Supporting Information

Nudicaulins, Yellow Flower Pigments of *Papaver nudicaule* – Revised Constitution and Assignment of Absolute Configuration

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S11. Computational Details of the Conformational Analyses

The starting geometries of the conformational searches of the authentic nudicaulins I (**3a**) and II (**3b**) and of the corresponding monoglucosidic forms **6a** and **6b** were obtained with the CAST program,[1] using the OPLS-AA force field.[2] Based on the force-field minimum geometries, further possible conformations were generated, and then optimized with B97-D/SVP[3,4] (density-fitting option) using Gaussian09.[5] The single-point energy calculations with SCS-MP2/def2-TZVP[6,7] ('chain-of-spheres exchange' approximation COSX,[8] and COSMO[9] solvent field of MeOH) were carried out with the ORCA software package.[10]

For the authentic structures possessing *cis*-configuration in the central chromophore, four energetically relevant conformers were found for the (3*S*,11*R*)-diastereomer, and two for the (3*R*,11*S*)-diastereomer. Additionally, *trans*-configured conformations of the (3*R*,11*R*)-diastereomer were optimized. Within each configuration, a cut-off energy of $\Delta E < 2.5$ kcal·mol^{-1} was chosen (contributions according to the Boltzmann statistics > 5%), determining for which conformers spectra were calculated.

In the case of the monoglucosides, five relevant conformers were found for the (3*S*,11*R*)-diastereomer **6a**, and three for the (3*R*,11*S*)-diastereomer **6b** (energy cut-off at 1.80 kcal·mol^{-1} within one configuration, contributions according to the Boltzmann statistics > 3%).

The structures of the aglycon models were obtained by replacing the remaining glucose moiety by a hydrogen atom. The conformations of the hydroxy substituents were not further investigated, since no contribution to the CD spectrum was to be expected. Thus, two conformations were considered that differed in the orientation of the 4-hydroxy phenyl group relative to the chromophoric backbone. After optimization, no separate single-point energies were calculated for the aglycon, since the ones of the monoglucosidic forms were used for Boltzmann weighting of the UV and CD spectra (see section S13 for details on the Boltzmann weighting).

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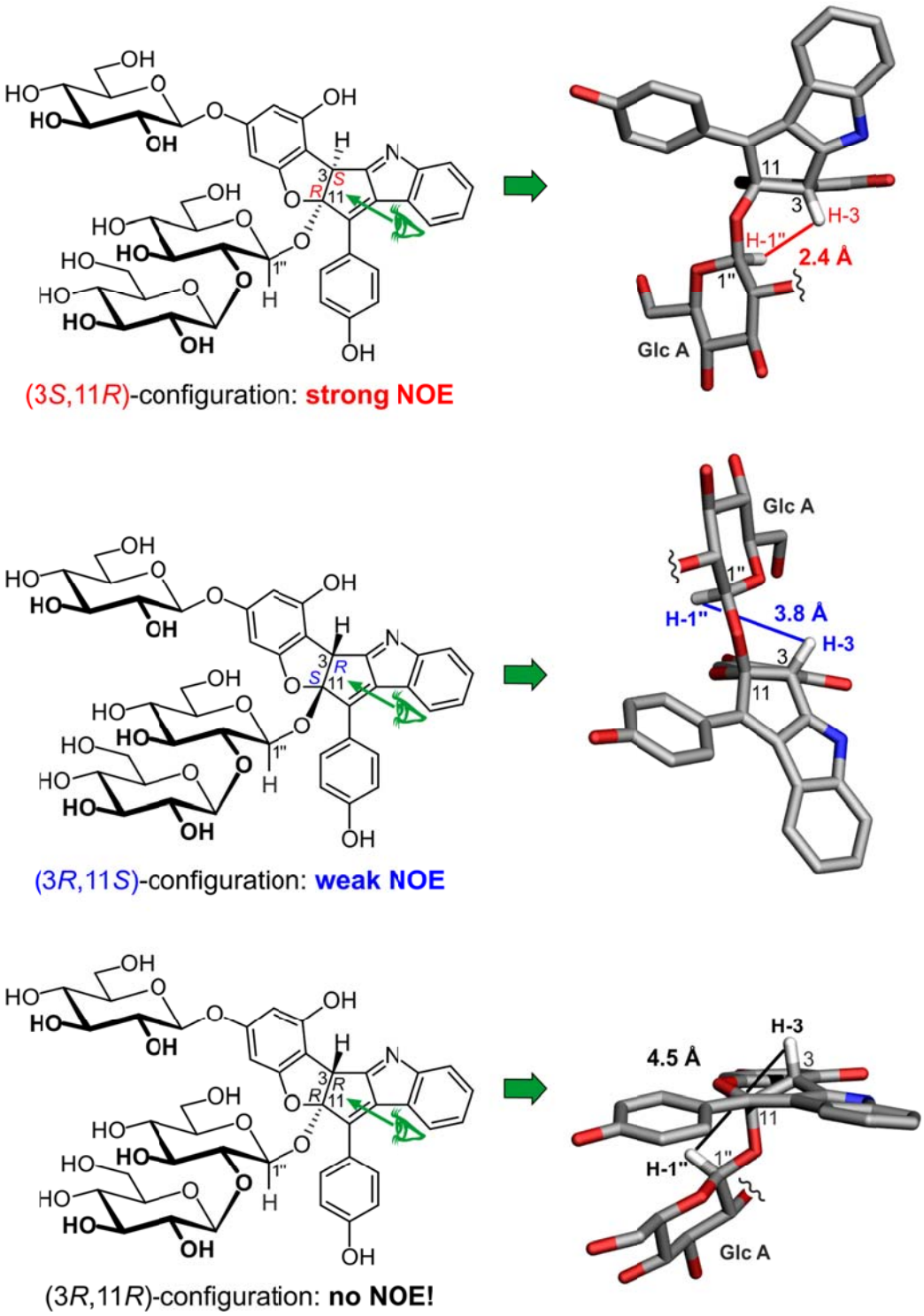


Figure S42. Comparison of the proton distances d(H-3–H-1") of the minimum structures of **3** of the (3*S*,11*R*)-, (3*R*,11*S*)- and (3*R*,11*R*)-diastereomers; glucose moieties glc B and glc C, and all hydrogen atoms, except for H-3 and H-1", were omitted for clarity.

S12. Experimental UV and CD Investigations

UV spectra. All experimental UV spectra used for the comparisons with the theoretical curves were measured offline in MeOH at room temperature, on a Varian Cary-50-conc spectrophotometer. For details on the experimental LC-UV spectra measured online with a linear gradient of MeCN–H_2O (0.1% TFA), see section S1 on p.**Error! Bookmark not defined.**.

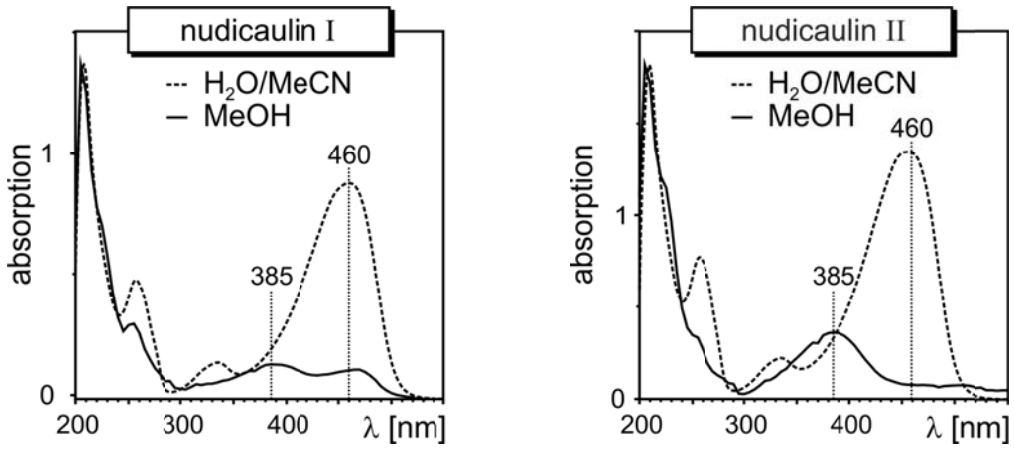


Figure S1. Comparison of the experimental UV spectra of nudicaulins I (**3a**, left) and II (**3b**, right) measured in MeOH, and MeCN–H_2O (0.1% TFA), demonstrating the strong influence of polar protic solvents capable of hydrogen bonding on the absorption properties of the nudicaulins.

CD spectra. The circular-dichroism (CD) spectra were recorded offline at ambient temperature on a Jasco J-715 spectropolarimeter (scanning rate: 200 nm/min, bandwidth: 1 nm, response time: 0.5 s, accumulations: 3). For nudicaulins I (**3a**) and II (**3b**), the wavelength-dependent differential absorption coefficients $\Delta\varepsilon$ [$M^{-1}cm^{-1}$] were determined for a concentration of c = 1.147 mmol·l^{-1}, using spectrophotometric grade MeOH, and 0.1 cm and 0.05 cm standard cells. In the case of the monoglucosides **6a** and **6b** of nudicaulins I and II, a concentration of c = 0.219 mmol·l^{-1} was used.

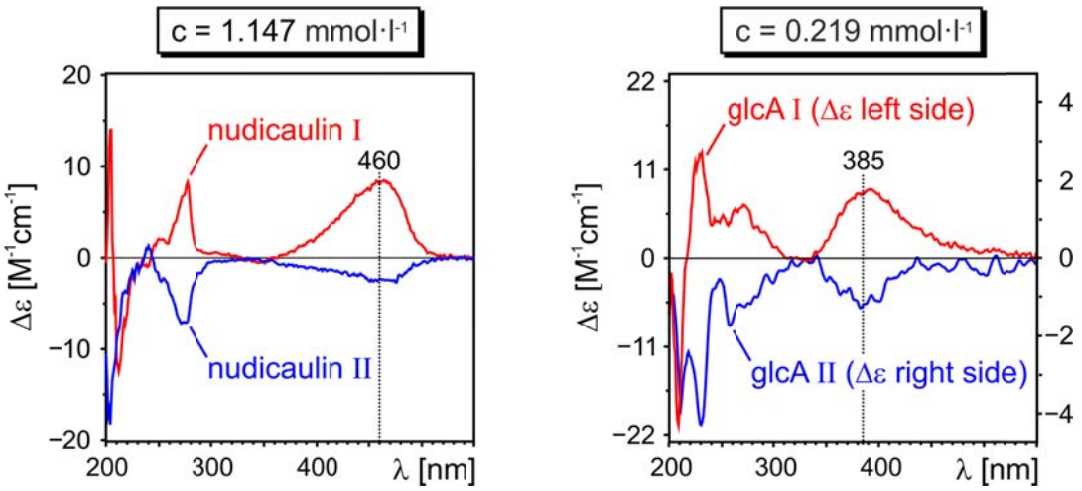


Figure S44. Comparison of the experimental CD spectra in MeOH of nudicaulins I (**3a**) and II (**3b**) (left) and their respective monoglucosidic derivatives **6a** and **6b** (right), from which the influence of the number of glucose moieties on the first CD effect becomes visible.

S13. Computational Details of the UV and CD Excited-States Calculations.

General. To gain line-shape UV and CD curves from the output files that were suited for comparison with the experimental data, the length representation of the oscillator and rotatory strengths was always selected and the 'bar type' spectra were overlain with Gaussian profiles that were in turn summed up to give, after Boltzmann weighting of the single spectra, the overall UV and CD spectra. These steps were performed with our software SpecDis,[1] as well as the determination of the UV correction[2] and the band width σ.

UV spectra with explicit H_2O inclusion. An arbitrarily chosen number of twelve water molecules were included into the conformational search of **3a** and **3b** within the CAST program. The result of the OPLS-AA run was submitted to a B97-D/SVP optimization, followed by an excited-states calculation with ZINDO/S-CI[3] (for 90 excitations). Additional ZINDO/S-CI calculations were then carried out for the same conformations, but without the water molecules.

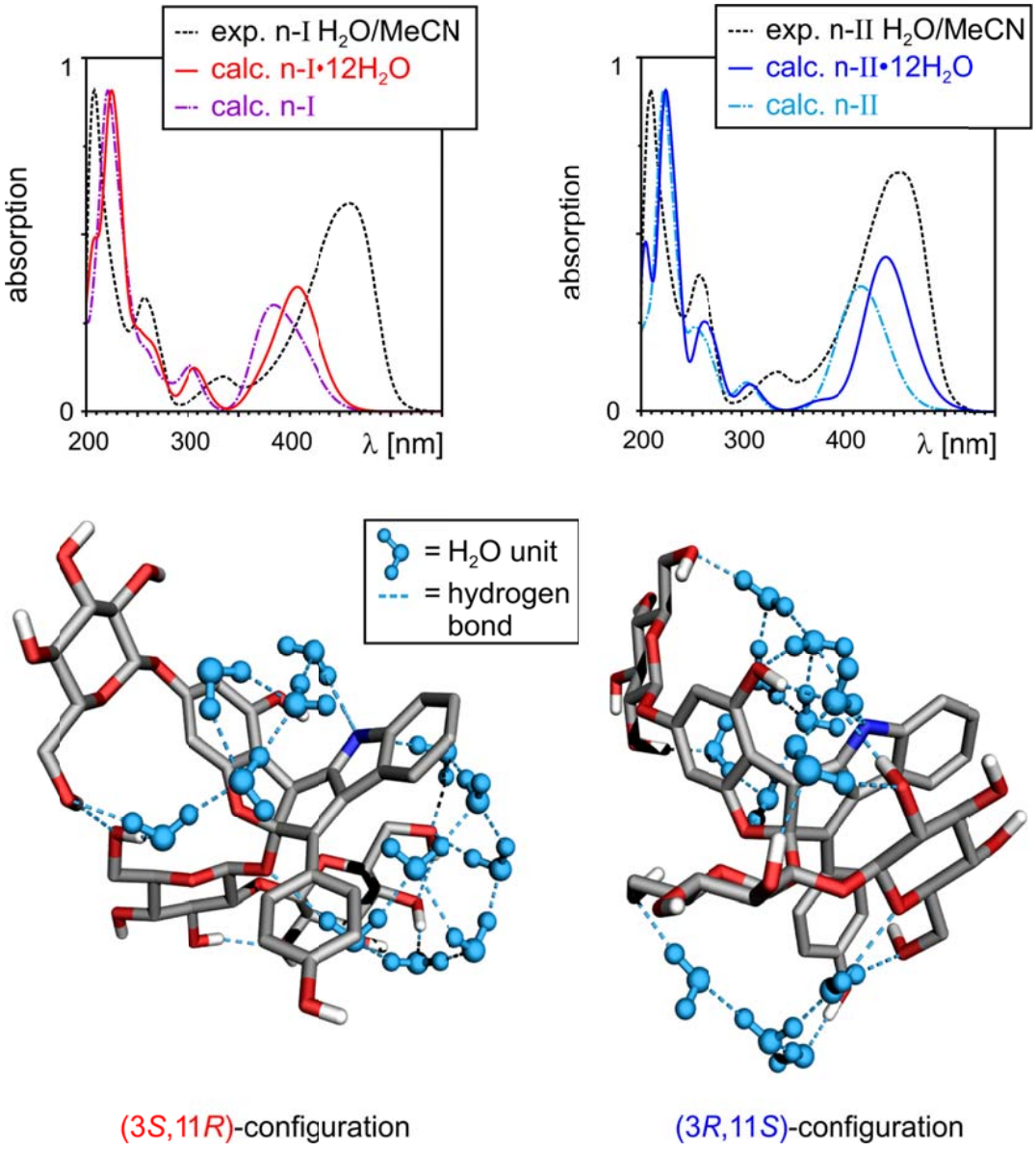


Figure S2. Comparison of the experimental UV spectra measured in MeCN–H_2O (0.1% TFA) (black dashed curves) of nudicaulins I (**3a**, left) and II (**3b**, right) with the ones obtained with ZINDO/S-CI (band width σ = 0.2 eV, no UV correction) for one (3*S*,11*R*)- and one (3*R*,11*S*)-configured structure with water (red and blue curves, corresponding structures below spectra), and without water (pink and light blue dashed-and-dotted lines).

