**S.Table 1.** The calculated molecular geometric parameters of BPT

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Selected Bond Lengths** | **Calculated** |  | **Selected Bond Lengths** | **Calculated** |
| C2-C1 /N12-N11 | 1.4068923/1.2838410 |  | N20-C18/ C31-C30 | 1.3597294/1.3984988 |
| C3-C2/ N13-C1 | 1.4015465/1.3671004 |  | N22-N20/ C32- C30 | 1.3679706/1.4001808 |
| C4-C3/ C14-N13 | 1.3832806/1.4420074 |  | C23-N22/ C33-C31 | 1.2976544/1.3943641 |
| C5-C4/ N17-C14 | 1.4146038/2.5397151 |  | C24-N17/ C35- C32 | 1.4632408/1.3929810 |
| C6-C5/ C18-N17 | 1.3851339/1.3898468 |  | C27-C24/ C37-C33 | 1.5405925/1.3932457 |
| N11-C2/ S19-C18 | 1.3796070/1.6683222 |  | C30-C27 | 1.5123607/ |
|  |  |  |  |  |
|  |  |  |  |  |
| **Selected Bond Angles** | **Calculated** |  | **Selected Bond Angles** | **Calculated** |
| C3-C2-C1/ N13-C1-C6 | 120.8301865/134.3827504 |  | N22-N20-C18/ C32- C30-C27 | 114.3170572/120.3675570 |
| C4-C3-C2/ C14-N13-C1 | 117.2973320/130.7069292 |  | C23-N22-N20/ C33-C31-C30 | 103.8927553/120.8434522 |
| C5-C4-C3/ N17-C14-N13 | 121.3883922 /140.1834183 |  | C24-N17-C14/ C35- C32-C30 | 98.5457276/120.7061524 |
| C6-C5-C4/ C18-N17-C14 | 122.0329470/137.5458150 |  | C27-C24-N17/ C37-C33-C31 | 112.7136214/120.0539618 |
| N11-C2-C1/ S19-C18-N17 | 108.5522469/128.9500806 |  | C30-C27-C24/ C31-C30-C27/ | 111.3564412/121.0299851 |
| N12-N11-C2/ N20-C18-N17 | 108.6885330/102.1430351 |  |  |  |
|  |  |  |  |  |
| **Selected Bond Dihedral Angles** | **Calculated** |  | **Selected Bond Dihedral Angles** | **Calculated** |
| C4-C3-C2-C1/ N13-C1-C6-C5 | 0.0825851/179.0589332 |  | N20-C18-N17-C14/ C30-C27-C24-N17 | 0.4567518/-178.0302611 |
| C5-C4-C3-C2/ C14-N13-C1-C6 | -0.1126026/-0.0470217 |  | N22-N20-C18-N17/ C31-C30-C27-C24 | 0.1189841/-98.6197479 |
| C6-C5-C4/ N17-C14-N13-C1 | -0.0763711/80.7575267 |  | C23-N22-N20-C18/ C32- C30-C27-C24 | 0.1140824/80.0054216 |
| N11-C2-C1-C6 / C18-N17-C14-N13 | 179.6844267/-7.9188506 |  | C24-N17-C14-N13/ C33-C31-C30-C27 | 170.4725491/178.6284845 |
| N12-N11-C2-C1/ S19-C18-N17-C14 | -0.0696815/-179.1307084 |  | C27-C24-N17-C14 C35- C32-C30-C27 | -93.5667092/-178.6081031 |
|  |  |  | C37-C33-C31-C30 | -0.0856134 |

