# Isolation and Absolute Configurations of Diversiform C<sub>17</sub>, C<sub>21</sub> and C<sub>25</sub> Terpenoids from the Marine Sponge *Cacospongia* sp.

Xingwang Zhang <sup>1,2,†</sup>, Ping-Lin Li <sup>1,3,†</sup>, Guo-Fei Qin <sup>1,3</sup>, Shengying Li <sup>2,4</sup>, Nicole J. de Voogd <sup>5</sup>, Xu-Li Tang <sup>6,\*</sup> and Guo-Qiang Li <sup>1,3,\*</sup>

- <sup>1</sup> Key Laboratory of Marine Drugs, Chinese Ministry of Education, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, China; zhangxw@qibebt.ac.cn (X.-W.Z.); ipinglin@ouc.edu.cn (P.-L.L.); qinguofei@126.com (G.-F.Q.)
- <sup>2</sup> Shandong Provincial Key Laboratory of Synthetic Biology, CAS Key Laboratory of Biofuels, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao, Shandong 266101, China
- <sup>3</sup> Laboratory of Marine Drugs and Biological Products, National Laboratory for Marine Science and Technology, Qingdao 266235, China
- <sup>4</sup> Laboratory for Marine Biology and Biotechnology, Qingdao National Laboratory for Marine Science and Technology, Qingdao, Shandong 266237, China
- <sup>5</sup> National Museum of Natural History, 2300 RA Leiden, The Netherlands; nicole.devoogd@naturalis.nl
- <sup>6</sup> College of Chemistry and Chemical Engineering, Ocean University of China, Qingdao 266100, China; tangxvli@ouc.ed.cn (X-L.T.)
- + These authors contributed equally to this paper.
- \* Correspondence: tangxuli@ouc.edu.cn (X.-L.T.); liguoqiang@ouc.edu.cn (G.-Q.L.); Tel.: +86-532-82032323 (X.-L.T.); +86-532-82032323 (G.-Q.L.)

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Figure S25. HMBC spectrum of compounds 3a/3b.

Figure S26. NOESY spectrum of compounds 3a/3b.

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Figure S28. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compounds 4a/4b.

Figure S29. <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of compounds 4a/4b.

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Figure S34. DEPT spectrum (125 MHz, CDCl<sub>3</sub>) of compounds 5a/5b.

Figure S35. HR-ESI-MS of compound 6.

Figure S36. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 6.

Figure S37. <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of compound 6.

Figure S38. DEPT spectrum (125 MHz, CDCl<sub>3</sub>) of compound 6.

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Figure S41. HMBC spectrum of compound 6.

Figure S42. NOESY spectrum of compound 6.

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Figure S45. <sup>13</sup>C NMR spectrum (125 MHz, DMSO-d<sub>6</sub>) of compound 7.

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Figure S47. HSQC spectrum of compound 7.

**Figure S48.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 7.

Figure S49. HMBC spectrum of compound 7.

### I. Photos of sponge specimen



### Cacospongia sp.

The sponge *Cacospongia* sp. was in irregular shaped, and with a detailed feather of tight encrusting, rough, blackbrownish crust with irregularity distributed holes on the surface, thick and solid, had the dimensions of around  $4 \times 5$  cm  $\sim 6 \times 8$  cm.

#### **II.** Computational details

The quantum chemical calculations were performed using the density functional theory (DFT) as carried out in the Gaussian 09 [1]. The initial structures of the key chiral structures in compounds **1**, **2**, and **6** were built with Spartan 10 software, and all trial structures were first minimized based on molecular mechanics calculations. Conformational search was performed by Spartan 10 software using MMFF force filed, and conformers occurring within a 10 kcal/mol energy window from the global minimum were chosen for geometry optimization in the gas phase with the DFT method at the B3LYP/DGDZVP level. The B3LYP/DGDZVP harmonic vibrational frequencies were further calculated to confirm their stability. The spin-allowed excitation energies and rotatory (*R*n) and oscillator strengths (*f*n) of the lowest excited states of stable conformers were calculated for ECD spectra using TD-DFT method with the basis set RB3LYP/DGDZVP. Solvent effects of methanol solution were evaluated at the same DFT level by using the SCRF/PCM method in agreement with the experiment condition. Electronic transitions were expanded as Gaussian curves with a FQHM (full width at half maximum) for each peak of 0.32 eV. The ECD spectra were combined after Boltzmann weighting according to their population contribution.

#### Reference

1. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; et al. *Gaussian 09*, Revision A.1; Gaussian, Inc.: Wallingford, CT, USA, 2009.





p1-a2 (24.9%)





p1-a1 (52.5%)



p1-b1 (57.0%)

p1-a3 (6.5%)

p1-a4 (5.9%)



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p1-b2 (27.1%)



p1-b3 (6.5%)



p1-b4 (5.7%)

p1-a5 (5.3%)



p1-01 (57.07

p1-c1 (72.9%)

p1-c5 (1.4%)



\*

p1-c2 (13.8%)



p1-d1 (71.7%)

p1-c3 (2.8%)

p1-d2 (13.5%)

p1-c4 (2.8%)



p1-d3 (8.7%)

p1-d4 (2.38%)

**Figure S1.** Stable conformers of the key chiral structure in compounds **1a/1b** and **2a/2b** with 4*R*,5*R* (**p1-a**), 4*S*,5*S* (**p1-b**), 4*R*,5*S* (**p1-c**), and 4*S*,5*R* (**p1-d**) configurations.

**Table S1**. Important thermodynamic parameters (a.u.) of the optimized o key chiral structure in compounds **1a/1b** and **2a/2b** at B3LYP/6-31G(d,p) level in the gas phase.

Conformations	E+ZPE	G	Conformations	E+ZPE	G
p1-a1	-538.775574	-538.812577	p1-b1	-538.775574	-538.812577
p1-a2	-538.774784	-538.811876	p1-b2	-538.774784	-538.811876
p1-a3	-538.773475	-538.810603	p1-b3	-538.772980	-538.810536
p1-a4	-538.773266	-538.810519	p1-b4	-538.772705	-538.810404
p1-a5	-538.772705	-538.810404	p1-d1	-538.775222	-538.812165
p1-c1	-538.775223	-538.812166	p1-d2	-538.773373	-538.810593
p1-c2	-538.773373	-538.810594	p1-d3	-538.772821	-538.810171
p1-c3	-538.772135	-538.809101	p1-d4	-538.772003	-538.808919
p1-c4	-538.772033	-538.809104			
p1-c5	-538.771025	-538.808496			

n1-a1					p1-a2				n1-a3			
C	3 039	_0 5952	0.0608	C	2 9196	_0 5972	-0 2572	C	2 668	_0.9015	-1.0558	
C	1 9738	0.3702	0.3252	C	1 9236	0.3772	0.1215	C C	1 4076	-0.0781	-1 1745	
C	0 7704	-0.1377	-0 397	C	0.6038	-0 1479	-0.3022	C	0.4403	-0.8481	-0.3007	
0	0.9166	_1 5588	_0 2199	0	0.7841	_1 5514	-0.0442	0	1 2573	-1 3676	0.564	
C	2 231	-1.8546	0.0037	C	2 1173	-1.8463	-0.0619	C	2 5518	-1 4472	0.3352	
C	-0.6114	0.3233	0.1374	C	-0.6424	0.37	0.4567	C	-0.753	-0.0488	0.2833	
C	-1 7449	-0.4126	-0.6172	C	-1 9256	-0 4205	0.109	C	-1 6416	0 4935	-0.8566	
C	-3.1549	-0.0684	-0.1495	C	-2.3428	-0.387	-1.3538	C	-2.9111	1.2002	-0.393	
0	-0.7047	-0.0128	1.5286	0	-0.4296	0.1935	1.8691	0	-1.5425	-0.9746	1.0498	
C	-0.751	1.845	0.025	C	-0.837	1.8724	0.2306	C	-0.3112	1.0614	1.2464	
0	2.6698	-2.9873	0.1075	0	2,5696	-2.9744	0.037	0	3.4637	-1.921	0.9912	
Н	3.5309	-0.4378	-0.9033	Н	3.7934	-0.5826	0.3984	Н	3.5623	-0.2841	-1.1646	
Н	3.7726	-0.632	0.8688	Н	3.2189	-0.5236	-1.3064	Н	2.6808	-1.7319	-1.7675	
Н	2.252	1.4354	-0.0328	Н	2.1228	1.4302	-0.3659	Н	1.5986	0.9254	-0.779	
Н	1.7986	0.5052	1.4059	Н	1.9643	0.6299	1.2055	Н	1.0635	0.0259	-2.2073	
Н	0.8363	0.0664	-1.474	Н	0.4662	-0.0263	-1.3839	Н	0.0519	-1.7241	-0.8385	
Н	-1.6248	-1.4956	-0.4877	Н	-1.8106	-1.4674	0.4183	Н	-1.9512	-0.3443	-1.4949	
Н	-1.6706	-0.2085	-1.6923	Н	-2.7544	-0.0396	0.721	Н	-1.0714	1.1855	-1.4878	
Н	-3.4116	0.9694	-0.3799	Н	-2.5082	0.6352	-1.7049	Н	-2.6792	2.1216	0.1492	
Н	-3.8816	-0.706	-0.6635	Н	-1.5948	-0.8606	-1.9956	Н	-3.5166	0.5577	0.2534	
Н	-3.2719	-0.2272	0.9265	Н	-3.2812	-0.9364	-1.4835	Н	-3.5218	1.4743	-1.2596	
Н	-0.6063	-0.9817	1.5936	Н	-0.2911	-0.7607	2.0184	Н	-0.9376	-1.4019	1.6866	
Н	-1.6812	2.198	0.4822	Н	-0.008	2.4482	0.6569	Н	0.1835	1.8853	0.724	
Н	-0.7252	2.1739	-1.019	Н	-0.9158	2.1199	-0.8321	Н	0.3734	0.6764	2.0101	
Н	0.0491	2.3584	0.5691	Н	-1.7422	2.227	0.737	Н	-1.1656	1.4671	1.7995	
Н	-0.7252	2.1739	-1.019	С	2.9196	-0.5972	-0.2572	С	2.668	-0.9015	-1.0558	
Н	0.0491	2.3584	0.5691	С	1.9236	0.4716	0.1215	С	1.4076	-0.0781	-1.1745	
		p1-a4			1	p1-a5				p1-b1		
С	2.3185	-1.2024	-1.2472	С	2.6886	-0.5104	0.4861	С	-3.0366	-0.6101	0.055	
С	1.1523	-0.243	-1.2643	С	1.9784	0.5337	-0.3389	С	-1.9766	0.4286	0.3281	
С	0.304	-0.7549	-0.1192	С	0.607	-0.066	-0.6036	С	-0.77	-0.1369	-0.3991	
0	1.2603	-1.223	0.8501	0	0.8439	-1.4849	-0.6014	0	-0.9096	-1.5602	-0.2357	
С	2.4302	-1.5246	0.2123	С	1.9929	-1.7692	0.0772	С	-2.2224	-1.8645	-0.0159	
С	-0.6614	0.2651	0.5328	С	-0.512	0.2826	0.4199	С	0.6098	0.3242	0.1409	
С	-1.6517	0.8888	-0.4729	С	-1.8035	-0.5433	0.1929	С	1.7468	-0.3989	-0.6213	
С	-2.5061	-0.1222	-1.2301	С	-2.4659	-0.3643	-1.1653	С	3.1551	-0.0511	-0.1507	
0	-1.4336	-0.4423	1.5192	0	-0.0519	-0.0169	1.7489	0	0.705	-0.0256	1.5289	
С	0.0744	1.385	1.2838	С	-0.8207	1.785	0.4042	С	0.7433	1.8474	0.0461	
0	3.4044	-2.0112	0.7608	0	2.368	-2.9012	0.3339	0	-2.6555	-3.0006	0.075	
Н	3.2311	-0.7319	-1.6195	Н	3.7526	-0.5556	0.2418	Н	-3.5294	-0.447	-0.9076	
Н	2.1007	-2.1197	-1.8019	Н	2.551	-0.35	1.5583	Н	-3.7693	-0.6586	0.8635	
Η	1.5211	0.7706	-1.073	Η	2.5088	0.6426	-1.2943	Η	-2.2605	1.4251	-0.0216	
Η	0.6234	-0.2342	-2.2214	Η	1.9697	1.5188	0.1324	Η	-1.8013	0.486	1.409	

