Supporting Information

Selective induced polarization through electron transfer in acetone and pyrazole ester derivatives via C-H···O=C interaction

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Content

Figure S1. Interaction energy vs C-H...O distances in vacuum

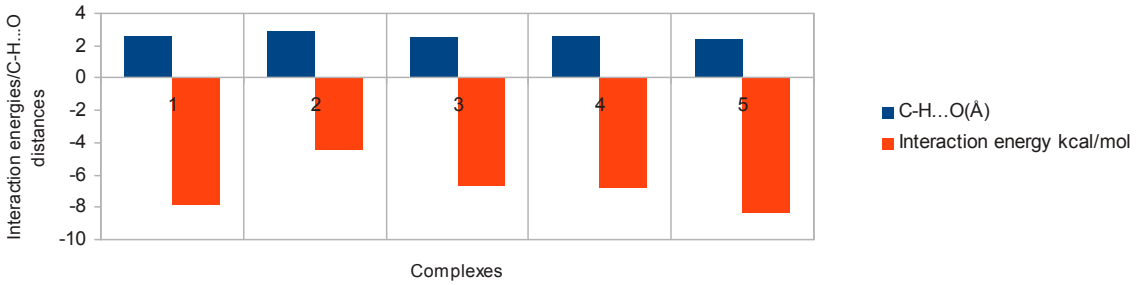


Figure S2. Interaction energy vs C-H stretching frequency shift in vacuum

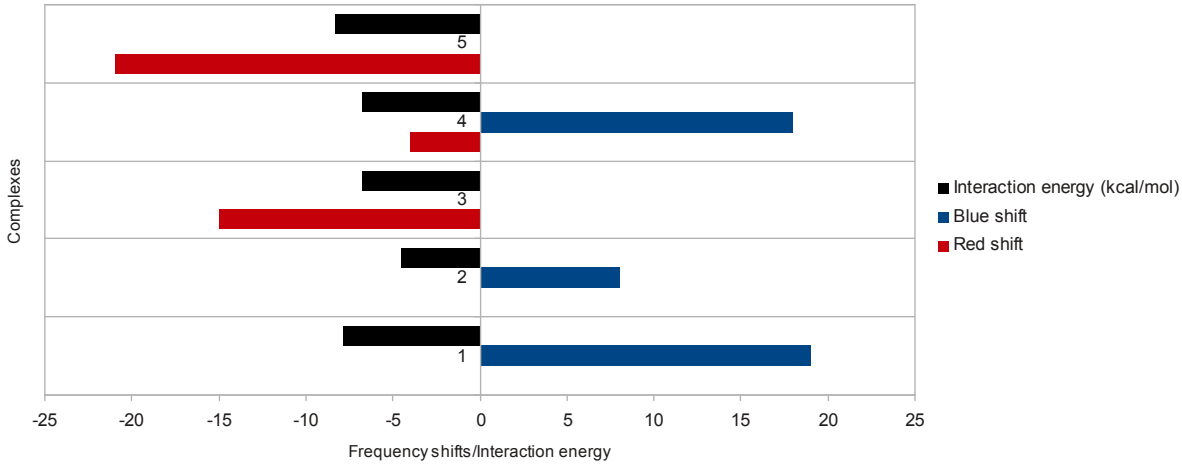
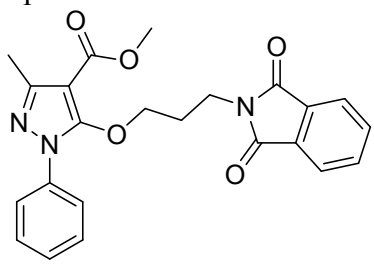


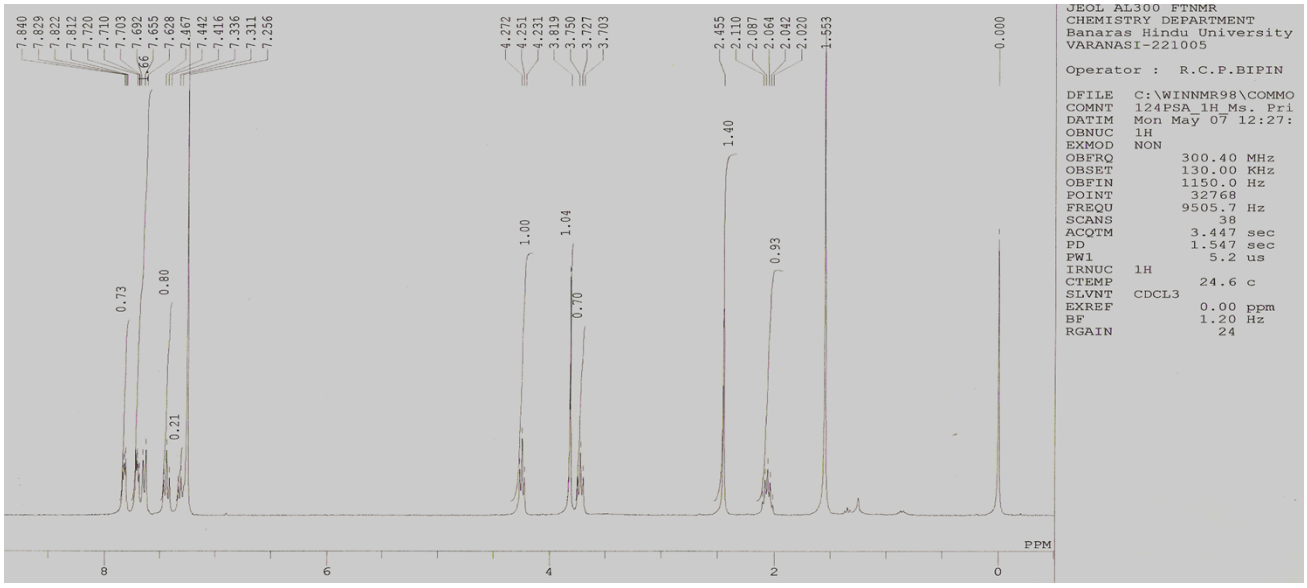
Table S1. ΔC-H distance and stretching frequencies (ν C-H) Vs Interaction Energy (ΔE) (In Vacuum)

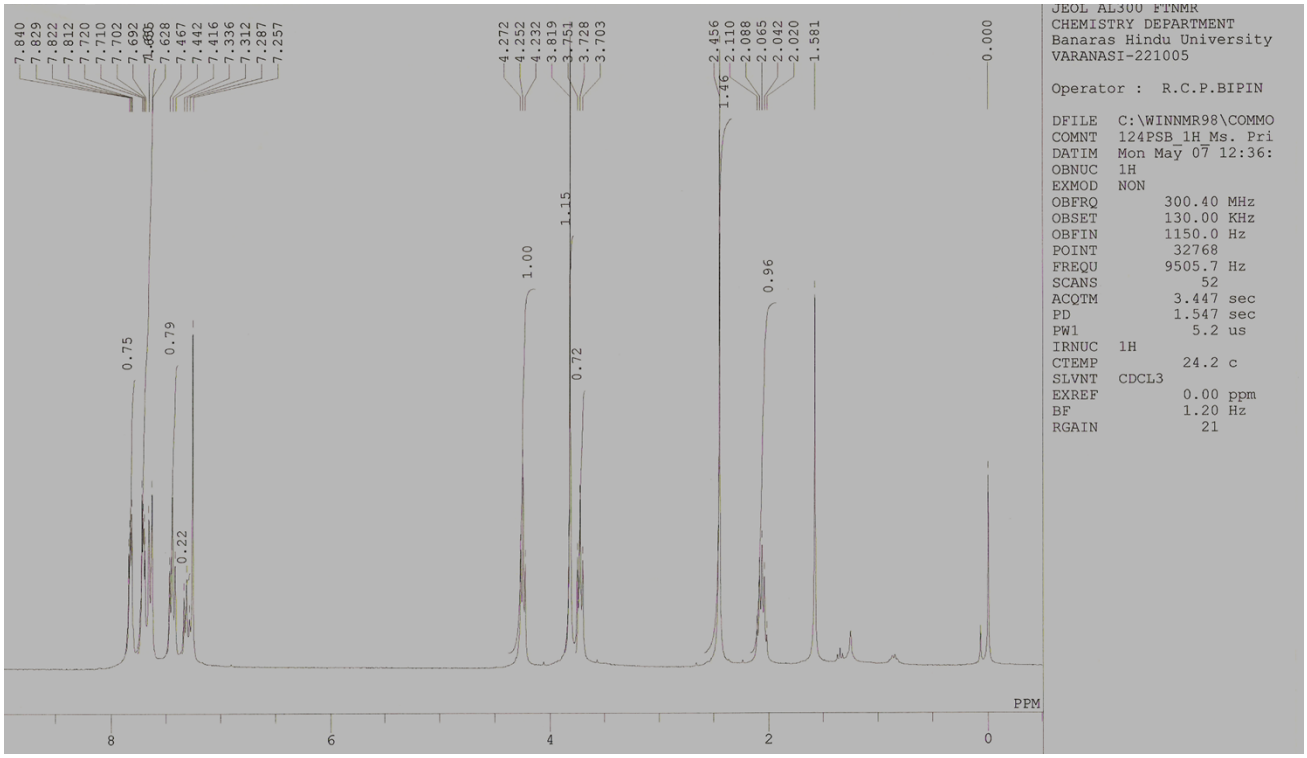
Compound No.	ΔC-H_1 (Å)	ΔC-H_2 (Å)	ΔC-H_3 (Å)	νC-H cm^{-1}	ΔE kcal/mol
1	0.001	-0.001	0.000	+19a	-7.8640
2	-0.001	0.001	0.001	+8s	-4.5058
3	-0.001	0.001	0.000	-15a	-6.7296
4	0.000	-0.001	0.000	-4a, +18a	-6.7600
5	0.003	0.000	0.000	-21a	-8.3693

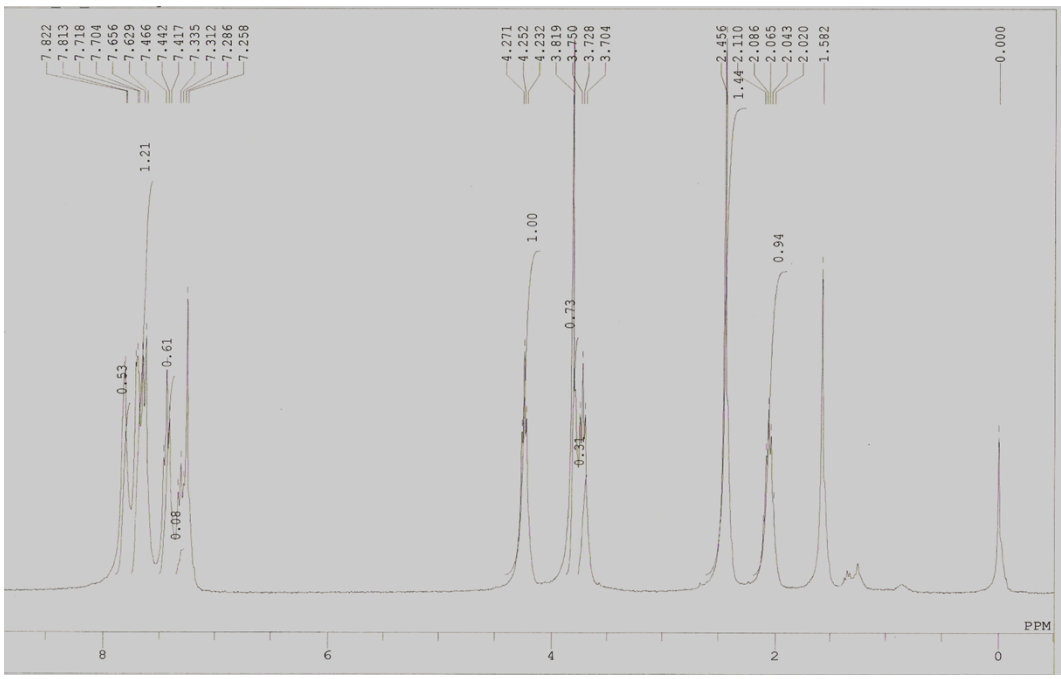
s = symmetry; a= asymmetry; '+' = blue shift; '-'= red shift

S3. ^{1}H NMR titration spectra of compound **1**









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CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

