Electronic supplementary materials *Mendeleev Commun.*, 2019, **29**, 584–586

Syntheses of chiral fused 4,5-diazafluorene–bis(nopinane) derivatives

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General experimental

NMR spectra were recorded at 25–28 °C for 10–15 mg ml^{-1} solutions using a Bruker Avance 400 and a Bruker Avance 300 spectrometers locked to the deuterium resonance of $CDCl_3$ solvent. The chemical shifts were calculated relative to the signals of $CDCl_3$ solvent used as the internal standard: δ_C 76.90 ppm and δ_H 7.24 ppm. The spectra were recorded after keeping the purified product solvates *in vacuo* to remove the bulk of the solvent.

IR spectra were recorded using a Bruker TENSOR 27 spectrophotometer in KBr at concentration 0.25%. UV-spectra were recorded on an Agilent 8453 instrument. Optical rotation was measured using a PolAAr 3005 polarimeter. Mass spectra were obtained on a Thermo electron DFS mass spectrometer in EI mode, 70 eV.

X-ray crystallographic data were obtained using a Bruker Apex Duo diffractometer with CCDs with graphite monochromated MoKα radiation (λ = 0.71073 Å). Experimental data editing was performed using APEX2 suite. The structures were solved by direct methods and refined by the full-matrix least-squares technique against F^2 in the anisotropic–isotropic approximation. The H atoms positions were calculated with the riding model. All calculations were performed using SHELXTL-2014/7 assisted with OLEX2 GUI.

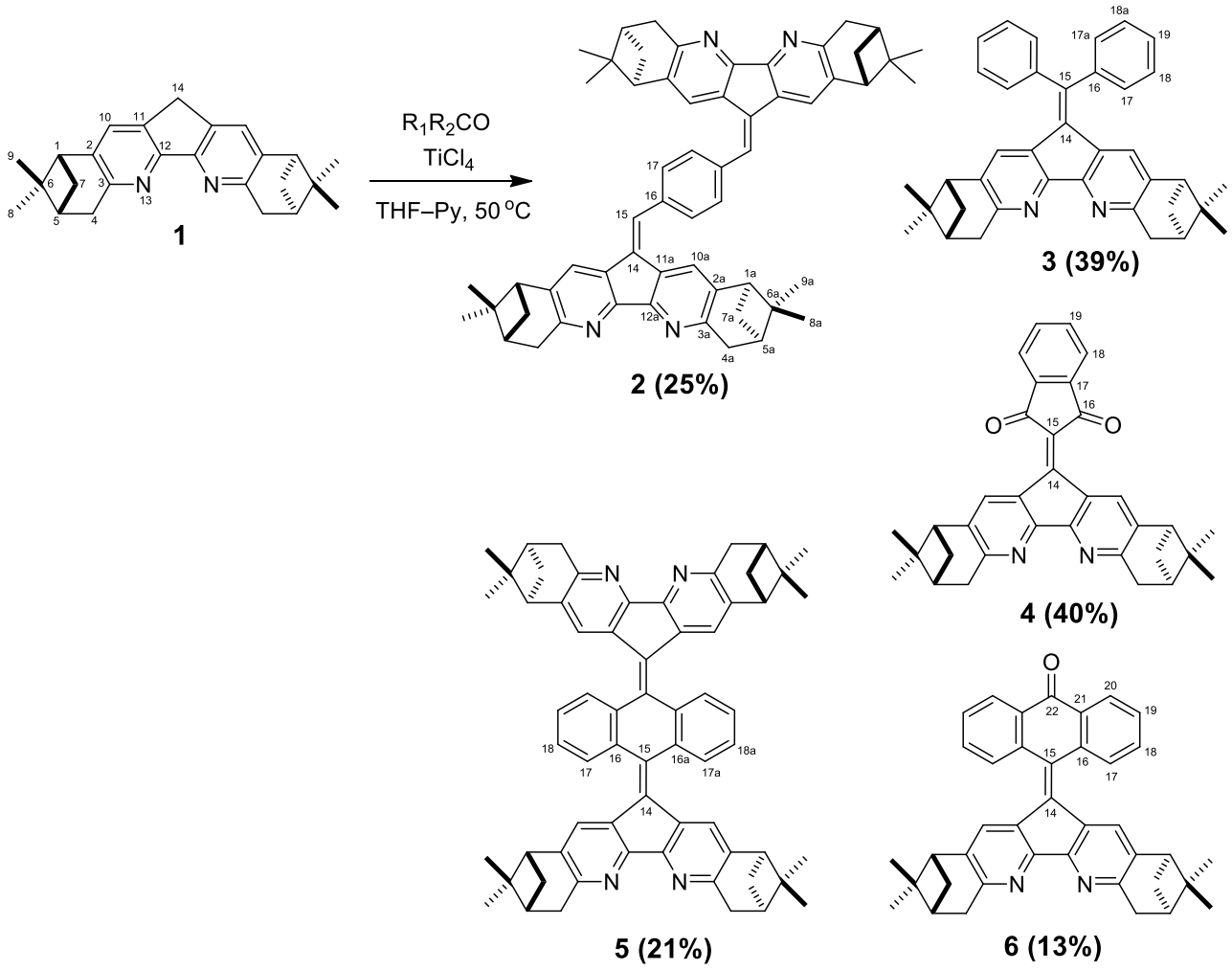
Geometry optimization and electronic spectra at the DFT level were obtained using ORCA program system. Geometry optimization was carried out using the BP86 functional (composed of the Becke 1988 exchange functional and the Perdew 86 correlation functional) and the valence triple-zeta polarization basis set def2-TZVP with the conductor-like screening solvation model (COSMO). Excitation energies, absorption intensities and CD intensities were calculated at the TD-DFT level (single excitation model) using hybrid exchange correlation functional B3LYP and the def2-TZVP basis set with COSMO solvation model.

General synthetic procedure for compounds 2–6.

Preparation of $TiCl_4$ complex of carbonyl compounds. $TiCl_4$ was added dropwise to the corresponding carbonyl compound under Ar, and the mixture was kept at room temperature for 24 h. The following ratios were used:

(*a*) $TiCl_4$ (0.159 g, 0.84 mmol) + terephthalaldehyde (0.056 g, 0.42 mmol)
(*b*) $TiCl_4$ (0.159 g, 0.84 mmol) + benzophenone (0.153 g, 0.84 mmol)
(*c*) $TiCl_4$ (0.478 g, 2.52 mmol) + ninhydrin (0.150 g, 0.84 mmol)
(*d*) $TiCl_4$ (0.159 g, 0.84 mmol) + anthraquinone (0.087 g, 0.42 mmol)

Preparation of the condensation products. A solution of dipinodiazafluorenone (0.30 g, 0.84 mmol) in THF (2 ml) was added dropwise at stirring to the above $TiCl_4$ complex. Then pyridine (2.65 g, 33.5 mmol) was added in 10 min. The reaction mixture was stirred at 50 °C for 4 days. Then the mixture was cooled down to room temperature and purified using a silica gel column with pyridine as eluent. The eluate was concentrated *in vacuo* affording the crude product as a dark red oil, which was purified by column chromatography (SiO_2, 0→10 vol% THF in benzene).



1,4-bis({(1*R*,3*R*,8*R*,10*R*)-2,2,9,9-tetramethyl-2,3,4,7,8,9,10,12-octahydro-1,3:8,10-dimethanocyclopenta[1,2-*b*:5,4-*b*']diquinolin-12-ylidene}methyl)benzene (2)

Yield 0.085 g (25%). R_f 0.19 (benzene–chloroform 2 : 1 v/v).

Yellow crystals, $[\alpha]_D^{24}$ –3.9 (*c* 0.30, $CHCl_3$), $[\alpha]_{546}^{24}$ –3.3.

HREIMS *m/z*: 810.4647 (calcd for $C_{58}H_{68}N_4^{+\bullet}$: 810.4656).

