# Supplementary materials

## The Influence of Flavonoids with -Br, -Cl Atoms and -$NO_2$, -$CH_3$ Groups on The Growth Kinetics and The Number of Pathogenic and Probiotic Microorganisms

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Compound name: 2′-Hydroxy-5′-methyl-3′-nitrochalcone
Symbol number: **1**
Molecular Formula: $C_{16}H_{13}NO_4$
Formula Weight: 283.279
SMILE: O=[N+]([O-])c1cc(C)cc(C(=O)/C=C/c2ccccc2)c1O

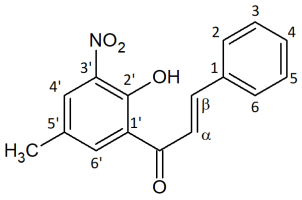



*Table S 1. 2′-Hydroxy-5′-methyl-3′-nitrochalcone (**1**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.722 | 0.060 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.545 | 0.020 | K562 | Erythroleukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 3 | 0.507 | 0.007 | RCC4 | Clear cell renal cell carcinoma | Kidney | Carcinoma |
| 4 | 0.471 | 0.024 | SNU-475 | Hepatocellular carcinoma | Liver | Carcinoma |
| 5 | 0.425 | 0.055 | YAPC | Pancreatic carcinoma | Pancreas | Carcinoma |
| 6 | 0.393 | 0.033 | HEK293 | Embryonic kidney fibroblast | Kidney | Normal |
| 7 | 0.388 | 0.054 | CAL-51 | Breast carcinoma | Breast | Carcinoma |
| 8 | 0.373 | 0.123 | NCI-H441 | Papillary adenocarcinoma | Lung | Adenocarcinoma |
| 9 | 0.351 | 0.169 | SW48 | Colorectal Adenocarcinoma | Colon | Adenocarcinoma |
| 10 | 0.346 | 0.023 | RL | Non-Hodgkin's Lymphoma | Ascites | Lymphoma |

