Supporting Information

Structure and Absolute Configuration of Jurassic Polyketide-Derived Spiroborate Pigments Obtained from Microgram Quantities

Klaus Wolkenstein,*[,†,⊥] Han Sun,[‡,∥,⊥] Heinz Falk,[§] and Christian Griesinger[‡]

[†]Department of Geobiology, Geoscience Centre, University of Göttingen, Goldschmidtstraße 3, 37077 Göttingen, Germany

[‡]Department of NMR Based Structural Biology, Max Planck Institute for Biophysical Chemistry, Am Fassberg 11, 37077 Göttingen, Germany

[§]Institute of Organic Chemistry, University of Linz, Altenbergerstraße 69, 4040 Linz, Austria

[∥]Present address: Leibniz-Institut für Molekulare Pharmakologie, Robert-Rössle-Str. 10, 13125 Berlin, Germany

[⊥]These authors contributed equally to this work

*Corresponding author E-mail: klaus.wolkenstein@geo.uni-goettingen.de

Table of Contents

Experimental Section

Fossil Material. Specimens of *S. jurassica* with distinct pink coloration were collected at Les Petites-Armoises (Département Ardennes, France), one of the original localities where borolithochromes have been discovered.[1] A voucher specimen of the analyzed material has been deposited in the Staatliches Museum für Naturkunde Stuttgart, Germany (SMNS P24204).

Extraction and Isolation of Pigments. The combined material of several pink-colored specimens of *S. jurassica* was broken into small pieces (2–3 cm) and cleaned with acetone. After treatment of the fossil material (830 g) with 10 M HCl, the residue was separated by centrifugation, washed thoroughly with distilled water, and dried overnight at room temperature under vacuum. Residues were then sequentially extracted by sonication (10 min at 40 °C) and centrifugation in toluene (3×) and dimethyl sulfoxide (DMSO) (3×). The dark, reddish-brown DMSO extract was further purified by solid-phase extraction. The DMSO extract was diluted 1:5 in acetonitrile/20 mM aqueous ammonium acetate (50:50) and the precipitate separated by centrifugation. The procedure comprising DMSO extraction, dilution, and separation of precipitate was repeated twice and the diluted extracts were combined. The sorbent (Bondesil C18, 40 µm) was conditioned by washing with acetonitrile, followed by acetonitrile/20 mM aqueous ammonium acetate (50:50). The diluted DMSO extract then was loaded onto the column, and the sorbent was washed with acetonitrile/20 mM aqueous ammonium acetate (50:50) to remove organic matrix compounds and then with water. The pink-colored compounds were eluted with acetonitrile, and the solvent was removed under vacuum, leaving an intensely crimson-colored residue (8.1 mg). Individual borolithochromes were isolated by semipreparative HPLC using a Phenomenex Gemini C18 column (250 × 10 mm i.d., 5 µm) at 30 °C. The HPLC program consisted of a linear gradient of acetonitrile/20 mM aqueous ammonium acetate (65:35) to 85% acetonitrile in 40 min, followed by a linear gradient to 100% acetonitrile in 2 min and isocratic elution at 100% acetonitrile at a flow rate of 4.5 mL min^{-1}. Fractions were concentrated and desalted by solid-phase extraction. Analytic HPLC measurements were carried out using an Agilent 1200 Series HPLC system with a diode array detector.

NMR Spectroscopy. Borolithochrome samples were dissolved in 35-50 µL 99.96% DMSO-d_6 and transferred into 1.7 mm NMR tubes. 1D and 2D NMR spectra were recorded at 298 K on a Bruker Avance III 800 MHz spectrometer equipped with a 1.7 mm cryo CP-TCI probe or a Bruker Avance III 700 MHz spectrometer with a 1.7 mm room temperature CP-TXI probe. 1D ^{1}H and 2D double quantum filtered correlated spectroscopy (DQF-COSY) and total correlation spectroscopy (TOCSY) experiments were carried out using the 700 MHz NMR spectrometer, whereas nuclear Overhauser effect spectroscopy (NOESY), ^{1}H-^{13}C heteronuclear single quantum coherence (HSQC) and ^{1}H-^{13}C heteronuclear multiple-bond correlation (HMBC) spectra, as well as all spectra of **3b** were acquired on the 800 MHz spectrometer. Pre-saturation pulses were employed in the 1D experiments to suppress strong water signals. The ^{1}H and ^{13}C chemical shifts were referenced to DMSO (δ_H = 2.50 ppm, δ_C = 39.5 ppm). NMR spectra were processed with Topspin 2.1 (Bruker). The following acquisition parameters were used for the 2D NMR experiments:

*2D NMR spectra of **2a***

COSY: 4k × 380 data points, 64 scans per increment, 2 s relaxation delay and pre-saturation for water suppression

TOCSY: 4k × 369 data points, 64 scans per increment, 2 s relaxation delay and pre-saturation for water suppression, DIPSI2 mixing sequence, 80 ms mixing time

NOESY: 4k × 558 data points, 128 scans per increment, 2 s relaxation delay and pre-saturation for water suppression, 300 ms mixing time

^{1}H-^{13}C HSQC: 2k × 457 data points, 84 scans per increment, 2 s relaxation delay

^{1}H-^{13}C HMBC: 4k × 623 data points, 128 scans per increment, 2 s relaxation delay, 62.5 ms delay for evolution of long-range coupling, phase sensitive mode, no decoupling during acquisition

*2D NMR spectra of **3a***

COSY: 4k × 219 data points, 48 scans per increment, 2 s relaxation delay and pre-saturation for water suppression

TOCSY: 4k × 400 data points, 64 scans per increment, 2 s relaxation delay and pre-saturation for water suppression, DIPSI2 mixing sequence, 80 ms mixing time

^{1}H-^{13}C HSQC: 2k × 289 data points, 84 scans per increment, 2 s relaxation delay

^{1}H-^{13}C HMBC: 4k × 516 data points, 88 scans per increment, 2 s relaxation delay, 62.5 ms delay for evolution of long-range coupling, phase sensitive mode, no decoupling during acquisition

*2D NMR spectra of **3b***

COSY: 4k × 219 data points, 48 scans per increment, 2 s relaxation delay and pre-saturation for water suppression

TOCSY: 4k × 512 data points, 56 scans per increment, 2 s relaxation delay and pre-saturation for water suppression, DIPSI2 mixing sequence, 80 ms mixing time

ROESY: 4k × 100 data points, 8 scans per increment, 2 s relaxation delay and pre-saturation for water suppression, spin lock with a mixing time of 250 ms

^{1}H-^{13}C HSQC: 2k × 317 data points, 128 scans per increment, 2 s relaxation delay

UV-visible and CD Spectroscopy. UV-visible absorption spectra were recorded in acetonitrile on a Jasco V-630 spectrophotometer. CD spectra were recorded at 20 °C on a Jasco J-810 spectropolarimeter using 1-mm quartz cuvettes and were smoothed using a 25-point Savitzky-Golay filter. Because of the significant errors in the weighing of microgram amounts, the concentrations of the sample solutions were determined based on the long-wavelength absorption maximum of **3a**.

Fluorescence Spectroscopy. Fluorescence was determined for the highly substituted borolithochrome C2 (**3b**). Fluorescence emission spectra were recorded at 25 °C on a Jasco FP-6200 spectrofluorometer. For the determination of the fluorescence quantum yield rhodamine 6G in ethanol was used as a reference.[2]

IR Spectroscopy. IR spectra were measured on a Jasco 4100 FT-IR spectrometer equipped with a Pike Gladi ATR (attenuated total reflection) accessory.

Mass Spectrometry. High-resolution ESI-MS spectra were obtained on a Bruker micrOTOF mass spectrometer with electrospray ionization in the negative-ion mode.

Spectroscopic Data

Borolithochrome G (**1**): red solid (6 µg); UV (acetonitrile) λ_{max} (log ε) 244 (4.58), 281 (4.37), 339 (4.02), 393 (3.75), 507 (4.20) nm; IR (ATR) ν_{max} 1566 cm^{-1}; ^{1}H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 747.2194 $[M]^-$ (calcd for $C_{48}H_{32}O_8{}^{11}B$, 747.2196).

Borolithochrome H1 (**2a**): red solid (31 µg); UV (acetonitrile) λ_{max} (log ε) 244 (4.57), 282 (4.34), 340 (3.98), 393 (3.74), 506 (4.21) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 283 (+11.2), 310 (+14.4), 351 (–5.5), 469 (+12.6), 520 (–26.2) nm; CD (DMSO) λ ($\Delta\varepsilon$) 285 (+11.0), 313 (+16.0), 354 (–4.7), 474 (+15.2), 527 (–27.9) nm; IR (ATR) ν_{max} 1566 cm^{-1}; ^{1}H NMR (DMSO-d_6, 700 MHz), see Table S2; HR-ESI-MS *m/z* 761.2365 $[M]^-$ (calcd for $C_{49}H_{34}O_8{}^{11}B$, 761.2352).

Borolithochrome H2 (**2b**): red solid (48 µg); UV (acetonitrile) λ_{max} (log ε) 244 (4.55), 282 (4.34), 340 (3.99), 393 (3.74), 507 (4.21) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 283 (–9.1), 310 (–13.5), 350 (+5.3), 468 (–11.8), 519 (+24.8) nm; CD (DMSO) λ ($\Delta\varepsilon$) 284 (–8.9), 313 (–14.8), 354 (+5.0), 474 (–13.9), 527 (+27.9) nm; IR (ATR) ν_{max} 1566 cm^{-1}; ^{1}H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 761.2354 $[M]^-$ (calcd for $C_{49}H_{34}O_8{}^{11}B$, 761.2352).

Borolithochrome C1 (**3a**): red solid (38 µg); UV (acetonitrile) λ_{max} (log ε) 274 (4.61), 303 (4.32), 336 (4.20), 419 (4.03), 518 (4.26) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 281 (+16.6), 486 (+17.2), 531 (–34.9) nm; CD (DMSO) λ ($\Delta\varepsilon$) 284 (+17.1), 497 (+15.7), 545 (–33.3) nm; IR (ATR) ν_{max} 1578 cm^{-1}; ^{1}H NMR (DMSO-d_6, 700 MHz), see Table S2; HR-ESI-MS *m/z* 867.2610 $[M]^-$ (calcd for $C_{52}H_{40}O_{12}{}^{11}B$,) 867.2618.

Borolithochrome C2 (**3b**): red solid (53 µg); UV (acetonitrile) λ_{max} (log ε) 245 (4.66), 269 (4.62), 302 (4.34), 336 (4.20), 419 (4.04), 517 (4.26) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 281 (–17.6), 485 (–16.6), 531 (+34.7) nm; CD (DMSO) λ ($\Delta\varepsilon$) 284 (–16.8), 499 (–15.5), 544 (+29.8) nm; Fluorescence (ethanol, λ_{exc} 490 nm) λ_{em} 565 nm, Φ 0.01; IR (ATR) ν_{max} 1578 cm^{-1}; ^{1}H NMR (DMSO-d_6, 800 MHz), see Table S1; HR-ESI-MS *m/z* 867.2616 $[M]^-$ (calcd for $C_{52}H_{40}O_{12}{}^{11}B$,) 867.2618.

Borolithochrome A (**4**): red solid (23 µg); UV (acetonitrile) λ_{max} (log ε) 245 (4.62), 270 (4.60), 302 (4.32), 336 (4.18), 419 (4.04), 516 (4.25) nm; IR (ATR) ν_{max} 1577 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 839.2300 $[M]^-$ (calcd for $C_{50}H_{36}O_{12}{}^{11}B$, 839.2305).

Borolithochrome B1 (**5a**): red solid (57 µg); UV (acetonitrile) λ_{max} (log ε) 246 (4.61), 272 (4.59), 303 (4.31), 336 (4.18), 419 (4.04), 518 (4.26) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 280 (+17.3), 486 (+15.4), 531 (–31.1) nm; IR (ATR) ν_{max} 1578 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 853.2470 $[M]^-$ (calcd for $C_{51}H_{38}O_{12}{}^{11}B$, 853.2462).

Borolithochrome B2 (**5b**): red solid (51 µg); UV (acetonitrile) λ_{max} (log ε) 242 (4.62), 274 (4.60), 303 (4.31), 338 (4.20), 419 (4.02), 518 (4.26) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 280 (–14.5), 485 (–14.3), 531 (+30.7) nm; IR (ATR) ν_{max} 1577 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 853.2452 $[M]^-$ (calcd for $C_{51}H_{38}O_{12}{}^{11}B$, 853.2462).

Borolithochrome D (**6**): red solid (19 µg); UV (acetonitrile) λ_{max} (log ε) 244 (4.63), 264 (4.57), 337 (4.14), 423 (3.88), 512 (4.24) nm; IR (ATR) ν_{max} 1575 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 793.2248 $[M]^-$ (calcd for $C_{49}H_{34}O_{10}{}^{11}B$, 793.2251).

Borolithochrome E (**7**): red solid (7 µg); UV (acetonitrile) λ_{max} (log ε) 244 (4.60), 264 (4.55), 337 (4.11), 424 (3.91), 511 (4.24) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 285 (+13.2), 476 (+12.4), 527 (–25.5) nm; IR (ATR) ν_{max} 1571 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 807.2405 $[M]^-$ (calcd for $C_{50}H_{36}O_{10}{}^{11}B$, 807.2407).

Borolithochrome F (**8**): red solid (9 µg); UV (acetonitrile) λ_{max} (log ε) 245 (4.60), 264 (4.55), 337 (4.11), 422 (3.88), 512 (4.24); CD (acetonitrile) λ ($\Delta\varepsilon$) 285 (–10.8), 478 (–11.5), 527 (+23.8); IR (ATR) ν_{max} 1576 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 821.2543 $[M]^-$ (calcd for $C_{51}H_{38}O_{10}{}^{11}B$, 821.2564).

Borolithochrome I1 (**9a**): red solid (31 µg); UV (acetonitrile) λ_{max} (log ε) 244 (4.56), 282 (4.33), 339 (4.00), 393 (3.74), 507 (4.22) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 284 (+9.2), 310 (+12.4), 351 (–4.3), 469 (+10.9), 521 (–21.8) nm; IR (ATR) ν_{max} 1566 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 775.2506 $[M]^-$ (calcd for $C_{50}H_{36}O_8{}^{11}B$, 775.2509).

Borolithochrome I2 (**9b**): red solid (30 µg); UV (acetonitrile) λ_{max} (log ε) 244 (4.55), 282 (4.30), 339 (3.98), 393 (3.73), 507 (4.22) nm; CD (acetonitrile) λ ($\Delta\varepsilon$) 281 (–2.5), 309 (–4.9), 351 (+2.4), 468 (–2.2), 518 (+5.6) nm (the CD spectrum of **9b** is likely affected by a CD active borolithochrome impurity with opposite sign as suggested by the compared to **9a** low $\Delta\varepsilon$ values); IR (ATR) ν_{max} 1566 cm^{-1}; ^1H NMR (DMSO-d_6, 700 MHz), see Table S1; HR-ESI-MS *m/z* 775.2504 $[M]^-$ (calcd for $C_{50}H_{36}O_8{}^{11}B$, 775.2509).

Table S1. ^{1}H NMR spectroscopic data for borolithochromes [^{1}H chemical shift (δ_H) in ppm, multiplicity, values in parentheses indicate *J* in Hz]. s, singlet; d, doublet; dd, doublet of doublets; t, triplet; m, multiplet; n.d., not determined. Spectra were recorded in DMSO-d_6 at 700 MHz with the exception of compound **3b** recorded at 800 MHz. All chemical shifts were referenced to DMSO (δ_H = 2.50 ppm).

Position	**1**	**2b**	**3b**	**4**	**5a**	**5b**	**6**	**7**	**8**	**9a**	**9b**
2	7.18, d (7.7)	7.18, d (7.7)	6.58, d (2.1)	6.57, s	6.58, d (2.1)	6.57, d (2.1)	6.60, d (2.1)	6.61, d (2.1)	6.59[a]	7.19, d (7.7)	7.16, d (7.7)
3	7.76, t (8.0)	7.75[a]								7.74[a]	7.75, t (7.8)
4	8.37, d (8.2)	8.36, d (8.2)	7.45, d (2.1)	7.43, s	7.45, d (2.1)	7.45, d (2.1)	7.48, d (2.1)	7.49, d (2.1)	7.48[a]	8.38, d (8.3)	8.36, d (8.2)
5	9.17, dd (8.3, 1.4)	9.17, dd (8.2, 1.8)								9.17, dd (8.2, 1.2)	9.16, dd (8.2, 1.3)
6	7.76, t (8.0)	7.75[a]	6.99, s	6.98, s	6.99, s	6.99, s	7.00, s	7.00, s	6.99, s	7.74[a]	7.75, t (7.8)
7	8.63, dd (7.6, 1.3)	8.63 or 8.64, dd (7.6, 1.2)								8.62, dd (7.6, 1.2)	8.63, dd (7.5, 1.3)
10	6.45, d (1.5)	6.47, d (1.6)	6.47, d (1.4)	6.50, s	6.50, d (1.5)	6.52, d (1.5)	6.50, d (1.6)	6.50, d (1.5)	6.48, d (1.5)	6.37, d (1.2)	6.42, d (1.5)
12	8.60, d (1.4)	8.67, d (1.5)	8.72, d (1.4)	8.74, s	8.75, d (1.5)	8.78, d (1.5)	8.71, d (1.5)	8.69, d (1.5)	8.67, d (1.2)	8.54, d (1.2)	8.59, d (1.5)
14	1.87, m	1.95, m	1.93, m	1.66, m	n.d.[a]	n.d.[a]	n.d.[a]	n.d.[a]	n.d.[a]	1.52, m	1.65, m
15	0.55, d (6.9)	0.59, d (6.9)	0.69, d (6.7)	0.71 or 0.72, d (6.9)	0.72, d (6.8)	0.77, d (6.9)	0.63, d (6.9)	0.65, d (6.8)	0.61, d (6.9)	0.39, d (6.9)	0.50, d (6.9)
16	0.48, d (6.9)	0.54, d (6.9)	1.14 and 1.21, m	0.71 or 0.72, d (6.9)	0.71, d (6.8)	0.76, d (6.9)	0.63, d (6.9)	0.63, d (6.8)	n.d.[a]	0.79, m	0.90 and 1.02, m
17			0.31, t (7.1)						0.27, t (7.3)	0.19, t (7.4)	0.13, t (7.4)
18			3.02, s	3.01, s	3.02, s	3.02, d (2.2)	3.05, s	3.05, s	3.05, s		
7-OH			n.d.	14.42, s	14.48, s	14.49, s	14.48, s	14.48, s	n.d.		
9-OH	14.39, s	14.39, s	13.37, s	13.37, s	13.34 or 13.35, s	13.34 or 13.36, s	13.33, s	13.32, s	n.d.	14.38, s	14.40, s
2'	7.18, d (7.7)	7.16, d (7.8)	6.58, d (2.1)	6.57, s	6.59, d (2.1)	6.60, d (2.1)	7.15, d (7.8)	7.14, d (7.8)	7.14, d (7.8)	7.19, d (7.7)	7.16, d (7.7)
3'	7.76, t (8.0)	7.75[a]					7.74 or 7.75, t (7.8)	7.74 or 7.75, t (7.8)	7.73 or 7.75, t (7.8)	7.74[a]	7.75, t (7.8)
4'	8.37, d (8.2)	8.36, d (8.2)	7.45, d (2.1)	7.43, s	7.46, d (2.1)	7.45, d (2.1)	8.34, d (7.9)	8.34, d (8.0)	8.33. d (8.5)	8.38, d (8.3)	8.36, d (8.2)
5'	9.17, dd (8.3, 1.4)	9.17, dd (8.2, 1.8)					9.15, dd (8.2, 1.4)	9.15, dd (8.1, 1.3)	9.15, dd (8.2, 1.4)	9.17, dd (8.2, 1.2)	9.16, dd (8.2, 1.3)

Table S1. (Continued)

Position	**1**	**2b**	**3b**	**4**	**5a**	**5b**	**6**	**7**	**8**	**9a**	**9b**
6'	7.76, t (8.0)	7.75[a]	6.99, s	6.98, s	7.00, s	6.99, s	7.74 or 7.75, t (7.8)	7.74 or 7.75, t (7.8)	7.73 or 7.75, t (7.8)	7.74[a]	7.75, t (7.8)
7'	8.63, dd (7.6, 1.3)	8.63 or 8.64, dd (7.6, 1.2)					8.63, dd (7.6, 1.2)	8.64, d (1.5)	8.64, dd (7.6, 1.4)	8.62, dd (7.6, 1.2)	8.63, dd (7.5, 1.3)
10'	6.45, d (1.5)	6.40, d (1.5)	6.47, d (1.4)	6.50, s	6.44, d (1.5)	6.45, d (1.4)	6.46, d (1.4)	6.39, d (1.5)	6.41[a]	6.37, d (1.2)	6.42, d (1.5)
12'	8.60, d (1.4)	8.54, d (1.5)	8.72, d (1.4)	8.74, s	8.69, d (1.5)	8.66, d (1.4)	8.66, d (1.5)	8.64, d (1.4)	8.66[a]	8.54, d (1.2)	8.59, d (1.5)
14'	1.87, m	1.57, m	1.93, m	1.66, m	1.87, m	1.85, m	n.d.[a]	n.d.[a]	n.d.[a]	1.52, m	1.65, m
15'	0.55, d (6.9)	0.46, d (6.9)	0.69, d (6.7)	0.71 or 0.72, d (6.9)	0.65, d (6.9)	0.64, d (7.0)	0.64, d (7.0)	0.48, d (6.9)	0.57, d (6.9)	0.39, d (6.9)	0.50, d (6.9)
16'	0.48, d (6.9)	0.85 and 0.97, m	1.14 and 1.21, m	0.71 or 0.72, d (6.9)	1.01, m	1.06 and 1.17, m	0.61, d (6.8)	n.d.[a]	n.d.[a]	0.79, m	0.90 and 1.02, m
17'		0.08, t (7.3)	0.31, t (7.1)		0.33, t (7.4)	0.25, t (7.4)		0.23, t (7.3)	0.15, t (7.4)	0.19, t (7.4)	0.13, t (7.4)
18'			3.02, s	3.01, s	3.03, s	3.02, d (2.2)					
7-OH'			n.d.	14.42, s	14.48, s	14.49, s					
9-OH'	14.39, s	14.41, s	13.37, s	13.37, s	13.34 or 13.35, s	13.34 or 13.36, s	14.43, s	14.43, s	14.43, s	14.38, s	14.40, s

[a]Overlapped signals.

Table S2. NMR spectroscopic data for borolithochrome H1 (**2a**) and C1 (**3a**). Spectra were recorded in DMSO-d_6 at 700 MHz for ^{1}H NMR and 800 MHz for ^{13}C NMR. All chemical shifts were referenced to DMSO (δ_H = 2.50 ppm, δ_C = 39.5 ppm).

