In-silico Studies of Simulated IR Spectra of Some Selected Pyrazolone Compounds

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Abstract: Pyrazolone compounds are a class of heterocyclic compounds which have their utility in pharmaceutical / medicinal fields and these compounds were of the interest for studies since past because of this quality. So many references related to the studies of different aspects of such compounds are available in literature which is related to explore their structural, medicinal, pharmaceutical and other related properties. Simulation of spectra and related studies using different softwares, methods are matter of interest of various workers. The present communication contains the studies of simulation of Infra-red (IR) spectra of some selected pyrazolone compounds based on the different quantum- chemical semi-empirical methods which include different AM1, PM3, MNDO and ZINDO methods using HYPAERCHEM 8.0 professional version. Comparison of the results obtained with the experimental spectra of the compounds is also reported. The results obtained using these different methods are in good agreement with the experimental data. So far as the comparison among the employed methods is concern, AM1 method gives comparatively reasonable good results. Geometrical parameters are also obtained after optimizations of the compounds under study which are also reported in this paper. Author has also tried to study and report parameters related to FMO approach theoretically on the basis of HOMO and LUMO energy values that are obtained using these methods. Other related parameters obtained after FMO studies are also reported.

Keywords: Pyrazolones, Simulation of Spectral Studies, Semi-Empirical Methods, HOMO-LUMO

1. Introduction

It is one of the key objectives of organic, medicinal and pharmaceutical chemistry that workers working in these areas and branches are extensively and actively involved in the designing and synthesis of molecules that possess potent therapeutic values and applications. The rapid development of resistance towards any present antimicrobial drugs puts a serious challenge before the scientific community. Consequently, there is utmost requirement to develop new antimicrobial agents with potent activity against resistant microorganism [1-5]. To achieve this goal, structural investigations of any compound or a series of compound is important and has significance in the establishment of that compound [6-10].

Pyrazolone derivatives have a long history of application in medicinal and pharmaceutical industry. Due to their wide range of biological activity, pyrazolones have received a considerable interest in the field of drug discovery and therefore, these heterocyclic ring compounds have been a relevant synthetic target of choice for a number of workers working in this field in pharmaceutical industry. In fact, these heterocyclic compounds have been a core structure of a number of medicines and drugs which are in use now-a- days.

Spectral studies of any series of compounds / compound are among important tools in their structural establishment [11-12]. Simulation of spectra of different compounds along with the computations of related parameters were of field of interest of various workers [13-19].

Keeping the above facts in mind and in continuation to the efforts in such type of study's author is hereby reporting the *in-silico* semi-empirical quantum chemical based spectral simulation studies of some selected pyrazolone compounds in this present paper.

Compounds that are selected for the studies in the present work are shown in the figure 1 below along with their names in the Table 1.

Compound I

Compound II

Compound III

Compound IV

Compound V

Compound VI
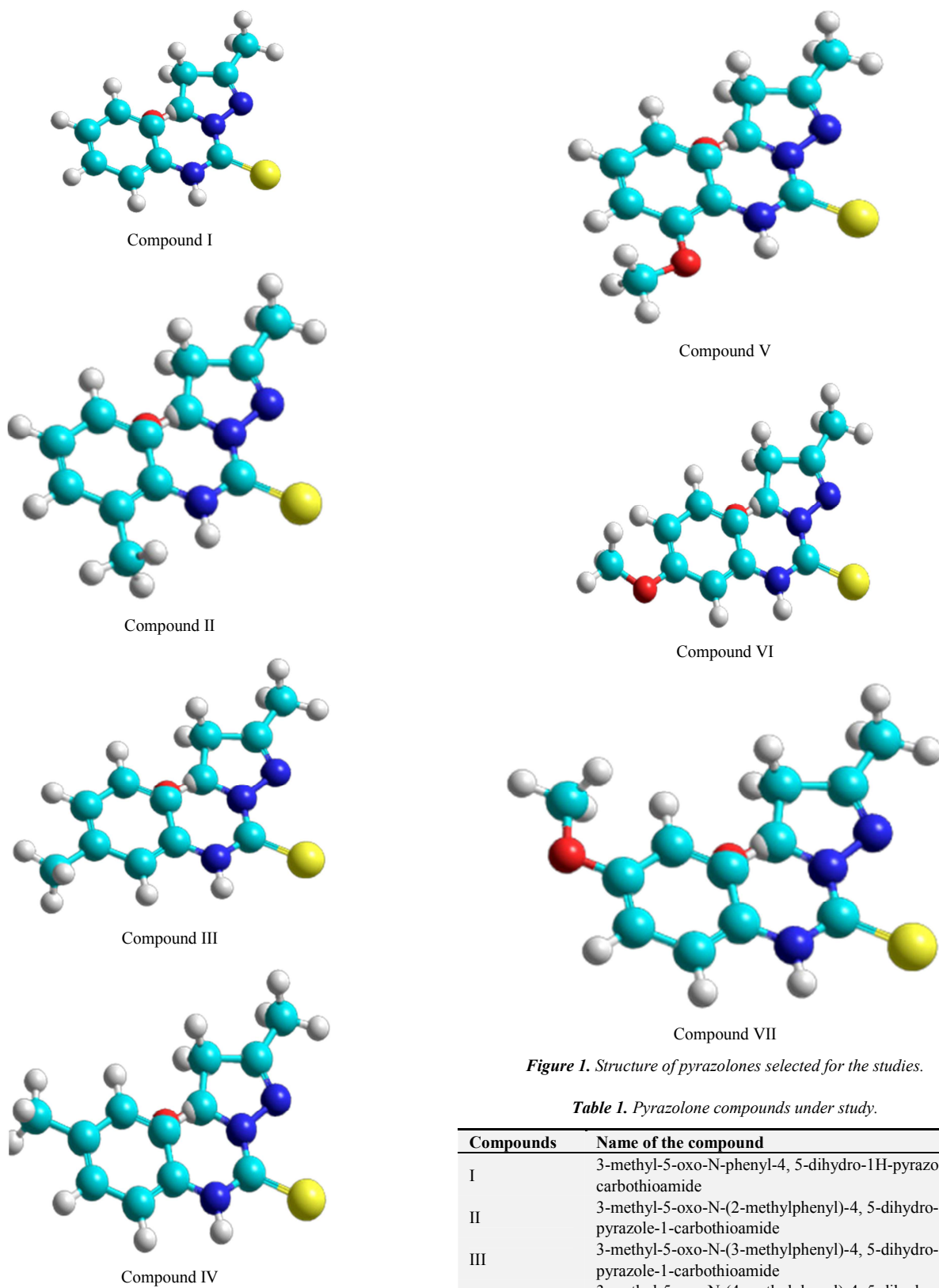
Compound VII

Figure 1. *Structure of pyrazolones selected for the studies.*

Table 1. *Pyrazolone compounds under study.*

Compounds	Name of the compound
I	3-methyl-5-oxo-N-phenyl-4, 5-dihydro-1H-pyrazole-1-carbothioamide
II	3-methyl-5-oxo-N-(2-methylphenyl)-4, 5-dihydro-1H-pyrazole-1-carbothioamide
III	3-methyl-5-oxo-N-(3-methylphenyl)-4, 5-dihydro-1H-pyrazole-1-carbothioamide
IV	3-methyl-5-oxo-N-(4-methylphenyl)-4, 5-dihydro-1H-pyrazole-1-carbothioamide
V	N-(2-methyoxyphenyl)-3-methyl-5-oxo-4, 5-dihydro-1H-pyrazole-1-carbothioamide
VI	N-(3-methyoxyphenyl)-3-methyl-5-oxo-4, 5-dihydro-1H-pyrazole-1-carbothioamide
VII	N-(4-methyoxyphenyl)-3-methyl-5-oxo-4, 5-dihydro-1H-pyrazole-1-carbothioamide

2. Experimental

The spectral data for the pyrazolone compounds for which studies are reported in this communication were obtained as reported earlier [20]. The FTIR spectral data of these pyrazolone compounds under study were taken and recorded as reported by authors previously [20].

Details for Computational Studies

The computational studies were carried out on Intel based Pentium core-2 Duo machine with configuration Intel (R) core TM 2 Duo CPU, T5450@1.66 GHZ, 2 GB RAM, 250 GB HDD. All computations were carried out on it.

Semi-empirical methods viz. AM1, PM3, MNDO and ZINDO1 were employed for various quantum chemical calculations. These computations were carried out by the computer software HYPERCHEM 8.0 professional version. The computed parameters such as normal modes or vibration frequencies were also obtained on the same platform. All the methods viz. AM1, PM3, MNDO and ZINDO were employed for studies of these pyrazolones. These have their usual meanings and these may be considered as Hamiltonians or key words for the methods under studies. The simulated spectral diagrams, and all other related statistical calculations were carried out on MS-Excel as usually carried out by other workers [18-19].

3. Results and Discussion

3.1. Computed Structural Parameters

All the structural parameters of the interest viz. heat of formation (HF); core-core interaction (CC), Total energy (TE), zero-point energy (ZPE) and electronic energy (EE) which are computed using above mentioned software on the basis of the methods mentioned in the experimental section are given in the Tables 2-5.

***Table 2.** AM1 computed parameters for the compounds under study.*

Compd	Total Energy (TE) (kcal/ mol)	Binding Energy (BE) (k cal/mol)	Isolated atomic energy (IAE) (kcal/mol)	Electronic energy (EE) (kcal/mol)	Core-Core repulsion energy (CC)	Heat of Formation (HF) (kcal/mol)	Dipole Moment (DM) (Debye)
I	-62023.917	-2771.2607	-59252.66	-351236.9	289213.02	146.6102	1.097
II	-65700.193	-3135.7928	-62564.40	-420678.5	354978.38	157.17216	6.041
III	-65592.585	-3028.1849	-62564.40	-381613.9	316021.35	164.7801	2.248
IV	-65600.729	-3036.3292	-62564.40	-400881.7	335280.99	156.6357	4.497
V	-72975.920	-3121.9379	-69853.98	-428920.9	355945.01	130.5860	1.547
VI	-73050.910	-3196.9275	-69853.98	-447991.3	374940.44	55.59646	6.709
VII	-72978.923	-3124.9411	-69853.98	-444443.6	371464.70	127.5828	4.749

***Table 3.** PM3 computed parameters for the compounds under study.*

Compd.	Total Energy (TE) (kcal/ mol)	Binding Energy (BE) (k cal/mol)	Isolated atomic energy (IAE) (kcal/mol)	Electronic energy (EE) (kcal/mol)	Core-Core repulsion energy (CC)	Heat of Formation (HF) (kcal/mol)	Dipole Moment (DM) (Debye)
I	-56132.289	-2792.8257	-53339.42	-342201.2	286068.86	125.0052	1.892
II	-59662.713	-3155.2614	-56507.45	-409195.2	349532.53	137.70355	7.155
III	-59583.981	-3076.5293	-56507.45	-378969.3	319385.32	116.4356	1.999
IV	-59566.059	-3058.6074	-56507.45	-387915.3	328349.25	134.3575	5.222
V	-66343.558	-3163.5906	-63179.96	-427856.6	361513.10	88.93336	2.359
VI	-66392.424	-3212.4562	-63179.96	-433673.4	367281.06	40.06773	7.028
VII	-66325.382	-3145.4144	-63179.96	-430689.8	364364.44	107.1095	5.677

