FABAD J. Pharm. Sci., 49, 1, s1-s28, 2024
Doi: 10.55262/fabadeczacilik.1340872
SUPPLEMENT ARTICLE

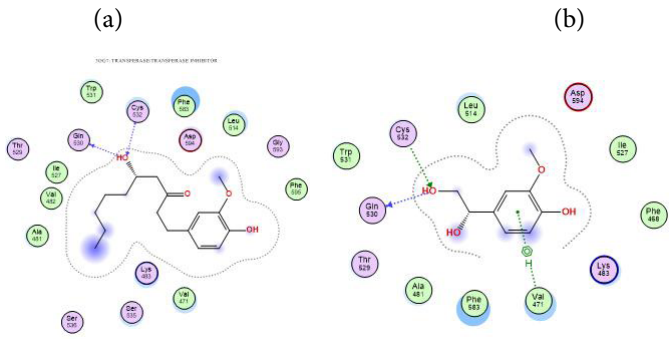


Figure S1. Predicted interaction of (a) N-G-1 and (b) N-G-42 with BRAF: PDB:ID: 3OG7.

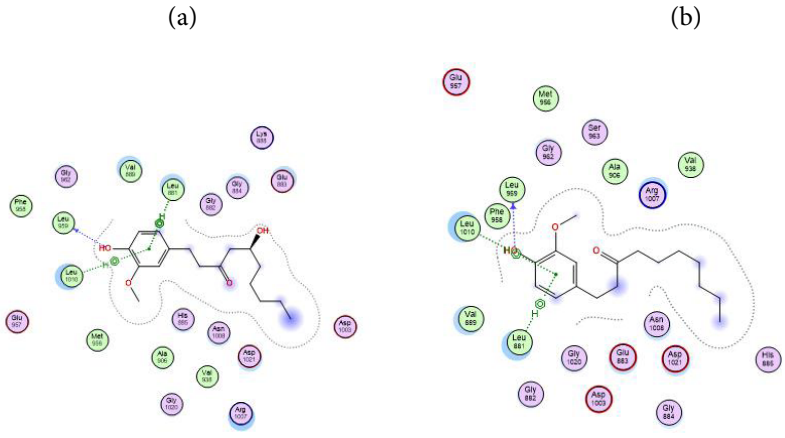


Figure S2. Predicted interaction of (a) N-G-1 and (b) N-G-30 with JAK 1: PDB:ID: 3EYG.

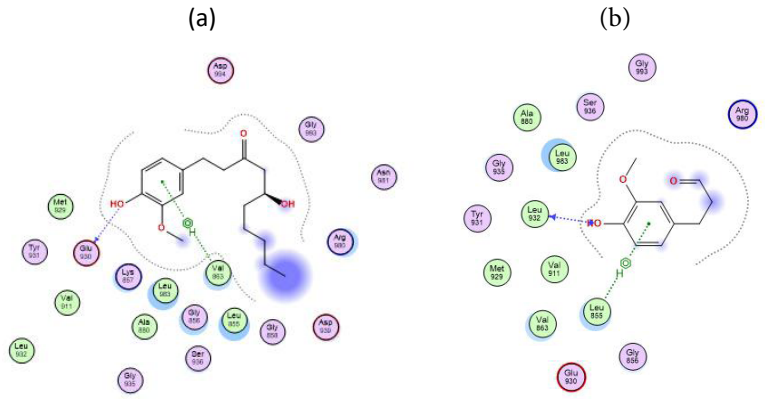


Figure S3. Predicted interaction of (a) N-G-1 and (b) N-G-43 with JAK 2: PDB:ID: 2B7A.

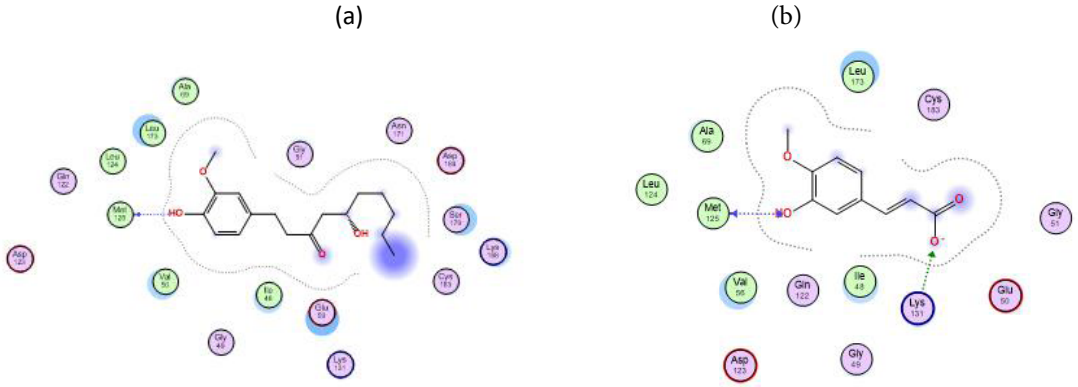
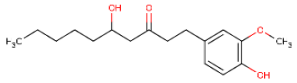
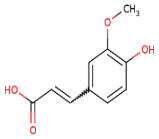
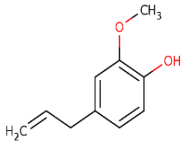
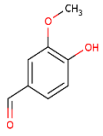
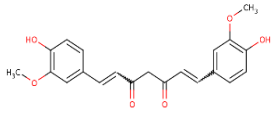
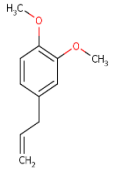
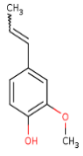
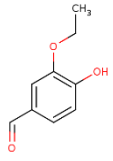
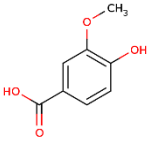
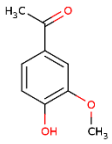
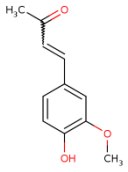
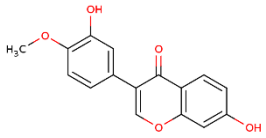
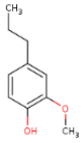
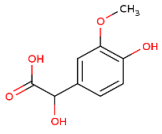
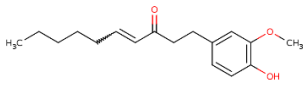
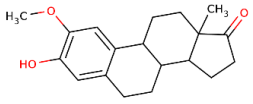
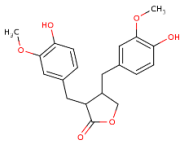
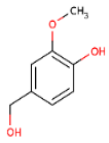
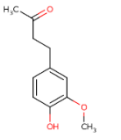
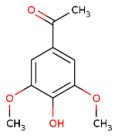
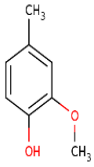
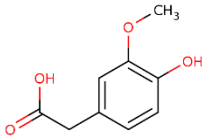
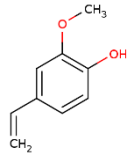
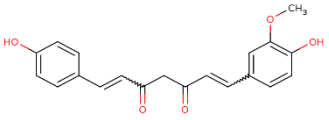
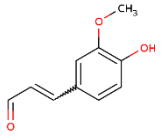
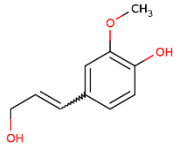
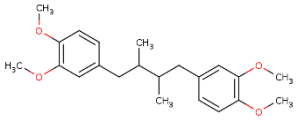
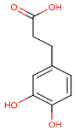
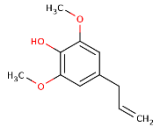


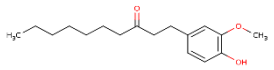
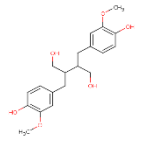
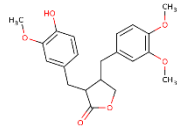
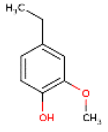
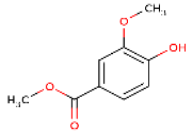
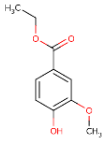
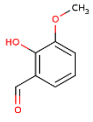
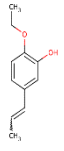
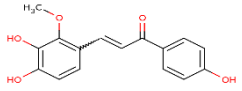
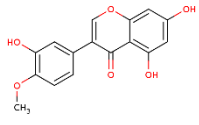
Figure S4. Predicted interaction of (a) N-G-1 and (b) N-G-47 with Erk 1 : PDB:ID: 2ZOQ

Table S1. ID and structure information of 6-gingerol and structurally similar compounds

Compound code	Compound name	CAS no	Structure
N-G-1	6-Gingerol	23513-14-6	
N-G-2	Ferulic acid	537-98-4	
N-G-3	Eugenol	97-53-0	
N-G-4	Vanillin	121-33-5	
N-G-5	Curcumin	458-37-7	
N-G-6	Methyl eugenol	93-15-2	
N-G-7	(E)Isoeugenol	97-54-1	
N-G-8	Ethyl vanillin	121-32-4	
N-G-9	Vanillic acid	121-34-6	

Compound code	Compound name	CAS no	Structure
N-G-10	Acetovanillone	498-02-2	
N-G-11	Dehydrozingerone	1080-12-2	
N-G-12	Calycosin	20575-57-9	
N-G-13	2-methoxy-4-propylphenol (Dihydroeugenol)	2785-87-7	
N-G-14	Vanillylmandelic acid	55-10-7	
N-G-15	Shogaol	555-66-8	
N-G-16	2-methoxyestrone	362-08-3	
N-G-17	Matairesinol	580-72-3	
N-G-18	Vanillyl alcohol	498-00-0	
N-G-19	Zingerone	122-48-5	

Compound code	Compound name	CAS no	Structure
N-G-20	Acetosyringone	2478-38-8	
N-G-21	2-methoxy-4-methylphenol (Cresol)	93-51-6	
N-G-22	Homovanillic acid	306-08-1	
N-G-23	2-methoxy-4-vinylphenol	7786-61-0	
N-G-24		22608-11-3	
N-G-25	Coniferaldehyde	20649-42-7	
N-G-26	Coniferyl alcohol	32811-40-8	
N-G-27	Terameprocol	24150-24-1	
N-G-28	Dihydrocaffeic acid	1078-61-1	
N-G-29	4-allyl-2,6-dimethoxyphenol ((Methoxyeugenol)	6627-88-9	