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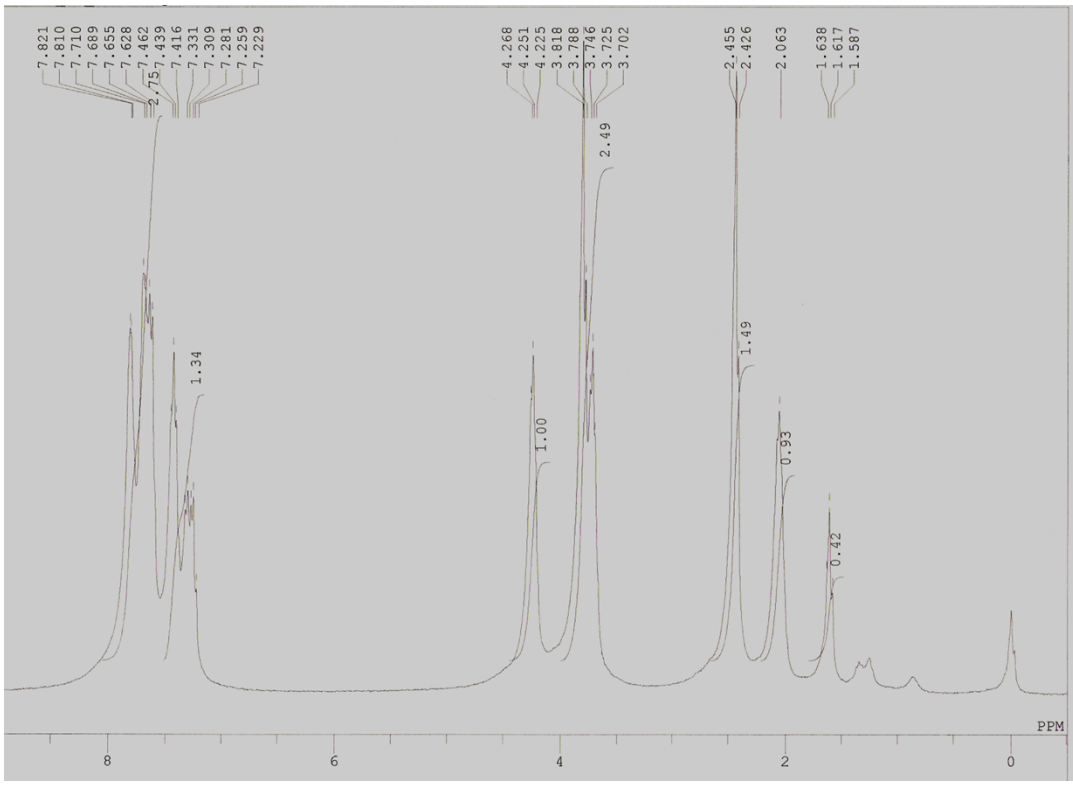

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

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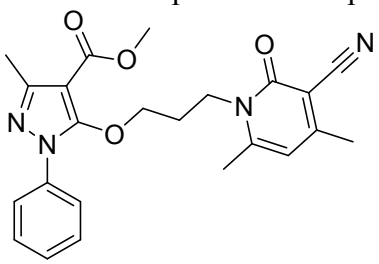
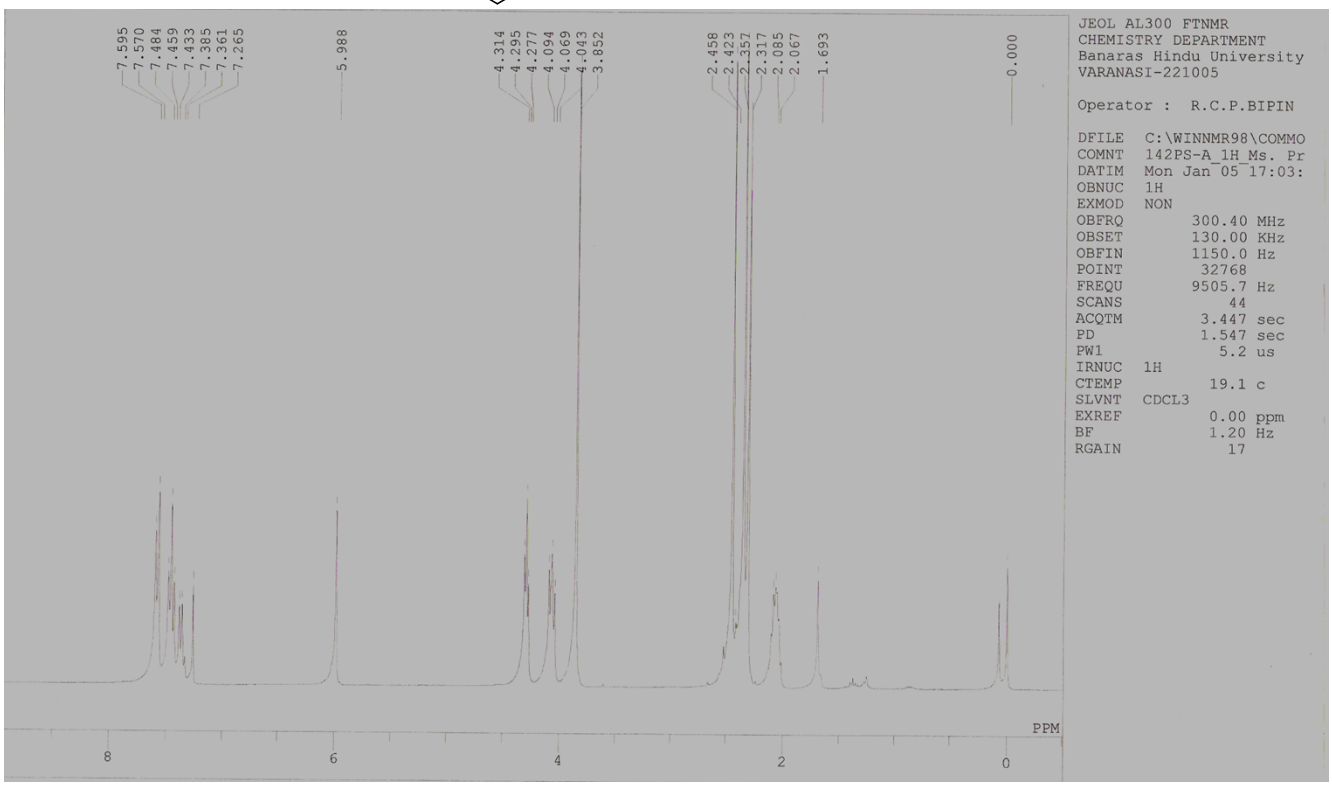
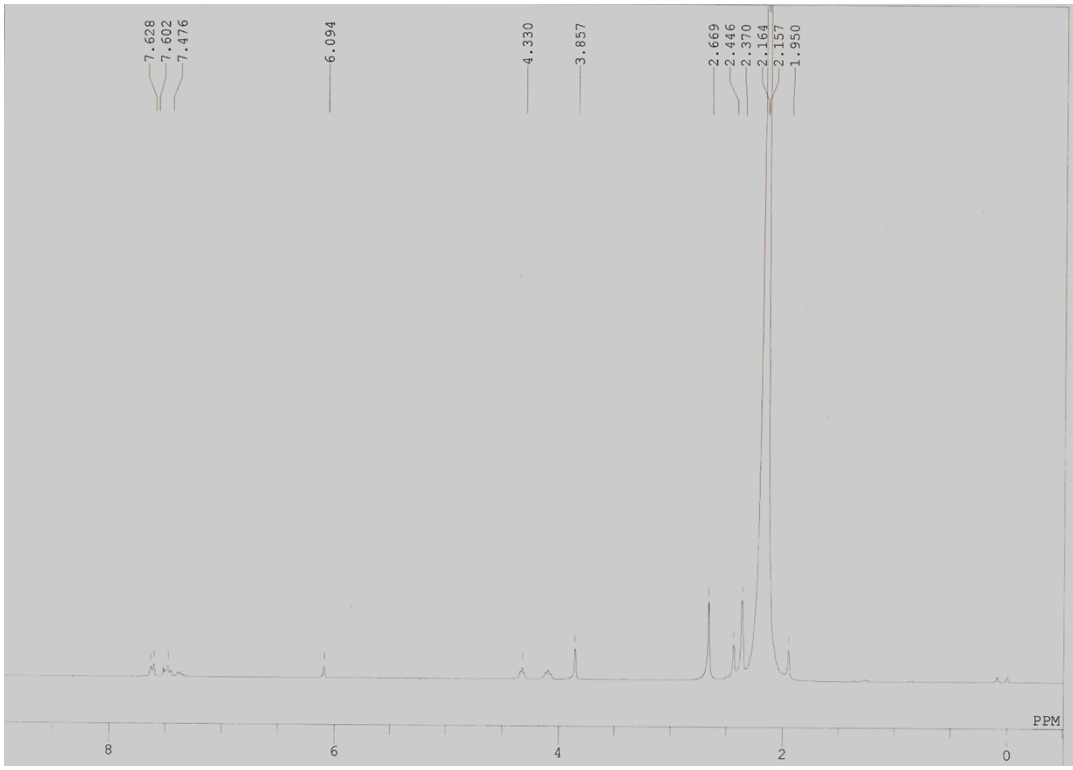
^{1}H NMR titration spectra of compound **2**







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Banaras Hindu University
VARANASI-221005

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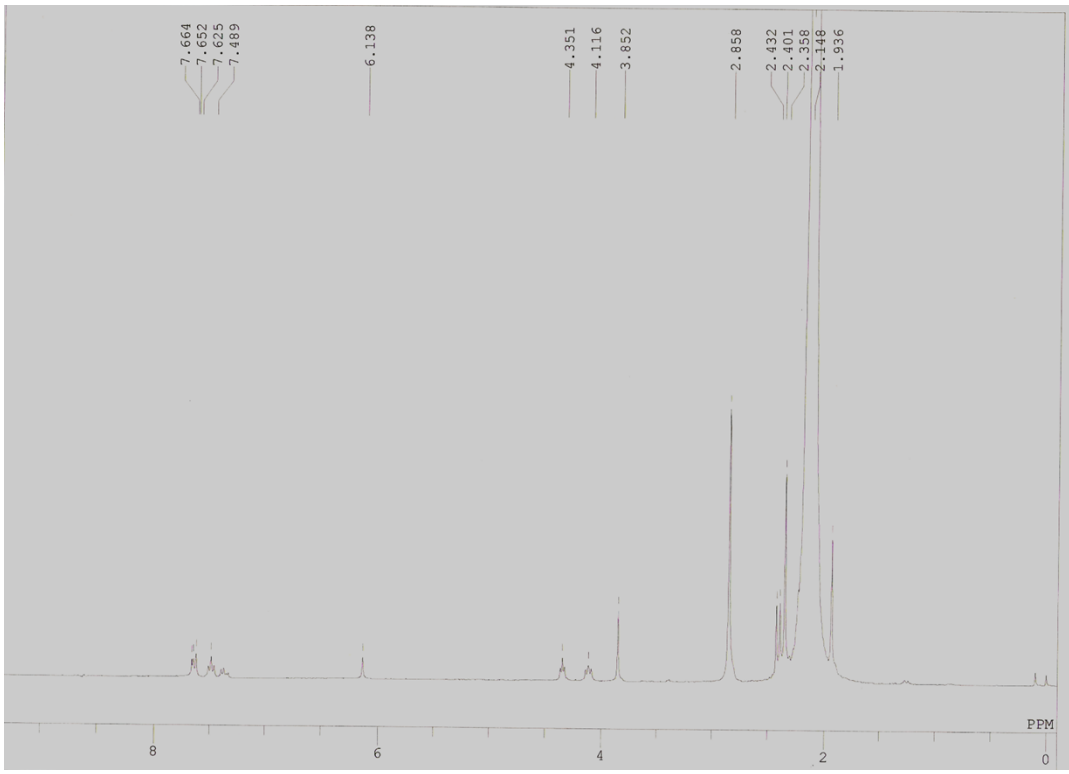

