Supplementary Materials

Reductive Metabolism of Ellagitannins in the Young Leaves of *Castanopsis sieboldii*

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		9u		100	
	position	1 H	¹³ C	$^{1}\mathrm{H}$	¹³ C
triterpene	1	2.21 (dd, 12.7, 4.9)	47.5	2.27 (dd, 13.0, 4.6)	48.0
_		1.25 (m)		1.37 (m)	
	2	4.23 (m)	68.3	4.47 (m)	66.5
	3	3.42 (d, 9.0)	78.6	5.40 (d, 9.5)	79.1
	4		48.9		48.6
	5	1.41 (m)	57.40	1.54 (m)	57.3
	6	2.45 (m)	20.0	2.46 (d, 13.2)	19.9
		1.62 (m)		1.66 (m)	
	7	1.57 (m)	33.05	1.50 (m)	32.5
		1.25 (m)		1.24 (m)	
	8		39.7		39.4
	9	1.70 (m)	47.6	1.76 (m)	47.6
	10		38.1		38.2
	11	1.95 (m)	24.0	1.95 (2H, m)	24.1
	12	5.37 (m)	125.8	5.37 (t, 3.4)	122.5
	13		138.6		144.3
	14		42.4		42.0
	15	2.41 (m)	28.7	2.34 (td,13.9, 4.6)	28.4
		1.09 (m)		1.09 (m)	
	16	2.03 (m)	24.6	2.06 (td, 13.7, 3.8)	23.3
				2.00 (m)	
	17		48.3		46.9
	18	2.49 (d, 11.0)	53.1	3.18 (dd, 13.7, 5.1)	41.6
	19	1.38 (m)	39.3	1.72 (m)	46.1
	• •	0.00 ()		1.21 (m)	
	20	0.88 (m)	39.1		30.8
	21	1.34 (m)	30.8	1.37 (m)	34.0
	22	1.02 ()	26.0	1.09 (m)	22.6
	22	1.92 (m)	36.8	1.77 (2H, m)	32.6
	22	1.69 (m)	71.4		(0 7
	23	6.04 (d, 11.2)	/1.4	5.54 (d, 11.5)	69.7
	24	3.73 (d, 11.2)	(2.4	3.82 (d, 11.5)	(1.0
	24	5.31 (d, 11.2)	62.6	5.46 (d, 11.7)	61.8
	25	4.40 (m)	167	4.33 (d, 11.5)	16.5
	25	0.8/(3H, s)	16.7	0.96 (3H, s)	16.5
	26	1.05 (3H, s)	17.5	1.02 (3H, s)	17.3
	27	1.12 (5H, S)	25.8	1.50 (5H, 8)	20.2
	28	0.02(1.6.4)	170.2	$0.01(2U_{c})$	170.4
	29	0.92(d, 0.4)	17.4	0.91 (3H, 8)	55.1 22.6
aluassa	50	0.90(d, 7.1)	21.5	0.89 (3H, 8)	25.0
giucose	1	4.20(t, 8.1)	74.2	4.21 (t, 8.3)	74.3
	2	4.20(t, 8.3)	74.2	4.21 (t, 8.3)	74.3
	3	4.20 (l, 0.9)	70.9	4.26 (t, 8.8)	79.0
	4	4.00 (m)	71.1	4.37 (t, 9.0)	71.0
	5	4.02 (m)	62 20	4.05 (m) 4.47 (m)	62.2
	0	4.44 (III)	02.20	4.42 (dd 11.7.4.5)	02.2
HHDP	1.1'		1165(2C)	$\tau.\tau_2$ (uu, 11.7, $\tau.J$)	116.7(2C)
IIIDI	2.2'		127 5 127 8		127 4 126 8
	3 3'	7 16 (s) 7 29 (s)	107 3 108 36	7.08(s), $7.56(s)$	107 5 108 6
	4.4'	(110 (5), (12) (5)	146.8, 146.6	100 (0), 100 (0)	146.8, 145.91
	5.5'		137.8, 137.7		137.8 (2C)
	6.6'		146.19. 146.24		145.94 (2C)
	7.7'		169.6. 169.8		169.0. 169.6
gallovl	1		,		121.4
U	2.6			8.03 (s)	111.9
	3.5				146.3
	4				141.6
	СО				167.4
	1'				
	2'.6'				
	3',5'				
	4'				
	СО				

Table S1. ¹H (500 MHz) and ¹³C (125 MHz) NMR Data for **9u** and **10o** (δ in ppm, J in Hz, Measured in pyridine-d5)

		110		120	
	position	¹ H ¹³ C		¹ H ¹³ C	
triterpene	1	2.23 (dd, 4.5, 12.8)	47.82	2.28 (m)	48.4
		1.37 (m)		1.36 (m)	
	2	4.12 (m)	65.3	4.47 (m)	66.5
	3	5.74 (d, 10.3)	84.8	5.38 (m)	79.0
	4		47.80		48.4
	5	1.18 (m)	50.8	1.52 (m)	57.5
	6	2.04 (m)	20.7	2.40 (m)	19.9
		1.75 (m)		1.59 (m)	
	7	1.22 (m)	33.3	1.52 (m)	32.7
		1.01 (m)		1.17 (m)	
	8		39.9		39.4
	9	1.75 (m)	48.5	1.73 (m)	47.6
	10		38.8		38.0
	11	1.93 (2H, m)	23.9	1.95 (m)	24.0
	12	5.40 (m)	122.3	5.37 (m)	122.6
	13		144.2		143.9
	14		42.2		42.2
	15	2.17 (m)	28.1	2.18 (m)	28.2
		1.08 (m)		1.16 (m)	
	16	2.02 (m)	23.5	2.08 (m)	24.6
		1.91 (m)			
	17		47.0		47.0
	18	3.15 (dd, 4.9, 13.9)	41.7	3.16 (dd, 13.6, 5.3)	41.7
	19	1.68 (m)	46.2	1.73 (m)	46.1
		1.19 (m)		1.22 (m)	
	20		30.7		30.6
	21	1.33 (m)	34.0	1.37 (m)	34.0
		1.05 (m)		1.11 (m)	
	22	1.82 (m)	32.5	1.81 (m)	32.6
	22	1.75 (m)	<i>c</i> 0 <i>c</i>	1.76 (m)	<0 7
	23	5.51 (d, 11.2)	69.6	5.54 (d, 11.5)	69.7
	24	4.15 (d, 11.0)	62 1	3.78 (d, 11.5)	(1.0
	24	5.48 (m)	63.1	5.41 (m)	61.8
	25	4.48 (m)	17.7	4.32 (m)	167
	25	1.12(3H, S)	17.7	0.94 (3H,8)	16.7
	20	1.05(3H, S) 1.14(2H, s)	17.5	0.96 (3H, \$)	17.5
	27	1.14 (5H, 8)	20.0	1.21 (3H, 8)	20.0
	28	0.87 (3H s)	33.1	0.01 (3 H s)	170.5
	29	0.87(3H, s) 0.84(3H, s)	23.50	0.91 (3H, 8)	23.6
glucosa	50	6.32 (d. 7.8)	25.59	6 30 (d. 8 3)	25.0
glucose	2	4.22 (t, 8.4)	74.14	4.30 (m)	72.3
	2	4.22(t, 8.4)	74.14	4.50 (m) 6 15 (t 9 3)	80.10
	3 4	4.27(t, 0.0)	71.1	4.55(t, 9.3)	68.90
	+ 5	4.06 (m)	79.4	4.04 (m)	79.1
	5	4.00 (m) 4.42 (m)	62.3	441 (dd 3268)	61.7
	0	4 47 (m)	02.5	1. 11 (dd, 5.2, 6.6)	01.7
HHDP	1.1'		116.3. 116.56		116.7 (2C)
	2.2'		126.6. 127.2		127.4. 126.8
	3,3'	7.14 (s), 6.90 (s)	106.7, 108.0	7.07 (s), 7.53 (s)	107.6, 108.6
	4,4'		146.7, 146.5		146.8, 145.9
	5,5'		137.57, 137.8		137.8, 137.9
	6,6'		146.0, 146.4		146.0 (2C)
	7,7'		169.9, 169.8		169.00, 169.5
galloyl	1		121.74		121.3
	2,6	7.93 (s)	110.4	8.01 (s)	111.9
	3,5		147.4		146.5
	4		140.8		141.5
	CO		168.0		167.3
	1'				121.6
	2',6'			7.86 (s)	110.5
	3',5'				147.4
	4'				140.7
	CO				167.2

Table S2. ¹H (500 MHz) and ¹³C (125 MHz) NMR Data for **110** and **120** (δ in ppm, J in Hz, Measured in pyridine-d5)



Figure S1. ¹H NMR spectrum of **10** (pyridine-*d*₅, 500 MHz)



Figure S2. ¹³C NMR spectrum of 10 (pyridine d_5 , 126 MHz)



Figure S3. ¹H⁻¹H COSY spectrum of **10** (pyridine-*d*₅, 500 MHz)