	2a			**3a**		
Position	δ_C, mult.[a]	δ_H, mult. (*J* in Hz)	HMBC[b]	δ_C, mult.[a]	δ_H, mult. (*J* in Hz)	HMBC[b]
1	155.4, qC			157.1, qC		
2	113.9, CH	7.18 or 7.19, d (8.4)	1, 4, 13a	101.1, CH	6.59, d (2.1)	1, 3, 4, 13a
3	131.2, CH	7.76[c]	1, 4a	160.2, qC		
4	113.1, CH	8.37, dd (2.8, 8.5)	1, 2, 4a, 4b, 13a	103.7, CH	7.47, d (2.1)	2, 3, 4b, 13a
4a	132.4, qC			not observed		
4b	125.0, qC			115.9, qC		
5	129.8, CH	9.16 or 9.18, dd (1.5, 8.2)	4a, 7, 12c	147.3, qC		
6	123.2, CH	7.76[c]	4b, 5, 7a	116.1, CH	6.99, s	4b, 7, 7a, 18
7	127.6, CH	8.62 or 8.63, dd (1.4, 7.5)	5, 8	163.4, qC		
7a	125.6, qC			107.7, qC		
8	186.1, qC			not observed		
8a	112.5, qC			111.5, qC		
9	163.0, qC			161.3, qC		
10	110.2, CH	6.44, d (1.6)	8a, 9, 12, 14	109.8, CH	6.44, d (1.5)	8a, 9, 12, 14
11	156.9, qC			155.1, qC		
12	116.8, CH	8.61, d (1.5)	8a, 10, 12b, 14	116.7, CH	8.70, d (1.5)	8a, 10, 12b, 14
12a	not observed			not observed		
12b	103.3, qC			102.1, qC		
12c	130.0, qC			not observed		
13	not observed			not observed		
13a	115.2, qC			108.6, qC		
14	34.1, CH	1.87, m	10, 11, 12, 15, 16	41.5, CH	1.85, m	10, 11, 12, 15, 16
15	22.5, CH_3	0.53, d (6.9)	11, 14, 16	20.8, CH_3	0.65, d (6.9)	11, 14, 16
16	22.6, CH_3	0.48, d (6.9)	11, 14, 15	29.4, CH_2	0.99 and 1.02, m[d]	11, 14, 15, 17
17				11.5, CH_3	0.33, t (7.3)	14, 16
18				27.3, CH_3	3.04, s	4b, 5, 6
7-OH					14.49, s	6, 7, 7a
9-OH		14.39, s	8a, 9, 10		13.34, s	8a, 9, 10
1'	155.4, qC			157.1, qC		
2'	113.9, CH	7.18 or 7.19, d (8.4)	1', 4', 13a'	101.1, CH	6.59, d (2.1)	1', 3', 4', 13a'
3'	131.2, CH	7.76[c]	1', 4a'	160.2, qC		

Table S2. (Continued)

Position	2a			3a		
	δ_C, mult.[a]	δ_H, mult. (*J* in Hz)	HMBC[b]	δ_C, mult.[a]	δ_H, mult. (*J* in Hz)	HMBC[b]
4'	113.1, CH	8.37, dd (2.8, 8.5)	1', 2', 4a', 4b', 13a'	103.7, CH	7.47, d (2.1)	2', 3', 4b', 13a'
4a'	132.4, qC			not observed		
4b'	125.0, qC			115.9, qC		
5'	129.8, CH	9.16 or 9.18, dd (1.5, 8.2)	4a', 7', 12c'	147.3, qC		
6'	123.2, CH	7.76[c]	4b', 5', 7a'	116.1, CH	6.99, s	4b', 7', 7a', 18'
7'	127.6, CH	8.62 or 8.63, dd (1.4, 7.5)	5', 8'	163.4, qC		
7a'	125.6, qC			107.7, qC		
8'	186.1, qC			not observed		
8a'	112.5, qC			111.5, qC		
9'	163.0, qC			161.3, qC		
10'	110.8, CH	6.38, d (1.5)	8a', 9', 12', 14'	109.8, CH	6.44, d (1.5)	8a', 9', 12', 14'
11'	156.0, qC			155.1, qC		
12'	117.2, CH	8.53, d (1.5)	8a', 10', 12b', 14'	116.7, CH	8.70, d (1.5)	8a', 10', 12b', 14'
12a'	not observed			not observed		
12b'	103.3, qC			102.1, qC		
12c'	130.0, qC			not observed		
13'	not observed			not observed		
13a'	115.2, qC			108.6, qC		
14'	41.5, CH	1.53, m	10', 11', 12', 15', 16', 17'	41.5, CH	1.85, m	10', 11', 12', 15', 16'
15'	20.8, CH_3	0.39, d (6.9)	11', 14', 16'	20.8, CH_3	0.65, d (6.9)	11', 14', 16'
16'	29.3, CH_2	0.79 and 0.81, m[d]	11', 14', 15', 17'	29.4, CH_2	0.99 and 1.02, m[d]	11', 14', 15', 17'
17'	11.6, CH_3	0.19, t (7.4)	14', 16'	11.5, CH_3	0.33, t (7.3)	14', 16'
18'				27.3, CH_3	3.04, s	4b', 5', 6'
7-OH'					14.49, s	6', 7', 7a'
9-OH'		14.39, s	8a', 9', 10'		13.34, s	8a', 9', 10'

[a] δ_C values determined from HSQC and HMBC spectra.

[b] HMBC correlations are from proton(s) stated to the indicated carbon.

[c] Overlapped signals.

[d] δ_H values determined from HMBC spectra.

Determination of Constitutions by 2D NMR

Borolithochrome H1 (**2a**):

COSY and TOCSY data of **2a** showed the presence of three isolated spin systems in each of the two ligands (Figure S1), and HMBC and HSQC data indicated that these spin systems result from three benzene rings respectively (Figure S1, Table S2) accounting for twelve of the sixteen degrees of unsaturation of a single ligand. HMBC correlations also revealed a carbonyl signal at δ_C 186.8 ppm accounting for one additional degree of unsaturation. The remaining degrees of unsaturation were ascribed to two further rings and one double bond, suggesting a pentacyclic carbon skeleton for the ligands, which was identified as a benzo[*gh*]tetraphene based on the HMBC correlations and also confirmed by key NOESY correlations between H4 and H5 (H4' and H5') (Figure S1). The positions of the hydroxy groups at C9 and C9', hydrogen bonded to the adjacent carbonyl groups at C8 and C8', and the positions of the isopropyl and *sec*-butyl group at C11 and C11' respectively were determined by HMBC correlations.

Borolithochrome C1 (**3a**):

HMBC and HSQC data of **3a** were in agreement with a benzo[*gh*]tetraphene carbon skeleton for the ligands and HMBC correlations indicated the presence of hydroxy groups at C3, C3', C7, C7', C9, and C9', methyl groups at C5 and C5', and *sec*-butyl groups at C11 and C11' (Figure S1, Table S2).

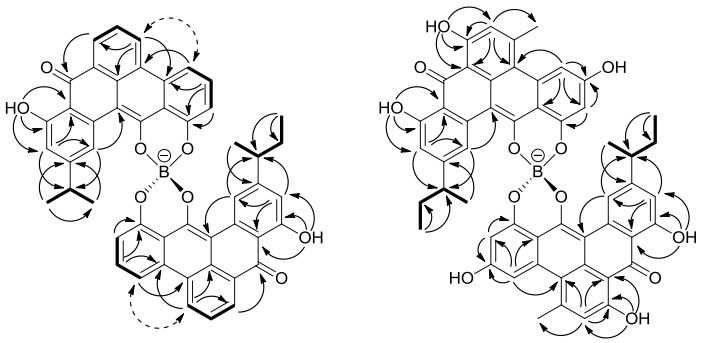


Figure S1. ^{1}H-^{1}H COSY (bold), key HMBC (H→C), and key NOESY (dashed arrows) correlations of borolithochrome H1 (**2a**) and C1 (**3a**).

COCON Simulations and Exclusion of Alternative Constitutions

Using the program COCON,[3] based on the molecular formula and experimental HMBC and COSY correlations, 234 theoretical constitutions were generated for the smaller ligand of **2a**. After discarding duplicates, non-sense proposals, and constitutions where two hydroxy groups cannot bind to a common boron atom due to geometrical restrictions, from the 234 constitutions 54 remained. After discarding constitutions where the ring containing the isopropyl group was generated as a five-membered ring, which would lead to unconventional aromatic chemical shifts, and discarding constitutions where no hydroxy proton can be hydrogen-bonded to the carbonyl group, from the 54 constitutions 7 remained. From these constitutions two constitutions containing a cyclooctatetraene ring were discarded, because the expected chemical shifts for the non-aromatic cyclooctatetraene ring would be not in agreement with the experimentally observed aromatic protons. Two further constitutions were discarded after structure minimization, one in which no complexation with boron was possible and the other with an unstable non-planar constitution. From the remaining three constitutions (Figure S2) one was discarded (left constitution), because for this constitution a strong HMBC correlation from the indicated aromatic proton to a hydroxy group-bearing carbon would be expected instead of the experimentally observed correlation to a quaternary carbon. Comparison of experimental ^{13}C chemical shifts of **2a** with those calculated by DFT for the two remaining constitutions (see below, Figure S3A, B) confirmed the proposed structure of **2a**.

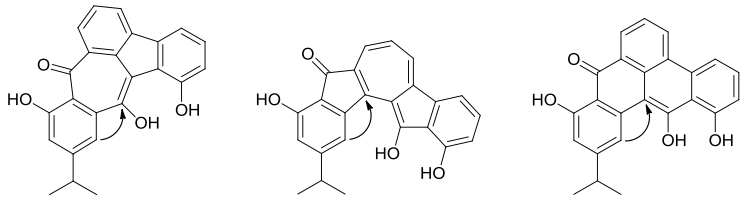


Figure S2. Exclusion of one (left constitution) of the remaining three theoretical constitutions for the smaller ligand of **2a** by comparison of expected HMBC (H→C) and experimentally observed correlations.

Density Functional Theory (DFT) Calculations

DFT calculations were performed with Gaussian09 on the B3LYP/6-31G(d) level of theory for the geometry optimization, chemical shift, and the CD calculations of rotatory strengths.[4] The shielding tensors for the calculation of the chemical shifts were calculated using the gauge-including atomic orbitals (GIAO) method.[5,6] In all calculations the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM) was used as solvent model with DMSO as solvent.

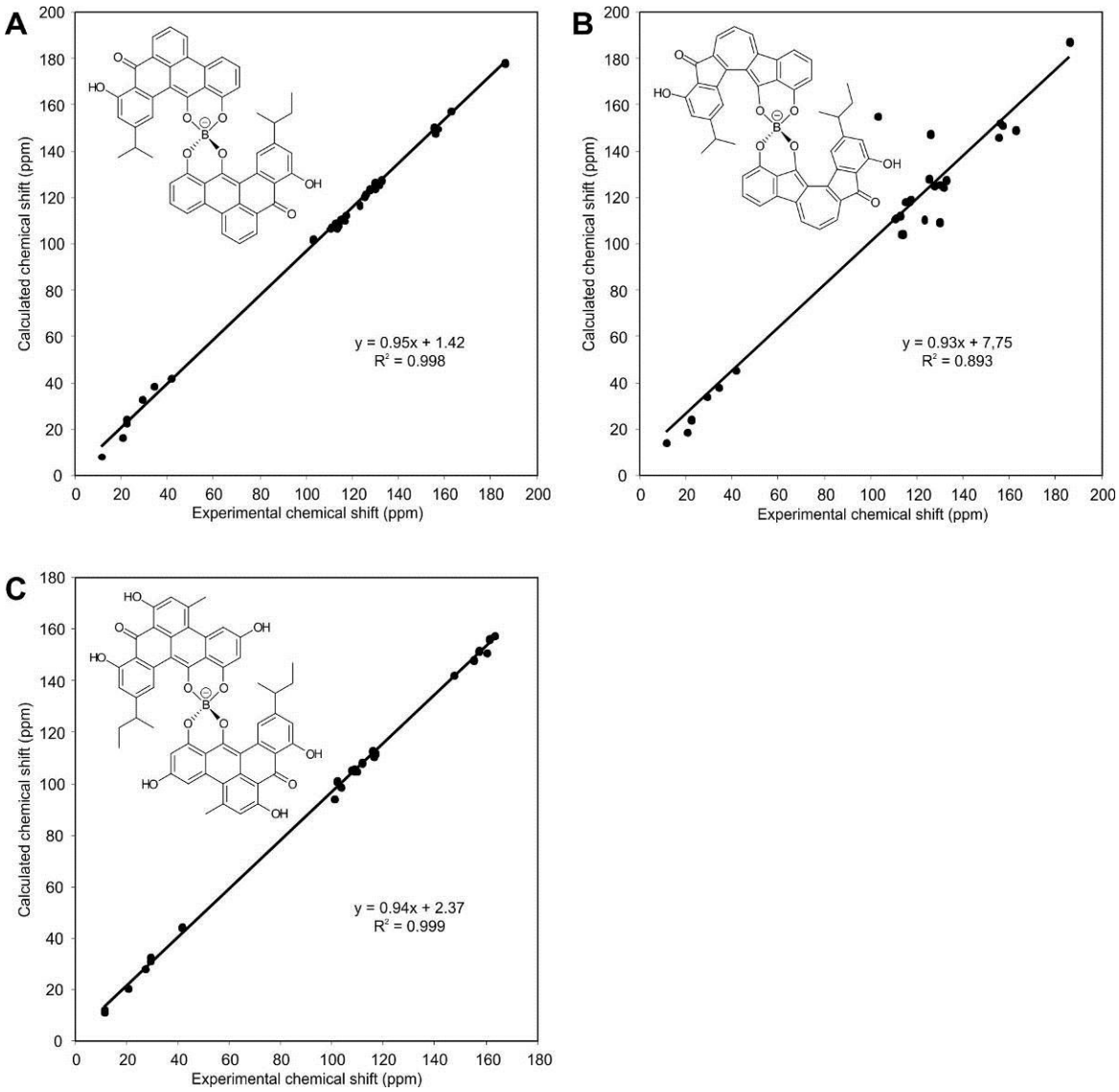


Figure S3. Comparison of experimental ^{13}C chemical shifts of **2a** and **3a** with those calculated by DFT. (A) Proposed structure of **2a**. (B) Constitutional alternative based on COCON calculations showing lower agreement with experimental data than **2a**. (C) Proposed structure of **3a**.

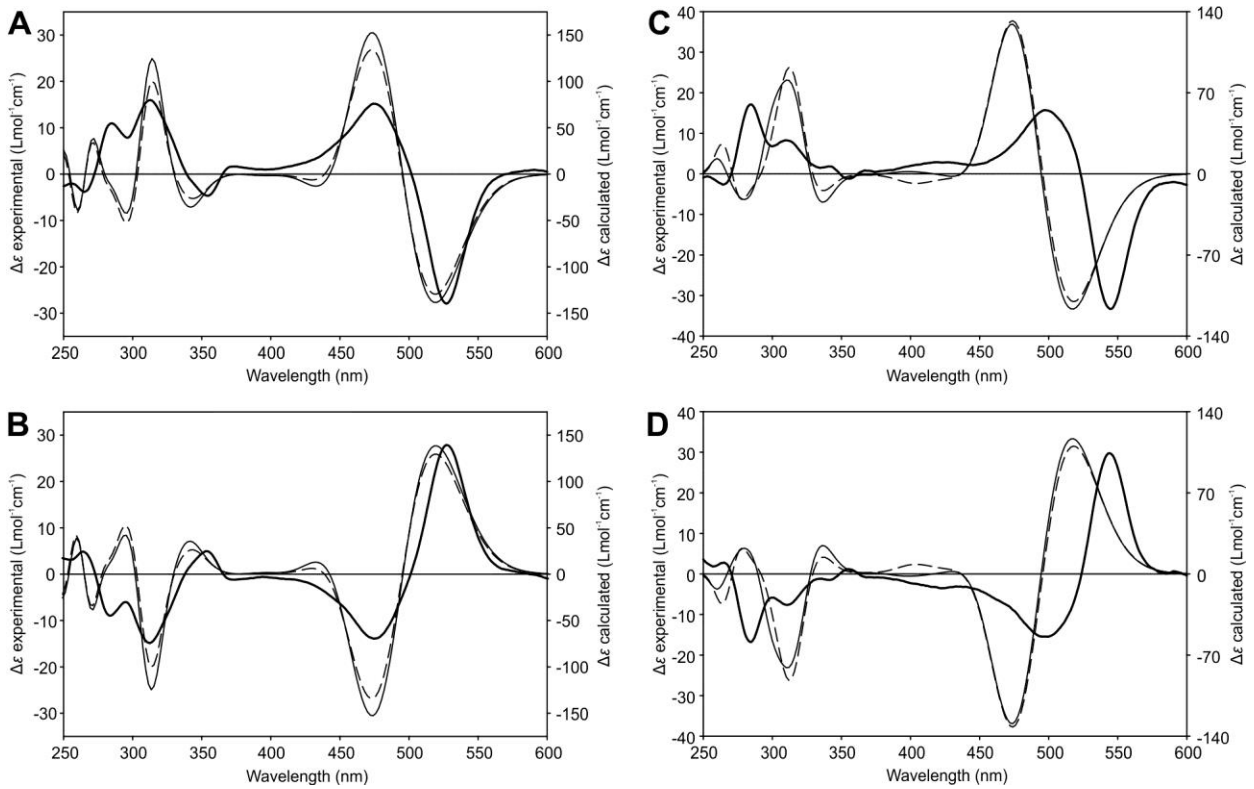


Figure S4. Assignment of axial chirality of the diastereomers borolithochrome H1 (**2a**) and borolithochrome H2 (**2b**) as well as the diastereomers borolithochrome C1 (**3a**) and borolithochrome C2 (**3b**) by comparison of experimental (bold solid lines) and calculated CD spectra. (A) Experimental CD spectrum of **2a** in DMSO and calculated CD spectra of the stereoisomers (*M*,14'*R*) (dashed line) and (*M*,14'*S*) (solid line). (B) Experimental CD spectrum of **2b** in DMSO and calculated CD spectra of the stereoisomers (*P*,14'*R*) (solid line) and (*P*,14'*S*) (dashed line). (C) Experimental CD spectrum of **3a** in DMSO and calculated CD spectra of the stereoisomers (*M*,14*R*,14'*R*) (solid line) and (*M*,14*S*,14'*S*) (dashed line). (D) Experimental spectrum of **3b** in DMSO and calculated CD spectra of the stereoisomers (*P*,14*R*,14'*R*) (dashed line) and (*P*,14*S*,14'*S*) (solid line).

Conformational and Configurational Analysis of *sec*-Butyl Group

The absolute configuration of the *sec*-butyl group was determined based on the determined absolute configuration of the borate. The strategy relies on the exceptional constitution of the borolithochromes with two large chromophores that are oriented perpendicular to each other with the *sec*-butyl groups situated just above the aromatic ring plane of the respective opposite ligand. The ring currents of the condensed aromatic system influence the chemical shifts of the two methyl groups of the *sec*-butyl group. Since, as shown below, these chemical shifts depend on the relative configuration of the borate and the *sec*-butyl group, they were calculated by DFT methods and used for the determination of the relative configuration and hence the absolute configuration of the *sec*-butyl groups. It is important to note that due to the similarity of the compounds and the distance of the *sec*-butyl group from the rest of the molecule, the conformational analysis of **2a/2b** and **3a/3b** is applicable for the *sec*-butyl groups of all borolithochromes. Since in the symmetric compounds **3a**/**3b** both ligands are identical, only the denotation for one of the ligands is used in the following discussion.

In order to accurately calculate the influence of the ring currents on the chemical shifts of the two methyl groups of the *sec*-butyl group, it was necessary to conduct a conformational analysis of the *sec*-butyl group. There are two rotatable bonds that define the conformation of the *sec*-butyl group, the bond C11' to C14' and the bond C14' to C16' (Figure S5). The torsion angle of the former bond (χ_1) was measured between H14' and C10' in order to make the torsion angle independent of the configuration of C14'. From first principles, χ_1 can adopt values of 0 (conformer a1) and 180° (conformer a2). It is expected that the populations of both conformers a1 and a2 are equal within a range of ± 10% due to the similarity of the ligands of C11'. In order to test this assumption, we evaluated the HMBC cross peaks of **2a** and **3a** between H14' and C12' and between H14' and C10'. Indeed, in agreement with an expected ratio of close to 1:1 populations for conformations a1 and a2, both HMBC cross peaks are of similar size, with a slightly larger cross peak between H14' and C12' than between H14' and C10' in the spectrum of **2a** (Figure S6A) and cross peaks of almost the same size in the spectrum of **3a** (Figure S6B). For further evaluation of the populations, a rotating-frame Overhauser effect spectroscopy (ROESY) spectrum was recorded for the symmetric compound **3b**. In the ROESY spectrum the cross peak between H14' and H10' has a larger integral than the cross peak between H14' and H12' (Figure

S6C). We measured the integral from the peak where the chemical shift of H14' has evolved during t_1 in order to make the ratio of the cross peaks independent of T_1 relaxation during the waiting time between scans in the ROESY. The ratio of integrals was determined as 1.4. The used pulse sequence employed a spin lock field $\gamma B_1/2\pi$ = 2756 Hz, the center of the spectrum was at 4.7 ppm. The scaling factor assuming small NOE contribution is dominated by the ROE which is scaled by: $(\gamma B_1)^2/((\gamma B_1)^2 + \Omega^2)$.[7] Compensating for this offset effect with the chemical shifts of 6.5 and 8.7 ppm for H10' and H12', respectively, the corrected ratio of the cross peaks was determined as 0.77, indicating that $\chi_1 = 0°$ (conformer a1) has a population of 44% and $\chi_1 = 180°$ (conformer a2) of 56%. Considering the low signal to noise ratio of the spectrum, the results obtained from the ROESY measurement are also in agreement with approximately equal populations (± 10%) for conformations a1 and a2.

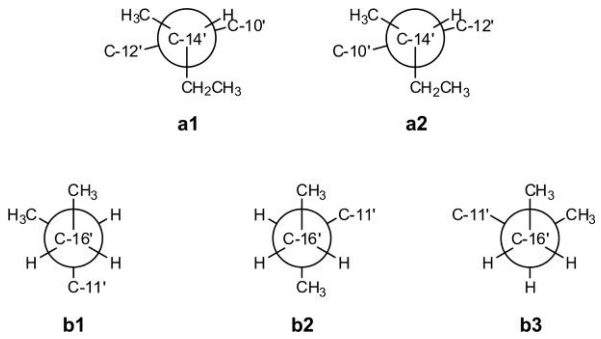


Figure S5. Newman projections for possible *sec*-butyl group conformations [(*S*)-configuration]; a1 and a2: conformations along the C11' to C14' bond; b1 to b3: conformations along the C14' to C16' bond.

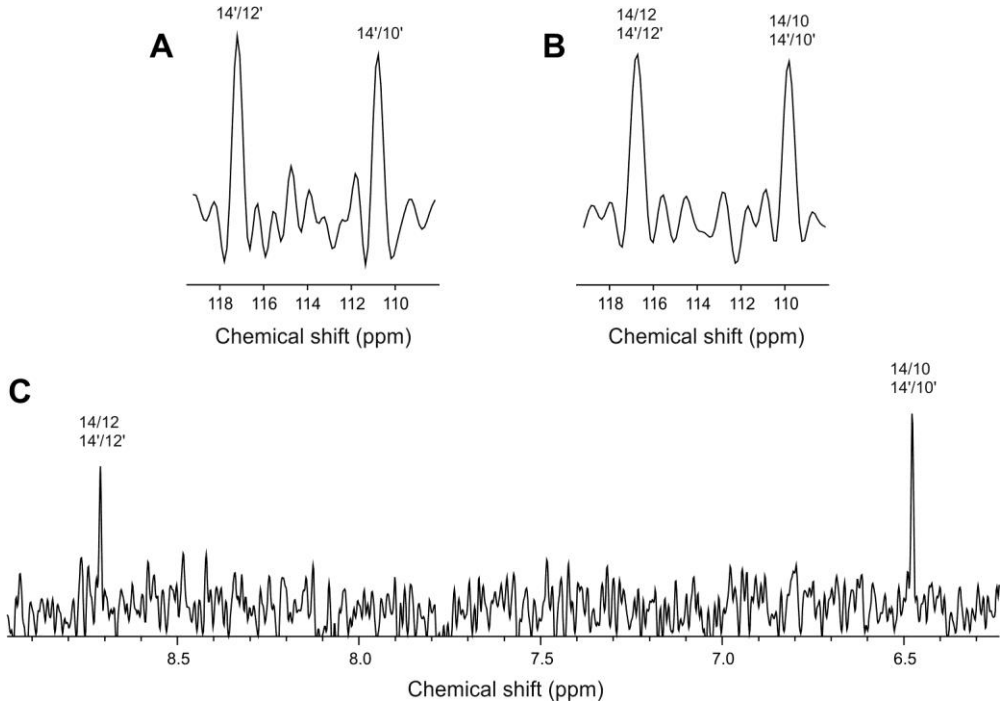


Figure S6. (A) HMBC trace of borolithochrome H1 (**2a**) showing the cross peaks between H14' and C12' and between H14' and C10'. (B) HMBC trace of borolithochrome C1 (**3a**) showing the cross peaks between H14' and C12' and between H14' and C10'. (C) ROESY trace of borolithochrome C2 (**3b**) showing the cross peaks between H14' and H12' and between H14' and H10'. Both HMBC and corrected ROESY peak ratios are in agreement with an expected ratio of close to 1:1 populations for conformations a1 and a2.

