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Structural, vibrational and electronic properties of the glucoalkaloid strictosidine: a combined experimental and theoretical study

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Table S1. 1D and 2D NMR signals of strictosidine

Position	$\delta_c, type$	δ_H (J in Hz)	HMBC
1	-	-	-
2	130.4	-	-
3	53.4	4.68 (d,J= 11.4Hz, 1H)	2, 15
4	-	-	-
5	42.3	3.74(d, J=6Hz, 1H) e 3,1 (m, 1H)	3, 6, 7
6	23.2	3.4(t,J= 4.8Hz, 1H) e 3.0(d, J= 6.6 Hz, 1H)	7, 2
7	108.0	-	-
8	127.2	-	-
9	119.1	7.47	7, 11, 13
10	120.2	7.04	8, 12
11	123.3	7.13	9, 13
12	112.2	7.33	8, 10
13	137.8	-	-
14	34.7	2.3 (ddd,J=1.8; 11.4; 13.2, 1H) e 2.2(ddd,J=3.6; 12; 13.2Hz,1H)	16
15	32.5	3.12 (d, J=4.8Hz, 1H)	3, 16, 21
16	108.6	-	-
17	156.6	7.8(s, 1H)	15, 16, 21, 22
18	119.4	5.2 e 5.3 (m, 2H)	19, 20
19	134	5.851 (dd, J= 3:12 Hz, 1H)	15, 21
20	45.3	2.7(dd, J= 3;8.4 Hz, 1H)	14, 16, 18, 21,C1’
21	97.5	5.853(d, J= 8.4Hz, 1H)	15, 19, 20, 1’
22	171.3	-	-
1’	100.1	4.82(m, 1H)	3’

2’	74	3.6(m, 1H)	4’
3’	78	3.5(m, 1H)	2’, 4’, 5’
4’	73	3.6(m, 1H)	2’
5’	71	3.2(m, 1H)	3’, 1’
6’	62.7	3.6 e 3.5(m, 1H)	4’
CH_3O-	52.7	3.8(s,3H)	22

