Supplementary Data

Site-selective biotransformation of ursane triterpenes by *Streptomyces griseus* ATCC 13273

Shao-Hua Xu, [a] Chao Zhang, [a] Wei-Wei Wang,[b] Bo-Yang Yu*[b] and Jian Zhang*[a]

[a] *State Key Laboratory of Natural Medicines, China Pharmaceutical University, Nanjing, Jiangsu 210009, China*

[b] *Jiangsu Key Laboratory of TCM Evaluation and Translational Research, China Pharmaceutical University, Nanjing, Jiangsu 211198, China*

* Corresponding author: E-mail: 1020071849@cpu.edu.cn Tel: 86-25-86185157 (Jian Zhang)

Content

Table S1. ^{13}C NMR spectral data of the substrates (recorded in C_5D_5N, 125 MHz)

Table S2. ^{13}C NMR spectral data of the metabolites (recorded in C_5D_5N, 125 MHz)

Fig.S1. ^{13}C NMR spectral of **1b** (C_5D_5N, 125 MHz)
Fig.S2. ^{1}H NMR spectral of **1b** (C_5D_5N, 500 MHz)
Fig.S3. HMBC spectral of **1b** (C_5D_5N, 500 MHz)
Fig.S4. HSQC spectral of **1b** (C_5D_5N, 500 MHz)
Fig.S5. DEPT spectral of **1b** (C_5D_5N, 125 MHz)
Fig.S6. NOESY spectral of **1b** (C_5D_5N, 500 MHz)
Fig.S7. ^{13}C NMR spectral of **1a** (C_5D_5N, 125 MHz)
Fig.S8. HMBC spectral of **1a** (C_5D_5N, 500 MHz)
Fig.S9. ^{13}C NMR spectral of **2a** (C_5D_5N, 125 MHz)
Fig.S10. HMBC spectral of **2a** (C_5D_5N, 500 MHz)
Fig.S11. ^{13}C NMR spectral of **2b** (C_5D_5N, 125 MHz)
Fig.S12. HMBC spectral of **2b** (C_5D_5N, 500 MHz)
Fig.S13. ^{13}C NMR spectral of **3a** (C_5D_5N, 125 MHz)
Fig.S14. HMBC spectral of **3a** (C_5D_5N,500 MHz)
Fig.S15. ^{13}C NMR spectral of **3b** (C_5D_5N, 125 MHz)
Fig.S16. HMBC spectral of **3b** (C_5D_5N, 500 MHz)
Fig.S17. ^{13}C NMR spectral of **5a** (C_5D_5N, 125 MHz)
Fig.S18. HMBC spectral of **5a** (C_5D_5N, 500 MHz)
Fig.S19. ^{13}C NMR spectral of **5b** (C_5D_5N, 125 MHz)
Fig.S20. HMBC spectral of **5b** (C_5D_5N, 500 MHz

Fig.S21. Time-course analysis of the biotransformation of ursolic acid (**1**).

Table S1. ^{13}C NMR spectral data of the substrates (recorded in C_5D_5N, 125MHz)

Carbon	**1**	**2**	**3**	**4**	**5**
1	39.13	39.79	48.51	48.42	48.56
2	28.15	34.83	69.07	69.37	69.54
3	78.17	216.60	84.32	78.79	78.84
4	39.39	47.58	40.29	44.09	43.56
5	55.87	55.83	56.40	48.45	49.18
6	18.82	19.51	19.31	19.01	68.03
7	33.62	33.41	33.99	33.68	39.89
8	40.02	40.36	40.53	40.56	41.76
9	48.09	47.84	48.58	48.58	50.81
10	37.46	37.31	38.92	38.81	38.59
11	23.66	24.28	24.21	24.27	24.48
12	125.68	125.89	126.04	126.07	126.49
13	139.30	139.81	139.78	139.79	139.16
14	42.54	43.08	43.03	43.06	44.96
15	28.73	29.15	29.12	29.15	29.13
16	24.95	25.38	25.37	25.38	25.43
17	48.09	48.57	48.46	48.52	49.12
18	53.60	54.10	54.01	54.04	54.15
19	39.52	39.99	39.95	39.94	40.00
20	39.43	39.89	39.87	39.89	39.99
21	31.11	31.57	31.55	31.56	31.58
22	37.33	37.89	37.90	37.93	37.95
23	28.83	27.20	29.83	67.14	66.74
24	15.69	22.07	18.13	14.84	16.39
25	16.56	15.63	17.43	17.95	19.61
26	17.48	17.79	17.95	17.98	19.35
27	23.93	24.17	24.37	24.27	24.37
28	179.84	180.29	180.32	180.33	180.32
29	17.52	17.97	17.95	18.03	17.93
30	21.41	21.86	21.85	21.84	21.82

Table S2. ^{13}C NMR spectral data of the metabolites (recorded in C_5D_5N, 125 MHz)

Carbon	**1a**	**1b**	**2a**	**2b**	**3a**	**3b**	**4a**	**5a**	**5b**
1	39.52	39.29	39.70	40.72	48.0	48.35	48.21	48.56	48.27
2	28.59	28.88	34.81	36.05	68.6	69.13	69.35	69.53	69.53
3	78.57	80.60	216.63	215.02	83.8	86.15	78.80	78.86	78.84
4	39.84	43.66	47.53	55.44	39.8	44.45	44.07	43.56	43.50
5	56.26	56.83	55.73	58.24	55.9	56.92	48.33	49.22	49.24
6	19.43	19.55	20.27	21.47	18.8	19.69	18.99	68.02	68.01
7	34.00	34.29	33.32	34.02	33.5	34.25	33.58	40.01	40.02
8	40.48	40.47	40.36	40.44	40.1	40.50	40.55	41.74	41.67
9	48.49	48.54	47.82	47.96	48.1	48.60	48.48	50.78	50.75
10	37.78	37.53	37.29	37.53	38.5	38.73	38.81	38.60	38.61
11	24.14	24.36	24.36	24.40	23.7	24.44	24.26	24.48	24.58
12	126.57	126.45	126.32	126.21	126.0	126.35	126.50	126.66	126.90
13	139.09	139.06	139.14	139.18	138.7	139.10	139.13	139.07	138.52
14	42.95	42.88	43.02	42.93	42.5	42.91	42.99	44.94	44.96
15	29.11	29.08	29.06	29.08	28.6	29.04	29.07	29.16	29.07
16	25.38	25.36	25.35	25.30	24.9	25.35	25.35	25.52	25.42
17	48.24	48.22	48.26	48.21	47.6	48.21	48.52	49.12	49.08
18	53.05	53.02	53.06	53.02	52.6	53.01	53.05	54.19	53.18
19	35.20	35.20	35.19	35.17	34.7	35.19	35.19	34.48	35.27
20	53.10	53.09	53.09	53.06	52.7	53.15	53.13	47.97	53.20
21	26.55	26.54	26.54	26.50	26.1	26.55	26.54	26.17	26.59
22	37.25	37.23	37.21	37.20	36.8	37.23	37.25	37.94	37.30
23	29.25	24.04	27.18	20.45	29.3	24.44	67.24	66.80	66.84
24	16.14	65.04	22.05	65.66	17.7	66.12	14.79	16.38	16.37
25	17.04	16.58	15.61	16.16	16.9	17.74	17.96	19.60	19.59
26	17.90	17.73	17.73	17.79	17.5	17.79	17.96	19.35	19.38
27	24.48	24.45	24.17	24.40	24.0	24.59	24.45	24.39	24.39
28	179.94	179.93	179.91	179.89	179.5	179.95	179.97	180.39	179.98
29	19.25	19.42	19.38	19.37	18.9	19.40	19.37	17.66	19.28
30	179.02	179.02	178.97	178.95	178.6	179.09	179.03	65.66	179.16

Fig.S1. ^{13}C NMR spectral of **1b** (C_5D_5N, 125 MHz)

