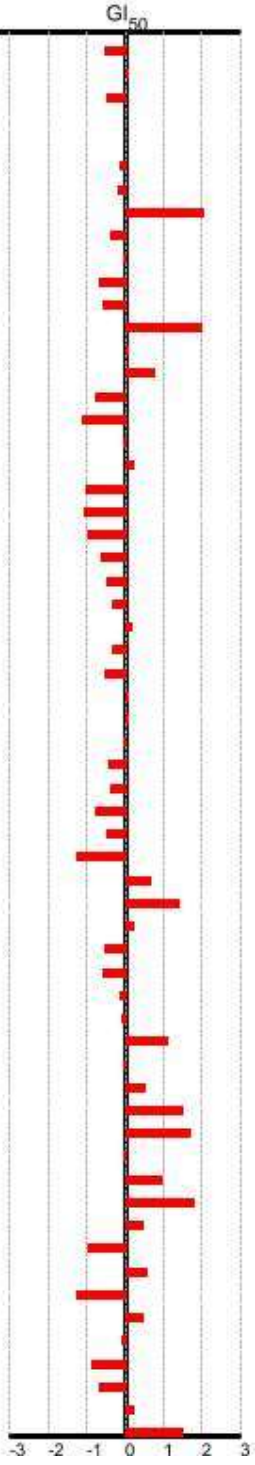
**Supplementary data**

**S1.** The explanation for the Mean Graph of $GI_{50}$: the mean $GI_{50}$ graph demonstrated the selective nature of growth inhibition of human derived cancer cell lines. The positive and negative values means resistance and sensitivity of a particular cell line, respectively.

## Erlotinib

$GI_{50}$ Mean Graph for Compound 718781
NCI Cancer Screen Current Data, May 2009
Average $GI_{50}$ over all cell lines is 5.51E-6

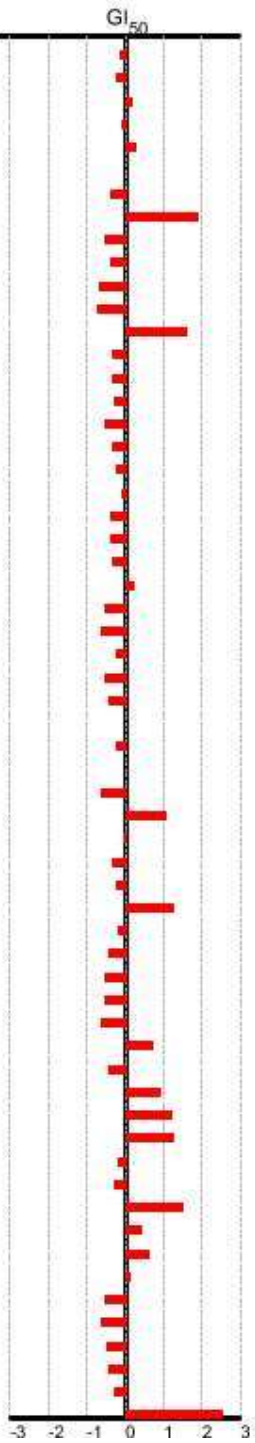
| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | CCRF-CEM | -4.8 |
| | HL-60(TB) | -5.3 |
| | K-562 | -4.8 |
| | MOLT-4 | -5.3 |
| | RPMI-8226 | -5.3 |
| | SR | -5.2 |
| Non-Small Cell Lung | A549/ATCC | -5.1 |
| | EKVX | -7.3 |
| | HOP-62 | -4.9 |
| | HOP-92 | -5.2 |
| | NCI-H226 | -4.6 |
| | NCI-H23 | -4.7 |
| | NCI-H322M | -7.3 |
| | NCI-H460 | -5.3 |
| | NCI-H522 | -6.0 |
| Colon | COLO 205 | -4.5 |
| | HCC-2998 | -4.1 |
| | HCT-116 | -5.2 |
| | HCT-15 | -5.5 |
| | HT29 | -4.3 |
| | KM12 | -4.2 |
| | SW-620 | -4.3 |
| Central Nervous System | SF-268 | -4.7 |
| | SF-295 | -4.8 |
| | SF-539 | -4.9 |
| | SNB-19 | -5.4 |
| | SNB-75 | -4.9 |
| | U251 | -4.7 |
| Melanoma | LOX IMVI | -5.3 |
| | MALME-3M | -5.3 |
| | M14 | -5.2 |
| | MDA-MB-435 | -4.8 |
| | SK-MEL-2 | -4.9 |
| | SK-MEL-28 | -4.5 |
| | SK-MEL-5 | -4.8 |
| | UACC-257 | -4.0 |
| | UACC-62 | -5.9 |
| Ovarian | IGROV1 | -6.6 |
| | OVCAR-3 | -5.5 |
| | OVCAR-4 | -4.7 |
| | OVCAR-5 | -4.7 |
| | OVCAR-8 | -5.1 |
| | NCI/ADR-RES | -5.2 |
| | SK-OV-3 | -6.4 |
| Renal | 786-0 | -5.3 |
| | A498 | -5.8 |
| | ACHN | -6.8 |
| | CAKI-1 | -7.0 |
| | RXF 393 | -5.2 |
| | SN12C | -6.2 |
| | TK-10 | -7.0 |
| | UO-31 | -5.7 |
| Prostate | PC-3 | -4.3 |
| | DU-145 | -5.8 |
| Breast | MCF7 | -4.0 |
| | MDA-MB-231/ATCC | -5.7 |
| | HS 578T | -5.2 |
| | MDA-N | -4.4 |
| | BT-549 | -4.6 |
| | T-47D | -5.5 |
| | MDA-MB-468 | -6.7 |