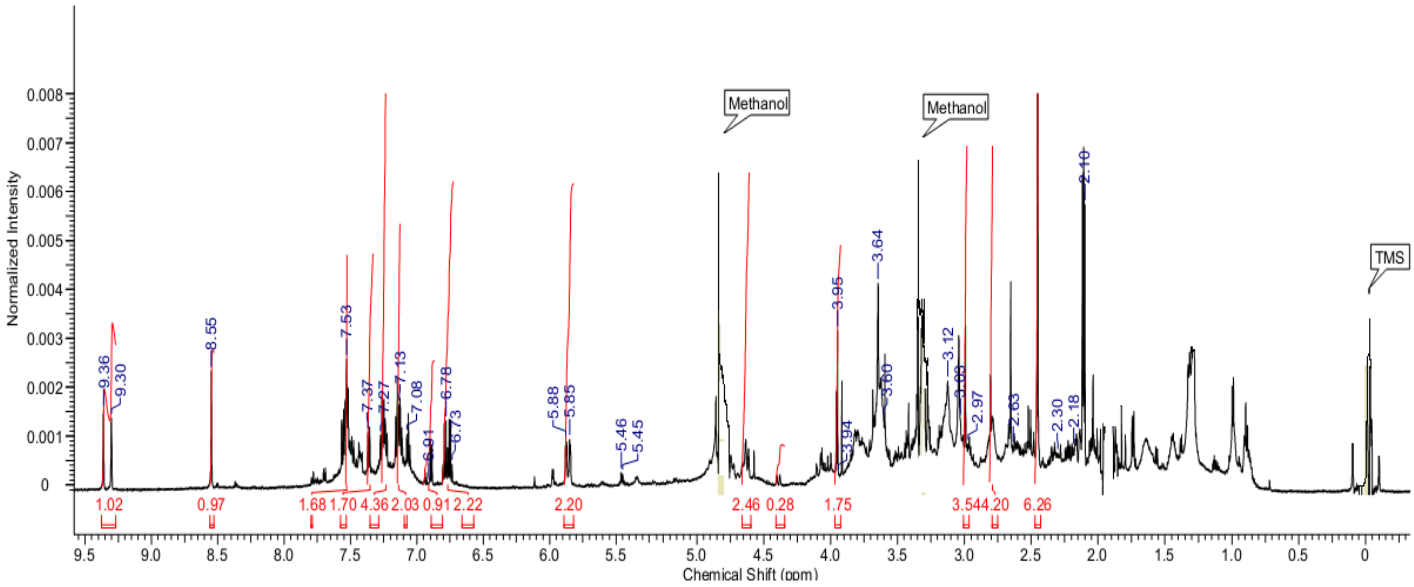


Figure S1. H^1 NMR spectrum of strictosidine

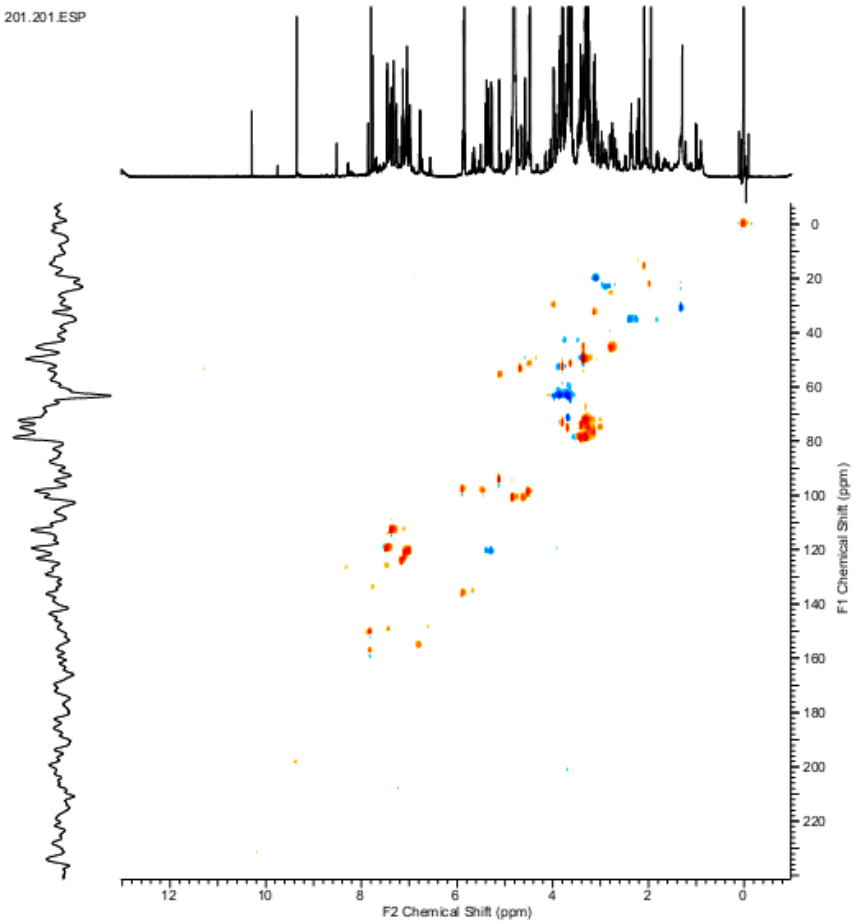


