

Supporting Information for

Oxytrodiflavanone A and Oxytrochalcoflavanones A,B: New
Biflavonoids from *Oxytropis chiliophylla*

Yang Liu ¹, Norbo Kelsang ¹, Jianghai Lu ², Yingtao Zhang ¹, Hong Liang ¹, Pengfei Tu ¹,
Dexin Kong ^{3,4,*} and Qingying Zhang ^{1,*}

¹ State Key Laboratory of Natural and Biomimetic Drugs and Department of Natural Medicines, School of Pharmaceutical Sciences, Peking University Health Science Center, Beijing 100191, China;

² National Anti-Doping Laboratory, China Anti-Doping Agency, Beijing 100029, China;

³ Tianjin Key Laboratory on Technologies Enabling Development of Clinical Therapeutics and Diagnostics, School of Pharmacy, Tianjin Medical University, Tianjin 300070, China

⁴ Research Center, School of Medicine, Tianjin Tianshi College, Tianyuan University, Tianjin 301700, China

Contents of Supporting Information

Figures

- Figure S1. ^1H NMR spectrum of oxytrodiflavanone A (**1**) in CDCl_3
- Figure S2. ^{13}C NMR spectrum of oxytrodiflavanone A (**1**) in CDCl_3
- Figure S3. ^1H - ^1H COSY spectrum of oxytrodiflavanone A (**1**) in CDCl_3
- Figure S4. HSQC spectrum of oxytrodiflavanone A (**1**) in CDCl_3
- Figure S5. HMBC spectrum of oxytrodiflavanone A (**1**) in CDCl_3
- Figure S6. ^1H NMR spectrum of oxytrodiflavanone A (**1**) in Pyridine- d_5
- Figure S7. NOESY spectrum of oxytrodiflavanone A (**1**) in Pyridine- d_5
- Figure S8. ^1H NMR spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3
- Figure S9. ^{13}C NMR spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3
- Figure S10. ^1H - ^1H COSY spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3
- Figure S11. HSQC spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3
- Figure S12. HMBC spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3
- Figure S13. Targeted MS/MS spectra of oxytrodiflavanone A (**1**), oxytrochalcoflavanones A (**2**) and B (**3**) at CE of 25 eV in negative ion mode
- Figure S14. Chiral analysis of oxytrochalcoflavanones A–B (**2-3**)
- Figure S15. ^1H NMR spectra of the epimers of oxytrochalcoflavanones A–B (**2-3**)
- Figure S16. Cell growth inhibitory activities of oxytrodiflavanone A (**1**) and oxytrochalcoflavanones B (**3**) on PC3 cells

Table

- Table S1. Raw data of cell growth inhibitory activities of oxytrodiflavanone A (**1**) and oxytrochalcoflavanones B (**3**)