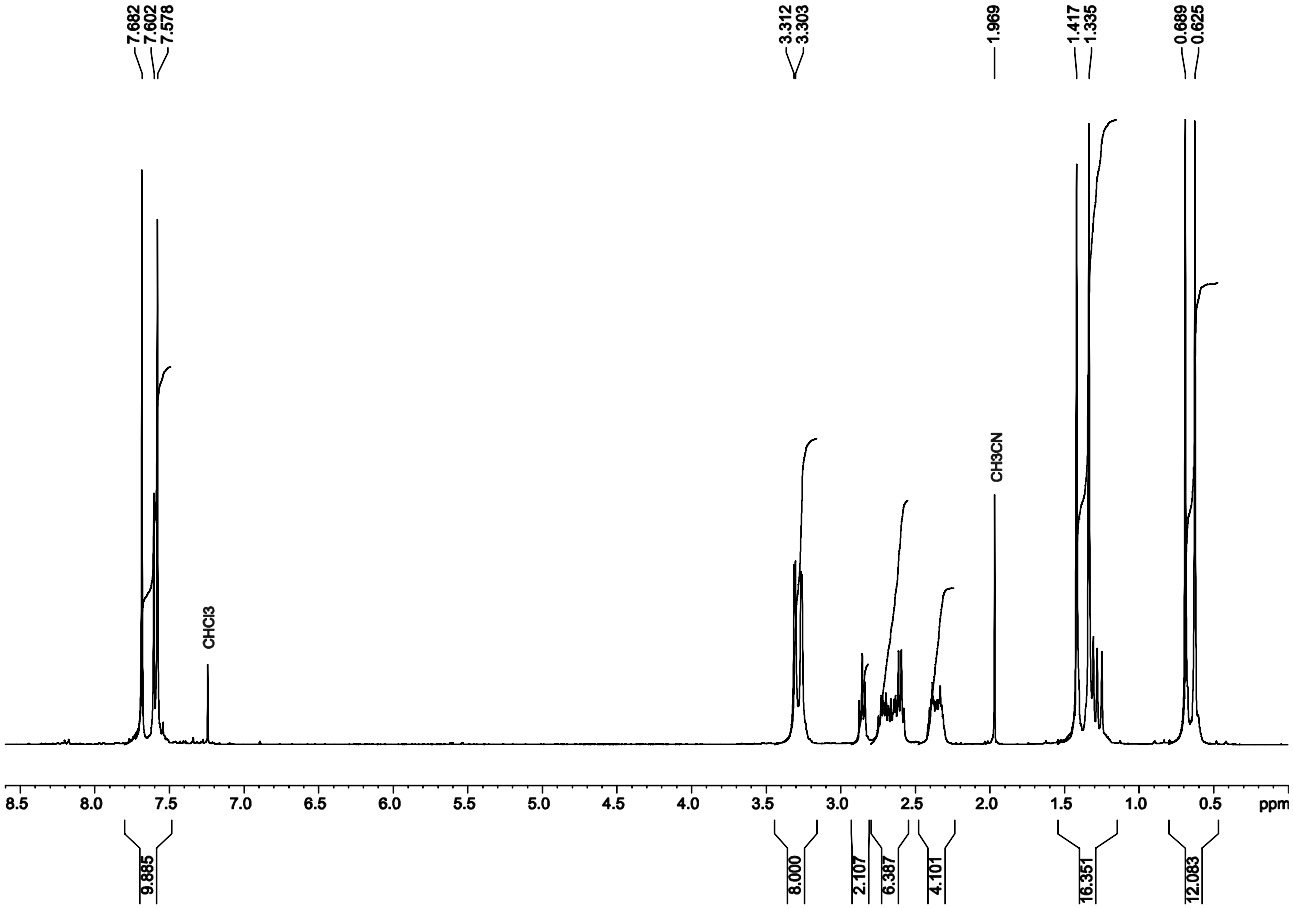
EI MS *m/z*: 810 $[M]^+$ (11), 370 (14), 295 (13), 265 (16), 249 (11), 242 (10), 239 (28), 206 (34), 193 (35), 90 (23), 76 (10), 69 (12), 57 (15), 54 (18), 43 (29), 42 (20), 40 (25), 38 (14), 37 (33), 36 (10), 35 (100), 34 (31).

UV ($CHCl_3$) λ_{max} (lg ε) 668 (2.68), 529 (2.62), 367 (4.46), 340 (4.77), 326 (4.70), 245 (4.78), 243 (4.77) nm.

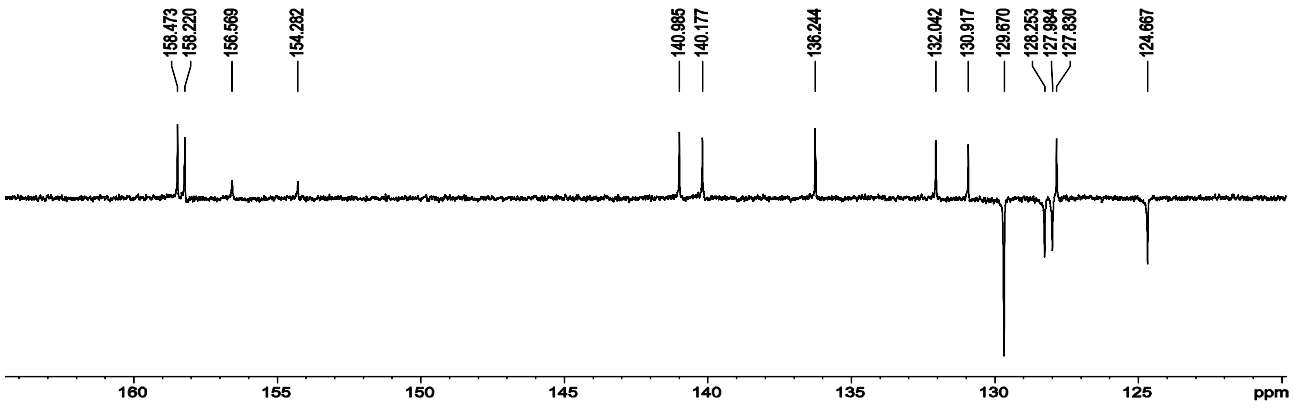
IR (KBr) ν_{max} 3040–2850 ($\nu_{C–H}$), 1607, 1555, 1503, 1470, 1425, 1395, 1260, 1215, 1100, 1050, 950, 930, 775, 750, 730 cm^{-1}.

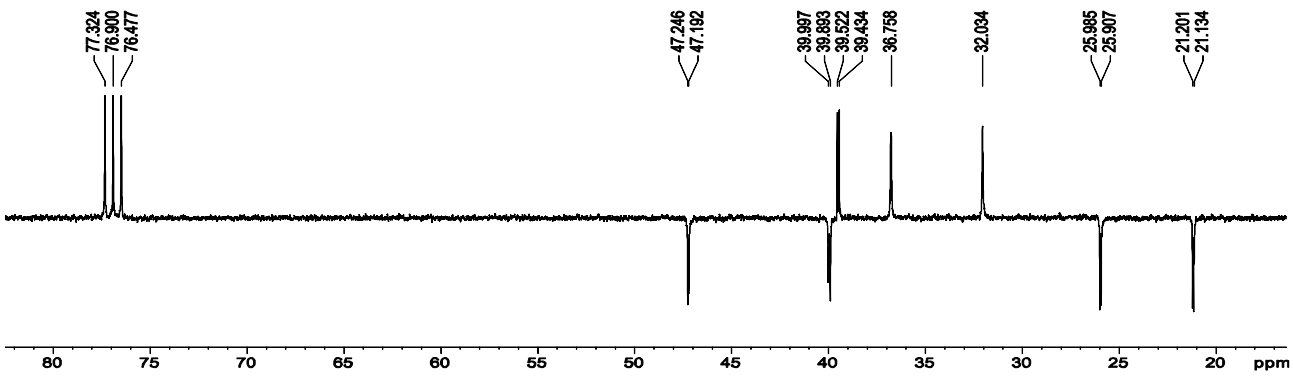
^1H NMR ($CDCl_3$) δ 0.63 (s, 3H, H8 or H8a), 0.69 (s, 3H, H8a or H8), 1.26 (d, 1H, *J* 9.3 Hz, *pro*-*R*-H7), 1.32 (d, 1H, *J* 9.3 Hz, *pro*-*R*-H7a), 1.34 (s, 3H, H9 or H9a), 1.42 (s, 3H, H9a or H9), 2.33 (dddd, 2H, *J* 5.7, 5.7, 2.4, 2.4 Hz, H5), 2.39 (dddd, 2H, *J* 5.7, 5.7, 2.4, 2.4 Hz, H5), 2.59 (dd, 1H, *J* 5.6, 5.6 Hz, H1), 2.64 (m, 1H, *pro*-*S*-H7), 2.71 (ddd, 2H, *J* 9.3, 5.6, 5.6 Hz, *pro*-*S*-H7a), 2.86 (dd, 1H, *J* 5.6, 5.6 Hz, H1a), 3.26 (d, 2H, *J* 2.6 Hz, H4), 3.31 (d, 2H, *J* 2.6 Hz, H4a), 7.58 (s, 4H) 7.60 (s, 2H) and 7.68 (s, 4H) are signals of 2H10, 2H10a, 2H15 and 4H17.

^{13}C NMR ($CDCl_3$) δ: 21.13 (C8 or C8a), 21.20 (C8a or C8), 25.91 (C9 or C9a), 25.99 (C9a or C9), 32.03 (C4 and C4a), 36.76 (C7 and C7a), 39.43 (C6 or C6a), 39.52 (C6a or C6), 39.89 (C1 or C1a), 40.00 (C1a or C1), 47.19 (C5 or C5a), 47.25 (C5a or C5), 124.67 (C14), 127.83 (C11), 127.98 (C10), 128.25 (C10a), 129.67 (C17 and C17a), 130.92 (C14), 132.04 (C12a), 136.24 (C16), 140.18 (C2), 140.99 (C2a), 154.28 (C12), 156.57 (C12a), 158.22 (C3) 158.47 (C3a).



J-modulation with BB-decoupling at 1H
(C,CH2 - positive, CH,CH3 - negative)





(1*R*,3*R*,8*R*,10*R*)-12-diphenylmethylidene-2,2,9,9-tetramethyl-2,3,4,7,8,9,10,12-octahydro-1,3:8,10-dimethanocyclopenta[1,2-*b*:5,4-*b*']diquinoline (3)

Yield 0.170 g (39%). R_f 0.54 (benzene–chloroform 2 : 1 v/v).

Yellow solid, $[\alpha]_D^{24}$ –152 (*c* 0.44, $CHCl_3$), $[\alpha]_{546}^{24}$ –201.

HREIMS *m/z*: 520.2880 (calcd for $C_{38}H_{36}N_2^{+\bullet}$: 520.2873).

