IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861,
PP 73-79
www.iosrjournals.org

Theoretical Study on Indacaterol by DFT Study

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Abstract: *Quantum chemical calculations were carried out to study the molecular structure for indacaterol. To investigate the optimized molecular structure, bond length, bond angle and tetrahedral angels, Mullikan atomic charges, HOMO, LUMO energy levels, energy gap, dipole moment, total energy and some other physical parameters, DFT calculations were carried out using 6-31G basis set with B3LYP.*
Keywords: *Dipole moment, HOMO-LUMO energy gap, Indacaterol, Mullikan charges.*

I. Introduction

Indacaterol is a drug used for the treatment of chronic obstructive pulmonary disease (COPD). It's chemical name is 5-{(1R)-2-[(5,6-diethyl-2,3-dihydro-1H-inden-2-yl)amino]-1-hydroxyethyl}-8-hydroxy-2(1H)-quinolinone maleate. It is an ultra long acting beta adrenoceptor agonist. According to WHO, there are more than two hundred million people have moderate to severe COPD worldwide. It is in essential need of the theoretical properties. B3LYP/DFT/631-G basis set is used to calculate some physical properties of the target molecule with the help of Gaussian 09 software.

II. Computational details

The combination of quantum chemical calculation is very effective to understand the structure and behavior of the compound. The various analysis of the present study of the compound under investigation are carried out by DFT with three parameter hybrid [1,2] functional (B3) [3] for the exchange part and Lee Yang–Parr [4] (LYP) correlation functional using 6-31G basis set. The Gaussian 09 package is used for this calculation [5].

III. Result and Discussion

3.1 Optimized molecular structure

The list of atoms for the target molecule is shown in Table 1. The optimized molecular structure is shown in Fig 1. The optimized bond length, bond angle and tetrahedral angles for Indacaterol molecule at both levels of theory are listed in Tables 2,3 and 4 respectively.

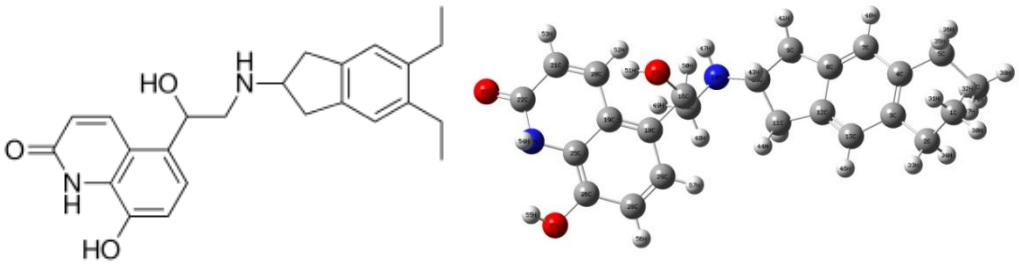


Fig 1: The 2D and 3D optimized molecular structure of Indacaterol

Table 1: The atom list of Indacaterol

1	2	3	4	5	6	7	8
C	**C**	**C**	**C**	**C**	**C**	**C**	**C**
9	10	11	12	13	14	15	16
C	**C**	**C**	**C**	**C**	**N**	**C**	**C**
17	18	19	20	21	22	23	24
O	**C**	**C**	**C**	**C**	**C**	**O**	**N**
25	26	27	28	29	30	31	32
C	**C**	**O**	**C**	**C**	**H**	**H**	**H**

33	34	35	36	37	38	39	40
H	**H**	**H**	**H**	**H**	**H**	**H**	**H**
41	42	43	44	45	46	47	48
H	**H**	**H**	**H**	**H**	**H**	**H**	**H**
49	50	51	52	53	54	55	56
H	**H**	**H**	**H**	**H**	**H**	**H**	**H**
57							
H							