***Table 4.** MNDO computed parameters for the compounds under study.*

Compd.	Total Energy (TE) (kcal/ mol)	Binding Energy (BE) (k cal/mol)	Isolated atomic energy (IAE) (kcal/mol)	Electronic energy (EE) (kcal/mol)	Core-Core repulsion energy (CC)	Heat of Formation (HF) (kcal/mol)	Dipole Moment (DM) (Debye)
I	-62909.758	-2765.3793	-60144.38	-356351.9	293442.16	152.49166	3.599
II	-66644.088	-3171.7066	-63472.38	-420394.5	353750.38	121.25830	5.757
III	-	-	-	-	-	-	-
IV	-66543.262	-3070.8806	-63472.38	-400558.3	334015.10	122.08436	4.221
V	-73940.794	-3138.0360	-70802.75	-448485.9	374545.06	114.48796	3.364
VI	-74040.304	-3237.5456	-70802.75	-445231.7	371191.48	14.978316	5.589
VII	-73964.028	-3161.2702	-70802.75	-445757.9	371793.97	91.253727	4.868

***Table 5.** ZINDO computed parameters for the compounds under study.*

Compd.	Total Energy (TE) (kcal/ mol)	Binding Energy (BE) (k cal/mol)	Isolated atomic energy (IAE) (kcal/mol)	Electronic energy (EE) (kcal/mol)	Core-Core repulsion energy (CC)	Heat of Formation (HF) (kcal/mol)	Dipole Moment (DM) (Debye)
I	-86905.866	-8620.1997	-78285.66	-464190.5	377284.63	-5702.33	19.921
II	-91964.869	-9543.8034	-82421.06	-485888.4	393923.51	-6350.838	11.162
III	-91895.187	-9474.1215	-82421.06	-522636.2	430741.00	-6281.156	10.454

Compd.	Total Energy (TE) (kcal/ mol)	Binding Energy (BE) (k cal/mol)	Isolated atomic energy (IAE) (kcal/mol)	Electronic energy (EE) (kcal/mol)	Core-Core repulsion energy (CC)	Heat of Formation (HF) (kcal/mol)	Dipole Moment (DM) (Debye)
IV	-92101.653	-9680.5873	-82421.06	-505165.7	413064.10	-6487.622	11.689
V	-102498.62	-9607.4047	-92891.22	-581347.6	478849.04	-6354.880	6.958
VI	-102623.08	-9731.8603	-92891.22	-532012.5	429389.46	-6479.336	12.562
VII	-102768.62	-9877.4050	-92891.22	-580056.4	477287.79	-6624.881	5.384

Comparison of various parameters have been done. Some of the comparative figures for the parameters viz. Heat of formation and dipole moment of these pyrazolone compounds are presented in the Figures 2-3.
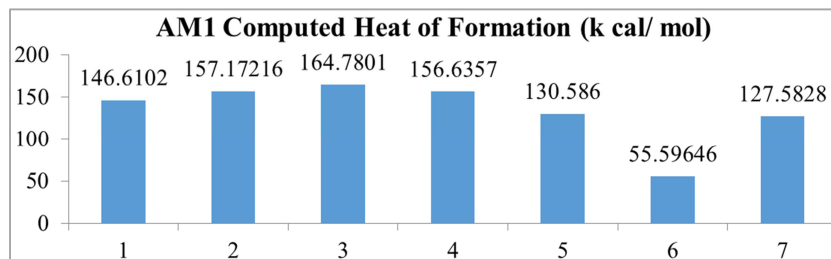
AM1 computed heat of formation for pyrazolone compounds
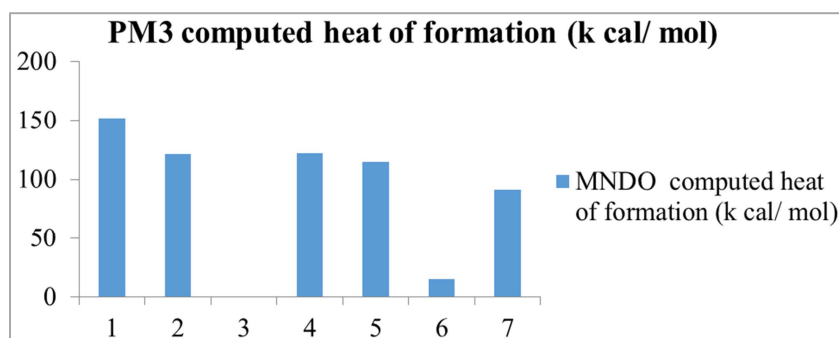
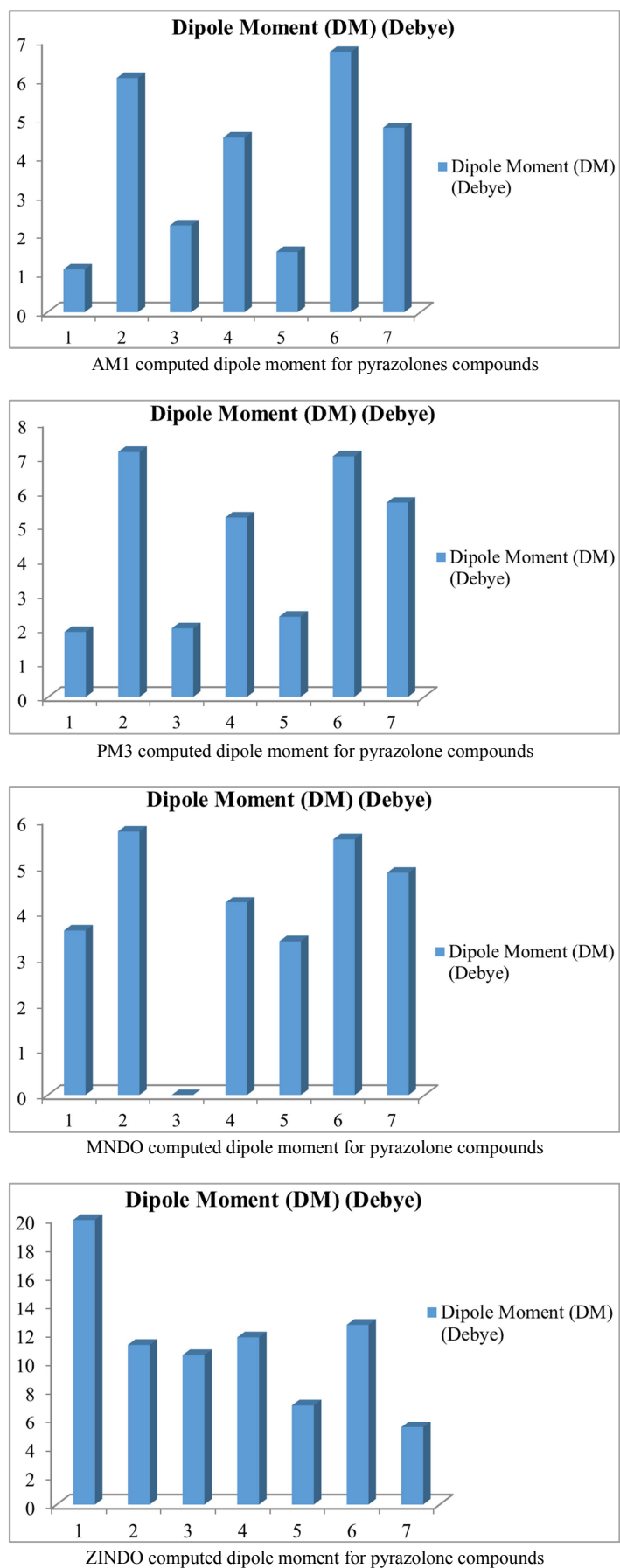PM3 COMPUTED HEAT OF FORMATION FOR PYRAZOLONE COMPOUNDS
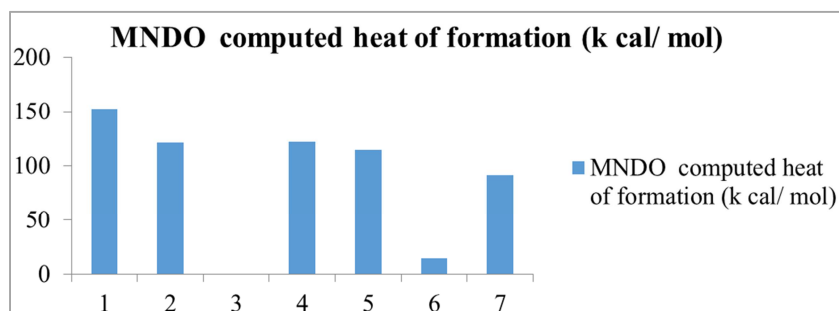
MNDO COMPUTED HEAT OF FORMATION FOR PYRAZOLONE COMPOUNDS
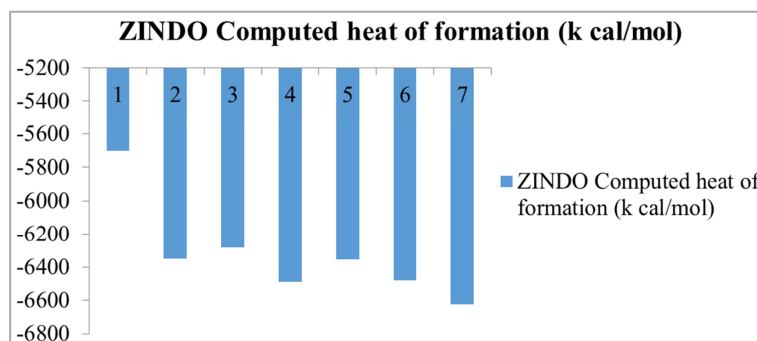
ZINDO computed heat of formation for pyrazolone compounds

Figure 2. *Comparison of Heat of formation of different pyrazolone compounds under study.*

AM1 computed dipole moment for pyrazolones compounds

PM3 computed dipole moment for pyrazolone compounds

MNDO computed dipole moment for pyrazolone compounds

ZINDO computed dipole moment for pyrazolone compounds

Figure 3. *Comparison of computed dipole moment values for different pyrazolone compounds under study.*

Heat of formation as computed using ZINDO method shows negative values which is indicative of the fact that the ZINDO method may not be reliable for such type of computations for pyrazolone compounds. Results for all other parameters that are obtained using these methods are fair enough with slight permissible error as it is indicative from the comparison of dipole moments for pyrazolone compounds.

