**Table S1:** Scaffold, structures, and corresponding bioactive phytochemicals organization.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Scaffold** | Alkaloids | Betalains | Coumarins | Flavonoids | Organics | Phenolics | Steroids | Terpenoids | Xanthenones |
| **Structures** | A-1 to A-7 | B-1 to B-13 | C-1 to C-23 | F-1 to F-130 | O-1 to O-64 | P-1 to P-158 | S-1 to S-15 | T-1 to T-58 | X-1 to X-19 |
| **Table** | Table S2 | Table S3 | Table S4 | Table S5 | Table S6 | Table S7 | Table S8 | Table S9 | Table S10 |