Supporting data
Nitrophenyl-group-containing Heterocycles. Part I. Synthesis, Characterization, Crystal Structure, Anticancer Activity and Antioxidant Properties of Some New 5,6,7,8-Tetrahydroisoquinolines Bearing 3(4)-Nitrophenyl Group

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Figure S1: $^1$H NMR Spectrum of 7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinoline-3(2H)-thione (2a) in DMSO-$d_6$. 
Figure S2: $^1$H NMR Spectrum of 7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinoline-3(2H)-thione (2b) in DMSO-$d_6$. 
Figure S3: IR Spectrum of 7-Acetyl-4-cyano-1,6-dimethyl-3-ethylthio-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinoline (3).
Figure S4: $^1$H NMR Spectrum of 7-Acetyl-4-cyano-1,6-dimethyl-3-ethylthio-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinoline (3) in CDCl$_3$. 
Figure S5: IR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]acetamide (5a).
Figure S6: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]acetamide (5a) in CDCl₃.
Figure S7: $^{13}$C NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]acetamide (5a) in CDCl$_3$. 
Figure S8: IR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-phenylacetamide (5b) in DMSO-$d_6$. 
Figure S9: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-phenylacetamide (5b) in DMSO-$d_6$. 
Figure S10: IR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-ylthio]-N-(4-tolyl)acetamide (5c).
Figure S11: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-tolyl)acetamide (5c) in DMSO-$d_6$. 


Figure S12: $^{13}$C NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-tolyl)acetamide (5c) in DMSO-$d_6$. 

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Figure S13: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-chlorophenyl)acetamide (5d) in DMSO-$d_6$. 
Figure S14: $^{13}$C NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(3-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-chlorophenyl)acetamide (5d) in DMSO-$d_6$. 
Figure S15: IR Spectrum of 2-[[7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl]thio]acetamide (5e)
Figure S16: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]acetamide (5e) in DMSO-$d_6$. 
Figure S17: IR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-phenylacetamide (5f).
Figure S18: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-ylthio]-N-phenylacetamide (5f) in DMSO-d$_6$. 
**Figure S19: $^{13}$C NMR** Spectrum of 2-((7-Acetyl-4-cyano-6-hydroxy-1,6-dimethyl-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio)-N-phenylacetamide (5f) in DMSO-$d_6$. 
Figure S20: IR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-tolyl)acetamide (5g).
Figure S21: \(^1\)H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-tolyl)acetamide (5g) in DMSO-\(d_6\).
Figure S22: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-chlorophenyl)acetamide (5h) in DMSO-$d_6$. 
Figure S23: $^{13}$C NMR Spectrum of 22-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-chlorophenyl)acetamide (5h) in DMSO-$d_6$. 
Figure S24: $^1$H NMR Spectrum of 2-[(7-Acetyl-4-cyano-1,6-dimethyl-6-hydroxy-8-(4-nitrophenyl)-5,6,7,8-tetrahydroisoquinolin-3-yl)thio]-N-(4-acetylphenyl)acetamide (5i) in DMSO-$d_6$. 
Figure S25: IR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-N-phenyl-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6b).
Figure S26: $^1$H NMR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-N-phenyl-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6b) in DMSO-$d_6$. 
Figure S27: $^{13}$C NMR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-N-phenyl-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoine-2-carboxamide (6b) in DMSO-$d_6$. 

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**Figure S28**: IR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-N-(4-tolyl)-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6c).
Figure S29: $^1$H NMR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-N-(4-tolyl)-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6c) in DMSO-$d_6$. 
Figure S30: $^{13}$C NMR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-N-(4-tolyl)-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6c) in DMSO-$d_6$. 
Figure S31: IR Spectrum of 7-Acetyl-1-amino-N-(4-chlorophenyl)-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6d).
Figure S32: $^1$H NMR Spectrum of 7-Acetyl-1-amino-N-(4-chlorophenyl)-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6d) in DMSO-$d_6$. 
Figure S33: $^{13}$C NMR Spectrum of 7-Acetyl-1-amino-$N$-(4-chlorophenyl)-5,8-dimethyl-8-hydroxy-6-(3-nitrophenyl)-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6d) in DMSO-$d_6$. 
Figure S34: $^1$H NMR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(4-nitrophenyl)-N-phenyl-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6f) in DMSO-d$_6$. 
Figure S35: $^{13}$C NMR Spectrum of 7-Acetyl-1-amino-5,8-dimethyl-8-hydroxy-6-(4-nitrophenyl)-N-phenyl-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6f) in DMSO-$d_6$. 
Figure S36: $^1$HNMR Spectrum of 7-Acetyl-1-amino-8-hydroxy-5,8-dimethyl-6-(4-nitrophenyl)-N-(4-tolyl)-6,7,8,9-tetrahydrothieno[2,3-c]isoquinoline-2-carboxamide (6g) in DMSO-$d_6$. 
Figure S37: $^{13}$ C NMR Spectrum of 7-Acetyl-1-amino-8-hydroxy-5,8-dimethyl-6-(4-nitrophenyl)-$N$-(4-tolyl)-6,7,8,9-tetrahydrothieno[2,3-$c$]isoquinoline-2-carboxamide (6g) in DMSO-$d_6$. 
## Supporting Information

### Table S1. Crystal and refinement data for 5d.

| Identification code | 5d |
|---------------------|----|
| **Chemical formula** | \( \text{C}_{28}\text{H}_{25}\text{ClN}_4\text{O}_5\text{S} \) |
| **Formula weight**   | 565.03 g/mol |
| **Temperature**      | 170(2) K |
| **Wavelength**       | 0.71073 Å |
| **Crystal size**     | 0.188 x 0.379 x 0.423 mm |
| **Crystal habit**    | colorless block |
| **Crystal system**   | monoclinic |
| **Space group**      | \( \text{P} 1 \ 21/c \ 1 \) |
| **Unit cell dimensions** | \( a = 17.7900(3) \ \text{Å} \ \ \ \alpha = 90^\circ \)
|                     | \( b = 14.2484(3) \ \text{Å} \ \ \ \beta = 95.3460(10)^\circ \)
|                     | \( c = 10.3782(2) \ \text{Å} \ \ \ \gamma = 90^\circ \) |
| **Volume**           | \( 2619.21(9) \ \text{Å}^3 \) |
| **Z**                | 4 |
| **Density (calculated)** | 1.433 g/cm\(^3\) |
| **Absorption coefficient** | 0.273 mm\(^{-1}\) |
| **F(000)**           | 1176 |
| **Diffractometer**   | Bruker D8 QUEST PHOTON 3 diffractometer |
Radiation source  
- fine-focus sealed tube (MoKα, λ = 0.71073 Å)

