Supporting Information

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Penioxalone A: A new isocoumarine derivative from *Penicillium oxalicum* with potent cytotoxic effects on A549 cells

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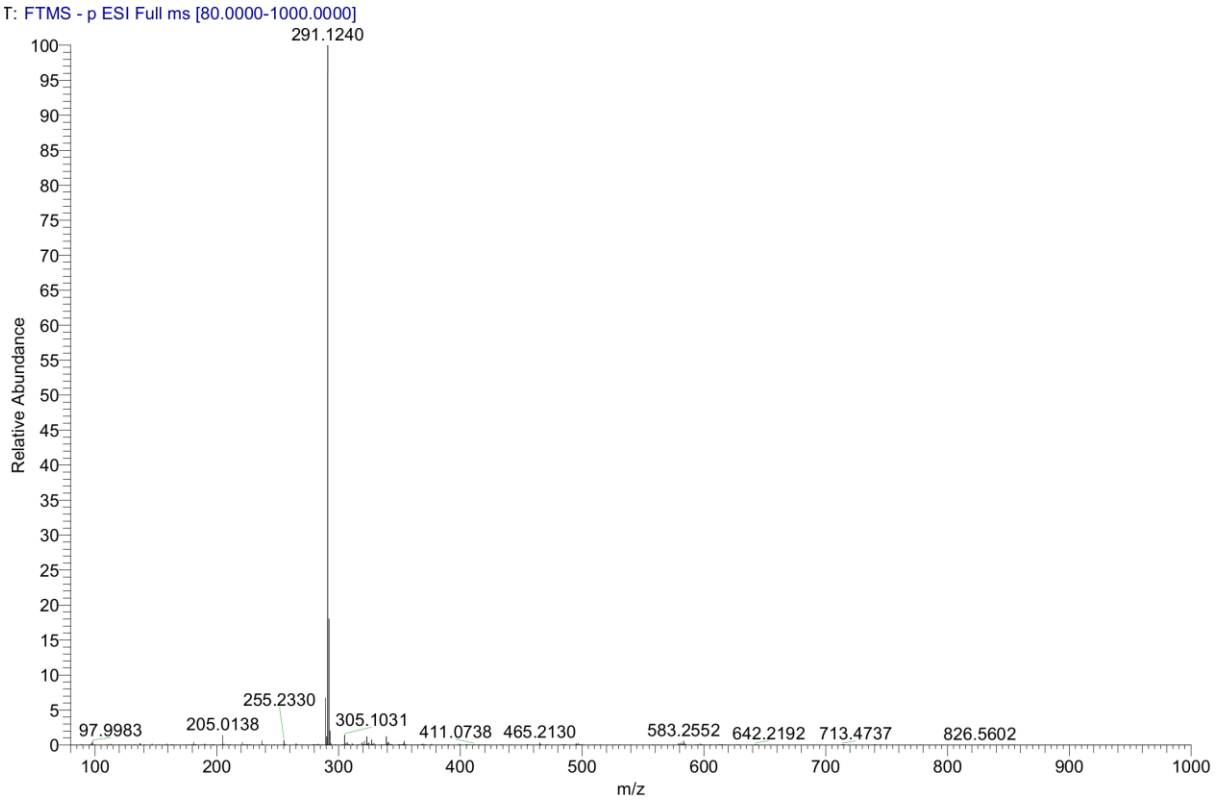

Figure S1: HR-ESI-MS spectrum of **1** (penioxalone A)