**S.Table 2.** Natural charge and Mulliken distribution of **BPT**

|  |  |  |
| --- | --- | --- |
| ATOM Mulliken Charge NBO Charge  B3LYP/6-311+G(d,p) B3LYP/6-311+G(d,p) | | |
| 1C | -0.253134 | 0.13928 |
| 2 C | -0.212698 | 0.07455 |
| 3 C | -0.016310 | -0.18123 |
| 4 C | -0.290754 | -0.21475 |
| 5 C | -0.294299 | -0.18110 |
| 6 C | 0.399582 | -0.24179 |
| 7 H | 0.142549 | 0.22988 |
| 8 H | 0.136649 | 0.21521 |
| 9 H | 0.136975 | 0.21446 |
| 10 H | 0.050312 | 0.19644 |
| 11 N | 0.014865 | -0.21109 |
| 12 N | -0.016613 | 0.00211 |
| 13 N | 0.329566 | -0.27918 |
| 14 C | -1.015373 | -0.22936 |
| 15 H | 0.226638 | 0.26172 |
| 16 H | 0.155242 | 0.22523 |
| 17 N | 0.310150 | -0.47140 |
| 18 C | 0.345671 | 0.20359 |
| 19 S | -0.604405 | -0.17856 |
| 20 N | -0.131046 | -0.38752 |
| 21 H | 0.331291 | 0.42264 |
| 22 N | -0.044332 | -0.26684 |
| 23 C | 0.543668 | 0.37208 |
| 24 C | -0.830807 | -0.18821 |
| 25 H | 0.196344 | 0.25357 |
| 26 H | 0.153137 | 0.20543 |
| 27 C | -0.749170 | -0.40177 |
| 28 H | 0.149450 | 0.22398 |
| 29 H | 0.157816 | 0.19527 |
| 30 C | 0.965476 | -0.04154 |
| 31 C | -0.233429 | -0.20860 |
| 32 C | -0.122941 | -0.19612 |
| 33 C | -0.118245 | -0.19176 |
| 34 H | 0.141920 | 0.18984 |
| 35 C | -0.360206 | -0.19039 |
| 36 H | 0.119273 | 0.21107 |
| 37 C | -0.102175 | -0.20689 |
| 38 H | 0.127338 | 0.20959 |
| 39 H | 0.131573 | 0.21103 |
| 40 H | 0.130450 | 0.21112 |

**S.Table 3.** Calculated energy values of BPT

|  |  |
| --- | --- |
| Different parameters | B3LYP/6-311++G(d, p) |
| HOMO | -6,07 eV |
| LUMO | -1,75 eV |
| HOMO-1 | -6,26 eV |
| LUMO+1 | -0,84 eV |
| ∆E(HOMO-LUMO) | -4,32 eV |
| ∆E (HOMO-1-LUMO+1) | -5,41 eV |
| Χ | 3,91 eV |
| Η | 2,16 eV |
| Σ | 342,51 eV |
| Pi | -3,91 eV |
| Ω | 0,022 eV |
| S | 1,08 eV |
| ΔNmax | 49,27 eV |

**S.Table 4.** Theoretical and experimental 13C and 1H-NMR chemical shifts for BPT

|  |  |  |
| --- | --- | --- |
| Atom | Chemical shifts (ppm) in DMSO | |
|  | **Experimental** | **B3LYP/6-311+G(d,p)** |
| C1 | 132 | 139 |
| C2 | 146 | 152 |
| C3 | 120 | 125 |
| C4 | 127 | 128 |
| C5 | 127 | 133 |
| C6 | 109 | 112 |
| C14 | 46 | 45 |
| C18 | 168 | 178 |
| C23 | 146 | 152 |
| C24 | 41 | 49 |
| C27 | 33 | 37 |
| C30 | 137 | 144 |
| C31 | 129 | 134 |
| C32 | 128 | 134 |
| C33 | 129 | 133 |
| C35 | 129 | 134 |
| C37 | 128 | 131 |
| H7 | 8.1 | 8.3 |
| H8 | 7.4 | 7.61 |
| H9 | 7.4 | 7.75 |
| H10 | 7.52 | 7.63 |
| H15 | 5.12 | 6.26 |
| H16 | 5.19 | 5.67 |
| H21 | 12.5 | 8.87 |
| H25 | 3.32 | 3.39 |
| H26 | 3.32 | 3.62 |
| H28 | 3 | 3.49 |
| H29 | 3 | 2.75 |
| H34 | 7.24 | 7.60 |
| H36 | 7.24 | 7.87 |
| H38 | 7.4 | 7.61 |
| H39 | 7.4 | 7.71 |