 Theta range for data collection  
- 2.30 to 30.59°

 Index ranges  
- -25 ≤ h ≤ 25, -20 ≤ k ≤ 20, -14 ≤ l ≤ 14

 Reflections collected  
- 113030

 Independent reflections  
- 7964 [R(int) = 0.0406]

 Coverage of independent reflections  
- 98.8%

 Absorption correction  
- Numerical μ Calculated

 Max. and min. transmission  
- 0.9500 and 0.8930

 Structure solution technique  
- direct methods

 Structure solution program  
- SHELXT/5

 Refinement method  
- Full-matrix least-squares on F²

 Refinement program  
- SHELXL 2018/3

 Function minimized  
- Σ w(Fo² - Fc²)²

 Data / restraints / parameters  
- 7964 / 5 / 363

 Goodness-of-fit on F²  
- 1.029

 Δ/σmax  
- 0.001

 Final R indices  
- 6810 data; R1 = 0.0401, wR2 = 0.1059
- I>2σ(I)
- all data R1 = 0.0485, wR2 = 0.1133

 Weighting scheme  
- w=1/[σ²(Fo²)+(0.0586P)²+1.0979P]
where \( P = (\overline{F}^2 + 2\overline{F}^2) / 3 \)

Largest diff. peak and hole 0.553 and -0.695 e\(\text{Å}^{-3}\)

R.M.S. deviation from mean 0.051 e\(\text{Å}^{-3}\)

Table S2. Bond lengths (Å) and interbond angles (°) for 8c.

|          | Bond Lengths (Å) |          | Bond Lengths (Å) |
|----------|------------------|----------|------------------|
| C11-C26  | 1.7436(13)       | N3-C23   | 1.4170(14)       |
| S1-C21   | 1.7966(12)       | N4-C15   | 1.4794(18)       |
| O2-C5    | 1.4296(15)       | C1-C10   | 1.5035(15)       |
| O3-C22   | 1.2266(14)       | C2-C3    | 1.5222(15)       |
| O5-N4    | 1.2292(18)       | C3-C4    | 1.5524(16)       |
| N1-C1    | 1.3473(14)       | C4-C17   | 1.5313(17)       |
| N3-C22   | 1.3556(14)       | C5-C19   | 1.5263(16)       |
| N3-H3    | 0.895(9)         | C7-C8    | 1.4004(15)       |
| C1-C2    | 1.4063(15)       | C8-C20   | 1.4386(15)       |
| C2-C7    | 1.3976(14)       | C11-C12  | 1.3943(17)       |
| C3-C11   | 1.5259(15)       | C12-C13  | 1.3935(18)       |
| C4-C5    | 1.5453(16)       | C13-C14  | 1.382(2)         |
| C5-C6    | 1.5183(16)       | C14-C15  | 1.378(2)         |
| C6-C7    | 1.5036(15)       | C15-C16  | 1.3875(17)       |
| C8-C9    | 1.3994(15)       | C17-C18  | 1.499(2)         |
| C11-C16  | 1.3946(16)       | C21-C22  | 1.5158(16)       |
| S1-C9    | 1.7678(11)       | C23-C24  | 1.3906(17)       |
| O1-C17   | 1.214(2)         | C23-C28  | 1.3922(16)       |
| O2-H2    | 0.838(9)         | C24-C25  | 1.3933(17)       |
| O4-N4    | 1.220(2)         | C25-C26  | 1.384(2)         |
| N1-C9    | 1.3272(14)       | C26-C27  | 1.378(2)         |
| N2-C20   | 1.1449(17)       | C27-C28  | 1.3856(18)       |
| C9-S1-C21| 99.91(5)         | C5-O2-H2 | 107.2(14)        |
| C9-N1-C1 | 118.95(9)        | C22-N3-C23| 123.45(10)     |
| C22-N3-H3| 119.6(11)        | C23-N3-H3| 115.4(11)       |
| O4-N4-O5 | 124.03(14)       | O4-N4-C15| 118.36(13)      |
| O5-N4-C15| 117.60(16)       | N1-C1-C2 | 122.69(10)      |
| N1-C1-C10| 114.43(10)       | C2-C1-C10| 122.86(10)      |
| C7-C2-C1 | 117.75(10)       | C7-C2-C3 | 121.57(9)       |
| C1-C2-C3 | 120.60(9)        | C2-C3-C11| 114.07(9)       |
Table S3. Hydrogen bond distances (Å) and angles (°) for 8c.

| Donor–H | Acceptor···H | Donor···Acceptor | Angle |
|---------|--------------|------------------|-------|
| O2-H2  | O1           | 0.838(9)         | 2.239(15) | 2.9035(14) | 136.3(17) |
| N3-H3  | O3"          | 0.895(9)         | 2.208(12) | 2.9175(13) | 143.5(14) |
| C21-H21B | O2"       | 0.99             | 2.54      | 3.3068(14) | 134.4     |
| C27-H27" | O4"        | 0.95             | 2.49      | 3.4124(18) | 164.9     |

Symmetry transformations used to generate equivalent atoms: (i) -x, -y+1, -z+1; (ii) -x+1, -y+1, -z+1; (iii) x, -y+3/2, z+1/2.
Table S4: Probit Analysis and raw data for cytotoxicity of compound 3 against PACA2 (Pancreatic cancer cell line)

Parameter Estimates

| Parameter | Estimate | Std. Error | Z      | Sig. | Lower Bound | Upper Bound |
|-----------|----------|------------|--------|------|-------------|-------------|
| PROBIT conc | 3.588    | .304       | 11.808 | .000 | 2.993       | 4.184       |
| Intercept | -6.202   | .514       | -12.056| .000 | -6.716      | -5.688      |

a. PROBIT model: PROBIT(p) = Intercept + BX (Covariates X are transformed using the base 10.000 logarithm.)

Chi-Square Tests

|                      | Chi-Square | df \( ^a \) | Sig. |
|----------------------|------------|-------------|------|
| PROBIT Pearson Goodness-of-Fit Test | 3.513 | 6 | .742 \( ^b \) |

a. Statistics based on individual cases differ from statistics based on aggregated cases.
b. Since the significance level is greater than .150, no heterogeneity factor is used in the calculation of confidence limits.

