|  |
| --- |
| C:\Users\Abir\Desktop\RDGscatter.png |
|  |
| **Figure S2:** Reduced density gradient of MBPPC dimer structure. |

|  |
| --- |
| C:\Users\Abir\Desktop\KH23\dimmm.tif |
| **Figure S1:** N-H...O and C-H...O Hydrogen bonding interactions in dimer conformation. |

**Geometrical and spectroscopic characterization combined with molecular docking study of N'-(4-Methoxybenzylidene)-5-phenyl-1H-pyrazole-3-carbohydrazide**

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | |  |
| ***dnorm*** | ***di*** | | ***de*** |
|  | |  | |
| ***Shape index*** | | ***Curvedness*** | |
| **Figure S3:** The dnorm, de, di, shape index, curvedness 2D surfaces of MBPPC. | | | |

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| --- |
|  |
| **Figure S4:** 2D fingerprint plots of the most powerful contributions. |

|  |
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|  |
| **Figure S5:** The HOMO and LUMO orbitals computed at B3LYP/6-311++G(d,p) basis set for N'-(4-Methoxybenzylidene)-5-phenyl-1H-pyrazole-3-carbohydrazide. |

|  |
| --- |
| C:\Users\Abir\Desktop\Benzothiophene\Multiwfn_3.7_dev_bin_Win64\Multiwfn_3.7_dev_bin_Win64\dislin_4.png |
| **Figure S6:** The variation of OPDOS (right side) and TDOS as well PDOS (left side) in term of energy (a.u). |

|  |
| --- |
| C:\Users\Abir\Desktop\NLO.tif |
| **Figure S7:** The first and second non linear optical parameters of MBPPC and urea. |

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|  |
|  |
| **Figure S8:** The experimental and theoretical FT-IR spectra of MBPPC compound. |

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|  |
| **Figure S9:** The theoretical Raman spectrum of MBPPC performed in gas phase. |

|  |
| --- |
| **(a)** |
| **C:\Users\Abir\Desktop\KH23\1H NMR-KH23.jpg** |
| **(b)** |
| **C:\Users\Abir\Desktop\KH23\13C NMR-KH23.jpg** |
| **Figure S10:** Experimental 1H (a) and 13C (b) NMR spectra of N'-(4-Methoxybenzylidene)-5-phenyl-1H-pyrazole-3-carbohydrazide recorded in DMSO solvent. |

|  |  |
| --- | --- |
| C:\Users\Abir\Desktop\KH23\KH23MONOMERB3LYP6311G+2DP_NMR_scf_giaoH.jpg | C:\Users\Abir\Desktop\KH23\KH23DIMERNMR_scf_giaoH.jpg |
| **(a)** | **(b)** |
| C:\Users\Samsung\Desktop\KH23\KH23MONOMERB3LYP6311G+2DP_NMR_scf_giaoC.jpg | C:\Users\Samsung\Desktop\KH23\KH23DIMERNMR_scf_giaoC.jpg |
| **(c)** | **(d)** |
| **Figure S11:** 1H (a) and 13C (c) monomeric NMR spectra along with 1H (b) and 13C (d) dimeric spectra of the studied compound. | |

**Table S1:** Electronic parameters of the studied compound obtained via TD-DFT calculation.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Energy** | **EHOMO** | **ELUMO** | **EHOMO-LUMO** | **I (eV)** | **A (eV)** | **χ (eV)** | **η (eV)** | **S (eV-1)** | **μ (eV)** | **ѱ (eV)** |
| **Monomer** | -6.0191 | -1.8664 | -4.1527 | 6.0191 | 1.8664 | 3.9427 | 2.0763 | 0.2408 | -3.9427 | 3.7434 |
| **Dimer** | -5.1301 | -1.5056 | -3.6245 | 5.1301 | 1.5056 | 3.3178 | 1.8122 | 0.2759 | -3.3178 | 3.0370 |

I :Ionization potential, (A) : Electronic affinity, χ : Electronegativity, η : Chemical hardness, S : Global softness, μ : Chemical potential, ѱ : Electrophilicity.