3.2. Spectral Simulation Studies

The vibration modes for the pyrazolone compounds under study were computed on the software HYPERCHEM 8.0 professional version. These were computed using semi-empirical AM1, PM3, MNDO and ZINDO methods. In all the cases vibration modes were obtained and spectra are simulated except MNDO computation for compound C, where computation was abort. These computed vibration frequencies are given in the table 6-12 along with the experimentally observed vibration modes and with assignments to these vibration modes. The experimental spectral data for these compounds is recorded as reported in the literature [20].

Table 6. Spectral data for the compound A.

Exp. Obs. Freq. (cm⁻¹)	Assignment	AM1 computed spectral peaks		PM3 computed spectral peaks		MNDO computed spectral peaks		ZINDO computed spectral peaks	
		Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity
3250	N-H str	3164	26.7522	3166	3.67592	3260	3.75097	2836	51.51505
1693	C=O str	1578	43.0894	1772	86.1566	1796	23.40594	1696	14.05793
1425	C-N str	1458	49.9579	1445	1.96301	1434	36.37600	1480	0.80925
1159	C=S	1129	7.35157	1148	1.01566	1187	2.95807	1161	22.81347
1610	C=N	1562	4.3789	-	-	1570	8.01173	1650	32.56234

Table 7. Spectral data for the compound B.

Exp. Obs. Freq. (cm⁻¹)	Assignment	AM1 computed spectral peaks		PM3 computed spectral peaks		MNDO computed spectral peaks		ZINDO computed spectral peaks	
		Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity
3178	N-H str	3179	13.01994	3163	3.29531	3254	5.2730	2652	6.11177
1699	C=O str	1765	19.85500	1786	15.11036	1723	96.34459	1694	4.66286
1452	C-N str	1450	21.11305	1464	48.84407	1455	52.41419	1448	1.76432
1157	C=S	1140	20.56179	1137	15.67019	1180	23.13411	1163	16.53502
1602	C=N	1637	1.30878	1615	9.31836	1610	43.4006	1602	1.65330

Table 8. Spectral data for the compound C.

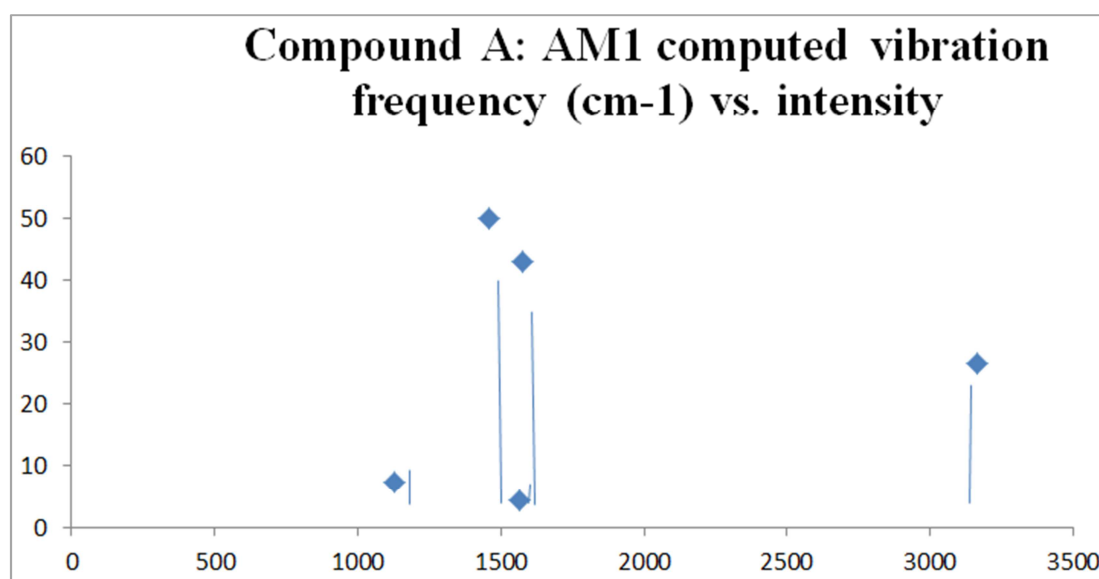| Exp. Obs. Freq. (cm⁻¹)	Assignment	AM1 computed spectral peaks		PM3 computed spectral peaks		MNDO computed spectral peaks		ZINDO computed spectral peaks	
		Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity
3265	N-H str	3177	17.49842	3167	3.70904	-	-	2637	42.76653
1672	C=O str	1725	13.65545	1774	85.78651	-	-	1681	5.42910
1476	C-N str	1438	9.90935	1476	20.56680	-	-	1465	14.55704
1166	C=S	1140	11.18259	1172	22.01321	-	-	1159	23.49492
1620	C=N	1658	67.80726	-	-	-	-	1610	5.90907

Table 9. Spectral data for the compound D.

Exp. Obs. Freq. (cm⁻¹)	Assignment	AM1 computed spectral peaks		PM3 computed spectral peaks		MNDO computed spectral peaks		ZINDO computed spectral peaks	
		Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity
3256	N-H str	3183	21.7159	3342	10.83551	3257	6.65073	2652	18.56735
1668	C=O str	1617	88.7560	1795	33.27678	1790	9.01049	1662	13.29531
1482	C-N str	1490	52.0506	1479	66.20783	1464	48.38817	1478	4.82767
1141	C=S	1109	7.18817	1135	74.73008	1136	3.16343	1148	18.89881
1605	C=N	1537	31.3571	1580	42.18705	1554	77.87932	1608	6.48599

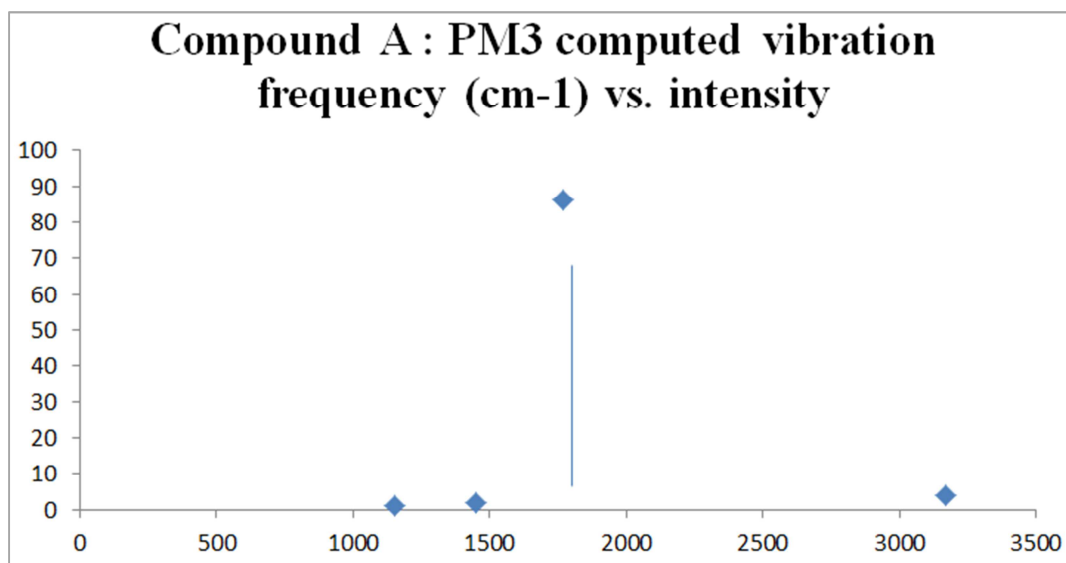***Table 10.** Spectral data for the compound E.*

Exp. Obs. Freq. (cm⁻¹)	Assignment	AM1 computed spectral peaks		PM3 computed spectral peaks		MNDO computed spectral peaks		ZINDO computed spectral peaks	
		Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity
3300	N-H str	3188	21.5193	3319	5.55814	3304	4.17813	2561	99.60681
1686	C=O str	1659	43.9456	1779	95.83850	1792	12.52494	1669	12.83180
1463	C-N str	1443	32.4626	1459	26.38128	1446	26.80243	1477	1.50574
1163	C=S	1186	6.81968	1171	5.41712	1196	6.76421	1153	22.75494
1615	C=N	1543	80.3143	-	-	1596	32.68214	1630	9.51217

***Table 11.** Spectral data for the compound F.*

Exp. Obs. Freq. (cm⁻¹)	Assignment	AM1 computed spectral peaks		PM3 computed spectral peaks		MNDO computed spectral peaks		ZINDO computed spectral peaks	
		Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity
3245	N-H str	3200	32.94534	3352	10.07711	3235	10.06939	2632	6.60610
1660	C=O str	1654	72.72335	1624	90.38378	1679	94.72584	1662	9.64059
1455	C-N str	1464	13.55929	1433	7.42262	1423	69.20970	1440	2.02141
1145	C=S	1164	21.10722	1143	8.77507	1160	31.96598	1137	33.89239
1612	C=N	1619	6.73961	1590	13.36299	1614	60.24741	1618	5.24232

***Table 12.** Spectral data for the compound G.*

Exp. Obs. Freq. (cm⁻¹)	Assignment	AM1 computed spectral peaks		PM3 computed spectral peaks		MNDO computed spectral peaks		ZINDO computed spectral peaks	
		Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity	Freq. (cm⁻¹)	Intensity
3223	N-H str	3206	23.1835	3343	10.93404	3216	16.36472	2786	27.58250
1630	C=O str	1615	92.5168	1581	42.16482	1607	87.54977	1635	3.67832
1435	C-N str	1432	81.9594	1436	9.66802	1464	47.34495	1449	9.17702
1159	C=S	11170	1.36505	1158	16.19762	1138	1.95983	1157	9.92444
1606	C=N	1550	9.21687	-	-	1550	44.94788	1602	6.53159