The second rotatable bond C14' to C16' can assume the three staggered conformations due to the torsional (Pitzer) strain. According to Cahn-Ingold-Prelog priorities this torsion angle (χ_2) was measured between C11' and C17'. The signs of the angles depend on the choice of the configuration for C14'. In principle this is arbitrary and we choose the (*S*)-configuration for the discussion. In the ^{1}H NMR spectrum of **3b**, showing clearly distinguished deshielded and shielded signals for the diastereotopic protons at C16', the H14' signal is close to a sextet, however, the couplings are not entirely identical as can be seen from the COSY and TOCSY correlations between H14' and the H16' deshielded and shielded protons with a stronger deshielded cross peak (larger coupling) (Figure S21, Figure S22). Since all other couplings to the two methylene protons are identical, this interpretation is justified. The coupling between H14' and the H16' deshielded proton is about 8.5 Hz (± 0.3 Hz) and the coupling between H14' and the

H16'-shielded proton is about 7 Hz (± 0.3 Hz). In the HMBC spectra of **2a** and **3a**, the shielded proton at C16' shows a stronger cross peak to C11' than the deshielded proton, in accordance with the conformation b2 as the highest populated. With a coupling of 13.6 Hz for *trans* and 2.6 Hz for *gauche*,[8–10] the populations of the conformers b2, b1, and b3 are determined as 54%, 40%, and 6%, respectively.

Based on this conformational analysis, the populations of the six possible conformations were calculated by multiplication of the population distributions of χ_1 and χ_2. For determination of the configurations of **2a**/**2b** and **3a**/**3b** then population-weighted average chemical shift differences of the *sec*-butyl group were calculated as detailed below. Chemical shift differences were used rather than absolute chemical shifts in order to average out systematic errors from the DFT calculation. The resulting chemical shift differences are predominantly determined by the population distribution of χ_1 and thus any population distribution of χ_2 would not change the configurational results for **2a**/**2b** and **3a**/**3b**.

*Configurational analysis of **2a**/**2b***

In order to assign the absolute configuration of C14', the observed experimental chemical shift differences between the methyl protons H15' and H17' in **2a** and **2b** (Table S3):

$$\Delta\delta^{exp} = (\delta_H\ 15' - \delta_H\ 17';\ \mathbf{2b}) - (\delta_H\ 15' - \delta_H\ 17';\ \mathbf{2a})$$

were compared with the corresponding population-weighted average chemical shift differences that were calculated by DFT for the configurations (*M*,14'*S*) and (*P*,14'*S*) (Tables S4 and S5):

$$\Delta\delta^{calc} = (\delta_H\ 15' - \delta_H\ 17';\ P,14'S) - (\delta_H\ 15' - \delta_H\ 17';\ M,14'S)$$

Since the configuration of the chiral axis of **2a** and **2b** was determined by CD spectroscopy as (*M*) and (*P*), respectively, and because the difference (δ_H 15' – δ_H 17') is identical for the enantiomers (*P*,14'*S*) and (*M*,14'*R*) [analogous (*M*,14'*S*) and (*P*,14'*R*)], $\Delta\delta^{calc}$ will have the same sign as $\Delta\delta^{exp}$ when C14' has the (*S*)-configuration, whereas $\Delta\delta^{calc}$ will have the opposite sign as $\Delta\delta^{exp}$ when C14' has the (*R*)-configuration. Because $\Delta\delta^{exp}$ = 0.18 ppm and $\Delta\delta^{calc}$ adopt values in

the range between 0.17 to 0.41 ppm for populations of χ_1 = 0° from 40 to 60%, the absolute configuration of C14' is assigned as (*S*).

*Configurational analysis of **3a**/**3b***

In order to assign the absolute configuration of C14', the observed experimental chemical shift differences between the methyl protons H15' and H17' in **3a** and **3b** (Table S3):

$$\Delta\delta^{exp} = (\delta_H\ 15' - \delta_H\ 17';\ \mathbf{3b}) - (\delta_H\ 15' - \delta_H\ 17';\ \mathbf{3a})$$

were compared with the corresponding population-weighted average chemical shift differences that were calculated by DFT for the configurations (*M*,14*S*,14'*S*) and (*P*,14*S*,14'*S*) (Tables S6 and S7):

$$\Delta\delta^{calc} = (\delta_H\ 15' - \delta_H\ 17';\ P,14S,14'S) - (\delta_H\ 15' - \delta_H\ 17';\ M,14S,14'S)$$

Since the configuration of the chiral axis of **3a** and **3b** was determined by CD spectroscopy as (*M*) and (*P*), respectively, and because the difference (δ_H 15' – δ_H 17') is identical for the enantiomers (*P*,14*S*,14'*S*) and (*M*,14*R*,14'*R*) [analogous (*M*,14*S*,14'*S*) and (*P*,14*R*,14'*R*)], $\Delta\delta^{calc}$ will have the same sign as $\Delta\delta^{exp}$ when C14' has the (*S*)-configuration, whereas $\Delta\delta^{calc}$ will have the opposite sign as $\Delta\delta^{exp}$ when C14' has the (*R*)-configuration. Because $\Delta\delta^{exp}$ = 0.06 ppm and $\Delta\delta^{calc}$ adopt values in the range between –0.08 to 0.28 ppm for populations of χ_1 = 0° from 40 to 60%, the absolute configuration of C14' is assigned as (*S*). The fraction of the range that suggests the opposite configuration is only 22%. It should also be noted that the experimental difference $\Delta\delta^{exp}$ of **3a**/**3b** is only 1/3 of $\Delta\delta^{exp}$ of **2a**/**2b**.

Table S3. Chemical shifts of *sec*-butyl group methyl protons showing characteristic differences in dependence of the configuration of the borate.

Compound	Configuration of borate	δ_H 15' (ppm)[a]	δ_H 17' (ppm)[a]	δ_H 15' – δ_H 17' (ppm)
2a	(*M*)	0.39	0.19	0.20
2b	(*P*)	0.69	0.31	0.38
3a	(*M*)	0.65	0.33	0.32
3b	(*P*)	0.69	0.31	0.38
5a	(*M*)	0.65	0.33	0.32
5b	(*P*)	0.64	0.25	0.39
7	(*M*)	0.48	0.23	0.25
8	(*P*)	0.57	0.15	0.42
9a	(*M*)	0.39	0.19	0.20
9b	(*P*)	0.50	0.13	0.37

[a]Compiled data from Tables S1 and S2.

Table S4. Chemical shift differences of *sec*-butyl group conformers for (*M*,14'*S*)-**2a** calculated by DFT.

Conformer	Population[a]	δ_H 15' (ppm)	δ_H 17' (ppm)	δ_H 15' – δ_H 17' (ppm)
a1, b1	0.20	0.44	0.72	–0.28
a2, b1	0.20	1.12	0.39	0.73
a1, b2	0.27	0.44	0.79	–0.35
a2, b2	0.27	1.15	0.39	0.76
a1, b3	0.03	0.75	0.74	0.01
a2, b3	0.03	1.27	0.75	0.52
Average		0.80[b]	0.59[b]	0.22[b]

[a]Populations of conformations were calculated by multiplication of the population distributions of χ1 (a1 and a2: both 50%) and χ2 (b2, b1, and b3: 54%, 40%, and 6%, respectively).

[b]Population-weighted average.

Table S5. Chemical shift differences of *sec*-butyl group conformers for (*P*,14'*S*)-**2b** calculated by DFT.

Conformer	Population[a]	δ_H 15' (ppm)	δ_H 17' (ppm)	δ_H 15' – δ_H 17' (ppm)
a1, b1	0.20	1.08	0.34	0.74
a2, b1	0.20	0.90	0.72	0.18
a1, b2	0.27	1.04	0.57	0.47
a2, b2	0.27	1.21	0.61	0.60
a1, b3	0.03	1.07	0.14	0.93
a2, b3	0.03	1.07	0.81	0.26
Average		1.07[b]	0.56[b]	0.51[b]

[a]Populations of conformations were calculated by multiplication of the population distributions of χ1 (a1 and a2: both 50%) and χ2 (b2, b1, and b3: 54%, 40%, and 6%, respectively).

[b]Population-weighted average.

Table S6. Chemical shift differences of *sec*-butyl group conformers for (*M*,14*S*,14'*S*)-**3a** calculated by DFT.

Conformer	Population[a]	δ_H 15' (ppm)	δ_H 17' (ppm)	δ_H 15' – δ_H 17' (ppm)
a1, b1	0.20	0.51	0.86	–0.35
a2, b1	0.20	1.29	0.65	0.64
a1, b2	0.27	0.57	0.82	–0.25
a2, b2	0.27	1.29	0.38	0.91
a1, b3	0.03	0.75	0.79	–0.04
a2, b3	0.03	1.37	0.81	0.56
Average		0.93[b]	0.67[b]	0.25[b]

[a]Populations of conformations were calculated by multiplication of the population distributions of χ1 (a1 and a2: both 50%) and χ2 (b2, b1, and b3: 54%, 40%, and 6%, respectively).

[b]Population-weighted average.

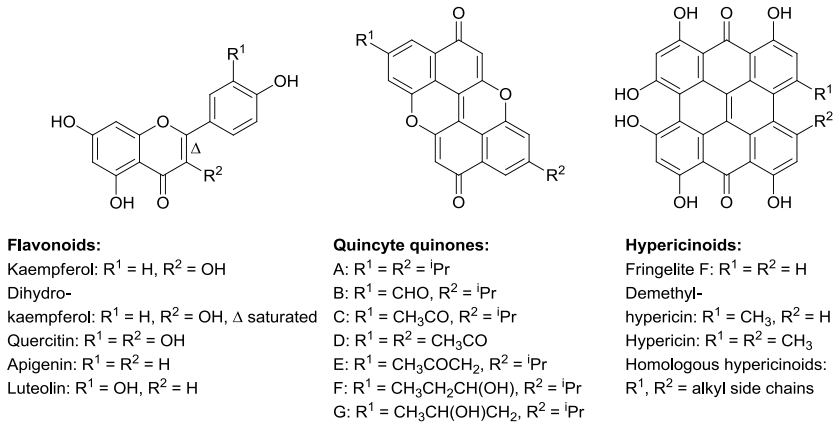
Table S7. Chemical shift differences of *sec*-butyl group conformers for (*P*,14*S*,14'*S*)-**3b** calculated by DFT.

Conformer	Population[a]	δ_H 15' (ppm)	δ_H 17' (ppm)	δ_H 15' – δ_H 17' (ppm)
a1, b1	0.20	1.16	0.52	0.64
a2, b1	0.20	0.84	1.00	–0.16
a1, b2	0.27	1.18	0.43	0.75
a2, b2	0.27	0.83	0.75	0.08
a1, b3	0.03	1.07	0.14	0.93
a2, b3	0.03	1.14	0.94	0.20
Average		1.01[b]	0.65[b]	0.35[b]

[a]Populations of conformations were calculated by multiplication of the population distributions of χ1 (a1 and a2: both 50%) and χ2 (b2, b1, and b3: 54%, 40%, and 6%, respectively).

[b]Population-weighted average.

Supporting Figures S7–S9

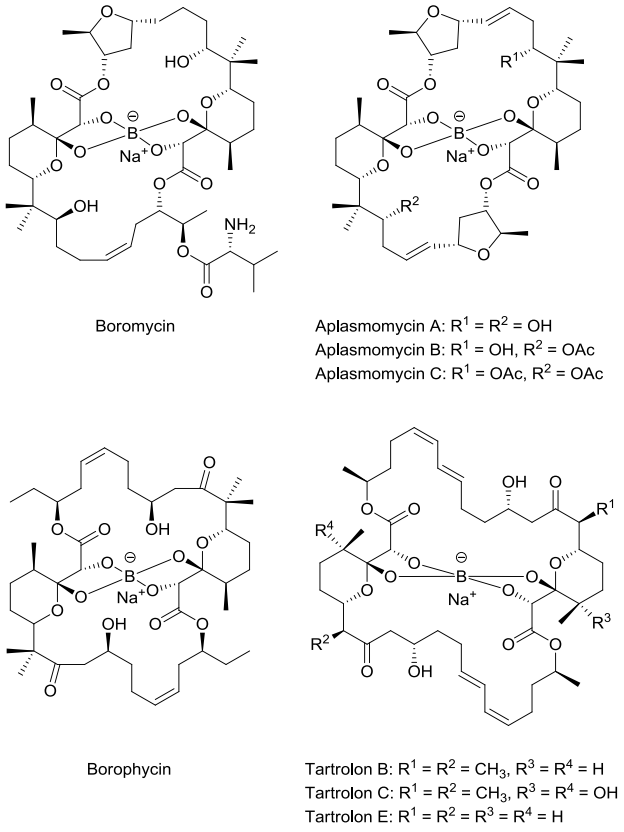


Flavonoids:
Kaempferol: R^1 = H, R^2 = OH
Dihydro-
kaempferol: R^1 = H, R^2 = OH, Δ saturated
Quercitin: R^1 = R^2 = OH
Apigenin: R^1 = R^2 = H
Luteolin: R^1 = OH, R^2 = H

Quincyte quinones:
A: R^1 = R^2 = ^{i}Pr
B: R^1 = CHO, R^2 = ^{i}Pr
C: R^1 = CH_3CO, R^2 = ^{i}Pr
D: R^1 = R^2 = CH_3CO
E: R^1 = CH_3COCH_2, R^2 = ^{i}Pr
F: R^1 = $CH_3CH_2CH(OH)$, R^2 = ^{i}Pr
G: R^1 = $CH_3CH(OH)CH_2$, R^2 = ^{i}Pr

Hypericinoids:
Fringelite F: R^1 = R^2 = H
Demethyl-
hypericin: R^1 = CH_3, R^2 = H
Hypericin: R^1 = R^2 = CH_3
Homologous hypericinoids:
R^1, R^2 = alkyl side chains

Figure S7. Chemical structures of previously known classes of fossil polyketides.



Boromycin

Aplasmomycin A: R^1 = R^2 = OH
Aplasmomycin B: R^1 = OH, R^2 = OAc
Aplasmomycin C: R^1 = OAc, R^2 = OAc

Borophycin

Tartrolon B: R^1 = R^2 = CH_3, R^3 = R^4 = H
Tartrolon C: R^1 = R^2 = CH_3, R^3 = R^4 = OH
Tartrolon E: R^1 = R^2 = R^3 = R^4 = H

Figure S8. Chemical structures of previously known boronated polyketides.

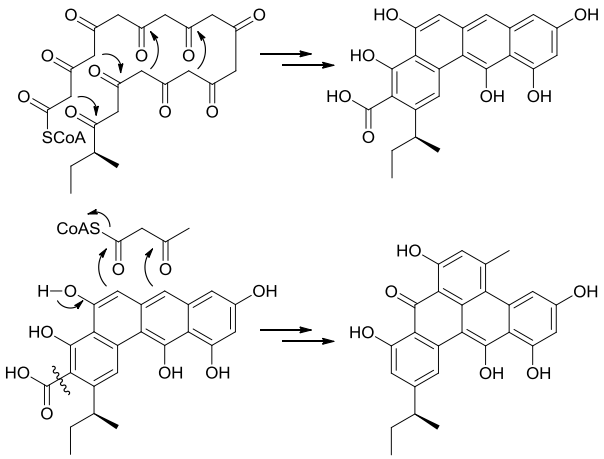


Figure S9. Proposed pathway for the biosynthesis of the ligand of borolithochrome C inferred from the pathway proposed for clostrubin A, with a (*S*)-2-methylbutyryl-coenzyme A starter unit in borolithochrome C instead of the conventional acetate starter unit in clostrubin A.

References

(1) Wolkenstein, K.; Gross, J. H.; Falk, H. *Proc. Natl. Acad. Sci. U. S. A.* **2010**, *107*, 19374.

(2) Fischer, M.; Georges, J. *Chem. Phys. Lett.* **1996**, *260*, 115.

(3) Lindel, T.; Junker, J.; Köck, M. *Eur. J. Org. Chem.* **1999**, 573.

(4) 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.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09 Revision A.1*., Gaussian Inc, Wallingford, CT, **2009**.

(5) Wolinski, K.; Hinton, J. F.; Pulay, P. *J. Am. Chem. Soc.* **1990**, *112*, 8251.

(6) Häser, M.; Ahlrichs, R.; Baron, H. P.; Weis, P.; Horn, H. *Theor. Chim. Acta* **1992**, *83*, 455.

(7) Griesinger, C.; Ernst, R. R. *J. Magn. Reson.* **1987**, *75*, 261.

(8) Bystrov, V. F. *Prog. Nucl. Magn. Reson. Spectrosc.* **1976**, *10*, 41.

(9) Pachler, K. G. R. *Spectrochim. Acta* **1963**, *19*, 2085.

(10) Pachler, K. G. R. *Spectrochim. Acta* **1964**, *20*, 581.

Appendix 1: NMR Spectra

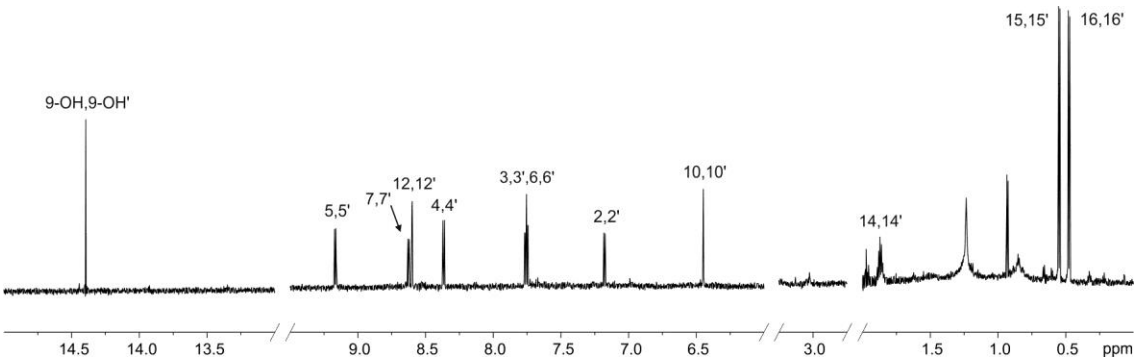


Figure S10. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome G (**1**).

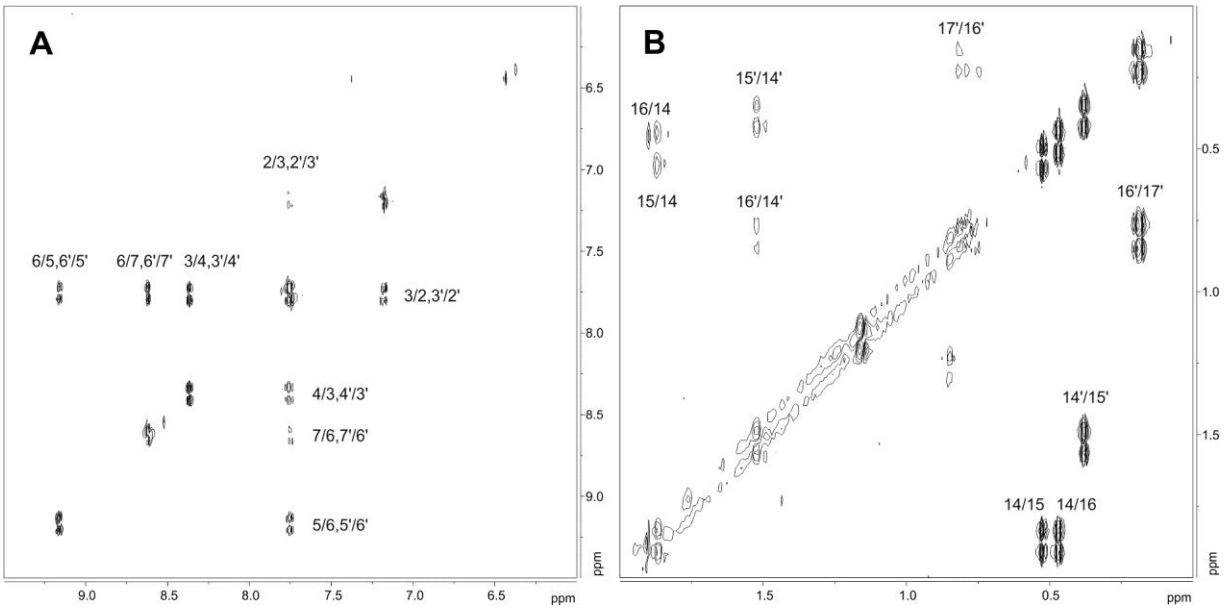


Figure S11. COSY spectrum (700 MHz, DMSO-d_6) of borolithochrome H1 (**2a**). (A) Aromatic area. (B) Aliphatic area.

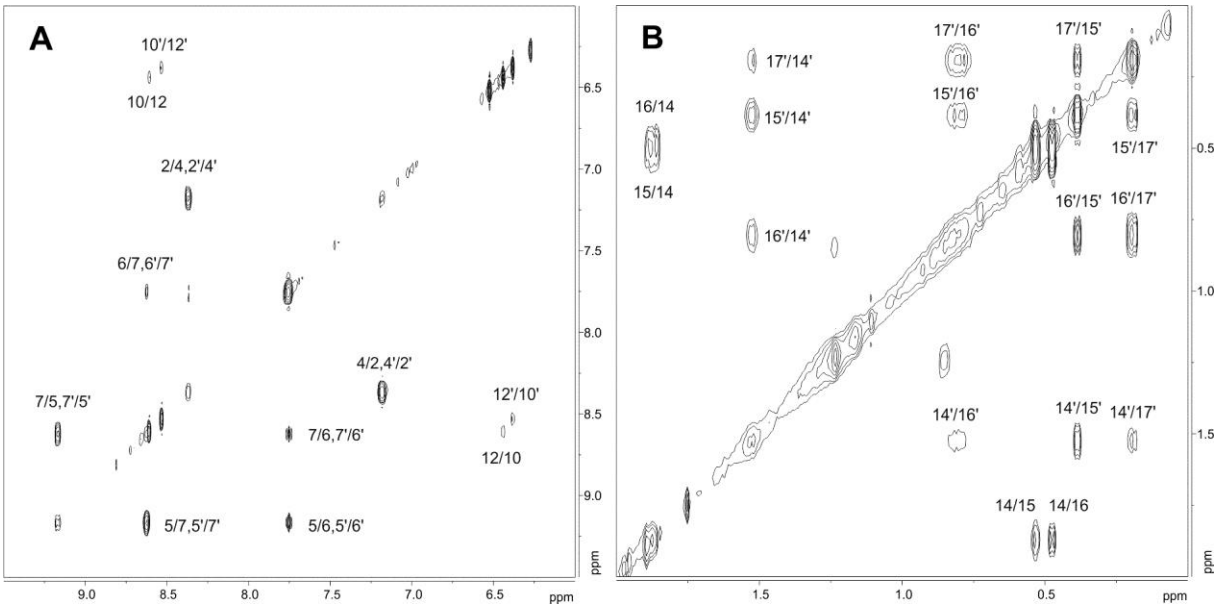


Figure S12. TOCSY spectrum (700 MHz, DMSO-d_6) of borolithochrome H1 (**2a**). (A) Aromatic area. (B) Aliphatic area.

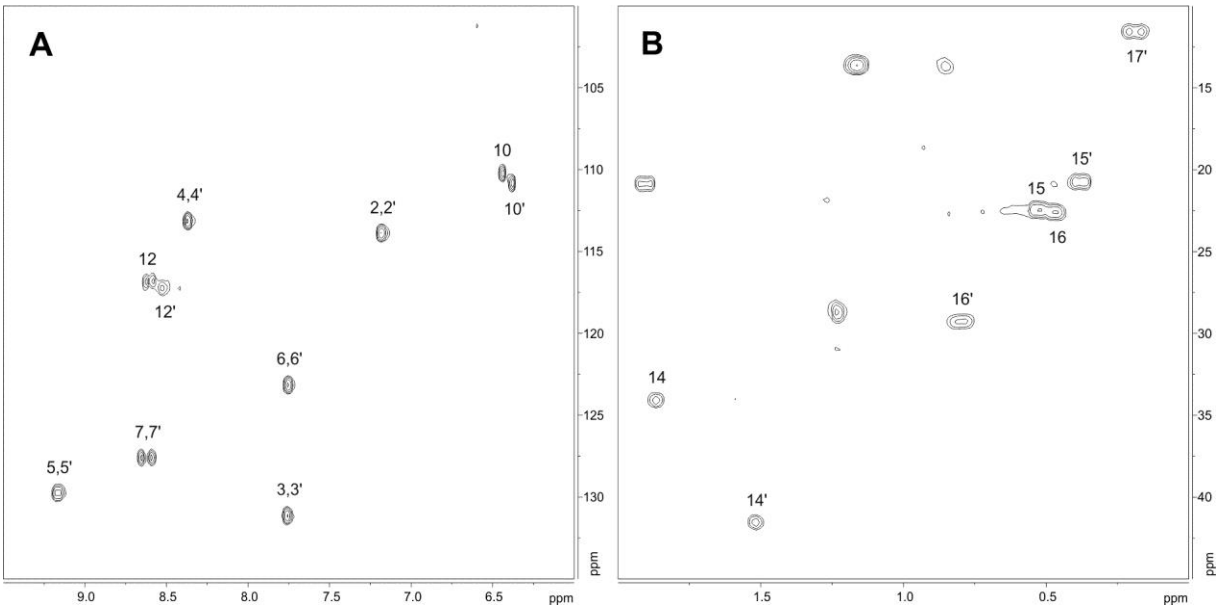


Figure S13. HSQC spectrum (800 MHz, DMSO-d_6) of borolithochrome H1 (**2a**). (A) Aromatic area. (B) Aliphatic area.