Figure S4. HSQC spectrum of 10 (pyridine d_5)



Figure S5. HMBC spectrum of 10 (pyridine d_5)



Figure S6. ¹H NMR spectrum of **1u** (pyridine-*d*₅, 500 MHz)



Figure S7. $^{13}\mathrm{C}$ NMR spectrum of $1\mathrm{u}$ (pyridine- d_5 , 126 MHz)



Figure S8. ¹H⁻¹H COSY spectrum of **1u** (pyridine⁻*d*₅, 500 MHz)



Figure S9. HSQC spectrum of 1u (pyridine d_5)



Figure S10. HMBC spectrum of **1u** (pyridine-*d*₅, 500 MHz)



Figure S11. NOESY spectrum of **10,u** (pyridine-*d*₅, 500 MHz)



Figure S12. ¹³H NMR spectrum of **2** (pyridine-*d*₅, 500 MHz)



Figure S13. $^{13}\mathrm{C}$ NMR spectrum of **2** (pyridine- d_5 , 126 MHz)



Figure S14. ¹H⁻¹H COSY spectrum of **2** (pyridine-*d*₅, 500 MHz)



Figure S15. HSQC spectrum of 2 (pyridine d_5)



Figure S16. HMBC spectrum of 2 (pyridine d_5)



Figure S17. ¹H NMR spectrum of **4** (pyridine-*d*₅, 500 MHz)



Figure S18. $^{13}\mathrm{C}$ NMR spectrum of **4** (pyridine- d_5 , 126 MHz)



Figure S19. ¹H⁻¹H COSY spectrum of **4** (pyridine *d*₅, 500 MHz)



Figure S20. HSQC spectrum of 4 (pyridine- d_5)



Figure S21. HMBC spectrum of 4 (pyridine d_5)



Figure S22. HMBC spectrum of 4 (CD₃OD, 500 MHz)



Figure S23. ¹H NMR spectrum of **9** (pyridine *d*₅, 500 MHz)

Figure S24. $^{13}\mathrm{C}$ NMR spectrum of **9** (pyridine- d_5 , 126 MHz)

Figure S25. ¹H⁻¹H COSY spectrum of **9** (pyridine⁻*d*₅, 500 MHz)

Figure S26. HSQC spectrum of 9 (pyridine d_5)

Figure S27. HMBC spectrum of 9 (pyridine d_5)

Figure S28. ¹H NMR spectrum of **10** (pyridine-*d*₅, 500 MHz)

Figure S29. $^{\rm 13}{\rm C}$ NMR spectrum of ${\bf 10}$ (pyridine- $d_5,\,126$ MHz)

Figure S30. ¹H-¹H COSY spectrum of **10** (pyridine-*d*₅, 500 MHz)

Figure S31. HSQC spectrum of 10 (pyridine- d_5)

Figure S32. HMBC spectrum of 10 (pyridine- d_5)

Figure S33. ¹H NMR spectrum of **11** (pyridine-*d*₅, 500 MHz)

Figure S34. ¹³C NMR spectrum of **11** (pyridine-*d*₅, 126 MHz)

Figure S35. ¹H-¹H COSY spectrum of **11** (pyridine-*d*₅, 500 MHz)

Figure S36. HSQC spectrum of 11 (pyridine d_5)

Figure S37. HMBC spectrum of 11 (pyridine d_5)

Figure S38. ¹H NMR spectrum of **12** (pyridine *d*₅, 500 MHz)

Figure S39. ¹³C NMR spectrum of **12** (pyridine- d_5 , 126 MHz)

Figure S40. ¹H-¹H COSY spectrum of **12** (pyridine- d_5 , 500 MHz)

Figure S41. HSQC spectrum of 12 (pyridine- d_5)

Figure S42. HMBC spectrum of 12 (pyridine d_5)

Figure S43. Experimental ECD spectra of $\mathbf{1o}$ and $\mathbf{1u}$

Figure S44. Experimental ECD spectra of 2o,u

Figure S45. Lowest-energy conformers of 3,24-(R)-HHDP ester of methyl $2\alpha,3\beta,23,24-$ tetrahydroxyolean-12-en-28-oate (**4'oA**) and 3,23-(R)-HHDP ester of methyl $2\alpha,3\beta,23,24-$ tetrahydroxyolean-12-en-28-oate (**4'oB**) at the B3LYP/6-31G(d,p) level in pyridine.

4'oB (3,23-(*R*)-HHDP ester)

										calculated ^a										experimental ^b
Position	40A-1	40A-2	40A-3	40A-4	40A-5	40A-6	4oA-7	40A-8	40A-9	4oA-10	40A-11	40A-12	40A-13	40A-14	40A-15	40A-16	40A-17	averaged- 40A ^c	averaged- 40A (corrected) ^d	40
1	2.11	2.12	2.01	1.99	2.03	2.01	2.05	1.97	2.04	2.18	2.04	2.09	2.15	2.14	1.95	2.01	2.00	2.07	2.03	2.02
	0.89	0.89	0.89	0.91	0.93	0.94	0.97	0.87	1.04	0.98	0.97	0.93	0.98	0.93	0.89	1.03	0.91	0.91	0.82	1.16
2	3.95	3.96	3.42	3.39	3.49	3.46	3.53	3.33	4.20	3.89	3.53	4.03	3.89	4.23	3.32	4.20	3.45	3.76	3.78	4.17
3	5.38	5.39	4.20	4.21	5.15	5.15	4.96	4.49	5.65	4.98	4.98	5.39	4.97	5.45	4.50	5.63	4.21	5.08	5.15	5.82
5	1.75	1.76	1.41	1.38	1.85	1.82	1.18	1.39	1.79	1.19	1.19	1.76	1.18	1.79	1.41	1.80	1.39	1.64	1.58	1.97
6	1.53	1.52	2.96	2.94	1.71	1.70	1.46	2.86	1.57	1.48	1.47	1.54	1.49	1.56	2.87	1.57	2.98	1.86	1.80	1.66
	1.54	1.54	1.64	1.61	1.54	1.52	1.54	1.63	1.55	1.56	1.56	1.54	1.58	1.58	1.65	1.56	1.60	1.56	1.50	1.34
7	1.82	1.82	1.80	1.83	1.78	1.80	1.72	1.83	1.83	1.75	1.69	1.80	1.75	1.83	1.83	1.83	1.84	1.81	1.75	1.59
	1.44	1.43	1.40	1.46	1.41	1.45	1.43	1.45	1.44	1.44	1.39	1.45	1.42	1.47	1.44	1.43	1.46	1.43	1.36	1.30
9	1.85	1.83	1.79	1.77	1.83	1.81	1.74	1.76	1.86	1.80	1.77	1.86	1.82	1.87	1.80	1.87	1.77	1.82	1.77	1.73
11	2.17	2.17	2.08	2.06	2.11	2.10	2.07	2.04	2.18	2.14	2.08	2.18	2.14	2.21	2.06	2.16	2.06	2.13	2.09	1.89
12	5.87	5.92	5.87	5.85	5.89	5.90	5.84	5.86	5.93	5.90	5.87	5.85	5.84	5.88	5.79	5.89	5.85	5.88	5.98	5.34
15	2.01	1.72	1.90	1.64	1.91	1.63	1.62	1.66	1.65	1.63	1.88	2.00	1.90	1.98	1.89	1.97	1.64	1.83	1.77	2.27
	1.18	1.26	1.14	1.23	1.14	1.22	1.22	1.22	1.26	1.21	1.13	1.16	1.13	1.15	1.15	1.22	1.24	1.20	1.12	1.05
16	2.06	2.18	2.01	2.17	2.02	2.14	2.17	2.17	2.12	2.12	2.01	2.05	2.01	2.06	2.05	2.07	2.18	2.10	2.06	1.97
	1.77	1.78	1.76	1.78	1.75	1.78	1.78	1.78	1.79	1.77	1.77	1.77	1.75	1.80	1.79	1.79	1.78	1.77	1.72	1.89
18	3.19	3.21	3.18	3.23	3.18	3.24	3.27	3.26	3.24	3.28	3.22	3.20	3.22	3.20	3.21	3.21	3.23	3.21	3.21	3.13
19	1.81	1.82	1.81	1.81	1.82	1.83	1.80	1.76	1.80	1.75	1.83	1.80	1.75	1.80	1.83	1.86	1.81	1.81	1.76	1.63
	1.23	1.27	1.18	1.27	1.18	1.26	1.27	1.26	1.27	1.26	1.21	1.24	1.23	1.25	1.25	1.24	1.27	1.24	1.16	1.16
21	1.52	1.53	1.53	1.54	1.53	1.51	1.53	1.56	1.51	1.54	1.52	1.52	1.51	1.54	1.50	1.50	1.54	1.53	1.46	1.30
	1.36	1.35	1.38	1.25	1.38	1.30	1.25	1.33	1.31	1.28	1.34	1.35	1.29	1.34	1.27	1.33	1.25	1.34	1.26	1.04
22	1.74	1.72	1.74	1.71	1.74	1.71	1.71	1.75	1.76	1.72	1.70	1.75	1.72	1.76	1.69	1.72	1.71	1.73	1.67	1.63
23	3.56	3.55	3.47	3.44	3.54	3.54	4.65	3.50	3.46	4.16	4.66	3.61	4.17	3.68	3.51	3.46	3.44	3.61	3.62	
	3.69	3.68	3.99	3.99	4.00	3.97	3.40	4.13	3.68	3.30	3.44	3.71	3.30	3.76	4.16	3.68	4.00	3.77	3.79	
24	4.58	4.58	5.34	5.33	5.15	5.16	5.32	5.25	4.53	4.97	5.31	4.61	4.98	4.62	5.24	4.52	5.29	4.87	4.93	
	4.15	4.17	4.71	4.70	4.43	4.42	4.58	4.65	4.17	4.62	4.59	4.12	4.61	4.18	4.65	4.18	4.68	4.35	4.39	
25	1.31	1.33	0.86	0.86	0.87	0.88	0.84	0.85	1.37	1.32	0.83	1.30	1.29	1.37	0.85	1.35	0.84	1.14	1.06	1.12
26	0.99	1.03	0.89	0.92	0.89	0.94	0.91	0.92	1.06	1.01	0.86	0.98	0.95	1.03	0.87	1.02	0.92	0.97	0.88	1.16
27	1.26	1.26	1.22	1.24	1.20	1.22	1.23	1.24	1.27	1.25	1.20	1.25	1.22	1.26	1.25	1.27	1.25	1.24	1.17	1.09
29	0.99	0.99	0.99	0.99	0.99	0.99	0.98	0.96	0.98	0.97	1.01	0.99	0.97	0.99	0.99	1.00	0.99	0.99	0.90	0.84
30	1.05	1.00	1.05	1.02	1.05	1.02	1.02	1.00	1.02	1.01	1.06	1.05	1.04	1.06	1.06	1.03	1.02	1.03	0.95	0.84
HHDP 3	7.49	7.49	7.74	7.73	7.75	7.74	7.81	7.62	7.74	7.62	7.81	7.14	7.61	7.22	7.62	7.71	7.67	7.59	7.75	7.72
HHDP 3	7.35	7.36	7.06	7.07	6.98	6.98	7.05	7.11	7.38	7.51	7.04	7.09	7.50	7.53	7.12	7.36	6.84	7.23	7.38	7.08

