Supplementary data

Two New Phomaligols from the Marine-Derived Fungus *Aspergillus flocculosus* and their Anti-Neuroinflammatory Activity in BV-2 Microglial Cells

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Elemental Composition Report

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 39 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass) Elements Used: C: 0-15 H: 0-30 O: 0-10 Na: 0-1 Minimum: -1.5 5.0 10.0 50.0 Maximum: mDa PPM DBE i-FIT Norm Conf(%) Mass Calc. Mass Formula 279.1209 279.1208 0.1 0.4 3.5 1477.8 0.006 99.41 C13 H20 O5 Na



Figure S1. HRESIMS data of deketo-phomaligol A (1).



Figure S3. ¹³C NMR spectrum of deketo-phomaligol A (1).



Figure S4. ¹H-¹H COSY spectrum of deketo-phomaligol A (1).



Figure S5. HSQC spectrum of deketo-phomaligol A (1).



Figure S6. HMBC spectrum of deketo-phomaligol A (1).



Figure S7. ROESY spectrum of deketo-phomaligol A (1).



Elemental Composition Report

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 45 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) Elements Used: C: 0-15 H: 0-30 O: 0-10 Na: 0-1 Minimum: -1.5 Maximum: 5.0 10.0 50.0 PPM DBE Norm Conf(%) Formula Mass Calc. Mass mDa i-FIT 209.0791 209.0790 0.1 0.5 1654.2 C9 H14 O4 Na 2.5 n/a n/a



Figure S9. HRESIMS data of phomaligol E (2).



Figure S11. ¹³C NMR spectrum of phomaligol E (**2**).



Figure S12. ¹H-¹H COSY spectrum of phomaligol E (**2**).



Figure S13. HSQC spectrum of phomaligol E (2).



Figure S14. HMBC spectrum of phomaligol E (2).



Figure S15. ROESY spectrum of phomaligol E (2).

Elemental Composition Report

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 42 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass) Elements Used: C: 0-15 H: 0-30 O: 0-10 Na: 0-1 Minimum: -1.5 5.0 Maximum: 10.0 50.0 PPM DBE Norm Conf(%) Calc. Mass mDa i-FIT Formula Mass 29.35 C12 H18 O4 Na 249.1104 249.1103 0.1 0.4 3.5 1382.9 1.226



Figure S16. HRESIMS data of sydowione A (3).



Figure S18. ¹³C NMR spectrum of sydowione A (**3**).



Figure S19. ¹H NMR spectrum of (S) and (R) MTPA (**3a** and **3b**).



Figure S20. ¹H NMR spectrum of oxidation of **3** (**3c**).



Figure S21. LRMS data of 2,6-dimethyl-3-O -methyl-4-(2-methylbutyryl)phloroglucinol (4).





Figure S24. LRMS data of phomaligol A (5).



Figure S25. ¹H NMR spectrum of phomaligol A (**5**).



Figure S26. ¹³C NMR spectrum of phomaligol A (**5**).



Figure S27. LRMS data of phomaligol A₁ (6).



Figure S29. ¹³C NMR spectrum of phomaligol A_1 (6).



Figure S30. LRMS data of saccharonol A (7).





F: {0,3} - c ESI corona sid=50.00 det=1600.00 Full ms [1.00-1999.00]







Figure S36. DFT optimized conformers and populations of **1** (*2R*, *5R*, *7S*) above 5% population.

Table S1. Gibbs free energies and Boltzmann distribution of conformers of compound 1.