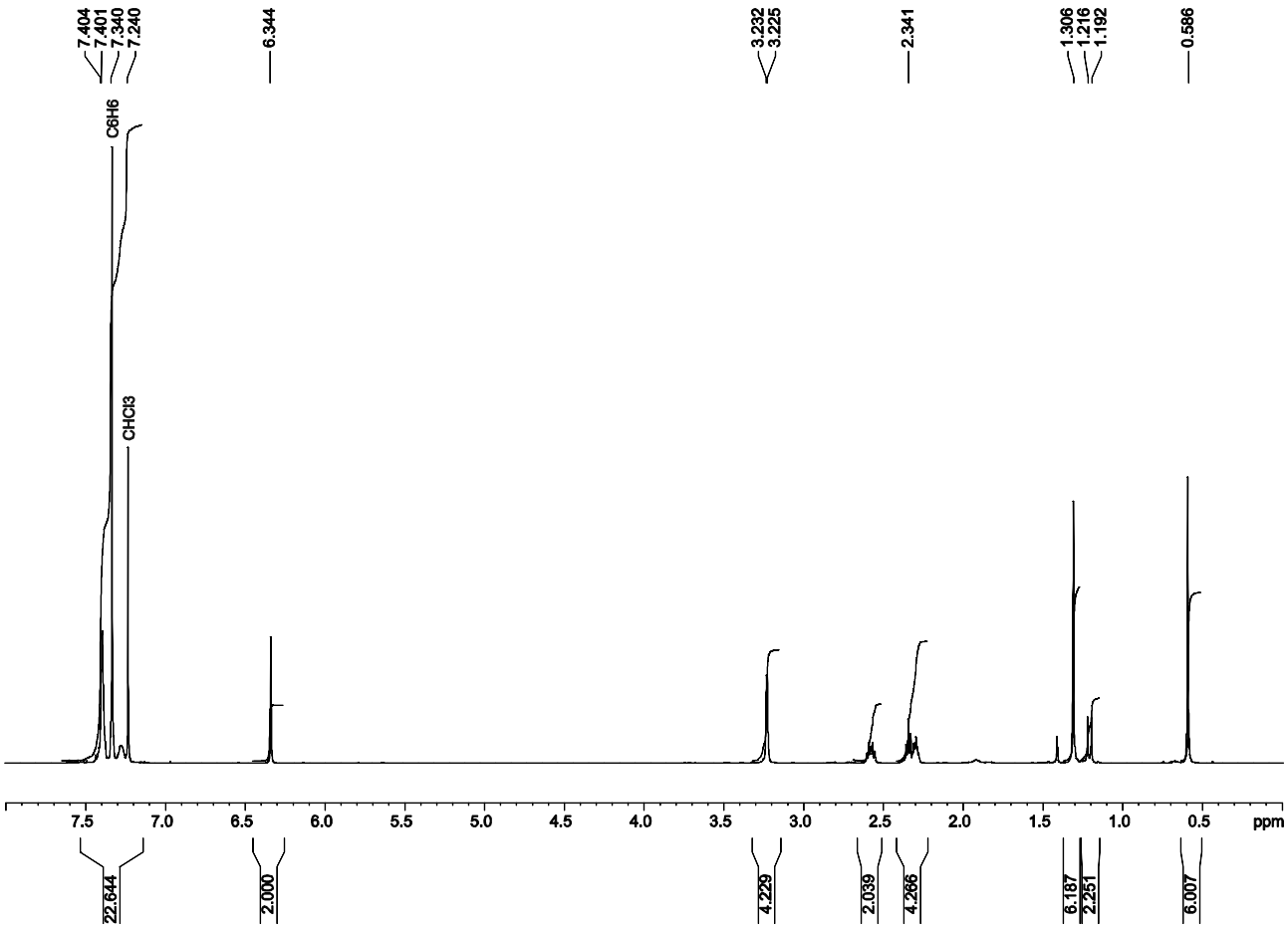
EI MS *m/z*: 520 $[M]^+$ (33), 505 (16), 491 (5), 479 (8), 370 (4), 86 (8), 84 (72), 82 (100), 48 (7), 47 (10), 46 (25).

UV ($CHCl_3$) λ_{max} (lg ε) 339 (4.45), 334 (4.44), 326 (4.41), 242 (4.52) nm.

IR (KBr) ν_{max} 1597, 1555, 1490, 1470, 1425, 1395, 1260, 1215, 1100, 1050, 950, 930, 775, 750, 695 cm^{-1}.

^1H NMR ($CDCl_3$) δ: 0.59 (s, 6H, H8), 1.20 (d, 2H, *J* 9.6 Hz, *pro*-*R*-H7), 1.31 (s, 6H, H8), 2.30 (dddd, 2H, *J* 5.7, 5,7, 2.4, 2.4 Hz, H5), 2.34 (dd, 2H, *J* 5.7, 5.7 Hz, H1), 2.57 (ddd, 2H, *J* 9.7, 5.7, 5.7 Hz, *pro*-*S*-H7), 3.23 (m, 4H, H4), 6.34 (s, 2H, H10), 7.25–7.44 (m, 10H, H17, H17a, H18, H18a, H19).

^{13}C NMR ($CDCl_3$) δ: 21.10 (C8), 25.87 (C9), 32.07 (C4), 36.62 (C7), 39.37 (C6), 39.93 (C1), 47.09 (C5), 128.19 (C19), 128.47 (C17), 128.63 (C17a), 128.70 (C10), 129.48 (C11), 129.54 (C18), 129.86 (C18a), 130.16 (C13), 139.79 (C14), 142.02 (C2), 146.51 (C15), 155.45 (C12), 156.25 (C3).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CHCl3
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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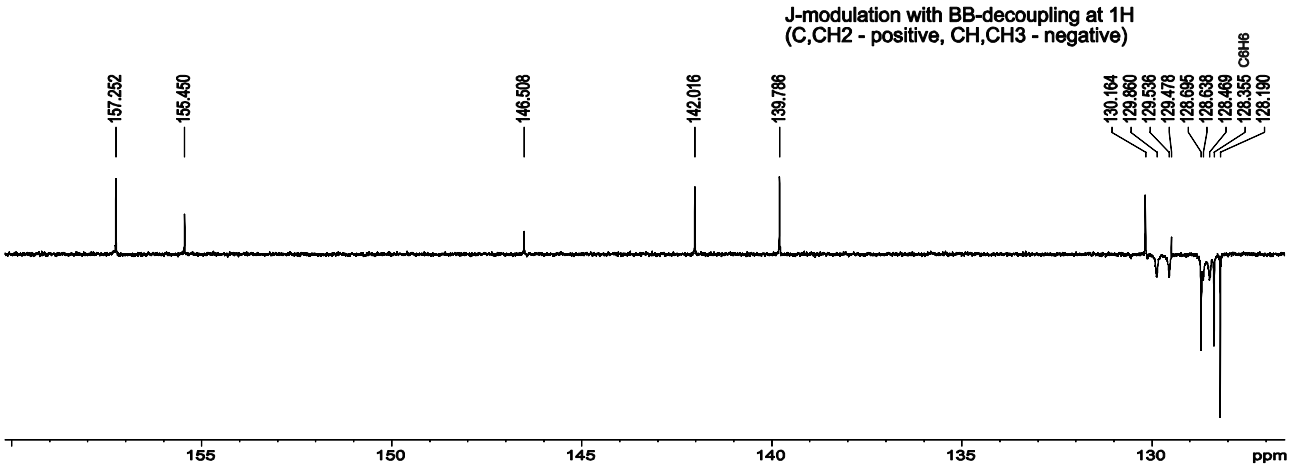
6.007


J-modulation with BB-decoupling at 1H
(C,CH2 - positive, CH,CH3 - negative)
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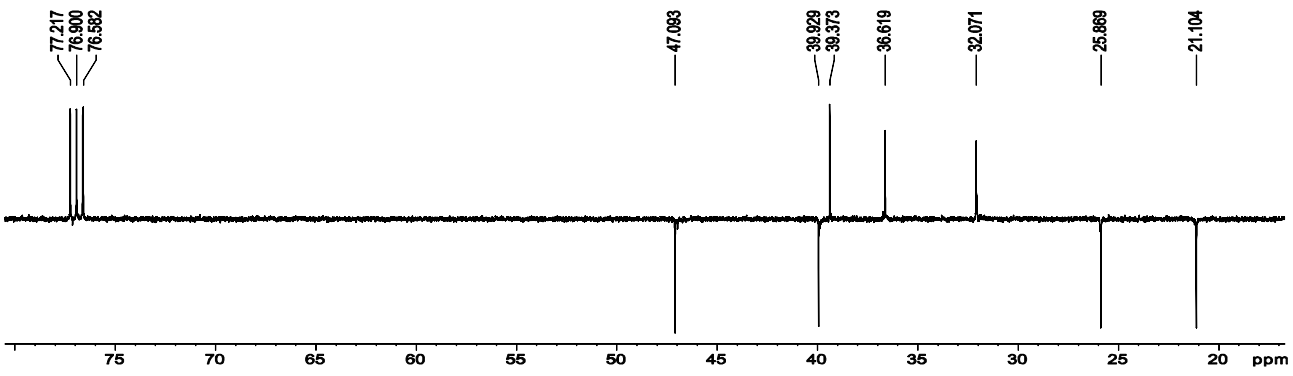
140
135
130
ppm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60
55
50
45
40
35
30
25
20
ppm

2-{(1*R*,3*R*,8*R*,10*R*)-2,2,9,9-tetramethyl-2,3,4,7,8,9,10,12-octahydro-1,3:8,10-dimethanocyclopenta[1,2-*b*:5,4-*b*']diquinolin-12-ylidene}indane-1,3-dione (4)

Yield 0.167 g (40%). R_f 0.51 (benzene–chloroform 2 : 1 v/v).

Red-purple crystals, $[\alpha]_D^{24}$ –46 (c 0.052, $CHCl_3$), $[\alpha]_{546}^{24}$ –19.

HREIMS *m/z*: 498.2301 (calcd for $C_{30}H_{34}N_2O_2^{+\bullet}$: 498.2302).