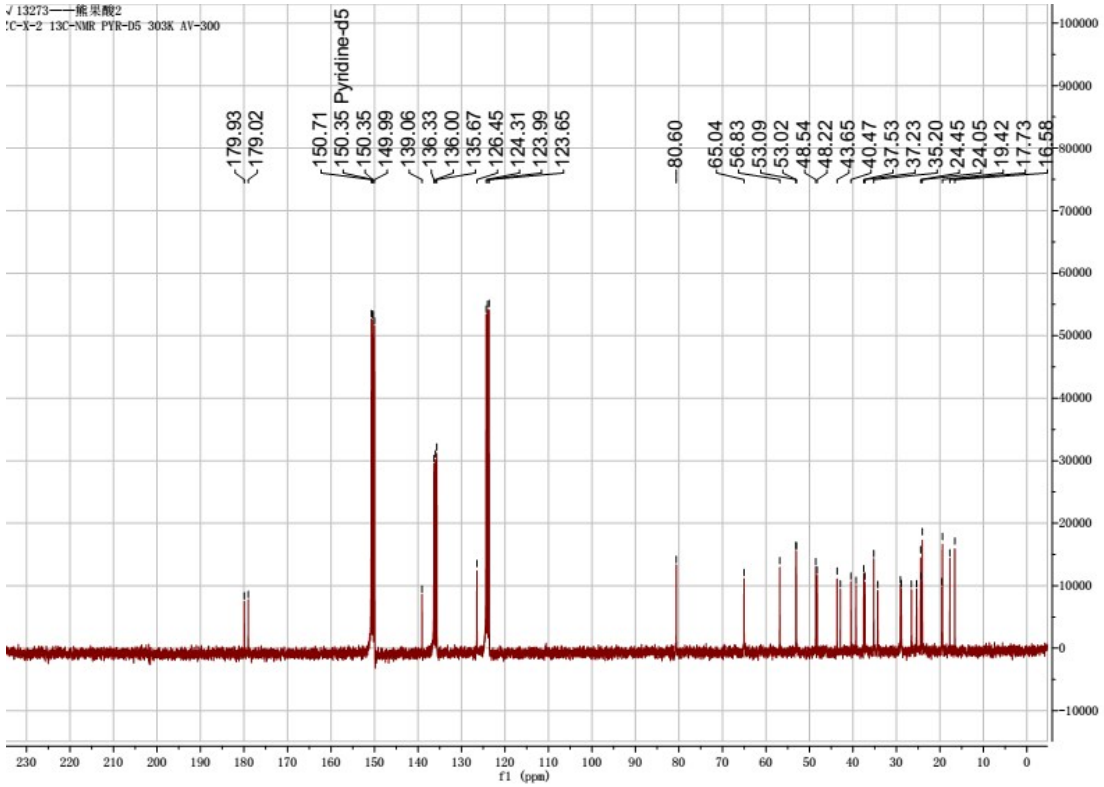

Fig.S2. ^{1}H NMR spectral of **1b** (C_5D_5N, 500 MHz)

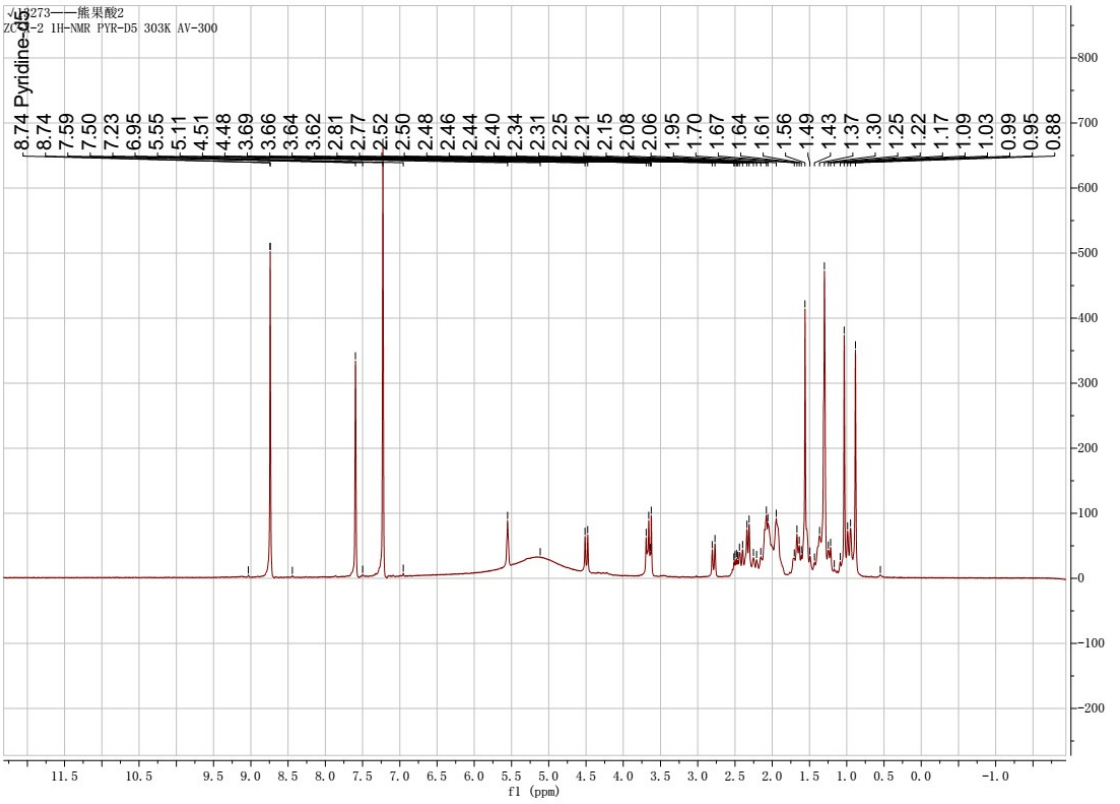

Fig.S3. HMBC spectral of **1b** (C_5D_5N, 500 MHz)

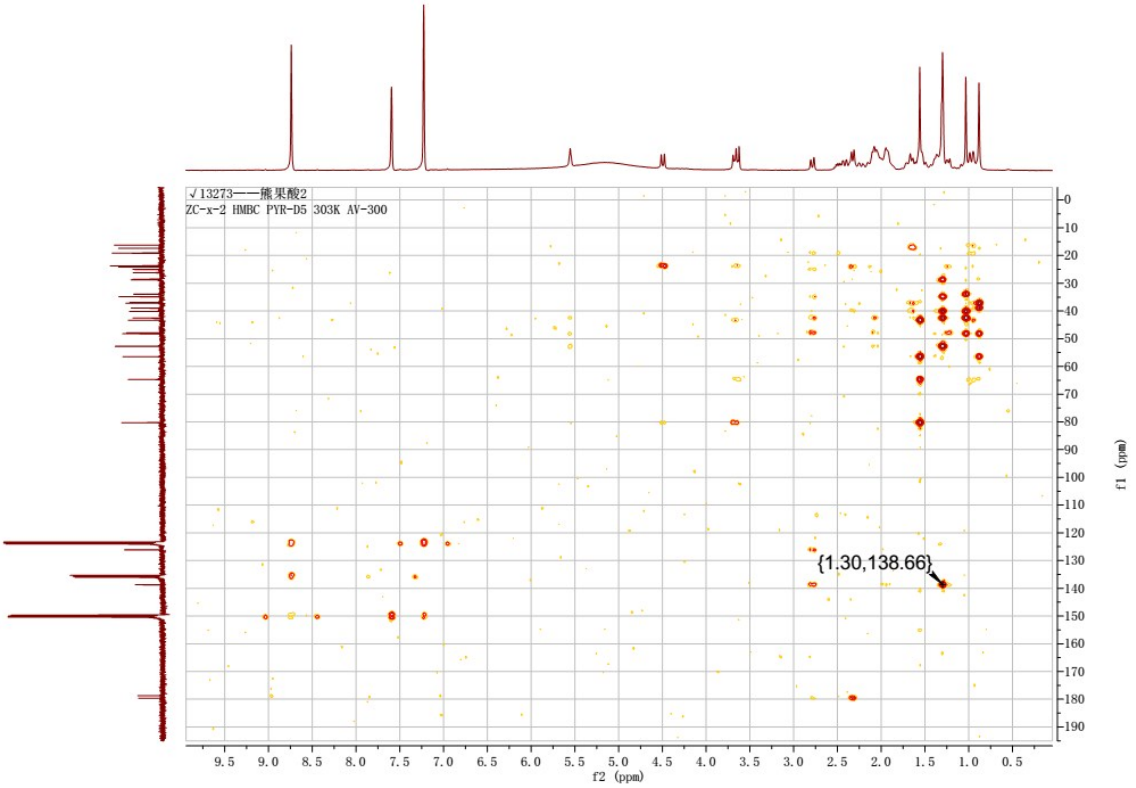

Fig.S4. HSQC spectral of **1b** (C_5D_5N, 500 MHz)

