Pharm2D2Point Fingerprint Features with Bit Positions

Table 1: Pharm2D2 Fingerprint Features and Properties

Bit Position	**Feature/Property**
0	Alkyl chain
1	Primary carbon
2	Secondary carbon
3	Tertiary carbon
4	Quaternary carbon
5	Methyl group (CH_3)
6	Methylene group (CH_2)
7	Alkene
8	Alkyne
9	Aromatic ring
10	Alcohol group (OH)
11	Ether group (C–O–C)
12	Amine group (NH_2)
13	Amide group (C=O-NH_2)
14	Carboxyl group (COOH)
15	Carbonyl group (C=O)
16	Ester group (RCOOR')
17	Thiol group (SH)
18	Sulfide group (C-S-C)
19	**Hydrogen bond acceptor (HBA)**
20	**Hydrogen bond donor (HBD)**
21	Halogen (Cl, Br, I)
22	Fluorine atom (F)
23	Nitrogen atom
24	Oxygen atom
25	Sulfur atom
26	Phosphorus atom
27	Benzene ring
28	Aromatic nitrogen

Bit Position	Feature/Property
29	Aromatic oxygen
30	Aromatic sulfur
31	Aromatic phosphorus
32	Pyrrole-like nitrogen (aromatic N-H)
33	Pyridine-like nitrogen (aromatic N)
34	Indole group
35	Pyrimidine group
36	Alcohol group in hydroxyl (-OH)
37	Hydrogen attached to carbon
38	Carbonyl oxygen (C=O)
39	C-H bond
40	C=C double bond
41	CC triple bond
42	C-O single bond
43	C-N single bond
44	C-S single bond
45	C-F bond
46	C-Cl bond
47	C-Br bond
48	C-I bond
49	Hydrogen attached to oxygen (in OH)
50	Hydrogen attached to nitrogen
51	Hydrogen attached to sulfur
52	Hydrophobic group (general)
53	Hydrophilic group (general)
54	Acidic group
55	Basic group
56	Polar group
57	Non-polar group
58	Positively charged group
59	Negatively charged group
60	Neutral group
61	Aromatic carbon (in aromatic ring)
62	Aliphatic carbon
63	Unsaturated carbon
64	Saturated carbon
65	Aromatic CH group
66	Hydrophobic ring
67	Polar ring
68	Electron-rich region
69	Electron-poor region
70	Sterically hindered region

Bit Position	Feature/Property
71	Linear chain
72	Branched chain
73	Cyclic structure
74	Double bond (bond)
75	Triple bond
76	Aromatic system
77	Heteroatom in aromatic ring
78	- stacking interaction
79	Cationic center
80	Anionic center
81	Hydrogen attached to carbon in alkyl
82	**Hydrophobic region (ethyl group)**
83	**Hydrophobic region (ethyl group)**
84	Hydrophobic alkyl chain
85	Hydrophobic ethyl chain
86	Hydrophobic methyl group
87	Hydrophobic methylene group
88	Hydrophobic aromatic system
89	Hydrophobic aliphatic system
90	Hydrophobic cyclic system
91	Non-polar surface
92	Polar surface
93	Hydrophobic alkane
94	Hydrophobic alkene
95	Hydrophobic alkyne
96	Hydrophobic saturated chain
97	Hydrophobic unsaturated chain
98	Hydrophobic tail
99	Hydrophilic head
100	Hydrophobic head
101	Van der Waals interaction site
102	Hydrogen bond interaction site
103	Electrostatic interaction site
104	Hydrophobic interaction site
105	Aromatic hydrophobic interaction
106	Aliphatic hydrophobic interaction
107	C-H interaction
108	N-H interaction
109	O-H interaction
110	S-H interaction
111	Cation-pi interaction
112	Anion-pi interaction

Bit Position	Feature/Property
113	Hydrophobic aromatic ring interaction
114	Hydrophobic carbon interaction
115	Hydrophobic heteroatom interaction
116	Hydrophobic backbone interaction
117	Hydrophobic residue interaction
118	Hydrophobic loop interaction
119	Hydrophobic side chain interaction
120	Hydrophilic backbone interaction
121	Hydrophilic side chain interaction
122	Hydrophilic loop interaction
123	Hydrophilic tail interaction
124	Hydrophilic aliphatic system
125	Hydrophilic aromatic system
126	Hydrophilic region
127	Hydrophobic branch
128	Hydrophobic surface
129	Hydrophilic surface
130	Hydrophobic interaction distance (short)
131	Hydrophobic interaction distance (medium)
132	Hydrophobic interaction distance (long)
133	Water-excluded surface
134	Hydrophilic-water interaction