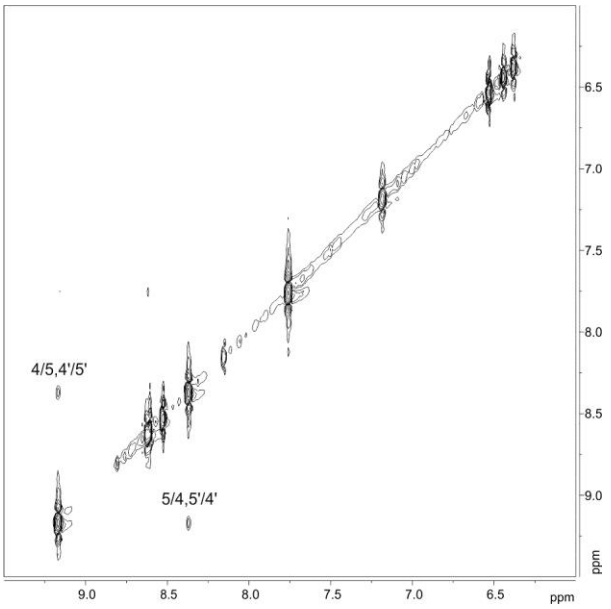


Figure S14. NOESY spectrum (aromatic area) (800 MHz, DMSO-d_6) of borolithochrome H1 (**2a**).

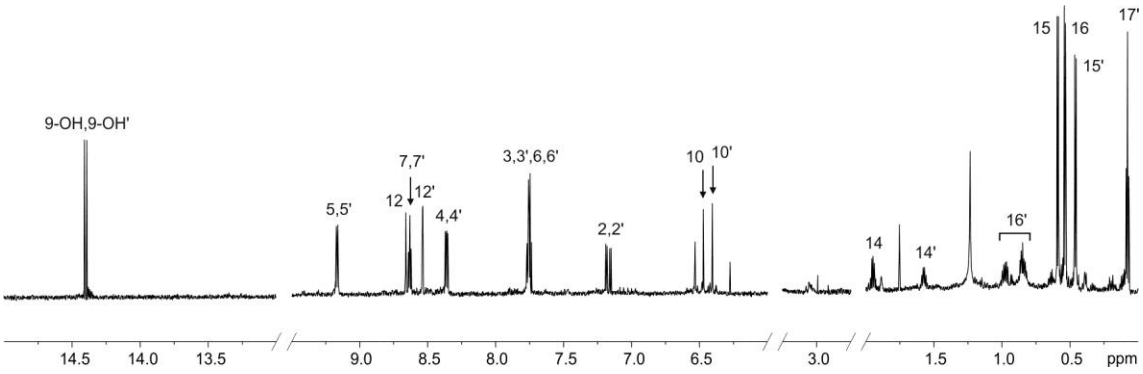


Figure S15. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome H2 (**2b**).

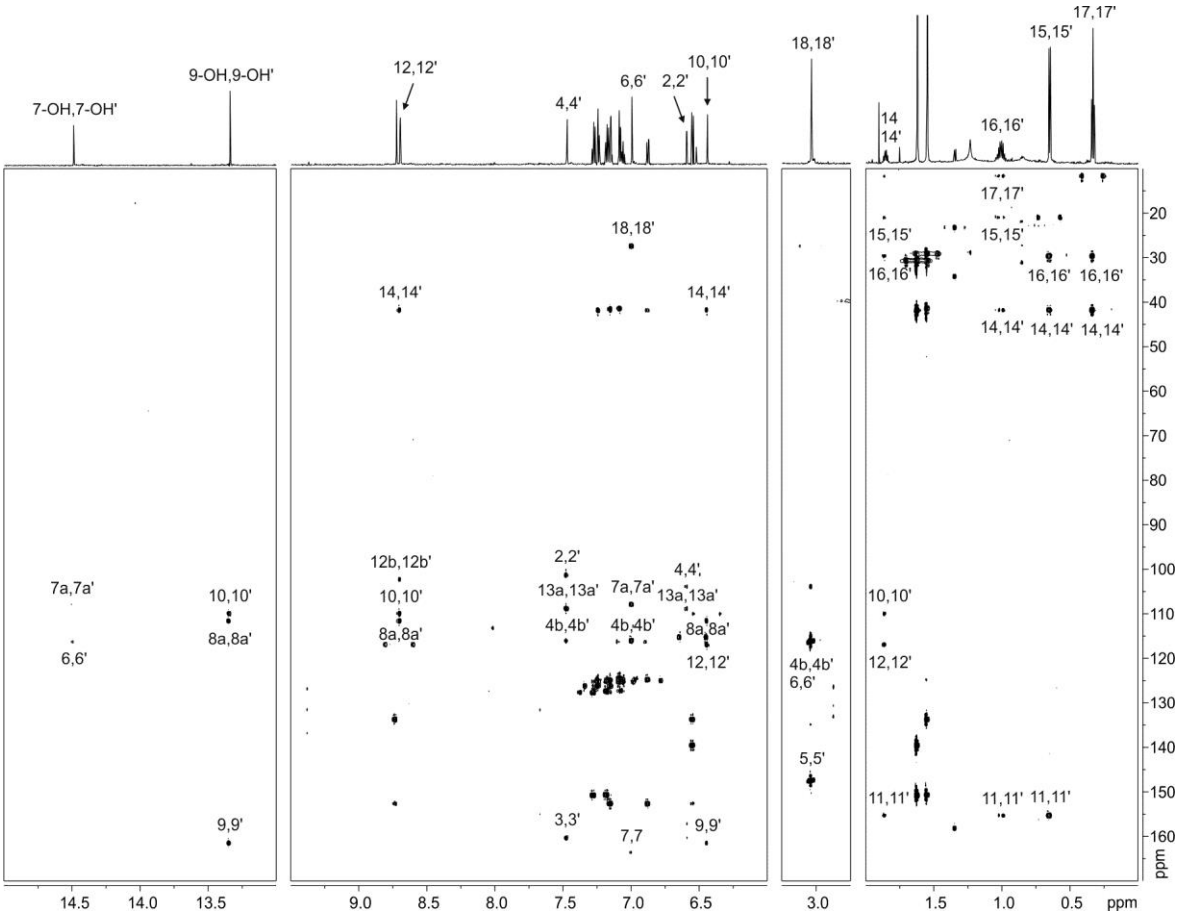


Figure S16. ^{1}H NMR spectrum (upper) and HMBC spectrum (lower) (800 MHz, DMSO-d_6) of borolithochrome C1 (**3a**).

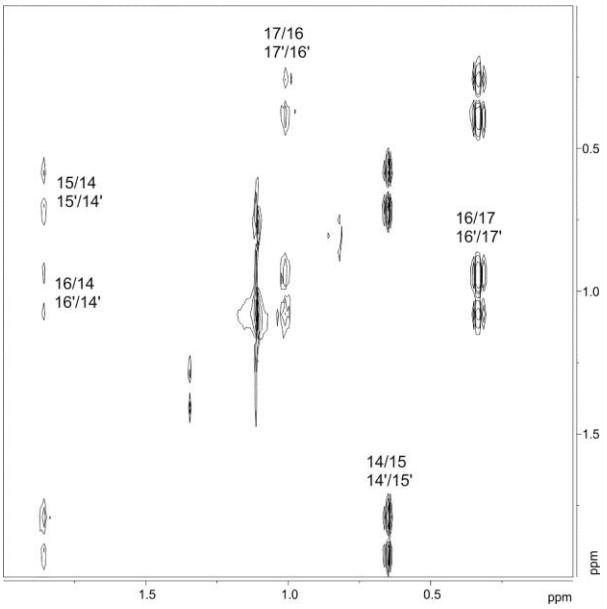


Figure S17. COSY spectrum (aliphatic area) (700 MHz, DMSO-d_6) of borolithochrome C1 (**3a**).

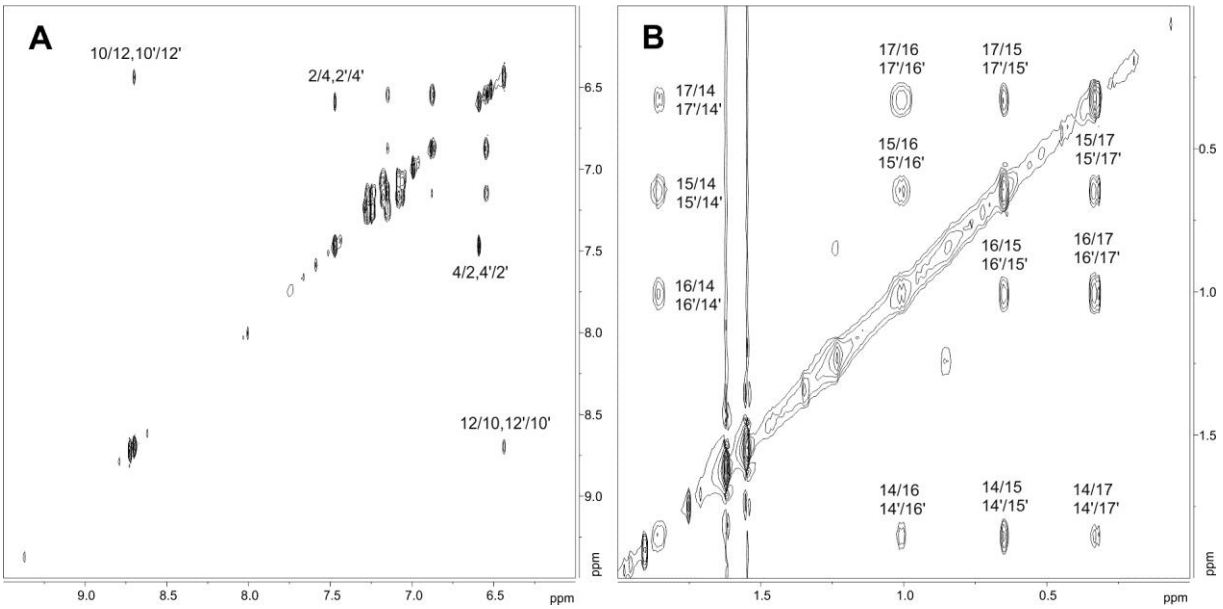


Figure S18. TOCSY spectrum (700 MHz, DMSO-d_6) of borolithochrome C1 (**3a**). (A) Aromatic area. (B) Aliphatic area.

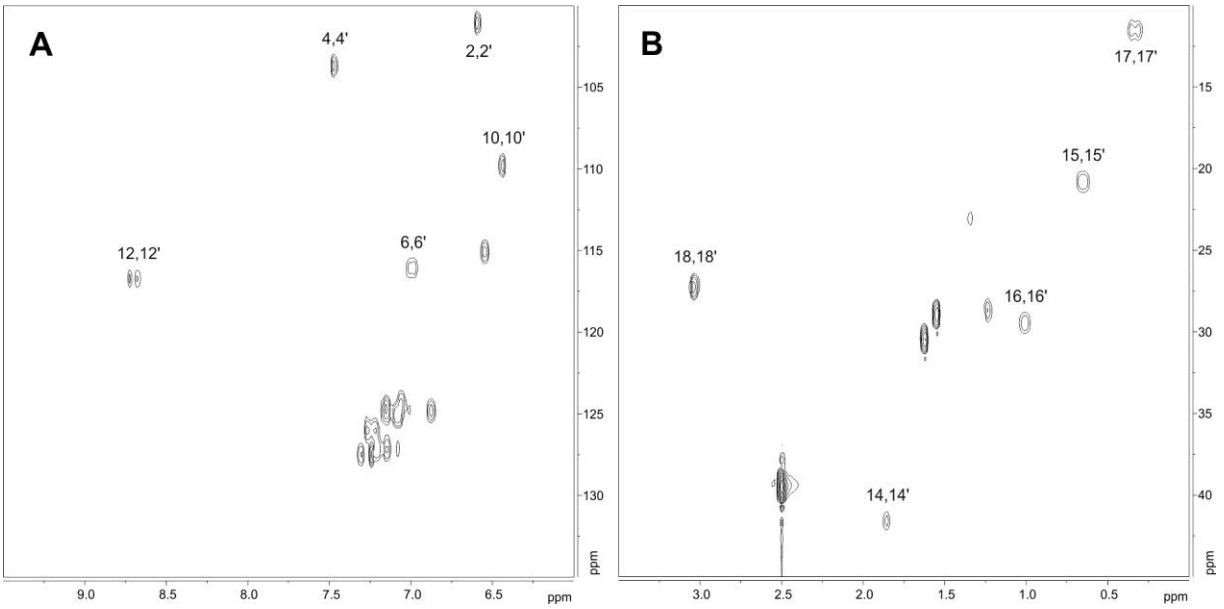


Figure S19. HSQC spectrum (800 MHz, DMSO-d_6) of borolithochrome C1 (**3a**). (A) Aromatic area. (B) Aliphatic area.

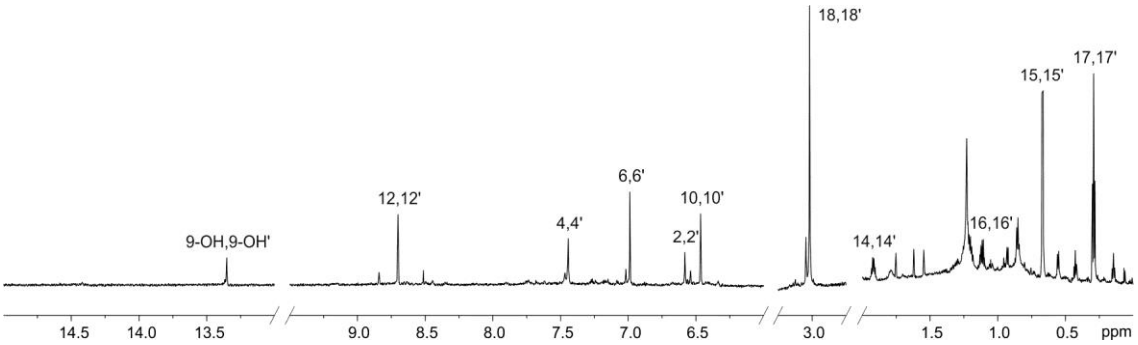


Figure S20. ^{1}H NMR spectrum (800 MHz, DMSO-d_6) of borolithochrome H2 (**3b**).

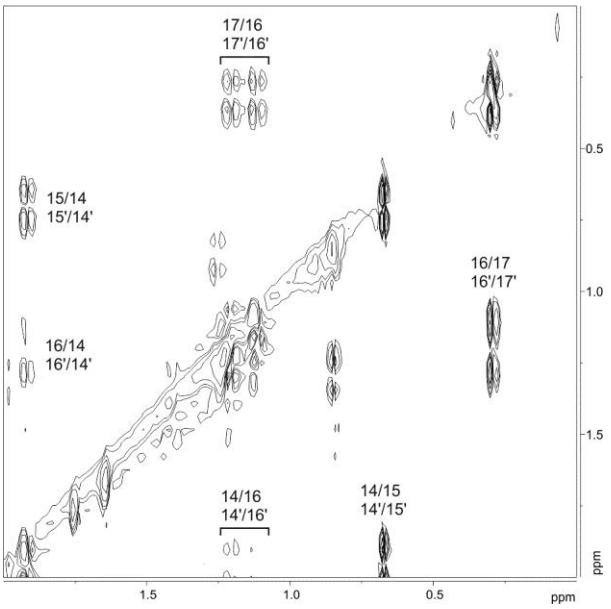


Figure S21. COSY spectrum (aliphatic area) (800 MHz, DMSO-d_6) of borolithochrome C2 (**3b**).

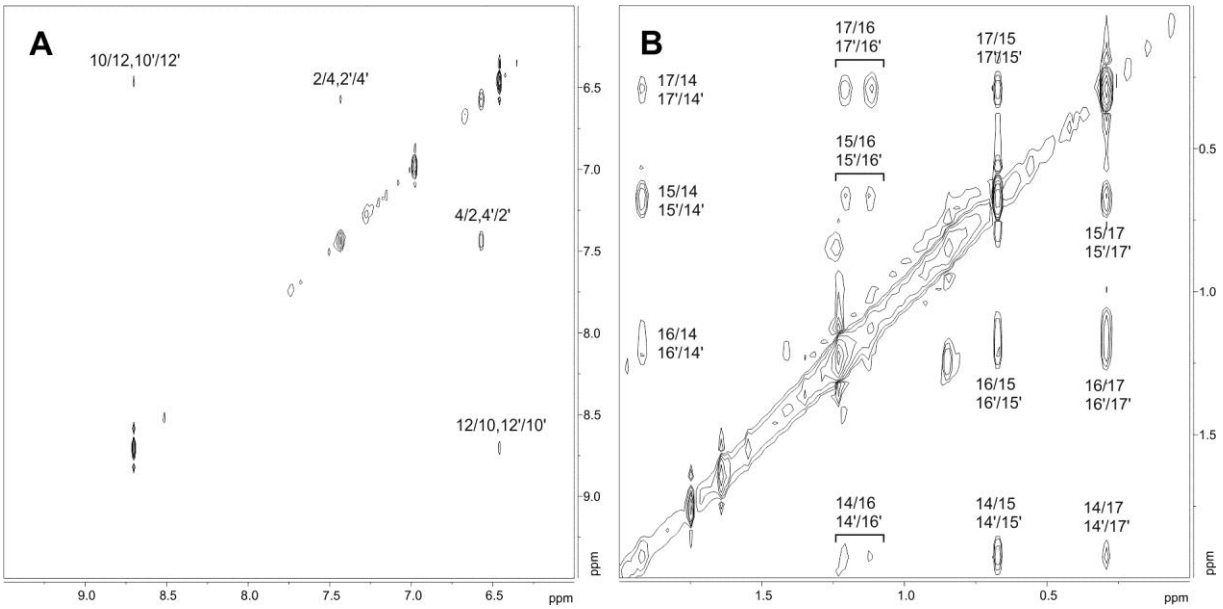


Figure S22. TOCSY spectrum (800 MHz, DMSO-d_6) of borolithochrome C2 (**3b**). (A) Aromatic area. (B) Aliphatic area.

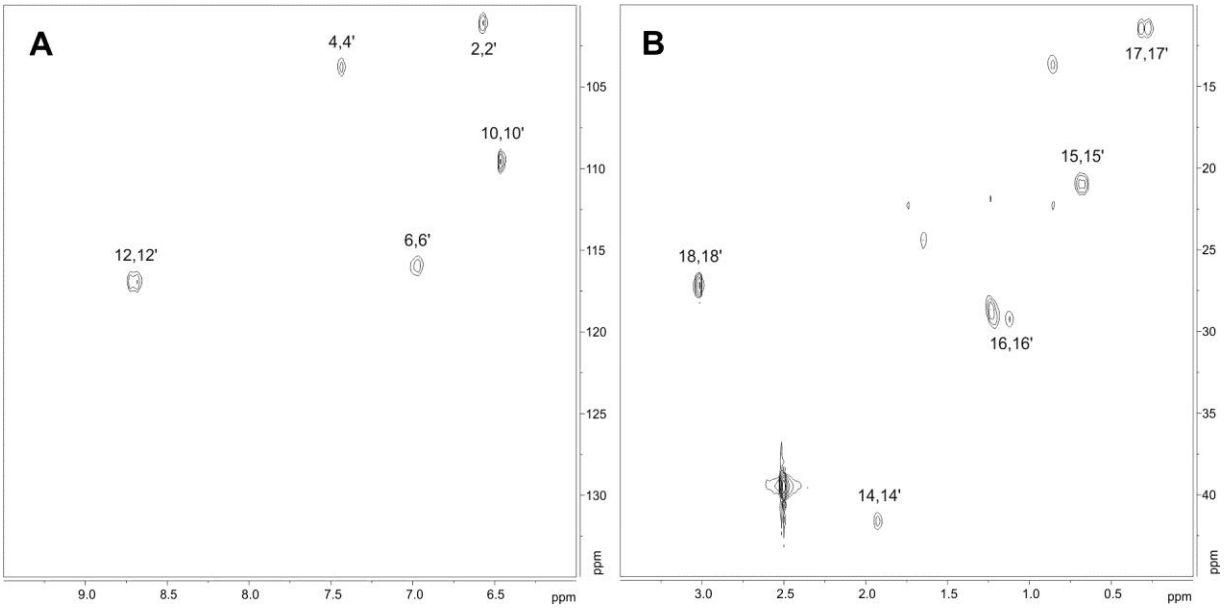


Figure S23. HSQC spectrum (800 MHz, DMSO-d_6) of borolithochrome C2 (**3b**). (A) Aromatic area. (B) Aliphatic area.

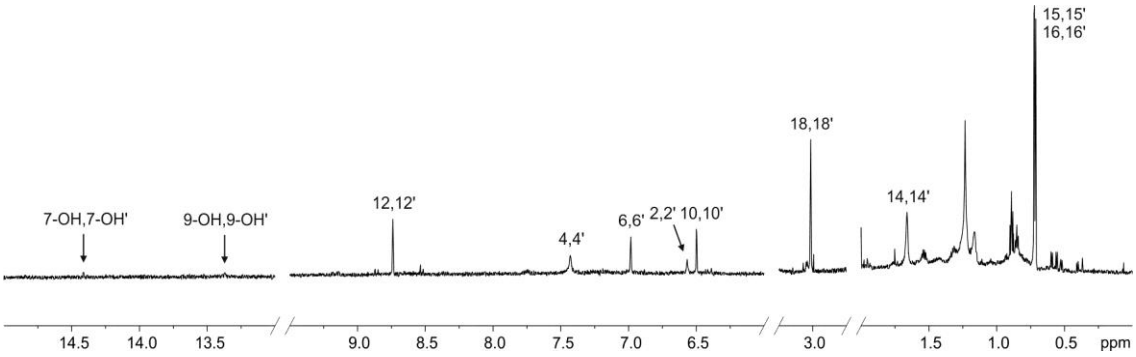


Figure S24. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome A (**4**).

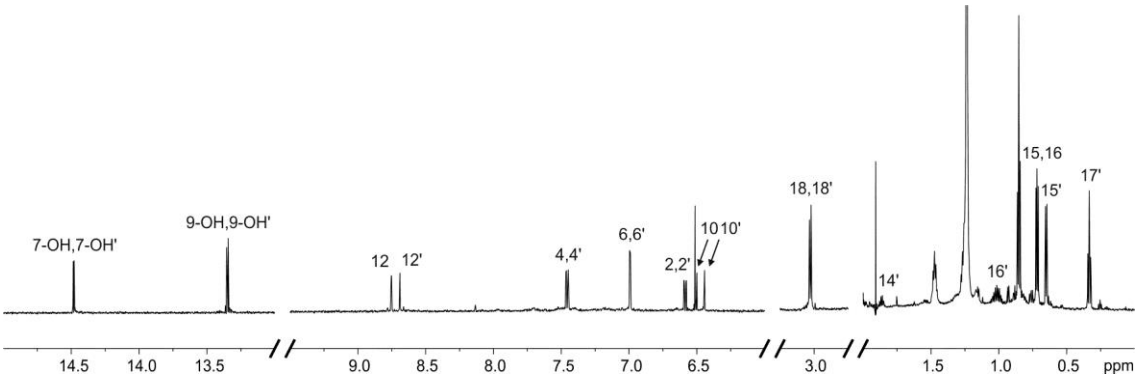


Figure S25. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome B1 (**5a**).

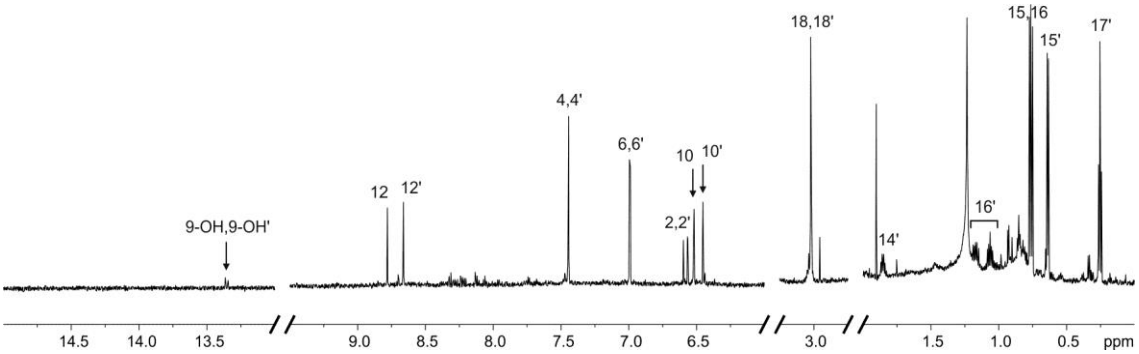


Figure S26. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome B2 (**5b**).

