

## Supplementary Data

A	<b>CNS Cancer</b>		
	<b>Drug</b>	<b>Indication</b>	<b>Mechanism of Action</b>
	Temozolomide	glioblastoma concomitantly with radiotherapy and refractory anaplastic astrocytoma	DNA and RNA Alkylation
	Lomustine	primary and metastatic brain tumors	DNA and RNA Alkylation
	Carmustine	brain tumors glioblastoma, brainstem glioma, medulloblastoma, astrocytoma, ependymoma, and metastatic brain tumors	DNA and RNA alkylation; Enzymatic Carbamoylation
B	Everolimus	subependymal giant cell astrocytoma (SEGA) that requires therapeutic intervention	mTOR inhibitor; HIF inhibitor
	<b>Prostate Cancer</b>		
	<b>Drug</b>	<b>Indication</b>	<b>Mechanism of Action</b>
	Rucaparib	metastatic Castration-Resistant Prostate Cancer (mCRPC)	PARP Inhibitor
	Enzalutamide	mCRPC and metastatic Castration-Sensitive Prostate Cancer (mCSPC)	Androgen Receptor Inhibitor
	Abiraterone Acetate	mCRPC and mCSPC	CYP17 Inhibitor
	<u>Cabazitaxel</u>	mCRPC	Antimicrotubular Antineoplastic Agent
	Docetaxel	mCRPC	Antimicrotubular Antineoplastic Agent
	Leuprolide Acetate	palliative treatment of advanced prostate cancer	GnRH Agonist
	Mitoxantrone	advanced prostate cancer not responding to hormone treatment	Topoisomerase Inhibitor
C	Olaparib	mCRPC	PARP Inhibitor
	<b>Non-Small Cell Lung Cancer</b>		
	<b>Drug</b>	<b>Indication</b>	<b>Mechanism of Action</b>
	Alectinib	ALK-positive metastatic NSCLC	ALK and RET Inhibitor
	Pemetrexed	locally advanced or metastatic, non-squamous NSCLC	Antimetabolite
	Carboplatin	chemotherapeutic treatment for NSCLC	Alkylating Agent
	Crizotinib	ALK or ROS1-positive metastatic NSCLC	ALK and ROS1 Inhibitor
	Docetaxel	locally advanced or metastatic NSCLC after failure of prior platinum-based chemotherapy	Taxoid
	Doxorubicin	chemotherapeutic treatment for NSCLC	Anthracycline Antibiotic
	Erlotinib	EGFR gene mutated metastatic NSCLC	EGFR Tyrosine Kinase Inhibitor
	Everolimus	unresectable, locally advanced, or metastatic NSCLC	mTOR Kinase Inhibitor
	Gefitinib	EGFR gene mutated metastatic NSCLC; in combination with Everolimus	EGFR Tyrosine Kinase Inhibitor
	Lorlatinib	ALK-positive metastatic NSCLC	ALK and ROS1 Inhibitor
	Mechlorethamine	NSCLC	Alkylating Agent
	Trametinib	in combination with dabrafenib for BRAF V600E mutated metastatic NSCLC	MEK Kinase Inhibitor
	Methotrexate	NSCLC	Folate Analog Metabolic Inhibitor
	Paclitaxel	chemotherapeutic treatment for NSCLC	Taxane; Plant Alkaloid
	Vinorelbine	alone or in combination with Cisplatin for locally advanced or metastatic NSCLC	Plant Alkaloid

**Table S1** The indication and mechanism of FDA-approved anticancer drugs for (A) CNS cancer, (B) prostate cancer (C) NSCLC. Literature review of indication, mechanism of FDA-approved CNS, prostate, NSCLC cancers.

A

	Cell Lines	NMI	Temozolomide	Lomustine	Carmustine	Everolimus	Max	Min	Max-Min
GI50 (µM)	SF-268	1.820	100.000	20.900	31.600	0.269	100.000	0.269	99.731
Min-max normalization		0.016	1.000	0.207	0.314	0.000	(GI50 - Min) / (Max - Min)		
		e.g. Min-max normalization of GI50 of NMI: (1.820-0.269)/99.731=0.016							
GI50 (µM)	SF-295	1.910	100.000	91.200	39.800	0.010	100.000	0.010	99.990
Min-max normalization		0.019	1.000	0.912	0.398	0.000	(GI50 - Min) / (Max - Min)		
GI50 (µM)	SF-539	1.200	100.000	16.600	31.600	0.010	100.000	0.010	99.990
Min-max normalization		0.012	1.000	0.166	0.316	0.000	(GI50 - Min) / (Max - Min)		
GI50 (µM)	SNB-19	1.120	100.000	100.000	63.100	0.257	100.000	0.257	99.743
Min-max normalization		0.009	1.000	1.000	0.630	0.000	(GI50 - Min) / (Max - Min)		
GI50 (µM)	SNB-75	1.290	63.000	23.400	50.100	0.010	63.000	0.010	62.990
Min-max normalization		0.020	1.000	0.371	0.795	0.000	(GI50 - Min) / (Max - Min)		
GI50 (µM)	U251	0.740	100.000	15.800	31.600	0.011	100.000	0.011	99.989
Min-max normalization		0.007	1.000	0.158	0.316	0.000	(GI50 - Min) / (Max - Min)		
TGI (µM)	SF-268	6.760	100.000	57.500	100.000	20.900	100.000	6.760	93.240
Min-max normalization		0.000	1.000	0.544	1.000	0.152	(TGI - Min) / (Max - Min)		
TGI (µM)	SF-295	4.070	100.000	100.000	251.000	17.300	251.000	4.070	246.930
Min-max normalization		0.000	0.388	0.388	1.000	0.054	(TGI - Min) / (Max - Min)		
TGI (µM)	SF-539	2.690	100.000	33.900	100.000	17.300	100.000	2.690	97.310
Min-max normalization		0.000	1.000	0.321	1.000	0.150	(TGI - Min) / (Max - Min)		
TGI (µM)	SNB-19	3.630	100.000	100.000	251.000	19.500	251.000	3.630	247.370
Min-max normalization		0.000	0.390	0.390	1.000	0.064	(TGI - Min) / (Max - Min)		
TGI (µM)	SNB-75	3.890	100.000	64.600	126.000	14.100	126.000	3.890	122.110
Min-max normalization		0.000	0.787	0.497	1.000	0.084	(TGI - Min) / (Max - Min)		
TGI (µM)	U251	2.090	100.000	51.300	63.100	18.200	100.000	2.090	97.910
Min-max normalization		0.000	1.000	0.503	0.623	0.165	(TGI - Min) / (Max - Min)		
LC50 (µM)	SF-268	100.000	100.000	100.000	251.000	53.700	251.000	53.700	197.300
Min-max normalization		0.235	0.235	0.235	1.000	0.000	(LC50 - Min) / (Max - Min)		
LC50 (µM)	SF-295	8.710	100.000	100.000	251.000	63.100	251.000	8.710	242.290
Min-max normalization		0.000	0.377	0.377	1.000	0.224	(LC50 - Min) / (Max - Min)		
LC50 (µM)	SF-539	6.030	100.000	70.800	251.000	41.700	251.000	6.030	244.970
Min-max normalization		0.000	0.384	0.264	1.000	0.146	(LC50 - Min) / (Max - Min)		
LC50 (µM)	SNB-19	28.200	100.000	100.000	251.000	44.700	251.000	28.200	222.800
Min-max normalization		0.000	0.322	0.322	1.000	0.074	(LC50 - Min) / (Max - Min)		
LC50 (µM)	SNB-75	13.800	100.000	100.000	251.000	38.900	251.000	13.800	237.200
Min-max normalization		0.000	0.363	0.363	1.000	0.106	(LC50 - Min) / (Max - Min)		
LC50 (µM)	U251	5.010	100.000	100.000	126.000	42.700	126.000	5.010	120.990
Min-max normalization		0.000	0.785	0.785	1.000	0.312	(LC50 - Min) / (Max - Min)		
Cumulative Score	SF-268	0.250	2.235	0.986	2.314	0.152	GI50+TGI+LC50 Min-max normalization		
	SF-295	0.019	1.765	1.677	2.398	0.278			
	SF-539	0.012	2.384	0.751	2.316	0.296			
	SNB-19	0.009	1.712	1.712	2.630	0.138			
	SNB-75	0.020	2.150	1.232	2.795	0.189			
	U251	0.007	2.785	1.446	1.939	0.476			
		e.g. Cumulative score of min-max normalization of GI50, TGI and LC50 of NMI: 0.016+0.000+0.235=0.250							