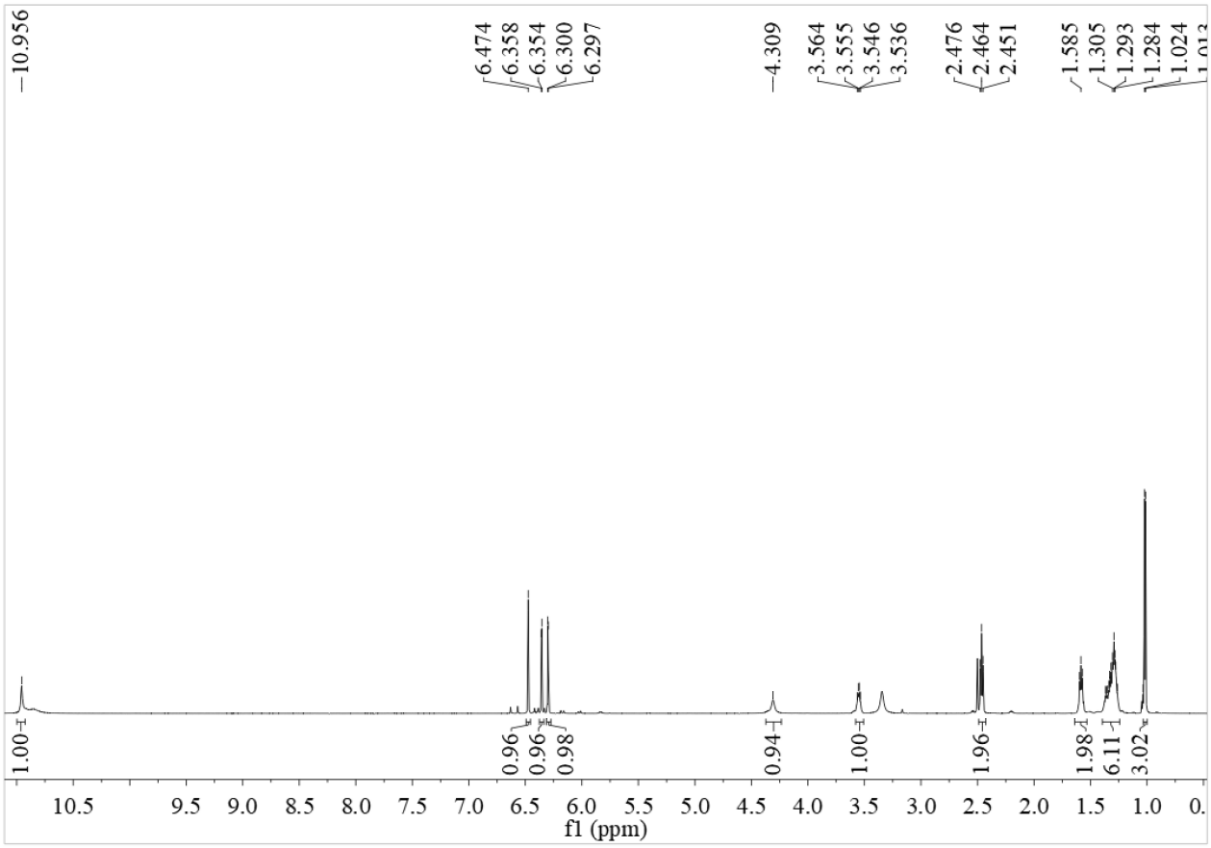

Figure S2: ^{1}H-NMR (600 MHz, DMSO-d_6) spectrum of **1** (penioxalone A)

