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Full Length Research Paper

Nanotechnology approach on anticancer and antiviral properties of *Consolida* Sp.: The study of dipole moment and nuclear magnetic resonance (NMR)

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14-O-demethyledelboxine is one of the most important alkaloids in *Consolida* species. It is toxic and has many effects in body. In this article, we used dipole moment and nuclear magnetic resonance (NMR) to describe this molecule properties. Nanoparameters and chemical shift calculations, geometry optimization and energies have been performed with *ab initio* method at HF/Sto-3G, B3Lyp/6-31G and B3Lyp/6-31G* levels with magnetic properties of the gauge-including atomic orbital method. According to this study this molecule has polarity, therefore it can highly react with microtubules. So it is recommended that more study in this molecule and the groups can be bound to evaluate these characters so it could be useful. Dipole moment calculations approve *ab initio* methods according to these results.

Key words: 14-o-demethyldelboxine, nuclear magnetic resonance (NMR), B3lyp, isotropy, anisotropy.

INTRODUCTION

Diterpene alkaloids are one of the most important substance with pharmacological and economical significance, it can be extracted from some species of Ranunculaceae family such as *Consilida, Aconitum* and *Delphinium* (Alva et al., 2004; Sener et al., 2007). These alkaloids are toxic for cattle and human beings. Antimicrobial compounds in these plants can protect them from biotic attack that could be essential for microbial infection resistance (Sener et al., 2007).

The norditerpenoid alkaloids are a group of highly oxygenated and complex natural products. They have many practical actions such as analgesic, local anesthetic, anti-inflammatory and antiarrhythmetic activities. The alkaloids obtained from these plants are neurotoxic, causing bradycardia, muscle system strokes, hypotension and cardiac arrest. Some of these alkaloids have different properties such as insect repellent, antioxidant, antiinflammatory and tyrosinase inhibition activities (Wang et al., 2000).

Methyllycaconitine (MLA), one of the many norditerpenoid alkaloids found in these plants, have effect on neuromuscular transmission. It acts as a competitive antagonist for nicotinic acetylecholine receptors (nAChRs) at mammalian neuromuscular junctions. They are bound to nicotinic receptors in central nervous system, reduce synaptic efficacy and block neuromuscular transmission (Dobelis et al., 1999).

One of these alkaloids is 14-O-demethyldelboxine, that is belonging to 7,8-methylenedioxylycoctonine type (MDL-type) norditerpenoids alkaloids. Welch et al. (2010) suggested that MDL-type alkaloids may play a larger role in larkspur toxicity more than others. The cattle were poisoned by larkspur which have significant increases in heart rate. The toxicity effects of 14-O-demethldelboxine against insect-derived SF9cells was known (Alva et al., 2004; Green et al., 2010).

COMPUTATIONAL DETAILS

The quantum chemical calculations have been performed using Gaussian 98 program (Frisch et al., 1998). Full

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geometry optimizations and frequency calculations of the fundamental vibrational frequencies of all possible 14-O-demethyldelboxine derivatives have been carried out employing Hartree-Fock (RHF) (Roothan, 1951; Pople and Nesbet, 1954) and density functional theory (B3LYP) (Becke, 1993; Lee et al., 1998) with 6-31 G and 6-31 G* basis sets (Frisch et al., 1985) and HFSTO methods (Vosko et al., 1980) with 3 G basis sets (Frisch et al., 1985).

For further investigation of the substituent effects, the frequency calculations as well as their corresponding thermochemical parameters including thermal energies, and entropies, Gibbs free energies and entropies of the derivatives of 1,4-benzodiapazine have been performed (Monajjemi et al., 2010).

Then isotropic part σiso of σ was determined by averaging σ over orientations in the magnetic field, that is, σiso = (σ11 + σ22 + σ33)/3. The anisotropy is δ =|σ33–σiso|, and the asymmetry is η = (σ22 – σ33)/δ (Monajjemi et al., 2007) nuclear magnetic resonance (NMR) calculations on vinblastine using Hartree-Fock (HF) and density functional theory (DFT) reveal that methods including electron correlation show significant improvements in the NMR shielding over results. The NMR measurements were carried out using HF,B3LYP/sto-3 g, 3-21 g and 3-21 g* of NMR at theoretical concepts (Monajjemi et al., 2010).

