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Synthesis, Computational, FT- IR, NMR and UV-Vis Spectral Studies of Bioactive 2-(4-fluorophenyl)-4-(4-(4-methoxyphenyl)-5-(3-nitrophenyl)-4H-1,2,4-triazol-3-yl)quinoline

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SUPPLEMENTARY INFORMATION

Table S1 — Comparison of calculated and experimental optimized structural parameters for title compound using B3LYP/6-31G (d, p) method.

Bondlength	B3LYP	Exp	Bond Angle	B3LYP	Exp	Dihedral Angle	B3LYP	Exp
N1-N2	1.414	1.390(2)	N2-N1-C5	106.9562	113.45(16)	C5-N1-N2-C3	12.3621	0
N1-C5	1.3856	1.311(2)	N2-N1-H40	114.4923	118.6(16)	C5-N1-N2-H41	142.246	
N1-H40	1.024	0.88(3)	C5-N1-H40	114.8677	128(16)	H40-N1-N2-C3	140.825	
N2-C3	1.3906	1.299(3)	N1-N2-C3	107.2419	103.63(16)	H40-N1-N2-H41	-89.291	
N2-H41	1.0181		N1-N2-H41	113.3911		N2-N1-C5-N4	-10.787	0
C3-N4	1.3724	1.370(3)	C3-N2-H41	116.3857		N2-N1-C5-C20	167.438	
C3-N7	1.4399		N2-C3-N4	106.5591	110.99(17)	H40-N1-C5-N4	-139.03	
N4-C5	1.364	1.371(2)	N2-C3-C7	129.4464		H40-N1-C5-C20	39.1931	
N4-C26	1.4495		C3-C4-C5	110.574	108.65(17)	N1-N2-C3-C7	168.679	180
C5-C20	1.4399		C3-N4-C26	124.4725		H41-N2-C3-N4	-137.25	
C6-C26	1.3998	1.378(3)	N1-C5-N4	107.2149	103.28(16)	H41-N2-C3-C7	40.5093	
C6-C27	1.3855		N1-C5-C20	119.6781		N2-C3-N4-C5	2.4699	0
C6-H42	1.0852		C26-C6-C27	119.2223		N2-C3-N4-C26	-174.88	
C7-C8	1.4476	1.46	C26-C6-H42	120.4419		C7-C3-N4-C5	-175.13	180
C7-C12	2.395	1.398	C27-C6-H42	120.3356		C7-C3-N4-C26	7.5267	
C8-C9	1.4366	1.399	C3-C7-C12	120.0043		N2-C3-C7-C8	31.1294	
C8-C31	1.4175	1.399	C8-C7-C12	118.439	117.6	N2-C3-C7-C12	-143.98	
C9-N10	1.357	1.399	C7-C8-C9	115.8669	120	N4-C3-C7-C8	-151.65	
C9-C34	1.4212	1.401	C7-C8-C31	118.2919	120.5	N4-C3-C7-C12	33.24	
N10-C11	1.357	1.393	C8-C9-N10	123.6857	119.5	C3-N4-C5-N1	5.3004	
C11-C12	1.4212	1.432	C8-C9-C34	117.008	119.4	C3-N4-C5-C20	-172.59	
C12-H43	1.3288		N10-C9-C34	117.008	121.5	C26-N4-C5-N1	-177.34	
C13-C14	1.4174		C9-N10-C11	119.6596	122.9	C26-N4-C5-C20	4.7706	
C14-C15	1.0801		N10-C11-C12	121.4282	117.5	C3-N4-C5-N1	-112.75	0
C14-H44	1.4063		N10-C11-C13	117.4248		C3-N4-C26-C30	67.8167	
C15-C16	1.3898		C12-C11-C13	121.113		C5-N4-C26-C6	70.2645	
C16-C17	1.0835		C7-C12-C11	120.8433	122.6	C5-N4-C26-C30	-109.17	
C16-F19	1.392		C7-C12-H43	119.0309		N1-C5-C20-C21	-158.4	
C17-C18	1.3908		C11-C12-H43	119.0309		N1-C5-C20-C25	14.8343	
C17-H46	1.3429		C11-C12-H43	119.0309		N4-C5-C20-C21	19.2812	
C18-H47	1.392		C11-C13-C14	119.443		C27-C6-C26-N4	-179.22	
C20-C21	1.4019		C11-C13-C18	122.0127		C27-C6-C26-C30	0.2025	
C20-C25	1.4207		C14-C13-C18	118.5403		H42-C6-C26-N4	0.6269	

