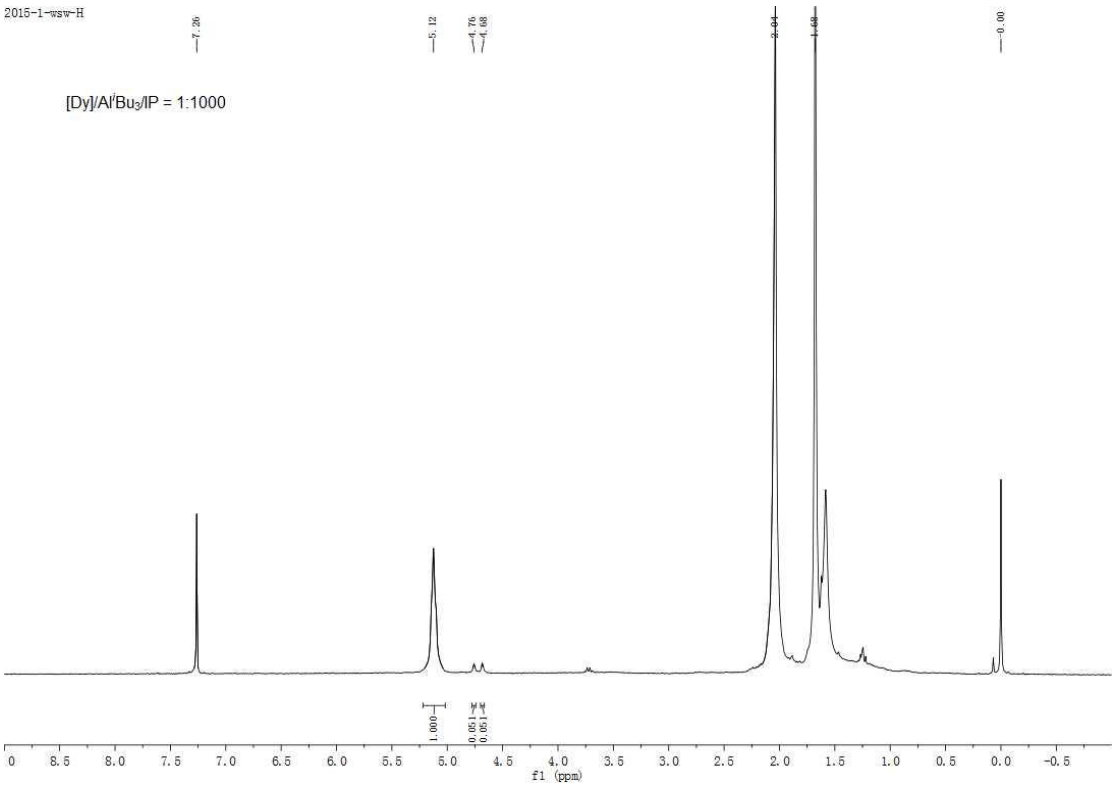

Fig. S34. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 6 (Table 3).