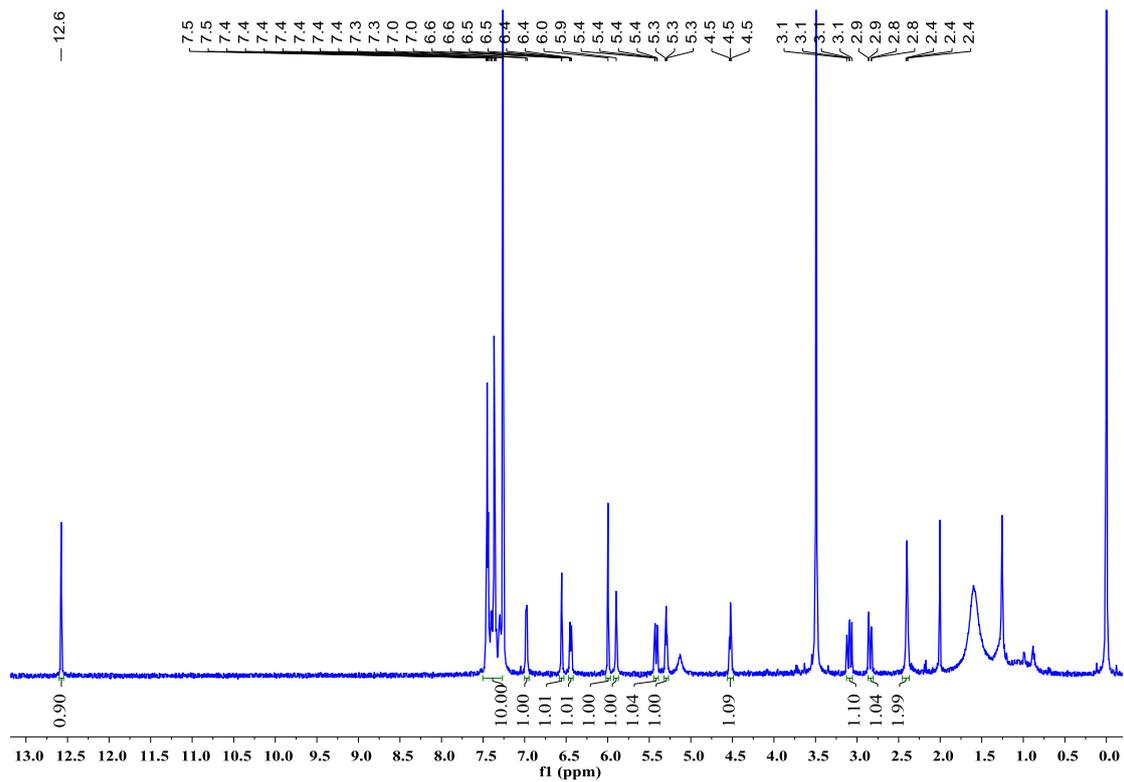


Figure S1. ^1H NMR spectrum of oxytrodidflavanone A (**1**) in CDCl_3

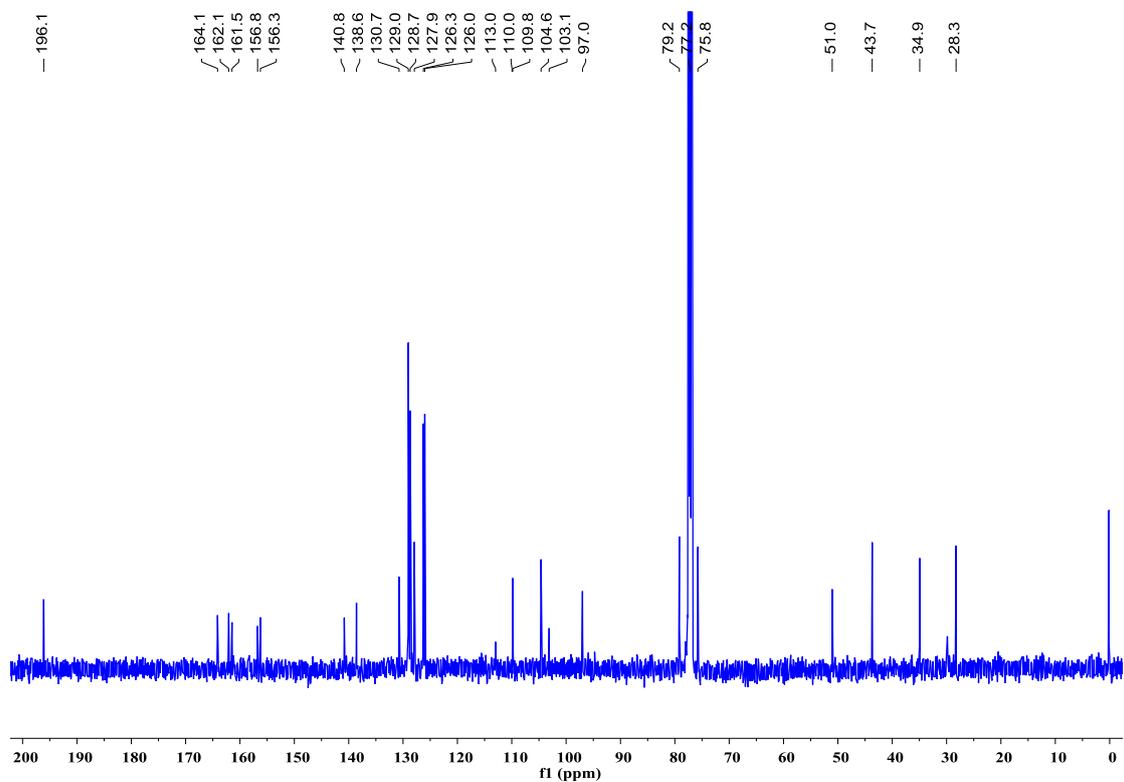


Figure S2. ^{13}C NMR spectrum of oxytrodidflavanone A (**1**) in CDCl_3