C21-C22	1.4028		C13-C14-C15	121.0479		H42-C6-C26-C30	-179.95	
C21-H48	1.08		C13-C14-H44	118.676		C26-C6-C27-C28	-0.0599	
C22-C23	1.4212		C15-C14-H44	120.2761		C26-C6-C27-H52	179.737	
C22-N35	1.385		C14-C15-C16	118.7581		H42-C6-C27-C28	-179.91	
C23-C24	1.3842		C14-C15-H45	121.649		H42-C6-C27-H52	-0.1109	
C23-H49	1.0804		C16-C15-H45	119.611		C3-C7-C8-C9	-172.93	
C24-C25	1.3994		C15-C16-C17	121.8962		C3-C7-C8-C31	8.8773	
C24-H50	1.0804		C15-C16-F19	119.1611		C12-C7-C8-C9	2.2618	1.7
C25-H51	1.30832		C17-C16-F19	118.9423		C12-C7-C8-C31	-175.94	
C26-C30	1.3921		C16-C17-H46	121.7437		C3-C7-C12-C11	174.982	
C27-C28	1.4099		C18-C17-H46	121.0636		C3-C7-C12-H43	-0.5127	
C27-H52	1.0841		C13-C18-C17	120.5584		C8-C7-C12-C11	-0.2735	0.9
C28-C29	1.4033		C13-C18-H47	118.3544		C8-C7-C12-H43	-175.77	
C28-O38	1.3449	1.359(2)	C17-C18-H47	118.7616		C7-C8-C9-N10	-2.1755	-1.6
C29-C30	1.3939		C5-C20-C25	119.7192		C7-C8-C9-C34	178.962	179
C29-H53	1.0823		C21-C20-C25	119.4598		C31-C8-C9-N10	176.164	177
C30-H54	1.0851		C20-C21-H48	122.4414		C31-C8-C9-C34	-2.6986	-2.4
C31-C32	1.3808	1.381	C22-C21-H48	118.0733		C7-C8-C31-C32	-179.86	180
C31-H55	1.0835	0.93	C21-C22-N35	115.6304		C7-C8-C31-H55	1.3759	
C32-C33	1.4125	1.392	C23-C22-N35	122.854		C9-C8-C31-C32	1.9857	
C32-H56	1.0854	0.93	C22-C23-C24	117.7043		C9-C8-C31-H55	-176.78	1
C33-C34	1.3751	1.376	C22-C23-H49	120.5312		C8-C9-N10-C11	-0.1365	-1.2
C33-H57	1.0852	0.93	C24-C23-H49	121.7643		C34-C9-N10-C11	178.75	178
C34-H58	1.0843	0.93	C23-C24-C25	122.4141		C8-C9-C34-C33	1.4791	1.4
N35-O36	1.2442		C23-C24-H50	118.7712		C8-C9-C34-H58	-179.42	
N35-O37	1.3844		C25-C24-H50	118.8143		N10-C9-C34-C33	-177.46	
O37-H59	0.9761		C20-C25-C24	119.1852		N10-C9-C34-H56	1.6393	3.7
O38-C39	1.4306	1.426(2)	C20-C25-H51	120.6087		C9-N10-C11-C12	2.3584	
C30-H60	1.0891		C24-C25-H51	120.0741		C9-CN10-C11-C13	-17974	-3.6
C39-H61	1.0954		N4-C26-C6	119.3776		N10-C11-C12-C7	-2.1693	
C39-H62	1.0955		N4-C26-C30	119.4477		N10-C11-C12-H43	173.368	
			C6-C26-C30	121.1722		C13-C11-C12-C7	-179.99	
			C6-C27-C28	120.4137		C13-C11-C12-H43	-4.4566	
			C6-C27-H52	118.4906		N10-C11-C13-C14	-18.351	
			C28-C27-H52	11804906		N10-C11-C13-C18	161.046	
			C27-C28-C29	119.6665		C12-C11-C13-C14	159.517	
			C27-C28-O38	115.5054		C12-C11-C14-C15	-21.045	
			C28-C29-C30	124.8281		C11-C13-C14-C15	-179.83	
			C28-C29-H53	119.844		C11-C13-C14-H44	0.0957	
			C30-C29-H53	121.0017		C18-C13-C14-C15	0.7497	
			C26-C30-C29	119.1534		C18-C13-C14-H44	-179.32	
			C26-C30-H54	119.6806		C11-C13-C18-C17	-179.97	
			C29-C30-H54	120.3388		C11-C13-C18-H47	-1.7699	
			C8-C31-C32	119.9807	120.7	C14-C13-C18-C17	-0.5711	
			C8-C31-C32	120.8453	119.7	C14-C13-C18-H47	177.633	
			C8-C31-H55	120.1979	119.7	C13-C14-C15-C16	-0.3546	
			C32-C31-H55	118.9456	119.4	C13-C14-C15-H45	179.494	
			C31-C32-C33	120.7736	120.3	H44-C14-C15-C16	179.719	
			C31-C32-H56	119.5124	119.7	H44-C14-C15-H45	-0.4327	
			C33-C32-H56	119.7127	119.7	C14-C15-C16-C17	-0.2388	
			C32-C33-C34	119.8954	119.4	C14-C15-C19-H45	-179.99	
			C32-C33-H57	119.817	119.7	H45-C15-C16-C17	-179.91	
			C34-C33-H57	120.2819	119.7	H45-C15-C16-C19	0.1573	
			C9-C34-C33	120.8416	120.2	C15-C16-C17-C18	0.412	
			C9-C34-H58	117.1089	119.8	C15-C16-C17-H46	-179.06	
			C33-C31-H58	122.0431	119.8	C19-C16-C17-C18	-179.84	
			C22-C35-O36	127.7597		C19-C16-C17-H46	0.698	
			C22-C35-O37	113.9861		C16-C17-C18-C13	0.0043	
			O36-C35-O37	118.2501		C16-C17-C18-H47	-178.24	
			C35-O37-H59	102.3091		H46-C17-C18-C13	179.459	
			C28-038-C39	119.2492	117.94(14)	H46-C17-C18-H47	1.2162	