Compound code	Compound name	CAS no	Structure
N-G-30	Paradol	27113-22-0	
N-G-31	Secoisolariciresinol	29388-59-8	
N-G-32	Arctigenin	7770-78-7	
N-G-33	4-ethyl-2-methoxyphenol	2785-89-9	
N-G-34	Methyl vanillate	3943-74-6	
N-G-35	Ethyl vanillate	617-05-0	
N-G-36	2-hydroxy-3-methoxybenzaldehyde	148-53-8	
N-G-37	Vanitrope	63477-41-8	
N-G-38	Licochalcone B	58749-23-8	
N-G-39	Pratensein	2284-31-3	

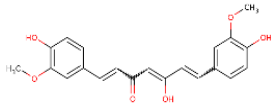
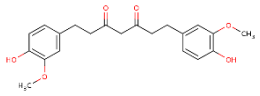
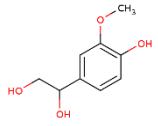
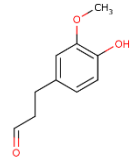
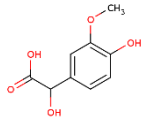
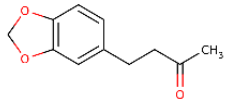
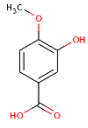
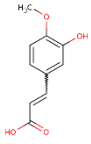
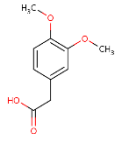
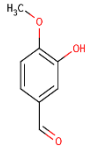
Compound code	Compound name	CAS no	Structure
N-G-40	Curcumin PE	NG	
N-G-41		36062-04-1	
N-G-42	Vanylglycol	534-82-7	
N-G-43	3-(4-Hydroxy-3-methoxyphenyl) propanal [dihydroconiferyl aldehyde]	80638-48-8	
N-G-44	L-(+)-vanilmandelic acid	13244-77-4	
N-G-45	Piperonyl acetone	55418-52-5	
N-G-46	3-hydroxy-4-methoxybenzoic acid (Isovanillic acid)	645-08-9	
N-G-47	Isoferulic acid	25522-33-2	
N-G-48	Homoveratric acid	93-40-3	
N-G-49	(3-hydroxy-4	621-59-0	

Table S2. Common anti-cancer targets for 6-gingerol and similar compounds via four different web servers

PASSonline	SwissTargetPrediction	MolTarPred	SEA
MAP Kinase Stimulant	MAP Kinase ERK1		
Apoptosis Agonist	MAP2K1		
Caspase3 Stimulant	mTOR		
Caspase8 Stimulant	STAT3		
	SYK		
JAK2 expression Inhibitor	JAK2		
	(PIK3CB) \ (PIK3CA)		
BRAF expression Inhibitor	BRAF		
AR expression Inhibitor	Androgen Receptor (AR)		
TP53 expression enhancer	p53-binding protein Mdm-2 (MDM2)		
Transcription Factor NFκB Inhibitor			NF-kappa B essential modulator
			Nuclear factor NF-kappa B p105 subunit (NF-$_{\kappa}$B1)
Beta Tubulin Antagonist	Tubulin beta-1 chain (TUBB1)		Beta-tubulin
Histone acetyltransferase Inhibitor			Histone acetyltransferase p300 (EP300)
Toll-like receptor Antagonist			Toll-like receptor 1
Beta-adrenergic receptor kinase Inhibitor			Beta-1 adrenergic receptor (ADRB1)
5-lipoxygenase Inhibitor	Arachidonate 5-lipoxygenase (ALOX5)	Arachidonate 5-lipoxygenase	Arachidonate 5-lipoxygenase (ALOX5)
	Arachidonate 15-lipoxygenase (ALOX15)		Arachidonate 15-lipoxygenase (ALOX15)

Table S3. Results of PASSonline server

Compounds	Gluconate 2-dehydrogenase (acceptor) inhibitor	TP53 expression enhancer	Preneoplastic conditions treatment	GST A substrate	GST M substrate	Lipid peroxidase inhibitor	JAK2 expression inhibitor	NOS2 expression inhibitor	TNF expression inhibitor
N-G-1	0,765	0,600	0,772	0,717	0,687	0,670	0,679	0,632	0,633
N-G-2	0,833	0,788	0,903	0,768	0,673	0,618	0,915	0,560	0,819
N-G-3	0,797	0,724	0,803	0,633	0,543	0,501	0,873	0,618	0,525
N-G-4	0,737	0,608	0,777	0,532	0,572	0,711	0,886	0,465	0,546
N-G-5	0,833	0,671	0,676	0,778	0,777	0,598	0,369	0,649	0,764
N-G-6	0,825	0,649	0,748	0,632	0,437	0,383	0,819	0,545	0,437
N-G-7	0,772	0,766	0,879	0,719	0,730	0,613	0,942	0,724	0,852
N-G-8	0,496	0,549	0,637	0,622	0,439	0,729	0,710	0,378	0,433
N-G-9	0,794	0,713	0,905	0,537	0,535	0,564	0,871	0,485	0,670
N-G-10	0,780	0,681	0,798	0,584	0,542	0,467	0,883	0,531	0,691
N-G-11	0,927	0,745	0,905	0,861	0,888	0,582	0,953	0,801	0,847
N-G-12	0,759	0,797	0,571	0,314	0,541	0,734	0,837	0,567	0,453
N-G-13	0,747	0,686	0,861	0,638	0,630	0,535	0,876	0,527	0,638
N-G-14	0,823	0,652	0,794	0,560	0,472	0,426	0,821	0,418	0,758
N-G-15	0,759	0,757	0,873	0,730	0,707	0,603	0,828	0,544	0,754
N-G-16	0,698	0,755	0,351		0,246	0,501	0,964	0,505	0,568
N-G-17	0,646	0,536	0,683	0,304	0,395	0,371	0,709	0,426	0,483
N-G-18	0,747	0,720	0,796	0,523	0,549	0,587	0,876	0,591	0,618
N-G-19	0,921	0,744	0,841	0,655	0,641	0,602	0,870	0,600	0,715
N-G-20	0,768	0,680	0,740	0,594	0,468	0,463	0,845	0,474	0,618
N-G-21	0,772	0,739	0,814	0,544	0,585	0,614	0,924	0,606	0,723
N-G-22	0,831	0,775	0,878	0,668	0,560	0,517	0,836	0,512	0,647
N-G-23	0,916	0,723	0,824	0,700	0,609	0,462	0,922	0,597	0,613
N-G-24	0,822	0,693	0,950	0,751	0,802	0,627	0,978	0,674	0,901
N-G-25	0,706	0,830	0,834	0,830	0,864	0,438	0,925	0,540	0,634
N-G-26	0,715	0,735	0,867	0,711	0,661	0,560	0,919	0,595	0,804
N-G-27	0,755	0,584	0,593	0,480	0,431	0,339	0,798	0,389	0,549
N-G-28	0,801	0,699	0,816	0,771	0,574	0,507	0,747	0,405	0,580
N-G-29	0,788	0,723	0,746	0,642	0,468	0,496	0,832	0,559	0,451
N-G-30	0,797	0,760	0,892	0,646	0,625	0,726	0,811	0,577	0,678
N-G-31	0,658	0,633	0,859	0,468	0,459	0,420	0,801	0,458	0,589
N-G-32	0,646	0,536	0,683	0,304	0,395	0,371	0,709	0,426	0,483
N-G-33	0,765	0,725	0,848	0,598	0,622	0,497	0,888	0,548	0,620
N-G-34	0,757	0,652	0,872	0,531	0,548	0,584	0,871	0,501	0,628
N-G-35	0,727	0,652	0,825	0,469	0,416	0,631	0,784	0,453	0,605
N-G-36	0,770	0,541	0,706	0,568	0,498	0,580	0,848	0,387	0,447
N-G-37	0,525	0,711	0,786	0,767	0,614	0,616	0,868	0,620	0,749
N-G-38	0,706	0,657	0,754	0,584	0,569	0,697	0,882	0,640	0,563
N-G-39	0,727	0,857	0,507	0,244	0,464	0,797	0,792	0,612	0,492
N-G-40	0,825	0,686	0,883	0,721	0,720	0,403	0,941	0,589	0,788
N-G-41	0,822	0,744	0,874	0,555	0,573	0,405	0,913	0,599	0,639
N-G-42	0,688	0,647	0,727	0,469	0,460	0,543	0,827	0,459	0,736
N-G-43	0,672	0,716	0,783	0,670	0,670	0,375	0,839	0,444	0,478
N-G-44	0,823	0,652	0,794	0,560	0,472	0,426	0,821	0,418	0,758
N-G-45	0,902	0,572	0,479	0,569	0,324	0,468	0,546	0,330	0,587
N-G-46	0,794	0,713	0,905	0,537	0,535	0,564	0,871	0,485	0,670
N-G-47	0,833	0,788	0,903	0,768	0,673	0,618	0,915	0,560	0,819
N-G-48	0,864	0,738	0,851	0,694	0,482	0,422	0,784	0,457	0,581
N-G-49	0,737	0,608	0,777	0,532	0,572	0,711	0,886	0,465	0,546

Table S3. Results of PASSonline server (continued)