**S.Table 5.** Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis for BPT

|  |  |  |
| --- | --- | --- |
| Donor NBO | Acceptor NBO | E2 (kcal/mol) |
| BD (1) C1 - C2 | BD\*(1) N13 - C14 | 5.15 |
| BD (2) C1 - N13 | LP (1) C2 | 11.90 |
| BD (2) C1 - N13 | BD\*(2) C5 - C6 | 5.03 |
| BD (2) C1 - N 13 | BD\*(2) N11 - N12 | 19.56 |
| BD (1) C3 - C4 | BD\*(1) C2 - N11 | 6.09 |
| BD (2) C3 - C4 | LP (1) C2 | 46.59 |
| BD (2) C3 - C4 | BD\*(2) C5 - C6 | 20.78 |
| BD (1) C5 - C6 | BD\*(1) C1 - N13 | 6.81 |
| BD (2) C5 - C6 | BD\*(2) C1 - N13 | 36.01 |
| BD (2) C5 - C6 | BD\*(2) C3 - C4 | 17.26 |
| BD (2) N 11 - N12 | LP (1) C2 | 17.73 |
| BD (1) C 14 - H16 | BD\*(1) N12 - N13 | 5.00 |
| BD (1) C14 - H16 | BD\*(1) N18 - C19 | 5.41 |
| BD (1) N17 - N27 | BD\*(1) N27 - H28 | 7.29 |
| BD (1) N27 - H28 | BD\*(1) N17 - C19 | 11.88 |
| BD (1) N27 - H28 | BD\*(1) N17 - N27 | 8.72 |
| BD (1) S29 - C30 | BD\*(1) S29 - C30 | 8.48 |
| LP (1) C2 | BD\*(2) C1 - N13 | 280.01 |
| LP (1) C2 | BD\*(2) C3 - C4 | 61.07 |
| LP (1) C2 | BD\*(2) N11 - N12 | 72.44 |
| LP (1) N11 | BD\*(1) N12 - N13 | 12.38 |
| LP (1) N12 | BD\*(1) C1 - N13 | 5.71 |
| LP (1) N12 | BD\*(1) C2 - N11 | 7.97 |
| LP (1) N17 | BD\*(1) N27 - H28 | 13.50 |
| LP (1) N17 | BD\*(1) N27 - C30 | 5.32 |
| LP (1) N18 | BD\*(2) N17 - C19 | 50.18 |
| LP (1) N18 | BD\*(1) S29 - C30 | 68.20 |
| LP (1) N27 | BD\*(2) N17 - C19 | 45.54 |
| LP (1) N27 | BD\*(1) S29 - C30 | 80.63 |
| LP (2) S29 | BD\*(1) N27 - C30 | 10.14 |
| BD\*(2) C1 - N13 | BD\*(2) C5 - C6 | 70.39 |
| BD\*(2) C1 - N13 | BD\*(2) N11 - N12 | 36.61 |

