Supplementary Information

Design, synthesis, *in silico* and *in vitro* evaluation of pyrrole-indole hybrids as dual tubulin and aromatase inhibitors with potent anticancer activities

Rungroj Saruengkhanphasit,^{1, 2*} Jaruwan Chatwichien,^{1, 3} Lukana Ngiwsara,⁴ Kriengsak Lirdprapamongkol,^{2, 4} Worawat Niwetmarin,¹ Chatchakorn Eurtivong,⁵ Prasat Kittakoop,^{1, 2, 6} ⁶ Jisnuson, Svasti,⁴ Somsak Ruchirawat^{1, 2, 7}

¹Chulabhorn Graduate Institute, Program in Chemical Sciences, 54 Kamphaeng Phet 6, Talat Bang Khen, Lak Si, Bangkok 10210, Thailand.

²Center of Excellence On Environmental Health and Toxicology (EHT), OPS, Ministry of Higher Education, Science, Research and Innovation, Bangkok, Thailand.

³Chulabhorn Royal Academy, Bangkok 10210, Thailand.

⁴Laboratory of Biochemistry, Chulabhorn Research Institute, Bangkok 10210, Thailand.

⁵Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mahidol University, 447 Si Ayutthaya Road, Ratchathewi, Bangkok 10400, Thailand.

⁶Laboratory of Natural Products, Chulabhorn Research Institute, Bangkok 10210, Thailand.

⁷Laboratory of Medicinal Chemistry, Chulabhorn Research Institute, Bangkok 10210, Thailand.

Table of content

Synthesis of various aldehydes	page 2-8
¹ H and ¹³ C Spectra	page 9-55
Figure S1. NCI60 one dose screen for compounds 3a-x	page 56-79
Table S2. GI_{50} and LC_{50} screen for compounds 3a-b , 3n , and 3p-3x	page 80-83
Figure S3. NCI60 five dose screen for compounds 3a-b , 3n , and 3p-3x	page 84-119
Figure S4. Screening derivatives 3a-x against T-47D	page 120
Figure S5. Correlations between IC_{50} values and GI_{50} values	page 121
Figure S6. Overlay between the co-crystallized colchicine	page 122
Figure S7. Overlay between the co-crystallized exemestane	page 122
Figure S8. Physicochemical properties of compounds 3a-x	page 123
Table S9. Toxicity evaluation of the most active compounds.	page 124

Synthesis of various aldehyde



4-bromo-1*H*-pyrrole-2-carbaldehyde

To a solution of pyrrole-2-carboxaldehyde (0.302 g, 3.18 mmol) in MeCN (5 mL) was added *N*-bromosuccinimide (0.566 g, 3.18 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 15 min. The mixture was diluted by H₂O (5 mL) and was extracted with Et₂O (3 x 10 mL). The combined organic layers were dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (3:7), gave 4-bromo-1*H*-pyrrole-2-carbaldehyde (0.305 g, 1.76 mmol, 55%) as a white solid; R_f 0.6 [EtOAc-Hexane (3:7)]; m.p. 123–125 °C, lit.¹ m.p. 122–124 °C; ¹H NMR (600 MHz, CDCl₃) δ 9.73 (br. s, 1H), 9.50 (s, 1H), 7.14–7.13 (m, 3H), 6.99 (m, 1H) Data were in agreement to those reported in the literature.^[1]



4,5-dibromo-1*H*-pyrrole-2-carbaldehyde

To a solution of pyrrole-2-carboxaldehyde (0.316 g, 3.32 mmol) in MeCN (5 mL) was added *N*-bromosuccinimide (1.21 g, 6.80 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 1 h. The mixture was diluted by H₂O (5 mL) and was extracted with Et₂O (3 x 10 mL). The combined organic layers were dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (3:7), gave 4,5-dibromo-1*H*-pyrrole-2-carbaldehyde (0.765 g 3.02 mmol, 91%) as a white solid; R_f 0.6 [EtOAc-Hexane (3:7)]; m.p. 148–150 °C, lit.¹ m.p. 144–146 °C; ¹H NMR (300 MHz, CDCl₃) δ 10.09 (br. s, 1H), 9.35 (s, 1H), 6.96 (s, 1H) Data were in agreement to those reported in the literature.^[2]



3-chloro-1H-pyrrole-2-carbaldehyde and 4-chloro-1H-pyrrole-2-carbaldehyde

To a solution of pyrrole-2-carboxaldehyde (0.249 g, 2.62 mmol) in THF (5 mL) was added *N*-chlorosuccinimde (0.390 g, 2.92 mmol) at room temperature. The reaction mixture was stirred at room temperature for 48 h. The mixture was dilute by MeOH (3 mL) and was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (0:100 to 1.5:8.5), gave 3-chloro-1*H*-pyrrole-2-carbaldehyde (0.156 g) as a white solid and 4-chloro-1*H*-pyrrole-2-carbaldehyde (0.051 g) as a yellow solid. The compounds were used in the next step without characterisation.

$$(H)$$
 CO_2Et $POCI_3$, DMF (H) CO_2Et (H) CO_2Et (H) (CO_2Et)

Ethyl 5-formyl-1*H*-pyrrole-2-carboxylate and ethyl 4-formyl-1*H*-pyrrole-2-carboxylate

To a solution of ethyl 1*H*-pyrrole-2-carboxylate (1.06 g, 7.62 mmol) in anhydrous DMF (14 mL) was added POCl₃ (2.1 mL, 15.7 mmol) at 0 °C. The reaction mixture was allowed to warm to room temperature 15 min and stirred at room temperature for 16 h. The mixture was diluted by H_2O (8 mL) and was added 25% aqueous NH₃ until the pH of solution adjust to 7. The aqueous layer was extracted with CH₂Cl₂ (3 x 20 mL). The combind organic layers were washed with saturated aqueous NaHCO₃ (25 mL), brine (25 mL), was dried (Na₂SO₄), and was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (3:7 to 1:1), gave ethyl 5-formyl-1*H*-pyrrole-2-carboxylate (0.514 g, 3.07 mmol, 40%) as a yellow solid and ethyl 4-formyl-1*H*-pyrrole-2-carboxylate (0.544 g, 3.25 mmol, 43%) as a yellow solid.

Ethyl 5-formyl-1*H*-pyrrole-2-carboxylate; R_f 0.6 [EtOAc-Hexane (3:7)]; m.p. 71–74 °C, lit.³ m.p. 122–124 °C; ¹H NMR (300 MHz, CDCl₃) δ 9.83 (br. s, 1H), 9.68 (s, 1H), 6.97 (d, *J* = 2.5 Hz, 2H), 4.44 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H) Data were in agreement to those reported in the literature.^[3]

Ethyl 4-formyl-1*H*-pyrrole-2-carboxylate; $R_f 0.3$ [EtOAc-Hexane (3:7)]; m.p. 100–102 °C, lit.³ m.p. 101–102 °C; ¹H NMR (300 MHz, CDCl₃) δ 9.89 (br. s, 1H), 9.85 (s, 1H), 7.58 (dd, *J* = 3.4, 1.6 Hz, 2H), 7.33–7.31 (m, 1H), 4.44 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H) Data were in agreement to those reported in the literature.^[3]



Ethyl 1H-pyrrole-3-carboxylate

Under Argon atmosphere, anhydrous Et₂O (20 mL) was added to NaH (60% in oil, 1.11 g, 27.72 mmol) at room temperature. With a magnetic stirring, TosMIC (3.0 g, 15.4 mmol) and ethyl acrylate (1.8 mL, 16.5 mmol) in anhydrous Et₂O-DMSO (20 mL: 10 mL) was added dropwise. The reaction mixture was stirred at room temperature for 5h. The mixture was diluted by H₂O (20 mL) and was extract with Et₂O (3 x 30 mL). The combined organic layers were dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (1:9 to 3:7), gave ethyl 1*H*-pyrrole-3-carboxylate (0.883 g, 6.35 mmol, 41%) as a yellow oil; R_f 0.4 [EtOAc-Hexane (3:7)]; ¹H NMR (400 MHz, CDCl₃) δ 8.58 (br. s, 1H), 7.44–7.42 (m, 1H), 6.76–6.75 (m, 1H), 6.67–6.65 (m, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H) Data were in agreement to those reported in the literature.^[4]

Ethyl 5-formyl-1*H*-pyrrole-3-carboxylate and ethyl 2-formyl-1*H*-pyrrole-3-carboxylate

To a solution of ethyl 1*H*-pyrrole-3-carboxylate (0.883 g, 6.35 mmol) in anhydrous DMF (20 mL) was added (Chloromethylene)dimethyliminium chloride (1.3 g, 10.16 mmol) at 0 °C. The reaction mixture was allowed to warm to room temperature 15 min and stirred at room temperature for 16 h. The mixture was diluted by H_2O (10 mL) and was added saturated aqueous Na₂CO₃ until the pH of solution adjust to 7. The aqueous layer was extracted with CH₂Cl₂ (3 x 20 mL). The combind organic layers were washed with saturated aqueous NaHCO₃

(25 mL), brine (25 mL), was dried (Na₂SO₄), and was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (1:9 to 3:7), gave ethyl 5-formyl-1*H*-pyrrole-3-carboxylate (0.847 g, 5.07 mmol, 80%) as a yellow solid and ethyl 2-formyl-1*H*-pyrrole-3-carboxylate (0.137 g, 0.82 mmol, 13%) as a yellow solid.

Ethyl 5-formyl-1*H*-pyrrole-3-carboxylate; R_f 0.4 [EtOAc-Hexane (3:7)]; m.p. 90–93 °C, lit.^[5] m.p. 84.1–85.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.18 (br. s, 1H), 9.56 (d, J = 1.1 Hz, 1H), 7.71 (dt, J = 3.3, 1.3 Hz, 1H), 7.40 (dd, J = 2.5, 1.4 Hz, 1H), 4.35 (q, J = 7.1 Hz, 2H), 1.38 (t, J = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 180.10, 163.74, 133.20, 129.92, 121.57, 119.36, 60.54, 14.52; v_{max}/cm⁻¹ 3254, 3051, 2838, 1699, 1651, 1189; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₈H₁₀O₃N 168.0655; found 168.0654.

Ethyl 2-formyl-1*H*-pyrrole-3-carboxylate; R_f 0.6 [EtOAc-Hexane (3:7)]; m.p. 116_119 °C, lit.^[6] m.p. 84.1–85.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.23 (d, *J* = 1.0 Hz, 1H), 10.13 (br. s, 1H), 7.05 (td, *J* = 2.8, 1.0 Hz, 1H), 6.78 (t, *J* = 2.7 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 182.06, 163.73, 132.94, 124.13, 123.06, 113.85, 60.93, 14.47; v_{max} /cm⁻¹ 3205, 3123, 2901, 1697, 1633, 1118; HRMS (ESI) *m*/*z* [M+H]⁺ calcd for C₈H₁₀O₃N 168.0655; found 168.0654.

5-formyl-1*H*-pyrrole-2-carboxylic acid

To a solution of ethyl 5-formyl-1*H*-pyrrole-2-carboxylate (0.45 g, 2.69 mmol) and KOH (166 mg, 2.96 mmol) in EtOH/H₂O (4:1, 5 mL) was heated to 90 °C. The reaction mixture was stirred for 3-6 h. The reaction mixture was cooled to room temperature, and the solvent was evaporated. The residue was dissolved in H₂O (3 mL), acidified with conc. HCl until the pH of solution adjusted to 1–2. The percipitate product was filtered, washed with H₂O (3 x 10 mL) and dried over night to gave 5-formyl-1*H*-pyrrole-2-carboxylic acid (0.347 g, 2.49 mmol, 93%) as brown solid; m.p. decomposed; ¹H NMR (300 MHz, (CD₃)₂SO) δ 13.13 (br. s, 1H), 12.87 (br. s, 1H), 9.68 (s, 1H), 6.95–6.93 (m, 1H), 6.84–6.82 (m, 1H) Data were in agreement to those reported in the literature.^[7] Compounds below were synthesized following the procedure described here.

4-formyl-1*H*-pyrrole-2-carboxylic acid

Brown solid (0.256 g, 1.84 mmol, 95%); m.p. decomposed; ¹H NMR (300 MHz, (CD₃)₂SO) δ 12.84 (br. s, 1H), 12.53 (br. s, 1H), 9.74 (s, 1H), 7.77 (dd, J = 3.4, 1.6 Hz, 1H), 7.08–7.06 (m, 1H); ¹³C NMR (75 MHz, (CD₃)₂SO) δ 185.90, 161.62, 130.90, 126.67, 125.67, 112.70; $v_{\text{max}}/\text{cm}^{-1}$ 3287, 3119, 2877, 2766, 1677, 1436, 1119; HRMS (ESI) m/z [M–H]⁻ calcd for C₆H₄O₃N 138.0186; found 138.0182.

5-formyl-1*H*-pyrrole-3-carboxylic acid

To a solution of ethyl 5-formyl-1*H*-pyrrole-3-carboxylate (0.238 g, 1.42 mmol) and KOH (239 mg, 4.26 mmol) in EtOH/H₂O (1:1, 5 mL) was heated to 90 °C. The reaction mixture was stirred for 17 h. The reaction mixture was cool to room temperature, and the solvent was evaporated. The residue was dissolved in H₂O (3 mL), acidified with conc. HCl until the pH of solution adjusted to 1–2. The percipitate product was filtered, washed with H₂O (3 x 10 mL) and dried over night to gave 5-formyl-1*H*-pyrrole-2-carboxylic acid (0.139 g, 1.0 mmol, 70%)

as an orange solid; m.p. decomposed; ¹H NMR (400 MHz, $(CD_3)_2SO$) δ 12.59 (br. s, 1H), 12.25 (br. s, 1H), 9.55 (d, J = 1.0 Hz, 1H), 7.68–7.66 (m, 1H), 7.33–7.32 (m, 1H); ¹³C NMR (100 MHz, $(CD_3)_2SO$) δ 180.36, 164.61, 133.31, 130.18, 120.92, 118.31; v_{max}/cm^{-1} 3236, 3122, 2893, 2720, 1649, 1564, 1232; HRMS (ESI) m/z [M–H]⁻ calcd for C₆H₄O₃N 138.0186; found 138.0182.



5-(morpholine-4-carbonyl)-1H-pyrrole-2-carbaldehyde

To a solution of 5-formyl-1*H*-pyrrole-2-carboxylic acid (0.119 g, 0.86 mmol), EDCI (0.247 g, 1.29 mmol), and HOBt (0.174 g, 1.29 mmol) in DMF (10 mL) was added morpholine (0.08 mL, 0.92 mmol) and NEt₃ (0.3 mL, 2.16 mmol) at roomtemperature. The reaction mixture was stirred at room temperature for 18 h. The mixture was diluted by H₂O (10 mL) and was extract with CH₂Cl₂ (3 x 30 mL). The combined organic layers were dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with MeOH-CH₂Cl₂ (1:99 to 1:19), gave 5-(morpholine-4-carbonyl)-1H-pyrrole-2-carbaldehyde (0.127 g, 0.61 mmol, 71%) as a white solid; R_f 0.6 [MeOH-CH₂Cl₂ (1:19)]; m.p. 160–162 °C; ¹H NMR (400 MHz, (CD₃)₂SO) δ 12.58 (br. s, 1H), 9.61 (s, 1H), 6.97 (d, *J* = 3.9 Hz, 1H), 6.57 (d, *J* = 4.0 Hz, 1H), 3.61 (s, 8H); ¹³C NMR (100 MHz, (CD₃)₂SO) δ 180.55, 160.97, 133.54, 131.23, 117.52, 112.55, 66.10; v_{max}/cm⁻¹ 3183, 3086, 2856, 2819, 1673, 1589, 1233; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₁₀H₁₃O₃N₂ 209.0921; found 209.0917. Compounds below were synthesized following the procedure described here.

5-(morpholine-4-carbonyl)-1H-pyrrole-3-carbaldehyde

White solid (0.091 g, 0.44 mmol, 51%); $R_f 0.5$ [MeOH-CH₂Cl₂ (1:19)]; m.p. 172–175 °C; ¹H NMR (400 MHz, CDCl₃) δ 11.29 (br. s, 1H), 9.81 (s, 1H), 7.51 (dd, J = 3.4, 1.4 Hz, 1H), 6.94–6.93 (m, 1H), 3.87 (s, 4H), 3.77–3.74 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 185.73, 161.50, 128.95, 127.14, 126.37, 110.63, 66.83; v_{max} /cm⁻¹ 3138, 3126, 2843, 1665, 1599, 1115; HRMS (ESI) *m*/*z* [M–H]⁻ calcd for C₁₀H₁₁O₃N₂ 207.0764; found 207.0766.

4-(morpholine-4-carbonyl)-1*H*-pyrrole-2-carbaldehyde

Yellow solid (0.058 g, 0.29 mmol, 48%); $R_f 0.4$ [MeOH-CH₂Cl₂ (1:19)]; m.p. 180–182 °C decomposed; ¹H NMR (400 MHz, (CD₃)₂SO) δ 12.49 (br. s, 1H), 9.52 (d, J = 1.0 Hz, 1H), 7.51–7.50 (m, 1H), 7.20 (t, J = 7.9 Hz, 1H), 3.60 (s, 8H); ¹³C NMR (100 MHz, (CD₃)₂SO) δ 180.02, 164.12, 132.42, 128.34, 120.34, 119.90, 66.19; v_{max} /cm⁻¹ 3172, 3001, 2923, 2858, 1658, 1591, 1114; HRMS (ESI) *m*/z [M–H]⁻ calcd for C₁₀H₁₁O₃N₂ 207.0764; found 138.0765.



5-nitro-1*H*-pyrrole-2-carbaldehyde and 4-nitro-1*H*-pyrrole-2-carbaldehyde

To acetic anhydride (4 mL) was added conc. HNO_3 (0.6 mL) at room temperature. After complete the addition, the nitration reagent was added dropwise to the solution of pyrrole-2-carboxaldehyde (0.511 g, 5.37 mmol) in acetic anhydride (5 mL) at -30 °C. The reaction

mixture was stirred at -30 °C for 1 h. The mixture was poured in H₂O (20 mL), basic dified with saturated aqueous Na₂CO3 until the pH of solution adjusted to 8, and was extracted with EtOAc (3 x 30 mL). The combined organic layers were dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (1:9 to 3:7), gave 5-nitro-1*H*-pyrrole-2-carbaldehyde (0.097 g, 0.69 mmol, 13%) as a yellow solid and 4-nitro-1*H*-pyrrole-2-carbaldehyde (0.276 g, 1.97 mmol, 37%) as a yellow solid.

5-nitro-1*H*-pyrrole-2-carbaldehyde; R_f 0.4 [EtOAc-Hexane (3:7)]; m.p. 176–178 °C decomposed; ¹H NMR (400 MHz, (CD₃)₂CO) δ 9.83 (s, 1H), 7.20 (d, *J* = 4.2 Hz, 1H), 7.11 (d, *J* = 4.3 Hz, 1H); ¹³C NMR (100 MHz, (CD₃)₂SO) δ 182.12, 134.70, 118.12, 111.23; v_{max}/cm^{-1} 3418, 3127, 2890, 2853, 1680, 1279; HRMS (ESI) *m/z* [M-H]⁻ calcd for C₅H₃O₃N₂ 139.0138; found 139.0138.

4-nitro-1*H*-pyrrole-2-carbaldehyde; R_f 0.3 [EtOAc-Hexane (3:7)]; m.p. 135–137 °C decomposed; ¹H NMR (400 MHz, (CD₃)₂CO) δ 12.05 (br. s, 1H), 9.69 (d, *J* = 1.1 Hz, 1H), 8.13_8.12 (m, 1H), 7.58 (d, *J* = 1.7 Hz, 1H); ¹³C NMR (100 MHz, (CD₃)₂SO) δ 181.02, 138.98, 133.14, 126.01, 144.35; v_{max} /cm⁻¹ 3216, 3134, 2813, 2702, 1660, 1306; HRMS (ESI) *m*/z [M-H]⁻ calcd for C₅H₃O₃N₂ 139.0138; found 139.0137.



3,5-dimethyl-4-nitro-1*H*-pyrrole-2-carbaldehyde

3,5-Dimethyl-1H-pyrrole-2-carbaldehyde (0.22 g, 1.79 mmol) was added into conc. H₂SO₄ (10 mL) slowly at -20 °C, and the mixture was stirred until it become homogeneous. Subsequently, KNO₃ (0.198 g, 1.96 mmol) was added in portion below -10 °C. The mixture was stirred at -10 °C for 20 min and then stirred at room temperature for another 20 min. After completion, cold H₂O (20 mL) was added in portions. The parcipitate was filtered washed with H2O (20 mL), and dried over night to gave 3,5-dimethyl-4-nitro-1*H*-pyrrole-2-carbaldehyde (0.178 g, 1.06 mmol, 59%) as a brown solid; m.p. decomposed; ¹H NMR (400 MHz, (CD₃)₂SO) δ 12.79 (br. s, 1H), 9.73 (s, 1H), 2.55 (s, 3H), 2.54 (s, 3H) Data were in agreement to those reported in the literature.^[8]



5-ethyl-1*H*-pyrrole-2-carbaldehyde

To a solution of 2-ethylpyrrole (0.3 mL, 2.93 mmol) in $C_2H_4Cl_2$ (10 mL) was added (Chloromethylene)dimethyliminium chloride (0.451 g, 3.52 mmol) at 0 °C. The reaction mixture was allowed to warm to room temperature 15 min. The reaction mixture was heated to 85 °C and stirred for 30 min. The mixture was cooled to room temperature, a solution of NaOAc (1.32 g, 16.11 mmol) in H₂O (10 mL) was added. The mixture was heated to 85 °C and stirred for 30 min. The mixture was with H₂O (10 mL), saturated Na₂CO₃ (2 x 10 mL), and brine (10 mL). The organic layer was dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (1:9 to 3:7), gave 5-

ethyl-1*H*-pyrrole-2-carbaldehyde (0.331 g, 2.69 mmol, 92%) as a yellow solid; $R_f 0.6$ [EtOAc-Hexane (3:7)]; m.p. 38-41 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.18 (br. s, 1H), 9.36 (s, 1H), 6.92 (dd, *J* = 3.8, 2.4 Hz, 1H), 6.10-6.09 (m, 1H), 2.76 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 178.66, 145.42, 132.31, 123.51, 109.27, 21.54, 13.54; v_{max}/cm^{-1} 3252, 3128, 2880, 2818, 1630, 1495; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₇H₁₀ON 124.0757; found 124.0759.



3-ethyl-1*H*-pyrrole

To a solution of LiAlH₄ (0.572 g, 15.08 mmol) in anhydrous THF (10 mL) was added 3acetylpyrrole (0.822 g, 7.53 mmol) at 0 °C. The reaction mixture was allowed to warm to room temperature 15 min. The reaction mixture was heated to 72 °C and stirred for 17 h. The reaction was cooled to room temperature and quenched with a few drops of EtOAc followed by MeOH and H₂O until no bubbles were released. The mixture was extracted by CH₂Cl₂ (3 x 20 mL). The combined organic layers were dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with Et₂O-Pentane (3:7), gave 3-ethyl-1*H*-pyrrole (0.544 g) as colourless oil. The compounds were used in the next step without characterisation.

4-ethyl-1*H*-pyrrole-2-carbaldehyde and 3-ethyl-1*H*-pyrrole-2-carbaldehyde

To a solution of 3-ethyl-1*H*-pyrrole (0.544 g, 5.72 mmol) in CH₂Cl₂ (10 mL) was added (Chloromethylene)dimethyliminium chloride (1.46 g, 11.44 mmol) at 0 °C. The reaction mixture was allowed to warm to room temperature 15 min. The mixture was stirred at room temperature for 16 h. The solvent was evaporated, the residue was added H₂O (10 mL) followed by NaOH (1.83 g, 45.76 mmol) and the mixture was stirred at room temperature for 1 h. EtOAc (20 mL) was added, the layers were separated and the aqueous layer was extracted by EtOAc (2 x 20 mL). The combined organic layers were dried (Na₂SO₄), filtered, and the solvent was evaporated. Purification by flash column chromatography, eluted with EtOAc-Hexane (1:9 to 3:7), gave 4-ethyl-1*H*-pyrrole-2-carbaldehyde (0.130 g, 1.06 mmol, 19%) as a yellow oil and 3-ethyl-1*H*-pyrrole-2-carbaldehyde (0.297 g, 2.41 mmol, 42%) as a yellow oil.

4-Ethyl-1*H*-pyrrole-2-carbaldehyde; R_f 0.5 [EtOAc-Hexane (3:7)]; ¹H NMR (300 MHz, CDCl₃) δ 9.45 (s, 1H), 6.93 (~t, 1H), 6.82 (t, *J* = 2.2 Hz, 1H), 2.54 (q, *J* = 7.6 Hz, 2H), 1.21 (t, *J* = 7.6 Hz, 3H) Data were in agreement to those reported in the literature.^[9]

3-Ethyl-1*H*-pyrrole-2-carbaldehyde; R_f 0.5 [EtOAc-Hexane (3:7)]; ¹H NMR (300 MHz, CDCl₃) δ 9.64 (s, 1H), 9.34 (br. S, 1H), 7.02 (~t, 1H), 6.19j (t, *J* = 2.6 Hz, 1H), 2.82 (q, *J* = 7.6 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H) Data were in agreement to those reported in the literature.^[9]

References

[1] M. A. Buil, M. Calbet, M. Castillo, J. Castro, C. Esteve, M. Ferrer, P. Forns, J. González, S. López, R. S. Roberts, S. Sevilla, B. Vidal, L. Vidal, P. Vilaseca, *Eur. J. Med. Chem.* **2016**, *113*, 102–103.

[2] J. K. Laha, S. Sharma, S. Kira, U. C. Banerjee, J. Org. Chem. 2017, 82, 9350-9359.

[3] T. Warashina, D. Matsuura, T. Sengoku, M. Takahashi, H. Yoda, Y. Kimura, Org. Process Res. Dev. 2019, 23, 614–618.

[4] K. C. Nguyen, P. Wang, R. D. Sommer, J. S. Lindsey, J. Org. Chem. 2020, 85, 6605-6619.

[5] Y.-Z. Jin, D.-X. Fu, N. Ma, Z.-C. Li, Q.-H. Liu, L. Xiao, R.-H. Zhang, *Molecules*. 2011, 16, 9368–9385.

[6] H. Jing, P. Wang, B. Chen, J. Jiang, P. Vairaprakash, S. Liu, J. Rong, C.-Y, Chen, P. Nalaoh, J. S. Lindsey, *New J. Chem.* **2022**, *46*, 5534–5555.

[7] C. Schmuck, V. Bickert, M. Merschky, L. Geiger, D. Rupprecht, J. Dudaczek, P. Wich, T. Rehm, U. Machon, *Eur. J. Org. Chem.* **2008**, *2*, 324–329.

[8] Q. Li, X. Pan, D. Wang, Q. Rong, B. Ma, X. Xie, Y. Zhang, J. Wang, L. Hu, *J. Med. Chem.* **2021**, *64*, 17184–17208.

[9] A. Sailer, J. C. M. Meiring, C. Heise, L. N. Pettersson, A. Akhmanova, J. Thorn-Seshold, O. Thorn-Seshold, *Angew. Chem. Int. Ed.* **2021**, *60*, 23695–23704.



1H and 13C spectra

4,5-dibromo-1*H*-pyrrole-2-carbaldehyde spectra in CDCl₃



Ethyl 5-formyl-1*H*-pyrrole-2-carboxylate spectra in CDCl₃



Ethyl 4-formyl-1*H*-pyrrole-2-carboxylate spectra in CDCl₃









00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 (f1 (ppm)

5-formyl-1*H*-pyrrole-2-carboxylic acid spectra in dmso-d₆



4-formyl-1*H*-pyrrole-2-carboxylic acid spectra in dmso-d₆





190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 (f1 (ppm)

5-(morpholine-4-carbonyl)-1*H*-pyrrole-2-carbaldehyde spectra in dmso-d₆



5-(morpholine-4-carbonyl)-1*H*-pyrrole-3-carbaldehyde spectra in CDCl₃



4-(morpholine-4-carbonyl)-1*H*-pyrrole-2-carbaldehyde spectra in dmso-d₆



240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

5-nitro-1*H*-pyrrole-2-carbaldehyde spectra in acetone-d₆



4-nitro-1*H*-pyrrole-2-carbaldehyde spectra in acetone-d₆



3,5-dimethyl-4-nitro-1*H*-pyrrole-2-carbaldehyde spectra in dmso-d₆



5-ethyl-1*H*-pyrrole-2-carbaldehyde spectra in CDCl₃





3-ethyl-1*H*-pyrrole-2-carbaldehyde spectra in CDCl₃



 $(E)-N'-((1H-pyrrol-2-yl)methylene)-5-bromo-3-phenyl-1H-indole-2-carbohydrazide~(3a) spectra in dmso-d_6$



 $(E)-N'-((1H-pyrrol-3-yl)methylene)-5-bromo-3-phenyl-1H-indole-2-carbohydrazide~(3b) spectra in dmso-d_6$



(E)-5-bromo-N'-((3,5-dimethyl-1H-pyrrol-2-yl)methylene)-3-phenyl-1H-2-carbohydrazide (3c) spectra in dmso-d₆



(*E*)-5-bromo-N'-((1-methyl-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2carbohydrazide (3d) spectra in dmso-d₆





(*E*)-5-bromo-*N*'-((4-bromo-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2carbohydrazide (3e) spectra in dmso-d₆



f1 (ppm)

(E)-5-bromo-N'-((4,5-dibromo-1H-pyrrol-2-yl)methylene)-3-phenyl-1H-indole-2-carbohydrazide (3f) spectra in dmso-d $_6$



34

(*E*)-5-bromo-*N*²-((3-chloro-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2carbohydrazide (3g) spectra in dmso-d₆



f1 (ppm)

(*E*)-5-bromo-*N*'-((4-chloro-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2carbohydrazide (3h) spectra in dmso-d₆


Ethyl (*E*)-5-((2-(5-bromo-3-phenyl-1*H*-indole-2-carbonyl)hydrazono)methyl)-1*H*-pyrrole-2-carboxylate (3i) spectra in dmso-d₆



00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 (f1 (ppm)

¹H NMR of compound (3i) at 90 °C in dmso-d₆



Ethyl (*E*)-5-((2-(5-bromo-3-phenyl-1*H*-indole-2-carbonyl)hydrazono)methyl)-1*H*-pyrrole-3-carboxylate (3j) spectra in dmso-d₆



Ethyl (*E*)-2-((2-(5-bromo-3-phenyl-1*H*-indole-2-carbonyl)hydrazono)methyl)-1*H*-pyrrole-3-carboxylate (3k) spectra in dmso-d₆



(*E*)-5-((2-(5-bromo-3-phenyl-1*H*-indole-2-carbonyl)hydrazono)methyl)-1*H*-pyrrole-2-carboxylic acid (31) spectra in dmso-d₆



 $(E)-5-((2-(5-bromo-3-phenyl-1H-indole-2-carbonyl)hydrazono)methyl)-1H-pyrrole-3-carboxylic acid (3m) spectra in dmso-d_6$



(*E*)-5-bromo-*N*'-((5-(morpholine-4-carbonyl)-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2-carbohydrazide (3n) spectra in dmso-d₆



(*E*)-5-bromo-*N*'-((4-(morpholine-4-carbonyl)-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2-carbohydrazide (30) spectra in dmso-d₆



(*E*)-5-bromo-*N*'-((5-nitro-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2-carbohydrazide (3p) spectra in dmso-d₆



f1 (ppm)



(E)-5-bromo-N'-((4-nitro-1H-pyrrol-2-yl)methylene)-3-phenyl-1H-indole-2-carbohydrazide (3q) spectra in dmso- d_6



(*E*)-5-bromo-*N*²-((3,5-dimethyl-4-nitro-1*H*-pyrrol-2-yl)methylene)-3-phenyl-1*H*-indole-2-carbohydrazide (3r) spectra in dmso-d₆



(E)-5-bromo-N'-((5-ethyl-1H-pyrrol-2-yl)methylene)-3-phenyl-1H-indole-2-carbohydrazide (3s) spectra in dmso- d_6



(E)-5-bromo-N'-((4-ethyl-1H-pyrrol-2-yl)methylene)-3-phenyl-1H-indole-2-carbohydrazide (3t) spectra in dmso-d₆