Compounds	Free radical scavenger	Prostaglandin-A1 DELTA-isomerase inhibitor	Antimutagenic	Caspase 3 stimulant	GST P substrate	GST P1-1 substrate	Nitric oxide antagonist	Apoptosis agonist
N-G-1	0,617	0,602	0,597	0,575	0,546	0,511	0,494	0,518
N-G-2	0,731	0,431	0,900	0,749	0,541	0,521	0,324	0,702
N-G-3	0,563	0,309	0,878	0,873	0,491	0,467	0,335	0,743
N-G-4	0,546	0,387	0,618	0,754	0,379	0,350	0,247	0,705
N-G-5	0,766	0,294	0,814	0,747	0,184	0,188	0,346	0,803
N-G-6	0,536	0,362	0,807	0,840	0,465	0,438	0,297	0,726
N-G-7	0,717	0,365	0,805	0,778	0,538	0,517	0,329	0,733
N-G-8	0,481	0,380	0,469	0,651	0,356	0,305	0,189	0,588
N-G-9	0,643	0,731		0,640	0,358	0,330	0,258	0,512
N-G-10	0,560	0,446	0,609	0,658	0,384	0,356	0,284	0,547
N-G-11	0,704	0,322	0,848	0,819	0,654	0,640	0,280	0,760
N-G-12	0,506	0,221	0,864	0,603	0,220	0,216	0,454	0,779
N-G-13	0,528	0,477	0,783	0,734	0,393	0,364	0,249	0,482
N-G-14	0,482		0,575	0,439	0,386	0,351	0,220	0,405
N-G-15	0,743	0,344	0,851	0,551	0,676	0,663	0,475	0,711
N-G-16	0,440		0,335	0,737			0,253	0,484
N-G-17	0,330	0,249	0,372	0,582	0,202	0,192	0,207	0,422
N-G-18	0,579	0,394	0,816	0,787	0,364	0,325	0,270	0,562
N-G-19	0,551	0,376	0,796	0,659	0,364	0,336	0,315	0,488
N-G-20	0,547	0,439	0,573	0,534	0,323	0,299	0,282	0,578
N-G-21	0,546	0,447	0,730	0,756	0,375	0,346	0,271	0,600
N-G-22	0,612	0,530	0,748	0,634	0,393	0,364	0,266	0,471
N-G-23	0,540	0,342	0,791	0,768	0,784	0,772	0,362	0,663
N-G-24	0,785	0,269	0,834	0,719	0,813	0,803	0,356	0,861
N-G-25	0,487	0,276	0,752	0,945	0,765	0,754	0,277	0,871
N-G-26	0,565	0,281	0,796	0,784	0,529	0,491	0,305	0,590
N-G-27	0,340	0,454	0,356	0,529	0,200	0,199	0,138	0,326
N-G-28	0,516	0,758	0,818	0,401	0,413	0,384	0,249	0,363
N-G-29	0,652	0,304	0,868	0,816	0,459	0,432	0,336	0,794
N-G-30	0,631	0,438	0,789	0,544	0,420	0,392	0,350	0,538
N-G-31	0,439	0,303	0,523	0,543	0,315	0,269	0,194	0,436
N-G-32	0,330	0,249	0,372	0,582	0,202	0,192	0,207	0,422
N-G-33	0,529	0,456	0,769	0,761	0,366	0,338	0,284	0,516
N-G-34	0,575	0,542	0,700	0,728	0,356	0,329	0,263	0,521
N-G-35	0,539	0,462	0,628	0,657	0,318	0,271	0,243	0,440
N-G-36	0,503	0,387	0,435	0,647	0,285	0,267	0,175	0,889
N-G-37	0,643	0,336	0,715	0,698	0,520	0,480	0,275	0,648
N-G-38	0,737	0,276	0,650	0,805	0,389	0,361	0,640	0,829
N-G-39	0,593		0,896	0,660	0,178	0,181	0,590	0,844
N-G-40	0,562	0,269	0,736	0,626	0,632	0,618	0,253	0,799
N-G-41	0,710	0,353	0,718	0,539	0,675	0,662	0,406	0,625
N-G-42	0,518	0,315	0,486	0,483	0,361	0,304	0,216	0,513
N-G-43	0,390	0,324	0,650	0,700	0,530	0,509	0,220	0,435
N-G-44	0,482	0,475	0,575	0,439	0,386	0,351	0,220	0,405
N-G-45	0,408	0,401	0,245	0,646			0,243	0,371
N-G-46	0,643	0,731	0,834	0,640	0,358	0,330	0,258	0,512
N-G-47	0,731	0,431	0,900	0,749	0,541	0,521	0,324	0,702
N-G-48	0,520	0,638	0,630	0,570	0,350	0,323	0,223	0,394
N-G-49	0,546	0,387	0,618	0,754	0,379	0,350	0,247	0,705

Table S3. Results of PASSonline server (continued)

Compounds	Platelet derived growth factor receptor kinase inhibitor	Histone acetyltransferase inhibitor	MAP kinase stimulant	Prostaglandin-E2 9-reductase inhibitor	Caspase 8 stimulant	Histidine kinase inhibitor	Anticarcinogenic	Myc inhibitor
N-G-1	0,509	0,470	0,482	0,461	0,433	0,390	0,364	0,350
N-G-2		0,555	0,709	0,464	0,551	0,400	0,616	0,357
N-G-3		0,457	0,735	0,298	0,598	0,331	0,459	0,476
N-G-4		0,284	0,744	0,240	0,525	0,473	0,388	0,307
N-G-5		0,305	0,737	0,235	0,487	0,317	0,611	0,313
N-G-6		0,350	0,663	0,285	0,566		0,362	0,492
N-G-7		0,524	0,806	0,324	0,545	0,344	0,408	0,350
N-G-8		0,432	0,597	0,195	0,449	0,443	0,353	0,278
N-G-9		0,619	0,717	0,702	0,573	0,405	0,413	0,358
N-G-10		0,470	0,764	0,510	0,519	0,467	0,341	0,343
N-G-11	0,400	0,584	0,756	0,241	0,491	0,315	0,609	0,319
N-G-12		0,170	0,794	0,167	0,536	0,937	0,703	0,327
N-G-13	0,346	0,561	0,781	0,435	0,566	0,435	0,367	0,390
N-G-14		0,333	0,608	0,389	0,505	0,433	0,370	0,464
N-G-15	0,559	0,614	0,564	0,454	0,536	0,389	0,475	0,386
N-G-16			0,547	0,875	0,521	0,259	0,496	0,444
N-G-17		0,210	0,578		0,487	0,251	0,566	0,337
N-G-18		0,357	0,720	0,342	0,649	0,372	0,469	0,392
N-G-19	0,854	0,399	0,728	0,257	0,478	0,360	0,419	0,346
N-G-20		0,390	0,691	0,513	0,474	0,473	0,341	0,350
N-G-21	0,379	0,397	0,838	0,438	0,606	0,407	0,402	0,398
N-G-22		0,414	0,733	0,705	0,608	0,706	0,453	0,389
N-G-23		0,502	0,810	0,324	0,610	0,342	0,402	0,370
N-G-24		0,703	0,760	0,248	0,461	0,388	0,649	0,299
N-G-25		0,362	0,735	0,196	0,498	0,385	0,498	0,286
N-G-26		0,565	0,711	0,332	0,550	0,298	0,595	0,369
N-G-27		0,227	0,721	0,439	0,470		0,270	0,431
N-G-28		0,501	0,652	0,705	0,482	0,553	0,412	0,367
N-G-29		0,378	0,660	0,301	0,553	0,326	0,459	0,488
N-G-30	0,630	0,471	0,647	0,350	0,507	0,438	0,415	0,359
N-G-31		0,344	0,691	0,379	0,506	0,307	0,477	0,407
N-G-32		0,210	0,578		0,487	0,251	0,566	0,337
N-G-33	0,286	0,377	0,826	0,401	0,644	0,410	0,394	0,471
N-G-34		0,567	0,717	0,453	0,608	0,376	0,364	0,392
N-G-35	0,268	0,684	0,630	0,386	0,511	0,323	0,341	0,339
N-G-36		0,218	0,660	0,271	0,461	0,493	0,353	0,391
N-G-37		0,624	0,673	0,237	0,461	0,326	0,367	0,302
N-G-38		0,511	0,644	0,315	0,351	0,457	0,382	0,219
N-G-39			0,744		0,570	0,954	0,781	0,329
N-G-40		0,503	0,682	0,187	0,432	0,289	0,455	0,284
N-G-41	0,680	0,475	0,733	0,241	0,472	0,359	0,495	0,330
N-G-42		0,344	0,610	0,268	0,504	0,331	0,421	0,475
N-G-43	0,251	0,277	0,707	0,208	0,484	0,430	0,341	0,316
N-G-44		0,333	0,608	0,389	0,505	0,433	0,370	0,464
N-G-45	0,850	0,159	0,658		0,481	0,235	0,251	
N-G-46		0,619	0,717	0,702	0,573	0,405	0,413	0,358
N-G-47		0,555	0,709	0,464	0,551	0,400	0,616	0,357
N-G-48		0,348	0,675	0,735	0,579	0,675	0,381	0,396
N-G-49		0,284	0,744	0,240	0,525	0,473	0,388	0,307

Table S3. Results of PASSonline server (continued)