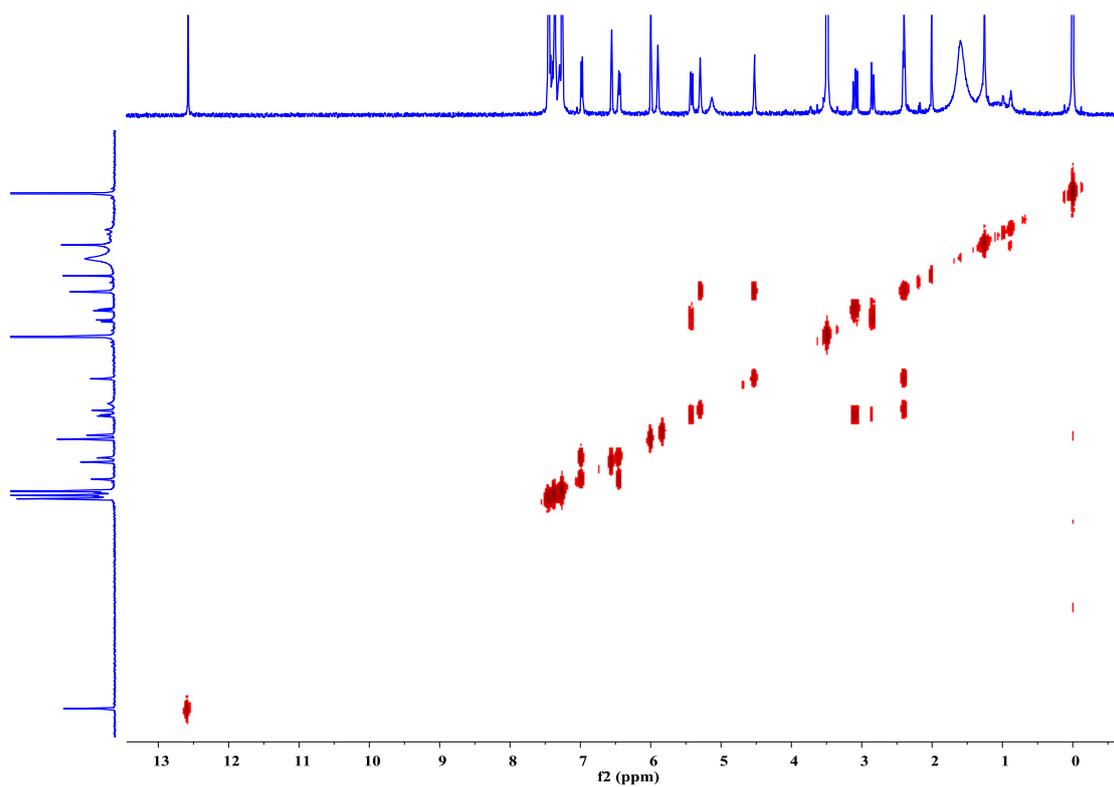


Figure S3. ^1H - ^1H COSY spectrum of oxytrodiflavanone A (**1**) in CDCl_3

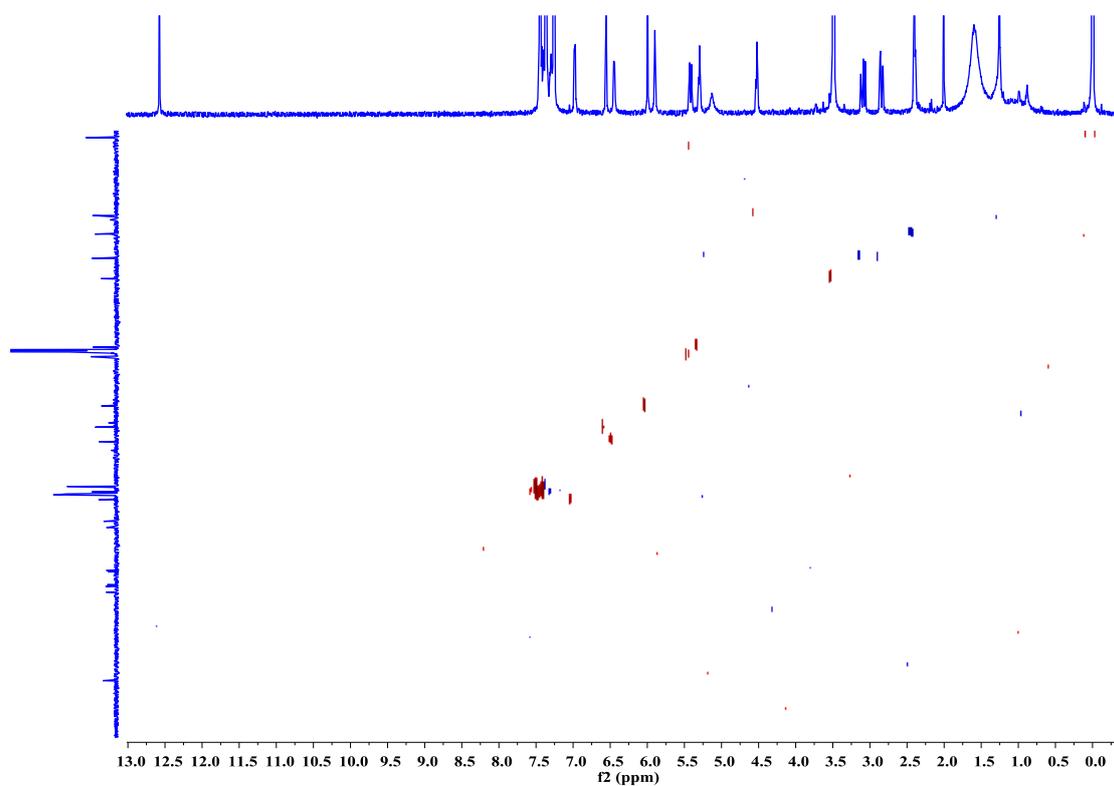


Figure S4. HSQC spectrum of oxytrodiflavanone A (**1**) in CDCl_3