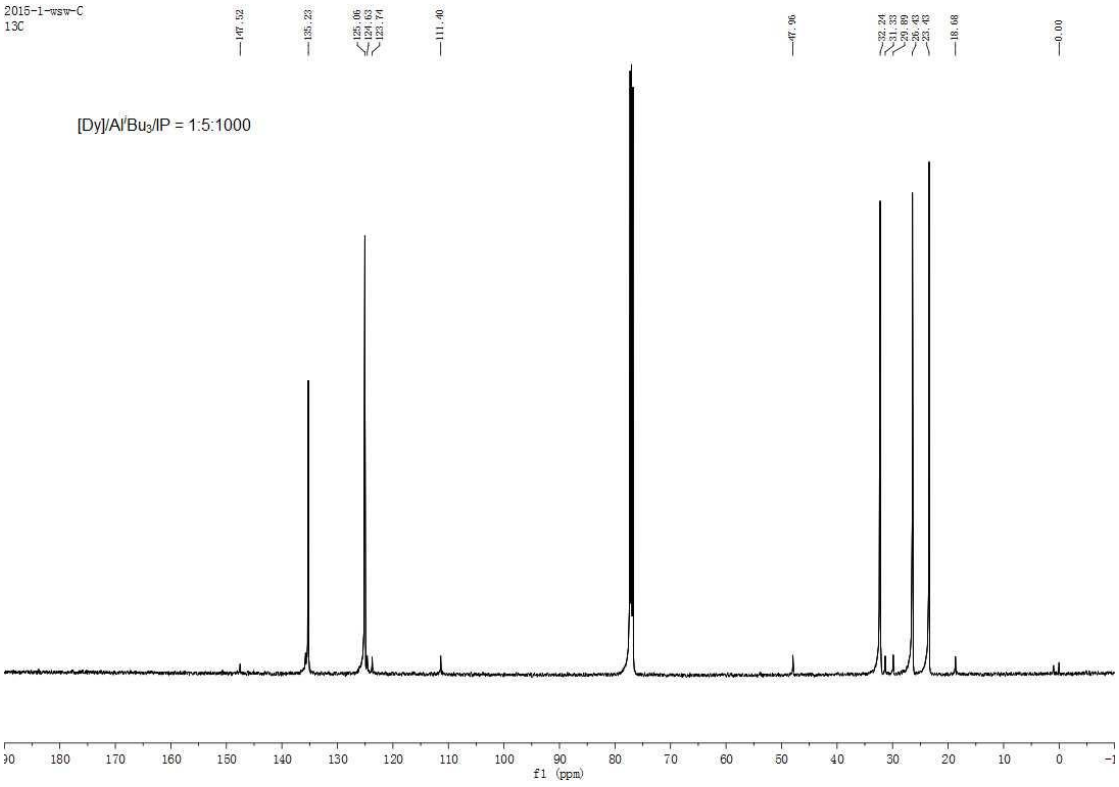

Fig. S35. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 6 (Table 3). Scan 8000 times. No 1, 4-*trans*-polymer.

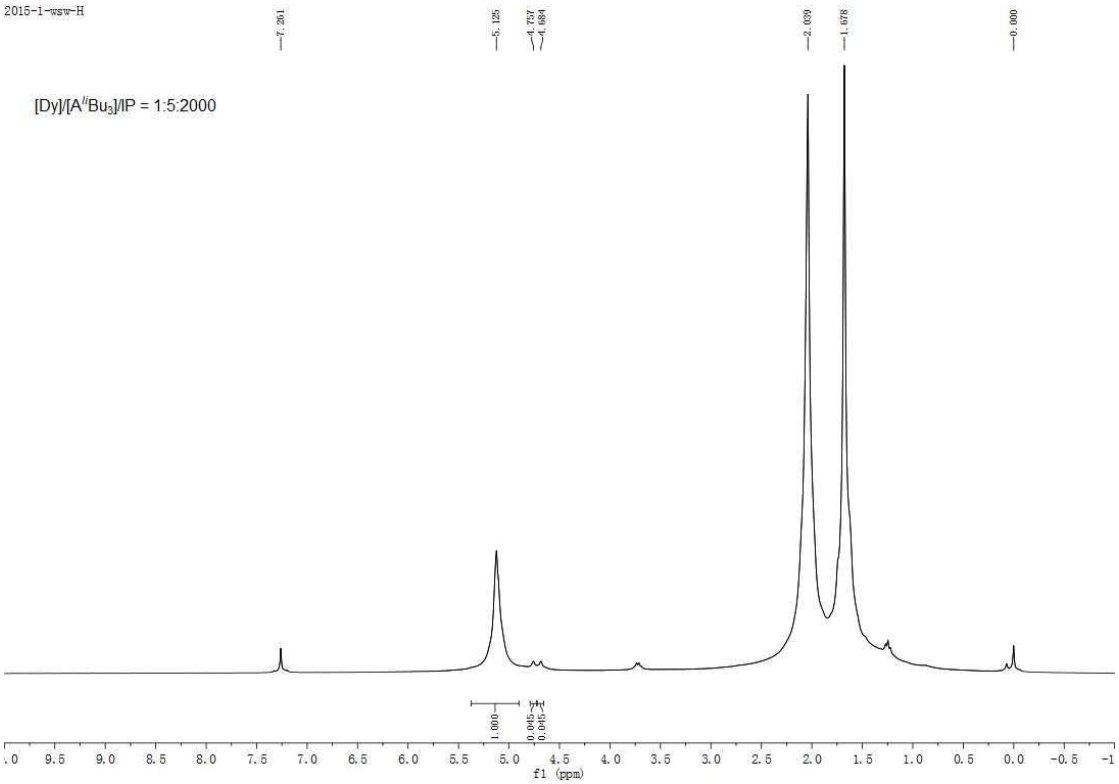

Fig. S36. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 7 (Table 3).