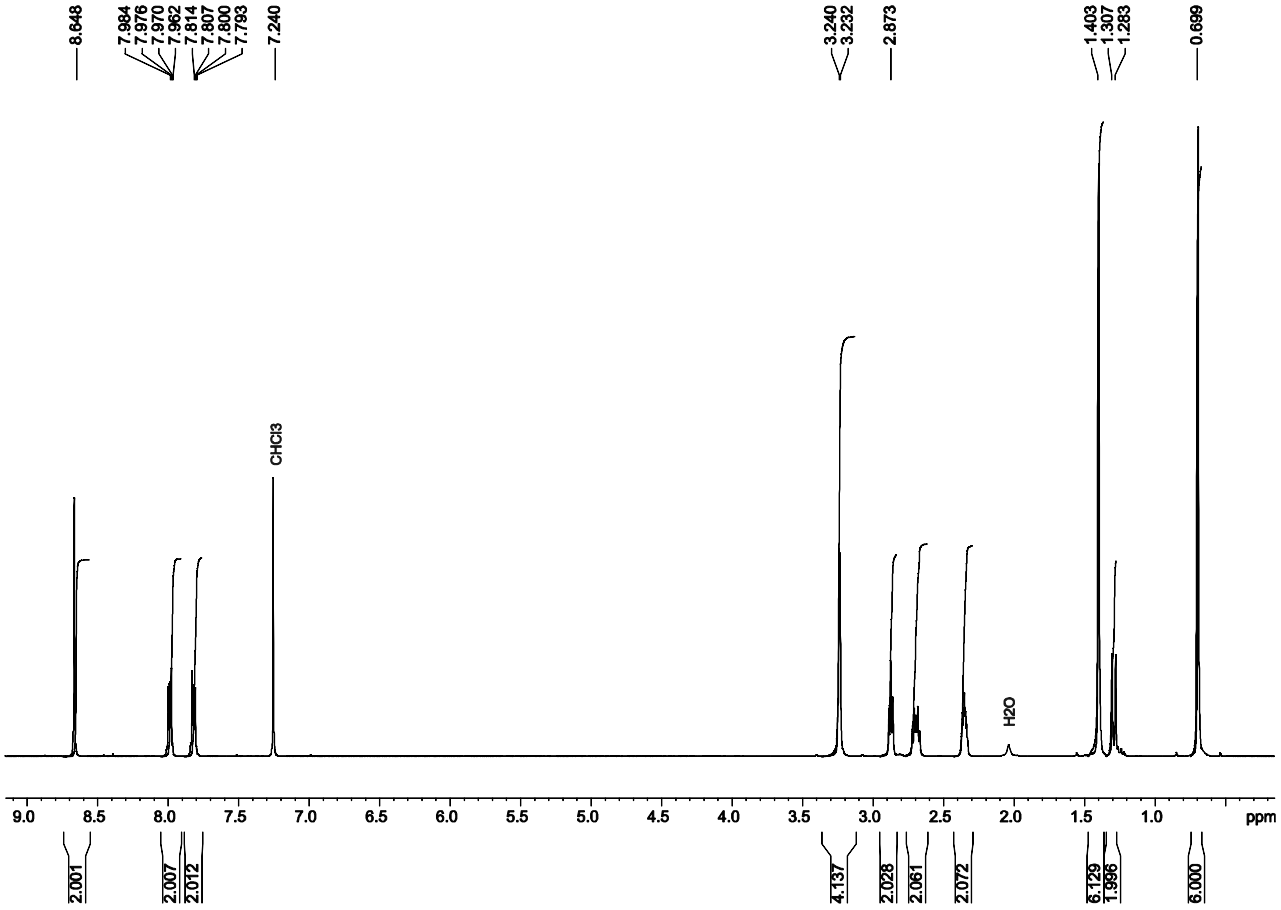
EI MS *m/z*: 498 $[M]^+$ (9), 408 (15), 355 (8), 334 (9), 325 (25), 281 (10), 268 (22), 267 (10), 256 (18), 227 (52), 200 (19), 133 (18), 97 (24), 95 (27), 86 (23), 85 (21), 83 (35), 82 (18), 81 (32), 73 (28), 71 (34), 69 (52), 67 (20), 59 (25), 57 (69), 56 (20), 55 (54), 44 (96), 43 (100), 43 (66), 42 (53), 40 (74), 38 (28), 35 (21).

UV ($CHCl_3$) λ_{max} (lg ε) 598 (2.37), 473 (3.29), 375 (4.59), 292 (4.49), 281 (4.46), 249 (4.29) nm.

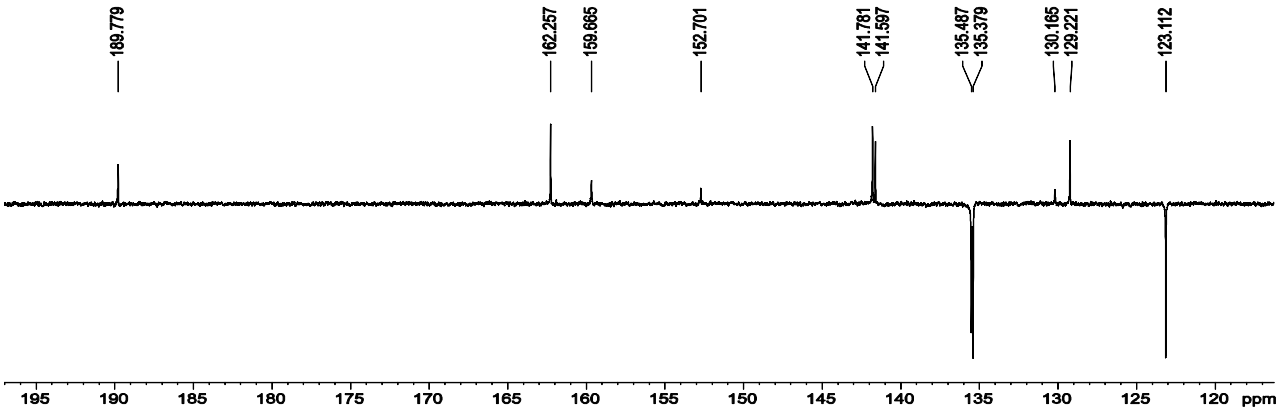
IR (KBr) ν_{max} 3040–2850 ($\nu_{C–H}$), 1715, 1685, 1555, 1470, 1425, 1400, 1350, 1260, 1215, 1186, 1070, 950, 930, 770, 750 cm^{-1}.

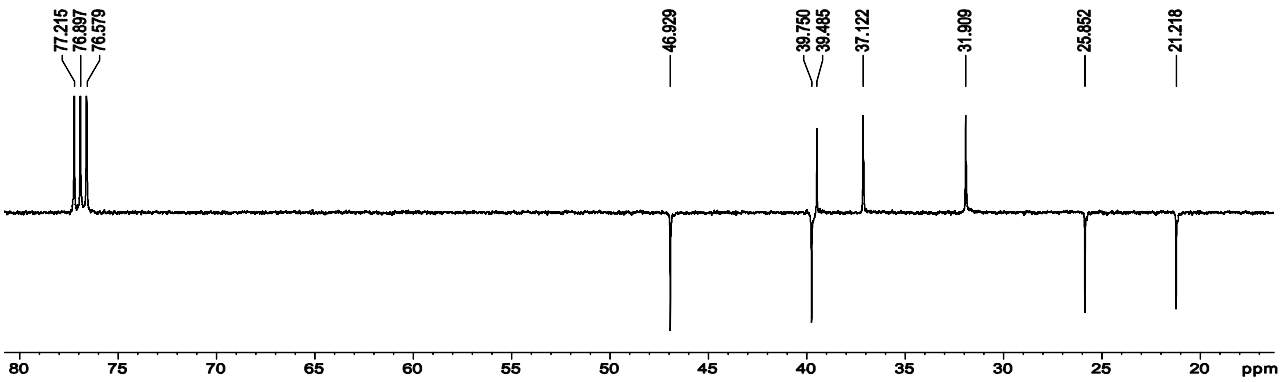
^1H NMR ($CDCl_3$) δ: 0.70 (s, 6H, H8), 1.29 (d, 2H, *J* 9.7 Hz, *pro-R*-H7), 1.40 (s, 6H, H9), 2.35 (dddd, 2H, *J* 5.6, 5.6, 2.7, 2.7 Hz, H5), 2.69 (ddd, 2H, *J* 9.7, 5.6, 5.6 Hz, *pro-S*-H7), 2.87 (dd, 2H, *J* 5.6, 5.6 Hz, H1), 3.24 (m, 4H, H4), 7.80 (dd, 2H, *J* 5.5, 3.0 Hz, H18), 7.97 (dd, 1H, *J* 5.5, 3.0 Hz, H17), 8.65 (s, 2H, H10),

^{13}C NMR ($CDCl_3$) δ: 21.22 (C8), 25.86 (C9), 31.91 (C4), 37.12 (C7), 39.49 (C6), 39.75 (C1), 46.93 (C5), 123.11 (C10), 129.22 (C13), 130.17 (C16), 135.38 (C17 or C18), 135.49 (C18 or C17), 141.60 (C2 or C14), 141.78 (C14 or C2), 152.70 (C14), 159.67 (C3), 162.26 (C12), 189.78 (C15).



J-modulation with BB-decoupling at 1H
(C,CH2 - positive, CH,CH3 - negative)





9,10-bis{(1*R*,3*R*,8*R*,10*R*)-2,2,9,9-tetramethyl-2,3,4,7,8,9,10,12-octahydro-1,3:8,10-dimethanocyclopenta[1,2-*b*:5,4-*b*']diquinolin-12ylidene}-9,10-dihydroanthracene (5)

Yield 0.078 g (21%). R_f 0.13 (benzene–chloroform 2 : 1 v/v).

Yellow crystals, $[\alpha]_D^{24}$ +9.1 (c 0.29, $CHCl_3$), $[\alpha]_{546}^{24}$ +14.

HREIMS *m/z*: 884.4807 (calcd for $C_{64}H_{60}N_4^{+\bullet}$: 884.4813).

