

**Two New Aristolochic Acid Analogues from the Roots of *Aristolochia contorta*
with Significant Cytotoxic Activity**

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Supporting Information Content:

S1. The HR-ESI-MS spectrum of compound **9**.

S2. The UV spectrum of compound **9** (methanol).

S3. The IR spectrum of compound **9**.

S4. The ¹H NMR spectrum of compound **9** (DMSO-*d*₆, 500 MHz).

S5. The ¹³C NMR spectrum of compound **9** (DMSO-*d*₆, 125 MHz).

S6. The HSQC spectrum of compound **9** (DMSO-*d*₆, 500 MHz).

S7. The HMBC spectrum of compound **9** (DMSO-*d*₆, 500 MHz).

S8. A: tR of compound **9**;

B: *m/z* of compound **9** at the same retention time;

C: TIC of the methanol extract from root of *A. contorta* by LC-Q-TOF/MS;

D: EIC of *m/z* 397.03 from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions;

E: Compound **9** was identified from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions. As indicated by symbols # and *.

S9. The HR-ESI-MS spectrum of compound **10**.

S10. The UV spectrum of compound **10** (methanol).

S11. The ¹H NMR spectrum of compound **10** (DMSO-*d*₆, 500 MHz).

S12. The ¹³C NMR spectrum of compound **10** (DMSO-*d*₆, 125 MHz).

S13. The HSQC spectrum of compound **10** (DMSO-*d*₆, 500 MHz).

S14. F: tR of compound **10**;

G: *m/z* of compound **10** at the same retention time;

H: TIC of the methanol extract from root of *A. contorta* by LC-Q-TOF/MS;

I: EIC of *m/z* 413.035 from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions;

J: Compound **10** was identified from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions. As indicated by symbols δ and ϵ .

S15. ^1H NMR (DMSO- d_6 , 500 MHz) and ^{13}C NMR (DMSO- d_6 , 125 MHz) spectral data for compounds **1, 3, 5, 6**, and **7**.

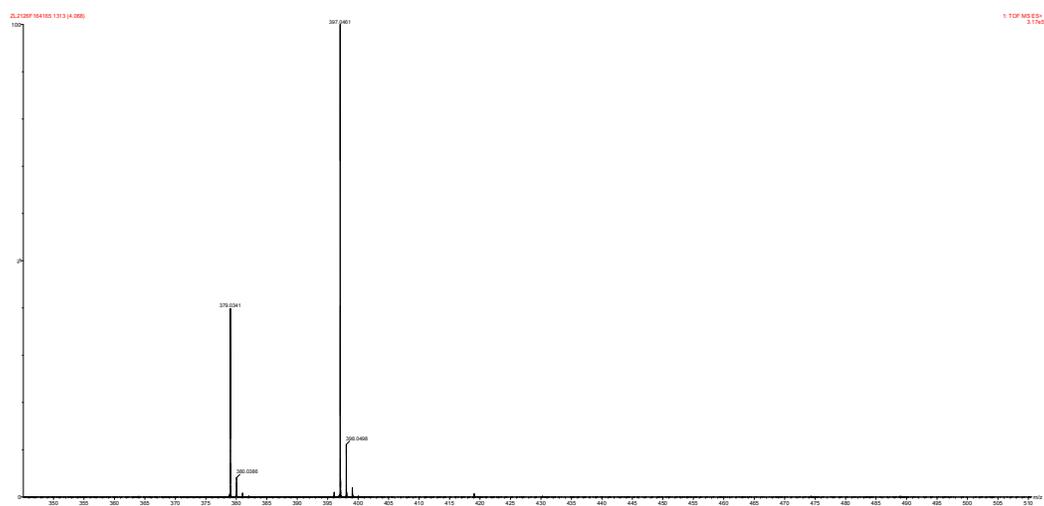
S16. ^1H NMR (DMSO- d_6 , 500 MHz) and ^{13}C NMR (DMSO- d_6 , 125 MHz) spectral data for compounds **2, 4, 8, 11**, and **12**.

S17. Structure of PDB code **4NOG**.

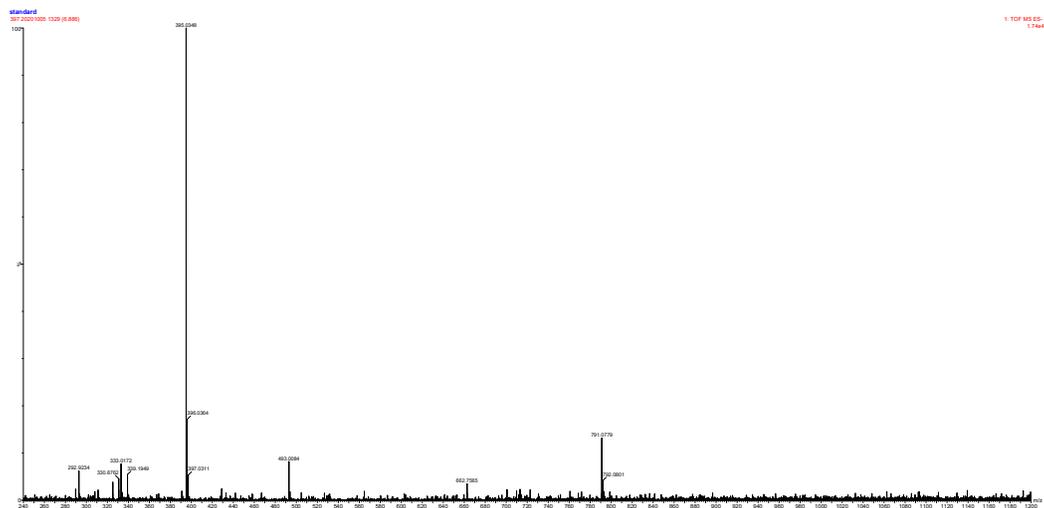
S18. **4NOG** generated with ligand by SWISS-MODEL software get 45.39% identity with OAT1.

S1. HR-ESI-MS spectrum of compound **9**.