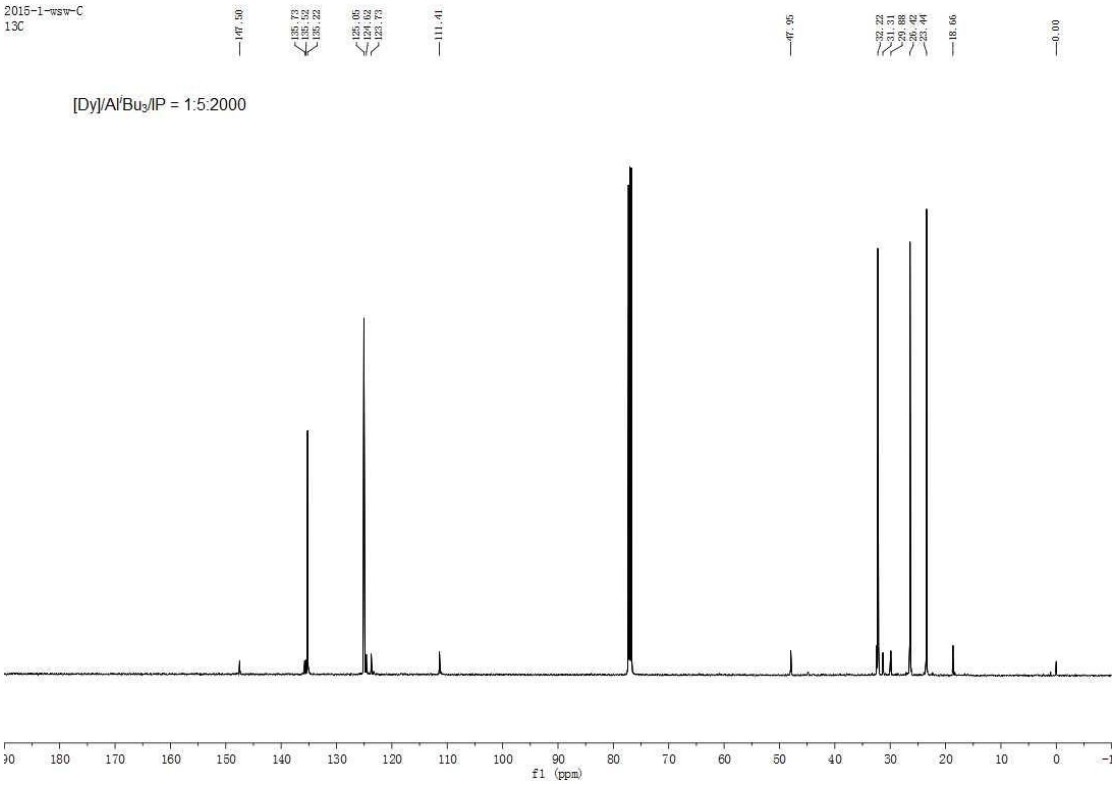

Fig. S37. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 7 (Table 3). Scan 10000 times. No 1, 4-*trans*-polymer.