(E)-5-bromo-N'-((3-ethyl-1H-pyrrol-2-yl)methylene)-3-phenyl-1H-indole-2-carbohydrazide (3u) spectra in dmso-d $_6$



Ethyl (*E*)-4-((2-(5-bromo-3-phenyl-1*H*-indole-2-carbonyl)hydrazono)methyl)-1*H*-pyrrole-2-carboxylate (3v) spectra in dmso-d₆



(*E*)-4-((2-(5-bromo-3-phenyl-1*H*-indole-2-carbonyl)hydrazono)methyl)-1*H*-pyrrole-2-carboxylic acid (3w) spectra in dmso-d₆



(*E*)-5-bromo-*N*'-((5-(morpholine-4-carbonyl)-1*H*-pyrrol-3-yl)methylene)-3-phenyl-1*H*-indole-2-carbohydrazide (3x) spectra in dmso-d₆



5-bromo-3-phenyl-1*H*-2-carbohydrazide (5) spectra in dmso-d₆



Figure S1. NCI60 one dose screen

Compound **3a**



Developmental Ther	apeutics Program	NSC: D-832482 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 30, 2021
One Dose Me	an Graph	Experiment ID: 2108	OS84	Report Date: Jan 25, 2022
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
One Dose Mea Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H322M NCI-H322M NCI-H322M NCI-H322 Colon Cancer COLO 205 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-62 Ovarian Cancer IGROV1 OVCAR-4 OVCAR-5 OVCAR-5 OVCAR	Growth Percent 5.27 -39.08 3.06 5.94 -1.05 17.57 24.44 22.15 15.54 35.92 32.40 2.17 -20.17 6.05 17.18 0.02 9.42 6.16 10.36 22.82 25.31 7.67 14.23 30.60 27.28 21.30 45.12 13.17 2.21 31.95 61.18 -34.25 30.29 13.40 8.52 22.19 33.23 43.70 12.98 14.76 36.74 13.74 12.28 15.17 20.63	Experiment ID: 2108	OS84 Percent - Growth Perc	Report Date: Jan 25, 2022
MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	3.98 13.98 29.49 -12.45 14.10 -0.63		-	
Mean Delta Range	15.97 55.05 100.26			
	150	100 50	0 -50	-100 -150

Compound **3b**



Developmental Therapeutics Program		NSC: D-843103 / 1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Me	an Graph	Experiment ID: 230)3OS10	Report Date: Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Per	cent
One Dose Me Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H228 NCI-H220 NCI-H220 NCI-H220 NCI-H220 NCI-H220 NCI-H220 NCI-H220 NCI-H220 SColon Cancer COLO 2005 HCT-116 HCT-125 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-5 UACC-25	an Graph Growth Percent 10.60 -8.20 7.33 13.28 11.94 11.85 27.71 -3.01 50.21 55.51 52.94 15.96 3.20 -25.46 -10.61 20.29 8.13 7.26 8.01 8.22 23.40 20.86 4.74 -20.84 43.16 18.40 18.76 12.64 16.56 34.26 -29.41 50.14 48.99 -9.09 67.41 43.83 38.91 -2.36 53.80 32.37 6.73 -35.86	Experiment ID: 230	Percent - Growth Per	cent
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 Mean Delta Range	49.27 80.76 34.08 30.90 -0.72 15.23 57.10 26.66 20.28 8.66 10.62 33.30 5.02 -6.95 71.36 -4.53 20.18 56.04 116.62			
	150	100 50	0 -50	-100 -150

Compound **3c**



Developmental The	rapeutics Program	NSC: D-843105/1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Me	ean Graph	Experiment ID: 230	3OS10	Report Date: Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean Growth	n Percent - Growth Per	cent
Leukemia	10.29			
HL-60(TB)	-29.94			
K-562	1.83		-	
MOLT-4	-4.88		_	
RPMI-8226 SR	-3.01			
Non-Small Cell Lung Cancer	-0.01			
A549/ATCC	16.15			
HOP-62	22.47			
NCI-H226	18.17			
NCI-H23	0.47		-	
NCI-H460	1.40			
Colon Cancer	-13.81			
COLO 205	2.58		-	
HCC-2998	17.84			
HCT-116 HCT-15	6.28			
HT29	12.39		- I	
KM12	2.51			
SW-620 CNS Cancer	13.08			
SF-268	20.71		_	
SF-295	3.24			
SF-539	7.09			
SNB-75	-0.96			
U251	7.16			
Melanoma	0.57			
MALME-3M	2.47		-	
M14	29.28			
MDA-MB-435	8.60			
SK-MEL-28	29.49			
SK-MEL-5	-12.99			
UACC-257	30.88			
Ovarian Cancer	14.14			
IGROV1	27.09			
OVCAR-3	20.93			
OVCAR-4 OVCAR-5	29.41			
OVCAR-8	8.09			
NCI/ADR-RES	-27.09			
Renal Cancer	21.34			
786-0	19.96		_	
	37.96			
CAKI-1	18.62		-	
RXF 393	-11.39			
SN12C	-33.61			
UO-31	12.36			
Prostate Cancer				
PC-3	7.50			
Breast Cancer	20.00			
MCF7	-20.33			
MDA-MB-231/ATCC HS 578T	16.84			
BT-549	12.45			
T-47D	11.09			
MDA-MB-468	-8.76			
Mean	8.87			
Delta	42.48			
Range	/1.5/			
	150	100 50	0 -50) -100 -150



Developmental Therapeutics Program		NSC: D-843112/1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Me	an Graph	Experiment ID: 2303	3OS10	Report Date: Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC HOP-92 NCI-H226 NCI-H23 NCI-H423 NCI-H522 Colon Cancer COLO 205 HCC-2998 HCT-116 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M	Growth Percent	Mean Growth	Percent - Growth Perc	ent
M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62 Ovarian Cancer IGROV1 OVCAR-3 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	20.83 -18.15 12.80 60.90 10.46 59.20 48.50 48.50 -8.15 46.22 43.23 21.14 -14.62 48.79			
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 Mean Delta Range	58.28 86.25 10.48 43.42 -12.24 26.90 45.55 38.65 33.52 15.05 7.52 44.14 -0.04 41.84 23.18 -5.26 21.79 52.43 116.89			
	150	100 50	0 -50	

Compound 3e



Developmental Therapeutics Program		NSC: D-843104 / 1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Me	an Graph	Experiment ID: 230	3OS10	Report Date: Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.95 -21.64 5.69 -11.31 -16.62 -11.68		-	
A549/ATCC HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H460 NCI-H522	11.07 32.23 -5.68 7.32 1.42 3.94 0.10 -24.45			
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer	0.52 -24.60 4.80 -30.73 -4.75 -28.37 7.06		[≓]	
SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma	14.42 -11.98 4.62 14.46 12.32 0.87			
LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	-75.05 16.83 18.97 3.53 12.17 37.16 -57.10 25.12 9.00		-	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Benal Carcer	14.45 -21.05 23.37 16.89 -8.45 -41.21 41.32		1	
786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer	13.29 42.05 0.72 4.62 -2.74 -71.29 22.83 6.16			
PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	11.08 1.24 -5.01 2.84 0.06 -27.80 22.65 -21.53			
Mean Deita Range	93 74.12 117.10			=
	150	100 50	0 -50	-100 -150



Developmental Therapeutics Program		NSC: D-843	111/1	Conc: 1.00E-5	Molar	Test Date: Ma	ar 20, 2023
One Dose Mea	an Graph	Experiment	D: 23030	OS10		Report Date:	Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean C	Browth I	Percent - Grow	h Perce	ent	
Leukemia CCRF-CEM	13 52						
HL-60(TB)	-6.85			-			
K-562	6.49						
MOL1-4 RPMI-8226	-0.74						
SR	7.79			-			
Non-Small Cell Lung Cancer							
A549/A1CC	13.01						
HOP-92	10.06			-			
NCI-H226	11.38			-			
NCI-H23	4.96						
NCI-H522	-34.42				-		
Colon Cancer							
	-28.52						
HCT-116	9.78			-			
HCT-15	-14.96						
HT29	-15.22				1		
SW-620	12.40						
CNS Cancer							
SF-268	15.02				_		
SF-295 SF-539	-22.71				_		
SNB-19	17.97			_			
SNB-75	1.02						
Melanoma	0.65						
LOX IMVI	-48.20						
MALME-3M M14	-3.27						
MDA-MB-435	2.21						
SK-MEL-2	2.57						
SK-MEL-28 SK-MEL-5	32.62						
UACC-257	14.22						
UACC-62	13.49						
Uvarian Cancer	12 33						
OVCAR-3	-24.68						
OVCAR-4	16.63						
OVCAR-5 OVCAR-8	0.70						
NCI/ADR-RES	-27.98						
SK-OV-3	35.63						
786-0	16.43						
A498	36.83		13				
ACHN CAKL1	3.38			_			
RXF 393	-10.19						
SN12C	-11.26						
TK-10	26.17						
Prostate Cancer	1.55						
PC-3	18.61						
DU-145 Breast Cancer	5.80						
MCF7	0.50						
MDA-MB-231/ATCC	18.99						
HS 5781 BT-549	-1.02						
T-47D	10.76						
MDA-MB-468	-16.08						
Mean	1.22						
Delta	66.27						
Kange	101.88					-	
	150	100	50	0	-50	-100	-150



Developmental Therapeutics Program		NSC: D-843106/1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Mea	an Graph	Experiment ID: 2303	OS10	Report Date: Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC HOP-92 HCI-H23 NCI-H460 NCI-H226 NCI-H226 NCI-H460 NCI-H522 Colon Cancer COLO 205 HCC-2998 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-28 SK-MEL-28 SK-MEL-5 UACC-257 UACC-257 UACC-62 OvcAR-3 OvCAR-4 OvCAR	Growth Percent 10.40 -8.65 7.66 9.70 1.80 5.05 18.82 28.21 18.13 12.23 8.71 4.55 -22.86 0.60 -8.53 8.72 -1.50 3.811 -10.17 21.97 32.86 -21.84 -27.29 14.73 14.57 8.58 -70.73 6.81 22.29 8.63 18.55 12.59 -61.99 39.15 -11.01 8.77 10.19 28.65 7.21 0.03 -3.4.00 27.44 11.77 40.72 -17.19 7.75 75.52 31.	Mean Growth	Percent - Growth Perc	
Mean Delta Range	3.24 78.76 116.24			=
	150	100 50	0 -50	-100 -150



Developmental Therapeutics Program		NSC: D-845424 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 05, 2023
One Dose Mea	an Graph	Experiment ID: 2306	50S32	Report Date: Jul 16, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
One Dose Mea Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H522 Colon Cancer COLO 2005 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-5 UAC-257 UAC-62 OVCAR-	an Graph Growth Percent 1.71 -30.35 1.36 -0.92 -17.10 -15.99 8.30 2.15 -9.31 -10.85 -12.85 -4.40 21.03 1.89 -33.46 -46.39 -33.93 5.55 -46.34 -64.25 -27.48 8.98 7.92 -6.11 -22.00 8.05 14.94 -65.46 -34.80 15.37 8.46 2.10 12.51 41.71 -36.98 13.93 5.68 6.30 -31.16 21.32 4.39 -46.38 -35.91 22.53 18.65 4.815 4.48 12.61 <tr< th=""><th>Experiment ID: 2300</th><th>Percent - Growth Perc</th><th>Report Date: Jul 16, 2023</th></tr<>	Experiment ID: 2300	Percent - Growth Perc	Report Date: Jul 16, 2023
PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T T-47D MDA-MB-468	9.15 -16.94 -13.44 -20.75 27.19 18.46 -13.22			
Mean Delta Range	-4.87 60.59 124.61			•
	150	100 50	0 -50	-100 -150

Compound 3i



Developmental Therapeutics Program		NSC: D-843107 / 1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Mea	an Graph	Experiment ID: 2303	3OS10	Report Date: Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC HOP-92 NCI-H226 HOP-92 NCI-H23 NCI-H226 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-28 SK-MEL-28 SK-MEL-28 SK-MEL-28 SK-MEL-50 UACC-62 OvcaR-3 OVCAR-4 OVCAR-5 OVCAR-5 OVCAR-62 </th <th>Growth Percent 12.09 1.13 10.45 9.96 -0.39 6.78 27.57 51.78 37.24 29.81 16.20 12.68 -9.26 9.53 19.50 12.52 6.34 3.96 8.47 32.74 37.74 -16.28 -4.90 20.43 51.25 14.82 1.86 15.79 31.49 7.61 26.40 20.22 -50.66 47.34 24.30 26.38 17.38 42.65 33.25 9.65 -25.61 45.34 27.97 7.8.68 8.41 27.97 7.8.68 8.41 27.97 7.5.36 2.20 43.23 23.81 18.72 18.84 4.85 30.87 16.85 9.37 42.38 1.84</th> <th>Mean Growth</th> <th>Percent - Growth Perc</th> <th>cent</th>	Growth Percent 12.09 1.13 10.45 9.96 -0.39 6.78 27.57 51.78 37.24 29.81 16.20 12.68 -9.26 9.53 19.50 12.52 6.34 3.96 8.47 32.74 37.74 -16.28 -4.90 20.43 51.25 14.82 1.86 15.79 31.49 7.61 26.40 20.22 -50.66 47.34 24.30 26.38 17.38 42.65 33.25 9.65 -25.61 45.34 27.97 7.8.68 8.41 27.97 7.8.68 8.41 27.97 7.5.36 2.20 43.23 23.81 18.72 18.84 4.85 30.87 16.85 9.37 42.38 1.84	Mean Growth	Percent - Growth Perc	cent
Mean Delta Range	17.69 68.35 129.34			=
	150	100 50	0 -50	-100 -150

Compound 3j



Developmental Therapeutics Program		NSC: D-845426 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 05, 2023
One Dose Me	an Graph	Experiment ID: 2306	50S32	Report Date: Jul 16, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H228 NCI-H228 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H522 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-268	14.34 -18.05 2.46 10.77 3.75 0.00 31.68 22.52 39.83 23.30 8.04 15.75 65.68 9.80 -18.44 8.69 3.43 20.00 5.94 0.76 17.02 31.35 35.67			
SI-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62 Ovarian Cancer IGROV1 OVCAR-3 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Banal Cancer	14.82 -89.78 15.77 36.83 18.49 17.59 81.08 18.10 5.98 33.06 14.90 -17.02 50.54 28.21 37.48 12.99 47.48 12.82 10.51 -36.41 -5.07			
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T T-47D MDA-MB-468 Mean Delta Range	27.86 82.53 22.71 40.12 -2.39 18.92 -37.39 31.20 17.22 20.23 9.28 3.32 35.89 31.06 20.76 16.34 106.12 172.31			
	150	100 50	0 -50	-100 -150

Compound 3k



Developmental Therapeutics Program		NSC: D-845428 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 05, 2023
One Dose Mea	an Graph	Experiment ID: 230	060\$32	Report Date: Jul 16, 2023
Panel/Cell Line	Growth Percent	Mean Growt	h Percent - Growth Pe	rcent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	35.74 30.70 22.92 20.11 41.26 18.78			
Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H23 NCI-H322M NCI-H322M NCI-H460 NCI-H522 Colon Cancer	44.15 38.66 50.35 81.49 45.24 50.30 67.50 31.81 58.29			
COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	38.29 56.00 48.47 18.34 43.07 41.30 40.43			
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma	56.41 27.03 48.99 50.85 65.01 46.68		-	
LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	41.73 94.35 59.09 56.66 67.01 72.55 4.98 88.49 43.74		-	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-5 NCI/ADR-RES SK-OV-3	47.61 65.59 51.42 80.59 51.42 41.98 68.69			
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Protetor Cancer	77.02 82.61 39.12 59.78 65.46 41.60 71.10 40.81			
PC-3 DU-145 Breast Cancer MCF7	36.36 63.03 21.99		-	
MDA-MB-231/ATCC HS 578T T-47D MDA-MB-468	55.53 67.17 15.39 20.62			
Mean Delta Range	49.35 44.37 89.37			
	150	100 50	0 -5	D -100 -150
Compound 3 l				
		\square		



One Dose Mean Graph Experiment ID: 2000510 Report Date: Apr 24, 200 Panel/Cell Line Growth Percent Mean Growth Percent - Growth Percent Leikerning 65.76 65.76 MOLT-2 85.76 65.77 MOLT-2 95.26 95.26 MOLT-2 95.76 95.76 MOLT-226 97.765 95.76 Color Cancer 95.77 96.83 MOLT-28 96.83 95.77 MOLT-28 96.83 95.77 MOLT-28 96.83 95.77 MALM-23 96.83 95.75 MALM-23 96.83 <th>Developmental Ther</th> <th>apeutics Program</th> <th>NSC: D-843109/1</th> <th>Conc: 1.00E-5 Molar</th> <th>Test Date: Mar 20, 2023</th>	Developmental Ther	apeutics Program	NSC: D-843109/1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
Panel/Cell Line Growth Percent Mean Growth Percent - Growth Percent Lewienig CCRP-CEM H-GOTB) 70.06 70.06 70.06 70.06 70.06 70.06 70.06 70.06 70.02 70.0205 65.26 70.07 70.05 70.00 70.0205 100.70 70.05 70.00 70.0205 100.70 70.05 70.00 70.05 7	One Dose Mea	an Graph	Experiment ID: 2303	OS10	Report Date: Apr 24, 2023
Levienia CCRF-CCM H-GOTED MOLT-4 RPM-M3226 SR SR NO SR SR SR Cellung Cancer HC-F226 HC-F2	Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Delta Range 32.64 60.72 150 100 50 0 -50 -100 -150 Compound 3m	Panien/Cent Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Smail Cell Lung Cancer A549/ATCC HOP-62 HOP-62 NCI-H230 NCI-H230 NCI-H230 NCI-H230 NCI-H460 NCI-H232 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62 Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-4 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-0V-3 Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	65.26 77.06 63.91 86.77 98.69 56.88 105.70 96.12 98.28 92.19 98.58 112.05 71.65 100.70 92.17 95.74 64.64 105.27 90.83 96.58 89.63 68.09 85.94 77.42 109.39 83.13 66.90 89.03 90.30 93.37 95.20 86.18 105.05 85.50 79.53 105.46 94.45 75.24 103.32 94.89 117.60 94.79 85.66 97.22 86.19 115.91 74.87 88.33 <			
Compound 3m	Delta Range	32.64 60.72			
Compound 3m		 150	100 50	0 -50	-100 -150
-	Compound 3m				



Developmental Therapeutics Program		NSC: D-845429/	1 Conc: 1.00E-5 Molar	Test Date: Jun 05, 2023	
One Dose Mean Graph		Experiment ID: 2	2306OS32	Report Date: Jul 16, 2023	
Panel/Cell Line	Growth Percent	Mean Grow	vth Percent - Growth Per	cent	
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	45.01 70.81 46.23 64.89 100.87 40.10				
Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522	103.62 88.86 72.38 48.67 80.85 95.42 99.62 96.15 68.53				
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNIS Concor	76.38 69.97 88.94 59.68 105.91 93.20 94.56		<u></u>		
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma	62.16 85.35 49.95 66.30 74.44 66.58		Ē		
MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	93.25 74.56 89.67 67.47 51.55 74.79 99.32 54.66		1		
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer	94.07 57.74 68.30 99.67 77.85 72.96 94.71				
786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	85.95 96.04 84.60 83.97 75.36 68.71 95.32 91.58				
PIOSIAIC Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T T-47D MDA-MB-468	62.12 97.05 62.36 68.34 73.38 51.39 29.20				
Mean Delta Range	75.93 46.73 76.71				
Compound 3n	150	100 5	50 0 -50) -100 -150	
	Br		N O		

69

Developmental Therapeutics Program		NSC: D-845	5425 / 1 Co	nc: 1.00E-5 Molar	Test Date:	Jun 05, 2023	
One Dose Mean Graph		Experiment ID: 2306OS32			Report Date	Report Date: Jul 16, 2023	
Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Percent					
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	10.59 -9.97 5.19 9.68 11.01 1.99			հու			
Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H23 NCI-H322M NCI-H460 NCI-H522	28.73 23.41 39.03 -7.11 3.88 14.29 62.78 10.38 -16.86		_	 			
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer	15.83 6.98 15.26 7.67 2.40 18.47 34.87			սոր			
SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma	32.00 7.15 2.13 24.08 18.28 18.91			_111			
MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-28 SK-MEL-5 UACC-257 UACC-257 UACC-257	76.05 34.48 2.05 15.34 47.01 -13.91 73.53 38.57						
IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer	44.37 11.90 40.51 42.54 8.82 -36.23 60.17		_		-		
786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3	14.37 73.29 38.05 39.01 -26.01 24.27 51.99 40.64 9.87		_				
DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T T-47D MDA-MB-468	18.53 8.75 17.48 29.68 32.02 16.26			la la			
Mean Delta Range	21.03 57.26 112.28						
	150	100	50	0 -5	0 -100	-150	
Compound 30							
	(
	Br	ļ,					



Developmental Ther	apeutics Program	NSC	: D-845431 / 1	Conc: 1	1.00E-5 Molar	Test Date:	Jun 12, 2023	
One Dose Mean Graph		Expe	Experiment ID: 2306OS36				Report Date: Jul 18, 2023	
Panel/Cell Line	Growth Percent		Mean Growth	Percent	- Growth Perc	cent		
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	15.34 14.03 20.31 15.43 22.02 15.48							
A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H230 NCI-H460 NCI-H522	58.15 31.41 54.25 41.39 48.55 51.14 47.98 46.10							
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer	80.75 55.51 36.11 27.31 70.58 51.39 75.29			Ξ	-			
SF-268 SF-295 SF-539 SNB-19 U251 Melanoma	47.09 35.07 51.98 32.91 21.75			-	_			
LOX IMVI M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	32.82 42.03 46.82 69.46 59.50 1.89 78.91 26.78			Ξ				
Ovarian Cancer OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer	53.96 33.51 82.58 54.02 53.40 81.63				-			
786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10	44.62 61.25 60.68 52.84 18.90 54.93 79.67			_				
Pictate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D	24.14 62.59 25.73 51.21 47.34 48.61 56.16							
MDA-MD-468 Mean Delta Range	-9.08 44.80 53.88 91.66							
	150	10	50	() -50	-10	0 -150	

Compound **3p**



Developmental Therapeutics Program		NSC: D-845422 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 05, 2023
One Dose Mean Graph		Experiment ID: 230	Report Date: Jul 16, 2023	
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer	5.79 -14.01 5.37 6.03 -9.11 2.98			
A549/A1CC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H322M NCI-H522 Colon Cancer	14.15 13.16 14.91 -9.49 -12.09 2.69 53.42 7.49 -34.97			
COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer	-24.27 2.96 12.42 3.20 2.64 4.14 27.86			
SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma	22.80 -4.92 3.73 13.59 6.35 6.46			
LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-257	6.80 57.75 23.83 18.28 -1.31 42.52 -48.69 22.98 27.08	-		.
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	26.87 17.57 30.92 56.19 -13.19 -36.29 32.84	-	<u> </u>	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	21.49 68.79 12.89 18.89 11.51 25.21 -0.57 20.38			
Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T T-47D MDA-MB-468	11.46 13.65 3.71 4.22 37.34 30.67 -17.71			
Mean Delta Range	11.01 59.70 117.48			
Company 12-	150	100 50	0 -50	-100 -150
Compound 3q	(


One Dose Mean Graph		Experiment ID: 2306OS32	Report Date: Jul 16, 2023
Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Perc	cent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H23 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-62 OvcAR-3 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 3933 SN12C TK-10 UD-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T T-47D MDA-MB-468 Mean Delta Range	13.40 -1.13 8.78 23.30 21.26 11.20 41.49 40.87 35.58 35.65 30.03 60.55 12.68 0.81 9.57 53.64 25.79 10.26 4.38 17.04 24.39 30.58 17.29 10.67 14.33 -1.73 14.65 16.08 42.47 20.22 -39.71 44.01 23.38 37.21 23.67 52.77 11.55 49.80 38.48 35.69 -2.06 47.80 32.86 76.90 27.25 42.65 8.05 41.77 33.28 41.87 -9.85 <th></th> <th>-100 -150</th>		-100 -150
Compound 3r		~	
	Br、 へ		
		/ NO ₂ Me	

Developmental Therapeutics Program NSC: D-845423 / 1 Conc: 1.00E-5 Molar Test Date: Jun 05, 2023

Developmental Therapeutics Program		NSC: D-845430 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 05, 2023
One Dose Mea	in Graph	Experiment ID: 230	06OS32	Report Date: Jul 16, 2023
Panel/Cell Line	Growth Percent	Mean Growth	h Percent - Growth Perc	ent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H223 NCI-H322M NCI-H322M NCI-H322 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2	Growth Percent 1.38 -17.20 -9.46 2.47 2.69 -20.99 3.34 5.20 -73.99 -57.45 -1.11 -26.53 7.66 -0.29 -28.80 -74.33 -26.36 -52.23 -40.1 -70.82 -31.11 17.17 17.00 -18.02 13.38 11.42 8.15 -41.90 -90.72 18.34 21.35 4.89 -7.88 13.01 -0.58 13.68 -32.48 13.31 -71.50 13.61 -0.32 1.27 41.75 4.55 19.75 19.26 -48.81 35.35 17.01 <td< th=""><th>Mean Growth</th><th>h Percent - Growth Perc</th><th>100 -150</th></td<>	Mean Growth	h Percent - Growth Perc	100 -150
	Br	, , , , , , , , , , , , , , , , , , ,		
	Ľ	Ń HN-N N H	Et	

Developmental Therapeutics Program		NSC: D-847584 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 14, 2023		
One Dose Mea	in Graph	Experiment ID: 230	08OS60	Report Date: Sep 07, 2023		
Panel/Cell Line	Growth Percent	Mean Growth	h Percent - Growth Per	cent		
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H23 NCI-H322M NCI-H322M NCI-H322M NCI-H460 NCI-H522 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62 Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer 786-0 A498 ACHN CAKI-1 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 Mean Delta Range	$\begin{array}{c} 2.11 \\ -26.99 \\ -2.16 \\ 0.97 \\ 6.45 \\ -12.97 \\ 11.38 \\ 23.88 \\ 32.28 \\ 32.28 \\ 16.42 \\ 19.00 \\ 18.05 \\ 32.43 \\ 4.52 \\ -1.18 \\ 1.69 \\ 3.82 \\ 5.44 \\ 7.89 \\ 3.05 \\ -1.80 \\ 23.21 \\ 27.43 \\ 8.27 \\ 8.14 \\ 22.60 \\ 46.64 \\ 8.57 \\ 8.89 \\ 43.70 \\ 25.58 \\ 13.48 \\ 44.02 \\ 58.75 \\ -41.85 \\ 40.32 \\ 20.03 \\ 11.92 \\ 17.41 \\ 38.20 \\ 24.07 \\ 8.21 \\ -15.48 \\ 52.34 \\ 12.52 \\ 53.64 \\ 10.65 \\ 3.59 \\ 6.52 \\ 37.86 \\ 13.75 \\ 17.42 \\ 10.84 \\ 13.58 \\ 3.36 \\ 9.86 \\ 11.88 \\ 42.41 \\ -12.09 \\ 14.82 \\ 56.67 \\ 100.60 \\ \end{array}$					
	150	100 50	0 -50	-100 -150		
Compound 3t						
		\bigcirc				
	Br	, o 	1			
		4	Ét			

Developmental Therapeutics Program		NSC: D-847585 / 1 Conc: 1.00E-5 Molar	Test Date: Aug 14, 2023
One Dose Mea	an Graph	Experiment ID: 2308OS60	Report Date: Sep 07, 2023
Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Per	cent
Once Dose mea Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H233 NCI-H226 NCI-H220 NCI-H322M NCI-H322M NCI-H432 NCI-H322M NCI-H432 NCI-H322M NCI-H432 NCI-H322M NCI-H432 NCI-H426 NCI-H432 NCI-H322M NCI-H432 NCI-H322M NCI-H432 NCI-H322 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 <t< th=""><th>Growth Percent -8.75 -32.19 -12.00 -6.19 1.01 -25.07 4.32 14.39 -4.14 -24.69 -15.57 2.86 27.66 -15.70 -8.86 27.66 -15.70 -8.86 -23.33 -4.36 11.00 5.04 1.72 -13.54 11.49 7.63 3.37 -26.11 11.28 16.25 -17.58 -56.08 14.17 11.05 18.33 34.44 49.63 -28.95 35.89</th><th>Mean Growth Percent - Growth Per</th><th>cent</th></t<>	Growth Percent -8.75 -32.19 -12.00 -6.19 1.01 -25.07 4.32 14.39 -4.14 -24.69 -15.57 2.86 27.66 -15.70 -8.86 27.66 -15.70 -8.86 -23.33 -4.36 11.00 5.04 1.72 -13.54 11.49 7.63 3.37 -26.11 11.28 16.25 -17.58 -56.08 14.17 11.05 18.33 34.44 49.63 -28.95 35.89	Mean Growth Percent - Growth Per	cent
UACC-257 UACC-62 Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer 786-0 A498 ACHN CAKI-1 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 Mean Delta Range	35.89 -4.08 8.23 -22.98 32.03 21.62 -22.76 -41.06 27.35 2.46 81.41 -0.99 -26.11 -15.18 41.82 -6.65 8.42 6.84 6.84 6.86 -2.61 0.23 -13.82 20.47 -41.40 31 56.39 137.49		
Compound 3u	150	100 50 0 -50	-100 -150
	Br	$ \begin{array}{c} $	

Developmental Therapeutics Program		NSC: D-847586 / 1 Conc: 1.00E-5 Molar	Test Date: Aug 14, 2023
One Dose Mea	in Graph	Experiment ID: 2308OS60	Report Date: Sep 07, 2023
Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Per	rcent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H322M NCI-H322 Colon Cancer	-10.62 -20.36 0.57 -5.68 22.55 -28.22 20.64 23.32 22.71 60.75 0.33 19.37 43.79 5.17 16.20		
COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295	-12.83 35.01 22.32 22.58 25.13 10.90 30.95 20.97 20.41		
SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435	6.05 22.82 48.31 17.59 2.13 28.07 6.36 26.23 26.23		
SK-WEL-28 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62 Ovarian Cancer IGROV1 OVCAR-3 OVCAR-3 OVCAR-4 OVCAR-8 NC/ADR-RES	34.39 34.39 8.98 37.75 6.99 38.07 31.59 35.51 51.60 20.05 -19.56		
SK-OV-3 Renal Cancer 786-0 A498 ACHN CAKI-1 SN12C TK-10 UO-31 Prostate Cancer	60.91 22.18 104.29 14.70 22.45 -18.13 63.77 12.09 21.91		
DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 Mean	21.97 13.33 18.72 41.83 39.73 23.90 15.34 21.90		
Delta Range	50.12 132.51 150	100 50 0 -5	0 -100 -150
Compound 3 v	Br		

Developmental Therapeutics Program	NSC: D-843108 / 1 Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Mean Graph	Experiment ID: 2303OS10	Report Date: Apr 24, 2023
Panel/Cell Line Growth Percent	Mean Growth Percent - Growth Pe	ercent
Panel/Cell Line Growth Percent Leukemia CCRF-CEM 19.34 HL-60(TB) 6.00 K-552 MOLT-4 24.04 RPMI-8226 25.68 SR Non-Smail Cell Lung Cancer A549/ATCC 36.15 HOP-62 43.25 HOP-92 NCI-H226 53.37 NCI-H23 28.47 NCI-H23 NCI-H226 53.37 NCI-H23 28.47 NCI-H460 COLO 205 11.44 HCC-29988 45.46 HCT-115 HCT-15 16.78 HT29 11.31 KM12 CNS Cancer 30.07 CNS Cancer 53.56 SF-295 SF-268 53.56 SF-295 SF-268 53.56 SF-295 SNB-75 32.26 U251 U251 27.81 Melanoma 20.01 MV1 LOX INV1 33.89 MALME-30 MALME-335 -15.44 SK-MEL-2 SK-MEL-25 -3.99 UACC-257 UACC-257 70.07 UACC-62 UACC-257 70.07 UACC-62 OVCAR-8 28.50 NCI/ADR-RES MDA-MB-435 -15.44 SK-MEL-2 OVCAR-8 28.50 NCI/ADR-RES OVCAR-8 28.50 NCI/ADR-RES	Mean Growth Percent - G	
Mean 29.76 Delta 45.20 Range 108.58		
Compound 3w	100 50 0 -5	jo -100 -150