B

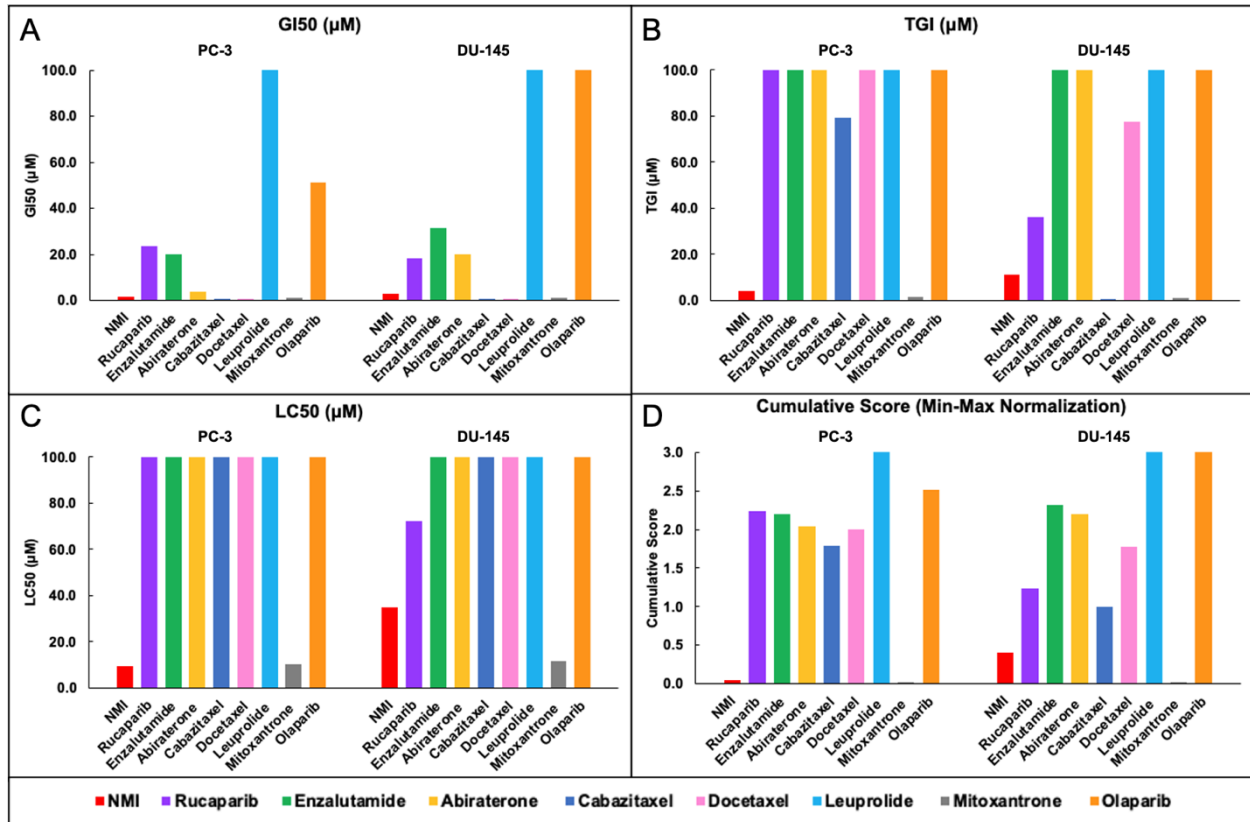
	Cell Lines	NMI	Rucaparib	Enzastamide	Abiraterone Acetate	Cabazitaxel	Docetaxel	Leuprolide Acetate	Mitoxantrone	Olaparib	Max	Min	Max-Min
GI50 (µM)	PC-3	1.700	23.400	20.000	3.980	0.010	0.010	100.000	0.141	51.286	100.000	0.010	99.990
Min-max normalization		0.017	0.234	0.200	0.040	0.000	0.000	1.000	0.001	0.513	(GI50 - Min) / (Max - Min)		
		e.g. Min-max normalization of GI50 of NMI: (1.700-0.010)/99.99=0.017											
GI50 (µM)	DU-145	3.020	18.200	31.800	20.000	0.010	0.010	100.000	0.018	100.000	100.000	0.010	99.990
Min-max normalization		0.030	0.182	0.316	0.200	0.000	0.000	1.000	0.000	1.000	(GI50 - Min) / (Max - Min)		
TGI (µM)	PC-3	3.980	100.000	100.000	100.000	79.400	100.000	100.000	1.445	100.000	100.000	1.445	98.555
Min-max normalization		0.026	1.000	1.000	1.000	0.791	1.000	1.000	0.000	1.000	(TGI - Min) / (Max - Min)		
TGI (µM)	DU-145	11.000	36.300	100.000	100.000	0.010	77.625	100.000	0.468	100.000	100.000	0.010	99.990
Min-max normalization		0.110	0.363	1.000	1.000	0.000	0.776	1.000	0.005	1.000	(TGI - Min) / (Max - Min)		
LC50 (µM)	PC-3	9.550	100.000	100.000	100.000	100.000	100.000	100.000	10.471	100.000	100.000	9.550	90.450
Min-max normalization		0.000	1.000	1.000	1.000	1.000	1.000	1.000	0.010	1.000	(LC50 - Min) / (Max - Min)		
LC50 (µM)	DU-145	34.700	72.400	100.000	100.000	100.000	100.000	100.000	11.482	100.000	100.000	11.482	88.518
Min-max normalization		0.262	0.888	1.000	1.000	1.000	1.000	1.000	0.000	1.000	(LC50 - Min) / (Max - Min)		
Cumulative Score	PC-3	0.043	2.234	2.200	2.040	1.791	2.000	3.000	0.011	2.513	GI50+TGI+LC50 Min-max normalization		
	DU-145	0.402	1.233	2.316	2.200	1.000	1.776	3.000	0.005	3.000			
		e.g. Cumulative score of min-max normalization of GI50, TGI and LC50 of NMI: 0.017+0.026+0.000+0.043											