Table S1. Calculated UV at the semiempirical ZINDO/S-CI level, wavelengths λ_k [nm], oscillator strengths f_{0k} and ratio f_{01} / f_{02} for the first two excited states of nudicaulins I (**3a**) and II (**3b**) and their respective monoglucosides (**6a** and **6b**) with and without explicit inclusion of twelve H_2O units; with f_{01} / f_{02} indicating the relative intensity between the first two UV absorptions.

compound	excited state				ratio
	λ_1 [nm]	f_{01}	λ_2 [nm]	f_{02}	f_{01} / f_{02}
3a•12H_2O	409.4	0.51	376.3	0.14	4
3a	409.4	0.25	378.6	0.40	1
6a•12H_2O	412.9	0.58	380.6	0.14	4
6a	409.0	0.25	384.1	0.47	1
3b•12H_2O	442.1	0.69	379.6	0.05	14
3b	426.3	0.44	402.4	0.28	2
6b•12H_2O	409.6	0.47	375.6	0.16	3
6b	406.6	0.28	381.1	0.36	1

TDDFT methods. The first 40 excited states of the authentic and monoglucosidic nudicaulins I (**3a**) and II (**3b**) were computed with the long-range corrected hybrid functional TD CAM-B3LYP[4] in combination with the 6-31G*[5] basis set and the CPCM[6] solvent field for MeOH. For the monoglucosides **6a** and **6b** of nudicaulins I and II, additionally, TD B2GP-PLYP/def2-TZVP(-f)[7,8] (TZVP auxiliary basis) calculations were carried out for again 40 vertical excitations, taking advantage of the 'chain-of-spheres exchange' approximation (COSX), and the COSMO solvent field for MeOH. In the case of the aglycon model, a total number of 50 excited states were computed with the TD B2GP-PLYP approach, using the same basis set and solvent field as for the monoglucosides.

To obtain the overall UV and CD spectra for the comparison with the experimental ones, the single spectra of the energetically relevant conformers were summed according to the Boltzmann factors that had been derived from the single-point energies. In order to ensure a better comparability

between the spectra of the aglycon and the monoglucoside, the single-point energies of the monoglucoside were used in the Boltzmann statistics.

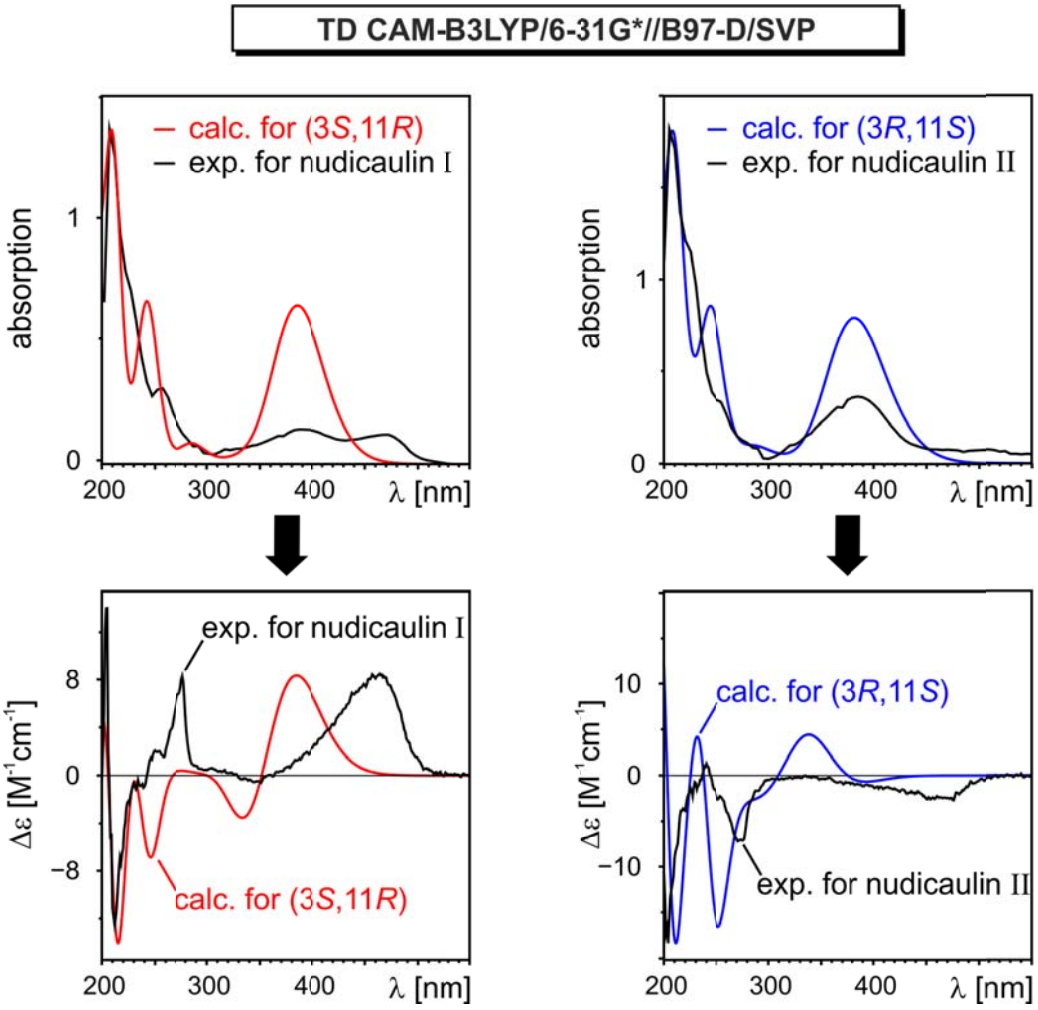


Figure S46. Nudicaulins I (**3a**) and II (**3b**): comparison of the experimental UV and CD curves with the ones obtained with TD CAM-B3LYP for the (3*S*,11*R*)- and (3*R*,11*S*)-configuration; prior to comparison, UV corrections of 15 nm and 17 nm, respectively, were applied, the band width was adjusted to the experiment using values of σ = 0.30 eV and σ = 0.36 eV, respectively.

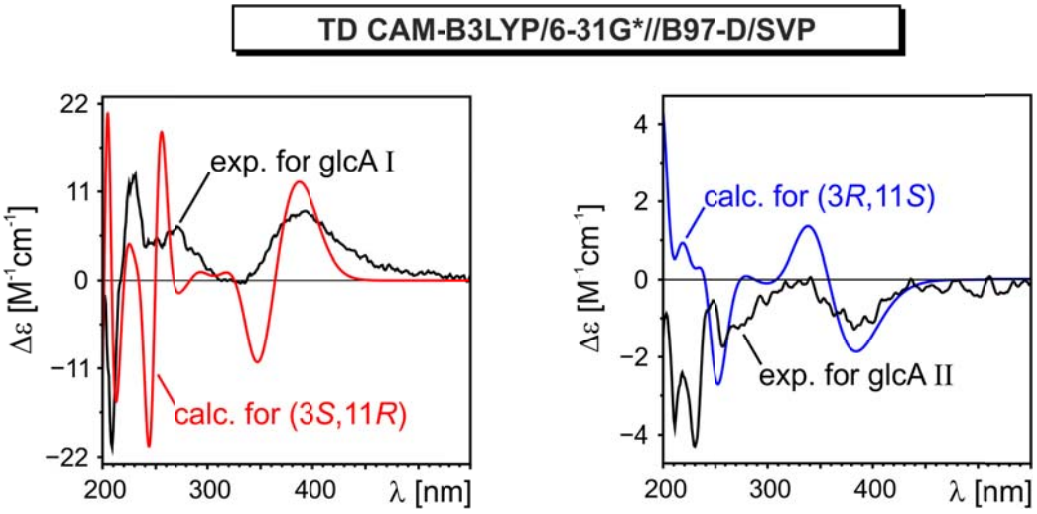


Figure S47. Monoglucosidic nudicaulins I (**6a**) and II (**6b**): comparison of the experimental CD curves with the ones obtained with TD CAM-B3LYP for the (3*S*,11*R*)- and (3*R*,11*S*)-configured diastereomers; UV correction = 20 nm in both cases, band width σ = 0.20 eV for (3*S*,11*R*) and σ = 0.20 eV for (3*R*,11*S*).

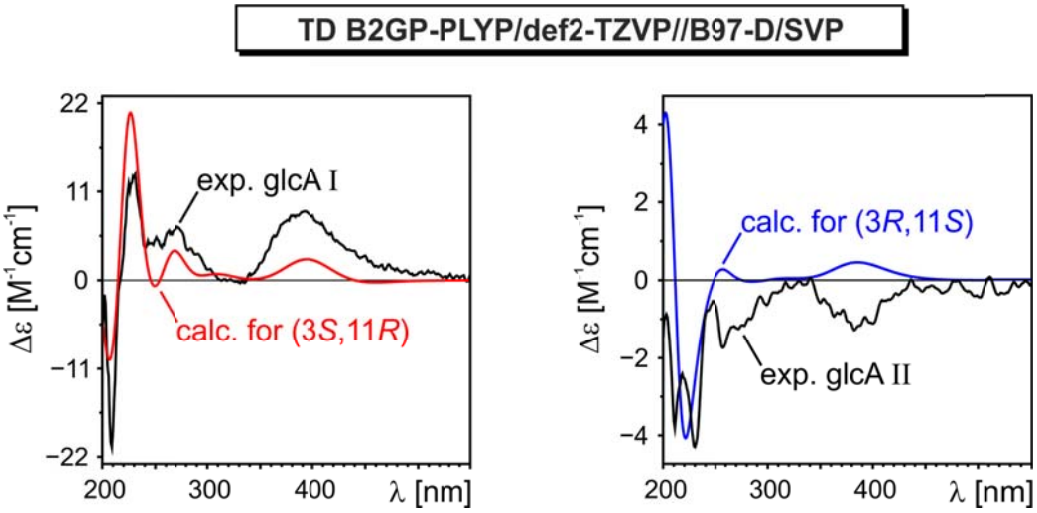


Figure S48. Monoglucosidic nudicaulins I (**6a**) and II (**6b**): experimental CD curves in comparison to the ones simulated for the (3*S*,11*R*)- and (3*R*,11*S*)-configuration using TD B2GP-PLYP; UV shift = 26 nm for (3*S*,11*R*) and 17 nm for (3*R*,11*S*), band width σ = 0.30 eV for both.

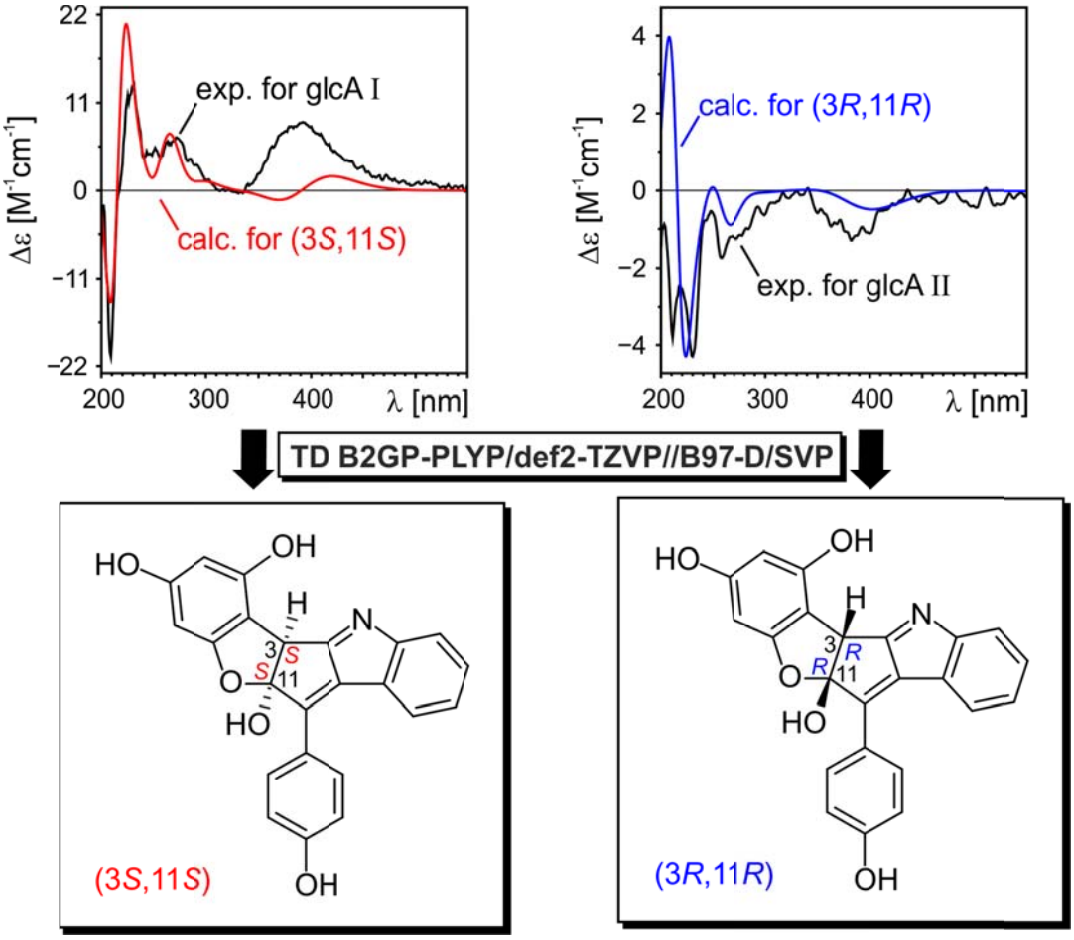


Figure S49. Aglycon model: experimental CD spectra of monoglucosidic nudicaulins I (**6a**) and II (**6b**) in comparison to the ones simulated for the (3*S*,11*S*)- and (3*R*,11*R*)-configured aglycon backbone using TD B2GP-PLYP (UV shift = 25 nm, band width σ = 0.30 eV).

