TABLE-S1-A. Calculated activity values for the full population with the different models

| Iden | Activity | MLR | | | | SVM | | | | PPR | | | | ANN | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | PaDEL | | CODESSA | | PaDEL | | CODESSA | | PaDEL | | CODESSA | | PaDEL | | CODESSA | |
| | | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred |
| 1 | 2.10 | 2.34 | 2.37 | 2.13 | 2.13 | 2.36 | 2.34 | 2.13 | 2.14 | 2.35 | 2.44 | 2.16 | 2.03 | 2.36 | 2.36 | 2.14 | 2.12 |
| 2 | 1.97 | 2.05 | 1.99 | 2.08 | 2.12 | 2.09 | 2.00 | 2.07 | 2.14 | 2.01 | 1.94 | 1.99 | 2.02 | 2.02 | 1.97 | 2.09 | 2.13 |
| 3 | 1.51 | 2.10 | 2.16 | 2.00 | 2.04 | 2.15 | 2.18 | 2.01 | 2.02 | 2.05 | 2.24 | 1.83 | 1.97 | 2.08 | 2.15 | 2.01 | 2.07 |
| 4 | 2.25 | 2.39 | 2.41 | 2.12 | 2.00 | 2.44 | 2.47 | 2.11 | 2.01 | 2.39 | 2.54 | 2.12 | 1.98 | 2.43 | 2.43 | 2.12 | 1.99 |
| 5 | 2.34 | 2.31 | 2.30 | 2.30 | 2.27 | 2.34 | 2.31 | 2.29 | 2.27 | 2.31 | 2.33 | 2.34 | 2.32 | 2.33 | 2.32 | 2.29 | 2.25 |
| 6 | 2.30 | 2.09 | 2.11 | 2.23 | 2.24 | 2.11 | 2.08 | 2.23 | 2.25 | 2.03 | 2.07 | 2.32 | 2.33 | 2.09 | 2.11 | 2.23 | 2.22 |
| 7 | 1.76 | 1.90 | 1.92 | 1.96 | 1.95 | 1.90 | 1.92 | 1.98 | 1.97 | 1.84 | 1.96 | 1.98 | 2.04 | 1.89 | 1.92 | 1.97 | 1.97 |
| 8 | 2.09 | 2.11 | 2.14 | 1.96 | 1.99 | 2.13 | 2.14 | 1.97 | 1.95 | 2.04 | 2.10 | 2.01 | 2.02 | 2.10 | 2.13 | 1.97 | 2.01 |
| 9 | 2.01 | 2.21 | 2.21 | 1.88 | 1.80 | 2.25 | 2.27 | 1.87 | 1.80 | 2.21 | 2.24 | 2.15 | 1.89 | 2.22 | 2.24 | 1.89 | 1.80 |
| 10 | 2.09 | 2.14 | 2.13 | 1.96 | 1.94 | 2.16 | 2.12 | 1.96 | 1.94 | 2.09 | 2.24 | 2.02 | 1.94 | 2.13 | 2.13 | 1.97 | 1.95 |
| 11 | 1.71 | 1.87 | 1.88 | 1.83 | 1.86 | 1.91 | 1.99 | 1.84 | 1.92 | 1.86 | 1.83 | 1.83 | 1.92 | 1.84 | 1.87 | 1.83 | 1.86 |
| 12 | 1.77 | 1.56 | 1.49 | 1.82 | 1.83 | 1.59 | 1.46 | 1.83 | 1.83 | 1.59 | 1.45 | 1.80 | 1.78 | 1.54 | 1.48 | 1.81 | 1.84 |
| 13 | 1.90 | 2.08 | 2.07 | 2.02 | 2.04 | 2.10 | 2.12 | 2.01 | 2.00 | 2.03 | 1.98 | 1.89 | 1.97 | 2.07 | 2.07 | 2.03 | 2.06 |
| 14 | 2.29 | 2.15 | 2.13 | 2.03 | 2.01 | 2.18 | 2.16 | 2.04 | 2.04 | 2.10 | 1.93 | 1.91 | 1.87 | 2.15 | 2.14 | 2.03 | 2.01 |
| 15 | 1.62 | 1.92 | 1.86 | 1.74 | 1.71 | 1.96 | 1.90 | 1.76 | 1.72 | 1.90 | 1.79 | 1.63 | 1.71 | 1.89 | 1.80 | 1.72 | 1.70 |
| 16 | 2.13 | 2.37 | 2.40 | 2.39 | 2.36 | 2.40 | 2.41 | 2.39 | 2.35 | 2.40 | 2.51 | 2.35 | 2.46 | 2.40 | 2.39 | 2.37 | 2.35 |
| 17 | 2.43 | 2.25 | 2.23 | 2.36 | 2.38 | 2.27 | 2.22 | 2.39 | 2.35 | 2.27 | 2.21 | 2.33 | 2.39 | 2.25 | 2.23 | 2.34 | 2.37 |
| 18 | 2.04 | 1.97 | 1.94 | 2.15 | 2.15 | 2.00 | 2.03 | 2.12 | 2.11 | 1.91 | 1.86 | 2.08 | 2.08 | 1.96 | 1.93 | 2.18 | 2.19 |
| 19 | 2.11 | 2.18 | 2.17 | 2.38 | 2.38 | 2.20 | 2.19 | 2.40 | 2.45 | 2.19 | 2.11 | 2.36 | 2.40 | 2.18 | 2.18 | 2.35 | 2.37 |
| 20 | 2.48 | 1.99 | 1.94 | 2.30 | 2.27 | 2.04 | 2.00 | 2.32 | 2.27 | 1.95 | 1.84 | 2.34 | 2.32 | 1.97 | 1.90 | 2.29 | 2.25 |
| 21 | 1.01 | 1.03 | 1.01 | 1.18 | 1.23 | 1.05 | 1.17 | 1.16 | 1.21 | 1.02 | 1.09 | 1.18 | 1.31 | 1.12 | 1.19 | 1.22 | 1.29 |
| 22 | 1.37 | 1.44 | 1.43 | 1.62 | 1.70 | 1.41 | 1.46 | 1.62 | 1.75 | 1.49 | 1.44 | 1.54 | 1.68 | 1.44 | 1.42 | 1.61 | 1.75 |
| 23 | 1.19 | 1.34 | 1.35 | 1.24 | 1.26 | 1.34 | 1.32 | 1.23 | 1.20 | 1.35 | 1.36 | 1.24 | 1.11 | 1.35 | 1.37 | 1.26 | 1.27 |
| 24 | 1.39 | 1.38 | 1.38 | 1.44 | 1.51 | 1.38 | 1.36 | 1.44 | 1.50 | 1.38 | 1.37 | 1.43 | 1.45 | 1.39 | 1.40 | 1.43 | 1.50 |
| 25 | 2.28 | 2.29 | 2.29 | 2.31 | 2.29 | 2.29 | 2.28 | 2.31 | 2.29 | 2.33 | 2.32 | 2.34 | 2.32 | 2.32 | 2.31 | 2.29 | 2.26 |
| 26 | 2.54 | 2.31 | 2.32 | 2.46 | 2.43 | 2.30 | 2.32 | 2.48 | 2.45 | 2.36 | 2.40 | 2.50 | 2.35 | 2.34 | 2.32 | 2.41 | 2.40 |
| 27 | 1.98 | 1.98 | 1.99 | 1.89 | 1.97 | 1.95 | 2.03 | 1.90 | 2.02 | 1.95 | 1.87 | 1.91 | 2.01 | 1.97 | 1.98 | 1.90 | 2.03 |
| 28 | 2.11 | 2.10 | 2.12 | 2.13 | 2.17 | 2.09 | 2.11 | 2.12 | 2.17 | 2.08 | 2.12 | 2.11 | 2.12 | 2.10 | 2.12 | 2.13 | 2.18 |
| 29 | 2.33 | 2.13 | 2.10 | 2.23 | 2.19 | 2.11 | 2.11 | 2.24 | 2.18 | 2.16 | 1.89 | 2.33 | 2.22 | 2.12 | 2.09 | 2.22 | 2.19 |
| 30 | 1.66 | 1.57 | 1.59 | 1.31 | 1.25 | 1.54 | 1.57 | 1.28 | 1.27 | 1.64 | 1.62 | 1.35 | 1.19 | 1.56 | 1.56 | 1.31 | 1.25 |
| 31 | 1.99 | 2.11 | 2.12 | 2.15 | 2.14 | 2.10 | 2.10 | 2.15 | 2.17 | 2.10 | 2.12 | 2.20 | 1.96 | 2.11 | 2.12 | 2.15 | 2.13 |
| 32 | 2.26 | 2.09 | 2.07 | 2.32 | 2.40 | 2.08 | 2.11 | 2.34 | 2.37 | 2.05 | 2.02 | 2.34 | 2.40 | 2.09 | 2.06 | 2.30 | 2.38 |
| 33 | 1.55 | 1.48 | 1.47 | 1.48 | 1.37 | 1.51 | 1.46 | 1.49 | 1.38 | 1.44 | 1.09 | 1.48 | 1.14 | 1.45 | 1.48 | 1.50 | 1.37 |
| 34 | 1.85 | 2.15 | 2.23 | 1.71 | 1.61 | 2.17 | 2.19 | 1.67 | 1.59 | 2.10 | 2.27 | 1.71 | 1.58 | 2.14 | 2.22 | 1.69 | 1.58 |
| 35 | 2.67 | 2.42 | 2.35 | 2.40 | 2.34 | 2.45 | 2.33 | 2.40 | 2.34 | 2.59 | 2.33 | 2.47 | 2.34 | 2.43 | 2.29 | 2.37 | 2.32 |
| 36 | 2.61 | 2.45 | 2.45 | 2.52 | 2.48 | 2.46 | 2.45 | 2.55 | 2.42 | 2.60 | 2.63 | 2.63 | 2.34 | 2.48 | 2.42 | 2.46 | 2.45 |
| 37 | 1.84 | 1.96 | 1.99 | 1.93 | 2.04 | 1.99 | 2.01 | 1.90 | 2.02 | 1.90 | 1.88 | 1.86 | 1.99 | 1.95 | 1.98 | 1.94 | 2.09 |
| 38 | 2.16 | 2.16 | 2.22 | 1.98 | 2.03 | 2.19 | 2.20 | 1.96 | 2.07 | 2.07 | 2.05 | 2.08 | 1.98 | 2.17 | 2.22 | 2.00 | 2.08 |
| 39 | 1.63 | 1.67 | 1.78 | 1.73 | 1.72 | 1.67 | 1.68 | 1.71 | 1.74 | 1.72 | 1.85 | 1.59 | 1.61 | 1.65 | 1.76 | 1.72 | 1.72 |
| 40 | 1.29 | 1.28 | 1.22 | 1.31 | 1.34 | 1.30 | 1.24 | 1.30 | 1.32 | 1.26 | 1.25 | 1.30 | 1.29 | 1.32 | 1.32 | 1.31 | 1.32 |
| 41 | 2.07 | 2.05 | 2.03 | 1.84 | 1.77 | 2.07 | 2.09 | 1.79 | 1.72 | 1.97 | 1.92 | 2.06 | 1.97 | 2.03 | 2.02 | 1.87 | 1.75 |
| 42 | 1.89 | 1.92 | 1.98 | 2.33 | 2.49 | 1.93 | 1.95 | 2.34 | 2.41 | 1.83 | 2.01 | 2.34 | 2.47 | 1.92 | 1.98 | 2.34 | 2.45 |
| 43 | 1.22 | 1.54 | 1.60 | 1.32 | 1.35 | 1.55 | 1.53 | 1.31 | 1.37 | 1.54 | 1.58 | 1.33 | 1.29 | 1.53 | 1.59 | 1.34 | 1.35 |
| 44 | 2.09 | 2.06 | 2.01 | 2.09 | 2.06 | 2.11 | 2.11 | 2.07 | 2.06 | 2.01 | 1.99 | 1.97 | 1.93 | 2.04 | 1.99 | 2.10 | 2.08 |