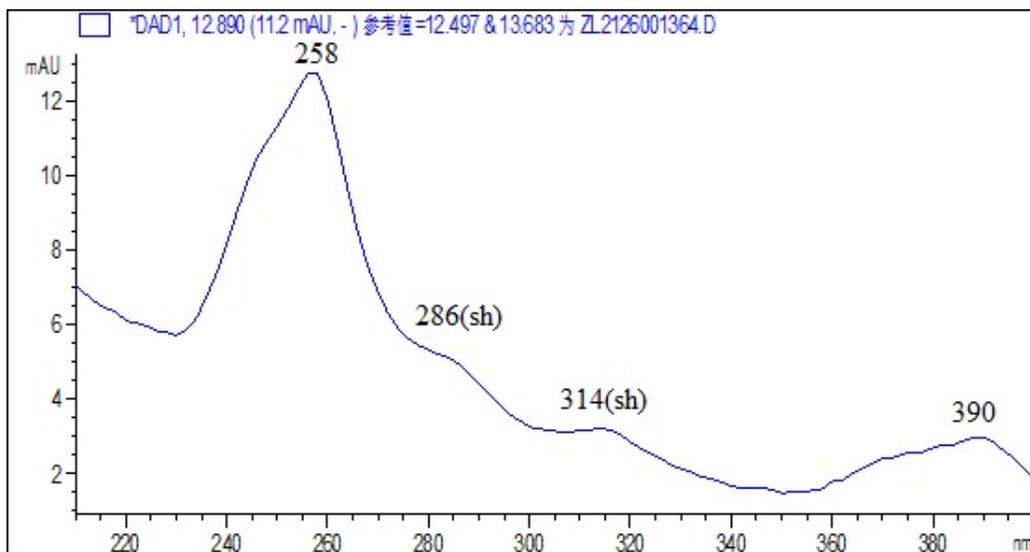
HR-ESI(+)-MS spectrum of compound **9**.



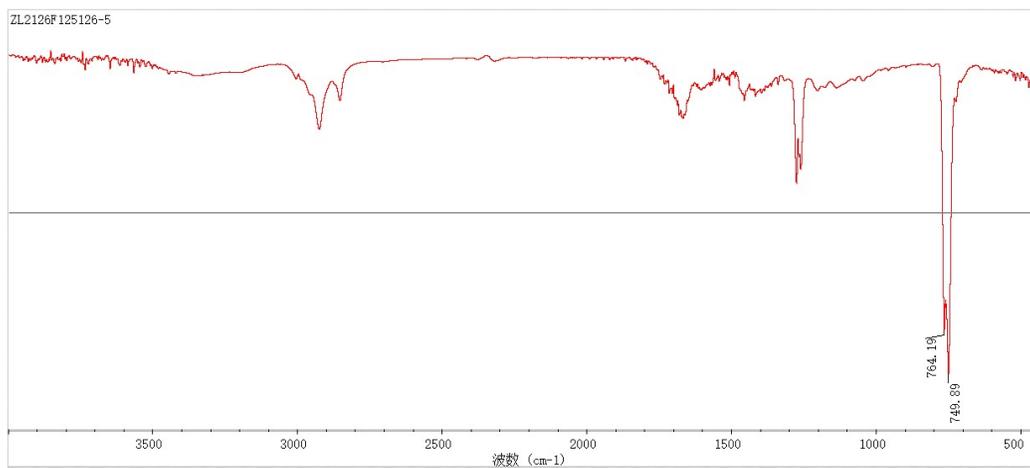
HR-ESI(-)-MS spectrum of compound **9**.



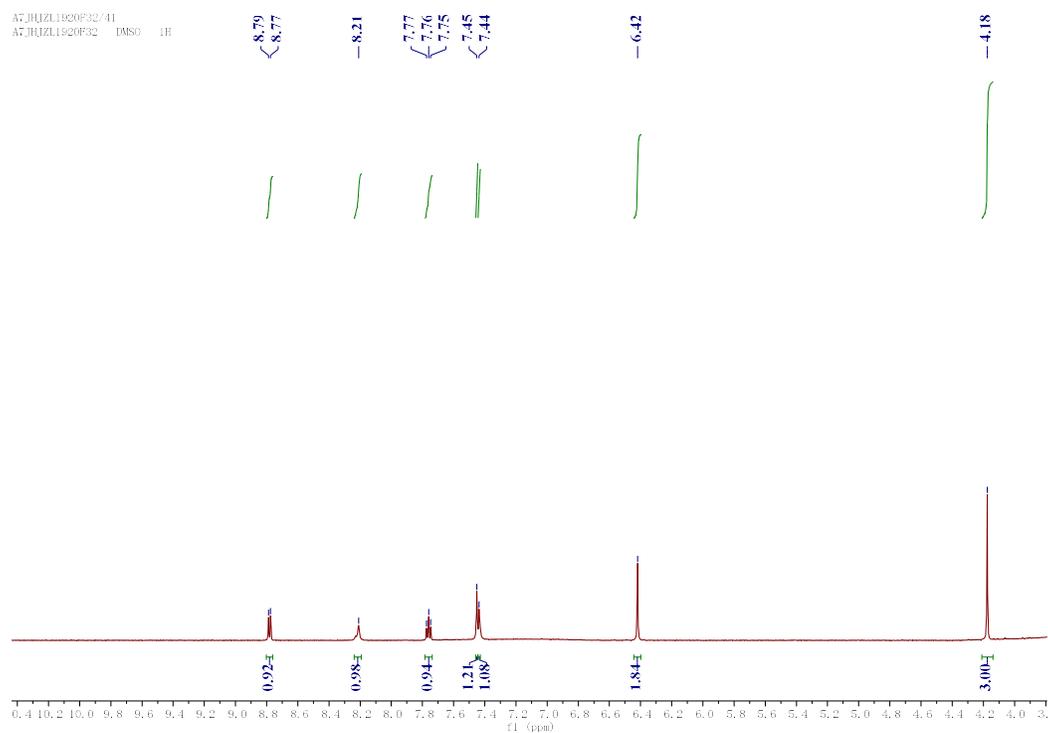
S2. UV spectrum of compound **9** (methanol).



