

Probing New Antileukemia Agents That Target FLT3 and BCL-2 from Traditional Concoctions through a Combination of Mass Spectrometry Analysis and Consensus Docking Methods

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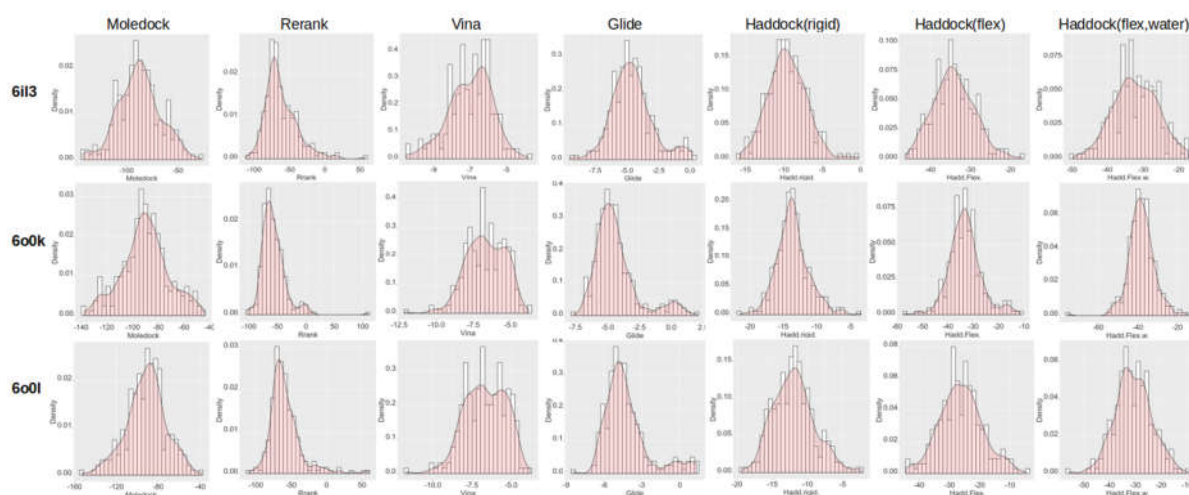


Figure S1. The distribution of the docking scores of the 262 molecules from the three samples of traditional concoctions with the two known drugs Venetoclax and Gilteritinib according to the seven docking scores Molodock, Rerank, Vina, Glide, Haddock(rigid), Haddock(Flex) and Haddock(flex,water)