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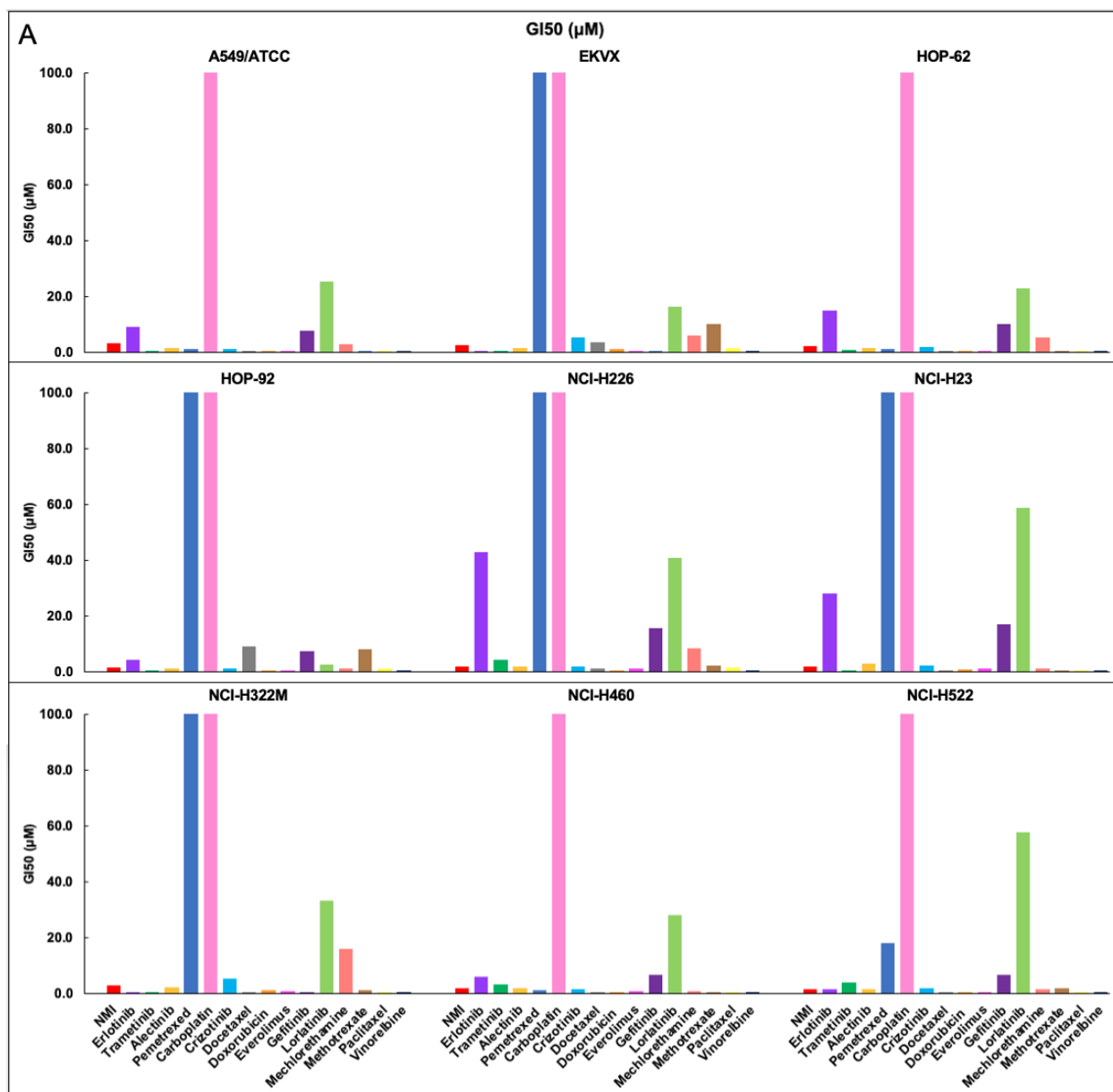
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C