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **S.Tablo.****6.** Potential Energy Distribution (PED) analysis of BPT by VEDA software   |  |  |  | | --- | --- | --- | | Vibrations | Atom | PED % | | STRE | N20H21 | 3668(100) | | STRE | C3H7 | 3203(70), 3196(14), 3185(13) | | STRE | C4H8 | 3203(20), 3185(47), 3173(31) | | STRE | C5H9 | 3196(24), 3185(14), 3173(56) | | STRE | C6H10 | 3196(60), 3185(25), 3173(10) | | STRE | C15H14 | 3093(89), 3032(10) | | STRE | C33H38 | 3190(23), 3179(42), 3170(20), 3151(13) | | STRE | C35H39 | 3190(25), 3179(43), 3159(25) | | STRE | C37H40 | 3190(47), 3170(44) | | STRE | C14H16 | 3093(10), 3032(89) | | STRE | C24H25 | 3117(54), 3083(12), 3065(31) | | STRE | C24H26 | 3117(37), 3065(61) | | STRE | C27H28 | 3083(66), 3038(28) | | STRE | C27H29 | 3083(22), 3038(68) | | STRE | C31H34 | 3151(84) | | STRE | C32H36 | 3179(10), 3170(20), 3159(66) | | STRE | N22C23 | 1625(59) | | STRE | C4C3 | 1655(21), 1524(17), 1415(10) | | STRE | C5C6 | 1655(14), 1624(11), 1524(11), 1415(15) | | STRE | N11N12 | 1485(10), 1378(13), 1359(25) | | STRE | C32C35 | 1644(30), 1342(17) | | STRE | C33C31 | 1342(15), 1107(10) | | STRE | C35C37 | 1342(15), 1050(24), 1017(13) | | STRE | C37C33 | 1623(27), 1050(18), 1017(11) | | STRE | C3C2 | 1655(14), 1415(10), 638(11) | | STRE | C6C1 | 1655(17), 1415(10), 784(14), 638(11) | | STRE | C31C30 | 1623(19), 1342(16) | | STRE | N20C18 | 1496(20), 1249(39) | | STRE | N13C1 | 1524(13), 1430(21), 1152(10) | | STRE | N11C2 | 1263(41) | | STRE | N17C23 | 1482(11), 1455(12), 976(16) | | STRE | N12N13 | 1093(17), 912(34) | | STRE | N20N22 | 1124(34), 1107(19) | | STRE | N13C14 | 1430(21) | | STRE | C14C23 | 1625(10), 1455(11), 794(11) | | STRE | C30C27 | 1222(35), 852(12) | | STRE | N17C24 | 1348(16) | | STRE | C27C24 | 1029(66) | | STRE | S19C18 | 588(14), 538(10), 447(12) | | BEND | C5C6C1 | 1129(14), 961(16), 912(14) | | BEND | C1N13N12 | 1624(10), 814(14), 638(11) | | BEND | N17C23N22 | 721(11) | | BEND | C30C27C24 | 269(17), 95(12), 62(18) | | BEND | H21N20N22 | 1496(26), 1455(10), 1249(24) | | BEND | H7C3C4 | 1485(15), 1324(10), 1152(26), 1023(11) | | BEND | H8C4C5 | 1524(20), 1324(12), 1152(21) | | BEND | H9C5C6 | 1524(12), 1430(15), 1184(17), 1183(15) | | BEND | H10C6C5 | 1485(15), 1324(12) | | BEND | H15C14C23 | 1304(12), 1298(15), 1093(23) | | BEND | H38C33C37 | 1527(17), 1484(10), 1363(10), 1204(16) 1182(10), 1050(11) | | BEND | H39C35C37 | 1527(17), 1484(11), 1204(20) | | BEND | H40C37C35 | 1484(26), 1183(13), 1182(16) | | BEND | H16C14H15 | 1470(48), 1455(21) | | BEND | H25C24C27 | 1400(11), 1348(16) | | BEND | H26C24H25 | 1499(23), 1482(28), 1455(12), 1400(13) | | BEND | H28C27C30 | 1216(16), 1048(24) | | BEND | H29C27H28 | 1499(48), 1496(21), 1482(11) | | BEND | H34C31C33 | 1527(14), 1363(19), 1204(19) | | BEND | H36C32C35 | 1527(16), 1363(18), 1204(19) | | BEND | C4C3C2 | 1624(13), 1263(10), 1023(10), 961(11), 912(13), 538(14) | | BEND | N11N12N13 | 1129(21), 1023(10), 