**Ranking of Descriptors according to their frequency**

|  |  |  |
| --- | --- | --- |
| **Descriptor Number** | **Name of Descriptor** | **Frequency** |
| 21 | aryl\_halide\_.C1\_electrostatic\_charge | 0 |
| 115 | ligand\_V7\_intensity | 1 |
| 41 | aryl\_halide\_electronegativity | 3 |
| 80 | ligand\_.C4\_electrostatic\_charge | 3 |
| 23 | aryl\_halide\_.C2\_electrostatic\_charge | 4 |
| 39 | aryl\_halide\_V3\_intensity | 4 |
| 119 | ligand\_V9\_intensity | 4 |
| 1 | additive\_.C3\_NMR\_shift | 5 |
| 53 | base\_molecular\_volume | 5 |
| 58 | ligand\_.C10\_electrostatic\_charge | 5 |
| 67 | ligand\_.C15\_NMR\_shift | 5 |
| 87 | ligand\_.C8\_NMR\_shift | 5 |
| 111 | ligand\_V5\_intensity | 5 |
| 11 | additive\_V1\_frequency | 6 |
| 27 | aryl\_halide\_.C4\_electrostatic\_charge | 6 |
| 69 | ligand\_.C16\_NMR\_shift | 6 |
| 75 | ligand\_.C2\_NMR\_shift | 6 |
| 90 | ligand\_.C9\_electrostatic\_charge | 6 |
| 116 | ligand\_V8\_frequency | 6 |
| 3 | additive\_.C4\_NMR\_shift | 7 |
| 5 | additive\_.C5\_NMR\_shift | 7 |
| 15 | additive\_hardness | 7 |
| 29 | aryl\_halide\_.H2\_electrostatic\_charge | 7 |
| 32 | aryl\_halide\_E\_HOMO | 7 |
| 46 | aryl\_halide\_surface\_area | 7 |
| 86 | ligand\_.C7\_electrostatic\_charge | 7 |
| 89 | ligand\_.C9\_NMR\_shift | 7 |
| 114 | ligand\_V7\_frequency | 7 |
| 16 | additive\_molecular\_volume | 8 |
| 79 | ligand\_.C4\_NMR\_shift | 8 |
| 105 | ligand\_V2\_intensity | 8 |
| 33 | aryl\_halide\_E\_LUMO | 9 |
| 40 | aryl\_halide\_dipole\_moment | 9 |
| 49 | base\_E\_LUMO | 9 |
| 54 | base\_molecular\_weight | 9 |
| 94 | ligand\_.H3\_electrostatic\_charge | 9 |
| 102 | ligand\_V1\_frequency | 9 |
| 9 | additive\_E\_HOMO | 10 |
| 30 | aryl\_halide\_.H3\_NMR\_shift | 10 |
| 44 | aryl\_halide\_molecular\_weight | 10 |
| 55 | base\_ovality | 10 |
| 96 | ligand\_.H4\_electrostatic\_charge | 10 |
| 104 | ligand\_V2\_frequency | 10 |
| 10 | additive\_E\_LUMO | 11 |
| 26 | aryl\_halide\_.C4\_NMR\_shift | 11 |
| 68 | ligand\_.C15\_electrostatic\_charge | 11 |
| 100 | ligand\_V10\_frequency | 11 |
| 103 | ligand\_V1\_intensity | 11 |
| 108 | ligand\_V4\_frequency | 11 |
| 118 | ligand\_V9\_frequency | 11 |
| 17 | additive\_molecular\_weight | 12 |
| 61 | ligand\_.C12\_NMR\_shift | 12 |
| 78 | ligand\_.C3\_electrostatic\_charge | 12 |
| 81 | ligand\_.C5\_NMR\_shift | 12 |
| 84 | ligand\_.C6\_electrostatic\_charge | 12 |
| 35 | aryl\_halide\_V1\_intensity | 13 |
| 48 | base\_E\_HOMO | 13 |
| 59 | ligand\_.C11\_NMR\_shift | 13 |
| 63 | ligand\_.C13\_NMR\_shift | 13 |
| 65 | ligand\_.C14\_NMR\_shift | 13 |