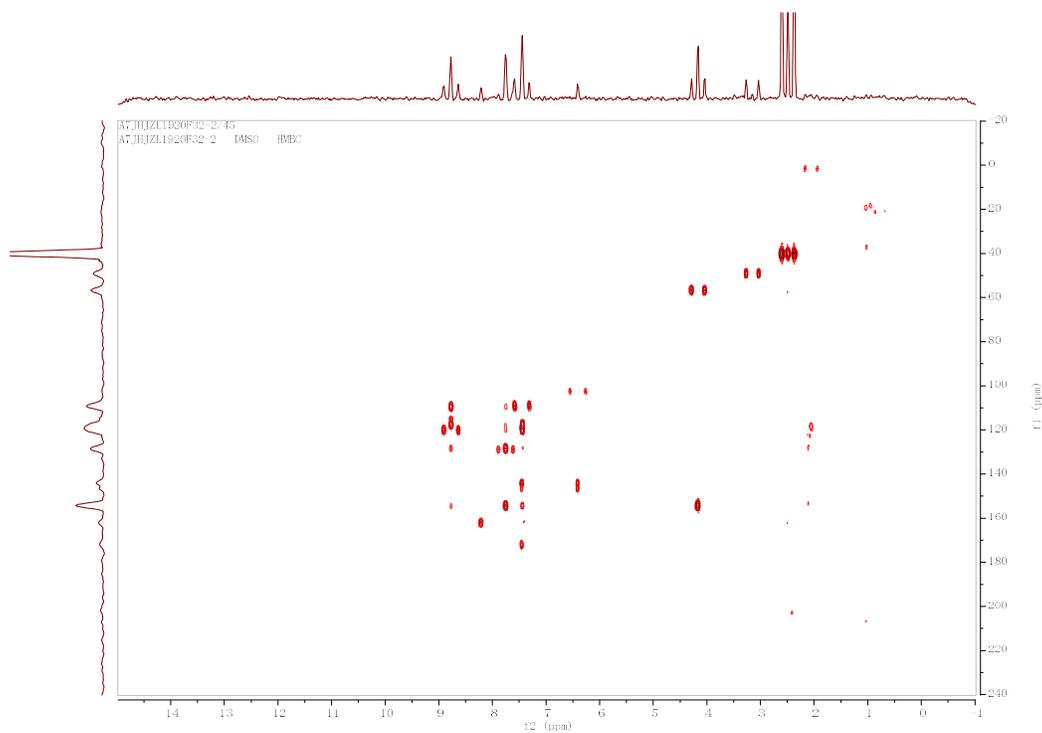
S3. IR spectrum of compound **9**.



S4. ^1H NMR spectrum of compound **9** (DMSO- d_6 , 500 MHz).



S5. ^{13}C NMR spectrum of compound **9** (DMSO- d_6 , 125 MHz).



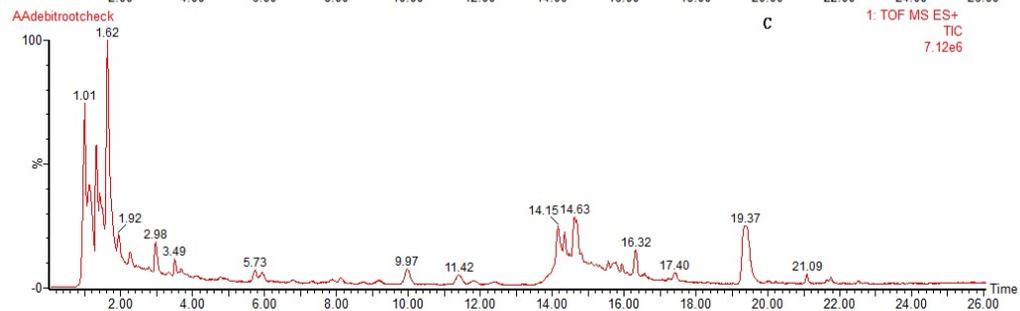
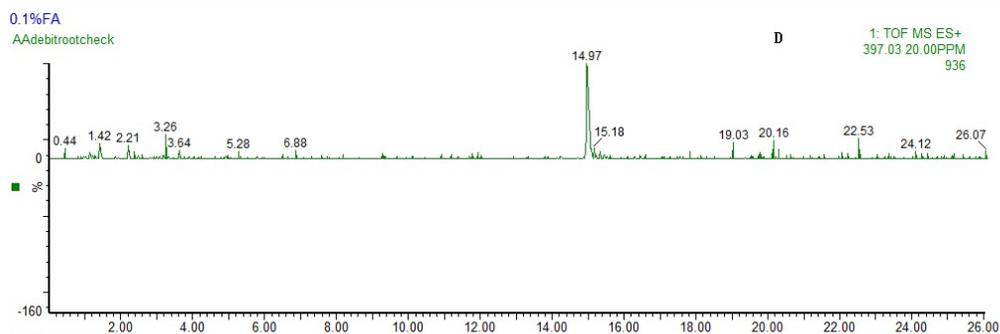
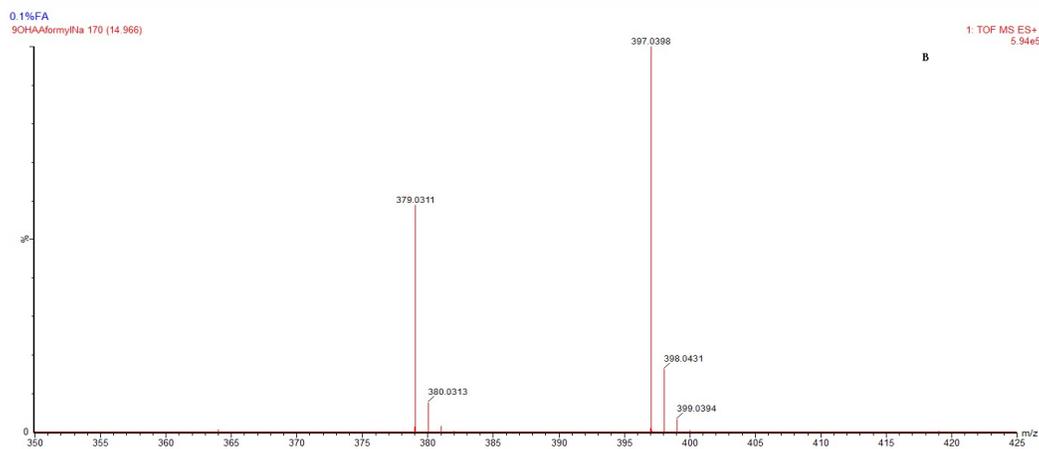
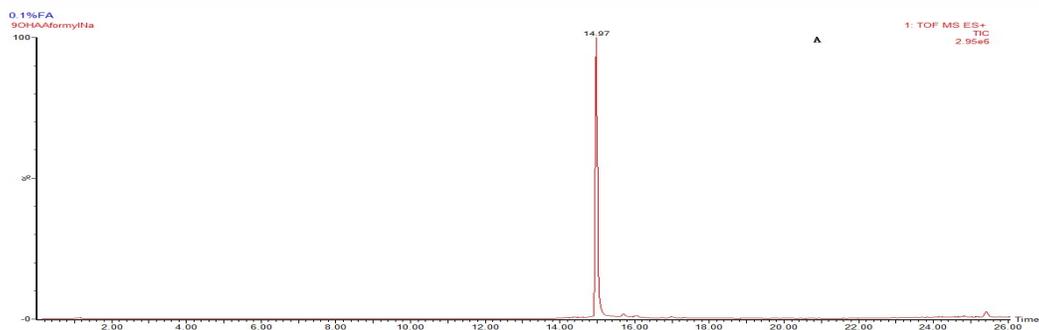
S8. A: tR of compound 9;