Developmental Therapeutics Program		NSC: D-843110/1	Conc: 1.00E-5 Molar	Test Date: Mar 20, 2023
One Dose Mea	an Graph	Experiment ID: 2303	OS10	Report Date: Apr 24, 2023
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC HOP-62 HOP-92 NCI-H226 NCI-H223 NCI-H23 NCI-H23 NCI-H460 NCI-H522 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-2	Growth Percent	Mean Growth	Percent - Growth Perc	Sent
Additional Calcel 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 Mean Delta Range	74.76 100.31 68.31 70.42 66.62 61.32 92.50 53.20 60.87 89.90 37.95 62.39 64.68 99.95 60.17 19.00 67.53 48.53 81.31			
	150	100 50	0 -50	-100 -150

Compound 3x



Developmental Therapeutics Program		NSC: D-845427 / 1	Conc: 1.00E-5 Molar	Test Date: Jun 05, 2023
One Dose Mea	an Graph	Experiment ID: 23060	DS32	Report Date: Jul 16, 2023
Panel/Cell Line	Growth Percent	Mean Growth I	cent	
Leukemia CCRF-CEM	43.76			
HL-60(TB)	22.25			
K-562 MOLT-4	26.96			
RPMI-8226	54.54			
SR Non Small Call Lung Canaar	35.66			
A549/ATCC	86.45			
EKVX	67.58			
HOP-62	73.25			
NCI-H226	54.02			
NCI-H23	87.42			
NCI-H322M NCI-H460	81.57			
NCI-H522	70.35			
Colon Cancer	77.91			
HCC-2998	69.53			
HCT-116	35.93			
HC1-15 HT29	42.75 92.08			
KM12	75.73			
SW-620 CNS Capcer	86.76			
SF-268	62.61			
SF-295	55.29			
SNB-19	64.06			
SNB-75	58.04			
Melanoma	63.36			
LOX IMVI	57.58			
MALME-SM M14	49.57		_	
MDA-MB-435	70.90		_	
SK-MEL-28	77.28			
SK-MEL-5	55.76			
UACC-257 UACC-62	98.53 51.13			
Ovarian Cancer	100.10			
OVCAR-3	102.48			
OVCAR-4	54.94			
OVCAR-5 OVCAR-8	93.09			
NCI/ADR-RES	54.37			
SK-OV-3 Repair Cancer	89.96			
786-0	52.23		_	
	89.70			
CAKI-1	72.61			
RXF 393	65.62			
SN12C TK-10	70.53			
UO-31	70.76			
Prostate Cancer PC-3	43.67			
DU-145	84.38			
Breast Cancer MCF7	46.87			
MDA-MB-231/ATCC	64.94			
HS 578T T-47D	68.47 51.64			
MDA-MB-468	22.44			
Mean	66.24			
Delta	43.99			
Range	100.65			
	150	100 50	0 -50	-100 -150

Table S2.	GI_{50} and	LC_{50} screen	for compounds	5 3a–j, 3n, and 3p–v
-----------	---------------	------------------	---------------	-----------------------------

Disease	Cell line	GI ₅₀ , μΜ									
		3a	3b	3c	3d	3e	3f	3g	3h	3i	3j
leukemia	CCRF-CEM	0.345	0.821	3.07	0.429	0.341	2.89	1.53	0.132	3.04	2.41
	HL-60 (TB)	0.242	0.598	2.4	0.317	0.327	2.38	0.891	0.185	1.84	1.5
	K-562	0.202	0.429	2.43	0.327	0.393	1.93	0.413	0.234	1.08	1.9
	MOLT-4	0.384	1.52	2.29	0.438	0.375	3.38	1.71	0.283	2.49	2.1
	RPMI-8226	0.337	1.43	2.43	0.61	0.346	2.27	0.855	0.446	2.28	2.52
	SR	0.160							0.179		0.948
NSC lung	A549/ATCC	0.357	1.61	3.82	0.649	0.395	3.11	0.838	0.43	3.25	2.7

cancer	EKVX	1.23	4.41	3.24	0.641	0.62	3.45	2.66	1.28	4.29	4.57
	HOP-62	0.684	2.01	2.97	0.57	0.546	3.52	3.8	0.408	3.65	2.78
	HOP-92	0.992	1.87	2.61	0.429	1.51	1.88	2.79	1.19	2.33	4.56
	NCI-H226	0.323	2.52	2.58	0.603	0.382	2.28	1.44	0.604	3.13	3.07
	NCI-H23	0.504	1.87	2.59	0.447	0.298	2.62	0.884	0.317	2.59	3.06
	NCI-H322M	0.661	2.38	2.69	1.98	0.578	3.73	3.14	0.768	3.3	5.63
	NCI-H460	0.318	0.657	2.83	0.442	0.353	2.53	0.448	0.281	2.8	2.41
	NCI-H522	0.045	0.925	2.61	0.217	0.185	0.623	0.233	0.211	0.46	2.27
Colon	COLO 205	0.261	1.23	3.25	0.366	0.192	3.36	1.66	0.251	3.15	2.49
cancer	HCC-2998	0.415	1.55	3.55	0.402	0.296	2.3	1.23	0.224	2.51	2.18
	HCT-116	0.28	0.991	4.02	0.427	0.242	3.24	0.467	0.331	3.24	2.95
	HCT-15	0.269	0.918	2.91	0.228	0.28	2.7	0.465	0.302	2.48	2.93
	HT29	0.329	0.68	3.53	0.327	0.345	2.33	0.401	0.287	2.32	2.59
	KM12	0.388	0.996	2.96	0.357	0.301	2.46	0.488	0.328	2.22	2.21
	SW-620	0.352	0.548	3.06	0.432	0.405	2.96	0.499	0.328	3.93	3.36
CNS	SF-268	0.995	2.41	2.98	0.547	0.529	2.57	1.76	0.388	2.68	2.29
cancer	SF-295	0.224	1.94	2.76	0.321	0.254	2.2	0.501	0.237	1.8	2.34
	SF-539	0.202	0.869	2.93	0.217	0.214	1.78	0.378	0.231	1.6	2.26
	SNB-19	0.416	2.55	3.86	0.449	0.330	3.47	1.06	0.638	2.98	4.51
	SNB-75	0.136	0.88	2.68	0.259	0.475	1.08	0.325	0.247	0.399	1.09
	U251	0.375	2.08	3.21	0.477	0.418	2.95	0.63	0.349	2.82	2.66
Melanoma	LOX IMVI	0.244	0.916	2.43	0.494	0.36	2.31	0.555	0.37	2.26	2.82
	MALME-3M	0.320	3.46	3.16	0.409	0.665	2.97	0.596	0.645	3.83	6.06
	M14	0.304	1.58	4.45	0.324	0.27	2.81	0.689	0.305	2.73	2.39
	MDA-MB-435	0.105	0.463	2.84	0.151	0.207	1.01	0.222	0.185	0.464	1.09
	SK-MEL-2	0.357	2.48	3.37	0.366	0.322	2.68	1.07	0.26	2.38	2.8
	SK-MEL-28	0.488	5.75	3.81	4.7	0.612	5.1	0.909	0.582	2.65	4.56
	SK-MEL-5	0.302	1.1	2.52	0.196	0.195	1.72	0.427	0.228	1.48	1.44
	UACC-257	0.647	8.22	4.35	0.416	1.09	3.24	0.738	0.856	2.97	2.53
	UACC-62	0.099	1.03	2.36	0.283	0.439	1.2	0.411	0.559	0.614	2.92
Ovarian	IGROV1	0.404	1.27	2.47	0.621	0.44	0.53	0.734	0.538	2.02	3.91
Cancer	OVCAR-3	0.423	1.09	2.53	0.246	0.302	2.3	0.409	0.27	2.63	2.13
	OVCAR-4	0.814	4.82	3.55	0.637	1.35	5.2	3.09	0.555	4.26	2.28
	OVCAR-5	0.437	1.74	3.63	0.472	0.346	3.6	1.1	0.473	3.43	3.87
	OVCAR-8	0.323	1.21	3.1	0.39	0.304	1.98	0.481	0.214	2.49	2.37
	NCI/ADR-RES	0.44	0.636	2.11	0.186	0.197	1.14	0.219	0.2	0.897	1.89
	SK-OV-3	0.702	5.59	6.81	1.61	0.966	4.76	11.6	0.519	4.01	4.53
Renal	786-0	0.791	5.46	5.19	29.4	0.727	4.91	2.58	0.459	4.48	3.29
Cancer	A498	2.57	12.7	8.25	>100	5.47	11.1	10.6	1.45	10.5	3.53
	ACHN	0.355	1.71	3.03	0.175	0.418	2.59	0.627	0.493	1.86	3.39
	CAKI-1	0.257	0.776	3.17	0.255	0.329	1.38	0.445	0.253	0.961	1.46
	RXF 393	0.339	1.78	2.26	0.28	0.497	1.55	0.346	0.219	1.69	1.36
	SN12C	0.371	1.49	2.58	0.497	0.310	2.15	1.34	0.391	2.86	2.49
	TK-10	2.46	11.1	7.32	1.01	4.21	6.8	7.16	3.91	6.92	7.35
	UO-31	0.431	1.66	1.77	0.33	0.618	1.94	0.577		1.48	
Prostate	PC-3	0.344	2	2.06	0.564	0.382	2.29	0.826	0.426	2.28	3.76
Cancer	DU-145	0.429	1.95	4.07	0.399	0.352	3.18	1.58	0.352	3.32	3,48
Breast	MCF7	0.136	0.436	2.3	0.072	0.294	1.99	0.376	0.309	1.54	2,76
Cancer	MDA-MB-231/ATCC	0.396	1.62	2.78	0.237	0.215	2.49	2.07	0.296	2.63	2.85
	HS 578T	0.452	1.31	2.31	0.22	0.34	1.82	0.59	0.284	1.21	2.36
	BT-549	0.375	4.53	5.04	2.81	0.314	3.69	3.56	0.255	3.47	2,23
	T-47D	0.341	3.49	4.68	0.344	1.4	3.84	2.5	0.546	4.2	2.91
	MDA-MB-468	0.209	0.593	2.00	0.155	0.231	2.09	0.297	0.251	1.63	2.47

Disease	Cell line	GI ₅₀ , μΜ										
		3n	Зр	3q	3r	3s	3t	3u	3v			
leukemia	CCRF-CEM	3.45	0.382	0.799	1.89	0.375	0.368	2.35	3.7			
	HL-60 (TB)	1.84	0.374	0.633	2.31	0.235	0.237	2.03	4.68			
	K-562	1.27	0.365	0.387	2.69	0.338	0.348	2.27	4.59			
	MOLT-4	1.5	0.537	0.657	2.29	0.464	0.399	2.37	3.91			
	RPMI-8226	4.5	0.468	3.71	2.70	0.375	0.343	2.04	3.84			
	SR	0.405	0.354	0.405	2.04	0.419	0.446	2.02				
NSC lung	A549/ATCC	3.88	2.23	1.79	3.19	0.399	0.397	2	4.37			
cancer	EKVX	7.51	5.37	>100	3.34	0.453	0.448	2.79	7.14			
	HOP-62	3.36	0.606	1.26	2.09	0.861	1.35	3.77	6.66			

	HOP-92	6.14	1.79	11.6	2.51	2.01	2.57	3.8	7.99
	NCI-H226	3.39	2.43	3.39	3.78	0.506	0.33	1.97	4.21
	NCI-H23	2.83	1.45	2.57	2.46	0.484	0.408	2.66	3.42
	NCI-H322M	13.9	11	46.4	4.22	1.73	2.31	3.93	4.42
	NCI-H460	2.49	0.421	0.328	1.87	0.396	0.346	1.23	3.49
	NCI-H522	1.6	0.588	0.722	2.43	0.183	0.206	2.3	2.41
Colon	COLO 205	3.12	1.52	1.28	1.9	0.316	0.207	2.96	3.51
cancer	HCC-2998	2.31	1.67	3.66	2.41	1.45	0.342	4.11	4.17
	HCT-116	2.79	0.439	0.491	1.98	0.325	0.385	2.5	3.42
	HCT-15	2.62	0.607	0.504	2.41	0.349	0.319	1.03	3.21
	HT29	2.57	0.55	0.469	1.84	0.298	0.308	2.17	3.33
	KM12	2.91	1.17	1.39	1.92	0.289	0.325	3.17	3.37
	SW-620	3.26	0.249	0.38	2.06	0.558	0.431	3.82	4.41
CNS	SF-268	2.51	1.47	0.774	2.37	1.47	0.861	2.86	6.04
cancer	SF-295	1.63	0.413	0.623	2.32	0.246	0.319	2.29	3.04
	SF-539	2.23	0.389	0.822	3.51	0.225	0.203	3.17	2.02
	SNB-19	5.66	3.34	6.25	3.45	1.82	0.396	4.5	4.08
	SNB-75	0.809	0.482	0.242	2.19	0.285	0.44	4.94	1.95
	U251	3.1	0.987	0.574	1.85	0.329	0.373	2.15	3.8
Melanoma	LOX IMVI	3.06	0.519	0.647	1.63	0.722	0.427	2.42	4.31
	MALME-3M	11.7	3.23	0.83	1.99	0.88	1.72	3.5	4.32
	M14	1.92	0.652	0.574	2.54	0.318	0.337	1.62	3.54
	MDA-MB-435	0.392	0.253	0.226	1.77	0.227	0.23	4.12	1.54
	SK-MEL-2	2.8	2.18	1.3	2.11	0.647	0.454	6.77	4.37
	SK-MEL-28	6.1	2.24	0.89	3.56	0.979	0.839	3.46	4.73
	SK-MEL-5	1.48	1.02	0.671	1.5	0.381	0.279	2.54	2.01
	UACC-257	11.9	3.12	2.58	3.13	1.32	1.23	3.78	11.7
	UACC-62	0.864	0.451	0.538	2.9	0.381	0.442	2.48	3.18
Ovarian	IGROV1	6.69	1.48	2.06	3.83	0.612	0.888	3.52	3.75
Cancer	OVCAR-3	2.57	0.602	0.397	1.77	0.356	0.316	3.2	3.23
	OVCAR-4	2.93	0.679	1.06	1.97	2.41	2.17	3.33	9.00
	OVCAR-5	5.78	2.87	5.37	3.53	0.573	0.337	6.77	3.49
	OVCAR-8	2.86	1.02	10.2	3.08	0.337	0.316	3.02	3.65
	NCI/ADR-RES	1.92	0.285	0.434	1.89	0.253	0.247	2.68	2.23
	SK-OV-3	5.68	2.95	3.14	3.23	0.514	0.922	2.59	1.31
Renal	786-0	2.86	0.803	2.21	2.35	0.801	0.646	3.51	6.01
Cancer	A498	3.53	2.6	10.7	2.35	5.59	13.7	1.45	12.9
	ACHN	4.56	1.26	0.791	3.3	0.861	0.628	3.27	4.87
	CAKI-1	1.46	0.411	0.53	2.29	1.04	1.05	6.04	3.2
	RXF 393	1.06	0.411	0.734	1.7	0.194	0.217	1.19	2.56
	SN12C	3.14	1.24	2.58	1.74	0.392	0.372	2.26	3.63
	TK-10	10.4	12.2	76	5.1	2.91	2.83	5.05	12.5
	UO-31					0.644	1	2.94	4.21
Prostate	PC-3	3.44	1.2	0.724	2.85	0.532	0.529	3.09	4.07
Cancer	DU-145	3.72	1.84	3.87	3.48	0.418	0.38	4.3	3.36
Breast	MCF7	2.46	0.394	0.354	2.57	0.369	0.375	2.63	3.03
Cancer	MDA-MB-231/ATCC	4.81	2.14	17.4	3.56	0.63	0.311	5.02	3.27
	HS 578T	1.04	0.27	0.486	2.43	0.294	0.3	3.6	3.11
	BT-549	2.36	1.52	2.47	2.74	0.979	0.39	2.7	13.4
	T-47D	3.1	2.4	2.21	2.51	0.681	1.59	2.17	5.88
	MDA-MB-468	1.98	0.873	0.503	1.94	0.248	0.263	2.72	2.6

Disease	Cell line					LC ₅₀ ,	μΜ				
		3a	3b	3c	3d	3e	3f	3g	3h	3i	3j
leukemia	CCRF-CEM	>100	>100	>100	>100	>100	>100	>100	>100	>100	>100
	HL-60 (TB)	>100	>100	>100	>100	>100	88.8	>100	0.886	>100	9.88
	K-562	>100	97	>100	>100	>100	76.4	>100	5.64	>100	57.1
	MOLT-4	>100	>100	>100	>100	>100	>100	>100		>100	53.4
	RPMI-8226	>100	>100	>100	>100	>100	>100	>100	>100	>100	>100
	SR	>100							4.6		>100
NSC lung	A549/ATCC	33.6	52.6	45.4	>100	56.4	37.6	53.4	47.4	79.4	51.8
cancer	EKVX	33.4	41.7	35.4	>100	34.3	44.8	38.1	>100	>100	43.1
	HOP-62	32.6	61.4	69.3	>100	>100	>100	60.8	34.7	>100	54.4

	HOP-92	26.4	50.3	43.5	>100	26.3	46	50.1	55.4	>100	58.6
	NCI-H226	23.3	51.2	34.4	>100	29.9	32.5	32.1	>100	45.4	41 3
	NCI-H23	37.7	33.9	35.2	>100	26.9	34	34.4	36.5	43.2	46.4
	NCI-H322M	36.5	37.2	38.7	>100	38.8	62.8	48.8	92.3	>100	50
	NCI-H460	12 5	46	37.9	>100	43.2	32.7	34 3	9.24	41 4	23.1
	NCI-H522	22.5	24	32.7	>100	19.1	23.2	20.4	>100	82.2	33
Colon	COLO 205	35.1	20.4	52.7	>100	0.884	48.8	40.3	1.88	36.9	55.2
cancer	HCC-2998	19.5	32.7	37.2	>100	15.6	24	28.6	4.2	36.4	15.9
cancer	HCT-116	32.3	>100	>100	>100	85	>100	79.9	29.1	>100	45.6
	HCT-15	32.3	3/	37.2	>100	13 5	22.1	3/1 3	21.1	/0.5	51 0
	нт29	9 21	3/1 5	16.6	>100	8 24	20.8	58.5	7 2	22 9	27.5
	KM12	56.5	37.8	35 /	>100	16.3	20.0	34.6	20.7	38	27.5
	SW/ 620	27 /	10.1	12	>100	50.0	11 0	50.2	20.7	52.6	76.2
CNS	SW-020	56.4	49.4 50.1	42 52.2	>100	52.0	41.9	52	20.3	>100	16.2
civo	SE-205	20.4	22.9	20.5	>100	25.0	26.0	26	595	28.1	24.0.5
cancer	SE 520	11.6	17	29.5	>100	25.5	15 7	195	JO.J 22 1	36.1	10 /
	SNR_10	25	20.9	20.4	>100	20.5	20.2	25 /	61.0	62.8	19.4
	SND-19	16	22	12 0	>100	54.5	59.5 64.4	28.6	75 5	02.8 ∖100	25.9
	11251	12 /	10.9	43.9	>100	10.1	26	27.7	24.0	20.4	10.6
Molanoma		10	40.8	20.2	>100	6.09	21.9	20.4	16.7	25.2	40.0
Welanoma	MALME-3M	30.9	18.3	38.5	>100	32.5	12.0	18 /	16.1	54.8	5/ 9
		JU.J	40.5	10.0	>100	20.2	42.4 66.1	45.4	50.2	71.0	50.2
		41.4	45.0	24	>100	20.2	10.1	45.4	50.5	27.6	16.1
	SK-MEL-2	20.0	29.4	J4 /1 7	>100	24.3	26.2	29.5	17.0	55	22.9
	SK-MEL-28	27 /	11 1	20.0	>100	12 0	30.3 47	JO.7	47.9	04 5	15.0
	SK-MEL-20	15 7	14.4	20.0	>100	43.9	9 65	47.5	2 09	7 68	45.8
		13.7	14.0	10.2	>100	1.22	45.7	52	50.0	97 /	51.9
		9 02	47.0	49.Z	>100	47	40.7	27	56.2	87.4 18 5	12.6
Ovarian		14.6	41.5	20 /	>100	26.2	26.1	12	00.3 44 1	48.5	42.0
Concor		25.2	43.0 21.0	26.4	>100	17.2	24.5	24.0	10.7	41.5	40.1 22.1
Cancer	OVCAR-3	22.6	45.2	30.4 40.7	>100	10.5	24.J 15.9	12 5	24.1	40.7 \\100	23.1
	OVCAR-5	20.9	4J.Z 29 5	40.7	>100	26.5	40.2	43.5	26	28	12 0
	OVCAR-S	50.8 6 EE	28.5	15	>100	10.5	40.2	33.7	0 0 0 0	17.6	42.9
		50.2	38.0 27.1	4J 10 2	/0.0	0 071	0 72	10.5	0.300	47.0	10.4
		21.0	71.0	70.9	×100	52.9	72 5	10.J	15 1	>100	10.4
Ponal	786.0	22.0	71.9	62.0	>100	55.0	64.1	50.2	20.9	>100	43.3
Concor	730-0 A / 08	23.9 /1 6	54.6	16.0	>100	11 5	10.1	10.2	12 1	55.2	44.7
Cancer		21.0	20	24.2	>100	22 5	25.5	49.3	42.1	72 9	26.4
	CAKL1	20.0	35 11 1	20.1	>100	23.5	10.0	26.0	27 5	73.8	40.5
		25.1	44.1	25	>100	27 0	2/ 2	30.9 42.1	27.5	74.2 66.4	40.5
	NAT 333	2 07	40.5	22.2	>100	57.9	20.7	42.1	15 2	26.2	22
	JNIZC	27 1	57.7	52.5 4E 2	>100	5.49	30.7 40 E	29.2 40 E	15.5	>100	35.5
	10.21	20.2	J0 //1	45.2	>100	20 1	49.5 20 E	49.5	05.2	>100	40.2
Droctato	00-51	20.2	41 >100	33.0	>100	20.1	50.5	55.7	17 6	>100	>100
Cancor	DUL 145	23.0	24.7	280	>100	20.1	22.0	22.1	47.0	29.7	>100
Broast	DU-145 MCE7	20.1	54.7 40.9	30.9 27.2	>100	29.7	22.9	33.1 42.2	27.2 E2 E	56.7 >100	55.0
Cancor		29.1	49.0	27.2	>100	1/ 2	35.7 26.2	42.2	25.5	>100	26.0
Callel		>100	20.4	52.0 \100	>100	14.5 \100	20.5	>100	20.9	55.Z	50.0 \100
	PT 5/0	>100	>100	/7.0	>100	26.2	>100	AE 8	10 1	>100	20 E
	T. 17D	51.2	52.5 \100	47.9	>100	90.Z	7/ 2	40.0 91.0	10.1	>100	29.5
		JI.5 42.1	24.2	26.4	>100	12	74.5 22.0	24.7	92.0 27.0	26.6	21 2
	IVIDA-IVID-400	42.1	24.2	20.4	>100	12	22.0	24./	27.0	30.0	24.2

Disease	Cell line				LC ₅₀ , μ	.M			
		3n	Зр	3q	3r	3s	3t	3u	3v
leukemia	CCRF-CEM	>100	>100	>100	>100	>100	>100	63.8	>100
	HL-60 (TB)	8.56	>100	>100	>100	>100	91.9	24.3	>100
	K-562	42.7	>100	>100	>100	>100	>100	56.2	>100
	MOLT-4	20.8	>100	>100	>100	>100	94.2	55.1	>100
	RPMI-8226	>100	>100	>100	>100	>100	>100	78.6	>100
	SR	38.9	>100	>100	>100	>100	>100	>100	
NSC lung	A549/ATCC	>100	44.9	>100	35.6	70.3	38.8	41.5	44.2
cancer	EKVX	>100	45.7	>100	34.9	43	35.6	37.7	60.7
	HOP-62	69.2	39.5	>100	11.7	46.2	37.5	45.8	69.2

	HOP-92	>100	47.3	>100	45.8	40.1	33	44.3	>100
	NCI-H226	81.7	46.9	>100	40.6	32.3	28	37.7	46.2
	NCI-H23	69.8	35.4	>100	26.3	42.6	37.4	38.3	40.4
	NCI-H322M	>100	53.3	>100	89.5	64.6	49.8	43.4	76.1
	NCI-H460	54.1	45.9	>100	8.05	43.5	20.2	36.7	34.3
	NCI-H522	58.8	19.8	>100	29.6	28	29.5	34.1	61.2
Colon	COLO 205	37.5	8.08	>100	7.51	26.1		41.3	34.8
cancer	HCC-2998	42.9	19.6	>100	25.4	35.1	30.4	42.4	42.1
	HCT-116	66.7	33.8	>100	10.4	31.9	40.3	44	50.5
	HCT-15	>100	35.7	>100	26.4	37.4	35.6	38.8	35.7
	HT29	38.3	43.9	>100	6.67	33.8	21	39.3	35.3
	KM12	43.6	34.2	>100	11.6	37.5	34.4	42.3	35.5
	SW-620	>100	48.4	>100	19.1	43.2	42.5	43.3	40.1
CNS	SF-268	>100	44.2	>100	33.1	83	51.9	42.7	>100
cancer	SF-295	31	29.9	>100	21.2	31.9	24.7	37.1	37.2
	SF-539	34.9	28.1	>100	35.7	29.8	19.6	35.6	13.5
	SNB-19	>100	42.4	>100	43.1	51.8	41.3	42.2	43.4
	SNB-75	88.9	40.5	>100	21.5	54.1	37.8	43.4	90.6
	U251	84.7	39.2	66.8	13.4	36.7	38.2	37.8	37.6
Melanom	LOX IMVI	71.2	35.8	>100	5.73	36.1	8.27	32.3	41.1
а	MALME-3M	>100	56.2	>100	28.5	46.5	48	40	52.8
	M14	64.2	37	>100	36.3	38.7	38.4	23.7	41.3
	MDA-MB-435	55.4	29.8	8.78	17.9	34	38.7	41.6	9.53
	SK-MEL-2	48.3	36.5	>100	22.6	45.9	43.8	45.8	47.3
	SK-MEL-28	>100	43.5	>100	38.7	49.8	46.6	40.1	48.5
	SK-MEL-5	17	8.69	69.9	5.87	10.1	6.96	27.2	17.9
	UACC-257	94.4	48.2	>100	48.1	64.7	41.3	40.8	77.8
	UACC-62	63.7	40.9	>100	37.5	38.1	32.1	30.8	40.7
Ovarian	IGROV1	>100	88.8	>100	41.2	43.3	48.6	44	38.9
Cancer	OVCAR-3	47.4	34.8	>100	10.4	36.1	41.7	44	33.4
	OVCAR-4	>100	35.9	>100	18.8	53.7	43	43.7	52.8
	OVCAR-5	>100	40.9	>100	41.5	38.7	37.2	45.4	37.4
	OVCAR-8	43.1	39	>100	36.5	25.2	26	39.8	38.5
	NCI/ADR-RES	84.1	16.2	>100	9.15	30.2	22	34.6	21.2
	SK-OV-3	>100	43	>100	39.2	50.1	35.4	42.4	80.3
Renal	786-0	80.7	41.4	>100	17	47.4	38.5	44.3	53.3
Cancer	A498	59.9	43.7	>100	27.6	47.2	54.5	55.4	52.1
	ACHN	>100	38	>100	33.4	36.6	35.5	36.7	49.9
	CAKI-1	>100	34.9	>100	33.1	56.2	34.4	45.3	40.2
	RXF 393	14.7	41.2	>100	15.9	28.9	21	18.7	33
	SN12C	79.7	36.7	>100	6.73	30.3	30	34	38.1
	TK-10	>100	53.8	>100	41.2	46.3	42.1	41.6	80.7
	UO-31	100	0010	. 200		59.9	40.7	39.7	61.9
Prostate	PC-3	>100	78.5	>100	45.5	>100	57	47.6	>100
Cancer	DU-145	>100	32.5	>100	34.9	36.7	39.5	42.3	33.4
Breast	MCF7	77.8	39	>100	29.9	45.9	33.8	37.5	40.3
Cancer	MDA-MB-231/ATCC	83.2	46.6	>100	40.5	48.4	42.4	44 7	33.8
5011001	HS 578T	>100	94.3	>100	97.2	>100	87.3	61.8	>100
	BT-549	55.2	28.4	>100	30.6	30.3	23.9	34.2	60.2
	T-47D	>100	59.6	>100	33.5	52.7	39.3	41.9	>100
	MDA-MB-468	75 5	34.7	>100	26.1	25.9	9.22	32.1	34
					20.2	20.0		5	2.