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 45 | 1.99 | 1.91 | 1.84 | 1.89 | 1.82 | 1.95 | 1.81 | 1.93 | 1.87 | 1.85 | 1.81 | 2.02 | 2.02 | 1.91 | 1.85 | 1.90 | 1.84 |
| 46 | 1.77 | 2.09 | 2.10 | 1.72 | 1.58 | 2.12 | 2.07 | 1.71 | 1.60 | 2.04 | 2.06 | 1.68 | 1.48 | 2.09 | 2.10 | 1.73 | 1.55 |
| 47 | 2.42 | 2.22 | 2.22 | 2.41 | 2.47 | 2.28 | 2.27 | 2.40 | 2.48 | 2.26 | 2.25 | 2.35 | 2.45 | 2.23 | 2.23 | 2.38 | 2.43 |
| 48 | 1.66 | 1.97 | 2.00 | 1.80 | 1.85 | 2.02 | 2.03 | 1.77 | 1.87 | 1.90 | 1.86 | 1.77 | 2.11 | 1.97 | 2.00 | 1.80 | 1.88 |
| 49 | 2.15 | 1.84 | 1.85 | 1.88 | 1.82 | 1.88 | 1.86 | 1.88 | 1.85 | 1.87 | 1.84 | 1.87 | 1.67 | 1.84 | 1.84 | 1.89 | 1.82 |
| 50 | 2.06 | 1.81 | 1.78 | 2.14 | 2.17 | 1.88 | 1.83 | 2.12 | 2.17 | 1.88 | 1.75 | 2.11 | 2.15 | 1.77 | 1.72 | 2.15 | 2.17 |
| 51 | 1.88 | 1.81 | 1.80 | 1.66 | 1.58 | 1.84 | 1.71 | 1.62 | 1.60 | 1.86 | 1.89 | 1.55 | 1.62 | 1.81 | 1.81 | 1.65 | 1.56 |
| 52 | 1.66 | 1.91 | 1.93 | 2.14 | 2.18 | 1.95 | 1.97 | 2.12 | 2.19 | 1.87 | 1.97 | 2.04 | 2.11 | 1.89 | 1.92 | 2.15 | 2.19 |
| 53 | 2.44 | 2.14 | 2.15 | 2.29 | 2.30 | 2.18 | 2.21 | 2.27 | 2.30 | 2.14 | 2.14 | 2.34 | 2.31 | 2.14 | 2.14 | 2.28 | 2.30 |
| 54 | 2.30 | 2.20 | 2.18 | 2.25 | 2.17 | 2.26 | 2.28 | 2.24 | 2.21 | 2.23 | 2.14 | 2.31 | 2.17 | 2.20 | 2.17 | 2.24 | 2.18 |
| 55 | 1.80 | 2.02 | 1.99 | 2.07 | 2.02 | 2.08 | 2.02 | 2.05 | 2.04 | 1.95 | 1.92 | 1.99 | 1.94 | 2.01 | 1.99 | 2.08 | 2.05 |
| 56 | 1.70 | 1.57 | 1.57 | 1.80 | 1.82 | 1.65 | 1.74 | 1.77 | 1.81 | 1.58 | 1.57 | 1.84 | 1.80 | 1.54 | 1.56 | 1.79 | 1.81 |
| 57 | 1.53 | 1.57 | 1.68 | 1.69 | 1.79 | 1.57 | 1.73 | 1.66 | 1.76 | 1.62 | 1.77 | 1.57 | 1.71 | 1.58 | 1.68 | 1.68 | 1.80 |
| 58 | 1.43 | 1.43 | 1.43 | 1.68 | 1.73 | 1.47 | 1.47 | 1.65 | 1.76 | 1.42 | 1.35 | 1.55 | 1.68 | 1.44 | 1.44 | 1.67 | 1.75 |
| 59 | 2.69 | 2.45 | 2.40 | 2.22 | 2.13 | 2.49 | 2.49 | 2.20 | 2.17 | 2.67 | 2.52 | 2.27 | 2.15 | 2.47 | 2.39 | 2.22 | 2.14 |
| 60 | 2.45 | 2.34 | 2.29 | 2.14 | 2.10 | 2.39 | 2.31 | 2.13 | 2.12 | 2.37 | 2.30 | 2.08 | 2.00 | 2.35 | 2.28 | 2.15 | 2.11 |
| 61 | 2.48 | 2.32 | 2.33 | 1.83 | 1.71 | 2.36 | 2.34 | 1.82 | 1.72 | 2.33 | 2.38 | 2.19 | 1.59 | 2.33 | 2.32 | 1.84 | 1.68 |
| 62 | 2.35 | 2.19 | 2.21 | 2.46 | 2.58 | 2.23 | 2.21 | 2.41 | 2.66 | 2.19 | 2.16 | 2.42 | 2.59 | 2.20 | 2.22 | 2.43 | 2.49 |
| 63 | 2.05 | 2.30 | 2.34 | 2.14 | 2.14 | 2.36 | 2.39 | 2.12 | 2.24 | 2.32 | 2.36 | 2.03 | 2.07 | 2.30 | 2.34 | 2.13 | 2.13 |
| 64 | 1.81 | 1.73 | 1.68 | 1.57 | 1.48 | 1.77 | 1.75 | 1.53 | 1.39 | 1.85 | 1.79 | 1.55 | 1.49 | 1.70 | 1.64 | 1.55 | 1.46 |
| 65 | 2.13 | 1.72 | 1.66 | 1.92 | 1.84 | 1.76 | 1.67 | 1.93 | 1.86 | 1.80 | 1.66 | 2.16 | 2.03 | 1.70 | 1.64 | 1.95 | 1.87 |
| 66 | 1.91 | 2.12 | 2.13 | 2.18 | 2.18 | 2.18 | 2.22 | 2.16 | 2.18 | 2.04 | 2.08 | 2.13 | 2.37 | 2.11 | 2.13 | 2.20 | 2.19 |
| 67 | 1.73 | 2.08 | 2.11 | 1.97 | 2.04 | 2.12 | 2.11 | 1.95 | 1.99 | 2.02 | 1.96 | 1.83 | 2.00 | 2.08 | 2.10 | 1.99 | 2.05 |
| 68 | 1.10 | 1.08 | 1.05 | 1.27 | 1.48 | 1.13 | 1.09 | 1.16 | 1.29 | 1.08 | 0.98 | 1.24 | 1.36 | 1.14 | 1.13 | 1.28 | 1.52 |
| 69 | 1.87 | 1.86 | 1.93 | 1.88 | 1.80 | 1.87 | 1.90 | 1.86 | 1.82 | 1.86 | 1.88 | 1.86 | 2.06 | 1.86 | 1.92 | 1.86 | 1.76 |
| 70 | 2.35 | 2.28 | 2.27 | 2.19 | 2.19 | 2.31 | 2.29 | 2.18 | 2.19 | 2.31 | 2.29 | 2.21 | 2.23 | 2.27 | 2.24 | 2.20 | 2.20 |
| 71 | 1.25 | 1.23 | 1.21 | 1.16 | 1.16 | 1.29 | 1.47 | 1.06 | 1.04 | 1.25 | 1.24 | 1.20 | 1.24 | 1.24 | 1.26 | 1.16 | 1.26 |
| 72 | 1.60 | 1.58 | 1.56 | 1.66 | 1.80 | 1.60 | 1.58 | 1.66 | 1.70 | 1.62 | 1.55 | 1.60 | 1.74 | 1.58 | 1.55 | 1.64 | 1.82 |
| 73 | 1.50 | 1.39 | 1.45 | 1.62 | 1.72 | 1.40 | 1.37 | 1.56 | 1.65 | 1.38 | 1.49 | 1.53 | 2.13 | 1.39 | 1.44 | 1.54 | 1.68 |
| 74 | 2.46 | 2.36 | 2.33 | 2.29 | 2.27 | 2.39 | 2.39 | 2.28 | 2.30 | 2.38 | 2.42 | 2.34 | 2.30 | 2.37 | 2.32 | 2.28 | 2.27 |