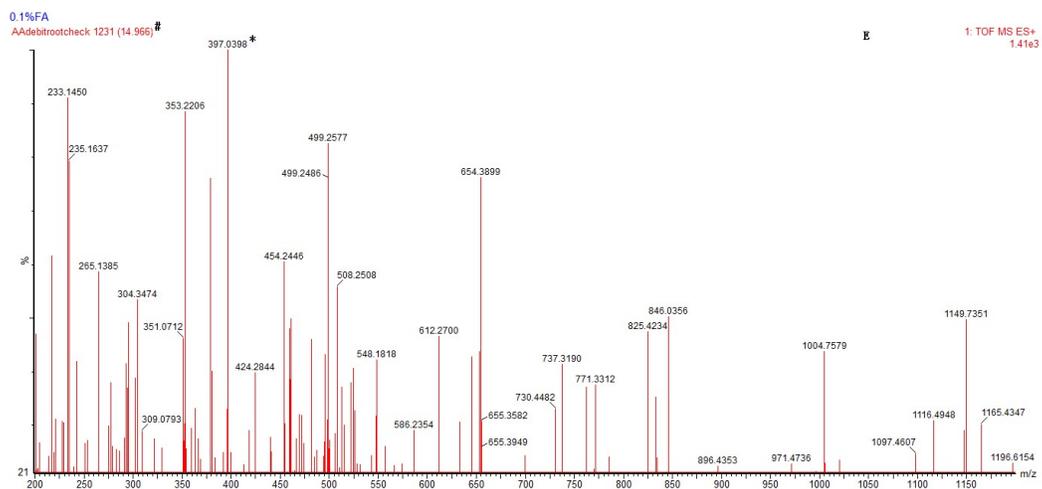
B: m/z of compound 9 at the same retention time;

C: TIC of the methanol extract from root of *A. contorta* by LC-Q-TOF/MS;

D: EIC of m/z 397.03 from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions;

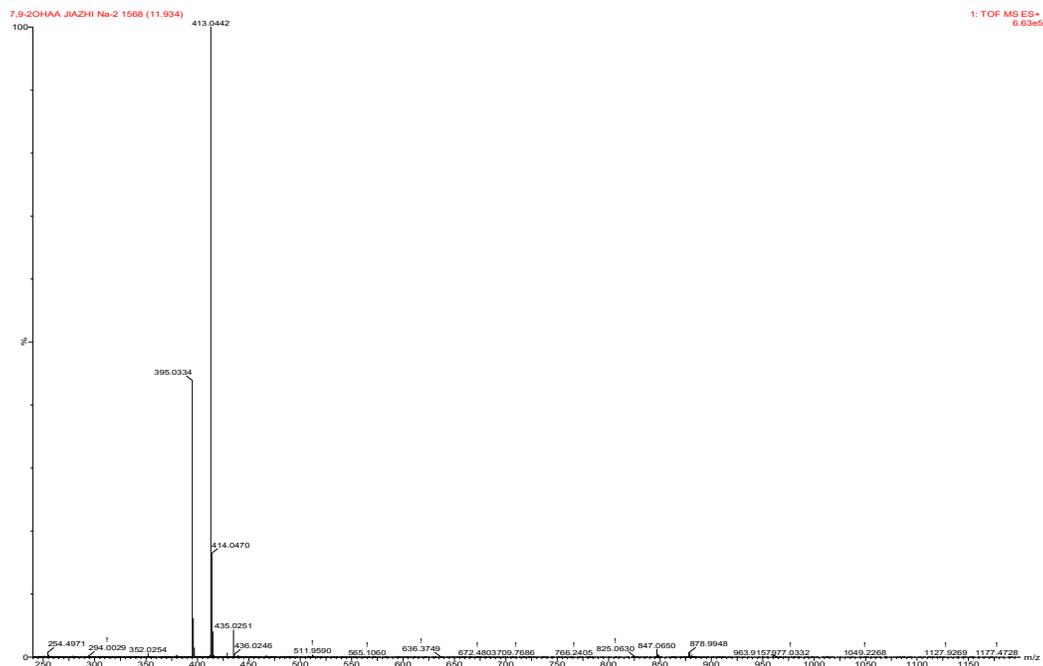
E: Compound 9 was identified from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions. As indicated by symbols # and *.



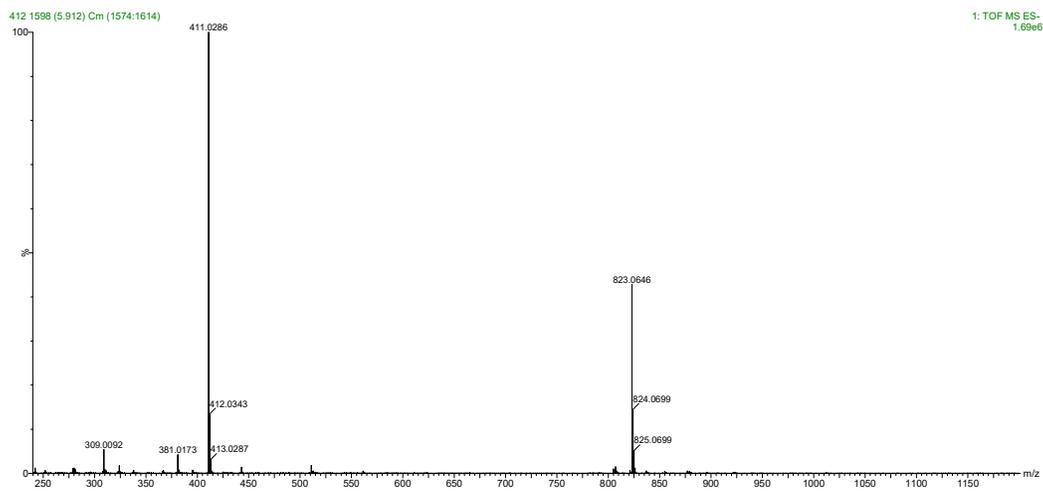


S9. HR-ESI-MS spectrum of compound **10**.