038-C39-H60	105.837	C5-C20-C21-C22	173.254
038-C39-H61	11.1037	C5-C20-C21-H48	-4.8703
038-C31-H62	111.1371	C25-C20-C21-C22	0.0862
H60-C39-H61	109.5068	C25-C20-C21-H48	-178.04
H61-C39-H62	109.9377	C5-C20-C25-C24	-173.8
		C5-C20-C25-H51	10.3724
		C21-C20-C25-C24	-0.0468
		C21-C20-C25-H51	-176.29
		C20-C21-C22-C23	0.1597
		C20-C21-C22-C35	-179.53
		H48-C21-C22-C23	178.366
		H48-C21-C22-C35	-1.3209
		C21-C22-C23-C24	-0.0171
		C21-C22-C23-H49	-179.87
		C35-C22-C23-C24	179.647
		C35-C22-C23-H49	-0.2071
		C21-C22-C35-C36	0.5809
		C21-C22-C35-C37	-178.66
		C23-C22-C35-C37	11.6577
		C22-C23-C24-C25	-0.3846
		C22-C23-C24-H50	179.385
		H49-C23-C24-C25	179.467
		H49-C23-C24-H50	-0.7629
		C23-C24-C25-H51	176.48
		H50-C24-C25-C20	-179.14
		H50-C21-C25-H51	-3.2901
		N4-C26-C30-C29	179.332
		N4-C26-C30-H54	-0.611
		C6-C26-C30-C29	-0.0906
		C6-C26-C30-H54	179.967
		C6-C27-C28-C29	-0.19
		C6-C27-C28-O38	179.857
		H52-C27-C28-C29	-179.99
		H52-C27-C28-O38	0.0548
		C27-C28-C29-C30	0.3018
		C27-C28-C29-H53	179.753
		O38-C28-C29-C30	-179.75
		O38-C28-C29-H53	-0.0984
		C27-C28-038-C39	-179.54
		C29-C28-O38-C39	0.5136
		C28-C29-C30-C26	-0.163
		C28-C29-C30-H54	179.78
		H53-C29-C30-C26	-179.82
		H53-C29-C30-H54	0.1225
		C8-C31-C32-C33	-0.0061
		C8-C31-C32-H56	-179.6
		H55-C31-C32-C33	178.777
		H55-C31-C32-H56	-0.8207
		C31-C32-C33-C34	-1.2905
		C31-C32-C33-H57	179.573
		H56-C32-C33-C34	178.307
		H56-C32-C33-H57	-0.8302
		C32-C33-C34-H58	-178.53
		H57-C33-C34-C9	179.658
		H57-C33-C34-H58	0.6052
		C22-C35-C37-H59	179.407
		C36-C35-C37-H59	0.0887
		C28-C38-C39-H60	179.655
		C28-C38-C39-H61	61.0207
		C28-C38-C39-H62	-61.738

