Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

for

Polymorphic Study and Anti-inflammatory Activity of 3-Cyano-2-pyridone Based Flexible Model

Sunil K. Rai, Praveen Singh, Shaziya Khanam and Ashish K. Tewari*

Department of Chemistry (Center of Advanced Study), Institute of Science, Banaras Hindu University, Varanasi 221005, India

E-mail: tashish2002@yahoo.com

Contents

1. Copies of NMR

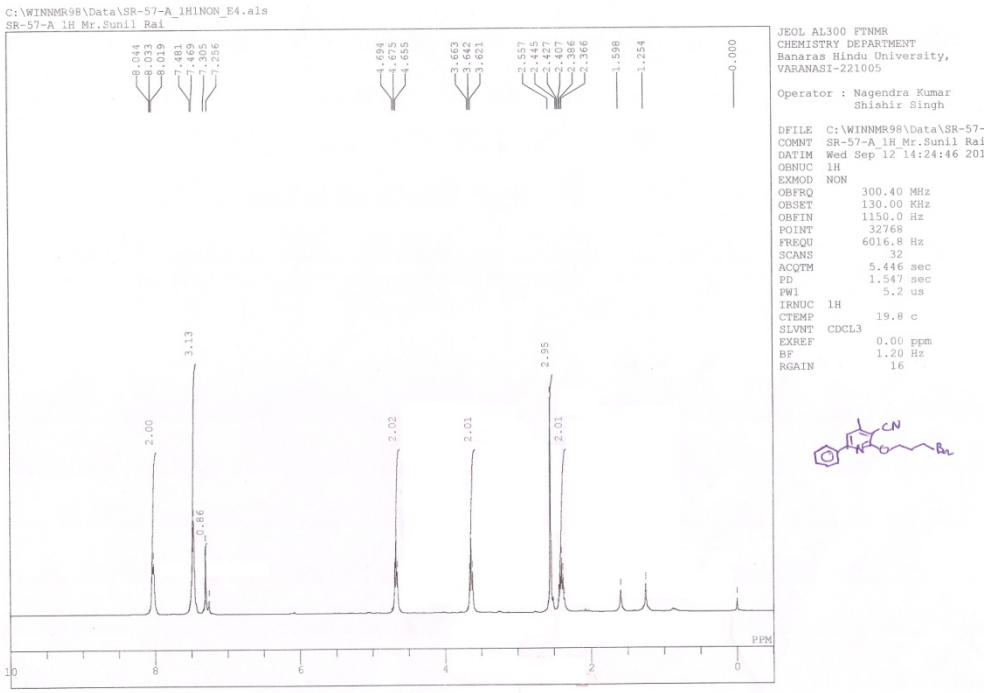


Figure S1. ^{1}H NMR of compound **1** in $CDCl_3$.