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CHEMISTRY DEPARTMENT
Banaras Hindu University
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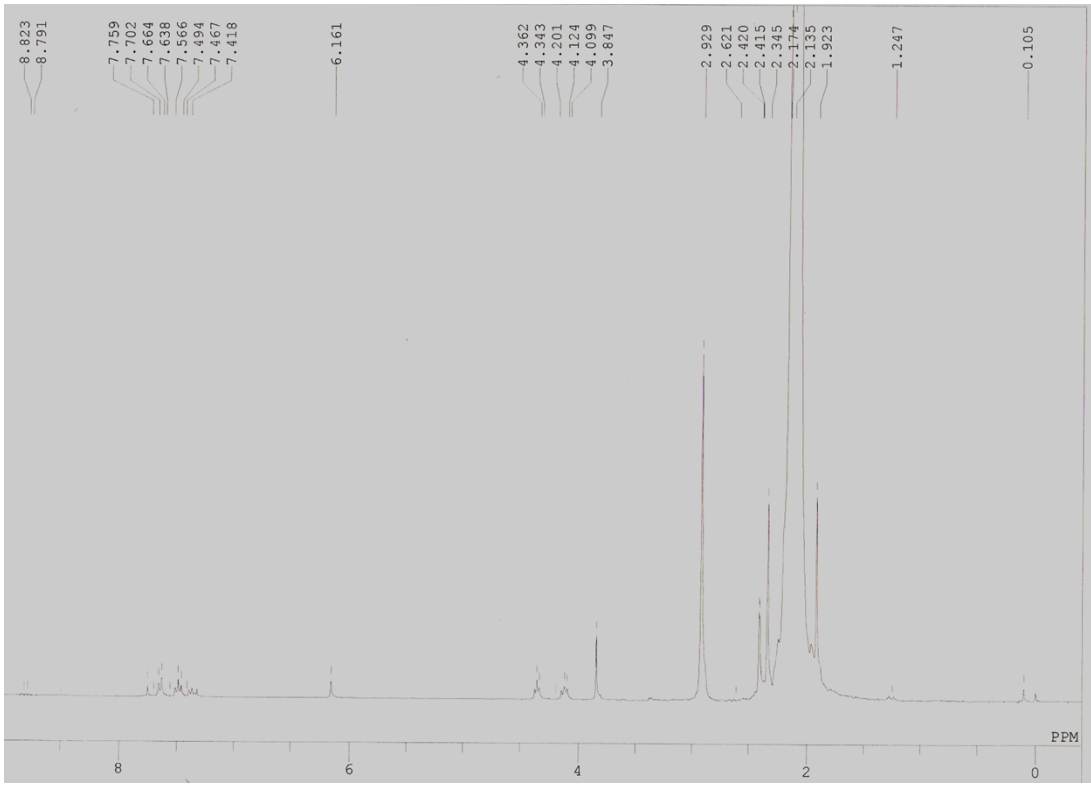

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CHEMISTRY DEPARTMENT
Banaras Hindu University
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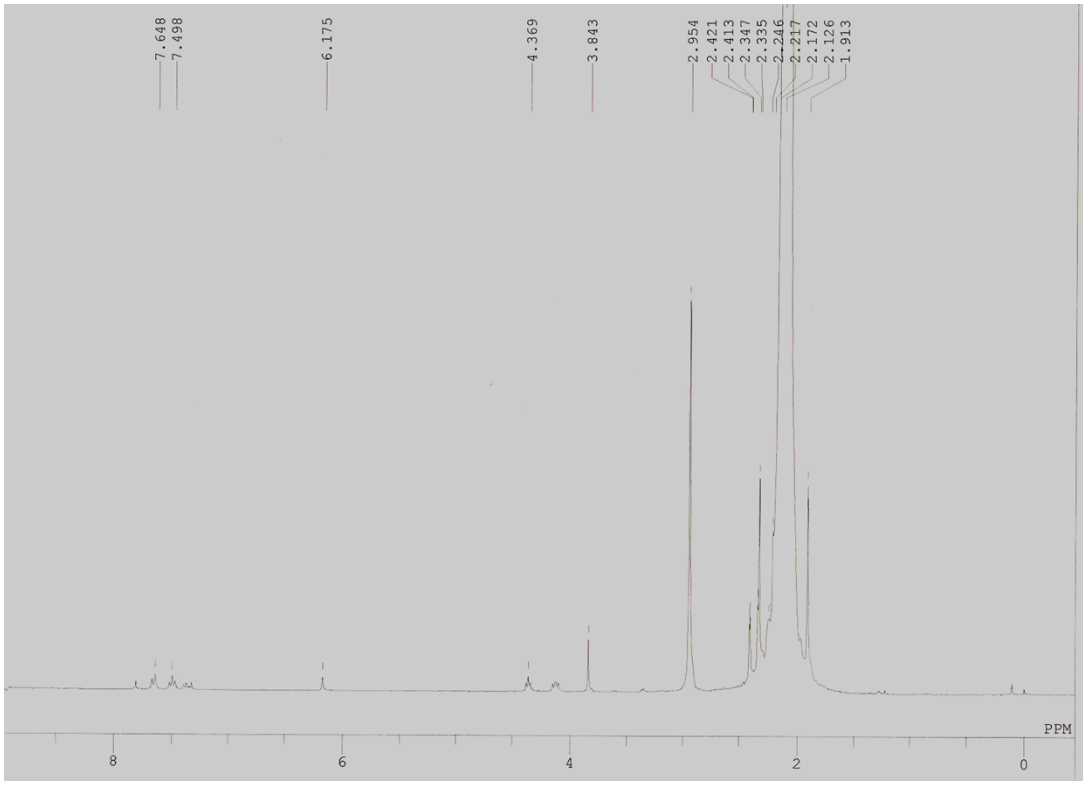

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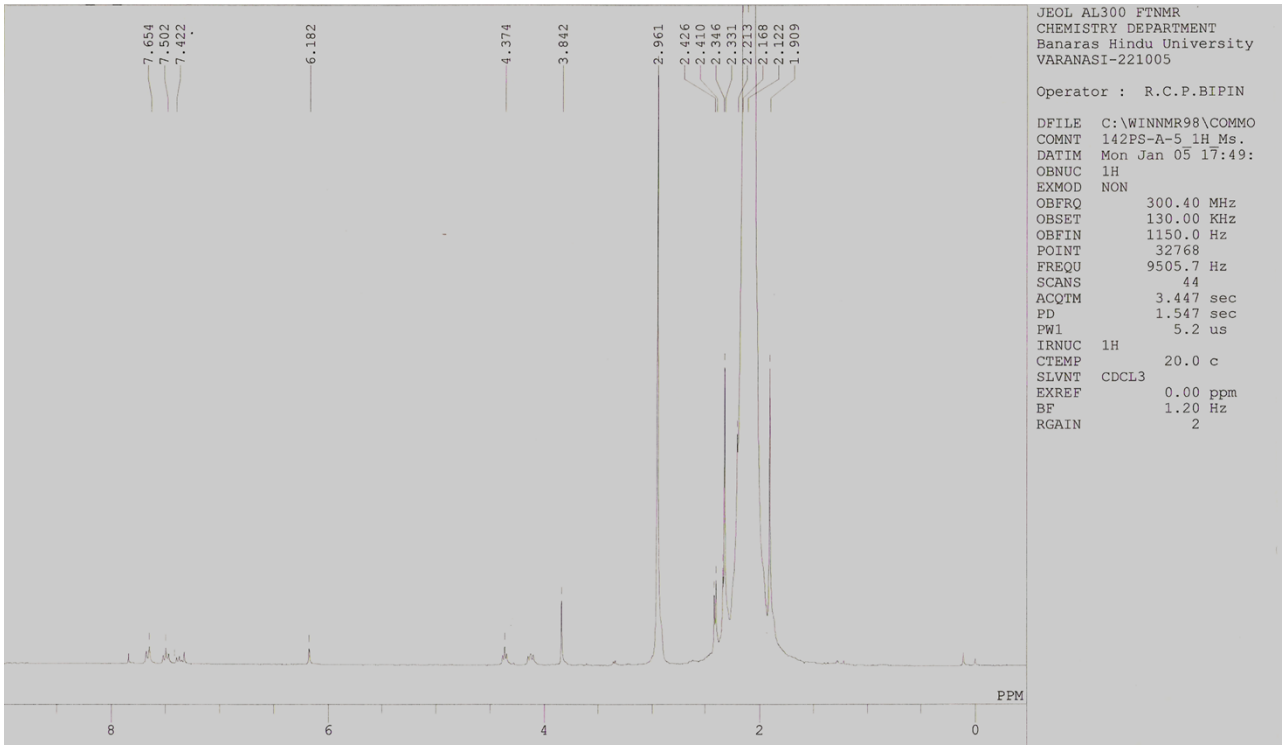

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Banaras Hindu University
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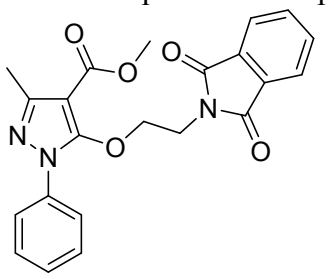
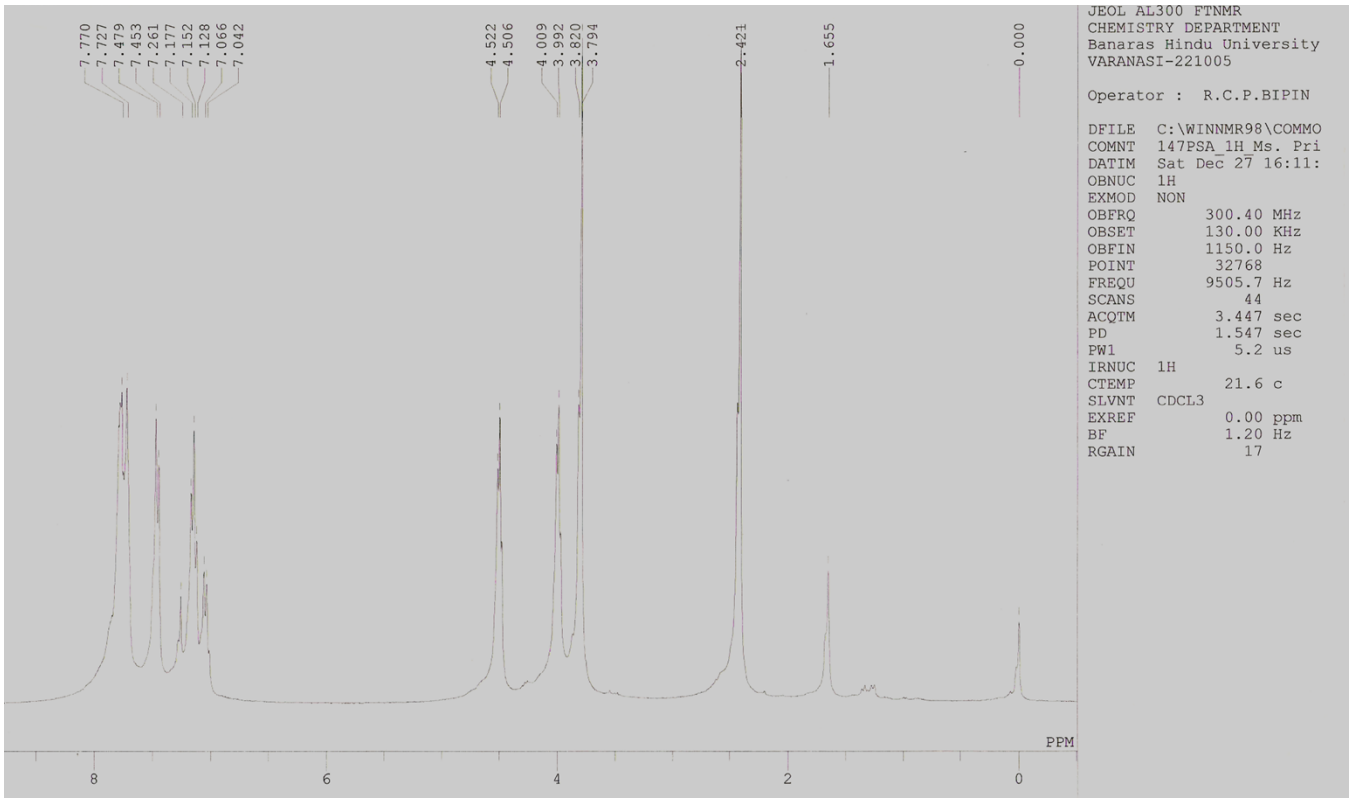
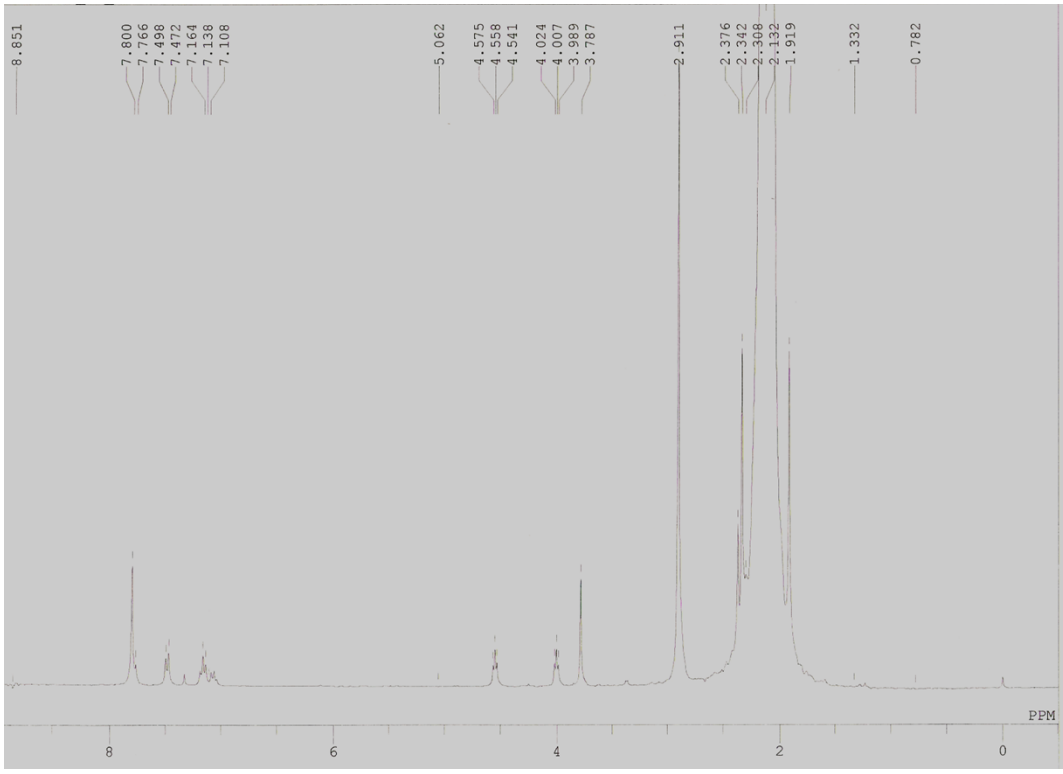
^{1}H NMR titration spectra of compound **3**







JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

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CTEMP	21.8 c
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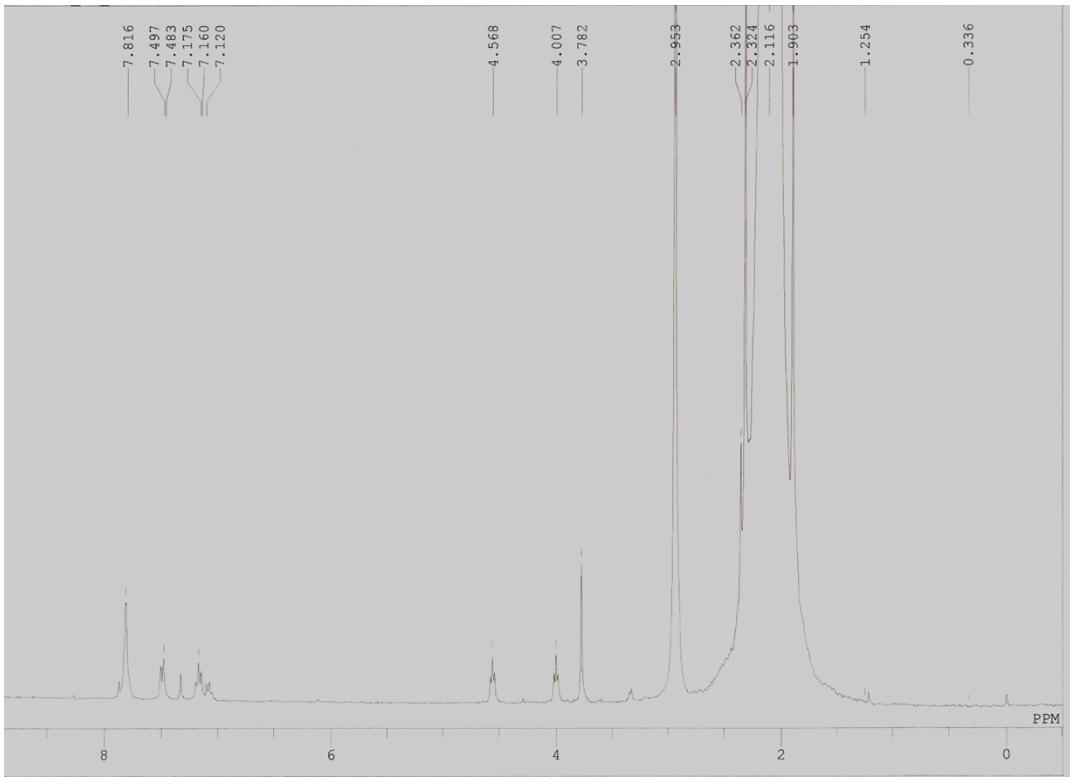
RGAIN	3



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
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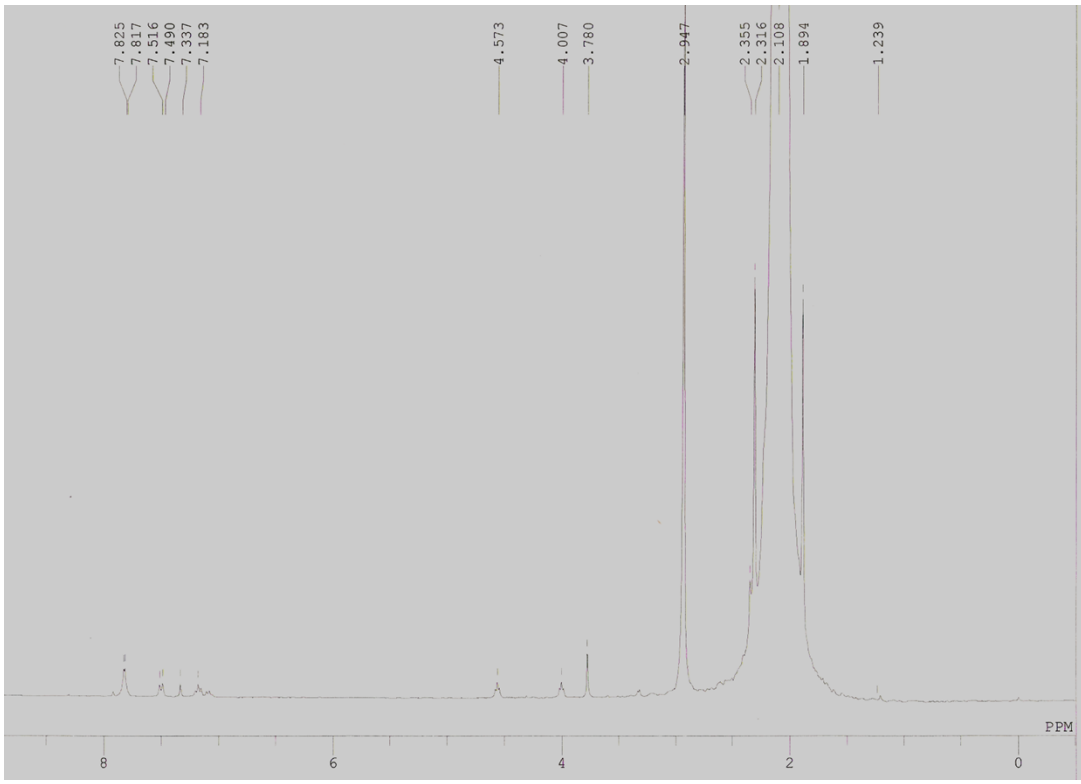


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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
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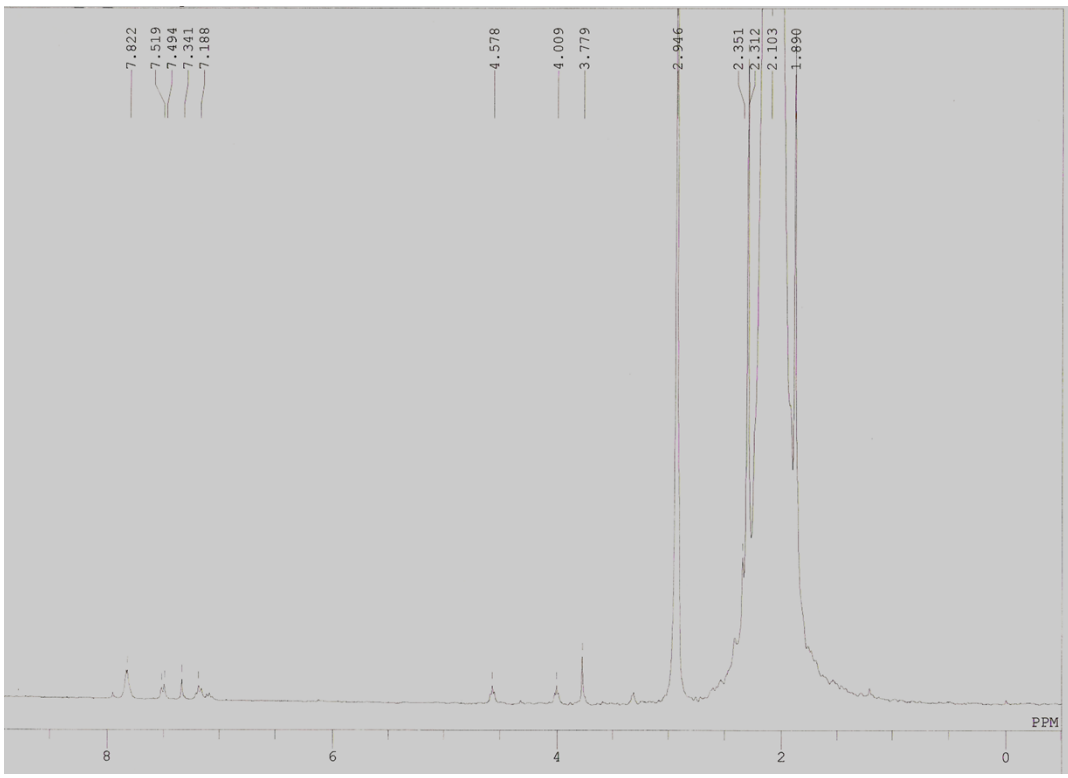