## Gefitinib

$GI_{50}$ Mean Graph for Compound 715055
NCI Cancer Screen Current Data, October 2009
Average $GI_{50}$ over all cell lines is 3.24E-6

| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | CCRF-CEM | -5.3 |
| | HL-60(TB) | -5.3 |
| | K-562 | -5.6 |
| | MOLT-4 | -5.4 |
| | RPMI-8226 | -5.8 |
| | SR | -5.5 |
| Non-Small Cell Lung | A549/ATCC | -5.1 |
| | EKVX | -7.3 |
| | HOP-62 | -5.0 |
| | HOP-92 | -5.1 |
| | NCI-H226 | -4.8 |
| | NCI-H23 | -4.8 |
| | NCI-H322M | -7.1 |
| | NCI-H460 | -5.2 |
| | NCI-H522 | -5.2 |
| Colon | COLO 205 | -5.2 |
| | HCC-2998 | -5.0 |
| | HCT-116 | -5.1 |
| | HCT-15 | -5.3 |
| | HT29 | -5.4 |
| | KM12 | -5.1 |
| | SW-620 | -5.1 |
| Central Nervous System | SF-268 | -5.1 |
| | SF-295 | -5.7 |
| | SF-539 | -5.0 |
| | SNB-19 | -4.9 |
| | SNB-75 | -5.2 |
| | U251 | -5.0 |
| Melanoma | LOX IMVI | -5.1 |
| | MALME-3M | -5.5 |
| | M14 | -5.3 |
| | MDA-MB-435 | -5.5 |
| | SK-MEL-2 | -4.9 |
| | SK-MEL-28 | -6.5 |
| | SK-MEL-5 | -5.4 |
| | UACC-257 | -5.2 |
| | UACC-62 | -5.3 |
| Ovarian | IGROV1 | -6.7 |
| | OVCAR-3 | -5.3 |
| | OVCAR-4 | -5.1 |
| | OVCAR-5 | -5.0 |
| | OVCAR-8 | -5.0 |
| | NCI/ADR-RES | -4.9 |
| | SK-OV-3 | -6.2 |
| Renal | 786-0 | -5.1 |
| | A498 | -6.4 |
| | ACHN | -6.7 |
| | CAKI-1 | -6.8 |
| | RXF 393 | -5.3 |
| | SN12C | -5.2 |
| | TK-10 | -7.0 |
| | UO-31 | -5.9 |
| Prostate | PC-3 | -6.1 |
| | DU-145 | -5.6 |
| Breast | MCF7 | -5.0 |
| | MDA-MB-231/ATCC | -4.9 |
| | HS 578T | -5.0 |
| | BT-549 | -5.1 |
| | T-47D | -5.2 |
| | MDA-MB-468 | -8.0 |