THEORETICAL BACKGROUND

Chemical shielding refers to the phenomenon associated with the secondary magnetic field created by the induced motions of the electrons surrounding the nuclei when in the presence of an applied magnetic field. The energy of a magnetic moment, μ, in a magnetic field, B, is:

$$E = -\mu (1-\alpha) B.$$

Where the shielding, σ, is the differential resonance shift due to the induced motion of the electrons. The chemical shielding is characterized by a real 3×3 Cartesian matrix. A 3×3 matrix can also represent the chemical shift tensor and in a special coordinate system called the principle axis system (PAS) it is diagonal:

$$\begin{bmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}$$

With, σ_{xx}, σ_{yy} and σ_{zz} as the three principle components. The isotropic shielding values, defined as:

$\sigma_{iso} = 1/3 (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$. (Monajjemi et al., 2008)

NANOPARAMETERS

In nanoparameters data calculations, according to chemical shift coefficients, can be used as an index for every studies in the future. Nanotechnology approach to this molecule can help us in anticancer properties calculations and increase or decrease these properties (Table 1).

RESULTS AND DISCUSSION

According to the Table 1, for C1 atom in HF/Sto-3G, B3Lyp/6-31G and B3Lyp/6-3G* methods, atomic charge decreases, iso increases and Aniso decreases. For C3 atom, atomic charge increases, iso and aniso from HF/Sto-3G to B3Lyp/6-31G decrease and from B3Lyp/6-31G to B3Lyp/6-31G* increase. For C4 atom, atomic charges increases from HF/Sto-3G to B3Lyp/6-31G and decreases from B3Lyp/6-31G to B3Lyp/6-31G*. iso and aniso increase. For C6 atom, atomic charges decreases from HF/Sto-3G to B3Lyp/6-31G and increases from B3Lyp/6-31G to B3Lyp/6-31G*. Iso is equal in different methods and aniso is equal too in HF/Sto-3G and B3Lyp/6-31G and decreases in B3Lyp/6-31G* method. For C7 atom, we see growth in atomic charges, iso and aniso (Figures 1 to 3).

For C8 atom, atomic charges and iso increase and aniso increases from HF/Sto-3G to B3Lyp/6-31G and decreases to B3Lyp/6-31G*. For C14 atom, atomic charges increase, iso decrease and aniso is equal in these methods. For C21 atom, atomic charges decreases, iso and aniso are equal. For C22 atom, atomic charges decreases, iso is equal in these methods. Aniso decreases from Sto-3G to B3Lyp/6-31G and decreases from B3Lyp/6-31G to B3Lyp/6-31G*. For C18 atom, atomic charges decrease, iso decrease and aniso is equal in these methods. For C24 atom, atomic charge, iso and aniso decrease. For C17 atom, atomic charge and iso decrease and aniso is equal. For C29 atom, atomic charge decreases, iso decreases from HF/Sto-3G to B3Lyp/6-31G and increase from B3Lyp/6-31G to B3Lyp/6-31G*. Aniso increases from HF/Sto-3G to B3Lyp/6-31 G and decreases from B3Lyp/6-31G to B3Lyp/6-31G*. Atomic charges decreases in different methods for C31 atom, iso is equal and aniso decreases from HF/Sto-3G to B3Lyp/6-31G and increase from B3Lyp/6-31G to B3Lyp/6-31G* (Figures 1 to 3).

C2, C5, C9, C10, C11, C13, C15, C27 and C30 atoms have atomic charges near to zero, so these atoms cannot be effective in plant characteristics. For O atoms, atomic charges and iso increase and aniso decrease from HF/Sto-3G to B3Lyp/6-31G and increase from B3Lyp/6-31G to B3Lyp/6-31G*. Atomic charge for N16 decrease from HF/Sto-3G to B3Lyp/6-31G and increase from B3Lyp/6-31G to B3Lyp/6-31G*. iso is equal and aniso increase from HF/Sto-3G to B3Lyp/6-31G and decrease from B3Lyp/6-31G to B3Lyp/6-31G*. H atoms have atomic charges about zero and nearly equal. They are nonpolar. If methyl and alkyl groups are substituted to

Table 1. The results of optimized geometry coordinate of 14-O-demethyldelboxine.