Figure S3. NCI60 five dose dcreen

Compound 3a





									.9		<u> </u>				
NSC : D - 832	482 / 1				Exp	erimer	nt ID : 2	111NS16				Test	t Type : 08	Units :	Molar
Report Date :	January	/ 25, 202	22		Tes	t Date	: Nover	nber 29, 2	2021			QNS	S :	MC :	
COMI : TO10					Stai	in Rea	gent : S	RB Dual-	Pass F	Related		SSF	PL:1BCH		
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	n Optica -6.0	Lo Densiti -5.0	og10 Con ies -4.0	centration -8.0	P -7.0	ercent G -6.0	irowth -5.0	-4.0	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.530 0.572 0.154 0.590 0.581 0.371	2.650 2.412 1.729 2.538 2.495 1.766	2.588 2.250 1.752 2.546 2.487 1.662	2.551 2.251 1.215 2.533 2.412 1.219	0.765 0.478 0.318 0.876 0.755 0.482	0.514 0.404 0.242 0.595 0.418 0.284	0.428 0.322 0.149 0.417 0.316 0.220	97 91 101 100 100 93	95 91 67 100 96 61	11 -16 10 15 9 8	-3 -29 6 0 -28 -23	-19 -44 -4 -29 -46 -41	3.45E-7 2.42E-7 2.02E-7 3.84E-7 3.37E-7 1.60E-7	6.04E-6 7.04E-7 4.06E-5 1.02E-5 1.75E-6 1.79E-6	 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522	Cancer 0.337 1.027 0.707 1.244 0.822 0.419 0.810 0.323 1.038	2.042 1.909 1.838 1.912 1.462 1.396 1.944 2.992 2.388	1.870 1.810 1.731 1.805 1.391 1.394 1.877 3.028 2.194	1.856 1.859 1.698 1.783 1.440 1.402 1.860 2.919 1.458	0.649 1.518 1.189 1.577 0.855 0.698 1.272 0.407 0.675	0.290 0.949 0.685 0.962 0.579 0.436 0.832 0.176 0.745	0.059 0.118 0.039 0.156 0.123 0.050 0.078 0.033 0.084	90 89 91 84 89 100 94 101 86	89 94 88 81 96 101 93 97 31	18 56 43 50 5 29 41 3 -35	-14 -8 -3 -23 -30 2 2 -46 -28	-82 -89 -94 -88 -85 -88 -90 -90 -92	3.57E-7 1.23E-6 6.84E-7 9.92E-7 3.23E-7 5.04E-7 6.61E-7 3.18E-7 4.50E-8	3.69E-6 7.58E-6 8.55E-6 4.87E-6 1.40E-6 1.05E-5 1.05E-5 1.16E-6 2.95E-7	3.36E-5 3.24E-5 2.64E-5 2.33E-5 3.77E-5 3.65E-5 1.25E-5 2.20E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.628 0.495 0.226 0.217 0.373 0.833 0.333	2.557 1.561 2.402 1.403 2.314 3.347 2.464	2.621 1.509 2.386 1.307 2.255 3.327 2.395	2.656 1.621 2.078 1.216 2.292 3.242 2.241	0.458 0.662 0.370 0.273 0.460 1.286 0.699	0.605 0.337 0.268 0.228 0.180 0.695 0.542	0.071 0.030 -0.019 0.002 -0.001 0.325 0.018	103 95 99 92 97 99 97	105 106 85 84 99 96 90	-27 16 7 5 4 18 17	-4 -32 2 1 -52 -17 10	-89 -94 -100 -99 -100 -61 -95	2.61E-7 4.15E-7 2.80E-7 2.69E-7 3.29E-7 3.88E-7 3.52E-7	6.23E-7 2.13E-6 1.04E-5 1.02E-5 1.20E-6 3.31E-6 1.24E-5	3.51E-5 1.95E-5 3.23E-5 3.32E-5 9.31E-6 5.65E-5 3.74E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.079 0.472 0.563 0.527 2.216 0.581	2.908 1.834 1.785 1.785 3.108 2.798	2.762 1.802 1.665 1.737 2.790 2.685	2.631 1.505 1.598 1.688 2.714 2.650	1.992 0.501 0.402 0.829 2.329 0.978	0.953 0.372 0.337 0.533 1.346 0.318	0.403 -0.012 -0.014 0.041 0.175 0.029	92 98 90 96 64 95	85 76 85 92 56 93	50 2 -29 24 13 18	-12 -21 -40 0 -39 -45	-63 -100 -100 -92 -92 -95	9.95E-7 2.24E-7 2.02E-7 4.16E-7 1.36E-7 3.75E-7	6.45E-6 1.23E-6 5.58E-7 1.01E-5 1.75E-6 1.92E-6	5.64E-5 2.32E-5 1.46E-5 3.50E-5 1.60E-5 1.24E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.163 0.726 0.470 0.779 1.232 0.523 0.640 0.948 0.837	1.211 1.433 1.929 3.060 2.657 1.667 2.673 2.522 2.807	1.149 1.344 1.910 3.000 2.530 1.677 2.555 2.404 2.699	0.899 1.261 1.723 1.976 2.596 1.470 2.484 2.347 1.817	0.351 0.902 0.639 0.354 1.416 0.925 0.760 1.593 1.051	0.113 0.703 0.495 0.960 1.315 0.700 0.389 1.065 0.365	-0.001 0.010 0.084 0.176 0.136 0.006 0.039 0.210 0.025	94 87 99 97 91 101 94 92 95	70 76 86 52 96 83 91 89 50	18 25 12 -55 13 35 6 41 11	-31 -3 2 8 6 15 -39 7 -56	-100 -99 -82 -77 -89 -99 -94 -78 -97	2.44E-7 3.20E-7 3.04E-7 3.57E-7 4.88E-7 3.02E-7 6.47E-7 9.86E-8	2.34E-6 7.71E-6 1.05E-5 1.37E-5 1.37E-5 1.35E-6 1.22E-5 1.45E-6	1.90E-5 3.09E-5 4.14E-5 3.88E-5 3.74E-5 1.57E-5 4.71E-5 8.03E-6
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-5 NCI/ADR-RES SK-OV-3	0.501 1.057 0.841 0.567 0.512 0.370 0.967	2.080 2.865 1.937 1.640 2.500 1.358 1.876	2.069 2.796 1.866 1.618 2.474 1.334 1.844	2.022 2.825 1.837 1.598 2.467 1.318 1.858	0.815 1.447 1.345 0.826 0.580 0.613 1.343	0.300 1.076 0.837 0.554 0.195 0.358 0.930	-0.003 0.083 0.045 -0.006 0.086 0.134 0.043	99 96 93 98 99 98 98	96 98 91 96 98 96 98	20 22 46 24 3 25 41	-40 1 0 -2 -62 -3 -4	-100 -92 -95 -100 -83 -64 -96	4.04E-7 4.23E-7 8.14E-7 3.23E-7 4.40E-7 7.02E-7	2.14E-6 1.03E-5 9.77E-6 8.19E-6 1.13E-6 7.64E-6 8.21E-6	1.46E-5 3.53E-5 3.36E-5 6.55E-6 5.92E-5 3.18E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.578 1.326 0.286 0.680 0.651 0.520 1.216 0.500	2.426 2.103 1.117 2.230 1.193 1.823 2.045 2.092	2.377 1.993 1.148 2.111 1.147 1.759 1.915 1.996	2.291 2.030 0.948 1.668 1.090 1.802 2.017 1.874	1.413 1.843 0.500 1.148 0.773 0.696 1.882 0.963	0.455 1.530 0.211 0.667 0.657 0.039 1.239 0.360	0.017 0.042 0.004 -0.015 0.049 0.006 0.123 -0.021	97 86 104 92 92 95 84 94	93 91 80 64 81 98 97 86	45 66 26 30 23 14 80 29	-21 26 -26 -2 1 -93 3 -28	-97 -97 -100 -92 -99 -90 -100	7.91E-7 2.57E-6 3.55E-7 2.57E-7 3.39E-7 3.71E-7 2.46E-6 4.31E-7	4.77E-6 1.63E-5 3.11E-6 8.67E-6 1.03E-5 1.34E-6 1.07E-5 3.23E-6	2.39E-5 4.16E-5 2.12E-5 3.09E-5 3.51E-5 3.71E-5 2.02E-5
Prostate Cancer PC-3 DU-145	0.628 0.333	2.212 1.647	2.175 1.668	2.066 1.732	0.861 0.559	0.521 0.380	0.082 0.004	98 102	91 106	15 17	-17 4	-87 -99	3.44E-7 4.29E-7	2.90E-6 1.08E-5	2.96E-5 3.33E-5
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.186 0.554 1.525 1.016 1.368 0.702	0.894 1.370 2.757 2.015 3.119 1.384	0.841 1.345 2.578 2.031 2.934 1.346	0.595 1.368 2.519 1.992 2.975 1.158	0.191 0.689 1.942 1.163 1.602 0.801	0.154 0.398 1.613 0.350 1.281 0.537	0.023 0.023 0.874 0.052 0.440 0.239	93 97 85 102 89 94	58 100 81 98 92 67	1 16 34 15 13 14	-17 -28 7 -66 -6 -24	-88 -96 -43 -95 -68 -66	1.36E-7 3.96E-7 4.52E-7 3.75E-7 3.41E-7 2.09E-7	1.10E-6 2.34E-6 1.39E-5 1.52E-6 4.74E-6 2.40E-6	2.91E-5 2.10E-5 > 1.00E-4 6.39E-6 5.13E-5 4.21E-5

Compound 3b





NSC : D - 843	103 / 1				Exp	erimer	nt ID : 2	308NS66				Tes	t Type : 08	Units :	Molar
Report Date :	October	r 15, 202	23		Tes	t Date	: Augus	st 28, 202	3			QNS	S :	MC :	
COMI : TO41					Stai	n Rea	gent : S	RB Dual-	Pass	Related	I	SSF	PL : 1BCH		
	Time			Mear	n Optica	Lo Densiti	og10 Con es	centration	F	Percent G	irowth				
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	Zero 0.489 0.609 0.255 0.491 0.768	Ctrl 2.589 2.652 2.249 2.462 2.466	-8.0 2.613 2.719 2.115 2.510 2.399	-7.0 2.596 2.338 1.902 2.337 2.398	-6.0 1.440 1.428 0.875 1.644 1.766	-5.0 0.625 0.462 0.411 0.718 0.807	-4.0 0.306 0.406 0.126 0.275 0.773	-8.0 101 103 93 102 96	-7.0 100 85 83 94 96	-6.0 45 40 31 59 59	-5.0 6 -24 8 11 2	-4.0 -38 -33 -51 -44 0	GI50 8.21E-7 5.98E-7 4.29E-7 1.52E-6 1.43E-6 >	TGI 1.40E-5 4.21E-6 1.36E-5 1.61E-5 1.00E-4	LC50 > 1.00E-4 > 1.00E-4 9.70E-5 > 1.00E-4 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H322M NCI-H322M NCI-H460 NCI-H522	Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	2.261 2.556 2.490 1.844 1.914 1.937 2.219 2.709 3.048	2.025 2.402 2.327 1.739 1.804 1.838 1.999 2.690 3.009	2.228 2.489 2.387 1.656 1.858 1.876 2.008 2.706 2.924	1.451 2.367 1.694 1.569 1.726 1.517 1.803 1.211 2.145	0.614 1.423 1.258 1.284 1.101 0.590 1.039 0.262 0.924	0.072 0.017 0.174 0.228 0.276 0.035 0.003 0.064 0.198	88 90 91 85 88 93 84 99 98	98 96 94 73 94 95 85 100 93	59 88 57 61 79 69 70 39 48	16 29 34 20 7 0 16 0 -29	-76 -98 -73 -80 -73 -94 -100 -75 -85	1.61E-6 4.41E-6 2.01E-6 2.52E-6 1.87E-6 2.52E-6 1.87E-6 2.38E-6 6.57E-7 9.25E-7	1.50E-5 1.69E-5 2.07E-5 1.60E-5 1.23E-5 9.92E-6 1.38E-5 1.00E-5 4.25E-6	5.26E-5 4.17E-5 6.14E-5 5.03E-5 5.12E-5 3.39E-5 3.72E-5 4.60E-5 2.40E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.564 2.576 2.705 2.525 1.692 2.606 2.095	2.582 2.367 2.879 2.330 1.590 2.527 2.036	2.500 2.539 2.991 2.416 1.732 2.617 2.008	1.726 1.844 1.498 1.380 0.798 1.548 0.890	0.369 0.677 0.465 0.385 0.194 0.570 0.606	0.068 0.016 0.219 0.009 0.035 0.054 0.053	101 89 107 91 93 96 97	97 98 112 95 103 101 95	58 62 50 48 39 50 34	-33 0 7 3 -11 4 19	-88 -98 -27 -97 -84 -89 -80	1.23E-6 1.55E-6 9.91E-7 9.18E-7 6.80E-7 9.96E-7 5.48E-7	4.35E-6 1.01E-5 1.59E-5 1.08E-5 6.14E-6 1.09E-5 1.54E-5	2.04E-5 3.27E-5 > 1.00E-4 3.40E-5 3.45E-5 3.78E-5 4.94E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.934 3.247 2.463 2.009 2.796 1.923	2.776 3.056 2.367 1.931 2.445 1.854	2.750 3.110 2.400 1.944 2.631 1.820	2.458 2.630 1.591 1.546 2.264 1.386	1.266 1.412 0.530 0.908 1.648 0.608	0.344 0.008 0.005 0.004 0.142 0.028	92 90 94 95 66 96	90 93 96 96 84 93	74 68 47 68 48 66	10 5 -35 24 -7 16	-68 -99 -99 -99 -92 -92	2.41E-6 1.94E-6 8.69E-7 2.55E-6 8.80E-7 2.08E-6	1.36E-5 1.12E-5 3.73E-6 1.56E-5 7.45E-6 1.41E-5	5.91E-5 3.38E-5 1.70E-5 3.98E-5 3.20E-5 4.08E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.908 1.675 2.419 3.019 1.947 2.026 3.255 2.466 2.837	2.748 1.536 2.467 2.946 1.929 1.992 2.965 2.329 2.679	2.783 1.596 2.615 3.007 1.967 2.058 3.078 2.368 2.678	1.612 1.286 1.649 1.265 1.725 1.761 2.170 2.001 1.910	0.793 1.025 0.947 0.414 0.900 1.271 0.540 1.664 1.517	0.017 0.056 0.088 0.034 0.096 0.005 0.004 0.034 0.006	94 87 103 97 98 97 88 91 92	95 93 111 99 102 102 92 94 91	48 63 58 25 80 79 54 70 50	15 39 19 -39 5 41 -40 48 29	-96 -91 -85 -95 -89 -99 -100 -96 -99	9.16E-7 3.46E-6 1.58E-6 4.63E-7 2.48E-6 5.75E-6 1.10E-6 8.22E-6 1.03E-6	1.38E-5 1.99E-5 1.52E-5 2.47E-6 1.12E-5 1.95E-5 3.73E-6 2.15E-5 1.68E-5	3.87E-5 4.83E-5 4.58E-5 1.58E-5 3.84E-5 4.44E-5 1.46E-5 4.78E-5 4.13E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	2.066 2.045 1.957 1.562 2.001 1.372 2.026	1.953 2.033 1.866 1.559 1.759 1.295 1.759	1.877 2.017 1.950 1.657 1.998 1.373 1.918	1.322 1.365 1.727 1.126 1.254 0.741 1.819	0.636 0.613 1.154 0.623 0.312 0.219 1.301	0.065 0.018 0.036 0.015 0.068 0.126 0.294	93 99 93 100 85 92 78	88 99 109 100 100 91	54 52 61 55 38 83	12 -2 35 16 -7 -39 39	-85 -97 -95 -97 -80 -65 -65	1.27E-6 1.09E-6 4.82E-6 1.74E-6 1.21E-6 6.36E-7 5.59E-6	1.34E-5 9.12E-6 1.87E-5 1.38E-5 7.61E-6 3.11E-6 2.37E-5	4.36E-5 3.19E-5 4.52E-5 3.85E-5 3.86E-5 2.71E-5 7.19E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	2.913 2.189 1.724 1.853 1.549 2.236 2.126 2.093	2.815 2.104 1.649 1.727 1.497 2.107 2.003 1.828	2.919 2.199 1.724 1.740 1.512 2.136 2.068 1.842	2.622 2.049 1.168 1.104 1.238 1.579 1.987 1.504	1.568 1.858 0.657 0.761 0.887 0.743 1.669 0.936	0.303 0.104 0.003 0.058 0.125 0.051 0.186 0.043	95 91 94 93 92 88 81	100 101 100 92 95 94 94 82	86 86 59 45 61 59 87 59	37 66 21 20 17 7 56 19	-61 -91 -99 -88 -83 -92 -83 -94	5.46E-6 1.27E-5 1.71E-6 7.76E-7 1.78E-6 1.49E-6 1.11E-5 1.66E-6	2.39E-5 2.63E-5 1.49E-5 1.52E-5 1.48E-5 1.18E-5 2.53E-5 1.47E-5	7.72E-5 5.46E-5 3.90E-5 4.41E-5 4.65E-5 3.77E-5 5.80E-5 4.10E-5
Prostate Cancer PC-3 DU-145	0.562 0.375	2.300 1.742	2.178 1.719	2.295 1.765	1.707 1.318	0.793 0.425	0.405 0.016	93 98	100 102	66 69	13 4	-28 -96	2.00E-6 1.95E-6	2.10E-5 1.09E-5	> 1.00E-4 3.47E-5
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.450 C 0.566 1.374 1.398 0.747 0.773	2.371 1.153 2.554 2.755 2.102 1.624	2.187 1.128 2.366 3.081 1.874 1.558	2.156 1.170 2.400 2.905 1.847 1.577	0.990 0.965 2.029 2.737 1.605 1.088	0.542 0.466 1.473 1.730 1.274 0.590	0.118 0.032 0.798 0.291 0.393 0.062	90 96 84 124 83 92	89 103 87 111 81 94	28 68 56 99 63 37	5 -18 8 24 39 -24	-74 -94 -42 -79 -47 -92	4.36E-7 1.62E-6 1.31E-6 4.53E-6 3.49E-6 5.93E-7	1.15E-5 6.22E-6 1.47E-5 1.72E-5 2.82E-5 4.06E-6	4.98E-5 2.64E-5 > 1.00E-4 5.23E-5 > 1.00E-4 2.42E-5

Compound 3c





NSC : D - 843	105 / 1				Exp	erimer	nt ID : 2	308NS66				Tes	t Type : 08	Units :	Molar
Report Date :	Octobe	r 15, 202	23		Tes	t Date	: Augus	st 28, 202	3			QNS	S :	MC :	
COMI : To43					Sta	in Rea	gent : S	RB Dual-	Pass	Related		SSF	PL : 1BCH		
Papel/Cell Line	Time	Ctrl	8.0	Mear	n Optica	Lo I Densiti	og10 Con es	centration	P	ercent G	Frowth	10	GI50	TGI	1 C 50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.489 0.609 0.255 0.491 0.768	2.664 2.344 2.045 2.118 2.610	2.700 2.337 1.904 2.223 2.550	2.345 2.363 1.928 2.224 2.456	2.371 2.135 1.733 1.750 2.172	0.739 0.538 0.250 0.511 0.922	0.496 0.375 0.182 0.304 0.693	102 100 92 106 97	85 101 93 107 92	87 88 83 77 76	-3.0 -11 -12 -2 1 8	0 -38 -29 -38 -10	3.07E-6 > 2.40E-6 2.43E-6 2.29E-6 2.43E-6	1.00E-4 7.64E-6 9.48E-6 1.07E-5 2.89E-5	 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H322M NCI-H322M NCI-H460 NCI-H522	Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	1.931 2.552 2.170 1.692 1.779 1.941 2.367 2.523 3.028	1.876 2.490 2.141 1.612 1.653 1.854 2.212 2.528 2.930	2.007 2.493 2.131 1.604 1.686 1.933 2.131 2.600 3.014	1.883 2.442 1.955 1.545 1.670 1.706 1.991 2.313 2.854	0.561 1.098 1.031 1.234 1.031 0.641 1.055 0.272 1.217	0.046 0.018 0.226 0.137 0.076 0.033 0.032 0.034 0.111	97 96 98 85 83 94 90 100 94	105 96 97 84 87 99 85 103 99	97 93 86 73 85 83 76 91 90	16 9 26 17 0 4 16 1 -6	-85 -98 -64 -88 -93 -95 -95 -96 -87 -91	3.82E-6 3.24E-6 3.97E-6 2.61E-6 2.58E-6 2.59E-6 2.69E-6 2.83E-6 2.63E-6 2.61E-6	1.45E-5 1.21E-5 1.94E-5 1.46E-5 9.83E-6 1.09E-5 1.38E-5 1.01E-5 8.65E-6	4.54E-5 3.54E-5 6.93E-5 4.35E-5 3.44E-5 3.52E-5 3.87E-5 3.79E-5 3.27E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.505 2.575 2.498 2.500 1.583 2.409 1.932	2.507 2.388 2.764 2.413 1.748 2.338 1.873	2.422 2.489 2.734 2.484 1.620 2.348 1.883	2.327 2.445 2.594 2.257 1.700 2.238 1.703	0.765 0.948 0.616 0.423 0.240 0.569 0.462	0.144 0.008 0.151 0.027 0.053 0.029 0.034	100 90 112 96 112 96 96	96 96 111 99 103 97 97	91 93 104 89 109 91 86	11 15 14 5 2 4 12	-74 -99 -50 -91 -76 -94 -87	3.25E-6 3.55E-6 4.02E-6 2.91E-6 3.53E-6 2.96E-6 3.06E-6	1.35E-5 1.35E-5 1.67E-5 1.13E-5 1.05E-5 1.10E-5 1.31E-5	5.23E-5 3.72E-5 > 1.00E-4 3.72E-5 4.66E-5 3.54E-5 4.20E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.816 3.287 2.411 1.977 2.753 1.823	2.673 3.127 2.380 1.904 2.551 1.746	2.635 3.163 2.437 1.904 2.716 1.776	2.555 3.182 2.312 1.882 2.671 1.747	1.265 1.222 0.819 0.839 1.674 0.448	0.289 0.015 0.016 0.016 0.449 0.015	92 92 98 95 79 95	90 94 102 95 96 97	85 95 94 93 92 95	11 -7 0 19 -6 6	-73 -99 -98 -97 -75 -96	2.98E-6 2.76E-6 2.93E-6 3.86E-6 2.68E-6 3.21E-6	1.35E-5 8.60E-6 1.00E-5 1.47E-5 8.75E-6 1.16E-5	5.32E-5 2.95E-5 3.24E-5 3.94E-5 4.39E-5 3.57E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.825 1.715 2.421 2.923 1.956 2.060 3.243 2.386 2.843	2.672 1.607 2.307 2.846 1.975 2.043 3.001 2.330 2.724	2.682 1.602 2.453 2.929 1.984 2.162 3.102 2.358 2.748	2.447 1.519 2.325 2.634 1.888 1.960 2.984 2.249 2.452	0.386 0.811 1.070 0.793 0.968 1.006 0.833 1.315 0.994	0.005 0.013 0.104 0.009 0.110 0.012 0.005 0.145 0.011	94 90 94 97 102 99 90 96 94	94 90 102 100 103 108 94 98 95	84 82 95 87 94 92 89 91 79	-5 18 26 5 11 19 -8 27 1	-99 -98 -83 -99 -87 -98 -99 -84 -99	2.43E-6 3.16E-6 4.45E-6 3.37E-6 3.81E-6 2.52E-6 4.35E-6 2.36E-6	8.81E-6 1.42E-5 1.73E-5 1.12E-5 1.28E-5 1.46E-5 8.30E-6 1.75E-5 1.02E-5	3.02E-5 3.85E-5 3.40E-5 4.17E-5 3.88E-5 2.88E-5 4.92E-5 3.24E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	2.136 1.961 1.862 1.546 1.989 1.306 1.821	2.026 1.944 1.812 1.605 1.837 1.304 1.859	1.958 1.951 1.887 1.628 1.928 1.301 1.843	1.719 1.642 1.684 1.463 1.783 1.214 1.763	0.618 0.778 0.966 0.630 0.522 0.235 1.243	0.030 0.013 0.029 0.004 0.059 0.039 0.284	94 99 96 105 91 100 104	90 99 102 107 96 99 102	75 76 84 92 88 90 94	11 11 22 17 11 -34 41	-93 -98 -96 -99 -82 -89 -66	2.47E-6 2.53E-6 3.55E-6 3.63E-6 3.10E-6 2.11E-6 6.81E-6	1.27E-5 1.27E-5 1.53E-5 1.39E-5 1.32E-5 5.30E-6 2.42E-5	3.84E-5 3.64E-5 4.07E-5 3.76E-5 4.50E-5 1.93E-5 7.08E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	2.726 2.109 1.749 1.741 1.433 2.180 2.177 2.093	2.615 2.039 1.677 1.620 1.351 2.124 2.093 1.863	2.740 2.057 1.740 1.647 1.343 2.228 2.159 1.788	2.727 2.071 1.608 1.521 1.290 1.940 2.484 1.590	1.363 1.622 0.473 0.717 0.728 0.642 1.497 0.739	0.238 0.037 0.017 0.080 0.007 0.042 0.006	94 92 95 90 88 96 92 84	101 94 99 92 87 103 98 79	100 96 90 82 79 85 128 65	30 46 7 18 -3 1 38 5	-69 -97 -100 -97 -89 -99 -96 -99	5.19E-6 8.25E-6 3.03E-6 3.17E-6 2.26E-6 2.58E-6 7.32E-6 1.77E-6	2.01E-5 2.09E-5 1.17E-5 1.43E-5 9.21E-6 1.02E-5 1.91E-5 1.12E-5	6.39E-5 4.69E-5 3.42E-5 3.91E-5 3.50E-5 3.23E-5 4.52E-5 3.38E-5
Prostate Cancer PC-3 DU-145	0.562 0.375	2.463 1.592	2.220 1.644	2.129 1.647	1.889 1.520	0.691 0.641	0.129 0.001	87 104	82 104	70 94	7 22	-77 -100	2.06E-6 4.07E-6	1.20E-5 1.51E-5	4.76E-5 3.89E-5
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.450 0.566 1.374 1.398 0.747 0.773	2.370 1.122 2.554 2.712 1.937 1.477	2.248 1.094 2.342 2.691 1.897 1.397	2.190 1.096 2.362 2.714 1.950 1.413	2.041 1.071 2.294 2.743 1.887 1.326	0.415 0.559 1.387 1.764 1.075 0.645	0.082 0.025 0.791 0.189 0.302 0.031	94 95 82 98 97 89	91 95 84 100 101 91	83 91 78 102 96 79	-8 -1 28 28 -17	-82 -96 -42 -87 -60 -96	2.30E-6 2.78E-6 2.31E-6 5.04E-6 4.68E-6 2.00E-6	8.21E-6 9.67E-6 1.06E-5 1.75E-5 2.07E-5 6.70E-6	3.72E-5 3.28E-5 > 1.00E-4 4.79E-5 7.76E-5 2.64E-5

Compound 3d





NSC : D - 843	112/1				Exp	erimer	nt ID : 2	308NS66	;			Test	: Туре : 08	Units :	Molar
Report Date :	Octobe	r 15, 202	23		Tes	t Date	: Augus	st 28, 202	23			QNS	S :	MC :	
COMI : To50					Sta	in Rea	gent : S	RB Dual-	Pass	Related	1	SSP	L : 1BCH		
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	n Optica -6.0	Lo I Densiti -5.0	og10 Con ies -4.0	centration -8.0	P -7.0	Percent G -6.0	Frowth -5.0	-4.0	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.489 0.609 0.255 0.491 0.768	2.664 2.344 2.045 2.118 2.610	2.846 2.320 2.063 2.092 2.504	2.624 2.341 1.786 2.068 2.474	0.969 0.615 0.552 0.877 1.474	0.887 0.562 0.487 0.677 1.095	0.831 0.609 0.455 0.653 1.251	108 99 101 98 94	98 100 85 97 93	22 0 17 24 38	18 -8 13 11 18	16 0 11 10 26	4.29E-7 > 3.17E-7 3.27E-7 > 4.38E-7 > 6.10E-7 >	1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H322M NCI-H322M NCI-H460 NCI-H522	Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	1.931 2.552 2.170 1.692 1.779 1.941 2.367 2.523 3.028	2.029 2.487 2.262 1.665 1.777 1.847 2.414 2.661 2.904	1.839 2.406 2.062 1.711 1.686 1.854 2.300 2.712 2.612	0.945 1.601 1.188 1.244 1.330 0.951 1.700 0.666 1.280	0.648 1.498 1.182 1.122 1.174 0.798 1.326 0.337 1.126	0.484 1.514 0.974 1.149 1.183 0.783 1.172 0.292 1.171	106 96 106 95 100 93 103 106 93	94 91 93 103 87 94 96 108 76	40 40 36 19 39 27 57 18 -1	22 34 36 -2 18 15 33 3 -13	12 35 22 20 14 23 1 -10	6.49E-7 > 6.41E-7 > 5.70E-7 > 4.29E-7 6.03E-7 > 4.47E-7 > 4.42E-7 > 2.17E-7	1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4 9.66E-7	 > 1.00E-4
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.505 2.575 2.498 2.500 1.583 2.409 1.932	2.490 2.629 2.503 2.404 1.616 2.415 2.009	2.553 2.324 2.453 1.971 1.578 2.238 1.922	0.733 1.161 0.782 0.391 0.262 0.817 0.630	0.426 0.506 0.816 0.294 0.235 0.651 0.607	0.542 0.414 0.453 0.295 0.288 0.540 0.507	99 103 100 96 102 100 105	102 87 98 76 100 91 99	9 26 22 4 3 17 22	-23 -24 23 -6 1 8 20	-2 -38 7 -5 5 2 14	3.66E-7 4.02E-7 4.27E-7 2.28E-7 3.27E-7 3.57E-7 4.32E-7	1.95E-6 3.28E-6 1.00E-4 2.47E-6 1.00E-4 1.00E-4 1.00E-4	 > 1.00E-4
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.816 3.287 2.411 1.977 2.753 1.823	2.770 3.152 2.398 1.879 2.599 1.787	2.623 3.086 2.211 1.809 2.558 1.750	1.703 1.531 0.621 0.983 1.847 0.775	1.263 1.249 0.538 0.867 1.549 0.579	1.247 1.281 0.464 0.897 1.451 0.521	97 93 99 93 84 98	89 90 87 88 80 95	36 11 -24 30 7 29	11 -5 -34 21 -13 15	10 -2 -43 24 -18 11	5.47E-7 > 3.21E-7 2.17E-7 4.49E-7 > 2.59E-7 4.77E-7 >	1.00E-4 5.11E-6 6.08E-7 1.00E-4 2.35E-6 1.00E-4	 > 1.00E-4
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.825 1.715 2.421 2.923 1.956 2.060 3.243 2.386 2.843	2.710 1.679 2.375 2.859 1.986 1.990 3.033 2.307 2.645	2.446 1.623 2.248 2.311 1.982 1.784 2.744 2.127 2.371	1.249 0.875 0.807 0.302 0.955 1.433 0.727 1.360 1.346	0.859 0.823 0.691 0.403 0.969 1.393 0.587 1.264 1.484	0.655 0.830 0.745 0.389 1.027 1.272 0.511 1.243 1.375	95 97 97 103 95 91 95 89	84 90 73 102 79 79 82 75	35 24 11 -55 9 52 -20 30 20	19 19 5 -40 11 49 -35 23 27	10 19 8 -42 16 40 -43 22 21	4.94E-7 > 4.09E-7 > 3.24E-7 > 3.66E-7 > 4.70E-6 > 1.96E-7 4.16E-7 > 2.83E-7 >	1.00E-4 1.00E-4 1.00E-4 3.70E-7 1.00E-4 1.00E-4 6.32E-7 1.00E-4 1.00E-4	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	2.136 1.961 1.862 1.546 1.989 1.306 1.821	2.177 2.142 1.834 1.544 1.834 1.309 1.851	2.122 1.898 1.701 1.518 1.929 1.120 1.860	1.068 0.496 1.189 0.744 0.634 0.242 1.390	0.819 0.581 1.131 0.624 0.405 0.209 1.100	0.721 0.586 1.071 0.573 0.371 0.160 1.268	102 114 98 100 91 100 103	99 95 86 97 96 80 104	37 -21 41 27 18 -32 56	23 -7 36 16 4 -42 27	17 -6 31 11 2 -55 44	6.21E-7 > 2.46E-7 6.37E-7 > 4.72E-7 > 3.90E-7 > 1.86E-7 1.61E-6 >	1.00E-4 6.62E-7 1.00E-4 1.00E-4 1.00E-4 5.17E-7 1.00E-4	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 4.09E-5 > 1.00E-4
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	2.726 2.109 1.749 1.741 1.433 2.180 2.177 2.093	2.666 2.087 1.691 1.620 1.417 2.011 2.081 1.852	2.756 2.028 1.262 1.327 1.292 2.017 2.082 1.770	2.055 1.986 0.437 0.812 0.843 1.138 1.631 1.016	1.791 1.847 0.415 0.834 0.816 0.785 1.575 0.987	1.707 1.824 0.442 0.839 0.799 0.720 1.588 0.923	97 96 90 98 89 91 83	102 91 65 67 79 90 91 77	66 86 5 25 14 33 50 25	52 71 3 27 10 10 45 23	48 68 5 28 7 6 46 18	2.94E-5 > > 1.00E-4 > 1.75E-7 > 2.55E-7 > 2.80E-7 > 4.97E-7 > 1.01E-6 > 3.30E-7 >	1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4 1.00E-4	 > 1.00E-4
Prostate Cancer PC-3 DU-145	0.562 0.375	2.463 1.592	2.463 1.663	2.388 1.583	1.222 0.586	1.037 0.440	0.859 0.516	100 106	96 99	35 17	25 5	16 12	5.64E-7 > 3.99E-7 >	1.00E-4 1.00E-4	> 1.00E-4 > 1.00E-4
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.450 C 0.566 1.374 1.398 0.747 0.773	2.370 1.122 2.554 2.712 1.937 1.477	2.177 1.124 2.442 2.598 2.042 1.475	1.283 1.075 2.282 2.550 1.735 1.248	0.537 0.457 1.352 2.222 1.004 0.589	0.492 0.336 1.428 1.851 1.057 0.671	0.447 0.366 1.364 1.717 1.009 0.571	90 100 91 91 109 100	43 91 77 88 83 67	5 -19 -2 63 22 -24	2 -41 5 34 26 -13	0 -35 0 24 22 -26	7.21E-8 2.37E-7 2.20E-7 2.81E-6 3.44E-7 1.55E-7	5.84E-5 6.70E-7 1.00E-4 1.00E-4 5.48E-7	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4