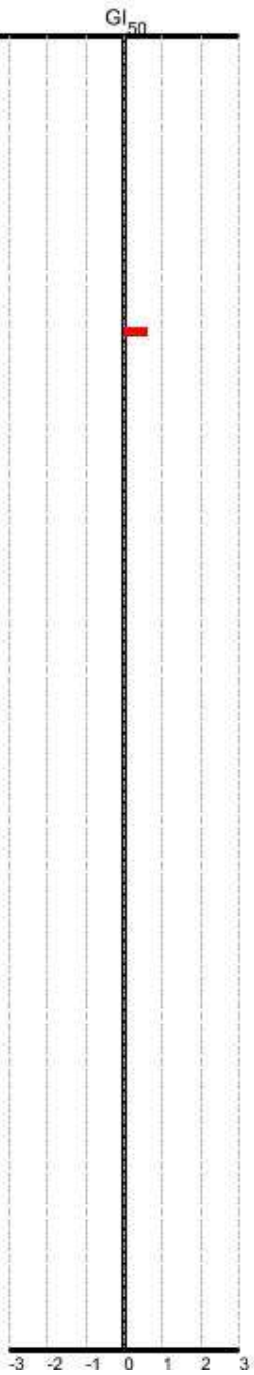
## Compound B

$GI_{50}$ Mean Graph for Compound 48283

NCI Cancer Screen Current Data, May 2009

Average $GI_{50}$ over all cell lines is 9.76E-5

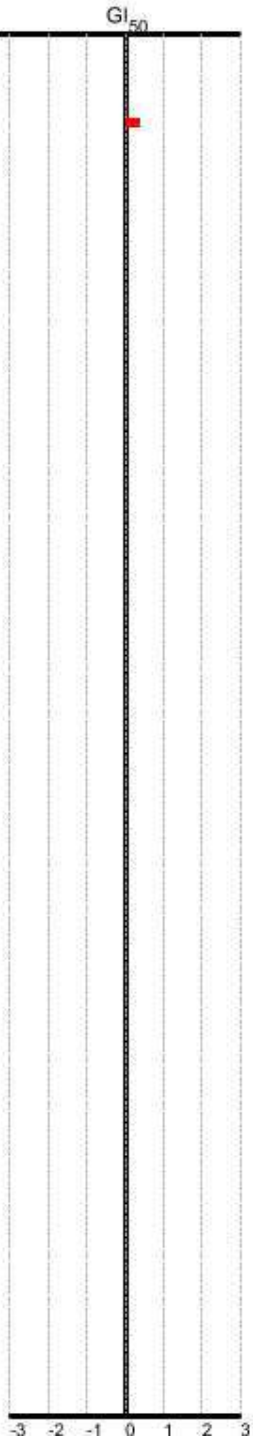
| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | CCRF-CEM | -4.0 |
| | K-562 | -4.0 |
| | MOLT-4 | -4.0 |
| | RPMI-8226 | -4.0 |
| | SR | -4.0 |
| Non-Small Cell Lung | A549/ATCC | -4.0 |
| | EKVX | -4.0 |
| | HOP-62 | -4.0 |
| | HOP-92 | -4.0 |
| | NCI-H23 | -4.0 |
| | NCI-H322M | -4.0 |
| | NCI-H460 | -4.0 |
| | NCI-H522 | -4.6 |
| Colon | COLO 205 | -4.0 |
| | HCT-116 | -4.0 |
| | HCT-15 | -4.0 |
| | HT29 | -4.0 |
| | KM12 | -4.0 |
| | SW-620 | -4.0 |
| Central Nervous System | SF-268 | -4.0 |
| | SF-295 | -4.0 |
| | SF-539 | -4.0 |
| | SNB-19 | -4.0 |
| | SNB-75 | -4.0 |
| | U251 | -4.0 |
| Melanoma | LOX IMVI | -4.0 |
| | MALME-3M | -4.0 |
| | M14 | -4.0 |
| | MDA-MB-435 | -4.0 |
| | SK-MEL-2 | -4.0 |
| | SK-MEL-28 | -4.0 |
| | SK-MEL-5 | -4.0 |
| | UACC-257 | -4.0 |
| | UACC-62 | -4.0 |
| Ovarian | IGROV1 | -4.0 |
| | OVCAR-3 | -4.0 |
| | OVCAR-4 | -4.0 |
| | OVCAR-5 | -4.0 |
| | OVCAR-8 | -4.0 |
| | NCI/ADR-RES | -4.0 |
| | SK-OV-3 | -4.0 |
| Renal | 786-0 | -4.0 |
| | A498 | -4.0 |
| | ACHN | -4.0 |
| | CAKI-1 | -4.0 |
| | RXF 393 | -4.0 |
| | SN12C | -4.0 |
| | TK-10 | -4.0 |
| | UO-31 | -4.0 |
| Prostate | PC-3 | -4.0 |
| | DU-145 | -4.0 |
| Breast | MCF7 | -4.0 |
| | MDA-MB-231/ATCC | -4.0 |
| | HS 578T | -4.0 |
| | MDA-N | -4.0 |
| | BT-549 | -4.0 |
| | T-47D | -4.0 |



## Compound G

$GI_{50}$ Mean Graph for Compound 125910
NCI Cancer Screen Current Data, May 2009
Average $GI_{50}$ over all cell lines is 9.86E-5

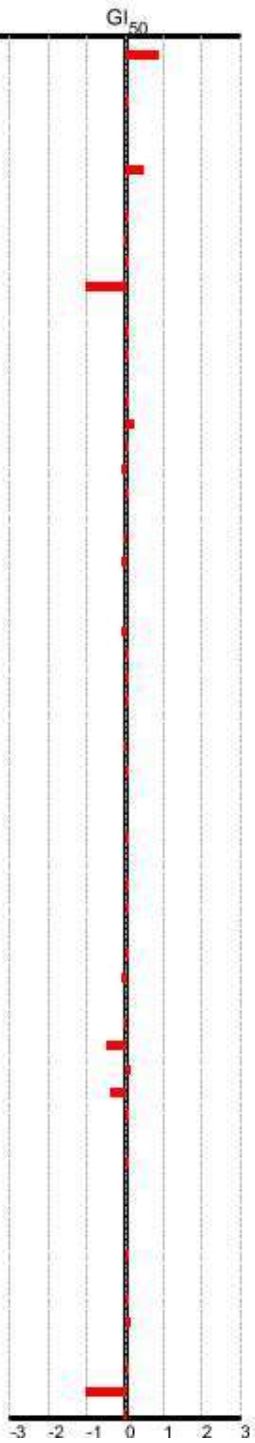
| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | CCRF-CEM | -4.0 |
| | HL-60(TB) | -4.0 |
| | K-562 | -4.0 |
| | MOLT-4 | -4.4 |
| | RPMI-8226 | -4.0 |
| | SR | -4.0 |
| Non-Small Cell Lung | A549/ATCC | -4.0 |
| | EKVX | -4.0 |
| | HOP-62 | -4.0 |
| | HOP-92 | -4.0 |
| | NCI-H226 | -4.0 |
| | NCI-H23 | -4.0 |
| | NCI-H322M | -4.0 |
| | NCI-H460 | -4.0 |
| | NCI-H522 | -4.0 |
| Colon | COLO 205 | -4.0 |
| | HCC-2998 | -4.0 |
| | HCT-116 | -4.0 |
| | HCT-15 | -4.0 |
| | HT29 | -4.0 |
| | KM12 | -4.0 |
| | SW-620 | -4.0 |
| Central Nervous System | SF-268 | -4.0 |
| | SF-295 | -4.0 |
| | SF-539 | -4.0 |
| | SNB-19 | -4.0 |
| | SNB-75 | -4.0 |
| | U251 | -4.0 |
| Melanoma | LOX IMVI | -4.0 |
| | MALME-3M | -4.0 |
| | M14 | -4.0 |
| | MDA-MB-435 | -4.0 |
| | SK-MEL-2 | -4.0 |
| | SK-MEL-28 | -4.0 |
| | SK-MEL-5 | -4.0 |
| | UACC-257 | -4.0 |
| | UACC-62 | -4.0 |
| Ovarian | IGROV1 | -4.0 |
| | OVCAR-3 | -4.0 |
| | OVCAR-4 | -4.0 |
| | OVCAR-5 | -4.0 |
| | OVCAR-8 | -4.0 |
| | NCI/ADR-RES | -4.0 |
| | SK-OV-3 | -4.0 |
| Renal | 786-0 | -4.0 |
| | A498 | -4.0 |
| | ACHN | -4.0 |
| | CAKI-1 | -4.0 |
| | RXF 393 | -4.0 |
| | SN12C | -4.0 |
| | TK-10 | -4.0 |
| | UO-31 | -4.0 |
| Prostate | PC-3 | -4.0 |
| | DU-145 | -4.0 |
| Breast | MCF7 | -4.0 |
| | MDA-MB-231/ATCC | -4.0 |
| | HS 578T | -4.0 |
| | MDA-N | -4.0 |
| | BT-549 | -4.0 |
| | T-47D | -4.0 |