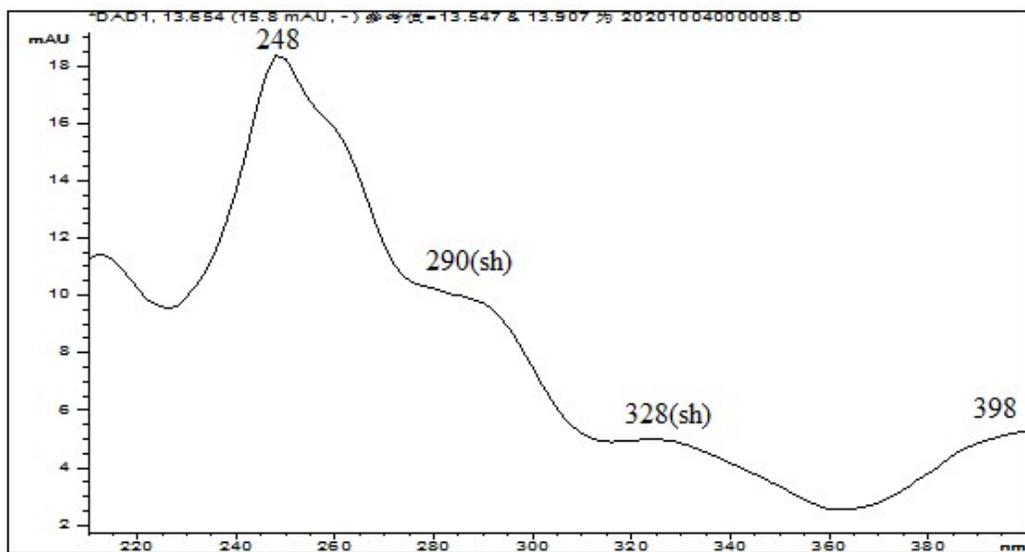
HR-ESI(+)-MS



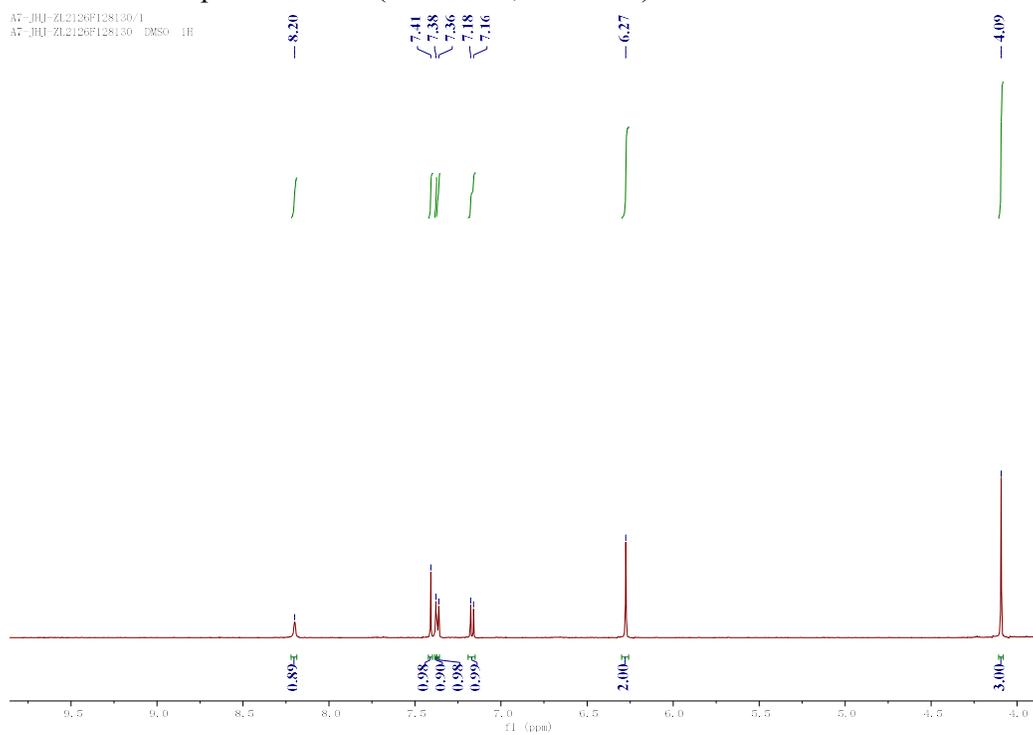
HR-ESI(-)-MS



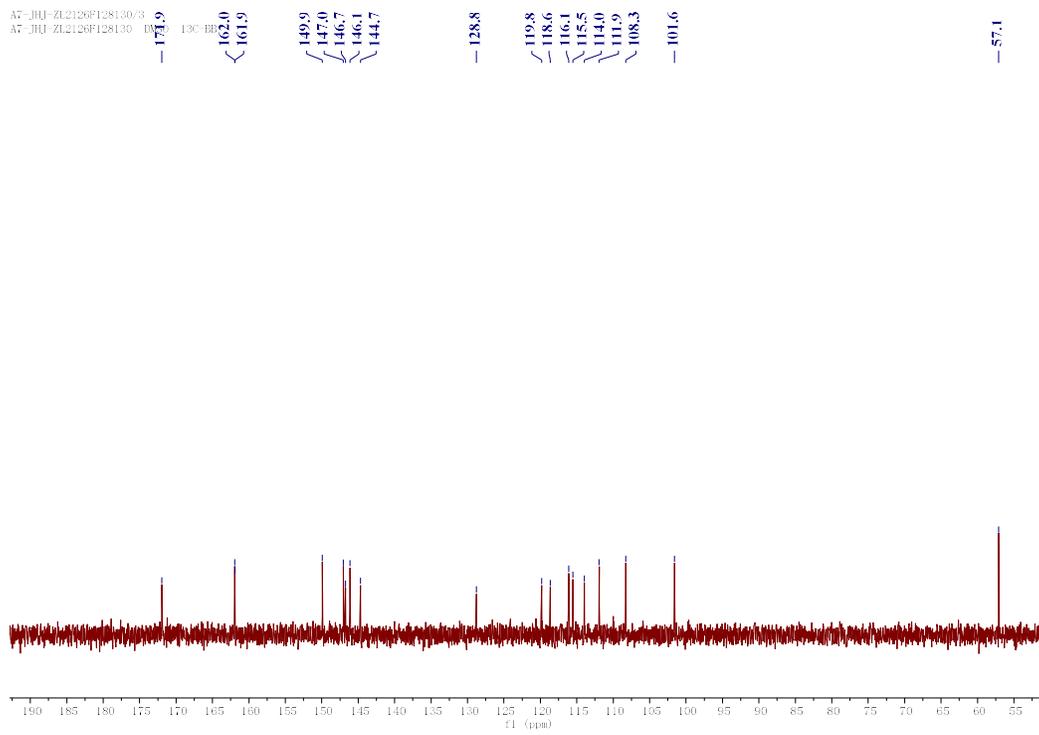
S10. UV spectrum of 10 (methanol).