**Table S2:**The dipole moments  (D), the isotropic polarizability (iso)(x10-24esu), the anisotropy of the polarizability (aniso) (x10-24esu), the first hyperpolarizability  (x10-30esu), and the second hyperpolarizability of MBPPC

|  |  |  |  |
| --- | --- | --- | --- |
|  | **MBPPC** | **Urea** | **Ratio** |
| μ | 3,88 | 4,38 | 0.89 |
| α(0,0) | 44,34 | 5,09 | 8.71 |
| (0,0) | 50,89 | 2,03 | 25.07 |
| α(-w;w) | 45,71 | 5,13 | 8.91 |
| α(-w;w) | 54,11 | 2,05 | 26.40 |
| β(0;0,0) || | 16,08 | 0,36 | 44.67 |
| β(-w;w,0) || | 19,68 | 0,38 | 51.79 |
| β(-2w;w,w) || | 31,99 | 0,41 | 78.02 |
| <γ(0;0,0,0)> | 179.12 | 3.45 | 51.92 |
| <γ(-w;w,0,0)> | 219,62 | 3,65 | 60.17 |
| <γ(-2w;w,w,0)> | 362,87 | 4,11 | 88.29 |

**Table S3:** Experimental and theoretical vibrational assignements of MBPPC.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Mode | Experimental frequency (cm-1) | Theoretical frequencies (cm-1) | | IR intensity | Raman activity | Assignments (%) |
| FT-IR | Unscaled | Scaled |  |
| 1 | 3014 | 3650 | 3496 | 74,57 | 81.68 | νNH(100) |
| 2 |  | 3485 | 3339 | 13,69 | 555.35 | νNH(100) |
| 3 |  | 3274 | 3136 | 3,88 | 38.44 | νCH(99) |
| 4 |  | 3206 | 3071 | 9,3 | 102.29 | νCH(91) |
| 5 |  | 3193 | 3058 | 11,2 | 366.90 | νCH(91) |
| 6 |  | 3191 | 3057 | 6,67 | 187.78 | νCH(86) |
| 7 |  | 3189 | 3055 | 3,02 | 20.19 | νCH (82) |
| 8 |  | 3185 | 3051 | 16,67 | 58.14 | νCH (94) |
| 9 |  | 3177 | 3043 | 10,19 | 111.66 | νCH (96) |
| 10 |  | 3168 | 3035 | 0,04 | 76.17 | νCH(91) |
| 11 |  | 3159 | 3026 | 7,39 | 25.72 | νCH(90) |
| 12 |  | 3158 | 3025 | 10,59 | 62.62 | νCH(94) |
| 13 |  | 3133 | 3001 | 23,2 | 183.56 | νCH(91) |
| 14 |  | 3068 | 2939 | 31,92 | 61.10 | νCH(100) |
| 15 |  | 3011 | 2884 | 30,64 | 89.66 | νCH(95) |
| 16 |  | 3010 | 2883 | 87,98 | 162.02 | νCH(87) |
| 17 | 1656 | 1747 | 1674 | 320,98 | 347.68 | νOC(84) |
| 18 |  | 1668 | 1639 | 15,67 | 2701.37 | νNC(67) |
| 19 |  | 1644 | 1616 | 2,2 | 597.72 | νCC(58), δHCC (22) |
| 20 | 1603 | 1641 | 1613 | 231,78 | 4748.09 | νCC(62) δHCC (18) |
| 21 |  | 1618 | 1590 | 2,78 | 36.15 | νCC (59) |
| 22 |  | 1602 | 1575 | 8,17 | 489.29 | νCC (68) |
| 23 |  | 1593 | 1566 | 5,25 | 241.57 | νCC (45) |
| 24 | 1564 | 1570 | 1543 | 335,91 | 717.71 | δHNN (53) |
| 25 | 1512 | 1543 | 1517 | 380,17 | 617.36 | δHCC(41 |
| 26 |  | 1527 | 1501 | 56,78 | 13.58 | δHCC(55),δCCC(16) |
| 27 |  | 1504 | 1478 | 57,14 | 10.41 | δHCO (91) |
| 28 |  | 1494 | 1469 | 9,29 | 13.44 | δHCH (93) |
| 29 |  | 1493 | 1467 | 22,5 | 10.05 | νCC (20),δHCC(42) |
| 30 |  | 1476 | 1451 | 12,04 | 11.16 | δHCH(83) |
| 31 |  | 1474 | 1449 | 2,63 | 211.42 | νCC (29),δHNN 32 |