Compounds	AR expression inhibitor	Transcription factor NF kappa B inhibitor	BRAF expression inhibitor	Endothelial growth factor antagonist	G-protein-coupled receptor kinase inhibitor	Beta-adrenergic receptor kinase inhibitor	Pin1 inhibitor	DNA polymerase I inhibitor
N-G-1	0,339	0,264	0,273	0,297	0,332	0,332	0,340	0,277
N-G-2	0,627	0,407	0,395	0,386	0,641	0,641	0,562	0,253
N-G-3	0,608	0,488	0,126	0,376	0,807	0,807	0,607	0,249
N-G-4	0,582	0,378	0,176	0,377	0,753	0,753	0,617	0,258
N-G-5	0,527	0,399	0,219	0,375	0,427	0,427	0,567	0,237
N-G-6	0,529	0,405	0,162	0,388	0,811	0,811	0,585	
N-G-7	0,702	0,520	0,296	0,414	0,539	0,539	0,612	0,252
N-G-8	0,465	0,451	0,185	0,290	0,882	0,882	0,479	0,237
N-G-9	0,594	0,296	0,172	0,393	0,698	0,698	0,606	0,289
N-G-10	0,666	0,290	0,188	0,424	0,388	0,388	0,631	0,292
N-G-11	0,697	0,422	0,230	0,479	0,407	0,407	0,556	0,229
N-G-12	0,871	0,332		0,264			0,680	0,245
N-G-13	0,559	0,246	0,230	0,490	0,447	0,447	0,674	0,302
N-G-14	0,560	0,133	0,183	0,370	0,562	0,562	0,507	0,303
N-G-15	0,570	0,452	0,217	0,382	0,406	0,406	0,428	0,271
N-G-16	0,846	0,255		0,216	0,256	0,256	0,398	0,315
N-G-17	0,393	0,155		0,383	0,290	0,290	0,467	0,240
N-G-18	0,529	0,288	0,148	0,416	0,617	0,617	0,654	0,354
N-G-19	0,551	0,272	0,145	0,747	0,309	0,309	0,620	0,260
N-G-20	0,664	0,278	0,243	0,487	0,392	0,392	0,620	0,268
N-G-21	0,634	0,356	0,270	0,685	0,541	0,541	0,660	0,318
N-G-22	0,544	0,207	0,206	0,447	0,515	0,515	0,668	0,288
N-G-23	0,639	0,375	0,152	0,349	0,551	0,551	0,630	0,235
N-G-24	0,810	0,560	0,193	0,343	0,425	0,425	0,534	
N-G-25	0,675	0,289	0,447	0,302	0,419	0,419	0,542	
N-G-26	0,598	0,458	0,181	0,370	0,675	0,675	0,589	0,276
N-G-27	0,526	0,189	0,172	0,411	0,323	0,323	0,631	
N-G-28	0,494	0,133	0,413	0,361	0,749	0,749	0,611	0,269
N-G-29	0,605	0,474	0,163	0,432	0,810	0,810	0,596	
N-G-30	0,504	0,267	0,193	0,433	0,319	0,319	0,522	0,292
N-G-31	0,492	0,177		0,356	0,401	0,401	0,630	0,294
N-G-32	0,393	0,155		0,383	0,290	0,290	0,467	0,240
N-G-33	0,619	0,281	0,196	0,481	0,417	0,417	0,715	0,291
N-G-34	0,561	0,350	0,141	0,418	0,628	0,628	0,606	0,316
N-G-35	0,496	0,547	0,115	0,355	0,655	0,655	0,580	0,266
N-G-36	0,566	0,253	0,176	0,413	0,755	0,755	0,657	0,233
N-G-37	0,612	0,559	0,260	0,311	0,788	0,788	0,492	0,230
N-G-38	0,648	0,497	0,170	0,259	0,359	0,359	0,542	
N-G-39	0,905	0,471		0,308			0,616	0,275
N-G-40	0,642	0,295	0,160	0,318	0,337	0,337	0,478	
N-G-41	0,596	0,406	0,122	0,552	0,305	0,305	0,638	0,260
N-G-42	0,524	0,141	0,107	0,354	0,598	0,598	0,534	0,323
N-G-43	0,575	0,188	0,227	0,359	0,316	0,316	0,605	0,247
N-G-44	0,560	0,133	0,183	0,370	0,562	0,562	0,507	0,303
N-G-45	0,242	0,130	0,187	0,422			0,487	
N-G-46	0,594	0,296	0,172	0,393	0,698	0,698	0,606	0,289
N-G-47	0,627	0,407	0,395	0,386	0,641	0,641	0,562	0,253
N-G-48	0,473	0,167	0,303	0,459	0,582	0,582	0,664	0,247
N-G-49	0,582	0,378	0,176	0,377	0,753	0,753	0,617	0,258

Table S3. Results of PASSonline server (continued)

Compounds	Leukopoiesis inhibitor	Toll-Like receptor antagonist	Transcription factor inhibitor	Tumour necrosis factor alpha release inhibitor	Glutamate decarboxylase inhibitor	Antineoplastic (breast cancer)	Transcription factor NF kappa A inhibitor	Antineoplastic (cervical cancer)
N-G-1	0,288	0,166	0,243	0,200	0,162	0,210	0,228	0,151
N-G-2	0,431		0,329		0,263	0,467	0,338	0,308
N-G-3	0,434		0,410	0,171	0,202	0,419	0,351	0,276
N-G-4	0,443		0,379		0,191	0,466	0,329	0,139
N-G-5	0,335		0,334		0,175	0,528	0,325	0,323
N-G-6	0,476		0,377	0,270	0,151	0,402	0,316	0,315
N-G-7	0,427		0,494	0,160	0,148	0,463	0,377	0,318
N-G-8	0,312		0,425		0,146	0,365	0,341	
N-G-9	0,570		0,304		0,513	0,298	0,371	0,155
N-G-10	0,582		0,415	0,176	0,225	0,413	0,382	0,264
N-G-11	0,348		0,339		0,153	0,552	0,342	0,512
N-G-12	0,300		0,361		0,097	0,565	0,294	0,355
N-G-13	0,499		0,254	0,158	0,183	0,252	0,366	0,181
N-G-14	0,443				0,360		0,292	
N-G-15	0,254		0,334		0,134	0,256	0,268	0,148
N-G-16	0,317		0,229			0,563	0,353	0,163
N-G-17	0,777					0,231	0,278	0,115
N-G-18	0,477		0,296		0,172	0,384	0,357	0,271
N-G-19	0,414		0,253	0,124	0,189	0,242	0,316	0,400
N-G-20	0,605		0,389	0,138	0,229	0,401	0,357	0,280
N-G-21	0,571		0,406	0,163	0,185	0,399	0,387	0,267
N-G-22	0,558		0,190		0,478	0,181	0,333	0,113
N-G-23	0,395		0,340	0,174	0,191	0,411	0,341	0,320
N-G-24	0,304		0,504		0,184	0,547	0,310	0,309
N-G-25	0,321		0,239		0,203	0,279	0,316	0,331
N-G-26	0,364		0,379		0,128	0,357	0,400	0,280
N-G-27	0,488	0,137	0,257	0,215	0,105	0,282	0,368	0,190
N-G-28	0,514	0,124	0,166		0,603		0,363	
N-G-29	0,465		0,384	0,136	0,206	0,410	0,327	0,292
N-G-30	0,305	0,121	0,255	0,137	0,194	0,227	0,288	0,254
N-G-31	0,381	0,122	0,181	0,131	0,126	0,179	0,398	0,103
N-G-32	0,777					0,231	0,278	0,115
N-G-33	0,588		0,305	0,171	0,192	0,302	0,371	0,229
N-G-34	0,647		0,382	0,145	0,248	0,349	0,404	0,259
N-G-35	0,652	0,145	0,519	0,140	0,177	0,309	0,357	0,164
N-G-36	0,510		0,295		0,173	0,437	0,298	0,177
N-G-37	0,307		0,535	0,159	0,120	0,391	0,379	0,179
N-G-38	0,283		0,449		0,183	0,597	0,320	0,537
N-G-39	0,252		0,468	0,131	0,092	0,602	0,267	0,376
N-G-40	0,293		0,245		0,146	0,727	0,307	0,406
N-G-41	0,423		0,375	0,134	0,202	0,250	0,305	0,156
N-G-42	0,374				0,195	0,174	0,348	
N-G-43	0,379				0,250		0,291	0,140
N-G-44	0,443				0,360		0,292	
N-G-45			0,210		0,172		0,231	0,345
N-G-46	0,570		0,304		0,513	0,298	0,371	0,155
N-G-47	0,431		0,329		0,263	0,467	0,338	0,308
N-G-48	0,597	0,119		0,137	0,358		0,307	0,107
N-G-49	0,443		0,379		0,191	0,466	0,329	0,139

Table S3. Results of PASSonline server (continued)

Compounds	Antineoplastic (endocrine cancer)	Phosphomevalonate kinase inhibitor	Tubulin antagonist	Nucleotidase inhibitor	Glutaminase inhibitor	Antineoplastic (thyroid cancer)	Antineoplastic (bone cancer)	Antineoplastic (non-Hodgkin's lymphoma)
N-G-1	0,171	0,115	0,121	0,126	0,180	0,161	0,205	0,295
N-G-2		0,482	0,283	0,137	0,335	0,163	0,219	0,424
N-G-3	0,172	0,170	0,344		0,214	0,189	0,206	
N-G-4		0,619	0,480		0,287		0,272	
N-G-5		0,267	0,238		0,274	0,160	0,211	0,387
N-G-6	0,174	0,115	0,315		0,201	0,188		
N-G-7		0,297	0,514		0,259	0,165	0,230	0,420
N-G-8		0,523	0,248		0,392	0,150	0,261	
N-G-9		0,320	0,254	0,194	0,594	0,168	0,235	0,388
N-G-10	0,187	0,171	0,347		0,316	0,176	0,222	0,432
N-G-11		0,264	0,272		0,313	0,163	0,208	0,426
N-G-12		0,129	0,327		0,178		0,274	
N-G-13	0,167	0,184	0,248		0,293	0,151	0,242	0,382
N-G-14		0,203	0,169	0,153	0,346	0,176	0,211	0,348
N-G-15		0,135	0,154		0,176		0,206	0,352
N-G-16			0,371			0,228	0,214	
N-G-17	0,187	0,112	0,172		0,162	0,173		0,336
N-G-18		0,205	0,271	0,120	0,322	0,160	0,251	0,467
N-G-19		0,164	0,203		0,351		0,209	0,356
N-G-20	0,205	0,138	0,383		0,309	0,172	0,192	0,444
N-G-21		0,197	0,447		0,352	0,178	0,246	0,415
N-G-22		0,233	0,231	0,150	0,390	0,150	0,225	0,362
N-G-23	0,189	0,233	0,521		0,254	0,208	0,232	0,316
N-G-24		0,286	0,234		0,253	0,153	0,209	0,375
N-G-25	0,175	0,292	0,288		0,202	0,179	0,253	0,320
N-G-26		0,313	0,384		0,305	0,159	0,227	0,442
N-G-27	0,155	0,093	0,176		0,227		0,258	0,315
N-G-28		0,344		0,226	0,618		0,206	0,400
N-G-29	0,186	0,140	0,377		0,208	0,187		
N-G-30		0,138	0,151		0,279	0,171	0,227	0,327
N-G-31		0,171	0,167		0,284		0,246	0,378
N-G-32	0,187	0,112	0,172		0,162	0,173		0,336
N-G-33	0,176	0,181	0,327		0,305	0,157	0,244	0,431
N-G-34		0,233	0,365	0,131	0,423	0,195	0,219	0,366
N-G-35	0,165	0,203	0,234	0,111	0,507	0,191	0,219	0,401
N-G-36		0,411	0,502		0,305		0,257	
N-G-37		0,260	0,326		0,351	0,165	0,216	0,391
N-G-38	0,166	0,229	0,353		0,202	0,184		0,319
N-G-39		0,114	0,386		0,171		0,272	
N-G-40		0,257	0,186		0,236			0,320
N-G-41		0,171	0,179		0,297	0,171	0,206	0,288
N-G-42		0,176	0,183		0,316	0,173	0,220	0,376
N-G-43	0,167	0,186	0,187		0,233	0,161	0,253	
N-G-44		0,203	0,169	0,153	0,346	0,176	0,211	0,348
N-G-45			0,179		0,282			0,339
N-G-46		0,320	0,254	0,194	0,594	0,168	0,235	0,388
N-G-47		0,482	0,283	0,137	0,335	0,163	0,219	0,424
N-G-48		0,201	0,184	0,163	0,410		0,212	0,297
N-G-49		0,619	0,480		0,287		0,272	