B3LYP/6-31+G(d,p) Gibbs free energy (298.15K)						
G (Hartree) Population (%)						
Conformer 1	-883.421988	41.48				
Conformer 2	-883.422344	17.88				
Conformer 3	-883.423125	16.88				
Conformer 4	-883.422103	7.65				
Conformer 5	-883.421843	5.99				

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Atom	Х	Y	Z	Atom	Х	Y	Z
C 0.9888 1.2109 0.0488 H 0.5433 3.1248 -1.7517 C 0.6175 0.1112 1.0196 C 1.4338 -1.0738 0.4532 C 2.4418 -0.5418 -0.5915 O -0.8083 -0.1603 1.0797 C 1.0167 0.4156 2.4643 C -1.4069 -0.6886 -0.0112 O -0.7999 -0.9808 -1.0251 C -2.9044 -0.8567 0.1805 C -3.4239 1.6594 -0.1401 O 1.3736 -2.2146 0.8565 C -3.4239 1.6594 -0.1401 O 1.3736 -2.2146 0.8565 C 2.4865 -1.3825 -1.8651 O 0.3034 2.3624 0.1772 C 0.6747 3.4274 -0.7077 H 2.4546 1.5329 -1.5113 H 0.705 1.2897 2.8265 H -3.0869 -2.4396 -1.3031 <td>С</td> <td>1.9936</td> <td>0.8811</td> <td>-0.7801</td> <td>Н</td> <td>1.7164</td> <td>3.7205</td> <td>-0.5405</td>	С	1.9936	0.8811	-0.7801	Н	1.7164	3.7205	-0.5405
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	0.9888	1.2109	0.0488	Н	0.5433	3.1248	-1.7517
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	С	0.6175	0.1112	1.0196				
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	С	1.4338	-1.0738	0.4532				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	2.4418	-0.5418	-0.5915				
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0	-0.8083	-0.1603	1.0797				
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	С	1.0167	0.4156	2.4643				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	-1.4069	-0.6886	-0.0112				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	-0.7999	-0.9808	-1.0251				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	-2.9044	-0.8567	0.1805				
C -3.6565 0.2268 -0.6295 C -3.4239 1.6594 -0.1401 O 1.3736 -2.2146 0.8565 C 2.4865 -1.3825 -1.8651 O 3.7327 -0.5310 0.0592 O 0.3034 2.3624 0.1772 C 0.6747 3.4274 -0.7077 H 2.4546 1.5329 -1.5113 H 0.7832 -0.4455 3.0954 H 2.0888 0.6172 2.5188 H 0.4705 1.2897 2.8265 H -3.1225 -0.7143 1.2440 H -4.4001 -2.4002 -0.1096 H -3.0869 -2.4396 -1.3031 H -2.8102 -3.0375 0.3412 H -3.3674 0.1344 -1.6837 H -4.7256 -0.0906 -0.5772 H -3.7469 1.7762 0.9003 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	С	-3.3230	-2.2717	-0.2486				
C -3.4239 1.6594 -0.1401 O 1.3736 -2.2146 0.8565 C 2.4865 -1.3825 -1.8651 O 3.7327 -0.5310 0.0592 O 0.3034 2.3624 0.1772 C 0.6747 3.4274 -0.7077 H 2.4546 1.5329 -1.5113 H 0.7832 -0.4455 3.0954 H 2.0888 0.6172 2.5188 H 0.4705 1.2897 2.8265 H -3.1225 -0.7143 1.2440 H -4.4001 -2.4002 -0.1096 H -3.0869 -2.4396 -1.3031 H -2.8102 -3.0375 0.3412 H -3.3674 0.1344 -1.6837 H -4.7256 -0.0096 -0.5772 H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	С	-3.6565	0.2268	-0.6295				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	-3.4239	1.6594	-0.1401				
C 2.4865 -1.3825 -1.8651 O 3.7327 -0.5310 0.0592 O 0.3034 2.3624 0.1772 C 0.6747 3.4274 -0.7077 H 2.4546 1.5329 -1.5113 H 0.7832 -0.4455 3.0954 H 2.0888 0.6172 2.5188 H 0.4705 1.2897 2.8265 H -3.1225 -0.7143 1.2440 H -4.4001 -2.4002 -0.1096 H -3.0869 -2.4396 -1.3031 H -2.8102 -3.0375 0.3412 H -3.3674 0.1344 -1.6837 H -4.7256 -0.0096 -0.5772 H -3.9927 2.3705 -0.7472 H -3.7469 1.7762 0.9003 H 2.7328 -2.4221 -1.6237 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	0	1.3736	-2.2146	0.8565				