Coupled-cluster RICC2 approach. All coupled-cluster excitations were computed with the Turbomole[9] software package and the implemented RICC2[10] module using the B97-D geometries. To make the calculations computationally more affordable, the def2-SV(P)8 basis set was employed. The core orbitals were kept frozen.

Table S2. Comparison of the electronic main configurations of the excited states 1–5 calculated with the coupled-cluster RICC2/def2-SV(P) method and TD B2GP-PLY/def-TZVP for one conformer of the (3*R*,11*S*)-configured monoglucoside (**6b**), and one conformer of the corresponding aglycon model **2** with (3*R*,11*R*)-configuration (identical orientation of the 4-hydroxy phenyl group relative to the chromophoric backbone).

RICC2: monoglucoside[a]

state	λ [nm]	main configuration	contribution [%]	rotatory strength	oscillator strength
1	383.7	H–1→L	92	–51	0.03
2	362.3	H, H–2→L	79, 11	–6	0.42
3	341.1	H–2, H–3, H→L	39, 38, 13	103	0.14
4	334.2	H–3, H–2→L	48, 36	–10	0.05
5	294.4	H–4, H–8, H–9→L	44, 19, 12	–14	0.06

RICC2: aglycon model[b]

state	λ [nm]	main configuration	contribution [%]	rotatory strength	oscillator strength
1	369.5	H–1→L	83	–58	0.10
2	350.3	H→L	86	18	0.58
3	328.6	H–2, H–3→L	54, 29	46	0.03
4	314.6	H–3, H–2→L	57, 24	–10	0.05
5	287.3	H–7, H–4, H–2→L	49, 17, 13	–5	0.02

TD B2GP–PLYP: monoglucoside[a]

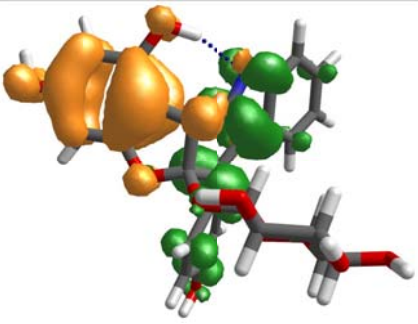
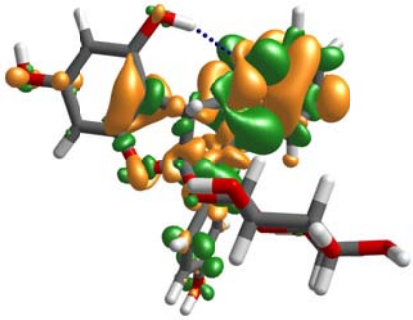
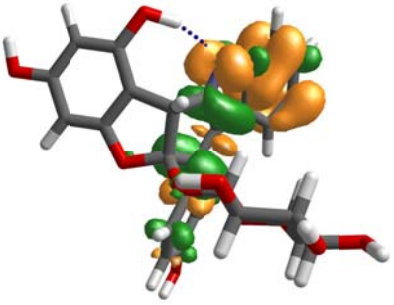
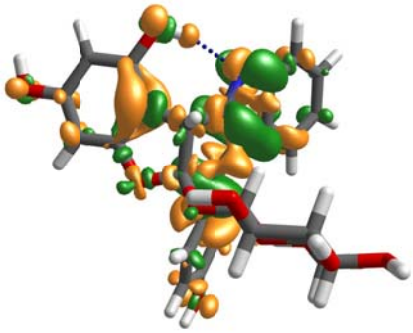
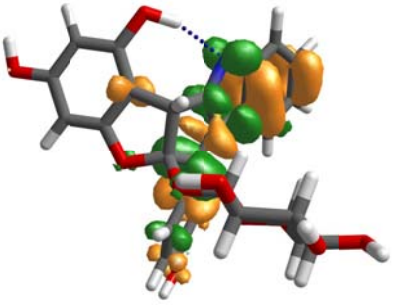
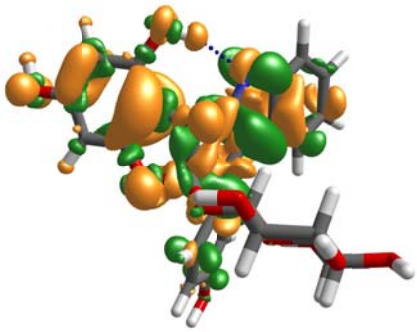
state	λ [nm]	main configuration	contribution [%]	rotatory strength	oscillator strength
1	393.3	H–2, H–1→L	58, 31	25	0.02
2	385.7	H–1, H–2, H→L	55, 23, 14	–32	0.20
3	368.5	H→L	79	89	0.46
4	362.1	H–3→L	77	–10	0.01
5	297.5	H–5, H–3, H–4→L H→L+2	43, 13,12 15	4	0.00

TD B2GP–PLYP: aglycon model[b]

state	λ [nm]	main configuration	contribution [%]	rotatory strength	oscillator strength
1	387.2	H–1, H–2→L	63, 24	–63	0.09
2	387.0	H–2, H–1→L	63, 26	11	0.01
3	356.8	H→L	88	52	0.71
4	312.7	H–3, H–4→L	45, 28	3	0.02
5	312.6	H–3, H–4→L	46, 31	–2	0.06

[a] Values of (3*R*,11*S*)-configured conf-1, for Cartesian coordinates see section S14.
[b] Values of (3*R*,11*R*)-configured conf-1, for Cartesian coordinates see section S14.

Density differences of the excited states. In order to further examine the nature of the excited states of the first broad CD effect, density-difference plots were generated exemplarily for the first five excitations of the monoglucosidic (3*R*,11*S*)-configured nudicaulin (conf-1) obtained from TD B2GP-PLYP and RICC2 calculations. All density differences were visualized with the software Chemcraft (*http://www.chemcraftprog.com*), using an isovalue of 0.0015.

B2GP-PLYP	ES-n	RICC2
	ES-1	
	ES-2	
	ES-3	

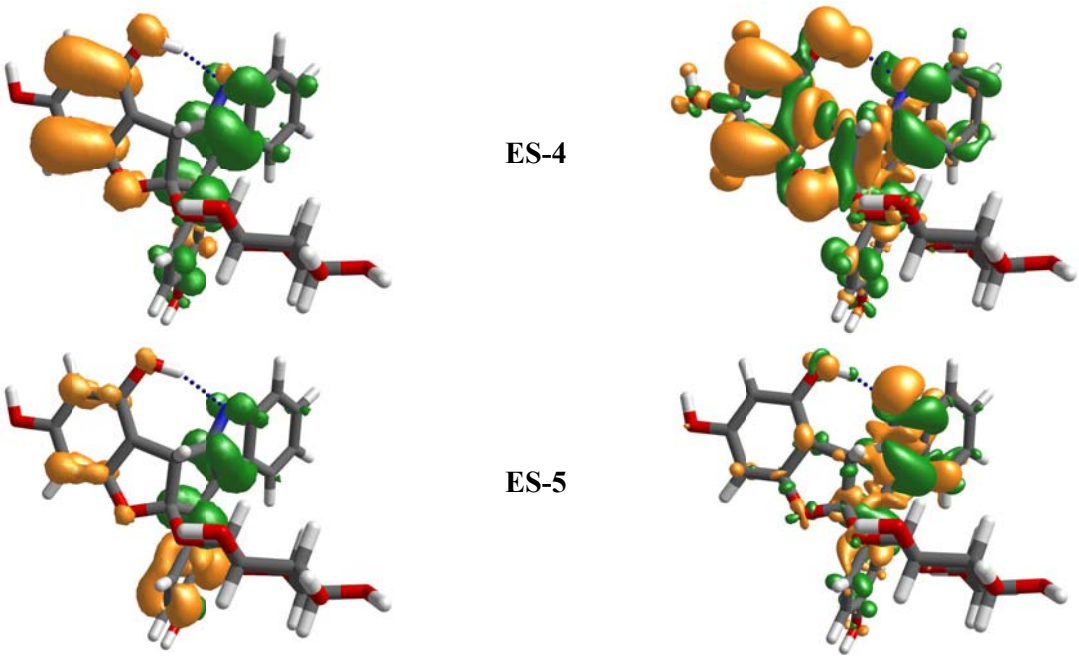


Figure S50. Density-difference plots of the first five excited states (ES-n, n=1–5) of the monoglucosidic (3*R*,11*S*)-configured nudicaulin (**6b**, conf-1) calculated with B2GP-PLYP (left) and RICC2 (right); green for increasing electron density, orange for dereasing electron density.

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S14. Cartesian Coordinates of the B97-D/SVP Optimized Structures

Nudicaulin I (3a):
(3*S*,11*R*) -configuration

conf-1
energy: -3144.3091981 Hartrees
no imaginary frequencies

C	-16.104091	2.937342	-9.736329
C	-15.211904	4.053605	-9.495650
C	-15.357811	5.403562	-9.774435
C	-14.238148	6.154271	-9.224743
C	-13.221894	5.276048	-8.591863
C	-13.868127	3.850871	-8.757486
C	-16.153991	6.428221	-10.444889
C	-15.415684	7.649760	-10.219396
N	-14.232585	7.436976	-9.465427
C	-11.980508	5.170930	-9.426075
C	-11.861943	3.861045	-9.897353
O	-12.931246	3.073336	-9.563901
C	-17.333922	6.463921	-11.206041
C	-17.781150	7.697842	-11.717807
C	-17.063487	8.885661	-11.475721
C	-15.869902	8.872173	-10.726042
C	-17.489410	3.160804	-9.976484
C	-18.368719	2.104069	-10.198359
C	-17.883928	0.775245	-10.189519
C	-16.516723	0.530352	-9.923023
C	-15.642424	1.590525	-9.687818
C	-11.047447	6.152742	-9.801345
C	-9.895839	5.730363	-10.504922
C	-9.748722	4.377843	-10.867851
C	-10.747679	3.408570	-10.608953
O	-8.561409	4.066049	-11.512210
O	-11.216137	7.461486	-9.502874
O	-18.772208	-0.221400	-10.421128
O	-8.046406	2.164715	-10.350240
C	-8.211016	2.720094	-11.643470
C	-6.423889	0.521354	-11.060908
C	-7.780148	0.758951	-10.376486
O	-6.188712	-0.870706	-11.125348
O	-5.158379	0.999564	-13.026036
O	-6.989984	3.092146	-13.741037
C	-7.850941	0.299382	-8.921777
C	-6.880954	2.629705	-12.406402
C	-6.449662	1.156425	-12.462281
O	-9.120783	0.601525	-8.355747
O	-12.889406	1.419452	-6.825484
C	-13.013351	2.817136	-6.790347
C	-11.901232	1.276289	-4.610900
C	-11.743831	0.938521	-6.110952
O	-10.748440	0.845598	-3.911508
O	-12.339651	3.088645	-3.090819
C	-11.607276	-0.564079	-6.388666
O	-14.129498	3.161444	-7.576627
C	-13.243277	3.285074	-5.349238
C	-12.102703	2.790950	-4.455124
O	-11.448551	-0.866952	-7.751479
O	-15.164479	5.687298	-6.026862
C	-14.392785	5.360759	-4.876132
C	-15.997911	7.762630	-5.109154
C	-16.370052	6.399657	-5.729322
O	-17.140450	8.526174	-4.727300
O	-14.723954	8.702525	-3.227979
O	-13.322530	6.219093	-2.926301
C	-17.163887	6.491885	-7.030870
O	-13.239714	4.712291	-5.284897
C	-13.969696	6.630577	-4.121433
C	-15.191283	7.507171	-3.829339
O	-17.571071	5.221962	-7.492709
H	-13.041207	5.517837	-7.529671
H	-17.902416	5.552278	-11.416937
H	-18.701374	7.731734	-12.314139
H	-17.435277	9.834606	-11.883315
H	-15.295165	9.788175	-10.544669
H	-17.878312	4.179334	-9.904681
H	-19.438578	2.277451	-10.360233
H	-16.145643	-0.503600	-9.892184
H	-14.593986	1.375286	-9.466311
H	-9.122072	6.454673	-10.777270
H	-10.669600	2.362668	-10.910518
H	-12.174978	7.649391	-9.358608
H	-18.313662	-1.075837	-10.369151
H	-8.993666	2.153209	-12.202782
H	-5.638987	1.044797	-10.467490
H	-8.570445	0.235841	-10.961419
H	-5.401601	-0.987977	-11.682411
H	-5.186899	1.419075	-13.901125
H	-7.239835	4.028784	-13.693697
H	-7.706094	-0.793133	-8.875559
H	-7.032769	0.792215	-8.352323
H	-6.126692	3.205083	-11.826539
H	-7.212274	0.607485	-13.062331
H	-9.330606	1.522479	-8.592707
H	-12.085073	3.297788	-7.176778
H	-12.820489	0.766765	-4.238412
H	-10.826964	1.451930	-6.482318