Cell Line	NMI	Griseofulvin	Trametinib	Alectinib	Pembrolizumab	Carboplatin	Cisplatin	Doxorubicin	Doxorubicin	Etoposide	Gefitinib	Lorazepam	Mechlorethamine	Methotrexate	Paclitaxel	Vincristine	Max	Min	Max-Min	
G50 (µM)	3.220	9.120	0.030	1.350	0.590	100.000	1.170	0.010	0.063	0.010	1.590	25.119	2.818	0.010	0.011	0.019	100.000	0.010	99.990	
Min-max normalization	0.032	0.091	0.000	0.013	0.006	1.000	0.012	0.000	0.001	0.000	0.016	0.251	0.028	0.000	0.000	0.000	(Min - Max) / (Max - Min)			
e.g. Min-max normalization of G50 of NMI: $(3.220 - 0.010) / (99.990 - 0.032)$																				
G50 (µM)	2.420	0.191	0.013	1.550	100.000	100.000	5.130	3.720	0.420	0.010	0.045	16.218	6.026	10.000	0.917	0.010	100.000	0.010	99.990	
Min-max normalization	0.024	0.002	0.000	0.015	1.000	1.000	0.051	0.037	0.004	0.000	0.000	0.162	0.060	0.100	0.010	0.000	(Min - Max) / (Max - Min)			
G50 (µM)	2.100	15.100	0.251	0.950	0.720	100.000	1.910	0.010	0.065	0.010	10.200	22.909	5.245	0.016	0.031	0.015	100.000	0.010	99.990	
Min-max normalization	0.021	0.151	0.002	0.005	0.007	1.000	0.019	0.000	0.001	0.000	0.102	0.229	0.052	0.000	0.000	0.000	(Min - Max) / (Max - Min)			
G50 (µM)	1.570	4.270	0.010	0.390	100.000	100.000	0.560	9.120	0.100	0.020	1.410	2.512	0.372	1.943	0.525	0.047	100.000	0.010	99.990	
Min-max normalization	0.016	0.043	0.000	0.004	1.000	1.000	0.006	0.091	0.001	0.000	0.014	0.025	0.004	0.019	0.005	0.000	(Min - Max) / (Max - Min)			
G50 (µM)	1.720	42.700	4.370	1.740	100.000	100.000	1.820	0.360	0.050	0.350	15.500	40.738	0.318	2.344	1.047	0.030	100.000	0.030	99.970	
Min-max normalization	0.011	0.427	0.043	0.017	1.000	1.000	0.018	0.003	0.000	0.003	0.155	0.407	0.003	0.023	0.010	0.000	(Min - Max) / (Max - Min)			
G50 (µM)	1.940	28.200	0.010	2.820	100.000	100.000	2.590	0.010	0.160	0.320	17.000	59.894	1.318	0.097	0.012	0.019	100.000	0.010	99.990	
Min-max normalization	0.019	0.282	0.000	0.028	1.000	1.000	0.021	0.000	0.001	0.003	0.170	0.589	0.013	0.001	0.000	0.000	(Min - Max) / (Max - Min)			
G50 (µM)	3.010	0.095	0.012	2.340	100.000	100.000	5.290	0.010	0.540	0.220	0.095	33.213	15.949	0.427	0.009	0.010	100.000	0.009	99.991	
Min-max normalization	0.030	0.001	0.000	0.023	1.000	1.000	0.052	0.000	0.005	0.002	0.001	0.331	0.159	0.004	0.000	0.000	(Min - Max) / (Max - Min)			
G50 (µM)	1.770	5.930	3.165	1.480	0.250	100.000	0.930	0.010	0.017	0.150	6.610	25.184	0.129	0.006	0.007	0.010	100.000	0.006	99.995	
Min-max normalization	0.018	0.059	0.032	0.015	0.003	1.000	0.009	0.000	0.000	0.001	0.066	0.282	0.001	0.000	0.000	0.000	(Min - Max) / (Max - Min)			
G50 (µM)	1.160	0.955	3.800	1.170	19.200	100.000	1.510	0.010	0.029	0.160	6.760	57.544	0.871	1.445	0.004	0.000	100.000	0.004	99.996	
Min-max normalization	0.012	0.010	0.039	0.012	0.182	1.000	0.015	0.000	0.000	0.002	0.068	0.575	0.009	0.014	0.000	0.000	(Min - Max) / (Max - Min)			
TGI (µM)	13.200	100.000	43.700	3.090	100.000	100.000	11.200	81.300	0.290	22.400	21.900	100.000	32.359	10.000	70.195	33.894	100.000	0.290	99.710	
Min-max normalization	0.129	1.000	0.435	0.028	1.000	1.000	0.109	0.813	0.000	0.222	0.217	1.000	0.322	0.097	0.707	0.337	(Min - Max) / (Max - Min)			
TGI (µM)	12.800	100.000	69.200	5.920	100.000	100.000	19.200	60.000	5.500	21.400	17.400	100.000	25.303	10.000	85.114	19.621	100.000	5.500	94.500	
Min-max normalization	0.071	1.000	0.591	0.015	1.000	1.000	0.134	1.000	0.000	0.165	0.126	1.000	0.230	0.045	0.843	0.139	(Min - Max) / (Max - Min)			
TGI (µM)	57.200	96.200	51.200	2.670	100.000	100.000	7.590	3.900	2.000	22.400	35.500	100.000	31.623	5.495	39.811	24.547	100.000	2.000	98.000	
Min-max normalization	0.035	0.553	0.503	0.006	1.000	1.000	0.097	0.018	0.000	0.208	0.342	1.000	0.302	0.036	0.386	0.230	(Min - Max) / (Max - Min)			
TGI (µM)	3.530	61.700	0.010	3.550	100.000	100.000	0.370	56.200	2.000	20.000	23.400	53.703	3.162	10.000	61.660	0.550	100.000	0.010	99.990	
Min-max normalization	0.035	0.617	0.000	0.035	1.000	1.000	0.033	0.562	0.020	0.200	0.234	0.537	0.032	0.100	0.617	0.005	(Min - Max) / (Max - Min)			