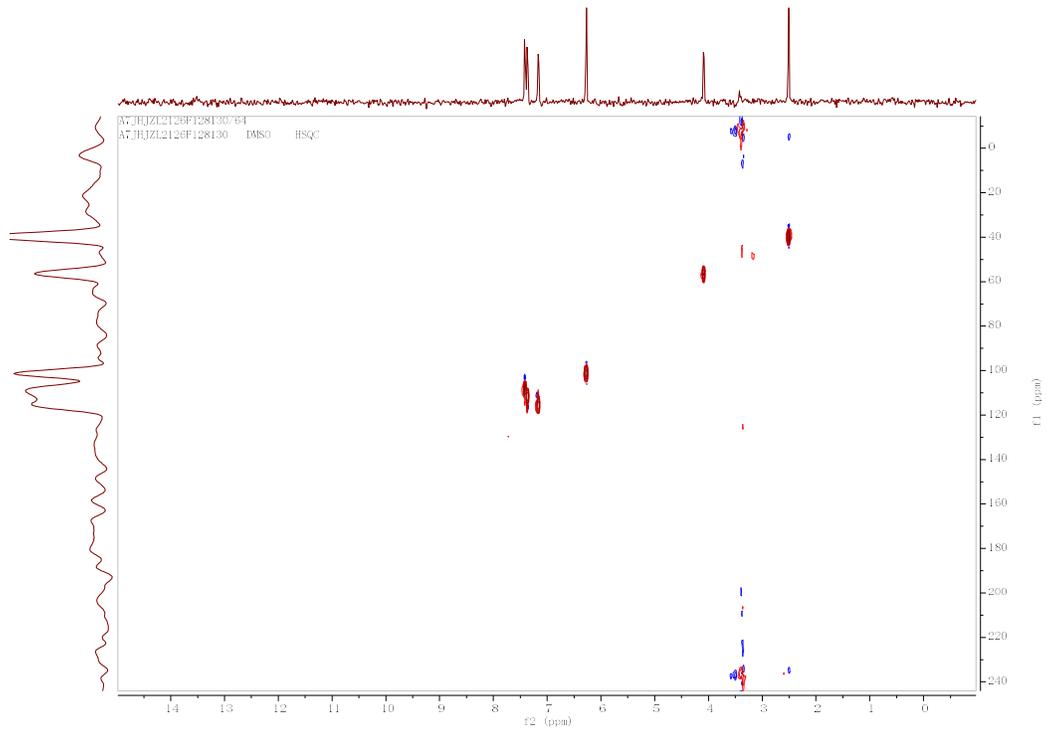
S11. ^1H NMR spectrum of 10 (DMSO- d_6 , 500 MHz).



S12. The ^{13}C NMR spectrum of compound 10 (DMSO- d_6 , 125 MHz).



S13. HSQC spectrum of compound **10** (DMSO-*d*₆, 500 MHz).



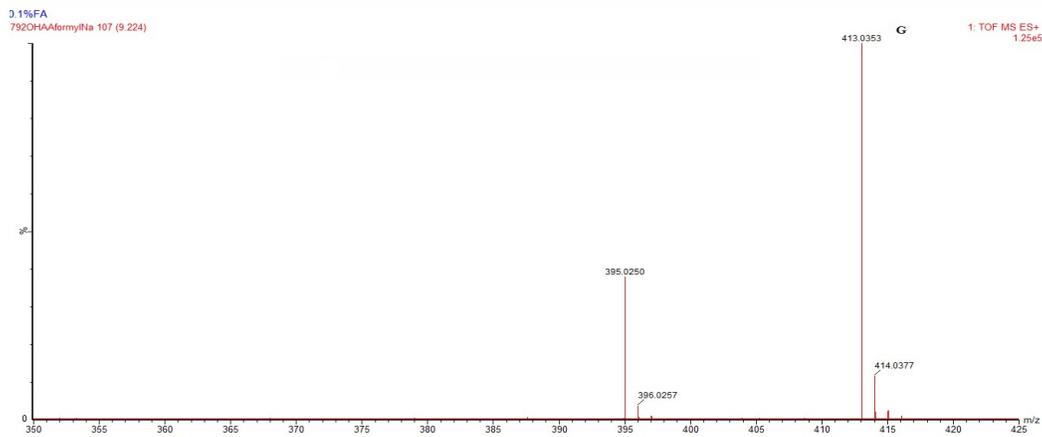
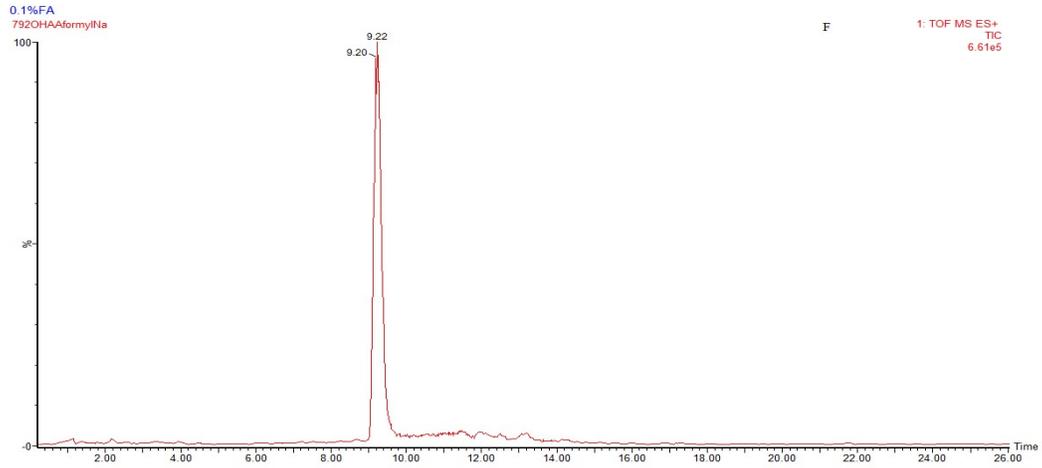
S14. F: tR of compound **10**;