Compound 3e





									-						
NSC : D - 843	3104 / 1				Exp	erimer	nt ID : 2	308NS66				Test	t Type : 08	Units :	Molar
Report Date :	Octobe	r 15, 202	23		Tes	t Date	: Augus	st 28, 202	3			QNS	S :	MC :	
COMI : TO42					Sta	in Rea	gent : S	RB Dual-	Pass I	Related	ĺ.	SSF	PL : 1BCH		
Deschlostilling	Time	011		Mear	Optica	Lo Densiti	og10 Cor es	centration	P	ercent G	Frowth	1.0	0150		1.050
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.489 0.609 0.255 0.491 0.768	2.112 2.572 2.236 2.517 2.366	-8.0 2.093 2.467 2.234 2.498 2.339	2.004 2.408 2.246 2.379 2.278	-6.0 0.684 0.819 0.562 0.854 0.959	-5.0 0.434 0.722 0.526 0.528 0.549	-4.0 0.460 0.661 0.500 0.876 0.658	-8.0 99 95 100 99 98	-7.0 93 92 101 93 94	-6.0 12 11 15 18 12	-5.0 -11 6 14 2 -29	-4.0 -6 3 12 19 -14	3.41E-7 3.27E-7 > 3.93E-7 > 3.75E-7 > 3.46E-7	3.28E-6 1.00E-4 1.00E-4 1.00E-4 1.97E-6	 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H228 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	2.072 2.567 2.468 1.758 1.772 1.905 2.201 2.695 3.086	2.079 2.499 2.505 1.664 1.740 1.839 2.185 2.709 3.010	1.983 2.516 2.279 1.589 1.696 1.821 2.031 2.716 2.727	0.642 1.567 1.291 1.543 1.195 0.612 1.342 0.457 0.883	0.419 1.052 0.698 0.918 0.945 0.496 0.950 0.285 0.843	0.092 0.015 0.346 0.089 0.050 0.030 0.066 0.054 0.150	100 96 102 85 96 95 99 101 96	95 97 90 73 90 94 88 101 80	20 38 36 65 22 2 38 8 -32	7 6 4 -19 -9 -16 10 1 -35	-69 -98 -45 -92 -95 -95 -92 -79 -88	3.95E-7 6.20E-7 5.46E-7 3.82E-7 2.98E-7 5.78E-7 3.53E-7 1.85E-7	1.24E-5 1.13E-5 1.18E-5 5.89E-6 5.09E-6 1.22E-6 1.25E-5 1.03E-5 5.19E-7	5.64E-5 3.43E-5 > 1.00E-4 2.63E-5 2.69E-5 3.88E-5 4.32E-5 1.91E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.530 2.526 2.952 2.556 1.695 2.521 2.110	2.615 2.465 2.562 2.398 1.681 2.555 2.127	2.387 2.408 2.422 2.275 1.684 2.390 2.025	0.231 0.688 0.355 0.396 0.332 0.545 0.650	0.159 0.413 0.542 0.179 0.097 0.307 0.288	0.091 0.007 0.137 0.003 0.099 0.026 0.094	104 97 85 93 99 102 101	93 94 80 87 99 94 95	-58 1 2 4 8 2 21	-71 -38 9 -43 -55 -38 1	-83 -99 -54 -99 -54 -95 -65	1.92E-7 2.96E-7 2.42E-7 2.80E-7 3.45E-7 3.01E-7 4.05E-7	4.12E-7 1.07E-6 1.39E-5 1.21E-6 1.33E-6 1.15E-6 1.04E-5	8.84E-7 1.56E-5 8.50E-5 1.35E-5 8.24E-6 1.63E-5 5.94E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.876 3.293 2.433 1.977 2.823 1.916	2.805 3.187 2.373 1.902 2.646 1.838	2.712 3.145 2.285 1.909 2.579 1.876	1.692 1.145 0.553 0.677 2.164 0.682	1.215 1.109 0.690 0.664 1.781 0.177	0.299 0.011 -0.001 0.005 0.515 0.093	96 95 96 95 83 95	91 93 91 95 77 97	34 -13 -32 8 37 21	8 -15 -16 7 1 -50	-72 -99 -100 -99 -71 -74	5.29E-7 2.54E-7 2.14E-7 3.30E-7 4.75E-7 4.18E-7	1.26E-5 7.59E-7 5.45E-7 1.17E-5 1.02E-5 1.98E-6	5.29E-5 2.59E-5 2.55E-5 3.45E-5 5.10E-5 1.01E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.840 1.684 2.512 2.967 2.014 2.059 3.195 2.357 2.799	2.791 1.707 2.499 2.908 1.923 2.000 3.012 2.294 2.584	2.544 1.654 2.196 2.832 1.950 1.841 2.961 2.217 2.475	0.887 1.042 0.714 0.372 0.929 1.287 0.474 1.659 1.559	0.151 0.574 0.380 0.535 0.894 1.259 0.220 1.074 0.644	0.004 0.055 0.119 0.024 0.096 0.005 0.012 0.187 0.012	98 102 99 97 92 95 92 96 88	88 97 83 94 95 83 90 90 82	20 40 6 -45 7 41 -48 51 32	-63 -7 -37 -21 4 39 -76 11 -34	-99 -91 -80 -96 -89 -99 -99 -80 -99	3.60E-7 6.65E-7 2.70E-7 3.22E-7 6.12E-7 1.95E-7 1.09E-6 4.39E-7	1.73E-6 7.14E-6 1.38E-6 4.75E-7 1.10E-5 1.91E-5 4.51E-7 1.31E-5 3.06E-6	6.98E-6 3.25E-5 2.02E-5 2.43E-5 3.81E-5 4.39E-5 1.22E-6 4.70E-5 1.77E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	1.986 1.971 1.930 1.578 1.885 1.310 2.125	2.020 2.078 1.888 1.523 1.798 1.352 1.977	2.029 2.012 1.861 1.478 1.821 1.238 2.193	0.758 0.579 1.380 0.614 0.350 0.172 1.471	0.387 0.406 0.941 0.387 0.196 0.148 0.911	0.085 0.016 0.041 0.001 0.092 0.027 0.247	102 108 97 95 94 104 88	103 103 94 91 96 92 105	21 -8 55 15 1 -52 49	-11 -35 19 -13 -42 -59 6	-81 -97 -94 -100 -73 -93 -71	4.40E-7 3.02E-7 1.35E-6 3.46E-7 3.04E-7 1.97E-7 9.66E-7	4.45E-6 8.54E-7 1.46E-5 3.34E-6 1.05E-6 4.37E-7 1.19E-5	3.62E-5 1.73E-5 4.05E-5 2.65E-5 1.82E-5 9.71E-7 5.38E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	2.862 2.202 1.749 1.813 1.437 2.173 2.166 2.098	2.741 2.190 1.719 1.690 1.484 2.089 2.136 1.871	2.705 2.182 1.669 1.519 1.357 1.986 2.254 1.740	1.677 2.213 0.692 0.814 0.979 0.797 2.044 1.286	0.875 1.525 0.297 0.453 0.853 0.181 1.374 0.601	0.245 0.069 -0.005 0.010 0.021 0.007 0.098 0.002	94 99 98 91 107 95 97 84	92 98 94 78 88 88 108 75	43 101 23 24 33 11 89 43	5 32 -21 -9 15 -71 27 -10	-68 -94 -100 -98 -97 -99 -91 -100	7.27E-7 5.47E-6 4.18E-7 3.29E-7 4.97E-7 3.10E-7 4.21E-6 6.18E-7	1.16E-5 1.79E-5 3.38E-6 5.47E-6 1.36E-5 1.35E-6 1.69E-5 6.60E-6	5.59E-5 4.45E-5 2.35E-5 2.90E-5 3.79E-5 5.49E-6 4.49E-5 2.81E-5
Prostate Cancer PC-3 DU-145	0.562 0.375	2.233 1.685	2.212 1.754	2.066 1.733	0.918 0.446	0.608 0.346	0.067 0.012	99 105	90 104	21 5	3-8	-88 -97	3.82E-7 3.52E-7	1.07E-5 2.56E-6	3.81E-5 2.97E-5
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.450 C 0.566 1.374 1.398 0.747 0.773	2.377 1.142 2.589 2.877 2.065 1.481	2.223 1.145 2.491 2.650 1.981 1.476	2.105 1.078 2.336 2.514 1.964 1.428	0.628 0.408 1.669 1.758 1.479 0.587	0.367 0.335 1.517 1.360 0.977 0.435	0.076 0.003 0.912 0.177 0.328 0.011	92 100 92 85 94 99	86 89 79 75 92 92	9 -28 24 24 56 -24	-18 -41 12 -3 17 -44	-83 -100 -34 -87 -56 -99	2.94E-7 2.15E-7 3.40E-7 3.14E-7 1.40E-6 2.31E-7	2.16E-6 5.76E-7 1.81E-5 7.93E-6 1.73E-5 6.22E-7	3.07E-5 1.43E-5 > 1.00E-4 3.62E-5 8.25E-5 1.30E-5

Compound 3f





NSC : D - 843	3111/1				Exp	erimer	nt ID : 2	308NS66				Test	Туре : 08	Units : N	Molar
Report Date :	Octobe	r 15, 202	23		Tes	t Date	: Augus	st 28, 202	3			QNS	:	MC :	
COMI : To49					Sta	in Rea	gent : S	RB Dual-	Pass	Related		SSP	L : 1BCH		
Papel/Coll Line	Time	Ctrl	8.0	Mear	Optica	Lo Densiti	og10 Cor es	ncentration	P	ercent G	rowth	10	C150	TCI	1.050
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.489 0.609 0.255 0.491 0.768	2.559 2.682 2.238 2.709 2.490	2.537 2.567 2.235 2.759 2.455	2.479 2.528 2.165 2.827 2.463	2.231 2.445 1.617 2.552 2.215	0.696 0.525 0.320 0.754 0.678	0.366 0.293 0.110 0.301 0.395	99 94 100 102 98	96 93 96 105 98	84 89 69 93 84	10 -14 3 12 -12	-25 -52 -57 -39 -49	2.89E-6 2.38E-6 1.93E-6 3.38E-6 2.27E-6	1.93E-5 7.33E-6 1.13E-5 1.71E-5 7.53E-6	 > 1.00E-4 8.88E-5 7.64E-5 > 1.00E-4 > 1.00E-4
Non-Small Cell Lun; A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H226 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	1.978 2.566 2.173 1.785 1.796 1.923 2.182 2.634 3.037	1.870 2.448 1.990 1.681 1.637 1.911 2.035 2.712 2.921	1.939 2.495 2.084 1.692 1.699 1.898 2.090 2.739 2.948	1.796 2.419 1.914 1.572 1.655 1.735 1.889 2.383 1.964	0.459 1.198 0.980 1.171 0.970 0.591 1.202 0.237 0.884	0.018 0.148 0.366 0.251 0.090 0.035 0.245 0.028 0.237	94 93 88 84 79 99 89 103 93	98 96 94 86 87 98 93 104 95	89 91 83 67 81 86 79 89 38	10 15 23 5 -7 0 29 -8 -32	-94 -85 -42 -78 -91 -94 -70 -89 -82	3.11E-6 3.45E-6 3.52E-6 1.88E-6 2.28E-6 2.62E-6 3.73E-6 2.53E-6 6.23E-7	1.24E-5 1.41E-5 2.23E-5 1.15E-5 8.43E-6 1.00E-5 1.95E-5 8.19E-6 3.53E-6	3.76E-5 4.48E-5 > 1.00E-4 4.60E-5 3.25E-5 3.40E-5 6.28E-5 3.27E-5 2.32E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.497 2.623 2.836 2.557 1.609 2.483 2.045	2.452 2.446 2.738 2.383 1.587 2.390 2.035	2.350 2.493 2.798 2.488 1.580 2.426 1.959	2.425 2.434 2.591 2.265 1.562 2.086 1.691	0.714 0.527 0.590 0.340 0.151 0.556 0.556	0.130 0.020 0.661 0.009 0.018 0.030 0.027	98 91 96 92 98 95 99	92 93 99 97 98 97 95	96 90 90 87 97 80 80	8 -21 11 -30 3 16	-76 -97 14 -97 -92 -94 -90	3.36E-6 2.30E-6 3.24E-6 2.70E-6 2.33E-6 2.46E-6 2.96E-6	1.25E-5 6.46E-6 > 1.00E-4 1.03E-5 5.76E-6 1.08E-5 1.42E-5	4.88E-5 2.40E-5 > 1.00E-4 3.31E-5 2.08E-5 3.53E-5 4.19E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.868 3.277 2.447 1.903 2.711 1.764	2.682 3.157 2.289 1.822 2.414 1.687	2.717 3.166 2.352 1.871 2.569 1.727	2.418 2.981 2.110 1.772 2.260 1.617	1.327 1.082 0.507 0.776 1.745 0.428	0.380 0.088 0.010 0.029 0.684 0.021	90 94 90 94 68 95	92 94 98 85 97	75 85 79 90 52 90	14 -17 -38 16 -2 5	-65 -93 -99 -95 -61 -94	2.57E-6 2.20E-6 1.78E-6 3.47E-6 1.08E-6 2.95E-6	1.51E-5 6.76E-6 4.74E-6 1.39E-5 9.33E-6 1.13E-5	6.53E-5 2.69E-5 1.57E-5 3.93E-5 6.44E-5 3.60E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.859 1.681 2.581 2.043 2.144 3.201 2.288 2.847	2.677 1.548 2.469 2.825 1.966 2.173 2.927 2.179 2.733	2.790 1.570 2.499 2.870 1.933 2.218 2.983 2.213 2.792	2.323 1.380 2.143 1.790 1.845 1.843 2.827 2.096 1.968	0.421 0.891 0.912 0.461 0.916 1.284 0.371 1.132 1.254	0.031 0.214 0.040 0.055 0.053 0.004 0.150 0.030	93 87 94 97 94 102 88 92 94	97 90 96 99 91 105 90 94 97	78 72 78 50 83 78 84 86 53	1 26 16 -32 5 38 -59 16 15	-100 -95 -64 -94 -94 -93 -100 -84 -97	2.31E-6 2.97E-6 2.81E-6 2.68E-6 5.10E-6 1.72E-6 3.24E-6 1.20E-6	1.01E-5 1.63E-5 1.57E-5 4.10E-6 1.14E-5 1.96E-5 3.86E-6 1.43E-5 1.36E-5	3.18E-5 4.24E-5 6.61E-5 1.96E-5 3.63E-5 4.70E-5 8.65E-6 4.57E-5 3.80E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	2.147 1.958 1.832 1.621 1.868 1.333 1.889	1.988 1.918 1.792 1.632 1.749 1.322 1.658	1.940 1.968 1.840 1.662 1.878 1.362 1.837	1.045 1.817 1.753 1.557 1.663 0.904 1.627	0.556 0.503 1.083 0.617 0.212 0.174 1.239	0.021 0.016 0.054 0.035 0.028 0.018 0.299	91 97 96 101 92 99 78	88 101 101 104 101 103 95	36 89 93 95 87 56 75	7 -20 33 14 -37 -51 38	-95 -97 -93 -92 -92 -95 -64	5.30E-7 2.30E-6 5.20E-6 3.60E-6 1.98E-6 1.14E-6 4.76E-6	1.17E-5 6.59E-6 1.83E-5 1.37E-5 5.01E-6 3.33E-6 2.36E-5	3.61E-5 2.45E-5 4.58E-5 4.02E-5 1.72E-5 9.73E-6 7.25E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	3.041 2.202 1.700 1.736 1.442 2.311 2.183 2.052	2.973 2.109 1.709 1.613 1.351 2.192 2.025 1.816	2.932 2.164 1.783 1.620 1.349 2.239 2.129 1.793	2.817 2.056 1.408 1.169 1.177 1.918 2.194 1.557	1.504 1.775 0.509 0.788 0.751 0.610 1.521 0.865	0.236 0.034 0.003 0.017 0.049 0.005 0.115 0.029	97 91 101 90 87 93 86 83	95 96 106 91 87 96 95 81	90 85 78 54 62 77 101 64	32 57 10 24 0 -3 40 14	-70 -97 -99 -97 -93 -99 -89 -96	4.91E-6 1.11E-5 2.59E-6 1.38E-6 1.55E-6 2.15E-6 6.80E-6 1.94E-6	2.07E-5 2.34E-5 1.24E-5 1.57E-5 1.00E-5 9.09E-6 2.03E-5 1.35E-5	6.41E-5 4.94E-5 3.55E-5 4.09E-5 3.43E-5 3.07E-5 4.95E-5 3.85E-5
Prostate Cancer PC-3 DU-145	0.562 0.375	2.244 1.634	2.060 1.643	2.161 1.668	1.796 1.573	0.706 0.440	0.200 0.005	89 101	95 103	73 95	9 5	-65 -99	2.29E-6 3.18E-6	1.31E-5 1.12E-5	6.33E-5 3.39E-5
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.450 C 0.566 1.374 1.398 0.747 0.773	2.385 1.111 2.564 2.929 1.941 1.451	2.208 1.085 2.408 2.896 1.881 1.414	2.242 1.095 2.455 2.733 1.856 1.432	1.833 1.075 2.173 2.639 1.849 1.356	0.450 0.474 1.389 1.801 0.985 0.567	0.024 0.021 1.017 0.653 0.296 0.062	91 95 87 98 95 95	93 97 91 87 93 97	71 93 67 81 92 86	0 -16 1 26 20 -27	-95 -96 -26 -53 -60 -92	1.99E-6 2.49E-6 1.82E-6 3.69E-6 3.84E-6 2.09E-6	9.96E-6 7.10E-6 1.11E-5 2.14E-5 1.77E-5 5.80E-6	3.37E-5 2.63E-5 > 1.00E-4 9.08E-5 7.43E-5 2.28E-5

Compound 3g





NSC : D - 843	106 / 1				Exp	erimer	nt ID : 2	308NS66	0			Test	t Type : 08	Units :	Molar
Report Date :	Octobe	15, 202	23		Tes	t Date	: Augus	st 28, 202	3			QNS	S :	MC :	
COMI : To44					Stai	in Rea	gent : S	RB Dual-	Pass I	Related		SSF	PL : 1BCH		
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	Optical	Lo Densiti -5.0	og10 Cor es -4.0	centration -8.0	P -7.0	ercent G -6.0	irowth -5.0	-4.0	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.489 0.609 0.255 0.491 0.768	2.450 2.329 1.971 2.198 2.438	2.409 2.231 2.053 2.275 2.323	2.406 2.158 1.919 2.178 2.266	1.616 1.433 0.610 1.561 1.555	0.824 0.446 0.344 0.630 0.746	0.465 0.324 0.196 0.274 0.709	98 94 105 105 93	98 90 97 99 90	57 48 21 63 47	17 -27 5 8 -3	-5 -47 -23 -44 -8	1.53E-6 8.91E-7 4.13E-7 1.71E-6 8.55E-7	5.93E-5 4.38E-6 1.52E-5 1.43E-5 8.74E-6	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522	Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	1.897 2.569 2.164 1.736 1.813 1.949 2.290 2.640 3.018	1.882 2.505 2.230 1.655 1.751 1.819 2.317 2.756 2.838	1.863 2.419 2.082 1.663 1.757 1.887 2.197 2.720 2.850	1.032 2.138 1.689 1.598 1.503 1.235 1.910 0.768 1.047	0.469 1.258 1.189 1.238 1.001 0.637 1.188 0.222 0.889	0.080 0.006 0.166 0.244 0.049 0.024 0.128 0.050 0.110	99 96 104 87 92 90 102 105 90	98 91 95 88 93 95 94 103 90	46 73 69 77 60 47 74 21 -19	11 19 36 17 -3 3 25 -14 -31	-73 -99 -74 -95 -96 -84 -81 -92	8.38E-7 2.66E-6 3.80E-6 2.79E-6 1.44E-6 8.84E-7 3.14E-6 4.48E-7 2.33E-7	1.35E-5 1.44E-5 2.14E-5 1.49E-5 8.82E-6 1.08E-5 1.71E-5 3.95E-6 6.68E-7	5.34E-5 3.81E-5 6.08E-5 5.01E-5 3.21E-5 3.44E-5 3.43E-5 3.43E-5 2.04E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.402 2.648 2.727 2.558 1.552 2.468 2.027	2.484 2.506 2.553 2.463 1.579 2.479 1.999	2.456 2.502 2.577 2.317 1.590 2.465 1.958	1.711 1.773 0.989 0.994 0.421 1.036 0.797	0.643 0.607 0.770 0.366 0.193 0.501 0.573	0.078 0.008 0.128 0.014 0.083 0.035 0.057	104 93 96 102 101 98	103 93 94 89 103 100 96	63 56 28 30 15 27 30	5 -9 19 2 -11 0 17	-86 -99 -57 -95 -62 -93 -79	1.66E-6 1.23E-6 4.67E-7 4.65E-7 4.01E-7 4.88E-7 4.99E-7	1.13E-5 7.23E-6 1.79E-5 1.06E-5 3.75E-6 1.01E-5 1.52E-5	4.03E-5 2.86E-5 7.99E-5 3.43E-5 5.85E-5 3.46E-5 5.02E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.841 3.281 2.464 1.998 2.794 1.742	2.875 3.212 2.379 1.928 2.729 1.705	2.836 3.116 2.327 1.855 2.522 1.672	2.151 1.944 1.139 1.295 2.056 0.891	1.358 1.112 0.556 0.695 1.813 0.423	0.266 0.009 0.006 0.008 0.214 0.034	102 97 95 95 94 97	100 92 92 90 73 95	61 32 19 51 28 39	16 -15 -32 9 4 5	-75 -99 -99 -99 -88 -90	1.76E-6 5.01E-7 3.78E-7 1.06E-6 3.25E-7 6.30E-7	1.50E-5 4.80E-6 2.39E-6 1.22E-5 1.10E-5 1.13E-5	5.30E-5 2.60E-5 1.85E-5 3.54E-5 3.86E-5 3.77E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.881 1.690 2.499 2.976 1.936 2.026 3.244 2.284 2.820	2.708 1.664 2.419 2.964 1.935 1.967 3.073 2.171 2.641	2.562 1.634 2.441 2.872 2.005 1.889 2.991 2.120 2.563	1.328 1.014 1.378 0.436 1.405 1.367 1.537 1.523 1.479	0.380 1.063 0.857 0.555 0.961 1.363 0.278 1.040 1.234	0.003 0.048 0.102 0.021 0.066 0.025 0.012 0.245 0.014	93 98 99 100 95 93 92 90	87 95 97 95 106 89 89 88 88	37 37 41 -36 51 48 27 44 27	-6 42 13 -18 10 48 -69 9 14	-99 -92 -83 -97 -92 -97 -99 -73 -99	5.55E-7 5.96E-7 6.89E-7 1.07E-6 9.09E-7 4.27E-7 7.38E-7 4.11E-7	7.13E-6 2.05E-5 1.38E-5 5.35E-7 1.26E-5 2.15E-5 1.91E-6 1.28E-5 1.33E-5	2.94E-5 4.84E-5 4.54E-5 2.55E-5 3.87E-5 4.75E-5 6.30E-6 5.20E-5 3.70E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	2.077 1.986 1.919 1.600 1.912 1.353 1.831	2.143 2.016 1.875 1.541 1.775 1.344 1.864	1.998 2.066 1.831 1.501 1.762 1.270 1.863	1.141 0.823 1.529 1.044 0.828 0.248 1.499	0.639 0.730 1.096 0.560 0.247 0.182 1.421	0.061 0.009 0.027 0.007 0.070 0.049 0.202	104 102 96 95 91 99 103	95 106 93 91 90 92 103	43 14 68 52 31 -31 67	12 8 32 10 -27 -49 59	-86 -99 -96 -98 -79 -86 -76	7.34E-7 4.09E-7 3.09E-6 1.10E-6 4.81E-7 2.19E-7 1.16E-5	1.33E-5 1.18E-5 1.77E-5 1.23E-5 3.45E-6 5.63E-7 2.73E-5	4.30E-5 3.49E-5 4.35E-5 3.57E-5 2.77E-5 1.05E-5 6.41E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	3.052 2.193 1.749 1.770 1.441 2.207 2.110 2.085	2.886 2.130 1.779 1.707 1.407 2.151 2.025 1.880	2.792 2.087 1.680 1.643 1.339 2.010 2.021 1.816	2.408 2.003 0.905 0.856 0.887 1.552 1.978 1.236	1.211 1.739 0.485 0.662 0.905 0.584 1.532 0.812	0.160 0.049 -0.001 0.009 0.049 0.008 0.096 0.007	93 94 102 95 95 96 92 86	89 95 90 85 87 91 81	72 81 39 28 20 58 87 40	19 54 8 13 22 -8 44 10	-79 -96 -100 -98 -93 -99 -91 -99	2.58E-6 1.06E-5 6.27E-7 4.45E-7 3.46E-7 1.34E-6 7.16E-6 5.77E-7	1.56E-5 2.29E-5 1.19E-5 1.31E-5 1.56E-5 7.69E-6 2.11E-5 1.24E-5	5.02E-5 4.93E-5 3.45E-5 3.69E-5 4.21E-5 2.92E-5 4.95E-5 3.57E-5
Prostate Cancer PC-3 DU-145	0.562 0.375	2.181 1.649	2.335 1.788	2.294	1.288 1.167	0.823	0.190 0.011	109 111	107 107	45 62	16 1	-66 -97	8.26E-7 1.58E-6	1.57E-5 1.03E-5	6.36E-5 3.31E-5
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.450 0.566 1.374 1.398 0.747 0.773	2.394 1.142 2.573 2.810 2.058 1.481	2.273 1.140 2.439 2.648 1.963 1.475	2.182 1.106 2.386 2.713 1.934 1.386	0.862 1.022 1.851 2.592 1.561 0.839	0.478 0.492 1.646 1.708 1.163 0.613	0.086 0.029 0.919 0.204 0.316 0.037	94 100 89 89 93 99	89 94 84 93 91 87	21 79 40 85 62 9	1 -13 23 22 32 -21	-81 -95 -33 -85 -58 -95	3.76E-7 2.07E-6 5.90E-7 3.56E-6 2.50E-6 2.97E-7	1.04E-5 7.20E-6 2.55E-5 1.60E-5 2.26E-5 2.04E-6	4.22E-5 2.82E-5 > 1.00E-4 4.68E-5 8.19E-5 2.47E-5

Compound 3h





NSC : D - 845424 / 1					Experiment ID : 2310NS86								Test Type : 08		Units : Molar		
Report Date : November 08, 2023					Test Date : October 02, 2023								QNS :		MC :		
COMI : TO53						Stain Reagent : SRB Dual-Pass Related							SSPL : 1CXF				
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	Log10 Concentration Optical Densities Percent Growth -6.0 -5.0 -4.0 -8.0 -7.0 -6.0 -5.0 -							-4.0	GI50	TGI	TGI LC50		
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.563 0.776 0.221 0.609 0.518 0.364	2.580 2.567 1.286 2.053 1.951 1.347	2.567 2.430 1.243 2.189 2.011 1.259	1.668 2.377 1.207 1.908 1.996 1.088	0.858 0.328 0.171 0.632 0.824 0.291	0.532 0.248 0.091 0.245 0.478 0.127	0.514 0.246 0.053 0.334 0.512 0.166	99 92 96 109 104 91	55 89 93 90 103 74	15 -58 -23 2 21 -20	-6 -68 -59 -60 -8 -65	-9 -68 -76 -45 -1 -54	1.32E-7 1.85E-7 2.34E-7 2.83E-7 4.46E-7 1.79E-7	5.32E-6 4.05E-7 6.36E-7 1.06E-6 5.39E-6 6.11E-7	> 1.00E-4 8.86E-7 5.64E-6 > 1.00E-4 4.60E-6		
Non-Small Cell Lun A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.333 1.086 0.559 1.079 1.191 0.621 0.862 0.359 1.404	1.903 2.487 1.541 1.763 2.326 2.296 2.331 2.328 2.894	1.745 2.360 1.540 1.678 2.243 2.208 2.231 2.308 2.766	1.926 2.428 1.556 1.657 2.321 2.254 2.346 2.383 2.727	0.651 1.849 0.728 1.454 1.601 0.668 1.500 0.306 0.968	0.397 1.272 0.392 0.991 1.181 0.719 1.244 0.175 0.805	0.080 0.623 0.184 0.384 0.610 0.041 0.408 0.123 0.730	90 91 100 88 93 95 93 99 91	101 96 102 84 100 97 101 103 89	20 54 17 55 36 3 43 -15 -31	4 13 -30 -8 0 6 26 -51 -43	-76 -43 -67 -64 -49 -93 -53 -66 -48	4.30E-7 1.28E-6 4.08E-7 1.19E-6 6.04E-7 3.17E-7 7.68E-7 2.81E-7 2.11E-7	1.12E-5 1.73E-5 2.31E-6 7.42E-6 9.49E-6 1.14E-5 2.14E-5 7.49E-7 5.51E-7	4.74E-5 > 1.00E-4 3.47E-5 5.54E-5 > 1.00E-4 3.65E-5 9.23E-5 9.24E-6 > 1.00E-4		
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.503 0.853 0.349 0.382 0.257 0.611 0.402	1.914 3.119 2.741 2.735 1.694 2.688 1.952	1.988 2.776 2.589 2.573 1.624 2.608 1.921	2.067 2.909 2.660 2.510 1.778 2.584 1.850	0.296 0.633 0.514 0.528 0.216 0.775 0.545	0.134 0.302 0.259 0.276 0.114 0.380 0.406	0.090 0.104 0.077 0.026 0.020 0.146 0.181	105 85 94 93 95 96 98	111 91 97 90 106 95 93	-41 -26 7 6 -16 8 9	-73 -65 -26 -28 -56 -38 0	-82 -88 -78 -93 -92 -76 -55	2.51E-7 2.24E-7 3.31E-7 3.02E-7 2.87E-7 3.28E-7 3.28E-7	5.36E-7 6.01E-7 1.63E-6 1.52E-6 7.37E-7 1.49E-6 1.01E-5	1.88E-6 4.20E-6 2.91E-5 2.19E-5 7.20E-6 2.07E-5 8.09E-5		
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.763 1.288 0.714 0.850 0.927 0.268	2.115 3.130 2.410 2.368 1.458 1.411	2.013 2.971 2.270 2.222 1.313 1.333	2.016 2.971 2.318 2.220 1.359 1.381	1.035 1.044 0.515 1.461 0.935 0.383	0.731 1.074 0.515 1.214 0.852 0.206	0.338 0.514 0.057 0.260 0.410 0.024	92 91 92 90 73 93	93 91 95 90 81 97	20 -19 -28 40 2 10	-4 -17 -28 24 -8 -23	-56 -60 -92 -69 -56 -91	3.88E-7 2.37E-7 6.38E-7 2.47E-7 3.49E-7	6.69E-6 6.73E-7 5.91E-7 1.81E-5 1.44E-6 2.01E-6	7.73E-5 5.85E-5 2.21E-5 6.19E-5 7.55E-5 2.49E-5		
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.464 0.739 0.494 0.751 1.244 0.803 1.062 1.089 1.130	2.633 1.671 1.782 2.341 2.432 2.295 3.211 2.637 3.072	2.481 1.588 1.736 2.287 2.396 2.256 3.059 2.525 2.922	2.403 1.595 1.730 2.140 2.375 2.227 3.003 2.545 2.865	0.901 1.113 0.508 0.355 1.072 1.341 0.822 1.814 1.843	0.295 0.828 0.543 0.535 1.206 1.384 0.228 1.093 1.136	0.012 0.147 0.134 0.087 0.348 0.066 0.016 0.381 0.442	93 91 97 97 97 93 93 92	89 92 96 87 95 95 90 94 89	20 40 1 -53 -14 36 -23 47 37	-36 9 4 -29 -3 39 -79 0 0	-98 -80 -73 -88 -72 -92 -98 -65 -61	3.70E-7 6.45E-7 3.05E-7 1.85E-7 2.60E-7 5.82E-7 2.28E-7 8.56E-7 5.59E-7	2.27E-6 1.28E-5 1.12E-5 4.20E-7 7.47E-7 1.99E-5 6.30E-7 1.01E-5 1.01E-5	1.67E-5 4.61E-5 5.03E-5 4.79E-5 3.08E-6 5.88E-5 6.63E-5		
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.598 0.648 0.950 0.593 0.526 0.585 0.720	2.066 1.918 2.156 1.464 2.524 2.053 1.622	1.967 1.888 2.085 1.419 2.337 2.026 1.588	2.003 1.950 2.160 1.410 2.517 1.970 1.610	1.085 0.523 1.345 0.845 0.259 0.275 0.996	0.563 0.440 0.880 0.635 0.165 0.297 0.772	0.154 0.046 0.120 0.038 0.044 0.075 0.151	93 98 94 95 91 98 96	96 103 100 94 100 94 99	33 -19 33 29 -51 -53 31	-6 -32 -7 5 -69 -49 6	-74 -93 -87 -94 -92 -87 -79	5.38E-7 2.70E-7 5.55E-7 4.73E-7 2.14E-7 2.00E-7 5.19E-7	7.08E-6 6.94E-7 6.53E-6 1.12E-5 4.60E-7 4.36E-7 1.17E-5	4.41E-5 1.97E-5 3.41E-5 3.60E-5 9.88E-7 4.54E-5		
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10	0.686 1.481 0.349 0.581 1.053 0.543 1.244	2.622 2.269 1.700 2.043 1.744 2.017 2.111	2.628 2.097 1.675 1.907 1.670 1.887 2.014	2.589 2.031 1.701 1.628 1.604 1.986 2.113	1.176 1.936 0.725 0.845 0.977 0.793 2.013	0.652 1.562 0.360 0.440 0.962 0.328 1.447	0.137 0.204 0.002 0.101 0.149 0.021 0.543	100 78 98 91 89 91 89	98 70 100 72 80 98 100	25 58 28 -7 17 89	-5 10 1 -24 -9 -40 23	-80 -86 -99 -83 -86 -96 -56	4.59E-7 1.45E-6 4.93E-7 2.53E-7 2.19E-7 3.91E-7 3.91E-6	6.82E-6 1.28E-5 1.02E-5 2.66E-6 8.25E-7 2.00E-6 1.96E-5	3.98E-5 4.21E-5 3.21E-5 2.75E-5 3.43E-5 1.53E-5 8.32E-5		
Prostate Cancer PC-3 DU-145	0.515 0.361	2.026 1.568	1.798 1.523	1.846 1.558	0.932 0.472	0.632 0.310	0.116 0.013	85 96	88 99	28 9	8 -14	-77 -97	4.26E-7 3.52E-7	1.23E-5 2.46E-6	4.76E-5 2.72E-5		
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.544 C 0.605 1.372 1.308 0.798 1.202	2.358 1.214 2.393 2.255 1.842 2.316	2.158 1.237 2.219 2.170 1.664 2.335	2.162 1.228 2.256 2.199 1.627 2.300	0.712 0.553 1.431 1.122 1.211 0.928	0.510 0.471 1.410 0.731 0.824 0.741	0.184 0.079 1.175 0.435 0.385 0.426	89 104 83 91 83 102	89 102 87 94 79 98	9 -9 6 -14 40 -23	-6 -22 4 -44 2 -38	-66 -87 -14 -67 -52 -65	3.09E-7 2.96E-7 2.84E-7 2.55E-7 5.46E-7 2.51E-7	3.92E-6 8.35E-7 1.61E-5 7.39E-7 1.11E-5 6.49E-7	5.35E-5 2.69E-5 > 1.00E-4 1.81E-5 9.26E-5 2.78E-5		