Method			HF						B3LYP									
Basis set			Sto-3G						6-31G						6-31G*			
Name	Atoms	Atomiccharges	Iso	Aniso	Determinant	η	iso	Atomiccharges	Iso	Aniso	Determinant	η	iso	Atomiccharges	Iso	Aniso	Determinant	η	iso
Cycles	C 1	-	219.1	17.6	10498800	0.77	17.61	-0.23	220.	14.1	107458	0.98	14.17	-0.29	220.7	15.4	107343	0.92	15.48
	H 32	0.0	32.82	16.2	32629.5	0.37	16.25	0.14	31.7	16.8	29126.	0.4	16.84	0.14	31.74	16.9	29084	0.4	16.95
	H 33	0.0	31.39	8.98	29702.6	0.86	-9.67	0.19	31.1	9.57	28748.	0.86	-10.31	0.18	31.26	9.25	29207.	-1.09	-10.15
	C 2	0.0	201.7	43.8	8056640	-0.9	-40.1	0.04	196.	27.8	747099	0.54	-36.19	0.06	201.7	38.9	807762	0.99	38.97
	H 34	0.0	32.19	15.6	30586.7	0.48	15.6	0.13	31.8	15.4	29857.	0.47	15.42	0.13	32.03	16.4	30062.	0.45	16.42
	C 3	0.0	201.4	52.2	10396100	0.9	-55.12	0.17	196.	35.1	737602	0.4	-50.15	0.29	202.2	46.7	805028	-1.13	-53.84
	C 4	-	199.7	15.4	7945690	0.69	-18.38	-0.1	202.	19.9	830644	0.95	19.94	-0.15	203.3	19.8	837202	0.97	19.84
	H 35	0.0	32.29	8.48	32993.3	0.81	-7.16	0.17	32.0	6.09	30639.	0.47	-8.32	0.15	32.11	6.07	32288.	0.45	-8.37
	C 5	0.0	197.9	11.5	7741880	0.29	-17.8	0.05	199.	11.8	790738	0.32	-17.98	0.08	200.3	11.4	802722	0.33	-17.16
	C 6	0.0	183.7	38.0	6103090	0.63	38.01	0.05	183.	38.1	602630	0.84	-38.11	0.08	184.6	35.9	619959	0.85	35.9
	H 36	0.0	31.64	7.78	30994.8	0.56	7.78	0.15	31.6	7.05	28264.	0.86	7.05	0.14	31.71	7.07	31253.	0.85	7.07
	C 7	0.0	172.6	41.9	5036100	0.6	8.42	0.12	177.	44.9	546076	0.78	44.91	0.13	178.7	44.7	557832	0.72	44.75
	H 37	0.0	31.52	5.82	30897.6	0.81	5.82	0.16	31.4	5.23	30805.	0.9	5.23	0.15	31.56	5.08	31089	0.99	5.08
	C 8	0.1	170.9	27.8	4463420	-	27.85	0.19	173.	30.8	519079	0.78	30.87	0.25	175.7	28.8	536897	0.83	28.81
	C 9	0.0	200.7	16.8	8070370	0.47	-16.87	0.07	201.	14.8	821386	0.3	14.87	0.11	203.2	15.5	837742	0.26	15.5
	C 10	-	204.7	14.9	8555140	0.51	-19.7	-0.16	204.	12.1	851420	0.67	-14.74	-0.18	205.0	11.5	860356	0.61	-14.35
	H 38	0.0	32.07	9.19	31843.2	0.9	9.19	0.14	32.3	8.91	32848.	0.53	8.91	0.14	32.41	8.96	33145.	0.54	8.96
	C 11	-	198.1	28.9	7714020	0.95	28.99	-0.13	197.	27.3	765343	0.94	-28.18	-0.14	198.7	27.6	778527	0.98	27.63
	H 39	0.0	32.29	9.41	32473.9	0.9	9.41	0.13	32.2	9.77	32192.	0.93	9.77	0.13	32.34	9.85	32485	0.93	9.85
	C 12	0.0	181.2	52.0	5777010	0.7	52.02	0.11	180.	52.2	573346	0.71	52.22	0.14	182.4	51.1	590132	0.68	51.14
	H 40	0.0	31.57	11.6	30045.7	0.5	11.61	0.12	31.5	11.7	29784.	0.53	11.72	0.11	31.56	11.8	29929.	0.54	11.87
	C 13	-	208.2	10.2	9013000	-	-14.4	-0.13	208.	9.53	905016	0.49	12.81	-0.14	209.5	9.08	919270	0.42	-12.76
	H 41	0.0	32.1	15.2	30637.2	0.14	15.22	0.14	31.9	15.3	30192.	0.42	15.33	0.14	32.01	15.3	30328.	0.45	15.38
	C 14	-	209.1	29.9	9068900	0.91	-31.32	-0.3	207.	28.8	884550	0.49	-29.05	-0.34	207.6	29.0	863080	0.1	-29.03
	H 42	0.0	32.01	14.6	30430.8	3.94	-11.37	0.12	32.2	14.7	31047.	0.53	14.71	0.13	32.27	14.7	31217.	0.54	14.75
	H 43	0.0	31.68	10.6	30154.3	0.98	-10.91	0.16	32.4	8.31	33327.	0.97	8.31	0.17	32.63	8.15	33937.	0.97	8.15
	C 15	0.0	185.3	27.2	6331740	-	27.24	0.02	185.	25.3	636093	0.49	25.38	-0.01	186.1	25.3	641490	0.32	25.36
	H 44	0.0	32.81	10.4	33770.6	0.94	10.49	0.13	32.7	10.2	33592.	0.97	10.27	0.12	32.94	10.1	34250.	0.99	10.15
	C 21	0.0	180.0	47.5	5698560	0.43	47.53	0.13	179.	47.4	569077	1.79	-33.97	0.17	181.7	46.2	587368	0.43	46.21
	H 52	0.0	31.36	7.43	29826.5	0.62	-9.18	0.15	31.4	7.13	30061.	0.57	-9.09	0.13	31.5	7.38	30242	0.59	-9.27
	C 22	-	216.2	24.1	10065300	0.83	24.17	-0.29	216.	22.8	100722	0.73	22.87	-0.34	217.3	23.5	102298	0.67	23.49
	H 53	0.0	33.13	9.44	35015.2	0.78	-9.76	0.1	32.9	9.92	34160.	0.88	-10.55	0.11	33.03	10.0	34442.	0.87	-10.71
		0.0	32.62	11.9	32880.9	0.85	11.95	0.17	32.4	12.0	32367.	0.82	12.05	0.17	32.51	11.9	32488	0.87	11.97