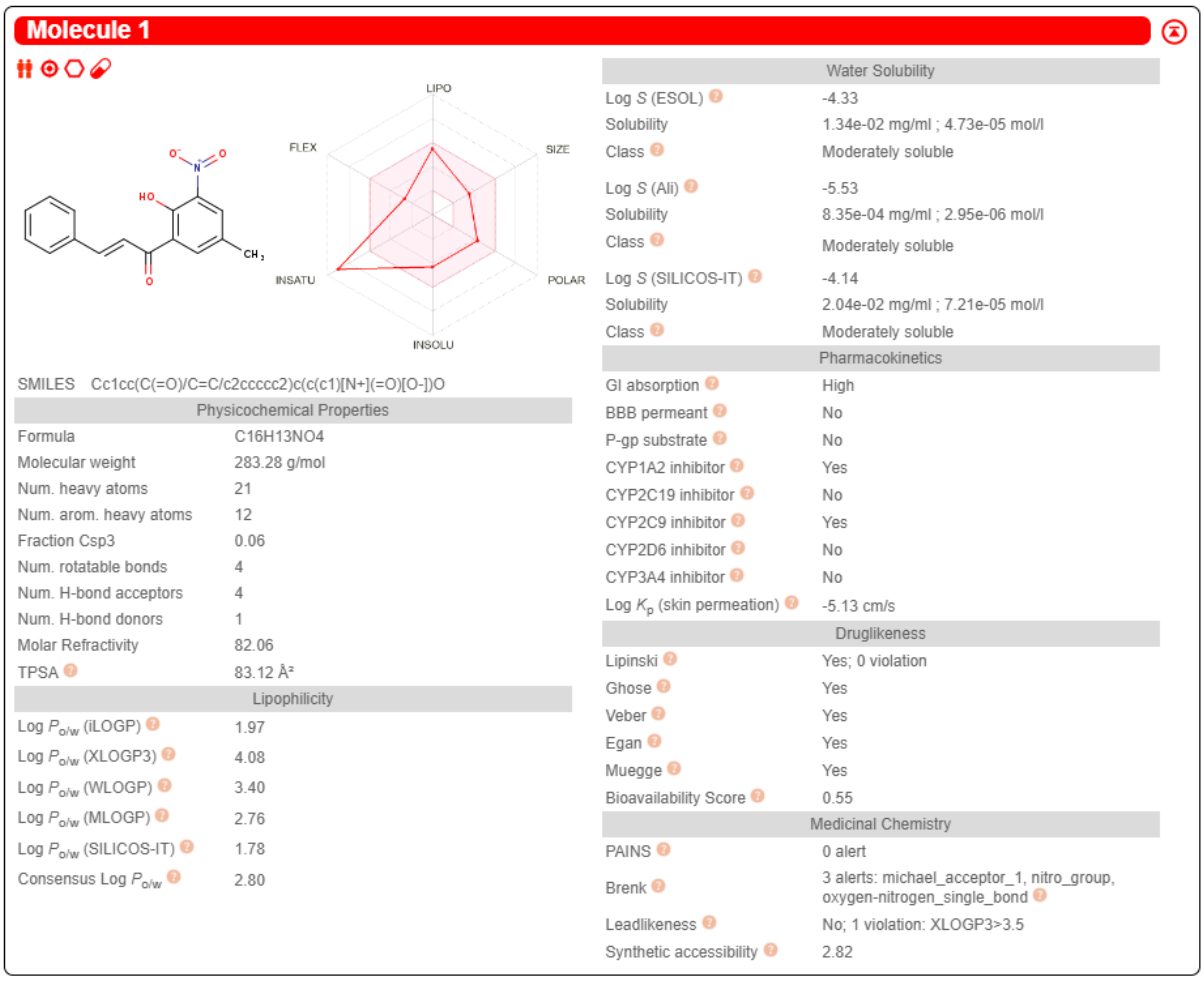



*Figure S 1. 2′-Hydroxy-5′-methyl-3′-nitrochalcone (**1**) activity prediction using SwissADME.*

Compound name: 6-Methyl-8-nitroflavanone
Symbol: **2**
Molecular Formula: $C_{16}H_{13}NO_4$
Formula Weight: 283.279
SMILE: [O-][N+](=O)c1cc(C)cc2c1OC(CC2=O)c1ccccc1

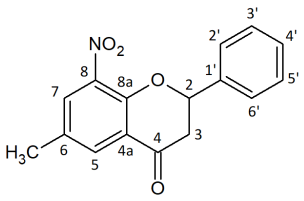



*Table S 2. 6-Methyl-8-nitroflavanone (**2**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.759 | 0.046 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.596 | 0.004 | MES-SA | Uterine corpus sarcoma | Uterus | Sarcoma |
| 3 | 0.396 | 0.087 | YAPC | Pancreatic carcinoma | Pancreas | Carcinoma |
| 4 | 0.391 | 0.044 | NCI-H187 | Small cell lung carcinoma | Lung | Carcinoma |
| 5 | 0.346 | 0.031 | 5637 | Urothelial bladder carcinoma | Urinary tract | Carcinoma |
| 6 | 0.324 | 0.036 | NALM-6 | Adult B acute lymphoblastic leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 7 | 0.321 | 0.150 | SK-MES-1 | Squamous cell lung carcinoma | Lung | Carcinoma |
| 8 | 0.313 | 0.114 | HCC1806 | Acantholytic Squamous Cell Carcinoma | Breast | Carcinoma |
| 9 | 0.305 | 0.037 | C8166 | Leukemic T-cells | Blood | Leukemia |
| 10 | 0.304 | 0.187 | SNU-475 | Hepatocellular carcinoma | Liver | Carcinoma |