Compound 3i





NSC : D - 843107 / 1					Exp	erimer	nt ID : 2	308NS66			Test	Test Type : 08		Units : Molar		
Report Date : October 15, 2023					Tes	t Date	: Augu	st 28, 202	3		QNS	QNS :		MC :		
COMI : To45						in Rea	gent : S	RB Dual-	Pass	Related	SSF	PL : 1BCH				
Panel/Cell Line	Time	Ctrl	8.0	Mear	Optica	Lo I Densiti	og10 Cor es	ncentration	F	Percent G	4.0	CI50				
-eukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.489 0.609 0.255 0.491 0.768	2.450 2.329 1.971 2.198 2.438	2.367 2.251 1.933 2.242 2.306	2.446 2.246 1.850 2.195 2.298	2.221 2.009 1.142 1.887 2.111	0.666 0.383 0.274 0.516 0.735	0.397 0.346 0.173 0.300 0.550	96 95 98 103 92	100 95 93 100 92	-0.0 88 81 52 82 80	-3.0 -37 1 -4	-19 -43 -32 -39 -28	3.04E-6 1.84E-6 1.08E-6 2.49E-6 2.28E-6	2.10E-5 4.86E-6 1.08E-5 1.09E-5 8.88E-6	 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 	
Von-Small Cell Lun; A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H322M NCI-H322M NCI-H460 NCI-H522	g Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	1.897 2.569 2.164 1.736 1.813 1.949 2.290 2.640 3.018	1.867 2.470 2.015 1.626 1.716 1.887 2.103 2.633 2.914	1.943 2.510 2.063 1.603 1.737 1.892 2.076 2.692 2.972	1.700 2.396 1.843 1.565 1.743 1.692 1.887 2.463 1.742	0.520 1.397 1.053 1.218 1.101 0.672 1.239 0.252 1.023	0.126 0.492 0.351 0.604 0.203 0.106 0.419 0.054 0.613	98 94 90 82 87 95 87 100 94	103 96 93 78 90 96 86 102 97	88 89 79 71 91 81 73 93 26	14 27 13 6 29 -3 -21	-57 -49 -45 -47 -80 -82 -82 -48 -79 -53	3.25E-6 4.29E-6 3.65E-6 3.13E-6 2.59E-6 3.30E-6 2.80E-6 4.60E-7	1.58E-5 2.28E-5 2.40E-5 1.66E-5 1.24E-5 1.17E-5 2.37E-5 9.37E-6 3.57E-6	7.94E-5 > 1.00E-4 > 1.00E-4 4.54E-5 4.32E-5 > 1.00E-4 4.14E-5 8.22E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.402 2.648 2.727 2.558 1.552 2.468 2.027	2.654 2.452 2.693 2.537 1.541 2.442 1.996	2.510 2.492 2.811 2.519 1.625 2.521 1.954	2.348 2.336 2.467 2.121 1.505 1.948 1.717	0.600 0.659 0.602 0.379 0.151 0.596 0.760	0.054 0.081 0.581 0.049 0.034 0.050 0.057	114 90 99 99 99 99 99	106 92 103 98 105 103 96	97 84 89 81 96 74 82	3 -1 12 3 -31 5 28	-90 -88 12 -84 -85 -90 -79	3.15E-6 2.51E-6 3.24E-6 2.32E-6 2.32E-6 3.93E-6	1.07E-5 9.63E-6 1.00E-4 1.08E-5 5.74E-6 1.13E-5 1.83E-5	3.69E-5 3.64E-5 > 1.00E-4 4.05E-5 2.29E-5 3.80E-5 5.36E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.841 3.281 2.464 1.998 2.794 1.742	2.720 3.181 2.356 1.893 2.475 1.644	2.765 3.199 2.350 1.919 2.523 1.701	2.443 2.762 1.979 1.745 2.125 1.532	1.308 1.062 0.572 0.766 1.726 0.455	0.702 0.361 0.183 0.191 0.911 0.039	93 95 93 93 69 93	96 96 93 95 73 97	77 74 71 82 34 85	13 -19 -30 14 -3 7	-35 -72 -78 -66 -49 -89	2.68E-6 1.80E-6 1.60E-6 2.98E-6 3.99E-7 2.82E-6	1.90E-5 6.25E-6 5.03E-6 1.50E-5 8.48E-6 1.19E-5	 > 1.00E-4 3.81E-5 2.62E-5 6.28E-5 > 1.00E-4 3.94E-5 	
Velanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.881 1.690 2.499 2.976 1.936 2.026 3.244 2.284 2.820	2.712 1.572 2.479 2.895 1.890 2.008 2.919 2.170 2.683	2.731 1.611 2.516 2.927 1.920 2.076 3.021 2.285 2.696	2.207 1.330 2.104 1.275 1.654 1.530 2.632 1.828 1.683	0.615 1.027 0.834 0.481 0.963 1.196 0.307 1.350 1.478	0.006 0.116 0.238 0.157 0.245 0.360 0.001 0.413 0.143	93 89 96 96 99 86 92 93	94 93 101 98 99 104 90 100 93	73 66 79 26 74 61 74 67 38	8 38 12 -29 10 35 -66 32 27	-99 -81 -60 -77 -71 -52 -100 -55 -85	2.26E-6 3.83E-6 2.73E-6 4.64E-7 2.38E-6 2.65E-6 1.48E-6 2.97E-6 6.14E-7	1.20E-5 2.09E-5 1.48E-5 2.98E-6 1.34E-5 2.52E-5 3.37E-6 2.31E-5 1.75E-5	3.52E-5 5.48E-5 7.19E-5 2.76E-5 5.50E-5 9.45E-5 7.68E-6 8.74E-5 4.85E-5	
Dvarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	2.077 1.986 1.919 1.600 1.912 1.353 1.831	1.940 1.931 1.857 1.638 1.782 1.312 1.750	1.976 1.942 1.890 1.619 1.963 1.357 1.814	1.524 1.769 1.688 1.497 1.735 0.830 1.684	0.650 0.668 1.099 0.614 0.307 0.166 1.105	0.049 0.101 0.631 0.015 0.103 0.107 0.896	92 96 95 103 92 96 92	94 97 98 102 103 100 98	66 84 81 91 89 48 85	13 32 14 -9 -54 27	-89 -84 -12 -97 -70 -70 6	2.02E-6 2.63E-6 4.26E-6 3.43E-6 2.49E-6 8.97E-7 4.01E-6 >	1.34E-5 1.09E-5 5.38E-5 1.35E-5 8.11E-6 2.95E-6 1.00E-4	4.15E-5 4.07E-5 > 1.00E-4 3.80E-5 4.76E-5 9.20E-6 > 1.00E-4	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	3.052 2.193 1.749 1.770 1.441 2.207 2.110 2.085	2.891 2.083 1.674 1.656 1.410 2.014 2.034 1.820	2.949 2.138 1.797 1.692 1.429 2.129 2.100 1.851	2.814 1.965 1.258 1.123 1.201 1.958 2.161 1.465	1.432 1.733 0.532 0.833 0.739 0.776 1.490 0.931	0.762 0.171 0.152 0.191 0.297 0.021 0.584 0.410	93 89 94 91 96 88 93 81	95 94 103 94 98 95 99 83	90 77 64 49 65 84 105 56	29 53 11 26 -2 9 40 19	-2 -86 -59 -61 -60 -97 -46 -38	4.48E-6 1.05E-5 1.86E-6 9.61E-7 1.69E-6 2.86E-6 6.92E-6 1.48E-6	8.61E-5 2.41E-5 1.45E-5 2.00E-5 9.48E-6 1.22E-5 2.89E-5 2.13E-5	> 1.00E-4 5.52E-5 7.38E-5 7.42E-5 6.64E-5 3.62E-5 > 1.00E-4	
Prostate Cancer PC-3 DU-145	0.562 0.375	2.181 1.649	2.049 1.644	2.057 1.650	1.718 1.583	0.749 0.487	0.310 0.033	92 100	92 100	71 95	12 9	-45 -91	2.28E-6 3.32E-6	1.60E-5 1.22E-5	> 1.00E-4 3.87E-5	
3reast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.450 C 0.566 1.374 1.398 0.747 0.773	2.394 1.142 2.573 2.810 2.058 1.481	2.188 1.130 2.412 2.784 1.841 1.456	2.245 1.146 2.457 2.689 1.805 1.465	1.642 1.106 2.017 2.522 1.831 1.262	0.473 0.507 1.496 1.748 1.144 0.615	0.240 0.078 1.048 0.888 0.697 0.210	89 98 87 98 83 96	92 101 90 91 81 98	61 94 54 80 83 69	1 -11 10 25 30 -20	-47 -86 -24 -36 -7 -73	1.54E-6 2.63E-6 1.21E-6 3.47E-6 4.20E-6 1.63E-6	1.06E-5 7.93E-6 2.00E-5 2.54E-5 6.57E-5 5.91E-6	 > 1.00E-4 3.32E-5 > 1.00E-4 > 1.00E-4 > 1.00E-4 3.66E-5 	

Compound 3j



NSC : D - 845426 / 1					Exp	erimer	nt ID:2	310NS86			Test	Test Type : 08		Units : Molar		
Report Date : November 08, 2023					Tes	Test Date : October 02, 2023							QNS :		MC :	
COMI : TO56					Stai	in Rea	gent : S	RB Dual-	Pass I	Related	SSF	PL : 1CXF				
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	Log10 Concentration n Optical Densities Percent Growth -6.0 -5.0 -4.0 -8.0 -7.0 -6.0 -5.0							-4.0	GI50	TGI	LC50	
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.563 0.776 0.221 0.609 0.518 0.364	2.634 2.697 1.759 2.259 2.021 1.688	2.801 2.553 1.600 2.261 2.067 1.609	2.680 2.438 1.680 2.078 2.029 1.580	2.095 2.147 1.465 1.999 1.801 1.013	0.797 0.383 0.156 0.474 0.503 0.248	0.457 0.387 0.096 0.241 0.450 0.225	108 92 90 100 103 94	102 87 95 89 101 92	74 71 81 84 85 49	11 -51 -30 -22 -3 -32	-19 -50 -57 -60 -13 -38	2.41E-6 1.50E-6 1.90E-6 2.10E-6 2.52E-6 9.48E-7	2.37E-5 3.85E-6 5.39E-6 6.19E-6 9.27E-6 4.04E-6	 > 1.00E-4 9.88E-6 5.71E-5 5.34E-5 > 1.00E-4 > 1.00E-4 	
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H227 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.333 1.086 0.559 1.079 1.191 0.621 0.862 0.359 1.404	1.992 2.483 1.632 1.656 2.315 2.299 2.098 2.288 3.169	1.796 2.365 1.555 1.659 2.171 2.261 1.928 2.293 3.014	1.668 2.475 1.654 1.738 2.273 2.278 2.069 2.415 3.070	1.616 2.472 1.445 1.643 2.195 2.139 1.941 2.343 2.907	0.564 1.431 0.658 1.225 1.288 0.741 1.327 0.232 1.217	0.082 0.076 0.161 0.294 0.161 0.133 0.106 0.088 0.225	88 92 93 101 87 98 86 100 91	80 99 102 114 96 99 98 107 94	77 99 83 98 89 90 87 103 85	14 25 9 25 9 7 38 -35 -13	-76 -93 -71 -73 -87 -79 -88 -76 -84	2.70E-6 4.57E-6 2.78E-6 3.07E-6 3.06E-6 5.63E-6 2.41E-6 2.27E-6	1.43E-5 1.62E-5 1.30E-5 1.81E-5 1.23E-5 1.21E-5 2.00E-5 5.55E-6 7.32E-6	5.18E-5 4.31E-5 5.44E-5 5.86E-5 4.13E-5 4.64E-5 5.00E-5 2.31E-5 3.30E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.503 0.853 0.349 0.382 0.257 0.611 0.402	1.916 3.101 2.690 2.806 1.628 2.536 1.887	1.990 2.692 2.490 2.609 1.566 2.386 1.843	2.062 3.081 2.546 2.714 1.643 2.454 2.055	1.867 3.029 2.545 2.587 1.674 2.217 1.734	0.398 0.500 0.364 0.460 0.191 0.529 0.614	0.201 0.137 0.083 0.110 0.050 0.107 0.167	105 82 91 92 95 92 97	110 99 94 96 101 96 111	96 97 94 91 103 83 90	-21 -41 1 3 -26 -13 14	-60 -84 -76 -71 -81 -82 -59	2.49E-6 2.18E-6 2.95E-6 2.93E-6 2.59E-6 2.59E-6 3.36E-6	6.64E-6 5.02E-6 1.02E-5 1.10E-5 6.31E-6 7.27E-6 1.57E-5	5.52E-5 1.59E-5 4.56E-5 5.19E-5 2.75E-5 3.39E-5 7.62E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.763 1.288 0.714 0.850 0.927 0.268	2.102 3.174 2.364 2.289 1.323 1.411	1.973 3.021 2.245 2.247 1.241 1.348	2.033 3.059 2.303 2.210 1.294 1.360	1.759 3.012 2.274 2.116 1.135 1.257	0.851 1.018 0.492 1.281 0.796 0.276	0.165 0.054 0.024 0.080 0.196 0.047	90 92 93 97 79 94	95 94 96 94 93 96	74 91 95 88 53 87	7 -21 -31 30 -14 1	-78 -96 -97 -91 -79 -83	2.29E-6 2.34E-6 2.26E-6 4.51E-6 1.09E-6 2.66E-6	1.19E-5 6.51E-6 5.66E-6 1.77E-5 6.13E-6 1.02E-5	4.63E-5 2.44E-5 1.94E-5 4.61E-5 3.58E-5 4.06E-5	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.464 0.739 0.494 0.751 1.244 0.803 1.062 1.089 1.130	2.625 1.616 1.745 2.235 2.506 2.344 3.058 2.575 3.011	2.449 1.519 1.749 2.170 2.474 2.290 2.481 2.389 2.856	2.506 1.557 1.718 2.180 2.489 2.359 2.509 2.395 2.888	2.278 1.411 1.480 1.544 2.382 1.949 2.434 2.162 2.624	0.650 1.113 0.527 0.444 1.247 1.380 0.534 1.342 1.434	0.060 0.129 0.137 0.114 0.036 0.042 0.045 0.253 0.125	92 89 100 96 97 96 71 87 92	94 93 98 96 99 101 72 88 93	84 77 53 90 74 69 72 79	9 43 3 -41 0 37 -50 17 16	-87 -83 -72 -85 -97 -95 -96 -77 -89	2.82E-6 6.06E-6 2.39E-6 2.80E-6 4.56E-6 4.56E-6 2.53E-6 2.53E-6 2.92E-6	1.23E-5 2.19E-5 1.08E-5 3.68E-6 1.01E-5 1.92E-5 3.80E-6 1.52E-5 1.42E-5	4.09E-5 5.49E-5 5.03E-5 1.61E-5 3.28E-5 4.58E-5 1.01E-5 5.18E-5 4.26E-5	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.598 0.648 0.950 0.593 0.526 0.585 0.720	1.926 1.874 2.034 1.544 2.370 2.074 1.567	2.126 1.815 1.935 1.408 2.315 2.026 1.596	1.940 1.957 2.036 1.453 2.379 2.086 1.607	1.939 1.736 1.852 1.410 2.271 1.896 1.577	0.795 0.460 0.861 0.829 0.398 0.295 0.916	0.103 0.088 0.149 0.039 0.039 0.164 0.085	115 95 91 86 97 97 103	101 107 100 90 101 101 105	101 89 83 86 95 88 101	15 -29 -9 25 -24 -50 23	-83 -86 -84 -93 -93 -72 -88	3.91E-6 2.13E-6 2.28E-6 3.87E-6 2.37E-6 1.89E-6 4.53E-6	1.42E-5 5.66E-6 7.91E-6 1.62E-5 6.23E-6 4.36E-6 1.61E-5	4.61E-5 2.31E-5 3.48E-5 4.29E-5 2.37E-5 1.04E-5 4.53E-5	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10	0.686 1.481 0.349 0.581 1.053 0.543 1.244	2.574 2.247 1.729 1.985 1.825 2.056 2.057	2.569 2.121 1.719 1.827 1.696 1.875 1.921	2.582 2.154 1.812 1.763 1.725 1.935 2.017	2.511 2.147 1.602 1.392 1.533 1.878 2.161	0.807 1.630 0.540 0.733 0.754 0.499 1.572	0.135 0.156 -0.001 0.062 0.090 0.064 0.056	100 84 99 83 83 88 83	100 88 106 84 87 92 95	97 87 91 58 62 88 113	6 19 14 11 -28 -8 40	-80 -89 -100 -89 -92 -88 -96	3.29E-6 3.53E-6 3.39E-6 1.46E-6 1.36E-6 2.49E-6 7.35E-6	1.18E-5 1.51E-5 1.32E-5 1.28E-5 4.86E-6 8.24E-6 1.98E-5	4.47E-5 4.34E-5 3.64E-5 4.05E-5 2.20E-5 3.33E-5 4.62E-5	
Prostate Cancer PC-3 DU-145	0.515 0.361	2.002 1.577	2.008 1.521	1.936 1.526	1.881 1.559	0.799 0.469	0.281 0.008	100 95	96 96	92 99	19 9	-46 -98	3.76E-6 3.48E-6	1.97E-5 1.21E-5	> 1.00E-4 3.56E-5	
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.544 C 0.605 1.372 1.308 0.798 1.202	2.461 1.235 2.322 2.211 1.803 2.268	2.250 1.212 2.152 2.122 1.655 2.256	2.267 1.246 2.256 2.342 1.736 2.261	2.230 1.202 2.163 2.067 1.677 2.239	0.577 0.583 1.293 1.127 0.866 0.923	0.152 0.087 0.737 0.120 0.370 0.084	89 96 82 90 85 99	90 102 93 114 93 99	88 95 83 84 87 97	2 -4 -6 -14 7 -23	-72 -86 -46 -91 -54 -93	2.76E-6 2.85E-6 2.23E-6 2.23E-6 2.91E-6 2.47E-6	1.06E-5 9.18E-6 8.61E-6 7.22E-6 1.29E-5 6.42E-6	5.02E-5 3.68E-5 > 1.00E-4 2.95E-5 8.69E-5 2.42E-5	

Compound 3n



NSC : D - 845425 / 1					Exp	erimer	nt ID : 2	310NS86			Tes	Test Type : 08		Units : Molar		
Report Date : November 08, 2023					Test Date : October 02, 2023								QNS :		MC :	
COMI : TO54					Stai	in Rea	gent : S	RB Dual-	Pass	Related	SSF	PL : 1CXF				
Time Mea Panel/Cell Line Zero Ctrl -8.0 -7.0						Log10 Concentration n Optical Densities Percent Growth -6.0 -5.0 -4.0 -8.0 -7.0 -6.0 -5.0							GI50	TGI	LC50	
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.563 0.776 0.221 0.609 0.518 0.364	2.580 2.567 1.286 2.053 1.951 1.347	2.569 2.427 1.399 2.031 2.110 1.314	2.779 2.438 1.390 1.653 1.957 1.199	2.436 2.380 0.854 1.594 2.114 0.633	0.828 0.310 0.154 0.393 0.769 0.244	0.629 0.286 0.085 0.114 0.505 0.139	99 92 111 98 111 97	110 93 110 72 100 85	93 90 59 68 111 27	13 -60 -30 -35 17 -33	3 -63 -62 -81 -3 -62	3.45E-6 > 1.84E-6 1.27E-6 1.50E-6 4.50E-6 4.05E-7	1.00E-4 3.97E-6 4.60E-6 4.55E-6 7.49E-5 2.84E-6	 > 1.00E-4 8.56E-6 4.27E-5 2.08E-5 > 1.00E-4 3.89E-5 	
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H226 NCI-H222 NCI-H322M NCI-H460 NCI-H522	Cancer 0.333 1.086 0.559 1.079 1.191 0.621 0.862 0.359 1.404	1.903 2.487 1.541 1.763 2.326 2.296 2.331 2.328 2.894	1.865 2.392 1.572 1.728 2.301 2.250 2.236 2.167 2.796	1.779 2.371 1.563 1.680 2.251 2.257 2.274 2.164 2.751	1.841 2.425 1.377 1.651 2.091 2.097 2.099 2.217 2.354	0.614 1.696 0.757 1.360 1.464 0.686 1.749 0.297 1.355	0.358 0.882 0.205 0.929 0.511 0.249 0.754 0.137 0.507	98 93 103 95 98 97 94 92 93	92 92 102 88 93 98 96 92 90	96 96 83 84 79 88 84 94 64	18 44 20 41 24 4 60 -17 -3	2 -19 -63 -14 -57 -60 -13 -62 -64	3.88E-6 > 7.51E-6 3.36E-6 6.14E-6 3.39E-6 2.83E-6 1.39E-5 2.49E-6 1.60E-6	1.00E-4 4.99E-5 1.74E-5 5.57E-5 1.98E-5 1.15E-5 6.73E-5 6.99E-6 8.87E-6	 > 1.00E-4 > 1.00E-4 6.92E-5 > 1.00E-4 8.17E-5 6.98E-5 > 1.00E-4 5.41E-5 5.88E-5 	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.503 0.853 0.349 0.382 0.257 0.611 0.402	1.914 3.119 2.741 2.735 1.694 2.688 1.952	1.943 2.988 2.695 2.557 1.676 2.618 1.835	1.900 2.953 2.692 2.537 1.658 2.622 1.844	1.940 2.956 2.446 2.287 1.702 2.315 1.670	0.487 0.639 0.421 0.543 0.199 0.880 0.710	0.077 0.304 0.135 0.210 0.079 0.089 0.360	102 94 98 92 99 97 92	99 93 98 92 97 97 93	102 93 88 81 101 82 82	-3 -25 3 7 -23 13 20	-85 -64 -61 -45 -69 -85 -11	3.12E-6 2.31E-6 2.79E-6 2.62E-6 2.57E-6 2.91E-6 3.26E-6	9.33E-6 6.12E-6 1.11E-5 1.35E-5 6.54E-6 1.35E-5 4.50E-5	3.75E-5 4.29E-5 6.67E-5 > 1.00E-4 3.83E-5 4.36E-5 > 1.00E-4	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.763 1.288 0.714 0.850 0.927 0.268	2.115 3.130 2.410 2.368 1.458 1.411	2.029 3.053 2.247 2.243 1.456 1.347	1.952 3.040 2.250 2.209 1.448 1.366	1.803 2.511 2.123 2.097 1.167 1.308	0.894 1.143 0.630 1.449 0.961 0.355	0.421 0.129 0.128 0.687 0.436 0.122	94 96 90 92 100 94	88 95 91 89 98 96	77 66 83 82 45 91	10 -11 -12 39 6 8	-45 -90 -82 -19 -53 -54	2.51E-6 1.63E-6 2.23E-6 5.66E-6 8.09E-7 3.10E-6	1.50E-5 7.16E-6 7.50E-6 4.71E-5 1.28E-5 1.33E-5	 > 1.00E-4 3.10E-5 3.49E-5 > 1.00E-4 8.89E-5 8.47E-5 	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.464 0.739 0.494 0.751 1.244 0.803 1.062 1.089 1.130	2.633 1.671 1.782 2.341 2.432 2.295 3.211 2.637 3.072	2.535 1.638 1.710 2.236 2.438 2.320 3.097 2.563 2.950	2.550 1.608 1.660 2.258 2.392 2.212 2.887 2.519 2.890	2.204 1.473 1.391 1.059 2.257 1.825 2.516 2.384 2.048	0.854 1.262 0.502 0.527 1.319 1.474 0.687 1.996 1.582	0.178 0.498 0.188 0.324 0.299 0.494 0.010 0.514 0.363	95 96 94 93 101 102 95 95 94	96 93 91 95 97 94 85 92 91	80 79 70 19 85 68 68 84 47	18 56 1 -30 6 45 -35 59 23	-62 -33 -62 -57 -76 -39 -99 -53 -68	3.06E-6 1.17E-5 1.92E-6 3.92E-7 2.80E-6 6.10E-6 1.19E-5 8.64E-7	1.68E-5 4.29E-5 1.02E-5 2.47E-6 1.19E-5 3.45E-5 4.54E-6 3.36E-5 1.80E-5	7.12E-5 > 1.00E-4 6.42E-5 5.54E-5 4.83E-5 > 1.00E-4 1.70E-5 9.44E-5 6.37E-5	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.598 0.648 0.950 0.593 0.526 0.585 0.720	2.066 1.918 2.156 1.464 2.524 2.053 1.622	2.049 1.882 2.152 1.400 2.428 2.047 1.692	2.191 1.832 2.086 1.363 2.410 2.008 1.701	2.059 1.767 1.931 1.382 2.319 1.838 1.602	1.179 0.618 1.122 0.918 0.577 0.354 1.031	0.359 0.183 0.516 0.511 0.104 0.288 0.473	99 97 100 93 95 100 108	109 93 94 88 94 97 109	99 88 81 91 90 85 98	40 -5 14 37 3 -39 34	-40 -72 -46 -14 -80 -51 -34	6.69E-6 2.57E-6 2.93E-6 5.78E-6 2.86E-6 1.92E-6 5.68E-6	3.14E-5 8.90E-6 1.73E-5 5.37E-5 1.07E-5 4.83E-6 3.17E-5	 > 1.00E-4 4.74E-5 > 1.00E-4 > 4.31E-5 8.41E-5 > 1.00E-4 	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10	0.686 1.481 0.349 0.581 1.053 0.543 1.244	2.622 2.269 1.700 2.043 1.744 2.017 2.111	2.576 2.216 1.679 1.903 1.693 1.948 2.008	2.490 2.158 1.654 1.933 1.633 1.902 2.035	2.414 2.071 1.622 1.406 1.415 1.804 2.161	0.747 1.713 0.715 0.831 0.575 0.749 1.688	0.306 0.403 0.194 0.318 0.285 0.234 1.044	98 93 98 90 93 95 88	93 86 97 92 84 92 91	89 75 94 56 52 86 106	3 29 27 17 -45 14 51	-55 -73 -44 -45 -73 -57 -16	2.86E-6 3.53E-6 4.56E-6 1.46E-6 1.06E-6 3.14E-6 1.04E-5	1.13E-5 1.94E-5 2.39E-5 1.88E-5 3.43E-6 1.57E-5 5.76E-5	8.07E-5 5.99E-5 > 1.00E-4 > 1.00E-4 1.47E-5 7.97E-5 > 1.00E-4	
Prostate Cancer PC-3 DU-145	0.515 0.361	2.026 1.568	1.965 1.594	2.011 1.530	1.760 1.538	0.849 0.533	0.584 0.351	96 102	99 97	82 97	22 14	5 -3	3.44E-6 > 3.72E-6	1.00E-4 6.87E-5	> 1.00E-4 > 1.00E-4	
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.544 C 0.605 1.372 1.308 0.798 1.202	2.358 1.214 2.393 2.255 1.842 2.316	2.268 1.242 2.286 2.364 1.758 2.296	2.229 1.221 2.239 2.219 1.707 2.229	1.983 1.255 1.892 2.047 1.692 2.066	0.620 0.748 1.254 1.334 0.935 1.022	0.236 0.264 0.867 0.414 0.718 0.543	95 105 89 112 92 98	93 101 85 96 87 92	79 107 51 78 86 78	4 23 -9 3 13 -15	-57 -56 -37 -68 -10 -55	2.46E-6 4.81E-6 1.04E-6 2.36E-6 3.10E-6 1.98E-6	1.17E-5 1.97E-5 7.16E-6 1.09E-5 3.69E-5 6.89E-6	7.78E-5 8.32E-5 > 1.00E-4 5.52E-5 > 1.00E-4 7.55E-5	