**Table S2.** Optimized Z-Matrixes of the key chiral structure in compounds **1a/1b** and **2a/2b** in the Gas Phase (Å) at B3LYP/6-31G(d,p) level.

H         -0.2623         -1.644         -0.4264         H         0.2827         0.2181         -1.6112         H         -0.3833         0.078         -1.4741           H         -1.1137         1.5303         0.0689         H         -1.6102         0.3437         H         1.6325         -1.4838         -0.5171           H         -2.5407         1.5503         0.0689         H         -2.503         0.0766         H         1.612         H         1.6855         H         -0.5431         H         -3.3784         -0.9644         -1.912         H         3.8857         -0.6823         1.6664           H         -0.3722         -0.8892         2.1094         H         -0.0712         -0.9823         1.8751         H         0.6619         -0.9955         1.5829           H         0.0648         2.0112         0.6127         H         -1.6626         2.0134         1.0684         H         0.7135         0.9995         2.3519         0.5826           H         -0.612         1.8074         H         0.0227         2.379         0.7835         H         -0.6039         2.1885         -0.999         2.3519         0.5826         -0.5211         0.4845         0.		1							1			
H         -1.1157         1.5139         -1.1972         H         -1.5928         -1.6102         0.3437         H         1.6225         -1.4838         -1.6014           H         -3.0639         -0.7681         H         -2.503         0.6766         -1.3419         H         3.0670         0.999         -0.3728           H         -1.897         -0.7529         -1.8845         H         -3.378         -0.0674         -1.2156         H         3.8857         H         0.9277           H         -0.772         -0.8982         2.1094         H         -0.1071         -0.9823         1.8751         H         -0.6975         1.8585         -0.9939         2.318         H         -0.6682         -0.9939         1.8998         -0.9939         2.3185         -0.9939         2.3185         -0.9939         2.318         -0.6602         2.0307         1.084         H         -0.7183         2.1885         -0.9939         2.318         H         -0.6071         2.1885         -0.9939         2.318         H         -0.602         -0.6126         -2.6323         -0.6181         C         -1.9930         0.2329         -0.3229         -0.4324         -0.6174         -0.6414         0.3339         -0.6181<	Н	-0.2623	-1.644	-0.4264	Η	0.2827	0.2181	-1.6112	Η	-0.8363	0.078	-1.4741
H         -2.3407         1.5503         0.0689         H         -2.5303         -0.2765         H         1.6701         -0.1885         -1.6495           H         -1.887         -0.7529         -1.884         H         -2.5703         0.6764         -1.2155         H         3.8857         -0.6823         -0.6823         -0.6811           H         -0.3729         -0.8842         2.1094         H         -1.0673         2.1429         -0.6011         H         0.6108         -0.999         0.3726           H         -0.6602         2.0004         H         -0.1063         2.1429         -0.6001         H         0.7183         2.1885         -0.9393           H         -0.6402         2.0307         H         -1.6626         2.0134         1.0684         H         0.7183         2.1885         -0.9393           H         -0.6177         -0.2629         C         -2.6055         -0.0085         0.7985         C         -2.6867         -0.5271         0.4842           C         -1.9577         -0.6065         C         -1.0303         C         -2.6864         -0.5271         0.4842           C         -2.1927         -0.4136         0.1128	Н	-1.1157	1.5139	-1.1972	Η	-1.5928	-1.6102	0.3437	Η	1.6325	-1.4838	-0.5017
H         -3.0639         -0.7681         -0.7581         H         -2.7303         0.6766         -1.3119         H         3.3087         -0.6823         -0.6823           H         -1.3871         -0.7722         -0.8892         2.1094         H         -0.771         -0.7982         H         3.3857         -0.6823         -0.6814           H         -0.7972         -0.8892         2.1094         H         -0.1071         -0.6924         H         J.3751         H         0.6109         -0.9955         1.5829           H         -0.6602         0.0121         H         -1.6626         2.0134         1.0684         H         -0.7599         2.318         0.5985         -0.9995           H         -0.6402         2.0307         1.8079         H         0.6223         -0.7832         H         -0.7599         2.318         0.7985         C         -2.6603         -0.2217         0.4615         0.1268         C         -0.7835         0.01618         C         -1.9867         -0.3292           C         -0.6032         -0.1477         -0.3355         C         -0.6038         -0.1787         0.4132         0.2881         0.07942         C         0.6132         0.29878 <td>Η</td> <td>-2.3407</td> <td>1.5503</td> <td>0.0689</td> <td>Η</td> <td>-2.5303</td> <td>-0.2904</td> <td>0.9765</td> <td>Η</td> <td>1.6701</td> <td>-0.1858</td> <td>-1.6945</td>	Η	-2.3407	1.5503	0.0689	Η	-2.5303	-0.2904	0.9765	Η	1.6701	-0.1858	-1.6945
H         -1.387         -0.7529         -1.884         H         -3.3784         -0.09674         -1.2156         H         3.2877         -0.0216         0.02481           H         -0.37972         -0.8892         2.1094         H         -0.0171         -0.9823         1.8751         H         0.6109         -0.9955         1.5829           H         0.6608         2.012         0.6127         H         -1.0623         2.1429         -0.6001         H         1.6716         2.1988         0.5995           H         -0.6402         2.0307         1.8079         H         -0.0222         2.3729         0.7832         H         -0.0599         2.3319         0.5986           C         -2.9171         -0.6077         -0.2629         C         -2.6085         0.0088         0.7885         C         -2.6867         -0.5271         0.4412           C         -1.9257         0.4615         0.1268         C         -2.1088         0.7975         O         -0.8389         -1.4826         0.6012         0.6012         0.6012         0.6012         0.6029         -0.6012         0.6029         0.6014         C         1.6014         0.4036         -1.1787         0.6051         C	Н	-3.0639	-0.7681	-0.5451	Н	-2.7503	0.6766	-1.3419	Η	3.4067	0.99	-0.3728
H         -3.215         0.4017         -1.8615         H         -1.612         -0.6914         -1.9782         H         0.2017         -0.2176         0.9247           H         0.0772         -0.8892         2.1094         H         -0.1071         -0.9233         1.8751         H         0.6109         -0.9355         1.5829           H         0.0632         0.6127         H         -1.6626         2.0134         1.0684         H         0.7133         2.1885         -0.9939           H         -0.6042         2.0307         1.8079         H         -0.622         2.0729         0.7832         H         -0.0599         2.3319         0.5946           C         -9.171         -0.0077         -0.2629         C         -2.6035         0.07985         C         -2.6867         -0.5271         0.4842           C         -1.9277         0.4615         0.1288         C         -2.1811         0.5319         -0.0618         C         -1.9805         0.1272         -0.6032         -0.1274         -1.5546         -0.6055         O         -0.6795         O         -0.8389         -1.4826         -0.6102           C         -0.4037         0.1641         C	Н	-1.897	-0.7529	-1.884	Η	-3.3784	-0.9674	-1.2156	Η	3.8857	-0.6823	-0.6681
H         -0.7972         -0.8820         2.1094         H         -0.1073         2.1429         -0.6001         H         1.6716         2.1988         0.5829           H         0.7649         0.9814         2.0877         H         -1.6673         2.1429         -0.6001         H         1.6716         2.1988         0.0939           H         -0.6402         2.0307         1.8079         H         0.0222         2.3729         0.7832         H         -0.0599         2.3319         0.0946           C         -2.9171         -0.6077         -0.2629         C         -2.035         -0.0608         0.7985         C         -2.6867         -0.3221         0.4481           C         -1.957         0.4615         0.1268         C         -2.088         -1.4787         0.0605           C         -0.6074         -1.554         -0.0805         O         -2.181         0.5319         -0.0184         C         -1.9867         -1.7777         0.0615           C         -0.6073         -0.4146         0.1649         C         1.681         -0.1846         -1.877         0.0131         -0.0277           C         -0.4136         0.1199         C         1.	Н	-3.2315	0.4017	-1.8615	Η	-1.812	-0.6914	-1.9782	Η	3.2717	-0.2176	0.9247
H         0.668         2.012         0.6127         H         -1.6673         2.1429         -0.6001         H         1.6716         2.1988         0.9092           H         -0.6402         2.0307         1.807         H         -1.662         2.0134         1.0684         H         0.7183         2.1885         -0.9993           C         -0.6402         2.0307         1.807         H         -0.022         2.3279         0.7855         C         -2.6867         -0.5271         0.4842           C         -9.9171         -0.6077         -0.2628         C         -0.6083         0.0795         O         -0.8329         -0.3226           C         -0.6032         -0.1477         -1.3035         C         -0.8335         0.0184         C         -0.6072         -0.6229         -0.3270           C         -0.6072         -1.551         -1.4088         -0.7758         O         -0.8389         -1.4143         C         -1.9867         -1.7787         0.0605           C         -1.853         -0.0612         C         -0.8481         0.0112         C         -0.848         -1.787         0.2783         0.2781           C         -0.4431         -0.36	Н	-0.7972	-0.8892	2.1094	Н	-0.1071	-0.9823	1.8751	Η	0.6109	-0.9955	1.5829
H         0.7349         0.9814         2.0587         H         -1.6626         2.0134         1.0644         H         0.7183         2.1885         -0.9399           H         0.6402         2.0371         1.8079         H         0.0222         2.3729         0.7832         H         -0.0599         2.1885         -0.9399           C         -2.9171         -0.6077         -0.2629         C         -2.6035         -0.0618         C         -1.9805         0.5289         -0.3292           C         -0.6012         -0.1477         -0.3055         C         -0.2335         0.0088         -0.6418         C         -0.6029         -0.0612           C         -1.0551         -1.4098         -0.7795         O         -0.8389         -1.4826         -0.6148           C         -1.9257         -0.4130         0.1049         C         -1.788         0.1154         C         -1.9867         -1.7787         0.0605           C         -2.443         -0.3629         -1.3574         C         3.0106         C         2.4648         -0.5340         0.331         -0.3724         1.2373           O         0.42829         0.3259         0.1846         1.4413	Η	0.668	2.012	0.6127	Η	-1.0673	2.1429	-0.6001	Η	1.6716	2.1988	0.5082
H         -0.6402         2.0307         1.8079         H         0.0222         2.379         0.7832         H         -0.0599         2.3519         0.5946           C         -2.9171         -0.6077         -0.2629         C         -2.6035         -0.6085         0.7985         C         -2.6827         0.4842           C         -0.6032         -0.1477         -0.3035         C         -0.8335         0.0098         -0.6845         C         -0.6029         -0.6029         -0.6029         -0.6148           C         -0.6074         -1.5546         -0.0605         O         -1.0551         -1.4098         -0.775         O         -0.8389         -1.4386         -0.6432         C         -0.6148           C         -0.6070         0.3674         0.4010         C         1.6681         -0.458         -0.546         C         1.8052         -0.5404         0.1885           C         2.3443         -0.3629         -1.3774         C         3.0196         -0.2813         0.1005         C         2.4648         -0.3727         1.7513           C         3.2481         1.7513         O         0.3794         -2.2694         -2.6546         2.4648         -0.3764	Н	0.7349	0.9814	2.0587	Η	-1.6626	2.0134	1.0684	Η	0.7183	2.1885	-0.9939
vp1-b2         p1-b3         p1-b4           C         -2.9171         -0.6077         -0.2629         C         -2.6035         -0.6085         0.7985         C         -2.6667         -0.5271         0.4482           C         -1.9257         0.4615         0.1268         C         -2.1181         0.5319         -0.0618         C         -0.6072         -0.0629         -0.629           O         -0.7774         -1.5546         -0.0605         O         -1.0551         -1.4098         -0.7795         O         -0.8389         -1.4826         -0.6148           C         -2.1092         -1.8553         -0.0813         C         -2.0888         -1.778         0.1154         C         -1.9867         -1.7777         0.0605           C         0.4647         0.3674         0.461         C         0.489         0.9841         C         0.1862         -0.5404         0.1855           C         1.2434         -0.3629         -1.3774         C         3.0196         -0.2813         0.1005         C         2.4648         -0.3463         -1.1691           O         0.2586         0.29862         0.0052         O         -2.2619         0.3373         O	Н	-0.6402	2.0307	1.8079	Η	0.0222	2.3729	0.7832	Η	-0.0599	2.3519	0.5946