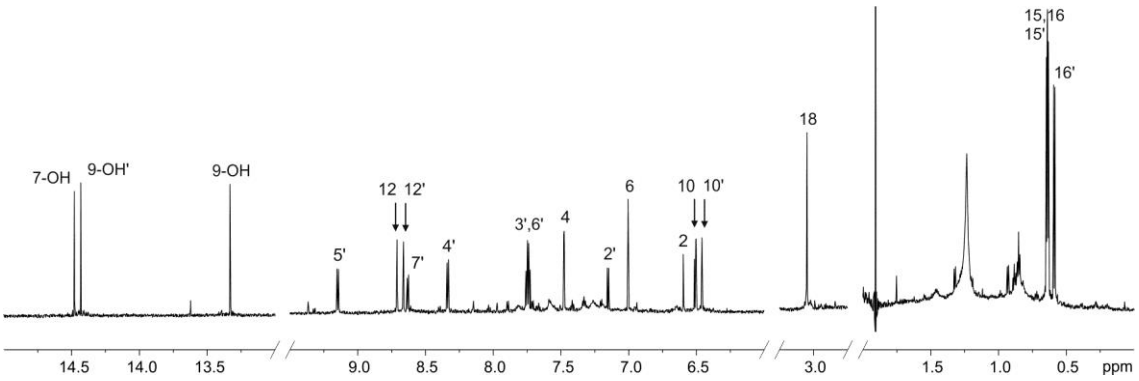


Figure S27. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome D (**6**).

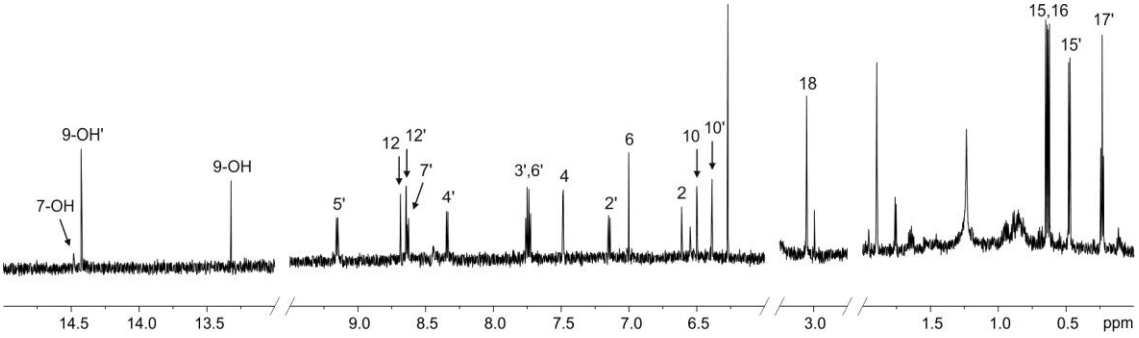


Figure S28. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome E (**7**).

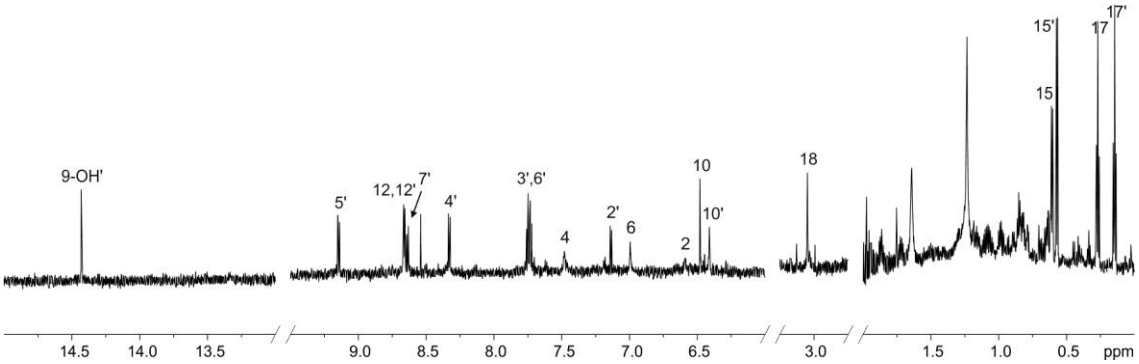


Figure S29. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome F (**8**).

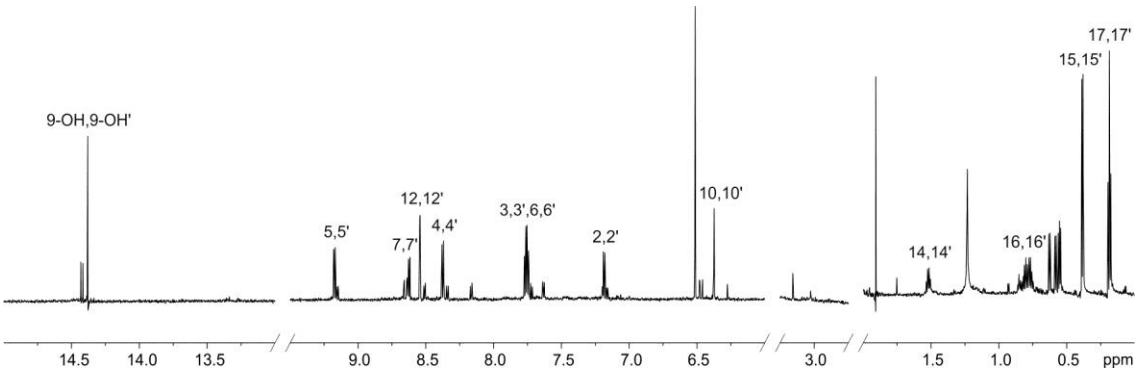


Figure S30. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome I1 (**9a**).

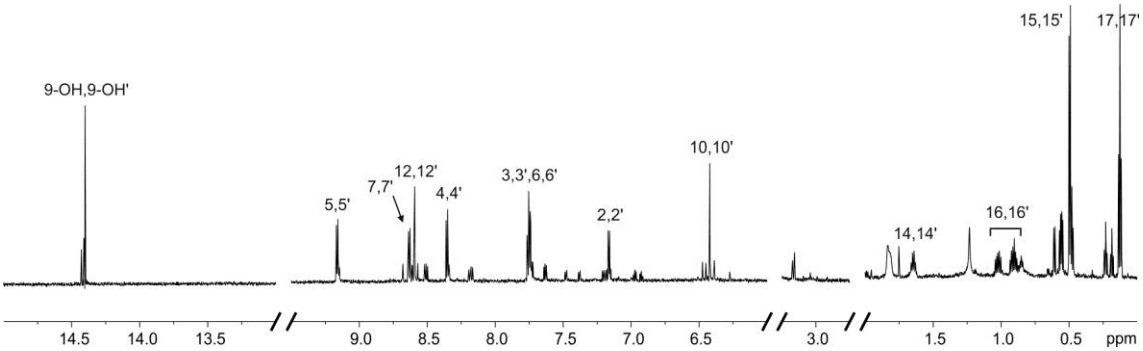


Figure S31. ^{1}H NMR spectrum (700 MHz, DMSO-d_6) of borolithochrome I2 (**9b**).

Appendix 2: Cartesian Coordinates of Stationary Points

(*M*,14'*S*)-**2a**, conformer a1b1

C	-1.118	-3.059	1.399
C	-1.552	-1.836	0.869
C	-2.916	-1.512	0.738
C	-3.869	-2.486	1.186
C	-3.416	-3.737	1.705
C	-2.053	-4.009	1.807
C	-3.400	-0.225	0.202
C	-5.294	-2.223	1.160
C	-5.745	-0.900	0.720
C	-4.814	0.077	0.261
C	-5.338	1.342	-0.158
C	-6.726	1.565	-0.104
C	-7.613	0.595	0.348
C	-7.117	-0.636	0.759
H	-0.812	-1.118	0.560
H	-1.744	-4.968	2.214
H	-8.679	0.800	0.373
C	-2.567	0.738	-0.395
C	-3.060	2.036	-0.785
C	-4.430	2.376	-0.635
C	-4.842	3.688	-0.946
C	-2.137	3.016	-1.255
C	-3.924	4.630	-1.388
C	-2.574	4.304	-1.548
H	-5.877	3.986	-0.827
H	-1.850	5.034	-1.897
O	-6.140	-3.089	1.523

O	-4.282	-4.682	2.121
H	-5.195	-4.289	1.975
C	0.370	-3.365	1.520
H	0.458	-4.333	2.035
C	1.100	-2.317	2.395
H	1.107	-1.348	1.878
H	0.519	-2.170	3.315
C	1.009	-3.523	0.126
H	0.483	-4.287	-0.457
H	2.059	-3.824	0.203
O	-1.274	0.494	-0.596
O	-0.829	2.733	-1.402
B	-0.413	1.346	-1.455
O	0.945	1.276	-0.912
O	-0.476	0.867	-2.834
C	1.880	0.428	-1.338
C	1.611	-0.311	-2.545
C	3.087	0.289	-0.632
C	0.418	-0.033	-3.275
C	2.544	-1.255	-3.049
C	3.993	-0.745	-1.079
C	0.176	-0.676	-4.486
C	2.269	-1.890	-4.277
C	3.741	-1.515	-2.261
C	1.106	-1.597	-4.978
H	-0.735	-0.444	-5.028
H	2.965	-2.604	-4.699
C	5.167	-1.051	-0.330
C	3.452	1.111	0.538
C	6.047	-2.059	-0.739

C	5.796	-2.792	-1.893
H	6.478	-3.575	-2.210
C	4.654	-2.518	-2.635
C	5.483	-0.328	0.905
C	4.619	0.768	1.297
C	4.972	1.542	2.443
C	2.728	2.248	0.942
C	3.093	3.012	2.060
C	4.207	2.647	2.815
H	4.507	3.216	3.691
H	1.868	2.553	0.373
O	6.498	-0.653	1.583
O	6.051	1.240	3.190
H	6.462	0.435	2.752
C	2.281	4.242	2.446
H	2.725	4.646	3.366
C	0.813	3.891	2.756
H	0.744	3.130	3.541
H	0.273	4.782	3.096
C	2.370	5.340	1.369
H	3.411	5.618	1.170
H	1.833	6.238	1.695
H	1.923	5.007	0.425
H	-7.778	-1.420	1.112
H	-7.127	2.515	-0.435
H	-4.259	5.638	-1.616
H	0.967	-2.583	-0.436
H	6.922	-2.251	-0.128
H	0.914	-2.094	-5.925
H	4.463	-3.110	-3.522

H	0.298	3.507	1.867
C	2.535	-2.704	2.769
H	2.562	-3.672	3.286
H	2.974	-1.956	3.439
H	3.185	-2.777	1.890

(*M*,14'*S*)-**2a**, conformer a1b2

C	-1.142	-3.049	1.378
C	-1.550	-1.815	0.852
C	-2.908	-1.476	0.693
C	-3.881	-2.442	1.111
C	-3.454	-3.704	1.626
C	-2.097	-3.993	1.754
C	-3.365	-0.179	0.157
C	-5.302	-2.159	1.062
C	-5.727	-0.825	0.632
C	-4.774	0.142	0.197
C	-5.274	1.419	-0.218
C	-6.658	1.663	-0.181
C	-7.567	0.703	0.249
C	-7.095	-0.541	0.654
H	-0.796	-1.102	0.568
H	-1.807	-4.960	2.156
H	-8.630	0.924	0.261
C	-2.509	0.774	-0.424
C	-2.978	2.081	-0.814
C	-4.344	2.442	-0.676
C	-4.731	3.763	-0.982
C	-2.035	3.048	-1.271

C	-3.793	4.693	-1.409
C	-2.447	4.345	-1.559
H	-5.761	4.077	-0.871
H	-1.708	5.065	-1.897
O	-6.166	-3.019	1.398
O	-4.339	-4.643	2.013
H	-5.245	-4.237	1.852
C	0.340	-3.379	1.513
H	0.409	-4.348	2.029
C	1.117	-2.353	2.367
H	2.175	-2.646	2.364
H	1.076	-1.367	1.886
C	0.991	-3.548	0.126
H	0.475	-4.315	-0.462
H	2.041	-3.846	0.228
O	-1.218	0.510	-0.610
O	-0.730	2.744	-1.409
B	-0.338	1.349	-1.464
O	1.016	1.255	-0.917
O	-0.405	0.875	-2.844
C	1.937	0.389	-1.340
C	1.657	-0.344	-2.548
C	3.139	0.228	-0.632
C	0.471	-0.044	-3.282
C	2.573	-1.307	-3.050
C	4.028	-0.822	-1.078
C	0.220	-0.684	-4.493
C	2.287	-1.938	-4.277
C	3.764	-1.588	-2.259
C	1.132	-1.624	-4.980

H	-0.685	-0.435	-5.037
H	2.970	-2.667	-4.696
C	5.197	-1.147	-0.328
C	3.516	1.043	0.540
C	6.060	-2.168	-0.736
C	5.798	-2.898	-1.890
H	6.467	-3.693	-2.206
C	4.660	-2.606	-2.632
C	5.523	-0.429	0.907
C	4.677	0.681	1.299
C	5.042	1.448	2.446
C	2.809	2.190	0.946
C	3.185	2.946	2.064
C	4.294	2.565	2.819
H	4.602	3.127	3.696
H	1.953	2.508	0.377
O	6.532	-0.771	1.586
O	6.116	1.129	3.193
H	6.514	0.318	2.755
C	2.391	4.187	2.453
H	2.841	4.585	3.372
C	0.919	3.856	2.763
H	0.839	3.095	3.547
H	0.391	4.754	3.105
C	2.493	5.285	1.376
H	3.538	5.548	1.176
H	1.970	6.191	1.703
H	2.041	4.959	0.432
H	-7.773	-1.318	0.988
H	-7.041	2.622	-0.509

H	-4.109	5.708	-1.634
H	0.961	-2.612	-0.443
H	6.931	-2.375	-0.125
H	0.932	-2.118	-5.927
H	4.460	-3.195	-3.520
H	0.397	3.481	1.875
C	0.628	-2.242	3.815
H	-0.413	-1.901	3.861
H	1.238	-1.529	4.381
H	0.684	-3.211	4.326

(*M*,14'*S*)-**2a**, conformer a1b3

C	-1.308	-3.130	1.307
C	-1.666	-1.875	0.799
C	-3.007	-1.514	0.558
C	-4.018	-2.479	0.871
C	-3.641	-3.767	1.359
C	-2.301	-4.078	1.568
C	-3.408	-0.191	0.045
C	-5.428	-2.168	0.744
C	-5.804	-0.804	0.365
C	-4.811	0.162	0.029
C	-5.260	1.469	-0.348
C	-6.639	1.743	-0.367
C	-7.589	0.785	-0.031
C	-7.165	-0.489	0.331
H	-0.890	-1.158	0.595
H	-2.050	-5.066	1.944
H	-8.646	1.030	-0.061

C	-2.505	0.760	-0.463
C	-2.924	2.096	-0.810
C	-4.285	2.488	-0.710
C	-4.624	3.833	-0.963
C	-1.938	3.056	-1.179
C	-3.644	4.755	-1.303
C	-2.303	4.378	-1.417
H	-5.650	4.169	-0.878
H	-1.532	5.093	-1.687
O	-6.325	-3.028	0.977
O	-4.563	-4.710	1.638
H	-5.449	-4.286	1.431
C	0.141	-3.491	1.620
H	0.207	-4.585	1.541
C	0.507	-3.161	3.096
H	-0.190	-3.700	3.751
H	1.502	-3.582	3.291
C	1.160	-2.910	0.628
H	0.917	-3.198	-0.401
H	2.162	-3.290	0.858
O	-1.216	0.465	-0.616
O	-0.638	2.720	-1.280
B	-0.284	1.315	-1.399
O	1.046	1.151	-0.812
O	-0.328	0.914	-2.801
C	2.035	0.422	-1.326
C	1.823	-0.170	-2.621
C	3.237	0.260	-0.615
C	0.618	0.119	-3.326
C	2.813	-0.992	-3.221

C	4.223	-0.629	-1.191
C	0.413	-0.404	-4.600
C	2.574	-1.505	-4.512
C	4.028	-1.258	-2.464
C	1.395	-1.211	-5.182
H	-0.510	-0.168	-5.119
H	3.311	-2.127	-5.006
C	5.429	-0.927	-0.489
C	3.527	0.920	0.674
C	6.385	-1.796	-1.022
C	6.184	-2.398	-2.259
H	6.925	-3.075	-2.673
C	5.016	-2.126	-2.961
C	5.702	-0.337	0.823
C	4.740	0.598	1.369
C	5.031	1.225	2.619
C	2.683	1.880	1.265
C	2.984	2.498	2.486
C	4.155	2.163	3.164
H	4.410	2.622	4.115
H	1.775	2.162	0.761
O	6.763	-0.640	1.439
O	6.155	0.940	3.304
H	6.641	0.259	2.747
C	2.027	3.523	3.083
H	2.500	3.914	3.994
C	0.693	2.872	3.496
H	0.855	2.046	4.198
H	0.042	3.609	3.980
C	1.788	4.715	2.138

H	2.731	5.196	1.856
H	1.156	5.466	2.627
H	1.280	4.402	1.218
H	-7.876	-1.266	0.589
H	-6.984	2.727	-0.665
H	-3.924	5.789	-1.487
H	1.209	-1.818	0.664
H	7.280	-1.988	-0.442
H	1.231	-1.613	-6.178
H	4.868	-2.612	-3.919
H	0.160	2.473	2.625
C	0.504	-1.676	3.477
H	1.234	-1.100	2.897
H	0.760	-1.556	4.536
H	-0.480	-1.223	3.317

(*M*,14'*S*)-**2a**, conformer a2b1

C	-1.005	-2.979	1.344
C	-1.474	-1.757	0.848
C	-2.848	-1.467	0.722
C	-3.772	-2.476	1.147
C	-3.282	-3.727	1.635
C	-1.915	-3.967	1.728
C	-3.365	-0.183	0.214
C	-5.203	-2.249	1.129
C	-5.689	-0.929	0.721
C	-4.785	0.081	0.280
C	-5.342	1.341	-0.114
C	-6.734	1.527	-0.051

C	-7.596	0.527	0.384
C	-7.068	-0.700	0.768
H	-0.748	-1.013	0.565
H	-1.588	-4.928	2.113
H	-8.666	0.704	0.416
C	-2.557	0.812	-0.366
C	-3.083	2.103	-0.735
C	-4.461	2.405	-0.576
C	-4.906	3.711	-0.866
C	-2.186	3.111	-1.194
C	-4.013	4.682	-1.297
C	-2.655	4.393	-1.466
H	-5.948	3.981	-0.741
H	-1.951	5.145	-1.806
O	-6.026	-3.144	1.474
O	-4.124	-4.704	2.029
H	-5.047	-4.331	1.895
C	0.495	-3.217	1.464
H	0.997	-2.317	1.083
C	0.945	-4.403	0.576
H	0.488	-5.330	0.948
H	0.543	-4.247	-0.434
C	0.910	-3.392	2.938
H	0.567	-2.545	3.542
H	1.999	-3.453	3.038
O	-1.259	0.604	-0.571
O	-0.872	2.863	-1.351
B	-0.423	1.487	-1.423
O	0.939	1.440	-0.889
O	-0.481	1.024	-2.807

C	1.863	0.570	-1.296
C	1.586	-0.183	-2.494
C	3.066	0.424	-0.585
C	0.401	0.104	-3.233
C	2.508	-1.146	-2.982
C	3.960	-0.627	-1.017
C	0.155	-0.551	-4.436
C	2.226	-1.795	-4.201
C	3.701	-1.410	-2.188
C	1.071	-1.495	-4.911
H	-0.751	-0.313	-4.985
H	2.912	-2.527	-4.610
C	5.131	-0.935	-0.264
C	3.438	1.256	0.575
C	6.002	-1.954	-0.661
C	5.746	-2.699	-1.806
H	6.421	-3.492	-2.114
C	4.605	-2.424	-2.551
C	5.453	-0.200	0.962
C	4.601	0.910	1.340
C	4.960	1.693	2.478
C	2.725	2.404	0.967
C	3.096	3.175	2.077
C	4.205	2.809	2.838
H	4.509	3.383	3.709
H	1.868	2.711	0.394
O	6.465	-0.528	1.646
O	6.036	1.388	3.230
H	6.438	0.574	2.801
C	2.294	4.416	2.451

H	2.736	4.822	3.370
C	0.821	4.082	2.755
H	0.739	3.327	3.545
H	0.288	4.981	3.088
C	2.399	5.505	1.366
H	3.444	5.772	1.172
H	1.870	6.411	1.683
H	1.955	5.170	0.422
H	-7.708	-1.507	1.106
H	-7.161	2.474	-0.363
H	-4.374	5.685	-1.509
H	0.482	-4.306	3.367
H	6.875	-2.147	-0.047
H	0.875	-2.002	-5.851
H	4.409	-3.025	-3.432
H	0.306	3.698	1.867
C	2.465	-4.583	0.486
H	2.952	-3.667	0.131
H	2.716	-5.386	-0.216
H	2.906	-4.844	1.454

(*M*,14'*S*)-**2a**, conformer a2b2

C	-1.025	-2.918	1.439
C	-1.468	-1.704	0.903
C	-2.835	-1.380	0.786
C	-3.780	-2.349	1.256
C	-3.317	-3.594	1.786
C	-1.955	-3.866	1.874
C	-3.325	-0.101	0.239

C	-5.205	-2.089	1.239
C	-5.664	-0.775	0.782
C	-4.739	0.198	0.302
C	-5.270	1.456	-0.132
C	-6.657	1.675	-0.072
C	-7.539	0.709	0.399
C	-7.037	-0.515	0.825
H	-0.727	-0.991	0.583
H	-1.647	-4.820	2.292
H	-8.605	0.911	0.428
C	-2.497	0.858	-0.372
C	-2.997	2.148	-0.780
C	-4.367	2.485	-0.630
C	-4.785	3.791	-0.960
C	-2.079	3.123	-1.270
C	-3.871	4.729	-1.421
C	-2.521	4.405	-1.581
H	-5.820	4.086	-0.843
H	-1.801	5.132	-1.945
O	-6.046	-2.952	1.623
O	-4.178	-4.534	2.224
H	-5.093	-4.144	2.082
C	0.470	-3.182	1.569
H	0.991	-2.350	1.077
C	0.919	-4.483	0.867
H	1.994	-4.612	1.053
H	0.425	-5.343	1.340
C	0.898	-3.187	3.051
H	0.618	-2.251	3.546
H	1.984	-3.306	3.136

O	-1.204	0.618	-0.570
O	-0.769	2.844	-1.419
B	-0.350	1.457	-1.448
O	1.011	1.397	-0.913
O	-0.416	0.953	-2.818
C	1.906	0.480	-1.282
C	1.607	-0.310	-2.450
C	3.102	0.322	-0.562
C	0.436	-0.011	-3.206
C	2.496	-1.323	-2.895
C	3.956	-0.781	-0.941
C	0.175	-0.699	-4.388
C	2.200	-2.006	-4.093
C	3.672	-1.602	-2.081
C	1.061	-1.690	-4.821
H	-0.719	-0.450	-4.951
H	2.863	-2.774	-4.470
C	5.107	-1.105	-0.165
C	3.503	1.192	0.560
C	5.936	-2.177	-0.508
C	5.656	-2.960	-1.622
H	6.298	-3.793	-1.889
C	4.535	-2.669	-2.390
C	5.449	-0.332	1.032
C	4.643	0.831	1.351
C	5.028	1.650	2.454
C	2.842	2.390	0.887
C	3.238	3.197	1.962
C	4.322	2.816	2.752
H	4.645	3.418	3.597