These tables show that the notable peaks in the case of these compounds are: υ(N-H) str; υ(C=O) str; υ(C-N) str; υ(C=S) and ν(C=N) which are also observed within permissible error on computations done for these compounds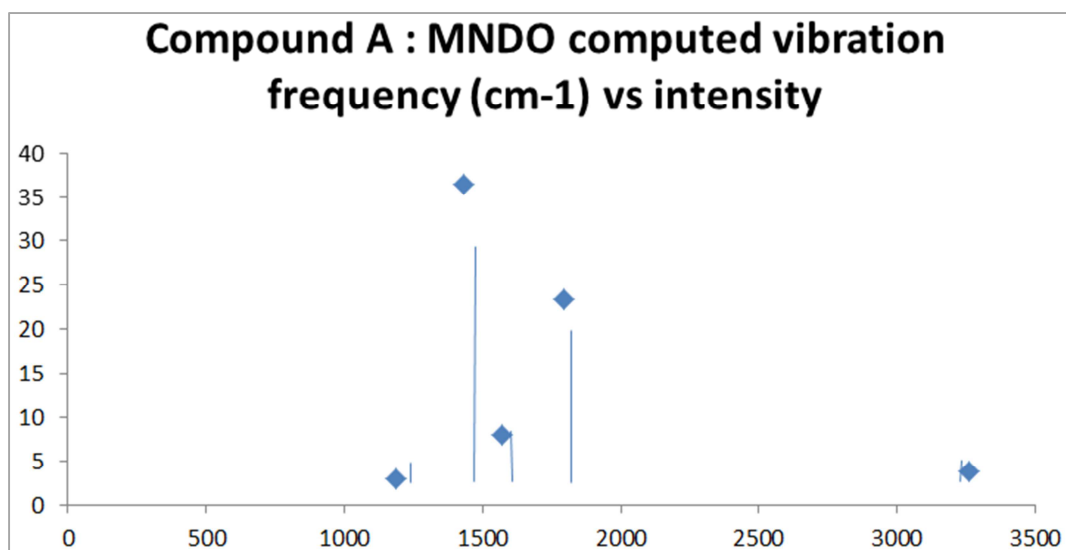 using these AM1, PM3, MNDO and ZINDO methods. All other peaks are also listed along with the experimental values in the tables 6-12. The spectra of these compounds are also simulated and designed on the basis of computed spectral values using these methods. These are shown in the Figure 4.
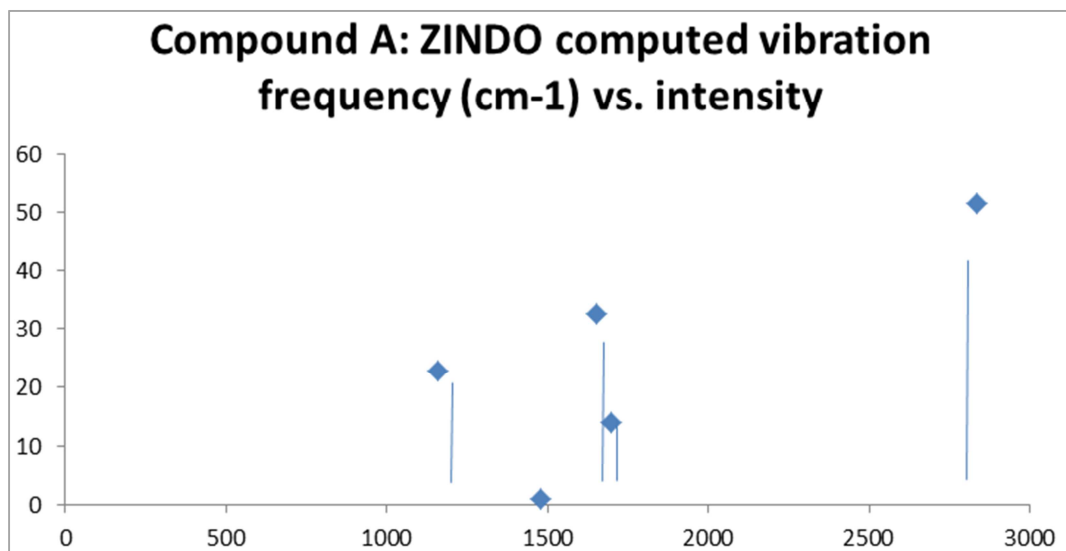

Simulated Spectra: AM1 computed vibration frequencies: Compound A

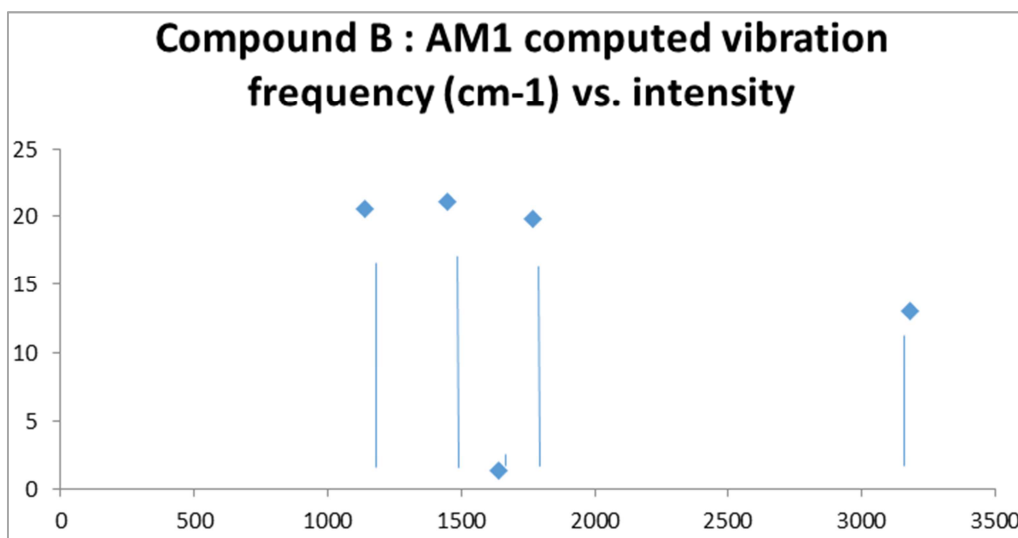Simulated Spectra: PM3 computed vibration frequencies: Compound A

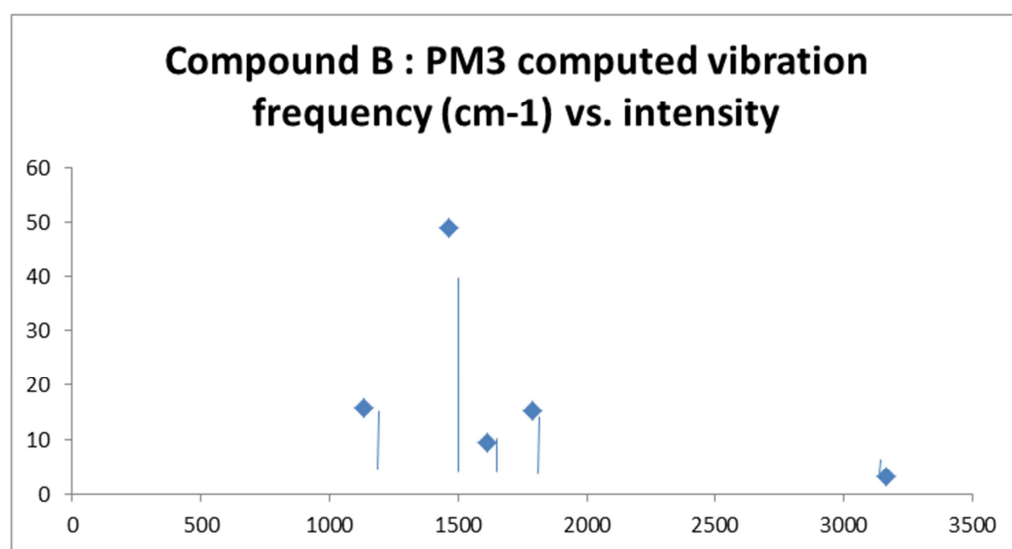Simulated Spectra: MNDO computed vibration frequencies: Compound A

