Revision of the Structure of Acremine P from a Marine-Derived Strain of *Acremonium persicinum*

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Figure 1. The image of the lowest energy optimized structure of **4d**.

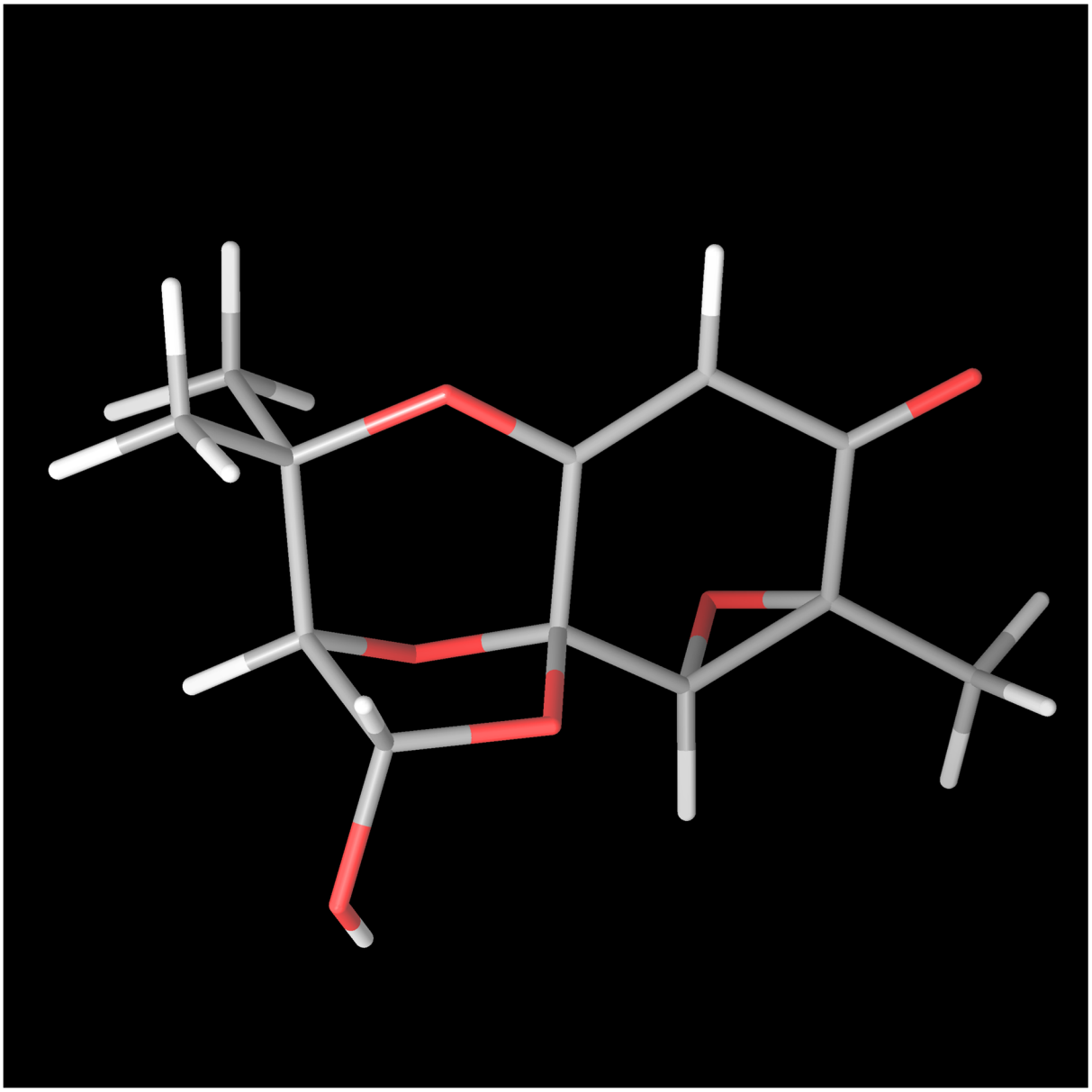

Table S1. Density functional theory calculations of coupling constants for **4a - 4d**

The ^{1}H-^{1}H and ^{1}H-^{13}C coupling constants were calculated using the DFT optimized structures as described by Kutateladze et al. (*J. Org. Chem.*, 2015, 80 (21), pp 10838–10848) using Gaussian 09W[#]. The data was extracted by the author supplied script and processed through the author's web site (http://kgroup.du.edu/nmr/).