Compound 3p





NSC : D - 845422 / 1					Exp	erimer	nt ID : 2	310NS86	U		Tes	Test Type : 08		Units : Molar		
Report Date : November 08, 2023					Test Date : October 02, 2023								QNS :		MC :	
COMI : TO51					Stai	n Reag	gent : S	RB Dual-	Pass I	Related	SSF	SSPL : 1CXF				
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	Optical	Log10 Concentration Optical Densities Percent Growth -6.0 -5.0 -4.0 -8.0 -7.0 -6.0 -5.0							GI50	TGI	LC50	
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.563 0.776 0.221 0.609 0.518 0.364	2.758 3.017 1.956 2.570 2.017 1.925	2.656 2.906 1.874 2.626 2.052 1.849	2.649 2.881 1.830 2.488 1.979 1.656	0.950 1.164 0.511 1.258 0.918 0.724	0.755 0.523 0.291 0.680 0.610 0.502	0.429 0.572 0.191 0.322 0.704 0.328	95 95 103 102 95	95 94 93 96 97 83	18 17 17 33 27 23	9 -33 4 4 6 9	-24 -26 -14 -47 12 -10	3.82E-7 3.74E-7 3.65E-7 5.37E-7 4.68E-7 > 3.54E-7	1.86E-5 2.22E-6 1.69E-5 1.18E-5 1.00E-4 2.94E-5	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4	
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H226 NCI-H322M NCI-H460 NCI-H522	Cancer 0.333 1.086 0.559 1.079 1.191 0.621 0.862 0.359 1.404	1.973 2.585 1.486 1.806 2.375 2.395 2.192 2.328 3.221	1.891 2.500 1.458 1.784 2.361 2.322 2.223 2.414 3.183	1.847 2.477 1.473 1.650 2.288 2.266 2.487 2.425 3.124	1.470 2.401 0.897 1.550 1.984 1.654 2.320 0.692 2.070	0.561 1.627 0.590 1.126 1.462 0.748 1.607 0.268 0.935	0.053 0.062 0.078 0.247 0.171 0.019 0.088 0.135 0.153	95 94 97 99 96 102 104 98	92 93 99 79 93 93 122 105 95	69 88 65 67 58 110 17 37	14 36 3 6 23 7 56 -25 -33	-84 -94 -77 -86 -97 -90 -63 -89	2.23E-6 5.37E-6 6.06E-7 1.79E-6 2.43E-6 1.45E-6 1.10E-5 4.21E-7 5.88E-7	1.39E-5 1.89E-5 1.09E-5 1.19E-5 1.62E-5 1.17E-5 2.42E-5 2.51E-6 3.33E-6	4.49E-5 4.57E-5 3.95E-5 4.73E-5 3.54E-5 3.54E-5 5.33E-5 4.59E-5 1.98E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.503 0.853 0.349 0.382 0.257 0.611 0.402	1.750 3.103 2.429 2.828 1.855 2.750 2.243	1.798 3.055 2.457 2.600 1.858 2.850 1.879	1.724 3.076 2.391 2.626 1.901 2.650 1.743	1.438 2.496 0.831 1.323 0.760 1.749 0.682	0.188 0.595 0.346 0.544 0.250 0.728 0.665	0.021 0.018 0.022 0.016 0.061 0.011 0.082	104 98 101 91 100 105 80	98 99 98 92 103 95 73	75 73 23 38 31 53 15	-63 -30 0 7 -3 5 14	-96 -98 -94 -96 -76 -98 -80	1.52E-6 1.67E-6 4.39E-7 6.07E-7 5.50E-7 1.17E-6 2.49E-7	3.50E-6 5.09E-6 9.21E-6 1.16E-5 8.32E-6 1.13E-5 1.42E-5	8.08E-6 1.96E-5 3.38E-5 3.57E-5 4.39E-5 3.42E-5 4.84E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.763 1.288 0.714 0.850 0.927 0.268	2.193 3.156 2.368 2.354 1.395 1.457	2.158 3.093 2.248 2.248 1.363 1.434	2.026 2.993 2.249 2.125 1.393 1.367	1.608 1.741 1.049 1.961 1.053 0.860	0.831 1.205 0.625 1.275 0.942 0.369	0.152 0.027 0.028 0.030 0.145 0.027	98 97 93 93 93 98	88 91 93 85 100 92	59 24 20 74 27 50	5 -6 -12 28 3 8	-80 -98 -96 -97 -84 -90	1.47E-6 4.13E-7 3.89E-7 3.34E-6 4.82E-7 9.87E-7	1.14E-5 6.15E-6 4.16E-6 1.68E-5 1.09E-5 1.22E-5	4.42E-5 2.99E-5 2.81E-5 4.24E-5 4.05E-5 3.92E-5	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.464 0.739 0.494 0.751 1.244 0.803 1.062 1.089 1.130	2.822 1.684 1.647 2.257 2.524 2.340 3.258 2.733 3.075	2.647 1.611 2.271 2.563 2.289 2.937 2.638 2.922	2.441 1.621 1.613 2.208 2.475 2.199 2.946 2.654 2.820	1.325 1.336 0.947 0.606 2.137 1.701 2.176 2.171 1.724	0.670 1.092 0.594 0.663 1.393 1.331 0.462 1.645 1.562	0.013 0.154 0.027 0.057 0.026 0.019 0.004 0.122 0.048	93 92 96 101 103 97 85 94 92	84 93 97 96 91 86 95 87	37 63 39 -19 70 58 51 66 31	9 37 9 -12 12 34 -57 34 22	-97 -79 -95 -92 -98 -100 -89 -96	5.19E-7 3.23E-6 6.52E-7 2.53E-7 2.18E-6 2.24E-6 1.02E-6 3.12E-6 4.51E-7	1.21E-5 2.09E-5 1.21E-5 6.81E-7 1.28E-5 1.82E-5 2.97E-6 1.89E-5 1.54E-5	3.58E-5 5.62E-5 3.70E-5 2.98E-5 3.65E-5 8.69E-6 4.82E-5 4.09E-5	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.598 0.648 0.950 0.593 0.526 0.585 0.720	2.205 1.970 2.012 1.433 2.558 2.176 1.462	2.158 1.952 2.027 1.366 2.488 2.172 1.556	2.049 1.963 1.958 1.313 2.448 2.144 1.488	1.468 1.124 1.385 1.168 1.555 0.541 1.270	1.081 0.756 0.982 0.830 0.477 0.313 0.889	0.273 0.006 0.071 0.003 0.116 0.215 0.058	97 99 101 92 97 100 113	90 99 95 86 95 98 103	54 36 41 68 51 -8 74	30 8 3 28 -9 -46 23	-54 -99 -93 -100 -78 -63 -92	1.48E-6 6.02E-7 6.79E-7 2.87E-6 1.02E-6 2.85E-7 2.95E-6	2.27E-5 1.19E-5 1.07E-5 1.66E-5 6.97E-6 8.49E-7 1.58E-5	8.88E-5 3.48E-5 3.59E-5 4.09E-5 3.90E-5 1.62E-5 4.30E-5	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10	0.686 1.481 0.349 0.581 1.053 0.543 1.244	2.451 2.327 1.710 2.010 1.801 2.105 2.251	2.353 2.302 1.779 1.869 1.789 2.032 2.137	2.393 2.200 1.694 1.750 1.697 2.018 2.139	1.482 2.048 1.077 1.010 1.258 1.399 2.209	0.850 1.701 0.607 0.597 1.130 0.601 1.882	0.090 0.108 -0.001 0.040 0.129 0.047 0.102	94 97 105 90 98 95 89	97 85 99 82 86 94 89	45 67 53 30 27 55 96	9 26 19 1 10 4 63	-87 -93 -100 -93 -88 -91 -92	8.03E-7 2.60E-6 1.26E-6 4.11E-7 4.11E-7 1.24E-6 1.22E-5	1.25E-5 1.66E-5 1.44E-5 1.03E-5 1.27E-5 1.09E-5 2.56E-5	4.14E-5 4.37E-5 3.80E-5 3.49E-5 4.12E-5 3.67E-5 5.38E-5	
Prostate Cancer PC-3 DU-145	0.515 0.361	2.183 1.801	2.122 1.758	2.033 1.697	1.398 1.333	0.795 0.383	0.217 0.003	96 97	91 93	53 67	17 2	-58 -99	1.20E-6 1.84E-6	1.68E-5 1.04E-5	7.85E-5 3.25E-5	
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.544 0.605 1.372 1.308 0.798 1.202	2.513 1.261 2.418 2.241 1.703 2.446	2.311 1.237 2.276 2.167 1.590 2.403	2.349 1.190 2.161 2.237 1.550 2.318	0.972 1.070 1.546 1.910 1.371 1.793	0.710 0.656 1.355 1.106 1.054 1.163	0.052 0.129 0.669 0.109 0.218 0.124	90 96 86 92 88 97	92 89 75 100 83 90	22 71 17 65 63 48	8 -1 -15 28 -3	-90 -79 -51 -92 -73 -90	3.94E-7 2.14E-6 2.70E-7 1.52E-6 2.40E-6 8.73E-7	1.22E-5 1.23E-5 8.49E-6 6.41E-6 1.90E-5 8.63E-6	3.90E-5 4.66E-5 9.43E-5 2.84E-5 5.96E-5 3.47E-5	
Compound **3q**





									·9 · ·	00011					
NSC : D - 845	5423 / 1				Exp	erimer	nt ID : 2	310NS86	c.			Test	Туре : 08	Units : I	Molar
Report Date :	Novem	oer 08, 2	2023		Tes	t Date	: Octob	er 02, 20	23			QNS	:	MC :	
COMI : TO52					Sta	n Rea	gent : S	RB Dual-	Pass F	Related	ł	SSPI	L : 1CXF		
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	n Optica -6.0	Lo Densiti -5.0	og10 Con es -4.0	centration -8.0	P -7.0	ercent G -6.0	Frowth -5.0	-4.0	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.563 0.776 0.221 0.609 0.518 0.364	2.708 2.875 1.937 2.640 2.210 1.896	2.666 2.780 1.939 2.583 2.295 1.922	2.625 2.783 1.820 2.408 2.169 1.646	1.529 1.589 0.560 1.449 1.691 0.797	1.125 0.762 0.436 1.055 1.117 0.662	0.884 0.641 0.399 0.629 0.959 0.512	98 95 100 97 105 102	96 93 89 98 84	45 39 20 41 69 28	26 -2 13 22 35 19	15 -17 10 1 26 10	7.99E-7 6.33E-7 3.87E-7 6.57E-7 3.71E-6 4.05E-7	 > 1.00E-4 8.99E-6 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Non-Small Cell Lun A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H226 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.333 1.086 0.559 1.079 1.191 0.621 0.862 0.359 1.404	2.100 2.450 1.609 1.815 2.391 2.299 2.366 2.348 2.984	2.009 2.409 1.636 1.816 2.341 2.294 2.406 2.136 2.885	1.885 2.350 1.648 1.764 2.230 2.157 2.465 2.069 2.847	1.271 2.319 1.106 1.654 1.885 1.654 2.068 0.684 2.086	1.056 2.023 0.890 1.462 1.708 1.181 1.729 0.455 1.718	0.653 1.837 0.423 1.236 1.475 0.514 1.556 0.303 1.829	95 97 103 100 96 100 103 89 94	88 93 104 93 87 92 107 86 91	53 90 52 78 58 62 80 16 43	41 69 31 52 43 33 58 5 20	18 55 -24 21 24 -17 46 -16 27	1.79E-6 > 1.00E-4 1.26E-6 1.16E-5 3.39E-6 2.57E-6 4.64E-5 3.28E-7 7.22E-7	 > 1.00E-4 > 1.00E-4 > 3.66E-5 > 1.00E-4 > 1.00E-4 4.57E-5 > 1.00E-4 1.72E-5 > 1.00E-4 	 > 1.00E-4
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.503 0.853 0.349 0.382 0.257 0.611 0.402	1.910 3.130 2.790 2.718 1.732 2.721 1.969	1.830 2.982 2.796 2.592 1.619 2.696 1.806	1.929 2.768 2.800 2.497 1.830 2.679 1.825	1.275 2.152 1.019 1.149 0.585 1.799 0.723	0.629 1.867 0.864 0.829 0.299 0.870 0.569	0.384 1.289 0.432 0.590 0.236 0.734 0.413	94 94 100 95 92 99 90	101 84 100 91 107 98 91	55 57 27 33 22 56 20	9 45 21 19 3 12 11	-24 19 3 9 -8 6 1	1.28E-6 3.66E-6 4.91E-7 5.04E-7 4.69E-7 1.39E-6 3.80E-7	1.88E-5 > 1.00E-4 > 1.00E-4 > 1.00E-4 1.79E-5 > 1.00E-4 > 1.00E-4	 > 1.00E-4
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.763 1.288 0.714 0.850 0.927 0.268	2.146 3.165 2.257 2.342 1.613 1.484	2.084 3.078 2.250 2.265 1.470 1.446	2.026 2.980 2.136 2.156 1.486 1.399	1.383 2.032 1.425 1.864 0.922 0.710	1.111 1.448 0.921 1.527 0.873 0.462	0.920 1.034 0.683 0.961 0.788 0.097	96 95 100 95 79 97	91 90 92 88 82 93	45 40 46 68 0 36	25 8 13 45 -6 16	11 -20 -4 7 -15 -64	7.74E-7 6.23E-7 8.22E-7 6.25E-6 2.42E-7 5.74E-7	 > 1.00E-4 2.00E-5 5.70E-5 > 1.00E-4 9.85E-7 1.58E-5 	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 6.68E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.464 0.739 0.494 0.751 1.244 0.803 1.062 1.089 1.130	2.632 1.684 1.802 2.268 2.432 2.435 3.271 2.793 3.089	2.545 1.745 1.739 2.264 2.469 2.365 3.081 2.661 2.959	2.372 1.702 1.736 2.210 2.440 2.235 3.010 2.540 2.872	1.357 1.169 0.961 0.492 1.885 1.586 1.990 2.124 1.829	1.021 0.930 0.606 0.369 1.469 1.336 0.900 1.681 1.619	0.657 1.019 0.439 0.228 1.075 0.967 0.463 1.326 1.212	96 106 95 100 103 96 91 92 93	88 102 95 96 101 88 88 85 89	41 45 36 -34 54 48 42 61 36	26 20 9 -51 19 33 -15 35 25	9 30 -11 -70 -14 10 -56 14 4	6.47E-7 8.30E-7 5.74E-7 2.26E-7 1.30E-6 8.90E-7 6.71E-7 2.58E-6 5.38E-7	 > 1.00E-4 > 1.00E-4 2.70E-5 5.45E-7 3.82E-5 > 1.00E-4 5.41E-6 > 1.00E-4 > 1.00E-4 > 1.00E-4 	> 1.00E-4 > 1.00E-4 > 1.00E-4 8.78E-6 > 1.00E-4 6.99E-5 > 1.00E-4 > 1.00E-4
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.598 0.648 0.950 0.593 0.526 0.585 0.720	2.230 1.924 2.239 1.490 2.519 2.090 1.685	2.372 2.001 2.234 1.365 2.436 2.080 1.653	2.509 1.859 2.140 1.314 2.374 2.021 1.651	1.521 0.903 1.600 1.246 1.908 0.949 1.276	1.179 0.634 1.405 0.966 1.525 0.571 1.129	0.745 0.528 1.144 0.717 1.197 0.519 0.764	109 106 100 86 96 99 97	117 95 92 80 93 95 96	57 20 50 73 69 24 58	36 -2 35 42 50 -2 42	9 -19 15 14 34 -11 5	2.06E-6 3.97E-7 1.06E-6 5.37E-6 1.02E-5 4.34E-7 3.14E-6	 > 1.00E-4 7.93E-6 > 1.00E-4 > 1.00E-4 > 1.00E-4 8.13E-6 > 1.00E-4 	 > 1.00E-4
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10	0.686 1.481 0.349 0.581 1.053 0.543 1.244	2.744 2.293 1.641 2.059 1.801 2.174 2.175	2.691 2.242 1.661 1.921 1.807 1.983 2.110	2.660 2.090 1.633 1.844 1.696 2.043 2.145	1.830 1.986 0.923 1.121 1.385 1.523 2.261	1.498 1.896 0.784 0.918 1.250 1.124 2.326	0.832 1.571 0.634 0.595 0.952 0.850 1.626	97 94 101 91 101 88 93	96 75 99 85 86 92 97	56 62 44 37 44 60 109	39 51 34 23 26 36 116	7 11 22 1 -10 19 41	2.21E-6 1.07E-5 7.91E-7 5.30E-7 7.34E-7 2.58E-6 7.60E-5	 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 5.39E-5 > 1.00E-4 > 1.00E-4 > 1.00E-4 	 > 1.00E-4
Prostate Cancer PC-3 DU-145	0.515	2.085	2.074	2.076	1.174	0.997	0.910	99 102	99 96	42 71	31	25 21	7.24E-7 3.87E-6	> 1.00E-4	> 1.00E-4
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.544 C 0.605 1.372 1.308 0.798 1.202	2.394 1.228 2.406 2.362 1.846 2.408	2.178 1.260 2.312 2.348 1.777 2.380	2.207 1.189 2.218 2.300 1.739 2.294	0.864 1.174 1.739 1.995 1.397 1.598	0.730 1.009 1.352 1.587 1.180 0.962	0.582 0.627 1.437 1.635 1.022 0.807	88 105 91 99 93 98	90 94 82 94 90 90	17 91 35 65 57 33	10 65 -1 26 36 -20	2 3 6 31 21 -33	3.54E-7 1.74E-5 4.86E-7 2.47E-6 2.21E-6 5.03E-7	 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 4.18E-6 	 > 1.00E-4

Compound 3r





NSC : D - 845430 / 1					Exp	Experiment ID : 2310NS86							: Туре : 08	Units : Molar	
Report Date :	Novem	oer 08, 2	2023		Tes	t Date	: Octob	oer 02, 20	23			QNS	S :	MC :	
COMI : TO59					Stain Reagent : SRB Dual-Pass Related							SSP	SSPL : 1CXF		
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	n Optica -6.0	Lo I Densiti -5.0	og10 Cor es -4.0	ncentration -8.0	P -7.0	ercent G -6.0	rowth -5.0	-4.0	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.563 0.776 0.221 0.609 0.518 0.364	2.779 3.029 1.956 2.594 2.030 1.947	2.115 2.865 1.955 2.628 2.082 1.747	2.363 2.889 1.967 2.302 2.134 1.755	2.024 2.824 1.665 2.184 1.768 1.586	0.743 0.608 0.323 0.595 0.623 0.325	0.448 0.605 0.275 0.473 0.433 0.289	70 93 100 102 103 87	81 94 101 85 107 88	66 91 83 79 83 77	8 -22 6 -2 7 -11	-21 -22 3 -22 -17 -21	1.89E-6 2.31E-6 2.69E-6 > 2.29E-6 2.70E-6 2.04E-6	1.92E-5 6.42E-6 1.00E-4 9.37E-6 1.97E-5 7.55E-6	 > 1.00E-4
Non-Small Cell Lun A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H227 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.333 1.086 0.559 1.079 1.191 0.621 0.862 0.359 1.404	1.973 2.587 1.521 1.834 2.429 2.422 2.225 2.009 3.221	1.946 2.479 1.569 1.796 2.293 2.372 2.032 2.180 3.106	1.897 2.577 1.508 1.779 2.422 2.399 2.151 2.192 3.142	1.860 2.528 1.480 1.724 2.339 2.283 2.167 1.891 3.053	0.458 1.208 0.296 1.043 1.423 0.524 1.170 0.126 1.193	0.011 0.013 0.051 0.282 0.070 0.016 0.400 0.037 0.153	98 93 105 95 89 97 86 110 94	95 99 93 99 99 99 95 111 96	93 96 85 93 92 96 93 91	8 -47 -3 19 -16 23 -65 -15	-97 -99 -91 -74 -94 -98 -54 -90 -89	3.19E-6 3.34E-6 2.09E-6 2.51E-6 3.78E-6 2.46E-6 4.22E-6 1.87E-6 2.43E-6	1.18E-5 1.19E-5 4.68E-6 9.16E-6 1.46E-5 7.15E-6 1.98E-5 3.88E-6 7.21E-6	3.56E-5 3.49E-5 4.58E-5 4.06E-5 2.63E-5 8.95E-5 8.05E-6 2.96E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.503 0.853 0.349 0.382 0.257 0.611 0.402	1.733 3.141 2.419 2.771 1.740 2.642 1.794	1.806 3.078 2.257 2.567 1.714 2.660 1.742	1.925 3.069 2.354 2.660 1.830 2.707 1.788	1.696 3.028 2.254 2.518 1.703 2.407 1.630	0.147 0.660 0.177 0.330 0.048 0.326 0.268	0.021 0.083 0.041 -0.005 -0.008 0.021 0.031	106 97 92 91 98 101 96	116 97 95 106 103 100	97 95 92 89 98 88 88	-71 -23 -49 -14 -82 -47 -33	-96 -90 -88 -100 -100 -97 -92	1.90E-6 2.41E-6 1.98E-6 2.41E-6 1.84E-6 1.92E-6 2.06E-6	3.78E-6 6.42E-6 4.48E-6 7.38E-6 3.50E-6 4.51E-6 5.31E-6	7.51E-6 2.54E-5 1.04E-5 2.64E-5 6.67E-6 1.16E-5 1.91E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.763 1.288 0.714 0.850 0.927 0.268	2.242 3.190 2.357 2.362 1.404 1.494	2.010 2.989 2.290 2.218 1.320 1.401	2.102 3.039 2.325 2.211 1.387 1.433	1.971 3.070 2.287 2.163 1.359 1.297	0.743 0.956 0.910 1.128 0.661 0.154	0.048 0.003 -0.002 0.090 0.066 -0.003	84 89 96 91 82 92	91 92 98 90 96 95	82 94 96 87 91 84	-3 -26 12 18 -29 -43	-94 -100 -100 -89 -93 -100	2.37E-6 2.32E-6 3.51E-6 3.45E-6 2.19E-6 1.85E-6	9.29E-6 6.08E-6 1.28E-5 1.48E-5 5.75E-6 4.60E-6	3.31E-5 2.12E-5 3.57E-5 4.31E-5 2.15E-5 1.34E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.464 0.739 0.494 0.751 1.244 0.803 1.062 1.089 1.130	2.847 1.699 1.642 2.340 2.512 2.314 3.341 2.845 3.069	2.653 1.518 1.584 2.296 2.426 2.264 3.000 2.737 2.880	2.743 1.558 1.590 2.255 2.475 2.329 2.982 2.735 2.947	2.589 1.468 1.498 1.997 2.326 2.187 2.876 2.613 2.866	0.026 0.657 0.470 0.481 0.954 1.049 0.117 1.311 1.206	0.004 0.026 0.072 0.067 0.017 0.028 -0.007 0.227 0.114	92 81 95 97 93 97 85 94 90	96 85 95 97 101 84 94 94	89 76 87 78 85 92 80 87 90	-94 -11 -5 -36 -23 16 -89 13 4	-99 -97 -86 -91 -99 -97 -100 -79 -90	1.63E-6 1.99E-6 2.54E-6 2.11E-6 3.56E-6 3.56E-6 3.13E-6 2.90E-6	3.06E-6 7.44E-6 8.86E-6 4.84E-6 6.10E-6 1.39E-5 2.97E-6 1.37E-5 1.10E-5	5.73E-6 2.85E-5 3.63E-5 1.79E-5 2.26E-5 3.87E-5 5.87E-6 4.81E-5 3.75E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.598 0.648 0.950 0.593 0.526 0.585 0.720	2.046 1.980 2.081 1.503 2.450 2.189 1.585	1.946 1.917 2.001 1.488 2.418 2.161 1.534	2.088 1.991 2.051 1.393 2.516 2.216 1.512	2.098 1.751 1.910 1.378 2.309 2.038 1.545	0.768 0.329 0.627 0.775 0.628 0.260 0.775	0.068 -0.007 0.074 0.040 0.037 0.043 0.083	93 95 93 98 98 98 98	103 101 97 88 103 102 92	104 83 85 86 93 91 95	12 -49 -34 20 5 -56 6	-89 -100 -92 -93 -93 -93 -89	3.83E-6 1.77E-6 3.53E-6 3.08E-6 1.89E-6 3.23E-6	1.31E-5 4.24E-6 5.18E-6 1.50E-5 1.13E-5 4.16E-6 1.17E-5	4.12E-5 1.04E-5 1.88E-5 4.15E-5 3.65E-5 9.15E-6 3.92E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10	0.686 1.481 0.349 0.581 1.053 0.543 1.244	2.384 2.250 1.742 2.022 1.870 2.111 2.171	2.318 2.106 1.713 1.880 1.738 1.968 2.034	2.439 2.117 1.766 1.939 1.773 2.033 2.212	2.411 2.152 1.719 1.760 1.677 1.968 2.364	0.431 1.287 0.418 0.543 0.657 0.113 1.436	0.051 0.049 -0.009 0.057 0.013 -0.007 0.071	96 81 98 90 84 91 85	103 83 102 94 88 95 104	102 87 98 82 76 91 121	-37 -13 5 -7 -38 -79 21	-93 -97 -100 -90 -99 -100 -94	2.35E-6 2.35E-6 3.30E-6 2.29E-6 1.70E-6 1.74E-6 5.10E-6	5.40E-6 7.40E-6 1.11E-5 8.43E-6 4.67E-6 3.42E-6 1.51E-5	1.70E-5 2.76E-5 3.34E-5 3.31E-5 1.59E-5 6.73E-6 4.12E-5
Prostate Cancer PC-3 DU-145	0.515	2.187 1.749	2.045 1.681	2.128	1.940 1.745	0.647	0.103 0.005	92 95	96 100	85 100	8	-80 -99	2.85E-6 3.48E-6	1.23E-5 1.19E-5	4.55E-5 3.49E-5
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.544 C 0.605 1.372 1.308 0.798 1.202	2.485 1.276 2.278 2.221 1.683 2.484	2.185 1.254 2.104 2.135 1.587 2.430	2.232 1.269 2.172 2.225 1.668 2.412	2.294 1.255 2.182 2.184 1.615 2.192	0.502 0.685 1.201 1.190 0.692 0.994	0.019 0.061 0.680 0.085 0.134 0.051	85 97 81 91 89 96	87 99 88 100 98 94	90 97 89 96 92 77	-8 12 -13 -9 -13 -17	-97 -90 -50 -94 -83 -96	2.57E-6 3.56E-6 2.43E-6 2.74E-6 2.51E-6 1.94E-6	8.34E-6 1.31E-5 7.54E-6 8.20E-6 7.48E-6 6.55E-6	2.99E-5 4.05E-5 9.72E-5 3.06E-5 3.35E-5 2.61E-5

Compound 3s





NSC : D - 847	/584 / 1				Experiment ID : 2311NS02							Test Type : 08		Units : Molar		
Report Date :	Decem	ber 04, 2	2023		Tes	Test Date : November 06, 2023					QNS	S :	MC :	MC :		
COMI : TO61					Sta	n Rea	gent : S	RB Dual-	Pass	Related		SSP	L : 1CXF			
						Lo	og10 Cor	centration						<u> </u>		
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	Optica -6.0	Densiti -5.0	es -4.0	-8.0	-7.0	ercent G -6.0	rowth -5.0	-4.0	GI50	TGI	LC50	
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.546 0.835 0.279 0.563 0.827 0.219	2.925 3.007 2.009 2.435 2.220 0.563	2.945 2.898 1.981 2.315 2.226 0.571	2.920 2.866 1.970 2.400 2.221 0.532	0.856 0.637 0.410 1.049 1.006 0.306	0.731 0.448 0.268 0.702 0.686 0.240	0.327 0.469 0.182 0.311 0.490 0.191	101 95 98 94 100 102	100 93 98 98 100 91	13 -24 8 26 13 25	8 -46 -4 7 -17 6	-40 -44 -35 -45 -41 -13	3.75E-7 2.35E-7 3.38E-7 4.64E-7 3.75E-7 4.19E-7	1.45E-5 6.28E-7 4.54E-6 1.39E-5 2.69E-6 2.09E-5	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4	
Non-Small Cell Lun; A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H227 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.217 0.536 0.641 1.403 0.894 0.505 0.560 0.286 1.112	1.198 1.764 1.775 1.718 1.655 1.722 2.071 2.453 2.814	1.138 1.643 1.725 1.657 1.551 1.717 2.046 2.468 2.515	1.140 1.612 1.743 1.634 1.604 1.723 1.952 2.519 2.476	0.420 0.908 1.171 1.643 1.137 0.833 1.377 0.596 0.721	0.316 0.736 0.913 1.261 0.824 0.708 1.121 0.287 0.887	0.085 0.063 0.082 0.333 0.083 0.054 0.166 0.062 0.149	94 90 96 81 86 100 98 101 82	94 88 97 73 93 100 92 103 80	21 30 47 76 32 27 54 14 -35	10 16 24 -10 -8 17 37 0 -20	-61 -88 -87 -76 -91 -89 -70 -78 -87	3.99E-7 4.53E-7 8.61E-7 5.06E-7 4.84E-7 1.73E-6 3.96E-7 1.83E-7	1.39E-5 1.43E-5 1.64E-5 7.63E-6 6.35E-6 1.44E-5 2.21E-5 1.00E-5 4.95E-7	7.03E-5 4.30E-5 4.62E-5 4.01E-5 3.23E-5 4.26E-5 6.46E-5 4.35E-5 2.80E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.476 0.821 0.267 0.311 0.201 0.615 0.279	2.080 2.699 2.090 2.050 1.335 2.374 1.981	2.001 2.450 1.911 1.940 1.268 2.290 1.946	1.970 2.724 1.939 2.019 1.286 2.163 1.957	0.585 1.933 0.454 0.474 0.200 0.712 0.850	0.377 0.862 0.241 0.359 0.189 0.686 0.603	0.045 0.053 0.028 0.033 0.022 0.061 0.029	95 87 90 94 94 95 98	93 101 92 98 96 88 99	7 59 10 9 0 5 34	-21 2 -10 3 -6 4 19	-91 -94 -90 -89 -89 -90 -90	3.16E-7 1.45E-6 3.25E-7 3.49E-7 2.98E-7 2.89E-7 5.58E-7	1.76E-6 1.05E-5 3.22E-6 1.07E-5 9.82E-7 1.10E-5 1.50E-5	2.61E-5 3.51E-5 3.19E-5 3.74E-5 3.38E-5 3.75E-5 4.32E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.838 0.431 0.637 0.692 1.075 0.199	2.283 1.904 2.043 1.919 2.104 1.132	2.187 1.682 1.937 1.825 1.889 1.067	2.237 1.629 1.961 1.836 1.924 1.058	1.661 0.447 0.439 1.389 1.188 0.300	1.065 0.416 0.566 1.069 1.071 0.265	0.371 0.019 0.045 0.123 0.343 0.012	93 85 92 92 79 93	97 81 94 93 82 92	57 1 -31 57 11 11	16 -3 -11 31 0 7	-56 -96 -93 -82 -68 -94	1.47E-6 2.46E-7 2.25E-7 1.82E-6 2.85E-7 3.29E-7	1.66E-5 1.73E-6 5.65E-7 1.87E-5 9.27E-6 1.17E-5	8.30E-5 3.19E-5 5.18E-5 5.41E-5 3.67E-5	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.472 0.602 0.428 0.562 1.611 0.646 1.258 0.788 0.740	3.086 1.682 1.515 2.514 3.189 1.975 3.300 2.063 2.662	2.952 1.611 1.533 2.346 3.131 1.950 3.201 1.953 2.397	2.915 1.651 1.486 2.368 3.154 1.965 3.164 2.038 2.379	1.592 1.112 0.462 0.411 2.225 1.305 1.641 1.464 1.211	0.718 1.100 0.495 0.610 1.905 1.211 0.631 1.153 0.952	0.014 0.013 0.046 0.022 0.241 0.063 0.008 0.250 0.045	95 93 102 91 96 98 95 91 86	93 97 93 98 99 93 98 85	43 47 3 -27 39 50 19 53 25	9 46 2 19 43 -50 29 11	-97 -98 -89 -96 -85 -90 -99 -68 -94	7.22E-7 8.80E-7 3.18E-7 2.27E-7 6.47E-7 9.79E-7 3.81E-7 3.81E-7	1.23E-5 2.09E-5 1.16E-5 1.51E-5 2.09E-5 1.88E-6 1.97E-5 1.27E-5	3.61E-5 4.65E-5 3.87E-5 3.40E-5 4.59E-5 1.01E-5 6.47E-5 3.81E-5	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.491 0.610 0.855 0.523 0.394 0.514 0.822	1.987 2.126 2.145 1.462 1.708 1.958 1.821	1.981 2.006 2.062 1.438 1.686 1.921 1.750	2.061 2.057 2.110 1.454 1.739 1.974 1.789	1.017 0.806 1.650 0.845 0.437 0.382 1.132	0.709 0.738 1.256 0.691 0.295 0.434 0.956	0.065 0.022 0.171 0.013 0.051 0.065 0.188	100 92 94 97 98 97 93	105 95 97 99 102 101 97	35 13 62 34 3 -26 31	15 8 31 18 -25 -16 13	-87 -96 -80 -98 -87 -87 -77	6.12E-7 3.56E-7 2.41E-6 5.73E-7 3.37E-7 2.53E-7 5.14E-7	1.39E-5 1.20E-5 1.91E-5 1.43E-5 1.30E-6 6.27E-7 1.41E-5	4.33E-5 3.61E-5 5.37E-5 3.87E-5 2.52E-5 3.02E-5 5.01E-5	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.606 1.529 0.357 0.633 1.036 0.558 1.130 0.596	2.332 2.366 1.506 2.110 1.278 2.056 2.103 2.297	2.176 2.288 1.419 1.987 1.248 1.987 1.980 2.115	2.302 2.281 1.512 1.931 1.238 1.947 1.999 2.115	1.380 2.172 0.891 1.380 0.700 0.868 1.832 1.289	0.804 1.872 0.500 0.935 0.902 0.527 1.368 0.898	0.125 0.093 0.006 0.168 0.069 0.012 0.142 0.183	91 92 92 88 95 87 89	98 90 101 88 83 93 89 89	45 77 46 51 -32 21 72 41	11 41 12 20 -13 -6 24 18	-79 -94 -98 -74 -93 -98 -87 -69	8.01E-7 5.59E-6 8.61E-7 1.04E-6 1.94E-7 3.92E-7 2.91E-6 6.44E-7	1.34E-5 2.01E-5 1.29E-5 1.65E-5 5.24E-7 6.11E-6 1.65E-5 1.60E-5	4.74E-5 4.72E-5 3.66E-5 5.62E-5 2.89E-5 3.03E-5 4.63E-5 5.99E-5	
Prostate Cancer PC-3 DU-145	0.500 0.494	1.836 1.676	1.844 1.575	1.832 1.632	0.918 0.751	0.764 0.484	0.320 0.065	101 91	100 96	31 22	20 -2	-36 -87	5.32E-7 4.18E-7	2.26E-5 8.22E-6	> 1.00E-4 3.67E-5	
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.445 C 0.643 1.428 1.245 0.725 0.842	1.907 1.341 2.417 2.025 1.670 1.366	1.902 1.303 2.169 1.926 1.604 1.306	1.834 1.338 2.273 2.010 1.703 1.332	0.672 0.905 1.525 1.632 1.096 0.702	0.529 0.737 1.404 1.066 0.951 0.652	0.096 0.134 0.796 0.145 0.156 0.092	100 94 75 87 93 89	95 100 85 98 103 94	16 38 10 50 39 -17	6 13 -2 -14 24 -23	-78 -79 -44 -88 -78 -89	3.69E-7 6.30E-7 2.94E-7 9.79E-7 6.81E-7 2.48E-7	1.17E-5 1.40E-5 7.09E-6 5.95E-6 1.71E-5 7.06E-7	4.59E-5 4.84E-5 > 1.00E-4 3.03E-5 5.27E-5 2.59E-5	