H	-10.824381	1.219010	-3.017796
H	-12.426809	4.057543	-3.015671
H	-10.769439	-0.929211	-5.753522
H	-12.535420	-1.060908	-6.040536
H	-14.208192	2.871709	-4.997086
H	-11.167329	3.280691	-4.812625
H	-10.620214	-0.435230	-8.044866
H	-14.997055	4.717880	-4.192594
H	-15.359953	8.318335	-5.829722
H	-16.974057	5.826589	-4.989829
H	-17.486693	8.957760	-5.521614
H	-15.508467	9.259240	-3.093540
H	-13.163153	7.023713	-2.406664
H	-18.081181	7.078867	-6.833908
H	-16.555764	7.037807	-7.785905
H	-13.281464	7.201177	-4.782601
H	-15.855727	6.946381	-3.131003
H	-16.759898	4.699746	-7.615320

conf-2
energy: -3144.3072508 Hartrees
no imaginary frequencies

C	-1.715905	-1.995763	2.644277
C	-1.605710	-1.625401	1.246850
C	-2.579947	-1.330329	0.303798
C	-1.981229	-1.230717	-1.020885
C	-0.508554	-1.416955	-0.993514
C	-0.228251	-1.587216	0.543854
C	-4.003245	-1.129345	0.042511
C	-4.083730	-1.013140	-1.395266
N	-2.811880	-1.100810	-2.018071
C	-0.056969	-2.734925	-1.546143
C	0.550416	-3.467619	-0.523030
O	0.469796	-2.852397	0.698460
C	-5.157236	-0.932182	0.817993
C	-6.382236	-0.680403	0.169827
C	-6.458244	-0.616105	-1.235574
C	-5.306105	-0.772732	-2.032458
C	-2.976023	-2.354935	3.201012
C	-3.107417	-2.732153	4.534383
C	-1.964835	-2.764498	5.368226
C	-0.699265	-2.435459	4.831402
C	-0.572451	-2.065011	3.493013
C	-0.173617	-3.272239	-2.839011
C	0.489024	-4.492853	-3.106544
C	1.184415	-5.156828	-2.077799
C	1.200300	-4.684176	-0.743082
O	1.846815	-6.312454	-2.462121
O	-0.875373	-2.656179	-3.818449
O	-2.138848	-3.128934	6.661136
O	3.823764	-5.910348	-1.382063
C	2.789478	-6.857194	-1.586046
C	5.521320	-7.572923	-0.958514
C	4.786598	-6.337187	-0.413626
O	6.440945	-8.019511	0.017061
O	5.188532	-9.745808	-1.885595
O	2.423500	-9.151367	-2.384888
C	5.676570	-5.123543	-0.153973
C	3.383500	-8.122021	-2.224102
C	4.487675	-8.660604	-1.301448
O	4.906577	-4.018250	0.305192
O	2.702046	-0.831713	1.723932
C	1.857530	-0.445023	0.669171
C	4.516954	0.630049	1.034771
C	4.090468	-0.819015	1.364582
O	5.873029	0.635809	0.629345
O	3.939593	2.541340	-0.305081
C	4.887375	-1.443450	2.516717
O	0.530198	-0.567055	1.122557
C	2.134064	1.012754	0.291927
C	3.610592	1.183124	-0.074517
O	4.507681	-2.764730	2.805855
O	-0.817624	1.856487	-0.382229
C	0.448235	2.412194	-0.716058
C	-2.069507	3.548653	-1.565240
C	-1.838072	2.847407	-0.210510
O	-3.037186	4.594005	-1.490127
O	-0.841059	4.787117	-3.298463
O	1.641077	3.786074	-2.257947
C	-3.072620	2.136456	0.340560
O	1.365298	1.383390	-0.853244
C	0.379244	3.167664	-2.051667
C	-0.753663	4.198430	-2.011902
O	-2.839021	1.547314	1.599820
H	0.028410	-0.545090	-1.410173
H	-5.112113	-0.929004	1.911742
H	-7.287399	-0.525480	0.770031
H	-7.426364	-0.425326	-1.716512
H	-5.348258	-0.693421	-3.125251
H	-3.855230	-2.376400	2.553068
H	-4.078641	-3.018284	4.953592
H	0.191367	-2.477366	5.473823
H	0.419390	-1.821271	3.103718
H	0.462397	-4.923395	-4.112249
H	1.704813	-5.199303	0.076152
H	-1.517462	-2.021187	-3.423220
H	-1.279912	-3.118357	7.114179
H	2.321052	-7.123663	-0.608126
H	6.032968	-7.283075	-1.905283
H	4.272137	-6.617131	0.533615
H	6.779422	-8.873488	-0.298744
H	4.522206	-10.415205	-2.110490
H	1.744693	-8.809489	-2.988412

H	6.416235	-5.371900	0.625737
H	6.217899	-4.871250	-1.091926
H	3.837655	-7.820887	-3.193194
H	4.002842	-8.971465	-0.347010
H	4.129563	-3.943780	-0.277193
H	2.037236	-1.086936	-0.223534
H	4.360168	1.250947	1.947720
H	4.245740	-1.438577	0.451564
H	6.044388	1.528304	0.285708
H	3.382389	2.855347	-1.041970
H	5.963066	-1.339410	2.249924
H	4.706878	-0.835748	3.426505
H	1.882876	1.648428	1.162818
H	3.799019	0.568416	-0.985031
H	4.662699	-3.291714	1.995463
H	0.762233	3.125968	0.082618
H	-2.359945	2.779657	-2.313282
H	-1.502823	3.605619	0.533060
H	-3.914547	4.185345	-1.510162
H	-1.590412	5.403935	-3.260305
H	1.546459	4.357447	-3.037268
H	-3.870226	2.892329	0.472945
H	-3.422176	1.394846	-0.411821
H	0.151957	2.426579	-2.848703
H	-0.490391	4.963392	-1.244272
H	-2.105283	0.921629	1.474804

conf-3
energy: -3144.3099798 Hartrees
no imaginary frequencies

C	0.147988	-0.018637	0.259003
C	0.154081	-0.021121	1.709092
C	1.214658	-0.028301	2.601814
C	0.735285	-0.282798	3.951706
C	-0.750454	-0.341588	4.026297
C	-1.160398	-0.139272	2.521758
C	2.662077	0.064937	2.771919
C	2.866964	-0.214409	4.176688
N	1.651835	-0.440665	4.867249
C	-1.326438	-1.691247	4.330104
C	-2.004074	-2.160679	3.200135
O	-1.878851	-1.325670	2.120544
C	3.762483	0.430256	1.972470
C	5.045655	0.482223	2.554995
C	5.235031	0.175021	3.917612
C	4.146273	-0.168420	4.741992
C	1.341899	-0.289231	-0.464221
C	1.361005	-0.308319	-1.857734
C	0.172911	-0.055584	-2.584373
C	-1.032699	0.185689	-1.886169
C	-1.045510	0.194117	-0.493759
C	-1.249816	-2.476980	5.491736
C	-1.990143	-3.677347	5.526647
C	-2.732767	-4.086363	4.399005
C	-2.745216	-3.346222	3.189397
O	-3.418251	-5.267794	4.554356
O	-0.493417	-2.119882	6.558760
O	0.130237	-0.049526	-3.936526
O	-5.142171	-5.200367	3.036970
C	-3.982434	-5.896661	3.430926
C	-6.207411	-7.188307	2.138991
C	-5.737276	-5.749733	1.850562
O	-6.740445	-7.740001	0.949197
O	-5.515287	-9.310670	2.993911
O	-3.199664	-8.101017	4.183158
C	-6.864837	-4.804982	1.425920
C	-4.342117	-7.333987	3.839756
C	-5.025374	-8.022013	2.654591
O	-6.391403	-3.522400	1.100581
O	-4.123464	0.356755	2.485688
C	-3.120380	1.223183	2.970545
C	-5.919788	1.959536	2.685474
C	-5.402200	0.572963	3.103561
O	-7.201098	2.162990	3.247352
O	-5.329893	4.283827	2.694119
C	-6.275302	-0.602301	2.681979
O	-1.934003	0.996243	2.251241
C	-3.493962	2.692116	2.717892
C	-4.917945	3.018709	3.176351
O	-5.794068	-1.824786	3.234275
O	-0.385064	3.414390	3.710068
C	-1.405461	3.880394	2.839317
C	1.188193	5.112187	2.866524
C	0.930677	3.619430	3.198291
O	2.406115	5.290926	2.164985
O	0.184069	7.086127	1.812635
O	-2.378686	5.815813	1.832510
C	1.900837	3.126747	4.284056
O	-2.632761	3.573480	3.428445
C	-1.291999	5.399041	2.646085
C	0.063774	5.684189	1.998034
O	3.262365	3.242220	3.872323
H	-1.130080	0.469200	4.678332
H	3.637344	0.701920	0.918513
H	5.905398	0.772453	1.938899
H	6.243674	0.223944	4.346340
H	4.278735	-0.375790	5.809975
H	2.253719	-0.538633	0.083522
H	2.291183	-0.534797	-2.397191
H	-1.949965	0.356424	-2.460757
H	-1.987593	0.368987	0.030602
H	-1.966046	-4.310214	6.418892
H	-3.318923	-3.652626	2.312294

H	0.203055	-1.491115	6.273954
H	1.014585	-0.238043	-4.290369
H	-3.242262	-5.918984	2.594479
H	-6.972074	-7.146922	2.948899
H	-4.977966	-5.782091	1.036551
H	-6.898936	-8.679739	1.136596
H	-4.757804	-9.808328	3.341758
H	-2.787962	-7.658518	4.942459
H	-7.344715	-5.247215	0.532961
H	-7.620859	-4.786218	2.245117
H	-5.064002	-7.265476	4.682580
H	-4.279459	-8.089248	1.828813
H	-6.181784	-3.069715	1.947090
H	-2.973880	1.063565	4.062492
H	-5.946632	1.998025	1.572278
H	-5.294376	0.549745	4.211495
H	-7.428884	3.091843	3.078362
H	-4.575414	4.894005	2.787377
H	-7.297817	-0.442034	3.064355
H	-6.314390	-0.645285	1.571812
H	-3.434418	2.875893	1.626278
H	-4.932134	2.987332	4.290928
H	-4.831829	-1.866510	3.080553
H	-1.306077	3.388498	1.846791
H	1.183735	5.677061	3.828166
H	1.075513	3.029484	2.263035
H	3.078330	4.799108	2.679536
H	1.078672	7.237487	1.465899
H	-2.169263	6.719182	1.542816
H	1.773798	3.770510	5.175142
H	1.645612	2.093127	4.575576
H	-1.326177	5.878895	3.648772
H	0.093180	5.154264	1.017182
H	3.475213	2.459955	3.335242

conf-4
energy: -3144.3122236 Hartrees
no imaginary frequencies

C	-1.916501	-0.951826	2.202405
C	-1.524023	-1.282965	0.847040
C	-1.920182	-2.330043	0.037854
C	-1.394213	-2.160568	-1.307127
C	-0.582809	-0.919123	-1.444563
C	-0.599699	-0.351922	0.023310
C	-2.663427	-3.581792	-0.042654
C	-2.488092	-4.003169	-1.415524
N	-1.693326	-3.099041	-2.162975
C	0.874433	-1.176921	-1.673764
C	1.585130	-0.823998	-0.522072
O	0.768066	-0.423515	0.503130
C	-3.417703	-4.376914	0.840707
C	-4.010293	-5.559376	0.354440
C	-3.849685	-5.949713	-0.990687
C	-3.083629	-5.178515	-1.886976
C	-3.151868	-1.419248	2.725493
C	-3.578773	-1.057528	4.003248
C	-2.766503	-0.226204	4.810270
C	-1.535304	0.253680	4.304797
C	-1.126774	-0.091922	3.018785
C	1.535617	-1.751620	-2.771926
C	2.944017	-1.806738	-2.738267
C	3.644500	-1.355826	-1.599860
C	2.981307	-0.866966	-0.444631
O	5.012114	-1.460574	-1.688079
O	0.864430	-2.252441	-3.838274
O	-3.122387	0.150563	6.060551
O	5.838703	0.169083	-0.304097
C	5.804157	-1.216258	-0.553720
C	8.047826	0.085072	0.694090
C	6.576909	0.500431	0.881720
O	8.753896	0.362016	1.889235
O	9.481560	-1.726472	0.084269
O	7.252069	-3.139643	-1.046536
C	6.382666	1.999330	1.126819
C	7.219166	-1.734869	-0.854906
C	8.121805	-1.407112	0.338652
O	5.030264	2.331552	1.315920
O	0.672890	2.350532	-0.239947
C	-0.637290	1.995124	-0.624627
C	0.364279	4.719829	-0.630872
C	1.201306	3.472272	-0.963183
O	0.892965	5.825266	-1.336330
O	-1.872657	5.570137	-0.610646
C	2.665991	3.580849	-0.556664
O	-1.078157	0.945943	0.194999
C	-1.613520	3.160812	-0.386094
C	-1.099438	4.456597	-1.018413
O	3.419076	2.448229	-0.978690
O	-3.902417	0.886850	-1.112140
C	-3.735491	2.033635	-0.285392
C	-6.062206	0.366955	-0.038958
C	-4.671446	-0.142189	-0.494051
O	-6.711588	-0.584446	0.791624
O	-7.207855	2.251806	1.027910
O	-4.870999	3.869767	0.740380
C	-4.815415	-1.269306	-1.529483
O	-2.893329	2.918307	-0.961748
C	-5.095800	2.689919	-0.012441
C	-5.941668	1.669321	0.756047
O	-5.564068	-2.370918	-1.011257
H	-1.045672	-0.222350	-2.169472
H	-3.540810	-4.095341	1.892223

H	-4.603835	-6.183895	1.033171
H	-4.328554	-6.871194	-1.344782
H	-2.948781	-5.479305	-2.932204
H	-3.813846	-2.020507	2.095666
H	-4.552612	-1.400535	4.378903
H	-0.922070	0.903526	4.939077
H	-0.180195	0.294435	2.630299
H	3.496658	-2.232967	-3.580934
H	3.512801	-0.515167	0.441840
H	-0.044510	-2.502224	-3.565557
H	-3.983948	-0.237959	6.283007
H	5.387699	-1.759604	0.329081
H	8.461340	0.658670	-0.167540
H	6.157518	-0.059154	1.748552
H	9.636412	-0.027245	1.776122
H	9.501208	-2.665300	-0.161928
H	6.693613	-3.327609	-1.817625
H	6.949614	2.262094	2.039112
H	6.840604	2.547931	0.270865
H	7.588443	-1.185525	-1.748248
H	7.740800	-1.979609	1.216035
H	4.597491	2.261020	0.436673
H	-0.659360	1.712878	-1.701561
H	0.403359	4.877584	0.471400
H	1.141844	3.277607	-2.057651
H	0.268980	6.557511	-1.203567
H	-2.807940	5.307085	-0.670231
H	3.102033	4.471724	-1.040093
H	2.721848	3.715529	0.545330
H	-1.699236	3.310268	0.709193
H	-1.128984	4.329581	-2.125825
H	2.920749	1.644540	-0.739169
H	-3.294062	1.733602	0.688642
H	-6.665049	0.589531	-0.950043
H	-4.144822	-0.519638	0.408853
H	-6.674885	-1.426244	0.292318
H	-7.737321	1.559179	1.455715
H	-5.736860	4.134013	1.092627
H	-5.374132	-0.868876	-2.397079
H	-3.819867	-1.587691	-1.886204
H	-5.582584	2.910168	-0.988315
H	-5.406441	1.434818	1.705878
H	-4.938170	-2.968355	-0.568070