C         -2.917         -0.6077         -0.2629         C         -2.6035         -0.7858         C         -2.6867         -0.5271         0.4842           C         -1.9257         0.6115         0.1268         C         -2.1181         0.5319         -0.66845         C         -1.06072         -0.6029         -0.6012           O         -0.7774         -1.5546         -0.0005         O         -1.0551         -1.4098         -0.7795         O         -0.8389         -1.4326         -0.61418           C         -2.1092         -1.8553         -0.0813         C         -2.0088         -1.798         0.1154         C         -1.9867         -1.7787         0.0605           C         0.4434         -0.3629         -1.3574         C         3.0186         -0.2813         0.1092         C         0.1845         -1.787         0.0403           O         0.4284         0.1752         0.813         0.1005         C         2.4648         -0.3737         1.7513           O         0.4284         0.1752         0.8148         1.7818         0.4256           O         -2.556         -2.9862         0.0052         O         -2.2294         -2.9619         0.3373 <td></td> <td></td> <td>p1-b2</td> <td></td> <td></td> <td></td> <td>p1-b3</td> <td></td> <td></td> <td></td> <td>p1-b4</td> <td>1</td>			p1-b2				p1-b3				p1-b4	1
C         -1.9257         0.4615         0.1268         C         -2.1181         0.5319         -0.0618         C         -1.9805         0.5299         -0.3292           C         -0.6032         -0.1477         -0.3035         C         -0.8335         0.0098         -0.6848         C         -0.6039         -0.6012         -0.6012           O         -0.7774         -1.5546         -0.0013         C         -2.0088         -1.798         0.1154         C         -1.9867         -1.7876         0.1154         C         -1.9867         -1.7870         0.0603           C         0.4647         0.3674         0.461         C         0.489         0.2881         0.0942         C         0.5112         0.2783         0.4253           C         2.3443         -0.329         -1.3713         O         0.3599         -0.1846         1.4413         O         0.0531         -0.0372         1.7513           C         0.4288         0.1752         0.2509         C         0.7606         1.796         0.0373         O         -2.358         -2.9151         0.3033           G         -2.5566         -2.9862         0.0052         O         -2.2044         -0.8753	С	-2.9171	-0.6077	-0.2629	С	-2.6035	-0.6085	0.7985	С	-2.6867	-0.5271	0.4842
C         -0.6032         -0.1477         -0.3035         C         -0.8335         0.0098         -0.6845         C         -0.6022         -0.0629         -0.0612           O         -0.7774         -1.5546         -0.0605         O         -1.0551         -1.4098         -0.7795         O         -0.8389         -1.4826         -0.6148           C         -2.1092         -1.8553         -0.0813         C         -2.0088         -1.798         0.1154         C         -1.9867         -1.7787         0.0603           C         0.6407         0.3674         0.4641         C         0.489         0.2881         0.0942         C         0.5112         0.2783         0.4253           C         1.3275         -0.1136         O         0.3599         -0.1846         1.4413         O         0.0351         -0.0372         1.7513           C         0.8289         1.8729         0.2509         C         0.7606         1.796         0.1712         C         0.8148         1.7818         0.4238         -2.9151         0.3033         D         -2.356         -0.2364         -0.6039         1.7514         0.2364         1.37507         -0.5734         0.2396           H	С	-1.9257	0.4615	0.1268	С	-2.1181	0.5319	-0.0618	С	-1.9805	0.5289	-0.3292
O         -0.7774         -1.5546         -0.0605         O         -1.0551         -1.4098         -0.7775         O         -0.8389         -1.4826         -0.6148           C         -2.1092         -1.8553         -0.0813         C         -2.0088         -1.798         0.1154         C         -1.7867         1.7787         0.0005           C         0.6407         0.3674         0.461         C         0.488         0.0281         0.0104         C         1.6681         -0.4584         0.5846         C         1.8052         -0.5404         0.1885           C         2.3443         -0.3629         -1.3574         C         3.0196         -0.2813         0.1005         C         2.4648         -0.3433         -1.1691           O         0.4288         0.1752         1.8713         O         0.3599         -0.1846         1.4413         O         0.0531         -0.0372         1.7513           C         0.2889         1.8729         0.2509         C         0.7606         1.796         0.373         O         -2.338         -2.9151         0.3033           H         -3.707         -0.5241         -1.3112         H         -2.2164         0.3786 <t< td=""><td>С</td><td>-0.6032</td><td>-0.1477</td><td>-0.3035</td><td>С</td><td>-0.8335</td><td>0.0098</td><td>-0.6845</td><td>С</td><td>-0.6072</td><td>-0.0629</td><td>-0.6012</td></t<>	С	-0.6032	-0.1477	-0.3035	С	-0.8335	0.0098	-0.6845	С	-0.6072	-0.0629	-0.6012
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0	-0.7774	-1.5546	-0.0605	0	-1.0551	-1.4098	-0.7795	0	-0.8389	-1.4826	-0.6148
C         0.6407         0.3674         0.461         C         0.489         0.2881         0.0942         C         0.5112         0.2783         0.4233           C         1.9275         -0.4136         0.1049         C         1.6681         -0.458         -0.5846         C         1.8052         -0.5404         0.1885           C         2.3443         -0.3629         -1.8713         O         0.3599         -0.1846         1.4413         O         0.0351         -0.0372         1.7513           C         0.8289         1.8729         0.2509         C         0.7606         1.796         0.1712         C         0.8148         1.7818         0.4256           O         -2.5566         -2.9862         0.0052         O         -2.2994         -2.9619         0.3373         O         -2.358         -2.9151         0.3043           H         -3.7906         -0.6039         0.3311         H         -2.22         -0.5452         1.8199         H         -2.5166         0.4885         H         -2.5116         0.6469         -1.2829           H         -1.9669         0.6084         1.2124         H         -2.0236         1.4704         0.4875         H	С	-2.1092	-1.8553	-0.0813	С	-2.0088	-1.798	0.1154	С	-1.9867	-1.7787	0.0605
C         1.9275         -0.4136         0.1049         C         1.6681         -0.458         -0.5846         C         1.8052         -0.5404         0.1885           C         2.3443         -0.3629         -1.3574         C         3.0196         -0.2813         0.1005         C         2.4648         -0.3463         -1.1691           O         0.4288         0.1752         1.8713         O         0.3599         -0.1846         1.4413         O         0.0531         -0.0372         1.7513           C         0.8289         1.8729         0.2509         C         0.7606         1.796         0.1712         C         0.8148         1.7818         0.4256           O         -2.5566         -2.9862         0.0039         1.4         -3.6944         -0.6669         0.8038         H         -2.7574         0.2376         -0.5734         0.2396           H         -2.1291         1.4243         -0.3505         H         -2.2284         1.4704         0.4875         H         -1.9752         1.5085         0.1335           H         -1.9669         0.6084         1.2124         H         -2.0236         1.4704         0.4875         H         -1.9752 <t< td=""><td>С</td><td>0.6407</td><td>0.3674</td><td>0.461</td><td>С</td><td>0.489</td><td>0.2881</td><td>0.0942</td><td>С</td><td>0.5112</td><td>0.2783</td><td>0.4253</td></t<>	С	0.6407	0.3674	0.461	С	0.489	0.2881	0.0942	С	0.5112	0.2783	0.4253
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	С	1.9275	-0.4136	0.1049	С	1.6681	-0.458	-0.5846	С	1.8052	-0.5404	0.1885
O         0.4288         0.1752         1.8713         O         0.3599         -0.1846         1.4413         O         0.0531         -0.0372         1.7513           C         0.8289         1.8729         0.2509         C         0.7606         1.776         0.1712         C         0.8148         1.7818         0.4256           O         -2.5566         -2.9862         0.0052         O         -2.2944         -2.9619         0.3373         O         -2.358         -2.9151         0.3043           H         -3.7906         -0.6039         0.3931         H         -3.6944         -0.6669         0.8038         H         -3.7507         -0.5734         0.2376           H         -3.2171         -0.5241         -1.3112         H         -2.22         -0.5452         1.8199         H         -2.5116         0.6469         -1.2829           H         -1.9669         0.6084         1.2124         H         -2.0236         0.4704         0.4875         H         -1.9752         1.5085         0.1337           H         -1.4643         0.4031         H         1.7572         -0.141         -1.613         H         -2.838         -0.2376         0.2377	С	2.3443	-0.3629	-1.3574	С	3.0196	-0.2813	0.1005	С	2.4648	-0.3463	-1.1691
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	0	0.4288	0.1752	1.8713	0	0.3599	-0.1846	1.4413	0	0.0531	-0.0372	1.7513
O         -2.5566         -2.9862         0.0052         O         -2.2994         -2.9619         0.3373         O         -2.358         -2.9151         0.3043           H         -3.7906         -0.6039         0.3931         H         -3.6944         -0.6669         0.8038         H         -3.7507         -0.5734         0.2396           H         -3.2171         -0.5241         -1.3112         H         -2.222         -0.5452         1.8199         H         -2.5494         -0.3786         1.5581           H         -2.1291         1.4243         -0.3505         H         -2.8526         0.7036         -0.8598         H         -2.5116         0.6469         -1.2829           H         -1.9669         0.6084         1.2124         H         -2.0236         1.4704         0.4875         H         -1.9752         1.5085         0.1535           H         -0.4661         -0.0139         -1.388         H         -0.7363         0.4003         -1.7047         H         1.4056         0.3237         -1.6095         0.3237           H         1.8171         -1.4643         0.4031         H         1.7572         -0.141         -1.631         H         2.528	С	0.8289	1.8729	0.2509	С	0.7606	1.796	0.1712	С	0.8148	1.7818	0.4256
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	0	-2.5566	-2.9862	0.0052	0	-2.2994	-2.9619	0.3373	0	-2.358	-2.9151	0.3043
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	-3.7906	-0.6039	0.3931	Н	-3.6944	-0.6669	0.8038	Н	-3.7507	-0.5734	0.2396
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	-3.2171	-0.5241	-1.3112	Н	-2.22	-0.5452	1.8199	Η	-2.5494	-0.3786	1.5581
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н	-2.1291	1.4243	-0.3505	Н	-2.8526	0.7036	-0.8598	Н	-2.5116	0.6469	-1.2829
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н	-1.9669	0.6084	1.2124	Н	-2.0236	1.4704	0.4875	Н	-1.9752	1.5085	0.1535
H         1.8171         -1.4643         0.4031         H         1.7572         -0.141         -1.631         H         1.5993         -1.6095         0.3297           H         2.7545         -0.0356         0.7207         H         1.4608         -1.5356         -0.5944         H         2.5328         -0.2917         0.973           H         2.5043         0.6637         -1.698         H         2.9738         -0.5603         1.1574         H         2.7424         0.6977         -1.3381           H         1.5988         -0.8338         -2.0042         H         3.3758         0.7501         0.0253         H         1.8114         -0.6708         -1.9839           H         0.2942         -0.7817         2.0103         H         0.4576         -1.1548         1.4266         H         0.1119         -1.004         1.8671           H         -0.026         2.4406         0.6834         H         -0.0523         2.3296         0.6737         H         -0.0293         2.3626         0.8123           H         0.9064         2.1323         -0.8091         H         0.8961         2.2301         -0.8247         H         1.0578         2.0058         1.090	Н	-0.4661	-0.0139	-1.3838	Η	-0.7363	0.4003	-1.7047	Η	-0.2846	0.2337	-1.6056
H         2.7545         -0.0356         0.7207         H         1.4608         -1.5356         -0.5944         H         2.5328         -0.2917         0.973           H         2.5043         0.6637         -1.698         H         2.9738         -0.5603         1.1574         H         2.7424         0.6977         -1.3381           H         1.5988         -0.8338         -2.0042         H         3.3758         0.7501         0.0253         H         1.8114         -0.6708         -1.9839           H         3.2856         -0.9061         -1.4929         H         3.7671         -0.9192         -0.3832         H         3.3808         -0.9435         -1.2259           H         0.2942         -0.7817         2.0103         H         0.4576         -1.1548         1.4266         H         0.1119         -1.004         1.8671           H         -0.0026         2.4406         0.6834         H         -0.0523         2.3296         0.6737         H         -0.0293         2.3626         0.8123           H         0.9064         2.1323         -0.8091         H         0.8961         2.2301         -0.8247         H         1.0578         2.0058	Н	1.8171	-1.4643	0.4031	Н	1.7572	-0.141	-1.631	Н	1.5993	-1.6095	0.3297