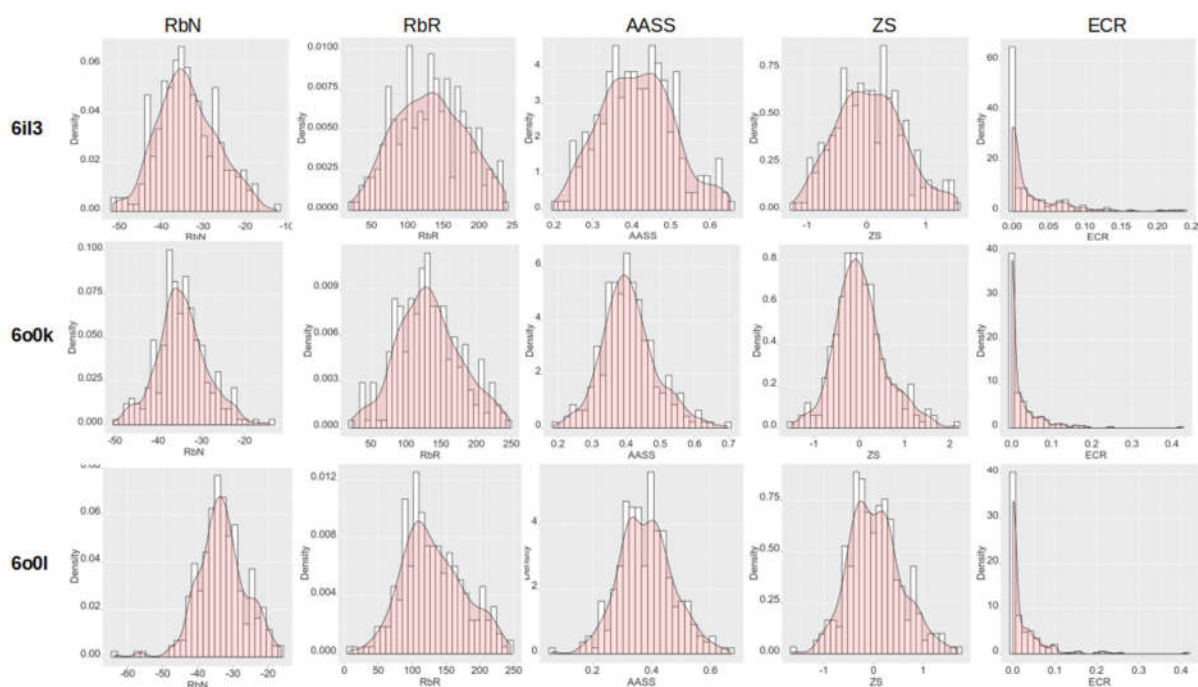


Figure S2. The distribution of the docking scores of the 262 molecules from the three samples of traditional concoctions with the two known drugs Venetoclax and Gilteritinib according to the five consensus methods RbN, RbR, AASS, ZS and ECR that were used for the combination of the seven docking scores

Table S1. The CAS number and the names of all the potential drugs candidates identified in NIST database to have similar structures with the LC-MS fragmentations obtained from the three traditional concoction using AMDIS package

CAS	Name	CAS	Name	CAS	Name
5003	Hydrocortisone	1315	Dioxybenzone	1662017	1,10-Phenanthroline, 4,7-diphenyl-
3	Acetate	33			
5014	Ergocalciferol	1315	Methanone, (2,4-dihydroxyphenyl)phenyl-	1713151	Acetic acid, (2,4-dichlorophenoxy)-, 2-methylpropyl ester
6		66			
5023	Hydrocortisone	1334	Benzenethiol, pentachloro-	1731799	Dodecanedioic acid, dimethyl ester
7		93			
5027	Estriol	1336	Trichlormethiazide	1771182	2-Methoxyphenothiazine
1		75			
5029	p,p'-DDT	1358	2-Naphthalenamine, N-phenyl-	1788314	Dibenzyl ketoxime
3		86			
5155	Atropine	1412	Ricinoleic acid	1807029	11.alpha.-Hydroxy-17.alpha.-methyl testosterone
8		20			
5221	Prednisolone Acetate	1429	Isopropyl palmitate	1843056	Octabenzone
1		16			
5239	Aldosterone	1432	9-Octadecen-1-ol, (Z)-	1918021	Picloram
1		82			