Cell Counts and Residuals

| Number | conc | Number of Subjects | Observed Responses | Expected Responses | Residual | Probability |
|--------|------|--------------------|--------------------|-------------------|----------|-------------|
| PROBIT | 1    | 2.000              | 100                | 87                | 83.502   | 3.498       | .835        |
|        | 2    | 1.699              | 100                | 39                | 45.782   | -6.782      | .458        |
|        | 3    | 1.398              | 100                | 13                | 11.780   | 1.220       | .118        |
|        | 4    | 1.097              | 100                | 2                 | 1.172    | .828        | .012        |
|        | 5    | .787               | 100                | 0                 | .037     | -.037       | .000        |
|        | 6    | .494               | 100                | 0                 | .000     | .000        | .000        |
|        | 7    | .193               | 100                | 0                 | .000     | .000        | .000        |
|        | 8    | -.108              | 100                | 0                 | .000     | .000        | .000        |
| Probability | 95% Confidence Limits for conc | 95% Confidence Limits for log(conc) |
|-------------|-------------------------------|-----------------------------------|
|             | Estimate | Lower Bound | Upper Bound | Estimate | Lower Bound | Upper Bound |
| PROBIT      |          |             |             |          |             |             |
| 0.01        | 12.027   | 8.973       | 14.922      | 1.080    | .953        | 1.174        |
| 0.02        | 14.326   | 11.035      | 17.387      | 1.156    | 1.043       | 1.240        |
| 0.03        | 16.007   | 12.578      | 19.166      | 1.204    | 1.100       | 1.283        |
| 0.04        | 17.401   | 13.875      | 20.629      | 1.241    | 1.142       | 1.314        |
| 0.05        | 18.624   | 15.025      | 21.905      | 1.270    | 1.177       | 1.341        |
| 0.06        | 19.732   | 16.077      | 23.057      | 1.295    | 1.206       | 1.363        |
| 0.07        | 20.758   | 17.057      | 24.121      | 1.317    | 1.232       | 1.382        |
| 0.08        | 21.722   | 17.982      | 25.118      | 1.337    | 1.255       | 1.400        |
| 0.09        | 22.637   | 18.865      | 26.963      | 1.355    | 1.276       | 1.416        |
| 0.1         | 23.514   | 19.714      | 26.968      | 1.371    | 1.295       | 1.431        |
| 0.15        | 27.520   | 23.622      | 31.102      | 1.440    | 1.373       | 1.493        |
| 0.2         | 31.184   | 27.218      | 34.908      | 1.494    | 1.435       | 1.543        |
| 0.25        | 34.715   | 30.676      | 38.618      | 1.541    | 1.487       | 1.587        |
| 0.3         | 38.225   | 34.086      | 42.367      | 1.582    | 1.533       | 1.627        |
| 0.35        | 41.793   | 37.510      | 46.257      | 1.621    | 1.574       | 1.665        |
| 0.4         | 45.487   | 40.996      | 50.377      | 1.658    | 1.613       | 1.702        |
| 0.45        | 49.371   | 44.591      | 54.817      | 1.693    | 1.649       | 1.739        |
| 0.5         | 53.517   | 48.349      | 59.677      | 1.728    | 1.684       | 1.776        |
| 0.55        | 58.012   | 52.333      | 65.080      | 1.764    | 1.719       | 1.813        |
| 0.6         | 62.965   | 56.628      | 71.184      | 1.799    | 1.753       | 1.852        |
| 0.65        | 68.530   | 61.348      | 78.208      | 1.836    | 1.788       | 1.893        |
| 0.7         | 74.928   | 66.661      | 86.477      | 1.875    | 1.824       | 1.937        |
| 0.75        | 82.503   | 72.820      | 96.505      | 1.916    | 1.862       | 1.985        |
| 0.8         | 91.844   | 80.255      | 109.177     | 1.963    | 1.904       | 2.038        |
| 0.85        | 104.075  | 89.774      | 126.216     | 2.017    | 1.953       | 2.101        |
| 0.9         | 121.803  | 103.231     | 151.690     | 2.086    | 2.014       | 2.181        |
| 0.91        | 126.520  | 106.754     | 158.605     | 2.102    | 2.028       | 2.200        |
| 0.92        | 131.851  | 110.710     | 166.486     | 2.120    | 2.044       | 2.221        |
| 0.93        | 137.973  | 115.222     | 175.617     | 2.140    | 2.062       | 2.245        |
| 0.94        | 145.146  | 120.469     | 186.423     | 2.162    | 2.081       | 2.270        |
| 0.95        | 153.784  | 126.733     | 199.580     | 2.187    | 2.103       | 2.300        |
| 0.96        | 164.591  | 134.496     | 216.252     | 2.216    | 2.129       | 2.335        |
Table S5: Probit Analysis and raw data for cytotoxicity of compound 5c against PACA2 (Pancreatic cancer cell line)

| Parameter Estimates | Estimate | Std. Error | Z   | Sig. | 95% Confidence Interval |
|---------------------|----------|------------|-----|------|-------------------------|
|                     |          |            |     |      | Lower Bound | Upper Bound |
| PROBIT\(^a\) conc   | 2.034    | .169       | 12.057 | .000 | 1.704 | 2.365 |
| Intercept            | -3.619   | .269       | -13.470 | .000 | -3.887 | -3.350 |

a. PROBIT model: PROBIT(p) = Intercept + BX (Covariates X are transformed using the base 10.000 logarithm.)

| Chi-Square Tests | Chi-Square | df\(^a\) | Sig. |
|------------------|------------|----------|------|
| PROBIT Pearson Goodness-of-Fit Test | 17.454 | 6 | .008\(^b\) |

a. Statistics based on individual cases differ from statistics based on aggregated cases.

b. Since the significance level is less than .150, a heterogeneity factor is used in the calculation of confidence limits.