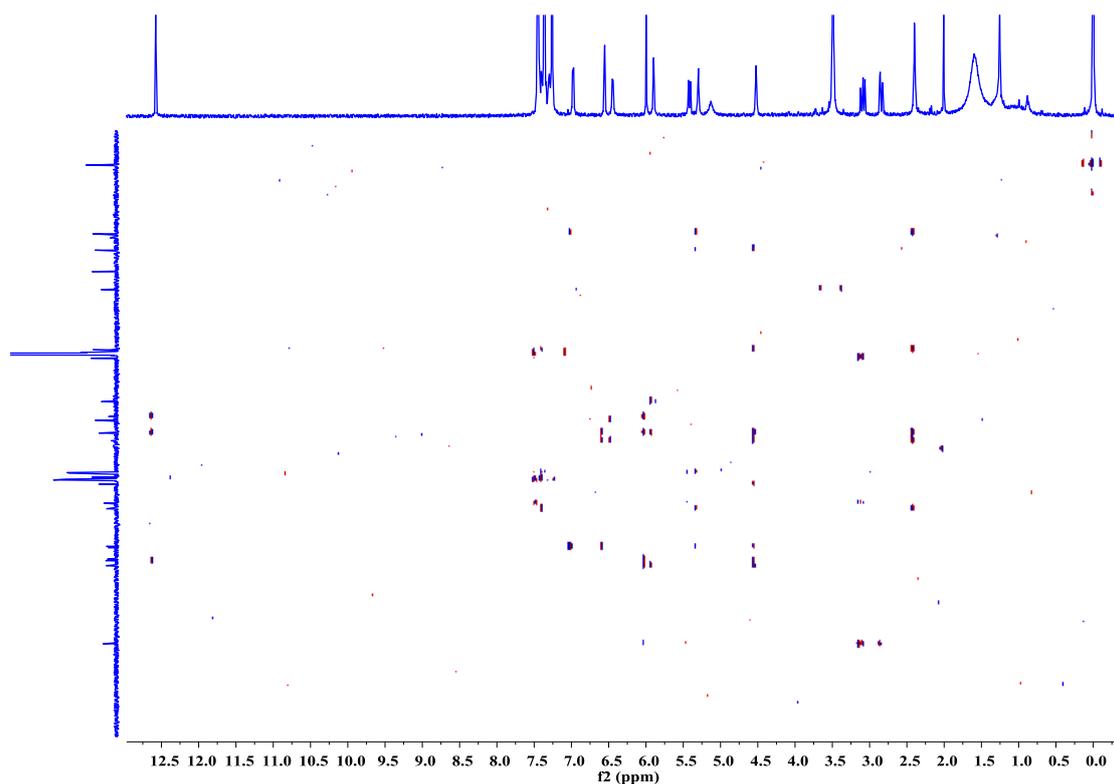


Figure S5. HMBC spectrum of oxytrodidflavanone A (**1**) in CDCl₃

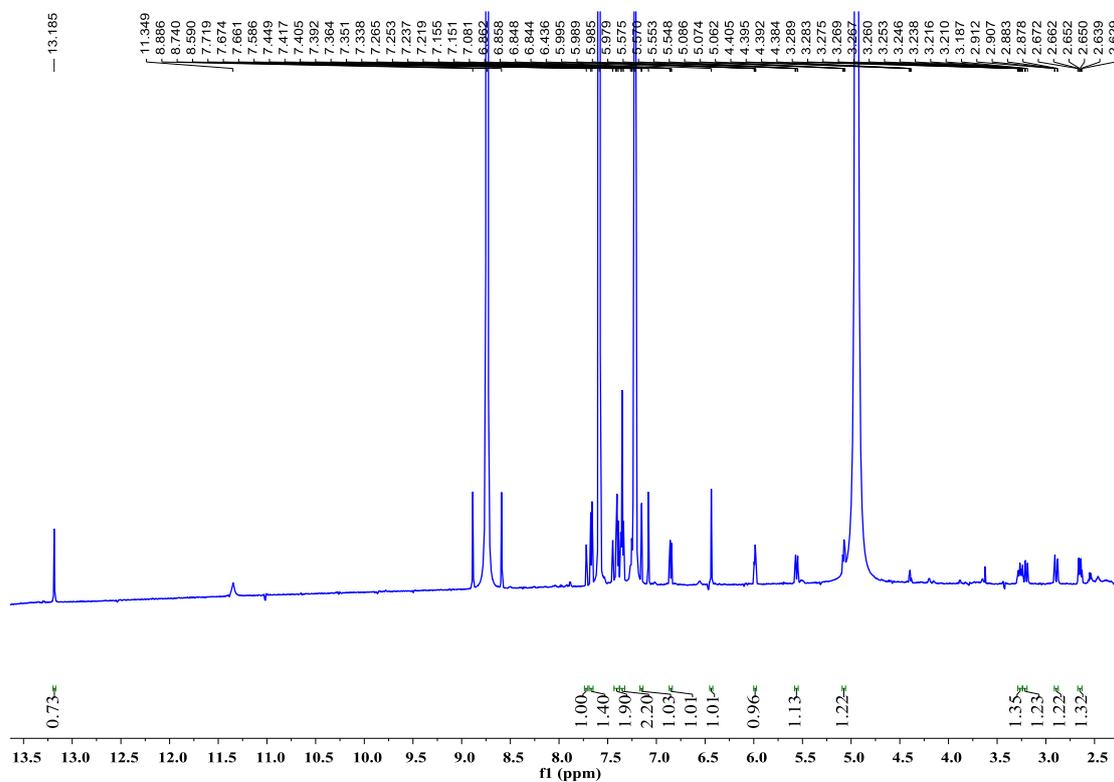


Figure S6. ¹H NMR spectrum of oxytrodidflavanone A (**1**) in Pyridine-*d*₅