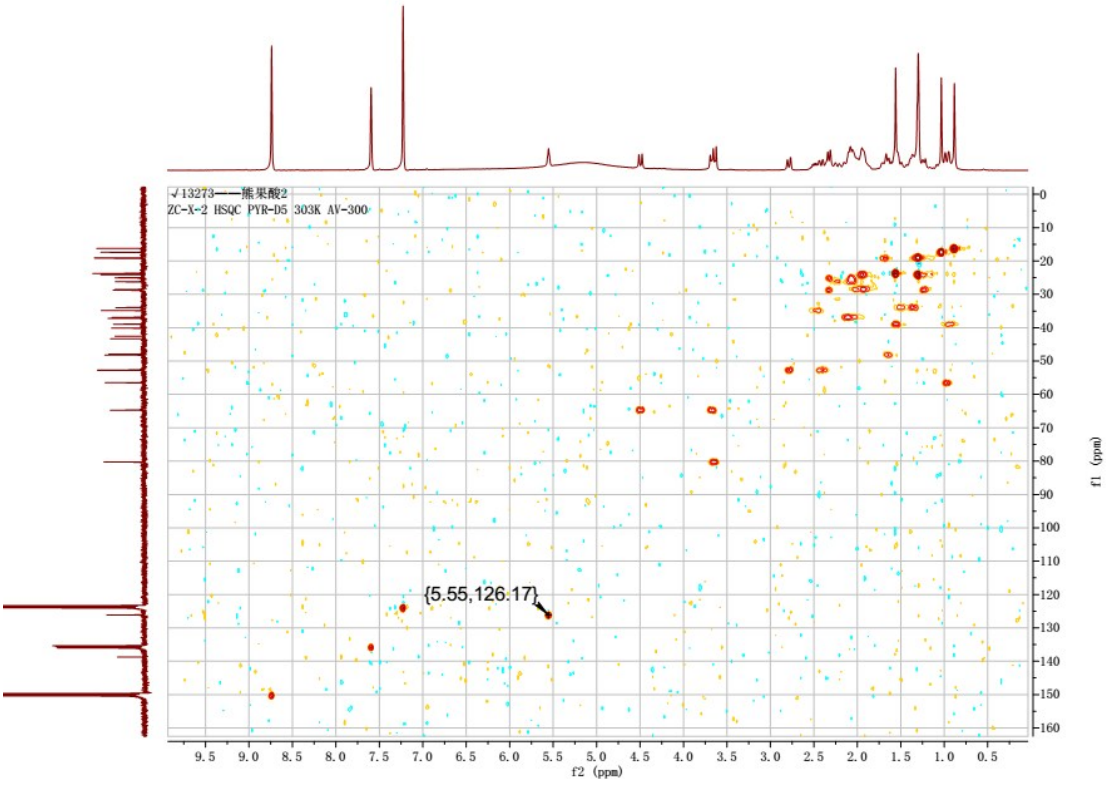

Fig.S5. DEPT spectral of **1b** (C_5D_5N, 125 MHz)

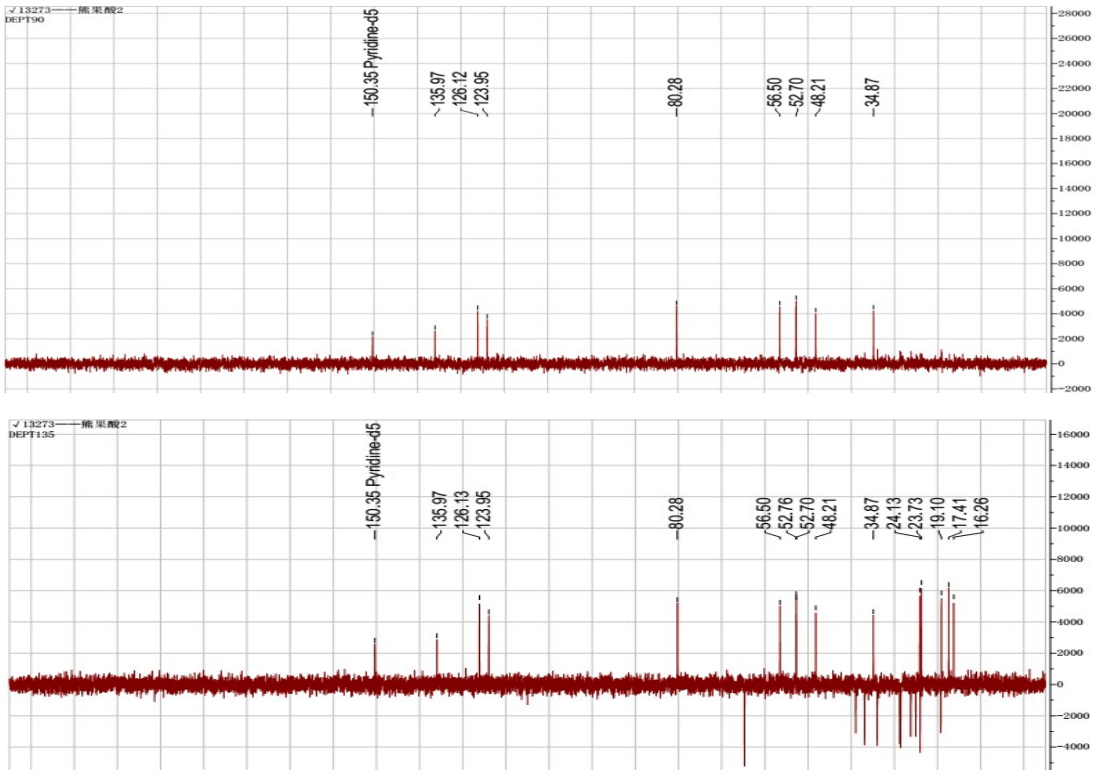

Fig.S6. NOESY spectral of **1b** (C_5D_5N, 500 MHz)

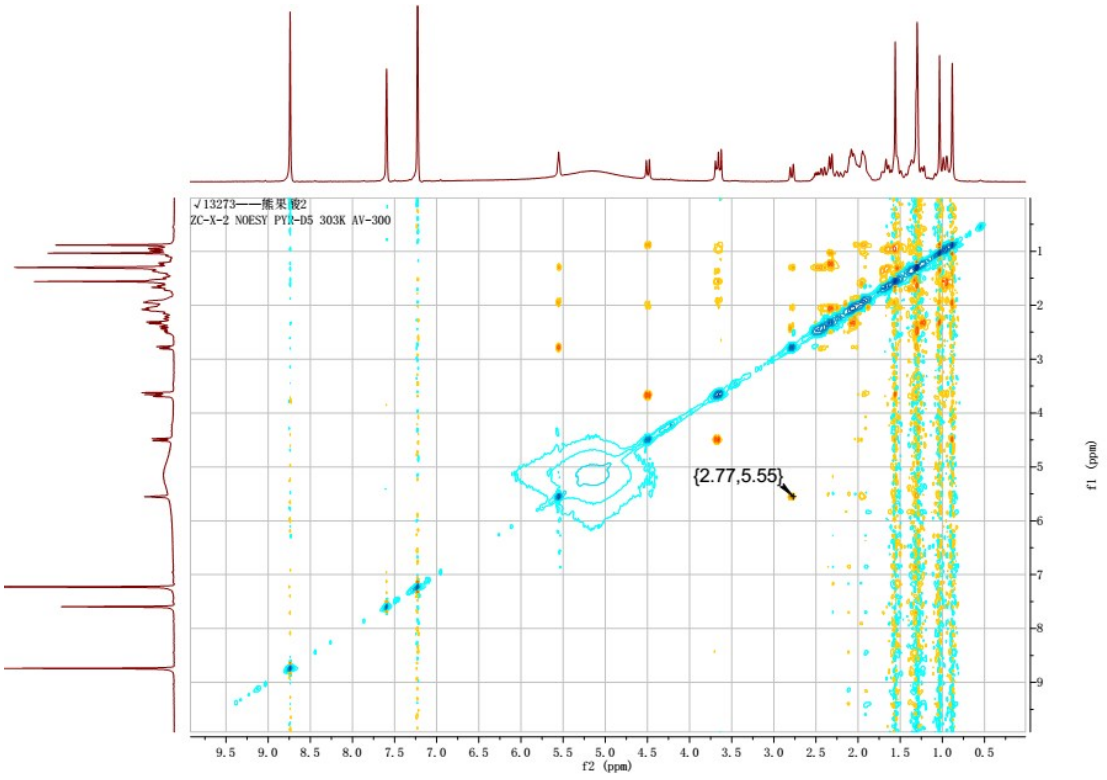

Fig.S7. ^{13}C NMR spectral of **1a** (C_5D_5N, 125 MHz)