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	2.7545	-0.0356	0.7207	Н	1.4608	-1.5356	-0.5944	Н	2.5328	-0.2917	0.973
H         1.5988         -0.8338         -2.0042         H         3.3758         0.7501         0.0253         H         1.8114         -0.6708         -1.9839           H         3.2856         -0.9061         -1.4929         H         3.7671         -0.9192         -0.3832         H         3.3808         -0.9435         -1.2259           H         0.2942         -0.7817         2.0103         H         0.4576         -1.1548         1.4266         H         0.1119         -1.004         1.8671           H         -0.0026         2.4406         0.6834         H         -0.0523         2.3296         0.6737         H         -0.0293         2.3626         0.8123           H         0.9064         2.1323         -0.8091         H         0.8961         2.2301         -0.8247         H         1.0554         2.1513         -0.575           H         1.7326         2.226         0.7612         H         1.6513         2.0132         0.7706         H         1.657         2.0058         1.0908           C         1.2183         -1.5555         -2.2604         C         -0.7771         -1.788         -2.3306         C         1.3409         -1.669         -2	Н	2.5043	0.6637	-1.698	Η	2.9738	-0.5603	1.1574	Η	2.7424	0.6977	-1.3381
H         3.2856         -0.9061         -1.4929         H         3.7671         -0.9192         -0.3832         H         3.3808         -0.9435         -1.2259           H         0.2942         -0.7817         2.0103         H         0.4576         -1.1548         1.4266         H         0.1119         -1.004         1.8671           H         -0.0026         2.4406         0.6834         H         -0.0523         2.3296         0.6737         H         -0.0293         2.3626         0.8123           H         0.9064         2.1323         -0.8091         H         0.8961         2.2301         -0.8247         H         1.0558         2.0058         1.0908           H         1.7326         2.226         0.7612         H         1.6513         2.0132         0.7706         H         1.657         2.0058         1.0908           V         P1-c1         P1-c2         P1-c3         P1-c3         P1-c3         P1-c3         P1-c3         P1-c3           C         1.2183         -1.5555         -2.2604         C         -1.1772         -1.3691         -0.9356         C         1.3409         -1.1669         -2.237           C         0.2917	Н	1.5988	-0.8338	-2.0042	Н	3.3758	0.7501	0.0253	Н	1.8114	-0.6708	-1.9839
H         0.2942         -0.7817         2.0103         H         0.4576         -1.1548         1.4266         H         0.1119         -1.004         1.8671           H         -0.0026         2.4406         0.6834         H         -0.0523         2.3296         0.6737         H         -0.0293         2.3626         0.8123           H         0.9064         2.1323         -0.8091         H         0.8961         2.2301         -0.8247         H         1.0584         2.1513         -0.575           H         1.7326         2.226         0.7612         H         1.6513         2.0132         0.7706         H         1.657         2.0058         1.0908 <b>p1-c1 p1-c2 p1-c3 p1-c3 p1-c3 p1-c3</b> C         1.3796         -0.9107         -0.9064         C         -1.1772         -1.3691         -0.9356         C         1.3409         -0.4352         -0.9175           C         0.2917         0.1489         -0.9103         C         0.1398         -0.8979         -0.3556         C         0.0496         0.2693         -0.8694           O         -0.7637         -0.4323         -1.6961	Н	3.2856	-0.9061	-1.4929	Н	3.7671	-0.9192	-0.3832	Н	3.3808	-0.9435	-1.2259
H         -0.0026         2.4406         0.6834         H         -0.0523         2.3296         0.6737         H         -0.0293         2.3626         0.8123           H         0.9064         2.1323         -0.8091         H         0.8961         2.2301         -0.8247         H         1.0584         2.1513         -0.575           H         1.7326         2.226         0.7612         H         1.6513         2.0132         0.7706         H         1.657         2.0058         1.0908           v         v1-c1         v1-c2         v1-c2         v1-c3         v1-c3         v1-c3         v1-c3           C         1.2183         -1.5555         -2.2604         C         -0.7771         -1.788         -2.3306         C         1.3409         -1.1669         -2.237           C         1.3796         -0.9107         -0.9064         C         -1.1772         -1.3691         -0.9356         C         1.3409         -0.4352         -0.9175           C         0.2917         0.1489         -0.9103         C         0.1398         -0.8979         -0.3556         C         0.0496         0.2693         -0.8694           O         -0.7637         -0.4323 </td <td>Н</td> <td>0.2942</td> <td>-0.7817</td> <td>2.0103</td> <td>Н</td> <td>0.4576</td> <td>-1.1548</td> <td>1.4266</td> <td>Н</td> <td>0.1119</td> <td>-1.004</td> <td>1.8671</td>	Н	0.2942	-0.7817	2.0103	Н	0.4576	-1.1548	1.4266	Н	0.1119	-1.004	1.8671
H       0.9064       2.1323       -0.8091       H       0.8961       2.2301       -0.8247       H       1.0584       2.1513       -0.575         H       1.7326       2.226       0.7612       H       1.6513       2.0132       0.7706       H       1.657       2.0058       1.0908 $\mathbf{V}$ $\mathbf{P}$ $\mathbf{P}$ $\mathbf{P}$ $\mathbf{P}$ $\mathbf{P}$ $\mathbf{P}$ $\mathbf{P}$ $\mathbf{P}$ $\mathbf{P}$ C       1.2183       -1.5555       -2.2604       C $-0.7771$ $-1.788$ $-2.3306$ C       1.3409 $-1.1669$ $-2.237$ C       1.3796 $-0.9107$ $-0.9064$ C $-1.1772$ $-1.3691$ $-0.9356$ C       1.3409 $-1.469$ $-2.237$ C       0.2917       0.1489 $-0.9103$ C $0.1398$ $-0.8979$ $-0.3556$ C $0.0496$ $0.2693$ $-0.8694$ O $-0.7637$ $-0.4323$ $-1.6961$ O $0.8339$ $-0.3101$ $-1.4698$ O $-0.837$ $-0.6465$ $-1.5464$ C $-0.2248$ 0.571       0.4949       C <td>Н</td> <td>-0.0026</td> <td>2.4406</td> <td>0.6834</td> <td>Н</td> <td>-0.0523</td> <td>2.3296</td> <td>0.6737</td> <td>Η</td> <td>-0.0293</td> <td>2.3626</td> <td>0.8123</td>	Н	-0.0026	2.4406	0.6834	Н	-0.0523	2.3296	0.6737	Η	-0.0293	2.3626	0.8123
H         1.7326         2.226         0.7612         H         1.6513         2.0132         0.7706         H         1.657         2.0058         1.0908 <b>p1-c1 p1-c2 p1-c3 p1-c3 p1-c3 p1-c3</b> C         1.2183         -1.5555         -2.2604         C         -0.7771         -1.788         -2.3306         C         1.3409         -1.1669         -2.237           C         1.3796         -0.9107         -0.9064         C         -1.1772         -1.3691         -0.9356         C         1.3905         -0.4352         -0.9175           C         0.2917         0.1489         -0.9103         C         0.1398         -0.8979         -0.3556         C         0.0496         0.2693         -0.8694           O         -0.7637         -0.4323         -1.6961         O         0.8339         -0.3101         -1.4698         O         -0.8377         -0.6465         -1.5464           C         -0.2502         -1.4014         -2.5059         C         0.3463         -0.8419         -2.6297         C         -0.1181         -1.4641         -2.3682           C         0.9112         1.2576         1.284	Н	0.9064	2.1323	-0.8091	Н	0.8961	2.2301	-0.8247	Н	1.0584	2.1513	-0.575
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Н	1.7326	2.226	0.7612	Н	1.6513	2.0132	0.7706	Η	1.657	2.0058	1.0908
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		L	p1-c1				p1-c2				p1-c3	
C       1.3796       -0.9107       -0.9064       C       -1.1772       -1.3691       -0.9356       C       1.3905       -0.4352       -0.9175         C       0.2917       0.1489       -0.9103       C       0.1398       -0.8979       -0.3556       C       0.0496       0.2693       -0.8694         O       -0.7637       -0.4323       -1.6961       O       0.8339       -0.3101       -1.4698       O       -0.8377       -0.6465       -1.5464         C       -0.2502       -1.4014       -2.5059       C       0.3463       -0.8419       -2.6297       C       -0.1181       -1.4641       -2.3682         C       -0.2248       0.571       0.4949       C       0.0606       0.1094       0.8206       C       -0.524       0.5823       0.5385         C       0.9112       1.2576       1.2884       C       -0.5091       1.4851       0.3991       C       0.3338       1.5787       1.3526         C       0.5199       1.7546       2.6767       C       -0.5219       2.5321       1.5101       C       1.5867       1.0187       2.0162         O       -0.6204       -0.6086       1.2091       O       1.4065 </td <td>С</td> <td>1.2183</td> <td>-1.5555</td> <td>-2.2604</td> <td>С</td> <td>-0.7771</td> <td>-1.788</td> <td>-2.3306</td> <td>С</td> <td>1.3409</td> <td>-1.1669</td> <td>-2.237</td>	С	1.2183	-1.5555	-2.2604	С	-0.7771	-1.788	-2.3306	С	1.3409	-1.1669	-2.237
C       0.2917       0.1489       -0.9103       C       0.1398       -0.8979       -0.3556       C       0.0496       0.2693       -0.8694         O       -0.7637       -0.4323       -1.6961       O       0.8339       -0.3101       -1.4698       O       -0.8377       -0.6465       -1.5464         C       -0.2502       -1.4014       -2.5059       C       0.3463       -0.8419       -2.6297       C       -0.1181       -1.4641       -2.3682         C       -0.2248       0.571       0.4949       C       0.0606       0.1094       0.8206       C       -0.524       0.5823       0.5385         C       0.9112       1.2576       1.2884       C       -0.5091       1.4851       0.3991       C       0.3338       1.5787       1.3526         C       0.5199       1.7546       2.6767       C       -0.5219       2.5321       1.5101       C       1.5867       1.0187       2.0162         O       -0.6204       -0.6086       1.2091       O       1.4065       0.3187       1.2823       O       -0.6541       -0.6366       1.2806	С	1.3796	-0.9107	-0.9064	С	-1.1772	-1.3691	-0.9356	С	1.3905	-0.4352	-0.9175
O         -0.7637         -0.4323         -1.6961         O         0.8339         -0.3101         -1.4698         O         -0.837         -0.6465         -1.5464           C         -0.2502         -1.4014         -2.5059         C         0.3463         -0.8419         -2.6297         C         -0.1181         -1.4641         -2.3682           C         -0.2248         0.571         0.4949         C         0.0606         0.1094         0.8206         C         -0.524         0.5823         0.5385           C         0.9112         1.2576         1.2884         C         -0.5091         1.4851         0.3991         C         0.3338         1.5787         1.3526           C         0.5199         1.7546         2.6767         C         -0.5219         2.5321         1.5101         C         1.5867         1.0187         2.0162           O         -0.6204         -0.6086         1.2091         O         1.4065         0.3187         1.2823         O         -0.6541         -0.6366         1.2806	С	0.2917	0.1489	-0.9103	С	0.1398	-0.8979	-0.3556	С	0.0496	0.2693	-0.8694
C       -0.2502       -1.4014       -2.5059       C       0.3463       -0.8419       -2.6297       C       -0.1181       -1.4641       -2.3682         C       -0.2248       0.571       0.4949       C       0.0606       0.1094       0.8206       C       -0.524       0.5823       0.5385         C       0.9112       1.2576       1.2884       C       -0.5091       1.4851       0.3991       C       0.3338       1.5787       1.3526         C       0.5199       1.7546       2.6767       C       -0.5219       2.5321       1.5101       C       1.5867       1.0187       2.0162         O       -0.6204       -0.6086       1.2091       O       1.4065       0.3187       1.2823       O       -0.6541       -0.6366       1.2806	0	-0.7637	-0.4323	-1.6961	0	0.8339	-0.3101	-1.4698	0	-0.837	-0.6465	-1.5464
C         -0.2248         0.571         0.4949         C         0.0606         0.1094         0.8206         C         -0.524         0.5823         0.5385           C         0.9112         1.2576         1.2884         C         -0.5091         1.4851         0.3991         C         0.3338         1.5787         1.3526           C         0.5199         1.7546         2.6767         C         -0.5219         2.5321         1.5101         C         1.5867         1.0187         2.0162           O         -0.6204         -0.6086         1.2091         O         1.4065         0.3187         1.2823         O         -0.6541         -0.6366         1.2806	С	-0.2502	-1.4014	-2.5059	С	0.3463	-0.8419	-2.6297	С	-0.1181	-1.4641	-2.3682
C         0.9112         1.2576         1.2884         C         -0.5091         1.4851         0.3991         C         0.3338         1.5787         1.3526           C         0.5199         1.7546         2.6767         C         -0.5219         2.5321         1.5101         C         1.5867         1.0187         2.0162           O         -0.6204         -0.6086         1.2091         O         1.4065         0.3187         1.2823         O         -0.6541         -0.6366         1.2806	С	-0.2248	0.571	0.4949	С	0.0606	0.1094	0.8206	С	-0.524	0.5823	0.5385
C         0.5199         1.7546         2.6767         C         -0.5219         2.5321         1.5101         C         1.5867         1.0187         2.0162           O         -0.6204         -0.6086         1.2091         O         1.4065         0.3187         1.2823         O         -0.6541         -0.6366         1.2806	С	0.9112	1.2576	1.2884	С	-0.5091	1.4851	0.3991	С	0.3338	1.5787	1.3526
O -0.6204 -0.6086 1.2091 O 1.4065 0.3187 1.2823 O -0.6541 -0.6366 1.2806	С	0.5199	1.7546	2.6767	С	-0.5219	2.5321	1.5101	С	1.5867	1.0187	2.0162
	0	-0.6204	-0.6086	1.2091	0	1.4065	0.3187	1.2823	0	-0.6541	-0.6366	1.2806