TGI (µM)	4.110	100.000	47.300	4.370	100.000	100.000	7.240	63.100	0.260	23.400	33.100	100.000	39.811	10.000	19.055	36.308	100.000	0.260	99.740	
Min-max normalization	0.039	1.000	0.473	0.041	1.000	1.000	0.070	0.630	0.000	0.232	0.329	1.000	0.397	0.098	0.189	0.361	(Min - Max) / (Max - Min)			
TGI (µM)	5.590	100.000	19.500	39.200	100.000	100.000	15.500	75.900	0.910	22.900	46.800	100.000	5.511	10.000	72.444	41.697	100.000	0.910	99.090	
Min-max normalization	0.042	1.000	0.195	0.393	1.000	1.000	0.147	0.759	0.000	0.222	0.463	1.000	0.097	0.092	0.722	0.412	(Min - Max) / (Max - Min)			
TGI (µM)	10.500	19.900	47.900	10.470	100.000	100.000	15.600	93.300	5.010	0.490	17.000	100.000	45.709	10.000	79.433	25.704	100.000	0.490	99.510	
Min-max normalization	0.105	0.134	0.475	0.100	1.000	1.000	0.182	0.933	0.046	0.000	0.166	1.000	0.454	0.096	0.793	0.253	(Min - Max) / (Max - Min)			
TGI (µM)	5.010	91.200	93.300	4.070	100.000	100.000	5.620	40.700	1.290	19.500	20.000	100.000	2.754	10.000	40.738	0.447	100.000	0.447	99.553	
Min-max normalization	0.046	0.912	0.933	0.036	1.000	1.000	0.052	0.404	0.008	0.191	0.196	1.000	0.023	0.096	0.405	0.000	(Min - Max) / (Max - Min)			
TGI (µM)	3.340	22.400	21.900	3.800	100.000	100.000	4.170	0.100	0.160	17.800	39.900	100.000	2.399	10.000	0.036	31.623	100.000	0.036	99.964	
Min-max normalization	0.033	0.224	0.219	0.038	1.000	1.000	0.041	0.001	0.001	0.178	0.389	1.000	0.024	0.100	0.000	0.316	(Min - Max) / (Max - Min)			
LC50 (µM)	38.300	100.000	89.100	6.920	100.000	100.000	36.300	100.000	100.000	70.800	46.800	100.000	100.000	10.000	91.201	66.059	100.000	6.920	93.080	
Min-max normalization	0.344	1.000	0.891	0.060	1.000	1.000	0.316	1.000	1.000	0.639	0.428	1.000	1.000	0.093	0.905	0.660	(Min - Max) / (Max - Min)			
LC50 (µM)	100.000	100.000	100.000	100.000	100.000	100.000	43.700	100.000	47.900	85.100	51.300	100.000	83.175	10.000	100.000	63.096	100.000	10.000	90.000	
Min-max normalization	1.000	1.000	1.000	1.000	1.000	1.000	0.374	1.000	0.421	0.834	0.459	1.000	0.813	0.000	1.000	0.590	(Min - Max) / (Max - Min)			
LC50 (µM)	22.800	100.000	100.000	6.460	100.000	100.000	28.800	93.300	67.600	55.000	74.100	100.000	100.000	10.000	85.114	85.114	100.000	6.460	93.540	
Min-max normalization	0.171	1.000	1.000	0.000	1.000	1.000	0.239	0.928	0.654	0.519	0.723	1.000	1.000	0.038	0.841	0.841	(Min - Max) / (Max - Min)			
LC50 (µM)	7.890	100.000	43.700	40.700	100.000	100.000	17.700	100.000	42.700	53.700	49.000	100.000	21.878	10.000	100.000	42.658	100.000	7.890	92.110	
Min-max normalization	0.000	1.000	0.389	0.356	1.000	1.000	0.107	1.000	0.378	0.497	0.446	1.000	0.152	0.023	1.000	0.277	(Min - Max) / (Max - Min)			
LC50 (µM)	9.850	100.000	100.000	14.500	100.000	100.000	20.900	100.000	6.460	64.600	70.800	100.000	100.000	10.000	81.283	81.283	100.000	14.500	93.500	
Min-max normalization	0.036	1.000	1.000	0.086	1.000	1.000	0.154	1.000	0.000	0.058	0.622	0.688	1.000	1.000	0.038	0.800	0.036	(Min - Max) / (Max - Min)		
LC50 (µM)	100.000	100.000	100.000	100.000	100.000	100.000	46.800	100.000	13.100	55.200	95.500	100.000	43.652	10.000	95.499	100.000	10.000	90.000	90.000	
Min-max normalization	1.000	1.000	1.000	1.000	1.000	1.000	0.409	1.000	0.035	0.513	0.950	1.000	0.374	0.000	0.950	1.000	(Min - Max) / (Max - Min)			
LC50 (µM)	39.000	75.900	100.000	91.200	100.000	100.000	46.800	100.000	67.600	39.900	59.900	100.000	100.000	10.000	100.000	69.183	100.000	10.000	90.000	
Min-max normalization	0.328	0.732	1.000	0.902	1.000	1.000	0.409	1.000	0.640	0.331	0.543	1.000	1.000	0.000	1.000	0.658	(Min - Max) / (Max - Min)			
LC50 (µM)	47.100	100.000	100.000	12.000	100.000	100.000	21.500	100.000	51.300	50.100	45.700	100.000	22.909	10.000	93.326	36.481	100.000	10.000	90.000	
Min-max normalization	0.412	1.000	1.000	0.022	1.000	1.000	0.194	1.000	0.459	0.446	0.397	1.000	0.143	0.000	0.926	0.283	(Min - Max) / (Max - Min)			
LC50 (µM)	9.660	97.700	100.000	28.800	100.000	100.000	12.600	85.100	2.820	47.900	87.100	100.000	6.026	10.000	74.131	107.956	100.000	2.820	97.180	
Min-max normalization	0.070	0.976	1.000	0.267	1.000	1.000	0.101	0.847	0.000	0.464	0.867	1.000	0.033	0.074	0.734	0.699				

