

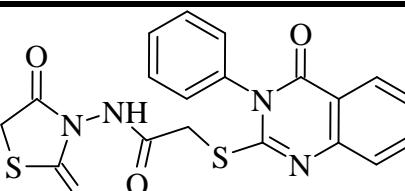
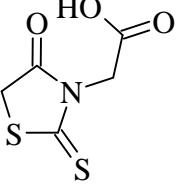
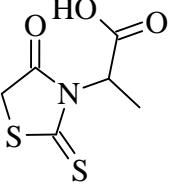
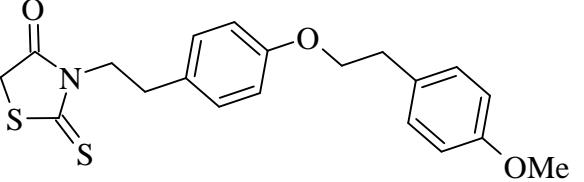
Supplemental materials for

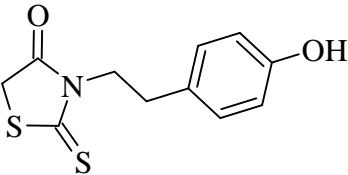
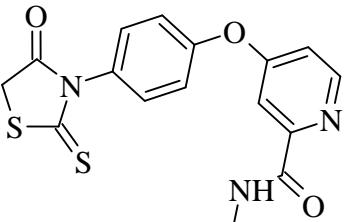
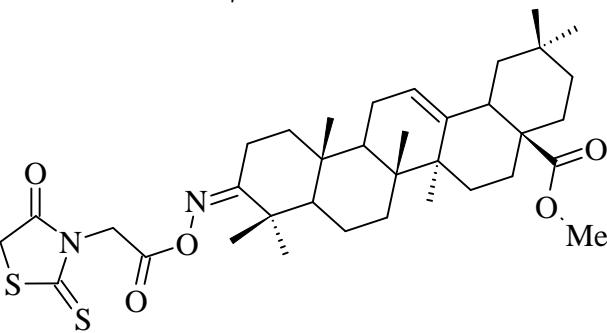
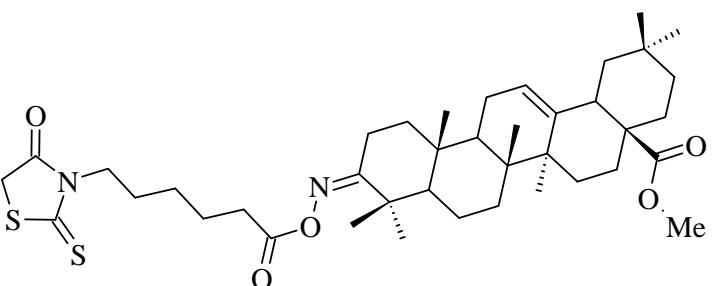
Anticancer profile of rhodanines: structure-activity relationship (SAR) and molecular targets. A review

Jacek Szczepański, Helena Tuszeńska and Nazar Trotsko *

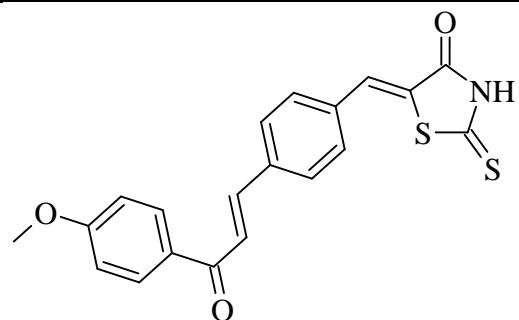
Chair and Department of Organic Chemistry, Faculty of Pharmacy, Medical University of Lublin, 4a Chodźki Street, 20-093 Lublin, Poland; jaacek.szczeński.93@gmail.com
(J.S.); tuszeńska.helena93@gmail.com (H.T.); nazar.trotsko@umlub.pl (N.T.)
* Correspondence: nazar.trotsko@umlub.pl (N.T.); Tel.: +48 81 448 7244

Table S1. The most potent 3-or 5-substituted, and 3,5-disubstituted rhodanine derivatives as anticancer agents

Nr.	Structure	Cell lines	IC ₅₀ , % inhibition	References
1		MCF-7	64.4%	[25]
2		K-562	14.6 µg/mL	[26]
3		K-562, HeLa	11.1 µg/mL, < 200 µg/mL	[25,26]
4		HCT 116	10 µM	[28]