O 3.7327 -0.5310 0.0592 O 0.3034 2.3624 0.1772 C 0.6747 3.4274 -0.7077 H 2.4546 1.5329 -1.5113 H 0.7832 -0.4455 3.0954 H 2.0888 0.6172 2.5188 H 0.4705 1.2897 2.8265 H -3.1225 -0.7143 1.2440 H -4.4001 -2.4002 -0.1096 H -3.0869 -2.4396 -1.3031 H -2.8102 -3.0375 0.3412 H -3.3674 0.1344 -1.6837 H -4.7256 -0.0096 -0.5772 H -3.9927 2.3705 -0.7472 H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	С	2.4865	-1.3825	-1.8651				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	0	3.7327	-0.5310	0.0592				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	0	0.3034	2.3624	0.1772				
H 2.4546 1.5329 -1.5113 H 0.7832 -0.4455 3.0954 H 2.0888 0.6172 2.5188 H 0.4705 1.2897 2.8265 H -3.1225 -0.7143 1.2440 H -4.4001 -2.4002 -0.1096 H -3.0869 -2.4396 -1.3031 H -2.8102 -3.0375 0.3412 H -3.3674 0.1344 -1.6837 H -4.7256 -0.0096 -0.5772 H -3.9927 2.3705 -0.7472 H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	С	0.6747	3.4274	-0.7077				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Η	2.4546	1.5329	-1.5113				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Η	0.7832	-0.4455	3.0954				
H 0.4705 1.2897 2.8265 H -3.1225 -0.7143 1.2440 H -4.4001 -2.4002 -0.1096 H -3.0869 -2.4396 -1.3031 H -2.8102 -3.0375 0.3412 H -3.3674 0.1344 -1.6837 H -4.7256 -0.0096 -0.5772 H -3.9927 2.3705 -0.7472 H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Η	2.0888	0.6172	2.5188				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Η	0.4705	1.2897	2.8265				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Η	-3.1225	-0.7143	1.2440				
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Η	-4.4001	-2.4002	-0.1096				
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Η	-3.0869	-2.4396	-1.3031				
H -3.3674 0.1344 -1.6837 H -4.7256 -0.0096 -0.5772 H -3.9927 2.3705 -0.7472 H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Η	-2.8102	-3.0375	0.3412				
H -4.7256 -0.0096 -0.5772 H -3.9927 2.3705 -0.7472 H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Н	-3.3674	0.1344	-1.6837				
H -3.9927 2.3705 -0.7472 H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Н	-4.7256	-0.0096	-0.5772				
H -3.7469 1.7762 0.9003 H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Н	-3.9927	2.3705	-0.7472				
H -2.3686 1.9452 -0.1923 H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Н	-3.7469	1.7762	0.9003				
H 2.7328 -2.4221 -1.6237 H 1.5177 -1.3678 -2.3689 H 3.2512 -0.9879 -2.5402 H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Н	-2.3686	1.9452	-0.1923				
H1.5177-1.3678-2.3689H3.2512-0.9879-2.5402H4.0047-1.45600.1636H0.01234.2602-0.4755	H	2.7328	-2.4221	-1.6237				
H3.2512-0.9879-2.5402H4.0047-1.45600.1636H0.01234.2602-0.4755	Н	1.5177	-1.3678	-2.3689				
H 4.0047 -1.4560 0.1636 H 0.0123 4.2602 -0.4755	Н	3.2512	-0.9879	-2.5402				
H 0.0123 4.2602 -0.4755	Н	4.0047	-1.4560	0.1636				
	Н	0.0123	4.2602	-0.4755				