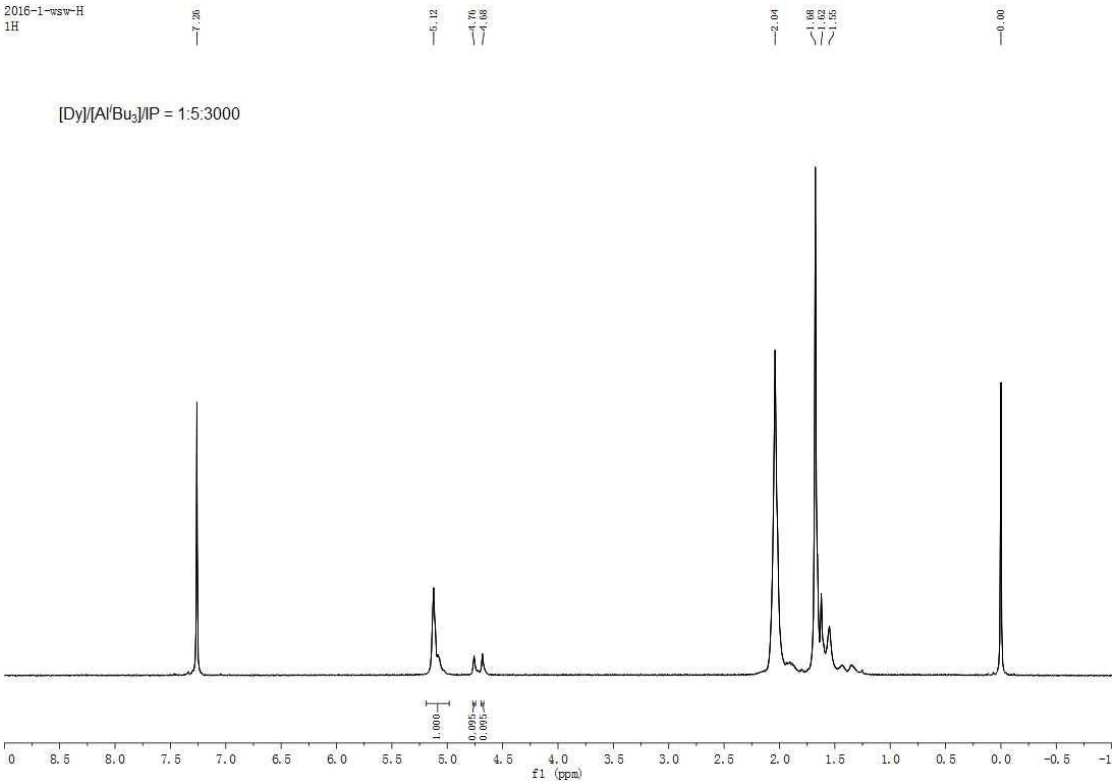

Fig. S38. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 8 (Table 3).

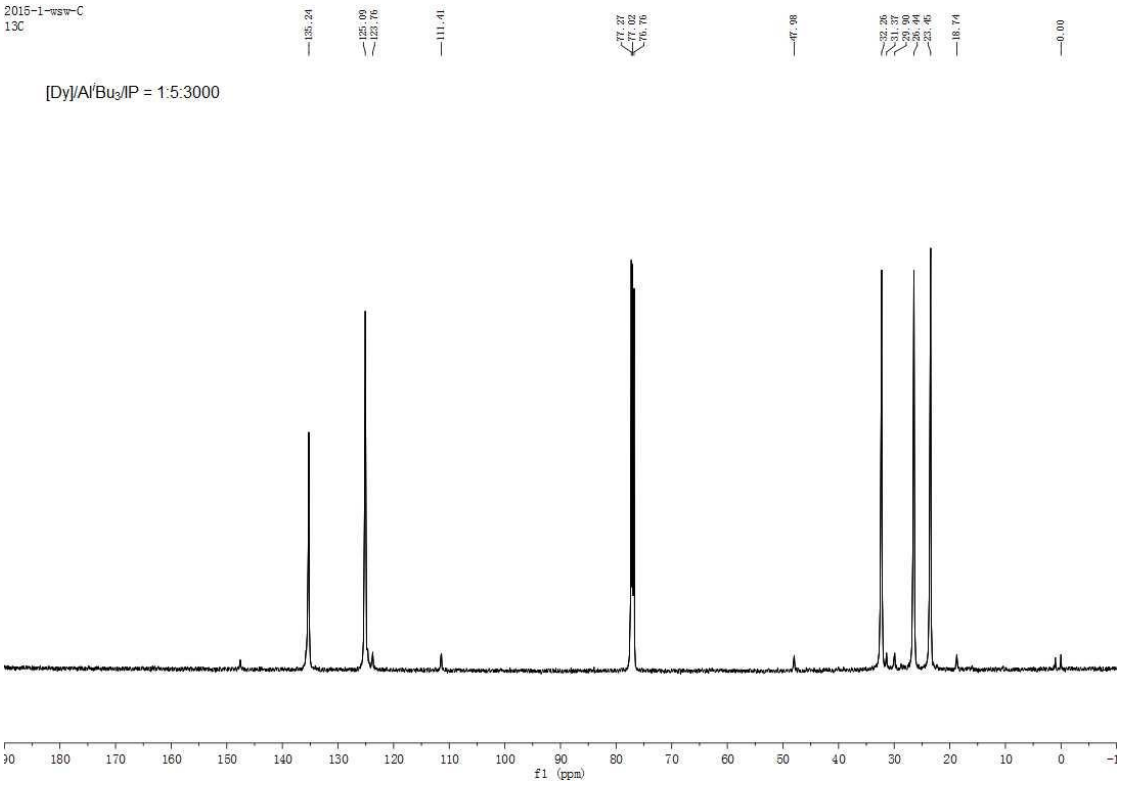

Fig. S39. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 8 (Table 3). Scan 10000 times. No 1, 4-*trans*-polymer.