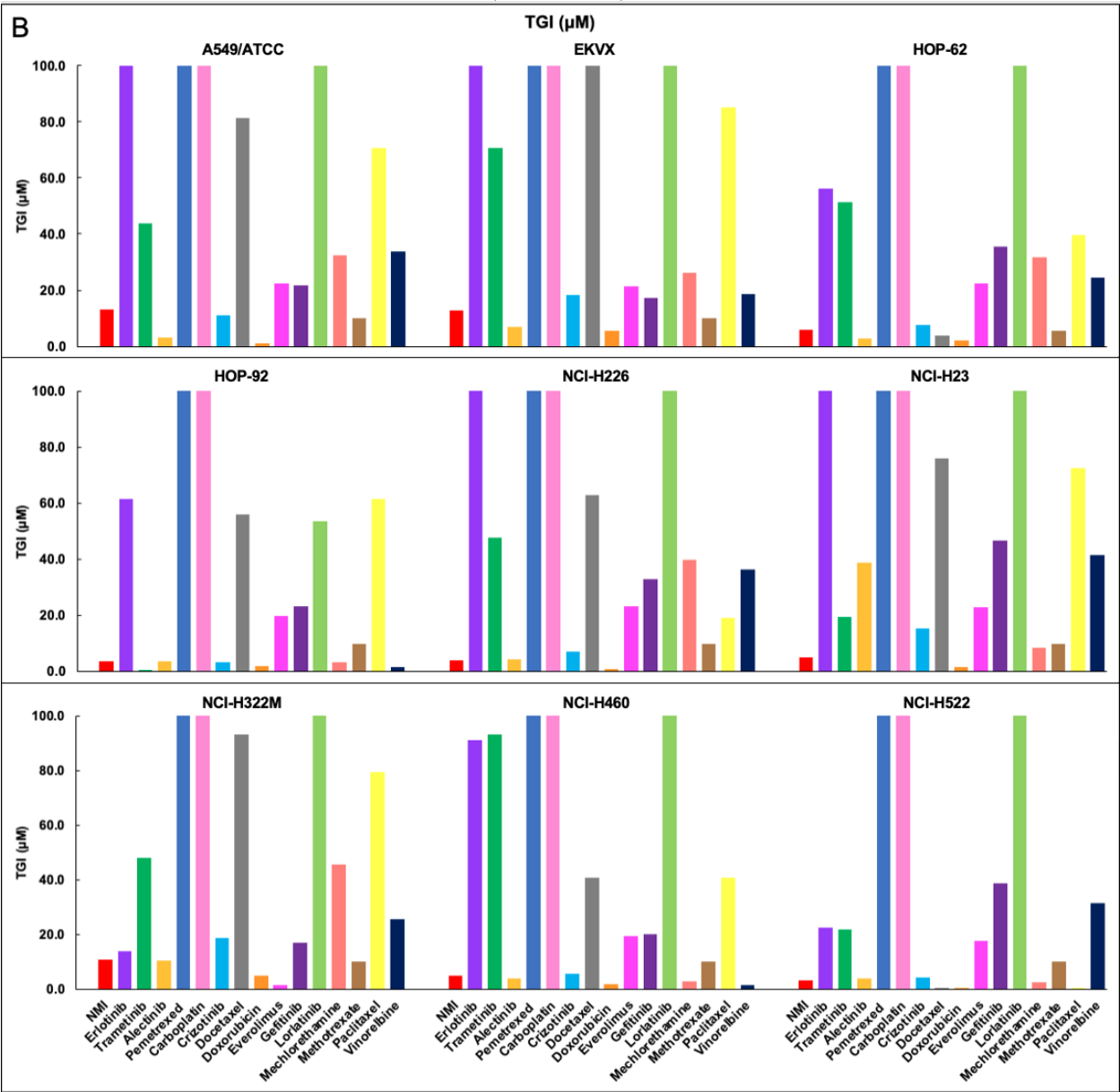


**Figure S1** The comparison of (A)GI<sub>50</sub>, (B)TGI, (C) LC<sub>50</sub>, (D)cumulative score of NMI to FDA-approved prostate cancer drugs. NMI shows higher potency to prostate cancer cell lines than most FDA-approved prostate cancer drugs. Y-axis indicates concentration of GI<sub>50</sub>, TGI, LC<sub>50</sub> (0  $\mu\text{M}$  to 100  $\mu\text{M}$ ), and cumulative score (0.0 to 3.0). Drugs are color-coded: NMI (red); Rucaparib (purple), Enzalutamide (green), Abiraterone (yellow), Cabazitaxel (blue), Docetaxel (pink), Leuprolide (cyan), Mitoxantrone (grey), and Olaparib (orange).



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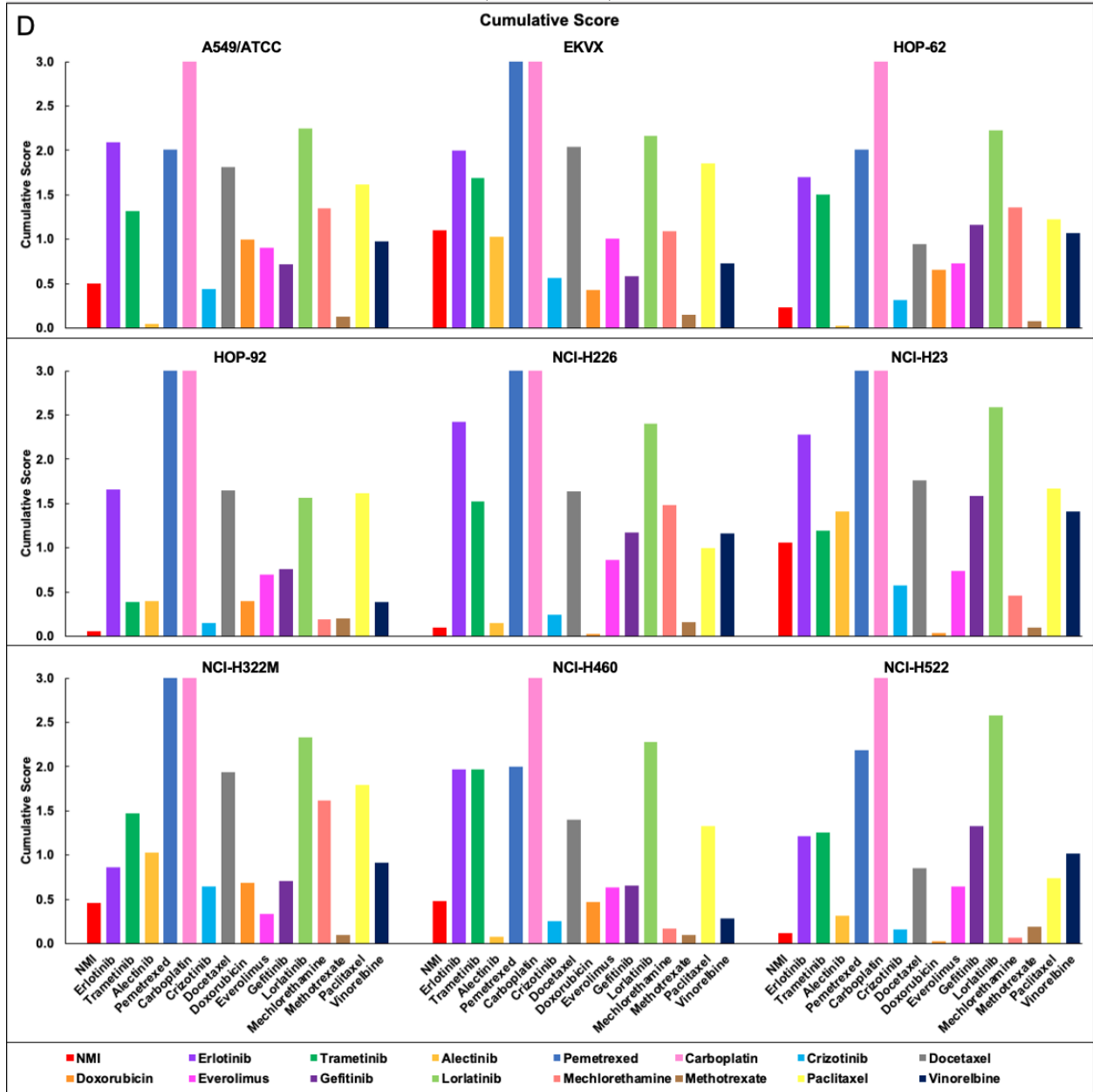
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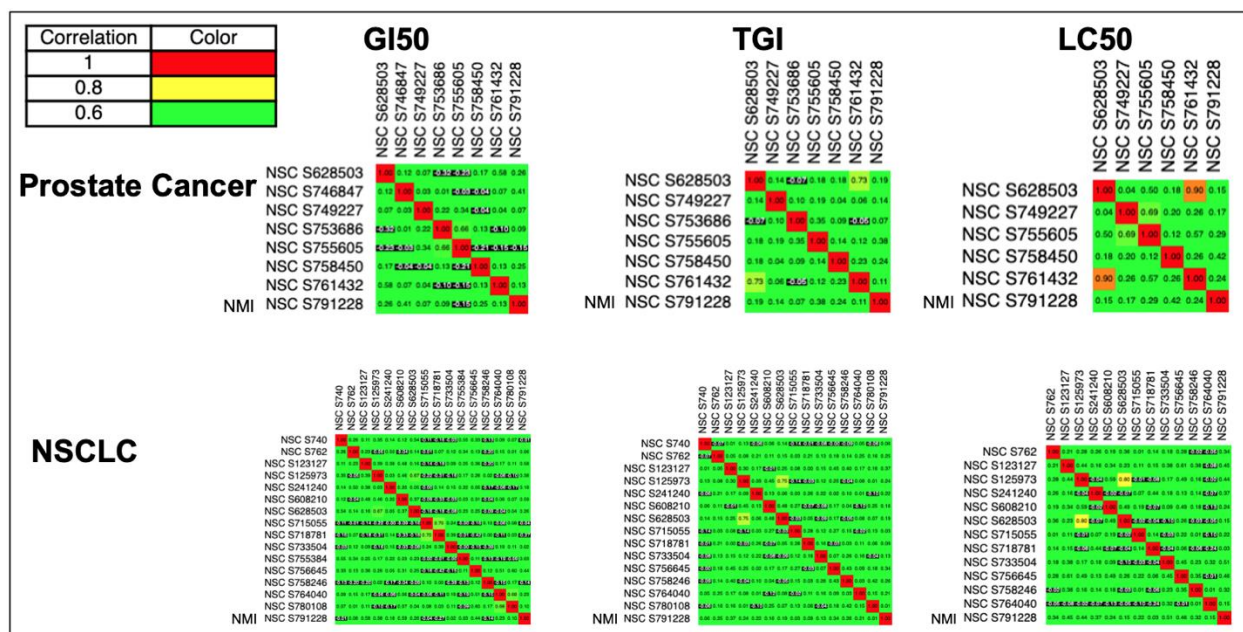