Nudicaulin II (3b):
(3*R*,11*S*)-configuration

conf-1
energy: -3144.2946569 Hartrees
no imaginary frequencies

C	-2.694543	1.874140	1.281547
C	-1.801462	1.945377	0.135492
C	-1.679510	2.912957	-0.846726
C	-0.499687	2.648649	-1.668628
C	0.157864	1.364708	-1.309993
C	-0.739717	0.849910	-0.130862
C	-2.184885	4.174555	-1.384707
C	-1.210048	4.545302	-2.383894
N	-0.177388	3.579315	-2.520606
C	1.496771	1.487882	-0.657402
C	1.416705	0.986983	0.643041
O	0.124529	0.657679	1.004609
C	-3.334978	4.962026	-1.212856
C	-3.480384	6.135937	-1.978793
C	-2.497270	6.516105	-2.912672
C	-1.356045	5.717460	-3.132440
C	-2.865191	0.678405	2.035065
C	-3.746542	0.619274	3.113293
C	-4.486404	1.760873	3.488484
C	-4.307144	2.969506	2.775913
C	-3.425908	3.018403	1.696074
C	2.713305	1.937341	-1.181492
C	3.876063	1.761647	-0.400942
C	3.773230	1.176606	0.874316
C	2.539245	0.811381	1.451510
O	4.888030	0.937035	1.672468
O	2.807316	2.518717	-2.404749
O	-5.343959	1.646697	4.534125
O	5.939421	-0.584180	0.323246
C	6.094927	0.625703	1.045531
C	8.274996	-1.200131	0.573852
C	7.103509	-0.955263	-0.402182
O	9.440146	-1.486508	-0.177078
O	9.492235	-0.271924	2.400644
O	7.408939	1.650370	2.848955
C	6.767484	-2.194840	-1.229061
C	7.162853	0.450588	2.135799
C	8.474330	0.036720	1.461544
O	5.741838	-1.965378	-2.191157
O	0.337400	-1.598618	-1.174245
C	-0.751315	-1.552478	-0.278341
C	0.316052	-3.982162	-1.455167
C	1.147990	-2.767116	-0.996586
O	1.072341	-5.166905	-1.286581
O	-1.798610	-5.077310	-1.116309

C	2.457925	-2.560142	-1.744756
O	-1.436353	-0.344096	-0.429199
C	-1.720110	-2.692233	-0.611695
C	-0.973903	-4.032820	-0.617252
O	3.165982	-1.525086	-1.113052
O	-4.306143	-1.142247	0.023079
C	-4.061349	-2.530892	-0.045996
C	-6.671987	-1.429765	0.503856
C	-5.620257	-0.759498	-0.400916
O	-7.959734	-1.095695	0.023792
O	-7.394323	-3.518341	1.415344
O	-4.823793	-4.692515	0.821971
C	-5.660869	0.770367	-0.350059
O	-2.760368	-2.799791	0.368561
C	-5.013259	-3.278254	0.899592
C	-6.456438	-2.952590	0.513282
O	-4.721432	1.362539	-1.220643
H	0.165514	0.641838	-2.145733
H	-4.132785	4.655958	-0.528123
H	-4.377059	6.755324	-1.851920
H	-2.631113	7.438044	-3.493226
H	-0.602467	5.986540	-3.881885
H	-2.330600	-0.225600	1.744656
H	-3.888001	-0.310962	3.674983
H	-4.858636	3.869334	3.082525
H	-3.270668	3.967350	1.178400
H	4.834660	2.084681	-0.815152
H	2.494710	0.370180	2.450557
H	1.926817	2.858762	-2.676752
H	-5.783215	2.499696	4.681507
H	6.422602	1.438011	0.353640
H	7.996751	-2.050419	1.238373
H	7.408086	-0.129561	-1.091633
H	10.175606	-1.492516	0.457611
H	9.581749	0.506496	2.973902
H	6.566138	1.907895	3.256255
H	7.702036	-2.556681	-1.703161
H	6.384193	-2.980833	-0.553104
H	6.822293	-0.369282	2.805405
H	8.791391	0.876471	0.800212
H	6.015224	-1.229082	-2.760971
H	-0.379050	-1.666030	0.764295
H	0.031575	-3.825298	-2.520963
H	1.393858	-2.886497	0.082004
H	0.468742	-5.902680	-1.479449
H	-2.620645	-5.068591	-0.596172
H	2.999439	-3.530801	-1.729675
H	2.213658	-2.333418	-2.812021
H	-2.145225	-2.497794	-1.615353
H	-0.661936	-4.241394	0.432237
H	4.094113	-1.565637	-1.419221
H	-4.225764	-2.892343	-1.091440
H	-6.514782	-1.063397	1.545140
H	-5.787757	-1.093818	-1.449499
H	-8.586950	-1.633746	0.534002
H	-7.222093	-4.473655	1.425313
H	-4.039860	-4.888551	1.357571
H	-6.669080	1.095878	-0.662533
H	-5.505488	1.083604	0.707266
H	-4.829004	-2.905344	1.928329
H	-6.629126	-3.324918	-0.523120
H	-3.851522	1.002836	-0.978121

conf-2
energy: -3144.2967473 Hartrees
no imaginary frequencies

C	-2.779267	2.073872	1.221509
C	-1.674590	2.085331	0.279434
C	-0.749101	3.073719	0.002547
C	0.072209	2.693277	-1.141841
C	-0.278796	1.342696	-1.659651
C	-1.410097	0.888035	-0.665290
C	-0.175392	4.348977	0.422911
C	0.908727	4.568226	-0.506840
N	1.028458	3.521017	-1.458473
C	0.805327	0.346939	-1.394878
C	0.363301	-0.568320	-0.438886
O	-0.878880	-0.242499	0.068562
C	-0.399941	5.268406	1.460585
C	0.431537	6.401691	1.560432
C	1.473835	6.616139	0.637501
C	1.725401	5.698998	-0.403635
C	-3.399424	0.860590	1.633525
C	-4.500840	0.865654	2.485728
C	-5.032264	2.090675	2.943029
C	-4.426489	3.306156	2.554733
C	-3.321977	3.294104	1.702760
C	2.096188	0.258745	-1.928331
C	2.869363	-0.875699	-1.602541
C	2.348348	-1.842406	-0.723277
C	1.103194	-1.693526	-0.076501
O	3.037166	-3.008178	-0.405686
O	2.611339	1.216393	-2.740508
O	-6.152198	2.045979	3.711682
O	3.198454	-3.863016	-2.522156
C	3.921401	-3.531819	-1.350082
C	4.715712	-5.652421	-3.134813
C	4.026734	-4.341927	-3.572060
O	5.593516	-6.071574	-4.162861
O	6.006320	-6.667945	-1.406670
O	5.356029	-4.519503	0.382586
C	3.154674	-4.522985	-4.813508
C	4.558447	-4.797416	-0.755465

C	5.471206	-5.420066	-1.817455
O	2.560838	-3.307893	-5.261711
O	-1.817048	-0.875669	-2.897328
C	-2.727144	-0.751036	-1.825484
C	-3.151844	-2.409844	-4.173267
C	-1.802302	-2.195331	-3.458552
O	-3.189378	-3.702296	-4.749248
O	-5.527179	-2.332045	-3.807047
C	-0.572405	-2.332597	-4.345320
O	-2.630145	0.530333	-1.271460
C	-4.153141	-0.930195	-2.350719
C	-4.276157	-2.242739	-3.136892
O	0.564433	-2.311387	-3.522373
O	-5.923142	1.068174	-0.695513
C	-6.188942	-0.159628	-1.346854
C	-8.262792	1.438428	-0.156447
C	-6.996802	2.006782	-0.826951
O	-9.325179	2.352250	-0.350245
O	-9.709566	-0.459647	-0.034372
O	-7.683320	-2.097909	-1.315789
C	-6.514994	3.309988	-0.182547
O	-5.080387	-0.988188	-1.259321
C	-7.374190	-0.858586	-0.667393
C	-8.596362	0.057351	-0.746088
O	-5.291926	3.758221	-0.720401
H	-0.639414	1.332725	-2.703755
H	-1.197333	5.110230	2.195347
H	0.264219	7.125241	2.368040
H	2.105125	7.508900	0.734207
H	2.544060	5.851485	-1.116740
H	-3.006278	-0.092582	1.272999
H	-4.986201	-0.068088	2.791006
H	-4.858419	4.260387	2.885968
H	-2.910063	4.241952	1.345738
H	3.861211	-0.973053	-2.051135
H	0.740145	-2.448770	0.625429
H	2.169022	2.075293	-2.548267
H	-6.418137	2.951171	3.940470
H	4.733364	-2.806674	-1.598495
H	3.921367	-6.409319	-2.940073
H	4.831217	-3.598914	-3.797148
H	6.109621	-6.807411	-3.793974
H	6.453365	-6.509510	-0.559433
H	4.768424	-4.115465	1.041255
H	3.773402	-4.994731	-5.603389
H	2.317653	-5.201077	-4.565869
H	3.733833	-5.506099	-0.522793
H	6.288334	-4.690572	-2.025861
H	3.265539	-2.656329	-5.404393
H	-2.508115	-1.528880	-1.060841
H	-3.266257	-1.613612	-4.944318
H	-1.706941	-2.944355	-2.641179
H	-4.099644	-3.828060	-5.064009
H	-6.230548	-2.325383	-3.133159
H	-0.683354	-3.284125	-4.909677
H	-0.588604	-1.500009	-5.091116
H	-4.377231	-0.073544	-3.014190
H	-4.158140	-3.076379	-2.407033
H	1.327369	-2.628863	-4.045851
H	-6.456404	0.035401	-2.414102
H	-8.039497	1.294283	0.926487
H	-7.208947	2.180770	-1.906092
H	-10.126302	1.908807	-0.026365
H	-9.896633	-1.333336	-0.413456
H	-7.023108	-2.734980	-1.000383
H	-7.278889	4.087270	-0.361727
H	-6.449876	3.138987	0.915808
H	-7.113561	-1.021832	0.398286
H	-8.846749	0.202310	-1.822602
H	-4.665304	3.019240	-0.628317

trans-configured diastereomer:
(3*R*,11*R*)-configuration

conf-1
energy: -3144.2512716 Hartrees
no imaginary frequencies

C	-1.148760	-2.128712	1.459877
C	-0.762068	-2.232264	0.064160
C	-1.242815	-3.007970	-0.984270
C	-0.596134	-2.642880	-2.278573
C	0.619974	-1.845807	-1.927016
C	0.100929	-1.172956	-0.644185
C	-2.250802	-3.986743	-1.386357
C	-2.153980	-4.013567	-2.826927
N	-1.118865	-3.184362	-3.333751
C	1.533497	-0.757186	-2.427722
C	1.925824	-0.074619	-1.253925
O	1.251855	-0.537811	-0.108017
C	-3.174806	-4.830461	-0.745342
C	-4.011614	-5.654470	-1.525554
C	-3.931478	-5.643779	-2.930762
C	-2.994208	-4.825431	-3.594561
C	-0.331771	-1.434685	2.391987
C	-0.732686	-1.265357	3.719423
C	-1.972486	-1.780009	4.159598
C	-2.799701	-2.473455	3.245874
C	-2.390561	-2.638373	1.924618
C	2.163304	-0.428324	-3.638770
C	3.108689	0.626841	-3.636399
C	3.441607	1.300438	-2.453323

C	2.856982	0.955326	-1.212778
O	4.344112	2.339611	-2.597459
O	1.929521	-1.047354	-4.815514
O	-2.428216	-1.623291	5.425541
O	3.053201	3.965724	-1.664180
C	4.335987	3.369484	-1.648697
C	3.933267	6.130025	-1.023416
C	2.925837	5.006733	-0.706772
O	3.931564	7.145601	-0.031755
O	6.262910	6.578386	-1.557443
O	6.714616	3.764592	-1.918881
C	1.462877	5.465078	-0.769746
C	5.444797	4.369547	-2.037232
C	5.371504	5.582486	-1.101829
O	1.182658	6.532209	0.138723
O	-2.169879	0.677034	0.639799
C	-1.058886	0.932593	-0.225260
C	-2.672593	3.031173	0.925490
C	-2.336180	1.692735	1.624368
O	-2.764045	4.055414	1.910845
O	-1.947440	4.548285	-0.795848
C	-3.429127	1.247246	2.608546
O	-0.844262	-0.144786	-1.057358
C	-1.404774	2.172494	-1.066934
C	-1.596053	3.355600	-0.111439
O	-3.415288	2.014287	3.794773
O	-0.802338	1.124978	-3.744408
C	-0.688332	2.472772	-3.319989
C	-0.003459	1.542123	-5.961388
C	-1.174024	1.007496	-5.116813
O	-0.303809	1.347655	-7.340497
O	1.332037	3.483834	-6.358062
O	0.380327	4.632279	-3.814428
C	-1.560696	-0.450550	-5.444543
O	-0.358576	2.508938	-1.973281
C	0.397307	3.230741	-4.106810
C	0.217015	3.016153	-5.620395
O	-0.483574	-1.266951	-5.888360
H	1.311372	-2.639009	-1.559946
H	-3.238503	-4.886863	0.346713
H	-4.729981	-6.317152	-1.026900
H	-4.597472	-6.290750	-3.516195
H	-2.901822	-4.822491	-4.687033
H	0.627907	-1.022668	2.066830
H	-0.090880	-0.721649	4.426381
H	-3.772258	-2.842353	3.590858
H	-3.070098	-3.111174	1.212782
H	3.565483	0.938045	-4.580900
H	3.074151	1.481342	-0.281589
H	0.982668	-1.327402	-4.925332
H	-1.815558	-1.056135	5.920861
H	4.558124	2.979052	-0.626098
H	3.672909	6.538197	-2.027366
H	3.152896	4.623706	0.319355
H	3.001410	7.426606	0.060611
H	6.124331	7.341202	-0.972298
H	6.717366	3.017533	-2.538476
H	1.252957	5.835959	-1.787242
H	0.816929	4.582755	-0.596538
H	5.234803	4.711796	-3.075018
H	5.645972	5.232638	-0.078249
H	1.272125	6.178722	1.038217
H	-0.163064	1.153133	0.395466
H	-3.641808	2.903632	0.392749
H	-1.393032	1.829613	2.202501
H	-2.895863	4.889865	1.430887
H	-1.191466	4.761810	-1.368961
H	-4.413059	1.281097	2.083068
H	-3.232165	0.195908	2.880207
H	-2.346264	1.960422	-1.608519
H	-0.642267	3.495102	0.446920
H	-3.442344	2.946726	3.515601
H	-1.675805	2.981805	-3.495150
H	0.904389	0.976830	-5.672709
H	-2.071229	1.641534	-5.312595
H	0.410301	1.780522	-7.837276
H	1.548270	4.365879	-6.013223
H	-0.466925	4.977641	-4.144364
H	-1.961578	-0.926645	-4.533451
H	-2.354794	-0.427873	-6.217670
H	1.382914	2.849989	-3.787321
H	-0.714325	3.559670	-5.925680
H	-0.174824	-0.883925	-6.728866