| 32 |  | 1452 | 1427 | 6,57 | 154.20 | νCC(44), δHCC (26) |
| 33 | 1406 | 1443 | 1419 | 24,69 | 336.12 | νNC(38),νCC(16),δHNN(13) |
| 34 |  | 1418 | 1394 | 14,5 | 842.61 | νNC (40), δCNN (11) |
| 35 | 1313 | 1387 | 1363 | 28,48 | 198.61 | νNC(11),δHCN(55) |
| 36 |  | 1361 | 1338 | 0,32 | 20.84 | δHCC(76) |
| 37 |  | 1340 | 1318 | 19,79 | 152.42 | δHCC(66) |
| 38 |  | 1331 | 1309 | 54,44 | 199.28 | νCC(66) |
| 39 |  | 1326 | 1303 | 0,96 | 42.39 | νCC(65) |
| 40 | 1250 | 1280 | 1259 | 326,76 | 16.42 | νOC (68) |
| 31 |  | 1279 | 1257 | 24,81 | 19.13 | νCC (62) |
| 42 |  | 1254 | 1232 | 162,72 | 137.02 | νCC(47),δHCC(13),δHCN(16) |
| 43 | 1169 | 1236 | 1215 | 301,22 | 493.82 | νNN (17), δHCC (19) |
| 44 |  | 1208 | 1188 | 0,6 | 36.96 | νCC(21),δHCC(71) |
| 45 |  | 1203 | 1183 | 14,66 | 11.56 | δHCO(77) |
| 46 |  | 1196 | 1176 | 61,21 | 3.29 | νNN(42),δHCC(11) |
| 47 | 1057 | 1193 | 1173 | 119,92 | 406.91 | νCC(20),δHCC(65) |
| 48 |  | 1186 | 1165 | 1,63 | 14.57 | νCC(14),δHCC(75 |
| 49 |  | 1170 | 1150 | 1,19 | 4.32 | δHCO(92) |
| 50 | 1032 | 1169 | 1149 | 164 | 1009.08 | νNN(55) |
| 51 |  | 1137 | 1118 | 21,48 | 13.40 | νCC(20),δHCC(59) |
| 52 |  | 1103 | 1084 | 1,97 | 14.25 | νCC(54),δHCC(27) |
| 53 |  | 1097 | 1078 | 12,65 | 90.71 | νNN(46) |
| 54 |  | 1068 | 1050 | 18,72 | 6.28 | νNC(13),δHCC(30) |
| 55 | 1016 | 1055 | 1038 | 76,48 | 16.07 | νCH(81) |
| 56 |  | 1049 | 1031 | 0,53 | 5.88 | νCC(45),δHCC(21),δCCC(15) |
| 57 |  | 1025 | 1008 | 0,25 | 7.90 | δCCC(79) |
| 58 |  | 1019 | 1001 | 5,48 | 113.69 | νCC(26),δCCC(46) |
| 59 |  | 1015 | 997 | 24,03 | 5.04 | δCNN(31),νCC(37) |
| 60 |  | 1001 | 984 | 0,05 | 0.38 | τHCCC(91) |
| 61 | 962 | 984 | 968 | 34,45 | 41.89 | δCNN(72) |
| 62 |  | 979 | 962 | 4,07 | 1.89 | τHCCC (73) |
| 63 |  | 978 | 962 | 0,08 | 5.96 | τHCCH(88) |
| 64 |  | 967 | 951 | 4,06 | 2.92 | τHCCN(83) |
| 65 |  | 944 | 928 | 7,29 | 3.19 | τHCNN(75) |
| 66 |  | 928 | 912 | 1,96 | 0.12 | τHCCC(81) |
| 67 | 900 | 915 | 899 | 91,76 | 3.99 | νCC(19),δNCO(47) |
| 68 | 848 | 856 | 841 | 57,53 | 14.61 | νCC(39),δNCO(37) |
| 69 |  | 850 | 836 | 2,83 | 3.04 | τHCCC(90) |
| 70 |  | 846 | 831 | 4,68 | 6.85 | τHCCC(68) |
| 71 | 827 | 844 | 829 | 56,67 | 0.49 | τHCCC(67),γOCCC(17) |
| 72 |  | 821 | 807 | 0,04 | 0.64 | τHCCC (93) |
| 73 |  | 786 | 773 | 3,05 | 44.36 | δCCC(43) |
| 74 |  | 781 | 768 | 8,32 | 6.21 | τHCCC(20),τCCCO(58) |
| 75 |  | 774 | 761 | 56,1 | 0.75 | τHCCC(47),τCCCO(22) |
| 76 |  | 737 | 724 | 0,17 | 2.25 | γOCCC(15),τCCCC(69) |
| 77 | 767 | 707 | 695 | 33,85 | 0.38 | τHCCC(12),τCCCC(73) |
| 78 |  | 703 | 691 | 3,09 | 3.80 | δCCC(51),τCCCC(11) |
| 79 |  | 696 | 684 | 6,4 | 1.20 | δCCC(10),τCCCC(54) |