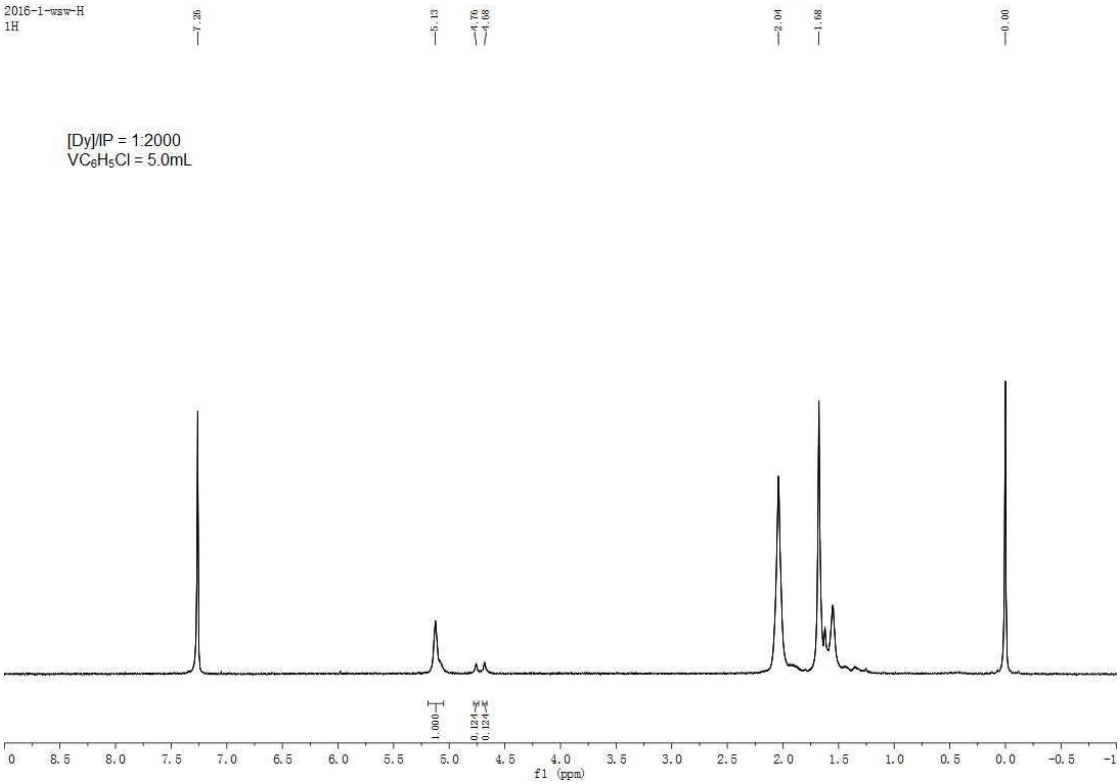

Fig. S40. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 9 (Table 3).