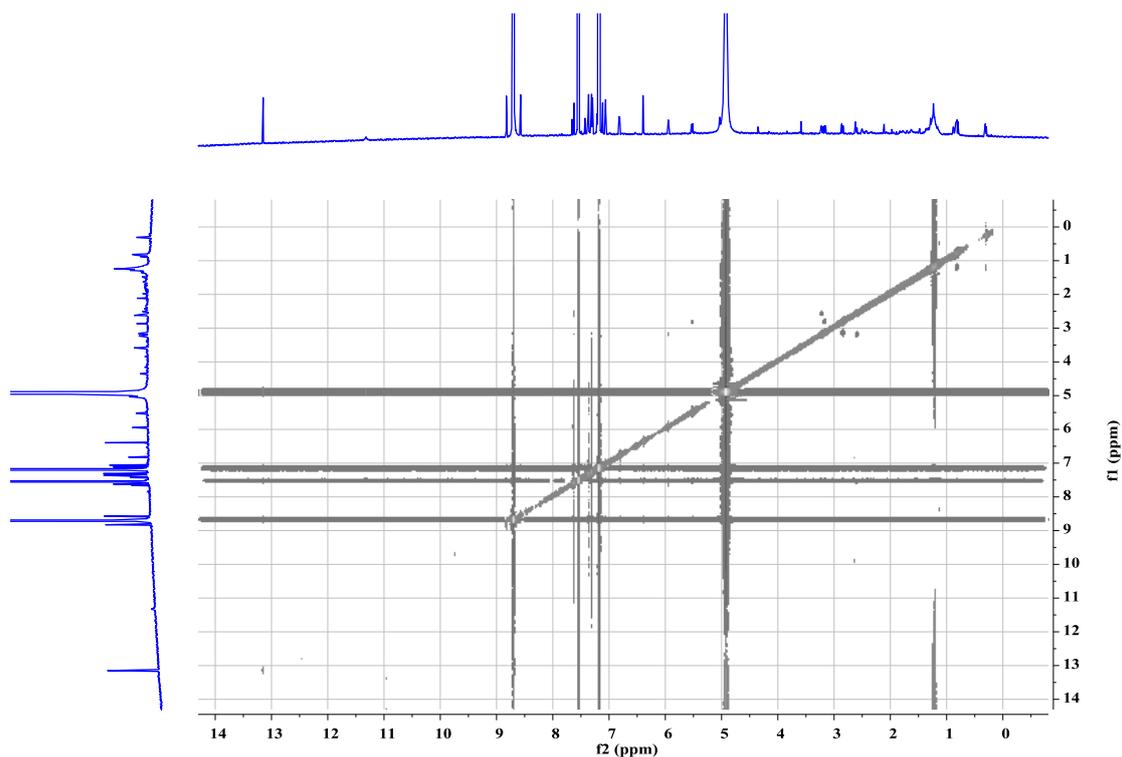


Figure S7. NOESY spectrum of oxytrodiflavanone A (**1**) in Pyridine-*d*₅

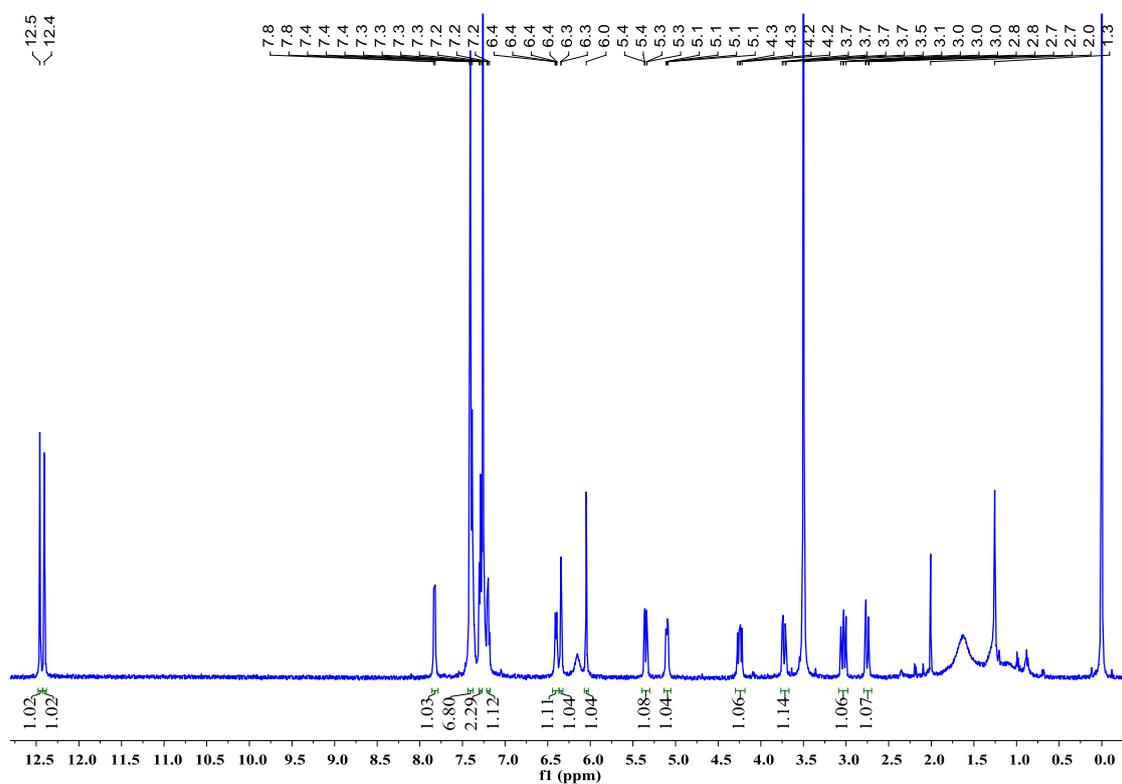


Figure S8. ¹H NMR spectrum of oxytrochalconflavanones A (**2**) and B (**3**) in CDCl₃