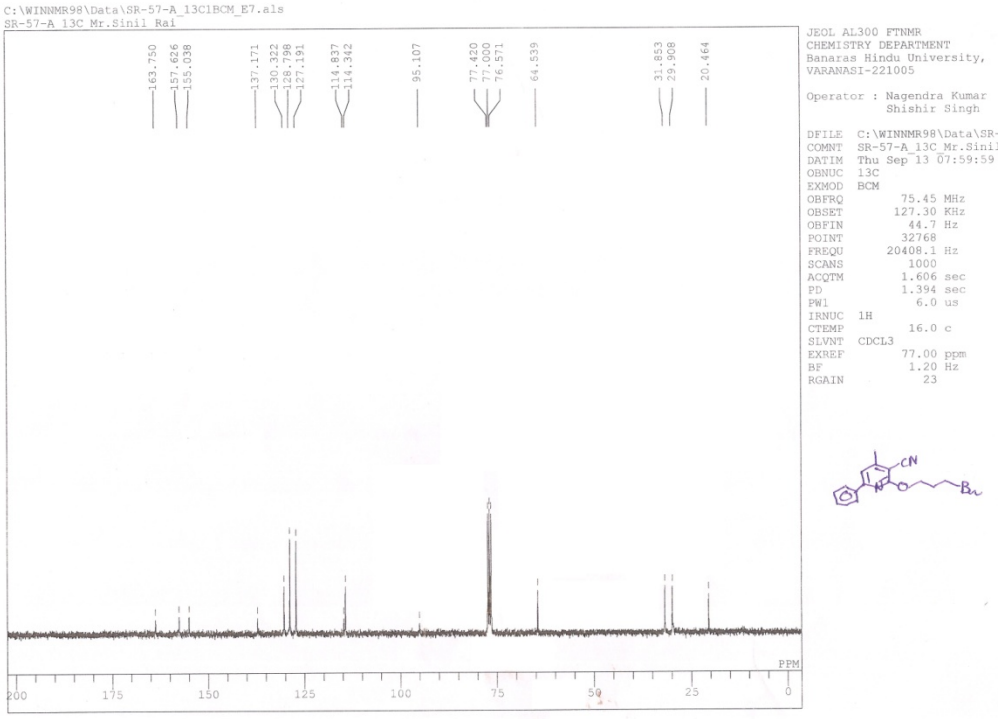


Figure S2. ^{13}C NMR of compound **1** in $CDCl_3$.

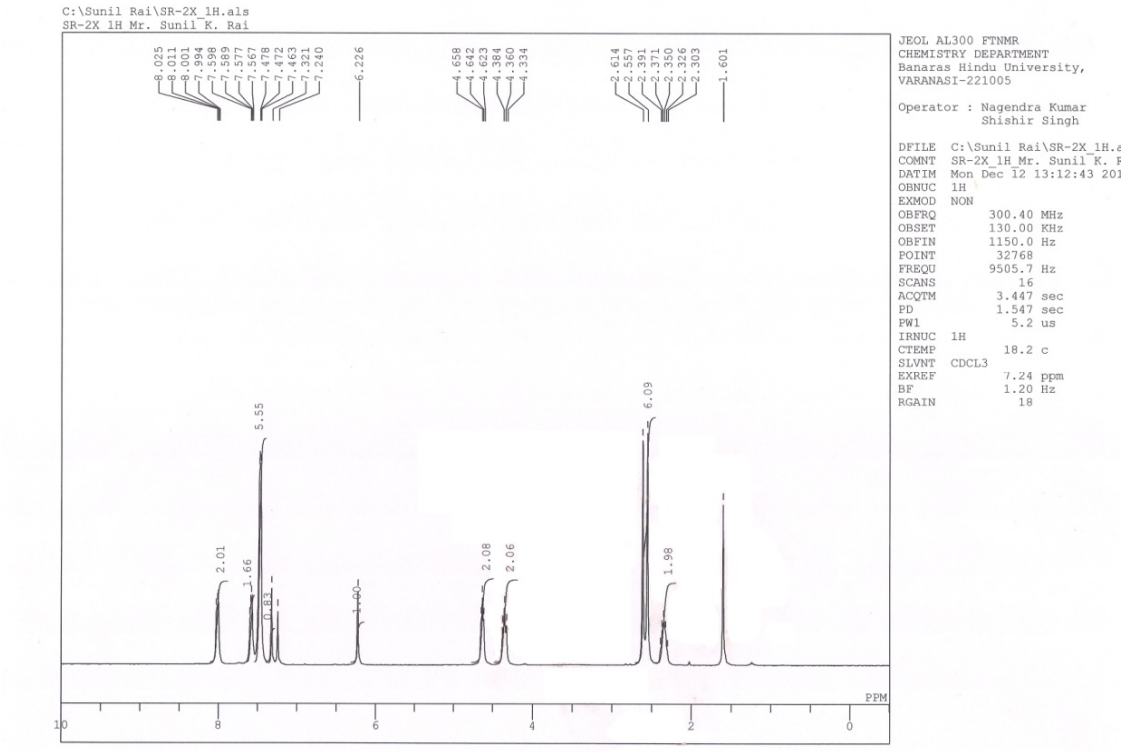


Figure S3. ^{1}H NMR of compound **2** in $CDCl_3$.