| 66 | ligand\_.C14\_electrostatic\_charge | 13 |
| 70 | ligand\_.C16\_electrostatic\_charge | 13 |
| 74 | ligand\_.C1\_electrostatic\_charge | 13 |
| 76 | ligand\_.C2\_electrostatic\_charge | 13 |
| 77 | ligand\_.C3\_NMR\_shift | 13 |
| 109 | ligand\_V4\_intensity | 13 |
| 37 | aryl\_halide\_V2\_intensity | 14 |
| 62 | ligand\_.C12\_electrostatic\_charge | 14 |
| 73 | ligand\_.C1\_NMR\_shift | 14 |
| 82 | ligand\_.C5\_electrostatic\_charge | 14 |
| 85 | ligand\_.C7\_NMR\_shift | 14 |
| 107 | ligand\_V3\_intensity | 14 |
| 110 | ligand\_V5\_frequency | 14 |
| 113 | ligand\_V6\_intensity | 14 |
| 117 | ligand\_V8\_intensity | 14 |
| 120 | ligand\_dipole\_moment | 14 |
| 28 | aryl\_halide\_.H2\_NMR\_shift | 15 |
| 38 | aryl\_halide\_V3\_frequency | 15 |
| 51 | base\_electronegativity | 15 |
| 71 | ligand\_.C17\_NMR\_shift | 15 |
| 72 | ligand\_.C17\_electrostatic\_charge | 15 |
| 88 | ligand\_.C8\_electrostatic\_charge | 15 |
| 91 | ligand\_.H11\_NMR\_shift | 15 |
| 99 | ligand\_.P1\_electrostatic\_charge | 15 |
| 12 | additive\_V1\_intensity | 16 |
| 25 | aryl\_halide\_.C3\_electrostatic\_charge | 16 |
| 31 | aryl\_halide\_.H3\_electrostatic\_charge | 16 |
| 47 | base\_.N1\_electrostatic\_charge | 16 |
| 83 | ligand\_.C6\_NMR\_shift | 16 |
| 98 | ligand\_.H9\_electrostatic\_charge | 16 |
| 101 | ligand\_V10\_intensity | 16 |
| 14 | additive\_electronegativity | 17 |
| 34 | aryl\_halide\_V1\_frequency | 17 |
| 36 | aryl\_halide\_V2\_frequency | 17 |
| 42 | aryl\_halide\_hardness | 17 |
| 45 | aryl\_halide\_ovality | 17 |
| 56 | base\_surface\_area | 17 |
| 64 | ligand\_.C13\_electrostatic\_charge | 17 |
| 112 | ligand\_V6\_frequency | 17 |
| 2 | additive\_.C3\_electrostatic\_charge | 18 |
| 8 | additive\_.O1\_electrostatic\_charge | 18 |
| 18 | additive\_ovality | 18 |
| 20 | aryl\_halide\_.C1\_NMR\_shift | 18 |
| 57 | ligand\_.C10\_NMR\_shift | 18 |
| 60 | ligand\_.C11\_electrostatic\_charge | 18 |
| 4 | additive\_.C4\_electrostatic\_charge | 19 |
| 6 | additive\_.C5\_electrostatic\_charge | 19 |
| 50 | base\_dipole\_moment | 19 |
| 52 | base\_hardness | 19 |
| 95 | ligand\_.H4\_NMR\_shift | 19 |
| 106 | ligand\_V3\_frequency | 19 |
| 43 | aryl\_halide\_molecular\_volume | 20 |
| 92 | ligand\_.H11\_electrostatic\_charge | 20 |
| 13 | additive\_dipole\_moment | 21 |
| 19 | additive\_surface\_area | 21 |
| 93 | ligand\_.H3\_NMR\_shift | 21 |
| 97 | ligand\_.H9\_NMR\_shift | 21 |
| 7 | additive\_.N1\_electrostatic\_charge | 22 |
| 22 | aryl\_halide\_.C2\_NMR\_shift | 25 |
| 24 | aryl\_halide\_.C3\_NMR\_shift | 34 |