Table 2: Bond length of optimized Indacaterol molecule by 631-G calculation

Sl .no	Code	Bond	Bond distance (Å)	Sl .no	Code	Bond	Bond distance (Å)
1	R1	R(1,2)	1.5464	31	R31	R(12,13)	1.3937
2	R2	R(1,30)	1.0965	32	R32	R(13,46)	1.0879
3	R3	R(1,31)	1.0959	33	R33	R(14,15)	1.4659
4	R4	R(1,32)	1.0959	34	R34	R(14,47)	1.0193
5	R5	R(2,3)	1.5207	35	R35	R(15,16)	1.5351
6	R6	R(2,33)	1.0977	36	R36	R(15,48)	1.0976
7	R7	R(2,34)	1.0964	37	R37	R(15,49)	1.1044
8	R8	R(3,4)	1.421	38	R38	R(16,17)	1.4839
9	R9	R(3,13)	1.4066	39	R39	R(16,18)	1.5186
10	R10	R(4,5)	1.5265	40	R40	R(16,50)	1.0957
11	R11	R(4,7)	1.407	41	R41	R(17,51)	0.9789
12	R12	R(5,6)	1.5361	42	R42	R(18,19)	1.4295
13	R13	R(5,35)	1.1009	43	R43	R(18,29)	1.3943
14	R14	R(5,36)	1.099	44	R44	R(19,20)	1.4487
15	R15	R(6,37)	1.0961	45	R45	R(19,25)	1.4144
16	R16	R(6,38)	1.0955	46	R46	R(20,21)	1.3602
17	R17	R(6,39)	1.0962	47	R47	R(20,52)	1.0838
18	R18	R(7,8)	1.3952	48	R48	R(21,22)	1.459
19	R19	R(7,40)	1.0845	49	R49	R(21,53)	1.0826
20	R20	R(8,9)	1.5159	50	R50	R(22,23)	1.2532
21	R21	R(8,12)	1.4036	51	R51	R(22,24)	1.3985
22	R22	R(9,10)	1.572	52	R52	R(24,25)	1.3831
23	R23	R(9,41)	1.0961	53	R53	R(24,54)	1.0129
24	R24	R(9,42)	1.1021	54	R54	R(25,26)	1.4105
25	R25	R(10,11)	1.5565	55	R55	R(26,27)	1.3935
26	R26	R(10,14)	1.4635	56	R56	R(26,28)	1.3851
27	R27	R(10,43)	1.0991	57	R57	R(27,55)	0.9747
28	R28	R(11,12)	1.5145	58	R58	R(28,29)	1.4079
29	R29	R(11,44)	1.0953	59	R59	R(28,56)	1.0864
30	R30	R(11,45)	1.1022	60	R60	R(29,57)	1.0826

It is predicted that the longest and possibly weakest bonds are R1, R5, R10, R12, R20, R25, R28, R35 and R39 involving C-C bonds. The shortest and possibly strongest bonds are R41and R57 involving O-H bond.

Table 3: Bond angle of optimized Indacaterol molecule by 6-31G calculation

Sl .no	Code	Bond	Bond angle (°)	Sl .no	Code	Bond	Bond angle (°)
1	A1	A(2,1,30)	110.8945	55	A55	A(8,12,11)	110.6888
2	A2	A(2,1,31)	110.6033	56	A56	A(8,12,13)	119.7246
3	A3	A(2,1,32)	111.401	57	A57	A(11,12,13)	129.585
4	A4	A(30,1,31)	108.1923	58	A58	A(3,13,12)	120.7643
5	A5	A(30,1,32)	108.0415	59	A59	A(3,13,46)	118.931
6	A6	A(31,1,32)	107.5726	60	A60	A(12,13,46)	120.3035
7	A7	A(1,2,3)	113.1311	61	A61	A(10,14,15)	116.6752
8	A8	A(1,2,33)	108.5676	62	A62	A(10,14,47)	112.2483
9	A9	A(1,2,34)	109.1776	63	A63	A(15,14,47)	110.1864
10	A10	A(3,2,33)	108.8281	64	A64	A(14,15,16)	112.0089
11	A11	A(3,2,34)	110.7046	65	A65	A(14,15,48)	108.8955
12	A12	A(33,2,34)	106.1729	66	A66	A(14,15,49)	112.562
13	A13	A(2,3,4)	121.9505	67	A67	A(16,15,48)	109.3157
14	A14	A(2,3,13)	118.4691	68	A68	A(16,15,49)	106.933