961(12) | | BEND | C32C35C37 | 1050(11), 1017(27), 635(24) | | BEND | C33C31C30 | 635(20) | | BEND | C35C37C33 | 1017(19), 852(18) | | BEND | C37C33C31 | 1017(14), 635(35) | | BEND | C3C2N11 | 1624(11), 1023(16), 481(25) | | BEND | C6C1C2 | 1023(19), 538(11), 481(10) | | BEND | C31C30C27 | 351(46), 337(19) | | BEND | C18N20N22 | 1182(18) | | BEND | C2N11N12 | 1624(13), 1023(13), 961(10) | | BEND | N12N13C14 | 481(25), 240(23) | | BEND | N20N22C23 | 976(27) | | BEND | N13C14C23 | 814(14), 322(10), 156(11), 43(19) | | BEND | C14C23N22 | 156(20) | | BEND | C24N17C23 | 447(23), 253(26) | | BEND | C27C24N17 | 337(22), 110(10), 62(12) | | BEND | S19C18N20 | 447(25), 253(17), 240(14) | | TORS | H21N20N22C23 | 662(22), 515(65) | | TORS | H10C6C5C4 | 994(11), 958(31), 856(27), 752(14), 432(12) | | TORS | H15C14C23N17 | 1470(16), 961(14) | | TORS | H38C33C37C35 | 1006(14), 988(32), 860(22) | | TORS | H39C35C37C33 | 1006(26), 988(20), 860(24) | | TORS | H40C37C35C32 | 1006(32), 930(27), 721(11) | | TORS | H16C14C23N17 | 1470(19), 1359(13) | | TORS | H25C24N17C18 | 1400(19) | | TORS | H26C24N17C18 | 1400(20), 1378(11) | | TORS | H28C27C30C31 | 1322(21), 768(10) | | TORS | H29C27C30C31 | 1322(17) | | TORS | H34C31C33C37 | 988(16), 930(25), 860(27), 413(13) | | TORS | H36C32C35C37 | 988(20), 930(24), 860(24), 413(12) | | TORS | C4C3C2C1 | 994(12), 432(22) | | TORS | C5C6C1N13 | 577(26), 226(42) | | TORS | N11N12N13C14 | 322(19), 156(16), 43(28) | | TORS | C32C35C37C33 | 1006(14), 709(13), 413(40) | | TORS | C33C31C30C27 | 509(14), 269(10), 95(22), 62(18) | | TORS | CC37C33C31 | 709(11), 509(21), 413(27), 269(11) | | TORS | C37C33C31C30 | 768(18), 760(13), 709(29) | | TORS | C31C30C27C24 | 67(10), 26(27), 20(30) | | TORS | C18N20N22C23 | 678(17), 662(12), 298(22), 110(10), 95(13) | | TORS | C2N11N12N13 | 764(19), 752(10), 668(25) | | TORS | N17C23N22N20 | 662(45), 515(12) | | TORS | N12N13C14C23 | 26(44), 20(10), 16(21) | | TORS | N13C14C23N17 | 10(65) | | TORS | C30C27C24N17 | 20(35), 16(39) | | TORS | C27C24N17C18 | 67(35) | | OUT | S19N20N17C18 | 678(42), 515(10), 298(15), 110(10) | | OUT | C3C1N11C2 | 764(12), 577(15), 432(12), 322(11) | | OUT | C6N13C2C1 | 752(17), 432(39), 226(20) | | OUT | C1C14N12N13 | 668(16), 577(10), 322(23), 156(11), 43(10) | | OUT | C14N17N22C23 | 298(44), 110(10) | | OUT | C24C18C23N17 | 337(12), 95(14), 62(32) | |  |  |
|  |  |  |
| **S.Table 7.** Temperature dependence of thermodynamic properties of BPT at B3LYP / 6-311+G(d,p)   |  |  |  |  | | --- | --- | --- | --- | | (K) | Som (J/mol K) | Cop.m(J/mol K) | Hom (J/mol K) | | 100 | 198,852 | 30,901 | 102,734 | | 200 | 202,965 | 52,13 | 131,793 | | 298,15 | 209,262 | 76,448 | 157,868 | | 400 | 218,325 | 101,066 | 184,425 | | 500 | 229,495 | 121,661 | 209,71 | | 600 | 242,524 | 138,3 | 233,777 | | 700 | 257,045 | 151,649 | 256,449 | | 800 | 272,77 | 162,478 | 277,69 | | 900 | 289,477 | 171,392 | 297,598 | | 1000 | 306,999 | 178,823 | 316,255 | |  |  |