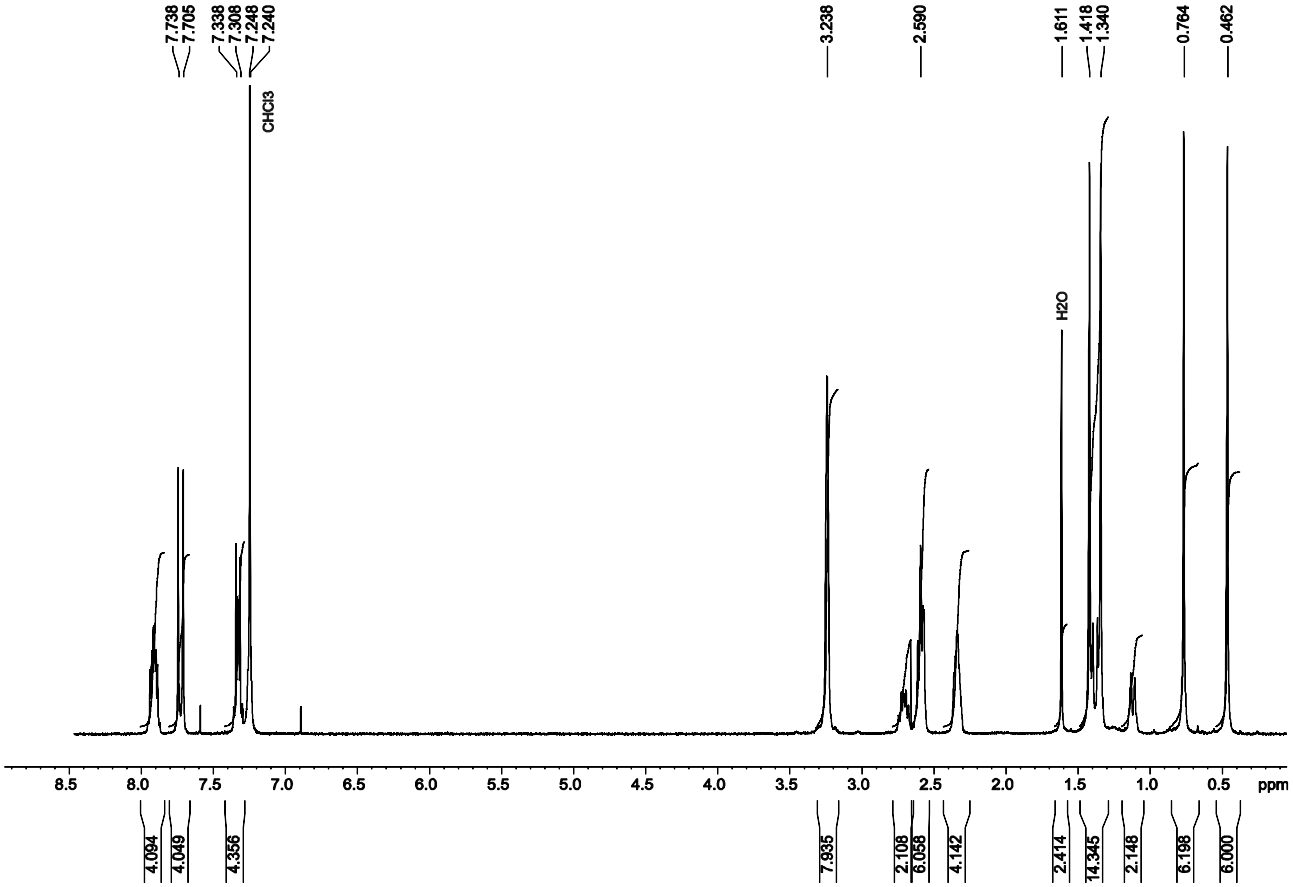
EI MS *m/z*: 884 $[M]^+$ (100), 812 (87), 489 (9), 356 (24), 341 (10), 207 (28), 83 (10), 57 (9), 43 (12).

UV ($CHCl_3$) λ_{max} (lg ε) 625 (2.86), 486 (2.54), 367 (4.40), 334 (4.74) nm.

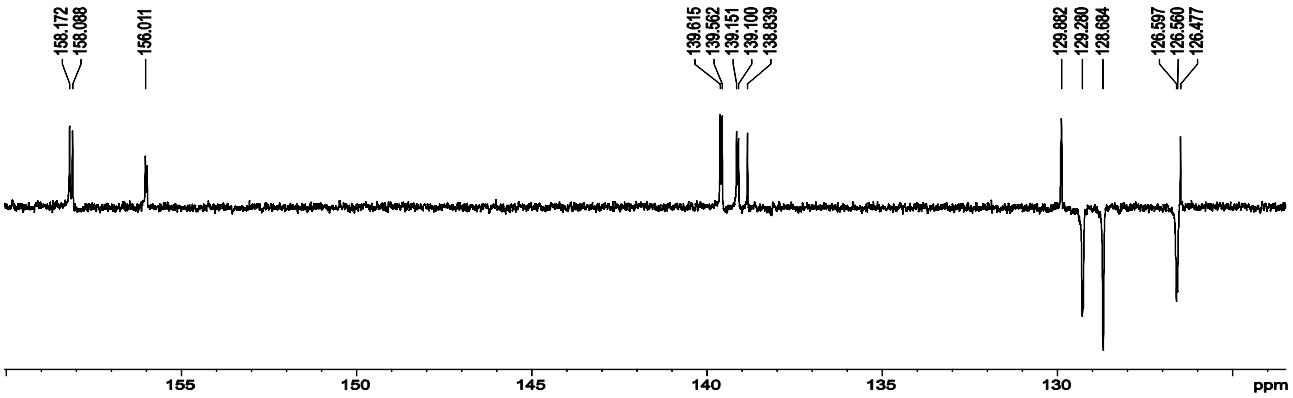
IR (KBr) ν_{max} 3040–2850 ($\nu_{C–H}$), 1615, 1592, 1555, 1478, 1470, 1425, 1395, 1260, 1215, 1186, 1070, 950, 930, 775, 755, 742 cm^{-1}.

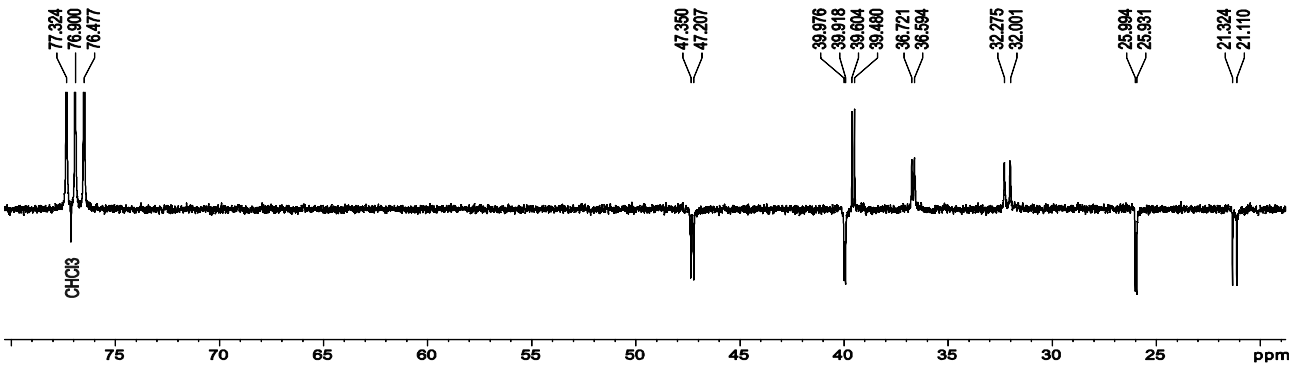
^1H NMR ($CDCl_3$) δ: 0.46 (s, 6H, H8 or H8a), 0.76 (s, 6H, H8a or H8), 1.12 (d, 2H, *J* 8.6 Hz, *pro*-*R*-H7 or *pro*-*R*-H7), 1.34 (s, 6H, H9 or H9a), 1.38 (d, 2H, *J* 9.4 Hz, *pro*-*R*-H7a or *pro*-*R*-H7a), 1.42 (s, 6H, H9a or H9), 2.34 (dddd, 4H, *J* 5.7, 5.7, 2.4, 2.4 Hz, H5 and H5a), 2.59 (m, 6H, H1, H1a and *pro*-*S*-H7), 2.57 (ddd, 2H, *J* 9.4, 5.7, 5.7 Hz, *pro*-*S*-H7a), 3.24 (m, 8H, H4 and H4a), 7.32 (m, 4H, H18), 7.71 (s, 2H, H10 or H10a), 7.74 (s, 2H, H10a or H10), 7.72 (m, 4H, H17).

^{13}C NMR ($CDCl_3$) δ: 21.10 (C8 or C8a), 21.32 (C8a or C8), 25.93 (C9 or C9a), 25.99 (C9a or C9), 32.00 (C4 or C4a), 32.28 (C4a or C4), 36.59 (C7 or C7a), 36.72 (C7a or C7), 39.48 (C6 or C6a), 39.60 (C6a or C6), 39.92 (C1 or C1a), 39.98 (C1a or C1), 47.21 (C5 or C5a), 47.35 (C5a or C5), 126.47 (C14), 126.56 (C18 or C18a), 126.59 (C18a or C18), 128.68 (C17 and C17a), 129.28 (C10 and C10a), 129.88 (C15), 138.84 (C13 and C13a), 139.10 (C11 or C11a), 139.15 (C11a or C11), 139.56 (C2 or C2a), 139.62 (C2a or C2), 155.96 (C12 or C12a), 156.01 (C12a or C12), 158.09 (C3 or C3a), 158.17 (C3a or C3).



J-modulation with BB-decoupling at 1H
(C,CH2 - positive, CH,CH3 - negative)





10-{(1*R*,3*R*,8*R*,10*R*)-2,2,9,9-tetramethyl-2,3,4,7,8,9,10,12-octahydro-1,3:8,10-dimethanocyclopenta[1,2-*b*:5,4-*b*']diquinolin-12ylidene)anthracen-9(10*H*)-one (6)

Yield 0.060 g (13%). R_f 0.38 (benzene–chloroform 2 : 1 v/v).

Yellow orange crystals, $[\alpha]_D^{24}$ −114 (c 0.0071, $CHCl_3$), $[\alpha]_{546}^{24}$ −452.

HREIMS *m/z*: 546.2661 (calcd for $C_{39}H_{34}N_2O^{+\bullet}$: 546.2666).