5303 2	Prednisone	1435 00	Kepone	1940574	9H-Fluorene, 9-bromo-
5306 5	Cortisone	1448 09	Sulfacetamide	1947586	dl-2,3-Dibromo-1,4-butanediol
5363 4	Estra-1,3,5(10)-trien-3-ol	1478 20	Benzenamine, 2,4,6-tribromo-	1948921	4-Nitro-4'-aminodiphenylsulfone
5580 1	Benzenamine, N,N-dimethyl-4-[(3-methylphenyl)azo]-	1542 12	Lincomycin	1985122	4-Bromophenyl isothiocyanate
5649 5	3-Methylcholanthrene	2134 67	Picene	1989522	Cholest-5-en-3-ol (3.beta.)-, tetradecanoate
5653 1	Diethylstilbestrol	2155 87	Benzo[b]triphenylene	2015567	Phosphoramidic acid, diphenyl ester
5675 7	Chloramphenicol	2390 10	11H-Benzo[a]carbazole	2016424	1-Tetradecanamine
5711 4	Octadecanoic acid	3153 77	Testosterone enanthate	2104963	Bromophos
5724 9	Strychnine	3391 62	Retinoic acid, methyl ester	2136756	(Triphenylphosphoranylidene) acetaldehyde
5766 9	Probenecid	3575 73	Brucine	2207274	1,3-Cyclopentadiene, 1,2,3,4-tetrachloro-5,5-dimethoxy-
5785 2	Testosterone propionate	4233 81	Butane, 1,1,3,4-tetrachloro-1,2,2,3,4,4-hexafluoro-	2227170	Dienochlor
5787 4	Ergosterol	4270 09	Desomorphine	2259963	Cyclothiazide
5818 4	17.alpha.-Methyltestosterone	4719 54	Bufotalin	2300881	3'-Trifluoromethylpropionanilide
5820 8	Testosterone cypionate	4789 44	Lysergamide	2303175	Triallate
5861 7	9-.alpha.-d-Arabinofuranosyladenine	4864 75	Isoquinoline, 1-[(3,4-diethoxyphenyl)methyl]-6,7-diethoxy-	2385855	Mirex
5893 5	Hydrochlorothiazide	5130 20	Triisopropylphosphate	2432908	Didodecyl phthalate
5894 6	Chlorothiazide	5182 07	2H,5H-Pyrano[3,2-c][1]benzopyran-5-one, 3,4-dihydro-2-methoxy-2-methyl-4-phenyl-	2440224	Drometrizole
5905 2	Methotrexate	5202 85	4H-1-Benzopyran-4-one, 5-hydroxy-7-methoxy-2-phenyl-	2475458	Disperse Blue 1
6011 7	Benzenamine, N,N-dimethyl-4-(phenylazo)-	5217 44	Broxyquinoline	2588058	O,O-Diethyl S-eththionylmethyl phosphorothioate

6325 2	Carbaril	5304 49	Methanone, [4-(dimethylamino)phenyl]phenyl-	2631370	Phenol, 3-methyl-5-(1-methylethyl)-, methylcarbamate
6486 8	Colchicine	5319 19	[1,1'-Biphenyl]-4,4'-diamine, N,N'-diphenyl-	2642800	1-Chloro-2,2-Bis(p-chlorophenyl)ethane
6797 0	Cholecalciferol	5403 85	Phenol, 4-iodo-	2673407	Vobassan-17-oic acid, 4-demethyl-3-oxo-, methyl ester
6826 8	Retinol	5424 49	Glycerol 1-palmitate	2834051	11-Bromoundecanoic acid
6876 8	Triaziquone	5447 63	Hexadecane	2850193	Acetic acid, [(4-methylphenyl)sulfonyl]-, ethyl ester
7030 4	Hexachlorophene	5484 36	Ergoline-8-methanol, 8,9-didehydro-6-methyl-	2872482	Disperse Red 11
7163 6	Digitoxin	5496 88	Octaverine	2958363	Methanone, (2-amino-5-chlorophenyl)(2-chlorophenyl)-
7214 0	Sulfathiazole	5630 42	Phosphoric acid, tris(3-methylphenyl) ester	3001158	4,4'-Diiododiphenyl
7248 0	Alizarin	5652 08	Acetamide, N-[4-[(4-aminophenyl)sulfonyl]phenyl]-	3058397	Benzonitrile, 4-iodo-
7706 5	Gibberellic acid	5934 53	Octadecane	3118976	2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]-
7709 8	Phenolphthalein	6015 47	Cholest-5-en-3-one	3342981	Benz[j]aceanthrylen-1-ol, 1,2-dihydro-3-methyl-
7830 8	Phosphoric acid, tris(2-methylphenyl) ester	6035 09	Bisacodyl	3383219	3,5-Cyclohexadiene-1,2-dione, 3,5-bis(1,1-dimethylethyl)-
8035 3	Sulfamethoxypyridazine	6043 20	Cholesteryl benzoate	3457485	Ethandione, bis(p-tolyl)-
8038 6	Benzenesulfonic acid, 4-chlorophenyl ester	6079 98	Benzene, 1,3,5-tribromo-2-methoxy-	3648213	1,2-Benzenedicarboxylic acid, diheptyl ester
8074 0	Sulfisoxazole Acetyl	6089 35	Benzene, pentachloro-	3848519	Phosphoramidic acid, phenyl-, diphenyl ester
8123 2	Dehydrocholic acid	6142 66	Diazene, bis(4-chlorophenyl)-, 1-oxide	4108616	7-Amino-3-phenylcoumarin
8163 0	9,10-Anthracenedione, 1,4-diamino-2,3-dihydro-	6155 54	3,4-Dibromoaniline	4419390	Beclomethasone
8164 1	9,10-Anthracenedione, 1,4-dihydroxy-	6155 76	Benzenamine, 2,4-dibromo-	4659476	2,3,6-Trichlorobenzaldehyde