Table S3. Calculated ¹H NMR chemical shifts of **4'oA**.

^a Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in pyridine (PCM). ^b Measured in pyridine-d 5. ^cAveraged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. ^d Linearly corrected for the experimental data.

Table S4. Calculated ¹H NMR chemical shifts of **4'oB**.

												calculated ^a											experimental ^b
Position		4oB-1	4oB-2	4oB-3	4oB-4	4oB-5	4oB-6	4oB-7	4oB-8	4oB-9	4oB-10	4oB-11	4oB-12	4oB-13	4oB-14	4oB-15	4oB-16	4oB-17	4oB-18	4oB-19	averaged- 40B ^c	averaged- 40B (corrected) ^d	40
	1	2.29	2.26	2.21	2.27	2.20	2.21	2.15	2.20	2.19	2.09	2.24	2.32	2.30	2.16	2.17	2.17	2.38	2.26	2.22	2.23	2.18	2.02
		1.19	1.19	1.19	1.20	1.19	1.19	1.19	1.22	1.19	1.23	1.16	1.19	1.20	1.15	1.20	1.11	0.98	1.16	1.15	1.19	1.15	1.16
	2	4.62	4.44	4.50	4.46	4.44	4.66	4.51	4.54	4.46	4.61	4.30	4.29	4.68	4.49	4.54	4.14	4.21	4.44	4.50	4.51	4.43	4.17
	3	5.17	5.21	5.13	5.19	5.20	5.08	5.13	5.16	5.20	5.09	5.06	5.08	5.17	5.09	5.16	4.98	4.93	5.15	5.09	5.15	5.07	5.82
	5	1.12	1.17	1.18	1.17	1.15	1.12	1.17	1.19	1.16	1.11	1.06	1.10	1.13	1.17	1.18	1.01	1.19	1.16	1.18	1.15	1.12	1.97
	6	1.63	1.50	1.51	1.51	1.52	1.63	1.53	1.52	1.54	1.65	2.03	2.02	1.64	1.54	1.54	1.92	1.51	1.51	1.52	1.58	1.54	1.66
		1.21	1.31	1.33	1.35	1.32	1.22	1.33	1.40	1.35	1.22	1.42	1.43	1.23	1.35	1.38	1.60	1.43	1.36	1.34	1.31	1.27	1.34
	7	1.68	1.65	1.65	1.66	1.61	1.68	1.63	1.68	1.63	1.53	1.44	1.47	1.69	1.63	1.66	1.52	1.67	1.66	1.65	1.64	1.60	1.59
		1.43	1.39	1.40	1.40	1.31	1.43	1.32	1.41	1.34	1.36	1.28	1.33	1.44	1.34	1.39	1.33	1.38	1.40	1.41	1.38	1.35	1.30
	9	1.83	1.81	1.79	1.83	1.83	1.80	1.80	1.79	1.86	1.89	1.85	1.84	1.84	1.79	1.82	1.85	1.75	1.82	1.77	1.82	1.78	1.73
	11	2.19	2.14	2.11	2.15	2.13	2.17	2.11	2.13	2.16	2.21	2.19	2.21	2.19	2.11	2.14	2.16	2.14	2.14	2.11	2.15	2.10	1.89
	12	5.90	5.87	5.86	5.88	5.79	5.90	5.78	5.89	5.81	5.75	5.81	5.88	5.91	5.78	5.84	5.78	5.92	5.87	5.86	5.86	5.76	5.34
	15	1.70	1.66	1.66	1.67	1.87	1.71	1.85	1.68	1.90	2.08	1.88	1.63	1.71	1.84	1.86	1.90	1.65	1.66	1.67	1.74	1.70	2.27
		1.19	1.20	1.21	1.19	1.05	1.20	1.05	1.21	1.04	1.04	1.05	1.17	1.20	1.06	1.08	1.05	1.22	1.20	1.22	1.15	1.12	1.05
	16	2.15	2.14	2.14	2.14	2.02	2.15	2.01	2.15	2.03	2.05	2.00	2.16	2.15	2.02	2.05	2.01	2.14	2.14	2.14	2.11	2.06	1.97
		1.80	1.78	1.79	1.77	1.72	1.80	1.72	1.76	1.75	1.75	1.72	1.82	1.78	1.73	1.79	1.73	1.76	1.77	1.79	1.77	1.73	1.89
	18	3.23	3.21	3.21	3.21	3.20	3.22	3.20	3.23	3.23	3.17	3.18	3.24	3.21	3.20	3.22	3.19	3.24	3.18	3.21	3.21	3.15	3.13
	19	2.15	2.11	2.10	2.13	2.11	2.14	2.09	2.12	2.13	2.21	2.16	2.20	2.16	2.10	2.13	2.18	2.12	2.13	2.10	2.13	2.08	1.63
		1.19	1.20	1.21	1.19	1.05	1.20	1.05	1.21	1.04	1.04	1.05	1.17	1.20	1.06	1.08	1.05	1.22	1.20	1.22	1.15	1.12	1.16
	21	1.53	1.52	1.52	1.53	1.47	1.53	1.46	1.52	1.47	1.46	1.47	1.51	1.54	1.46	1.50	1.47	1.52	1.54	1.53	1.51	1.47	1.30
		1.30	1.29	1.29	1.30	1.32	1.30	1.31	1.32	1.31	1.31	1.33	1.29	1.30	1.31	1.30	1.33	1.33	1.30	1.29	1.30	1.27	1.04
	22	1.69	1.69	1.69	1.67	1.71	1.69	1.69	1.67	1.68	1.72	1.70	1.70	1.68	1.69	1.67	1.71	1.70	1.67	1.69	1.69	1.65	1.63
	23	3.20	3.55	3.54	3.47	3.55	3.23	3.56	3.52	3.44	3.24	3.19	3.20	3.20	3.53	3.49	3.22	3.51	3.46	3.51	3.41	3.35	
		4.48	5.01	5.13	5.56	5.02	4.47	5.10	5.57	5.61	4.48	5.30	5.32	4.82	5.18	5.61	5.67	5.54	5.53	5.17	5.03	4.95	
	24	3.74	3.58	3.61	3.62	3.59	3.74	3.62	3.63	3.64	3.76	4.12	4.13	3.83	3.62	3.65	3.99	3.61	3.62	3.61	3.68	3.61	
		3.70	4.41	4.41	4.45	4.41	3.69	4.41	4.45	4.43	3.71	4.02	4.00	3.79	4.39	4.43	3.91	4.40	4.43	4.39	4.18	4.11	
	25	1.48	0.98	0.97	1.02	0.94	1.49	0.93	1.00	0.98	1.43	1.20	1.27	1.50	0.93	0.99	1.18	1.01	1.00	0.97	1.14	1.10	1.12
	26	1.05	0.85	0.85	0.86	0.77	1.03	0.77	0.87	0.77	0.77	0.79	0.87	1.05	0.78	0.81	0.82	0.92	0.85	0.85	0.88	0.85	1.16
	27	1.24	1.21	1.21	1.21	1.18	1.23	1.19	1.21	1.22	1.22	1.17	1.19	1.24	1.19	1.22	1.18	1.19	1.20	1.21	1.21	1.18	1.09
	29	0.98	0.97	0.97	0.97	0.98	0.98	0.98	0.97	0.99	0.99	0.97	0.98	0.98	0.98	0.98	0.98	0.98	0.97	0.97	0.98	0.95	0.84
	30	1.02	1.01	1.01	1.01	1.06	1.02	1.06	1.01	1.06	1.08	1.06	1.02	1.01	1.06	1.05	1.06	1.00	1.01	1.01	1.03	1.00	0.84
н	HDP 3	7.71	7.76	7.79	7.85	7.74	7.82	7.80	8.22	7.80	7.84	7.51	7.49	7.83	7.64	8.17	7.37	8.07	7.71	7.63	7.79	7.67	7.72
HI	IDP 3	7.53	7.58	7.62	7.57	7.59	7.54	7.63	7.57	7.57	7.54	7.51	7.50	7.36	7.58	7.58	8.13	7.59	7.41	7.56	7.57	7.46	7.08