Nudicaulins I (3a) and II (3b) including H_2O:
(3*S*,11*R*)- and (3*R*,11*S*)-configuration

(3*S*,11*R*)-H_2O
energy: -4060.4734096 Hartrees
no imaginary frequencies

C	-0.779956	-0.624269	2.611305
C	-0.738880	-0.817244	1.182475
C	-0.954581	-1.959098	0.426179
C	-0.889284	-1.664127	-0.994662
C	-0.514427	-0.234863	-1.259171
C	-0.313391	0.299883	0.221016
C	-1.124011	-3.402258	0.488575
C	-1.162571	-3.805715	-0.891795
N	-1.029026	-2.709689	-1.780810
C	0.888738	-0.153962	-1.806991

C	1.756503	0.189108	-0.760788
O	1.102746	0.449090	0.404504
C	-1.208143	-4.367150	1.506212
C	-1.325944	-5.723196	1.142708
C	-1.368170	-6.108981	-0.216092
C	-1.285959	-5.153906	-1.247326
C	-1.589579	-1.471312	3.420234
C	-1.641641	-1.305578	4.801185
C	-0.862278	-0.296923	5.422343
C	-0.054511	0.555868	4.631473
C	-0.032049	0.413885	3.248008
C	1.434418	-0.500769	-3.052641
C	2.834942	-0.458057	-3.218539
C	3.668553	-0.106921	-2.129929
C	3.140056	0.242514	-0.869448
O	5.016897	-0.162500	-2.347704
O	0.669197	-0.947904	-4.090721
O	-0.860491	-0.099312	6.756426
O	6.087852	0.739302	-0.503430
C	5.830005	-0.454668	-1.221121
C	8.169635	-0.139476	0.397490
C	6.791476	0.477264	0.721805
O	8.819608	-0.462415	1.613141
O	9.286332	-1.859903	-0.820620
O	6.959346	-2.257536	-2.448129
C	6.911360	1.788955	1.497089
C	7.150076	-1.054192	-1.721196
C	7.989207	-1.385061	-0.482617
O	5.688284	2.257769	2.031372
O	0.604044	3.135192	0.776309
C	-0.393817	2.650188	-0.080572
C	0.340578	5.444622	0.209759
C	1.306354	4.247922	0.198543
O	0.996551	6.588591	-0.301337
O	-1.838314	6.103728	-0.553253
C	2.622050	4.404245	0.958439
O	-0.967257	1.497305	0.522589
C	-1.480829	3.707819	-0.283479
C	-0.876552	5.073945	-0.658162
O	3.444645	3.277447	0.737932
O	-3.455465	1.397418	-1.660998
C	-3.527773	2.704242	-1.090312
C	-5.895579	1.305294	-1.950678
C	-4.623415	0.612826	-1.406846
O	-7.053976	0.559724	-1.583672
O	-7.048579	3.465420	-2.056062
O	-4.676519	4.796943	-1.159283
C	-4.383689	-0.744761	-2.067987
O	-2.332396	3.348789	-1.368069
C	-4.682937	3.493881	-1.725653
C	-5.987628	2.752567	-1.442544
O	-5.530695	-1.594055	-2.016077
H	-1.291073	0.351803	-1.785929
H	-1.178517	-4.078949	2.562512
H	-1.383966	-6.489900	1.924778
H	-1.463260	-7.171396	-0.471816
H	-1.313967	-5.449650	-2.301620
H	-2.242356	-2.203983	2.935645
H	-2.298261	-1.939732	5.412300
H	0.548818	1.327147	5.122172
H	0.599932	1.085542	2.661311
H	3.281363	-0.729703	-4.180779
H	3.761203	0.564252	-0.034738
H	-0.231046	-1.125602	-3.769799
H	-1.464258	-0.728750	7.184195
H	5.313423	-1.191380	-0.567220
H	8.754367	0.607120	-0.189956
H	6.221332	-0.258216	1.330293
H	9.591596	-0.999046	1.368556
H	9.150143	-2.649705	-1.367711
H	6.424481	-2.027219	-3.223679
H	7.600027	1.602959	2.341155
H	7.378410	2.544805	0.829532
H	7.673658	-0.283407	-2.329021
H	7.424643	-2.141267	0.106125
H	5.161817	2.729670	1.348103
H	0.037347	2.388355	-1.074019
H	-0.008103	5.602569	1.256107
H	1.570890	4.010117	-0.855923
H	0.310769	7.267108	-0.414255
H	-2.654827	5.800498	-0.994924
H	3.131190	5.305384	0.570952
H	2.404682	4.561727	2.038459
H	-2.053310	3.818511	0.659099
H	-0.496684	4.980522	-1.702503
H	3.085684	2.520540	1.279208
H	-3.706214	2.623227	0.004562
H	-5.853805	1.334593	-3.058288
H	-4.752928	0.472118	-0.319783
H	-7.056379	0.563375	-0.566938
H	-7.855052	2.950915	-1.884713
H	-5.523126	5.207208	-1.402363
H	-4.081859	-0.564550	-3.124190
H	-3.558324	-1.269975	-1.554311
H	-4.509615	3.525783	-2.823828
H	-6.126604	2.718307	-0.339795
H	-6.335115	-1.007976	-2.038299
O	1.606606	-3.545195	-2.571189
H	2.130714	-2.913169	-3.092089
H	0.688338	-3.207630	-2.657228
O	-6.689195	-1.620424	2.328265
H	-5.728943	-1.659158	2.470150
H	-6.803904	-2.227617	1.543055
O	-6.772814	-3.114868	0.075656

H	-6.283853	-2.530493	-0.541372
H	-6.139691	-3.851367	0.190933
O	3.142117	1.267594	2.471246
H	4.117100	1.349524	2.564134
H	2.973695	0.326777	2.235071
O	-3.958208	-1.903777	1.096876
H	-3.029056	-1.813580	0.833457
H	-4.193165	-2.807425	0.747534
O	-6.836846	0.734787	1.051322
H	-5.959781	1.077300	1.313000
H	-6.888725	-0.127126	1.565774
O	-4.302032	-4.369409	0.057327
H	-3.643696	-5.002434	0.385733
H	-4.115153	-4.265593	-0.922858
O	4.875574	-2.820692	0.999202
H	4.471245	-2.354365	1.751960
H	4.076948	-3.096913	0.509143
O	2.572186	-1.447457	2.165951
H	1.767072	-1.448432	2.706237
H	2.301212	-1.854820	1.307861
O	2.062988	-3.104693	0.042399
H	1.571365	-3.855804	0.409790
H	1.943144	-3.206767	-0.945824
O	-3.977245	0.807473	1.886435
H	-4.079227	-0.140580	1.657187
H	-3.109609	1.043835	1.516750
O	-3.984711	-3.839783	-2.541750
H	-4.703852	-3.171309	-2.600276
H	-3.164885	-3.327848	-2.658289

(3*R*,11*S*)-H_2O
energy: -4060.4718797 Hartrees
no imaginary frequencies

C	-1.464464	1.023329	-2.435188
C	-1.077973	0.076597	-1.434841
C	-0.877832	-1.308306	-1.453493
C	-0.529365	-1.771348	-0.135240
C	-0.415309	-0.676747	0.876536
C	-0.929177	0.547285	0.034697
C	-0.995309	-2.534098	-2.239404
C	-0.720312	-3.590983	-1.294118
N	-0.436137	-3.082384	-0.013631
C	0.974482	-0.251597	1.257058
C	1.210009	1.029998	0.737445
O	0.119473	1.556952	0.091815
C	-1.368874	-2.888219	-3.550675
C	-1.441874	-4.245753	-3.905888
C	-1.155744	-5.262906	-2.973231
C	-0.797125	-4.943489	-1.652142
C	-1.603674	0.670300	-3.815968
C	-2.186763	1.531942	-4.738746
C	-2.661728	2.815349	-4.319325
C	-2.384553	3.231169	-2.987440
C	-1.811985	2.367454	-2.078063
C	1.997591	-0.924632	1.937072
C	3.261653	-0.315234	2.040553
C	3.473612	0.952818	1.466472
C	2.447077	1.666729	0.814506
O	4.711733	1.531095	1.516477
O	1.843728	-2.190218	2.452154
O	-3.337327	3.573954	-5.162207
O	6.435090	0.037440	1.277973
C	5.645260	1.012945	0.594512
C	8.423079	0.475357	-0.050184
C	7.406120	-0.578487	0.416311
O	9.383704	-0.159613	-0.877142
O	8.572390	2.574519	-1.195950
O	5.804433	3.137466	-0.629943
C	8.022267	-1.722994	1.212772
C	6.527446	2.164568	0.079585
C	7.654125	1.570854	-0.793014
O	7.016815	-2.641537	1.657329
O	-1.443837	2.058051	2.319018
C	-2.548574	1.484946	1.672719
C	-2.388543	1.886329	4.512504
C	-1.830157	2.842129	3.455997
O	-2.802605	2.618688	5.641813
O	-4.137940	0.243380	4.876138
C	-0.597411	3.658023	3.831664
O	-2.170270	1.060667	0.378788
C	-3.151150	0.390817	2.600562
C	-3.584530	1.094578	3.908486
O	-0.145719	4.419163	2.707672
O	-4.798796	-0.630830	-0.127534
C	-4.035406	-1.121244	0.962029
C	-4.934423	-2.791119	-1.234237
C	-4.535676	-1.307391	-1.359701
O	-4.578435	-3.449120	-2.437019
O	-4.646630	-4.746464	0.107680
O	-3.663178	-3.160576	2.319029
C	-5.299818	-0.593120	-2.473114
O	-4.281161	-0.274109	2.044713
C	-4.426115	-2.582073	1.253817
C	-4.211258	-3.404070	-0.028450
O	-4.814047	0.717449	-2.736739
H	-1.048397	-0.876670	1.752659
H	-1.630117	-2.136077	-4.299648
H	-1.736885	-4.515400	-4.926878
H	-1.221614	-6.314430	-3.278849
H	-0.597055	-5.726616	-0.910284
H	-1.229385	-0.298164	-4.152071
H	-2.315277	1.240938	-5.787468
H	-2.702051	4.221203	-2.663334

H	-1.678897	2.730100	-1.060126
H	4.086147	-0.822560	2.547554
H	2.669825	2.631140	0.349973
H	0.889529	-2.440179	2.548520
H	-3.742741	4.370086	-4.657894
H	5.122960	0.528167	-0.258494
H	8.898190	0.932494	0.849335
H	6.898246	-0.989027	-0.478756
H	9.849658	0.554920	-1.341763
H	8.020488	3.307549	-1.521441
H	5.333291	2.654803	-1.374605
H	8.724494	-2.276500	0.567821
H	8.581580	-1.310241	2.079801
H	6.986964	2.649765	0.964303
H	7.179320	1.096064	-1.681890
H	6.365146	-2.090858	2.125848
H	-3.327068	2.245922	1.462827
H	-1.588552	1.148474	4.767504
H	-2.633734	3.542843	3.147765
H	-3.378358	2.013941	6.144918
H	-3.557791	-0.557192	4.943768
H	0.204152	2.983142	4.199476
H	-0.860458	4.363232	4.638406
H	-2.379439	-0.354306	2.868911
H	-4.365538	1.838755	3.646393
H	0.168667	3.766697	2.057146
H	-2.962514	-1.125957	0.682348
H	-6.030496	-2.851695	-1.042458
H	-3.448667	-1.268715	-1.580958
H	-4.642107	-4.402893	-2.265843
H	-4.282779	-5.072916	0.946840
H	-2.707476	-3.141745	2.097442
H	-6.357435	-0.486849	-2.167619
H	-5.257293	-1.228797	-3.379150
H	-5.483907	-2.620274	1.568482
H	-3.121143	-3.370280	-0.261242
H	-3.941268	0.643854	-3.157870
O	4.614708	1.690988	-2.519861
H	4.897562	0.746536	-2.454969
H	3.632083	1.632584	-2.512292
O	5.491232	-3.196278	-0.653895
H	4.604169	-3.456007	-0.344434
H	6.025163	-3.087951	0.166221
O	-4.910902	2.393213	-0.527900
H	-5.216743	1.774123	0.152039
H	-4.777709	1.808749	-1.310256
O	-4.416642	5.503315	-3.764738
H	-3.960175	6.357093	-3.817495
H	-4.458462	5.313008	-2.775053
O	4.930701	-1.024221	-2.235265
H	3.965536	-1.181867	-2.209675
H	5.278932	-1.773675	-1.687604
O	-2.479013	4.896592	1.052672
H	-3.057324	5.441324	1.608191
H	-1.636932	4.862089	1.561627
O	-4.390896	5.013083	-1.117204
H	-4.701163	4.100888	-0.882922
H	-3.560144	5.079734	-0.605497
O	-2.732404	-2.085402	4.722565
H	-3.284425	-2.442312	3.989452
H	-1.838940	-2.124120	4.345293
O	1.824186	1.150105	-2.446417
H	1.916684	0.276191	-2.007981
H	1.269276	1.657953	-1.835365
O	-0.724289	-3.271397	2.555399
H	-0.628517	-4.135070	2.987324
H	-0.584752	-3.431111	1.543716
O	2.184231	-1.512679	-1.707230
H	2.371938	-2.152287	-0.971812
H	1.609781	-1.999879	-2.318995
O	2.645818	-3.486591	0.132545
H	2.435757	-3.146198	1.034647
H	1.880080	-4.043025	-0.085466