TABLE-S1-B. Calculated activity values for the reduced population with the different models

| | | **MLR** | | **SVM** | | | **PPR** | | **ANN** | |
|---|---|---|---|---|---|---|---|---|---|---|
| Iden | **Activity** | **PaDEL** | **CODESSA** | **PaDEL** | **CODESSA** | | **PaDEL** | **CODESSA** | **PaDEL** | **CODESSA** |

| | | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred | Recall | Pred |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.10 | 2.21 | 2.21 | 2.04 | 2.01 | 2.20 | 2.21 | 2.03 | 2.00 | 2.20 | 2.34 | 2.09 | 2.08 | 2.21 | 2.22 | 2.05 | 2.02 |
| 2 | 1.97 | 1.98 | 1.96 | 1.93 | 1.93 | 1.98 | 1.94 | 1.92 | 1.91 | 2.01 | 2.00 | 1.94 | 1.95 | 1.99 | 1.98 | 1.95 | 1.95 |
| 3 | 1.51 | 1.80 | 1.83 | 1.85 | 1.91 | 1.81 | 1.79 | 1.85 | 1.90 | 1.74 | 1.85 | 1.88 | 1.96 | 1.78 | 1.83 | 1.86 | 1.95 |
| 4 | 2.25 | 2.28 | 2.28 | 2.11 | 2.08 | 2.26 | 2.25 | 2.09 | 2.03 | 2.26 | 2.28 | 2.17 | 2.10 | 2.28 | 2.28 | 2.12 | 2.09 |
| 5 | 2.34 | 2.31 | 2.31 | 2.37 | 2.35 | 2.30 | 2.30 | 2.34 | 2.32 | 2.32 | 2.38 | 2.35 | 2.37 | 2.31 | 2.30 | 2.35 | 2.33 |
| 6 | 2.30 | 2.14 | 2.13 | 2.41 | 2.40 | 2.14 | 2.14 | 2.40 | 2.41 | 2.23 | 2.34 | 2.28 | 2.32 | 2.16 | 2.16 | 2.38 | 2.38 |
| 7 | 1.76 | 1.83 | 1.80 | 1.80 | 1.82 | 1.84 | 1.84 | 1.79 | 1.69 | 1.76 | 1.74 | 1.81 | 1.70 | 1.80 | 1.80 | 1.80 | 1.82 |
| 8 | 2.09 | 2.14 | 2.14 | 2.22 | 2.27 | 2.13 | 2.13 | 2.20 | 2.23 | 2.17 | 2.15 | 2.22 | 2.33 | 2.14 | 2.13 | 2.24 | 2.28 |
| 9 | 2.01 | 2.07 | 2.07 | 1.93 | 1.89 | 2.05 | 2.08 | 1.92 | 1.88 | 2.07 | 2.08 | 1.90 | 1.91 | 2.07 | 2.07 | 1.94 | 1.90 |
| 10 | 2.09 | 2.04 | 1.99 | 1.86 | 1.84 | 2.03 | 1.99 | 1.86 | 1.83 | 2.02 | 1.98 | 1.85 | 1.82 | 2.03 | 1.96 | 1.87 | 1.83 |
| 11 | 1.71 | 1.79 | 1.82 | 1.66 | 1.66 | 1.81 | 1.84 | 1.68 | 1.69 | 1.71 | 1.64 | 1.64 | 1.59 | 1.77 | 1.80 | 1.65 | 1.65 |
| 12 | 1.77 | 1.80 | 1.82 | 1.69 | 1.69 | 1.82 | 1.86 | 1.70 | 1.64 | 1.79 | 1.78 | 1.67 | 1.66 | 1.78 | 1.80 | 1.68 | 1.67 |
| 13 | 1.90 | 1.85 | 1.85 | 2.09 | 2.11 | 1.86 | 1.84 | 2.09 | 2.08 | 1.85 | 1.89 | 2.12 | 2.18 | 1.84 | 1.86 | 2.12 | 2.16 |
| 14 | 2.29 | 2.20 | 2.18 | 2.17 | 2.14 | 2.19 | 2.17 | 2.15 | 2.14 | 2.23 | 2.20 | 2.20 | 2.33 | 2.20 | 2.18 | 2.18 | 2.15 |
| 15 | 1.62 | 1.61 | 1.61 | 1.65 | 1.65 | 1.64 | 1.64 | 1.68 | 1.64 | 1.56 | 1.56 | 1.64 | 1.63 | 1.58 | 1.57 | 1.65 | 1.63 |
| 16 | 2.13 | 2.20 | 2.22 | 2.22 | 2.23 | 2.18 | 2.20 | 2.24 | 2.30 | 2.21 | 2.34 | 2.22 | 2.20 | 2.21 | 2.23 | 2.23 | 2.24 |
| 17 | 2.43 | 2.38 | 2.39 | 2.30 | 2.26 | 2.35 | 2.41 | 2.32 | 2.30 | 2.38 | 2.35 | 2.44 | 2.29 | 2.36 | 2.36 | 2.30 | 2.26 |
| 18 | 2.04 | 2.28 | 2.31 | 2.28 | 2.31 | 2.26 | 2.26 | 2.27 | 2.31 | 2.28 | 2.32 | 2.26 | 2.36 | 2.29 | 2.32 | 2.26 | 2.29 |
| 19 | 2.11 | 2.40 | 2.40 | 2.40 | 2.43 | 2.37 | 2.37 | 2.41 | 2.40 | 2.39 | 2.38 | 2.31 | 2.34 | 2.37 | 2.37 | 2.36 | 2.38 |
| 20 | 2.48 | 2.19 | 2.15 | 2.29 | 2.28 | 2.17 | 2.13 | 2.30 | 2.29 | 2.23 | 2.15 | 2.42 | 2.35 | 2.19 | 2.15 | 2.29 | 2.28 |
| 21 | 1.01 | 1.17 | 1.22 | 1.15 | 1.17 | 1.20 | 1.23 | 1.12 | 1.13 | 1.17 | 1.23 | 1.10 | 1.23 | 1.21 | 1.26 | 1.19 | 1.24 |
| 22 | 1.37 | 1.46 | 1.48 | 1.54 | 1.59 | 1.47 | 1.52 | 1.48 | 1.57 | 1.45 | 1.46 | 1.53 | 1.61 | 1.44 | 1.45 | 1.51 | 1.55 |