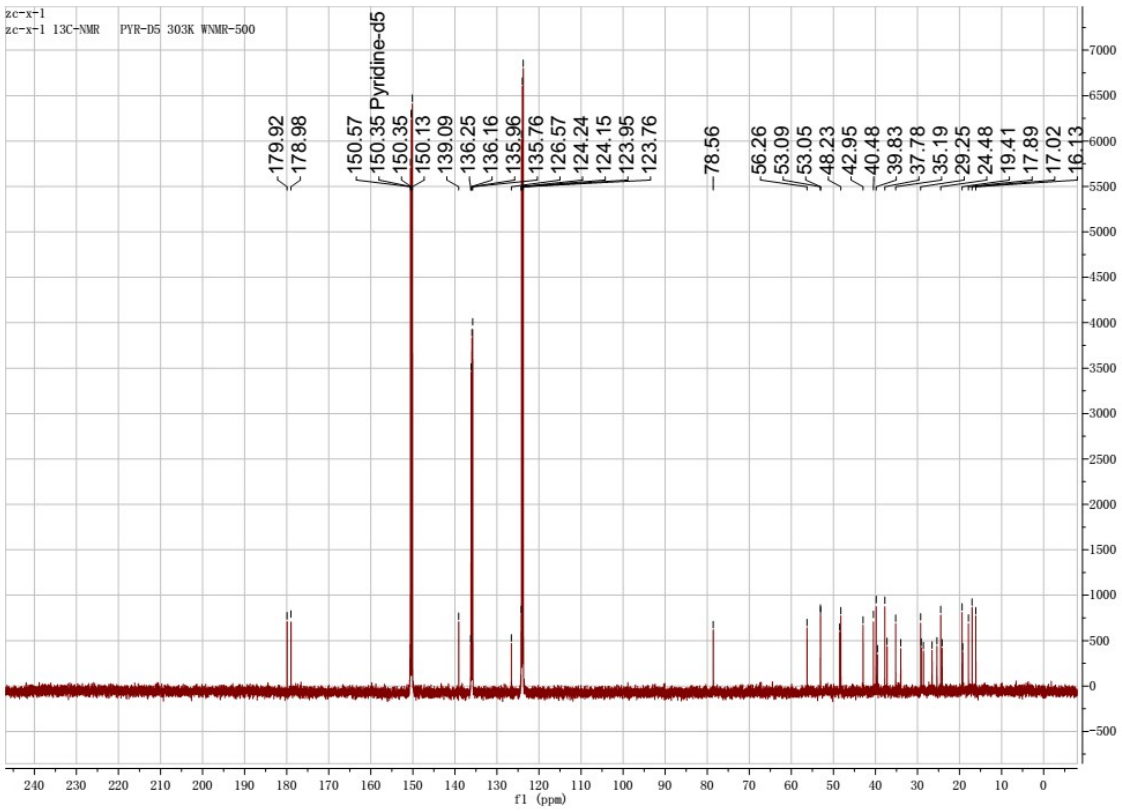

Fig.S8. HMBC spectral of **1a** (C_5D_5N, 500 MHz)

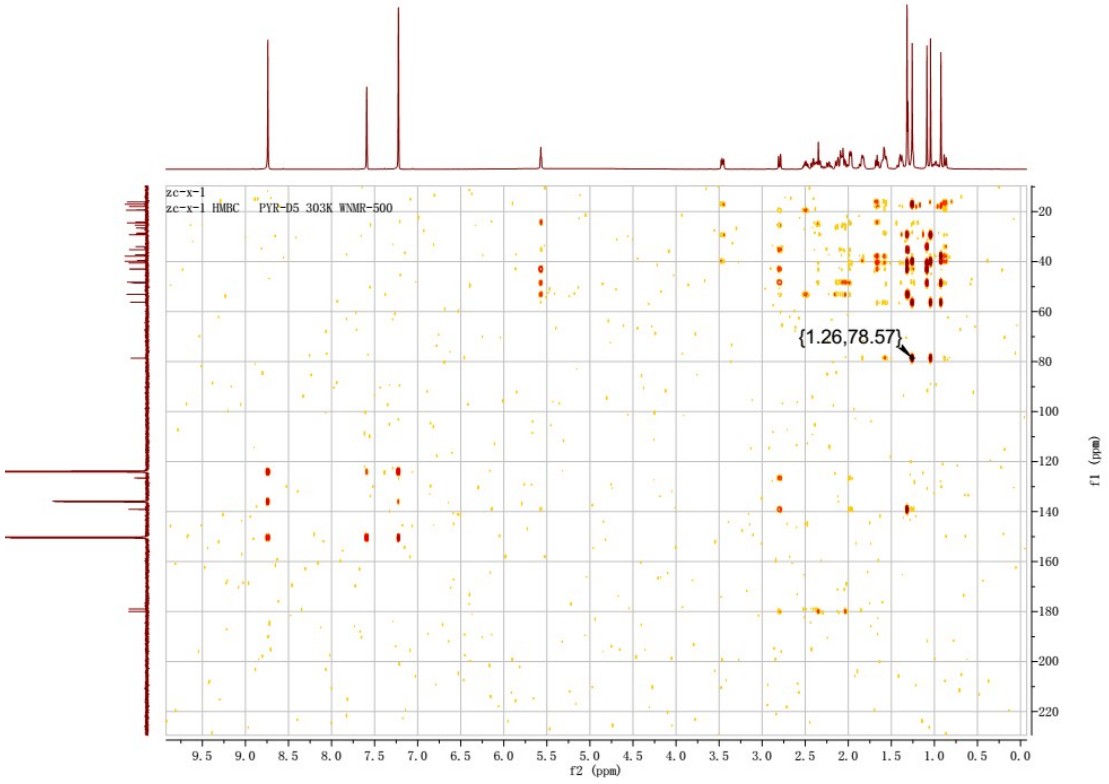

Fig.S9. ^{13}C NMR spectral of **2a** (C_5D_5N, 125 MHz)

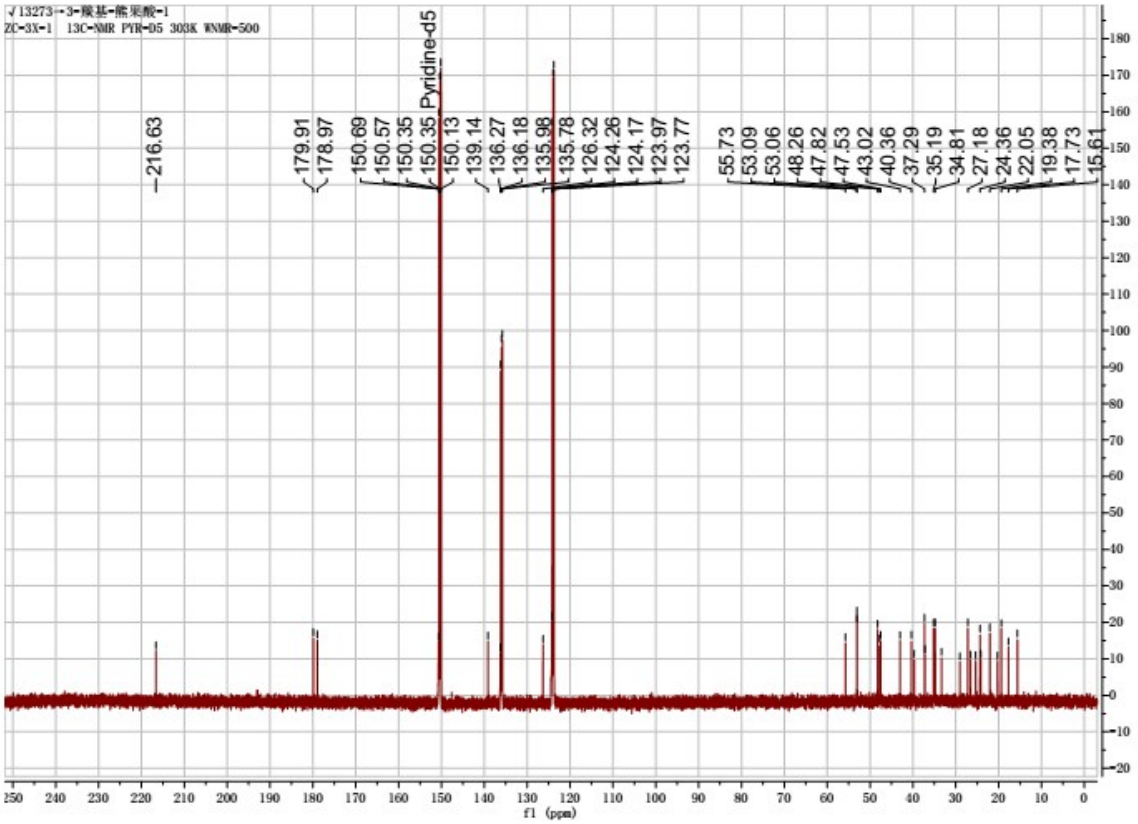

Fig.S10. HMBC spectral of **2a** (C_5D_5N, 500 MHz)