**Figure S2** The comparison of (A)  $GI_{50}$ , (B) TGI, (C)  $LC_{50}$ , (D) cumulative score of NMI to FDA-approved NSCLC drugs. NMI shows higher potency to NSCLC cell lines than most FDA-approved NSCLC cancer drugs. Y-axis indicates concentration of  $GI_{50}$ , TGI,  $LC_{50}$  (0  $\mu$ M to 100  $\mu$ M), and cumulative score (0.0 to 3.0). Drugs are color-coded: NMI (red); Erlotinib (purple); Trametinib (green); Alectinib (yellow); Pemetrexed (blue); Carboplatin (pink); Crizotinib (cyan); Docetaxel (grey); Doxorubicin (orange); Everolimus (magenta); Gefitinib (dark purple); Lorlatinib (light green); Mechlorethamine (light red); Methotrexate (brown); Paclitaxel (yellow-green); Vinorelbine (dark blue).

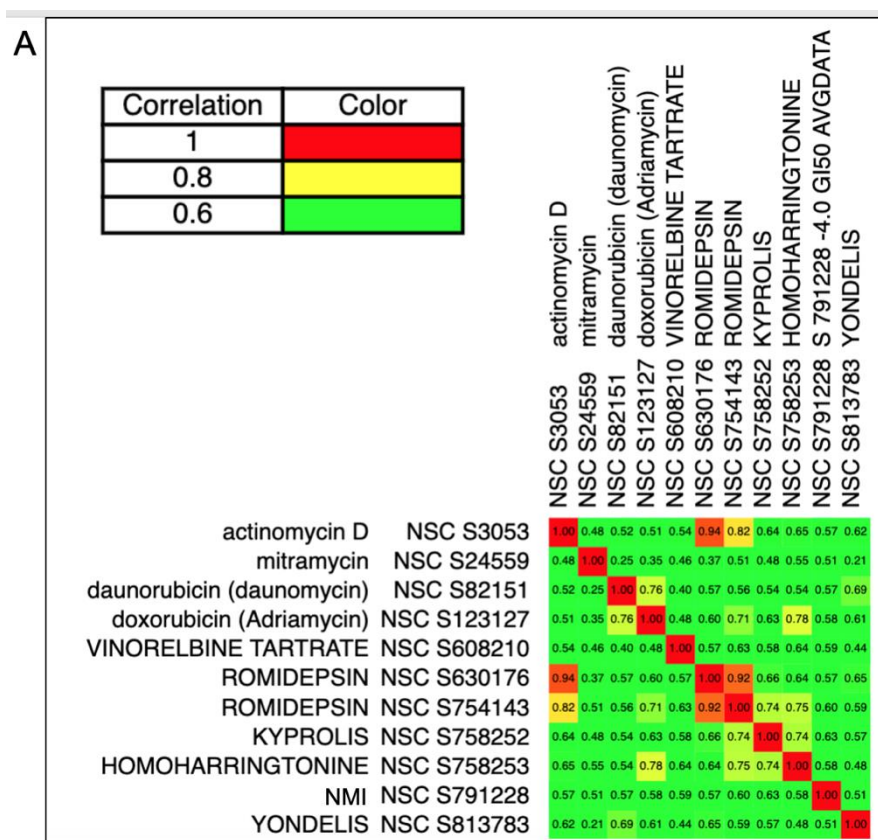
**Table S3.** The COMPARE results between NMI and FDA-approved CNS cancer, prostate cancer, and NSCLC drugs. All PCC values lower than 0.8, NMI has unique mechanisms than FDA-approved CNS, prostate, and NSCLC cancer drugs. Table of COMPARE results of Figure 5 and Figure S3. Exact values generated by COMPARE algorithm are provided.