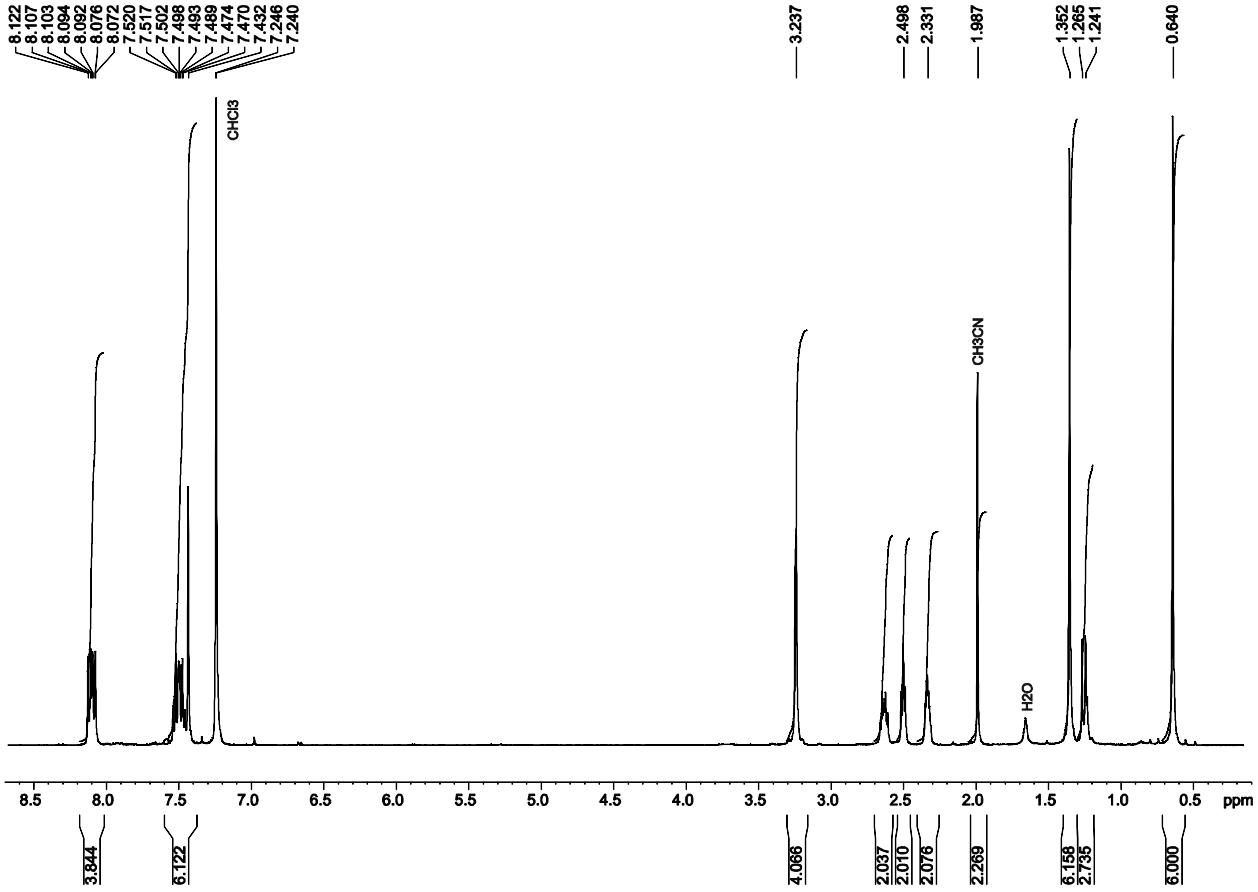
EI MS *m/z*: 546 $[M]^+$ (100), 531 (23), 505 (11), 503 (12), 356 (16), 355 (23), 83 (13).

UV ($CHCl_3$) λ_{max} (lg ε) 521 (3.36), 368 (4.10), 335 (4.37), 251 (4.53) nm.

IR (KBr) ν_{max} 3040–2850 (ν_{C-H}), 1719, 1677, 1592, 1555, 1478, 1470, 1425, 1395, 1300, 1260, 1215, 1186, 1070, 950, 930, 790, 775, 735 cm^{-1}.

^1H NMR ($CDCl_3$) δ: 0.64 (s, 6H, H8), 1.25 (d, 2H, *J* 9.6 Hz, *pro*-*R*-H7), 1.35 (s, 6H, H9), 2.33 (dddd, 2H, *J* 5.7, 5.7, 2.4, 2.4 Hz, H5), 2.50 (dd, 2H, *J* 5.6, 5.6 Hz, H1), 2.63 (ddd, 2H, *J* 9.6, 5.7, 5.7 Hz, *pro*-*S*-H7), 3.24 (m, 4H, H4), 7.43 (s, 2H, H10), 7.47 (ddd, 2H, *J* 7.4, 7.4, 1.5 Hz, H18 or H19), 7.52 (ddd, 2H, *J* 7.5, 7.5, 1.4 Hz, H19 or H18), 8.08 (d.d., 2H, *J* 7.4, 1.4 Hz, H17 or H20), 8.11 (dd, 2H, *J* 7.5, 1.5 Hz, H20 or H17).

^{13}C NMR ($CDCl_3$) δ: 21.26 (C8), 25.91 (C9), 32.04 (C4), 36.74 (C7), 39.56 (C6), 39.93 (C1), 47.12 (C5), 127.07 (C10), 129.04 and 129.54 and 129.64 and 130.16 (C17, C18, C19 and C20), 130.63 (14), 131.94 (15), 133.90 (13), 135.11 (21), 138.99 (C2), 139.63 (C11), 156.37 (C12), 158.79 (C3) 185.79 (C22).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7.246
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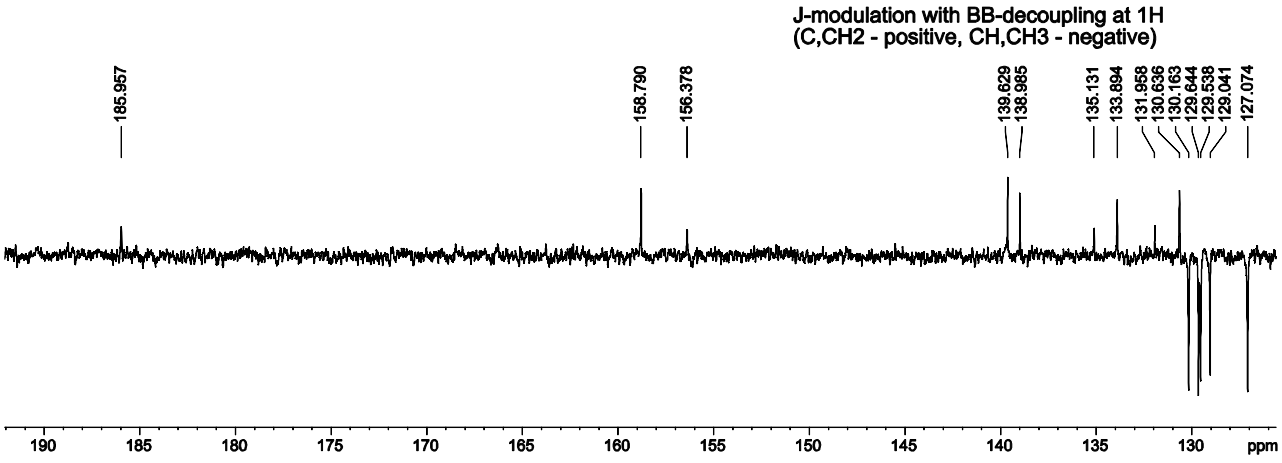
J-modulation with BB-decoupling at 1H
(C,CH2 - positive, CH,CH3 - negative)
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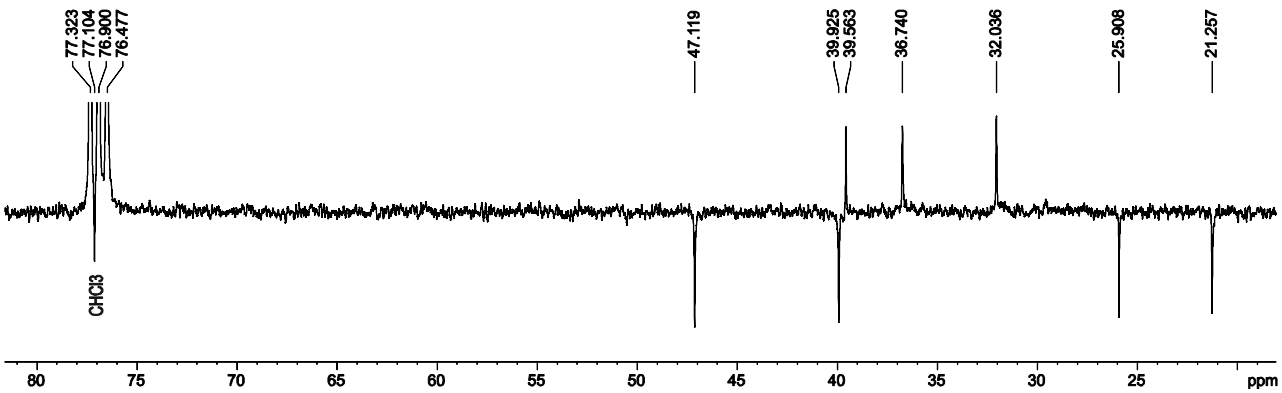
158.790
156.378
139.629
138.985
135.131
133.894
131.958
130.636
130.163
129.644
129.538
129.041
127.074
ppm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77.104
76.900
76.477
47.119
39.925
39.563
36.740
32.036
25.908
21.257
CHCl3
ppm

Calculated data for the *M*-helix conformer 6'

CARTESIAN COORDINATES (ANGSTROEM)