Table S3. Results of PASSonline server (continued)

Compounds	Prostaglandin F2 alpha antagonist	Antineoplastic (liver cancer)	Aspartate kinase inhibitor	Antineoplastic	Dual specificity protein phosphatase VHR inhibitor	Glutamate dehydrogenase (NADP+) inhibitor	Prostaglandin EP2 antagonist	Adenylate kinase inhibitor	Glutamate-tRNA ligase inhibitor	Glutamate synthase (ferredoxin) inhibitor	Beta tubulin antagonist	5-Lipoxygenase inhibitor
N-G-1	0,063	0,175	0,115	0,241	0,062	0,081	0,043	0,127	0,198	0,129	0,050	0,064
N-G-2	0,051	0,241	0,121	0,601		0,133	0,055	0,148	0,291	0,172	0,163	0,172
N-G-3		0,239		0,461	0,057		0,029	0,135	0,203		0,237	0,154
N-G-4		0,190	0,115	0,636	0,050	0,160		0,136	0,254	0,149	0,462	0,094
N-G-5	0,045	0,194		0,672		0,065			0,217	0,143	0,168	0,156
N-G-6		0,245		0,417			0,037	0,144	0,221		0,195	0,113
N-G-7	0,046	0,205	0,097	0,679				0,121	0,225	0,136	0,387	0,210
N-G-8			0,148	0,448		0,192		0,148	0,239	0,145	0,227	0,089
N-G-9		0,250	0,193	0,326	0,079	0,207		0,258	0,457	0,274	0,150	0,105
N-G-10		0,234	0,117	0,404	0,075			0,132	0,264	0,161	0,169	0,166
N-G-11	0,043	0,216		0,773		0,078		0,146	0,199	0,138	0,189	0,135
N-G-12				0,708							0,145	0,156
N-G-13	0,042	0,208	0,126	0,222	0,071	0,072		0,129	0,255	0,152	0,173	0,131
N-G-14	0,042		0,134			0,090		0,149	0,324	0,180	0,058	0,068
N-G-15	0,015	0,230		0,338	0,066	0,062	0,019	0,152			0,085	0,141
N-G-16				0,731							0,251	
N-G-17		0,183		0,574	0,056						0,074	0,086
N-G-18		0,258	0,121	0,509	0,062	0,082		0,157	0,292	0,163	0,168	0,122
N-G-19		0,190	0,100	0,383	0,055	0,090		0,143	0,226	0,155	0,095	0,089
N-G-20		0,213	0,134	0,513	0,079	0,076		0,151	0,284	0,174	0,180	0,165
N-G-21		0,244	0,117	0,478	0,065	0,070		0,145	0,279	0,179	0,321	0,138
N-G-22	0,043	0,217	0,145		0,054	0,118		0,225	0,337	0,197	0,104	0,121
N-G-23		0,220		0,617	0,057			0,143	0,231	0,135	0,442	0,150
N-G-24	0,045	0,193		0,678					0,202	0,133	0,169	0,152
N-G-25	0,042	0,202	0,113	0,551		0,060		0,150	0,191		0,218	0,140
N-G-26	0,046	0,232	0,107	0,674		0,069		0,118	0,204	0,151	0,312	0,158
N-G-27		0,160	0,118						0,313	0,156	0,063	0,102
N-G-28	0,058	0,165	0,214		0,050	0,262	0,070	0,252	0,501	0,280		0,118
N-G-29		0,220		0,564	0,059		0,031	0,155	0,219	0,127	0,265	0,153
N-G-30	0,042	0,219	0,110	0,268	0,076	0,109		0,127		0,157	0,060	0,095
N-G-31		0,230	0,114	0,247					0,235	0,159	0,071	0,072
N-G-32		0,183		0,574	0,056						0,074	0,086
N-G-33		0,259	0,116	0,329	0,063	0,064		0,130	0,262	0,157	0,219	0,115
N-G-34		0,242	0,148	0,378	0,116	0,099		0,239	0,335	0,194	0,208	0,116
N-G-35		0,196	0,185	0,270	0,088	0,091		0,214	0,277	0,186	0,139	0,120
N-G-36		0,187	0,115	0,693	0,052	0,166		0,141	0,259	0,151	0,498	0,104
N-G-37	0,046		0,117	0,545		0,066		0,129	0,217	0,131	0,226	0,190
N-G-38	0,043			0,786			0,030		0,191		0,251	0,378
N-G-39		0,161		0,775							0,203	0,193
N-G-40	0,042			0,888						0,125	0,107	0,102
N-G-41				0,260	0,053	0,064		0,118	0,233	0,153	0,096	0,090
N-G-42		0,170	0,118	0,287		0,065		0,119	0,229	0,158	0,071	0,086
N-G-43		0,174	0,153	0,250	0,050			0,146	0,217	0,124	0,125	0,077
N-G-44	0,042		0,134			0,090		0,149	0,324	0,180	0,058	0,068
N-G-45				0,236		0,088		0,144	0,245	0,132	0,049	
N-G-46		0,250	0,193	0,326	0,079	0,200		0,258	0,457	0,274	0,150	0,105
N-G-47	0,051	0,241	0,121	0,601		0,133	0,055	0,148	0,291	0,172	0,163	0,172
N-G-48	0,042	0,218	0,164			0,143	0,019	0,261	0,387	0,212	0,059	0,091
N-G-49		0,190	0,115	0,636	0,050	0,160		0,136	0,254	0,149	0,462	0,094

Table S4. SwissTarget prediction results

Target																										
	N-G-1	N-G-2	N-G-3	N-G-4	N-G-5	N-G-6	N-G-7	N-G-8	N-G-9	N-G-10	N-G-11	N-G-12	N-G-13	N-G-14	N-G-15	N-G-16	N-G-17	N-G-18	N-G-19	N-G-20	N-G-21	N-G-22	N-G-23	N-G-24	N-G-25
ESR1	+						+		+		+	+	+		+	+	+		+		+				+
ALOX5	+	+			+		+			+	+	+	+	+	+	+	+		+			+		+	+
ALOX15	+	+	+			+					+	+	+			+	+		+		+	+			
LYPLA1	+															+	+		+						
LYPLA2	+															+	+		+						
PDE4B	+																								
PPARG	+											+				+	+								
MAP2K1	+																+		+						
NR3C1	+												+			+	+		+		+				
CHEK1	+		+		+		+			+	+	+	+		+		+		+	+	+			+	
WEE1	+				+						+	+			+		+		+					+	
PTGES	+			+	+						+													+	+
KIF11	+																								
PIK3CB	+					+									+										
PIK3CG	+			+						+	+				+		+		+	+					
PIK3CA	+			+		+									+				+	+					
CDK2	+		+										+	+			+		+		+				
MTOR	+														+									+	
KDR	+		+			+	+			+					+	+				+	+		+		
ERN1	+							+	+	+					+					+	+		+		
RET	+									+						+				+					
ITK	+																								
PDK1	+				+										+		+								
PARP1	+	+	+	+		+	+				+		+		+		+		+			+	+		+
PIK3C2B	+																								
STAT3	+	+			+		+				+		+											+	+
PIM2	+							+		+	+	+			+		+		+	+		+			+
PIM3	+			+				+		+	+	+								+					+
IGF1R	+								+				+			+	+		+		+				
PIK3CD	+			+											+		+			+					
SYK	+																+						+		
MAPK3	+															+									
LIMK1	+																								
LRRK2	+			+		+		+		+						+				+					
AR	+		+			+	+						+		+										
CDK2 CCNA1 CCNA2	+				+			+		+	+					+			+	+	+		+	+	+
JAK3	+					+				+					+	+			+	+					
JAK1	+		+		+	+	+			+										+	+		+		
JAK2	+		+		+	+	+			+						+			+	+	+		+		
TYK2	+		+			+	+			+										+	+		+		
CDK5R1 CDK5	+				+			+		+	+				+	+					+		+	+	+
CCNE1 CDK2	+																		+		+				
CDK7 CCNH	+																								
CDK9 CCNT1	+									+											+		+		
PRKDC	+			+											+				+	+	+				
PDPK1	+							+							+						+		+		
FLT1	+																			+					
ROCK2	+														+	+									
ROCK1	+																+							+	
TUBB1	+	+	+	+			+		+		+		+						+	+			+		+
BRAF	+		+		+	+	+					+	+		+	+	+							+	
TNK2	+																								
EPHB4	+																								
HSP90AA1	+								+			+					+		+						
GAK	+																								
MDM2	+																								
CCND1 CDK4	+																				+				
CDK1 CCNB1	+						+	+			+													+	+
CCNE2 CDK2 CCNE1	+					+		+			+					+					+		+		+
GSK3B	+	+			+					+	+					+	+							+	+
GSK3A	+							+			+				+				+	+	+		+		

Table S4. SwissTarget prediction results (continued)