| Cell Counts and Residuals | Number | conc | Number of Subjects | Observed Responses | Expected Responses | Residual | Probability |
|---------------------------|--------|------|--------------------|--------------------|--------------------|----------|-------------|
| PROBIT                    |        |      |                    |                    |                    |          |             |
| 1                          | 2.000  | 100  | 73                 | 67.364             | 5.636              | .674     |
| 2                          | 1.699  | 100  | 38                 | 43.549             | -5.549             | .435     |
| 3                          | 1.398  | 100  | 20                 | 21.922             | -1.922             | .219     |
| 4                          | 1.097  | 100  | 9                  | 8.268              | .732               | .083     |
| Probability | Estimate | Lower Bound | Upper Bound | Estimate | Lower Bound | Upper Bound |
|-------------|----------|-------------|-------------|----------|-------------|-------------|
| PROBIT      |          |             |             |          |             |             |
| 0.01        | 4.318    | 1.338       | 7.899       | .635     | .126        | .898        |
| 0.02        | 5.879    | 2.122       | 10.039      | .769     | .327        | 1.002       |
| 0.03        | 7.150    | 2.838       | 11.710      | .854     | .453        | 1.069       |
| 0.04        | 8.284    | 3.528       | 13.165      | .918     | .548        | 1.119       |
| 0.05        | 9.339    | 4.207       | 14.494      | .970     | .624        | 1.161       |
| 0.06        | 10.341   | 4.882       | 15.744      | 1.015    | .689        | 1.197       |
| 0.07        | 11.308   | 5.559       | 16.942      | 1.053    | .745        | 1.229       |
| 0.08        | 12.250   | 6.240       | 18.103      | 1.088    | .795        | 1.258       |
| 0.09        | 13.175   | 6.927       | 19.242      | 1.120    | .841        | 1.284       |
| 0.1         | 14.089   | 7.621       | 20.365      | 1.149    | .882        | 1.306       |
| 0.15        | 18.593   | 11.225      | 25.971      | 1.269    | 1.050       | 1.414       |
| 0.2         | 23.180   | 15.074      | 31.919      | 1.365    | 1.178       | 1.504       |
| 0.25        | 28.007   | 19.163      | 38.591      | 1.447    | 1.282       | 1.586       |
| 0.3         | 33.193   | 23.476      | 46.341      | 1.521    | 1.371       | 1.666       |
| 0.35        | 38.851   | 28.009      | 55.543      | 1.589    | 1.447       | 1.745       |
| 0.4         | 45.110   | 32.783      | 66.630      | 1.654    | 1.516       | 1.824       |
| 0.45        | 52.124   | 37.854      | 80.135      | 1.717    | 1.578       | 1.904       |
| 0.5         | 60.091   | 43.310      | 96.761      | 1.779    | 1.637       | 1.986       |
| 0.55        | 69.275   | 49.277      | 117.488     | 1.841    | 1.693       | 2.070       |
| 0.6         | 80.046   | 55.929      | 143.750     | 1.903    | 1.748       | 2.158       |
| 0.65        | 92.942   | 63.514      | 177.739     | 1.968    | 1.803       | 2.250       |
| 0.7         | 108.787  | 72.392      | 222.996     | 2.037    | 1.860       | 2.348       |
| 0.75        | 128.929  | 83.139      | 285.639     | 2.110    | 1.920       | 2.456       |
| 0.8         | 155.777  | 96.745      | 377.280     | 2.193    | 1.986       | 2.577       |
| 0.85        | 194.206  | 115.147     | 523.152     | 2.288    | 2.061       | 2.719       |
| 0.9         | 256.301  | 142.950     | 791.530     | 2.409    | 2.155       | 2.898       |
| Parameter | Estimate | Std. Error | Z    | Sig.  | 95% Confidence Interval | 49% Confidence Interval |
|-----------|----------|------------|------|-------|-------------------------|-------------------------|
| PROBIT*   | conc     | 3.195      | .222 | 14.394| .000                    | 2.760                   | 3.630                   |
| Intercept | -4.517   | .317       | -14.250 | .000  | -4.834                  | -4.200                  |

a. PROBIT model: \( \text{PROBIT}(p) = \text{Intercept} + BX \) (Covariates X are transformed using the base 10.000 logarithm.)

### Chi-Square Tests

| Test                          | Chi-Square | df | Sig.  |
|-------------------------------|------------|----|-------|
| PROBIT Pearson Goodness-of-Fit Test | 10.858     | 6  | .093  |

a. Statistics based on individual cases differ from statistics based on aggregated cases.

b. Since the significance level is less than .150, a heterogeneity factor is used in the calculation of confidence limits.

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**Table S6: Probit Analysis and raw data for cytotoxicity of compound 5h against PACA2 (Pancreatic cancer cell line).**

a. Logarithm base = 10.

PROBIT dead OF total WITH conc
/LOG 10
/MODEL PROBIT
/PRINT FREQ CI
/CRITERIA P(0.15) ITERATE(20) STEPLIMIT(.1).
### Cell Counts and Residuals

| Number | conc  | Number of Subjects | Observed Responses | Expected Responses | Residual | Probability |
|--------|-------|--------------------|--------------------|--------------------|----------|-------------|
| PROBIT | 1     | 2.000              | 100                | 100                | 96.951   | 3.049       | .970        |
|        | 2     | 1.699              | 100                | 82                 | 81.905   | .095        | .819        |
|        | 3     | 1.398              | 100                | 38                 | 48.000   | -10.000     | .480        |
|        | 4     | 1.097              | 100                | 17                 | 15.576   | 1.424       | .156        |
|        | 5     | .787               | 100                | 5                  | 2.264    | 2.736       | .023        |
|        | 6     | .494               | 100                | 0                  | .165     | -1.165      | .002        |
|        | 7     | .193               | 100                | 0                  | .005     | -1.005      | .000        |
|        | 8     | -.108              | 100                | 0                  | .000     | .000        | .000        |