15	A15	A(4,3,13)	119.5664	69	A69	A(48,15,49)	106.9627
16	A16	A(3,4,5)	120.006	70	A70	A(15,16,17)	108.299
17	A17	A(3,4,7)	118.9815	71	A71	A(15,16,18)	117.3853
18	A18	A(5,4,7)	121.0051	72	A72	A(15,16,50)	106.6921
19	A19	A(4,5,6)	116.2799	73	A73	A(17,16,18)	111.0973
20	A20	A(4,5,35)	108.8641	74	A74	A(17,16,50)	103.928
21	A21	A(4,5,36)	109.0978	75	A75	A(18,16,50)	108.5141
22	A22	A(6,5,35)	108.4027	76	A76	A(16,17,51)	109.0385
23	A23	A(6,5,36)	108.4157	77	A77	A(16,18,19)	118.851
24	A24	A(35,5,36)	105.2162	78	A78	A(16,18,29)	122.1208
25	A25	A(5,6,37)	111.757	79	A79	A(19,18,29)	119.0269
26	A26	A(5,6,38)	110.0556	80	A80	A(18,19,20)	124.2265
27	A27	A(5,6,39)	111.605	81	A81	A(18,19,25)	119.2921
28	A28	A(37,6,38)	107.5817	82	A82	A(20,19,25)	116.481
29	A29	A(37,6,39)	107.9654	83	A83	A(19,20,21)	121.6817
30	A30	A(38,6,39)	107.7003	84	A84	A(19,20,52)	118.4848
31	A31	A(4,7,8)	120.7492	85	A85	A(21,20,52)	119.7913
32	A32	A(4,7,40)	119.8168	86	A86	A(20,21,22)	122.4013
33	A33	A(8,7,40)	119.4335	87	A87	A(20,21,53)	121.7888
34	A34	A(7,8,9)	129.1896	88	A88	A(22,21,53)	115.8073
35	A35	A(7,8,12)	120.2124	89	A89	A(21,22,23)	125.0916
36	A36	A(9,8,12)	110.5972	90	A90	A(21,22,24)	113.9689
37	A37	A(8,9,10)	102.9867	91	A91	A(23,22,24)	120.938
38	A38	A(8,9,41)	113.4793	92	A92	A(22,24,25)	125.2027
39	A39	A(8,9,42)	111.0859	93	A93	A(22,24,54)	116.8442
40	A40	A(10,9,41)	112.7322	94	A94	A(25,24,54)	117.9529
41	A41	A(10,9,42)	109.5127	95	A95	A(19,25,24)	120.2448
42	A42	A(41,9,42)	107.0519	96	A96	A(19,25,26)	120.2644
43	A43	A(9,10,11)	104.4006	97	A97	A(24,25,26)	119.4906
44	A44	A(9,10,14)	117.2919	98	A98	A(25,26,27)	114.9554
45	A45	A(9,10,43)	107.5829	99	A99	A(25,26,28)	120.0758
46	A46	A(11,10,14)	111.9368	100	A100	A(27,26,28)	124.9675
47	A47	A(11,10,43)	108.1677	101	A101	A(26,27,55)	112.474
48	A48	A(14,10,43)	107.1117	102	A102	A(26,28,29)	120.1199
49	A49	A(10,11,12)	103.4178	103	A103	A(26,28,56)	120.075
50	A50	A(10,11,44)	111.9544	104	A104	A(29,28,56)	119.8051
51	A51	A(10,11,45)	109.5582	105	A105	A(18,29,28)	121.1875
52	A52	A(12,11,44)	114.1293	106	A106	A(18,29,57)	118.9597
53	A53	A(12,11,45)	111.0329	107	A107	A(28,29,57)	119.8227
54	A54	A(44,11,45)	106.7575				

From the Table 3, it is clear that A37, carbon atoms – 8,9,10 present in the five membered ring system shows the shortest angle while A57, carbons atoms 11,12,13 shows the largest angle.

From the tetrahedral values in Table 4, it is clear that the atoms of D1, D8, D19, D22, D23, D30, D31, D32, D33, D35, D43, D44, D45, D46, D53, D54, D55, D56, D87, D88, D89, D90, D131, D132, D135, D136, D137, D139, D140, D141, D142, D143, D144, D145, D146, D147, D148, D149, D150, D151, D152, D153, D154, D155, D156 and D157 lie in same plane.