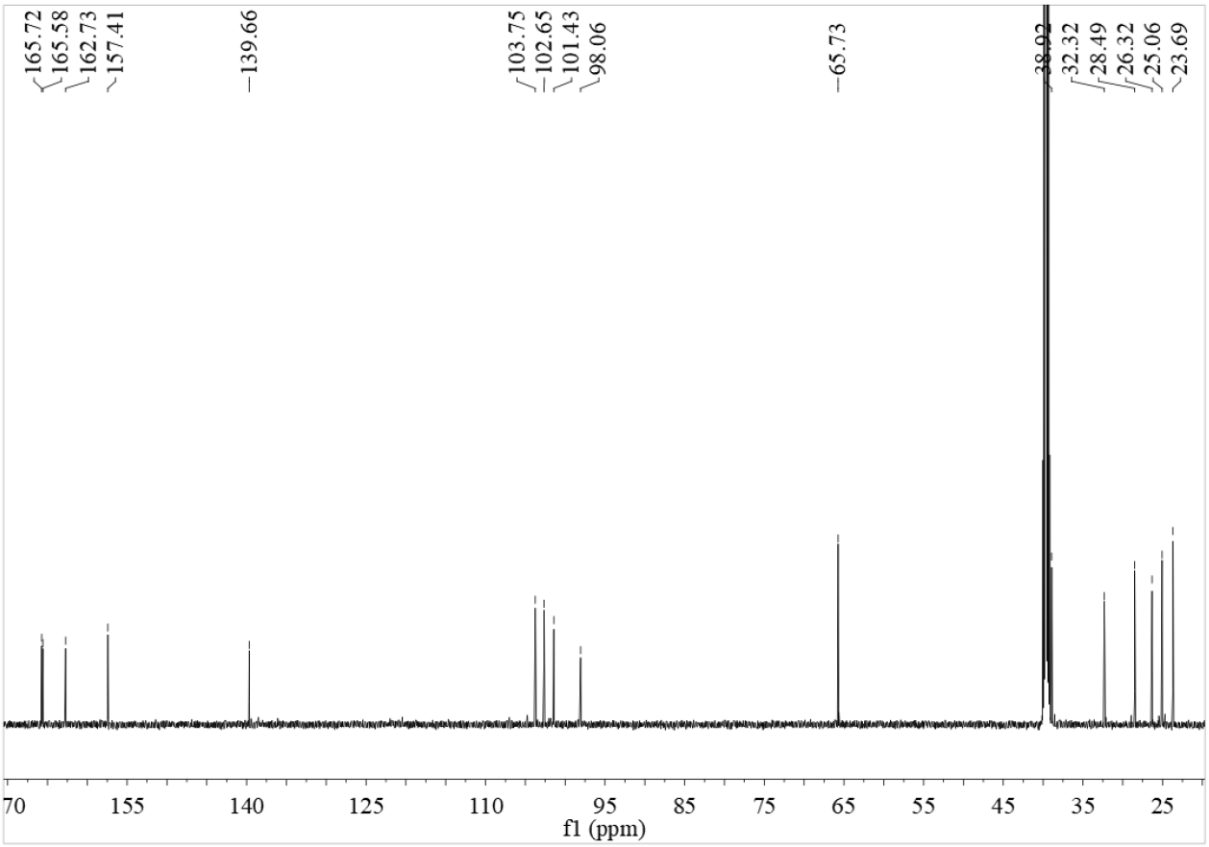

Figure S3: ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum of **1** (penioxalone A)