Figure S2. HSQC spectrum of strictosidine

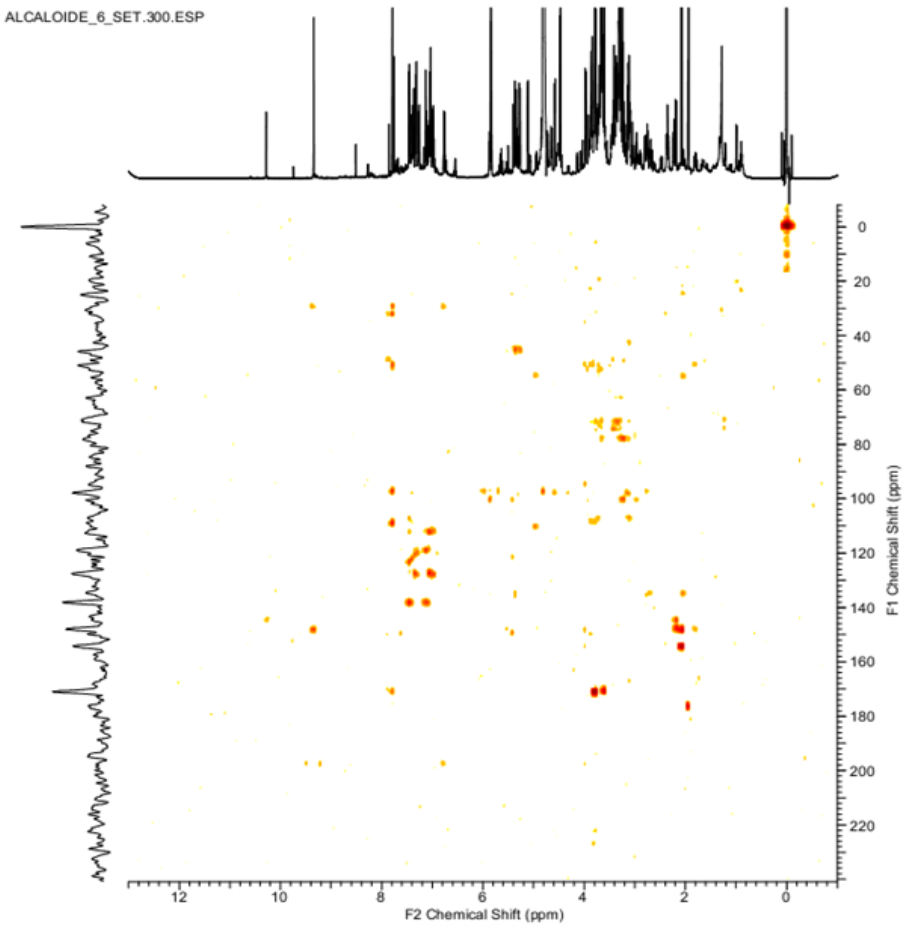
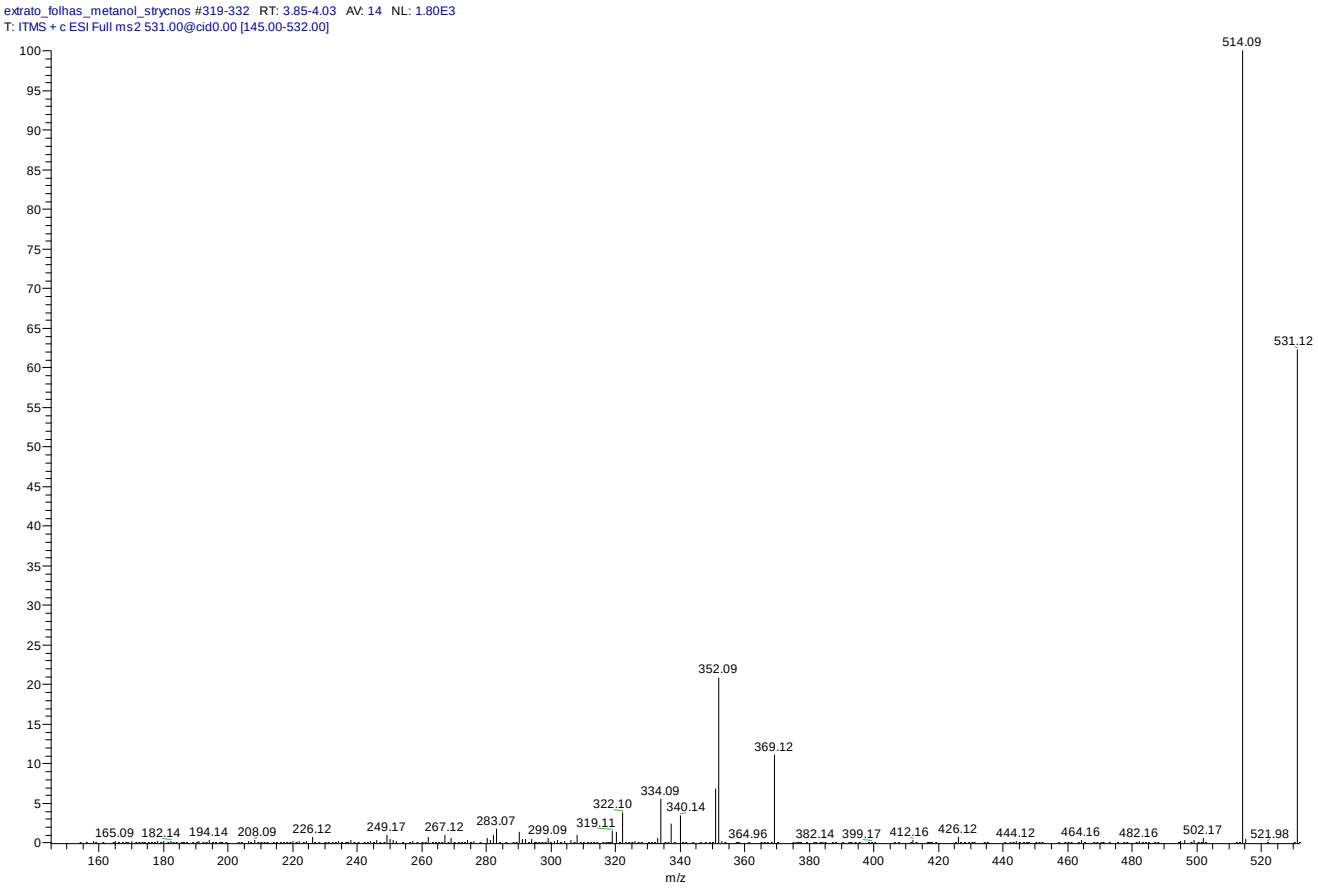