Table: 4 Tetrahedral angle of optimized Indacaterol molecule by 631-G calculation

Sl .no	Code	Bond	Bond angle (°)	Sl .no	Code	Bond	Bond angle (°)
1	D1	D(30,1,2,3)	179.6524	81	D81	D(10,11,12,8)	17.085
2	D2	D(30,1,2,33)	58.7415	82	D82	D(10,11,12,13)	-163.3913
3	D3	D(30,1,2,34)	-56.5944	83	D83	D(44,11,12,8)	138.9567
4	D4	D(31,1,2,3)	59.6169	84	D84	D(44,11,12,13)	-41.5196
5	D5	D(31,1,2,33)	-61.294	85	D85	D(45,11,12,8)	-100.3317
6	D6	D(31,1,2,34)	-176.6299	86	D86	D(45,11,12,13)	79.192
7	D7	D(32,1,2,3)	-59.9717	87	D87	D(8,12,13,3)	0.0259
8	D8	D(32,1,2,33)	179.1174	88	D88	D(8,12,13,46)	-179.5661
9	D9	D(32,1,2,34)	63.7815	89	D89	D(11,12,13,3)	-179.4609
10	D10	D(1,2,3,4)	87.9956	90	D90	D(11,12,13,46)	0.947
11	D11	D(1,2,3,13)	-90.6379	91	D91	D(10,14,15,16)	177.9432
12	D12	D(33,2,3,4)	-151.2412	92	D92	D(10,14,15,48)	56.9156