5		MDA-MB231, HCT 116, Caco 2	2 μM, 2 μM, 3 μM	[28]
6		A549	43.6 μM	[12]
7		CCRF-CEM/L	56.34%	[29]
8		T-47D/BC	76.91%	[29]

9

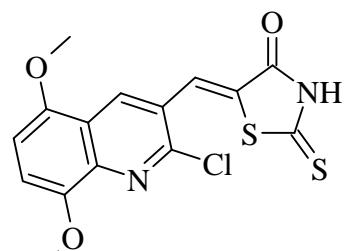


HeLa,
HT29,
A549,
MCF-7

28.3 μ M,
24.5 μ M,
26.6 μ M,
28.6 μ M

[11]

10

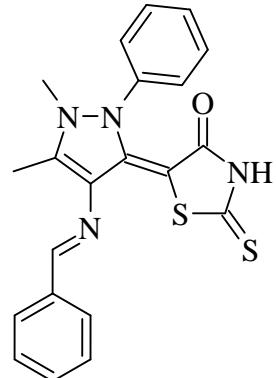


HGC,
DU-145,
MCF-7

7.2 μ M,
15.3 μ M,
9.5 μ M

[30]

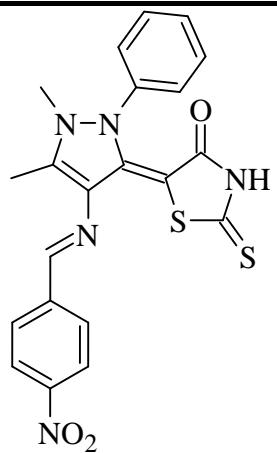
11



MCF-7

7.67 μ g/mL

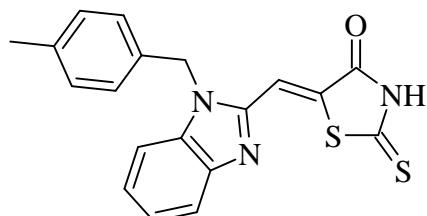
[34]

12

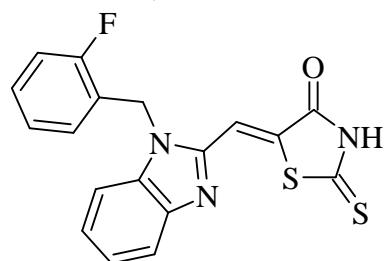
MCF-7

11.7 µg/mL

[34]

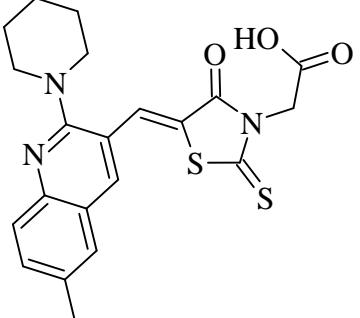
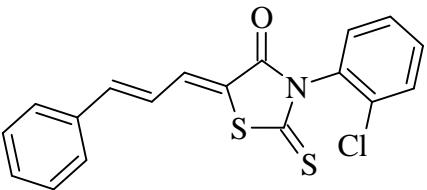
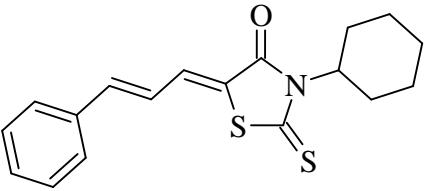
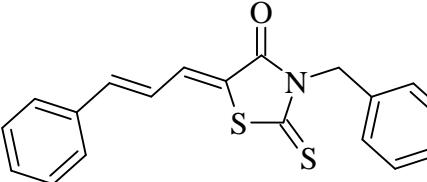
13HL-60,
A549,
Raji,
MDA-MB2012.66 µM,
5.31 µM,
4.48 µM,
6.42 µM

[35]

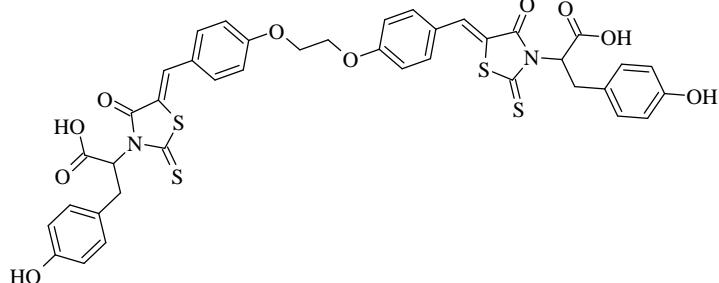
14HL-60,
A549,
Raji,
MDA-MB2018.42 µM,
> 50 µM,
25.48 µM,
21.33 µM