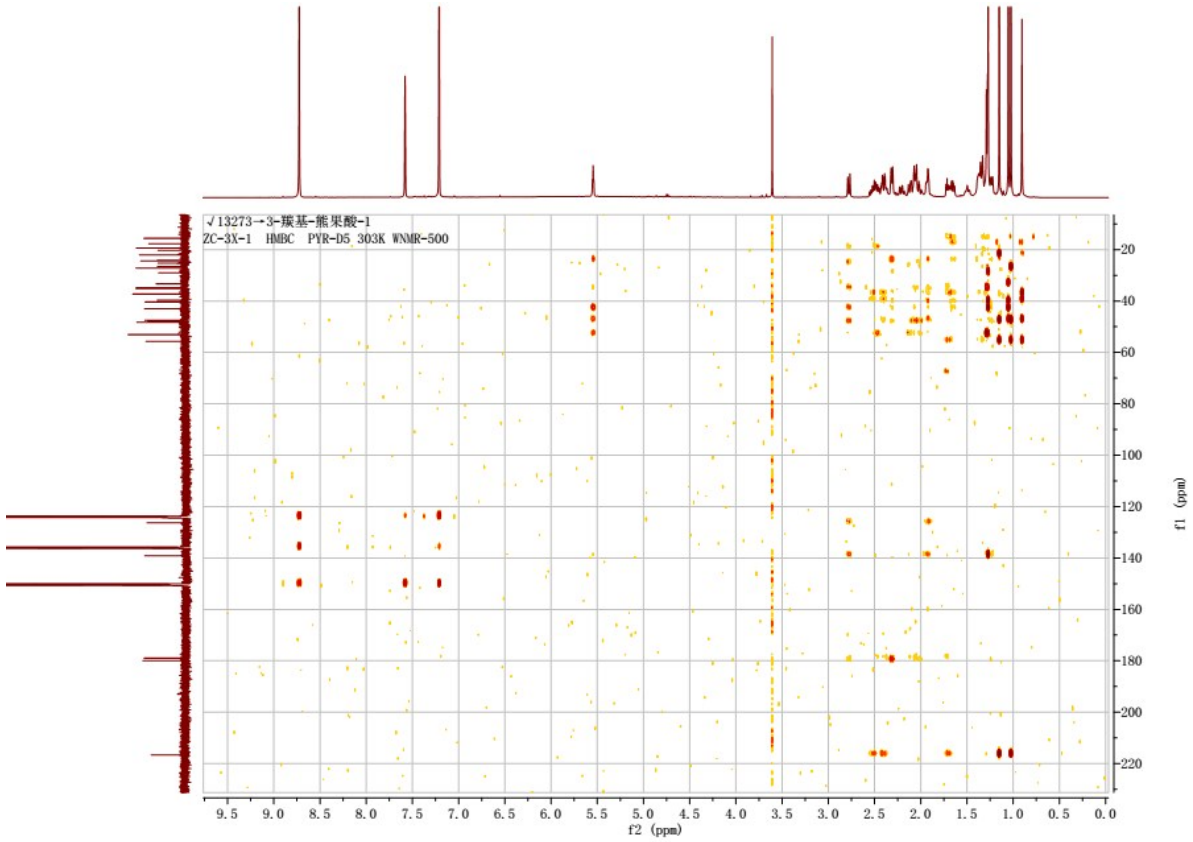

Fig.S11. ^{13}C NMR spectral of **2b** (C_5D_5N, 125 MHz)

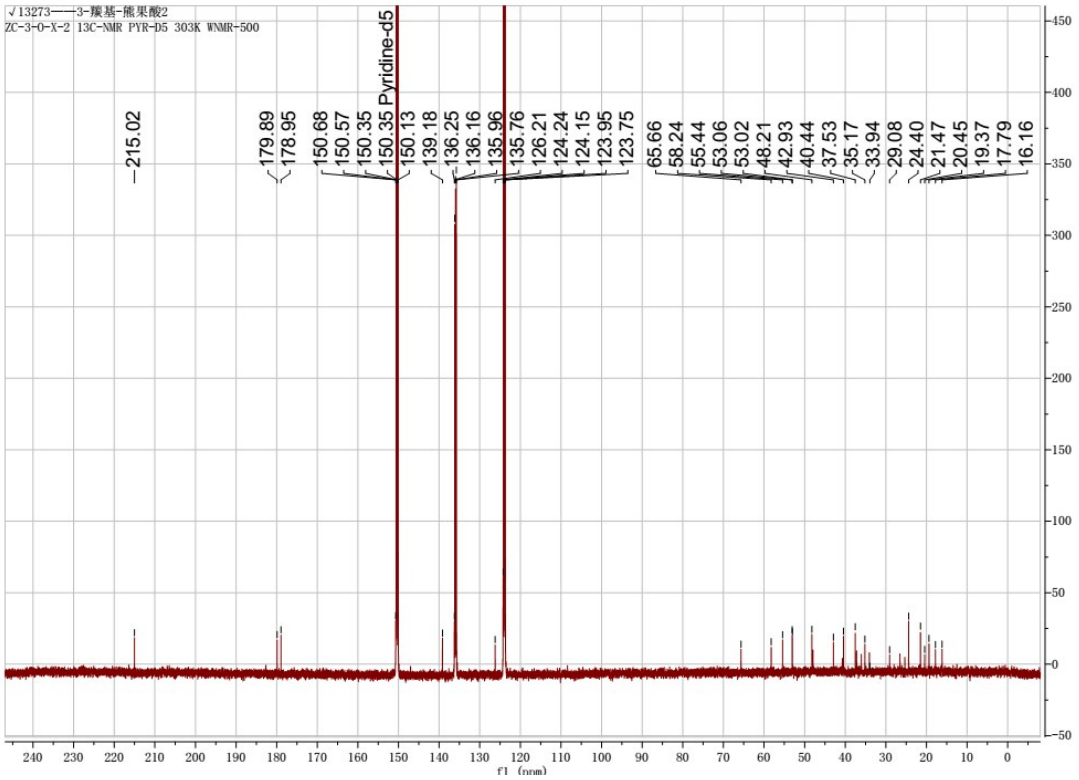

Fig.S12. HMBC spectral of **2b** (C_5D_5N, 500 MHz)

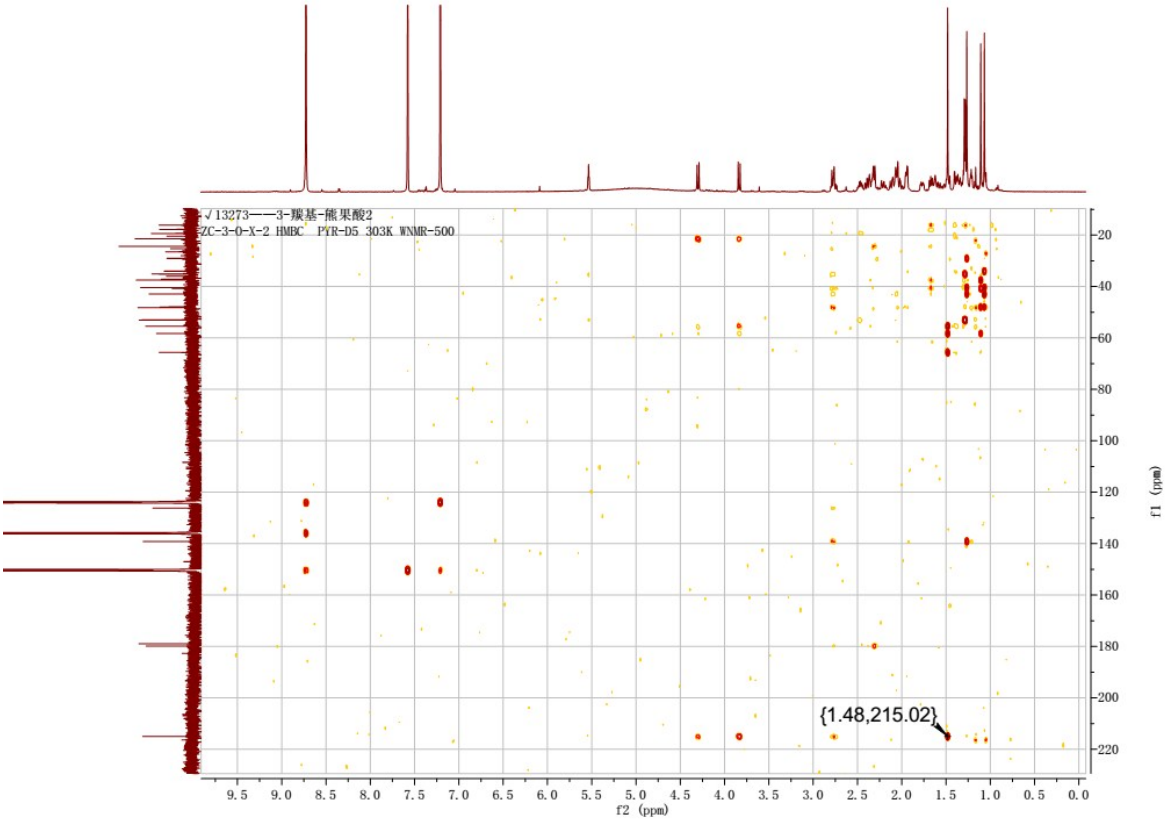

Fig.S13. ^{13}C NMR spectral of **3a** (C_5D_5N, 125 MHz)