С	-1.4536	1.4808	0.3488	С	-0.7178	-0.5016	1.9896	С	-1.9422	1.1692	0.394
0	-0.8951	-2.0111	-3.3433	0	0.7909	-0.5941	-3.7377	0	-0.6129	-2.288	-3.1182
Н	1.5067	-2.6089	-2.2413	Н	-1.5992	-1.6628	-3.0388	Н	1.9317	-2.0848	-2.209
Н	1.7698	-1.016	-3.0356	Н	-0.3966	-2.813	-2.355	Н	1.6522	-0.5291	-3.0692
Н	1.207	-1.6642	-0.1293	Н	-1.9061	-0.5547	-1.0022	Н	1.488	-1.1639	-0.1043
Н	2.3793	-0.4944	-0.7523	Н	-1.6315	-2.1823	-0.3617	Н	2.2367	0.2551	-0.8668
Н	0.6331	1.0406	-1.453	Н	0.7462	-1.7597	-0.0431	Н	0.0813	1.1903	-1.4664
Н	1.7363	0.5476	1.4265	Н	-1.5301	1.3777	0.0175	Н	-0.2802	1.978	2.1715
Н	1.3066	2.1045	0.7144	Н	0.0977	1.8969	-0.4167	Н	0.6028	2.4377	0.7255
Н	0.0925	0.9533	3.2866	Н	0.4766	2.6836	1.9307	Н	2.3429	0.7171	1.2904
Н	1.4051	2.1348	3.1974	Н	-1.2024	2.2507	2.3191	Н	1.3551	0.1627	2.6574
Н	-0.2022	2.5744	2.6196	Н	-0.8657	3.4926	1.1119	Н	2.0407	1.7887	2.6495
Н	-1.2294	-0.3497	1.9218	Н	1.9271	0.6132	0.5105	Н	-1.2311	-1.2264	0.7588
Н	-2.2594	0.9741	-0.1936	Η	-0.3356	-1.5015	2.2273	Η	-2.6178	0.4732	-0.1152
Н	-1.8806	1.7422	1.3226	Η	-1.7862	-0.5854	1.7671	Н	-1.9305	2.1124	-0.162
Н	-1.2046	2.4054	-0.1811	Η	-0.5959	0.088	2.9049	Η	-2.3898	1.3511	1.3784
		p1-c4				p1-c5				p1-d1	
С	-1.1056	-1.0431	-2.2284	С	1.0744	-1.6642	-1.7586	С	-2.8433	-1.2034	-0.2404
С	-1.0342	-1.6809	-0.8629	С	1.607	-0.3919	-1.1439	С	-1.4406	-0.9905	-0.7529
С	0.2323	-1.1241	-0.2419	С	0.3615	0.4269	-0.8555	С	-0.7261	-0.4205	0.4596
0	1.0482	-0.7033	-1.3513	0	-0.5581	0.0246	-1.8879	0	-1.74	0.3397	1.1408
С	0.3136	-0.6588	-2.4977	С	-0.2214	-1.2121	-2.3556	С	-2.9735	-0.1102	0.7738
С	0.0744	0.0458	0.7716	С	-0.2775	0.2236	0.5502	С	0.5142	0.462	0.1416
С	-0.5959	1.2958	0.1601	С	0.6281	0.7109	1.7043	С	1.6127	-0.396	-0.5276
С	-0.6595	2.5037	1.0903	С	1.0181	2.1807	1.661	С	2.9003	0.3493	-0.8627
0	1.3981	0.4169	1.1939	0	-0.4821	-1.1834	0.7656	0	0.1203	1.486	-0.7826
С	-0.662	-0.4343	2.0278	С	-1.6563	0.8992	0.6094	С	1.0179	1.1384	1.4258
0	0.7553	-0.3058	-3.5784	0	-0.889	-1.8444	-3.1587	0	-4.0224	0.2915	1.2505
Н	-1.7265	-0.1439	-2.2277	Η	0.8844	-2.438	-1.0112	Η	-3.5836	-1.0938	-1.036
Н	-1.4658	-1.75	-2.98	Η	1.7471	-2.0414	-2.5328	Η	-2.9514	-2.17	0.2596
Н	-1.9403	-1.5252	-0.272	Η	2.2525	-0.5686	-0.2807	Η	-1.4675	-0.2723	-1.5807
Η	-0.9217	-2.7656	-0.9869	Η	2.2115	0.1332	-1.8947	Η	-0.982	-1.9114	-1.1243
Η	0.785	-1.9341	0.251	Η	0.5701	1.4902	-1.0152	Η	-0.4301	-1.2298	1.1404
Η	-1.6155	1.0575	-0.1624	Η	1.5394	0.1017	1.7457	Η	1.2288	-0.8035	-1.4709
Η	-0.037	1.6132	-0.7283	Η	0.1236	0.5125	2.66	Η	1.8617	-1.2493	0.1153
Η	0.3353	2.7907	1.4439	Η	0.1397	2.8317	1.6686	Η	2.7075	1.2273	-1.4857
Н	-1.2964	2.309	1.9576	Η	1.619	2.4128	0.7775	Η	3.5778	-0.3092	-1.4162
Н	-1.0837	3.3611	0.5573	Η	1.6209	2.4302	2.5405	Η	3.4252	0.6705	0.0415
Η	1.9266	0.5567	0.3842	Η	-1.0492	-1.2915	1.5498	Η	0.7633	2.2137	-0.7306
Η	-0.2165	-1.3615	2.4067	Η	-2.3688	0.4032	-0.0595	Η	0.2369	1.7585	1.8793
Η	-1.7239	-0.6161	1.838	Η	-1.6038	1.9572	0.3349	Η	1.8485	1.8226	1.2225
Η	-0.5742	0.2903	2.8445	Η	-2.0842	0.8247	1.6157	Η	1.3477	0.3992	2.1631
		p1-d2				p1-d3			-	p1-d4	
С	-2.6745	-1.3554	0.8776	С	-2.6051	-0.6154	-0.7152	С	-2.5557	-0.6515	-0.6938
С	-1.1648	-1.3729	0.9283	С	-1.3775	-1.4421	-0.4234	С	-1.2044	-1.3069	-0.5536
C	-0.8302	0.1036	0.9075	С	-0.6559	-0.6684	0.6674	С	-0.5109	-0.5048	0.5336