C	1.054333	5.541783	-2.126682
C	-0.007506	5.253617	-3.248917
C	0.053914	3.795239	-3.720608
C	0.042909	2.843699	-2.544812
C	0.048516	3.393711	-1.244320
C	-0.008810	4.894791	-1.154069
N	0.021888	1.530727	-2.779219
C	0.051214	0.729656	-1.718608
C	0.126221	1.164061	-0.379296
C	0.085205	2.541448	-0.151801
C	-1.100262	5.375652	-2.155492
C	1.226436	7.041091	-1.866808
C	2.439319	4.911979	-2.234089
C	-1.054700	-5.541445	-2.126183
C	0.007479	-5.253719	-3.248212
C	-0.053450	-3.795391	-3.720134
C	-0.042496	-2.843679	-2.544472
C	-0.048539	-3.393512	-1.243905
C	0.008383	-4.894588	-1.153418
N	-0.021167	-1.530742	-2.779052
C	-0.085284	-2.541102	-0.151506
C	1.099945	-5.375879	-2.154512
C	-1.227271	-7.040664	-1.866111
C	-2.439491	-4.911287	-2.234009
C	-0.050579	-0.729517	-1.718544
C	-0.125905	-1.163743	-0.379196
C	0.000140	0.000205	0.518180
C	0.000102	0.000138	1.912751
C	-0.952009	-0.823204	2.675633
C	-0.928353	-0.850138	4.089266
C	0.000713	-0.001263	4.859511
C	0.929162	0.848668	4.089668
C	0.952215	0.823190	2.675984
O	0.001171	-0.002055	6.087652
C	-2.033032	-1.478386	2.050202
C	-2.950831	-2.220766	2.767323
C	-2.858023	-2.310674	4.157656
C	-1.865711	-1.603778	4.806512
C	1.866502	1.601971	4.807276
C	2.858211	2.309985	4.158733
C	2.950507	2.221497	2.768277
C	2.032761	1.479403	2.050786
H	-0.039359	5.943347	-4.094649
H	-0.798770	3.569838	-4.369187
H	0.948053	3.608592	-4.324523
H	-0.039452	5.246992	-0.121851
H	0.081605	2.952953	0.849381
H	-1.417270	6.399892	-1.978231
H	-1.984418	4.744430	-2.257290
H	1.795407	7.207163	-0.947254
H	1.785131	7.506051	-2.684423
H	0.282314	7.576829	-1.770514
H	2.418045	3.836674	-2.405655
H	3.010136	5.085251	-1.316644
H	3.000761	5.366400	-3.056075
H	0.039351	-5.943582	-4.093835
H	0.799452	-3.570306	-4.368535
H	-0.947392	-3.608604	-4.324295
H	0.038691	-5.246640	-0.121140
H	-0.082026	-2.952475	0.849730
H	1.416646	-6.400174	-1.977024
H	1.984288	-4.744900	-2.256194

H	-1.796530	-7.206427	-0.946681
H	-1.785877	-7.505607	-2.683796
H	-0.283319	-7.576643	-1.769476
H	-3.010546	-5.084211	-1.316648
H	-3.000874	-5.365731	-3.056024
H	-2.417892	-3.836028	-2.405802
H	-2.168451	-1.386296	0.984363
H	-3.758957	-2.716016	2.243109
H	-3.577342	-2.892069	4.720485
H	-1.803415	-1.593858	5.886678
H	1.804665	1.590959	5.887450
H	3.577492	2.891178	4.721820
H	3.758200	2.717622	2.244206
H	2.167821	1.388415	0.984814

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	15277.7	654.5	0.004396100	0.09473	-0.01698	0.30731	-0.00053
2	19705.8	507.5	0.613664315	10.25211	0.00009	-0.00015	3.20189
3	21140.5	473.0	0.002235490	0.03481	0.00010	0.00007	-0.18658
4	22906.3	436.6	0.002001563	0.02877	0.10177	0.13568	-0.00075
5	25770.2	388.0	0.017993383	0.22986	-0.00007	-0.00004	0.47944
6	23912.1	418.2	0.022168128	0.30520	-0.00011	-0.00011	-0.55245
7	25113.5	398.2	0.000234473	0.00307	0.01862	-0.05222	0.00004
8	26968.7	370.8	0.042064891	0.51349	-0.64752	-0.30695	-0.00005
9	28520.5	350.6	0.004454550	0.05142	0.00011	0.00035	-0.22676
10	26528.1	377.0	0.015972443	0.19822	-0.08682	0.43666	0.00223
11	29030.5	344.5	0.264832697	3.00326	0.00013	-0.00109	1.73299
12	29688.8	336.8	0.003620329	0.04014	0.17241	0.10208	0.00098
13	31061.1	321.9	0.000806922	0.00855	-0.00012	0.00083	-0.09248
14	29915.7	334.3	0.001249087	0.01375	-0.04259	0.10923	0.00001
15	33017.6	302.9	0.143200531	1.42782	0.21629	1.17518	0.00047
16	30793.0	324.7	0.001487758	0.01591	-0.00016	-0.00100	0.12611

CD SPECTRUM

State	Energy (cm-1)	Wavelength (nm)	R (1e40*sgs)	MX (au)	MY (au)	MZ (au)
1	15277.7	654.5	2.29475	-0.20847	0.00432	-0.00003
2	19705.8	507.5	378.61240	-0.00003	-0.00015	0.25081
3	21140.5	473.0	-13.23175	0.00002	-0.00008	0.15042
4	22906.3	436.6	2.17065	0.09426	-0.03677	-0.00005
5	25770.2	388.0	11.71787	0.00038	-0.00036	0.05184
6	23912.1	418.2	-2.77212	0.00000	-0.00003	0.01064
7	25113.5	398.2	-10.42607	-0.31732	0.31036	0.00023
8	26968.7	370.8	-39.05457	0.13523	-0.01538	0.00015
9	28520.5	350.6	-5.52118	-0.00002	0.00004	0.05165
10	26528.1	377.0	-18.90057	0.05785	-0.08031	-0.00005
11	29030.5	344.5	-37.69730	-0.00027	0.00011	-0.04614
12	29688.8	336.8	-1.26910	-0.02541	0.01655	-0.00008
13	31061.1	321.9	-1.19426	0.00003	0.00004	0.02739
14	29915.7	334.3	-0.96110	0.08177	0.01322	0.00002
15	33017.6	302.9	-36.08588	0.04811	-0.07399	-0.00000
16	30793.0	324.7	-2.24567	-0.00011	0.00006	-0.03777

Calculated data for the *P*-helix conformer 6''

CARTESIAN COORDINATES (ANGSTROEM)

C	0.990040	5.518264	-2.113512
C	-0.059114	5.255001	-3.253892
C	-0.021839	3.795832	-3.725679
C	-0.056493	2.843888	-2.550628
C	-0.081991	3.393154	-1.250236
C	-0.103539	4.895009	-1.159638
N	-0.023242	1.530977	-2.784975
C	-0.053750	0.729213	-1.725136
C	-0.132849	1.162571	-0.385497
C	-0.107167	2.540068	-0.157808
C	-1.167117	5.400889	-2.179054
C	1.190959	7.012904	-1.848095
C	2.362726	4.858623	-2.197452
C	-0.990660	-5.518293	-2.114384
C	0.058553	-5.255203	-3.254751
C	0.021749	-3.795946	-3.726301
C	0.056717	-2.844208	-2.551094
C	0.082088	-3.393684	-1.250793
C	0.103156	-4.895559	-1.160438
N	0.023772	-1.531252	-2.785219
C	0.107553	-2.540788	-0.158220
C	1.166536	-5.401629	-2.179967
C	-1.192081	-7.012903	-1.849191
C	-2.363121	-4.858169	-2.198200
C	0.054511	-0.729659	-1.725253
C	0.133620	-1.163255	-0.385659
C	0.000538	-0.000377	0.512041
C	0.000459	-0.000244	1.906505
C	-0.958404	0.815465	2.669378
C	-0.935221	0.842444	4.082932
C	0.001032	0.001783	4.853566
C	0.936441	-0.840544	4.083691
C	0.959171	-0.815520	2.670067
O	0.001473	0.002836	6.081628
C	-2.044710	1.461776	2.043722
C	-2.969001	2.196330	2.760370
C	-2.877450	2.286376	4.150941
C	-1.879338	1.587850	4.799923
C	1.880283	-1.585598	4.801393
C	2.877718	-2.285675	4.153062
C	2.969004	-2.197447	2.762361
C	2.045026	-1.463186	2.045001
H	-0.061097	5.945657	-4.099456
H	-0.875564	3.587978	-4.379298
H	0.871267	3.591491	-4.324821
H	-0.143915	5.248363	-0.128184
H	-0.111745	2.951372	0.843445
H	-1.464164	6.431867	-2.006034
H	-2.063293	4.789569	-2.296391
H	1.753497	7.164527	-0.922109
H	1.768551	7.467998	-2.658080
H	0.257796	7.568930	-1.760154
H	2.322862	3.785746	-2.380179
H	2.917103	5.010634	-1.266198
H	2.951925	5.308270	-3.002538
H	0.060279	-5.945723	-4.100425
H	0.875533	-3.588261	-4.379895
H	-0.871296	-3.591217	-4.325399
H	0.143441	-5.249095	-0.129044
H	0.112029	-2.952279	0.842955
H	1.463245	-6.432732	-2.007117
H	2.062911	-4.790587	-2.297232

H	-1.754654	-7.164478	-0.923218
H	-1.769841	-7.467677	-2.659236
H	-0.259105	-7.569257	-1.761349
H	-2.917502	-5.009997	-1.266918
H	-2.952505	-5.307582	-3.003281
H	-2.322895	-3.785303	-2.380899
H	-2.178696	1.369156	0.977733
H	-3.780512	2.685658	2.235875
H	-3.601907	2.861433	4.713698
H	-1.817895	1.578950	5.880144
H	1.819216	-1.575188	5.881613
H	3.601958	-2.860503	4.716332
H	3.780065	-2.687936	2.238248
H	2.178873	-1.371904	0.978884