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CHEMISTRY DEPARTMENT
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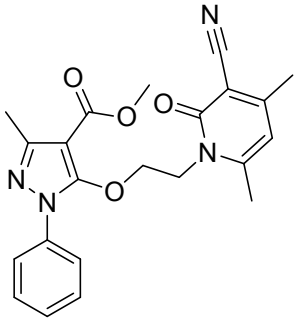
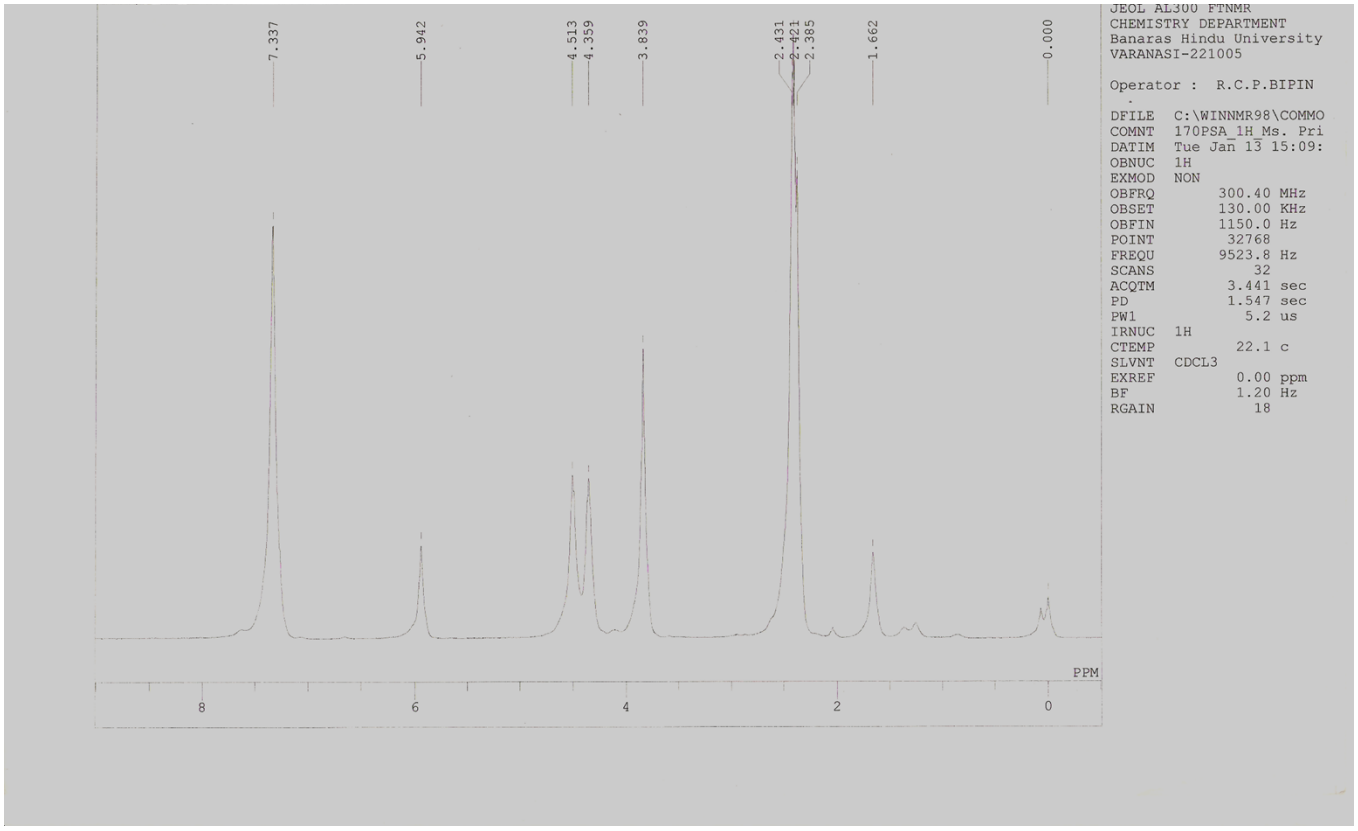
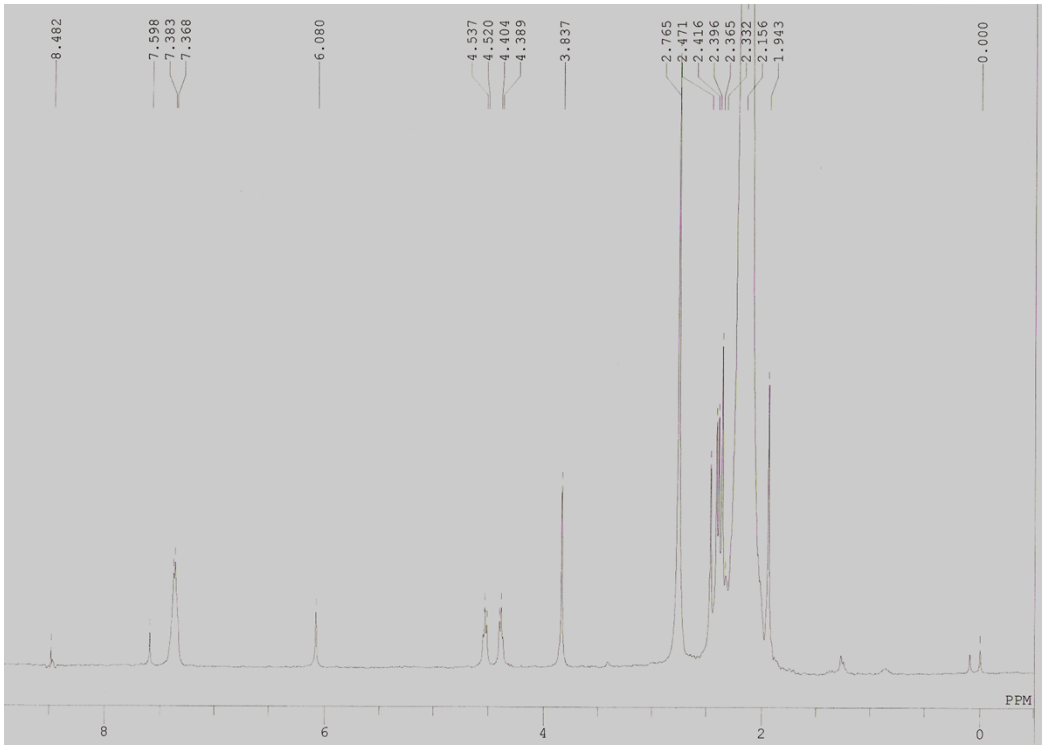
^{1}H NMR titration spectra of compound **4**







JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

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PD	1.547 sec
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CTEMP	21.9 c
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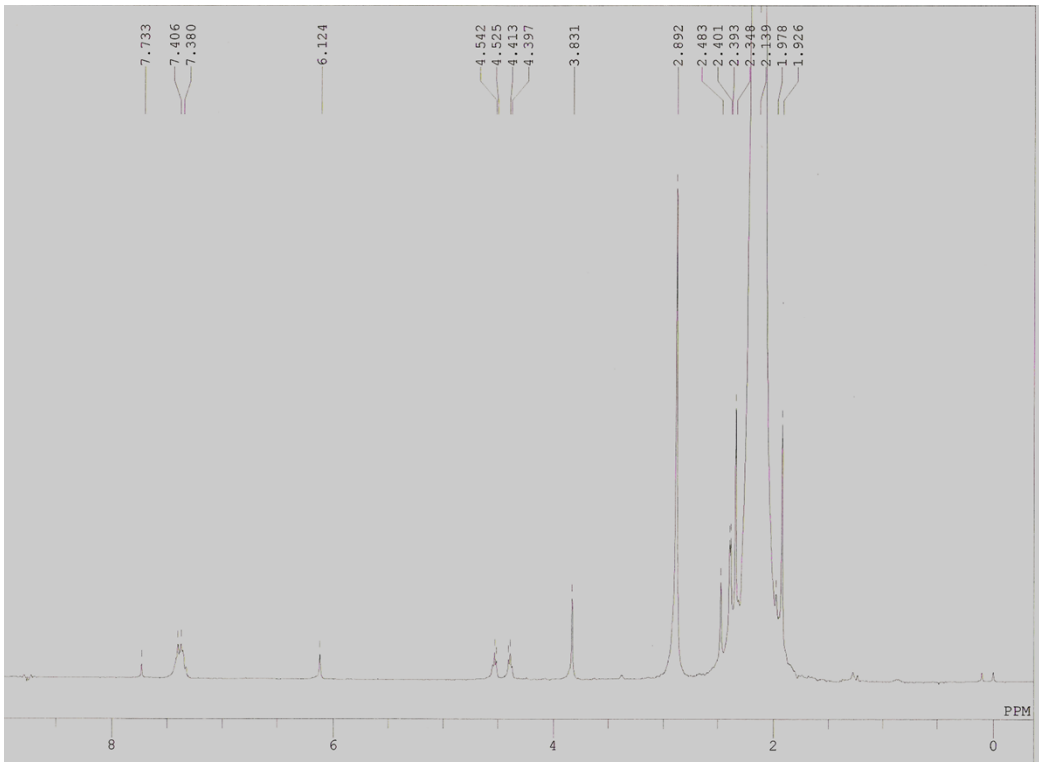

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

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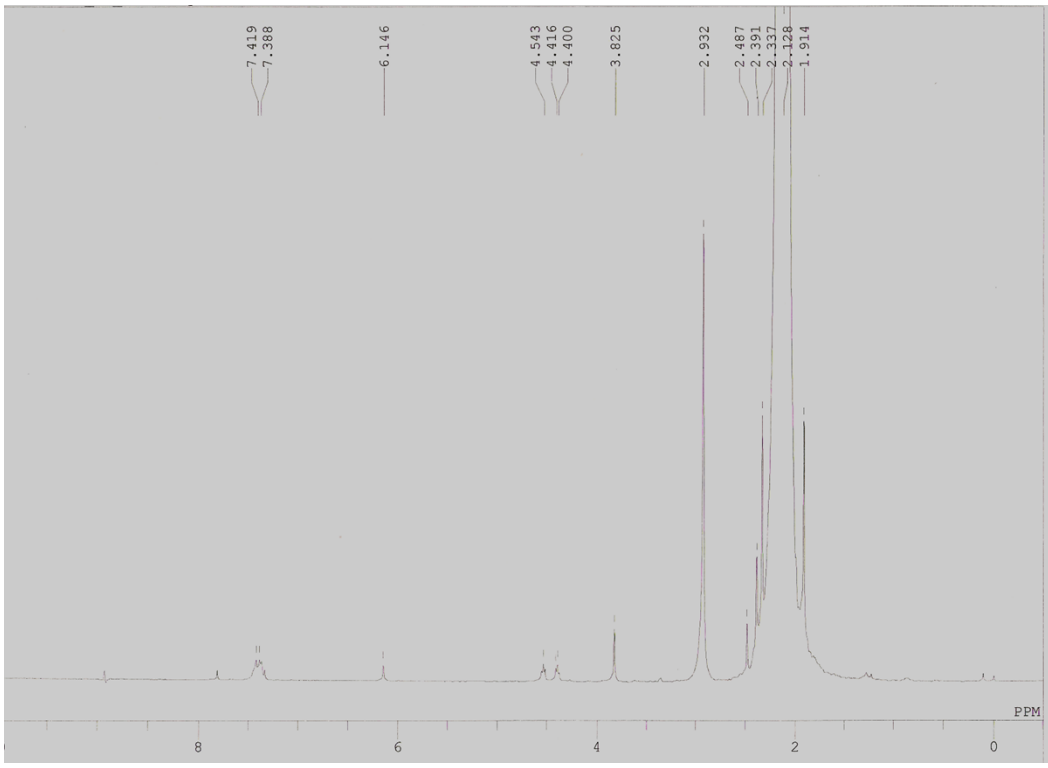


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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

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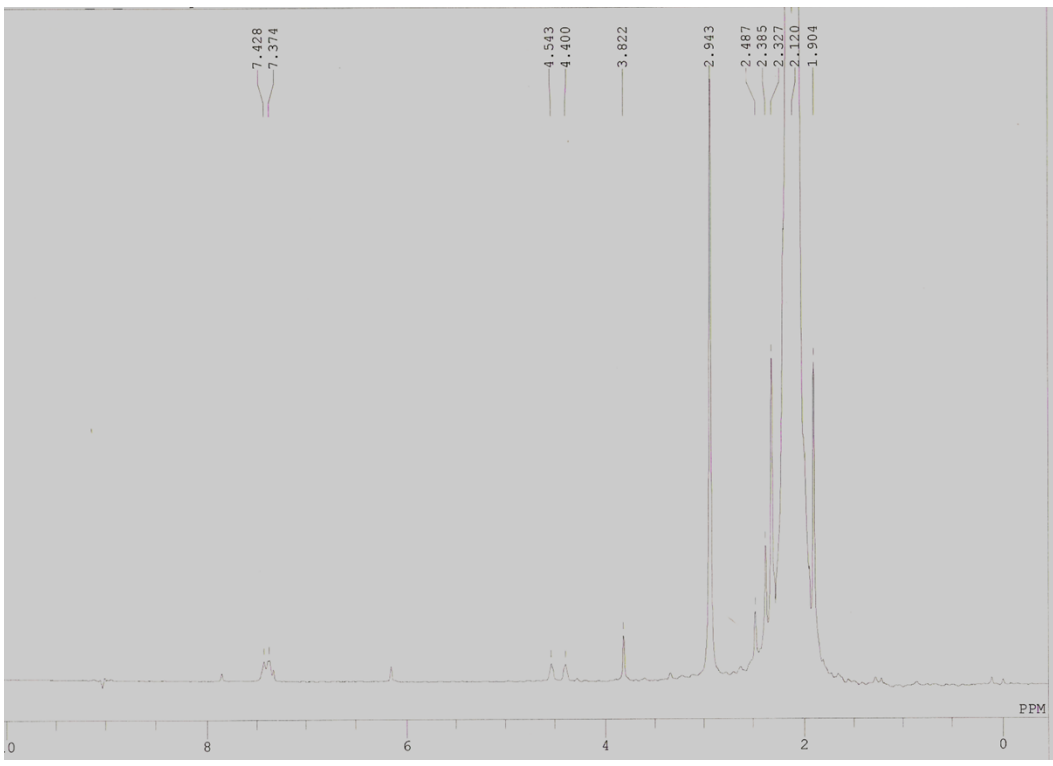