^a Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in pyridine (PCM). ^b Measured in pyridine-d 5. ^c Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. ^d Linearly corrected for the experimental data.

Posizion 4nA-1 4nA-3 4nA-4 4nA-5 4nA-6 4nA-7 4nA-8 4nA-9 4nA-11 4nA-12 4nA-13 4nA-14 4nA-15 4nA-1 4nA-15 4nA-1 4nA-15 4nA-15 4nA-15 4nA-15 4nA 4nA-15	40
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HIND-2 1280 1280 1255 1255 1258 1259 1261 1246 1269 1275 1275 1267 1265 1777 1245 1270 1250 1269 1261	110.0
HINDE-7 1312 1312 1247 1245 1251 1248 1243 1237 1317 1298 1247 1294 1296 1289 1241 1318 1247 1285 1276	
HHDP-3 1117 1117 1133 1134 1130 1132 1137 1107 1133 1137 1072 1132 1100 1105 1133 1125 1120	112.1
HHDP-3' 1075 1075 1043 1043 1040 1040 1040 1069 1073 1087 1042 1040 1087 1100 1069 1073 1017 1063 1061	106.6
HHDP-4 1466 1466 1471 1466 1470 1471 1440 1463 1465 1467 1431 1466 1431 1439 1463 1459 1464 1450	145.7
HHDP-4' 147.3 147.2 145.8 145.9 145.8 145.9 145.8 145.9 145.3 146.8 147.1 145.8 143.4 147.1 145.6 145.1 147.0 143.2 146.5 145.1	145.9
HHDP-5 135.9 136.0 141.1 141.8 141.1 141.5 141.7 137.2 136.4 136.7 141.0 135.8 136.8 135.7 137.2 136.3 140.9 137.9 136.8	139.8
HHDP-5' 135.6 135.5 135.0 135.5 134.7 135.4 135.4 135.4 135.4 136.2 135.0 135.2 136.3 140.0 134.8 134.9 135.5 134.4	137.7
HHDP-6 1432 1433 1460 1461 1461 1462 1460 1462 1433 1458 1466 1434 1433 1461 1428 1445 1444 1431	147.1
HHDE-6' 144.0 143.9 143.9 143.7 143.8 144.1 143.6 143.7 143.6 143.6 143.6 143.6 143.6 143.6 143.7 143.5 143.3 146.9 143.0 143.6	146.9
HHP-7 1736 1737 1743 1744 1747 1747 1750 1736 1736 1736 1748 1747 1737 1710 1757 1740 1748	168.9
HHDP-7 1739 1739 1745 1786 1793 1792 1791 1744 1740 1758 1790 1741 1758 1738 1743 1740 1781 1758 1735	170.7

^a Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in pyridine (PCM).^b Measured in pyridine-d 5.^c Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies.^d Linearly corrected for the experimental data.

Table S6. Calculated ¹³C NMR chemical shifts of **4'oB**.