Coupling Constant	Expt (Hz)	**4a** (Hz)	**4b** (Hz)	**4c** (Hz)	**4d** (Hz)
H7-H8	0	0.2	4.1	3.9	0.3
C4-H8	5.4	5.4	5	4.9	5.6

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Table S2. Computed coordinates of the lowest energy conformers of **4a** – **4d**

Compound **4a**

32
3a lower Energy

C	-0.24740	-0.76690	-1.97120
C	-0.47940	-0.83450	0.39420
O	0.77410	0.92400	-0.57720
C	-0.19280	0.65580	0.41700
C	-0.00700	0.73660	-1.76460
O	-0.91870	-1.29970	-0.79570
C	0.25430	1.18850	1.75130
C	0.47080	0.30130	2.90520
C	0.21840	-1.18720	2.72620
C	-0.33370	-1.64800	1.44760
C	1.08470	-1.49870	-2.12840
C	-1.17360	-1.05730	-3.14230
C	-1.26360	1.55070	-1.39930
O	-1.35610	1.35070	0.00060
O	0.51300	-1.96130	3.61730
O	-0.71720	1.09230	2.76830
C	1.39620	0.68050	4.02750
O	-1.15020	2.89710	-1.71320
H	-2.18220	1.20600	-1.87240
H	0.53250	1.16700	-2.60940
H	0.79170	2.13490	1.68910
H	-0.54120	-2.70840	1.35500
H	1.74440	-1.29490	-1.28170
H	0.90540	-2.57570	-2.18520
H	1.58990	-1.17950	-3.04570
H	-0.75700	-0.64640	-4.06720
H	-1.28030	-2.13870	-3.26260
H	-2.17010	-0.63800	-2.98700
H	2.39420	0.26740	3.85560
H	1.46510	1.76840	4.10640
H	1.02230	0.27380	4.96980
H	-0.38660	3.24030	-1.22810

32
3a higher Energy

C	-0.20670	-0.75970	-1.97590
C	-0.42840	-0.84400	0.39680
O	0.80140	0.91950	-0.57460
C	-0.15020	0.64810	0.42420
C	0.01980	0.74510	-1.75870
O	-0.86220	-1.30780	-0.79640
C	0.29960	1.18330	1.75540
C	0.51920	0.29400	2.90710
C	0.27040	-1.19570	2.72730

C	-0.27680	-1.65970	1.44780
C	1.13320	-1.47370	-2.14720
C	-1.13690	-1.05910	-3.14140
C	-1.24640	1.52350	-1.37950
O	-1.33180	1.32560	0.01730
O	0.56490	-1.96860	3.62000
O	-0.67140	1.08200	2.77470
C	1.44530	0.67350	4.02870
O	-1.04740	2.86140	-1.70400
H	-2.17100	1.13860	-1.82180
H	0.55040	1.19760	-2.59680
H	0.83130	2.13190	1.68960
H	-0.47360	-2.72200	1.35320
H	1.79650	-1.26440	-1.30480
H	0.96770	-2.55260	-2.20820
H	1.62670	-1.14250	-3.06660
H	-0.72940	-0.64160	-4.06750
H	-1.23180	-2.14150	-3.26330
H	-2.13720	-0.65130	-2.98050
H	2.44420	0.26360	3.85430
H	1.51170	1.76150	4.10850
H	1.07420	0.26440	4.97110
H	-1.75520	3.37070	-1.28890

Compound **4b**

32
3b

C	-1.65950	-0.37750	-1.68180
C	-0.54970	-0.82090	0.41290
O	-1.04170	1.43170	-0.25720
C	-0.09170	0.63060	0.40260
C	-0.91380	0.96700	-1.59870
O	-1.06760	-1.29970	-0.73060
C	0.20510	1.19400	1.76350
C	0.43540	0.30620	2.91080
C	0.28600	-1.19270	2.69520
C	-0.34760	-1.64120	1.45640
C	-1.59120	-1.06140	-3.04020
C	-3.11910	-0.16750	-1.26790
C	0.63050	0.94610	-1.73360
O	1.07390	0.73270	-0.40010
O	0.66870	-1.96470	3.55570
O	-0.79920	1.02250	2.73690
C	1.29590	0.72770	4.06840
O	1.08250	-0.03590	-2.59700
H	0.99840	1.93440	-2.03940
H	0.68360	2.17210	1.72870
H	-0.61740	-2.68920	1.38840
H	-0.57010	-1.33650	-3.29450
H	-2.21380	-1.96050	-3.02020
H	-1.98400	-0.39170	-3.81240
H	-3.63390	0.47190	-1.99300
H	-3.18700	0.29710	-0.28240
H	-3.62530	-1.13610	-1.24030
H	1.28040	1.81560	4.17160
H	2.32600	0.39410	3.91530
H	0.92980	0.27190	4.99110
H	2.04740	-0.02230	-2.58160
H	-1.37710	1.69800	-2.26360