Monoglucoside of nudicaulin I (6a):
(3*S*,11*R*)-configuration

conf 1
energy: -1924.4231232 Hartrees
no imaginary frequencies

C	2.512042	0.045757	2.164539
C	2.057917	0.882733	1.066045
C	2.501427	2.120826	0.646635
C	1.891402	2.466407	-0.633256
C	0.827477	1.508954	-1.025771
C	1.015294	0.358129	0.031649
C	3.407233	3.239342	0.902040
C	3.259224	4.084061	-0.258995
N	2.309471	3.571597	-1.184896
C	-0.532708	2.033275	-0.660584
C	-1.102552	1.183709	0.293169
O	-0.267618	0.144668	0.642519
C	4.268624	3.635841	1.939356
C	4.992710	4.837301	1.805771
C	4.861769	5.636741	0.653853
C	3.988059	5.269286	-0.390148
C	3.799114	0.245657	2.737150
C	4.288890	-0.582918	3.744558
C	3.493946	-1.649355	4.225050
C	2.216838	-1.872677	3.662590
C	1.737500	-1.044992	2.644932

C	-1.200687	3.206556	-1.059666
C	-2.499288	3.435803	-0.556928
C	-3.074194	2.532681	0.361389
C	-2.375816	1.388743	0.827339
O	-4.329857	2.826511	0.807033
O	-0.645987	4.113250	-1.898975
O	4.008224	-2.424024	5.211322
O	3.188950	0.070649	-1.565119
C	2.712811	-1.075807	-0.896451
C	4.779474	-1.114534	-2.918322
C	4.579942	0.009331	-1.887218
O	6.161682	-1.226235	-3.201703
O	4.344744	-3.428566	-3.342872
C	5.008700	1.409922	-2.352528
O	1.359756	-0.886254	-0.541039
C	2.787706	-2.282903	-1.842246
C	4.232436	-2.432137	-2.338715
O	4.187465	1.936944	-3.371090
O	2.420144	-3.497471	-1.207227
H	0.919016	1.137051	-2.061750
H	4.369715	3.041142	2.853944
H	5.665059	5.153925	2.612689
H	5.441802	6.564679	0.571131
H	3.867747	5.891523	-1.284471
H	4.438815	1.038788	2.340457
H	5.288423	-0.434615	4.168797
H	1.601203	-2.705014	4.031710
H	0.746890	-1.230320	2.222011
H	-3.050655	4.333033	-0.854018
H	-2.807572	0.710197	1.572018
H	-4.605066	2.145957	1.440152
H	0.329554	4.004923	-1.922694
H	3.368425	-3.116714	5.442297
H	3.328933	-1.262042	0.014094
H	4.191316	-0.848761	-3.824020
H	5.169977	-0.250397	-0.977812
H	6.256554	-2.000338	-3.779892
H	3.987110	-4.245795	-2.960001
H	5.034745	2.073949	-1.461235
H	6.037490	1.317631	-2.748217
H	2.134079	-2.056462	-2.712230
H	4.864143	-2.689231	-1.456574
H	3.405988	2.312861	-2.931959
H	1.489070	-3.404749	-0.950217

conf 2
energy: -1924.4244496 Hartrees
no imaginary frequencies

C	-0.183331	1.868549	1.455210
C	0.435783	0.878793	0.594188
C	0.154708	-0.462993	0.436158
C	1.133683	-1.084905	-0.450596
C	2.213512	-0.140008	-0.834871
C	1.636546	1.235247	-0.332240
C	-0.788143	-1.542437	0.712397
C	-0.256974	-2.667491	-0.019345
N	0.942314	-2.347627	-0.713115
C	3.438579	-0.263311	0.027835
C	3.650481	0.954111	0.685360
O	2.676195	1.887386	0.401730
C	-2.012201	-1.669831	1.389985
C	-2.686088	-2.906917	1.353838
C	-2.148469	-4.003081	0.651455
C	-0.928588	-3.892683	-0.047440
C	-0.939178	1.467780	2.591737
C	-1.545460	2.399888	3.431483
C	-1.415834	3.781108	3.155936
C	-0.653865	4.201659	2.041559
C	-0.040415	3.261720	1.211593
C	4.289066	-1.358512	0.264676
C	5.404251	-1.166324	1.108093
C	5.621247	0.084866	1.721759
C	4.732410	1.175719	1.538788
O	6.717338	0.191814	2.527545
O	4.078863	-2.580325	-0.283014
O	-2.030505	4.650882	3.994300
O	-0.076457	0.588052	-2.414352
C	0.066339	1.933725	-2.017468
C	-1.469724	1.073745	-4.309785
C	-1.360139	0.304829	-2.981940
O	-2.749920	0.838223	-4.865284
O	-1.278501	3.255116	-5.279907
C	-1.499745	-1.222751	-3.088347
O	1.313847	2.117663	-1.391973
C	0.033545	2.837368	-3.258742
C	-1.263198	2.574791	-4.034798
O	-0.385077	-1.847484	-3.684983
O	0.074068	4.218111	-2.925674
H	2.418471	-0.127909	-1.921122
H	-2.454976	-0.823655	1.927073
H	-3.643411	-3.015624	1.878401
H	-2.692433	-4.956144	0.640093
H	-0.514731	-4.732608	-0.617149
H	-1.008772	0.402268	2.831322
H	-2.115141	2.087429	4.313993
H	-0.546680	5.275328	1.832734
H	0.545015	3.602813	0.353040
H	6.089119	-1.995915	1.308131
H	4.880366	2.135487	2.046984
H	6.748048	1.087730	2.896480
H	3.162685	-2.650010	-0.622220
H	-1.858245	5.559121	3.697839
H	-0.760707	2.207737	-1.319817

H	-0.656079	0.714313	-4.977651
H	-2.165097	0.676799	-2.306617
H	-2.815136	1.411968	-5.645720
H	-1.135718	4.194377	-5.080384
H	-1.697593	-1.620703	-2.070327
H	-2.387973	-1.423481	-3.715986
H	0.894017	2.543106	-3.896787
H	-2.111877	2.908609	-3.392950
H	0.297026	-1.907604	-2.994646
H	0.956801	4.387062	-2.560662

conf 3
energy: -1924.4252962 Hartrees
no imaginary frequencies

C	0.091461	1.266407	0.652793
C	0.348520	0.447932	1.825492
C	1.514043	0.263561	2.539868
C	1.255051	-0.530037	3.737565
C	-0.160445	-0.985696	3.816782
C	-0.805774	-0.303281	2.549524
C	2.960158	0.464582	2.568361
C	3.387127	-0.232190	3.758102
N	2.303681	-0.837872	4.449474
C	-0.245430	-2.442024	3.451176
C	-0.941610	-2.571398	2.243113
O	-1.331065	-1.353246	1.729358
C	3.911906	1.084247	1.742415
C	5.271670	1.025552	2.107740
C	5.676234	0.357470	3.280034
C	4.737897	-0.282162	4.116216
C	-1.036049	1.041865	-0.188115
C	-1.317546	1.891180	-1.258916
C	-0.480244	2.999792	-1.524883
C	0.640346	3.240001	-0.697428
C	0.917782	2.383989	0.369380
C	0.358705	-3.563084	4.047783
C	0.100865	-4.829003	3.473564
C	-0.671085	-4.937983	2.295885
C	-1.191941	-3.799256	1.633048
O	-0.922596	-6.147394	1.717570
O	1.169998	-3.470421	5.126896
O	-0.803718	3.795553	-2.572339
O	-2.159668	1.176296	4.962197
C	-1.723467	1.604312	3.680553
C	-2.847031	3.417452	5.633934
C	-2.019835	2.169100	5.991588
O	-2.598311	4.401094	6.622073
O	-3.304802	5.019947	3.926221
C	-2.485529	1.504230	7.291885
O	-1.913011	0.545440	2.782039
C	-2.553676	2.806513	3.199177
C	-2.459977	3.923957	4.241355
O	-3.822615	1.052470	7.214251
O	-2.069084	3.336990	1.977284
H	-0.684498	-0.713074	4.750503
H	3.614696	1.594632	0.819275
H	6.024265	1.504304	1.469073
H	6.741160	0.328672	3.543988
H	5.047473	-0.815787	5.022368
H	-1.687263	0.185222	0.005547
H	-2.180002	1.713936	-1.911551
H	1.277890	4.114793	-0.886788
H	1.757841	2.608019	1.034224
H	0.552025	-5.719174	3.929786
H	-1.745188	-3.897261	0.695287
H	-0.513181	-6.840722	2.258085
H	1.594528	-2.577759	5.150805
H	-0.158352	4.517581	-2.640646
H	-0.650638	1.905314	3.732246
H	-3.916658	3.115084	5.616808
H	-0.952456	2.471423	6.090968
H	-3.069410	5.198423	6.330910
H	-3.067505	5.297311	3.026619
H	-1.777052	0.678314	7.532159
H	-2.434047	2.258112	8.097362
H	-3.610430	2.470484	3.118282
H	-1.394093	4.249241	4.285716
H	-3.863732	0.464419	6.441999
H	-2.130733	2.641574	1.301226

conf 4
energy: -1924.423293 Hartrees
no imaginary frequencies

C	-0.136606	2.255133	-0.777922
C	0.534984	1.012898	-0.441856
C	0.365470	0.172233	0.640673
C	1.395995	-0.860326	0.649048
C	2.371087	-0.682054	-0.458641
C	1.697172	0.452771	-1.318242
C	-0.417052	-0.116077	1.839635
C	0.256763	-1.247198	2.432517
N	1.385798	-1.663010	1.678217
C	3.614048	0.018645	0.013635
C	3.736793	1.235084	-0.672569
O	2.688684	1.457094	-1.539264
C	-1.586804	0.386903	2.433741
C	-2.065676	-0.214684	3.614605
C	-1.387790	-1.303903	4.196893
C	-0.221512	-1.834421	3.608590
C	-0.133397	2.770653	-2.106244
C	-0.792180	3.959243	-2.415994
C	-1.458175	4.687400	-1.404332

C	-1.449332	4.204878	-0.074342
C	-0.801049	3.006715	0.227301
C	4.525530	-0.327560	1.024846
C	5.627588	0.532817	1.237268
C	5.760219	1.723138	0.489115
C	4.798662	2.116216	-0.474618
O	6.810313	2.573117	0.683757
O	4.388132	-1.434781	1.793117
O	-2.079994	5.839012	-1.759474
O	0.238418	-1.916780	-2.057467
C	0.083418	-0.645139	-2.684293
C	-1.413522	-2.988285	-3.435778
C	-0.980780	-2.664292	-1.990611
O	-2.654401	-3.687518	-3.488612
O	-1.881899	-1.905254	-5.584905
C	-0.704284	-3.904884	-1.140017
O	1.293299	0.038437	-2.608954
C	-0.316632	-0.816822	-4.155390
C	-1.586825	-1.682150	-4.215831
O	0.208920	-4.794516	-1.759419
O	-0.541917	0.460370	-4.716549
H	2.556260	-1.597081	-1.048819
H	-2.133559	1.225418	1.987567
H	-2.978213	0.171217	4.085894
H	-1.777503	-1.750725	5.120595
H	0.304145	-2.690497	4.047675
H	0.364548	2.214857	-2.905291
H	-0.805454	4.345190	-3.441437
H	-1.943955	4.784291	0.717963
H	-0.765059	2.659572	1.264324
H	6.356635	0.279013	2.017202
H	4.893055	3.063644	-1.011830
H	7.386936	2.200075	1.368385
H	3.452632	-1.744540	1.781012
H	-2.486287	6.239406	-0.974027
H	-0.728857	-0.089843	-2.160878
H	-0.602054	-3.580844	-3.903688
H	-1.775729	-2.058027	-1.499131
H	-2.458204	-4.623756	-3.335348
H	-2.659820	-2.486683	-5.598494
H	-0.353310	-3.571419	-0.138823
H	-1.656260	-4.452837	-1.007184
H	0.506615	-1.359319	-4.671053
H	-2.406234	-1.105754	-3.725360
H	1.030256	-4.292524	-1.887587
H	-0.938172	0.304704	-5.589417

conf 5
energy: -1924.4224497 Hartrees
no imaginary frequencies

C	0.491810	1.143884	1.102968
C	-0.489126	0.662897	0.133957
C	-1.500423	1.396802	-0.448858
C	-2.333571	0.549210	-1.291678
C	-1.877056	-0.868397	-1.271577
C	-0.571814	-0.796400	-0.405871
C	-2.210550	2.673870	-0.436657
C	-3.377088	2.431750	-1.250184
N	-3.424391	1.099357	-1.745285
C	-2.776649	-1.707395	-0.405781
C	-2.042838	-2.194492	0.680191
O	-0.739703	-1.741287	0.686512
C	-2.027941	3.927484	0.168207
C	-2.994088	4.931293	-0.044587
C	-4.122961	4.689186	-0.851329
C	-4.328334	3.434298	-1.461314
C	0.993126	2.467198	0.982859
C	1.939990	2.974859	1.870834
C	2.413258	2.167380	2.930280
C	1.919617	0.851812	3.073300
C	0.977605	0.347237	2.170375
C	-4.162450	-1.949300	-0.498322
C	-4.745883	-2.814995	0.452481
C	-3.966642	-3.354123	1.497200
C	-2.592859	-3.033730	1.651305
O	-4.605945	-4.174673	2.380219
O	-4.937290	-1.386827	-1.452246
O	3.334203	2.704403	3.768350
O	2.392951	0.083549	-1.001882
C	1.811142	-1.155036	-0.654457
C	4.650483	-0.847427	-0.967058
C	3.710912	0.262222	-0.455364
O	5.892364	-0.702020	-0.299866
O	4.905771	-3.197495	-1.290458
C	4.168603	1.659893	-0.884977
O	0.513379	-1.201711	-1.197037
C	2.617442	-2.317729	-1.250551
C	4.045398	-2.231832	-0.706856
O	4.185474	1.810971	-2.291770
O	2.087426	-3.574904	-0.868933
H	-1.677204	-1.295202	-2.273703
H	-1.157991	4.127693	0.803149
H	-2.863970	5.914254	0.424803
H	-4.857828	5.489704	-1.005160
H	-5.210615	3.235209	-2.080671
H	0.659538	3.082029	0.140554
H	2.341772	3.988048	1.757497
H	2.276351	0.226350	3.903455
H	0.589487	-0.666529	2.303472
H	-5.816287	-3.037037	0.403770
H	-2.001029	-3.412770	2.492504
H	-3.973655	-4.460680	3.057037
H	-4.530811	-0.540808	-1.766887