											calculated ^a											experimental ^b
																					averaged-	
Position	4oB-1	4oB-2	4oB-3	4oB-4	4oB-5	4oB-6	4oB-7	4oB-8	4oB-9	4oB-10	4oB-11	4oB-12	4oB-13	4oB-14	4oB-15	4oB-16	4oB-17	4oB-18	4oB-19	averaged-	4oB	40
																				40B	(corrected) ^d	
1	42.1	41.4	44.3	41.2	41.3	45.1	44.2	44.8	41.0	45.1	41.8	42.0	42.1	44.3	44.6	40.7	44.6	41.3	44.5	42.8	43.9	48.3
2	68.7	67.5	67.7	67.5	67.5	69.0	67.7	67.9	67.5	68.7	67.5	67.6	68.6	68.0	67.9	67.7	68.7	67.6	67.9	68.0	68.4	67.4
3	92.7	91.2	88.5	90.1	91.4	89.4	88.6	87.2	90.2	89.4	90.4	90.4	91.3	88.5	87.2	89.0	89.6	89.8	88.3	90.2	90.0	79.1
4	48.7	47.7	47.5	47.6	47.6	48.6	47.4	47.7	47.4	48.6	47.2	47.4	48.1	47.4	47.6	47.9	48.7	47.5	47.5	47.9	48.9	48.3
3	51.8	53.1	52.4	52.9	52.7	51.5	52.2	52.3	52.8	51.2	52.4	52.8	51.6	52.2	52.4	51.8	52.2	52.9	52.5	52.3	53.2	47.0
6	18.5	21.2	21.2	21.4	17.2	18.4	17.3	21.4	20.8	18./	19.6	19.7	18.0	17.2	20.4	19.8	21.4	17.0	21.2	17.6	19.5	18.2
/	31.0	31.5	51.2 40.4	51.4 40.5	29.8	40.0	29.9	51.4 40.5	29.8	20.0	40.0	40.1	31.0	29.9	50.4 40.6	40.0	40.2	31.4	31.2 40.5	30.9	52.4	32.7
c	40.9	40.4	40.4	40.5	40.0	40.9	40.1	40.5	40.4	40.8	40.0	40.1	40.9	40.2	40.6	40.0	40.5	40.6	40.5	40.5	41.7	59.9 47.5
20	40.0	40.5	40.2	40.0	29.5	43.2	40.2	28.2	40.0	43.7	40.7	40.7	29.5	40.2	40.5	47.0	20.2	40.0	40.3	40.1	47.1	47.5
11	22.7	22.5	22.4	22.5	22.5	22.7	22.5	22.4	22.6	22.0	22.4	22.3	22.7	22.5	22.6	22.3	22.2	22.5	22.4	22.6	24.2	24.0
12	127.6	127.1	127.0	127.4	126.6	127.5	126.6	127.5	126.9	127.0	126.8	127.1	127.9	126.5	127.1	126.6	127.4	127.3	127.0	127.2	125.9	122.7
13	149.6	149.3	149.5	149.5	150.3	149.6	150.3	149.6	150.2	150.8	150.2	149.5	149.6	150.3	150.2	150.4	149.9	149.6	149.5	149.8	147.9	144.1
14	43.8	43.4	43.3	43.5	42.6	43.8	42.8	43.5	42.8	42.7	42.3	43.1	44.0	42.9	43.1	42.5	43.6	43.5	43.3	43.3	44.4	42.2
15	25.5	25.7	25.6	25.7	24.6	25.5	24.6	25.6	24.6	24.7	24.7	25.3	25.5	24.6	24.6	24.5	25.5	25.6	25.6	25.3	26.9	28.1
16	21.6	21.6	21.6	21.6	20.5	21.6	20.6	21.5	20.7	20.4	20.4	21.3	21.5	20.6	20.8	20.5	21.5	21.5	21.6	21.3	23.0	23.4
17	48.1	47.9	47.9	47.6	48.3	48.1	48.2	47.5	48.1	47.8	48.1	47.8	47.8	48.2	47.9	48.3	47.4	47.6	47.9	48.0	49.0	47.0
18	41.3	41.0	41.0	41.2	41.3	41.2	41.3	41.2	41.3	41.5	41.3	40.9	41.4	41.3	41.4	41.3	41.2	41.1	41.0	41.2	42.4	41.7
19	42.8	43.0	43.0	43.2	43.0	42.8	42.9	43.3	42.8	42.6	43.3	43.0	43.0	42.9	43.0	43.2	43.4	43.2	43.0	43.0	44.1	46.1
20	31.6	31.7	31.7	31.4	31.5	31.6	31.6	31.2	31.8	31.9	31.4	31.8	31.4	31.7	31.7	31.4	31.2	31.4	31.7	31.6	33.0	30.7
21	31.4	31.4	31.3	31.3	30.9	31.3	31.0	31.3	30.9	30.8	30.9	31.4	31.4	31.0	31.0	30.9	31.4	31.3	31.3	31.2	32.7	33.9
22	30.7	30.7	30.7	30.9	30.9	30.7	30.9	30.9	30.9	31.0	31.1	30.8	30.9	30.9	30.7	31.0	30.7	30.9	30.7	30.8	32.3	33.0
23	71.0	73.4	72.8	72.9	73.4	71.0	72.9	73.0	72.7	71.0	68.6	68.6	71.3	72.4	72.8	68.8	73.3	72.6	72.3	72.2	72.5	62.2
24	58.3	63.4	63.4	63.8	63.4	58.3	63.4	63.8	63.8	58.3	59.3	59.4	58.7	63.4	63.8	56.3	63.4	63.7	63.4	61.7	62.3	62.4
25	10.6	11.8	11.6	11.9	11.7	10.4	11.5	11.7	11.9	10.3	10.8	11.0	10.4	11.5	11.7	11.7	11.6	11.8	11.6	11.3	13.3	17.5
26	13.6	12.6	12.6	12.5	11.4	13.5	11.6	12.6	11.5	12.0	10.8	12.2	13.5	11.7	11.8	11.3	12.9	12.5	12.6	12.5	14.5	17.7
27	20.0	20.1	20.2	20.3	20.7	20.0	20.7	20.3	21.0	22.2	20.7	20.1	20.2	20.7	20.8	20.8	20.4	20.3	20.2	20.4	22.1	25.9
28	183.8	183.8	183.8	183.6	183.5	183.8	183.4	183.7	183.6	183.9	183.5	183.8	183.7	183.4	183.6	183.4	183.8	183.7	183.8	183.7	180.8	176.4
29	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	28.3	29.8	33.0
30	18.7	18.7	18.7	18.6	18.8	18.7	18.8	18.6	18.8	18.9	18.8	18.7	18.6	18.8	18.8	18.8	18.6	18.6	18.7	18.7	20.5	23.6
HHDP-1	114.2	114.3	114.0	116.2	114.4	113.9	114.2	115.9	115.9	114.5	113.9	114.1	115.4	117.3	115.7	114.6	116.2	119.2	117.4	114.8	113.9	118.0
HHDP-1	115.8	115.5	116.1	113.4	115.5	116.0	115.9	113.6	113.5	116.0	115.9	115.9	113.3	120.3	113.6	117.7	113.5	118.0	120.3	115.4	114.5	118.4
HHDP-2	126.2	126.6	127.3	123.8	126.4	126.5	127.0	124.2	123.8	126.3	126.8	127.1	124.6	127.1	124.2	127.8	123.9	124.0	127.2	126.0	124.8	
HHDP-2	127.9	128.1	127.9	125.8	128.0	127.9	128.0	126.0	125.6	127.9	128.6	128.5	126.6	127.0	125.8	119.6	125.8	124.1	126.9	127.3	126.0	
HHDP-3	107.0	107.3	107.2	108.7	107.2	107.2	107.2	109.4	108.5	107.0	106.4	106.2	108.6	104.8	109.1	106.8	108.9	106.1	105.0	107.5	106.8	106.6
HHDP-3	111.8	112.4	112.5	110.4	112.4	111.8	112.5	110.2	110.6	111.8	111.2	111.2	109.2	111.6	110.5	113.4	110.5	108.8	111.6	111.6	110.8	112.1
HHDP-4	145.7	146.0	145.7	145.0	145.8	145.6	145.7	145.0	144.9	145.4	145.8	145.7	144.9	145.1	144.9	142.8	144.8	142.4	143.1	145.4	143.6	145.7
HHDP-4	147.2	147.1	146.9	143.8	147.1	147.1	147.0	143.6	144.1	147.3	147.0	147.0	144.1	145.8	143.9	145.7	143.6	143.4	145.8	146.2	144.4	145.9
HHDP-5	134.6	134.8	134.2	135.6	134.8	134.2	134.2	135.0	135.5	134.1	134.5	134.7	135.1	134.0	135.0	134.3	135.1	135.5	134.2	134.7	133.2	137.7
HHDP-5	140.1	139.9	140.1	130.0	140.0	140.2	140.2	136.4	1.56.8	140.6	139.6	139.7	136.5	139.9	136.7	138.5	136.4	136.5	139.8	139.2	137.6	139.8
HHDP-6	143.3	143.2	142.7	143.5	143.2	142.9	142.7	143.1	143.3	143.4	143.3	143.8	143.5	145.3	143.0	145.5	143.2	146.5	145.5	143.3	141.6	146.9
HHDP-6	145.6	145.5	145.5	145.3	145.6	145.6	145.7	145.4	145.4	146.0	145.6	145.5	145.8	144.3	145.4	143.2	145.2	145.6	144.3	145.5	143.7	147.1
HHDP-7	178.1	178.1	178.9	174.3	178.1	178.6	178.9	174.4	174.2	178.5	178.4	178.3	173.5	178.5	174.4	172.5	175.1	174.0	178.5	177.3	1/4.6	170.7
nnDP-/	1/1.4	1/0.0	1/0.2	1/1/1	1/0.0	1/1.5	1/0.4	1/0.5	1/0/0	1/1.5	1/1./	1/1.0	1/1.4	1/01/	1/0.2	171.0	1/0.5	1/0.0	1/11/	1/11/	100.1	106.9

^a Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in pyridime (PCM). ^b Measured in pyridine-d 5. ^c Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. ^d Linearly corrected for the experimental data.

Figure S46. Correlation plots of experimental ¹H NMR chemical shifts versus corresponding calculated ¹H NMR chemical shifts of **4'o**.

Figure S47. Correlation plots of experimental ¹³C NMR chemical shifts versus corresponding calculated ¹³C NMR chemical shifts of **4'o**.

	4'0A	4'oB
$sDP4+(^{1}H)$	48.77%	51.23%
$sDP4+(^{13}C)$	100.00%	0.00%
$sDP4+(^{1}H+^{13}C)$	100.00%	0.00%
$uDP4+(^{1}H)$	0.58%	99.42%
$uDP4+(^{13}C)$	99.90%	0.10%
$uDP4+(^{1}H+^{13}C)$	85.66%	14.34%
$DP4+(^{1}H)$	0.55%	99.45%
$DP4+(^{13}C)$	100.00%	0.00%
$DP4+(^{1}H+^{13}C)$	100.00%	0.00%

Table S7. The DP4+ probability analysis of **4'o**.

Cartesian coordinates of the lowest-energy conformer of **4'oA** (**4'oA-1**) at the B3LYP/6-31G(d,p) level in pyridine (PCM).