### Confidence Limits

| y     | 95% Confidence Limits for conc | 95% Confidence Limits for log(conc) |
|-------|-------------------------------|-------------------------------------|
|       | Estimate | Lower Bound | Upper Bound | Estimate | Lower Bound | Upper Bound |
| PROBIT|          |            |            |          |            |            |
| 0.01  | 4.848    | 2.884      | 6.816      | .686     | .460       | .834       |
| 0.02  | 5.901    | 3.703      | 8.036      | .771     | .569       | .905       |
| 0.03  | 6.684    | 4.337      | 8.926      | .825     | .637       | .951       |
| 0.04  | 7.341    | 4.882      | 9.665      | .866     | .689       | .985       |
| 0.05  | 7.923    | 5.373      | 10.313     | .899     | .730       | 1.013      |
| 0.06  | 8.454    | 5.829      | 10.902     | .927     | .766       | 1.038      |
| 0.07  | 8.949    | 6.260      | 11.449     | .952     | .797       | 1.059      |
| 0.08  | 9.417    | 6.671      | 11.963     | .974     | .824       | 1.078      |
| 0.09  | 9.864    | 7.067      | 12.453     | .994     | .849       | 1.095      |
| 0.1   | 10.294   | 7.451      | 12.924     | 1.013    | .872       | 1.111      |
| 0.15  | 12.282   | 9.258      | 15.100     | 1.089    | .967       | 1.179      |
| 0.2   | 14.133   | 10.971     | 17.136     | 1.150    | 1.040      | 1.234      |
| 0.25  | 15.942   | 12.658     | 19.149     | 1.203    | 1.102      | 1.282      |
| 0.3   | 17.763   | 14.356     | 21.214     | 1.250    | 1.157      | 1.327      |
| 0.35  | 19.636   | 16.090     | 23.386     | 1.293    | 1.207      | 1.369      |
| 0.4   | 21.595   | 17.881     | 25.720     | 1.334    | 1.252      | 1.410      |
| 0.45  | 23.676   | 19.751     | 28.275     | 1.374    | 1.296      | 1.451      |
| 0.5   | 25.920   | 21.724     | 31.121     | 1.414    | 1.337      | 1.493      |
| 0.55  | 28.377   | 23.831     | 34.343     | 1.453    | 1.377      | 1.536      |
| 0.6   | 31.111   | 26.115     | 38.057     | 1.493    | 1.417      | 1.580      |
Table S7: Probit Analysis and raw data for cytotoxicity of compound 5i against PACA2 (Pancreatic cancer cell line).

| Parameter Estimates |
|---------------------|
| Parameter | Estimate | Std. Error | Z    | Sig.  | 95% Confidence Interval |
| PROBIT$^a$  |
| conc      | 2.381    | .224       | 10.649 | .000  | 1.942 - 2.819           |
| Intercept | -4.441   | .376       | -11.817 | .000  | -4.817 - 4.065          |

a. PROBIT model: PROBIT(p) = Intercept + BX (Covariates X are transformed using the base 10.000 logarithm.)

Chi-Square Tests

| Chi-Square Test | Chi-Square | df$^b$ | Sig.  |
|-----------------|------------|-------|-------|
| PROBIT          | 1.342      | 6     | .969$^c$ |

a. Logarithm base = 10.

PROBIT dead OF total WITH conc
/LOG 10
/MODEL PROBIT
/PRINT FREQ CI
/CRITERIA P(0.15) ITERATE(20) STEPLIMIT(.1).
a. Statistics based on individual cases differ from statistics based on aggregated cases.

b. Since the significance level is greater than .150, no heterogeneity factor is used in the calculation of confidence limits.

| Number | conc | Number of Subjects | Observed Responses | Expected Responses | Residual | Probability |
|--------|------|--------------------|--------------------|-------------------|----------|-------------|
| PROBIT | 1    | 2.000              | 100                | 65                | 62.559   | 2.441       | .626       |
|        | 2    | 1.699              | 100                | 32                | 34.590   | -.250       | .346       |
|        | 3    | 1.398              | 100                | 12                | 13.285   | -1.285      | .133       |
|        | 4    | 1.097              | 100                | 4                 | 3.365    | .635        | .034       |
|        | 5    | .787               | 100                | 1                 | .513     | .487        | .005       |
|        | 6    | .494               | 100                | 0                 | .055    | -.055       | .001       |
|        | 7    | .193               | 100                | 0                 | .003    | -.003       | .000       |
|        | 8    | -.108              | 100                | 0                 | .000    | .000        | .000       |

| Probabil | 95% Confidence Limits for conc | 95% Confidence Limits for log(conc)* |
|-----------|-------------------------------|------------------------------------|
| y        | Estimate | Lower Bound | Upper Bound | Estimate | Lower Bound | Upper Bound |
| PROBIT    |          |             |             |          |             |             |
| 0.01      | 7.731    | 5.060       | 10.449      | .888     | .704        | 1.019       |
| 0.02      | 10.064   | 6.958       | 13.116      | 1.003    | .842        | 1.118       |
| 0.03      | 11.897   | 8.509       | 15.163      | 1.075    | .930        | 1.181       |
| 0.04      | 13.492   | 9.895       | 16.921      | 1.130    | .995        | 1.228       |
| 0.05      | 14.946   | 11.181      | 18.508      | 1.175    | 1.048       | 1.267       |
| 0.06      | 16.307   | 12.403      | 19.983      | 1.212    | 1.094       | 1.301       |
| 0.07      | 17.602   | 13.579      | 21.380      | 1.246    | 1.133       | 1.330       |
| 0.08      | 18.848   | 14.722      | 22.720      | 1.275    | 1.168       | 1.356       |
| 0.09      | 20.058   | 15.839      | 24.019      | 1.302    | 1.200       | 1.381       |
| 0.1       | 21.240   | 16.938      | 25.288      | 1.327    | 1.229       | 1.403       |
| 0.15      | 26.923   | 22.280      | 31.406      | 1.430    | 1.348       | 1.497       |
| 0.2       | 32.505   | 27.546      | 37.523      | 1.512    | 1.440       | 1.574       |
| 0.25      | 38.209   | 32.861      | 43.955      | 1.582    | 1.517       | 1.643       |
| 0.3       | 44.178   | 38.301      | 50.934      | 1.645    | 1.583       | 1.707       |
| 0.35      | 50.540   | 43.933      | 58.664      | 1.704    | 1.643       | 1.768       |
| 0.4       | 57.421   | 49.838      | 67.354      | 1.759    | 1.698       | 1.828       |
| Parameter Estimate | Std. Error | Z    | Sig.  |
|--------------------|------------|------|-------|
| PROBIT conc        | 2.419      | .169 | 14.331| .000  |
| Interception       | -3.731     | .254 | -14.685| .000  |

**Chi-Square Tests**

| Chi-Square | df<sup>b</sup> | Sig. |
|------------|----------------|------|
| PROBIT     | Pearson Goodness-of-Fit Test | 8.623 | 6 | .196<sup>a</sup> |

<sup>a</sup> Statistics based on individual cases differ from statistics based on aggregated cases.