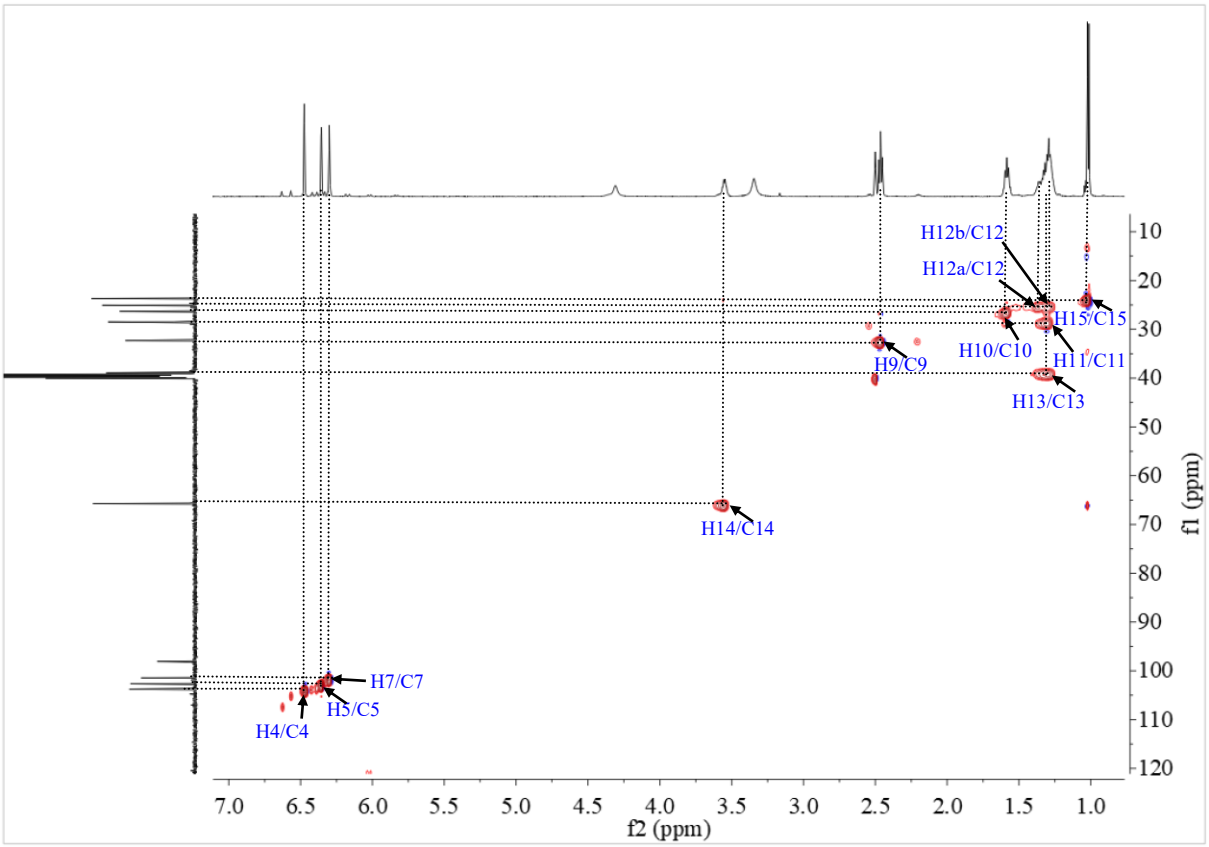

Figure S4: HSQC spectrum of **1** (penioxalone A)

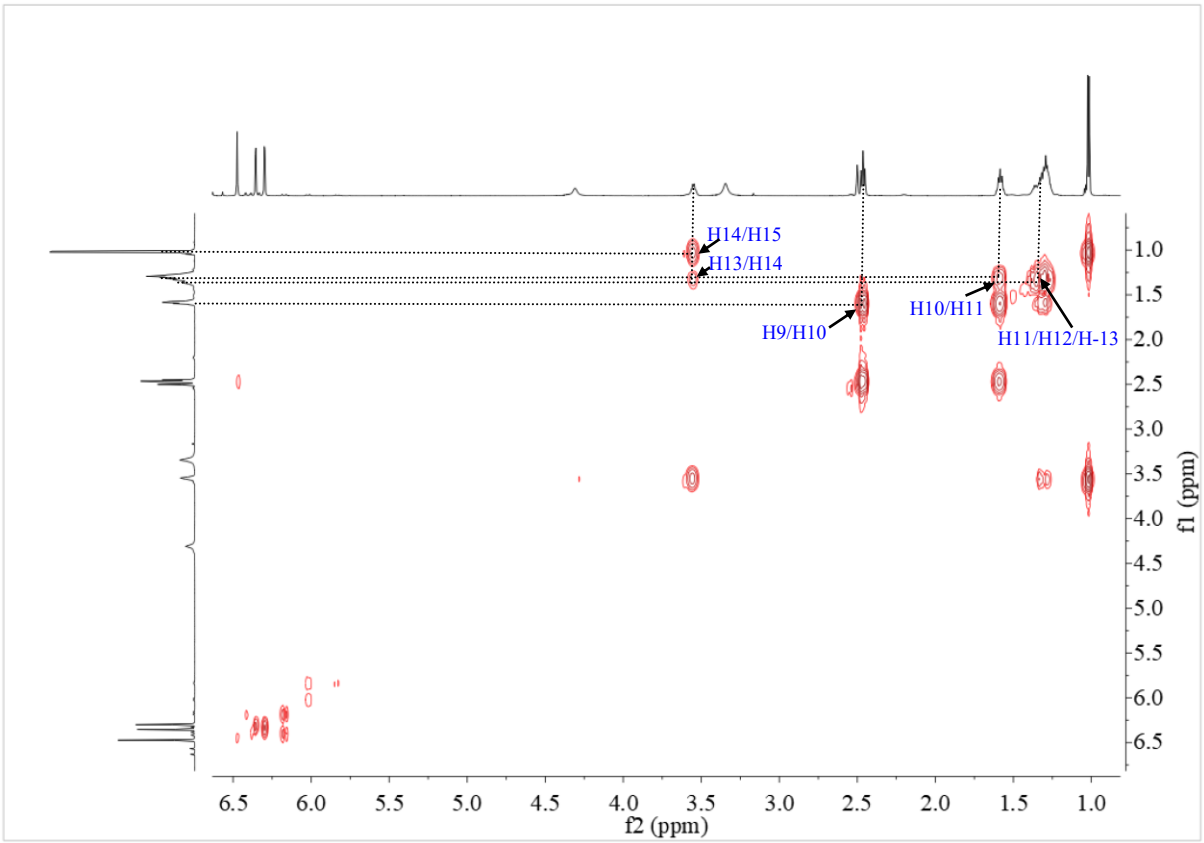

Figure S5: ^{1}H-^{1}H COSY spectrum of **1** (penioxalone A)