0	-1.8437	0.6893	0.0717	0	-1.7232	-0.015	1.3803	0	-1.5939	-0.0483	1.3668
С	-2.9454	-0.1183	0.0756	С	-2.8242	0.095	0.582	С	-2.765	-0.0637	0.6655
С	0.5805	0.4911	0.3933	С	0.3942	0.3869	0.204	С	0.3379	0.7125	0.0678
С	0.7864	0.1683	-1.1056	С	1.5643	-0.3006	-0.5373	С	1.4794	0.3305	-0.9001
С	2.1212	0.6401	-1.6774	С	2.6659	0.6434	-1.0111	С	2.4648	-0.7064	-0.3811
0	0.7072	1.9145	0.5559	0	-0.2224	1.3069	-0.7065	0	-0.502	1.6293	-0.6553
С	1.6584	-0.1516	1.2713	С	0.9005	1.1904	1.4141	С	0.8943	1.472	1.284
0	-3.9981	0.1554	-0.4749	0	-3.827	0.7182	0.889	0	-3.8188	0.3771	1.0931
Н	-3.1141	-1.2399	1.8724	Н	-3.4615	-1.2465	-0.9639	Н	-3.3326	-1.3838	-0.9257
Н	-3.0699	-2.2439	0.38	Н	-2.4288	0.1179	-1.5061	Н	-2.55	0.148	-1.4388
Н	-0.775	-1.8888	1.8107	Η	-1.6968	-2.4107	-0.0167	Η	-1.3504	-2.3344	-0.1946
Н	-0.7844	-1.8881	0.0401	Н	-0.7863	-1.6545	-1.3158	Н	-0.6607	-1.377	-1.4977
Н	-0.9743	0.5392	1.9061	Н	-0.1756	-1.3707	1.3596	Н	0.1093	-1.172	1.1429
Н	-0.0003	0.6546	-1.6957	Н	1.1876	-0.8049	-1.4339	Н	2.0364	1.2388	-1.168
Н	0.7	-0.9094	-1.2813	Η	2.0115	-1.0703	0.1036	Η	1.0606	-0.02	-1.8514
Н	2.1595	0.4315	-2.7518	Η	3.2013	1.0924	-0.1695	Η	1.9767	-1.6664	-0.1904
Н	2.2575	1.7171	-1.542	Н	2.2632	1.4444	-1.6378	Н	2.9544	-0.3745	0.539
Н	2.9641	0.1206	-1.2127	Η	3.3994	0.0893	-1.6069	Η	3.2469	-0.8801	-1.1278
Н	-0.0432	2.3205	0.0804	Η	-0.7692	1.9222	-0.1836	Η	-1.0729	2.0834	-0.0079
Н	2.6471	0.2744	1.0696	Η	1.45	0.5542	2.1151	Η	1.5109	0.8301	1.9198
Н	1.7082	-1.2355	1.1261	Η	0.0729	1.6619	1.9559	Η	0.0878	1.8854	1.9
Η	1.4609	0.0456	2.3317	Η	1.5479	2.0172	1.103	Η	1.4978	2.3288	0.9635