Table 1.Contd.

	C 18	-	223.3	26.7	11071900	0.75	26.69	-0.41	222.	26.2	110236	0.68	26.29	-0.48	222.9	26.8	110136	0.73	26.87
	H 48	0.0	32.61	11.9	32851.3	0.8	11.93	0.16	31.8	11.4	30714.	0.73	11.48	0.17	31.87	11.8	30757.	0.64	11.83
	H 49	0.0	32.49	8.45	33137.2	0.92	-9.09	0.14	32.2	8.7	32206.	0.8	9.66	0.15	32.23	8.57	32166.	0.69	-10.1
	H 50	0.0	32.79	16.1	32459.5	-	16.19	0.15	32.4	16.7	31257.	0.43	16.77	0.15	32.47	16.9	31225.	0.39	16.97
	C 27	-	196.1	64.1	7296920	0.23	64.14	-0.17	195.	65.0	717363	0.14	65.58	-0.21	196.1	64.3	802769	0.16	64.39
	H 60	0.0	31.18	14.8	28179.4	0.29	14.84	0.15	31.2	14.7	28536.	0.07	14.57	0.15	31.23	15.1	28342.	0.05	15.19
	H 61	0.0	32.02	9.87	31793.2	-	9.87	0.17	31.2	7.32	29524.	0.72	-8.49	0.16	31.23	7.69	29510.	0.74	-8.82
	H 62	0.0	31.63	9.39	30365.9	0.84	9.39	0.13	31.7	9.72	30941.	0.52	9.72	0.14	31.79	9.99	31056.	0.48	9.99
	C 24	-0.2	219.3	31.5	10474000	0.67	31.52	-0.43	217.	30.3	102203	0.58	30.36	-0.49	217.7	30.2	102595	0.59	30.25
	H 56	0.0	32.6	12.2	32688.7	0.86	12.22	0.12	32.5	12.2	32508.	0.89	12.23	0.14	32.62	12.2	51306.	0.88	69.68
	H 57	0.0	32.63	12.5	33123.3	0.35	12.58	0.13	32.2	11.8	32100.	0.3	11.86	0.14	32.27	12.0	32134.	0.3	12.04
	H 58	0.0	31.53	11.8	28646.9	0.61	-14.7	0.17	31.8	10.8	30413.	1.16	10.82	0.17	31.95	10.8	30775.	0.85	-11.68
	C 17	-	202.3	53.6	8090330	0.35	53.65	-0.31	201.	54.2	794075	0.4	54.21	-0.36	201.4	53.4	798223	0.39	53.47
	H 45	0.0	32.4	11.9	33034.0	0.34	10.51	0.11	32.0	10.9	31748.	0.3	10.9	0.11	32.18	10.8	32098.	0.28	10.89
	H 46	0.0	30.72	8.65	2749740000	0.59	-10.92	0.22	30.7	8.72	27703.	0.54	-11.31	0.21	30.96	8.57	28214.	0.53	-11.21
	H 47	0.0	32.29	14.7	31797.8	0.09	14.7	0.14	32.0	14.6	30782.	0.14	14.65	0.14	31.1	14.9	30636.	0.13	14.91
	C 29	-	201.5	53.0	8007340	0.2	53.02	-0.16	200.	54.6	784067	0.16	54.64	-0.2	201.6	52.9	802130	0.17	52.9
	H 63	0.0	31.76	7.52	31012.9	0.62	-9.09	0.16	31.5	6.7	30500.	0.45	-9.25	0.15	31.71	7.76	30845.	-0.71	-9.09