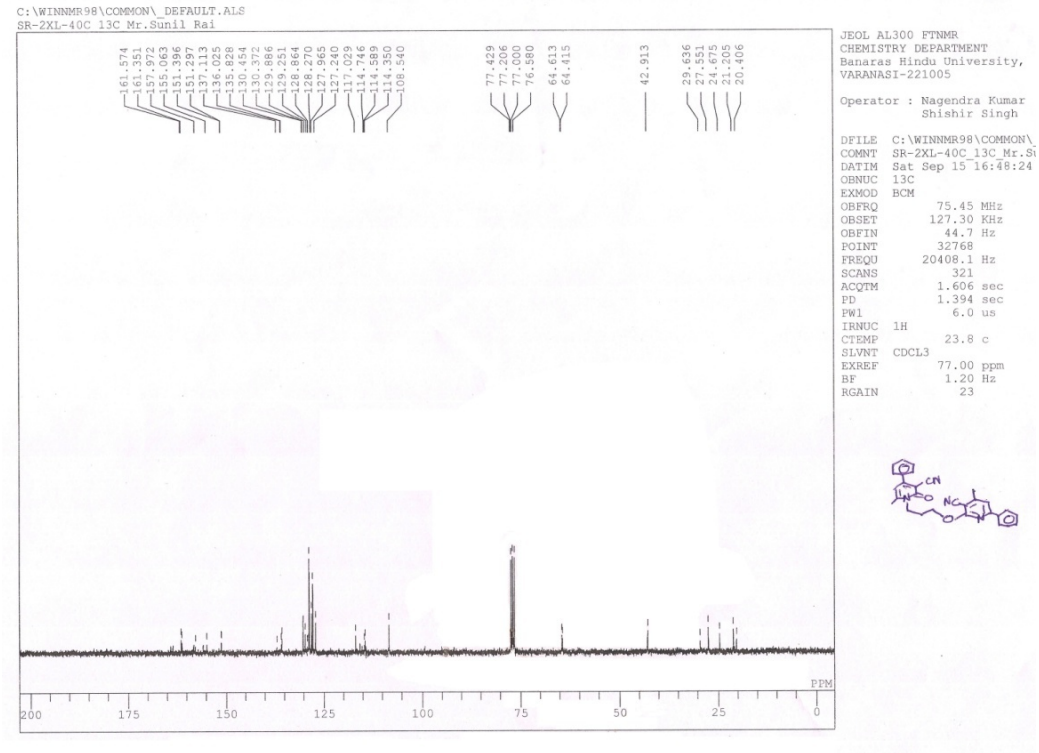
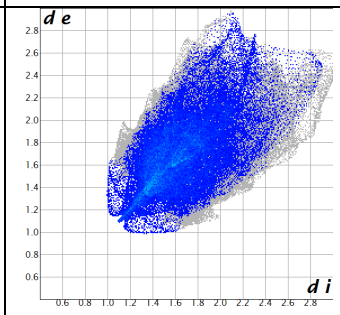
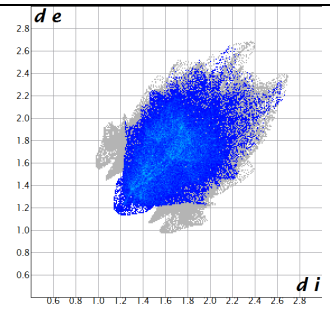
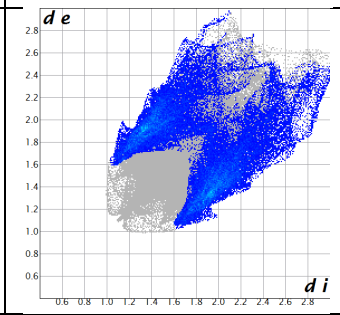
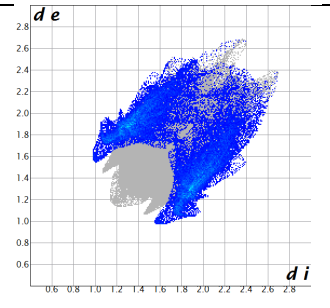
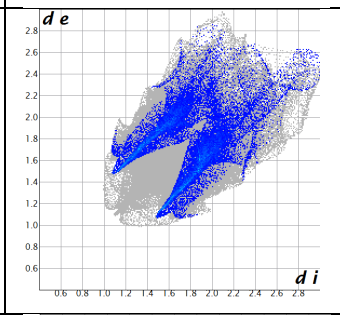
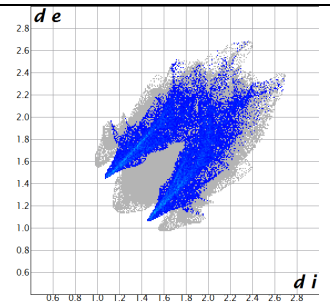
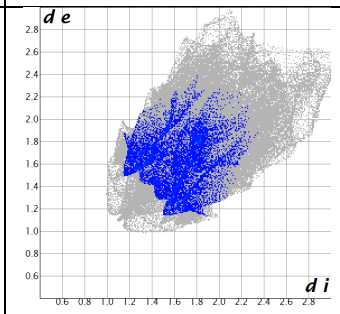
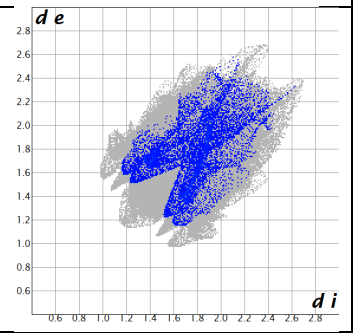