6a1 (89.0%)



**6a5** (1.4%)



**6b1** (78.2%)





**6a2** (1.9%)







**6a3** (1.9%)

**6a7** (0.6%)

**6b4** (2.0%)



**6b5** (1.6%) **6b6** (1.3%) **6b7** (1.3%) 6b8 (1.3%) Figure S2. Stable conformers of the key chiral structure in compound 6 with 3*R*,4*R* (6a) and 3*S*,4*S* (6b) configurations, respectively.



**6a4** (1.8%)



**Table S3**. Important thermodynamic parameters (a.u.) of the optimized o key chiral structure in compound **6** at B3LYP/6-31G(d,p) level in the gas phase.

Conformations	E+ZPE	G	Conformations	E+ZPE	G
6a1	-691.345018	-691.386499	6b1	-691.345018	-691.386499
6a2	-691.340558	-691.382891	6b2	-691.341496	-691.384024
6a3	-691.340555	-691.382887	6b3	-691.340878	-691.383480
6a4	-691.340675	-691.382808	6 <b>b</b> 4	-691.341527	-691.383035
6a5	-691.340039	-691.382567	6b5	-691.340571	-691.382820
6a6	-691.339726	-691.382111	6b6	-691.339730	-691.382657
6a7	-691.339544	-691.381846	6b7	-691.342095	-691.383581
			6b8	-691.382656	-691.382656

# Table S4. Optimized Z-Matrixes of the key chiral structure in compound 6 in the Gas Phase (Å) at B3LYP/6-31G(d,p) level.

		6a1				6a2			6a3           1.726980         -0.3257           1.770275         1.18375           0.531114         1.70233           0.185847         0.83125           0.950781         -0.40286           -0.108255         2.70469           3.088629         -1.02959           3.059299         -0.49842           -2.260895         -0.97829           -3.196986         -1.10368           -1.091284         -1.63832           -0.033102         -1.57358           1.657278         -0.39090           -2.758680         -0.04458           -2.958926         1.28165		
С	1.021268	0.860014	-0.370334	С	1.726955	-0.326185	0.573242	С	1.726980	-0.325757	0.573247
С	2.395320	0.513100	-0.954254	С	1.770536	1.183251	0.851220	С	1.770275	1.183755	0.851060
С	2.736706	-0.823711	-0.307541	С	0.531616	1.702328	0.14404	С	0.531114	1.702334	0.143931
0	1.943340	-1.002672	0.788104	0	0.185971	0.831347	-0.835339	0	0.185847	0.831254	-0.835415
С	1.064114	0.136807	0.991840	С	0.950670	-0.403060	-0.763941	С	0.950781	-0.402860	-0.763990
0	3.558614	-1.633600	-0.648525	0	-0.107300	2.704971	0.352667	0	-0.108255	2.704691	0.352623
C	0.718684	2.357888	-0.271990	С	3.088588	-1.030104	0.519510	С	3.088629	-1.029591	0.519894
0	-0.503516	2.638670	0.382816	0	3.959235	-0.498222	-0.471791	0	3.959299	-0.498421	-0.471755
С	-2.178895	-1.142594	0.047652	С	-2.261218	-0.978097	0.195910	С	-2.260895	-0.978298	0.195910
С	-2.771730	-2.208181	-0.844945	С	-3.197398	-1.103610	1.370746	С	-3.196986	-1.103681	1.370827
С	-0.996775	-1.320104	0.659433	С	-1.091604	-1.638107	0.159673	С	-1.091284	-1.638329	0.159650
С	-0.272809	-0.357109	1.560438	С	-0.033550	-1.573423	-0.919435	С	-0.033102	-1.573553	-0.919363
Н	1.540322	0.784710	1.740806	Н	1.657126	-0.391163	-1.601168	Н	1.657278	-0.390909	-1.601193
C	-2.992657	0.129838	0.173236	С	-2.758953	-0.044257	-0.894083	С	-2.758680	-0.044554	-0.894125
0	-2.619931	1.141990	-0.787555	0	-2.958823	1.281996	-0.418182	0	-2.958926	1.281650	-0.418207
Н	0.244063	0.384098	-0.981391	Н	1.129472	-0.807900	1.356680	Н	1.129363	-0.807309	1.356687
Н	2.436345	0.430912	-2.041897	Н	1.766023	1.466679	1.904810	Н	1.765802	1.467244	1.904631
Н	3.159954	1.240866	-0.648830	Н	2.638948	1.652504	0.370209	Н	2.638492	1.653221	0.369916
Н	1.505228	2.851138	0.313535	Н	2.941043	-2.083685	0.257279	Н	2.941149	-2.083303	0.258185
Н	0.751010	2.799127	-1.282067	Н	3.554375	-1.011031	1.514998	Н	3.554438	-1.010024	1.515377
Н	-1.226742	2.246242	-0.141516	Н	4.403369	0.276827	-0.106808	Н	4.402175	0.277852	-0.107826
Н	-3.732113	-2.565811	-0.451579	Н	-4.151644	-1.551349	1.062852	Н	-4.151147	-1.551671	1.063044
Н	-2.977057	-1.825304	-1.854608	Н	-3.432923	-0.109117	1.763482	Н	-3.432683	-0.109136	1.763324
Н	-2.105284	-3.068075	-0.947851	Н	-2.775578	-1.714538	2.173601	Н	-2.775011	-1.714362	2.173782
Н	-0.472509	-2.259426	0.487134	Н	-0.855140	-2.278991	1.009452	Н	-0.854845	-2.279291	1.009378
Н	-0.058934	-0.852162	2.516735	Н	0.553432	-2.500481	-0.921266	Н	0.554197	-2.500397	-0.920849
Η	-0.859826	0.538750	1.772892	Η	-0.478571	-1.497766	-1.916311	Н	-0.478011	-1.498291	-1.916322
Н	-4.062572	-0.094561	0.064942	Н	-3.748336	-0.387244	-1.224280	Н	-3.747947	-0.387773	-1.224441
Н	-2.855907	0.607165	1.144530	Н	-2.098108	-0.058407	-1.766871	Н	-2.097720	-0.058534	-1.766813
Η	-2.653386	0.751543	-1.670764	Η	-2.090019	1.702503	-0.316809	Н	-2.090240	1.702499	-0.317090
		6a4				6a5		6a6			
С	-1.757981	0.864267	0.312133	С	1.975704	-0.383931	0.255445	С	1.808200	-0.230822	0.111615