Target	N-G-26	N-G-27	N-G-28	N-G-29	N-G-30	N-G-31	N-G-32	N-G-33	N-G-34	N-G-35	N-G-36	N-G-37	N-G-38	N-G-39	N-G-40	N-G-41	N-G-42	N-G-43	N-G-44	N-G-45	N-G-46	N-G-47	N-G-48	N-G-49
ESR1		+	+		+	+	+					+	+	+		+		+			+			+
ALOX5		+	+		+	+	+					+	+	+	+	+		+	+	+		+		
ALOX15		+	+	+	+	+	+	+	+	+				+	+	+		+		+		+	+	
LYPLA1			+			+	+									+								
LYPLA2			+			+	+									+								
PDE4B							+																	
PPARG			+		+		+							+		+					+			
MAP2K1		+	+		+	+	+									+								
NR3C1		+	+		+	+		+								+		+		+				
CHEK1					+	+	+		+	+	+		+	+	+	+		+		+				
WEE1					+	+	+						+	+		+		+						
PTGES					+		+								+	+								
KIF11																								
PIK3CB		+			+	+	+						+											+
PIK3CG		+			+	+	+				+							+		+				+
PIK3CA		+			+	+	+				+	+	+			+				+				+
CDK2			+	+	+	+	+									+			+	+				
MTOR						+	+						+							+				+
KDR		+		+	+	+				+		+			+	+					+			+
ERN1			+			+	+	+	+	+	+		+								+			+
RET					+		+		+	+						+		+						
ITK					+	+																		
PDK1													+			+								
PARP1			+	+	+	+	+	+				+						+		+		+	+	
PIK3C2B																								
STAT3															+	+						+		
PIM2							+				+							+					+	+
PIM3									+		+							+		+				+
IGF1R		+	+		+	+							+	+		+		+		+	+			
PIK3CD		+				+	+				+									+				+
SYK							+					+				+								
MAPK3						+																		
LIMK1																				+				
LRRK2																								+
AR			+	+	+	+				+						+								
CDK2 CCNA1 CCNA2				+	+			+	+	+	+					+		+		+				
JAK3				+			+		+	+		+								+				
JAK1				+			+	+	+											+				
JAK2				+			+	+	+	+										+				
TYK2				+				+	+											+				
CDK5R1 CDK5				+	+		+	+	+			+		+				+		+				
CCNE1 CDK2				+		+							+					+		+				
CDK7 CCNH						+																		
CDK9 CCNT1				+		+		+	+	+		+								+				
PRKDC		+									+									+				+
PDPK1		+		+			+	+										+						
FLT1					+		+																	
ROCK2						+																		
ROCK1																		+						
TUBB1		+		+	+		+	+	+	+	+	+	+			+		+		+	+	+		+
BRAF					+		+	+					+		+	+		+		+				
TNK2																								
EPHB4																								
HSP90AA1				+	+	+	+							+		+		+			+		+	
GAK																								
MDM2																								
CCND1 CDK4				+										+						+		+		
CDK1 CCNB1													+					+						
CCNE2 CDK2 CCNE1				+			+								+			+		+				
GSK3B						+	+			+					+						+			
GSK3A				+	+				+	+	+									+				+

Table S5. MolTarPred (Compounds 1-25)

Compounds	Targets	
	Vanilloid receptor (Homo sapiens)	Arachidonate 5-lipoxygenase (Homo sapiens)
N-G-1	+	+
N-G-2		
N-G-3		+
N-G-4		+
N-G-5		+
N-G-6		
N-G-7		+
N-G-8		
N-G-9		
N-G-10		+
N-G-11		+
N-G-12		
N-G-13		+
N-G-14		
N-G-15	+	+
N-G-16		
N-G-17		
N-G-18		+
N-G-19	+	+
N-G-20		+
N-G-21		
N-G-22		+
N-G-23		+
N-G-24		+
N-G-25		+
N-G-26		+
N-G-27		
N-G-28		
N-G-29		+
N-G-30	+	+
N-G-31		
N-G-32		
N-G-33		+
N-G-34		
N-G-35		
N-G-36		
N-G-37		
N-G-38		+
N-G-39		
N-G-40		+
N-G-41	+	+
N-G-42		
N-G-43	+	+
N-G-44		
N-G-45	+	
N-G-46		
N-G-47		+
N-G-48		
N-G-49		

Table S6. SEA online

Compounds	Targets																									
	APP	NDUFAB1	Adrb1	ADRB1	EP300	GPR174	LPAR1	IKBKG	NFE2L2	NFKB1	Ptger2	beta-tubulin	CXCL12	MAPT	TLR1	Tlr1	Tlr2	YWHAG	NDUFAF1	Enpp2	FOS	ALOX15	ALOX5	Alox5	Trpv2	
N-G-1	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	
N-G-2	+	+			+			+	+	+			+	+					+		+	+	+	+	+	
N-G-3	+	+	+		+			+	+	+		+	+	+		+	+		+		+	+	+	+	+	
N-G-4	+		+		+			+	+	+		+	+	+		+	+				+	+	+	+	+	
N-G-5	+	+	+		+			+	+	+			+	+		+	+		+		+	+	+	+	+	
N-G-6	+		+	+				+	+	+											+	+				
N-G-7	+				+			+	+	+			+	+							+	+	+	+	+	
N-G-8	+				+			+	+	+			+	+							+		+	+	+	
N-G-9	+	+	+		+		+	+	+	+		+	+	+	+	+	+		+		+		+	+	+	
N-G-10	+	+	+		+			+	+	+		+	+	+		+	+		+		+	+	+	+	+	
N-G-11	+	+			+			+	+	+			+	+					+		+	+	+	+	+	
N-G-12														+								+	+	+		
N-G-13	+	+	+		+			+	+	+		+	+	+	+	+	+	+	+		+	+	+	+	+	
N-G-14	+	+	+		+			+	+	+			+	+		+	+		+		+			+	+	
N-G-15	+	+	+		+		+	+	+	+	+	+	+	+	+	+	+	+	+		+	+	+	+	+	
N-G-16																+	+									
N-G-17	+	+	+	+	+			+	+	+			+	+			+		+		+		+	+	+	
N-G-18	+	+	+		+			+	+	+		+	+	+		+	+	+	+		+	+	+	+	+	
N-G-19	+	+	+	+	+			+	+	+		+	+	+		+	+	+	+		+	+	+	+	+	
N-G-20	+							+	+	+		+	+	+	+	+	+				+		+	+		
N-G-21	+	+	+		+			+	+	+		+	+	+		+	+		+		+	+	+	+	+	
N-G-22	+	+	+		+			+	+	+		+	+	+	+	+	+	+	+		+	+	+	+	+	
N-G-23	+		+		+			+	+	+			+	+							+		+	+	+	
N-G-24	+	+	+		+			+	+	+		+	+	+							+	+	+	+	+	
N-G-25	+		+		+			+	+	+			+	+							+	+	+	+	+	
N-G-26	+	+	+		+			+	+	+		+	+	+		+	+		+		+	+	+	+	+	
N-G-27	+		+	+										+							+	+				
N-G-28	+		+								+	+						+				+		+		
N-G-29	+							+	+	+				+		+	+				+	+	+			
N-G-30	+	+	+		+	+	+	+	+	+	+	+	+	+	+	+	+	+	+		+	+	+	+	+	
N-G-31	+	+	+		+			+	+	+		+	+	+		+	+		+		+	+		+	+	
N-G-32	+	+	+		+			+	+	+				+					+		+			+	+	
N-G-33	+	+	+	+	+			+	+	+		+	+	+	+	+	+	+	+		+	+	+	+	+	
N-G-34	+	+	+		+			+	+	+		+	+	+	+	+	+		+		+	+	+	+	+	
N-G-35	+	+	+	+	+			+	+	+		+	+	+	+	+	+	+	+		+	+	+	+	+	
N-G-36	+		+					+	+	+		+	+	+		+	+				+	+		+		
N-G-37	+							+	+	+			+	+										+		
N-G-38	+							+	+	+			+	+		+	+							+		
N-G-39																+	+					+	+	+		
N-G-40	+				+			+	+	+			+	+							+		+	+	+	
N-G-41	+	+	+	+	+			+	+	+		+	+	+		+	+	+	+		+	+	+	+	+	
N-G-42	+	+	+	+	+			+	+	+			+	+		+	+		+		+	+		+	+	
N-G-43	+	+	+	+	+			+	+	+		+	+	+		+	+	+	+		+	+	+	+	+	
N-G-44	+	+	+		+			+	+	+			+	+		+	+		+		+			+	+	
N-G-45											+		+					+						+		
N-G-46	+		+		+		+	+	+	+		+	+	+	+	+	+				+		+	+	+	
N-G-47	+				+			+	+	+			+	+							+	+	+	+	+	
N-G-48	+		+	+	+			+	+	+		+	+	+		+	+	+			+	+	+	+	+	
N-G-49	+		+		+			+	+	+			+	+		+	+				+		+	+	+	

Table S8. Predicted drug-likeness based on the RO5 including bioavailability (BA) and synthetic accessibility (SA) of the molecules

Compound code	Mol.wt	HBA	HBD	TPSA	iLOGP	NRB	BA Score	SA
N-G-1	294.39	4	2	66.76	3.48	10	0.55	2.81
N-G-2	194.18	4	2	66.76	1.62	3	0.85	1.93
N-G-3	164.2	2	1	29.46	2.37	3	0.55	1.58
N-G-4	152.15	3	1	46.53	1.57	2	0.55	1.15
N-G-5	368.38	6	2	93.06	3.27	8	0.55	2.97
N-G-6	178.23	2	0	18.46	2.65	4	0.55	1.71
N-G-7	164.2	2	1	29.46	2.38	2	0.55	1.81
N-G-8	166.17	3	1	46.53	1.82	3	0.55	1.37
N-G-9	168.15	4	2	66.76	1.4	2	0.55	1.42
N-G-10	166.17	3	1	46.53	1.77	2	0.55	1.36
N-G-11	192.21	3	1	46.53	2.11	3	0.55	2.13
N-G-12	284.26	5	2	79.9	2.4	2	0.55	2.95
N-G-13	166.22	2	1	29.46	2.46	3	0.55	1.4
N-G-14	198.17	5	3	86.99	1.21	3	0.55	2.2
N-G-15	276.37	3	1	46.53	3.28	9	0.55	2.51
N-G-16	300.39	3	1	46.53	2.92	1	0.55	3.52
N-G-17	358.39	6	2	85.22	2.47	6	0.55	3.3
N-G-18	154.16	3	2	49.69	1.79	2	0.55	1.26
N-G-19	194.23	3	1	46.53	2.09	4	0.55	1.52
N-G-20	196.2	4	1	55.76	1.98	3	0.55	1.65
N-G-21	138.16	2	1	29.46	1.94	1	0.55	1
N-G-22	182.17	4	2	66.76	1.18	3	0.85	1.49
N-G-23	150.17	2	1	29.46	2.14	2	0.55	1.45
N-G-24	338.35	5	2	83.83	2.78	7	0.55	2.82
N-G-25	178.18	3	1	46.53	1.75	3	0.55	1.88
N-G-26	180.2	3	2	49.69	2.16	3	0.55	1.86
N-G-27	358.47	4	0	36.92	4.31	9	0.55	3.32
N-G-28	182.17	4	3	77.76	0.86	3	0.55	1.2
N-G-29	194.23	3	1	38.69	2.46	4	0.55	1.87
N-G-30	278.39	3	1	46.53	3.65	10	0.55	2.28
N-G-31	362.42	6	4	99.38	2.98	9	0.55	3.21
N-G-32	372.41	6	1	74.22	2.8	7	0.55	3.43
N-G-33	152.19	2	1	29.46	2.21	2	0.55	1.18
N-G-34	182.17	4	1	55.76	2.13	3	0.55	1.67
N-G-35	196.2	4	1	55.76	1.98	4	0.55	1.85
N-G-36	152.15	3	1	46.53	1.6	2	0.55	1.16
N-G-37	178.23	2	1	29.46	2.63	3	0.55	1.89
N-G-38	286.28	5	3	86.99	1.7	4	0.55	2.8
N-G-39	300.26	6	3	100.13	2.38	2	0.55	3.02
N-G-40	368.38	6	3	96.22	3.21	7	0.55	3.42
N-G-41	372.41	6	2	93.06	3.21	10	0.55	2.45