[35]

15		HT-1080, HL-60, K-562, AG01523	8.7 μ M, 1.2 μ M, 1.5 μ M, > 100 μ M	[36]
16		CCRF-CEM, RPMI-8226, HOP-92, Normal human cell line	GI_{50} = 2.50 μ M, GI_{50} = 2.52 μ M, GI_{50} = 0.62 μ M, LC_{50} > 100 μ M	[32]
17		HeLa S3, Hep G2	EC_{50} = 7.9 μ M, EC_{50} = 6.1 μ M	[33]

18		HGC, MNK-74	11.2 μ M, 13.9 μ M	[30]
19		MCF-7	81%	[36]
20		MCF-7	77%	[36]
21		MCF-7	71%	[36]

22

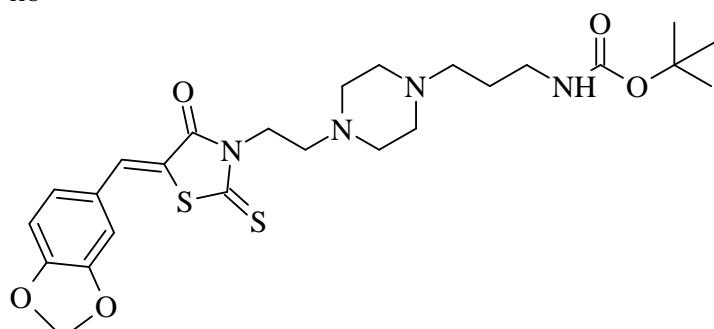


A549

 $CTC_{50} = 3.6 \mu\text{g/mL}$

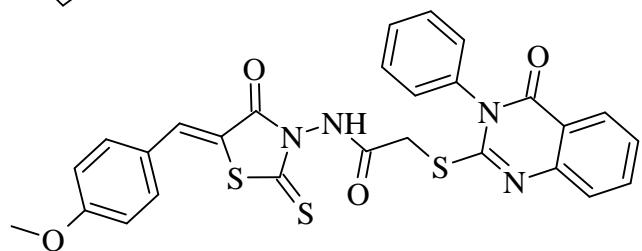
[37]

23

Huh7 D12,
Caco 28 μM ,
8 μM

[13]

24

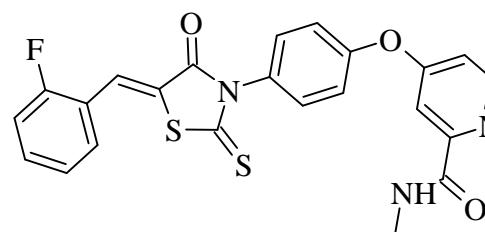


MCF-7

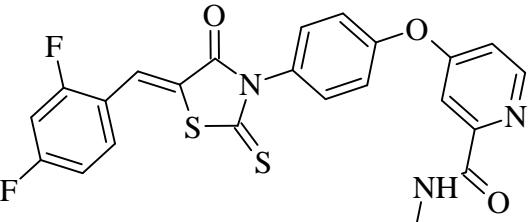
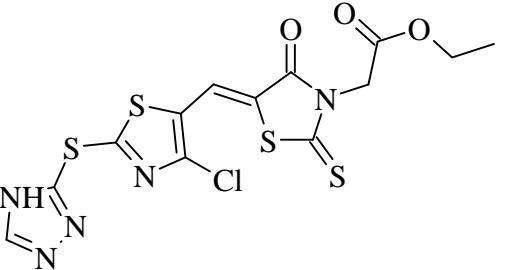
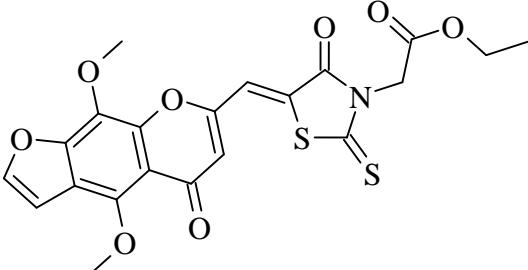
82.5%