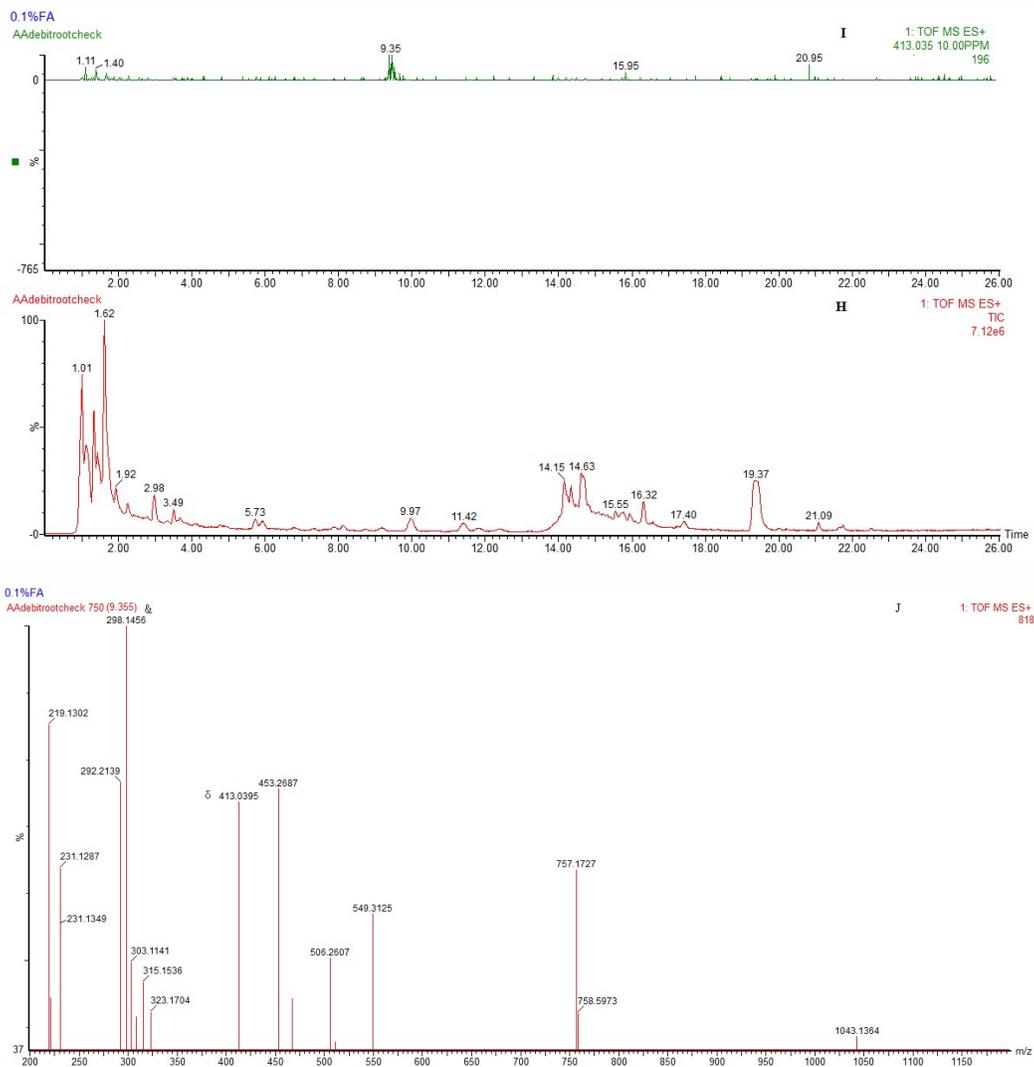
G: *m/z* of compound **10** at the same retention time;

H: TIC of the methanol extract from root of *A. contorta* by LC-Q-TOF/MS;

I: EIC of m/z 413.035 from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions;

J: Compound **10** was identified from the methanol extract from root of *A. contorta* by LC-Q-TOF/MS under the same liquid chromatography and mass spectrometry conditions. As indicated by symbols δ and δ .





S15. ¹H NMR (DMSO-*d*₆, 500 MHz) and ¹³C NMR (DMSO-*d*₆, 125 MHz) spectral data for compounds **1**, **3**, **5**, **6**, and **7** (δ in ppm, *J* in Hz).

	1		3		5		6		7	
C	δ_H	δ_C								
1		128.		124.		124.		120.		121.
		5		3		1		4		5
2	7.8, s	111.	7.8, s	112.	7.7, s	110.	7.74, s	112.	7.75, s	111.
		8		2		8		4		7
3		146		146		145.		145.		145.
						8		8		4
4		146.		146.		146.		146.		145.
		4		7		3		2		8
4a		117.		116.		117.		117.		117.
		2		8		8		1		3
4b		128.		129.		132.		132.		132.