Figure S4. ^{13}C NMR of compound **2** in $CDCl_3$.

2. Hirsfeld Surface Analysis.

Table S1. Decomposed fingerprints showing area of various interactions in form-I and II.

Interaction Type	Form-I	Form-II
H···H		
C···H		
N···H		
O···H		

3. Computational details

Table S2. Single point energy and optimized structure energy of form-I and II calculated at the B3LYP/6-31G (d, p) and ωB97X-D/6-311G (d, p) level of theory.

Compound name	B3LYP (kcal/mol)	ωB97X-D (kcal/mol)
Form-I (sp)	-934135.20	-934030.62
Form-I (op)	-934391.63	-934274.95
Form-II (sp)	-934125.47	-934019.71
Form-II (op)	-934391.63	-934274.95

Last Standard Orientation of Form-I optimized at ωB97X-D/6-311G(d,p) level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.178008	2.817987	0.563741
2	1	0	-0.821486	1.702573	0.771732
3	1	0	-1.232998	2.294368	-0.827729
4	8	0	1.793669	0.348943	0.334735
5	7	0	4.026675	-0.159331	0.226482
6	6	0	3.059809	0.728060	0.169229
7	7	0	-2.135559	-0.384845	-0.456734
8	8	0	-2.444527	-2.597804	-0.903559
9	6	0	3.273746	2.100865	-0.060871
10	6	0	5.291455	0.258253	0.062003
11	6	0	5.597930	1.594033	-0.185828
12	1	0	6.621723	1.897536	-0.358930
13	6	0	2.159733	2.987638	-0.124554
14	6	0	-2.947460	-1.529416	-0.610883
15	6	0	-4.864279	-0.080420	-0.023579
16	6	0	-4.368816	-1.307488	-0.406059
17	6	0	4.584208	2.544418	-0.248033
18	6	0	6.341127	-0.787280	0.136998
19	6	0	-2.618568	0.830427	-0.061591
20	6	0	1.494761	-1.048888	0.459190
21	1	0	1.996613	-1.453721	1.340003
22	1	0	1.873819	-1.575987	-0.421527
23	6	0	-0.011053	-1.143884	0.573743
24	1	0	-0.299839	-2.185905	0.726896
25	1	0	-0.333839	-0.577767	1.452984
26	6	0	-0.705870	-0.604885	-0.677893
27	1	0	-0.252417	0.331499	-0.992177
28	1	0	-0.616003	-1.327147	-1.488643
29	6	0	-6.307986	0.169755	0.206813
30	6	0	-3.957797	0.991213	0.154045