C 1.93986700 -0.84574500 -0.38158400 C 1.030883400 -1.9715400 -0.95209100 -0.85650800 C -0.24758100 -0.95309100 -0.85650800 C -0.75792700 0.3542500 -1.20080500 C -1.05555800 -1.74655100 -2.713403400 C -2.51799100 -1.53555100 -1.77671300 C -2.25724900 -0.38821800 -1.00330800 C -2.25724900 0.414041200 0.14474500 C -0.45262200 1.63360600 -0.98196700 C -4.58194200 -0.91318700 -0.32429100 C -4.58194200 -0.91318700 -0.32429100 C -5.56246900 -1.44622600 -1.41345500 C -7.05122300 -1.52551100 -0.98388900 C -7.56528600 -1.4622600 -0.4838900 C -7.05312300 -1.52551100 -0.98388900 C -7.56528600 -1.4622600 -0.46365900 C -7.05312300 -0.52737500 0.63722000 C -9.37533900 -1.3361400 -0.46365900 C -9.37533900 -0.52737500 2.4129700 C -9.37533900 -1.33401400 1.18674300 C -9.06001400 0.88501900 2.83183700 C -9.6601400 0.88501900 2.843183700 C -9.6601400 0.88501900 2.843183700 C -9.6601400 0.88501900 2.843183700 C -9.6601400 0.88501900 2.843183700 C -8.81205000 -1.4798400 3.59616000 C -4.33091300 -2.65388900 0.6178000 C -4.33091300 -2.6538900 0.5178400 C -5.5915000 -1.436543000 0.15748800 C -6.26093400 -2.65438200 0.5178400 C -5.5915000 -1.436543000 0.15748800 C -5.5915000 -1.436543000 0.15748800 C -5.5915000 -1.436543000 0.15748800 C -5.5934500 -2.8297000 -0.78534500 C -5.8945800 3.38094300 0.16582000 C -5.89458500 3.38094300 0.16582000 C 4.35609200 2.92970200 -0.74622800 C 4.35609200 2.9297020 -0.7462800 C 4.35649600 5.11694200 -0.38543300 C 4.6541900 -2.229700 -0.7462800 C 4.15459700 -2.84873000 -1.71524500 C 4.15459700 -2.8487200 -0.94873300 C 4.6541900 0.55114700 -1.7343200 C 4.6541900 -2.2297000 -0.7462800 C 4.15459700 -2.84873000 -1.71524500 C 4.15459700 -2.84873000 -1.71524500 C 4.16541900 -2.222090 -2.14827300 C 4.6541900 -2.21234400 -1.17842200 C 4.7436000 -2.12334000 -0.5717100 C 4.7436000 -1.7487900 -2.4873300 C 4.65240900 -2.12334000 -2.1823300 H -0.2969200 1.4075600 -1.70892400 C 4.7437000 0.55643000 -0.5717300 C 4.65240900 -2.17335000 -2.65163300 H -0.81252600 -1.76	С	1.50017600	0.42996600	1.09983100
C 1.30883400 -1.09715400 -0.1826508 C -0.75792700 0.35462500 -0.16542300 C -0.02803800 0.47625300 1.20080500 C -1.0554800 -1.24658100 -1.77671300 C -3.22262900 0.14041200 0.14474500 C -4.58194200 -0.93131700 -0.32429100 C -4.4423300 1.21135500 0.9979100 C -5.21297900 0.24060400 -0.432429100 C -4.4423300 -1.4462200 -1.41345600 C -5.66246900 -1.3750400 -0.46365900 C -6.71793300 -0.24770300 -0.6454200 C -9.07979200 -0.24770300 -0.2654800 C -9.07979200 -0.24770300 -2.02973000 C -8.58661600 -0.5237700 2.44249700 C -9.0601400 .88501900 -2.02973000 C -3.5874400 0.395800 0.66778000 C -9.1601400 -88	С	1.93986700	-0.84574500	0.38158400
C -0.24758100 -0.85309100 -0.85650800 C -0.02803900 0.47625300 1.20080500 C -1.05354800 -1.24658100 -2.13403400 C -2.51799100 -1.53565100 -1.77671300 C -2.25724900 1.63360600 -0.98196700 C -2.25724900 0.414041200 0.14474500 C -0.45262200 1.63360600 -0.98196700 C -4.58194200 -0.91318700 -0.32429100 C -5.262999400 1.34735500 0.83722000 C -4.44823300 -1.1435500 0.98779100 C -2.9599400 -1.44622600 -1.4134560 C -7.05512300 -1.52514100 -0.98388900 C -7.565246900 -1.44622600 -0.46365900 C -7.65358800 -0.23775000 0.76454200 C -9.0779200 -0.24770300 -0.09564800 C -9.07979200 -0.24770300 -0.09564800 C -9.07979200 -0.24770300 -0.29564800 C -9.075353900 -1.03401400 1.18674300 C -9.0601400 0.88501900 2.8138700 C -9.0601400 0.88501900 2.8138700 C -9.0601400 0.88501900 2.8138700 C -4.3091300 -2.09395800 0.66178000 C -4.3091300 -2.09395800 0.56178000 C -6.2469400 -0.3269300 0.15748800 C -4.3091300 -2.65438000 0.17548800 C -5.59315000 -1.43659100 0.7546900 C -6.2469400 -0.3269300 0.15748800 C -7.56218300 -1.75786900 0.015134100 C -7.5628200 -1.75786900 0.015134100 C -7.56728200 -1.75786900 0.015134100 C -7.56728200 -2.82344100 0.47774900 C -7.56728200 -2.82344100 0.47774900 C -7.56728200 -2.82344100 0.47774900 C 4.756785400 1.59105400 -0.75834600 C 4.43609200 2.92970200 -0.28739300 C 4.5649500 3.3401700 1.06817500 C 4.4564960 5.11694200 0.1751300 C 4.5649500 3.3401700 1.06817500 C 4.65045100 -0.18513600 -0.7854600 C 4.9390500 -2.40837900 0.16542000 C 7.19806600 1.48489200 -0.17342200 C 4.56494600 5.11694200 0.18439800 C 7.19806600 1.487600 -1.7342200 C 7.6173300 0.55646400 -1.7343200 C 7.642731100 1.9887300 -1.7342200 C 7.64373000 0.55646000 -1.7354000 C 7.64373000 0.55646000 -1.7354000 C 7.643746200 -0.23540200 -2.4837300 D 7.64270800 -2.5509600 -1.7452700 0.48481900 D 7.642746000 -0.58574000 -2.5433300 H 1.663	С	1.30883400	-1.09715400	-1.01920800
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C	c	-9.06001400	0.75594500	2 93193700
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0 3.72354100 -2.02220900 2.15547500 C 1.65411300 -2.56093600 -1.40562900 C 1.91352000 -0.23396000 -2.18237300 O 3.38519200 -0.84872000 0.24483100 O 1.04422000 -3.46472500 -0.49272500 O 2.10978700 0.52261000 2.38956300 O 9.48823600 -1.96029400 -0.59710100 O 9.48823600 -4.02052700 0.63421200 C -7.51235600 0.84794500 -1.61052700 O 9.74832600 2.12344200 -1.17840200 C -7.44336000 2.12344200 -1.17840200 C -7.49778300 3.13831300 -2.19987000 H 1.66932600 -1.70487900 1.00352200 H -0.50590600 -1.75910000 -0.15718600 H -0.34746200 -0.34540300 1.85734000 H -0.65240900 -2.12351500 -2.65163200 H -0.65240900	c	4.15459700	-1.45174400	1.16839800
C 1.65411300 -2.56093600 -1.40562900 C 1.91352000 -0.23396000 -2.18237300 O 3.38519200 -0.84872000 0.24483100 O 1.04422000 -3.46472500 -0.49272500 O 2.10978700 0.52261000 2.38956300 O 9.48823600 -1.96029400 -0.59710100 O 8.19420500 -4.02052700 0.63421200 C -7.51235600 0.84794500 -1.61052700 O -7.60817500 0.56664600 -2.79168600 O -7.44336000 2.12344200 -1.17840200 C -7.49778300 3.13831300 -2.19987000 H 1.66932600 -1.70487900 1.00352200 H 0.50590600 -1.75910000 -0.15718600 H -0.29692000 1.40756000 1.70894200 H -0.34746200 -0.34540300 1.85734000 H -0.65240900 -2.12351500 -2.65163200 H -0.65240900 -2.45336200 -1.18106900 H -2.51900600 -2.	0	3.72354100	-2.02220900	2.15547500
C 1.91352000 -0.23396000 -2.18237300 O 3.38519200 -0.84872000 0.24483100 O 1.04422000 -3.46472500 -0.49272500 O 2.10978700 0.52261000 2.38956300 O 9.48823600 -1.96029400 -0.59710100 O 8.19420500 -4.02052700 0.63421200 C -7.51235600 0.84794500 -1.61052700 O -7.60817500 0.56664600 -2.79168600 O -7.409778300 3.13831300 -2.19987000 C -7.49778300 3.13831300 -2.19987000 H 1.66932600 -1.70487900 1.00352200 H 0.50590600 -1.75910000 -0.15718600 H -0.29692000 1.40756000 1.70894200 H -0.34746200 -0.34540300 1.85734000 H -0.65240900 -2.12351500 -2.65163200 H -0.29692000 1.40756000 1.70894200 H -0.65240900 -2.12351500 -2.65163200 H -0.65240900 -2.	c	1.65411300	-2.56093600	-1.40562900
0 3.38519200 -0.84872000 0.24483100 0 1.04422000 -3.46472500 -0.49272500 0 2.10978700 0.52261000 2.38956300 0 9.48823600 -1.96029400 -0.59710100 0 8.19420500 -4.02052700 0.63421200 0 -7.51235600 0.84794500 -1.61052700 0 -7.60817500 0.56664600 -2.79168600 0 -7.44336000 2.12344200 -1.17840200 0 -7.49778300 3.13831300 -2.19987000 1 1.87639400 1.29674900 0.55433300 0 1.66932600 -1.70487900 1.00352200 0 +0.50590600 -1.75910000 -0.15718600 0 -0.29692000 1.40756000 1.70894200 0 -0.34746200 -0.34540300 1.85734000 0 -0.65240900 -2.12351500 -2.65163200 0 + -0.65240900 -2.45336200 -1.18106900 0 -2.519	c	1,91352000	-0.23396000	-2.18237300
0 1.04422000 -3.46472500 -0.49272500 0 2.10978700 0.52261000 2.38956300 0 9.48823600 -1.96029400 -0.59710100 0 8.19420500 -4.02052700 0.63421200 0 -7.51235600 0.84794500 -1.61052700 0 -7.60817500 0.56664600 -2.79168600 0 -7.44336000 2.12344200 -1.17840200 0 -7.49778300 3.13831300 -2.19987000 0 -7.49778300 3.13831300 -2.19987000 0 -7.49778300 1.29674900 0.55433300 1 1.66932600 -1.70487900 1.00352200 H 1.66932600 -1.75910000 -0.15718600 H -0.50590600 -1.75910000 1.07894200 H -0.34746200 -0.34540300 1.85734000 H -0.65240900 -2.12351500 -2.65163200 H -0.65240900 -2.12351500 -2.68993500 H -2.51900600 -2.45336200 -1.18106900 H -2.28029800 -	0	3.38519200	-0.84872000	0.24483100
0 2.10978700 0.52261000 2.38956300 0 9.48823600 -1.96029400 -0.59710100 0 8.19420500 -4.02052700 0.63421200 0 -7.51235600 0.84794500 -1.61052700 0 -7.60817500 0.56664600 -2.79168600 0 -7.44336000 2.12344200 -1.17840200 0 -7.49778300 3.13831300 -2.19987000 0 -7.49778300 3.1987900 1.0352200 1 1.86932600 -1.70487900 1.0352200 H 1.66922600 -1.75910000 -0.15718600 H -0.29692000 1.40756000 1.70894200 H -0.34746200 -0.34540300 1.85734000 H -0.65240900 -2.12351500 -2.65163200 H -0.65240900 -2.45336200 -1.18106900 H -2.51900600 -2.45336200 -1.18106900 H -2.28029800 -0.66574700 0.88586500 H -0.81252600 <	0	1.04422000	-3.46472500	-0.49272500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	2.10978700	0.52261000	2.38956300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	9.48823600	-1.96029400	-0.59710100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	8.19420500	-4.02052700	0.63421200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-7.51235600	0.84794500	-1.61052700
O-7.443360002.12344200-1.17840200C-7.497783003.13831300-2.19987000H1.876394001.296749000.55433300H1.66932600-1.704879001.00352200H-0.50590600-1.75910000-0.15718600H-0.296920001.407560001.70894200H-0.34746200-0.345403001.85734000H-0.98686200-0.41779500-2.84790200H-0.65240900-2.12351500-2.65163200H-2.51900600-2.45336200-1.18106900H-2.51900600-2.45336200-1.81806900H-0.812526001.58557400-2.01018100H0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	0	-7.60817500	0.56664600	-2.79168600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	-7.44336000	2.12344200	-1.17840200
H1.876394001.296749000.55433300H1.66932600-1.704879001.00352200H-0.50590600-1.75910000-0.15718600H-0.296920001.407560001.70894200H-0.34746200-0.345403001.85734000H-0.98686200-0.41779500-2.84790200H-0.65240900-2.12351500-2.65163200H-3.07987300-1.76207900-2.68993500H-2.51900600-2.45336200-1.18106900H-0.812526001.58557400-2.01018100H0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	C	-7.49778300	3.13831300	-2.19987000
H1.66932600-1.704879001.00352200H-0.50590600-1.75910000-0.15718600H-0.296920001.407560001.70894200H-0.34746200-0.345403001.85734000H-0.98686200-0.41779500-2.84790200H-0.65240900-2.12351500-2.65163200H-3.07987300-1.76207900-2.68993500H-2.51900600-2.45336200-1.18106900H-0.812526001.58557400-2.01018100H-0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	H	1.87639400	1.29674900	0.55433300
H-0.50590600-1.75910000-0.15718600H-0.296920001.407560001.70894200H-0.34746200-0.345403001.85734000H-0.98686200-0.41779500-2.84790200H-0.65240900-2.12351500-2.65163200H-3.07987300-1.76207900-2.68993500H-2.51900600-2.45336200-1.18106900H-0.812526001.58557400-2.01018100H0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	Н	1.66932600	-1.70487900	1.00352200
H-0.296920001.407560001.70894200H-0.34746200-0.345403001.85734000H-0.98686200-0.41779500-2.84790200H-0.65240900-2.12351500-2.65163200H-3.07987300-1.76207900-2.68993500H-2.51900600-2.45336200-1.18106900H-2.28029800-0.665747000.88586500H-0.812526001.58557400-2.01018100H0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	Н	-0.50590600	-1.75910000	-0.15718600
H-0.34746200-0.345403001.85734000H-0.98686200-0.41779500-2.84790200H-0.65240900-2.12351500-2.65163200H-3.07987300-1.76207900-2.68993500H-2.51900600-2.45336200-1.18106900H-2.28029800-0.665747000.88586500H-0.812526001.58557400-2.01018100H0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	Н	-0.29692000	1.40756000	1.70894200
H-0.98686200-0.41779500-2.84790200H-0.65240900-2.12351500-2.65163200H-3.07987300-1.76207900-2.68993500H-2.51900600-2.45336200-1.18106900H-2.28029800-0.665747000.88586500H-0.812526001.58557400-2.01018100H0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	Н	-0.34746200	-0.34540300	1.85734000
H-0.65240900-2.12351500-2.65163200H-3.07987300-1.76207900-2.68993500H-2.51900600-2.45336200-1.18106900H-2.28029800-0.665747000.88586500H-0.812526001.58557400-2.01018100H0.618899001.83223700-1.03135800H-0.910796002.51084300-0.51781500	Н	-0.98686200	-0.41779500	-2.84790200
H -3.07987300 -1.76207900 -2.68993500 H -2.51900600 -2.45336200 -1.18106900 H -2.28029800 -0.66574700 0.88586500 H -0.81252600 1.58557400 -2.01018100 H 0.61889900 1.83223700 -1.03135800 H -0.91079600 2.51084300 -0.51781500	Н	-0.65240900	-2.12351500	-2.65163200
H -2.51900600 -2.45336200 -1.18106900 H -2.28029800 -0.66574700 0.88586500 H -0.81252600 1.58557400 -2.01018100 H 0.61889900 1.83223700 -1.03135800 H -0.91079600 2.51084300 -0.51781500	Н	-3.07987300	-1.76207900	-2.68993500
H -2.28029800 -0.66574700 0.88586500 H -0.81252600 1.58557400 -2.01018100 H 0.61889900 1.83223700 -1.03135800 H -0.91079600 2.51084300 -0.51781500	Н	-2.51900600	-2.45336200	-1.18106900
H -0.81252600 1.58557400 -2.01018100 H 0.61889900 1.83223700 -1.03135800 H -0.91079600 2.51084300 -0.51781500	Н	-2.28029800	-0.66574700	0.88586500
H 0.61889900 1.83223700 -1.03135800 H -0.91079600 2.51084300 -0.51781500	Н	-0.81252600	1.58557400	-2.01018100
H -0.91079600 2.51084300 -0.51781500	Н	0.61889900	1.83223700	-1.03135800
	Н	-0.91079600	2.51084300	-0.51781500