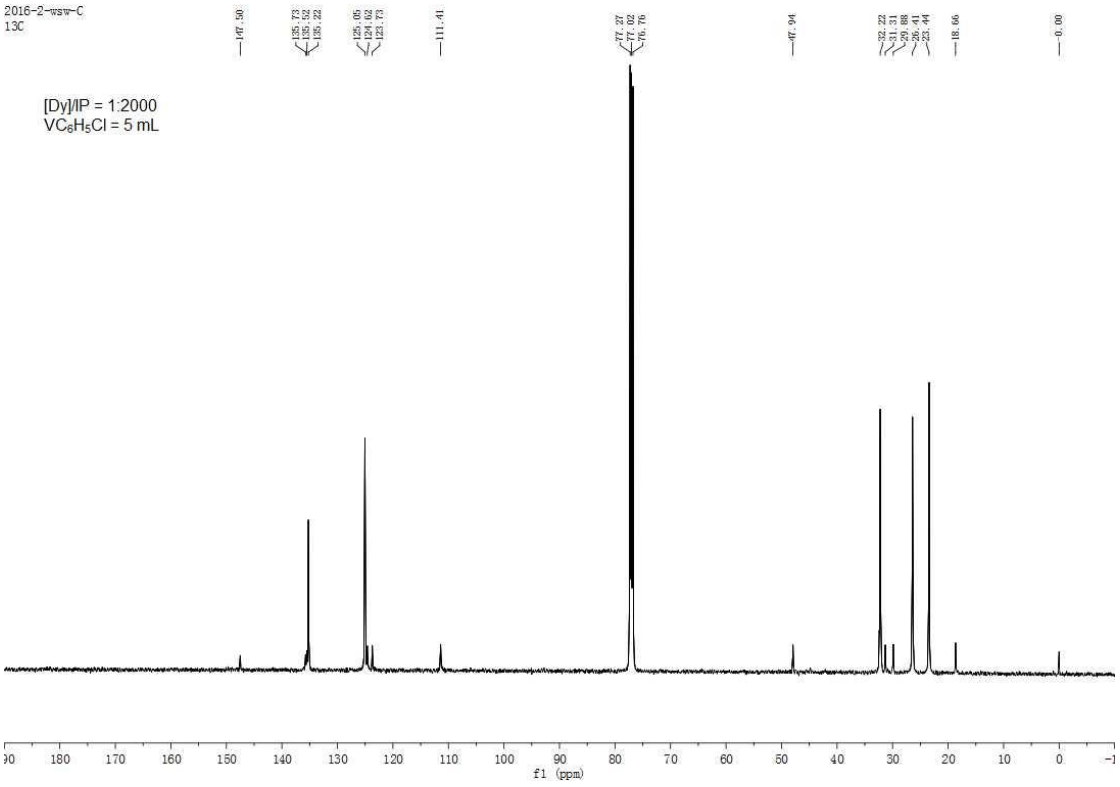

Fig. S41. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 9 (Table 3). Scan 10240 times. No 1, 4-*trans*-polymer.

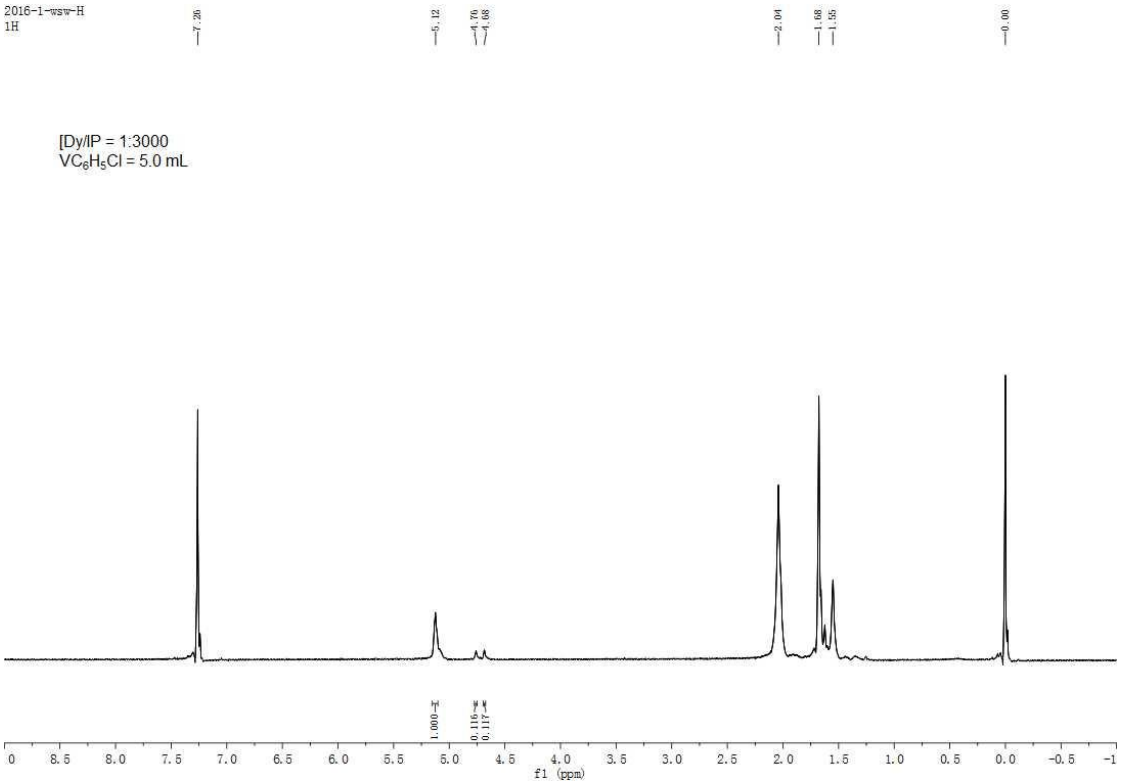

Fig. S42. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 10 (Table 3).