| 23 | 1.19 | 1.08 | 1.07 | 1.09 | 1.05 | 1.13 | 1.08 | 1.11 | 1.12 | 1.12 | 1.14 | 1.03 | 1.06 | 1.16 | 1.16 | 1.15 | 1.11 |
| 24 | 1.39 | 1.24 | 1.18 | 1.52 | 1.57 | 1.28 | 1.24 | 1.50 | 1.56 | 1.25 | 1.19 | 1.48 | 1.61 | 1.25 | 1.22 | 1.49 | 1.55 |
| 25 | 2.28 | 2.39 | 2.36 | 2.25 | 2.24 | 2.34 | 2.36 | 2.23 | 2.21 | 2.39 | 2.43 | 2.22 | 2.21 | 2.38 | 2.36 | 2.25 | 2.24 |
| 26 | 2.54 | 2.50 | 2.51 | 2.23 | 2.20 | 2.44 | 2.49 | 2.23 | 2.22 | 2.45 | 2.38 | 2.21 | 2.23 | 2.46 | 2.47 | 2.23 | 2.21 |
| 27 | 1.98 | 1.90 | 1.93 | 1.97 | 1.99 | 1.87 | 1.96 | 1.91 | 2.03 | 1.89 | 1.90 | 1.98 | 2.11 | 1.89 | 1.91 | 1.96 | 1.99 |
| 28 | 2.11 | 2.16 | 2.17 | 2.26 | 2.33 | 2.12 | 2.12 | 2.23 | 2.26 | 2.21 | 2.18 | 2.21 | 2.44 | 2.17 | 2.17 | 2.26 | 2.31 |
| 29 | 2.33 | 2.30 | 2.30 | 2.31 | 2.26 | 2.25 | 2.29 | 2.28 | 2.24 | 2.28 | 2.31 | 2.34 | 2.10 | 2.30 | 2.30 | 2.31 | 2.26 |
| 30 | 1.66 | 1.54 | 1.48 | 1.41 | 1.35 | 1.53 | 1.50 | 1.35 | 1.33 | 1.49 | 1.44 | 1.39 | 1.33 | 1.50 | 1.43 | 1.39 | 1.33 |
| 31 | 1.99 | 2.19 | 2.19 | 2.15 | 2.12 | 2.15 | 2.20 | 2.12 | 2.10 | 2.22 | 2.33 | 2.19 | 2.18 | 2.20 | 2.21 | 2.16 | 2.13 |
| 32 | 2.26 | 2.27 | 2.26 | 2.43 | 2.49 | 2.23 | 2.29 | 2.37 | 2.41 | 2.24 | 2.27 | 2.33 | 2.36 | 2.28 | 2.27 | 2.39 | 2.39 |
| 38 | 2.16 | 1.94 | 1.95 | 2.02 | 2.00 | 1.95 | 1.96 | 2.03 | 2.00 | 2.00 | 1.95 | 2.10 | 2.13 | 1.96 | 1.96 | 2.05 | 2.07 |
| 39 | 1.63 | 1.70 | 1.68 | 1.60 | 1.57 | 1.73 | 1.65 | 1.60 | 1.65 | 1.65 | 1.65 | 1.58 | 1.62 | 1.69 | 1.67 | 1.60 | 1.57 |
| 40 | 1.29 | 1.32 | 1.34 | 1.33 | 1.38 | 1.35 | 1.41 | 1.40 | 1.37 | 1.35 | 1.36 | 1.33 | 1.36 | 1.34 | 1.36 | 1.32 | 1.34 |
| 44 | 2.09 | 1.87 | 1.85 | 2.17 | 2.18 | 1.88 | 1.84 | 2.14 | 2.15 | 1.90 | 1.84 | 2.21 | 2.28 | 1.88 | 1.85 | 2.18 | 2.19 |
| 45 | 1.99 | 1.91 | 1.89 | 2.22 | 2.19 | 1.89 | 1.91 | 2.21 | 2.19 | 1.90 | 1.89 | 2.21 | 2.18 | 1.91 | 1.90 | 2.22 | 2.19 |
| 46 | 1.77 | 1.95 | 1.97 | 1.95 | 1.93 | 1.96 | 1.98 | 1.93 | 1.88 | 2.00 | 2.09 | 1.99 | 2.02 | 1.96 | 1.99 | 1.97 | 1.93 |
| 47 | 2.42 | 2.35 | 2.36 | 2.34 | 2.30 | 2.32 | 2.29 | 2.34 | 2.36 | 2.38 | 2.35 | 2.35 | 2.24 | 2.36 | 2.36 | 2.33 | 2.30 |
| 48 | 1.66 | 1.82 | 1.85 | 1.79 | 1.78 | 1.81 | 1.81 | 1.82 | 1.80 | 1.73 | 1.88 | 1.82 | 1.84 | 1.82 | 1.88 | 1.78 | 1.80 |
| 53 | 2.44 | 2.21 | 2.25 | 2.30 | 2.30 | 2.19 | 2.17 | 2.29 | 2.28 | 2.24 | 2.26 | 2.39 | 2.44 | 2.22 | 2.27 | 2.30 | 2.32 |
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| 60 | 2.45 | 2.43 | 2.46 | 2.19 | 2.16 | 2.40 | 2.43 | 2.15 | 2.13 | 2.41 | 2.38 | 2.22 | 2.16 | 2.41 | 2.44 | 2.20 | 2.17 |
| 61 | 2.48 | 2.41 | 2.40 | 2.08 | 2.05 | 2.38 | 2.40 | 2.04 | 2.00 | 2.40 | 2.35 | 2.15 | 2.18 | 2.39 | 2.39 | 2.10 | 2.06 |
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| 63 | 2.05 | 2.10 | 2.11 | 2.29 | 2.36 | 2.09 | 2.11 | 2.27 | 2.32 | 2.13 | 2.13 | 2.22 | 2.44 | 2.12 | 2.14 | 2.29 | 2.33 |
| 64 | 1.81 | 1.95 | 1.96 | 1.96 | 1.91 | 1.91 | 2.00 | 1.92 | 1.88 | 1.93 | 1.98 | 1.92 | 1.90 | 1.95 | 1.97 | 1.94 | 1.90 |
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| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
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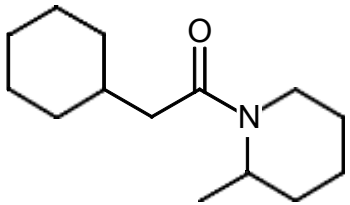