H	2.005	2.707	0.289
O	6.438	-0.672	1.741
O	6.083	1.333	3.231
H	6.452	0.483	2.844
C	2.496	4.493	2.263
H	2.944	4.918	3.171
C	1.002	4.251	2.552
H	0.867	3.536	3.372
H	0.513	5.190	2.836
C	2.679	5.523	1.131
H	3.740	5.726	0.947
H	2.191	6.469	1.393
H	2.236	5.165	0.194
H	-7.693	-1.295	1.195
H	-7.064	2.619	-0.415
H	-4.212	5.732	-1.664
H	0.425	-4.011	3.598
H	6.794	-2.380	0.122
H	0.853	-2.223	-5.745
H	4.319	-3.299	-3.246
H	0.483	3.857	1.671
C	0.660	-4.506	-0.643
H	-0.410	-4.425	-0.867
H	1.025	-5.439	-1.088
H	1.169	-3.674	-1.144

(*M*,14'*S*)-**2a**, conformer a2b3

C	-1.093	-2.888	1.526
C	-1.519	-1.663	0.993

C	-2.877	-1.343	0.815
C	-3.841	-2.318	1.234
C	-3.399	-3.569	1.759
C	-2.039	-3.844	1.898
C	-3.345	-0.057	0.264
C	-5.264	-2.049	1.180
C	-5.701	-0.720	0.743
C	-4.757	0.252	0.299
C	-5.267	1.520	-0.130
C	-6.653	1.753	-0.092
C	-7.553	0.791	0.350
C	-7.072	-0.446	0.763
H	-0.765	-0.941	0.724
H	-1.755	-4.805	2.314
H	-8.617	1.003	0.362
C	-2.498	0.893	-0.332
C	-2.977	2.189	-0.743
C	-4.344	2.543	-0.605
C	-4.741	3.857	-0.929
C	-2.042	3.154	-1.221
C	-3.811	4.785	-1.375
C	-2.463	4.444	-1.527
H	-5.774	4.165	-0.819
H	-1.731	5.163	-1.881
O	-6.120	-2.915	1.517
O	-4.275	-4.516	2.148
H	-5.184	-4.123	1.981
C	0.406	-3.138	1.653
H	0.865	-2.156	1.829
C	1.014	-3.645	0.314

H	0.795	-2.902	-0.463
H	2.106	-3.656	0.429
C	0.794	-4.033	2.841
H	0.404	-3.630	3.782
H	1.886	-4.089	2.924
O	-1.204	0.636	-0.512
O	-0.736	2.854	-1.364
B	-0.340	1.460	-1.395
O	1.023	1.380	-0.867
O	-0.423	0.957	-2.765
C	1.914	0.468	-1.257
C	1.599	-0.316	-2.424
C	3.121	0.309	-0.557
C	0.420	-0.010	-3.165
C	2.480	-1.330	-2.884
C	3.967	-0.796	-0.950
C	0.141	-0.695	-4.345
C	2.166	-2.008	-4.080
C	3.666	-1.614	-2.087
C	1.019	-1.687	-4.793
H	-0.759	-0.441	-4.897
H	2.823	-2.777	-4.468
C	5.126	-1.124	-0.188
C	3.542	1.177	0.558
C	5.947	-2.199	-0.544
C	5.651	-2.979	-1.656
H	6.287	-3.814	-1.932
C	4.520	-2.683	-2.409
C	5.486	-0.355	1.006
C	4.689	0.811	1.335

C	5.093	1.631	2.432
C	2.891	2.380	0.890
C	3.307	3.187	1.958
C	4.398	2.801	2.736
H	4.735	3.403	3.575
H	2.049	2.701	0.302
O	6.481	-0.701	1.703
O	6.156	1.309	3.195
H	6.515	0.457	2.805
C	2.578	4.490	2.264
H	3.038	4.913	3.166
C	1.085	4.261	2.568
H	0.952	3.549	3.390
H	0.607	5.205	2.855
C	2.758	5.516	1.128
H	3.819	5.710	0.934
H	2.281	6.467	1.393
H	2.304	5.160	0.196
H	-7.743	-1.226	1.104
H	-7.044	2.707	-0.428
H	-4.135	5.795	-1.613
H	0.422	-5.057	2.737
H	6.813	-2.407	0.075
H	0.797	-2.217	-5.715
H	4.292	-3.311	-3.263
H	0.553	3.870	1.693
C	0.542	-5.023	-0.161
H	0.806	-5.815	0.548
H	1.010	-5.273	-1.120
H	-0.544	-5.050	-0.304

(*P*,14'*S*)-**2b**, conformer a1b1

C	-2.898	2.897	2.253
C	-2.584	2.142	1.115
C	-3.439	1.145	0.608
C	-4.675	0.928	1.303
C	-4.983	1.699	2.465
C	-4.096	2.671	2.928
C	-3.135	0.338	-0.593
C	-5.641	-0.053	0.849
C	-5.336	-0.816	-0.364
C	-4.113	-0.616	-1.069
C	-3.895	-1.406	-2.245
C	-4.874	-2.334	-2.643
C	-6.057	-2.511	-1.936
C	-6.284	-1.748	-0.797
H	-1.655	2.341	0.611
H	-4.363	3.239	3.814
H	-6.790	-3.238	-2.272
C	-1.930	0.426	-1.312
C	-1.695	-0.330	-2.515
C	-2.668	-1.236	-3.013
C	-2.408	-1.914	-4.221
C	-0.485	-0.122	-3.241
C	-1.224	-1.695	-4.913
C	-0.260	-0.804	-4.433
H	-3.131	-2.606	-4.635
H	0.666	-0.626	-4.970
O	-6.727	-0.255	1.463
O	-6.131	1.520	3.146

H	-6.620	0.792	2.655
C	-1.926	3.957	2.758
H	-2.403	4.450	3.615
C	-0.613	3.323	3.259
H	-0.079	2.821	2.443
H	-0.804	2.583	4.043
H	0.050	4.094	3.670
C	-1.646	5.038	1.697
H	-1.002	5.821	2.115
H	-2.575	5.508	1.355
O	-0.962	1.246	-0.904
O	0.446	0.748	-2.816
B	0.388	1.291	-1.462
O	1.260	0.486	-0.569
O	0.805	2.682	-1.477
C	2.563	0.726	-0.436
C	3.053	1.994	-0.918
C	3.411	-0.210	0.180
C	2.120	2.960	-1.396
C	4.432	2.323	-0.847
C	4.830	0.065	0.140
C	2.555	4.230	-1.765
C	4.842	3.614	-1.236
C	5.350	1.297	-0.371
C	3.914	4.547	-1.678
H	1.824	4.951	-2.116
H	5.885	3.904	-1.175
C	5.769	-0.911	0.588
C	2.936	-1.448	0.826
C	7.145	-0.673	0.531

C	7.637	0.528	0.035
H	8.706	0.711	-0.014
C	6.742	1.494	-0.409
C	5.319	-2.203	1.112
C	3.894	-2.425	1.253
C	3.448	-3.630	1.874
C	1.578	-1.712	1.089
C	1.153	-2.886	1.726
C	2.090	-3.848	2.103
H	1.787	-4.771	2.590
H	0.839	-0.982	0.804
O	6.168	-3.076	1.452
O	4.317	-4.581	2.272
H	5.226	-4.226	2.033
C	-0.326	-3.132	1.998
H	-0.391	-4.048	2.602
C	-1.089	-3.405	0.678
H	-1.084	-2.495	0.063
H	-0.533	-4.163	0.109
C	-0.957	-1.992	2.820
H	-0.381	-1.804	3.732
H	-1.980	-2.244	3.117
H	-0.999	-1.057	2.249
C	-2.531	-3.887	0.873
H	-2.992	-4.125	-0.092
H	-3.156	-3.129	1.355
H	-2.565	-4.793	1.491
H	-7.193	-1.857	-0.217
H	-4.707	-2.941	-3.525
H	-1.044	-2.224	-5.845

H	-1.137	4.619	0.822
H	7.813	-1.454	0.878
H	4.249	5.540	-1.966
H	7.139	2.419	-0.811

(*P*,14'*S*)-**2b**, conformer a1b2

C	-2.712	3.000	2.168
C	-2.465	2.155	1.077
C	-3.404	1.210	0.622
C	-4.649	1.133	1.332
C	-4.891	2.001	2.440
C	-3.927	2.923	2.845
C	-3.172	0.313	-0.530
C	-5.677	0.183	0.961
C	-5.414	-0.720	-0.162
C	-4.193	-0.647	-0.894
C	-4.024	-1.559	-1.986
C	-5.046	-2.481	-2.277
C	-6.224	-2.536	-1.545
C	-6.405	-1.650	-0.490
H	-1.521	2.240	0.571
H	-4.147	3.568	3.691
H	-6.992	-3.262	-1.798
C	-2.004	0.327	-1.312
C	-1.814	-0.563	-2.430
C	-2.807	-1.512	-2.787
C	-2.579	-2.345	-3.902
C	-0.623	-0.458	-3.207
C	-1.412	-2.228	-4.643

C	-0.432	-1.289	-4.307
H	-3.314	-3.080	-4.203
H	0.482	-1.189	-4.885
O	-6.778	0.113	1.579
O	-6.049	1.960	3.127
H	-6.595	1.241	2.685
C	-1.650	3.998	2.615
H	-2.085	4.586	3.435
C	-0.403	3.283	3.169
H	0.085	2.680	2.394
H	-0.663	2.617	3.999
H	0.327	4.015	3.534
C	-1.270	4.980	1.491
H	-0.554	5.723	1.861
H	-2.150	5.513	1.115
O	-1.028	1.196	-1.052
O	0.325	0.449	-2.920
B	0.310	1.155	-1.642
O	1.192	0.449	-0.680
O	0.739	2.528	-1.835
C	2.493	0.706	-0.562
C	2.982	1.920	-1.169
C	3.340	-0.161	0.152
C	2.051	2.819	-1.767
C	4.358	2.266	-1.114
C	4.756	0.132	0.122
C	2.486	4.040	-2.274
C	4.767	3.507	-1.643
C	5.274	1.312	-0.504
C	3.841	4.374	-2.205

H	1.756	4.711	-2.717
H	5.806	3.809	-1.602
C	5.696	-0.772	0.700
C	2.866	-1.345	0.895
C	7.069	-0.515	0.661
C	7.559	0.634	0.053
H	8.626	0.832	0.019
C	6.663	1.529	-0.521
C	5.252	-2.009	1.345
C	3.827	-2.252	1.453
C	3.384	-3.406	2.166
C	1.505	-1.628	1.119
C	1.081	-2.754	1.838
C	2.023	-3.646	2.350
H	1.722	-4.530	2.905
H	0.760	-0.952	0.736
O	6.105	-2.820	1.808
O	4.257	-4.288	2.691
H	5.167	-3.931	2.460
C	-0.404	-3.004	2.075
H	-0.486	-3.930	2.662
C	-1.187	-3.225	0.760
H	-2.250	-3.332	1.015
H	-1.111	-2.323	0.139
C	-1.039	-1.873	2.907
H	-0.500	-1.723	3.849
H	-2.081	-2.114	3.146
H	-1.034	-0.922	2.362
C	-0.735	-4.446	-0.047
H	-1.342	-4.561	-0.952

H	-0.832	-5.367	0.541
H	0.313	-4.357	-0.356
H	-7.313	-1.658	0.103
H	-4.919	-3.177	-3.098
H	-1.256	-2.876	-5.501
H	-0.804	4.461	0.645
H	7.737	-1.241	1.112
H	4.175	5.330	-2.601
H	7.060	2.414	-1.006

(*P*,14'*S*)-**2b**, conformer a1b3

C	-3.910	-7.729	4.678
C	-4.232	-6.847	3.637
C	-3.881	-7.096	2.297
C	-3.158	-8.305	2.025
C	-2.838	-9.198	3.092
C	-3.216	-8.905	4.402
C	-4.215	-6.187	1.179
C	-2.730	-8.649	0.684
C	-3.042	-7.719	-0.403
C	-3.775	-6.521	-0.159
C	-4.049	-5.675	-1.282
C	-3.577	-6.047	-2.555
C	-2.859	-7.217	-2.766
C	-2.597	-8.052	-1.686
H	-4.772	-5.950	3.879
H	-2.956	-9.608	5.188
H	-2.510	-7.472	-3.762
C	-4.944	-4.994	1.330

C	-5.253	-4.134	0.217
C	-4.818	-4.452	-1.097
C	-5.165	-3.585	-2.154
C	-6.039	-2.964	0.439
C	-5.929	-2.451	-1.916
C	-6.371	-2.134	-0.628
H	-4.851	-3.795	-3.169
H	-6.972	-1.251	-0.435
O	-2.098	-9.716	0.437
O	-2.165	-10.345	2.873
H	-1.988	-10.365	1.884
C	-4.313	-7.399	6.110
H	-4.015	-8.252	6.734
C	-3.566	-6.157	6.634
H	-3.826	-5.264	6.054
H	-2.481	-6.294	6.574
H	-3.829	-5.967	7.681
C	-5.838	-7.228	6.256
H	-6.102	-7.056	7.306
H	-6.372	-8.121	5.912
O	-5.401	-4.629	2.528
O	-6.495	-2.647	1.661
B	-5.966	-3.318	2.845
O	-4.873	-2.498	3.427
O	-7.031	-3.528	3.807
C	-5.083	-1.540	4.327
C	-6.371	-1.518	4.977
C	-4.075	-0.613	4.644
C	-7.302	-2.563	4.705
C	-6.693	-0.521	5.935

C	-4.433	0.466	5.538
C	-8.512	-2.617	5.391
C	-7.929	-0.600	6.607
C	-5.716	0.533	6.172
C	-8.814	-1.635	6.339
H	-9.200	-3.427	5.172
H	-8.200	0.136	7.355
C	-3.515	1.525	5.801
C	-2.704	-0.670	4.099
C	-3.852	2.587	6.646
C	-5.099	2.639	7.257
H	-5.363	3.465	7.910
C	-6.013	1.620	7.014
C	-2.188	1.543	5.182
C	-1.802	0.414	4.359
C	-0.476	0.376	3.832
C	-2.210	-1.758	3.354
C	-0.899	-1.794	2.857
C	-0.040	-0.720	3.089
H	0.978	-0.719	2.710
H	-2.855	-2.599	3.164
O	-1.408	2.516	5.389
O	0.395	1.382	4.042
H	-0.104	2.054	4.597
C	-0.404	-3.004	2.075
H	0.642	-2.806	1.802
C	-1.187	-3.225	0.760
H	-1.035	-2.341	0.126
H	-0.749	-4.071	0.215
C	-0.421	-4.279	2.942

H	0.148	-4.136	3.868
H	0.025	-5.118	2.395
H	-1.443	-4.565	3.215
C	-2.689	-3.458	0.952
H	-3.190	-3.583	-0.015
H	-3.159	-2.610	1.465
H	-2.883	-4.357	1.547
H	-2.043	-8.976	-1.810
H	-3.776	-5.407	-3.406
H	-6.189	-1.798	-2.744
H	-6.202	-6.373	5.675
H	-3.115	3.367	6.804
H	-9.759	-1.683	6.873
H	-6.988	1.681	7.484

(*P*,14'*S*)-**2b**, conformer a2b1

C	-3.244	3.294	1.855
C	-2.815	2.479	0.799
C	-3.444	1.260	0.486
C	-4.584	0.885	1.269
C	-5.003	1.714	2.353
C	-4.329	2.901	2.639
C	-3.007	0.382	-0.616
C	-5.357	-0.303	0.961
C	-4.979	-1.090	-0.216
C	-3.829	-0.749	-0.986
C	-3.510	-1.581	-2.108
C	-4.337	-2.679	-2.405
C	-5.457	-2.989	-1.642

C	-5.772	-2.193	-0.547
H	-1.979	2.805	0.205
H	-4.676	3.509	3.469
H	-6.071	-3.847	-1.898
C	-1.805	0.555	-1.321
C	-1.476	-0.241	-2.477
C	-2.337	-1.281	-2.918
C	-2.017	-1.965	-4.108
C	-0.308	0.080	-3.229
C	-0.883	-1.625	-4.834
C	-0.024	-0.610	-4.404
H	-2.659	-2.753	-4.483
H	0.866	-0.343	-4.965
O	-6.348	-0.654	1.662
O	-6.060	1.386	3.122
H	-6.404	0.521	2.745
C	-2.538	4.614	2.141
H	-3.002	5.040	3.041
C	-1.040	4.417	2.440
H	-0.505	4.025	1.567
H	-0.889	3.719	3.271
H	-0.579	5.374	2.712
C	-2.744	5.622	0.993
H	-2.282	6.584	1.244
H	-3.809	5.794	0.803
O	-0.931	1.492	-0.952
O	0.520	1.066	-2.839
B	0.444	1.534	-1.456
O	1.255	0.643	-0.590
O	0.897	2.906	-1.378

C	2.545	0.845	-0.335
C	3.078	2.148	-0.650
C	3.334	-0.166	0.241
C	2.200	3.157	-1.144
C	4.442	2.458	-0.411
C	4.742	0.117	0.410
C	2.674	4.444	-1.377
C	4.894	3.770	-0.664
C	5.304	1.395	0.089
C	4.019	4.740	-1.133
H	1.985	5.195	-1.748
H	5.926	4.044	-0.484
C	5.631	-0.890	0.889
C	2.810	-1.485	0.648
C	6.998	-0.640	1.045
C	7.530	0.606	0.734
H	8.591	0.801	0.852
C	6.684	1.603	0.262
C	5.143	-2.230	1.223
C	3.722	-2.490	1.107
C	3.229	-3.778	1.487
C	1.441	-1.821	0.629
C	0.968	-3.081	1.009
C	1.868	-4.063	1.430
H	1.538	-5.054	1.727
H	0.721	-1.085	0.316
O	5.956	-3.117	1.612
O	4.060	-4.750	1.913
H	4.979	-4.345	1.887
C	-0.528	-3.367	0.963

H	-1.017	-2.460	0.582
C	-1.087	-3.625	2.383
H	-0.639	-4.543	2.788
H	-0.754	-2.808	3.037
C	-0.849	-4.512	-0.017
H	-0.426	-4.307	-1.007
H	-1.930	-4.636	-0.137
H	-0.438	-5.466	0.334
C	-2.615	-3.729	2.452
H	-2.948	-3.827	3.491
H	-2.993	-4.597	1.902
H	-3.092	-2.835	2.032
H	-6.632	-2.409	0.077
H	-4.095	-3.319	-3.246
H	-0.657	-2.160	-5.753
H	-2.288	5.263	0.063
H	7.625	-1.445	1.409
H	4.384	5.746	-1.317
H	7.115	2.565	0.011

(*P*,14'*S*)-**2b**, conformer a2b2

C	-3.266	3.205	1.878
C	-2.842	2.417	0.800
C	-3.442	1.184	0.488
C	-4.549	0.764	1.296
C	-4.962	1.565	2.402
C	-4.316	2.769	2.686
C	-3.008	0.332	-0.636
C	-5.297	-0.440	0.990

C	-4.931	-1.196	-0.212
C	-3.808	-0.815	-1.003
C	-3.495	-1.623	-2.144
C	-4.303	-2.735	-2.440
C	-5.398	-3.082	-1.658
C	-5.706	-2.312	-0.542
H	-2.033	2.777	0.188
H	-4.658	3.355	3.534
H	-5.999	-3.949	-1.915
C	-1.826	0.545	-1.364
C	-1.497	-0.235	-2.531
C	-2.342	-1.287	-2.970
C	-2.027	-1.951	-4.173
C	-0.344	0.115	-3.294
C	-0.912	-1.581	-4.912
C	-0.065	-0.555	-4.481
H	-2.659	-2.748	-4.546
H	0.813	-0.267	-5.051
O	-6.256	-0.831	1.713
O	-5.986	1.195	3.195
H	-6.315	0.326	2.816
C	-2.592	4.542	2.163
H	-3.049	4.946	3.077
C	-1.083	4.385	2.430
H	-0.556	4.015	1.543
H	-0.896	3.684	3.251
H	-0.643	5.352	2.700
C	-2.850	5.555	1.031
H	-2.410	6.528	1.282
H	-3.923	5.699	0.863

O	-0.973	1.507	-1.007
O	0.475	1.107	-2.901
B	0.403	1.556	-1.511
O	1.210	0.648	-0.658
O	0.860	2.924	-1.414
C	2.494	0.849	-0.379
C	3.034	2.152	-0.679
C	3.271	-0.165	0.207
C	2.163	3.168	-1.171
C	4.398	2.455	-0.427
C	4.680	0.108	0.384
C	2.644	4.455	-1.389
C	4.856	3.767	-0.666
C	5.252	1.384	0.071
C	3.987	4.744	-1.133
H	1.960	5.213	-1.758
H	5.887	4.036	-0.474
C	5.559	-0.907	0.863
C	2.735	-1.477	0.615
C	6.927	-0.667	1.025
C	7.469	0.576	0.721
H	8.531	0.763	0.843
C	6.633	1.581	0.249
C	5.060	-2.245	1.189
C	3.636	-2.492	1.074
C	3.129	-3.772	1.457
C	1.361	-1.795	0.602
C	0.873	-3.048	0.989
C	1.764	-4.041	1.407
H	1.423	-5.027	1.708

H	0.649	-1.051	0.292
O	5.864	-3.141	1.575
O	3.950	-4.753	1.882
H	4.874	-4.360	1.852
C	-0.625	-3.321	0.932
H	-1.109	-2.396	0.592
C	-1.222	-3.669	2.314
H	-2.284	-3.911	2.171
H	-0.750	-4.585	2.695
C	-0.953	-4.419	-0.099
H	-0.559	-4.163	-1.088
H	-2.038	-4.547	-0.188
H	-0.524	-5.385	0.195
C	-1.095	-2.551	3.353
H	-1.560	-2.843	4.302
H	-1.589	-1.634	3.008
H	-0.046	-2.308	3.555
H	-6.544	-2.560	0.099
H	-4.065	-3.356	-3.297
H	-0.690	-2.101	-5.840
H	-2.403	5.219	0.088
H	7.548	-1.478	1.387
H	4.358	5.751	-1.305
H	7.071	2.542	0.003

(*P*,14'*S*)-**2b**, conformer a2b3

C	-3.262	3.207	1.915
C	-2.844	2.420	0.833
C	-3.455	1.194	0.514

C	-4.565	0.779	1.320
C	-4.971	1.579	2.431
C	-4.315	2.775	2.720
C	-3.029	0.346	-0.615
C	-5.322	-0.418	1.009
C	-4.963	-1.170	-0.196
C	-3.839	-0.793	-0.988
C	-3.535	-1.595	-2.135
C	-4.352	-2.699	-2.437
C	-5.448	-3.043	-1.654
C	-5.747	-2.278	-0.532
H	-2.031	2.776	0.223
H	-4.653	3.360	3.571
H	-6.055	-3.904	-1.915
C	-1.847	0.554	-1.344
C	-1.529	-0.217	-2.520
C	-2.384	-1.261	-2.964
C	-2.079	-1.916	-4.174
C	-0.379	0.133	-3.287
C	-0.965	-1.546	-4.916
C	-0.110	-0.529	-4.481
H	-2.718	-2.705	-4.551
H	0.766	-0.240	-5.053
O	-6.284	-0.805	1.731
O	-5.998	1.213	3.222
H	-6.334	0.348	2.839
C	-2.576	4.536	2.207
H	-3.032	4.941	3.120
C	-1.070	4.363	2.478
H	-0.543	3.991	1.592

H	-0.892	3.658	3.297
H	-0.621	5.325	2.754
C	-2.819	5.556	1.077
H	-2.372	6.523	1.334
H	-3.891	5.711	0.906
O	-0.984	1.503	-0.980
O	0.446	1.119	-2.891
B	0.386	1.561	-1.498
O	1.209	0.656	-0.659
O	0.833	2.933	-1.400
C	2.494	0.866	-0.387
C	3.016	2.181	-0.667
C	3.287	-0.150	0.175
C	2.132	3.190	-1.151
C	4.374	2.500	-0.409
C	4.690	0.147	0.373
C	2.596	4.485	-1.357
C	4.815	3.821	-0.635
C	5.241	1.438	0.085
C	3.936	4.790	-1.096
H	1.903	5.237	-1.720
H	5.843	4.102	-0.439
C	5.583	-0.856	0.850
C	2.774	-1.484	0.545
C	6.944	-0.592	1.033
C	7.465	0.665	0.753
H	8.522	0.871	0.892
C	6.616	1.659	0.283
C	5.107	-2.208	1.153
C	3.692	-2.485	1.005