Table S2 — Dipole Moment μ, Polarizability α_{tot} ($^{x}10^{-24}$esu) and first order static hyperpolarizability β_{tot} (10^{-30}) data for compound

Dipole moment	B3LYP 6-31G (d,p)	Hyperpolarisability	B3LYP 6-31G (d,p)
μx	-7.6149	βxxx	0.000011
μy	4.2497	βxxy	0.003829
μz	0.9465	βxyy	-0.000208
μ	8.7693	βyyy	0.008068
polarisability			
αxx	0.09976	βxxz	0.000188
αxy	0.00123	βxyz	0.0037104
αyy	0.005325	βyyz	0.0080685
αxz	0.03421	βxzz	-0.001808
αyz	-0.17031	βyzz	-0.01268
αzz	0.002384	βzzz	0.093324
(α)	0.005723	βtotal	0.0087225

Table S3 — Calculated thermodynamic parameters of studied compound

Parameters	B3LYP 6-31 G (d,p)
Zero point vibrational energy(Kcal/mol)	299.5984
Rotational Temperature (K)	
	0.00577
	0.00295
	0.00217
Rotational Constant (GHZ)	
X	0.12033
Y	0.06143
Z	0.04528
Total Energy (E^{total}) (Kcal/mol)	319.719
Translational	0.889
Rotational	0.889
Vibrational	317.941

Table S4 — Thermodynamic functions at different temperatures at the B3LYP/6-31-G(d,p) level

Temp (T) (K)	Heat capacity (CV) (cal/mol K) B3LYP	Entropy (S) (cal/mol K) G-31G(d-p)
100	48.339	118.512
200	78.64	139.105
298.15	126.97	208.068
300	127.37	208.868
400	165.35	251.469
500	196.921	292.329
600	222.171	330.914