Figure S3. HMBC spectrum of strictosidine



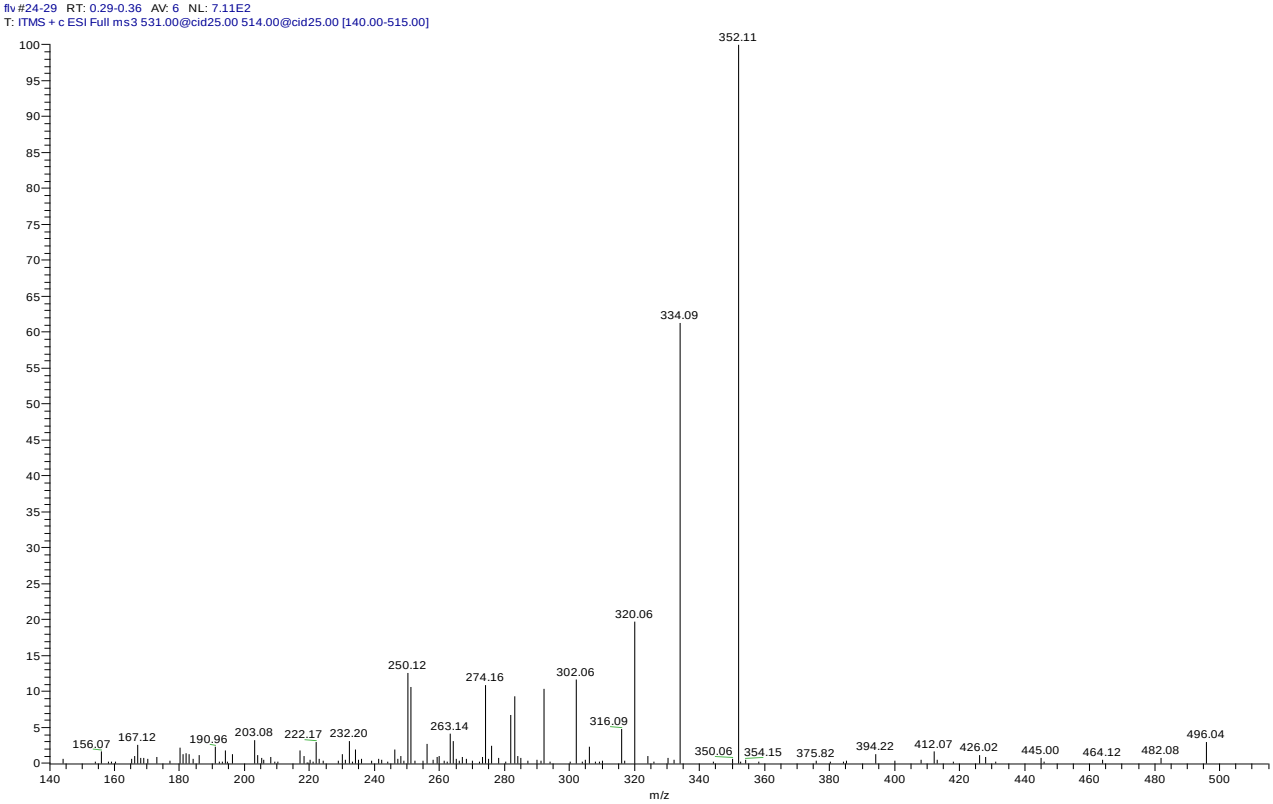


Figure S4. ESI-IT-MS spectra of strictosidine. Ms^2 spectrum of ion peak m/z 531 (top) ms^3 of ion peak m/z 514.