[25]

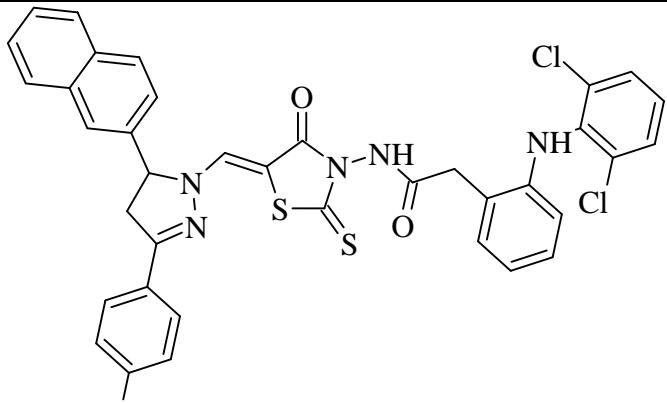
25

A549,
H460,
HT290.8 μM ,
1.3 μM ,
2.8 μM

[12]

26		A549, H460, HT29	3.1 μ M, 0.3 μ M, 2.8 μ M	[12]
27		Huh7, MCF-7	4.67 μ M, 2.30 μ M	[38]
28		MCF-7, MDA-MB-231, Huh7	EC ₅₀ = 1.732 μ M, EC ₅₀ = 2.912 μ M, EC ₅₀ = 3.797 μ M	[39]

29

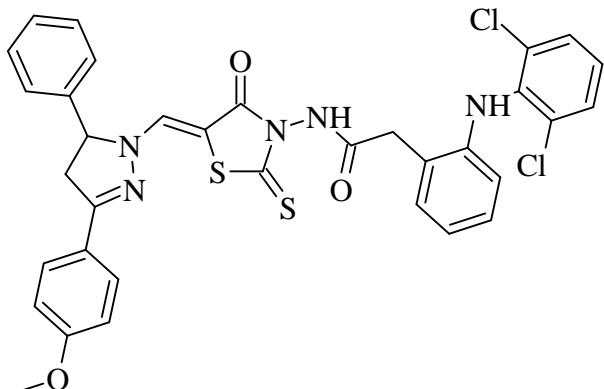


panel of approximately
sixty cancer cell lines¹

GP mean= 22.40%

[10]

30

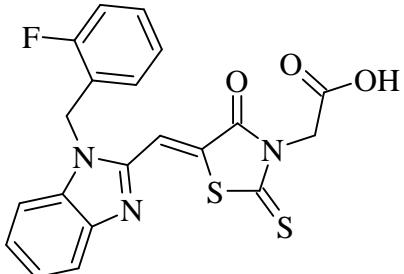


panel of approximately
sixty cancer cell lines¹

GP mean= 99.30%

[10]

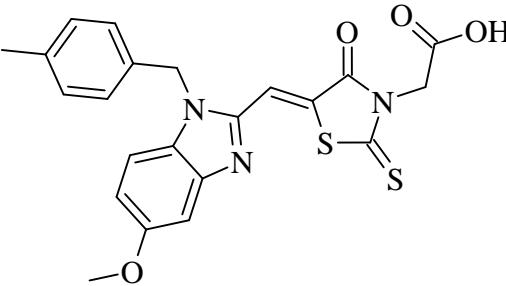
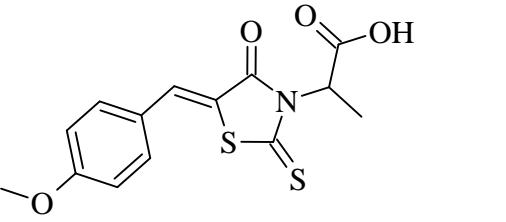
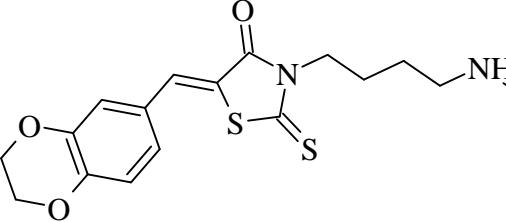
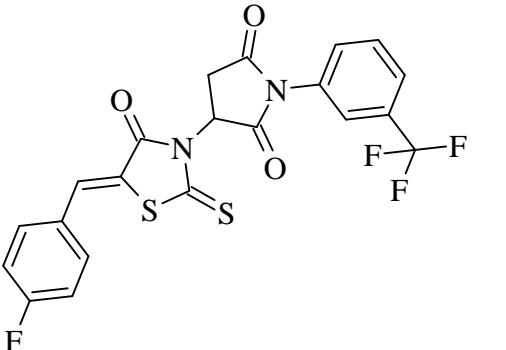
31