	H 64	0.0	31.54	15.7	29044.8	0.59	15.78	0.14	31.4	12.2	28859.	0.13	15.23	0.15	31.41	15.6	28214.	0.14	15.67
CH_3	H 65	0.0	31.71	7.67	30903.0	-	-9	0.13	31.6	8.47	30695.	0.93	-8.76	0.13	31.67	8.11	30747.	0.8	-8.99
	C 30	-	199.5	48.1	7783700	0.57	48.13	-0.06	199.	49.0	771374	0.6	49.02	-0.08	199.8	48.6	780866	0.59	48.68
	C 31	-	224.8	18.9	11342800	0.37	18.93	-0.41	223.	17.3	111367	0.5	17.39	-0.46	223.7	18.0	111725	0.41	18.09
	H 66	0.0	32.04	7.35	32111.8	0.94	-7.58	-0.1	31.7	7.7	31275.	0.96	7.7	0.11	31.95	7.65	31815.	0.99	-7.6
	H 67	0.0	32.24	13.3	31213.6	0.84	13.3	0.13	31.9	13.2	30369.	0.92	13.26	0.13	32.03	13.3	30460.	0.94	13.33
	H 68	0.0	32.76	17.0	32588.3	0.16	17.03	0.12	32.4	16.8	31290.	0.16	16.82	0.13	32.44	16.8	31381.	0.16	16.89
C_2H_5	H 69	0.0	32.69	9.08	33743.5	0.99	-9.13	0.13	32.3	8.95	32620.	0.99	8.95	0.14	32.29	9.52	32473.	0.14	9.52
	H 70	0.0	32.29	6.9	32720.1	0.59	8.68	0.16	32.1	7.43	31952.	0.55	-9.61	0.17	32.12	7.5	31969.	0.53	9.78
	O	-	360.3	119.	41168400	0.18	-16.87	-0.49	323.	150.	289027	0.85	-196.31	-0.5	360.2	106.	412338	0.05	-
	O	-0.3	351.5	95.2	-	0.41	-19.7	-0.61	352.	52	437244	0.07	52	-0.63	364.5	63.8	480236	0.31	63.83
	H 51	0.1	34.19	21.4	34850.7	0.62	21.45	0.36	33.9	16.9	35710.	0.6	16.94	0.4	34.42	18.8	36933.	0.81	16.88
	O	-	383.7	49.5	10474000	0.35	49.57	-0.54	371.	42.9	507657	-	-48.05	-0.5	392.6	43.8	602346	0.9	43.8
	O	-0.3	353.6	80.7	10474000	0.48	80.71	-0.63	353.	60.5	437417	-	60.5	-0.67	364.6	69.6	479803	0.36	69.68
	H 59	0.1	34.15	14.3	36811.6	0.96	14.35	0.37	34.2	14.7	36896.	0.92	14.75	0.4	34.62	15.2	38080.	0.94	15.21
	O	-0.3	357.5	86.4	3509550000	0.65	86.45	-0.61	355.	67	444075	0.24	67	-0.63	365.0	77.4	479820	-0.12	77.49
	H 55	0.1	34.23	10.5	35991.3	0.42	19.45	0.36	34.3	19.1	36736.	0.34	19.18	0.4	34.84	19.5	38128.	0.4	19.51
	O	-	367.5	81.6	5264100	0.21	81.67	-0.54	359.	91.8	456059	0.21	91.89	-0.5	385.3	92.6	562332	0.29	92.66
N O	N 16	-	290.7	39.4	24289800	-0.5	-52.69	-0.49	296.	46.4	255685	0.5	-62.09	-0.42	299.6	43.9	265135	0.47	-59.6