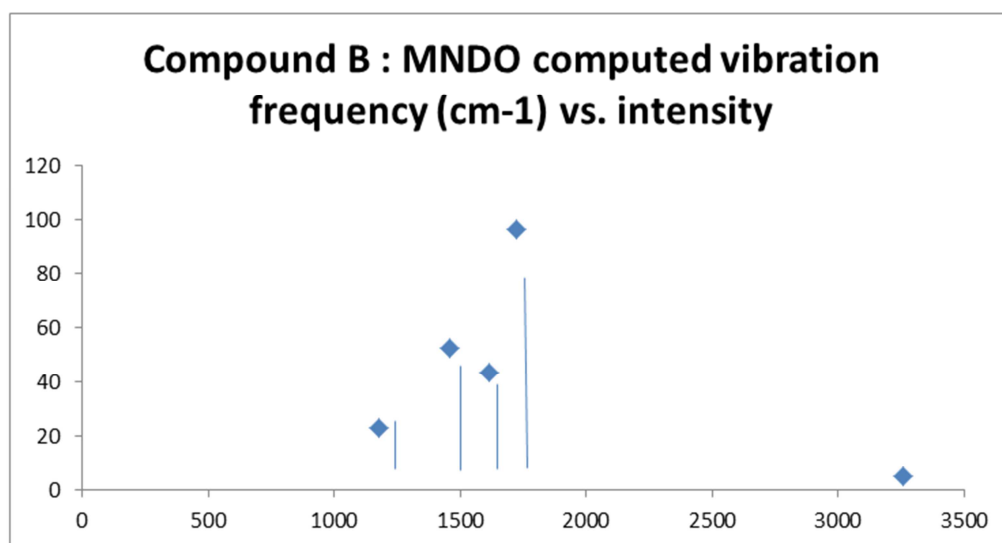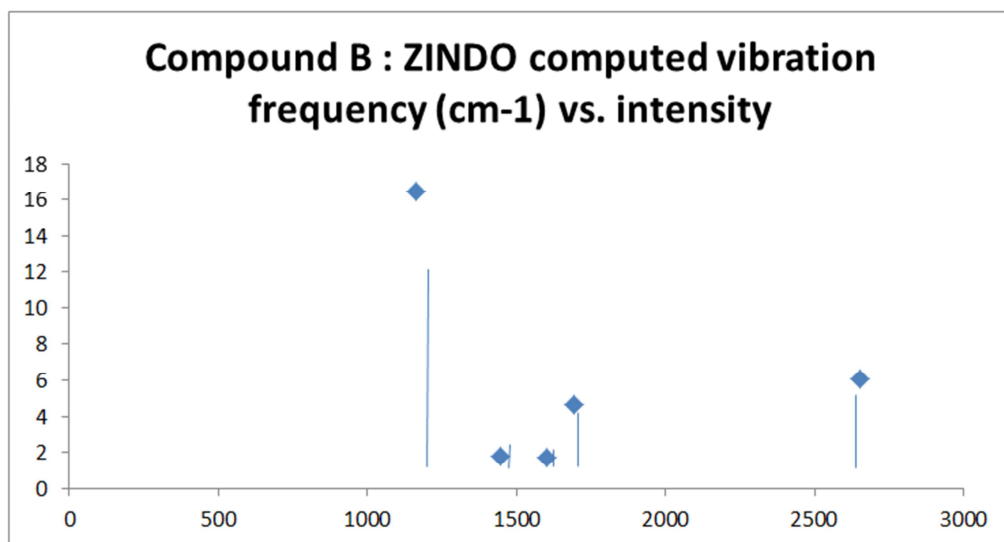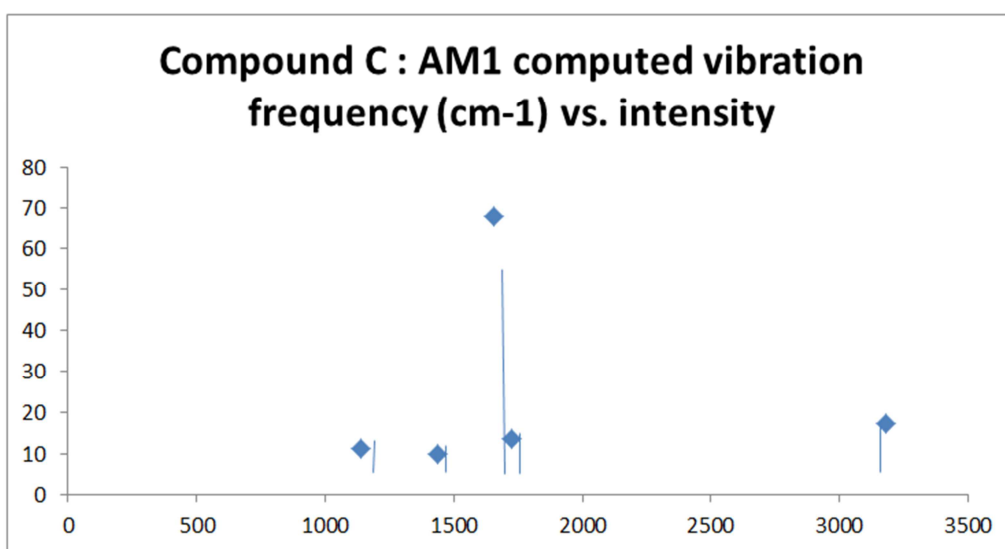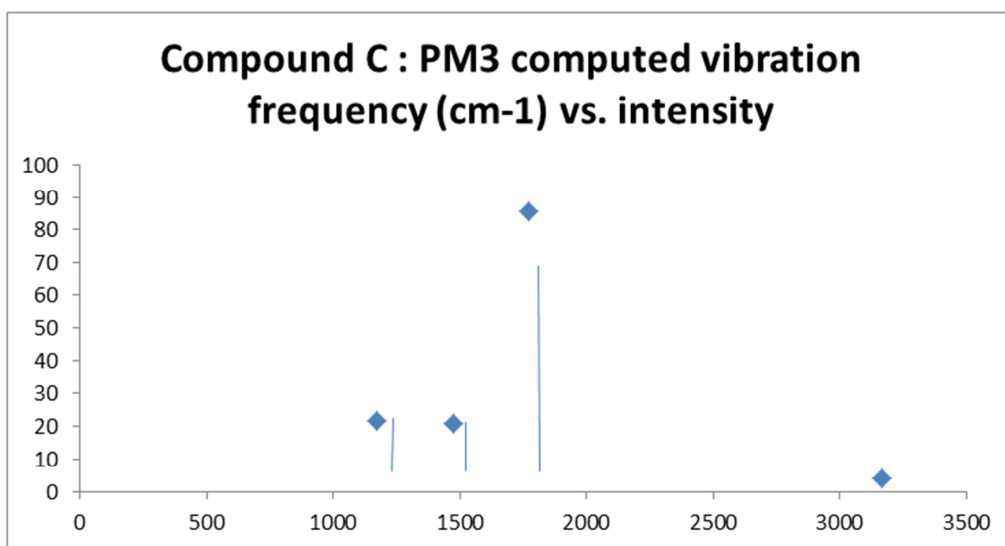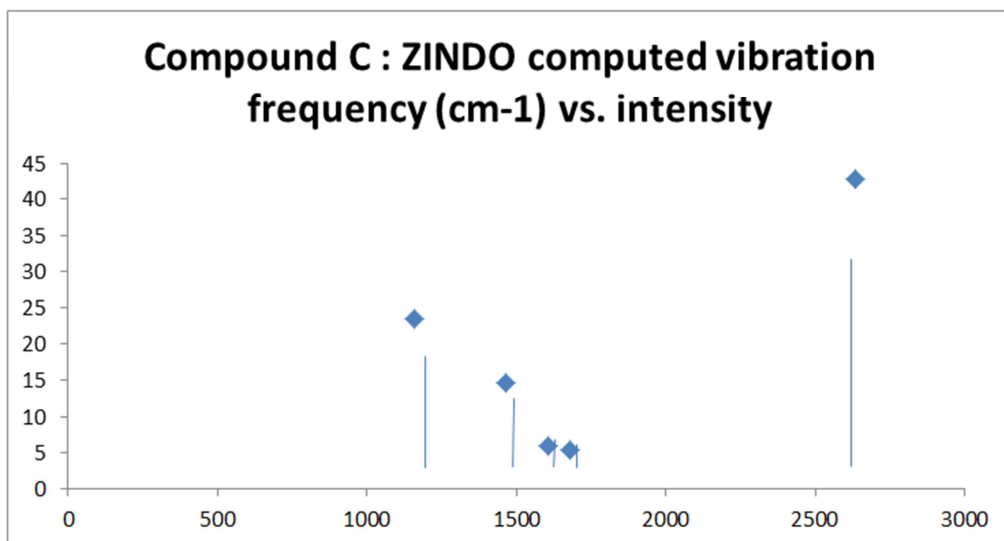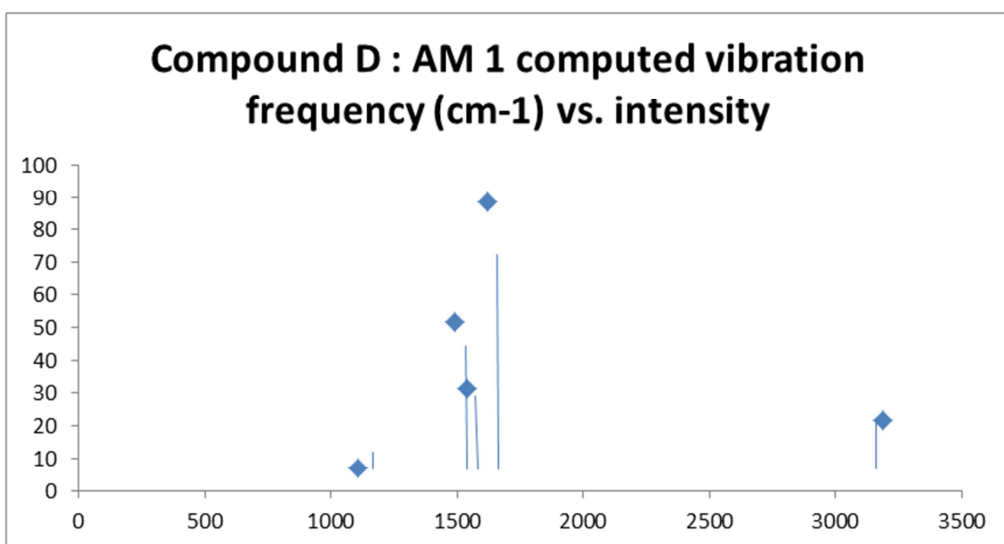Simulated Spectra: ZINDO computed vibration frequencies: Compound A

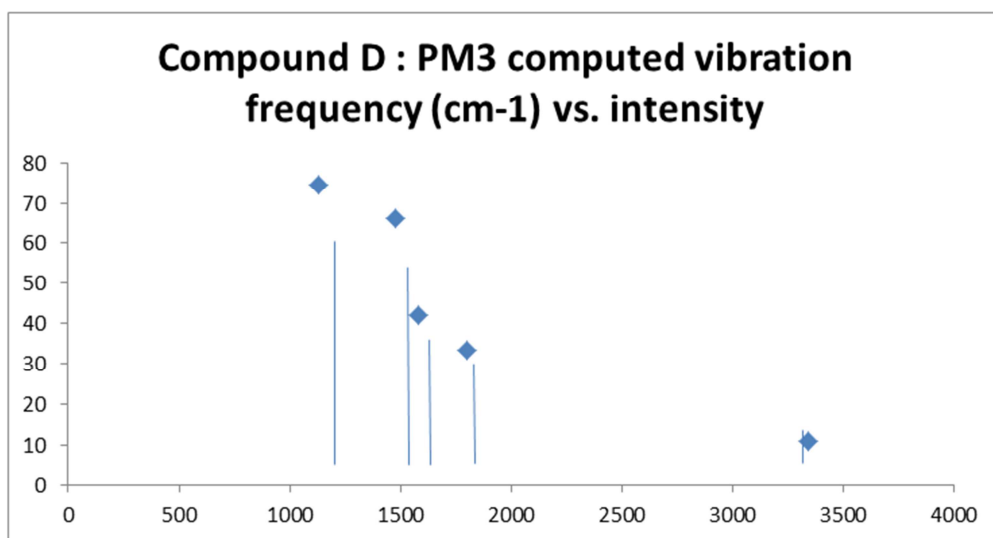Simulated Spectra: AM1 computed vibration frequencies: Compound B