13	D13	D(33,2,3,13)	30.1254	93	D93	D(10,14,15,49)	-61.5179
14	D14	D(34,2,3,4)	-34.9152	94	D94	D(47,14,15,16)	-52.5504
15	D15	D(34,2,3,13)	146.4514	95	D95	D(47,14,15,48)	-173.578
16	D16	D(2,3,4,5)	2.6785	96	D96	D(47,14,15,49)	67.9884
17	D17	D(2,3,4,7)	-178.305	97	D97	D(14,15,16,17)	55.4567
18	D18	D(13,3,4,5)	-178.7027	98	D98	D(14,15,16,18)	-71.2904
19	D19	D(13,3,4,7)	0.3138	99	D99	D(14,15,16,50)	166.793
20	D20	D(2,3,13,12)	178.3238	100	D100	D(48,15,16,17)	176.2411
21	D21	D(2,3,13,46)	-2.0786	101	D101	D(48,15,16,18)	49.494
22	D22	D(4,3,13,12)	-0.343	102	D102	D(48,15,16,50)	-72.4226
23	D23	D(4,3,13,46)	179.2545	103	D103	D(49,15,16,17)	-68.2993
24	D24	D(3,4,5,6)	-177.6214	104	D104	D(49,15,16,18)	164.9536
25	D25	D(3,4,5,35)	59.6414	105	D105	D(49,15,16,50)	43.0369
26	D26	D(3,4,5,36)	-54.6776	106	D106	D(15,16,17,51)	-106.512
27	D27	D(7,4,5,6)	3.3824	107	D107	D(18,16,17,51)	23.7938
28	D28	D(7,4,5,35)	-119.3548	108	D108	D(50,16,17,51)	140.303
29	D29	D(7,4,5,36)	126.3262	109	D109	D(15,16,18,19)	-165.2877
30	D30	D(3,4,7,8)	0.0282	110	D110	D(15,16,18,29)	14.286
31	D31	D(3,4,7,40)	-179.7115	111	D111	D(17,16,18,19)	69.3413
32	D32	D(5,4,7,8)	179.0345	112	D112	D(17,16,18,29)	-111.085
33	D33	D(5,4,7,40)	-0.7052	113	D113	D(50,16,18,19)	-44.3166
34	D34	D(4,5,6,37)	-61.4123	114	D114	D(50,16,18,29)	135.2571
35	D35	D(4,5,6,38)	179.1202	115	D115	D(16,18,19,20)	-2.8007
36	D36	D(4,5,6,39)	59.6019	116	D116	D(16,18,19,25)	177.4303
37	D37	D(35,5,6,37)	61.5658	117	D117	D(29,18,19,20)	177.6122
38	D38	D(35,5,6,38)	-57.9017	118	D118	D(29,18,19,25)	-2.1567
39	D39	D(35,5,6,39)	-177.42	119	D119	D(16,18,29,28)	-177.9588
40	D40	D(36,5,6,37)	175.2888	120	D120	D(16,18,29,57)	4.0389
41	D41	D(36,5,6,38)	55.8213	121	D121	D(19,18,29,28)	1.6142
42	D42	D(36,5,6,39)	-63.697	122	D122	D(19,18,29,57)	-176.3882
43	D43	D(4,7,8,9)	179.3098	123	D123	D(18,19,20,21)	178.9093
44	D44	D(4,7,8,12)	-0.3476	124	D124	D(18,19,20,52)	-3.4588
45	D45	D(40,7,8,9)	-0.9495	125	D125	D(25,19,20,21)	-1.3158
46	D46	D(40,7,8,12)	179.3931	126	D126	D(25,19,20,52)	176.3161
47	D47	D(7,8,9,10)	163.1545	127	D127	D(18,19,25,24)	-178.8929
48	D48	D(7,8,9,41)	40.977	128	D128	D(18,19,25,26)	1.2363
49	D49	D(7,8,9,42)	-79.6964	129	D129	D(20,19,25,24)	1.3205
50	D50	D(12,8,9,10)	-17.1618	130	D130	D(20,19,25,26)	-178.5502
51	D51	D(12,8,9,41)	-139.3393	131	D131	D(19,20,21,22)	0.2105
52	D52	D(12,8,9,42)	99.9873	132	D132	D(19,20,21,53)	179.5953
53	D53	D(7,8,12,11)	179.8979	133	D133	D(52,20,21,22)	-177.3911
54	D54	D(7,8,12,13)	0.3206	134	D134	D(52,20,21,53)	1.9938
55	D55	D(9,8,12,11)	0.1815	135	D135	D(20,21,22,23)	-179.5874
56	D56	D(9,8,12,13)	-179.3957	136	D136	D(20,21,22,24)	0.8649
57	D57	D(8,9,10,11)	26.7374	137	D137	D(53,21,22,23)	0.9934
58	D58	D(8,9,10,14)	151.2438	138	D138	D(53,21,22,24)	-178.5543
59	D59	D(8,9,10,43)	-88.0377	139	D139	D(21,22,24,25)	-0.8665
60	D60	D(41,9,10,11)	149.4167	140	D140	D(21,22,24,54)	179.2401
61	D61	D(41,9,10,14)	-86.0769	141	D141	D(23,22,24,25)	179.565
62	D62	D(41,9,10,43)	34.6416	142	D142	D(23,22,24,54)	-0.3284
63	D63	D(42,9,10,11)	-91.52	143	D143	D(22,24,25,19)	-0.2338
64	D64	D(42,9,10,14)	32.9864	144	D144	D(22,24,25,26)	179.6379
65	D65	D(42,9,10,43)	153.7049	145	D145	D(54,24,25,19)	179.6585
66	D66	D(9,10,11,12)	-26.6923	146	D146	D(54,24,25,26)	-0.4697
67	D67	D(9,10,11,44)	-150.0108	147	D147	D(19,25,26,27)	179.8699
68	D68	D(9,10,11,45)	91.7531	148	D148	D(19,25,26,28)	0.2725
69	D69	D(14,10,11,12)	-154.5542	149	D149	D(24,25,26,27)	-0.0018
70	D70	D(14,10,11,44)	82.1273	150	D150	D(24,25,26,28)	-179.5992
71	D71	D(14,10,11,45)	-36.1088	151	D151	D(25,26,27,55)	179.9594
72	D72	D(43,10,11,12)	87.6703	152	D152	D(28,26,27,55)	-0.4657
73	D73	D(43,10,11,44)	-35.6482	153	D153	D(25,26,28,29)	-0.8531
74	D74	D(43,10,11,45)	-153.8843	154	D154	D(25,26,28,56)	179.1297