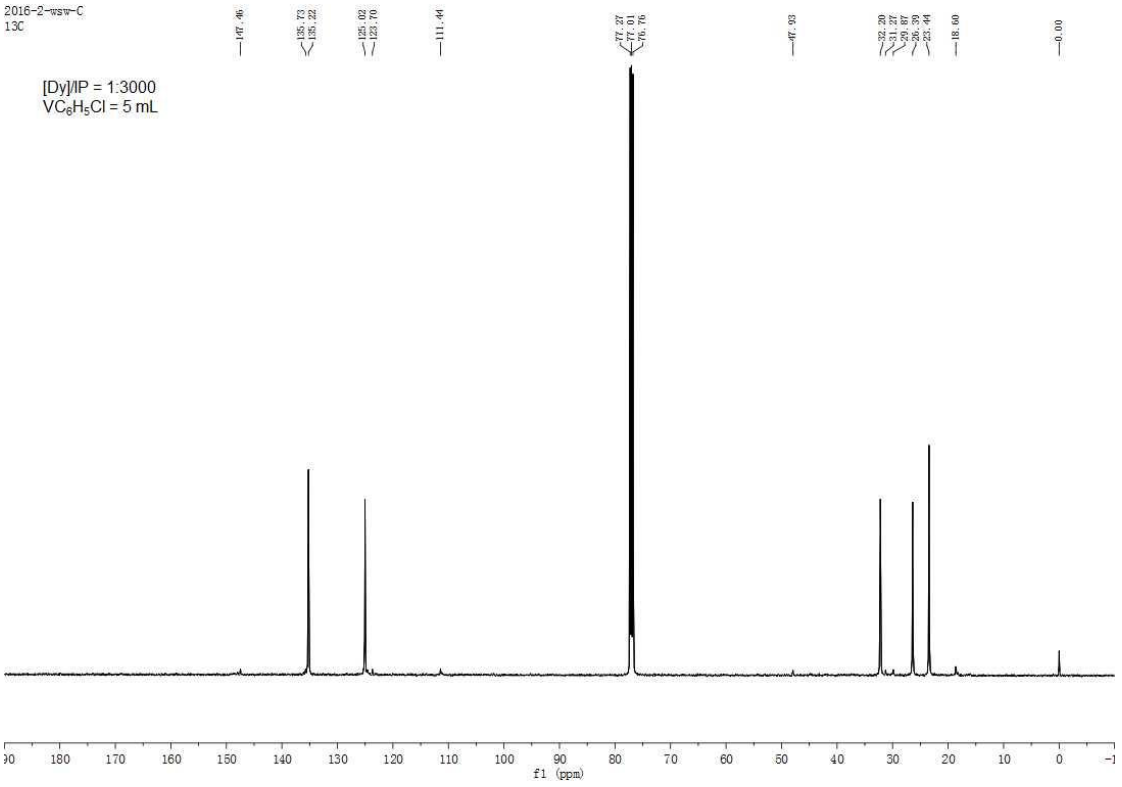

Fig. S43. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 10 (Table 3). Scan 10240 times. No 1, 4-*trans*-polymer.