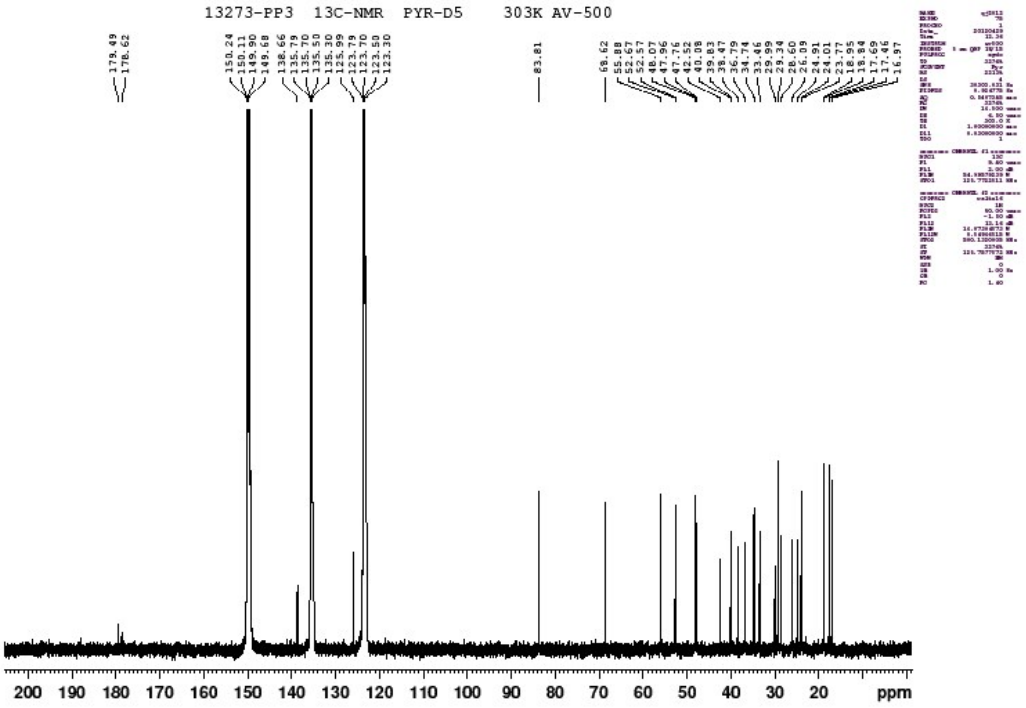

Fig.S14. ^{13}C NMR spectral of **3a** (C_5D_5N, 500 MHz)

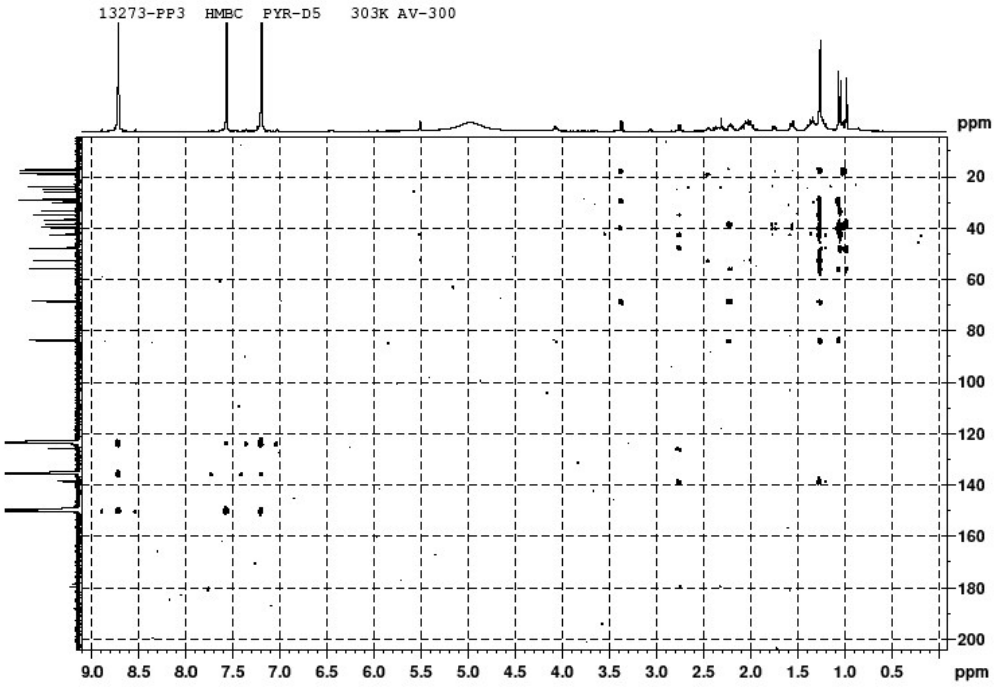

Fig.S15 ^{13}C NMR spectral of **3b** (C_5D_5N, 125 MHz)

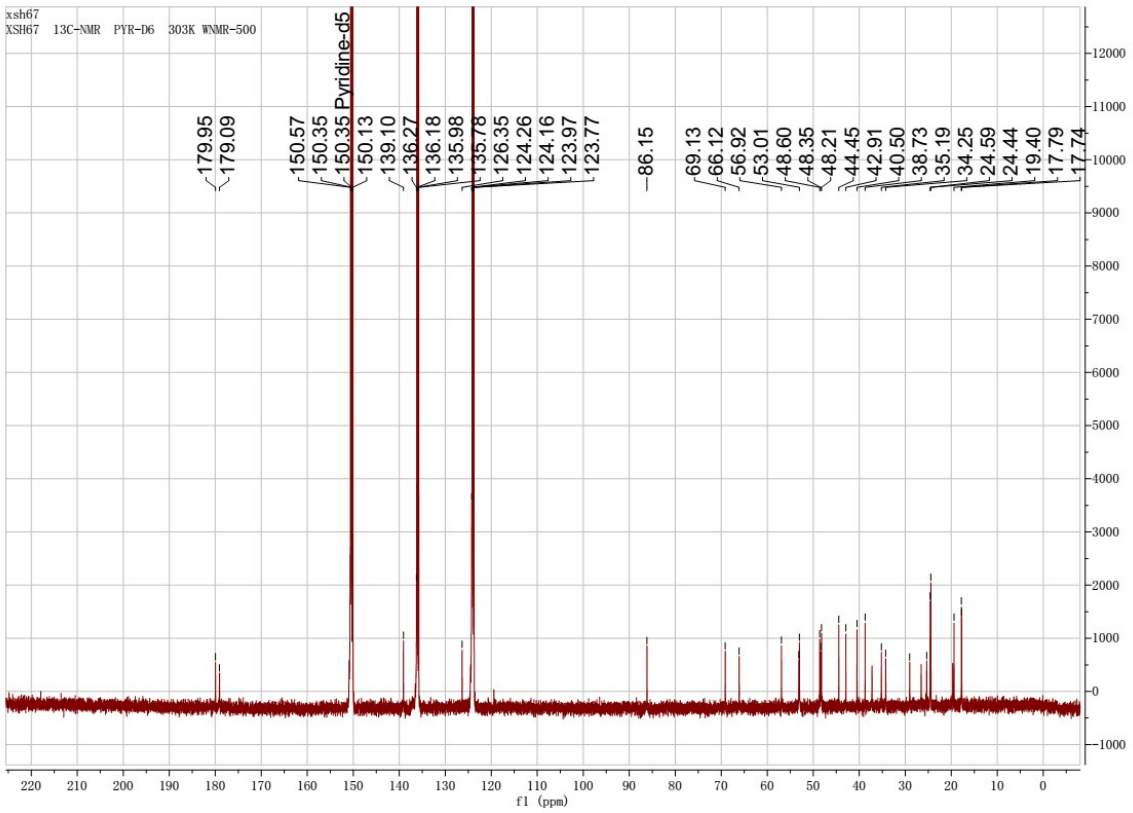

Fig.S16. HMBC spectral of **3b** (C_5D_5N, 500 MHz)