## Compound H

$GI_{50}$ Mean Graph for Compound 130813
NCI Cancer Screen Current Data, May 2009
Average $GI_{50}$ over all cell lines is 1.94E-6

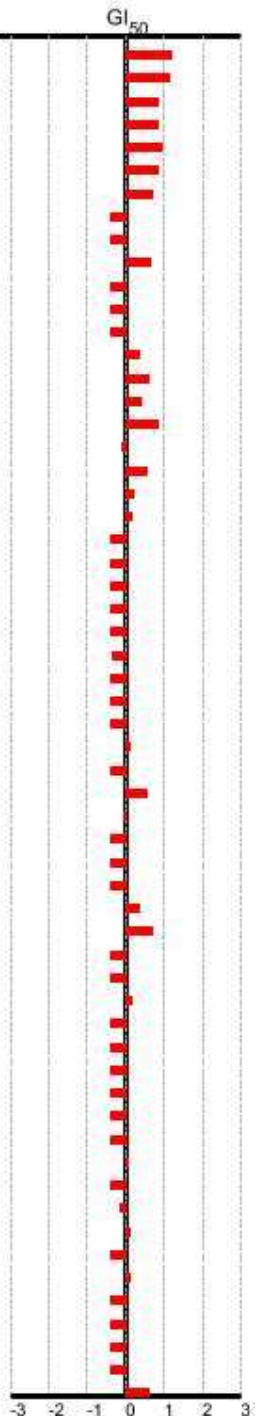
| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | CCRF-CEM | -6.6 |
| | HL-60(TB) | -5.7 |
| | K-562 | -5.8 |
| | MOLT-4 | -5.7 |
| | RPMI-8226 | -5.7 |
| | SR | -6.2 |
| Non-Small Cell Lung | A549/ATCC | -5.7 |
| | EKVX | -5.8 |
| | HOP-62 | -5.7 |
| | HOP-92 | -5.8 |
| | NCI-H226 | -4.7 |
| | NCI-H23 | -5.7 |
| | NCI-H322M | -5.8 |
| | NCI-H460 | -5.8 |
| | NCI-H522 | -5.8 |
| Colon | COLO 205 | -5.8 |
| | HCC-2998 | -5.9 |
| | HCT-116 | -5.8 |
| | HCT-15 | -5.6 |
| | HT29 | -5.8 |
| | KM12 | -5.7 |
| | SW-620 | -5.7 |
| Central Nervous System | SF-268 | -5.6 |
| | SF-295 | -5.7 |
| | SF-539 | -5.7 |
| | SNB-19 | -5.6 |
| | SNB-75 | -5.8 |
| | U251 | -5.8 |
| Melanoma | LOX IMVI | -5.8 |
| | MALME-3M | -5.7 |
| | M14 | -5.7 |
| | MDA-MB-435 | -5.8 |
| | SK-MEL-2 | -5.7 |
| | SK-MEL-28 | -5.7 |
| | SK-MEL-5 | -5.8 |
| | UACC-257 | -5.7 |
| | UACC-62 | -5.8 |
| Ovarian | IGROV1 | -5.8 |
| | OVCAR-3 | -5.7 |
| | OVCAR-4 | -5.8 |
| | OVCAR-5 | -5.6 |
| | OVCAR-8 | -5.7 |
| | NCI/ADR-RES | -5.7 |
| | SK-OV-3 | -5.2 |
| Renal | 786-0 | -5.8 |
| | A498 | -5.3 |
| | ACHN | -5.8 |
| | CAKI-1 | -5.7 |
| | RXF 393 | -5.8 |
| | SN12C | -5.7 |
| | TK-10 | -5.7 |
| | UO-31 | -5.7 |
| Prostate | PC-3 | -5.8 |
| | DU-145 | -5.7 |
| Breast | MCF7 | -5.8 |
| | MDA-MB-231/ATCC | -5.8 |
| | HS 578T | -5.7 |
| | MDA-N | -5.8 |
| | BT-549 | -4.7 |
| | T-47D | -5.7 |



## Compound I

$GI_{50}$ Mean Graph for Compound 135371
NCI Cancer Screen Current Data, May 2009
Average $GI_{50}$ over all cell lines is 3.95E-5

| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | CCRF-CEM | -5.6 |
| | HL-60(TB) | -5.5 |
| | K-562 | -5.3 |
| | MOLT-4 | -5.3 |
| | RPMI-8226 | -5.3 |
| | SR | -5.2 |
| Non-Small Cell Lung | A549/ATCC | -5.1 |
| | EKVX | -4.0 |
| | HOP-62 | -4.0 |
| | HOP-92 | -5.1 |
| | NCI-H226 | -4.0 |
| | NCI-H23 | -4.0 |
| | NCI-H322M | -4.0 |
| | NCI-H460 | -4.8 |
| | NCI-H522 | -5.0 |
| Colon | COLO 205 | -4.8 |
| | HCT-116 | -5.2 |
| | HCT-15 | -4.3 |
| | HT29 | -5.0 |
| | KM12 | -4.6 |
| | SW-620 | -4.5 |
| Central Nervous System | SF-268 | -4.0 |
| | SF-295 | -4.0 |
| | SF-539 | -4.0 |
| | SNB-19 | -4.0 |
| | SNB-75 | -4.0 |
| | U251 | -4.1 |
| Melanoma | LOX IMVI | -4.0 |
| | MALME-3M | -4.0 |
| | M14 | -4.0 |
| | MDA-MB-435 | -4.5 |
| | SK-MEL-2 | -4.0 |
| | SK-MEL-28 | -5.0 |
| | SK-MEL-5 | -4.3 |
| | UACC-257 | -4.0 |
| | UACC-62 | -4.0 |
| Ovarian | IGROV1 | -4.0 |
| | OVCAR-3 | -4.8 |
| | OVCAR-4 | -5.1 |
| | OVCAR-5 | -4.0 |
| | OVCAR-8 | -4.0 |
| | NCI/ADR-RES | -4.6 |
| | SK-OV-3 | -4.0 |
| Renal | 786-0 | -4.0 |
| | A498 | -4.0 |
| | ACHN | -4.0 |
| | CAKI-1 | -4.0 |
| | RXF 393 | -4.0 |
| | SN12C | -4.4 |
| | TK-10 | -4.0 |
| | UO-31 | -4.3 |
| Prostate | PC-3 | -4.5 |
| | DU-145 | -4.0 |
| Breast | MCF7 | -4.5 |
| | MDA-MB-231/ATCC | -4.0 |
| | HS 578T | -4.0 |
| | MDA-N | -4.0 |
| | BT-549 | -4.0 |
| | T-47D | -5.0 |



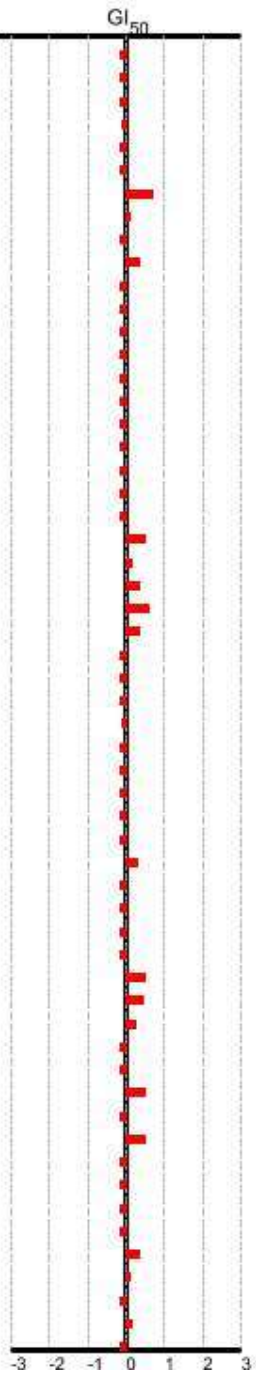
## Compound J

$GI_{50}$ Mean Graph for Compound 299137

NCI Cancer Screen Current Data, May 2009

Average $GI_{50}$ over all cell lines is 7.03E-5

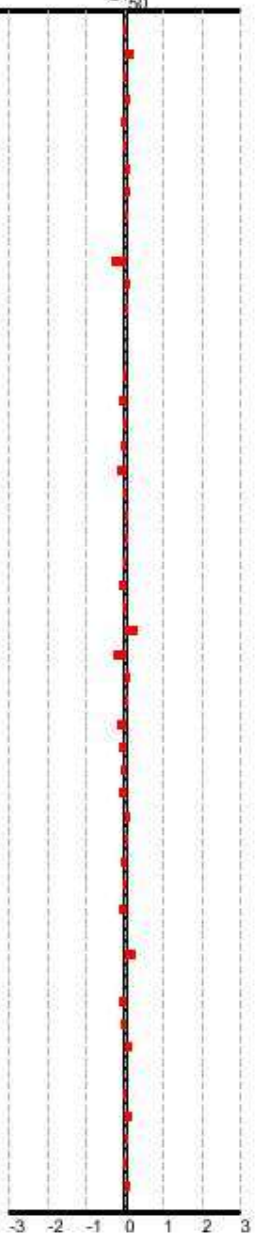
| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | K-562 | -4.0 |
| | MOLT-4 | -4.0 |
| | RPMI-8226 | -4.0 |
| | SR | -4.0 |
| Non-Small Cell Lung | A549/ATCC | -4.0 |
| | EKVX | -4.0 |
| | HOP-62 | -4.8 |
| | HOP-92 | -4.3 |
| | NCI-H226 | -4.0 |
| | NCI-H23 | -4.5 |
| | NCI-H322M | -4.0 |
| | NCI-H460 | -4.0 |
| | NCI-H522 | -4.0 |
| Colon | COLO 205 | -4.0 |
| | HCC-2998 | -4.0 |
| | HCT-116 | -4.0 |
| | HCT-15 | -4.0 |
| | HT29 | -4.0 |
| | KM12 | -4.0 |
| | SW-620 | -4.0 |
| Central Nervous System | SF-268 | -4.0 |
| | SF-295 | -4.6 |
| | SF-539 | -4.3 |
| | SNB-19 | -4.5 |
| | SNB-75 | -4.7 |
| | U251 | -4.5 |
| Melanoma | MALME-3M | -4.0 |
| | M14 | -4.0 |
| | MDA-MB-435 | -4.0 |
| | SK-MEL-2 | -4.0 |
| | SK-MEL-28 | -4.0 |
| | SK-MEL-5 | -4.0 |
| | UACC-257 | -4.0 |
| | UACC-62 | -4.0 |
| Ovarian | IGROV1 | -4.0 |
| | OVCAR-3 | -4.4 |
| | OVCAR-4 | -4.0 |
| | OVCAR-5 | -4.0 |
| | OVCAR-8 | -4.0 |
| | NCI/ADR-RES | -4.0 |
| | SK-OV-3 | -4.6 |
| Renal | 786-0 | -4.6 |
| | A498 | -4.4 |
| | ACHN | -4.0 |
| | CAKI-1 | -4.0 |
| | RXF 393 | -4.6 |
| | SN12C | -4.0 |
| | TK-10 | -4.7 |
| | UO-31 | -4.0 |
| Prostate | PC-3 | -4.0 |
| | DU-145 | -4.0 |
| Breast | MCF7 | -4.0 |
| | MDA-MB-231/ATCC | -4.5 |
| | HS 578T | -4.2 |
| | MDA-N | -4.0 |
| | BT-549 | -4.3 |
| | T-47D | -4.0 |