Compound **4c**

32
3c

C	-0.23270	-0.75490	-1.97880
C	-0.47030	-0.83760	0.38820
O	0.72840	0.95810	-0.59280
C	-0.20820	0.65880	0.42120
C	-0.06470	0.76310	-1.76780
O	-0.87830	-1.31760	-0.80310
C	0.26230	1.18670	1.75000
C	0.47650	0.30080	2.90410
C	0.20670	-1.18550	2.73050
C	-0.32940	-1.64720	1.44750
C	1.14920	-1.40200	-2.10830
C	-1.10380	-1.13640	-3.16650
C	-1.32370	1.55520	-1.35800
O	-1.38350	1.35530	0.04560
O	0.48110	-1.95680	3.63140
O	-0.70390	1.10460	2.77560
C	1.41440	0.67230	4.01860
O	-2.47420	1.12410	-1.99270
H	-1.16410	2.62870	-1.53160
H	0.46030	1.21130	-2.61310
H	0.80660	2.12800	1.67860
H	-0.52330	-2.70990	1.35110
H	1.03290	-2.48770	-2.16250
H	1.64490	-1.05950	-3.02250
H	1.78670	-1.15700	-1.25610
H	-1.09300	-2.22410	-3.28250
H	-0.70080	-0.69120	-4.08210
H	-2.12820	-0.79850	-3.02880
H	2.40740	0.25020	3.83890
H	1.49390	1.75960	4.09580
H	1.04420	0.26920	4.96380
H	-3.21830	1.60630	-1.61090

Compound **4d**

32
3d lower Energy

C	-1.64750	-0.39420	-1.68360
C	-0.53390	-0.82290	0.41070
O	-1.11640	1.41770	-0.20320
C	-0.11340	0.63640	0.40480
C	-1.00390	0.99290	-1.56090
O	-0.99390	-1.30450	-0.76070
C	0.21540	1.19370	1.76080
C	0.44320	0.30540	2.90870
C	0.27140	-1.19240	2.70260
C	-0.34520	-1.64420	1.45370
C	-1.46580	-1.00750	-3.06410
C	-3.12410	-0.32340	-1.29770
C	0.52860	1.05130	-1.75220
O	1.01350	0.75570	-0.44850
O	0.62920	-1.96490	3.57220
O	-0.78320	1.03590	2.74270
C	1.31800	0.71720	4.05880
O	0.97540	2.29100	-2.18070
H	0.92710	0.32370	-2.45860
H	-1.51630	1.71310	-2.20100
H	0.70710	2.16540	1.72330
H	-0.59750	-2.69590	1.37670
H	-1.96330	-1.98040	-3.10050
H	-1.91260	-0.36240	-3.82710
H	-0.41130	-1.16080	-3.30530
H	-3.54970	-1.33040	-1.29930
H	-3.67860	0.29140	-2.01440
H	-3.24240	0.11010	-0.30200
H	1.32600	1.80580	4.15510
H	0.94690	0.27480	4.98580
H	2.34030	0.36180	3.90260
H	0.68120	2.94260	-1.52840

32
3d higher Energy

C	-0.87110	0.11730	-2.00640
C	-0.83320	-0.40970	0.35100
O	0.68880	1.19560	-0.55210
C	0.57800	0.15400	0.37980
C	0.60180	0.48470	-1.78240
O	-1.33730	-0.66520	-0.87310
C	1.03610	0.61890	1.73220
C	0.31760	0.21430	2.94870
C	-0.93960	-0.62950	2.79430
C	-1.50780	-0.77120	1.45210
C	-1.08880	-0.76080	-3.22960

C	-1.72310	1.38330	-2.07800
C	1.53760	-0.70510	-1.50410
O	1.44400	-0.86850	-0.09780
O	-1.44390	-1.14370	3.77550
O	0.17990	1.52860	2.38540
C	1.01250	0.12510	4.27820
O	2.82100	-0.34750	-1.89630
H	1.22580	-1.64760	-1.96660
H	0.98160	1.11840	-2.58450
H	2.10180	0.84000	1.77560
H	-2.48280	-1.23890	1.37200
H	-2.15550	-0.97270	-3.34260
H	-0.74170	-0.24530	-4.13060
H	-0.56470	-1.71570	-3.14590
H	-2.77930	1.10860	-2.14190
H	-1.46050	1.97190	-2.96330
H	-1.56950	2.00180	-1.19100
H	1.86320	0.81070	4.30460
H	0.31690	0.38070	5.08060
H	1.36600	-0.89490	4.45280
H	3.42640	-1.03750	-1.59650