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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
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RGAIN              2
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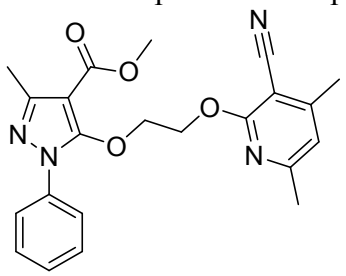
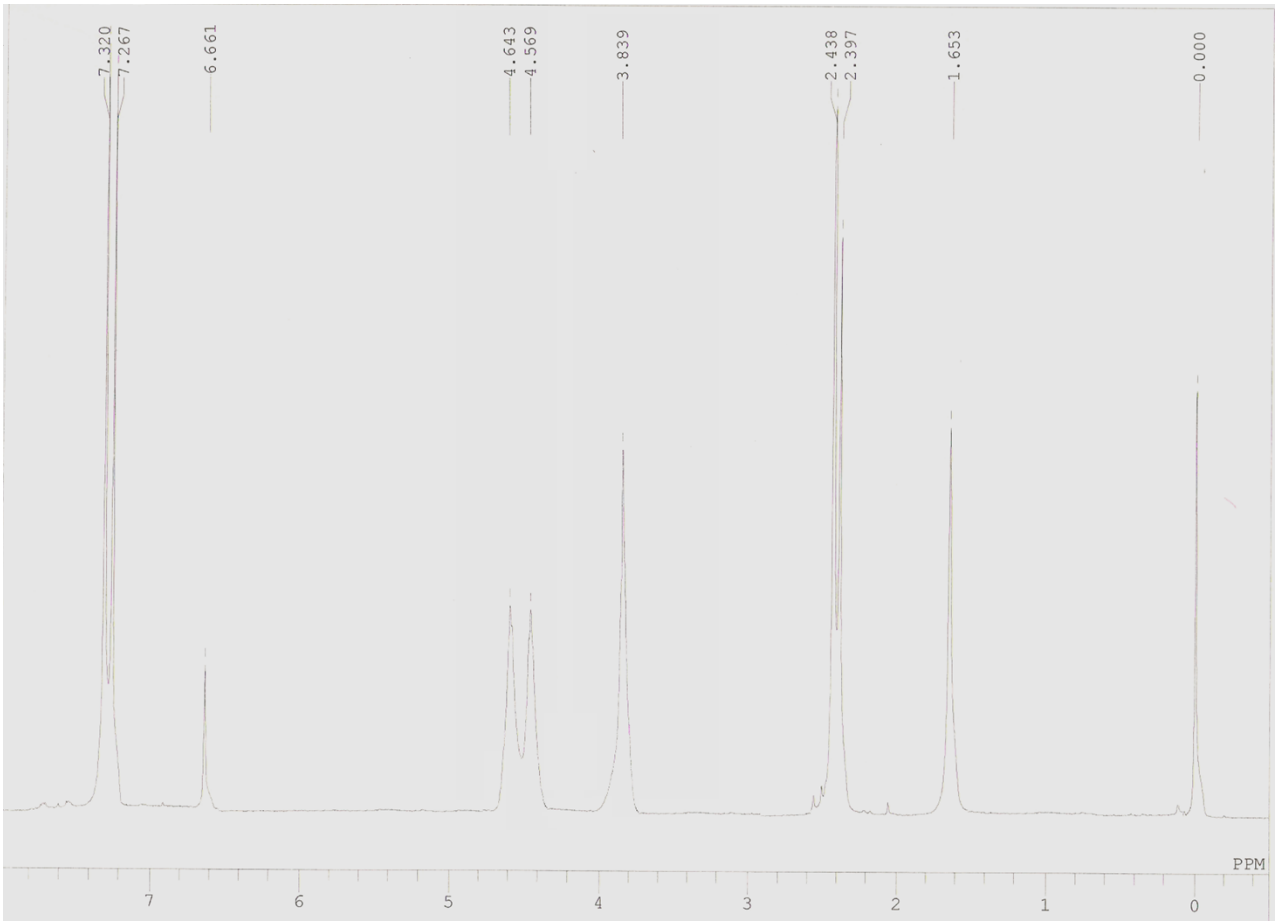
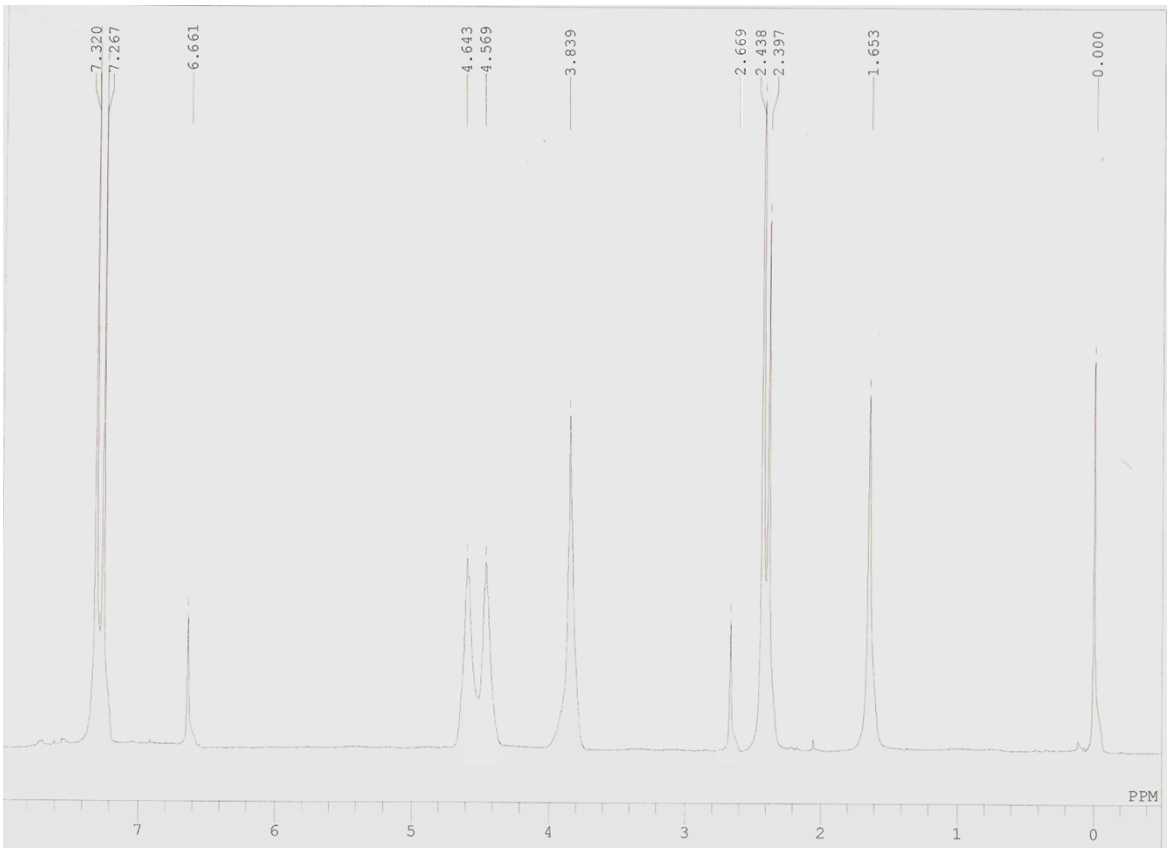
^{1}H NMR titration spectra of compound **5**



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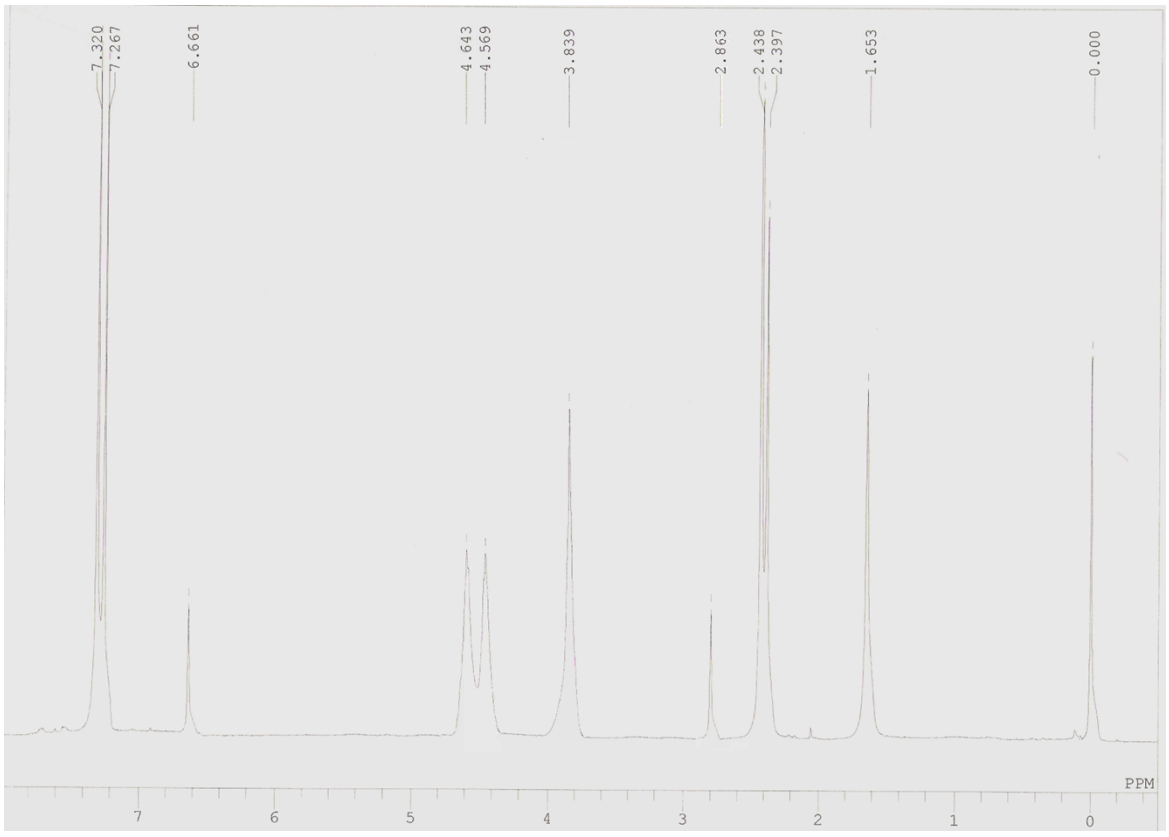
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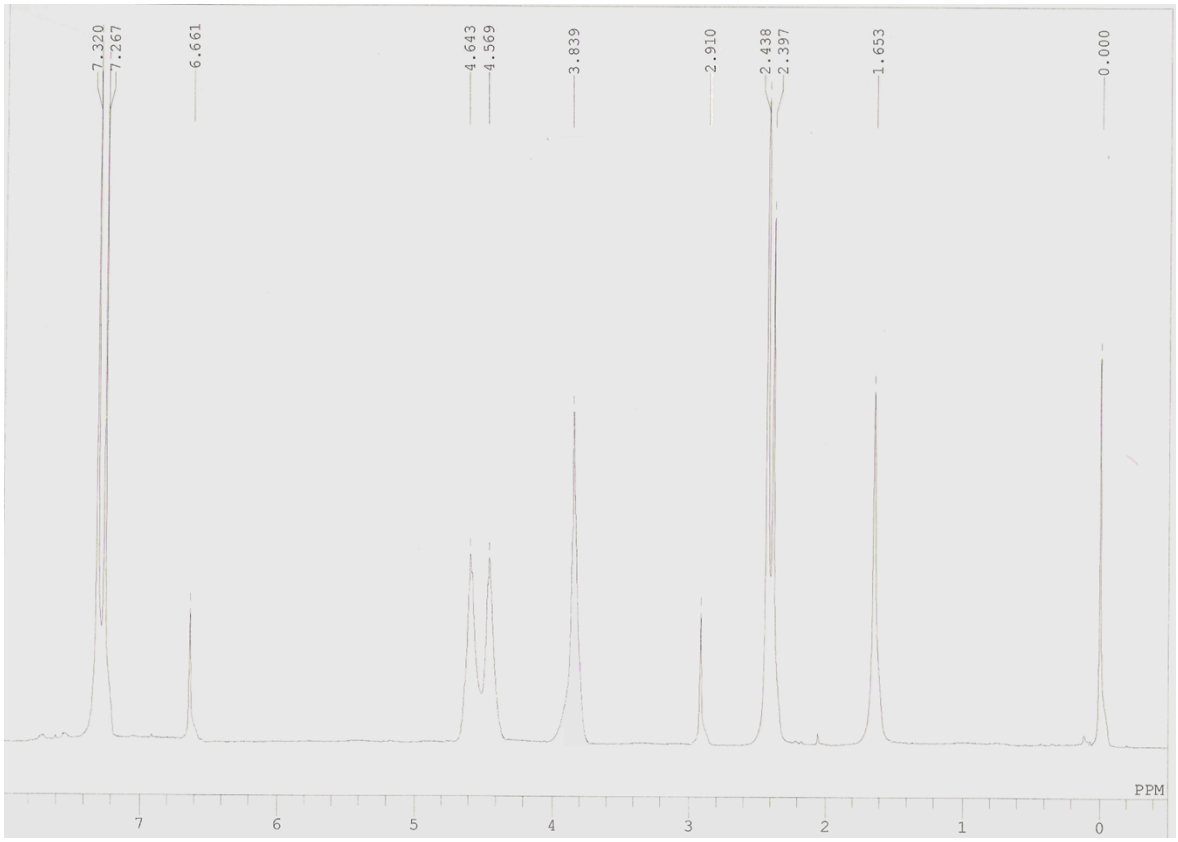
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7.267
6.661
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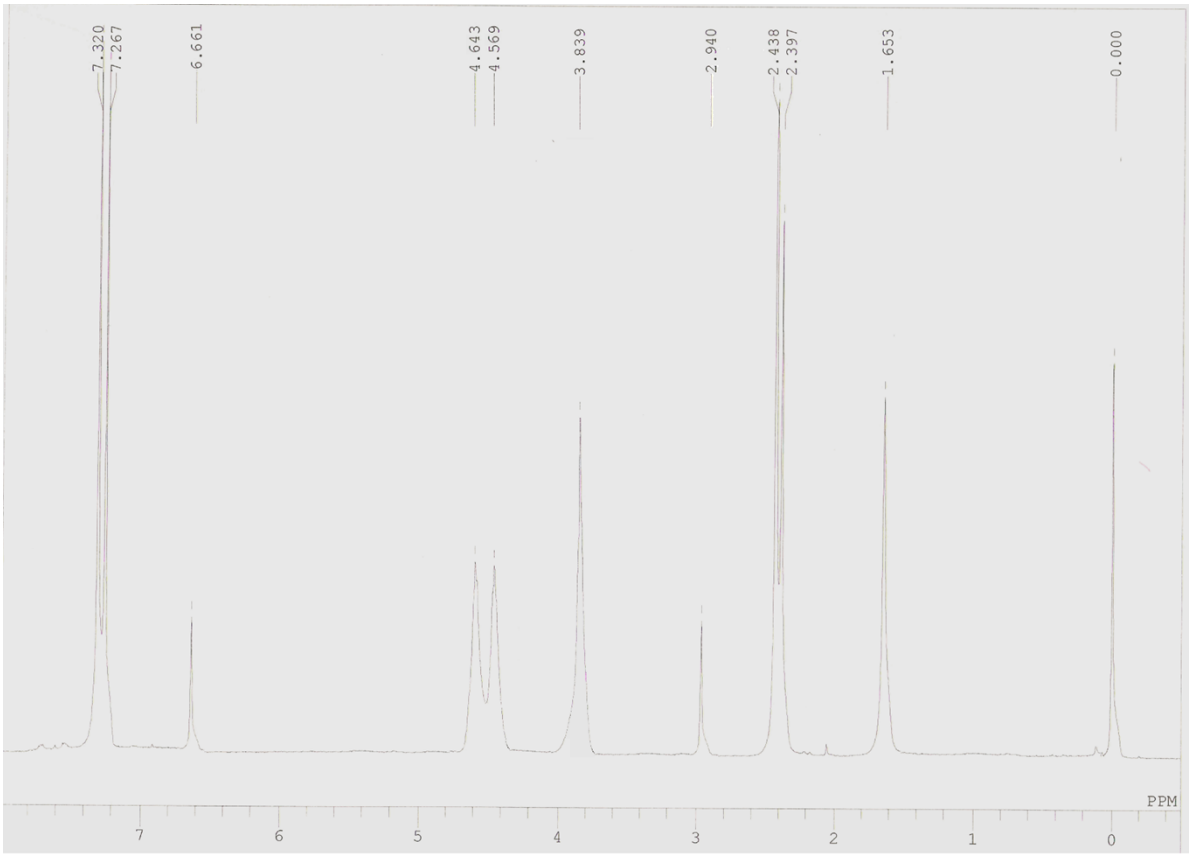
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3.839
2.940
2.438
2.397
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PPM
7
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0