Compound code	**Mol.wt**	**HBA**	**HBD**	**TPSA**	**iLOGP**	**NRB**	**BA Score**	**SA**
N-G-42	184.19	4	3	69.92	1.61	3	0.55	2.11
N-G-43	180.2	3	1	46.53	1.77	4	0.55	1.4
N-G-44	198.17	5	3	86.99	1.21	3	0.56	2.2
N-G-45	192.21	3	0	35.53	2.21	3	0.55	2.03
N-G-46	168.15	4	2	66.76	0.89	2	0.85	1.24
N-G-47	194.18	4	2	66.76	1.79	3	0.85	1.9
N-G-48	196.2	4	1	55.76	1.67	4	0.85	1.62
N-G-49	152.15	3	1	46.53	1.44	2	0.55	1.05

Table S9. Predicted ADME properties of molecules under study

Compound code	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
N-G-1	High	+	-	+	-	-	+	-
N-G-2	High	+	-	-	-	-	-	-
N-G-3	High	+	-	+	-	-	-	-
N-G-4	High	+	-	-	-	-	-	-
N-G-5	High	-	-	-	-	+	-	+
N-G-6	High	+	-	+	-	-	-	-
N-G-7	High	+	-	+	-	-	-	-
N-G-8	High	+	-	-	-	-	-	-
N-G-9	High	-	-	-	-	-	-	-
N-G-10	High	+	-	-	-	-	-	-
N-G-11	High	+	-	+	-	-	-	-
N-G-12	High	-	-	+	-	-	+	+
N-G-13	High	+	-	+	-	-	-	-
N-G-14	High	-	-	-	-	-	-	-
N-G-15	High	+	-	+	+	-	+	-
N-G-16	High	+	+	-	-	-	+	-
N-G-17	High	-	-	-	-	-	+	+
N-G-18	High	+	-	-	-	-	-	-
N-G-19	High	+	-	+	-	-	-	-
N-G-20	High	+	-	-	-	-	-	-
N-G-21	High	+	-	-	-	-	-	-
N-G-22	High	-	-	-	-	-	-	-
N-G-23	High	+	-	+	-	-	-	-
N-G-24	High	-	-	+	-	+	-	+
N-G-25	High	+	-	-	-	-	-	-
N-G-26	High	+	-	-	-	-	-	-
N-G-27	High	+	+	-	-	-	+	+
N-G-28	High	-	-	-	-	-	-	-
N-G-29	High	+	-	+	-	-	-	-
N-G-30	High	+	-	+	-	-	+	-
N-G-31	High	-	+	-	-	-	+	-
N-G-32	High	+	-	-	-	+	+	+
N-G-33	High	+	-	+	-	-	-	-
N-G-34	High	+	-	-	-	-	-	-
N-G-35	High	+	-	-	-	-	-	-
N-G-36	High	+	-	-	-	-	-	-
N-G-37	High	+	-	+	-	-	-	-
N-G-38	High	-	-	+	-	+	-	+
N-G-39	High	-	-	+	-	+	+	+
N-G-40	High	-	-	-	-	+	-	+
N-G-41	High	-	-	-	-	-	+	+
N-G-42	High	-	-	-	-	-	-	-
N-G-43	High	+	-	-	-	-	-	-
N-G-44	High	-	-	-	-	-	-	-
N-G-45	High	+	-	+	-	-	-	-
N-G-46	High	-	-	-	-	-	-	-
N-G-47	High	+	-	-	-	-	-	-
N-G-48	High	+	-	-	-	-	-	-
N-G-49	High	+	-	-	-	-	-	-

Table S10. The excretion properties of the studied compounds

Compound code	Total Clearance Log (ml/min/kg)	Renal OCT2 substrate
N-G-1	1.339	No
N-G-2	0.623	No
N-G-3	0.282	No
N-G-4	0.601	No
N-G-5	-0.002	No
N-G-6	0.338	No
N-G-7	0.221	No
N-G-8	0.642	No
N-G-9	0.628	No
N-G-10	0.62	No
N-G-11	0.16	No
N-G-12	0.18	No
N-G-13	0.244	No
N-G-14	0.446	No
N-G-15	1.44	No
N-G-16	0.719	No
N-G-17	0.147	No
N-G-18	0.215	No
N-G-19	0.307	No
N-G-20	0.641	No
N-G-21	0.202	No
N-G-22	0.246	No
N-G-23	0.233	No
N-G-24	0.026	No
N-G-25	0.183	No
N-G-26	0.233	No
N-G-27	0.197	No
N-G-28	0.245	No
N-G-29	0.293	No
N-G-30	1.411	No
N-G-31	0.248	No
N-G-32	0.214	No
N-G-33	0.232	No
N-G-34	0.687	No
N-G-35	0.769	No
N-G-36	0.159	No

Compound code	Total Clearance Log (ml/min/kg)	Renal OCT2 substrate
N-G-37	0.268	No
N-G-38	0.555	No
N-G-39	0.165	No
N-G-40	0.089	No
N-G-41	0.230	No
N-G-42	0.206	No
N-G-43	0.325	No
N-G-44	0.446	No
N-G-45	0.158	No
N-G-46	0.626	No
N-G-47	0.621	No
N-G-48	0.304	No
N-G-49	0.599	No

Table S11. Results of the cytotoxicity predictions by Way2Drug server on the tumor and non-tumor cell lines

	Cell-line	NCI-H322M	NCI-H226	PC-6	HOP-18	NCI-H187	DMS-114	Malme-3M	M14	SK-MEL-	M19-MEL
	Full name	Non-small cell l	Non-small cell l	Small cell lun	Non-small cell	Small cell lung ca	Lung carcin	Melanoma	Melanoma	Melanoma	Melanoma
Compound code	Tissue	Lung	Lung	Lung	Lung	Lung	Lung	Skin	Skin	Skin	Skin
	N-G-1	-									
	N-G-2	-									
	N-G-3	-									
	N-G-4	-				0.537					
	N-G-5	-									
	N-G-6	-									
	N-G-7	-									
	N-G-8	-									
	N-G-9	-									
	N-G-10	-									
	N-G-11	-									
	N-G-12	-									
	N-G-13	-									
	N-G-14	-					0.539				
	N-G-15	-									
	N-G-16	-									
	N-G-17	-									
	N-G-18	-									
	N-G-19	-									
	N-G-20	-									
	N-G-21	-			0.587						0.514
	N-G-22	-									
	N-G-23	-									
	N-G-24	-									
	N-G-25	0.7	0.64					0.646	0.564	0.514	
	N-G-26	-									
	N-G-27	-									
	N-G-28	-									
	N-G-29	-									
	N-G-30	-									
	N-G-31	-									
	N-G-32	-									
	N-G-33	-		0.628							
	N-G-34	-		0.534							
	N-G-35	-									
	N-G-36	-				0.741					
	N-G-37	-									
	N-G-38	-									
	N-G-39	-									
	N-G-40	-									
	N-G-41	-									
	N-G-42	-					0.512				
	N-G-43	-									
	N-G-44	-					0.539				
	N-G-45	-									
	N-G-46	-									
	N-G-47	-									
	N-G-48	-									
	N-G-49	-									

Table S11. Results of the cytotoxicity predictions by Way2Drug server on the tumor and non-tumor cell lines (Continued)

Cell-line	RPMI-8226	K562	Hs 683	SF-539	MDA-MB	MCF7	OVCAR-3	IGROV-1	PC-3	DU-145	SN12C	SNB-75	cytoxicity on non-tumor cell line when pa>0.5
Full name	Multiple myeloma	Erythroleu	Oligodendr	Glioblastor	Breast ade	nocarcinor	Ovarian ad	Ovarian ad	Prostate c	Prostate c	Renal carc	Glioblastor	
Tissue	Haematopoietic and lymph	Haematop	Brain	Brain	Breast	Breast	Ovarium	Ovarium	Prostate	Prostate	Kidney	Nervous s	
N-G-1													no
N-G-2		0.542						0.529					no
N-G-3													no
N-G-4													no
N-G-5													no
N-G-6													no
N-G-7													no
N-G-8													no
N-G-9													no
N-G-10		0.53											no
N-G-11		0.586											no
N-G-12													no
N-G-13													no
N-G-14													no
N-G-15					0.601								no
N-G-16				0.528	0.53						0.524		yes (on endothelium)
N-G-17													yes (on lung)
N-G-18			0.612										no
N-G-19													no
N-G-20		0.517								0.503			no
N-G-21			0.591										no
N-G-22													yes (on lung)
N-G-23													no
N-G-24													no
N-G-25	0.578												no
N-G-26													no
N-G-27													no
N-G-28													no
N-G-29													no
N-G-30													no
N-G-31													no
N-G-32													yes (on lung)
N-G-33													no
N-G-34													no
N-G-35													no
N-G-36			0.512										no
N-G-37													no
N-G-38		0.646											no
N-G-39													no
N-G-40									0.733				no
N-G-41													no
N-G-42							0.53		0.747				no
N-G-43					0.551								no
N-G-44													no
N-G-45			0.598									0.535	yes (on lung)
N-G-46													no
N-G-47		0.542						0.529					no
N-G-48													yes (on lung)
N-G-49													no