8181 2	Warfarin	6166 82	Trimecaine	5060526	4(3H)-Quinazolinone, 3-(4-hydroxy-2-methylphenyl)-2-methyl-
8268 8	Benzene, pentachloronitro-	6243 17	Benzene, 1-iodo-4-methyl-	6259763	n-Hexyl salicylate
8373 8	Iodoquinol	6260 28	Phenol, 3-iodo-	6267023	Acridine, 9,10-dihydro-9,9-dimethyl-
8388 5	Riboflavine	6266 20	Cyclohexane, iodo-	7173844	Carbophenoxon
8436 6	Syrosingopine	6299 70	Docosane	7235407	.beta. Carotene
8451 5	9,10-Anthracenedione, 2-ethyl-	6300 13	Hexacosane	7507019	3,4-Hexanediol, 3,4-bis(4-hydroxyphenyl)-
8464 0	1,2-Benzenedicarboxylic acid, butyl cyclohexyl ester	6300 24	Octacosane	15318453	Thiamphenicol
8474 2	Dibutyl phthalate	6302 51	Ethane, 1,2-dibromo-1,1,2,2-tetrachloro-15597769	15358482	Hydroxylupanine
8476 4	1,2-Benzenedicarboxylic acid, dinonyl ester	6316 41	Acetic acid, dibromo-	5-Chlorosalicylidene aniline	
8478 6	1,2-Benzenedicarboxylic acid, butyl octyl ester	6320 08	Sulfasomizole	16655826	3-Hydroxycarbofuran
8569 8	1,2-Benzenedicarboxylic acid, butyl 2-ethylhexyl ester	6325 20	Hydrazine, tetraphenyl-	16965085	tert-Butyl 2,4,5-trichlorophenyl carbonate
8572 3	Benzoic acid, 2-[[[(3-methylphenyl)amino]carbonyl]-	6333 18	Cholest-5-en-3-ol (3.beta.)-, propanoate	18435455	1-Nonadecene
8573 4	Phthalylsulfathiazole	6426 59	Acetamide, N-acetyl-N-9H-fluoren-2-yl-	18713514	2-Propanol, 1,3-dibromo-, phosphate (3:1)
8688 4	Thiourea, 1-naphthalenyl-	6454 10	1-Butanamine, 3-methyl-N,N-bis(3-methylbutyl)-	19386459	Phenol, 2,2'-methylenebis(3,5,6-trichloro-
8700 3	Homatropine	6463 00	Nonadecanoic acid	22232719	Mazindol
8889 1	Picric acid	7052 15	3,5-Dichlorobenzenesulfonyl chloride	22248799	Tetrachlorvinphos
9223 9	Leucinocaine	8650 43	Methoserpidine	23095058	5-Bromo-2-methoxybenzenesulfonyl chloride
9376 5	Acetic acid, (2,4,5-trichlorophenoxy)-	8863 40	.alpha.-(4-Bromophenylimino)-	24323259	Undecanoic acid, 2-methyl-