H	3.581339	2.047810	4.439179
H	1.784338	-1.274294	0.448762
H	4.758725	-0.711754	-2.064992
H	3.669355	0.208557	0.655119
H	6.444462	-1.442488	-0.598894
H	4.490432	-4.062117	-1.141220
H	3.506552	2.404440	-0.391450
H	5.201043	1.806211	-0.520927
H	2.636332	-2.188143	-2.355293
H	3.988660	-2.371980	0.398055
H	3.294093	1.573792	-2.596713
H	1.157259	-3.584295	-1.147786

Monoglucoside of nudicaulin II (6b):
(3*R*,11*S*)-configuration

conf 1
energy: -1924.4282005 Hartrees
no imaginary frequencies

C	1.449659	-0.960392	-1.016268
C	1.389397	-0.467699	0.347347
C	2.355585	-0.462704	1.334252
C	1.947085	0.400008	2.436361
C	0.592031	0.976792	2.220114
C	0.125579	0.253069	0.902921
C	3.703045	-0.877865	1.708640
C	3.967267	-0.154056	2.928344
N	2.862824	0.644840	3.332631
C	0.640325	2.403915	1.756283
C	0.053682	2.488600	0.486365
O	-0.354517	1.256438	0.013887
C	4.641730	-1.801641	1.221432
C	5.857919	-1.957524	1.915194
C	6.129134	-1.210556	3.078926
C	5.181904	-0.307544	3.604606
C	2.701185	-1.226784	-1.637711
C	2.778914	-1.713727	-2.941091
C	1.592644	-1.950091	-3.673357
C	0.338861	-1.678167	-3.078127
C	0.268934	-1.185226	-1.774856
C	1.230934	3.532206	2.349571
C	1.094363	4.769861	1.678616
C	0.439421	4.839094	0.429522
C	-0.079412	3.686547	-0.212510
O	0.304915	6.020205	-0.239974
O	1.914842	3.478553	3.515810
O	1.715758	-2.429733	-4.934602
O	-0.152415	-2.766005	0.962573
C	-0.671728	-1.780611	1.834569
C	-0.846471	-4.597393	2.376565
C	0.338593	-3.913619	1.669483
O	-0.357336	-5.693063	3.124428
O	-2.703905	-4.230928	3.831269
C	1.044525	-4.796297	0.639968
O	-0.975589	-0.630880	1.096546
C	-1.942926	-2.309022	2.510512
C	-1.568969	-3.582387	3.280253
O	2.126830	-4.134531	0.018006
O	-2.471763	-1.379489	3.442851
H	-0.107449	0.798241	3.062412
H	4.419455	-2.422603	0.347282
H	6.599887	-2.677288	1.547910
H	7.087324	-1.347728	3.596425
H	5.373829	0.252419	4.527399
H	3.622955	-1.025414	-1.084496
H	3.744949	-1.913496	-3.417875
H	-0.582230	-1.859944	-3.649381
H	-0.705930	-0.990332	-1.321676
H	1.540199	5.667331	2.125709
H	-0.537152	3.751138	-1.203133
H	0.708779	6.724712	0.290193
H	2.229441	2.558833	3.688542
H	0.833107	-2.542029	-5.322954
H	0.079895	-1.557296	2.627868
H	-1.570789	-4.925487	1.594898
H	1.078744	-3.588052	2.433891
H	-1.104537	-6.013187	3.656137
H	-3.143555	-3.579592	4.401160
H	0.283396	-5.141370	-0.098539
H	1.438828	-5.685133	1.163283
H	-2.676731	-2.564684	1.715613
H	-0.854691	-3.285849	4.082839
H	1.763654	-3.339218	-0.406362
H	-2.728264	-0.593128	2.934596

conf 2
energy: -1924.4266181 Hartrees
no imaginary frequencies

C	1.892153	2.110872	0.540596
C	1.620091	0.783563	0.016086
C	2.478292	-0.150508	-0.532046
C	1.723916	-1.287089	-1.050350
C	0.264015	-1.161602	-0.787480
C	0.181625	0.212687	-0.023486
C	3.869456	-0.534583	-0.759238
C	3.776748	-1.837643	-1.376028
N	2.432743	-2.267408	-1.535838
C	-0.174118	-2.141490	0.259699
C	-0.495047	-1.445615	1.429777
O	-0.280638	-0.089907	1.317403

C	5.132441	0.012288	-0.477329
C	6.286167	-0.717502	-0.826403
C	6.183719	-1.977328	-1.447798
C	4.926642	-2.552819	-1.724882
C	0.978092	2.779666	1.404206
C	1.238447	4.064954	1.877786
C	2.421435	4.736710	1.492187
C	3.331878	4.098014	0.618756
C	3.068006	2.807189	0.156755
C	-0.153110	-3.550736	0.251128
C	-0.656268	-4.224998	1.383532
C	-1.072699	-3.494219	2.516531
C	-0.968888	-2.080128	2.578172
O	-1.544182	-4.215856	3.571267
O	0.327406	-4.255459	-0.799173
O	2.623752	5.985503	1.979028
O	-2.520633	-0.186932	-0.790591
C	-2.043131	1.069611	-0.358047
C	-4.737732	0.643401	-1.273273
C	-3.908770	-0.379141	-0.474489
O	-6.102926	0.482201	-0.940509
O	-4.976065	2.973744	-1.751616
C	-4.233534	-1.842154	-0.768282
O	-0.664551	1.170887	-0.612862
C	-2.735860	2.198804	-1.132884
C	-4.250588	2.063921	-0.939069
O	-3.564087	-2.721094	0.105814
O	-2.352639	3.481812	-0.662373
H	-0.365234	-1.152668	-1.695168
H	5.233239	0.982151	0.022419
H	7.276519	-0.298873	-0.608338
H	7.097617	-2.524121	-1.713082
H	4.838260	-3.540601	-2.191904
H	0.065030	2.268648	1.720568
H	0.539734	4.572729	2.552383
H	4.239773	4.627100	0.296976
H	3.757121	2.338809	-0.552276
H	-0.690167	-5.318344	1.400609
H	-1.237038	-1.519828	3.480984
H	-1.802935	-3.606313	4.279200
H	1.015456	-3.722415	-1.266226
H	3.465903	6.331190	1.641685
H	-2.245347	1.188444	0.729692
H	-4.555920	0.466894	-2.358807
H	-4.068432	-0.198999	0.611863
H	-6.571136	1.226651	-1.352738
H	-4.650370	3.860598	-1.528855
H	-5.320111	-1.983080	-0.626830
H	-3.999500	-2.037575	-1.841894
H	-2.496415	2.062911	-2.210146
H	-4.466134	2.240692	0.140081
H	-2.609227	-2.552903	0.021397
H	-1.392933	3.552067	-0.791334

conf 3
energy: -1924.425858 Hartrees
no imaginary frequencies

C	2.101217	1.883471	0.579697
C	1.599037	0.655770	-0.021104
C	1.957900	0.044007	-1.207686
C	1.345809	-1.277542	-1.302767
C	0.507567	-1.596677	-0.116188
C	0.630148	-0.282775	0.740713
C	2.769117	0.127985	-2.421340
C	2.586708	-1.157421	-3.054116
N	1.711380	-2.002675	-2.322008
C	1.155599	-2.614448	0.774017
C	1.504385	-2.005826	1.984506
O	1.218378	-0.658895	2.004792
C	3.559766	1.104730	-3.049785
C	4.181429	0.795846	-4.276074
C	4.018520	-0.470958	-4.870046
C	3.214429	-1.459486	-4.266806
C	1.391567	2.582886	1.597539
C	1.902367	3.749603	2.165911
C	3.155395	4.252948	1.749691
C	3.888354	3.559368	0.759211
C	3.364610	2.399205	0.186938
C	1.525470	-3.948567	0.512245
C	2.092475	-4.695295	1.566677
C	2.350370	-4.082093	2.811148
C	2.088999	-2.706278	3.039683
O	2.900480	-4.868008	3.778635
O	1.349408	-4.520502	-0.701511
O	3.606375	5.389641	2.335145
O	-1.699762	-1.454056	1.832479
C	-1.394273	-0.087813	2.019619
C	-3.789558	-1.315627	3.036181
C	-2.417496	-2.008510	2.946120
O	-4.483443	-1.825588	4.157764
O	-4.867957	0.815755	3.143905
C	-2.470270	-3.519717	2.730861
O	-0.601498	0.375099	0.955221
C	-2.687741	0.737251	2.030927
C	-3.587147	0.206125	3.153585
O	-1.195295	-4.113037	2.815731
O	-2.446474	2.117117	2.279804
H	-0.545365	-1.821740	-0.363160
H	3.685493	2.101245	-2.611357
H	4.799275	1.553381	-4.774139
H	4.519035	-0.689267	-5.822118
H	3.069074	-2.442419	-4.729879
H	0.416696	2.215703	1.927460

H	1.346617	4.291378	2.939765
H	4.876376	3.930941	0.453078
H	3.960517	1.848148	-0.546147
H	2.363283	-5.743943	1.412196
H	2.339127	-2.219398	3.989001
H	3.012111	-4.341608	4.584934
H	1.342831	-3.824813	-1.400755
H	4.472806	5.620807	1.963287
H	-0.858067	0.042569	2.985708
H	-4.341588	-1.511825	2.087872
H	-1.854445	-1.809983	3.884805
H	-5.280671	-1.279444	4.254697
H	-4.716485	1.772612	3.206694
H	-3.101857	-3.954076	3.526491
H	-2.971926	-3.710265	1.752336
H	-3.198766	0.579708	1.057310
H	-3.065316	0.395983	4.120039
H	-0.625052	-3.687893	2.151327
H	-2.010543	2.470261	1.488500

Aglycon model (2):
(3*R*,11*R*)-configuration

conf-1
energy: -1314.4854381 Hartrees
no imaginary frequencies

C	-2.694543	1.874140	1.281547
C	-1.801462	1.945377	0.135492
C	-1.679510	2.912957	-0.846726
C	-0.499687	2.648649	-1.668628
C	0.157864	1.364708	-1.309993
C	-0.739717	0.849910	-0.130862
C	-2.184885	4.174555	-1.384707
C	-1.210048	4.545302	-2.383894
N	-0.177388	3.579315	-2.520606
C	1.496771	1.487882	-0.657402
C	1.416705	0.986983	0.643041
O	0.124529	0.657679	1.004609
C	-3.334978	4.962026	-1.212856
C	-3.480384	6.135937	-1.978793
C	-2.497270	6.516105	-2.912672
C	-1.356045	5.717460	-3.132440
C	-2.865191	0.678405	2.035065
C	-3.746542	0.619274	3.113293
C	-4.486404	1.760873	3.488484
C	-4.307144	2.969506	2.775913
C	-3.425908	3.018403	1.696074
C	2.713305	1.937341	-1.181492
C	3.876063	1.761647	-0.400942
C	3.773230	1.176606	0.874316
C	2.539245	0.811381	1.451510
O	4.888030	0.937035	1.672468
O	2.807316	2.518717	-2.404749
O	-5.343959	1.646697	4.534125
H	5.674517	1.232927	1.187533
H	-0.764828	-1.021789	-0.617136
O	-1.436353	-0.344096	-0.429199
H	0.165514	0.641838	-2.145733
H	-4.132785	4.655958	-0.528123
H	-4.377059	6.755324	-1.851920
H	-2.631113	7.438044	-3.493226
H	-0.602467	5.986540	-3.881885
H	-2.330600	-0.225600	1.744656
H	-3.888001	-0.310962	3.674983
H	-4.858636	3.869334	3.082525
H	-3.270668	3.967350	1.178400
H	4.834660	2.084681	-0.815152
H	2.494710	0.370180	2.450557
H	1.926817	2.858762	-2.676752
H	-5.783215	2.499696	4.681507

conf-2
energy: -1314.4867401 Hartrees
no imaginary frequencies

C	-2.847621	2.039460	1.134287
C	-1.704232	2.277984	0.271898
C	-1.331592	3.414362	-0.420843
C	-0.194747	3.128741	-1.289703
C	0.272623	1.721820	-1.157271
C	-0.692389	1.152488	-0.052768
C	-1.552031	4.845368	-0.609946
C	-0.528587	5.235385	-1.552426
N	0.290039	4.144465	-1.947813
C	1.610063	1.640701	-0.492715
C	1.459171	1.072661	0.772815
O	0.135259	0.853104	1.097973
C	-2.417583	5.816217	-0.080028
C	-2.279099	7.155045	-0.497187
C	-1.290345	7.521822	-1.431004
C	-0.402206	6.565726	-1.965312
C	-2.883897	0.945278	2.044153
C	-4.012198	0.687079	2.818531
C	-5.153815	1.507997	2.695992
C	-5.136134	2.605182	1.806609
C	-4.001906	2.859805	1.035477
C	2.867048	2.056629	-0.946216
C	3.993674	1.728424	-0.162700
C	3.817800	1.050470	1.057353
C	2.544899	0.747645	1.585474
O	4.889790	0.650663	1.848144

O	3.027181	2.749937	-2.101977
O	-6.255103	1.170648	3.417407
H	5.708870	0.916209	1.401151
H	-0.767380	-0.683892	-0.642362
O	-1.418482	0.005164	-0.427393
H	0.206967	1.128689	-2.086885
H	-3.183302	5.550924	0.657550
H	-2.950259	7.920642	-0.088340
H	-1.205430	8.570745	-1.743173
H	0.379394	6.846155	-2.681157
H	-2.011811	0.293969	2.135481
H	-4.044312	-0.163751	3.508241
H	-6.035009	3.225670	1.688906
H	-4.027173	3.662860	0.293846
H	4.982420	2.010925	-0.532905
H	2.441416	0.246982	2.551668
H	2.196580	3.240052	-2.302481
H	-6.966620	1.803217	3.227564