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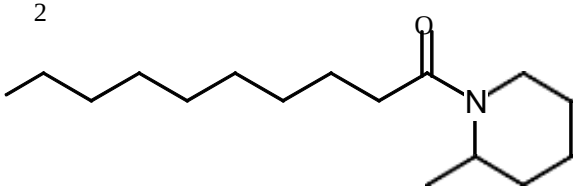

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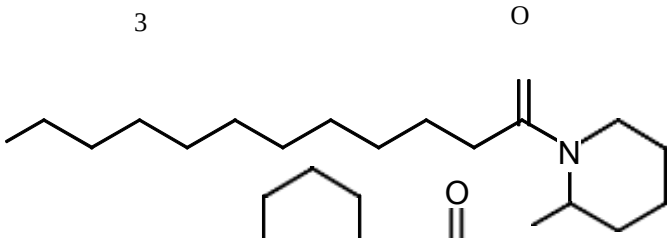

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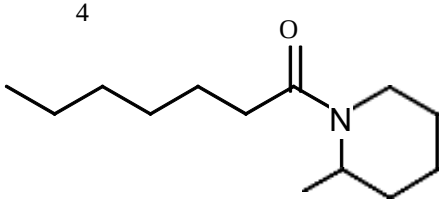

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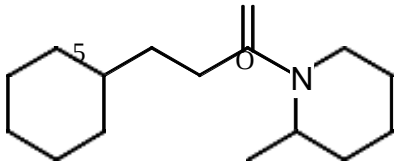

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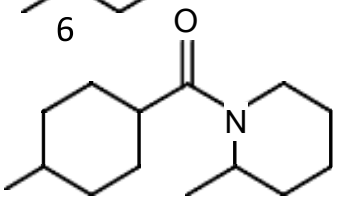

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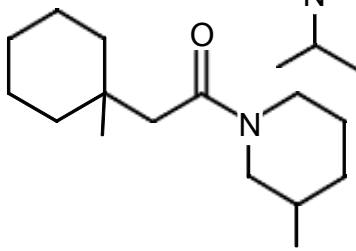

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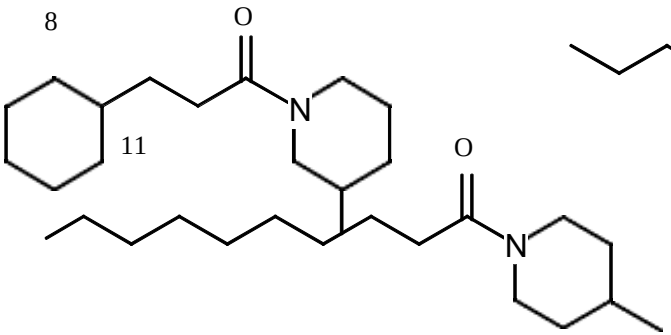

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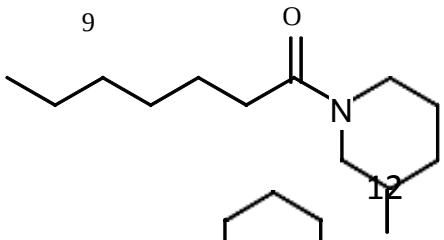

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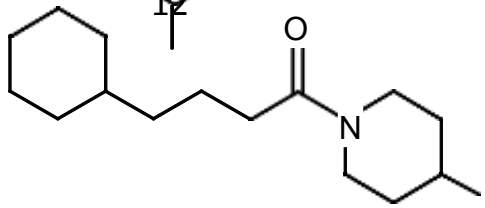

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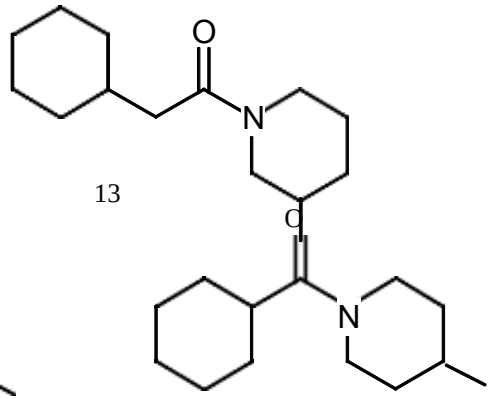

Fig S1-b

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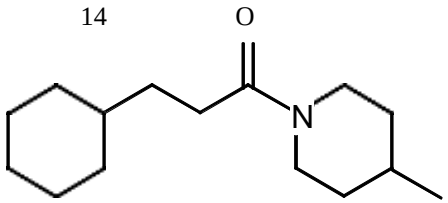

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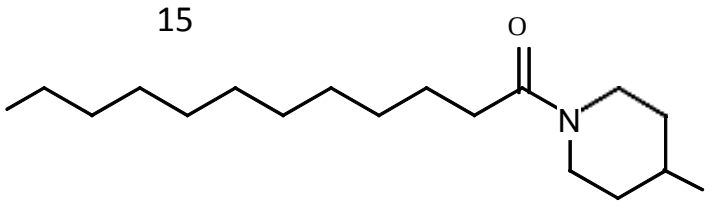

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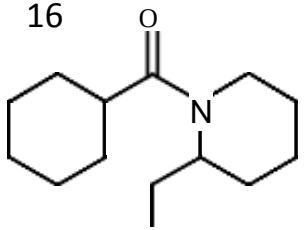

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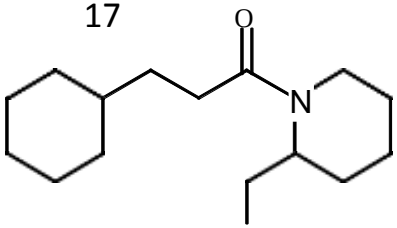

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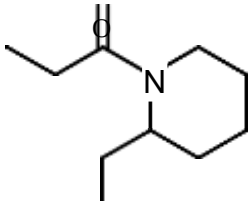