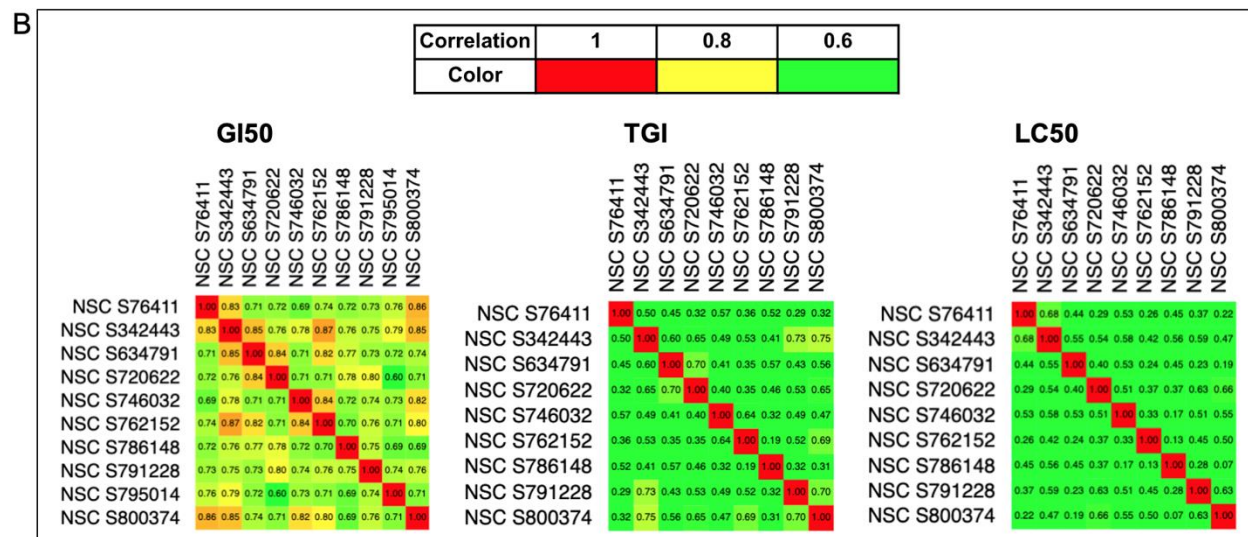


CNS Cancer				
Drug	NSC	PCC-GI50	PCC-TGI	PCC-LC50
Temozolomide	362856	0.00	-0.08	No data (StdDev = 0)
Lomustine	79037	0.48	0.04	0.23
Carmustine	409962	0.31	-0.04	0.27
Everolimus	733504	0.02	0.13	0.51
Prostate Cancer				
Drug	NSC	PCC-GI50	PCC-TGI	PCC-LC50
Rucaparib	756644	No data	No data	No data
Enzalutamide	755605	-0.15	0.38	0.29
Abiraterone Acetate	749227	0.07	0.14	0.17
Cabazitaxel	761432	0.13	0.11	0.24
Docetaxel	628503	0.26	0.19	0.15
Leuprolide Acetate	746847	0.41	No data (StdDev = 0)	No data (StdDev = 0)
Mitoxantrone	758450	0.25	0.24	0.42
Olaparib	753686	0.09	0.07	No data (StdDev = 0)
Non-Small Cell Lung Cancer				
Drug	NSC	PCC-GI50	PCC-TGI	PCC-LC50
Erlotinib	718781	-0.27	0.09	0.03
Trametinib	758246	-0.14	0.26	0.32
Alectinib	764040	0.23	0.15	0.21
Pemetrexed	755384	0.03	No data (StdDev = 0)	No data (StdDev = 0)
Carboplatin	241240	No data (StdDev = 0)	No data (StdDev = 0)	No data (StdDev = 0)
Crizotinib	756645	0.44	0.46	0.34
Docetaxel	628503	0.26	0.19	0.15
Doxorubicin	123127	0.58	0.37	0.45
Everolimus	733504	0.02	0.13	0.51
Gefitinib	715055	-0.04	0.03	0.22
Lorlatinib	780108	0.1	0.01	No data (StdDev = 0)
Mechlorethamine	762	0.06	0.25	0.34
Methotrexate	740	-0.01	0.06	No data (StdDev = 0)
Paclitaxel	125973	0.38	0.24	0.44
Vinorelbine	608210	0.59	0.16	0.24



**Figure S3.** Comparison of the mechanism of NMI to FDA-approved prostate cancer and NSCLC drugs by COMPARE plots. NMI has unique mechanism compared to FDA-approved prostate and NSCLC cancer drugs. High PCC (Pearson Pairwise correlation coefficient), > 0.8 shown in yellow (0.8), orange (0.6), or red (0.4) in the matrix COMPARE figure, indicates these 2 drugs have similar mechanisms for cancer therapy.





**Figure S4.** COMPARE plots of NMI (NSC 791228) to (A) marketed, (B) unmarked drugs in all cancers (top 10) PCC were shown. The result showed NMI has unique mechanism compared to all marketed anti-cancer drugs ; NMI might have similar mechanism with some unmarked drugs. The Pairwise Pearson Correlation Coefficient (PCC) was determined by searching PUBLIC COMPARE Web Site Navigation for all marketed or unmarked drugs in all different cancers in NCI60 database.

**Table S4.** Table of the COMPARE results of Figure S4A, with the drug names and their mechanisms.

NSC No.	Drug Name	PCC-GI50	Mechanism of Action
758252	Carfilzomib (Kyprolis)	0.63	Selective Proteasome Inhibitor
754143	Romidepsin	0.60	Histone Deacetylase Inhibitor
608210	Vinorelbine Tartrate	0.59	Antimicrotubular Antineoplastic Agent
123127	Doxorubicin	0.58	Topoisomerase Inhibitor
758253	Homoharringtonine	0.58	Protein Synthesis Inhibitor
3053	Actinomycin D	0.57	Transcription Inhibitor
82151	Daunorubicin	0.57	Topoisomerase Inhibitor
630176	Romidepsin	0.57	Histone Deacetylase Inhibitor
24559	Mitramycin	0.51	RNA Synthesis Inhibitor
813783	Trabectedin (Yondelis)	0.51	Alkylating Drug
791228	NMI	1.00	MAO A Inhibition; HIF1 $\alpha$ Stabilization