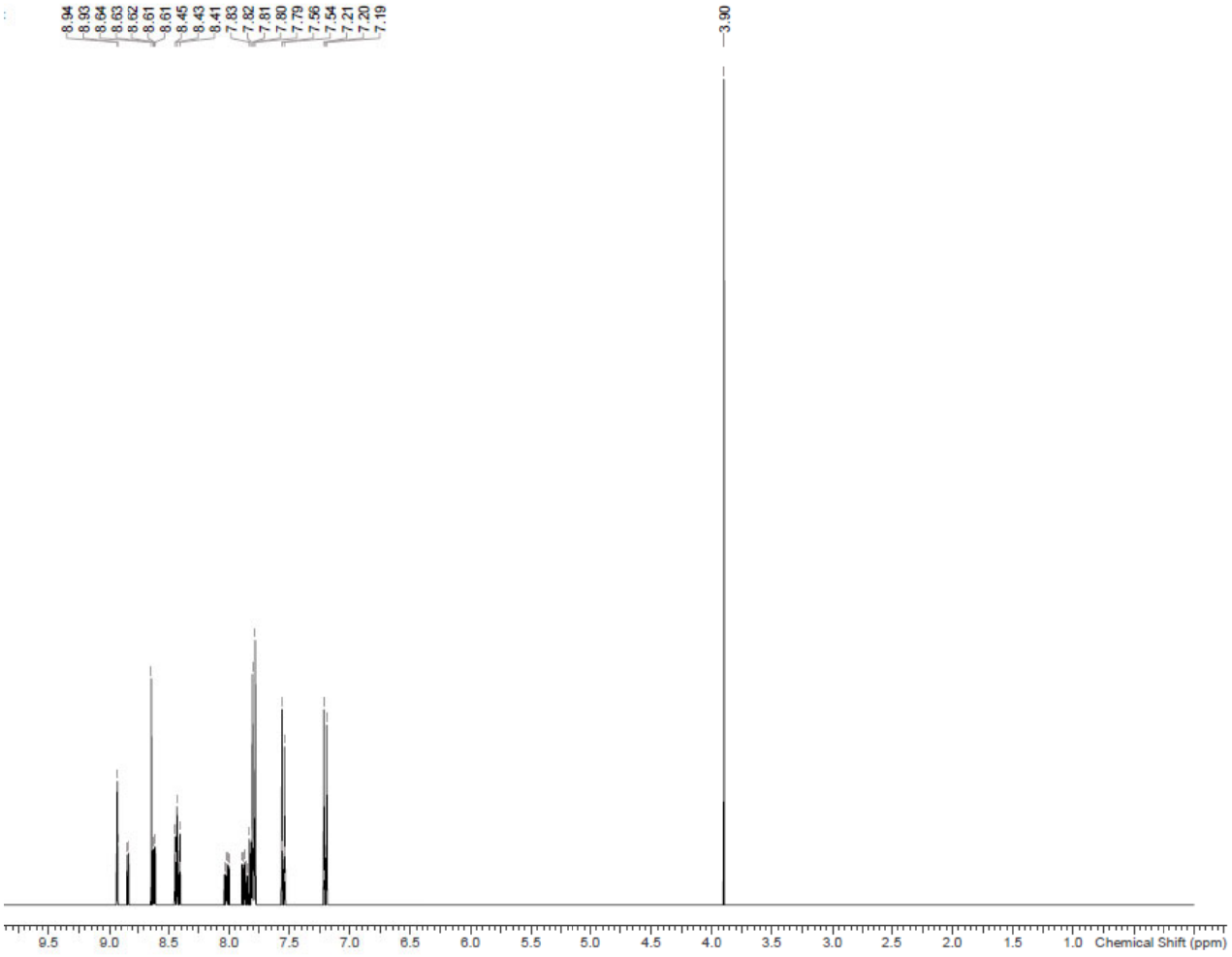

Fig. S1 Experimental ^{1}H-NMR spectra of compound 3

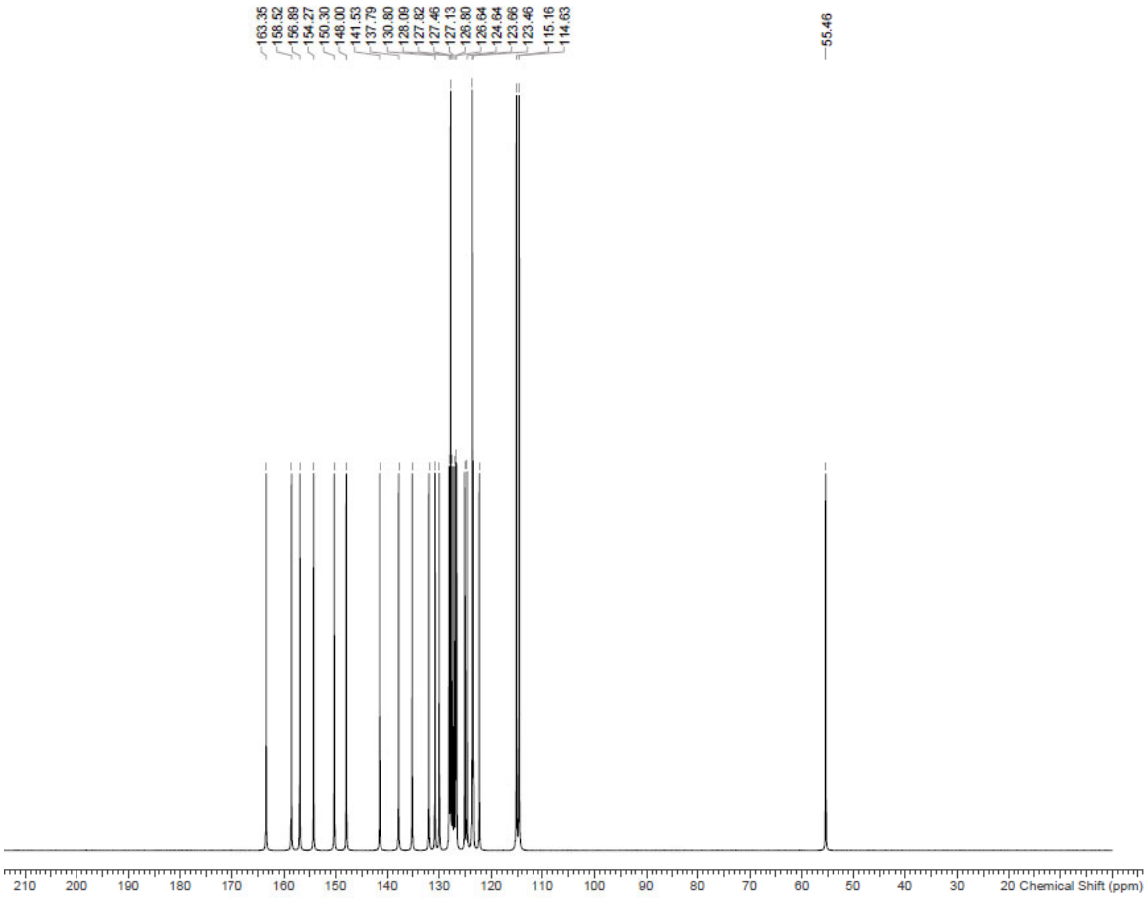