Table S2. ECD calculation and energy minimized coordinates of conformer 1 for all atoms (Å).

Atom	Х	Y	Z	Atom	Х	Y	Z
С	1.9553	0.9146	-0.8104	Н	1.4797	3.7364	-0.6894
С	0.9220	1.2092	-0.0034	Н	0.3680	3.0111	-1.8880
С	0.6192	0.1291	1.0128				
С	1.5135	-1.0221	0.4972				
С	2.4958	-0.4659	-0.5593				
0	-0.7837	-0.2303	1.0848				
С	0.9953	0.5198	2.4432				
С	-1.3508	-0.8265	0.0097				
0	-0.7222	-1.1181	-0.9899				
С	-2.8329	-1.0825	0.2347				
С	-3.4338	-1.8659	-0.9365				
С	-3.5912	0.2321	0.5562				
С	-3.5079	1.3116	-0.5284				
0	1.5205	-2.1496	0.9408				
С	2.6108	-1.3514	-1.7975				
0	3.7754	-0.3436	0.1026				
0	0.1546	2.3127	0.0682				
С	0.4635	3.3643	-0.8561				
Н	2.3769	1.5643	-1.5668				
Н	0.8155	-0.3268	3.1105				
Н	2.0523	0.7915	2.4888				
Н	0.3934	1.3718	2.7679				
Н	-2.8862	-1.7038	1.1389				
Н	-4.4902	-2.0718	-0.7413				
Н	-3.3593	-1.3101	-1.8747				
Н	-2.9193	-2.8200	-1.0763				
Н	-4.6394	-0.0341	0.7352				
Н	-3.2055	0.6346	1.4980				
Н	-4.0966	2.1872	-0.2375				
Н	-2.4758	1.6459	-0.6785				
Н	-3.8951	0.9600	-1.4897				
Н	2.9232	-2.3619	-1.5130				
Н	1.6488	-1.4216	-2.3098				
Н	3.3546	-0.9332	-2.4817				
Н	4.1046	-1.2439	0.2504				
Н	-0.2586	4.1573	-0.6663				
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Table S3. ECD calculation and energy minimized coordinates of conformer 2 for all atoms (Å).AtomXYZAtomXYZ

Atom	Х	Y	Z	Atom	Х	Y	Z
С	2.3587	0.5298	-0.4847	Н	2.8725	3.2984	0.0667
С	1.3370	1.1039	0.1732	Н	1.8734	3.1747	-1.4110
С	0.4492	0.1140	0.8950				
С	0.9755	-1.2250	0.3299				
С	2.3099	-0.9716	-0.4086				
0	-0.9648	0.3157	0.6483				
С	0.5933	0.1655	2.4169				
С	-1.4410	0.0811	-0.5963				
0	-0.7401	-0.3123	-1.5095				
С	-2.9308	0.3614	-0.6905				
С	-3.2112	1.8645	-0.5064				
С	-3.7310	-0.4965	0.3136				
С	-3.4979	-2.0042	0.1740				
0	0.4801	-2.3118	0.5371				
С	2.3982	-1.6929	-1.7510				
0	3.3576	-1.4190	0.4822				
0	1.0058	2.3988	0.3218				
С	1.8535	3.3522	-0.3307				
Н	3.1432	1.0492	-1.0200				
Н	-0.0223	-0.6169	2.8678				
Н	1.6367	0.0040	2.6969				
Н	0.2707	1.1406	2.7894				
Н	-3.2076	0.0675	-1.7086				
Н	-4.2786	2.0604	-0.6446				
Н	-2.9286	2.1945	0.4971				
Н	-2.6595	2.4672	-1.2342				
Н	-3.4829	-0.1734	1.3311				
Н	-4.7931	-0.2696	0.1632				
Н	-4.1281	-2.5597	0.8752				
Н	-3.7369	-2.3519	-0.8372				
Н	-2.4563	-2.2710	0.3835				
Н	2.2615	-2.7706	-1.6112				
Η	1.6224	-1.3346	-2.4310				
Η	3.3804	-1.5182	-2.1993				
Н	3.3172	-2.3878	0.5028				
Н	1.4257	4.3323	-0.1228				

Table S4. ECD calculation and energy minimized coordinates of conformer 3 for all atoms (Å).AtomXYZAtomXYZ