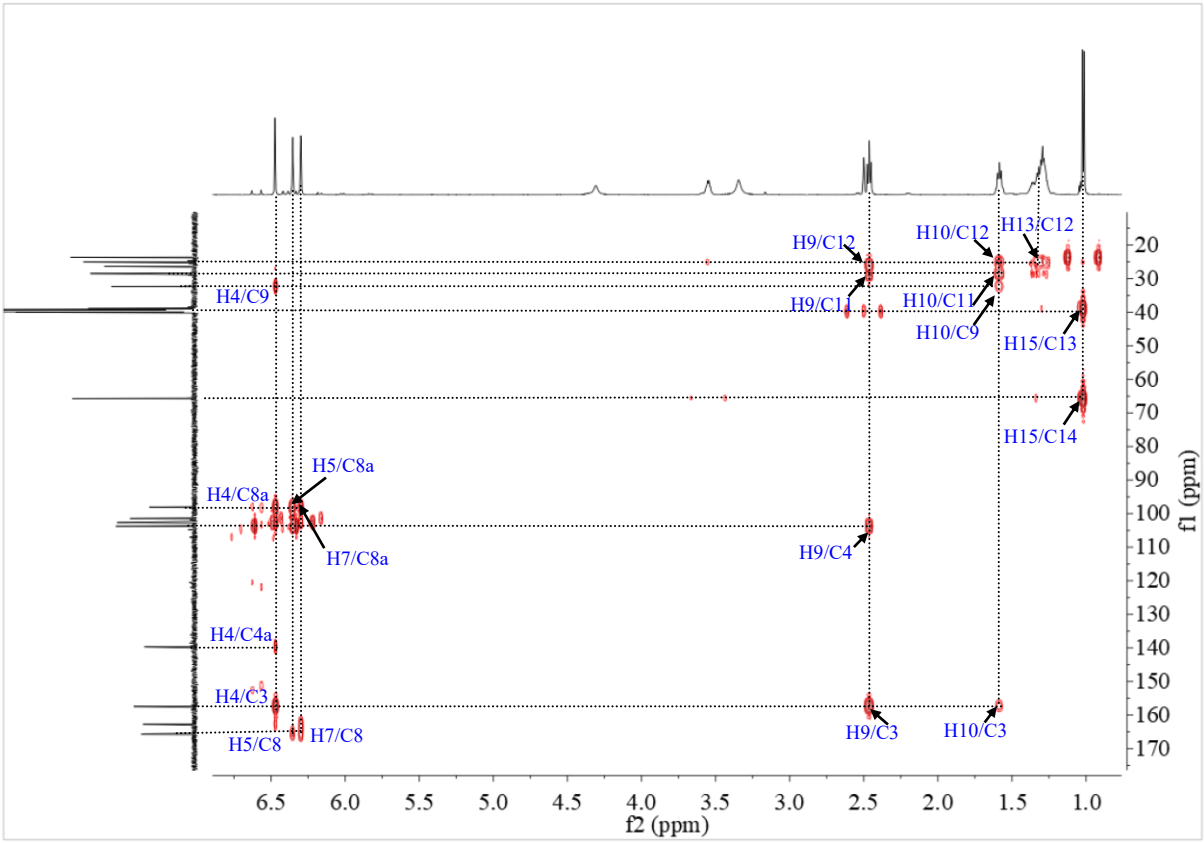

Figure S6: HMBC spectrum of **1** (penioxalone A)

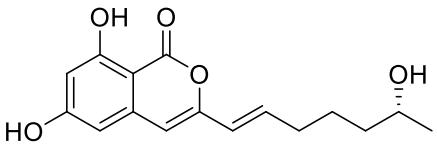

Figure S7: Chemical structure of the known stutter α-pyrone

Table S1. The coordinate for the lowest-energy conformer [(14*R*)-**1**] in ECD and ORD calculations