## Compound K

$GI_{50}$ Mean Graph for Compound 306698
NCI Cancer Screen Current Data, May 2009
Average $GI_{50}$ over all cell lines is 3.25E-6

| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | K-562 | -5.4 |
| | RPMI-8226 | -5.7 |
| Non-Small Cell Lung | A549/ATCC | -5.5 |
| | EKVX | -5.6 |
| | HOP-62 | -5.4 |
| | NCI-H226 | -5.5 |
| | NCI-H23 | -5.6 |
| | NCI-H322M | -5.6 |
| | NCI-H460 | -5.6 |
| | NCI-H522 | -5.5 |
| Colon | COLO 205 | -5.2 |
| | HCC-2998 | -5.6 |
| | HCT-116 | -5.6 |
| | HCT-15 | -5.5 |
| | HT29 | -5.5 |
| | KM12 | -5.5 |
| | SW-620 | -5.4 |
| Central Nervous System | SF-268 | -5.5 |
| | SF-295 | -5.4 |
| | SF-539 | -5.3 |
| | SNB-19 | -5.4 |
| | SNB-75 | -5.6 |
| | U251 | -5.5 |
| Melanoma | MALME-3M | -5.5 |
| | M14 | -5.4 |
| | MDA-MB-435 | -5.5 |
| | SK-MEL-2 | -5.8 |
| | SK-MEL-28 | -5.2 |
| | SK-MEL-5 | -5.6 |
| | UACC-257 | -5.5 |
| | UACC-62 | -5.3 |
| Ovarian | OVCAR-3 | -5.4 |
| | OVCAR-4 | -5.4 |
| | OVCAR-5 | -5.4 |
| | NCI/ADR-RES | -5.6 |
| | SK-OV-3 | -5.5 |
| Renal | 786-0 | -5.4 |
| | A498 | -5.5 |
| | ACHN | -5.4 |
| | CAKI-1 | -5.5 |
| | RXF 393 | -5.7 |
| | SN12C | -5.5 |
| | TK-10 | -5.3 |
| | UO-31 | -5.4 |
| Prostate | PC-3 | -5.7 |
| | DU-145 | -5.5 |
| Breast | MCF7 | -5.5 |
| | MDA-MB-231/ATCC | -5.6 |
| | HS 578T | -5.5 |
| | MDA-N | -5.5 |
| | BT-549 | -5.6 |
| | T-47D | -5.5 |