Table S2. Natural population analysis

Atom	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
C11	-0.257	1.999	4.244	0.0140	6.257
C10	-0.272	1.999	4.258	0.0139	6.271
C9	-0.232	1.999	4.258	0.0139	6.272
C8	-0.094	1.999	4.080	0.0146	6.094
C13	0.156	1.999	3.826	0.0186	5.844
C12	-0.271	1.999	4.259	0.0129	6.271
N1	-0.558	1.999	5.549	0.0101	7.558
C7	-0.115	1.999	4.101	0.0150	6.115
C2	0.167	1.999	3.812	0.0206	5.832
C6	-0.485	1.999	4.476	0.0102	6.485
C5	-0.260	1.999	4.243	0.0175	6.260
N4	-0.706	1.999	5.691	0.0158	7.706
C14	-0.457	1.999	4.444	0.0140	6.457
C15	-0.263	1.999	4.246	0.0173	6.263
C20	-0.323	1.999	4.307	0.0169	6.323
C19	-0.224	1.999	4.208	0.0173	6.224
C18	-0.433	1.999	4.422	0.0112	6.433
C16	-0.259	1.999	4.243	0.0175	6.259
C17	0.222	1.999	3.755	0.0228	5.777
O3	-0.537	1.999	6.525	0.0128	8.537
C21	0.411	1.999	3.560	0.0228	5.588
C22	0.812	1.999	3.145	0.0429	5.187
O4	-0.578	1.999	6.565	0.0131	8.578
C1’	0.397	1.999	3.572	0.0314	5.602
C5’	0.029	1.999	3.949	0.0225	5.970
C3’	0.048	1.999	3.927	0.0246	5.951
C4’	0.045	1.999	3.932	0.0235	5.955
H11	0.240	0.000	0.759	0.0007	0.760
H10	0.238	0.000	0.761	0.0009	0.762
H9	0.240	0.000	0.759	0.0009	0.760
H12	0.244	0.000	0.754	0.0094	0.755
H1	0.446	0.000	0.552	0.0015	0.553
H6b	0.245	0.000	0.752	0.0017	0.754
H6s	0.237	0.000	0.761	0.0019	0.763
H5b	0.224	0.000	0.773	0.0017	0.775
H5a	0.239	0.000	0.759	0.0012	0.761
H7	0.392	0.000	0.605	0.0021	0.607
H14S	0.237	0.000	0.761	0.0012	0.762
H14R	0.243	0.000	0.755	0.0017	0.757
H15	0.281	0.000	0.715	0.0028	0.718
H20	0.277	0.000	0.720	0.0024	0.722
H19	0.237	0.000	0.760	0.0014	0.762

H18	0.225	0.000	0.774	0.0007	0.775
H18	0.224	0.000	0.774	0.0023	0.776
H17	0.244	0.000	0.754	0.0012	0.755
H21	0.225	0.000	0.771	0.0031	0.774
H1’	0.213	0.000	0.783	0.0035	0.786
H3’	0.225	0.000	0.772	0.0034	0.775
O2	-0.649	1.999	6.631	0.0176	8.649
O1	-0.557	1.999	6.547	0.0103	8.557
CH3	-0.322	1.999	4.308	0.0142	6.322
H(CH3)	0.229	0.000	0.769	0.0005	0.770
H(CH3)	0.219	0.000	0.778	0.0015	0.780
H(CH3)	0.219	0.000	0.779	0.0015	0.781
O5	-0.626	1.999	6.613	0.0133	8.626
C2’	0.046	1.999	3.929	0.0250	5.953
O7	-0.777	1.999	6.765	0.0124	8.777
H3’’	0.501	0.000	0.496	0.0025	0.498
O8	-0.777	1.999	6.765	0.0127	8.777
H4’’	0.504	0.000	0.494	0.0009	0.495
H4’	0.233	0.000	0.764	0.0003	0.767
O6	-0.768	1.999	6.756	0.0127	8.768
H2’’	0.497	0.000	0.500	0.0021	0.502
H2’	0.228	0.000	0.767	0.0037	0.771
C6’	-0.111	1.999	4.092	0.0201	6.111
H6’b	0.206	0.000	0.791	0.0023	0.793
H6’a	0.232	0.000	0.766	0.0017	0.768
O9	-0.765	1.999	6.753	0.0125	8.765
H6”	0.487	0.000	0.510	0.0024	0.513
H5’	0.229	0.000	0.767	0.0037	0.771
C2	-0.088	1.999	4.070	0.0197	6.088
H3	0.265	0.000	0.732	0.0024	0.734