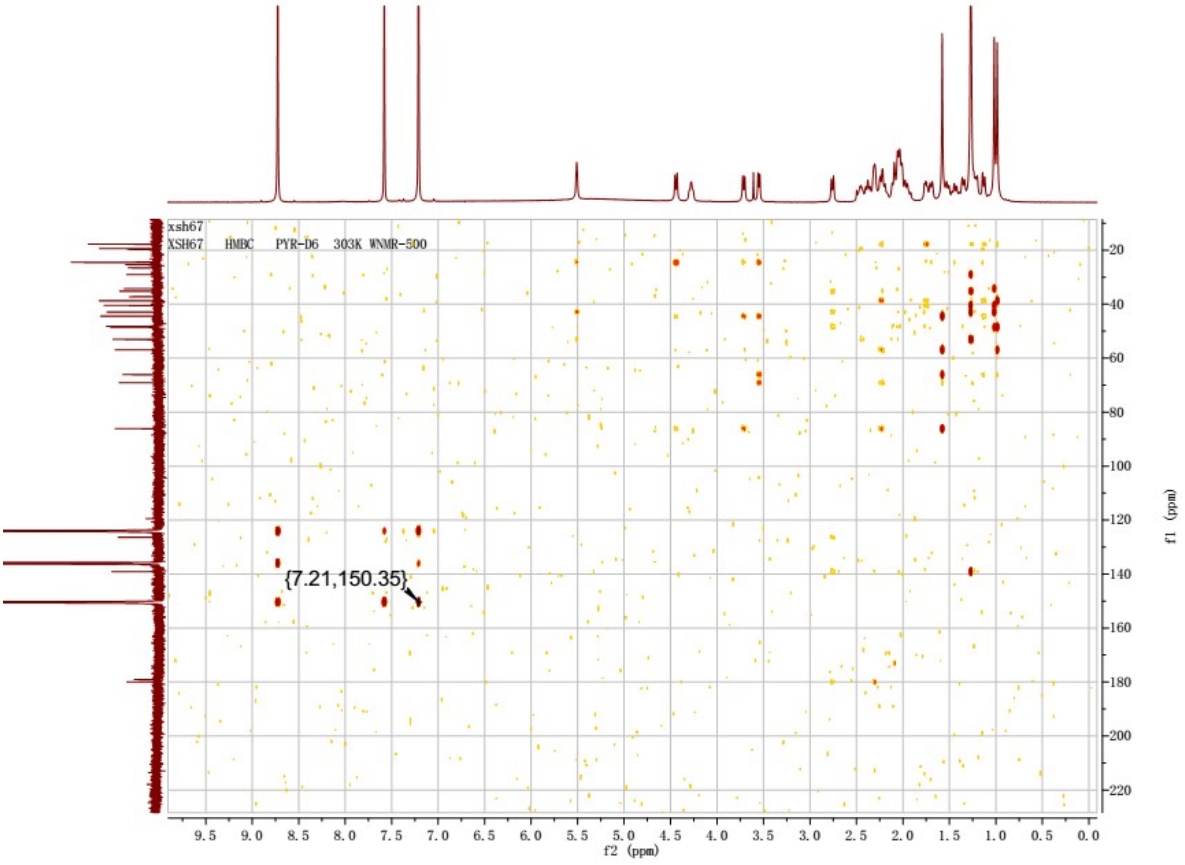

Fig.S17. ^{13}C NMR spectral of **5a** (C_5D_5N, 125 MHz)

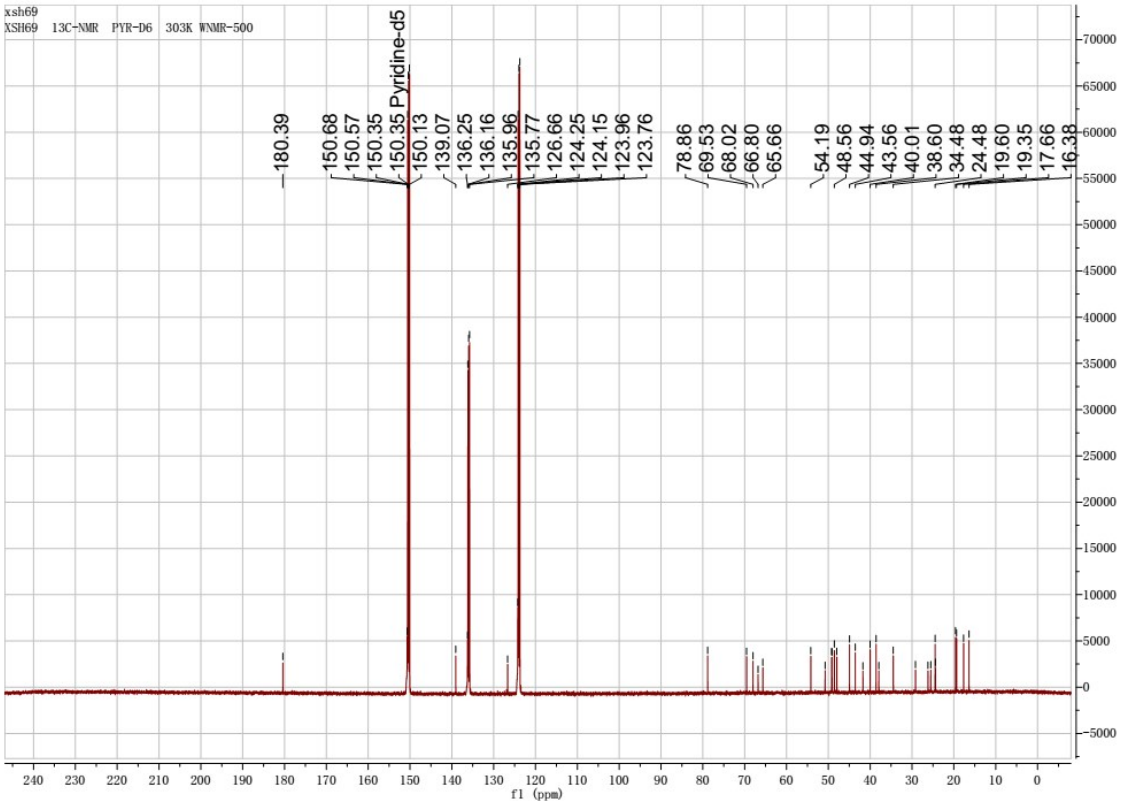

Fig.S18. HMBC spectral of **5a** (C_5D_5N, 500 MHz)