Simulated Spectra: PM3 computed vibration frequencies: Compound B

Simulated Spectra: MNDO computed vibration frequencies: Compound B

Simulated Spectra: ZINDO computed vibration frequencies: Compound B

Simulated Spectra: AM1 computed vibration frequencies: Compound C

Simulated Spectra: PM3 computed vibration frequencies: Compound C
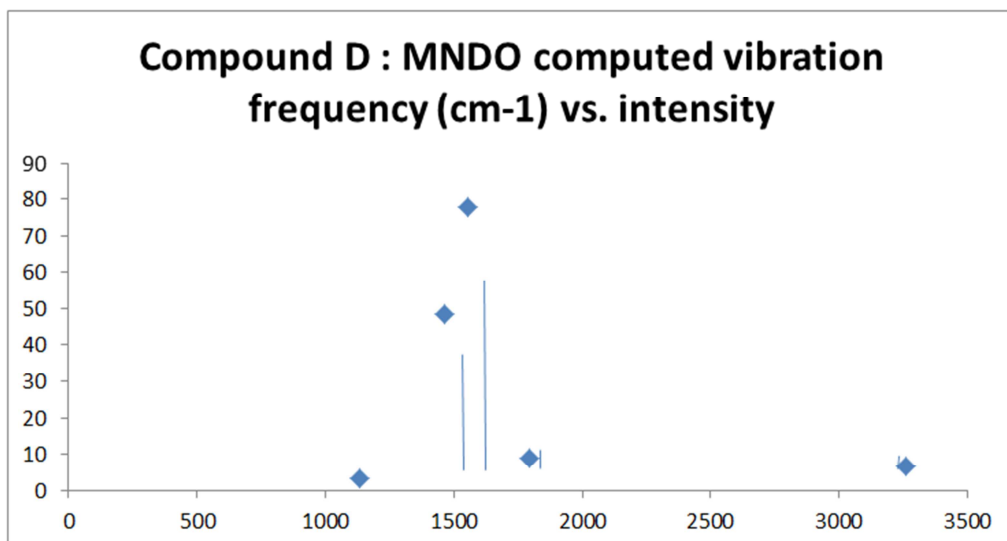
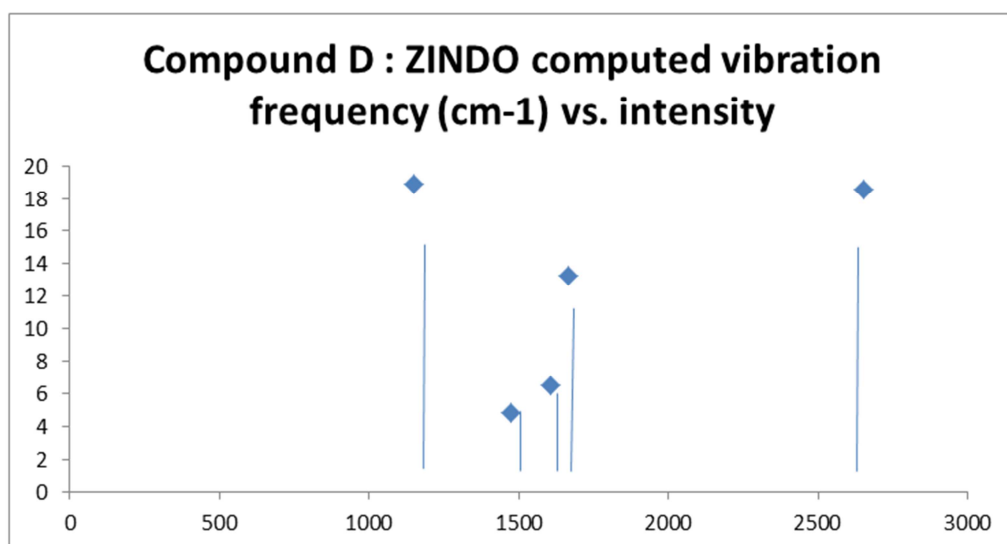Simulated Spectra: ZINDO computed vibration frequencies: Compound C

Simulated Spectra: AM1 computed vibration frequencies: Compound D
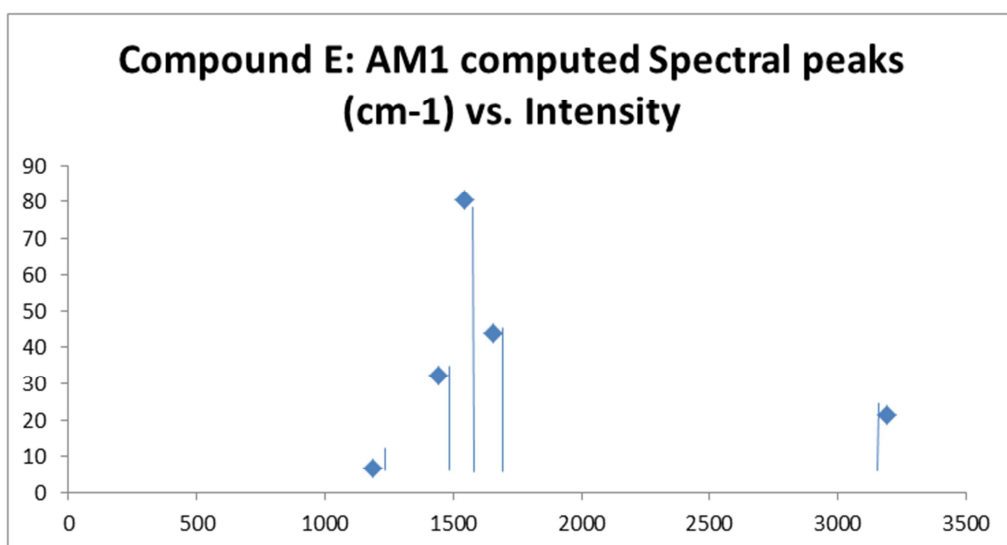

Simulated Spectra: PM3 computed vibration frequencies: Compound D

Simulated Spectra: MNDO computed vibration frequencies: Compound D

Simulated Spectra: ZINDO computed vibration frequencies: Compound D

Simulated Spectra: AM1 computed vibration frequencies: Compound E

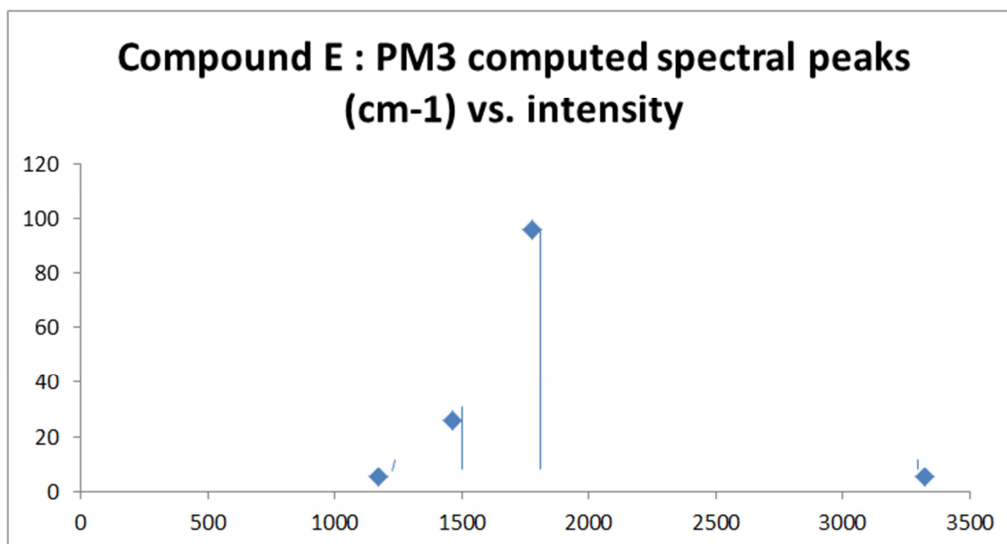Simulated Spectra: PM3 Computed vibration frequencies: Compound E

Simulated Spectra: MNDO computed vibration frequencies: Compound E
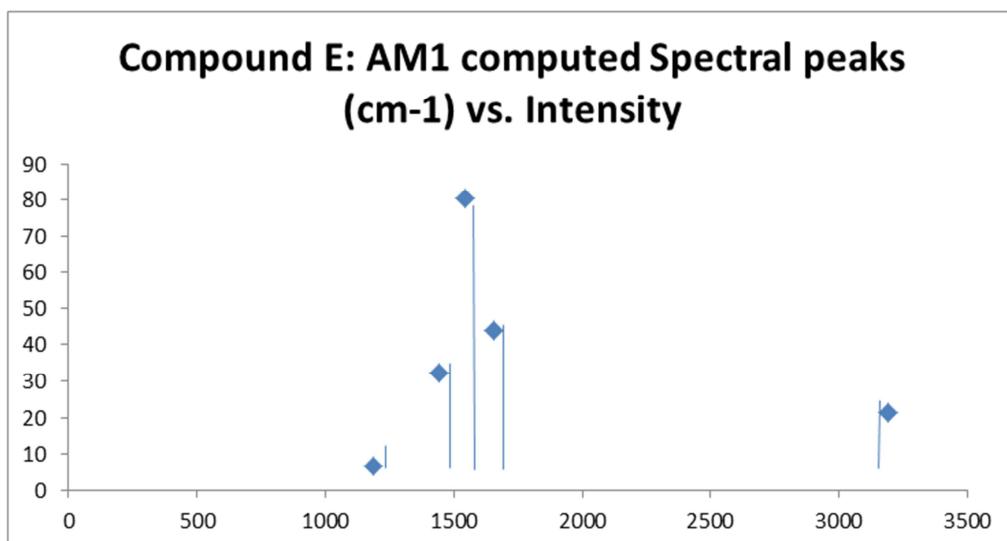

Simulated Spectra: ZINDO computed vibration frequencies: Compound E

Simulated Spectra: AM1 computed vibration frequencies: Compound F

Simulated Spectra: PM3 computed vibration frequencies: Compound F

Simulated Spectra: MNDO computed vibration frequencies: Compound F

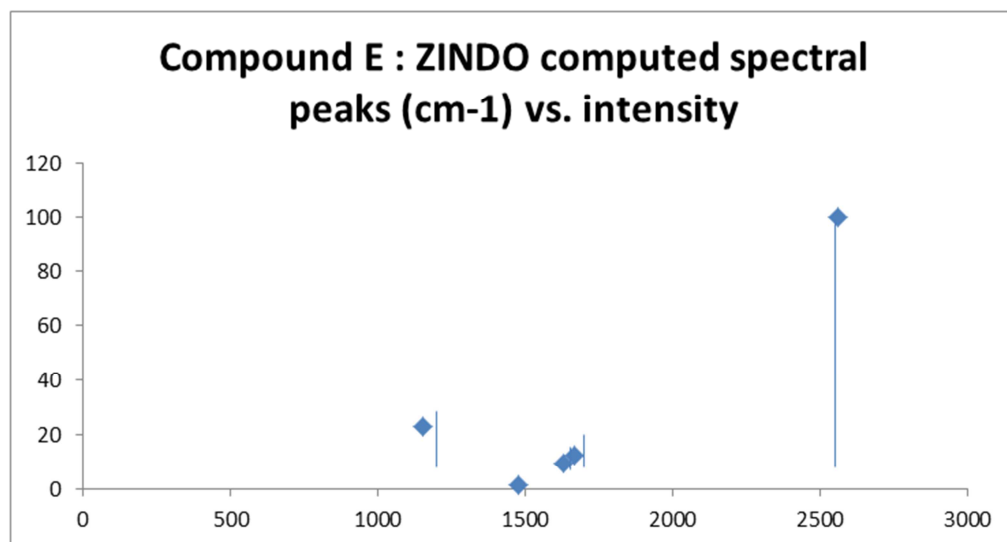Simulated Spectra: ZINDO computed vibration frequencies: Compound F