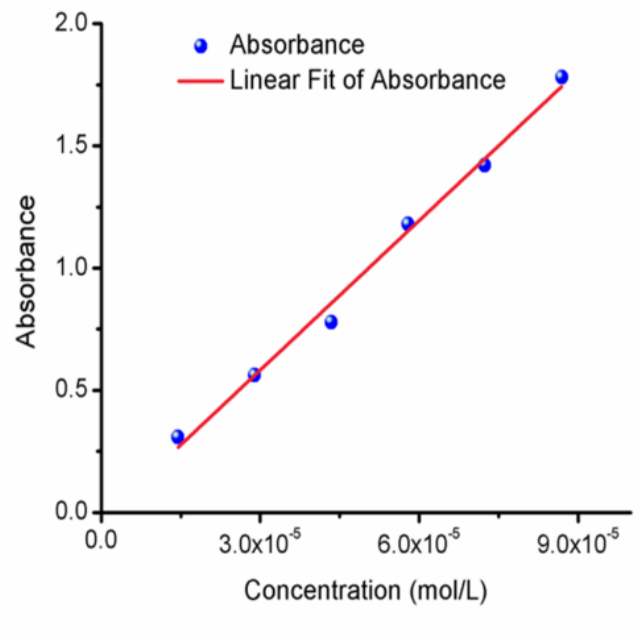
31	1	0	-4.324880	1.950492	0.490497
32	7	0	1.263263	3.709318	-0.187005
33	6	0	-6.910718	1.288877	-0.371744
34	1	0	-6.324429	1.943705	-1.007154
35	6	0	-5.207653	-2.436989	-0.646817
36	6	0	-1.659646	1.967603	0.124170
37	6	0	4.873393	3.990915	-0.519699
38	1	0	5.941034	4.158629	-0.660583
39	1	0	4.527755	4.613780	0.309553
40	1	0	4.345177	4.327794	-1.415397
41	6	0	-7.074198	-0.675574	1.009611
42	1	0	-6.618361	-1.544001	1.469271
43	6	0	-8.256914	1.550017	-0.161950
44	1	0	-8.716606	2.413693	-0.628390
45	6	0	-9.012814	0.704566	0.640997
46	1	0	-10.064345	0.908389	0.807359
47	6	0	6.005961	-2.119223	-0.115838
48	1	0	4.977089	-2.360876	-0.350647
49	6	0	-8.417671	-0.405240	1.227682
50	1	0	-9.001915	-1.067299	1.855846
51	6	0	6.974089	-3.110407	-0.066830
52	1	0	6.702287	-4.139201	-0.273090
53	7	0	-5.888323	-3.346211	-0.838496
54	6	0	8.289621	-2.788091	0.246320
55	1	0	9.045907	-3.563468	0.286596
56	6	0	7.663344	-0.474270	0.459836
57	1	0	7.940646	0.546373	0.696939
58	6	0	8.630033	-1.468077	0.514875
59	1	0	9.650955	-1.212126	0.773653

Last Standard Orientation of Form-II optimized at ωB97X-D/6-311G(d,p) level of theory.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.177082	2.817423	0.562567
2	1	0	-0.820844	1.701706	0.770465
3	1	0	-1.232577	2.293282	-0.828993
4	7	0	4.026699	-0.159269	0.225856
5	8	0	1.793515	0.348498	0.333266
6	7	0	-2.135660	-0.385728	-0.457066
7	6	0	-4.864206	-0.080476	-0.023494
8	6	0	3.059693	0.727937	0.168565
9	6	0	-6.307813	0.170185	0.206939
10	6	0	3.273490	2.100875	-0.060880
11	6	0	-2.947856	-1.530185	-0.610564
12	6	0	5.291510	0.258542	0.062062
13	8	0	-2.445180	-2.598803	-0.902854