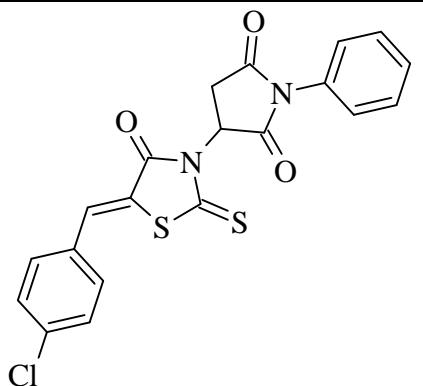
HL-60,
MDA-MB-201,
Raji,
A549

0.21 μ M,
0.33 μ M,
1.23 μ M,
2.67 μ M

[35]

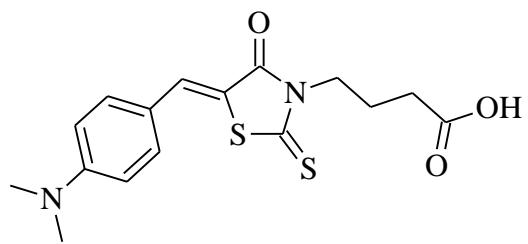
32		HL-60, MDA-MB-201, Raji, A549	0.77 μ M, 1.22 μ M, 1.79 μ M, 5.68 μ M	[35]
33		HeLa	52.00%	[27]
34		Huh7 D12, HaCat, MDA-MB231, normal fibroblasts	9 μ M, 8 μ M, 9 μ M, > 25 μ M	[40]
35		Dami	35.10%	[41]

36

Dami,
HL-6044.75%,
40.30%

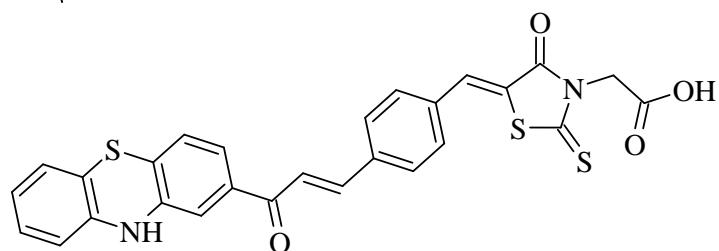
[41]

37

A2780,
A2780cisR4.4 nM,
3.3 nM

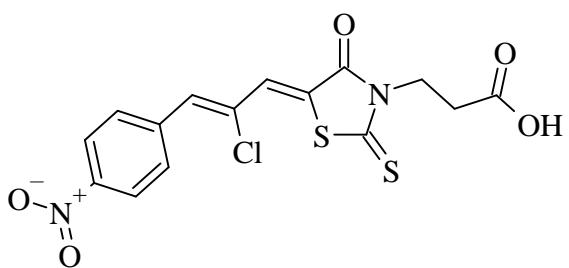
[42]

38

K562,
K5628.79 $\mu\text{g/mL}$ - T.B. assay,
19.62 $\mu\text{g/mL}$ - MTT assay

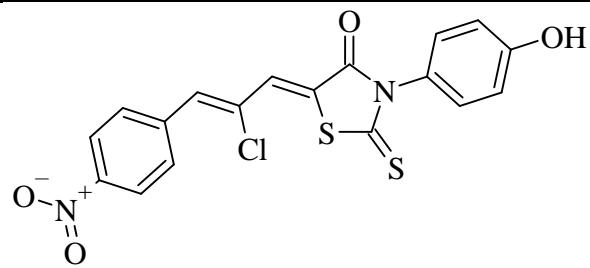
[43]

39

60 tumor cell lines MG_MID² $\text{GI}_{50}= 1.57 \mu\text{M}$

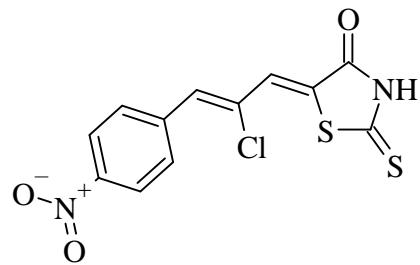
[44]