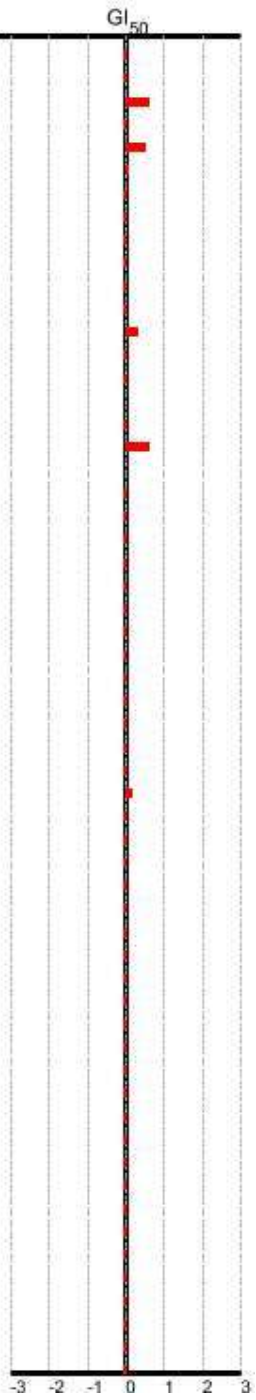
## Compound L

$GI_{50}$ Mean Graph for Compound 351123

NCI Cancer Screen Current Data, May 2009

Average $GI_{50}$ over all cell lines is 9.02E-5

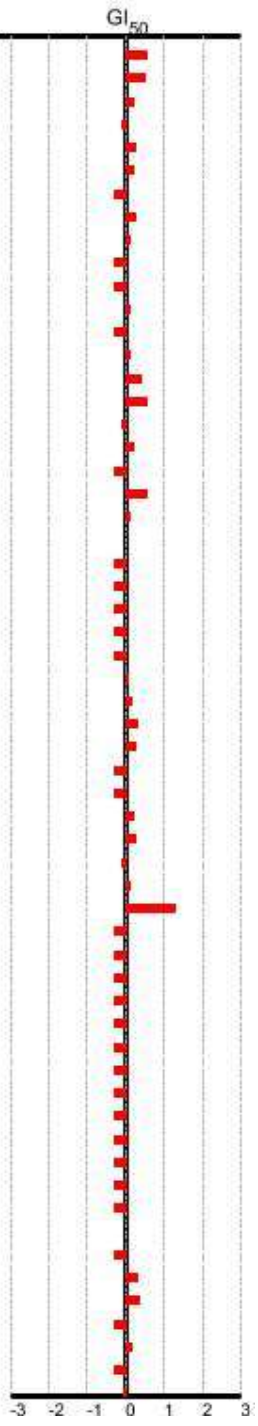
| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | HL-60(TB) | -4.0 |
| | K-562 | -4.0 |
| | MOLT-4 | -4.6 |
| | RPMI-8226 | -4.0 |
| | SR | -4.5 |
| Non-Small Cell Lung | A549/ATCC | -4.1 |
| | EKVX | -4.0 |
| | HOP-62 | -4.0 |
| | HOP-92 | -4.0 |
| | NCI-H226 | -4.0 |
| | NCI-H23 | -4.0 |
| | NCI-H322M | -4.0 |
| | NCI-H460 | -4.4 |
| | NCI-H522 | -4.0 |
| Colon | COLO 205 | -4.0 |
| | HCC-2998 | -4.1 |
| | HCT-116 | -4.0 |
| | HCT-15 | -4.6 |
| | HT29 | -4.1 |
| | KM12 | -4.0 |
| | SW-620 | -4.0 |
| Central Nervous System | SF-268 | -4.0 |
| | SF-295 | -4.0 |
| | SF-539 | -4.0 |
| | SNB-19 | -4.0 |
| | SNB-75 | -4.0 |
| | U251 | -4.0 |
| Melanoma | LOX IMVI | -4.0 |
| | M14 | -4.0 |
| | MDA-MB-435 | -4.0 |
| | SK-MEL-2 | -4.0 |
| | SK-MEL-28 | -4.0 |
| | SK-MEL-5 | -4.2 |
| | UACC-257 | -4.0 |
| | UACC-62 | -4.0 |
| Ovarian | IGROV1 | -4.0 |
| | OVCAR-3 | -4.0 |
| | OVCAR-4 | -4.0 |
| | OVCAR-5 | -4.0 |
| | OVCAR-8 | -4.0 |
| | NCI/ADR-RES | -4.0 |
| | SK-OV-3 | -4.0 |
| Renal | 786-0 | -4.0 |
| | A498 | -4.0 |
| | ACHN | -4.0 |
| | CAKI-1 | -4.0 |
| | RXF 393 | -4.0 |
| | SN12C | -4.0 |
| | TK-10 | -4.0 |
| | UO-31 | -4.0 |
| Prostate | PC-3 | -4.0 |
| | DU-145 | -4.0 |
| Breast | MCF7 | -4.0 |
| | MDA-MB-231/ATCC | -4.0 |
| | HS 578T | -4.0 |
| | MDA-N | -4.0 |
| | BT-549 | -4.0 |
| | T-47D | -4.0 |



## Compound M

$GI_{50}$ Mean Graph for Compound 402959
NCI Cancer Screen Current Data, May 2009
Average $GI_{50}$ over all cell lines is 5.5E-5

| Cell Panel | Cell Line | Log $GI_{50}$ |
|---|---|---|
| Leukemia | CCRF-CEM | -4.8 |
| | HL-60(TB) | -4.7 |
| | K-562 | -4.5 |
| | MOLT-4 | -4.2 |
| | RPMI-8226 | -4.5 |
| | SR | -4.5 |
| Non-Small Cell Lung | A549/ATCC | -4.0 |
| | EKVX | -4.5 |
| | HOP-62 | -4.4 |
| | HOP-92 | -4.0 |
| | NCI-H226 | -4.0 |
| | NCI-H23 | -4.4 |
| | NCI-H322M | -4.0 |
| | NCI-H460 | -4.4 |
| | NCI-H522 | -4.6 |
| Colon | COLO 205 | -4.8 |
| | HCC-2998 | -4.2 |
| | HCT-116 | -4.5 |
| | HCT-15 | -4.0 |
| | HT29 | -4.8 |
| | KM12 | -4.4 |
| | SW-620 | -4.3 |
| Central Nervous System | SF-268 | -4.0 |
| | SF-295 | -4.0 |
| | SF-539 | -4.0 |
| | SNB-19 | -4.0 |
| | SNB-75 | -4.0 |
| | U251 | -4.3 |
| Melanoma | MALME-3M | -4.4 |
| | M14 | -4.6 |
| | MDA-MB-435 | -4.5 |
| | SK-MEL-2 | -4.0 |
| | SK-MEL-28 | -4.0 |
| | SK-MEL-5 | -4.5 |
| | UACC-257 | -4.5 |
| | UACC-62 | -4.2 |
| Ovarian | IGROV1 | -4.4 |
| | OVCAR-3 | -5.5 |
| | OVCAR-4 | -4.0 |
| | OVCAR-5 | -4.0 |
| | OVCAR-8 | -4.0 |
| | NCI/ADR-RES | -4.0 |
| | SK-OV-3 | -4.0 |
| Renal | 786-0 | -4.0 |
| | A498 | -4.0 |
| | ACHN | -4.0 |
| | CAKI-1 | -4.0 |
| | RXF 393 | -4.0 |
| | SN12C | -4.0 |
| | TK-10 | -4.0 |
| | UO-31 | -4.0 |
| Prostate | PC-3 | -4.3 |
| | DU-145 | -4.0 |
| Breast | MCF7 | -4.6 |
| | MDA-MB-231/ATCC | -4.6 |
| | HS 578T | -4.0 |
| | MDA-N | -4.4 |
| | BT-549 | -4.0 |
| | T-47D | -4.2 |




*Sample Availability:* Samples are available from the authors.

**S2.** Diagram showing the interaction between the EGFR-TK and the eight candidate compounds using Ligand Interactions module in MOE package.