Fig. S2 Experimental ^{13}C-NMR spectra of compound 3

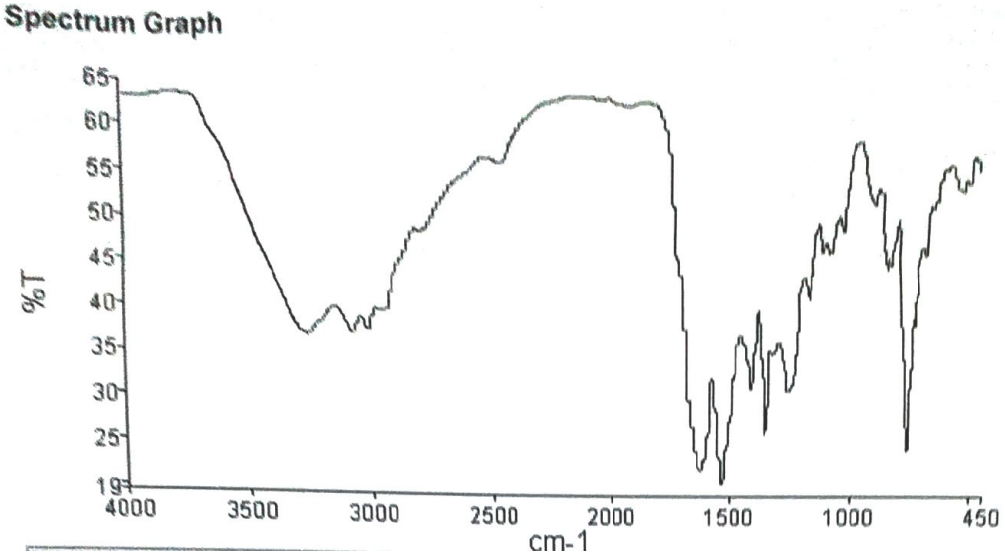