C	3.210	-3.785	1.347
C	1.415	-1.843	0.482
C	0.948	-3.119	0.828
C	1.854	-4.093	1.252
H	1.540	-5.096	1.517
H	0.690	-1.116	0.157
O	5.923	-3.090	1.545
O	4.045	-4.754	1.773
H	4.958	-4.336	1.776
C	-0.552	-3.382	0.745
H	-0.925	-2.766	-0.083
C	-1.292	-2.865	2.012
H	-1.076	-1.795	2.122
H	-2.371	-2.943	1.822
C	-0.916	-4.839	0.416
H	-0.427	-5.169	-0.507
H	-2.000	-4.928	0.275
H	-0.632	-5.535	1.211
C	-0.956	-3.582	3.324
H	-1.502	-3.126	4.158
H	0.114	-3.521	3.553
H	-1.231	-4.643	3.294
H	-6.586	-2.524	0.109
H	-4.121	-3.316	-3.298
H	-0.751	-2.059	-5.849
H	-2.372	5.219	0.135
H	7.575	-1.396	1.395
H	4.293	5.803	-1.258
H	7.038	2.632	0.058

(*M*,14*S*,14'*S*)-**3a**, conformer a1b1

C	-0.736	-2.805	2.232
C	-1.284	-1.768	1.470
C	-2.665	-1.681	1.197
C	-3.510	-2.698	1.749
C	-2.938	-3.763	2.512
C	-1.566	-3.806	2.742
C	-3.272	-0.584	0.429
C	-4.939	-2.645	1.565
C	-5.523	-1.524	0.868
C	-4.711	-0.468	0.338
C	-5.346	0.650	-0.309
C	-6.753	0.592	-0.559
C	-7.508	-0.458	-0.053
C	-6.932	-1.489	0.686
H	-0.626	-1.006	1.090
H	-1.165	-4.626	3.331
H	-8.575	-0.507	-0.245
C	-2.510	0.368	-0.282
C	-3.105	1.565	-0.789
C	-4.512	1.778	-0.707
C	-4.999	3.071	-0.975
C	-2.251	2.615	-1.239
C	-4.139	4.092	-1.374
C	-2.765	3.870	-1.535
H	-6.035	3.332	-0.834
H	-2.094	4.658	-1.862
O	-5.690	-3.579	2.032
O	-3.692	-4.749	3.041

H	-4.633	-4.545	2.775
O	-7.747	-2.442	1.162
H	-7.149	-3.105	1.619
O	-4.699	5.314	-1.603
H	-4.005	5.946	-1.853
C	-7.519	1.570	-1.428
H	-6.929	1.925	-2.276
H	-7.857	2.451	-0.868
H	-8.416	1.080	-1.816
C	0.764	-2.864	2.496
H	0.935	-3.696	3.193
C	1.532	-3.184	1.198
H	1.423	-2.377	0.465
H	1.154	-4.106	0.742
H	2.600	-3.321	1.392
C	1.274	-1.578	3.190
H	0.617	-1.362	4.042
H	1.178	-0.727	2.503
C	2.722	-1.667	3.687
H	2.997	-0.760	4.237
H	3.434	-1.778	2.862
H	2.857	-2.520	4.363
O	-1.200	0.206	-0.449
O	-0.923	2.434	-1.346
B	-0.402	1.078	-1.344
O	0.957	1.136	-0.809
O	-0.427	0.544	-2.706
C	1.934	0.320	-1.204
C	1.690	-0.540	-2.316
C	3.190	0.355	-0.566

C	0.511	-0.333	-3.093
C	2.672	-1.484	-2.743
C	4.095	-0.736	-0.846
C	0.334	-0.997	-4.299
C	2.485	-2.104	-3.992
C	3.818	-1.711	-1.867
C	1.342	-1.857	-4.751
H	-0.564	-0.814	-4.882
H	3.231	-2.746	-4.430
C	5.274	-0.872	-0.041
C	3.568	1.406	0.388
C	6.121	-1.998	-0.221
C	5.774	-2.984	-1.144
H	6.403	-3.866	-1.200
C	4.649	-2.873	-1.950
C	5.608	0.097	0.977
C	4.761	1.250	1.162
C	5.140	2.264	2.096
C	2.841	2.603	0.548
C	3.229	3.598	1.450
C	4.370	3.415	2.236
H	4.689	4.167	2.951
H	1.962	2.768	-0.052
O	6.664	-0.056	1.695
O	7.240	-2.184	0.496
H	7.291	-1.405	1.125
O	6.247	2.152	2.860
H	6.664	1.281	2.612
O	1.254	-2.496	-5.953
H	0.436	-2.227	-6.403

C	4.365	-4.081	-2.820
H	4.870	-4.955	-2.400
H	4.743	-3.957	-3.842
H	3.297	-4.303	-2.889
C	2.421	4.884	1.573
H	2.893	5.488	2.362
C	0.968	4.598	2.023
H	0.444	4.046	1.231
H	1.001	3.928	2.892
C	2.485	5.700	0.266
H	3.525	5.881	-0.029
H	1.997	6.673	0.382
H	1.989	5.170	-0.556
C	0.166	5.852	2.390
H	-0.828	5.579	2.763
H	0.023	6.515	1.530
H	0.670	6.428	3.176

(*M*,14*S*,14'*S*)-**3a**, conformer a1b2

C	-0.739	-2.780	2.166
C	-1.277	-1.744	1.396
C	-2.659	-1.638	1.132
C	-3.515	-2.635	1.703
C	-2.953	-3.698	2.477
C	-1.581	-3.759	2.698
C	-3.255	-0.542	0.355
C	-4.943	-2.566	1.524
C	-5.516	-1.449	0.811
C	-4.692	-0.410	0.265

C	-5.316	0.706	-0.395
C	-6.723	0.660	-0.646
C	-7.489	-0.375	-0.125
C	-6.924	-1.401	0.629
H	-0.610	-0.998	1.000
H	-1.187	-4.578	3.294
H	-8.557	-0.416	-0.316
C	-2.483	0.396	-0.364
C	-3.065	1.595	-0.881
C	-4.470	1.822	-0.805
C	-4.945	3.116	-1.088
C	-2.200	2.634	-1.336
C	-4.074	4.125	-1.494
C	-2.702	3.890	-1.647
H	-5.979	3.388	-0.953
H	-2.023	4.670	-1.977
O	-5.705	-3.483	2.009
O	-3.719	-4.665	3.025
H	-4.658	-4.452	2.762
O	-7.750	-2.338	1.121
H	-7.158	-3.000	1.589
O	-4.623	5.350	-1.737
H	-3.923	5.973	-1.991
C	-7.478	1.633	-1.529
H	-6.883	1.973	-2.380
H	-7.810	2.524	-0.981
H	-8.379	1.146	-1.913
C	0.766	-2.878	2.393
H	0.928	-3.672	3.135
C	1.479	-3.308	1.094

H	1.364	-2.551	0.310
H	1.071	-4.251	0.714
H	2.551	-3.448	1.272
C	1.392	-1.586	2.962
H	1.264	-0.765	2.244
H	2.475	-1.749	3.044
C	0.838	-1.169	4.328
H	1.344	-0.271	4.698
H	0.981	-1.963	5.072
H	-0.235	-0.952	4.276
O	-1.175	0.218	-0.531
O	-0.873	2.441	-1.434
B	-0.357	1.084	-1.412
O	0.990	1.141	-0.845
O	-0.351	0.543	-2.771
C	1.981	0.333	-1.220
C	1.768	-0.525	-2.341
C	3.221	0.373	-0.552
C	0.603	-0.324	-3.141
C	2.766	-1.459	-2.750
C	4.142	-0.709	-0.819
C	0.457	-0.985	-4.353
C	2.611	-2.075	-4.006
C	3.895	-1.681	-1.851
C	1.481	-1.835	-4.787
H	-0.430	-0.808	-4.954
H	3.371	-2.709	-4.430
C	5.307	-0.838	0.007
C	3.567	1.419	0.420
C	6.167	-1.955	-0.161

C	5.847	-2.939	-1.095
H	6.485	-3.816	-1.143
C	4.738	-2.834	-1.923
C	5.611	0.128	1.037
C	4.749	1.271	1.214
C	5.098	2.280	2.164
C	2.821	2.604	0.581
C	3.179	3.594	1.502
C	4.310	3.419	2.303
H	4.606	4.167	3.033
H	1.949	2.764	-0.030
O	6.655	-0.019	1.774
O	7.273	-2.135	0.577
H	7.304	-1.358	1.211
O	6.192	2.175	2.947
H	6.624	1.310	2.700
O	1.424	-2.469	-5.993
H	0.613	-2.206	-6.459
C	4.482	-4.041	-2.805
H	4.985	-4.913	-2.378
H	4.881	-3.909	-3.818
H	3.418	-4.271	-2.896
C	2.356	4.871	1.618
H	2.783	5.458	2.443
C	0.873	4.605	1.965
H	0.355	5.573	1.984
H	0.408	4.026	1.156
C	2.474	5.720	0.336
H	3.521	5.945	0.105
H	1.940	6.670	0.455

H	2.043	5.198	-0.526
C	0.661	3.888	3.302
H	-0.407	3.757	3.511
H	1.095	4.461	4.131
H	1.126	2.896	3.303

(*M*,14*S*,14'*S*)-**3a**, conformer a1b3

C	-0.909	-2.642	2.451
C	-1.388	-1.629	1.616
C	-2.741	-1.561	1.213
C	-3.630	-2.564	1.710
C	-3.125	-3.613	2.542
C	-1.782	-3.642	2.896
C	-3.274	-0.485	0.368
C	-5.039	-2.510	1.409
C	-5.561	-1.388	0.665
C	-4.701	-0.349	0.180
C	-5.273	0.768	-0.523
C	-6.664	0.734	-0.855
C	-7.466	-0.299	-0.387
C	-6.954	-1.335	0.391
H	-0.706	-0.869	1.277
H	-1.431	-4.452	3.530
H	-8.521	-0.332	-0.643
C	-2.450	0.424	-0.328
C	-2.988	1.618	-0.902
C	-4.391	1.869	-0.895
C	-4.828	3.168	-1.213
C	-2.084	2.634	-1.335

C	-3.921	4.157	-1.589
C	-2.549	3.895	-1.680
H	-5.863	3.460	-1.129
H	-1.842	4.658	-1.993
O	-5.829	-3.439	1.820
O	-3.922	-4.596	3.015
H	-4.834	-4.400	2.663
O	-7.811	-2.275	0.818
H	-7.253	-2.945	1.312
O	-4.436	5.389	-1.867
H	-3.715	5.997	-2.097
C	-7.359	1.720	-1.772
H	-6.716	2.052	-2.591
H	-7.704	2.615	-1.239
H	-8.247	1.248	-2.203
C	0.538	-2.683	2.932
H	0.791	-3.747	3.044
C	1.551	-2.087	1.944
H	1.422	-1.009	1.803
H	1.467	-2.560	0.959
H	2.570	-2.249	2.311
C	0.679	-2.072	4.355
H	1.705	-2.262	4.699
H	0.018	-2.625	5.035
C	0.376	-0.574	4.472
H	0.481	-0.244	5.512
H	-0.647	-0.346	4.151
H	1.059	0.031	3.865
O	-1.137	0.224	-0.421
O	-0.760	2.408	-1.381

B	-0.296	1.029	-1.340
O	1.062	1.043	-0.803
O	-0.348	0.459	-2.685
C	2.037	0.237	-1.222
C	1.771	-0.632	-2.321
C	3.309	0.288	-0.617
C	0.575	-0.432	-3.075
C	2.741	-1.583	-2.757
C	4.216	-0.797	-0.915
C	0.367	-1.119	-4.264
C	2.522	-2.225	-3.990
C	3.912	-1.791	-1.911
C	1.360	-1.991	-4.723
H	-0.543	-0.942	-4.829
H	3.257	-2.876	-4.434
C	5.428	-0.907	-0.157
C	3.702	1.347	0.321
C	6.279	-2.026	-0.352
C	5.905	-3.034	-1.238
H	6.539	-3.913	-1.302
C	4.748	-2.948	-2.002
C	5.790	0.082	0.832
C	4.930	1.220	1.043
C	5.324	2.246	1.959
C	2.952	2.528	0.513
C	3.351	3.531	1.399
C	4.534	3.377	2.131
H	4.868	4.140	2.829
H	2.047	2.666	-0.049
O	6.880	-0.043	1.503

O	7.429	-2.187	0.322
H	7.497	-1.394	0.933
O	6.469	2.165	2.671
H	6.894	1.302	2.408
O	1.241	-2.652	-5.910
H	0.412	-2.390	-6.345
C	4.437	-4.178	-2.832
H	4.956	-5.041	-2.406
H	4.784	-4.080	-3.868
H	3.368	-4.401	-2.861
C	2.511	4.786	1.620
H	3.210	5.572	1.936
C	1.522	4.609	2.807
H	2.102	4.348	3.702
H	1.069	5.589	3.009
C	1.807	5.298	0.352
H	2.529	5.473	-0.454
H	1.303	6.248	0.565
H	1.051	4.603	-0.025
C	0.411	3.571	2.611
H	-0.219	3.515	3.506
H	0.820	2.572	2.427
H	-0.241	3.823	1.767

(*M*,14*S*,14'*S*)-**3a**, conformer a2b1

C	-0.856	-2.700	-2.234
C	-1.383	-1.628	-1.511
C	-2.758	-1.522	-1.208
C	-3.619	-2.554	-1.697

C	-3.067	-3.661	-2.417
C	-1.703	-3.725	-2.673
C	-3.339	-0.389	-0.478
C	-5.045	-2.471	-1.500
C	-5.607	-1.302	-0.867
C	-4.774	-0.236	-0.392
C	-5.381	0.926	0.200
C	-6.790	0.917	0.441
C	-7.568	-0.141	-0.011
C	-7.014	-1.226	-0.688
H	-0.708	-0.851	-1.191
H	-1.326	-4.578	-3.230
H	-8.637	-0.154	0.176
C	-2.554	0.562	0.206
C	-3.117	1.792	0.667
C	-4.516	2.046	0.559
C	-4.962	3.363	0.770
C	-2.233	2.830	1.090
C	-4.073	4.370	1.141
C	-2.710	4.111	1.330
H	-5.988	3.653	0.607
H	-2.018	4.890	1.638
O	-5.815	-3.419	-1.906
O	-3.841	-4.666	-2.880
H	-4.774	-4.440	-2.609
O	-7.849	-2.188	-1.110
H	-7.265	-2.890	-1.525
O	-4.596	5.618	1.314
H	-3.884	6.237	1.548
C	-7.537	1.962	1.247

H	-6.948	2.339	2.087
H	-7.835	2.824	0.638
H	-8.457	1.522	1.643
C	0.634	-2.742	-2.546
H	1.084	-1.846	-2.096
C	0.884	-2.676	-4.066
H	0.514	-3.576	-4.571
H	0.376	-1.811	-4.505
H	1.953	-2.583	-4.287
C	1.307	-3.970	-1.886
H	1.034	-3.981	-0.823
H	0.889	-4.889	-2.319
C	2.835	-3.997	-2.010
H	3.252	-4.841	-1.448
H	3.161	-4.101	-3.050
H	3.281	-3.079	-1.609
O	-1.252	0.364	0.391
O	-0.914	2.607	1.227
B	-0.452	1.232	1.289
O	0.929	1.208	0.809
O	-0.552	0.748	2.666
C	1.829	0.323	1.239
C	1.485	-0.501	2.353
C	3.103	0.254	0.638
C	0.303	-0.194	3.091
C	2.375	-1.512	2.820
C	3.919	-0.892	0.973
C	0.038	-0.828	4.297
C	2.102	-2.104	4.067
C	3.529	-1.835	1.988

C	0.960	-1.760	4.788
H	-0.861	-0.570	4.849
H	2.784	-2.797	4.533
C	5.127	-1.116	0.233
C	3.589	1.255	-0.321
C	5.885	-2.295	0.464
C	5.421	-3.250	1.366
H	5.981	-4.175	1.457
C	4.267	-3.054	2.114
C	5.580	-0.180	-0.769
C	4.815	1.016	-1.019
C	5.304	1.985	-1.953
C	2.935	2.482	-0.566
C	3.428	3.428	-1.468
C	4.609	3.168	-2.172
H	5.017	3.876	-2.887
H	2.025	2.714	-0.038
O	6.667	-0.405	-1.418
O	7.028	-2.560	-0.188
H	7.167	-1.789	-0.814
O	6.448	1.793	-2.644
H	6.800	0.907	-2.350
O	0.784	-2.376	5.992
H	-0.024	-2.039	6.412
C	3.848	-4.236	2.965
H	4.290	-5.149	2.556
H	4.199	-4.150	4.000
H	2.763	-4.364	2.994
C	2.678	4.738	-1.669
H	1.785	4.700	-1.030

C	3.528	5.943	-1.195
H	4.407	6.045	-1.847
H	3.915	5.718	-0.192
C	2.200	4.892	-3.126
H	1.612	4.021	-3.437
H	1.570	5.779	-3.243
H	3.047	4.989	-3.816
C	2.767	7.272	-1.149
H	3.400	8.066	-0.736
H	2.442	7.596	-2.144
H	1.874	7.194	-0.516

(*M*,14*S*,14'*S*)-**3a**, conformer a2b2

C	-0.928	-2.714	2.201
C	-1.425	-1.629	1.477
C	-2.799	-1.479	1.184
C	-3.688	-2.483	1.679
C	-3.167	-3.601	2.405
C	-1.804	-3.707	2.655
C	-3.348	-0.330	0.453
C	-5.111	-2.364	1.479
C	-5.640	-1.187	0.831
C	-4.778	-0.144	0.357
C	-5.355	1.030	-0.242
C	-6.761	1.050	-0.500
C	-7.567	0.011	-0.051
C	-7.044	-1.081	0.640
H	-0.727	-0.876	1.149
H	-1.452	-4.568	3.214

H	-8.634	0.020	-0.250
C	-2.537	0.608	-0.221
C	-3.069	1.852	-0.681
C	-4.464	2.133	-0.589
C	-4.883	3.459	-0.802
C	-2.160	2.874	-1.086
C	-3.970	4.450	-1.157
C	-2.610	4.165	-1.329
H	-5.905	3.768	-0.651
H	-1.899	4.931	-1.624
O	-5.906	-3.288	1.892
O	-3.969	-4.579	2.878
H	-4.896	-4.328	2.606
O	-7.905	-2.020	1.062
H	-7.340	-2.730	1.491
O	-4.466	5.708	-1.333
H	-3.739	6.314	-1.553
C	-7.475	2.106	-1.320
H	-6.865	2.472	-2.149
H	-7.770	2.973	-0.717
H	-8.395	1.681	-1.733
C	0.561	-2.794	2.514
H	1.048	-1.963	1.986
C	0.817	-2.600	4.022
H	0.369	-3.411	4.609
H	0.394	-1.654	4.378
H	1.894	-2.591	4.230
C	1.213	-4.102	2.012
H	0.762	-4.958	2.533
H	2.269	-4.087	2.313

C	1.120	-4.312	0.498
H	1.623	-5.239	0.200
H	1.593	-3.486	-0.046
H	0.077	-4.375	0.166
O	-1.238	0.383	-0.396
O	-0.844	2.628	-1.202
B	-0.400	1.247	-1.261
O	0.965	1.201	-0.738
O	-0.465	0.775	-2.644
C	1.879	0.329	-1.162
C	1.571	-0.469	-2.305
C	3.135	0.249	-0.525
C	0.408	-0.150	-3.068
C	2.480	-1.464	-2.772
C	3.966	-0.886	-0.863
C	0.180	-0.756	-4.297
C	2.247	-2.024	-4.041
C	3.611	-1.803	-1.915
C	1.122	-1.669	-4.785
H	-0.705	-0.490	-4.867
H	2.945	-2.701	-4.505
C	5.150	-1.126	-0.092
C	3.588	1.227	0.473
C	5.920	-2.296	-0.329
C	5.489	-3.227	-1.272
H	6.056	-4.148	-1.369
C	4.359	-3.015	-2.051
C	5.568	-0.215	0.948
C	4.793	0.974	1.202
C	5.250	1.921	2.173

C	2.924	2.447	0.727
C	3.385	3.371	1.666
C	4.546	3.097	2.399
H	4.930	3.788	3.144
H	2.030	2.690	0.177
O	6.634	-0.455	1.627
O	7.040	-2.576	0.354
H	7.156	-1.821	1.004
O	6.374	1.716	2.893
H	6.736	0.836	2.590
O	0.985	-2.256	-6.008
H	0.186	-1.914	-6.443
C	3.975	-4.174	-2.949
H	4.412	-5.096	-2.554
H	4.357	-4.055	-3.970
H	2.893	-4.309	-3.015
C	2.613	4.664	1.897
H	1.763	4.661	1.202
C	3.452	5.926	1.590
H	2.842	6.804	1.837
H	4.320	5.959	2.263
C	2.042	4.723	3.328
H	1.417	3.849	3.541
H	1.428	5.622	3.458
H	2.843	4.754	4.077
C	3.923	6.030	0.136
H	4.485	6.956	-0.029
H	3.071	6.029	-0.556
H	4.573	5.191	-0.137

(*M*,14*S*,14'*S*)-**3a**, conformer a2b3

C	-0.958	-2.688	2.218
C	-1.451	-1.584	1.516
C	-2.819	-1.427	1.210
C	-3.716	-2.438	1.680
C	-3.202	-3.572	2.382
C	-1.839	-3.689	2.639
C	-3.360	-0.264	0.497
C	-5.138	-2.304	1.484
C	-5.659	-1.106	0.867
C	-4.789	-0.062	0.410
C	-5.355	1.128	-0.167
C	-6.764	1.169	-0.411
C	-7.577	0.131	0.024
C	-7.062	-0.981	0.687
H	-0.751	-0.821	1.216
H	-1.499	-4.562	3.184
H	-8.646	0.156	-0.166
C	-2.543	0.670	-0.172
C	-3.063	1.924	-0.620
C	-4.453	2.223	-0.510
C	-4.855	3.558	-0.703
C	-2.145	2.936	-1.030
C	-3.932	4.539	-1.060
C	-2.579	4.235	-1.255
H	-5.870	3.880	-0.535
H	-1.862	4.994	-1.554
O	-5.939	-3.231	1.876
O	-4.009	-4.557	2.831

H	-4.934	-4.296	2.565
O	-7.930	-1.920	1.094
H	-7.371	-2.647	1.501
O	-4.411	5.806	-1.215
H	-3.677	6.404	-1.433
C	-7.473	2.250	-1.204
H	-6.868	2.621	-2.035
H	-7.745	3.111	-0.582
H	-8.405	1.847	-1.611
C	0.543	-2.770	2.478
H	0.899	-1.733	2.541
C	0.912	-3.450	3.806
H	0.644	-4.512	3.825
H	0.409	-2.965	4.650
H	1.993	-3.383	3.972
C	1.299	-3.394	1.270
H	2.376	-3.288	1.463
H	1.086	-2.787	0.381
C	0.984	-4.862	0.963
H	1.553	-5.196	0.088
H	-0.080	-5.007	0.744
H	1.247	-5.522	1.797
O	-1.245	0.434	-0.353
O	-0.835	2.671	-1.169
B	-0.411	1.285	-1.234
O	0.963	1.221	-0.736
O	-0.505	0.811	-2.615
C	1.845	0.316	-1.159
C	1.495	-0.491	-2.284
C	3.108	0.208	-0.541

C	0.332	-0.148	-3.037
C	2.365	-1.522	-2.747
C	3.897	-0.959	-0.872
C	0.068	-0.766	-4.252
C	2.096	-2.095	-4.004
C	3.498	-1.882	-1.900
C	0.973	-1.717	-4.737
H	-0.816	-0.481	-4.814
H	2.767	-2.802	-4.465
C	5.084	-1.224	-0.112
C	3.606	1.187	0.435
C	5.810	-2.424	-0.337
C	5.334	-3.358	-1.255
H	5.867	-4.300	-1.341
C	4.201	-3.121	-2.022
C	5.546	-0.310	0.906
C	4.813	0.907	1.152
C	5.309	1.850	2.104
C	2.982	2.427	0.684
C	3.484	3.353	1.605
C	4.643	3.052	2.325
H	5.058	3.733	3.061
H	2.084	2.687	0.148
O	6.614	-0.572	1.573
O	6.930	-2.729	0.336
H	7.081	-1.967	0.970
O	6.434	1.621	2.815
H	6.767	0.728	2.519
O	0.800	-2.318	-5.949
H	0.006	-1.957	-6.378

C	3.763	-4.284	-2.891
H	4.173	-5.213	-2.483
H	4.132	-4.200	-3.920
H	2.675	-4.382	-2.937
C	2.751	4.681	1.770
H	1.692	4.474	1.563
C	3.190	5.715	0.694
H	2.997	5.282	-0.296
H	2.528	6.587	0.784
C	2.822	5.261	3.192
H	2.458	4.539	3.931
H	2.198	6.160	3.259
H	3.839	5.548	3.480
C	4.649	6.179	0.762
H	4.859	6.891	-0.045
H	5.344	5.339	0.653
H	4.877	6.681	1.709