	Coordinates (Angstroms)		
	X	Y	Z
C	4.03981900	-1.29893600	0.23550600
C	4.51593900	0.01008600	0.34716700
C	3.67156000	1.11221000	0.19968200
C	2.32134400	0.90511200	-0.06752100
C	1.81536700	-0.41848900	-0.18746000
C	2.69358400	-1.52473200	-0.03131300
C	1.38442200	1.98953700	-0.23332300
C	0.08669800	1.74890500	-0.49736000
O	-0.37791000	0.45905100	-0.61922200
C	0.42207800	-0.63636700	-0.46216500
C	-1.00314400	2.75471500	-0.69170700
C	-1.96931900	2.91751800	0.50846800
C	-2.76555000	1.67210300	0.92831500
C	-3.72816800	1.13311400	-0.13818200
C	-4.47937400	-0.13908300	0.27799600
C	-3.61096200	-1.40332600	0.34381700
O	-3.06718700	-1.65357600	-0.95576800
C	-4.41523900	-2.61817000	0.80468000
O	2.27191800	-2.79276300	-0.13181400
O	5.82324800	0.27286000	0.60585800
O	-0.12387400	-1.73528400	-0.56760300
H	4.69786100	-2.15421900	0.35202600
H	4.08131300	2.11052100	0.29528600
H	1.72595700	3.01407300	-0.15000900
H	-0.53588200	3.72173600	-0.89658700
H	-1.56636000	2.48058600	-1.58923300
H	-1.39285300	3.28107700	1.36687600
H	-2.66765000	3.72222900	0.24856400
H	-2.07170700	0.88603400	1.23962800
H	-3.33886700	1.93247200	1.82730700

H	-4.45910200	1.91558200	-0.37977100
H	-3.19130800	0.91442100	-1.06485900
H	-4.96694200	0.01169500	1.25009300
H	-5.28116200	-0.33133100	-0.44476800
H	-2.78736900	-1.24265500	1.05199200
H	-2.10697500	-1.76415600	-0.89545800
H	-4.85087200	-2.45928900	1.79677900
H	-5.22715300	-2.82216400	0.10066400
H	-3.77946800	-3.50612800	0.84804800
H	1.30786400	-2.79158300	-0.31765700
H	6.32677900	-0.54639400	0.68987000

Table S2. The coordinate for the lowest-energy conformer [(14*S*)-**1**] in ECD and ORD calculations

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.03982000	-1.29893400	0.23550600
C	-4.51593900	0.01008900	0.34716500
C	-3.67155900	1.11221100	0.19968000
C	-2.32134300	0.90511200	-0.06752100
C	-1.81536700	-0.41848900	-0.18745900
C	-2.69358500	-1.52473100	-0.03131200
C	-1.38442000	1.98953600	-0.23332200
C	-0.08669600	1.74890300	-0.49735900
O	0.37791100	0.45904900	-0.61922300
C	-0.42207800	-0.63636800	-0.46216300
C	1.00314600	2.75471200	-0.69170600
C	1.96932100	2.91751600	0.50847000
C	2.76555200	1.67210100	0.92831500
C	3.72817100	1.13311400	-0.13818200
C	4.47937500	-0.13908400	0.27799500
C	3.61096100	-1.40332500	0.34381600
O	3.06718500	-1.65357100	-0.95577000
C	4.41523300	-2.61817200	0.80467800
O	-2.27192000	-2.79276300	-0.13181000
O	-5.82324800	0.27286500	0.60585400
O	0.12387300	-1.73528600	-0.56760100
H	-4.69786300	-2.15421600	0.35202500
H	-4.08131100	2.11052300	0.29528400
H	-1.72595300	3.01407300	-0.15000800
H	1.56636300	2.48058300	-1.58923100
H	0.53588500	3.72173400	-0.89658800
H	2.66765100	3.72222700	0.24856600
H	1.39285400	3.28107400	1.36687700
H	3.33886700	1.93246800	1.82730900
H	2.07170900	0.88603100	1.23962600

H	3.19131100	0.91442200	-1.06485900
H	4.45910500	1.91558300	-0.37976900
H	5.28116300	-0.33133200	-0.44476900
H	4.96694300	0.01169300	1.25009200
H	2.78736800	-1.24265200	1.05199000
H	2.10697500	-1.76415800	-0.89545900
H	4.85086600	-2.45929300	1.79677800
H	5.22714900	-2.82216700	0.10066300
H	3.77946000	-3.50612800	0.84804400
H	-1.30786600	-2.79158600	-0.31764900
H	-6.32678000	-0.54638800	0.68986600