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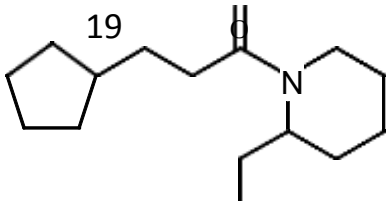

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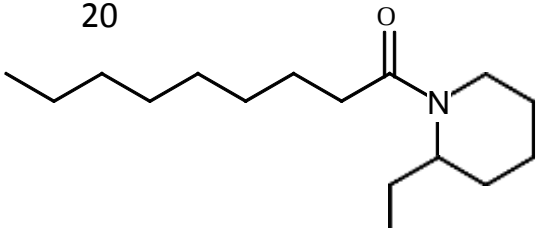

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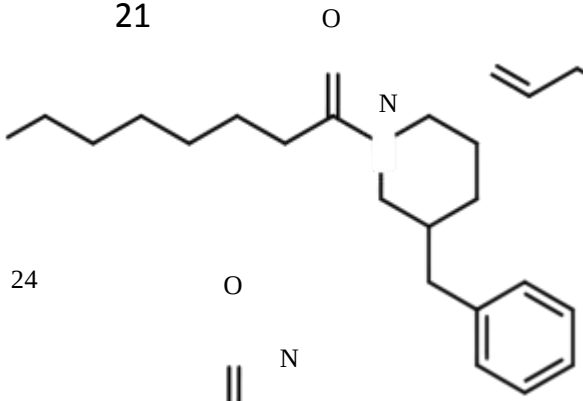

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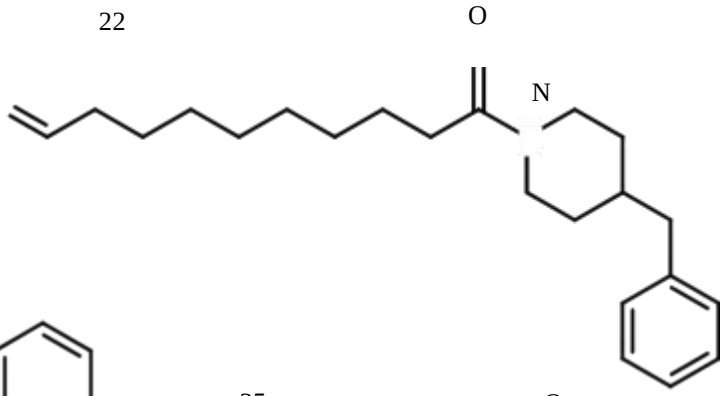

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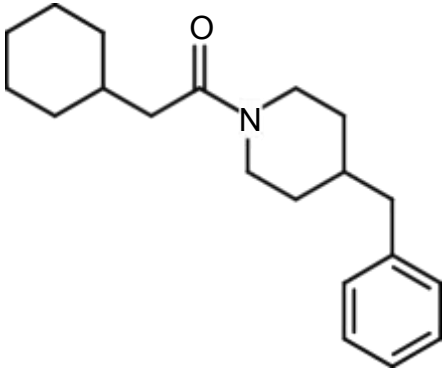

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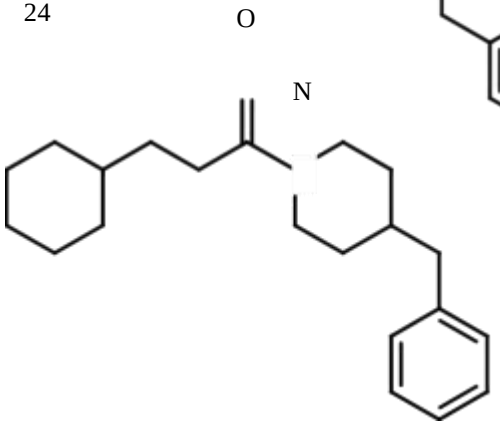

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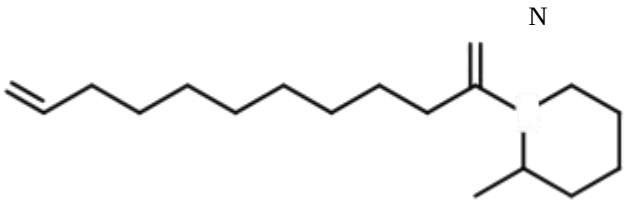

Fig S1-c

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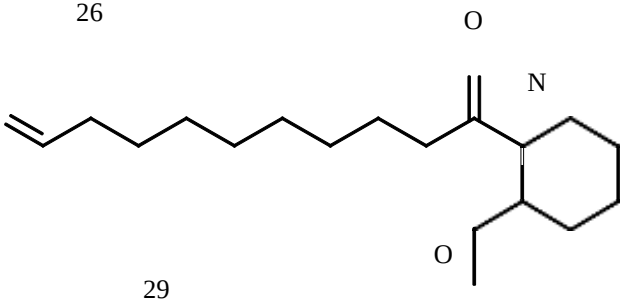

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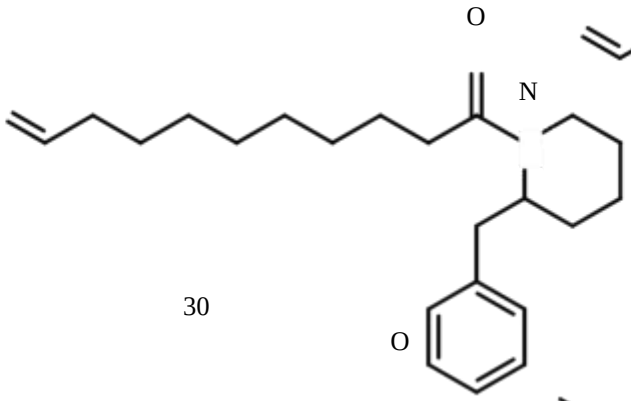

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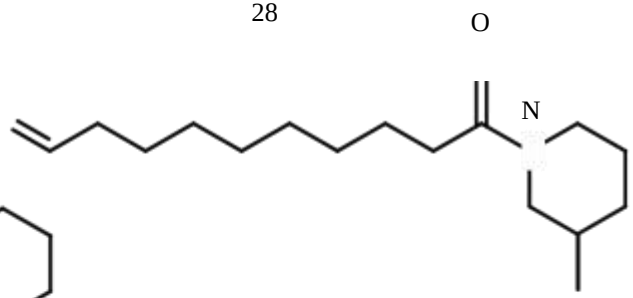

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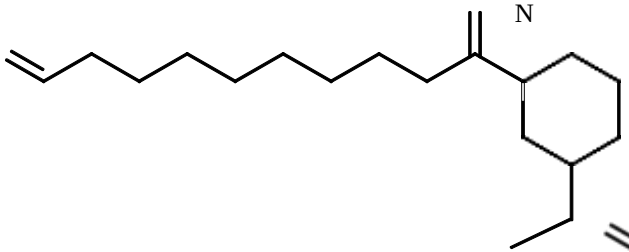

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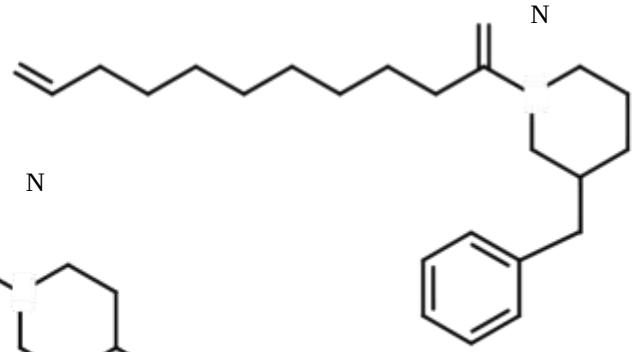