(*P*,14*S*,14'*S*)-**3b**, conformer a1b1

C	-3.364	3.401	1.704
C	-2.920	2.458	0.771
C	-3.635	1.275	0.495
C	-4.872	1.077	1.188
C	-5.310	2.038	2.151
C	-4.554	3.180	2.402
C	-3.201	0.281	-0.496
C	-5.698	-0.069	0.899
C	-5.297	-0.991	-0.138
C	-4.078	-0.806	-0.872

C	-3.738	-1.731	-1.920
C	-4.538	-2.904	-2.087
C	-5.701	-3.066	-1.344
C	-6.115	-2.119	-0.408
H	-2.003	2.653	0.241
H	-4.917	3.891	3.138
H	-6.310	-3.956	-1.466
C	-1.924	0.301	-1.092
C	-1.626	-0.492	-2.240
C	-2.567	-1.440	-2.741
C	-2.323	-2.001	-4.008
C	-0.433	-0.213	-2.972
C	-1.165	-1.690	-4.718
C	-0.200	-0.819	-4.200
H	-3.038	-2.643	-4.497
H	0.708	-0.583	-4.747
O	-6.794	-0.260	1.545
O	-6.461	1.886	2.839
H	-6.858	1.027	2.520
O	-7.269	-2.348	0.237
H	-7.368	-1.594	0.890
O	-1.019	-2.274	-5.942
H	-0.195	-1.964	-6.352
C	-4.184	-4.075	-2.982
H	-3.108	-4.262	-3.017
H	-4.529	-3.931	-4.013
H	-4.677	-4.977	-2.608
C	-2.565	4.675	1.950
H	-3.075	5.227	2.751
C	-1.137	4.361	2.439

H	-0.548	3.865	1.659
H	-1.162	3.700	3.312
H	-0.609	5.276	2.727
C	-2.576	5.580	0.693
H	-3.615	5.684	0.354
H	-2.036	5.074	-0.119
C	-1.981	6.975	0.914
H	-2.089	7.588	0.012
H	-0.914	6.934	1.157
H	-2.491	7.497	1.733
O	-0.975	1.111	-0.620
O	0.462	0.678	-2.521
B	0.390	1.142	-1.136
O	1.221	0.268	-0.272
O	0.850	2.520	-1.064
C	2.533	0.461	-0.151
C	3.075	1.695	-0.630
C	3.350	-0.496	0.484
C	2.174	2.740	-0.993
C	4.478	1.944	-0.594
C	4.779	-0.347	0.319
C	2.642	4.024	-1.240
C	4.918	3.263	-0.811
C	5.357	0.818	-0.297
C	4.014	4.277	-1.119
H	1.937	4.808	-1.501
H	5.951	3.547	-0.698
C	5.636	-1.418	0.737
C	2.808	-1.630	1.244
C	7.030	-1.347	0.476

C	7.548	-0.259	-0.224
H	8.604	-0.275	-0.475
C	6.749	0.806	-0.621
C	5.108	-2.588	1.398
C	3.696	-2.665	1.681
C	3.187	-3.766	2.437
C	1.454	-1.729	1.627
C	0.971	-2.797	2.390
C	1.840	-3.821	2.779
H	1.488	-4.665	3.365
H	0.769	-0.950	1.338
O	5.895	-3.541	1.754
O	7.885	-2.314	0.843
H	7.323	-3.016	1.288
O	3.982	-4.773	2.856
H	4.898	-4.553	2.527
O	4.530	5.526	-1.303
H	3.810	6.149	-1.492
C	7.450	1.855	-1.460
H	8.338	1.415	-1.923
H	7.796	2.707	-0.860
H	6.811	2.250	-2.253
C	-0.498	-2.874	2.787
H	-0.591	-3.702	3.504
C	-1.375	-3.235	1.562
H	-1.350	-2.403	0.845
H	-0.919	-4.094	1.053
C	-0.976	-1.593	3.496
H	-0.317	-1.340	4.334
H	-1.988	-1.721	3.895

H	-0.995	-0.736	2.812
C	-2.828	-3.577	1.910
H	-3.377	-3.888	1.014
H	-3.360	-2.722	2.339
H	-2.877	-4.400	2.635

(*P*,14*S*,14'*S*)-**3b**, conformer a1b2

C	-3.474	3.315	1.759
C	-3.006	2.405	0.806
C	-3.659	1.183	0.546
C	-4.862	0.911	1.271
C	-5.323	1.838	2.255
C	-4.625	3.019	2.493
C	-3.194	0.220	-0.460
C	-5.633	-0.275	0.990
C	-5.215	-1.158	-0.074
C	-4.025	-0.903	-0.833
C	-3.662	-1.795	-1.903
C	-4.418	-2.997	-2.081
C	-5.556	-3.223	-1.316
C	-5.986	-2.319	-0.347
H	-2.119	2.655	0.249
H	-5.005	3.703	3.246
H	-6.128	-4.137	-1.444
C	-1.924	0.300	-1.065
C	-1.603	-0.469	-2.223
C	-2.513	-1.444	-2.732
C	-2.258	-1.975	-4.010
C	-0.424	-0.139	-2.956

C	-1.115	-1.613	-4.721
C	-0.177	-0.717	-4.194
H	-2.951	-2.635	-4.504
H	0.720	-0.443	-4.742
O	-6.696	-0.534	1.665
O	-6.444	1.616	2.975
H	-6.802	0.741	2.658
O	-7.110	-2.615	0.324
H	-7.224	-1.880	0.997
O	-0.957	-2.172	-5.955
H	-0.145	-1.830	-6.363
C	-4.039	-4.131	-3.012
H	-2.958	-4.283	-3.064
H	-4.400	-3.969	-4.035
H	-4.498	-5.058	-2.658
C	-2.728	4.623	2.002
H	-3.264	5.160	2.797
C	-1.293	4.366	2.500
H	-0.689	3.864	1.736
H	-1.291	3.737	3.397
H	-0.800	5.313	2.748
C	-2.719	5.539	0.756
H	-2.197	5.027	-0.064
H	-2.116	6.426	0.995
C	-4.108	5.981	0.288
H	-4.035	6.650	-0.577
H	-4.640	6.520	1.082
H	-4.725	5.124	-0.003
O	-1.007	1.144	-0.591
O	0.444	0.772	-2.494

B	0.359	1.214	-1.102
O	1.208	0.347	-0.247
O	0.786	2.601	-1.008
C	2.516	0.569	-0.125
C	3.029	1.822	-0.584
C	3.356	-0.379	0.494
C	2.104	2.852	-0.929
C	4.426	2.104	-0.541
C	4.780	-0.198	0.323
C	2.541	4.151	-1.151
C	4.834	3.437	-0.731
C	5.331	0.992	-0.268
C	3.906	4.435	-1.021
H	1.818	4.923	-1.398
H	5.861	3.744	-0.611
C	5.659	-1.264	0.709
C	2.841	-1.534	1.240
C	7.049	-1.159	0.444
C	7.544	-0.042	-0.227
H	8.599	-0.030	-0.481
C	6.723	1.017	-0.594
C	5.156	-2.461	1.341
C	3.749	-2.566	1.639
C	3.265	-3.691	2.376
C	1.496	-1.655	1.645
C	1.038	-2.746	2.391
C	1.924	-3.770	2.739
H	1.592	-4.632	3.310
H	0.799	-0.874	1.389
O	5.961	-3.411	1.661

O	7.924	-2.120	0.779
H	7.378	-2.845	1.206
O	4.079	-4.698	2.758
H	4.987	-4.458	2.421
O	4.392	5.700	-1.177
H	3.656	6.310	-1.350
C	7.401	2.103	-1.404
H	8.301	1.695	-1.875
H	7.724	2.947	-0.782
H	6.755	2.502	-2.190
C	-0.414	-2.817	2.849
H	-0.530	-3.755	3.410
C	-1.411	-2.863	1.670
H	-2.427	-2.848	2.086
H	-1.312	-1.946	1.074
C	-0.752	-1.660	3.809
H	-0.066	-1.640	4.663
H	-1.773	-1.770	4.195
H	-0.688	-0.690	3.304
C	-1.254	-4.088	0.763
H	-2.005	-4.082	-0.034
H	-1.376	-5.019	1.332
H	-0.265	-4.113	0.292

(*P*,14*S*,14'*S*)-**3b**, conformer a1b3

C	-3.258	3.253	2.021
C	-2.861	2.344	1.036
C	-3.638	1.216	0.689
C	-4.881	1.037	1.375

C	-5.273	1.965	2.391
C	-4.463	3.051	2.703
C	-3.257	0.264	-0.365
C	-5.755	-0.059	1.037
C	-5.397	-0.944	-0.045
C	-4.180	-0.768	-0.784
C	-3.890	-1.648	-1.884
C	-4.735	-2.783	-2.097
C	-5.893	-2.939	-1.348
C	-6.261	-2.026	-0.361
H	-1.933	2.514	0.522
H	-4.789	3.733	3.483
H	-6.535	-3.801	-1.504
C	-1.993	0.278	-0.991
C	-1.745	-0.462	-2.186
C	-2.724	-1.356	-2.712
C	-2.520	-1.866	-4.007
C	-0.556	-0.188	-2.925
C	-1.362	-1.563	-4.721
C	-0.361	-0.747	-4.181
H	-3.263	-2.462	-4.512
H	0.545	-0.516	-4.733
O	-6.854	-0.237	1.682
O	-6.428	1.828	3.075
H	-6.862	1.004	2.716
O	-7.416	-2.243	0.286
H	-7.481	-1.516	0.975
O	-1.254	-2.097	-5.972
H	-0.424	-1.800	-6.379
C	-4.433	-3.922	-3.050

H	-3.364	-4.143	-3.110
H	-4.787	-3.720	-4.068
H	-4.951	-4.824	-2.710
C	-2.423	4.484	2.359
H	-2.691	4.760	3.388
C	-0.906	4.226	2.351
H	-0.525	3.963	1.360
H	-0.646	3.410	3.033
H	-0.374	5.126	2.681
C	-2.817	5.710	1.488
H	-2.296	6.586	1.898
H	-3.890	5.898	1.626
C	-2.517	5.603	-0.011
H	-2.832	6.517	-0.527
H	-3.047	4.762	-0.470
H	-1.447	5.469	-0.206
O	-1.009	1.030	-0.500
O	0.375	0.653	-2.455
B	0.334	1.106	-1.066
O	1.221	0.256	-0.236
O	0.755	2.499	-1.000
C	2.528	0.495	-0.146
C	3.017	1.744	-0.638
C	3.393	-0.433	0.471
C	2.073	2.761	-0.973
C	4.412	2.038	-0.644
C	4.811	-0.240	0.263
C	2.493	4.058	-1.234
C	4.804	3.369	-0.875
C	5.334	0.940	-0.372

C	3.859	4.355	-1.156
H	1.756	4.820	-1.472
H	5.831	3.685	-0.795
C	5.712	-1.283	0.658
C	2.910	-1.580	1.249
C	7.094	-1.171	0.355
C	7.558	-0.070	-0.364
H	8.606	-0.055	-0.646
C	6.715	0.969	-0.738
C	5.239	-2.466	1.339
C	3.839	-2.584	1.663
C	3.384	-3.697	2.438
C	1.568	-1.716	1.671
C	1.137	-2.795	2.445
C	2.051	-3.790	2.816
H	1.742	-4.640	3.418
H	0.859	-0.953	1.402
O	6.066	-3.393	1.676
O	7.989	-2.111	0.699
H	7.462	-2.827	1.164
O	4.223	-4.675	2.843
H	5.121	-4.428	2.487
O	4.330	5.619	-1.357
H	3.585	6.219	-1.524
C	7.359	2.037	-1.599
H	8.246	1.623	-2.088
H	7.696	2.900	-1.011
H	6.685	2.410	-2.374
C	-0.314	-2.950	2.894
H	-0.275	-3.361	3.912

C	-1.055	-4.019	2.042
H	-0.509	-4.968	2.129
H	-2.039	-4.188	2.499
C	-1.100	-1.632	2.977
H	-0.588	-0.907	3.620
H	-2.092	-1.819	3.403
H	-1.247	-1.164	1.999
C	-1.234	-3.680	0.559
H	-1.727	-4.507	0.035
H	-0.270	-3.501	0.070
H	-1.851	-2.787	0.415

(*P*,14*S*,14'*S*)-**3b**, conformer a2b1

C	-3.416	3.657	1.067
C	-2.914	2.653	0.237
C	-3.526	1.386	0.125
C	-4.720	1.165	0.881
C	-5.217	2.194	1.744
C	-4.564	3.418	1.831
C	-3.031	0.323	-0.760
C	-5.447	-0.074	0.758
C	-4.995	-1.071	-0.184
C	-3.818	-0.870	-0.979
C	-3.427	-1.877	-1.930
C	-4.134	-3.120	-1.943
C	-5.256	-3.293	-1.144
C	-5.720	-2.287	-0.298
H	-2.032	2.869	-0.343
H	-4.977	4.172	2.493

H	-5.791	-4.237	-1.148
C	-1.769	0.376	-1.387
C	-1.421	-0.531	-2.434
C	-2.297	-1.591	-2.809
C	-2.033	-2.266	-4.014
C	-0.251	-0.263	-3.208
C	-0.908	-1.956	-4.777
C	0.006	-0.977	-4.371
H	-2.706	-3.006	-4.416
H	0.894	-0.748	-4.952
O	-6.502	-0.283	1.463
O	-6.330	2.023	2.488
H	-6.655	1.102	2.286
O	-6.830	-2.537	0.414
H	-6.974	-1.725	0.984
O	-0.739	-2.657	-5.935
H	0.063	-2.346	-6.387
C	-3.711	-4.348	-2.726
H	-2.625	-4.458	-2.772
H	-4.087	-4.335	-3.756
H	-4.126	-5.240	-2.249
C	-2.708	5.004	1.134
H	-1.858	4.955	0.439
C	-3.630	6.146	0.664
H	-4.479	6.279	1.345
H	-4.030	5.937	-0.335
H	-3.088	7.096	0.614
C	-2.128	5.256	2.548
H	-1.572	4.361	2.857
H	-2.953	5.367	3.264

C	-1.201	6.473	2.639
H	-0.768	6.554	3.643
H	-1.729	7.410	2.433
H	-0.372	6.392	1.925
O	-0.885	1.316	-1.050
O	0.601	0.711	-2.854
B	0.508	1.252	-1.496
O	1.230	0.366	-0.553
O	1.045	2.597	-1.472
C	2.524	0.512	-0.288
C	3.168	1.704	-0.739
C	3.217	-0.457	0.467
C	2.361	2.764	-1.252
C	4.566	1.902	-0.541
C	4.659	-0.360	0.487
C	2.911	4.015	-1.499
C	5.084	3.192	-0.760
C	5.355	0.760	-0.088
C	4.268	4.223	-1.222
H	2.277	4.811	-1.877
H	6.107	3.444	-0.532
C	5.412	-1.441	1.054
C	2.538	-1.557	1.163
C	6.830	-1.422	0.983
C	7.476	-0.381	0.318
H	8.554	-0.441	0.212
C	6.776	0.690	-0.225
C	4.759	-2.572	1.671
C	3.319	-2.606	1.743
C	2.670	-3.685	2.423

C	1.138	-1.621	1.339
C	0.514	-2.671	2.015
C	1.286	-3.712	2.546
H	0.834	-4.549	3.069
H	0.519	-0.831	0.949
O	5.459	-3.530	2.168
O	7.593	-2.399	1.497
H	6.952	-3.065	1.887
O	3.368	-4.703	2.971
H	4.328	-4.505	2.788
O	4.856	5.441	-1.396
H	4.190	6.081	-1.696
C	7.623	1.674	-1.007
H	8.548	1.183	-1.322
H	7.915	2.544	-0.406
H	7.112	2.046	-1.898
C	-1.001	-2.670	2.171
H	-1.377	-1.774	1.659
C	-1.406	-2.551	3.660
H	-1.081	-3.452	4.198
H	-0.849	-1.713	4.102
C	-1.634	-3.894	1.481
H	-1.309	-3.962	0.437
H	-2.727	-3.827	1.484
H	-1.353	-4.827	1.983
C	-2.905	-2.328	3.890
H	-3.115	-2.175	4.955
H	-3.504	-3.182	3.556
H	-3.260	-1.441	3.350

(*P*,14*S*,14'*S*)-**3b**, conformer a2b2

C	-3.493	3.618	1.125
C	-2.987	2.630	0.278
C	-3.597	1.363	0.142
C	-4.795	1.129	0.889
C	-5.296	2.142	1.767
C	-4.644	3.364	1.880
C	-3.094	0.315	-0.755
C	-5.517	-0.111	0.745
C	-5.053	-1.096	-0.203
C	-3.874	-0.881	-0.989
C	-3.472	-1.876	-1.947
C	-4.169	-3.125	-1.974
C	-5.295	-3.311	-1.182
C	-5.771	-2.315	-0.331
H	-2.103	2.857	-0.293
H	-5.061	4.106	2.554
H	-5.823	-4.260	-1.196
C	-1.832	0.383	-1.380
C	-1.476	-0.510	-2.436
C	-2.343	-1.574	-2.821
C	-2.072	-2.237	-4.032
C	-0.309	-0.225	-3.208
C	-0.949	-1.912	-4.791
C	-0.045	-0.927	-4.376
H	-2.738	-2.980	-4.441
H	0.842	-0.685	-4.955
O	-6.576	-0.331	1.441
O	-6.413	1.957	2.502

H	-6.737	1.040	2.282
O	-6.883	-2.578	0.371
H	-7.036	-1.772	0.947
O	-0.772	-2.601	-5.954
H	0.028	-2.280	-6.402
C	-3.733	-4.343	-2.763
H	-2.646	-4.443	-2.808
H	-4.108	-4.328	-3.794
H	-4.141	-5.243	-2.293
C	-2.797	4.970	1.210
H	-1.930	4.931	0.536
C	-3.716	6.107	0.721
H	-4.592	6.219	1.371
H	-4.075	5.916	-0.296
H	-3.177	7.061	0.719
C	-2.259	5.273	2.628
H	-3.099	5.311	3.335
H	-1.826	6.282	2.615
C	-1.208	4.277	3.128
H	-0.841	4.561	4.121
H	-0.345	4.239	2.451
H	-1.617	3.263	3.200
O	-0.955	1.326	-1.032
O	0.533	0.755	-2.846
B	0.436	1.286	-1.485
O	1.178	0.409	-0.550
O	0.953	2.639	-1.456
C	2.477	0.566	-0.314
C	3.100	1.765	-0.778
C	3.197	-0.397	0.423

C	2.272	2.820	-1.267
C	4.501	1.974	-0.613
C	4.638	-0.292	0.402
C	2.804	4.076	-1.520
C	5.002	3.269	-0.840
C	5.310	0.836	-0.186
C	4.166	4.294	-1.277
H	2.154	4.869	-1.879
H	6.029	3.529	-0.638
C	5.412	-1.372	0.940
C	2.544	-1.500	1.138
C	6.828	-1.345	0.830
C	7.449	-0.294	0.157
H	8.525	-0.345	0.023
C	6.729	0.776	-0.359
C	4.782	-2.512	1.565
C	3.346	-2.551	1.683
C	2.721	-3.634	2.380
C	1.152	-1.561	1.367
C	0.553	-2.613	2.062
C	1.342	-3.660	2.554
H	0.910	-4.500	3.089
H	0.520	-0.767	1.006
O	5.500	-3.474	2.029
O	7.610	-2.322	1.314
H	6.984	-2.996	1.713
O	3.438	-4.656	2.895
H	4.391	-4.457	2.679
O	4.739	5.518	-1.461
H	4.061	6.153	-1.742

C	7.548	1.773	-1.154
H	8.471	1.293	-1.491
H	7.845	2.643	-0.555
H	7.015	2.144	-2.033
C	-0.957	-2.621	2.264
H	-1.347	-1.692	1.827
C	-1.362	-2.632	3.756
H	-2.457	-2.696	3.808
H	-0.981	-3.547	4.230
C	-1.612	-3.795	1.510
H	-1.358	-3.771	0.444
H	-2.704	-3.747	1.599
H	-1.285	-4.761	1.912
C	-0.888	-1.406	4.543
H	-1.228	-1.453	5.584
H	-1.280	-0.480	4.104
H	0.206	-1.333	4.551

(*P*,14*S*,14'*S*)-**3b**, conformer a2b3

C	-3.457	3.686	1.067
C	-2.973	2.690	0.211
C	-3.577	1.422	0.104
C	-4.759	1.190	0.877
C	-5.240	2.207	1.758
C	-4.585	3.433	1.851
C	-3.089	0.368	-0.794
C	-5.489	-0.046	0.744
C	-5.051	-1.030	-0.219
C	-3.880	-0.821	-1.021

C	-3.496	-1.817	-1.986
C	-4.208	-3.058	-2.012
C	-5.327	-3.236	-1.208
C	-5.780	-2.241	-0.344
H	-2.110	2.918	-0.392
H	-4.993	4.175	2.528
H	-5.865	-4.178	-1.221
C	-1.828	0.423	-1.420
C	-1.484	-0.473	-2.477
C	-2.365	-1.526	-2.863
C	-2.103	-2.190	-4.076
C	-0.315	-0.200	-3.250
C	-0.978	-1.876	-4.836
C	-0.061	-0.903	-4.420
H	-2.779	-2.923	-4.485
H	0.828	-0.671	-5.000
O	-6.535	-0.263	1.461
O	-6.341	2.029	2.518
H	-6.672	1.111	2.308
O	-6.884	-2.499	0.375
H	-7.020	-1.696	0.960
O	-0.811	-2.565	-6.000
H	-0.008	-2.252	-6.449
C	-3.795	-4.277	-2.812
H	-2.709	-4.394	-2.861
H	-4.171	-4.247	-3.842
H	-4.216	-5.173	-2.347
C	-2.706	5.014	1.119
H	-2.393	5.227	0.087
C	-3.558	6.205	1.584

H	-3.876	6.114	2.627
H	-4.459	6.311	0.969
H	-2.979	7.132	1.498
C	-1.388	4.886	1.935
H	-0.839	5.832	1.832
H	-0.766	4.115	1.464
C	-1.556	4.557	3.423
H	-0.577	4.466	3.906
H	-2.087	3.609	3.565
H	-2.114	5.335	3.955
O	-0.941	1.357	-1.073
O	0.540	0.769	-2.886
B	0.450	1.297	-1.523
O	1.177	0.404	-0.591
O	0.986	2.642	-1.487
C	2.474	0.544	-0.338
C	3.115	1.742	-0.782
C	3.174	-0.433	0.400
C	2.304	2.807	-1.276
C	4.514	1.938	-0.594
C	4.616	-0.335	0.410
C	2.852	4.060	-1.515
C	5.031	3.230	-0.803
C	5.307	0.792	-0.160
C	4.211	4.265	-1.248
H	2.214	4.861	-1.879
H	6.055	3.479	-0.582
C	5.375	-1.421	0.960
C	2.501	-1.542	1.090
C	6.793	-1.399	0.878

C	7.432	-0.352	0.218
H	8.510	-0.410	0.102
C	6.727	0.723	-0.309
C	4.729	-2.559	1.570
C	3.290	-2.596	1.652
C	2.647	-3.684	2.321
C	1.105	-1.615	1.270
C	0.484	-2.675	1.940
C	1.262	-3.718	2.452
H	0.821	-4.566	2.963
H	0.480	-0.826	0.887
O	5.433	-3.521	2.053
O	7.561	-2.380	1.377
H	6.924	-3.051	1.765
O	3.349	-4.708	2.852
H	4.308	-4.506	2.667
O	4.797	5.485	-1.414
H	4.128	6.129	-1.700
C	7.567	1.716	-1.089
H	8.489	1.228	-1.417
H	7.864	2.580	-0.483
H	7.048	2.095	-1.973
C	-1.032	-2.634	2.105
H	-1.421	-2.096	1.230
C	-1.451	-1.779	3.335
H	-1.038	-0.770	3.207
H	-2.544	-1.671	3.306
C	-1.698	-4.019	2.109
H	-1.430	-4.589	1.212
H	-2.788	-3.909	2.126

H	-1.416	-4.619	2.981
C	-1.033	-2.322	4.706
H	-1.360	-1.642	5.500
H	0.056	-2.425	4.783
H	-1.476	-3.303	4.911