Simulated Spectra: AM1 computed vibration frequencies: compound G
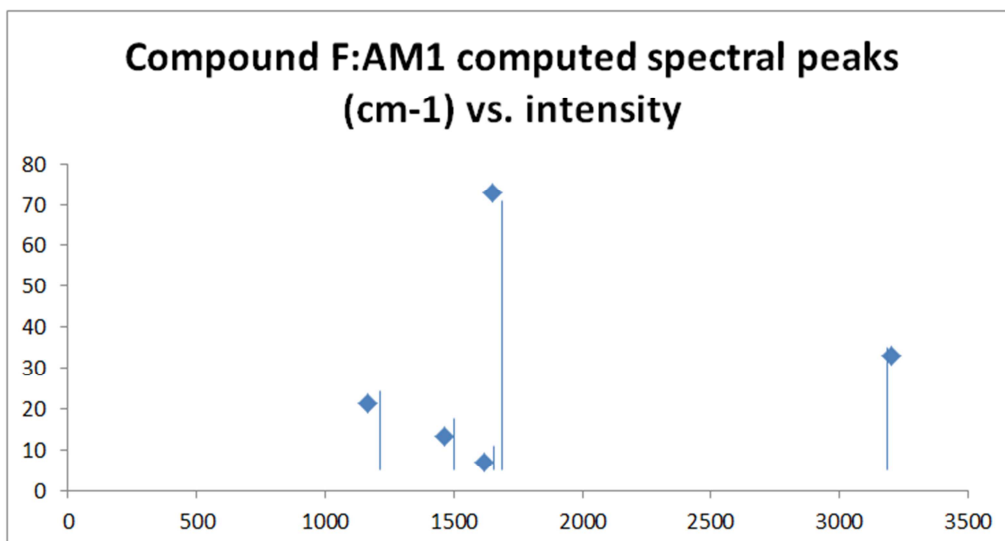

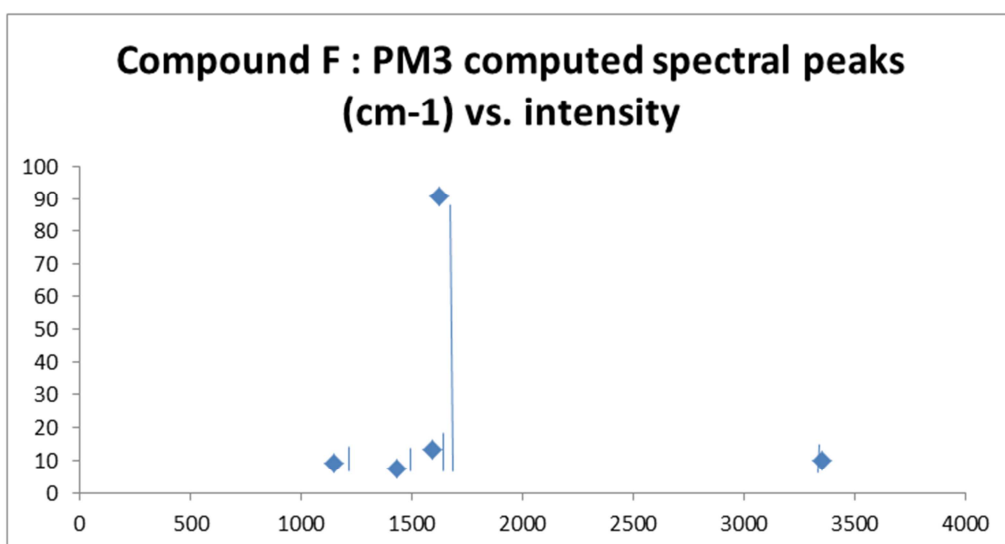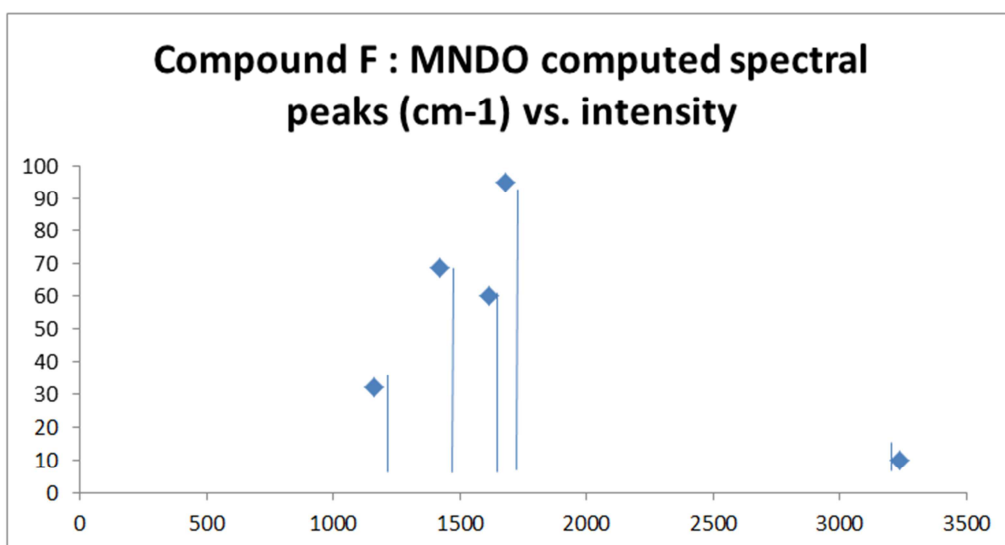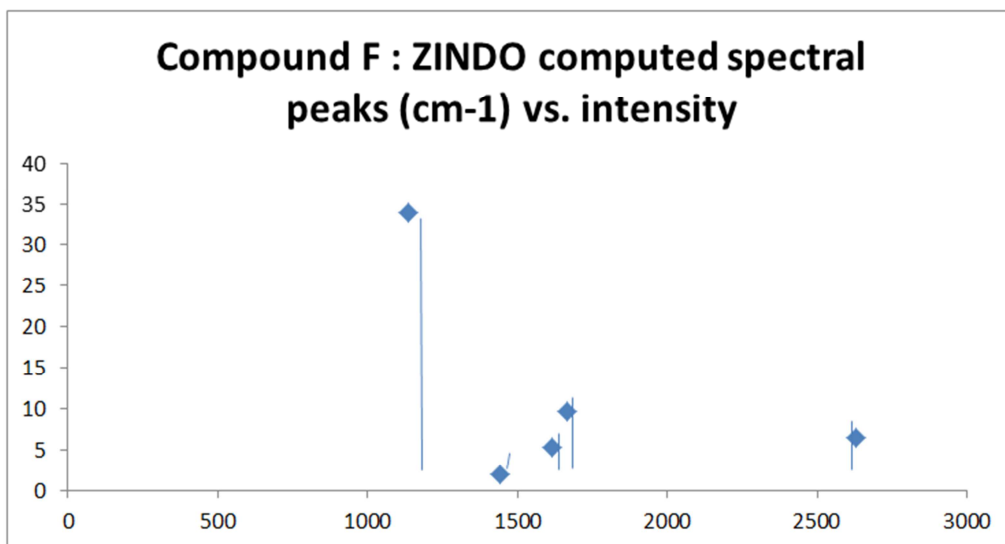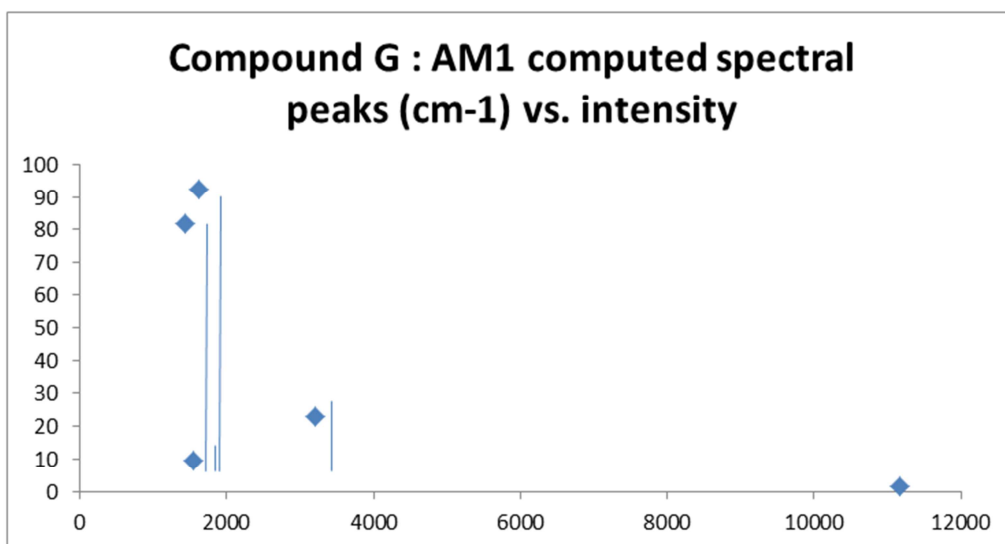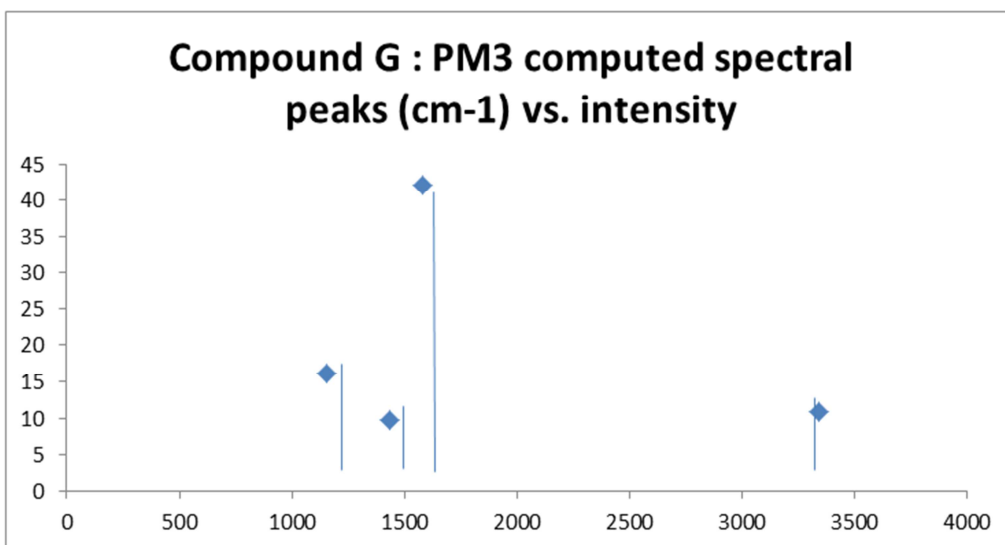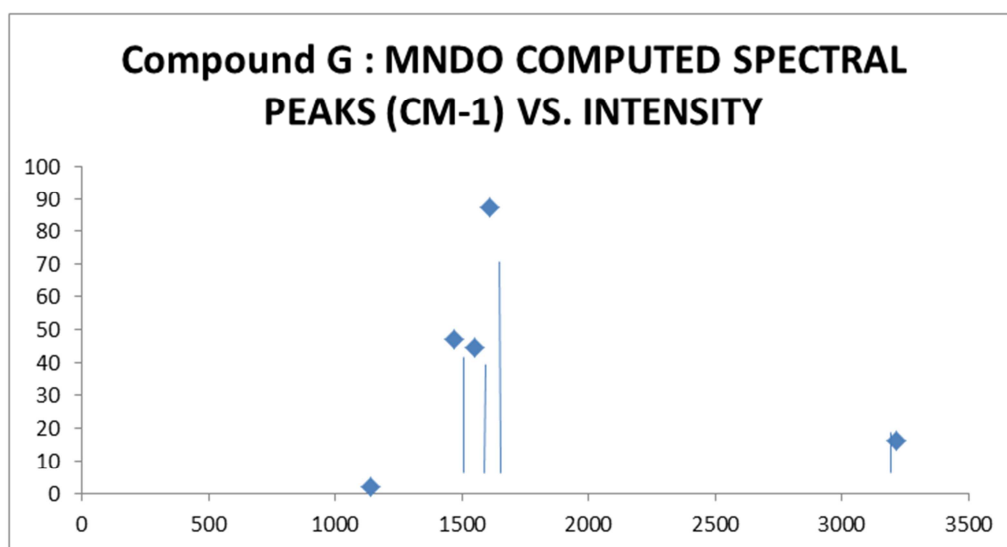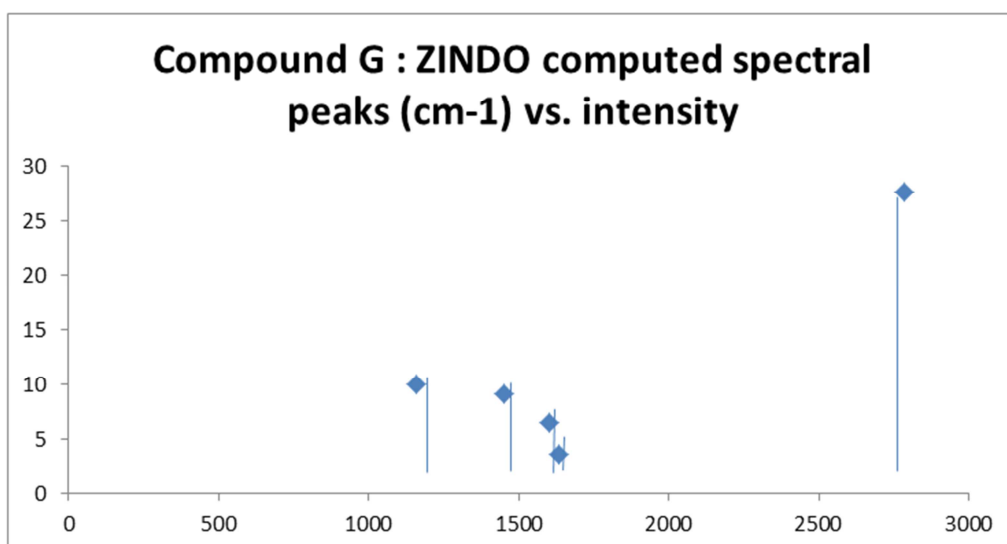Simulated Spectra: PM3 computed vibration frequencies: compound G