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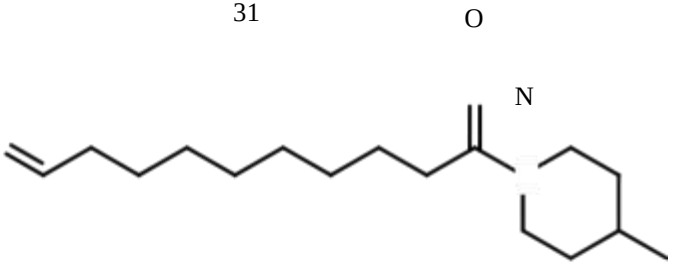

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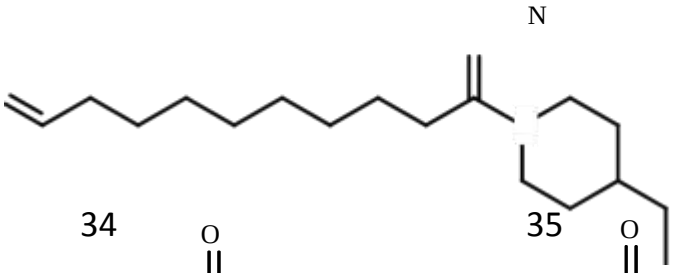

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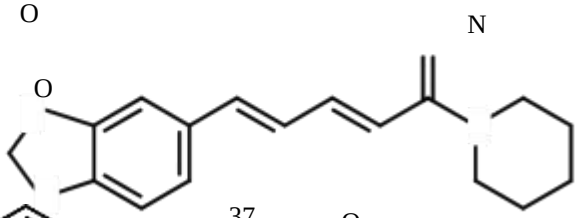

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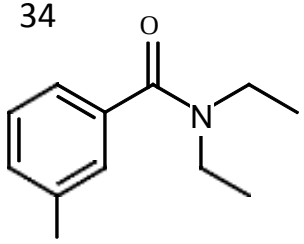

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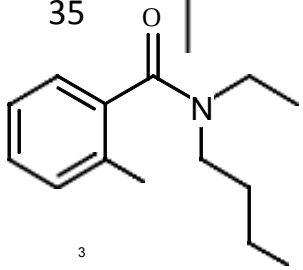

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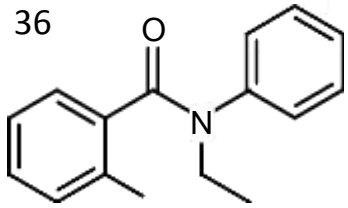

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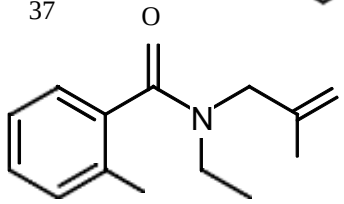

Fig S1-d

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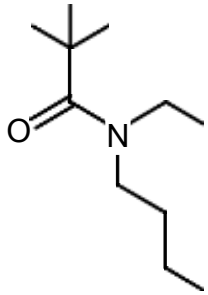

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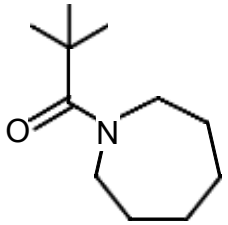

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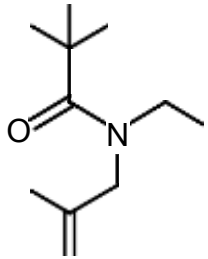

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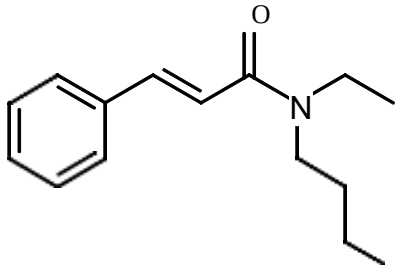

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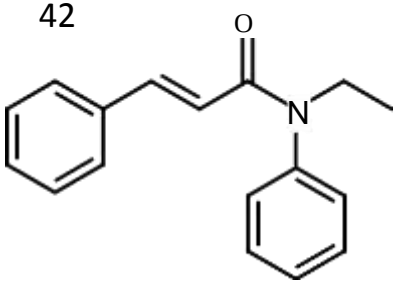

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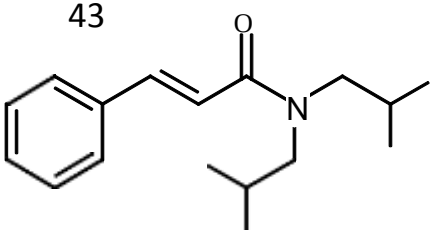

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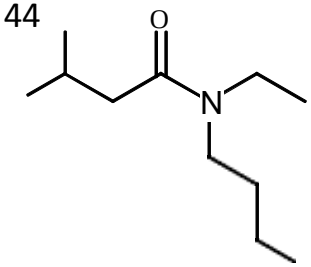

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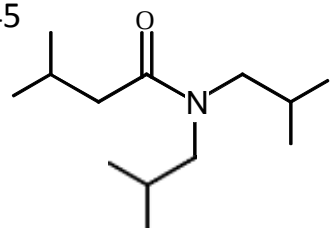

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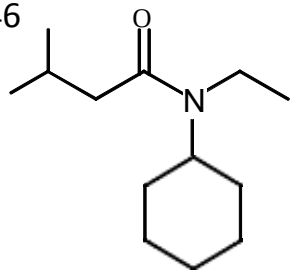

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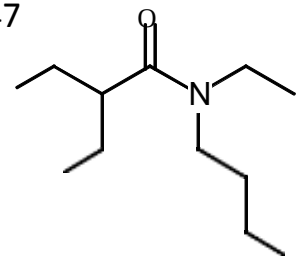

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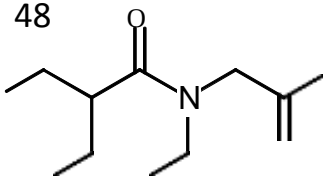

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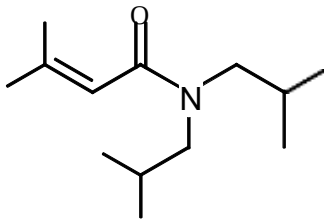

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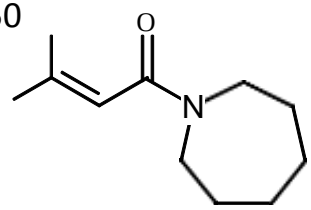

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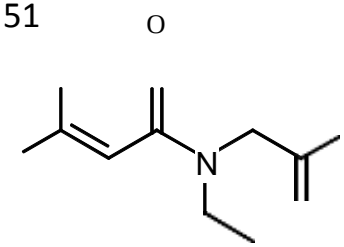

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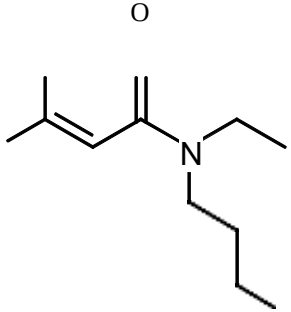

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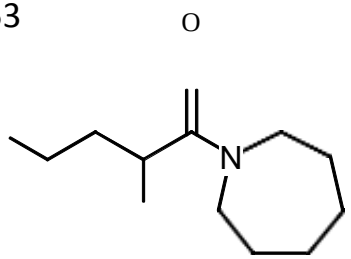

Fig S1-e

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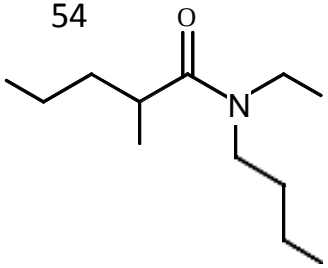

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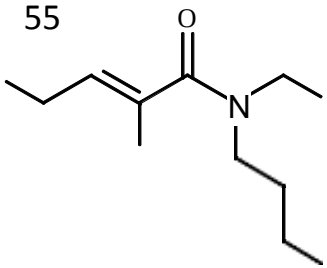