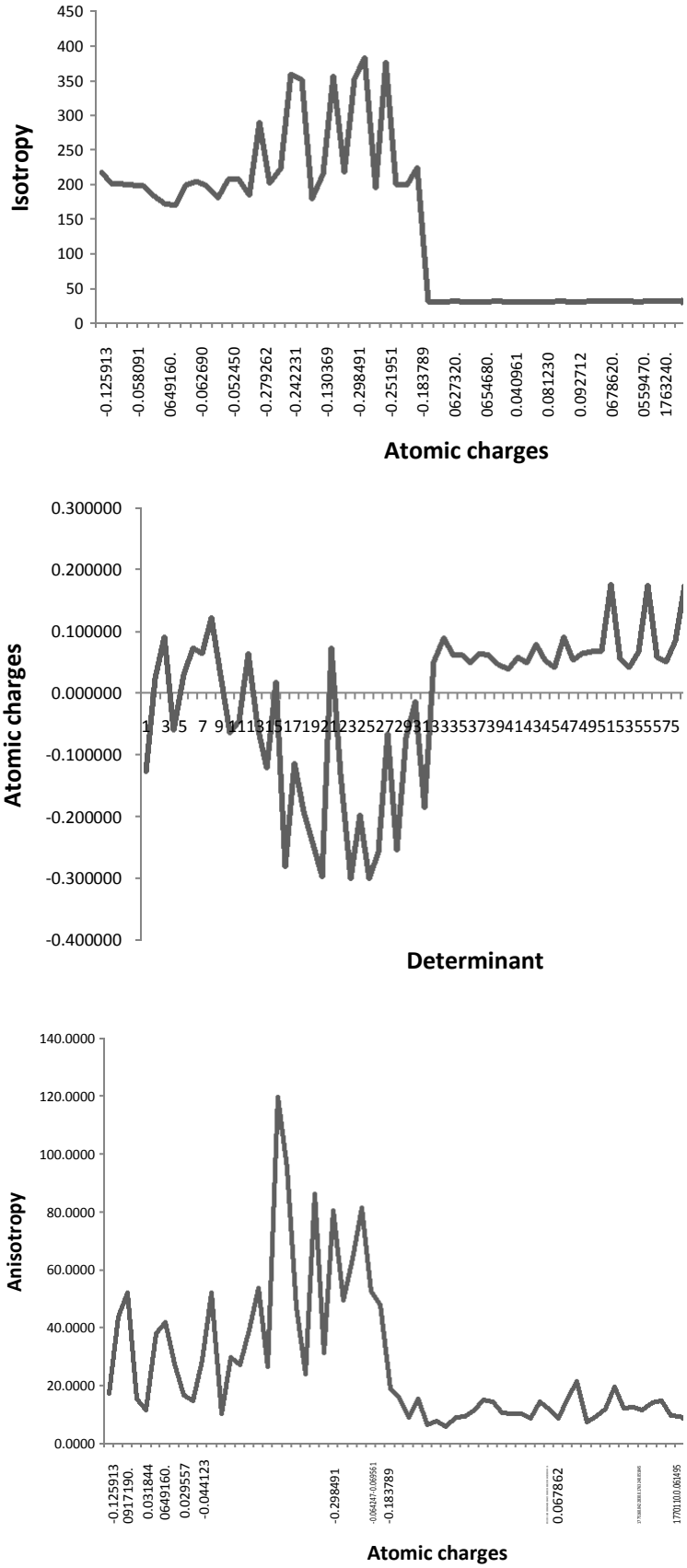
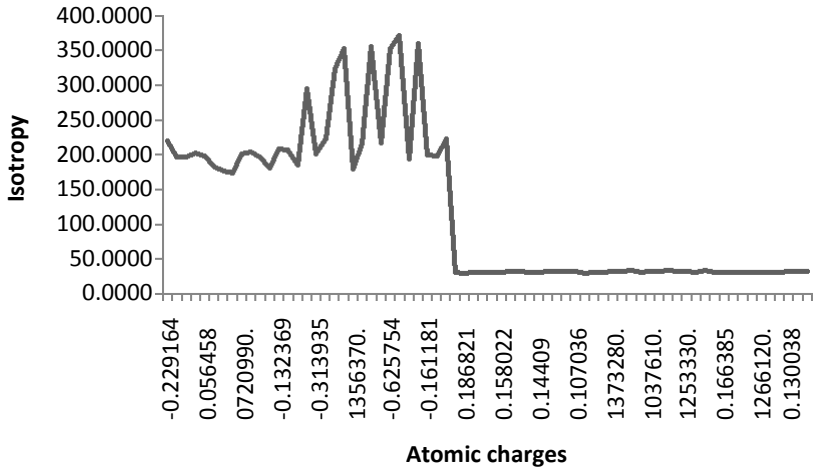
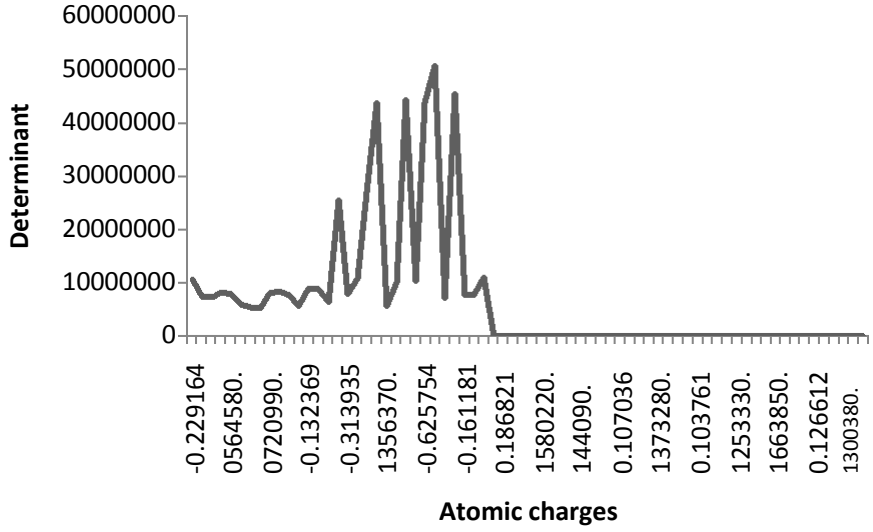