Fig. S3 Experimental FT-IR spectra of compound 3

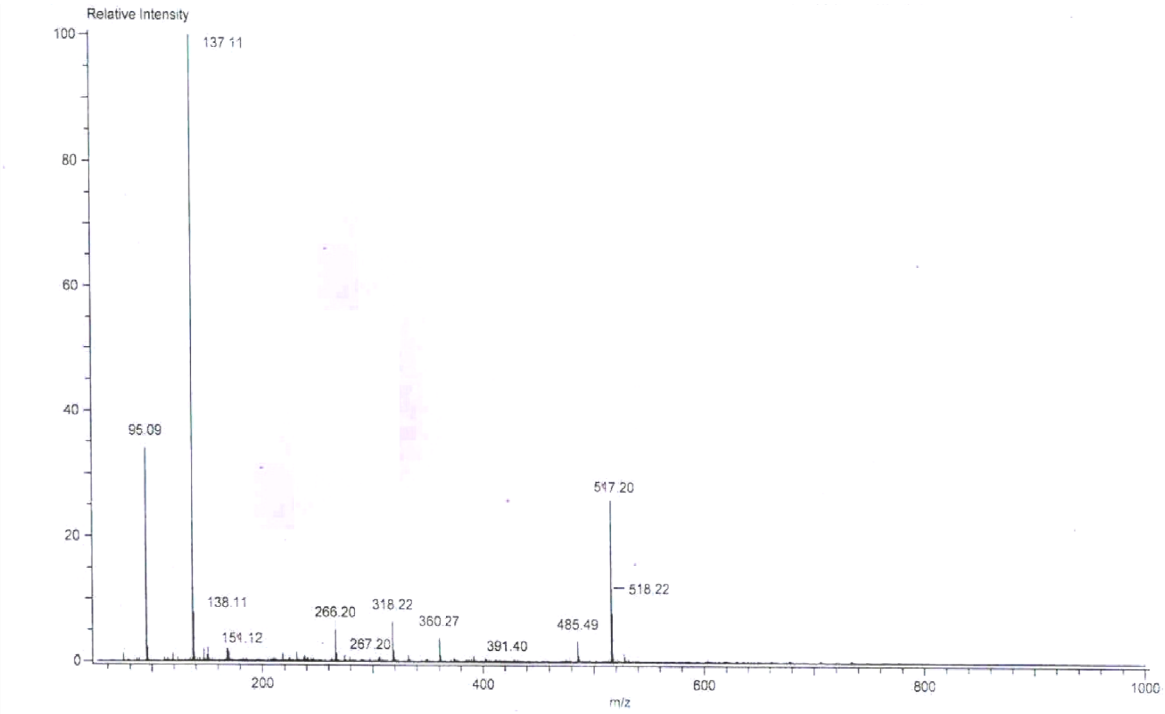

Fig. S4 Mass spectra of title compound