**Table S8: Probit Analysis and raw data for cytotoxicity of compound 6b against A549 (Lung carcinoma cell line)**

a. PROBIT model: PROBIT(p) = Intercept + BX (Covariates X are transformed using the base 10.000 logarithm.)

a. Logarithm base = 10.

/LOG 10
/MODEL PROBIT
/PRINT FREQ CI
/CRITERIA P(0.15) ITERATE(20) STEPLIMIT(.1).

PROBIT dead OF total WITH conc

| Parameter | Estimate | Std. Error | Z    | Sig.  |
|-----------|----------|------------|------|-------|
| PROBIT    | 2.419    | .169       | 14.331| .000  |
| Intercept | -3.731   | .254       | -14.685| .000  |

| Parameter  | Estimate | Std. Error | Z    | Sig.  | Lower Bound | Upper Bound |
|------------|----------|------------|------|-------|-------------|-------------|
| PROBIT     | 2.419    | .169       | 14.331| .000  | 2.088       | 2.750       |
| Intercept  | -3.731   | .254       | -14.685| .000  | -3.986      | -3.477      |

a. Statistics based on individual cases differ from statistics based on aggregated cases.
a. Statistics based on individual cases differ from statistics based on aggregated cases.

b. Since the significance level is greater than .150, no heterogeneity factor is used in the calculation of confidence limits.

### Cell Counts and Residuals

| Number | conc | Number of Subjects | Observed Responses | Expected Responses | Residual | Probability |
|--------|------|--------------------|--------------------|-------------------|----------|-------------|
| PROBIT |      |                    |                    |                   |          |             |
| 1      | 2.000| 100                | 89                 | 86.568            | 2.432    | .866        |
| 2      | 1.699| 100                | 68                 | 64.730            | 3.270    | .647        |
| 3      | 1.398| 100                | 27                 | 36.314            | -9.314   | -.363       |
| 4      | 1.097| 100                | 14                 | 14.047            | -.047    | -.140       |
| 5      | .787 | 100                | 4                  | 3.381             | .619     | .034        |
| 6      | .494 | 100                | 2                  | .560              | 1.440    | .006        |
| 7      | .193 | 100                | 0                  | .055              | -.055    | -.001       |
| 8      | -.108| 100                | 0                  | .003              | -.003    | -.000       |

### Confidence Limits

| Probability | 95% Confidence Limits for conc | 95% Confidence Limits for log(conc)* |
|-------------|-------------------------------|-------------------------------------|
|             | Estimate | Lower Bound | Upper Bound | Estimate | Lower Bound | Upper Bound |
| PROBIT      |          |             |             |          |             |             |
| 0.01        | 3.810    | 2.698       | 4.983       | .581     | .431        | .698        |
| 0.02        | 4.939    | 3.631       | 6.284       | .694     | .560        | .798        |
| 0.03        | 5.823    | 4.382       | 7.283       | .765     | .642        | .862        |
| 0.04        | 6.590    | 5.046       | 8.141       | .819     | .703        | .911        |
| 0.05        | 7.289    | 5.658       | 8.915       | .863     | .753        | .950        |
| 0.06        | 7.941    | 6.236       | 9.634       | .900     | .795        | .984        |
| 0.07        | 8.561    | 6.790       | 10.314      | .933     | .832        | 1.013       |
| 0.08        | 9.158    | 7.326       | 10.965      | .962     | .865        | 1.040       |
| 0.09        | 9.736    | 7.849       | 11.594      | .988     | .895        | 1.064       |
| 0.1         | 10.300   | 8.363       | 12.206      | 1.013    | .922        | 1.087       |
| 0.15        | 13.007   | 10.853      | 15.133      | 1.114    | 1.036       | 1.180       |
| 0.2         | 15.658   | 13.317      | 17.998      | 1.195    | 1.124       | 1.255       |
| 0.25        | 18.358   | 15.833      | 20.936      | 1.264    | 1.200       | 1.321       |
| 0.3         | 21.178   | 18.451      | 24.038      | 1.326    | 1.266       | 1.381       |
| 0.35        | 24.175   | 21.210      | 27.388      | 1.383    | 1.327       | 1.438       |
| 0.4         | 27.412   | 24.152      | 31.071      | 1.438    | 1.383       | 1.492       |
Table S9: Probit Analysis and raw data for cytotoxicity of compound 6d against A549 (Lung carcinoma cell line).

| Parameter | Estimate | Std. Error | Z   | Sig.  | 95% Confidence Interval |
|-----------|----------|------------|-----|-------|-------------------------|
| PROBIT<sup>a</sup> conc | 2.130 | .174 | 12.211 | .000 | 1.788 | 2.472 |
| Intercept | -3.751 | - .278 | -13.487 | .000 | -4.029 | -3.473 |

a. PROBIT model: PROBIT(p) = Intercept + BX (Covariates X are transformed using the base 10.000 logarithm.)
### Chi-Square Tests

|        | Chi-Square | df | Sig. |
|--------|------------|----|------|
| PROBIT | Pearson Goodness-of-Fit Test | 9.161 | 6 | .165 |

a. Statistics based on individual cases differ from statistics based on aggregated cases.

b. Since the significance level is greater than .150, no heterogeneity factor is used in the calculation of confidence limits.

### Cell Counts and Residuals

| Number | conc | Number of Subjects | Observed Responses | Expected Responses | Residual | Probability |
|--------|------|-------------------|--------------------|--------------------|----------|-------------|
| PROBIT | 1    | 2.000             | 100                | 77                 | 69.481   | 7.519 .695  |
|        | 2    | 1.699             | 100                | 38                 | 44.762   | -6.762 .448 |
|        | 3    | 1.398             | 100                | 18                 | 21.979   | -3.979 .220 |
|        | 4    | 1.097             | 100                | 7                  | 7.866    | -3.866 .079 |
|        | 5    | .787              | 100                | 4                  | 1.904    | 2.096 .19   |
|        | 6    | .494              | 100                | 1                  | .349     | .651 .003   |
|        | 7    | .193              | 100                | 0                  | .042     | -.042 .000  |
|        | 8    | -.108             | 100                | 0                  | .003     | -.003-.000  |