Figure 1. It shows the graphs were obtained from HF/Sto-3G method.





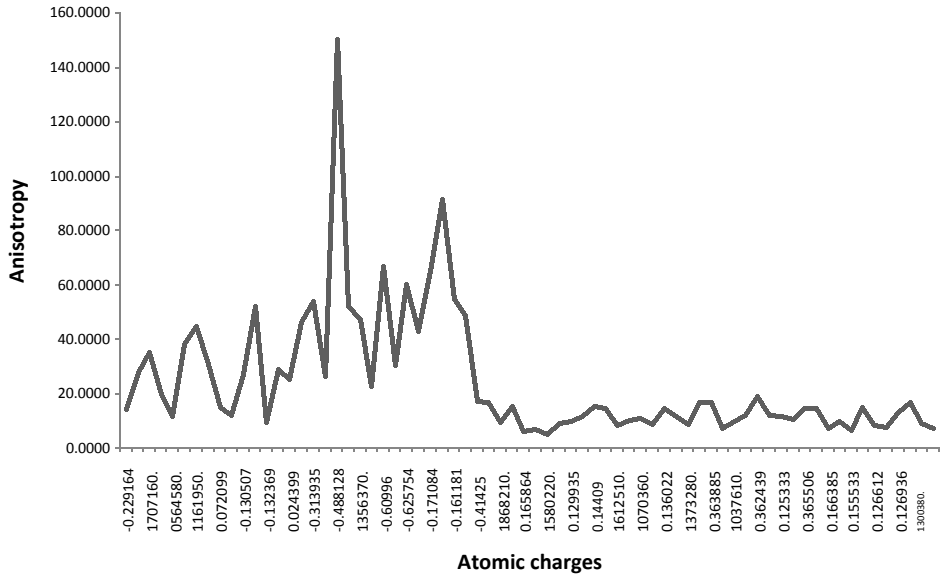


Figure 2. It shows the graphs were obtained from B3Lyp/6-31G method.