Compound 3t





					1							-		1		
NSC : D - 847585 / 1					Exp	erimer	nt ID : 2	311NS02				Test	Test Type : 08		Units : Molar	
Report Date :	Decem	ber 04, 2	2023		Tes	t Date	: Nover	mber 06,	2023			QNS	S :	MC :		
COMI : TO62					Stai	in Rea	gent : S	RB Dual-	Pass	Related	ł	SSF	PL:1CXF			
						Lo	og10 Cor	ncentration								
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	-6.0	-5.0	es -4.0	-8.0	-7.0	ercent G -6.0	-5.0	-4.0	GI50	TGI	LC50	
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.546 0.835 0.279 0.563 0.827 0.219	3.038 3.077 2.073 2.491 2.245 0.594	2.981 2.873 2.066 2.497 2.288 0.590	2.926 3.028 1.997 2.481 2.188 0.582	0.922 0.585 0.482 0.894 0.971 0.312	0.638 0.536 0.335 0.629 0.760 0.237	0.322 0.413 0.140 0.274 0.434 0.170	98 91 100 100 103 99	96 98 96 99 96 97	15 -30 11 17 10 25	4 -36 3 -8 5	-41 -51 -50 -51 -48 -22	3.68E-7 2.37E-7 3.48E-7 3.99E-7 3.43E-7 4.46E-7	1.21E-5 5.83E-7 1.14E-5 1.15E-5 3.58E-6 1.49E-5	 > 1.00E-4 9.19E-5 > 1.00E-4 9.42E-5 > 1.00E-4 > 1.00E-4 > 1.00E-4 	
Non-Small Cell Lun A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H227 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.217 0.536 0.641 1.403 0.894 0.505 0.560 0.286 1.112	1.313 1.764 1.783 1.855 1.679 1.709 2.127 2.283 2.848	1.258 1.736 1.712 1.812 1.626 1.706 2.183 2.374 2.733	1.222 1.682 1.819 1.758 1.633 1.633 1.636 2.030 2.293 2.658	0.460 0.865 1.289 1.821 0.966 0.771 1.508 0.424 0.716	0.294 0.663 0.698 1.242 0.767 0.629 1.056 0.196 1.001	0.022 0.006 0.059 0.199 0.052 0.026 0.082 0.022 0.053	95 98 94 91 93 100 104 105 93	92 93 103 79 94 94 94 100 89	22 27 57 93 9 22 61 7 -36	7 10 5 -11 -14 10 32 -31 -10	-90 -99 -91 -86 -94 -95 -85 -92 -95	3.97E-7 4.48E-7 1.35E-6 3.30E-7 4.08E-7 2.31E-6 3.46E-7 2.06E-7	1.18E-5 1.24E-5 1.13E-5 7.76E-6 2.47E-6 1.25E-5 1.86E-5 1.51E-6 5.18E-7	3.88E-5 3.56E-5 3.75E-5 3.30E-5 2.80E-5 3.74E-5 4.98E-5 2.02E-5 2.95E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.476 0.821 0.267 0.311 0.201 0.615 0.279	2.094 2.728 2.062 2.034 1.353 2.343 1.786	1.980 2.639 2.183 2.007 1.347 2.091 1.783	2.146 2.561 2.107 1.915 1.279 2.340 1.691	0.163 1.089 0.498 0.441 0.250 0.658 0.653	0.333 0.772 0.407 0.413 0.143 0.584 0.626	0.020 0.024 0.033 0.014 0.012 0.069 0.019	93 95 107 98 99 85 100	103 91 102 93 94 100 94	-66 14 13 8 4 2 25	-30 -6 8 6 -29 -5 23	-96 -97 -88 -95 -94 -89 -93	2.07E-7 3.42E-7 3.85E-7 3.08E-7 3.08E-7 3.25E-7 4.31E-7	4.08E-7 5.01E-6 1.21E-5 1.14E-5 1.34E-6 2.13E-6 1.58E-5	3.04E-5 4.03E-5 3.56E-5 2.10E-5 3.44E-5 4.25E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.838 0.431 0.637 0.692 1.075 0.199	2.192 1.922 2.041 1.913 1.955 1.125	2.096 1.897 1.912 1.811 1.905 1.123	2.087 1.912 1.875 1.796 1.868 1.127	1.476 0.450 0.409 0.971 1.320 0.314	1.003 0.351 0.449 1.022 1.179 0.221	0.212 0.007 0.002 0.014 0.052 0.025	93 98 91 92 94 100	92 99 88 90 90 100	47 1 -36 23 28 12	12 -19 -30 27 12 2	-75 -98 -100 -98 -95 -88	8.61E-7 3.19E-7 2.03E-7 3.96E-7 4.40E-7 3.73E-7	1.38E-5 1.16E-6 5.14E-7 1.65E-5 1.29E-5 1.06E-5	5.19E-5 2.47E-5 1.96E-5 4.13E-5 3.78E-5 3.82E-5	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-28 SK-MEL-28 SK-MEL-28 UACC-257 UACC-62	0.472 0.602 0.428 0.562 1.611 0.646 1.258 0.788 0.740	3.079 1.712 1.574 2.409 3.184 1.981 3.297 2.110 2.597	3.043 1.699 1.486 2.398 3.119 1.915 3.250 2.099 2.436	2.983 1.732 1.556 2.287 3.094 1.900 3.168 2.021 2.394	1.191 1.227 0.504 0.412 2.034 1.265 1.203 1.490 1.270	0.203 0.931 0.478 0.866 2.107 1.238 0.522 1.027 0.746	0.004 0.077 0.049 0.020 0.073 0.021 0.005 0.059 0.007	99 92 99 96 95 98 99 99	96 102 98 93 94 94 94 93 89	28 56 7 -27 27 46 -4 53 29	-57 30 4 16 32 44 -59 18 0	-99 -87 -89 -97 -95 -97 -100 -93 -99	4.72E-7 1.72E-6 3.37E-7 2.30E-7 4.54E-7 8.39E-7 2.79E-7 1.23E-6 4.42E-7	2.12E-6 1.79E-5 1.11E-5 2.06E-5 9.02E-7 1.46E-5 1.01E-5	8.27E-6 4.80E-5 3.84E-5 4.87E-5 4.66E-5 6.96E-6 4.13E-5 3.21E-5	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-0V-3	0.491 0.610 0.855 0.523 0.394 0.514 0.822	1.970 1.900 2.123 1.449 1.813 1.974 1.959	2.136 1.925 2.082 1.373 1.777 1.983 2.007	2.336 1.878 2.017 1.291 1.784 1.940 1.963	1.170 0.630 1.620 0.713 0.421 0.393 1.370	0.639 0.706 1.231 0.665 0.297 0.375 0.884	0.111 0.090 0.034 0.005 0.057 0.030 0.037	111 102 97 92 97 101 104	125 98 92 83 98 98 100	46 2 60 21 2 -24 48	10 7 30 15 -25 -27 5	-77 -85 -96 -99 -86 -94 -95	8.88E-7 3.16E-7 2.17E-6 3.37E-7 3.16E-7 2.47E-7 9.22E-7	1.30E-5 1.20E-5 1.72E-5 1.36E-5 1.18E-6 6.38E-7 1.13E-5	4.86E-5 4.17E-5 4.30E-5 3.72E-5 2.60E-5 2.20E-5 3.54E-5	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.606 1.529 0.357 0.633 1.036 0.558 1.130 0.596	2.390 2.333 1.507 2.124 1.348 2.041 2.170 2.364	2.316 2.215 1.551 2.072 1.327 1.993 2.055 2.119	2.252 2.096 1.483 2.012 1.298 1.963 1.971 2.105	1.321 2.098 0.793 1.392 0.860 0.800 1.830 1.481	0.726 2.115 0.484 0.721 0.742 0.527 1.431 0.749	0.060 0.093 -0.001 0.011 0.046 0.007 0.028 0.075	96 85 104 97 93 97 89 86	92 70 98 92 84 95 81 85	40 71 38 51 -17 16 67 50	7 73 11 6 -28 -6 29 9	-90 -94 -100 -98 -96 -99 -98 -98 -88	6.46E-7 1.37E-5 6.28E-7 1.05E-6 2.17E-7 3.72E-7 2.83E-6 1.00E-6	1.17E-5 2.74E-5 1.26E-5 1.14E-5 6.79E-7 5.57E-6 1.69E-5 1.23E-5	3.85E-5 5.45E-5 3.55E-5 3.44E-5 2.10E-5 3.00E-5 4.21E-5 4.07E-5	
Prostate Cancer PC-3 DU-145	0.500	1.998	1.987	1.948	0.982	0.815	0.136	99 101	97	32	21	-73	5.29E-7 3.80E-7	1.67E-5	5.70E-5	
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.445 C 0.643 1.428 1.245 0.725 0.842	1.981 1.333 2.372 2.110 1.697 1.396	1.806 1.319 2.355 2.079 1.616 1.384	1.893 1.288 2.277 1.998 1.599 1.350	0.709 0.680 1.486 1.457 1.307 0.779	0.458 0.847 1.417 0.961 0.833 0.408	0.021 0.018 0.670 0.068 0.060 0.025	89 98 96 92 98	94 94 90 87 90 92	17 5 6 24 60 -7	1 30 0 -23 11 -52	-95 -97 -53 -95 -92 -97	3.75E-7 3.11E-7 3.00E-7 3.90E-7 1.59E-6 2.63E-7	1.02E-5 1.71E-5 7.66E-6 3.29E-6 1.28E-5 8.40E-7	3.38E-5 4.24E-5 8.73E-5 2.39E-5 3.93E-5 9.22E-6	

Compound **3u**



NSC : D - 847586 / 1					Exp	Experiment ID : 2311NS02							Test Type : 08		Units : Molar	
Report Date :	Decem	oer 04, 2	2023		Tes	t Date	: Nover	mber 06, 2	2023			QNS	QNS :		MC :	
COMI : TO63					Stai	in Rea	gent : S	RB Dual-	Pass	Related		SSP	L:1CXF			
						Lo	og10 Cor	centration								
Panel/Cell Line Leukemia	Time Zero	Ctrl	-8.0	Mear -7.0	Optica -6.0	I Densiti -5.0	es -4.0	-8.0	F -7.0	ercent G -6.0	-5.0	-4.0	GI50	TGI	LC50	
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.546 0.835 0.279 0.563 0.827 0.219	3.038 3.077 2.073 2.491 2.245 0.594	2.980 2.981 2.083 2.479 2.218 0.616	2.968 2.984 2.036 2.392 2.200 0.619	2.411 2.803 1.623 2.021 1.781 0.474	0.746 0.544 0.365 0.704 0.989 0.254	0.196 0.217 0.089 0.169 0.354 0.213	98 96 101 99 98 106	97 96 98 95 97 107	75 88 75 76 67 68	8 -35 5 7 11 9	-64 -74 -68 -70 -57 -3	2.35E-6 2.03E-6 2.27E-6 2.37E-6 2.04E-6 2.02E-6	1.29E-5 5.20E-6 1.16E-5 1.24E-5 1.47E-5 5.90E-5	6.38E-5 2.43E-5 5.62E-5 5.51E-5 7.86E-5 > 1.00E-4	
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H232 NCI-H322M NCI-H460 NCI-H522	Cancer 0.217 0.536 0.641 1.403 0.894 0.505 0.560 0.286 1.112	1.313 1.764 1.783 1.855 1.679 1.709 2.127 2.283 2.848	1.135 1.645 1.733 1.794 1.612 1.674 2.113 2.193 2.595	1.286 1.715 1.744 1.792 1.642 1.687 1.998 2.312 2.671	0.913 1.483 1.593 1.781 1.445 1.410 1.802 1.376 2.466	0.425 0.735 0.933 1.519 0.908 0.699 1.031 0.364 1.121	0.016 0.007 0.072 0.121 0.106 0.015 0.026 0.024 0.064	84 90 96 86 91 97 99 95 85	97 96 97 86 95 98 92 101 90	63 77 83 84 70 75 79 55 78	19 16 26 2 16 30 4 1	-93 -99 -89 -91 -88 -97 -95 -92 -94	2.00E-6 2.79E-6 3.77E-6 3.80E-6 1.97E-6 2.66E-6 3.93E-6 1.23E-6 2.30E-6	1.48E-5 1.38E-5 1.67E-5 1.66E-5 1.05E-5 1.39E-5 1.74E-5 1.10E-5 1.01E-5	4.15E-5 3.77E-5 4.58E-5 4.43E-5 3.77E-5 3.83E-5 4.34E-5 3.67E-5 3.41E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.476 0.821 0.267 0.311 0.201 0.615 0.279	2.094 2.728 2.062 2.034 1.353 2.343 1.786	2.130 2.385 2.044 1.916 1.293 2.543 1.776	2.201 2.676 2.157 2.022 1.300 2.440 1.750	1.823 2.414 1.565 1.180 0.974 1.902 1.551	0.683 1.372 0.561 0.631 0.389 1.059 0.660	0.052 0.026 0.036 0.007 0.010 0.030 0.020	102 82 99 93 95 112 99	107 97 105 99 95 106 98	83 84 72 50 67 74 84	13 29 16 19 16 26 25	-89 -97 -87 -98 -95 -95 -93	2.96E-6 4.11E-6 2.50E-6 1.03E-6 2.17E-6 3.17E-6 3.82E-6	1.33E-5 1.70E-5 1.44E-5 1.44E-5 1.44E-5 1.40E-5 1.63E-5 1.64E-5	4.13E-5 4.24E-5 3.88E-5 3.93E-5 4.23E-5 4.23E-5 4.33E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.838 0.431 0.637 0.692 1.075 0.199	2.192 1.922 2.041 1.913 1.955 1.125	2.062 1.691 1.955 1.783 1.736 1.080	2.126 1.829 2.075 1.832 1.838 1.153	1.894 1.479 1.903 1.757 1.831 0.830	1.065 0.638 0.779 1.062 1.376 0.324	0.092 0.007 0.007 0.014 0.022 0.007	90 85 94 89 75 95	95 94 102 93 87 103	78 70 90 87 86 68	17 14 10 30 34 13	-89 -98 -99 -98 -98 -98	2.86E-6 2.29E-6 3.17E-6 4.50E-6 4.94E-6 2.15E-6	1.44E-5 1.33E-5 1.24E-5 1.72E-5 1.81E-5 1.33E-5	4.27E-5 3.71E-5 3.56E-5 4.22E-5 4.34E-5 3.78E-5	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.472 0.602 0.428 0.562 1.611 0.646 1.258 0.788 0.740	3.079 1.712 1.574 2.409 3.184 1.981 3.297 2.110 2.597	2.979 1.619 1.543 2.299 3.152 1.904 3.172 2.016 2.434	3.001 1.691 1.533 2.345 3.166 1.949 3.199 2.123 2.454	2.571 1.520 1.225 2.171 3.080 1.726 3.132 1.939 2.313	0.496 0.853 0.326 1.057 2.258 0.961 1.111 1.091 0.715	0.005 0.013 0.028 0.015 0.054 0.011 0.004 0.028 0.010	96 92 97 94 98 94 94 93 91	97 98 96 99 98 95 101 92	80 83 70 87 93 81 92 87 85	1 23 -24 27 41 24 -12 23 -3	-99 -98 -94 -97 -97 -98 -100 -96 -99	2.42E-6 3.50E-6 1.62E-6 4.12E-6 6.77E-6 3.46E-6 2.54E-6 3.78E-6 2.48E-6	1.02E-5 1.54E-5 5.56E-6 1.64E-5 1.99E-5 1.56E-5 7.71E-6 1.56E-5 9.14E-6	3.23E-5 4.00E-5 2.37E-5 4.16E-5 4.58E-5 4.01E-5 2.72E-5 4.08E-5 3.08E-5	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.491 0.610 0.855 0.523 0.394 0.514 0.822	1.970 1.900 2.123 1.449 1.813 1.974 1.959	2.045 1.784 2.040 1.415 1.699 1.943 1.810	2.023 1.854 2.049 1.416 1.839 2.019 1.851	1.710 1.477 1.763 1.292 1.559 1.778 1.630	0.832 1.037 1.239 0.924 0.611 0.532 1.050	0.047 0.025 0.043 0.007 0.026 0.032 0.069	105 91 93 96 92 98 87	104 96 94 102 103 90	82 67 72 83 82 87 71	23 33 30 43 15 1 20	-91 -96 -95 -99 -94 -94 -92	3.52E-6 3.20E-6 3.33E-6 6.77E-6 3.02E-6 2.68E-6 2.59E-6	1.60E-5 1.81E-5 1.74E-5 2.02E-5 1.38E-5 1.03E-5 1.51E-5	4.40E-5 4.40E-5 4.37E-5 4.54E-5 3.98E-5 3.46E-5 4.24E-5	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UC-31	0.606 1.529 0.357 0.633 1.036 0.558 1.130 0.596	2.390 2.333 1.507 2.124 1.348 2.041 2.170 2.364	2.231 2.215 1.467 2.002 1.281 1.847 2.050 2.140	2.334 2.271 1.550 2.014 1.326 1.916 2.053 2.175	2.194 2.201 1.368 2.010 1.213 1.667 2.151 1.988	0.919 2.154 0.521 1.201 0.697 0.632 1.438 0.905	0.079 0.090 0.022 0.025 0.037 0.009 0.011 0.029	91 85 96 92 79 87 88 88	97 92 104 93 93 92 89 89	89 84 88 92 57 75 98 79	18 78 14 -33 -33 5 30 17	-87 -94 -99 -96 -96 -98 -99 -99	3.51E-6 1.45E-5 3.27E-6 6.04E-6 1.19E-6 2.26E-6 2.26E-6 2.94E-6	1.47E-5 2.83E-5 1.33E-5 1.92E-5 4.31E-6 1.12E-5 1.70E-5 1.43E-5	4.43E-5 5.54E-5 3.67E-5 4.53E-5 1.87E-5 3.40E-5 4.16E-5 3.97E-5	
Prostate Cancer PC-3 DU-145	0.500 0.494	1.998 1.660	1.929 1.610	2.005 1.684	1.542 1.506	0.944 0.829	0.061 0.015	95 96	100 102	70 87	30 29	-88 -97	3.09E-6 4.30E-6	1.79E-5 1.69E-5	4.76E-5 4.23E-5	
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.445 C 0.643 1.428 1.245 0.725 0.842	1.981 1.333 2.372 2.110 1.697 1.396	1.965 1.302 2.180 1.970 1.573 1.326	1.867 1.313 2.263 2.103 1.638 1.309	1.665 1.225 2.224 1.990 1.404 0.872	0.590 0.887 1.642 1.265 0.831 0.815	0.026 0.026 0.440 0.055 0.095 0.038	99 96 80 84 87 87	93 97 89 99 94 84	79 84 84 86 70 5	9 35 23 2 11 -3	-94 -96 -69 -96 -87 -96	2.63E-6 5.02E-6 3.60E-6 2.70E-6 2.17E-6 2.72E-7	1.23E-5 1.86E-5 1.76E-5 1.06E-5 1.29E-5 4.20E-6	3.75E-5 4.47E-5 6.18E-5 3.42E-5 4.19E-5 3.21E-5	

Compound 3v



NSC : D - 843108 / 1						Experiment ID : 2308NS66							Test Type : 08		Units : Molar	
Report Date :	October	r 15, 202	23		Tes	t Date	: Augus	st 28, 202	3			QNS	S :	MC :		
COMI : To46					Stain Reagent : SRB Dual-Pass Related								PL : 1BCH			
Panel/Cell Line Leukemia	Time Zero	Ctrl	-8.0	Mear -7.0	n Optica -6.0	Lo I Densiti -5.0	og10 Cor es -4.0	ncentration -8.0	F -7.0	Percent G -6.0	Frowth -5.0	-4.0	GI50	TGI	LC50	
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.489 0.609 0.255 0.491 0.768	2.559 2.682 2.238 2.709 2.490	2.615 2.606 2.292 2.586 2.471	2.494 2.586 2.237 2.474 2.401	2.492 2.639 2.159 2.468 2.321	0.789 1.157 0.780 1.003 1.138	0.510 0.749 0.432 0.360 0.640	103 96 103 94 99	97 95 100 89 95	97 98 96 89 90	14 26 23 21	1 7 9 -27 -17	3.70E-6 > 4.68E-6 > 4.59E-6 > 3.91E-6 3.84E-6	1.00E-4 1.00E-4 1.00E-4 2.91E-5 3.65E-5	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4	
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H322M NCI-H322M NCI-H522	Cancer 0.294 0.960 0.633 1.139 1.037 0.591 0.811 0.259 1.295	1.978 2.566 2.173 1.785 1.796 1.923 2.182 2.634 3.037	1.893 2.503 2.106 1.748 1.758 1.893 2.224 2.697 2.946	1.825 2.484 2.059 1.696 1.703 1.829 2.105 2.670 2.934	1.906 2.474 2.055 1.692 1.697 1.804 2.053 2.644 2.700	0.704 1.641 1.263 1.437 1.248 0.780 1.191 0.438 1.304	0.027 0.234 0.207 0.601 0.112 0.049 0.321 -0.002 0.470	95 96 94 95 98 103 103 95	91 95 93 86 88 93 94 102 94	96 94 92 86 87 91 91 100 81	24 42 41 46 28 14 28 8 0	-91 -76 -67 -47 -89 -92 -60 -100 -64	4.37E-6 7.14E-6 6.66E-6 7.99E-6 4.21E-6 3.42E-6 3.42E-6 3.49E-6 2.41E-6	1.63E-5 2.29E-5 2.39E-5 3.12E-5 1.73E-5 1.36E-5 2.06E-5 1.17E-5 1.02E-5	4.42E-5 6.07E-5 6.92E-5 > 1.00E-4 4.62E-5 4.04E-5 7.61E-5 3.43E-5 6.12E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.551 0.668 0.301 0.311 0.217 0.494 0.268	2.497 2.623 2.836 2.557 1.609 2.483 2.045	2.402 2.551 2.614 2.401 1.584 2.525 2.101	2.383 2.516 2.512 2.364 1.621 2.443 2.077	2.505 2.427 2.575 2.317 1.653 2.347 1.935	0.707 1.166 0.693 0.573 0.236 0.719 0.727	0.006 0.031 0.068 -0.024 0.017 -0.002	95 96 91 93 98 102 103	94 95 87 91 101 98 102	100 90 99 103 93 94	8 25 15 12 1 11 26	-99 -95 -78 -100 -92 -100 -100	3.51E-6 4.17E-6 3.42E-6 3.21E-6 3.33E-6 3.37E-6 4.41E-6	1.19E-5 1.62E-5 1.47E-5 1.27E-5 1.03E-5 1.26E-5 1.60E-5	3.48E-5 4.21E-5 5.05E-5 3.57E-5 3.53E-5 3.55E-5 4.01E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	1.072 1.309 0.818 0.564 1.773 0.353	2.868 3.277 2.447 1.903 2.711 1.764	2.776 3.180 2.293 1.856 2.635 1.739	2.806 3.147 2.279 1.790 2.434 1.680	2.701 3.126 2.296 1.781 2.470 1.689	1.766 1.401 0.471 0.886 1.605 0.602	0.784 0.115 -0.040 0.045 0.855 -0.044	95 95 91 96 92 98	97 93 90 92 70 94	91 92 91 91 74 95	39 5 -42 24 -10 18	-27 -91 -100 -92 -52 -100	6.04E-6 3.04E-6 2.02E-6 4.08E-6 1.95E-6 3.80E-6	3.88E-5 1.12E-5 4.80E-6 1.61E-5 7.70E-6 1.41E-5	> 1.00E-4 3.72E-5 1.35E-5 4.34E-5 9.06E-5 3.76E-5	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.406 0.616 0.601 0.676 0.850 0.751 0.904 0.919 0.974	2.859 1.681 2.581 2.043 2.144 3.201 2.288 2.847	2.768 1.673 2.468 2.816 2.058 2.069 3.059 2.292 2.685	2.733 1.601 2.273 2.770 2.097 1.996 3.120 2.172 2.607	2.508 1.531 2.417 2.306 2.029 1.789 2.882 2.187 2.386	1.129 0.929 0.913 0.320 1.120 1.283 0.605 1.716 1.440	-0.076 0.120 0.054 0.179 0.128 0.073 -0.078 0.338 0.020	96 99 94 97 101 95 94 100 91	95 92 84 95 104 89 96 91 87	86 92 74 99 75 86 93 75	29 29 -53 23 38 -33 58 25	-100 -81 -91 -74 -85 -90 -100 -63 -98	4.31E-6 4.32E-6 3.54E-6 4.37E-6 4.37E-6 4.73E-6 2.01E-6 1.17E-5 3.18E-6	1.69E-5 1.85E-5 1.40E-5 3.83E-6 1.62E-5 1.98E-5 5.27E-6 3.01E-5 1.59E-5	4.11E-5 5.28E-5 4.13E-5 9.53E-6 4.73E-5 4.85E-5 1.79E-5 7.78E-5 4.07E-5	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.436 0.626 0.715 0.447 0.337 0.357 0.838	2.147 1.958 1.832 1.621 1.868 1.333 1.889	2.165 2.088 1.811 1.535 1.849 1.380 1.744	2.065 2.016 1.772 1.516 1.789 1.283 1.732	1.938 1.916 1.767 1.493 1.781 1.240 1.876	0.813 0.692 1.250 0.647 0.573 0.265 1.523	-0.028 -0.030 0.089 -0.069 0.013 -0.013 0.318	101 110 98 93 99 105 86	95 104 95 91 95 95 85	88 97 94 89 94 90 99	22 5 48 17 15 -26 65	-100 -100 -88 -100 -96 -100 -62	3.75E-6 3.23E-6 9.00E-6 3.49E-6 3.65E-6 2.23E-6 1.31E-5	1.51E-5 1.11E-5 2.26E-5 1.40E-5 1.37E-5 6.00E-6 3.25E-5	3.89E-5 3.34E-5 5.28E-5 3.74E-5 3.85E-5 2.12E-5 8.03E-5	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.777 1.209 0.374 0.495 0.750 0.631 1.084 0.664	3.041 2.202 1.700 1.736 1.442 2.311 2.183 2.052	2.832 2.186 1.673 1.613 1.452 2.106 2.122 1.855	2.774 2.131 1.611 1.612 1.444 1.988 2.037 1.809	2.784 2.145 1.569 1.413 1.334 2.129 2.146 1.825	1.661 1.885 0.795 0.823 0.752 0.955 1.766 1.077	0.129 0.042 0.055 -0.008 0.025 -0.062 0.417 0.193	91 98 90 101 88 94 86	88 93 90 100 81 87 83	89 94 90 74 84 89 97 84	39 68 32 26 0 19 62 30	-83 -97 -85 -100 -97 -100 -62 -71	6.01E-6 1.29E-5 4.87E-6 3.20E-6 2.56E-6 3.63E-6 1.25E-5 4.21E-6	2.08E-5 2.59E-5 1.87E-5 1.62E-5 1.01E-5 1.45E-5 3.18E-5 1.97E-5	5.33E-5 5.21E-5 4.99E-5 4.02E-5 3.30E-5 3.81E-5 8.07E-5 6.19E-5	
Prostate Cancer PC-3 DU-145	0.562 0.375	2.244 1.634	2.097 1.687	2.165 1.666	2.112 1.634	0.949 0.438	0.345 -0.036	91 104	95 103	92 100	23 5	-39 -100	4.07E-6 3.36E-6	2.36E-5 1.12E-5	> 1.00E-4 3.34E-5	
Breast Cancer MCF7 MDA-MB-231/ATCO HS 578T BT-549 T-47D MDA-MB-468	0.450 0.566 1.374 1.398 0.747 0.773	2.385 1.111 2.564 2.929 1.941 1.451	2.245 1.068 2.457 2.856 1.972 1.472	2.130 1.063 2.481 2.582 1.903 1.468	2.124 1.091 2.399 2.783 1.873 1.441	0.655 0.600 1.526 2.466 1.186 0.631	0.047 -0.003 0.985 0.226 0.593 0.171	93 92 91 95 103 103	87 91 93 77 97 102	87 96 86 90 94 99	11 6 13 70 37 -18	-90 -100 -28 -84 -21 -78	3.03E-6 3.27E-6 3.11E-6 1.34E-5 5.88E-6 2.60E-6	1.28E-5 1.14E-5 2.04E-5 2.84E-5 4.37E-5 6.96E-6	4.03E-5 3.38E-5 > 1.00E-4 6.02E-5 > 1.00E-4 3.40E-5	











IC50 (µM)

Figure S5. Correlations between IC₅₀ values and GI₅₀ values of the tested compounds against the T47D breast cancer cell line (R^2 =0.7884).

Fig. S6. Overlay between the co-crystallized colchicine (green) and the re-docked colchicine conformer using the GoldScore scoring function. The RMSD between the heavy atoms was calculated to be 1.33 Å.



Fig. S7. Overlay between the co-crystallized exemestane (green) and the re-docked exemestane conformer using the GoldScore scoring function. The RMSD between the heavy atoms was calculated to be 0.46 Å.



Derivatives	Molecular weight (g/mol)	MlogP	Hydrogen bond donor	Hydrogen bond acceptor	Topological polar surface area (Å ²)	Rotatable bond count
3a	407.29	3.112	3	3	73.04	4
3b	407.29	3.112	3	3	73.04	4
3c	435.35	3.542	3	3	73.04	4
3d	421.32	3.329	2	3	62.18	4
3 e	486.18	3.704	3	3	73.04	4
3f	565.07	4.019	3	3	73.04	4
3g	441.73	3.597	3	3	73.04	4
3h	441.73	3.597	3	3	73.04	4
3i	479.36	3.229	3	5	99.34	7
3j	479.36	3.229	3	5	99.34	7
3k	479.36	3.229	3	5	99.34	7
31	451.3	2.806	4	5	110.34	5
3m	451.3	2.806	4	5	110.34	5
3n	520.42	2.483	3	6	102.58	5
30	520.42	2.483	3	6	102.58	5
3 p	452.29	3.605	3	5	118.86	5
3q	452.29	3.199	3	5	118.86	5
3r	480.35	3.628	3	5	118.86	5
35	435.35	3.542	3	3	73.04	5
3t	435.35	3.542	3	3	73.04	5
<u>3u</u>	435.35	3.542	3	3	73.04	5
3v	479.36	3.229	3	5	99.34	7
3w	451.3	2.806	4	5	110.34	5
3x	520.42	2.483	3	6	102.58	5

Table S8. The physicochemical properties of the newly synthesised furanyl- and thiophenyl-3-phenyl-1*H*-indole-2-carbohydrazide derivatives.

	3 a	3 e	3h	3 p	3r	3t
hERG blocker	0.149	0.277	0.268	0.341	0.139	0.293
AMES mutagenicity	0.562	0.471	0.473	0.867	0.697	0.546
Human hepatotoxicity	0.898	0.841	0.885	0.868	0.939	0.857
RPMI-8226	0.157	0 1 2 1	0 1 2 5	0.002	0.060	0.000
immunotoxicity	0.137	0.121	0.123	0.082	0.000	0.090

 Table S9. Toxicity evaluation of the most active compounds.

^{*a*}All values represent toxicity probabilities within the range of 0 to 1.