40

60 tumor cell lines MG_MID² $GI_{50} = 2.8 \mu\text{M}$

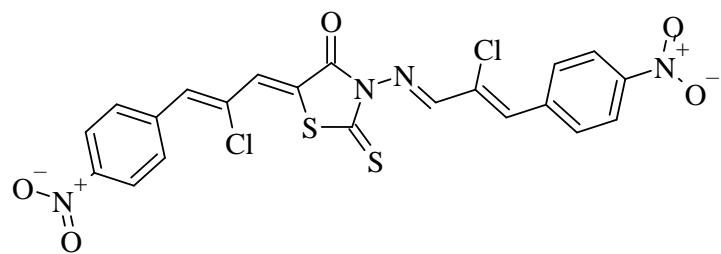
[44]

41

60 tumor cell lines MG_MID² $GI_{50} = 4.79 \mu\text{M}$

[44]

42

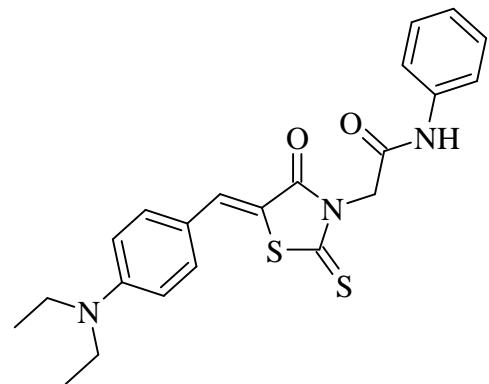


60 tumor cell lines MG_MID

 $GI_{50} = 18 \mu\text{M}$

[44]

43

A549,
NRK-52E $7 \mu\text{M},$
 $14.7 \mu\text{M}$

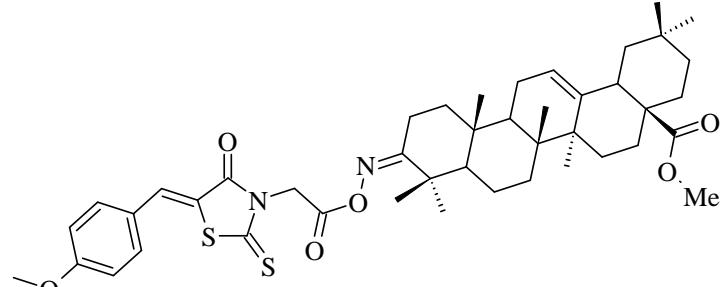
[46]

44

BT-549/BC

67.36%

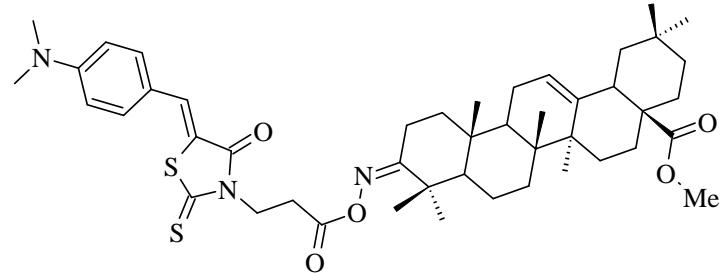
[29]

**45**

IGROV1/OC

82.21%

[29]



MG_MID - mean graph midpoint, arithmetical mean value for all tested cell lines.

^{1,2} panel of approximately sixty cancer cell lines and 60 tumor cell lines MG_MID the next cell lines were used: leukemia (CCRF-CEM, HL-60, K562, MOLT-4, RPMI-8226, SR), NSC lung cancer (A549, EKVV, HOP-62, HOP-92, NCI-H266, NCI-H23, NCI-H322M, NCI-H460, NCI-H522), colon cancer (COLO 205, HCT 116, HCT-15, HT29, KM12, SW-620, HCC-2998), CNS cancer (SF-268, SF-295, SF-539, SNB-19, SNB-75, U251), melanoma (LOX IMVI, MALME-3M, M14, MDA-MB-435, UACC-62, UACC-257, SK-MEL-2, SK-MEL-5, SK-MEL-28), 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, RXF 393, SN12C, TK-10, UO-31), prostate cancer (PC-3, DU-145), breast cancer (MCF-7, MDA-MB-231, HS 578T, BT-549, T-47D, MDA-MB-468).