			ortho-cresol		
9777 8	Disulfiram	8977 89	Cyclohexanone, 2,6-bis(phenylmethylene)-	24815245	Rescinnamine
9930 9	Botran	9566 27	Benzene, 1,1'-methylenebis[4-isocyano-	25216277	1-Naphthyl n-propylcarbamate
1013 15	Hyoscyamine	9580 98	Adenosine, 2'-deoxy-	25573437	Eseridine
1017 57	Benzenamine, N-phenyl-4-(phenylazo)-	1002 842	Pentadecanoic acid	27314132	Norflurazon
1032 31	Hexanedioic acid, bis(2-ethylhexyl) ester	1021 256	1-Phenyl-1,3,8-triazaspiro[4.5]decan-4-one	28322023	Acetamide, N-9H-fluoren-4-yl-
1061 16	Octadecanoic acid, 2-(2-hydroxyethoxy)ethyl ester	1031 932	Diphenyl(4-tolyl)phosphine	28782425	Difenoxin
1110 13	Squalane	1045 698	Testosterone acetate	29091212	1,3-Benzenediamine, 2,4-dinitro-N3,N3-dipropyl-6-(trifluoromethyl)-
1110 68	Hexadecanoic acid, butyl ester	1059 865	Cholesta-5,7-dien-3-ol, acetate, (3.beta.)-	32634687	(+)-di-O-4-Toluoyl-D-tartaric acid
1123 90	Hexadecanoic acid, methyl ester	1082 888	Phenethylamine, 3,4,5-trimethoxy-.alpha.-methyl-	38396393	Bupivacaine
1126 18	Methyl stearate	1085 127	Benzoic acid, 4-hydroxy-, n-heptyl ester	39208009	Benzaldehyde, 4-((4-(dimethylamino)phenyl)azo)-
1126 29	9-Octadecenoic acid (Z)-, methyl ester	1088 568	Lumiflavine	40817081	[1,1'-Biphenyl]-4-carbonitrile, 4'-pentyl-
1129 25	1-Octadecanol	11202 81	Eicosanoic acid, methyl ester	50782699	VX
1129 58	Eicosane	11641 65	N-Benzyloxycarbonyl-L-tyrosine	51234287	Benoxaprofen
1131 55	Ergotamine	11665 25	Lauryl gallate	52584391	5-Ethyl-5-p-tolylbarbituric acid
1161 65	Hexachloroacetone	11826 67	Cholest-5-en-3-ol (3.beta.)-, nonanoate54771607	52645531	Permethrine
1178 17	Bis(2-ethylhexyl) phthalate	1207 698	Acridine, 9-chloro-	4-Acetoxy-3-methoxyacetophenone	
1178 40	Di-n-octyl phthalate	1222 055	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-	55334515	1,4-Benzenedicarboxylic acid, [4-(methoxycarbonyl)phenyl]methyl methyl ester

1252 91	Hydrocodone	1223 310	hexamethyl- di(p-Nitrophenyl) sulfide	56534022	.alpha.-Chlordene
1261 47	Sucrose Octaacetate	1241 947	Octicizer	62373802	Benzaldehyde, 3-(4-methoxyphenoxy)-
1267 27	1-Propanol, 2,3-dibromo-, phosphate (3:1)	1330 865	Diisooctyl adipate	63077009	7H-Dibenzo(a,g)carbazole, 12,13-dihydro-
1267 38	Tributyl phosphate	1440 977	Phosphorodiamidic acid, tetramethyl-, pentachlorophenyl ester	65967013	N-Acetylcolchinel methyl ether
1276 95	Sulfisoxazole	1472 873	Tridecanedioic acid, dimethyl ester	67199660	Daniquidone
1290 00	Pyrene	16119 23	Benzene, 1,3-dibromo-5-methyl-	75520897	Colchicine, (+)-
1302 67	Clioquinol	1617 909	Vincamine	78725469	3-(3-[Trifluoromethyl]phenoxy)benzaldehyde
1308 03	Diethylstilbestrol dipropionate				