**S1.** Values of variables in experiments and results obtained for cefazolin.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| RUN | pH | Temperature  (˚C) | Contact Time  (min) | Init.Cons. Drug (mg/L) | Comp. Dosage (g) | response (% ) |
| 1 | 6 | 50 | 90 | 30 | 0.03 | 30 |
| 2 | 8 | 60 | 60 | 40 | 0.04 | 45 |
| 3 | 8 | 40 | 60 | 20 | 0.02 | 40 |
| 4 | 6 | 30 | 90 | 30 | 0.03 | 66 |
| 5 | 4 | 60 | 60 | 20 | 0.02 | 11 |
| 6 | 2 | 50 | 90 | 30 | 0.03 | 12 |
| 7 | 8 | 40 | 120 | 20 | 0.04 | 60 |
| 8 | 8 | 60 | 120 | 20 | 0.04 | 49 |
| 9 | 4 | 40 | 60 | 20 | 0.02 | 13 |
| 10 | 4 | 60 | 120 | 20 | 0.04 | 24 |
| 11 | 6 | 70 | 90 | 30 | 0.03 | 66 |
| 12 | 6 | 50 | 90 | 10 | 0.03 | 20 |
| 13 | 6 | 50 | 90 | 30 | 0.03 | 30.5 |
| 14 | 8 | 50 | 120 | 20 | 0.02 | 63 |
| 15 | 4 | 40 | 120 | 20 | 0.02 | 36 |
| 16 | 4 | 60 | 60 | 40 | 0.02 | 16 |
| 17 | 4 | 40 | 60 | 20 | 0.04 | 26 |
| 18 | 6 | 50 | 90 | 30 | 0.03 | 31 |
| 19 | 4 | 60 | 60 | 20 | 0.04 | 24 |
| 20 | 4 | 40 | 120 | 40 | 0.04 | 38 |
| 21 | 6 | 50 | 30 | 30 | 0.03 | 21 |
| 22 | 6 | 50 | 90 | 50 | 0.03 | 12.1 |
| 23 | 8 | 60 | 120 | 20 | 0.02 | 52 |
| 24 | 6 | 50 | 90 | 30 | 0.03 | 30.3 |
| 25 | 6 | 50 | 90 | 30 | 0.05 | 33 |
| 26 | 6 | 50 | 90 | 30 | 0.01 | 16 |
| 27 | 8 | 60 | 60 | 20 | 0.04 | 49 |
| 28 | 8 | 40 | 120 | 40 | 0.02 | 43 |
| 29 | 8 | 60 | 120 | 40 | 0.04 | 48 |
| 30 | 4 | 60 | 120 | 40 | 0.04 | 37 |
| 31 | 4 | 40 | 120 | 40 | 0.02 | 31 |
| 32 | 6 | 50 | 150 | 30 | 0.03 | 47 |
| 33 | 6 | 50 | 90 | 30 | 0.03 | 30.7 |
| 34 | 10 | 50 | 90 | 30 | 0.03 | 49 |
| 35 | 4 | 60 | 120 | 40 | 0.02 | 30 |
| 36 | 4 | 60 | 120 | 20 | 0.02 | 23 |
| 37 | 8 | 40 | 60 | 20 | 0.04 | 49 |
| 38 | 4 | 60 | 60 | 40 | 0.04 | 35 |
| 39 | 8 | 60 | 60 | 20 | 0.02 | 40 |
| 40 | 6 | 50 | 90 | 30 | 0.03 | 30.9 |
| 41 | 8 | 40 | 60 | 40 | 0.02 | 18 |
| 42 | 4 | 40 | 120 | 20 | 0.04 | 37 |
| 43 | 4 | 40 | 60 | 40 | 0.02 | 6 |
| 44 | 6 | 50 | 90 | 30 | 0.03 | 31.1 |
| 45 | 8 | 40 | 120 | 40 | 0.04 | 46 |
| 46 | 6 | 50 | 90 | 30 | 0.03 | 30.1 |
| 47 | 8 | 40 | 60 | 40 | 0.04 | 33 |
| 48 | 4 | 40 | 60 | 40 | 0.04 | 25 |
| 49 | 8 | 60 | 60 | 40 | 0.02 | 30 |
| 50 | 8 | 60 | 120 | 40 | 0.02 | 45 |