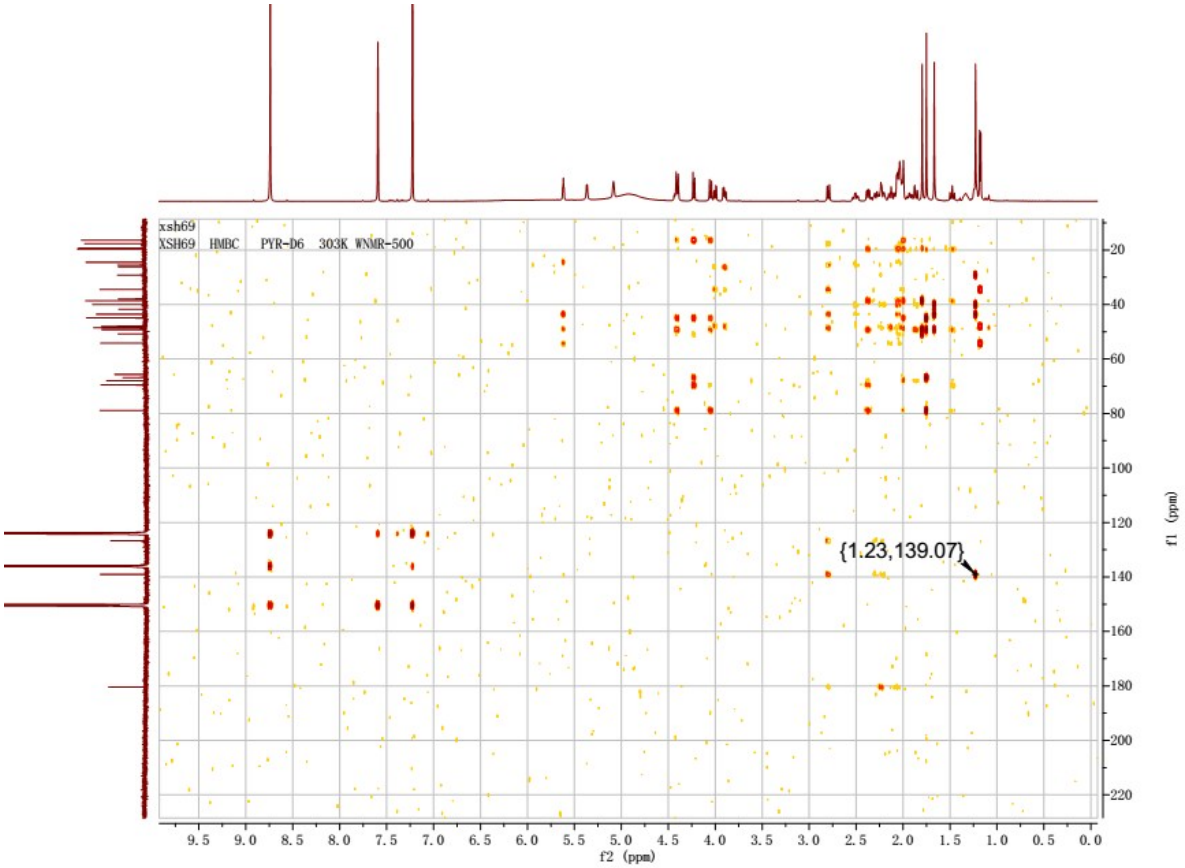

Fig.S19. ^{13}C NMR spectral of **5b** (C_5D_5N, 125 MHz)

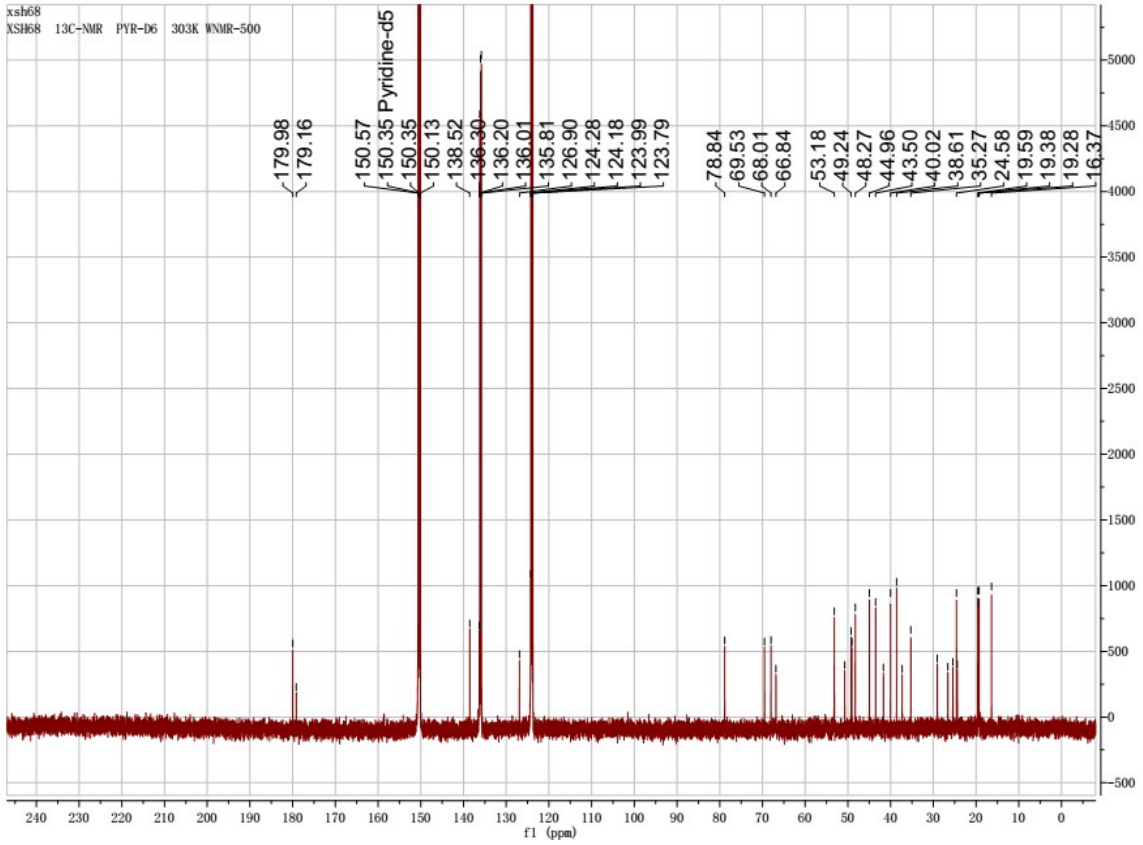

Fig.S20. HMBC spectral of **5b** (C_5D_5N, 500 MHz)

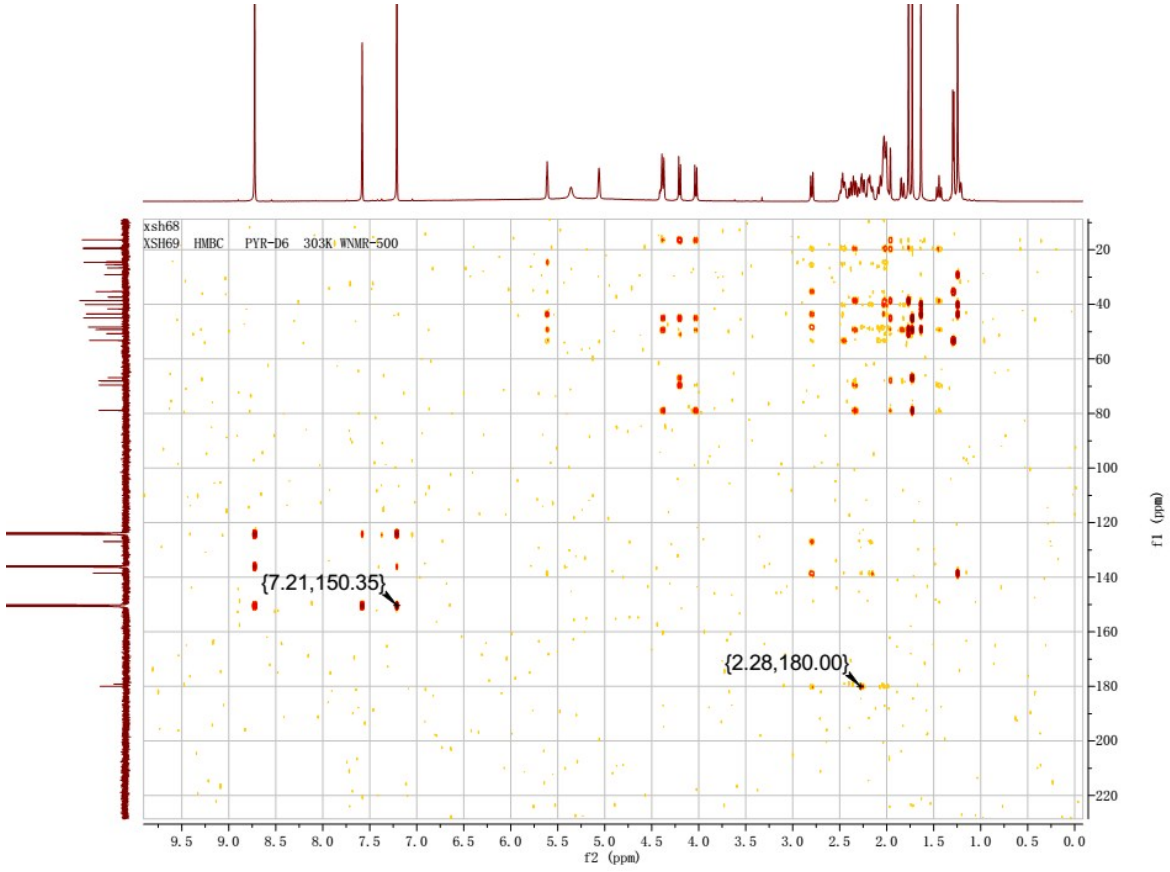

Fig.S21. Time-course analysis of the biotransformation of ursolic acid (**1**).