S4. Optimized Coordinates with acetone:

For compound 1.

HETATM	1	C	1	-4.428	4.414	-1.160
HETATM	2	C	1	-5.401	3.435	-0.992
HETATM	3	C	1	-5.993	2.796	-2.091
HETATM	4	C	1	-5.636	3.111	-3.397
HETATM	5	C	1	-4.651	4.100	-3.579
HETATM	6	C	1	-4.057	4.740	-2.478
HETATM	7	C	1	-5.984	2.854	0.254
HETATM	8	N	1	-6.914	1.883	-0.169
HETATM	9	C	1	-6.965	1.786	-1.579
HETATM	10	C	1	-7.679	1.021	0.733
HETATM	11	C	1	-6.805	-0.008	1.443
HETATM	12	O	1	-6.064	-0.731	0.400
HETATM	13	C	1	-5.264	-1.735	0.807
HETATM	14	N	1	-3.921	-1.701	0.545
HETATM	15	N	1	-3.300	-2.858	0.996
HETATM	16	C	1	-4.260	-3.592	1.570
HETATM	17	C	1	-5.533	-2.933	1.490
HETATM	18	C	1	-3.155	-0.656	-0.064
HETATM	19	C	1	-3.660	0.046	-1.169
HETATM	20	C	1	-2.897	1.071	-1.738
HETATM	21	C	1	-1.635	1.389	-1.221
HETATM	22	C	1	-1.131	0.671	-0.128
HETATM	23	C	1	-1.888	-0.349	0.457
HETATM	24	C	1	-6.899	-3.409	1.781
HETATM	25	O	1	-7.135	-4.215	2.858
HETATM	26	C	1	-6.327	-4.163	4.078
HETATM	27	C	1	-3.925	-4.949	2.115
HETATM	28	O	1	-7.677	1.012	-2.206
HETATM	29	O	1	-5.739	3.118	1.427
HETATM	30	O	1	-7.855	-3.138	1.057
HETATM	31	H	1	-4.630	-0.213	-1.581
HETATM	32	H	1	-3.290	1.617	-2.591
HETATM	33	H	1	-1.046	2.187	-1.669
HETATM	34	H	1	-0.150	0.909	0.278
HETATM	35	H	1	-1.503	-0.905	1.305
HETATM	36	H	1	-4.763	-5.642	1.988
HETATM	37	H	1	-3.690	-4.895	3.185
HETATM	38	H	1	-3.050	-5.353	1.595
HETATM	39	H	1	-7.439	-0.700	2.007
HETATM	40	H	1	-6.079	0.471	2.111
HETATM	41	H	1	-8.438	0.520	0.126
HETATM	42	H	1	-8.178	1.637	1.490

HETATM 43 H 1 -6.094 2.608 -4.245
HETATM 44 H 1 -4.342 4.371 -4.586
HETATM 45 H 1 -3.295 5.498 -2.649
HETATM 46 H 1 -3.966 4.904 -0.307
HETATM 47 H 1 -7.014 -3.913 4.892
HETATM 48 H 1 -5.892 -5.151 4.246
HETATM 49 H 1 -5.539 -3.412 4.016
HETATM 50 O 1 -3.347 -3.147 5.137
HETATM 51 C 1 -2.805 -2.257 4.482
HETATM 52 C 1 -3.542 -0.981 4.119
HETATM 53 C 1 -1.380 -2.393 3.986
HETATM 54 H 1 -3.092 -0.140 4.666
HETATM 55 H 1 -3.426 -0.759 3.052
HETATM 56 H 1 -4.601 -1.056 4.380
HETATM 57 H 1 -0.834 -1.445 4.070
HETATM 58 H 1 -0.859 -3.188 4.526
HETATM 59 H 1 -1.421 -2.655 2.918

END

Compound 2.

HETATM 1 C UNK 1 -6.877 3.089 -3.352
HETATM 1 C UNK 1 -5.897 2.915 -2.381
HETATM 3 C UNK 1 -4.917 3.891 -2.147
HETATM 4 C UNK 1 -4.882 5.074 -2.878
HETATM 5 C UNK 1 -5.868 5.258 -3.863
HETATM 6 C UNK 1 -6.850 4.281 -4.096
HETATM 7 C UNK 1 -4.024 3.411 -1.044
HETATM 8 N UNK 1 -4.536 2.146 -0.668
HETATM 9 C UNK 1 -5.666 1.776 -1.436
HETATM 10 C UNK 1 -3.957 1.314 0.387
HETATM 11 C UNK 1 -2.839 0.395 -0.145
HETATM 12 C UNK 1 -2.263 -0.455 0.982
HETATM 13 O UNK 1 -1.191 -1.272 0.395
HETATM 14 C UNK 1 -0.362 -1.914 1.243
HETATM 15 N UNK 1 0.996 -1.802 1.077
HETATM 16 N UNK 1 1.679 -2.540 2.039
HETATM 17 C UNK 1 0.743 -3.097 2.805
HETATM 18 C UNK 1 -0.577 -2.750 2.353
HETATM 19 C UNK 1 1.733 -1.024 0.133
HETATM 20 C UNK 1 2.966 -0.477 0.525
HETATM 21 C UNK 1 3.707 0.279 -0.386
HETATM 22 C UNK 1 3.228 0.501 -1.684
HETATM 23 C UNK 1 2.001 -0.053 -2.069

HETATM 24 C UNK 1 1.253 -0.822 -1.172
HETATM 25 C UNK 1 -1.866 -3.298 2.776
HETATM 26 O UNK 1 -2.910 -3.243 2.128
HETATM 27 C UNK 1 1.139 -4.024 3.913
HETATM 28 O UNK 1 -6.289 0.733 -1.311
HETATM 29 O UNK 1 -3.056 3.954 -0.536
HETATM 30 O UNK 1 -1.779 -3.930 3.984
HETATM 31 C UNK 1 -2.947 -4.708 4.370
HETATM 32 C UNK 1 -0.914 -5.867 0.854
HETATM 33 C UNK 1 -2.269 -5.905 0.166
HETATM 34 O UNK 1 -0.768 -6.260 2.005
HETATM 35 C UNK 1 0.241 -5.286 0.050
HETATM 36 H UNK 1 1.625 0.103 -3.079
HETATM 37 H UNK 1 -7.602 4.452 -4.864
HETATM 38 H UNK 1 -7.633 2.326 -3.522
HETATM 39 H UNK 1 -2.713 -5.101 5.361
HETATM 40 H UNK 1 0.311 -1.262 -1.480
HETATM 41 H UNK 1 3.806 1.095 -2.388
HETATM 42 H UNK 1 4.662 0.700 -0.077
HETATM 43 H UNK 1 3.329 -0.658 1.532
HETATM 44 H UNK 1 0.730 -5.024 3.725
HETATM 45 H UNK 1 0.737 -3.684 4.873
HETATM 46 H UNK 1 2.231 -4.079 3.971
HETATM 47 H UNK 1 -3.015 -1.122 1.417
HETATM 48 H UNK 1 -1.822 0.169 1.772
HETATM 49 H UNK 1 -2.045 1.006 -0.592
HETATM 50 H UNK 1 -3.246 -0.261 -0.924
HETATM 51 H UNK 1 -3.842 -4.077 4.399
HETATM 52 H UNK 1 -3.093 -5.527 3.657
HETATM 53 H UNK 1 -4.773 0.721 0.815
HETATM 54 H UNK 1 -3.564 1.991 1.154
HETATM 55 H UNK 1 -4.118 5.824 -2.687
HETATM 56 H UNK 1 -5.873 6.172 -4.454
HETATM 57 H UNK 1 -2.709 -4.900 0.236
HETATM 58 H UNK 1 -2.180 -6.162 -0.898
HETATM 59 H UNK 1 -2.932 -6.609 0.677
HETATM 60 H UNK 1 -0.060 -4.347 -0.431
HETATM 61 H UNK 1 1.111 -5.115 0.688
HETATM 62 H UNK 1 0.508 -5.986 -0.755