| 80 |  | 662 | 651 | 5,97 | 1.03 | τHNNC(77) |
| 81 |  | 651 | 640 | 1,3 | 7.80 | νCC(10),δCCC(71),δCCC(10) |
| 82 |  | 635 | 624 | 0,25 | 4.81 | δCCC(80) |
| 83 |  | 610 | 599 | 18,52 | 6.55 | δCCN(67) |
| 84 | 669 | 564 | 554 | 101,34 | 1.30 | τHNCC(88) |
| 85 |  | 539 | 529 | 6,7 | 0.05 | τHCCC(19),γOCCC(49),τCCCC(10 |
| 86 |  | 536 | 526 | 17,79 | 0.78 | δCOC(51) |
| 87 |  | 530 | 521 | 16,71 | 0.98 | δHNC(11), τHNCC(43) |
| 88 |  | 516 | 507 | 12,08 | 14.33 | δHNC(36),τHNNC(11),τHNCC(18) |
| 89 |  | 499 | 490 | 14,54 | 0.71 | τHNNC(39) |
| 90 |  | 457 | 449 | 0,73 | 4.88 | δNCO(12),νCC(11),δHNC(16)τHNNC(15) |
| 91 |  | 428 | 420 | 0,26 | 0.82 | τCCCC (77) |
| 92 |  | 424 | 417 | 0,1 | 1.22 | δNCO (65) |
| 93 |  | 412 | 405 | 0,37 | 1.33 | τCCCC(83) |
| 94 |  | 410 | 403 | 8,44 | 5.22 | δCCC (46) |
| 95 |  | 402 | 395 | 0,86 | 3.02 | τCCCC(77) |
| 96 |  | 326 | 320 | 17,19 | 2.23 | δCNN(22),γCCCC(13) |
| 97 |  | 314 | 309 | 2,81 | 1.63 | δCCC(15),γCCCC(13) |
| 98 |  | 272 | 267 | 5,65 | 1.09 | δCNN(19),τCCNN(36) |
| 99 |  | 270 | 265 | 2,49 | 4.74 | δCNN (33),τCCNN(15) |
| 100 |  | 235 | 231 | 2,39 | 1.53 | τHCOC (68) |
| 101 |  | 222 | 218 | 11,45 | 1.71 | δCCN (69) |
| 102 |  | 200 | 196 | 2,28 | 0.50 | τCCCN(79) |
| 103 |  | 197 | 194 | 0,76 | 2.16 | δCCC(14) |
| 104 |  | 182 | 179 | 4,93 | 1.39 | τCCNN(44) |
| 105 |  | 117 | 115 | 1,32 | 1.32 | δCCC(58) |
| 106 |  | 114 | 112 | 0,86 | 0.72 | τCCOC(66),τCCNN(12) |
| 107 |  | 94 | 93 | 1,64 | 3.01 | τNCCN(43),γCCCC(24) |
| 108 |  | 78 | 76 | 4,42 | 0.78 | τCCOC (68) |
| 109 |  | 75 | 73 | 5,87 | 1.50 | δCCN(66) |
| 110 |  | 46 | 45 | 3,15 | 1.78 | τCCCN(81) |
| 111 |  | 43 | 42 | 0,85 | 5.24 | τCCCN(60) |
| 112 |  | 27 | 26 | 0,72 | 0.37 | δCNN(85) |
| 113 |  | 21 | 21 | 0,06 | 1.95 | τCCCO(86) |
| 114 |  | 14 | 14 | 1,21 | 0.15 | τCCNN(73) |

(ν- stretching; δ- in plane bending; γ- out of plane bending; τ- torsion).

**Table S4:** Binding score of MBPPC,Bactrim, Rifampicine, Raloxifene with Vibrio cholerae, Mycobacterium tuberculosis and Estrogen receptor.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Protein** | **Properties** | **Code** | **Ligand** | **Eint (kcal/mol)** | **EVDW** | **EH-bond** | **EElectrost** |
| Vibrio cholerae | Anti-microbial | 5UL7 | MBPPC | -114.11 | -101.27 | -12.84 | 0 |
| Bactrim | -114.88 | -81.54 | -33.34 | 0 |
| Mycobacterium tuberculosis | Anti-tubercular | 6VW0 | MBPPC | -127.90 | -117.43 | -10.45 | 0 |
| Rifampicine | -137.08 | -103.67 | -33.40 | 0 |
| Estrogen receptor | Anti-cancer | 5TOA | MBPPC | -102.01 | -73.45 | -28.56 | 0 |
| Raloxifene | -116.21 | -116.21 | 0 | 0 |