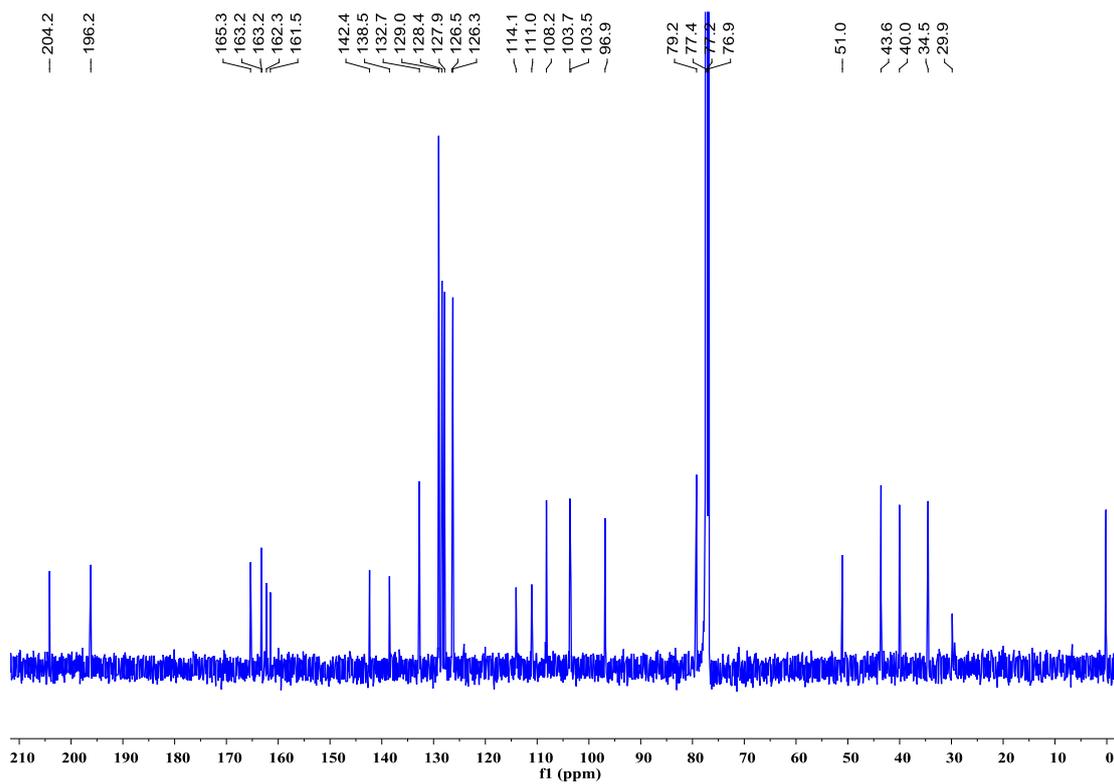


Figure S9. ^{13}C NMR spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3

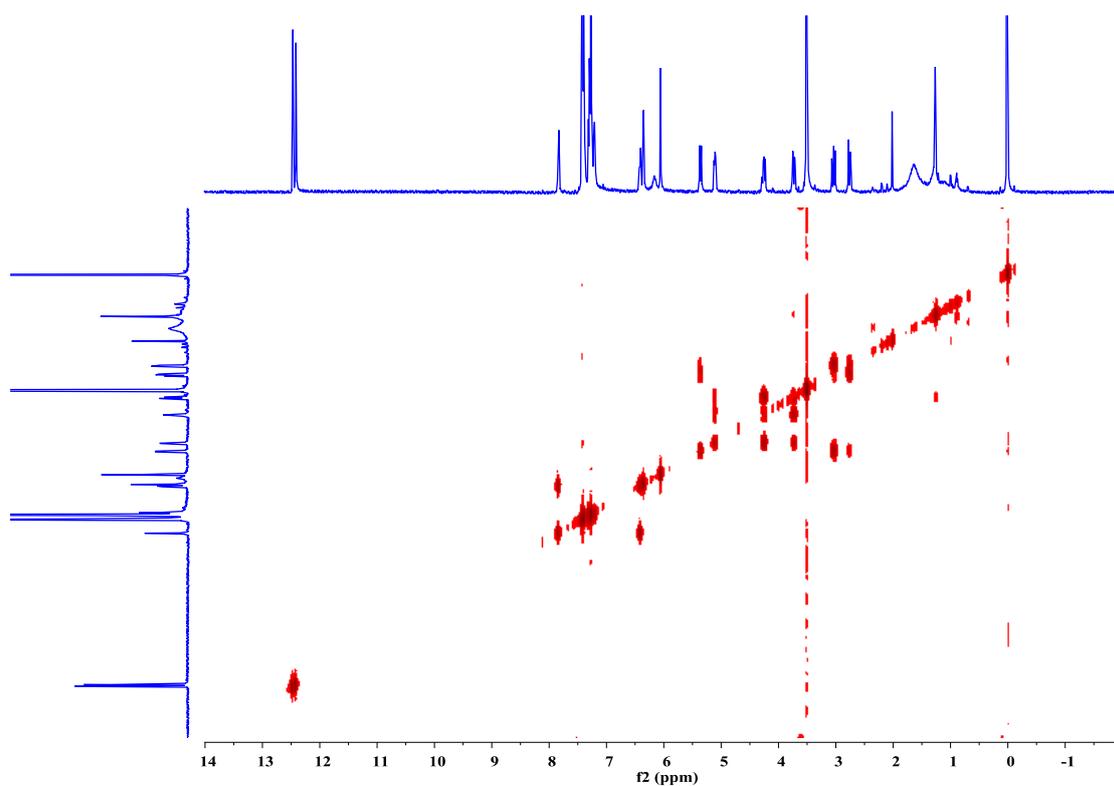


Figure S10. ^1H - ^1H COSY spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3