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	15290.7	654.0	0.004465003	0.09613	0.04132	0.30728	-0.00136
2	19671.0	508.4	0.612593596	10.25231	-0.00011	-0.00040	-3.20192
3	21113.8	473.6	0.002249237	0.03507	-0.00017	0.00011	0.18727
4	22815.7	438.3	0.001966371	0.02837	0.10313	-0.13318	0.00102
5	25713.4	388.9	0.000033627	0.00043	-0.00010	0.00039	-0.02075
6	23833.9	419.6	0.035672048	0.49273	0.00029	-0.00010	-0.70195
7	25061.0	399.0	0.000270531	0.00355	0.01697	0.05715	-0.00016
8	26939.6	371.2	0.043176794	0.52764	-0.66174	0.29956	-0.00112
9	28287.1	353.5	0.004423606	0.05148	0.00063	-0.00044	-0.22690
10	26643.7	375.3	0.016589538	0.20498	-0.12746	-0.43444	0.00011
11	29059.2	344.1	0.273953345	3.10362	-0.00014	-0.00137	-1.76171
12	29613.3	337.7	0.004157943	0.04622	0.17360	-0.12684	0.00011
13	30954.6	323.1	0.000669398	0.00712	-0.00018	0.00001	-0.08438
14	30113.9	332.1	0.006262196	0.06846	-0.03740	-0.25896	0.00022
15	33022.4	302.8	0.130218790	1.29820	0.14227	-1.13047	-0.00022
16	31089.1	321.7	0.006981693	0.07393	-0.00028	0.00079	-0.27190

CD SPECTRUM

State	Energy (cm-1)	Wavelength (nm)	R (1e40*sgs)	MX (au)	MY (au)	MZ (au)
1	15290.7	654.0	-11.15705	-0.20971	-0.04881	0.00008
2	19671.0	508.4	-157.83533	0.00028	0.00035	0.10456
3	21113.8	473.6	14.22125	0.00005	0.00014	0.16108
4	22815.7	438.3	-1.25256	-0.07013	-0.03436	0.00004
5	25713.4	388.9	-0.25525	0.00051	0.00053	0.02611
6	23833.9	419.6	2.37564	0.00002	0.00003	-0.00718
7	25061.0	399.0	10.81585	0.31365	0.30830	-0.00030
8	26939.6	371.2	37.70895	-0.12233	-0.00322	-0.00025
9	28287.1	353.5	5.77167	0.00002	0.00003	-0.05396
10	26643.7	375.3	9.21319	-0.05553	-0.02869	0.00003
11	29059.2	344.1	72.06525	-0.00034	-0.00008	-0.08677
12	29613.3	337.7	2.39106	0.02686	-0.00323	0.00001
13	30954.6	323.1	1.30663	0.00006	0.00005	-0.03285
14	30113.9	332.1	-4.66094	0.11854	0.02106	0.00001
15	33022.4	302.8	-6.56723	-0.06964	0.00356	0.00002
16	31089.1	321.7	1.16236	0.00010	0.00004	-0.00907

Calculated data for the folded conformer 6'''

CARTESIAN COORDINATES (ANGSTROEM)

C	-5.094550	-1.010722	2.116839
C	-4.491261	-2.455663	2.248908
C	-3.570013	-2.789254	1.067792
C	-2.567226	-1.680541	0.834649
C	-2.660151	-0.521355	1.627399
C	-3.709097	-0.533242	2.706811
N	-1.622846	-1.845008	-0.091325
C	-0.780735	-0.833153	-0.279810
C	-0.835133	0.408845	0.380896
C	-1.786234	0.533317	1.392794
C	-3.625369	-1.917192	3.417033
C	-6.243345	-0.770898	3.100942
C	-5.529381	-0.511243	0.743086
C	4.956846	-2.107528	-2.490124
C	4.045431	-2.689244	-3.630241
C	2.628971	-2.988563	-3.121265
C	2.075736	-1.815500	-2.341889
C	2.888873	-0.677216	-2.184482
C	4.251091	-0.734536	-2.822851
N	0.866960	-1.919217	-1.789307
C	2.398275	0.414456	-1.478038
C	4.056507	-1.276529	-4.270124
C	6.436159	-2.095701	-2.885383
C	4.843611	-2.678646	-1.080348
C	0.425064	-0.868537	-1.104339
C	1.108867	0.352401	-0.950573
C	0.270919	1.276208	-0.127244
C	0.454795	2.610338	0.084568
C	-0.400181	3.450621	0.963395
C	0.248628	4.259622	1.916070
C	1.729059	4.408776	1.865582
C	2.300366	4.202173	0.506473
C	1.613448	3.393282	-0.419298
O	2.389073	4.808085	2.810539
C	-1.788196	3.535589	0.852849
C	-2.517354	4.348051	1.713485
C	-1.875786	5.074334	2.714438
C	-0.492175	5.033484	2.809296
C	3.427771	4.924109	0.115692
C	3.837706	4.912009	-1.209669
C	3.107489	4.186294	-2.147867
C	2.011739	3.426309	-1.755725
H	-5.189335	-3.269852	2.452358
H	-3.031819	-3.723449	1.257029
H	-4.144348	-2.954154	0.150242
H	-3.696495	0.375742	3.310437
H	-1.850748	1.411914	2.015877
H	-4.139887	-1.933814	4.374511
H	-2.629295	-2.343844	3.541867
H	-6.492098	0.293287	3.147740
H	-7.141606	-1.301809	2.772869
H	-6.021212	-1.100444	4.115686
H	-4.763872	-0.617792	-0.024377
H	-5.799135	0.548022	0.790025
H	-6.414256	-1.057975	0.403760
H	4.444620	-3.524180	-4.209555
H	1.964366	-3.203747	-3.964285
H	2.611286	-3.880244	-2.487300
H	4.821069	0.183486	-2.670946
H	3.034973	1.273786	-1.337388
H	4.920474	-1.103038	-4.907290
H	3.155998	-0.957018	-4.796770

H	7.016566	-1.491183	-2.182577
H	6.845728	-3.109884	-2.859181
H	6.616117	-1.698085	-3.884449
H	5.435728	-2.083581	-0.378804
H	5.234709	-3.699976	-1.052566
H	3.824434	-2.709230	-0.696840
H	-2.300144	2.973498	0.083823
H	-3.592725	4.414987	1.600935
H	-2.450087	5.692736	3.392671
H	0.033661	5.629638	3.544266
H	3.947305	5.521723	0.853803
H	4.700768	5.488200	-1.518054
H	3.392277	4.211396	-3.192557
H	1.459290	2.862959	-2.495068

ABSORPTION SPECTRUM VIA TRANSITION ELECTRIC DIPOLE MOMENTS

State	Energy (cm-1)	Wavelength (nm)	fosc	T2 (au**2)	TX (au)	TY (au)	TZ (au)
1	19785.7	505.4	0.000325245	0.00541	-0.06294	0.00568	0.03765
2	24714.4	404.6	0.348025511	4.63593	-0.42398	-2.04583	-0.52032
3	26502.6	377.3	0.001322606	0.01643	0.10596	-0.00026	-0.07213
4	25191.6	397.0	0.005879254	0.07683	-0.23335	0.01613	0.14872
5	29817.9	335.4	0.004164086	0.04597	-0.17875	-0.01129	0.11787
6	28520.4	350.6	0.018147104	0.20947	0.00347	0.45622	-0.03643
7	29243.4	342.0	0.004401932	0.04956	0.14205	0.15468	-0.07384
8	30709.6	325.6	0.190167920	2.03863	-0.10507	-1.41465	-0.16231
9	31998.9	312.5	0.120890324	1.24375	-0.93439	0.01734	0.60857
10	32604.8	306.7	0.198904191	2.00835	-1.20500	0.06230	0.74326
11	33268.4	300.6	0.024246424	0.23993	0.01084	-0.48843	0.03541
12	34475.0	290.1	0.068584586	0.65493	-0.25225	-0.67935	-0.36026
13	34414.6	290.6	0.011051261	0.10572	-0.26243	-0.00951	0.19172
14	35440.7	282.2	0.015827578	0.14702	0.19601	0.14045	0.29812
15	36399.6	274.7	0.100831006	0.91195	-0.81395	-0.00413	0.49943
16	35044.2	285.4	0.013490514	0.12673	0.17402	0.29570	-0.09492

CD SPECTRUM

State	Energy (cm-1)	Wavelength (nm)	R (1e40*sgs)	MX (au)	MY (au)	MZ (au)
1	19785.7	505.4	-0.94844	0.10946	-0.04075	0.13570
2	24714.4	404.6	44.37608	-0.02009	-0.03692	-0.01935
3	26502.6	377.3	0.38451	0.02720	0.22581	0.02783
4	25191.6	397.0	-2.70801	0.05221	0.00657	0.04258
5	29817.9	335.4	-1.98542	-0.15701	0.32578	-0.24263
6	28520.4	350.6	0.40434	0.01802	0.00273	0.01237
7	29243.4	342.0	11.22484	-0.15499	0.17976	-0.24404
8	30709.6	325.6	18.66968	-0.04762	-0.01985	-0.04016
9	31998.9	312.5	-16.21547	0.10283	0.03684	0.10031
10	32604.8	306.7	-31.46858	-0.16079	0.14294	-0.36247
11	33268.4	300.6	0.16784	-0.02244	-0.00103	0.00273
12	34475.0	290.1	-0.36206	0.01993	0.00130	-0.01428
13	34414.6	290.6	7.73222	0.23540	-0.25888	0.39493
14	35440.7	282.2	3.11111	-0.10536	0.01558	0.08407
15	36399.6	274.7	-3.95686	-0.24066	0.14852	-0.40779
16	35044.2	285.4	27.80548	-0.04534	0.14241	-0.26084