		8		9		7		1		4
5	9.10, d (8.4)	126. 5	8.65, d(8.5)	118. 4	8.70, d(9.05)	121. 9	8.09, s	103. 1	8.48, d (2.2)	111. 1
6	7.83, t(7.3)	130. 4	7.85, t(8.2)	131. 6	7.50, d(9.05)	122. 8	10.86, br,s(- OH)	161. 7		159. 8
7	7.92, t(7.6)	128. 7	7.37, d(8.1)	108. 9	10.44, br,s(- OH)	148. 4	6.84, s	104. 2	7.29, dd (8.7, 2.2)	116. 6
8	8.27, d(7.9)	130. 4		156. 3		148. 9		158. 5	8.09, d(8.7)	130. 9
8a		129. 6		118. 8		122. 8		112. 6		121. 5
9	8.58, s	125. 8	8.58, s	119. 4	8.40, (1H, s)	121. 5	8.46, s	120. 5	8.48, s	126. 3
10		146		146		142. 9		143. 2		143. 5
10a		116. 6		117. 3		115. 5		118. 2		118. 7
-OCH 3			4.07, s	56.3	3.98, s	60.9	4.01, s	56.6		
-CH2 O-	6.51, s	102. 9	6.50, s	102. 9	6.45, s	102. 6	6.46, s	100. 2	6.49, s	102. 7

S16. ^1H NMR (DMSO- d_6 , 500 MHz) and ^{13}C NMR (DMSO- d_6 , 125 MHz) spectral data for compounds **2**, **4**, **8**, **11**, and **12** (δ in ppm, J in Hz).

	2		4		8		11		12	
C	δ_{H}	δ_{C}								
1		119. 3		122. 2		124. 1		118. 1		117. 3
2	7.66,s	105. 8	7.63,s	113. 4	7.77,s	106. 5	7.72,s	106	7.74,s	105. 6
3		148. 9		152. 3		149. 4		148. 8		148. 7
4		147. 2	10.77,s	148. 8		148. 1		147. 8		147. 5
4a		110		120. 3		111		111. 2		111. 3

4b		124. 9		126. 7		124. 8		126		125. 2
5	8.1,d(6.2)	118. 8	9.11,d(7.7)	126	8.21,d(8.05)	118. 2	8.01,d,(2.5)	118	8.08,d(8.1)	117. 6
6	7.52, t(6.6)	125	7.52-7.58, m	125. 2	7.60,t(8.05,8.0 5)	126. 9		156. 2	7.43,t(7.9,7. 8)	126. 4
7	7.21,d(6. 6)	108. 4	7.52-7.58, m	127. 2	7.26,d(8.05)	111. 6	7.13,dd(2.5,6. 1)	118. 2	7.12, d(7.8)	112. 5
8		155. 3	7.93,d(8.5 5)	128. 9		155. 9	7.87,d(8.7)	130. 9		154
8a		124		134. 8		119. 2		126. 9		122. 8
9	7.36,s	97.9	7.09,s	103. 8	7.66,s	109. 1	7.35,s	107. 9	7.64,s	101. 1
10		132. 8		135. 3		134. 1		131. 9		132. 7
10a		125. 8		121. 7		125. 4		125. 1		124. 5
CONR	10.77,s	168. 2		168. 4		166. 6		166. 5		166. 2
-OCH2 O-	6.48,s	103. 3			6.51,s	103. 9	6.52,s	103. 7	6.50,s	103. 3
-OCH3	4.00,s	55.9	4.02,s	59.4 3	4.02,s	56.5				
1"					5.35,d(9.3)	82.8	5.34,d(9.5)	82.3	5.35,d(9.3)	81.8
2"						70.9		70.6		69.9
3"						77.9		78		77.5
4"						72.8		70.3		70.4
5"						80.6		80.6		80.2
6"						61.8		61.8		61.3

S17. Structure of PDB code **4NOG**.



S18. 4NOG generated with ligand by SWISS-MODEL software get 45.39% identity with OAT1.

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[Templates 30](#)
[Models 0](#)

Template Results

Sort	Name	Title	Coverage	GMQE	QSQE	Identity	Method	Oligo State	Ligands
<input type="checkbox"/>	<input checked="" type="checkbox"/>	5eav1.B	Ornithine aminotransferase, mitochondrial, putative Unliganded structure of the ornithine aminotransferase from <i>Triclopsana gondi</i>	0.77	0.78	46.71	X-ray, 1.6Å	homo-dimer ✓	None
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	4hg9.1.A	Putative ornithine aminotransferase, mitochondrial Crystal structure of a putative ornithine aminotransferase from <i>Triclopsana gondi</i> ME48 in complex with pyrooxalyl-S-phosphate	0.74	0.75	45.39	X-ray, 1.2Å	homo-dimer ✓	2 x PLP ² , 1 x BTB ²
<input type="checkbox"/>	<input type="checkbox"/>	5eav1.B	Ornithine aminotransferase, mitochondrial, putative Unliganded structure of the ornithine aminotransferase from <i>Triclopsana gondi</i>	0.72	0.75	50.37	X-ray, 1.6Å	homo-dimer ✓	None
<input type="checkbox"/>	<input type="checkbox"/>	4hg9.1.A	Putative ornithine aminotransferase, mitochondrial Crystal structure of a putative ornithine aminotransferase from <i>Triclopsana gondi</i> ME48 in complex with pyrooxalyl-S-phosphate	0.72	0.74	50.37	X-ray, 1.2Å	homo-dimer ✓	2 x PLP ² , 1 x BTB ²
<input type="checkbox"/>	<input type="checkbox"/>	2oan.1.A	ORNITHINE AMINOTRANSFERASE HUMAN ORNITHINE AMINOTRANSFERASE COMPLEXED WITH L-CANAVINE	0.72	0.70	52.84	X-ray, 2.3Å	homo-dimer ✓	2 x CAN-PLP
<input type="checkbox"/>	<input type="checkbox"/>	2bpl.1.A	ORNITHINE AMINOTRANSFERASE Structure of ornithine aminotransferase from <i>Yersinia enterocolitica</i> mutant Y81-135A-G202F	0.73	0.67	52.57	X-ray, 2.1Å	homo-dimer ✓	2 x PLP ²
<input type="checkbox"/>	<input type="checkbox"/>	2bpl.1.A	ORNITHINE AMINOTRANSFERASE Ornithine aminotransferase mutant Y81	0.73	0.66	49.82	X-ray, 3.0Å	homo-dimer ✓	2 x PLP ²
<input type="checkbox"/>	<input type="checkbox"/>	1z74.1.A	ornithine aminotransferase Ornithine aminotransferase P702104 from <i>Pleurodium Yoellii</i>	0.68	0.70	46.38	X-ray, 2.1Å	homo-dimer ✓	None
<input type="checkbox"/>	<input type="checkbox"/>	6hg7.1.A	Ornithine aminotransferase, mitochondrial Crystal structure of human H1937 variant of ORNITHINE AMINOTRANSFERASE at 1.2 Angstrom	0.72	0.67	46.45	X-ray, 1.8Å	homo-dimer ✓	2 x PLP ²

Build Models 1

Clear Selection