END

Compound 3.

```
HETATM    1  C         2     -7.219   2.269  -1.075
HETATM    2  N         2     -5.975   1.799  -1.430
HETATM    3  C         2     -4.856   2.663  -1.671
HETATM    4  C         2     -5.136   4.082  -1.545
HETATM    5  C         2     -6.401   4.568  -1.193
HETATM    6  C         2     -7.430   3.634  -0.960
HETATM    7  C         2     -5.686   0.353  -1.562
HETATM    8  C         2     -5.063  -0.188  -0.272
HETATM    9  O         2     -4.550  -1.519  -0.619
HETATM   10  C         2     -3.926  -2.187   0.374
HETATM   11  N         2     -2.557  -2.252   0.464
HETATM   12  N         2     -2.179  -3.061   1.530
HETATM   13  C         2     -3.310  -3.493   2.092
HETATM   14  C         2     -4.456  -2.970   1.408
HETATM   15  C         2     -1.555  -1.546  -0.283
HETATM   16  C         2     -1.809  -1.071  -1.581
HETATM   17  C         2     -0.821  -0.345  -2.254
HETATM   18  C         2      0.424  -0.106  -1.660
HETATM   19  C         2      0.680  -0.606  -0.376
HETATM   20  C         2     -0.303  -1.319   0.316
HETATM   21  C         2     -5.889  -3.168   1.640
HETATM   22  O         2     -6.126  -4.123   2.586
HETATM   23  C         2     -7.532  -4.400   2.876
HETATM   24  C         2     -3.255  -4.393   3.289
HETATM   25  O         2     -3.750   2.176  -1.960
HETATM   26  C         2     -4.047   4.967  -1.783
HETATM   27  N         2     -3.165   5.706  -1.974
HETATM   28  C         2     -6.656   6.048  -1.056
HETATM   29  C         2     -8.333   1.288  -0.823
HETATM   30  O         2     -6.788  -2.560   1.060
HETATM   31  H         2     -2.762  -1.258  -2.059
HETATM   32  H         2     -1.032   0.033  -3.252
HETATM   33  H         2      1.187   0.460  -2.191
HETATM   34  H         2      1.645  -0.435   0.097
HETATM   35  H         2     -0.104  -1.702   1.310
HETATM   36  H         2     -3.775  -3.936   4.139
HETATM   37  H         2     -2.214  -4.579   3.569
HETATM   38  H         2     -3.751  -5.348   3.082
HETATM   39  H         2     -5.799  -0.288   0.533
HETATM   40  H         2     -4.226   0.445   0.044
HETATM   41  H         2     -4.969   0.234  -2.378
HETATM   42  H         2     -6.597  -0.188  -1.814
HETATM   43  H         2     -8.031  -3.496   3.241
HETATM   44  H         2     -8.040  -4.763   1.977
HETATM   45  H         2     -7.516  -5.171   3.649
HETATM   46  H         2     -8.419   3.983  -0.681
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HETATM 47 H 2 -6.015 6.477 -0.274
HETATM 48 H 2 -6.414 6.570 -1.990
HETATM 49 H 2 -7.701 6.250 -0.801
HETATM 50 H 2 -9.225 1.821 -0.485
HETATM 51 H 2 -8.059 0.550 -0.058
HETATM 52 H 2 -8.589 0.737 -1.738
HETATM 54 O 2 -2.245 -1.756 5.472
HETATM 55 C 2 -1.567 -1.315 4.544
HETATM 56 C 2 -2.084 -0.218 3.634
HETATM 57 C 2 -0.180 -1.856 4.252
HETATM 58 H 2 0.502 -1.066 3.917
HETATM 59 H 2 0.226 -2.370 5.128
HETATM 60 H 2 -0.275 -2.580 3.429
HETATM 61 H 2 -1.508 0.700 3.822
HETATM 62 H 2 -1.922 -0.481 2.582
HETATM 63 H 2 -3.145 -0.029 3.820

END

Compound 4.

HETATM 1 C 2 -4.639 3.190 -1.787
HETATM 2 N 2 -5.377 2.251 -1.105
HETATM 3 C 2 -6.691 1.856 -1.509
HETATM 4 C 2 -7.220 2.564 -2.663
HETATM 5 C 2 -6.480 3.528 -3.357
HETATM 6 C 2 -5.180 3.819 -2.899
HETATM 7 C 2 -4.829 1.545 0.083
HETATM 8 C 2 -4.102 0.246 -0.313
HETATM 9 C 2 -3.500 -0.425 0.914
HETATM 10 O 2 -2.666 -1.542 0.422
HETATM 11 C 2 -1.895 -2.145 1.349
HETATM 12 N 2 -0.540 -1.938 1.391
HETATM 13 N 2 0.041 -2.676 2.414
HETATM 14 C 2 -0.955 -3.346 3.000
HETATM 15 C 2 -2.210 -3.058 2.368
HETATM 16 C 2 0.261 -1.048 0.606
HETATM 17 C 2 -0.043 -0.811 -0.745
HETATM 18 C 2 0.749 0.079 -1.481
HETATM 19 C 2 1.848 0.714 -0.888
HETATM 20 C 2 2.154 0.455 0.455
HETATM 21 C 2 1.362 -0.417 1.209
HETATM 22 C 2 -3.546 -3.600 2.621
HETATM 23 O 2 -3.521 -4.607 3.543
HETATM 24 C 2 -4.807 -5.231 3.843
HETATM 25 C 2 -0.663 -4.252 4.158

HETATM 26 O 2 -7.297 0.968 -0.884
HETATM 27 C 2 -8.540 2.220 -3.070
HETATM 28 N 2 -9.622 1.957 -3.419
HETATM 29 C 2 -7.050 4.237 -4.560
HETATM 30 C 2 -3.254 3.535 -1.308
HETATM 31 O 2 -4.579 -3.222 2.069
HETATM 32 H 2 -0.879 -1.316 -1.214
HETATM 33 H 2 0.508 0.264 -2.526
HETATM 34 H 2 2.462 1.400 -1.467
HETATM 35 H 2 3.009 0.940 0.925
HETATM 36 H 2 1.589 -0.613 2.252
HETATM 37 H 2 -1.231 -3.943 5.043
HETATM 38 H 2 0.406 -4.227 4.390
HETATM 39 H 2 -0.958 -5.283 3.936
HETATM 40 H 2 -4.265 -0.833 1.584
HETATM 41 H 2 -2.850 0.264 1.470
HETATM 42 H 2 -3.299 0.469 -1.026
HETATM 43 H 2 -4.807 -0.433 -0.806
HETATM 44 H 2 -5.491 -4.498 4.285
HETATM 45 H 2 -5.252 -5.644 2.932
HETATM 46 H 2 -4.578 -6.025 4.555
HETATM 47 H 2 -5.672 1.325 0.740
HETATM 48 H 2 -4.158 2.226 0.610
HETATM 49 H 2 -4.578 4.556 -3.421
HETATM 50 H 2 -2.787 4.237 -2.003
HETATM 51 H 2 -2.615 2.648 -1.233
HETATM 52 H 2 -3.284 4.004 -0.316
HETATM 53 H 2 -7.346 3.515 -5.332
HETATM 54 H 2 -7.954 4.797 -4.283
HETATM 55 H 2 -6.326 4.935 -4.991
HETATM 56 O 2 0.451 -7.386 2.644
HETATM 57 C 2 0.360 -6.605 1.697
HETATM 58 C 2 1.546 -5.793 1.216
HETATM 59 C 2 -0.951 -6.397 0.962
HETATM 60 H 2 -0.841 -6.730 -0.079
HETATM 61 H 2 -1.758 -6.954 1.446
HETATM 62 H 2 -1.202 -5.329 0.927
HETATM 63 H 2 1.665 -5.890 0.129
HETATM 64 H 2 1.356 -4.730 1.425
HETATM 65 H 2 2.461 -6.107 1.728

END

Compound 5.

```
ATOM      1  N   UNK     1      -5.777   2.045  -1.794
ATOM      2  C   UNK     1      -4.724   2.628  -1.233
ATOM      3  C   UNK     1      -4.313   3.961  -1.526
ATOM      4  C   UNK     1      -5.067   4.703  -2.463
ATOM      5  C   UNK     1      -6.179   4.073  -3.037
ATOM      6  C   UNK     1      -6.511   2.757  -2.688
ATOM      7  O   UNK     1      -3.968   1.952  -0.332
ATOM      8  C   UNK     1      -4.243   0.536  -0.132
ATOM      9  C   UNK     1      -3.200   0.062   0.876
ATOM     10  O   UNK     1      -3.092  -1.392   0.680
ATOM     11  C   UNK     1      -2.242  -2.029   1.515
ATOM     12  N   UNK     1      -0.880  -2.062   1.335
ATOM     13  N   UNK     1      -0.278  -2.825   2.323
ATOM     14  C   UNK     1      -1.268  -3.296   3.087
ATOM     15  C   UNK     1      -2.539  -2.822   2.626
ATOM     16  C   UNK     1      -0.073  -1.406   0.351
ATOM     17  C   UNK     1      -0.566  -1.171  -0.943
ATOM     18  C   UNK     1       0.243  -0.516  -1.879
ATOM     19  C   UNK     1       1.540  -0.111  -1.540
ATOM     20  C   UNK     1       2.029  -0.365  -0.250
ATOM     21  C   UNK     1       1.228  -1.006   0.699
ATOM     22  C   UNK     1      -3.891  -2.895   3.218
ATOM     23  O   UNK     1      -4.357  -4.069   3.731
ATOM     24  C   UNK     1      -3.818  -5.377   3.342
ATOM     25  C   UNK     1      -0.952  -4.176   4.259
ATOM     26  C   UNK     1      -3.158   4.507  -0.901
ATOM     27  N   UNK     1      -2.210   4.966  -0.398
ATOM     28  C   UNK     1      -4.674   6.111  -2.832
ATOM     29  C   UNK     1      -7.710   2.057  -3.274
ATOM     30  O   UNK     1      -4.622  -1.911   3.298
ATOM     31  H   UNK     1      -1.566  -1.491  -1.217
ATOM     32  H   UNK     1      -0.145  -0.331  -2.878
ATOM     33  H   UNK     1       2.164   0.397  -2.272
ATOM     34  H   UNK     1       3.035  -0.055   0.024
ATOM     35  H   UNK     1       1.598  -1.195   1.702
ATOM     36  H   UNK     1      -0.960  -5.231   3.956
ATOM     37  H   UNK     1      -1.686  -4.046   5.061
ATOM     38  H   UNK     1       0.044  -3.942   4.648
ATOM     39  H   UNK     1      -3.500   0.255   1.912
ATOM     40  H   UNK     1      -2.231   0.533   0.669
ATOM     41  H   UNK     1      -4.125  -0.000  -1.081
ATOM     42  H   UNK     1      -5.266   0.393   0.232
ATOM     43  H   UNK     1      -4.675  -5.971   3.011
ATOM     44  H   UNK     1      -3.085  -5.299   2.537
ATOM     45  H   UNK     1      -3.363  -5.836   4.223
ATOM     46  H   UNK     1      -6.787   4.609  -3.761
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ATOM     47  H   UNK     1      -7.424   1.072  -3.665
ATOM     48  H   UNK     1      -8.171   2.642  -4.075
ATOM     49  H   UNK     1      -8.462   1.886  -2.490
ATOM     50  H   UNK     1      -5.373   6.541  -3.554
ATOM     51  H   UNK     1      -3.666   6.127  -3.269
ATOM     52  H   UNK     1      -4.646   6.754  -1.943
ATOM     53  O   UNK     1      -1.120  -6.252   1.413
ATOM     54  C   UNK     1      -0.751  -5.579   0.451
ATOM     55  C   UNK     1       0.716  -5.375   0.132
ATOM     56  C   UNK     1      -1.749  -4.919  -0.482
ATOM     57  H   UNK     1      -2.734  -4.848  -0.012
ATOM     58  H   UNK     1      -1.403  -3.931  -0.806
ATOM     59  H   UNK     1      -1.831  -5.538  -1.387
ATOM     60  H   UNK     1       0.904  -5.489  -0.943
ATOM     61  H   UNK     1       0.983  -4.343   0.402
ATOM     62  H   UNK     1       1.337  -6.066   0.708

END
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