|  |
| --- |
|  |
| **S1**. Molecular structure (with numbering) |

**S2: Computed molecular orbital calculations of sumatriptan**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Atom | **Atom Type(MM2)** | **Charge (MM2)** | **Atom Type (MMFF94)** | **Charge (MMFF94)** | **Mulliken Charges (Mopac Interface)** | **charge avarag** |
| C(3) | C Alkane | 0 | ALKYL CARBON, SP3 | 0.27 | -0.380745 | -0.05537 |
| N(4) | N Pyrrole | 0 | AROMATIC 5-RING NITROGEN WITH p LONE PAIR | 0.3172 | -0.734275 | -0.20854 |
| C(5) | C Alkene | 0 | AROMATIC 5-RING C, a TO N, O, OR S | -0.3016 | -0.031634 | -0.16662 |
| C(6) | C Alkene | 0 | AROMATIC 5-RING C, b TO N, O, OR S | -0.181 | -0.146458 | -0.16373 |
| C(7) | C Alkene | 0 | AROMATIC 5-RING C, b TO N, O, OR S | -0.15 | -0.253354 | -0.20168 |
| C(8) | C Alkene | 0 | AROMATIC 5-RING C, a TO N, O, OR S | -0.2046 | 0.119213 | -0.04269 |
| S(9) | S Sulfone | 0 | SULFONAMIDE SULFUR | 1.295 | 2.50373 | 1.899365 |
| O(10) | O Oxo | 0 | ONE OF 2 TERMINAL O'S ON SULFUR | -0.65 | -0.874269 | -0.76213 |
| O(11) | O Oxo | 0 | ONE OF 2 TERMINAL O'S ON SULFUR | -0.65 | -0.888736 | -0.76937 |
| C(12) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | 0.16 | 0.144389 | 0.152195 |
| C(13) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | -0.009 | -0.568528 | -0.28876 |
| C(14) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | -0.15 | -0.031789 | -0.09089 |
| C(15) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | -0.15 | -0.331819 | -0.24091 |
| C(16) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | 0.16 | 0.099835 | 0.129918 |
| N(17) | N Pyridine | 0 | AROMATIC NITROGEN WITH s LONE PAIR | -0.62 | -0.490766 | -0.55538 |
| C(18) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | 0.053 | -0.138461 | -0.04273 |
| C(19) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | 0.19 | 0.218984 | 0.204492 |
| C(20) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | -0.15 | -0.283203 | -0.2166 |
| C(21) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | -0.15 | -0.135921 | -0.14296 |
| C(22) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | -0.15 | -0.252573 | -0.20129 |
| C(23) | C Alkene | 0 | AROMATIC CARBON, E. G. IN BENZENE, PYRIDIN | -0.15 | -0.14189 | -0.14595 |
| F(24) | F | 0 | FLUORINE | -0.19 | -0.137847 | -0.16392 |
| H(25) | H | 0 | H ATTACHED TO C | 0 | 0.196761 | 0.098381 |
| H(26) | H | 0 | H ATTACHED TO C | 0 | 0.199807 | 0.099904 |
| H(27) | H Amine | 0 | GENERIC HYDROGEN ON SP3 NITROGEN, E. G., IN AMINES | 0.36 | 0.319057 | 0.339529 |
| H(28) | H | 0 | H ATTACHED TO C | 0 | 0.18502 | 0.09251 |
| H(29) | H | 0 | H ATTACHED TO C | 0 | 0.193431 | 0.096716 |
| H(30) | H | 0 | H ATTACHED TO C | 0 | 0.164282 | 0.082141 |
| H(31) | H | 0 | H ATTACHED TO C | 0.15 | 0.244081 | 0.197041 |
| H(32) | H | 0 | H ATTACHED TO C | 0.15 | 0.219664 | 0.184832 |
| H(33) | H | 0 | H ATTACHED TO C | 0.15 | 0.266468 | 0.208234 |
| H(34) | H | 0 | H ATTACHED TO C | 0.15 | 0.228459 | 0.18923 |
| H(35) | H | 0 | H ATTACHED TO C | 0.15 | 0.228801 | 0.189401 |
| H(36) | H | 0 | H ATTACHED TO C | 0.15 | 0.224924 | 0.187462 |
| H(37) | H | 0 | H ATTACHED TO C | 0.15 | 0.237327 | 0.193664 |
| H(38) | H | 0 | H ATTACHED TO C | 0.15 | 0.208661 | 0.179331 |
| H(39) | H | 0 | H ATTACHED TO C | 0.15 | 0.209594 | 0.179797 |
| H(40) | H | 0 | H ATTACHED TO C | 0.15 | 0.213752 | 0.181876 |

**S 3: Analytical methods for vonoprazan**

|  |  |  |  |
| --- | --- | --- | --- |
| **Method** | **Linear Range** | **LOD**  | **Ref.** |
| HPLC | 0.299–29.885 µg mL-1 | 0.090 µg mL-1 | Liu et al, 2016 |
| LC/ tandem mass spectrometry | 0.1 to 100 ng mL-1 | ND | Yoneyama, et al., 2016 |
| LC/ tandem mass spectrometry | 1–2000 ng mL-1 | ND | Qiao et al., 2017 |
| Differential pulse voltammetry | 0.99-20.00 µg mL-1 | 0.24 µg mL-1 | This work |