Simulated Spectra: MNDO computed vibration frequencies: compound G

Simulated Spectra: ZINDO computed vibration frequencies: compound G

Figure 4. *Simulated Spectra of the pyrazolone compounds under study.*

3.3. FMO Approach

The HOMO, LUMO and their energy gap i e., energy gap between HOMO-LUMO has also been computed for these pyrazolone compounds using semi-empirical AM1, PM3, MNDO and ZINDO methods. [18-20]. Associated with theseHOMO and LUMO parameters, within the framework of HF-SCF MO theory the ionization energy (IE) and electron affinity (EA) can be estimated and expressed utilizing HOMO and LUMO orbital energies [21] as

$$IE = -E_{HOMO} \text{ and } EA = -E_{LUMO}$$

Similarly, the hardness that corresponds to the gap between the HOMO and LUMO orbital energies which can also be computed as shown below. The larger the HOMO-LUMO energy gap implies the harder molecule. According

to Koopmans's theorem for global reactivity, the reactivity trends depend upon prediction of Chemical potential (μ), global hardness (η), electronegativity (χ), global softness (S) and electrophilicity index (ω). These may be considered as highly successful global reactivity descriptors and these descriptors may be calculated from the energies of frontier molecular orbitals viz. εHOMO, εLUMO [18-20] as per according to following formulae:

$$S = 1/2\eta$$

$$\omega = \mu^2/2\eta$$

$$\eta = 1/2 \ (\varepsilon HOMO - \varepsilon LUMO)$$

$$\chi = -1/2 \ (\varepsilon HOMO + \varepsilon LUMO)$$

$$\mu = -\chi = 1/2 \ (\varepsilon HOMO + \varepsilon LUMO)$$

All these parameters are also computed for the pyrazolone compounds under study in this present communication and are presented in the table 13-17 below.

Table 13. Computed HOMO – LUMO energy values for the compounds (A-G).

Compd.	AM1		PM3		MNDO		ZINDO	
	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
I	-0.28711	0.425378	-0.19547	0.23130	-0.73549	0.32990	-2.1363	5.76735
II	-0.22690	0.218430	-0.32606	0.12667	-0.49400	0.09836	-6.7735	6.37815
III	-0.15310	0.433256	-0.18089	0.24725	-	-	-4.50475	5.92903
IV	-0.00940	0.632653	-0.01333	0.15353	-0.18357	0.52964	-6.04917	6.59030
V	-0.16302	0.460270	-0.16886	0.32022	-0.82972	0.30877	-2.74208	5.25400
VI	-0.14253	0.265443	-0.40320	0.01461	-0.11052	0.75350	-6.83592	6.31062
VII	-0.03236	0.625167	-0.03820	0.13659	-0.22788	0.40487	-4.57723	5.97715

Table 14. AM1 computed HOMO-LUMO energy gap and other related parameters for the pyrazolone compounds under study.

Compound	HOMO (eV)	LUMO (eV)	Energy gap	η	S	χ	μ	HOMO-1	LUMO+1
I	-0.28711	0.425378	0.712488	0.356244	0.178122	-0.06913	0.069134	-8.3082	0.497587
II	-0.2269	0.21843	0.44533	0.222665	0.111333	0.004235	-0.00423	-0.6947	0.443379
III	-0.1531	0.433256	0.586356	0.293178	0.146589	-0.14008	0.140078	-0.3303	0.646275
IV	-0.0094	0.632653	0.642053	0.321027	0.160513	-0.31163	0.311627	-0.4239	0.752082
V	-0.16302	0.46027	0.62329	0.311645	0.155823	-0.14863	0.148625	-0.2608	0.701094
VI	-0.14253	0.265443	0.407973	0.203987	0.101993	-0.06146	0.061457	-0.2525	0.932204
VII	-0.03236	0.625167	0.657527	0.328764	0.164382	-0.2964	0.296404	-0.4914	0.745386

Table 15. PM3 computed HOMO-LUMO energy gap and other related parameters for the pyrazolone compounds under study.

Compound	HOMO (eV)	LUMO (eV)	Energy gap	η	S	χ	μ	HOMO-1	LUMO+1
I	-0.19547	0.2313	0.42677	0.213385	0.106693	-0.01792	0.017915	-0.3169	0.495935
II	-0.32606	0.12667	0.45273	0.226365	0.113183	0.099695	-0.0997	-0.5395	0.453445
III	-0.18089	0.24725	0.42814	0.21407	0.107035	-0.03318	0.03318	-0.2968	0.512554
IV	-0.01333	0.15353	0.16686	0.08343	0.041715	-0.0701	0.0701	-0.5435	0.739779
V	-0.16886	0.32022	0.48908	0.24454	0.12227	-0.07568	0.07568	-0.2484	0.571361
VI	-0.4032	0.01461	0.41781	0.208905	0.104453	0.194295	-0.1943	-0.7214	0.35442
VII	-0.0382	0.13659	0.17479	0.087395	0.043698	-0.0492	0.049195	-0.5833	0.716786

Table 16. MNDO computed HOMO-LUMO energy gap and other related parameters for the pyrazolone compounds under study.

Compound	HOMO (eV)	LUMO (eV)	Energy gap	η	S	χ	μ	HOMO-1	LUMO+1
I	-0.73549	0.3299	1.06539	0.532695	0.266348	0.202795	-0.2028	-8.7420	0.558710
II	-0.49400	0.09836	0.59236	0.29618	0.14809	0.19782	-0.19782	-0.6516	0.647550
III	-	-	-	-	-	-	-	-	-
IV	-0.18357	0.52964	0.71321	0.356605	0.178303	-0.17304	0.173035	-0.3130	0.940458
V	-0.82972	0.30877	1.13849	0.569245	0.284623	0.260475	-0.26048	-8.7785	0.373310
VI	-0.11052	0.7535	0.86402	0.43201	0.216005	-0.32149	0.32149	-0.1574	1.990090
VII	-0.22788	0.40487	0.63275	0.316375	0.158188	-0.0885	0.088495	-0.3753	0.896207

Table 17. ZINDO computed HOMO-LUMO energy gap and other related parameters for the pyrazolone compounds under study.

Compound	HOMO (eV)	LUMO (eV)	Energy gap	η	S	χ	μ	HOMO-1	LUMO+1
I	-2.1363	5.76735	7.90365	-3.95183	-1.97591	-1.81553	1.815525	-4.7794	6.105271
II	-6.7735	6.37815	13.15165	-6.57583	-3.28791	0.197675	-0.19768	-7.1571	6.717012
III	-4.50475	5.92903	10.43378	-5.21689	-2.60845	-0.71214	0.71214	-5.7590	6.713082
IV	-6.04917	6.5903	12.63947	-6.31974	-3.15987	-0.27057	0.270565	-6.4433	7.357150
V	-2.74208	5.254	7.99608	-3.99804	-1.99902	-1.25596	1.25596	-7.3538	6.434645
VI	-6.83592	6.31062	13.14654	-6.57327	-3.28664	0.26265	-0.26265	-7.2619	6.820849
VII	-4.57723	5.97715	10.55438	-5.27719	-2.6386	-0.69996	0.69996	-6.8254	6.979484

4. Conclusions

Semi-empirical studies using different AM1, PM3, MNDO and ZINDO were performed with the help of a computer software HYPERCHEM 8.0 professional version to compute the vibration frequency modes of selected pyrazolone compounds. This is also applied to draw theoretically simulated spectra. The computed results so obtained are presented and discussed in the relevant section of the paper. Results and discussion section of the present communication clearly shows that the computed normal modes frequency of vibrations on the basis of these methods viz. AM1, PM3, MNDO and ZINDO methods are in good agreement with experimental values. These are reported with appreciable correlation coefficient values. On the comparison of these

methods, this may be inferred that AM1 method is very good and provide reasonable results as compare to other one. The optimized molecular geometry of the pyrazolone compounds was also up to the mark and best with this AM1 method. HOMO-LUMO energy level gap and other related molecular descriptors on the basis of FMO approach are also computed, discussed and reported in this present paper.

The studies included in this present paper are less time consuming and provide reasonably good results. The methods may be considered as an alternative method of Studies so far as the study of chemistry of pyrazolones and related compounds is concern.

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