Н	-4.93036100	2.00485400	1.57136500
Н	-2.50960500	1.51214800	1.82434100
Н	-2.76779200	2.27473300	0.27946600
Н	-5.23015500	-2.44209700	-1.72769500
Н	-5.52371400	-0.81822300	-2.30371600
Н	-7.17525300	-2.28382400	-0.20796600
Н	-7.63611100	-1.84226500	-1.84177500
Н	-6.96752700	1.31776000	0.96945000
Н	-9.46185300	0.77371700	0.01285900
Н	-9.62061100	-0.69124500	-0.93993500
Н	-9.13769300	-2.09460000	1.03379500
Н	-10.45297800	-0.98878400	1.39057000
Н	-6.50035000	-0.10503400	2.87473200
H	-6.76517700	-1.56617800	1.94917400
Н	-4.15982000	1.52545400	-1.59441300
Н	-2.63983000	1.19546500	-2.41749100
H	-4.08326300	0.33894700	-2.89598100
Н	-8.93139600	1.63180000	2.04359500
Н	-8.50033400	1.23242500	3.70769200
H	-10.12257300	0.86927700	3.10024300
H	-8.24587400	-1.15755100	4.47759900
Н	-8.49503700	-2.49916100	3.34795900
Н	-9.87161000	-1.51663100	3.87484800
Н	-3.81695300	-1.78056100	1.57264000
Н	-5.28017600	-2.53637800	0.97030800
Н	-3.75285300	-2.89788000	0.19909300
Н	5.75169400	-3.48689700	1.40112700
Н	3.59972900	3.29940500	-1.42347300
H	7.75233800	1.20010800	-1.10786800
Н	7.30753500	0.68533200	2.00729800
H	7.01044700	3.74051300	2.56305800
Н	5.04897700	5.56047100	0.89841500
Н	2.74721300	-2.66276400	-1.39498700
H	1.32021000	-2.75854600	-2.43356500
Н	2.52023600	-0.85546000	-2.84327100
H	1.12697800	0.22725400	-2.77659800
Н	1.43488900	-4.33695600	-0.6324/800
Н	2.06713400	-0.35201100	2.80420600
Н	9.78714700	-1.15558500	-1.04945600
H	9.07946600	-3.95225100	0.24293900
H	-8.43438600	3.07069800	-2.75749700
H	-6.65955100	3.02977100	-2.89130200
Н	-7.43556200	4.08892700	-1.67200800

Cartesian coordinates of the lowest-energy conformer of **4'oB** (**4'oB-1**) at the B3LYP/6-31G(d,p) level in pyridine (PCM).