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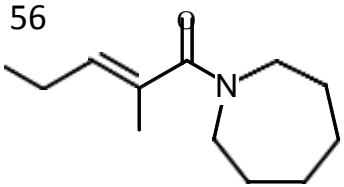

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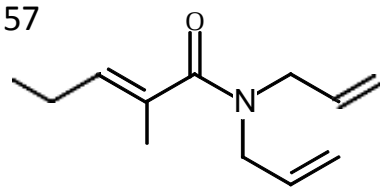

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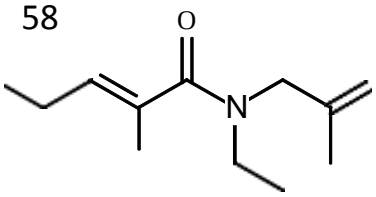

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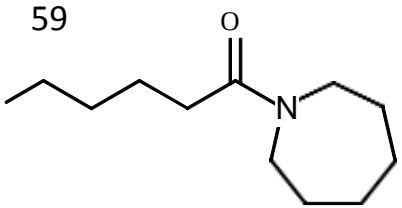

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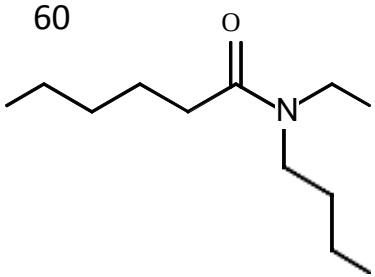

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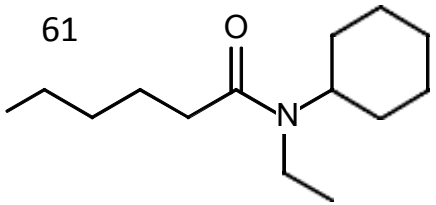

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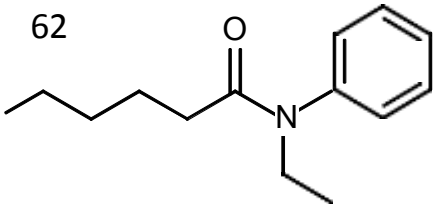

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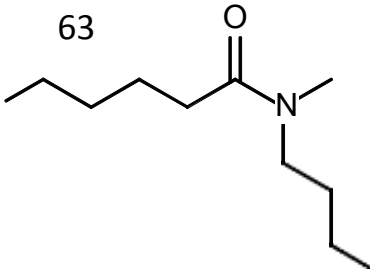

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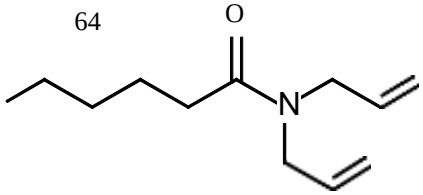

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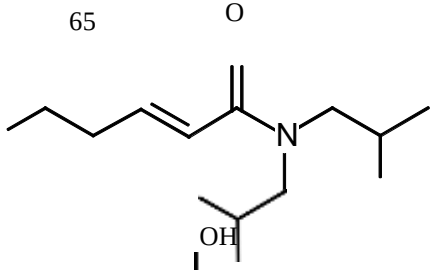

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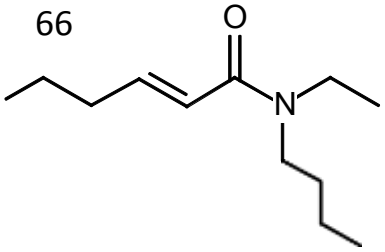

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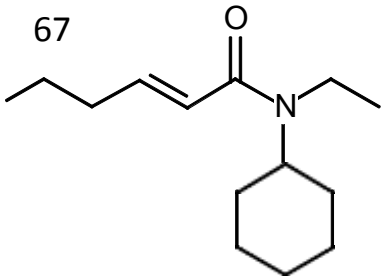

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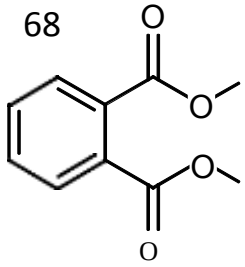

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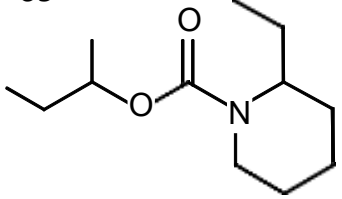

Fig S1-f

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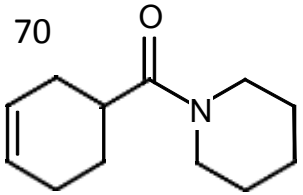


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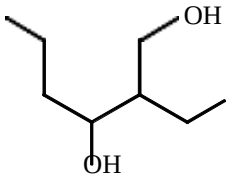


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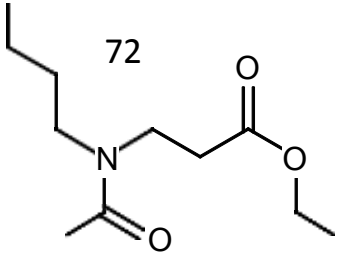


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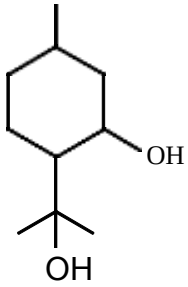


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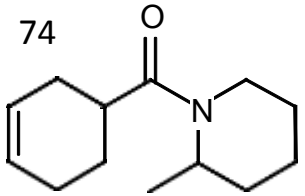


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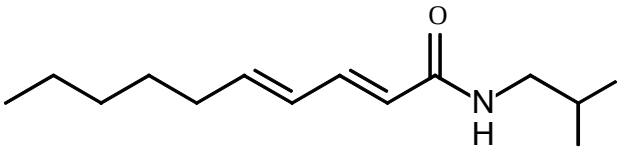


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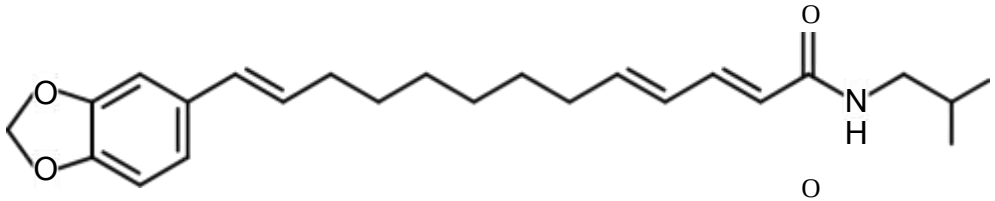


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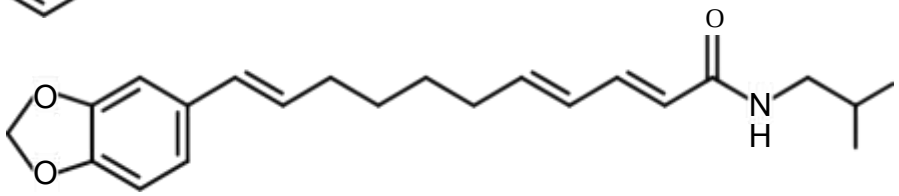


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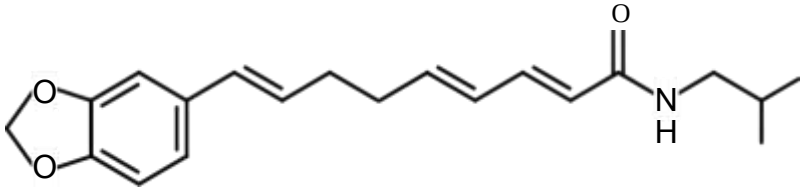

Fig S2