### Confidence Limits

| Probability | 95% Confidence Limits for conc | 95% Confidence Limits for log(conc) |
|-------------|--------------------------------|-----------------------------------|
|             | Estimate | Lower Bound | Upper Bound | Estimate | Lower Bound | Upper Bound |
| PROBIT      |          |             |             |          |             |             |
| 0.01        | 4.663    | 3.073       | 6.358       | .669     | .488        | .803        |
| 0.02        | 6.261    | 4.345       | 8.234       | .797     | .638        | .916        |
| 0.03        | 7.548    | 5.409       | 9.710       | .878     | .733        | .987        |
| 0.04        | 8.688    | 6.374       | 10.997      | .939     | .804        | 1.041       |
| 0.05        | 9.741    | 7.282       | 12.175      | .989     | .862        | 1.085       |
| 0.06        | 10.737   | 8.153       | 13.281      | 1.031    | .911        | 1.123       |
| 0.07        | 11.694   | 8.999       | 14.337      | 1.068    | .954        | 1.156       |
| 0.08        | 12.623   | 9.828       | 15.358      | 1.101    | .992        | 1.186       |
| 0.09        | 13.532   | 10.645      | 16.354      | 1.131    | 1.027       | 1.214       |
| x  | y1   | y2   | y3   | y4   | y5   | y6   |
|----|------|------|------|------|------|------|
| 0.1| 14.426| 11.455| 17.332| 1.159| 1.059| 1.239|
| 0.15| 18.803| 15.466| 22.116| 1.274| 1.189| 1.345|
| 0.2 | 23.210| 19.536| 26.977| 1.366| 1.291| 1.431|
| 0.25| 27.806| 23.757| 32.145| 1.444| 1.376| 1.507|
| 0.3 | 32.704| 28.189| 37.799| 1.515| 1.450| 1.577|
| 0.35| 38.010| 32.889| 44.111| 1.580| 1.517| 1.645|
| 0.4 | 43.838| 37.927| 51.267| 1.642| 1.579| 1.710|
| 0.45| 50.326| 43.393| 59.489| 1.702| 1.637| 1.774|
| 0.5 | 57.649| 49.404| 69.055| 1.761| 1.694| 1.839|
| 0.55| 66.036| 56.120| 80.344| 1.820| 1.749| 1.905|
| 0.6 | 75.810| 63.758| 93.884| 1.880| 1.805| 1.973|
| 0.65| 87.435| 72.630| 110.459| 1.942| 1.861| 2.043|
| 0.7 | 101.620| 83.204| 131.284| 2.077| 1.920| 2.118|
| 0.75| 119.520| 96.228| 158.381| 2.077| 1.983| 2.200|
| 0.8 | 143.187| 113.013| 195.412| 2.156| 2.053| 2.291|
| 0.85| 176.750| 136.151| 249.927| 2.247| 2.134| 2.398|
| 0.9 | 230.375| 171.886| 341.058| 2.362| 2.235| 2.533|
| 0.91| 245.601| 181.809| 367.715| 2.390| 2.260| 2.566|
| 0.92| 263.284| 193.22| 399.065| 2.420| 2.286| 2.601|
| 0.93| 284.200| 206.599| 436.660| 2.454| 2.315| 2.640|
| 0.94| 309.531| 222.611| 482.885| 2.491| 2.348| 2.684|
| 0.95| 341.188| 242.373| 541.655| 2.533| 2.384| 2.734|
| 0.96| 382.541| 267.813| 619.971| 2.583| 2.428| 2.792|
| 0.97| 440.311| 302.736| 732.037| 2.644| 2.481| 2.865|
| 0.98| 530.830| 356.235| 913.162| 2.725| 2.552| 2.961|
| 0.99| 712.741| 460.214| 1294.332| 2.853| 2.663| 3.112|

a. Logarithm base = 10.

PROBIT dead OF total WITH conc
/LOG 10
/MODEL PROBIT
/PRINT FREQ CI
/CRITERIA P(0.15) ITERATE(20) ST
EPLIMIT(.1).
Table S10: Probit Analysis and raw data for cytotoxicity of compound 6g against A549 (Lung carcinoma cell line).

### Parameter Estimates

| Parameter | Estimate | Std. Error | Z   | Sig. | 95% Confidence Interval |
|-----------|----------|------------|-----|------|-------------------------|
| PROBIT\(^a\) conc | 2.312 | .179 | 12.925 | .000 | 1.961 - 2.662 |
| Intercept | -3.851- | .282 | -13.649- | .000 | -4.133- - 3.568- |

a. PROBIT model: PROBIT(p) = Intercept + BX (Covariates X are transformed using the base 10.000 logarithm.)

### Chi-Square Tests

| PROBIT Pearson Goodness-of-Fit Test | Chi-Square | df\(^a\) | Sig. |
|-------------------------------------|------------|----------|------|
| PROBIT                             | 1.164      | 6        | .979\(^b\) |

a. Statistics based on individual cases differ from statistics based on aggregated cases.

b. Since the significance level is greater than .150, no heterogeneity factor is used in the calculation of confidence limits.

### Cell Counts and Residuals

| Number | conc | Number of Subjects | Observed Responses | Expected Responses | Residual | Probability |
|--------|------|--------------------|--------------------|--------------------|----------|-------------|
| PROBIT | 1    | 2.000              | 100                | 77                 | 78.013   | -1.013- .780 |
|        | 2    | 1.699              | 100                | 54                 | 53.059   | .941 .531   |
|        | 3    | 1.398              | 100                | 28                 | 26.793   | 1.207 .268  |
|        | 4    | 1.097              | 100                | 8                  | 9.426    | -1.426-.094 |
|        | 5    | .787               | 100                | 3                  | 2.112    | .888 .021   |
|        | 6    | .494               | 100                | 0                  | .338     | -.338-.003  |
|        | 7    | .193               | 100                | 0                  | .033     | -.033-.000  |
|        | 8    | -.108-             | 100                | 0                  | .002     | -.002-.000  |