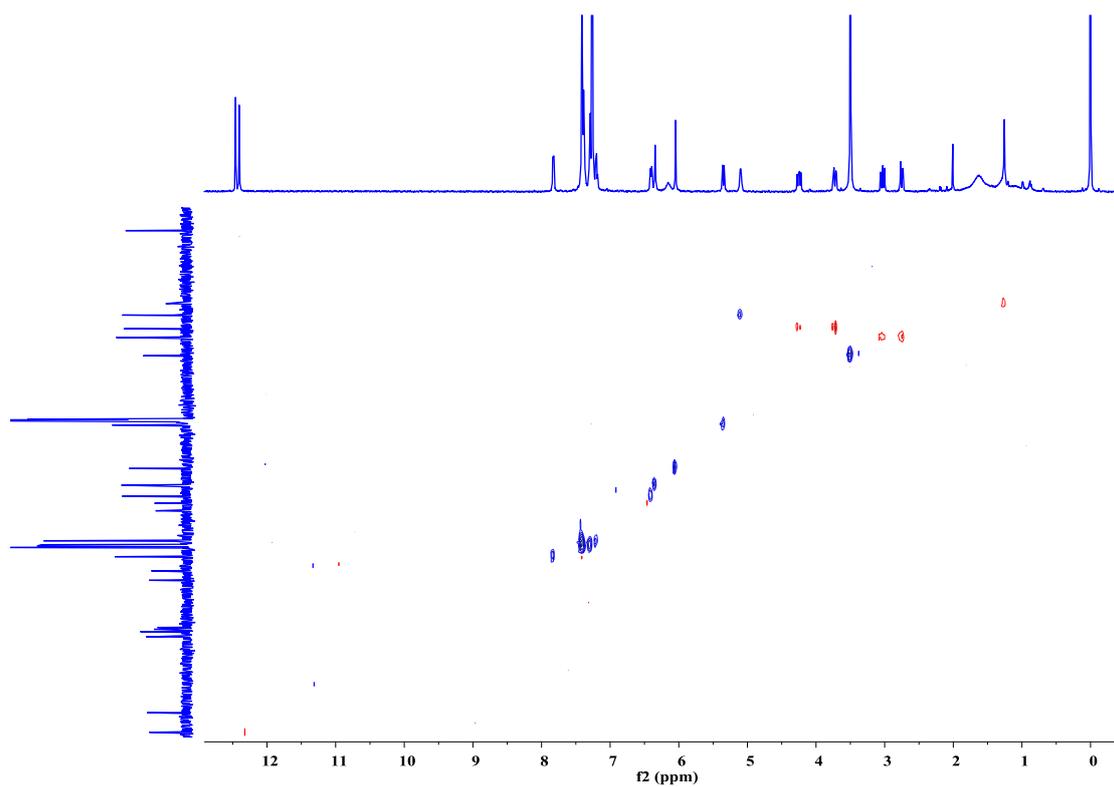


Figure S11. HSQC spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3

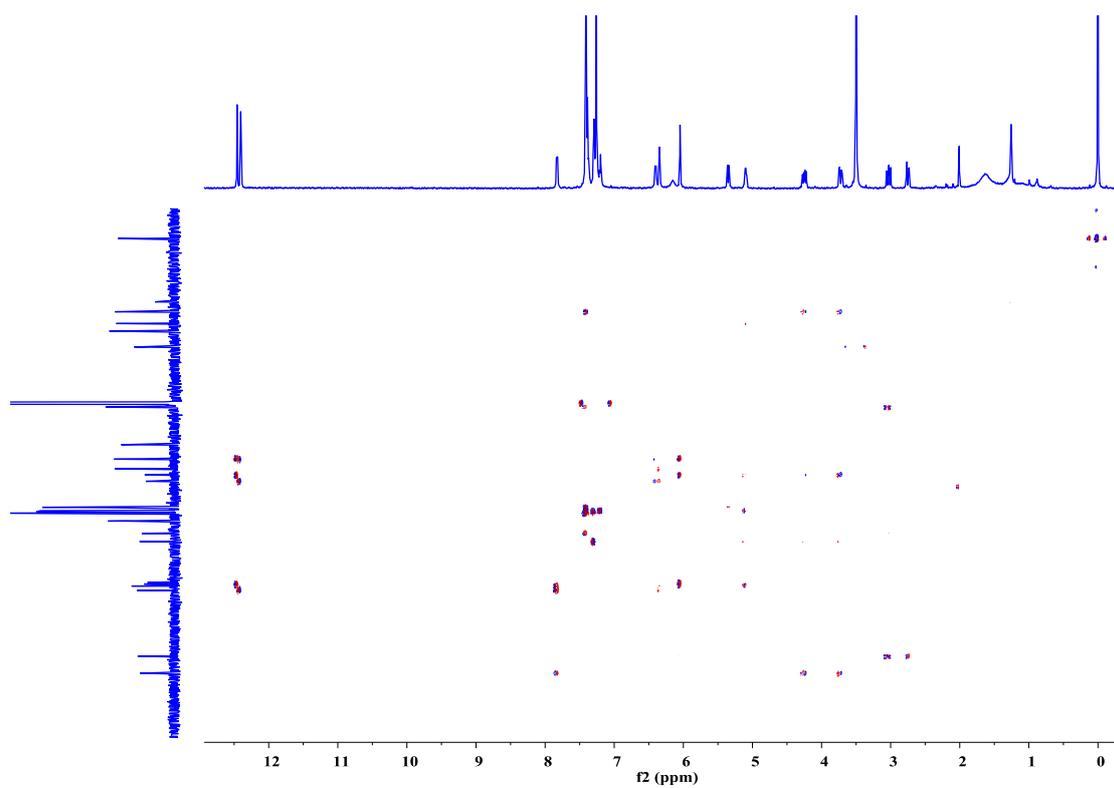


Figure S12. HMBC spectrum of oxytrochalcoflavanones A (**2**) and B (**3**) in CDCl_3

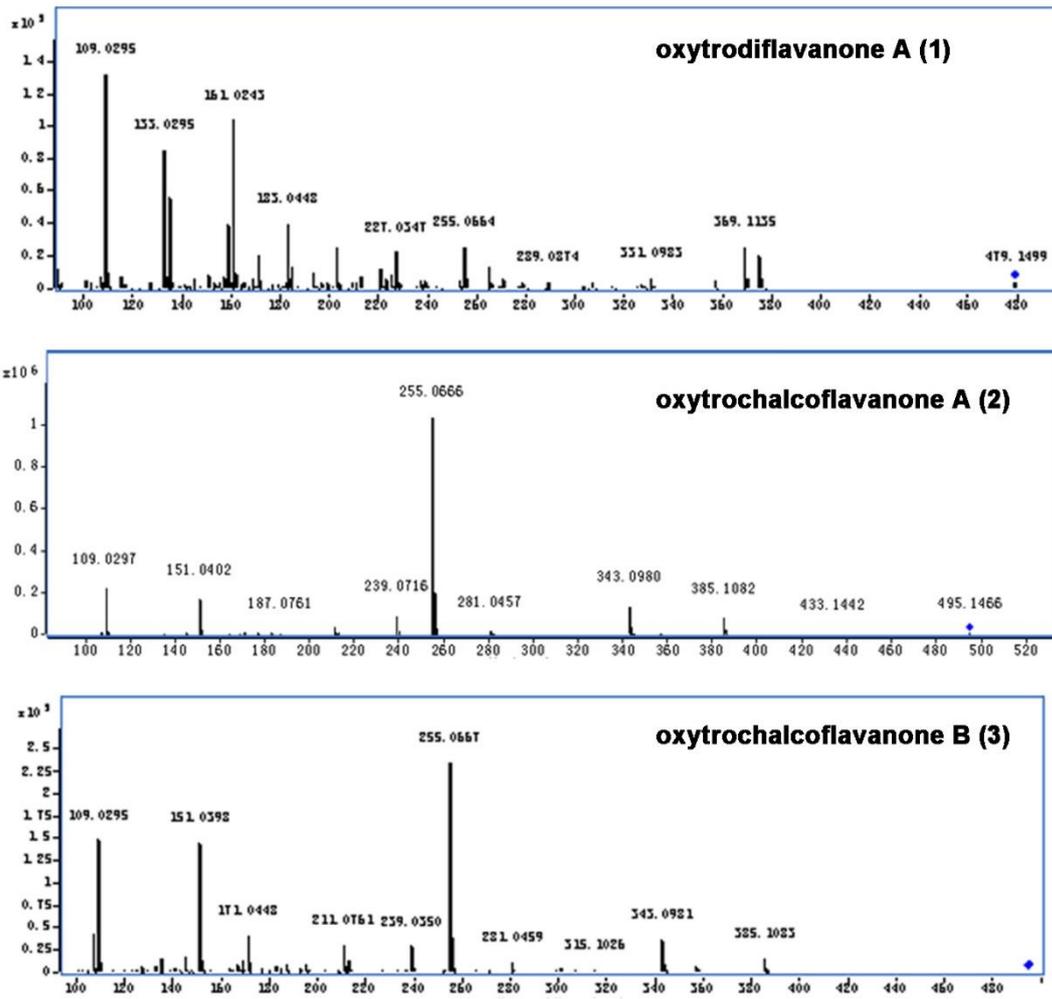


Figure S13. Targeted MS/MS spectra of oxytrodiflavanone A (1), oxytrochalcoflavanones A (2) and B (3) at CE of 25 eV in negative ion mode