Table S12. Results of the toxicity prediction by ProTox-II server

	Organ Toxicity	Toxicity end points				Tox21 Stress response pathways	
Compound code	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity	(MMP)	p53
N-G-1	inactive(0.83)	inactive(0.76)	active(0.95)	inactive(0.65)	inactive(0.88)	inactive(0.59)	inactive(0.69)
N-G-2	inactive(0.51)	inactive(0.61)	active(0.91)	inactive(0.96)	inactive(0.88)	inactive(0.92)	inactive(0.93)
N-G-3	inactive(0.67)	inactive(0.73)	inactive(0.83)	inactive(0.97)	inactive(0.90)	inactive(0.98)	inactive(0.99)
N-G-4	inactive(0.52)	inactive(0.60)	inactive(0.55)	inactive(0.98)	inactive(0.94)	inactive(0.99)	inactive(1.0)
N-G-5	inactive(0.61)	inactive(0.84)	active(0.92)	inactive(0.88)	inactive(0.88)	active(1.0)	active(1.0)
N-G-6	inactive(0.65)	active(0.76)	inactive(0.92)	inactive(0.86)	inactive(0.89)	inactive(0.99)	inactive(0.99)
N-G-7	inactive(0.67)	active(0.55)	active(0.85)	inactive(0.97)	inactive(0.85)	inactive(0.97)	inactive(0.99)
N-G-8	inactive(0.69)	inactive(0.70)	inactive(0.68)	inactive(0.92)	inactive(0.90)	inactive(0.97)	inactive(0.99)
N-G-9	inactive(0.55)	inactive(0.64)	inactive(0.97)	inactive(0.96)	inactive(0.93)	inactive(0.93)	inactive(0.98)
N-G-10	inactive(0.52)	inactive(0.57)	inactive(0.78)	inactive(0.99)	inactive(0.94)	inactive(0.97)	inactive(0.99)
N-G-11	active(0.51)	inactive(0.59)	active(0.87)	inactive(0.87)	inactive(0.91)	inactive(0.96)	inactive(0.98)
N-G-12	inactive(0.72)	inactive(0.59)	active(0.92)	inactive(0.71)	inactive(0.89)	active(0.89)	inactive(0.88)
N-G-13	inactive(0.65)	inactive(0.54)	inactive(0.72)	inactive(0.83)	inactive(0.87)	inactive(0.91)	inactive(0.98)
N-G-14	inactive(0.6)	inactive(0.52)	inactive(0.95)	inactive(0.95)	inactive(0.92)	inactive(0.95)	inactive(0.99)
N-G-15	inactive(0.72)	inactive(0.74)	active(0.86)	active(0.67)	inactive(0.75)	inactive(0.68)	inactive(0.92)
N-G-16	inactive(0.73)	inactive(0.68)	active(0.98)	inactive(0.86)	inactive(0.83)	inavtive(0.53)	inactive(0.76)
N-G-17	inactive(0.78)	inactive(0.61)	active(0.98)	inactive(0.72)	inactive(0.92)	active(0.63)	inactive(0.70)
N-G-18	inactive(0.87)	inactive(0.64)	inactive(0.78)	inactive(0.88)	inactive(0.93)	inactive(0.93)	inactive(0.98)
N-G-19	inactive(0.51)	inactive(0.73)	inactive(0.90)	inactive(0.89)	inactive(0.89)	inactive(0.93)	inactive(0.98)
N-G-20	inactive(0.55)	inactive(0.61)	inactive(0.78)	inactive(0.95)	inactive(0.94)	inactive(0.81)	inactive(0.99)
N-G-21	inactive(0.71)	active(0.61)	inactive(0.95)	inactive(0.98)	inactive(0.86)	inactive(0.99)	inactive(1.0)
N-G-22	inactive(0.61)	inactive(0.79)	inactive(0.94)	inactive(0.92)	inactive(0.91)	inactive(0.95)	inactive(0.98)
N-G-23	inactive(0.66)	inactive(0.61)	active(0.59)	inactive(0.97)	inactive(0.88)	inactive(0.98)	inactive(0.99)
N-G-24	inactive(0.61)	inactive(0.82)	active(0.94)	inactive(0.79)	inactive(0.85)	active(0.94)	active(0.80)
N-G-25	active(0.50)	inactive(0.63)	active(0.79)	inactive(0.85)	inactive(0.90)	inactive(0.97)	inactive(0.98)
N-G-26	inactive(0.82)	inactive(0.68)	active(0.76)	inactive(0.81)	inactive(0.93)	inactive(0.92)	inactive(0.96)
N-G-27	inactive(0.63)	inactive(0.57)	inactive(0.80)	inactive(0.75)	inactive(0.93)	active(0.52)	inactive(0.89)
N-G-28	inactive(0.67)	inactive(0.64)	inactive(0.99)	inactive(0.79)	inactive(0.86)	inactive(0.88)	inactive(0.95)
N-G-29	inactive(0.64)	inactive(0.63)	inactive(0.73)	inactive(0.72)	inactive(0.93)	inactive(0.97)	inactive(0.96)
N-G-30	inactive(0.71)	inactive(0.75)	active(0.62)	active(0.53)	inactive(0.80)	inactive(0.69)	inactive(0.93)
N-G-31	inactive(0.87)	inactive(0.70)	inactive(0.71)	inactive(0.80)	inactive(0.94)	inactive(0.58)	inactive(0.80)
N-G-32	inactive(0.74)	inactive(0.60)	active(0.98)	inactive(0.72)	inactive(0.94)	active(0.55)	inactive(0.84)
N-G-33	inactive(0.71)	active(0.53)	inactive(0.82)	inactive(0.93)	inactive(0.88)	inactive(0.98)	inactive(0.99)
N-G-34	active(0.52)	inactive(0.70)	inactive(0.92)	inactive(0.95)	inactive(0.96)	inactive(0.96)	inactive(0.99)
N-G-35	inactive(0.70)	inactive(0.74)	inactive(0.94)	inactive(0.87)	inactive(0.94)	inactive(0.91)	inactive(0.98)
N-G-36	inactive(0.55)	inactive(0.62)	inactive(0.68)	inactive(0.96)	inactive(0.93)	inactive(0.98)	inactive(1.0)
N-G-37	inactive(0.76)	inactive(0.62)	active(0.87)	inactive(0.78)	inactive(0.88)	inactive(0.92)	inactive(0.99)
N-G-38	inactive(0.62)	inactive(0.57)	active(0.97)	inactive(0.61)	inactive(0.86)	active(0.85)	inactive(0.53)
N-G-39	inactive(0.72)	inactive(0.68)	active(0.66)	inactive(0.94)	inactive(0.95)	active(0.92)	inactive(0.86)
N-G-40	inactive(0.58)	inactive(0.69)	active(0.93)	inactive(0.69)	inactive(0.97)	active(0.94)	active(0.56)
N-G-41	inactive(0.70)	inactive(0.71)	inactive(0.91)	inactive(0.75)	inactive(0.85)	active(0.78)	inactive(0.59)
N-G-42	inactive(0.94)	inactive(0.79)	active(0.52)	inactive(0.83)	inactive(0.92)	inactive(0.94)	inactive(0.97)
N-G-43	inactive(0.55)	inactive(0.72)	inactive(0.69)	inactive(0.87)	inactive(0.91)	inactive(0.92)	inactive(0.98)
N-G-44	inactive(0.6)	inactive(0.52)	inactive(0.95)	inactive(0.95)	inactive(0.92)	inactive(0.95)	inactive(0.99)
N-G-45	inactive(0.68)	active(0.64)	inactive(0.91)	inactive(0.79)	inactive(0.88)	inactive(0.96)	inactive(0.98)
N-G-46	inactive(0.55)	inactive(0.64)	inactive(0.96)	inactive(0.96)	inactive(0.93)	inactive(0.93)	inactive(0.98)
N-G-47	inactive(0.51)	inactive(0.61)	active(0.95)	inactive(0.96)	inactive(0.88)	inactive(0.92)	inactive(0.93)
N-G-48	active(0.50)	inactive(0.80)	inactive(0.97)	inactive(0.93)	inactive(0.92)	inactive(0.95)	inactive(0.97)
N-G-49	inactive(0.52)	inactive(0.60)	active(0.63)	inactive(0.98)	inactive(0.94)	inactive(0.99)	inactive(1.0)

Table S13. Results of the toxicity prediction by using pkCSM server

Compound code	Hepatotoxicity	hERG I inhibitor	hERG II inhibitor
N-G-1	no	no	no
N-G-2	no	no	no
N-G-3	no	no	no
N-G-4	no	no	no
N-G-5	no	no	no
N-G-6	no	no	no
N-G-7	yes	no	no
N-G-8	no	no	no
N-G-9	no	no	yes
N-G-10	no	no	no
N-G-11	no	no	no
N-G-12	no	no	no
N-G-13	yes	no	no
N-G-14	no	no	no
N-G-15	no	no	yes
N-G-16	no	no	no
N-G-17	no	no	yes
N-G-18	no	no	no
N-G-19	yes	no	no
N-G-20	no	no	no
N-G-21	no	no	no
N-G-22	no	no	no
N-G-23	no	no	no
N-G-24	no	no	yes
N-G-25	no	no	no
N-G-26	no	no	no
N-G-27	no	no	yes
N-G-28	yes	no	no
N-G-29	no	no	no
N-G-30	no	no	yes
N-G-31	no	no	yes
N-G-32	no	no	no
N-G-33	yes	no	no
N-G-34	no	no	no
N-G-35	no	no	no
N-G-36	no	no	no
N-G-37	no	no	no
N-G-38	no	no	no
N-G-39	no	no	no
N-G-40	no	no	no
N-G-41	no	no	yes
N-G-42	no	no	no
N-G-43	yes	no	no
N-G-44	no	no	no
N-G-45	yes	no	no
N-G-46	no	no	no
N-G-47	no	no	no
N-G-48	no	no	no
N-G-49	no	no	no