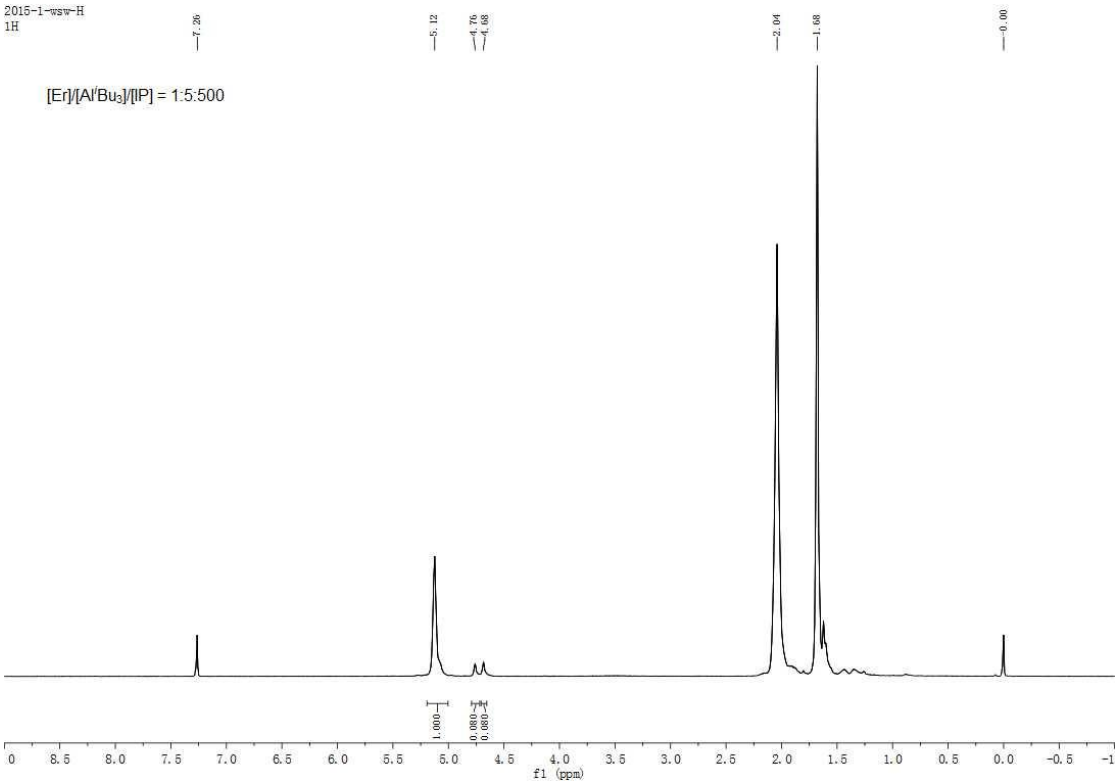

Fig. S44. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 11 (Table 3).

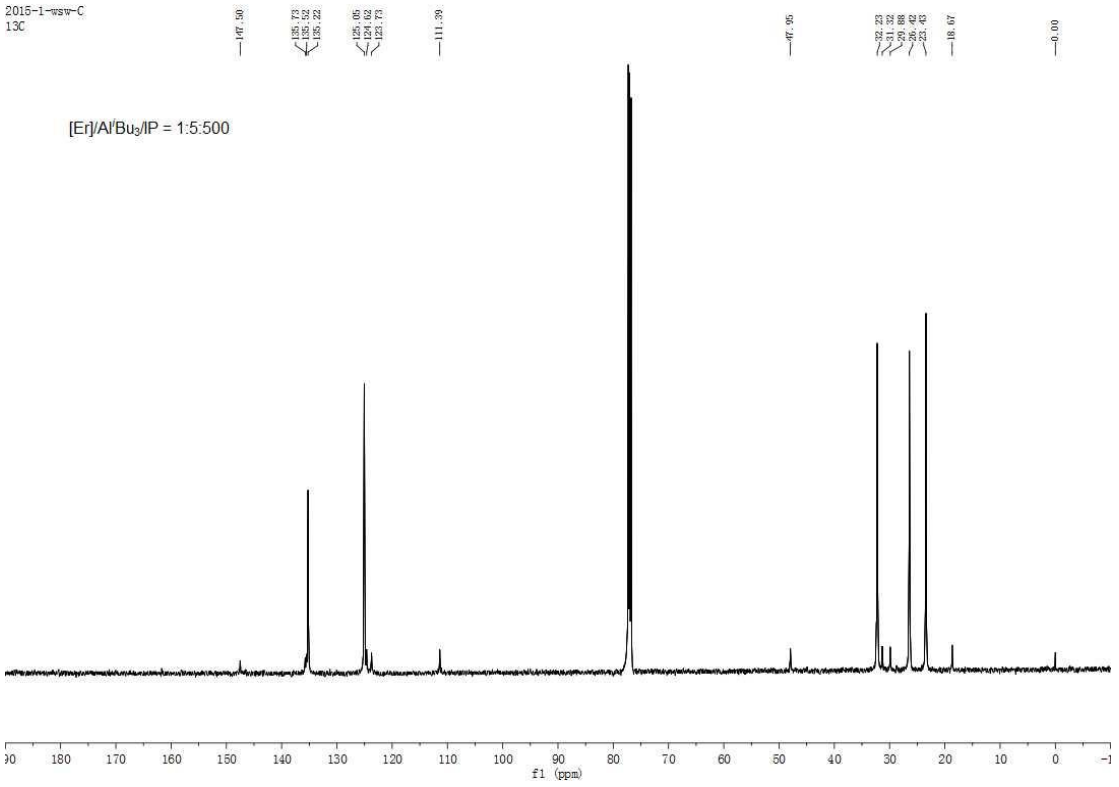

Fig. S45. ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) spectrum of PIP for entry 11 (Table 3). Scan 3000 times. No 1, 4-*trans*-polymer.