C C	-1.15850000 -2.01364900	0.11761900 -0.13011000	2.74122700 1.49169900
C	-1.49878700	-1.24638200	0.52914400
C	0.06252100	-1.05844600	0.33663200
C	0.94190700	-0.81968100	1.60621800
C	0.30309000	0.35592500	2.38922200
C	0.72953100	-2.10965100	-0.57289900
С	2.04539400	-1.54903000	-1.13124800
С	3.07178400	-1.14146000	-0.04280600
С	2.35827700	-0.32421500	1.09461400
С	1.00905700	-2.04917100	2.54075000
С	4.21769000	-0.19318200	-0.65867300
С	5.16067700	0.25513600	0.47719500
С	4.72713600	0.33001700	1.74288900
С	3.35548100	-0.04051100	2.23237300
С	5.00776900	-0.95252600	-1.76785000
С	6.36894900	-0.33832700	-2.12324200
С	7.28487200	-0.22621100	-0.88636400
С	6.60608500	0.67558200	0.18289100
С	8.70112800	0.31570300	-1.25782900
С	8.73247400	1.81306700	-1.58454900
С	8.13757600	2.69550400	-0.46470000
С	6.70881500	2.18371000	-0.16718000
С	3.71999500	-2.44161600	0.50632500
С	9.01963600	2.66369600	0.79998700
С	8.05351900	4.15129400	-0.95826900
С	3.63173500	1.08527400	-1.32862700

C	2 02064200	0 54450000	1 1 (= 4 2 (0 0
C	-3.83984200	2.34439600	1.10343000
С	-4.53119400	1.36762800	0.86402800
С	-5.37464300	1,26826200	-0.25943700
Ċ	-5 48669800	2 39625600	-1 08622100
C	-3.48889800	2.39023000	-1.00022100
С	-4.80681600	3.58292800	-0.78955300
С	-3.98592400	3.65942200	0.33850200
C	-6 15654100	0 04604900	-0 64057800
C	-0.13034100	0.04804900	-0.04037800
C	-5.70616100	-0.89463100	-1.59666700
C.	-6.57560100	-1.85029500	-2.13535300
	7 0022200	1 02207100	1 00705000
L	-7.89333200	-1.9320/100	-1.08/95000
С	-8.31989700	-1.08631300	-0.65552700
C	-7 45534400	-0 11590400	-0 13829900
8		0.11330100	0.13023300
0	-6.25062400	2.44//5800	-2.21/29100
0	-7.94321700	0.63605800	0.89901200
0	-9 58177300	-1 25219000	-0 17252900
0	5.50177500	1.25215000	0.1/252500
0	-8.73020100	-2.87341900	-2.20118700
С	-4.25791000	-1.04004100	-1.92355300
0	-3 52070200	-0 97993300	_0 70007300
0	-3.52070200	-0.87993300	-0.79887300
0	-3.79048000	-1.34918000	-3.00248200
C	-4 49372500	0 18241300	1 76699900
8	1.13372300	0.10211300	1.700333000
0	-5.51502200	-0.25100300	2.28182900
С	-1.97085500	-2.66884700	0.97108800
C	-2 08975100	-1 01035600	-0 88824000
-	2 241/2000	1.01000000	2 020023000
U	-3.34163900	-0.46443000	∠.0∠909800
0	-2.05791000	-2.90079500	2.37295400
0	-1 63504000	1 28191700	3 42810500
- -	1.00005000	1.20101/00	1 574671000
U	-4.90985300	4.69593900	-1.5/46/100
0	-3.32518100	4.81232300	0.63321700
C	7 55503200	-1 61201100	_0 27888700
C	7.33303200	1.01201100	0.27090700
0	7.61951400	-1.86584600	0.90940100
0	7.80666100	-2.53824400	-1.22909700
C	0 16205200	2 0 5 0 0 2 2 0 0	0 75216000
C	0.10393300	-3.83003300	-0.75218900
H	-1.24951400	-0.75248900	3.39701400
Н	-2.08592200	0.80871300	0.94042900
ц	0 13646400	-0 10652400	-0 21247000
11	0.13040400	0.10032400	0.2124/000
Н	0.83852500	0.54501200	3.3241/800
Н	0.36667900	1.27788200	1.79551800
н	0 90359700	-3 04215900	-0 02596100
11	0.00045700	2 27405100	1 41022000
н	0.08945700	-2.3/495100	-1.41933000
Н	2.49928000	-2.28410800	-1.80524800
н	1 78010700	-0 68817800	-1 75235100
	10001000	0.0001/000	1.75255100
Н	2.12601100	0.646/2400	0.64394000
Н	1.42558200	-2.93134400	2.05517800
н	0 01862100	-2 33329300	2 89575200
	0.01002100	2.33329300	2.05575200
Н	1.62935500	-1.83596900	3.41604800
Н	5.42730600	0.65320800	2.51417600
ц	2 97883500	0 76311300	2 87765800
11	2.97003300	0.70311300	2.07705000
Н	3.45522200	-0.91414500	2.89185800
Н	4.38909700	-1.00230900	-2.67102100
ц	5 18791600	-1 98708300	-1 16797500
11	5.10/51000	1.90700500	1.40797900
Н	6.24477600	0.65586200	-2.56395300
Н	6.85272400	-0.95493200	-2.88641000
ц	7 159/2700	0 52661900	1 11460500
11	7.13542700	0.52001500	1.11400500
H	9.38054700	0.11843500	-0.41979400
Н	9.08445900	-0.26190300	-2.10616100
н	8 176/5100	2 0008/100	-2 51231000
п	8.1/045100	2.00084100	-2.51251000
Н	9.76971000	2.11152900	-1.78455400
Н	6.27970800	2,74933600	0.66908800
11	6 09533300	2 41465200	1 02604000
п	0.00555200	2.41403200	-1.03894800
H	/ 6//69////	-2 23803500	1.11225600
Н	4.00400000	2.23003300	
ц	3.02509200	-3.01259000	1.11956500
11	3.02509200	-3.01259000	1.11956500
	4.00408000 3.02509200 4.02228800	-3.01259000 -3.10340500	1.11956500
Н	4.00408000 3.02509200 4.02228800 10.02621900	-3.01259000 -3.10340500 3.03576400	1.11956500 -0.30953400 0.57704600
H H	4.00408000 3.02509200 4.02228800 10.02621900 9.12591500	-3.01259000 -3.10340500 3.03576400 1.66060600	1.11956500 -0.30953400 0.57704600 1.22177000
H H H	4.00408000 3.02509200 4.02228800 10.02621900 9.12591500 8.59311400	-3.01259000 -3.10340500 3.03576400 1.66060600 3.0397400	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600
H H H	4.0040000 3.02509200 4.02228800 10.02621900 9.12591500 8.59311400	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600
Н Н Н	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900
н н н н	4.00438000 3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000
H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.5286000	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000
H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000
H H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500
H H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200 1.63218400	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200
H H H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500 2.87219600	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200 1.63218400 0.84384500	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200 -2.07666500
H H H H H H H H	4.00438000 3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500 2.87219600	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200 1.63218400 0.84384500	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200 -2.07666500
H H H H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500 2.87219600 -3.18523800	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200 1.63218400 0.84384500 2.60606100	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200 -2.07666500 2.02769000
H H H H H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500 2.87219600 -3.18523800 -6.21618800	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200 1.63218400 0.84384500 2.60606100 -2.56178500	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200 -2.07666500 2.02769000 -2.86977500
H H H H H H H H H H H	4.00438000 3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500 2.87219600 -3.18523800 -6.21618800	-3.01259000 -3.0340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200 1.63218400 0.84384500 2.60606100 -2.56178500 1.58774300	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200 -2.07666500 2.02769000 -2.86977500 -2.36038600
H H H H H H H H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500 2.87219600 -3.18523800 -6.21618800 -6.67500900	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.22917900 4.54386800 1.77774200 1.63218400 0.84384500 2.60606100 -2.56178500 1.58774300	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200 -2.07666500 2.02769000 -2.86977500 -2.36038600
H H H H H H H H H H H H	3.02509200 4.02228800 10.02621900 9.12591500 8.59311400 7.61047100 7.43964000 9.04951300 3.19593400 4.41657500 2.87219600 -3.18523800 -6.21618800 -6.67500900 -7.23893700	-3.01259000 -3.10340500 3.03576400 1.66060600 3.30397400 4.80135900 4.22917900 4.54386800 1.77774200 1.63218400 0.84384500 2.60606100 -2.56178500 1.58774300 0.64790100	1.11956500 -0.30953400 0.57704600 1.22177000 1.58045600 -0.19504900 -1.86283000 -1.19402000 -0.60578500 -1.85398200 -2.07666500 2.02769000 -2.86977500 -2.36038600 1.57938300

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Н	9.07160300	-3.80318600	-0.14649700