75	D75	D(9,10,14,15)	65.7398	155	D155	D(27,26,28,29)	179.5923
76	D76	D(9,10,14,47)	-62.7784	156	D156	D(27,26,28,56)	-0.4249
77	D77	D(11,10,14,15)	-173.6299	157	D157	D(26,28,29,18)	-0.107
78	D78	D(11,10,14,47)	57.8519	158	D158	D(26,28,29,57)	177.8783
79	D79	D(43,10,14,15)	-55.2252	159	D159	D(56,28,29,18)	179.9102
80	D80	D(43,10,14,47)	176.2566	160	D160	D(56,28,29,57)	-2.1045

3.2 Mullikan charges

The bonding ability of a molecule depends on the electronic charge on the chelating atoms. The atomic charge values have been obtained by the Mullikan population analysis [6]. To confirm the reliability of the result, the Mullikan population analysis of the target molecule has been calculated using B3LYP/6-31G basis set. The Mullikan charges are given in Table 5. From the results, it is clear 22 C is having very high value, since it attached with nitrogen atom and oxygen atom. Also 26 C shows higher value due to the attachment of oxygen atom. All the hydrogen atoms were found to possess positive charge.

Table 5: Mullikan atomic charges of Indacaterol (Hartree)

Sl. No	Atoms	Atomic charges with B3LYP	Sl. no	Atoms	Atomic charges with B3LYP	Sl. no	Atoms	Atomic charges with B3LYP
1	C	-0.398892	20	C	-0.092165	39	H	0.140695
2	C	-0.316669	21	C	-0.163114	40	H	0.120137
3	C	0.071831	22	C	0.506772	41	H	0.136876
4	C	0.085315	23	O	-0.470661	42	H	0.142955
5	C	-0.326371	24	N	-0.787431	43	H	0.138033
6	C	-0.410013	25	C	0.320134	44	H	0.142010
7	C	-0.195206	26	C	0.245138	45	H	0.139564
8	C	0.068281	27	O	-0.639857	46	H	0.116046
9	C	-0.317758	28	C	-0.129374	47	H	0.275737
10	C	0.023848	29	C	-0.157536	48	H	0.138440
11	C	-0.313620	30	H	0.131596	49	H	0.131058
12	C	0.082292	31	H	0.138839	50	H	0.148660
13	C	-0.199152	32	H	0.139910	51	H	0.363617
14	N	-0.589553	33	H	0.132681	52	H	0.173499
15	C	-0.085881	34	H	0.132069	53	H	0.154086
16	C	0.024189	35	H	0.145855	54	H	0.354835
17	O	-0.608652	36	H	0.145341	55	H	0.385164
18	C	0.002986	37	H	0.139700	56	H	0.127041
19	C	0.030804	38	H	0.131869	57	H	0.174004

3.3 Dipole moment, Quadrupole moment and various energies

The dipole moment is the first derivative of the energy with respect to an applied field. It is a measure of the asymmetry in the molecular charge distribution and is given as a vector in three dimensions. The theoretical dipole moment (in Debye) is shown in Table 6. The total dipole moment is found to be 7.0504 Debye.

Table 6: The Dipole moment (in Debye) of Indacaterol

B3LYP/6-31G			
X	**Y**	**Z**	**Total**
-6.0446	3.2090	-1.6949	7.0504

The predicted quadrupole moment for the target molecule is given in Table 7. It is clear that the molecule is slightly elongated along the XX axis in both levels of theory.

Table 7: The quadrupole moment of Indacaterol

B3LYP/6-31G		
XX	**YY**	**ZZ**
-229.5692	-155.9353	-171.2368

Thermo chemical analysis for the molecule is carried out at 298.15K and 1 atmospheric pressure. The energies of thermal, constant volume heat capacity and entropy due to electronic, translational, rotational and vibrational energies are given in Table 8. It is seen that vibrational energy accounts for almost all of the total energy. It is observed that the constant volume heat capacity due to vibrational energy is greater than all other. Similarly, the translational energy causes more entropy.