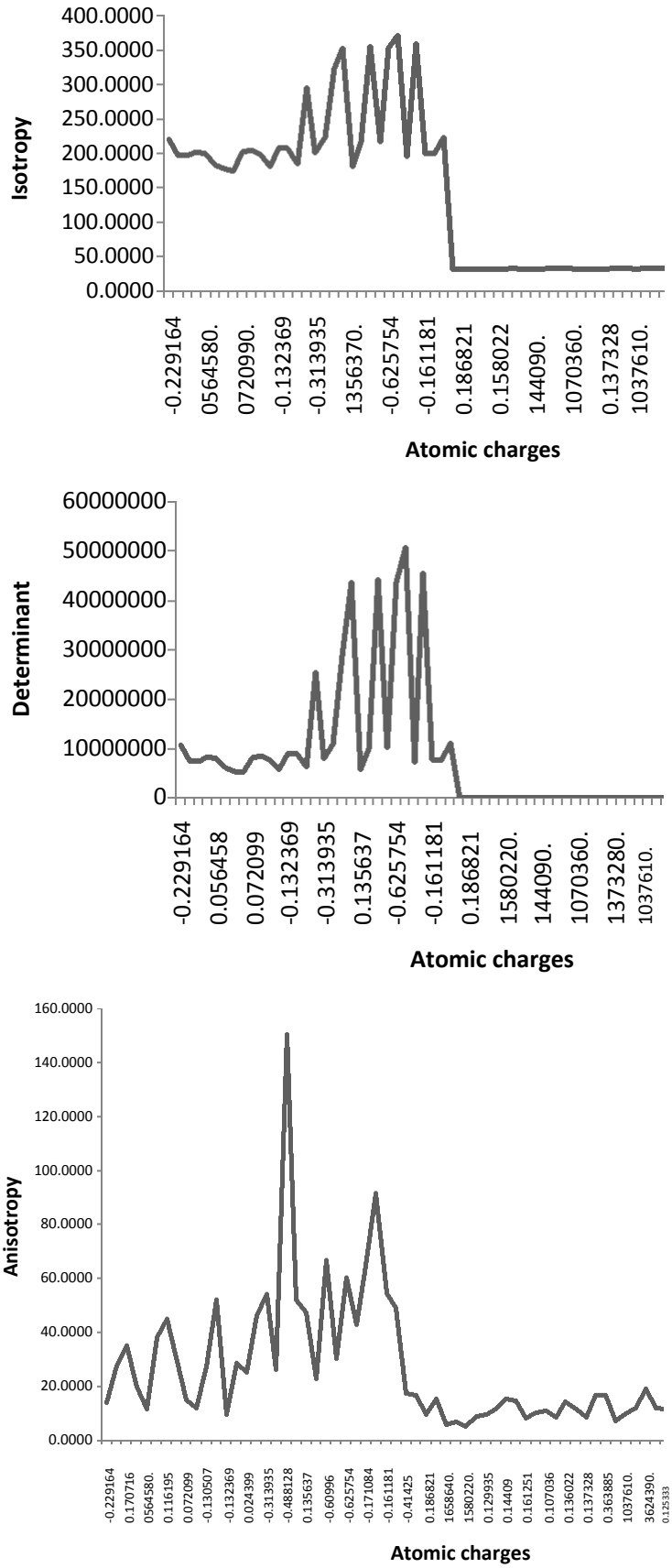


Figure 3. It shows the graphs were obtained from B3Lyp/6-31G* method

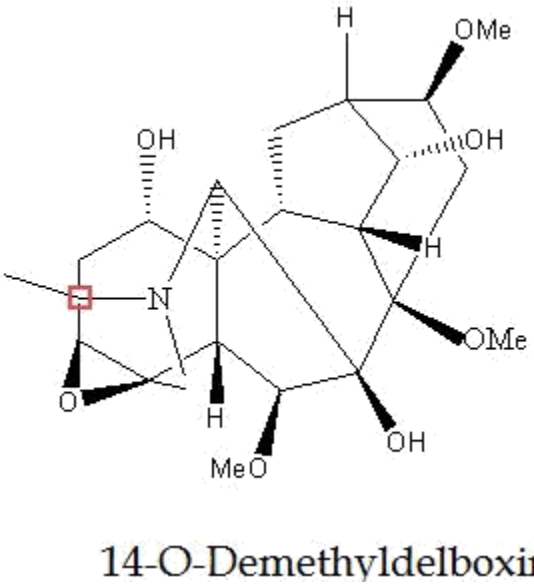


Figure 4. 14-o-demethyldelboxine.

these atoms, plant characteristics increase because of electron donor groups increasing.

In this research, we focus on two mechanisms to define anticancer and antiviral properties of *Consolida* species and effective material from this plant. One of these mechanisms is the study of NMR and the other one is dipole moment. We studied molecular stability in both methods for anticancer properties and understood that in *ab initio* calculation, in negative charges, minimum isotropy is about -0.3 degree and in positive charges, maximum isotropy is about 0.15 degree. These show that this molecule has polarity and alkaloidal properties that can highly reactions with microtubules and destroys there stability by polarity. It can be block cellular division and prevent from rapid growth in cancer.

Anisotropical calculations resulted exactly -0.3 degree too that emphasized in isotropical data. In the other hand, with drawing the atomic charges curve to determinant 3*3 based on NMR, we saw that these properties were formed in -0.3 degree. With changing the calculation from *ab initio* to DFT and B3Lyp instruction, we found this minimum for determinant in -0.6 degree too, that is two equal to -0.3. This result was not only for isotropy and anisotropy data. According to DFT that focuses in molecular density, these calculation show DFT methods can be the complementary of *ab initio* methods and feature in so small alkaloidal molecule from *Consolida* such as the pik in aniso curve and we can see it in Table 1.

The result of calculations show that 6-31G* order is more accurate than 6-31G, and 6-31G is more accurate than STO order especially for methyl groups. If methyl groups were substitute with other donor electron groups such as ethyl, demethyl, propyl,… , anticancer properties increase. Electron pulling groups such as phenyl and dephenyl decrease these properties. Different groups were discovered in *Consolida* that the most effective of them is 14-o-demethyldelboxine (Figure 4). These result can be inferred clearly in NMR result and *ab initio* calculations. η data for cycles characterize more details for us. Then it can be suggested that more concentration on η should be useful. Δiso can also be shown in total manner in aniso and iso. With the substitution of ethyl, propyle and phenyl groups, we can gain these data and hereby some indexes can get for demethyldelboxin molecules. Dipole moment calculations exactly approve *ab initio* methods.

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