Table S3. Natural bond orbital analysis

Cycle	Occupation Threshold	Occupancies		Dev
		lewis	Non-lewis	
1	1.90	273.8	8.13	0.68
2	1.90	273.8	8.13	0.68
3	1.90	275.9	6.05	0.49
4	1.80	275.9	6.05	0.49
5	1.80	277.3	4.67	0.37
6	1.70	277.3	4.67	0.37
7	1.70	277.4	4.52	0.49
8	1.60	277.1	4.91	0.37
9	1.60	277.4	4.52	0.49
10	1.60	277.1	4.91	0.37
11	1.60	277.4	4.52	0.49
12	1.60	277.1	4.91	0.37
13	1.60	277.4	4.52	0.49
14	1.60	277.1	4.91	0.37
15	1.60	277.4	4.52	0.49
16	1.50	275.2	6.76	0.91
17	1.50	276.5	5.50	0.73
18	1.50	276.5	5.50	0.73
19	1.60	277.4	4.52	0.49

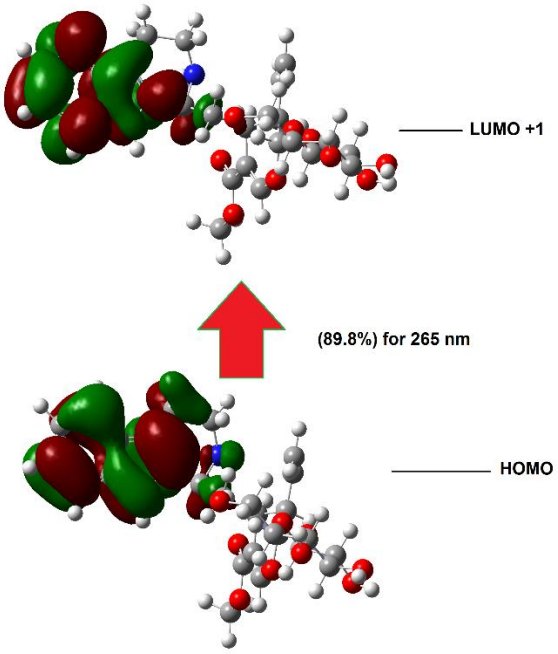


Figure S5. Most contributive electronic transition for 265 nm in B3LYP 6-31G(d)

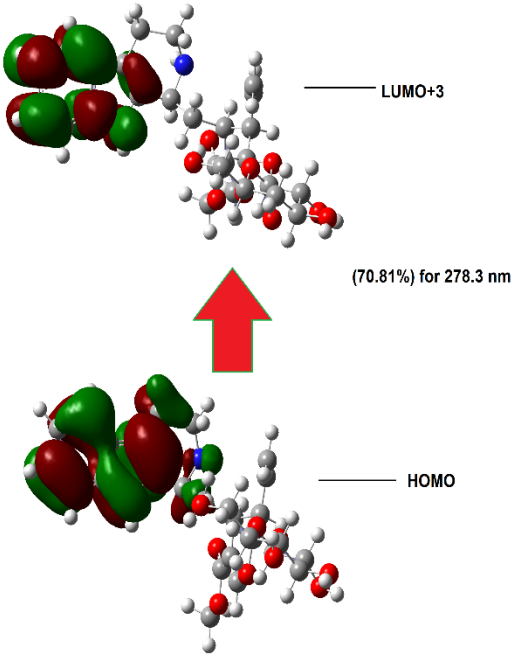


Figure S6. Most contributive electronic transition for 278 nm in B3LYP 6-311++G(2d,p)