

Supplementary file 3

Investigating the function and targeting of MET protein as an oncogene kinase in pancreatic ductal adenocarcinoma: A microarray data integration

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





³A. Nocivelli Institute for Molecular Medicine, Department of Molecular and Translational Medicine, University of Brescia, 25123 Brescia, Italy


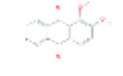
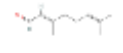
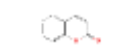
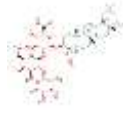
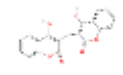
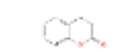
⁴Research Center for Pharmaceutical Nanotechnology, Biomedicine Institute, Tabriz University of Medical Sciences, Tabriz, Iran


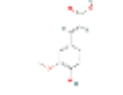


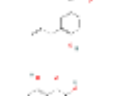
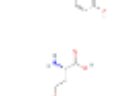
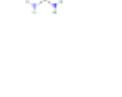
⁵Department of Molecular Genetics, Faculty of Biological Sciences, Tarbiat Modares University, Tehran, Iran

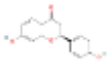
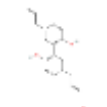
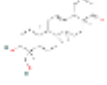
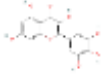
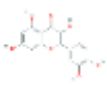
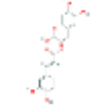
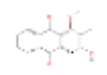
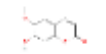
⁶Bioinformatics Research Group (BIRG), Department of Biosciences, Faculty of Science, Universiti Teknologi Malaysia, Skudai, Johor, Malaysia

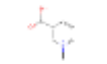
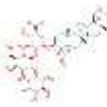
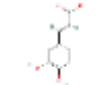
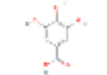
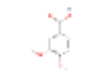
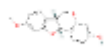
Table S3. List of 40 phytochemical compounds of the yellow sweet clover plant retrieved from both IMPPAT and Dr. Duke's databases.



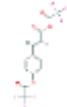



Phytochemical ID	Phytochemical name	Molecular formula	Chemical diagram	Binding affinity kcal/mol
CID:5280841	2-Coumarinate	C ₉ H ₈ O ₃		-4.9
CID: 18646	2-Methoxyanthraquinone	C ₁₅ H ₁₀ O ₃		-9.9
CID:446611	2,4-Dihydroxycinnamic acid	C ₉ H ₈ O ₄		-5.8
CID:8768	3,4-Dihydroxybenzaldehyde	C ₇ H ₆ O ₃		-5.5
CID:135	4-Hydroxybenzoic acid	C ₇ H ₆ O ₃		-5.7
CID: 100031	7-Oxabicyclo[4.1.0] heptan-2-one, 6-methyl-3-(1-methylethenyl)-	C ₁₀ H ₁₄ O ₂		-4.3

CID:101997831	Acetylsoyasaponin I	C ₆₇ H ₁₀₄ O ₃₃		-5.4
CID:80309	Alizarin 1-methyl ether	C ₁₅ H ₁₀ O ₄		-4.5
CID:638011	Citral	C ₁₀ H ₁₆ O		-5.1
CID:323	Coumarin	C ₉ H ₆ O ₂		-6.7
CID:656760	Dehydrosoyasaponin I	C ₄₈ H ₇₆ O ₁₈		-10.5
CID:54676038	Dicumarol	C ₁₉ H ₁₂ O ₆		-10.8
CID:660	Dihydrocoumarin	C ₉ H ₈ O ₂		-6.5

Phytochemical ID	Phytochemical name	Molecular formula	Chemical diagram	Binding affinity kcal/mol
CID:99474	Diosgenin	C ₂₇ H ₄₂ O ₃		-5.7
CID:445858	Ferulic acid	C ₁₀ H ₁₀ O ₄		-7.0
CID:16129616	Fortical	C ₁₄₅ H ₂₄₀ N ₄₄ O ₄₈ S ₂		-6.1
CID:439336	Galactomannan	C ₁₈ H ₃₂ O ₁₆		-7.4
CID:72303	Honokiol	C ₁₈ H ₁₈ O ₂		-6.3
CID:5280863	Kaempferol	C ₁₅ H ₁₀ O ₆		-6.0
CID:439202	L-canavanine	C ₅ H ₁₂ N ₄ O ₃		-5.9

CID:114829	Liquiritigenin	C ₁₅ H ₁₂ O ₄		-7.2
CID:72300	Magnolol	C ₁₈ H ₁₈ O ₂		-5.8
CID:14059499	Melilotigenin	C ₃₀ H ₄₆ O ₅		-11.9
CID:5281672	Myricetin	C ₁₅ H ₁₀ O ₈		-5.7
CID:5280343	Quercetin	C ₁₅ H ₁₀ O ₇		-9.5
CID:5281792	Rosmarinic acid	C ₁₈ H ₁₆ O ₈		-5.6
CID:96191	Rubiadin 1-methyl ether	C ₁₆ H ₁₂ O ₄		-5.8
CID:5280460	Scopoletin	C ₁₀ H ₈ O ₄		-5.9

Phytochemical ID	Phytochemical name	Molecular formula	Chemical diagram	
CID:5570	Trigonelline	C ₇ H ₇ NO ₂		-6.2
CID:189675	Azukisaponin-V	C ₄₈ H ₇₇ O ₁₈ ⁻		-9.0
CID:689043	Caffeic acid	C ₉ H ₈ O ₄		-6.8
CID:370	Gallic acid	C ₇ H ₆ O ₅		-5.9
CID: 8468	Vanillic acid	C ₈ H ₈ O ₄		-5.7
CID:336327	Medicarpin	C ₁₆ H ₁₄ O ₄		-7.1

CID: 131751575	Melilotin	$C_{54}H_{90}O_{21}$		-6.4
CID: 5280759	Melilotoside	$C_{15}H_{18}O_8$		-7.3
CID: 91738022	P-coumaric-acid	$C_{13}H_6F_6O_5$		-6.2
CID: 338	Salicylic-acid	$C_7H_6O_3$		-5.9
CID: 637775	Sinapic-acid	$C_{11}H_{12}O_5$		-7.0
CID: 122097	Soyasaponin I	$C_{48}H_{78}O_{18}$		-8.5