Atom	Х	Y	Z	Atom	Х	Y	Z
С	2.0723	0.8820	-0.8286	Н	1.6672	3.7210	-0.8067
С	1.0487	1.2314	-0.0310	Н	0.5271	2.9822	-1.9692
С	0.7047	0.1873	1.0081				
С	1.5712	-1.0030	0.5348				
С	2.5699	-0.5070	-0.5369				
0	-0.7123	-0.1199	1.0608				
С	1.0690	0.6009	2.4344				
С	-1.2784	-0.7273	-0.0079				
0	-0.6370	-1.1177	-0.9651				
С	-2.7869	-0.8079	0.1405				
С	-3.3459	-1.9835	-0.6675				
С	-3.3874	0.5638	-0.2721				
С	-4.8777	0.7041	0.0504				
0	1.5558	-2.1124	1.0217				
С	2.6621	-1.4304	-1.7490				
0	3.8520	-0.4038	0.1243				
0	0.3140	2.3578	0.0113				
С	0.6405	3.3683	-0.9508				
Н	2.5147	1.4967	-1.6022				
Н	0.8545	-0.2242	3.1182				
Н	2.1327	0.8429	2.4909				
Н	0.4875	1.4774	2.7293				
Н	-2.9939	-0.9554	1.2071				
Н	-4.4267	-2.0653	-0.5314				
Н	-3.1398	-1.8530	-1.7336				
Н	-2.8957	-2.9286	-0.3504				
Н	-2.8306	1.3557	0.2410				
Н	-3.2213	0.7092	-1.3471				
Н	-5.2329	1.7037	-0.2186				
Н	-5.4871	-0.0200	-0.4983				
Н	-5.0647	0.5594	1.1202				
Н	2.9403	-2.4419	-1.4343				
Н	1.7011	-1.4842	-2.2648				
Н	3.4229	-1.0559	-2.4398				
Η	4.1516	-1.3090	0.3022				
Н	-0.0595	4.1859	-0.7830				

Table S5. ECD calculation and energy minimized coordinates of conformer 4 for all atoms (Å).AtomXYZAtomXYZ

Atom	Х	Y	Z	Atom	Х	Y	Z
С	2.2784	0.6849	-0.7813	Н	2.6369	3.4954	-0.3375
С	1.3891	1.1648	0.1048	Н	1.3324	3.2602	-1.5376
С	0.7941	0.1023	1.0028				
С	1.3095	-1.1865	0.3219				
С	2.3956	-0.8128	-0.7132				
0	-0.6527	0.1643	1.0889				
С	1.2762	0.1902	2.4517				
С	-1.3781	-0.1374	-0.0133				
0	-0.8727	-0.4855	-1.0635				
С	-2.8682	-0.0161	0.2596				
С	-3.3108	-1.2023	1.1446				
С	-3.6534	0.0890	-1.0595				
С	-5.1389	0.4095	-0.8685				
0	0.9976	-2.3133	0.6401				
С	2.2300	-1.5383	-2.0461				
0	3.6652	-1.1448	-0.1055				
0	0.9789	2.4236	0.3419				
С	1.5524	3.4467	-0.4812				
Н	2.8609	1.2722	-1.4797				
Н	0.8624	-0.6437	3.0240				
Н	2.3668	0.1382	2.4843				
Н	0.9506	1.1332	2.8971				
Н	-3.0052	0.9061	0.8384				
Н	-4.3622	-1.0989	1.4225				
Н	-3.1904	-2.1504	0.6098				
Н	-2.7210	-1.2472	2.0633				
Н	-3.1936	0.8680	-1.6782				
Н	-3.5390	-0.8483	-1.6164				
Н	-5.6307	0.5342	-1.8381				
Н	-5.6673	-0.3856	-0.3337				
Н	-5.2752	1.3394	-0.3047				
Н	2.2347	-2.6225	-1.8903				
Н	1.2840	-1.2642	-2.5178				
Н	3.0558	-1.2757	-2.7135				
Н	3.7209	-2.1126	-0.0769				
Н	1.0941	4.3833	-0.1660				

Table S6. ECD calculation and energy minimized coordinates of conformer 5 for all atoms (Å).