### Confidence Limits

| Probability \(y\) | 95% Confidence Limits for conc | 95% Confidence Limits for log(conc)\(^a\) |
|-------------------|-------------------------------|------------------------------------------|
| PROBIT | Estimate | Lower Bound | Upper Bound | Estimate | Lower Bound | Upper Bound |
|--------|----------|-------------|-------------|----------|-------------|-------------|
| 0.01   | 4.564    | 3.102       | 6.111       | .659     | .492        | .786        |
| 0.02   | 5.988    | 4.255       | 7.765       | .777     | .629        | .890        |
| 0.03   | 7.114    | 5.198       | 9.046       | .852     | .716        | .956        |
| 0.04   | 8.099    | 6.040       | 10.150      | .908     | .781        | 1.006       |
| 0.05   | 8.999    | 6.822       | 11.151      | .954     | .834        | 1.047       |
| 0.06   | 9.844    | 7.565       | 12.083      | .993     | .879        | 1.082       |
| 0.07   | 10.650   | 8.281       | 12.967      | 1.027    | .918        | 1.113       |
| 0.08   | 11.427   | 8.978       | 13.816      | 1.058    | .953        | 1.140       |
| 0.09   | 12.183   | 9.661       | 14.638      | 1.086    | .985        | 1.165       |
| 0.1    | 12.923   | 10.333      | 15.442      | 1.111    | 1.014       | 1.189       |
| 0.15   | 16.497   | 13.623      | 19.307      | 1.217    | 1.134       | 1.286       |
| 0.2    | 20.030   | 16.913      | 23.137      | 1.302    | 1.228       | 1.364       |
| 0.25   | 23.658   | 20.295      | 27.112      | 1.374    | 1.307       | 1.433       |
| 0.3    | 27.473   | 23.825      | 31.363      | 1.439    | 1.377       | 1.496       |
| 0.35   | 31.555   | 27.552      | 36.014      | 1.499    | 1.440       | 1.556       |
| 0.4    | 35.989   | 31.527      | 41.192      | 1.556    | 1.499       | 1.615       |
| 0.45   | 40.870   | 35.812      | 47.048      | 1.611    | 1.554       | 1.673       |
| 0.5    | 46.319   | 40.490      | 53.765      | 1.666    | 1.607       | 1.731       |
| 0.55   | 52.496   | 45.671      | 61.587      | 1.720    | 1.660       | 1.789       |
| 0.6    | 59.616   | 51.510      | 70.846      | 1.775    | 1.712       | 1.850       |
| 0.65   | 67.991   | 58.225      | 82.030      | 1.832    | 1.765       | 1.914       |
| 0.7    | 78.095   | 66.146      | 95.883      | 1.893    | 1.821       | 1.982       |
| 0.75   | 90.688   | 75.797      | 113.634     | 1.958    | 1.880       | 2.056       |
| 0.8    | 107.115  | 88.091      | 137.479     | 2.030    | 1.945       | 2.138       |
| 0.85   | 130.055  | 104.818     | 171.891     | 2.114    | 2.020       | 2.235       |
| 0.9    | 166.023  | 130.253     | 228.019     | 2.220    | 2.115       | 2.358       |
| 0.91   | 176.108  | 137.244     | 244.171     | 2.246    | 2.137       | 2.388       |
| 0.92   | 187.760  | 145.254     | 263.037     | 2.274    | 2.162       | 2.420       |
| 0.93   | 201.464  | 154.590     | 285.489     | 2.304    | 2.189       | 2.456       |
| 0.94   | 217.954  | 165.714     | 312.864     | 2.338    | 2.219       | 2.495       |
| 0.95   | 238.415  | 179.363     | 347.340     | 2.377    | 2.254       | 2.541       |
| 0.96   | 264.922  | 196.819     | 392.776     | 2.423    | 2.294       | 2.594       |
| 0.97   | 301.580  | 220.588     | 456.929     | 2.479    | 2.344       | 2.660       |
| 0.98   | 358.281  | 256.628     | 558.844     | 2.554    | 2.409       | 2.747       |
| 0.99   | 470.058  | 325.617     | 767.882     | 2.672    | 2.513       | 2.885       |
| conc | 0.01 | 0.02 | 0.03 | 0.04 | 0.05 | 0.06 | 0.07 | 0.08 | 0.09 | 0.1 | 0.15 | 0.2 | 0.25 | 0.3 | 0.35 | 0.4 | 0.45 | 0.5 | 0.55 | 0.6 | 0.65 | 0.7 | 0.75 | 0.8 | 0.85 | 0.9 | 0.91 | 0.92 | 0.93 | 0.94 | 0.95 | 0.96 | 0.97 | 0.98 | 0.99 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
|      | 4.564 | 5.988 | 7.114 | 8.099 | 8.999 | 9.844 | 10.650 | 11.427 | 12.183 | 12.923 | 16.497 | 20.030 | 23.658 | 27.473 | 31.555 | 35.989 | 40.870 | 46.319 | 52.496 | 59.616 | 67.991 | 78.095 | 90.688 | 107.115 | 130.055 | 166.023 | 176.108 | 187.760 | 201.464 | 217.954 | 238.415 | 264.922 | 301.580 | 358.281 | 470.058 |
|      | 3.102 | 4.255 | 5.198 | 6.040 | 6.822 | 7.565 | 8.281 | 8.978 | 9.661 | 10.333 | 13.623 | 16.913 | 20.295 | 23.825 | 27.552 | 31.527 | 35.812 | 40.490 | 45.671 | 51.510 | 58.225 | 66.146 | 75.797 | 88.091 | 104.818 | 130.253 | 137.244 | 145.254 | 154.590 | 165.714 | 179.363 | 196.819 | 220.588 | 256.628 | 325.617 | 376.882 |
|      | 6.111 | 7.765 | 9.046 | 10.150 | 11.151 | 12.083 | 12.967 | 13.816 | 14.638 | 15.442 | 19.307 | 23.137 | 27.112 | 31.363 | 36.014 | 41.192 | 47.048 | 53.765 | 61.587 | 70.846 | 82.030 | 95.883 | 113.634 | 137.479 | 171.891 | 228.019 | 244.171 | 263.037 | 285.489 | 312.864 | 347.340 | 392.776 | 456.929 | 558.844 | 767.882 | 2.672 |
|      | .659  | .777  | .852  | .908  | .954  | .993  | 1.027  | 1.058  | 1.086  | 1.111  | 1.217  | 1.302  | 1.374  | 1.439  | 1.499  | 1.556  | 1.611  | 1.666  | 1.720  | 1.775  | 1.832  | 1.893  | 1.958  | 2.030  | 2.114  | 2.220  | 2.246  | 2.274  | 2.304  | 2.338  | 2.377  | 2.423  | 2.479  | 2.554  | 2.672  | 2.513  | 2.885 |
| a. Logarithm base = 10. PROBIT dead OF total WITH conc /LOG 10