Table 8: Various energies of Indacaterol

Parameters	B3LYP/6-31G		
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	321.175	104.734	183.275
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.792
Rotational	0.889	2.981	37.013
Vibrational	319.397	98.772	102.471

The zero point correction, thermal correction to energy, thermal correction to enthalpy, thermal correction to Gibbs free energy, sum of electronic and zero point energy, sum of electronic and thermal energies, sum of electronic and thermal enthalpies and sum of electronic and thermal free energies are shown in Table 9. It is clear that the data are well correlated for both levels of theories.

Table 9: Thermo-chemistry of Indacaterol

Parameters	**B3LYP/6-31G** (Hartree/Particle)
Zero-point correction	0.484975
Thermal correction to Energy	0.511825
Thermal correction to Enthalpy	0.512769
Thermal correction to Gibbs Free Energy	0.425689
Sum of electronic and zero-point Energies	-1265.789516
Sum of electronic and thermal Energies	-1265.762667
Sum of electronic and thermal Enthalpies	-1265.761723
Sum of electronic and thermal Free Energies	-1265.848803

3.4 Electrostatic Potential Map (ESP)

ESP gives the electrostatic potential at location on a particular surface most commonly a surface of electron density to over all molecular size. In this target molecule (Fig 3) the colors near red represent large negative values [electron rich] while the colors near blue represent large positive values [electron poor] and the colors green and yellow represent intermediate values of the potential. [7] In this case, red, green, and yellow colors appeared near –-OH, aromatic regions, -NH groups respectively.

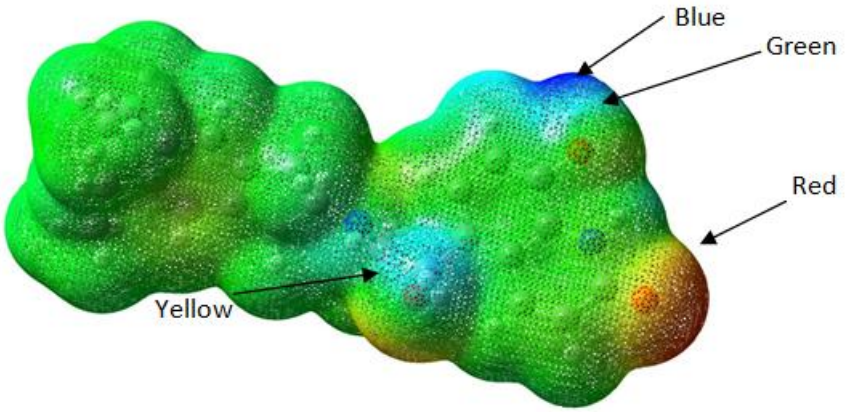
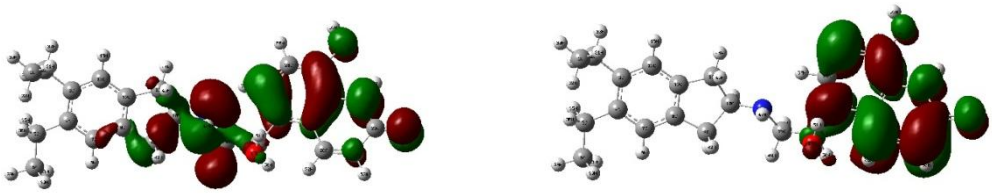


Fig 3: Electrostatic potential map of Indacaterol

3.5 HOMO – LUMO and total energy

From the Table 10, it is clear that the energy gap between HOMO and LUMO are high and hence the molecule is found to be stable. The total energy of the target molecule is found to be -1266.2744917 a.u.



a. (HOMO) b.(LUMO)

Fig 4: HOMO and LUMO of Indacaterol

Table 9: Physical parameters of Indacaterol

	6-31G
HOMO (a.u)	-0.21177
LUMO (a.u)	-0.05805
Energy gap (a.u)	-0.15372
Total energy (a.u)	-1266.2744917

IV. Conclusion

In this present study, computational methods are used to predict the molecular dynamics of indacaterol. The equilibrium geometry of Indacaterol molecule was analyzed at DFT/B3LYP/6-31G basis set. The HOMO, LUMO, energy gap, dipole moment and total energy etc., were calculated theoretically, The ESP has also been used to understand the activity of the molecule.

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