14	6	0	6.341258	-0.786924	0.137115
15	6	0	4.583959	2.544674	-0.247341
16	6	0	-3.957451	0.991002	0.153468
17	1	0	-4.324229	1.950493	0.489640
18	6	0	-2.618295	0.829787	-0.062266
19	6	0	5.597820	1.594460	-0.185144
20	1	0	6.621568	1.898304	-0.357844
21	6	0	6.006108	-2.118960	-0.115245
22	1	0	4.977208	-2.360698	-0.349773
23	6	0	1.494990	-1.049395	0.457807
24	1	0	1.997110	-1.454144	1.338506
25	1	0	1.873980	-1.576401	-0.422973
26	6	0	2.159443	2.987601	-0.124478
27	6	0	-4.369094	-1.307846	-0.405515
28	6	0	-0.706105	-0.606174	-0.678789
29	1	0	-0.252603	0.329987	-0.993632
30	1	0	-0.616810	-1.328754	-1.489305
31	6	0	8.289843	-2.787656	0.246616
32	1	0	9.046144	-3.563001	0.287041
33	6	0	-6.910318	1.289212	-0.372016
34	1	0	-6.323930	1.943635	-1.007730
35	6	0	-5.208252	-2.437249	-0.645624
36	6	0	-7.074162	-0.674574	1.010174
37	1	0	-6.618507	-1.542917	1.470161
38	6	0	7.663545	-0.473805	0.459501
39	1	0	7.940980	0.546881	0.696178
40	6	0	-0.010746	-1.144874	0.572680
41	1	0	-0.333509	-0.578835	1.451951
42	1	0	-0.299142	-2.186985	0.725984
43	7	0	-5.889166	-3.346351	-0.836975
44	6	0	6.974263	-3.110093	-0.066129
45	1	0	6.702451	-4.138943	-0.272053
46	6	0	8.630271	-1.467561	0.514638
47	1	0	9.651248	-1.211485	0.773052
48	6	0	-8.256423	1.550768	-0.162218
49	1	0	-8.715940	2.414367	-0.628961
50	6	0	-1.659072	1.966806	0.123047
51	6	0	-8.417550	-0.403844	1.228223
52	1	0	-9.001919	-1.065517	1.856666
53	6	0	4.873035	3.991343	-0.518243
54	1	0	5.940661	4.159171	-0.659045
55	1	0	4.527387	4.613691	0.311367
56	1	0	4.344786	4.328652	-1.413735
57	7	0	1.263033	3.709357	-0.186716
58	6	0	-9.012468	0.705841	0.641116
59	1	0	-10.063942	0.909956	0.807436

4. Solubility Experiment:



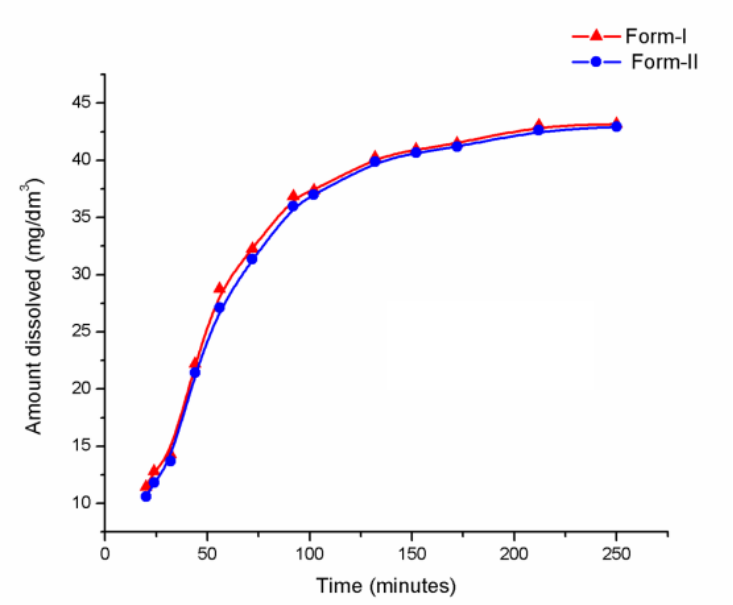


Figure S5. Linear fit of absorbance of compound **2** has been drawn at correlation coefficient R^2 = 0.99 which shows extension coefficient 20393 $M^{-1}cm^{-1}$ (upper). Solubility profile of form I and II in 50% MeOH-water mixture (lower).