**S.Table 8.** The UV-Vis. parameters of BPT in Different solvents.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| λ (nm) | | E (eV) | MOs contribution | Solvent |
| Experimental | Theoretical |  |  |  |
| 264 | 313 | 31925.0374087 | H->L (100%) | Dioxane |
| 290 | 34441.4872272 | H-1->L (100%) |
| 277 | 36010.2355916 | H-1->L+1 (49%), H-1->L+3 (37%),  H-1->L+2 (9%) |
| - | 316 | 31641.9368041 | H->L (100%) | CCl4 |
| 294 | 33963.2004508 | H-1->L (100%) |
| 281 | 35552.1126759 | H-1->L+1 (37%), H-1->L+3 (51%),  H-1->L+2 (6%) |
| - | 315 | 315.714377052 | H->L (100%) | Toluene |
| 293 | 293.97556138 | H-1->L (100%) |
| 280 | 280.91397728 | H-1->L+1 (38%), H-1->L+3 (49%), H-1->L+2 (6%) |
| 261 | 311 | 32136.3546691 | H->L (100%) | CH2Cl2 |
| 287 | 34804.4367202 | H-1->L (100%) |
| 275 | 36340.9229075 | H-1->L+1 (58%), H-1->L+2 (11%), H-1->L+3 (26%) |
| 262 | 312 | 31962.1389124 | H->L (100%) | Chloroform |
| 289 | 34503.5919182 | H-1->L (100%) |
| 277 | 36057.8223029 | H-1->L+1 (51%), H-1->L+2 (10%), H-1->L+3 (35%) |
| - | 311 | 32094.4138388 | H->L (100%) | THF |
| 287 | 34731.8468216 | H-1->L (100%) |
| 275 | 36275.5919987 | H-1->L+1 (56%), H-1->L+2 (11%), H-1->L+3 (28%) |
| - | 309 | 32308.1507625 | H->L (100%) | Acetonitrile |
| 284 | 35106.0880767 | H-1->L (100%) |
| 272 | 36632.8956108 | H-1->L+1 (65%), H-1->L+2 (12%), H-1->L+3 (19%) |
| - | 309 | 32262.9837144 | H->L (100%) | Acetone |
| 285 | 35026.2391882 | H-1->L (99%) |
| 273 | 36557.0794944 | H-1->L+1 (63%), H-1->L+2 (12%), H-1->L+3 (20%) |
| 270 | 309 | 32322.6687422 | H->L (100%) | DMSO |
| 284 | 35130.2847095 | H-1->L (99%) |
| 272 | 36649.0266993 | H-1->L+1 (65%), H-1->L+2 (13%), H-1->L+3 (18%) |
| 250 | 309 | 32281.5344663 | H->L (100%) | Ethanol |
| 285 | 35058.5013653 | H-1->L (99%) |
| 273 | 36586.9220083 | H-1->L+1 (64%), H-1->L+2 (12%), H-1->L+3 (20%) |
| 281 |  |  |  | Formic Acid |
| 304 |  |  |  | Pyridine |

**S.Table 9.** Docking analysis of BPT

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Name of proteins | Pub Chem ID | Conventional Hydrogen Bond | Docking Score( Binding Free Energy)Kcal/mol | RMSD (A) |
| Streptomyces  sp. | 1CHK | N(Benztriazole)…GLY4 | -4.7 | 2.349 |
| Hordeum  Vulgare | 1CNS | N-H…ASN199 | -7.3 | 1.828 |
| Aspergillus  niger | 3EQA | N(Benztriazole)…SER455  N(triazole)… ER455  S…ARG453 | -6.2 | 1.805 |
| Candida  albicans | 4HOE | N(Benzotriazole)…GLY23  N(triazole)… GLY23 | -7.6 | 51.691 |