С	-2.975665	0.168146	-0.305943	С	2.508169	0.969699	-0.228568	С	1.757259	1.228987	0.587260
С	-2.636465	-1.316047	-0.236469	С	1.254404	1.805922	-0.422866	С	0.419819	1.723385	0.072056
0	-1.300152	-1.460193	-0.005593	0	0.167578	0.969043	-0.487138	0	0.024930	0.941185	-0.966498
С	-0.636519	-0.173686	0.084697	С	0.561985	-0.428475	-0.364018	С	0.843371	-0.246144	-1.102734
0	-3.374270	-2.257871	-0.363912	0	1.140608	2.99834	-0.515029	0	-0.259972	2.644926	0.454022
С	-1.447992	2.242893	-0.285733	С	2.852436	-1.579671	-0.11897	С	3.211861	-0.735463	-0.226917
0	-0.310472	2.865183	0.282016	0	4.176315	-1.462012	0.381296	0	4.105892	-0.638450	0.871158
С	2.642937	-0.813213	0.005753	С	-2.942537	-0.634615	-0.135616	С	-2.157433	-1.065564	0.269192
С	3.698019	-1.851982	-0.299384	С	-4.167006	-0.98611	-0.948881	С	-2.895384	-1.332181	1.556240
С	1.618255	-1.093857	0.826742	С	-1.810848	-1.342311	-0.270653	С	-0.980334	-1.656929	0.004130
С	0.426671	-0.234277	1.185730	С	-0.49387	-1.179556	0.451217	С	-0.101944	-1.455384	-1.210942
Н	-0.153182	0.004380	-0.886315	Н	0.608746	-0.832059	-1.385752	Н	1.404071	-0.137646	-2.040987
С	2.868861	0.482142	-0.754365	С	-3.176429	0.54513	0.792334	С	-2.859071	-0.082229	-0.652984
0	2.256900	1.662548	-0.229937	0	-2.044059	1.128184	1.40333	0	-3.068207	1.182281	-0.036122
Н	-1.908464	0.982053	1.392723	Н	1.862766	-0.353399	1.349116	Н	1.382602	-0.868103	0.897218
Н	-3.926143	0.362700	0.194212	Н	3.200263	1.467806	0.450958	Н	1.833194	1.365977	1.666014
Н	-3.101852	0.433392	-1.364691	Н	3.014906	0.877191	-1.198116	Н	2.548213	1.832430	0.123436
Н	-2.296630	2.911364	-0.101845	Н	2.952874	-1.633855	-1.209208	Н	3.646331	-0.112304	-1.017225
Н	-1.350900	2.143764	-1.380347	Н	2.379352	-2.517908	0.210639	н	3.160781	-1.764723	-0.617080
н	0.490476	2 469619	-0.102570	н	4.138615	-1.527138	1.344828	н	3.814542	-1.260908	1.550668
н	4 692662	_1 523618	0.029853	н	-4 452929	-0.160757	-1 613459	н	-3 866857	-1 803724	1 357425
н	3 772562	-2.037122	_1 379400	н	-5.031588	-1 176518	_0 299342	н	-3 107502	_0 385335	2.063063
н	3.474436	-2.804682	0.185766	н	_4.005398	-1.876749	-1 561028	н	-2 330603	_1 981361	2.000000
н	1 606615	_2.004002	1 255707	н	-1 823548	-2 145091	_1.009249	н	_0 590860	_2 3/7191	0.752738
ш	-0.05(122	-2.094144	2.085222	и П	-1.823348	-2.145091	-1.009249	ш	-0.590800	-2.347191	1 274507
п	-0.056155	-0.031034	2.065255	п	-0.020137	-0.004300	0.661717	п	0.017270	-2.340424	-1.374307
п	0.709046	0.795620	1.404552	п	-0.063034	-2.176657	0.001/1/	п	-0.696039	-1.32/301	-2.120997
н	2.4/9262	0.382029	-1.//5346	п	-3.833354	0.221533	1.611829	п	-3.862970	-0.468302	-0.8/4260
H	3.951650	0.649103	-0.857937	Н	-3.754456	1.300191	0.23037	Н	-2.329566	0.021544	-1.605605
н	2.639823	1.833528	0.640863	н	-1.442623	1.412847	0.69656	н	-2.221799	1.657899	-0.012776
	1.0.11722	6a7	0.470070	-	1 0010 (0	6b1	0.05000.4	-	0.15(001	6b2	0.004770
С	1.841732	0.119573	0.472053	C	-1.021268	0.860014	-0.370334	C	-2.176031	-0.063884	0.304773
С	1.507341	1.577287	0.825274	С	-2.395320	0.513100	-0.954254	C	-2.430712	1.399230	-0.081533
С	0.214724	1.847613	0.077302	С	-2.736706	-0.823711	-0.307541	C	-1.034947	1.991661	-0.208981
0	0.089864	0.956416	-0.936977	0	-1.943340	-1.002672	0.788104	0	-0.131140	0.975160	-0.321153
С	1.043050	-0.129740	-0.836145	С	-1.064114	0.136807	0.991840	C	-0.779989	-0.330806	-0.302221
0	-0.621669	2.694626	0.278849	0	-3.558614	-1.633600	-0.648525	0	-0.701301	3.146691	-0.220741
С	3.340143	-0.160114	0.331682	C	-0.718684	2.357888	-0.271990	С	-3.262429	-1.029887	-0.171817
0	3.617134	-1.515481	-0.001486	0	0.503516	2.638670	0.382816	0	-2.986956	-2.390240	0.138501
С	-2.003645	-1.164325	0.265307	С	2.178895	-1.142594	0.047652	С	2.590480	-0.911875	-0.004562
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Н	3.837632	0.027756	1.288809	Н	-1.505228	2.851138	0.313535	Н	-3.337853	-0.984691	-1.264441
Н	3.780248	0.532015	-0.403969	Н	-0.751010	2.799127	-1.282067	Н	-4.236963	-0.716364	0.231823
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Н	-3.260026	-0.417721	1.831346	Н	2.977057	-1.825304	-1.854608	Н	4.182860	-0.283409	-1.289767
Н	-2.323739	-1.862212	2.296461	Н	2.105284	-3.068075	-0.947851	Н	3.634215	-1.947182	-1.602370
Н	-0.374603	-2.162710	1.090967	Н	0.472509	-2.259426	0.487134	Н	1.414404	-2.317311	-1.001529
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Н	3.799817	0.257936	1.547015	Н	-2.654466	1.266486	1.076815	Н	3.799877	0.257879	1.546921
Η	2.045980	0.271440	1.742243	Н	-3.921862	1.122111	-0.141264	Н	2.046045	0.271049	1.742470
Η	1.987400	1.644914	-0.093749	Н	-2.095761	1.082411	-1.685048	Н	1.987093	1.644749	-0.093578

# III. Chiral HPLC separation profiles of 1a/1b 5a/5b



Figure S3. Chiral HPLC separation of compounds 1a (left) and 1b (right).







Figure S5. Chiral HPLC analysis of compounds 3a/3b.



Figure S6. Chiral HPLC separation of the LAH reduction products of compound 3 (3a-r left and 3b-r right).



Figure S7. Chiral HPLC separation of compounds 4a/4b and 5a/5b.



Scheme S1. NaOH hydrolysis reaction of 3 and  $CH_2N_2$  diazotization of the hydrolyzates.

#### IV. HR-MS, 1D and 2D NMR spectra of the new compounds



Figure S8. HR-ESI-MS of compounds 1a/1b.



Figure S9. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compounds 1a/1b.



Figure S11. DEPT spectrum (125 MHz, CDCl<sub>3</sub>) of compounds 1a/1b.



Figure S13. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compounds 2a/2b.





Figure S15. DEPT spectrum (125 MHz, CDCl<sub>3</sub>) of compounds 2a/2b.



Figure S16. HMQC spectrum of compounds 2a/2b.



Figure S17. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compounds 2a/2b.



Figure S18. HMBC spectrum of compounds 2a/2b.



Figure S19. NOESY spectrum of compounds 2a/2b.



Figure S21. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compounds 3a/3b.



Figure S23. HSQC spectrum of compounds 3a/3b.



Figure S25. HMBC spectrum of compounds 3a/3b.



Figure S27. HR-ESI-MS of compounds 4a/4b.



Figure S28. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compounds 4a/4b.

-140



Figure S29. <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of compounds 4a/4b.



Figure S30. DEPT spectrum (125 MHz, CDCl3) of compounds 4a/4b.



Figure S31. HR-ESI-MS of compounds 5a/5b.



Figure S32. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compounds 5a/5b.



Figure S33. <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of compounds 5a/5b.



Figure S34. DEPT spectrum (125 MHz, CDCl<sub>3</sub>) of compounds 5a/5b.



Figure S35. HR-ESI-MS of compound 6.



Figure S36. 1H NMR spectrum (500 MHz, CDCl3) of compound 6.



Figure S37. <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of compound 6.



Figure S38. DEPT spectrum (125 MHz, CDCl<sub>3</sub>) of compound 6.







Figure S41. HMBC spectrum of compound 6.



Figure S43. -of compound 7.



Figure S44. <sup>1</sup>H NMR spectrum (500 MHz, DMSO-d<sub>6</sub>) of compound 7.



Figure S45. <sup>13</sup>C NMR spectrum (125 MHz, DMSO-d<sub>6</sub>) of compound 7.









10

·20 ·30

-150 -160 -170 -170

2.5

2.0

1.5

-40 -50 -60 -70 -90 -110 -120 -120 -120 -120



8

8.5