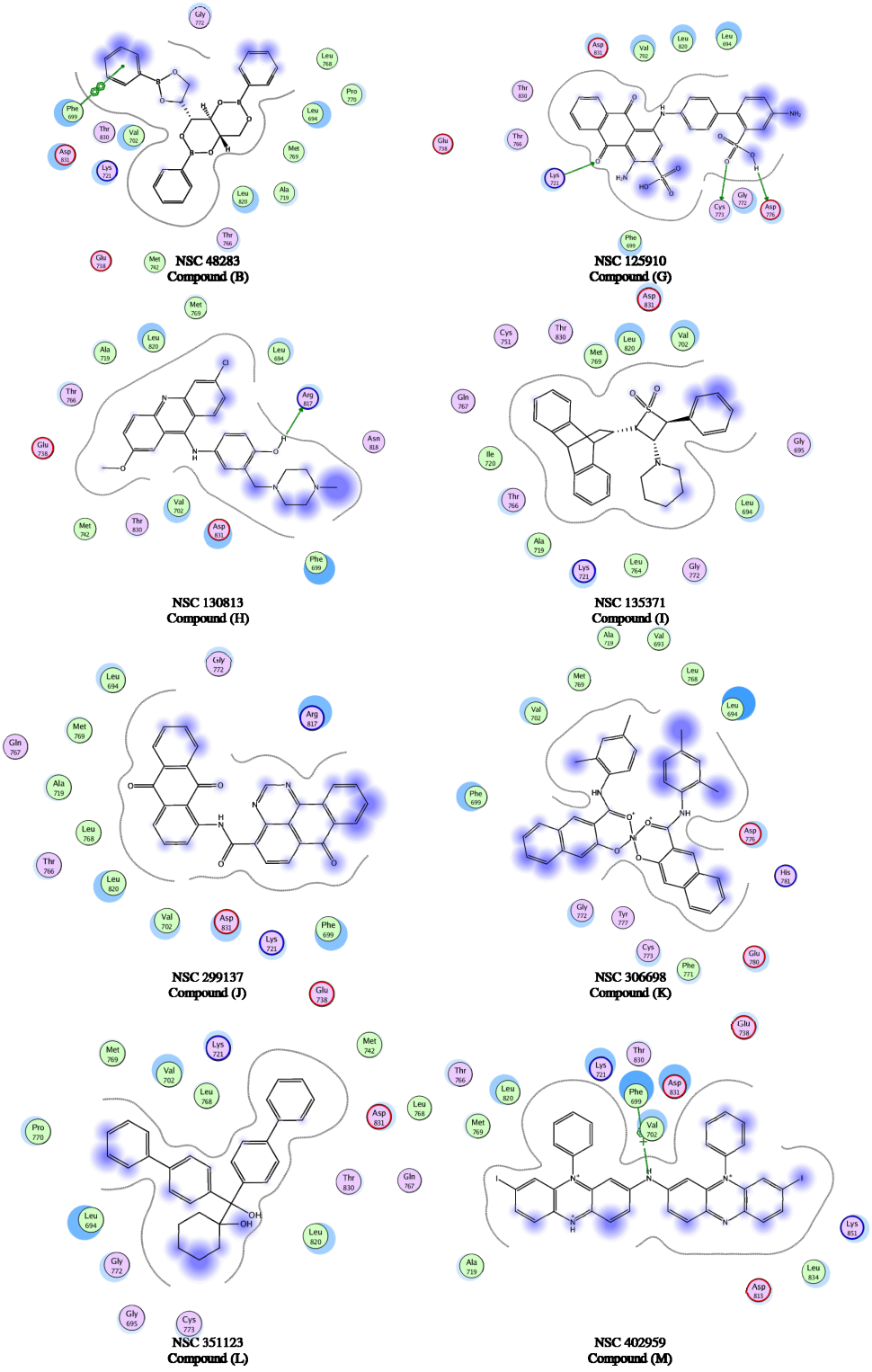
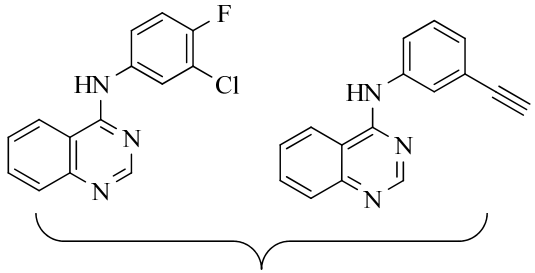


**Table S1.** The binding free energy and the score fitness value of the 3 known inhibitors from GOLD docking and scoring calculations.

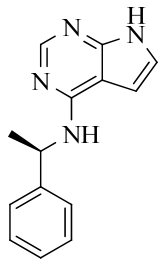
| Compounds | NSC no. | RMSD (Å) All heavy atom | RMSD (Å) Core structure | KCS score fitness value | GOLD Chemscore Hbond§ | GOLD Chemscore Lipo‡ | GOLD Chemscore DE Clash* | ΔG(kJ/mol) | Average $GI_{50}$† (μg/ml) |
|---|---|---|---|---|---|---|---|---|---|
| Gefitinib | 715055 | 3.67 | 0.81 | 30.05 | 0.70 | 229.62 | 0.26 | -31.00 | 3.24×10-6 |
| Erlotinib | 718781 | 1.74 | 0.34 | 28.65 | 0.61 | 237.36 | 1.49 | -31.03 | 5.51×10-6 |
| AEE788 | N/A | 1.37 | 0.68 | 32.55 | 1.65 | 220.57 | 0.80 | -34.04 | N/A |

†The average $GI_{50}$ overall cell line from NCI Cancer Screen Current Data, May 2009. The $GI_{50}$ means drug concentration causing 50% cell-growth inhibition; § and ‡ refer to protein-ligand H-bond and lipophilic contribution to the chemscore values, respectively, and * refer to protein-ligand clash penalty to the chemscore value.

**S3.** The core structure of the known inhibitors that used for calculate the RMSD values, the aniline-quinazoline group from gefitinib and erlotinib and the phenethyl-amino-pyrrolopyrimidine group from AEE 788.




anilino-quinazoline group from gefitinib (left) and erlotinib (right)




core structure of AEE 788

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