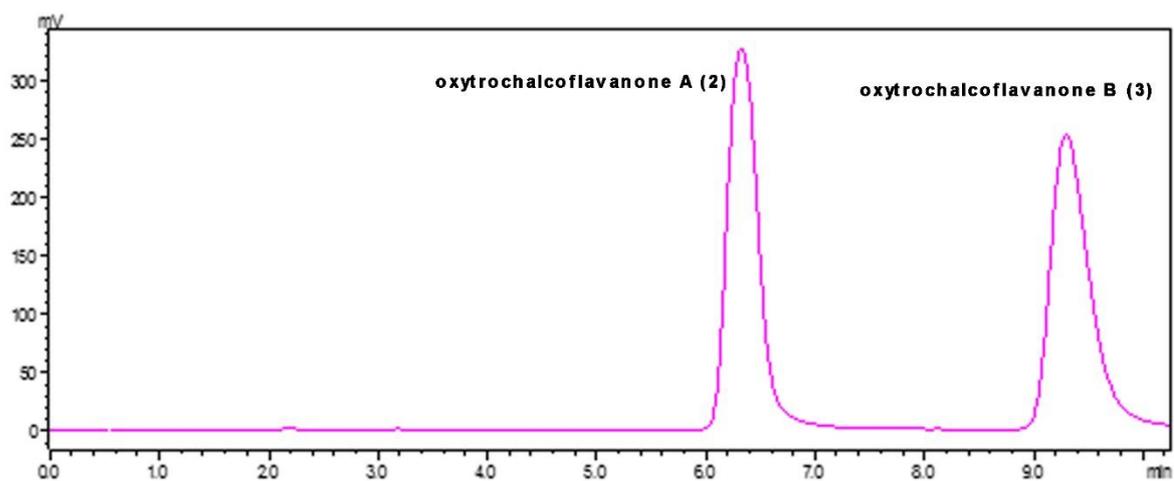


Figure S14. Chiral analysis of oxytrochalcoflavanones A–B (2-3)

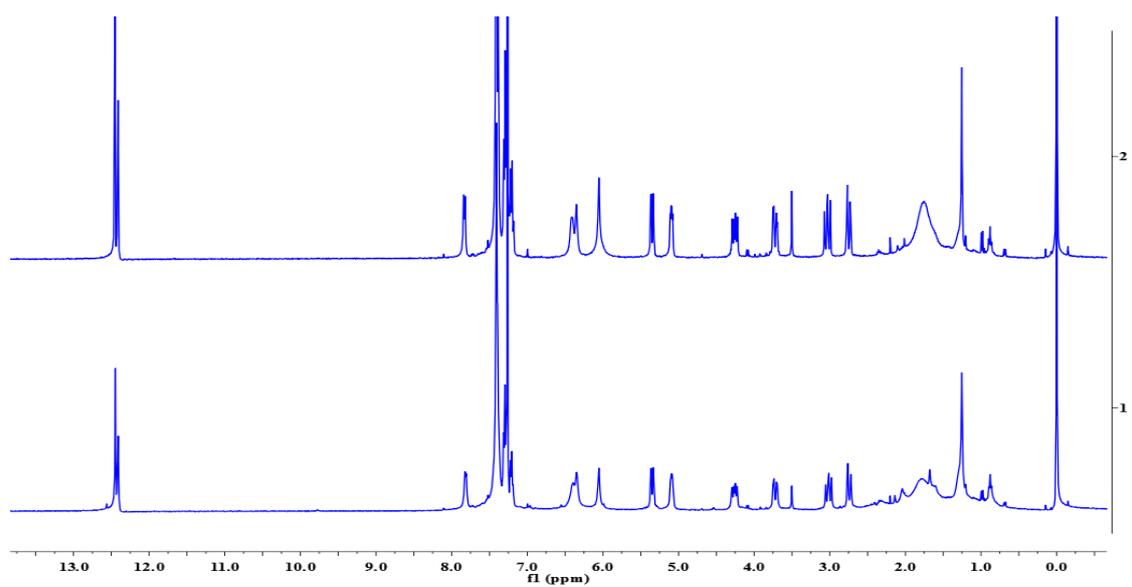


Figure S15. ¹H NMR spectra of the epimers of oxytrochalcoflavanones A–B (2-3)

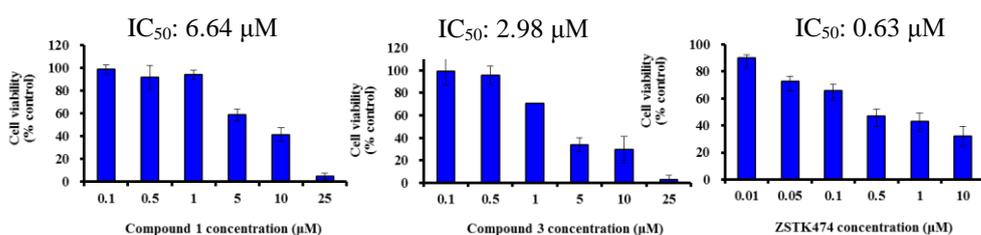


Figure S16. Cell growth inhibitory activities of oxytrodiflavanone A (**1**) and oxytrochalcoflavanone B (**3**) on PC3 cells. The activities of indicated concentrations of Compound 1, Compound 3 and ZSTK474 (positive control) on PC3 cells were determined by MTT assay. Data are presented as mean \pm SD, representative of three independent experiments.

Table S1. Raw data of cell growth inhibitory activities of oxytrodiflavanone A (**1**), oxytrochalcoflavanones B (**3**)

Compounds	Concentration (μM)	cell viability (mean \pm SD, %)
1	0.1	98.6 \pm 4.0
	0.5	91.4 \pm 10.7
	1	93.8 \pm 4.1
	5	58.6 \pm 5.1
	10	41.3 \pm 5.8
	25	4.9 \pm 2.9
	0.1	99.4 \pm 12.4
3	0.5	95.5 \pm 8.1
	1	70.5 \pm 0.4
	5	33.8 \pm 6.2
	10	29.4 \pm 12.1
	25	2.6 \pm 4.1
ZSTK474	0.01	90.0 \pm 2.5
	0.05	73.0 \pm 3.4
	0.1	66.0 \pm 4.4
	0.5	47.0 \pm 5.1
	1	43.0 \pm 6.3
	10	32.0 \pm 7.5