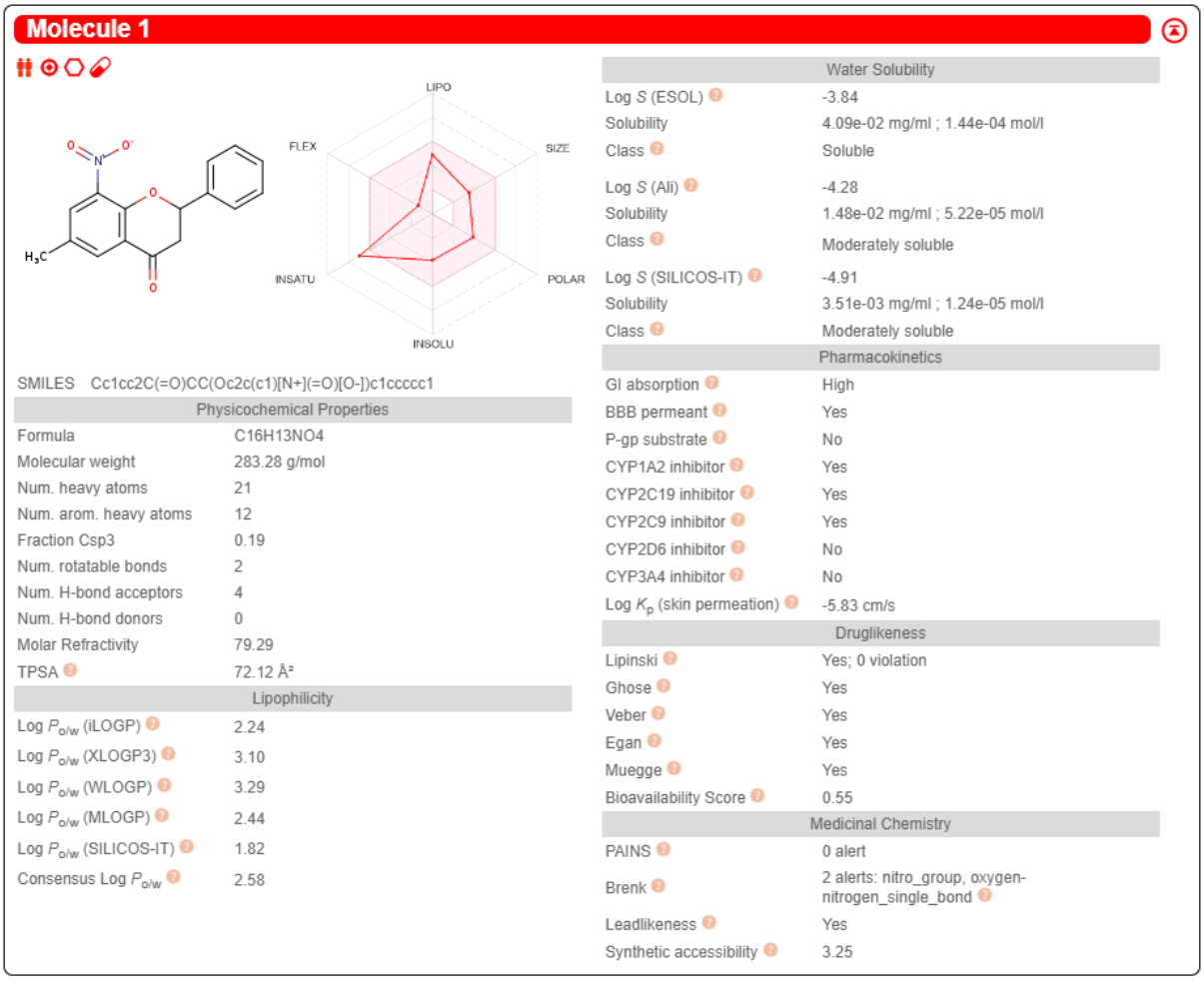



*Figure S 2. 6-Methyl-8-nitroflavanone (**2**) activity prediction using SwissADME.*

Compound name: 6-Methyl-8-nitroflavone
Symbol: **3**
Molecular Formula: $C_{16}H_{11}NO_4$
Formula Weight: 281.263
SMILE: [O-][N+](=O)c1cc(C)cc2c1OC(=CC2=O)c1ccccc1

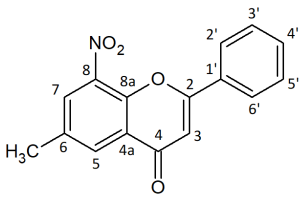



*Table S 3. 6-Methyl-8-nitroflavone (**3**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.725 | 0.003 | MES-SA | Uterine corpus sarcoma | Uterus | Sarcoma |
| 2 | 0.617 | 0.103 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 3 | 0.431 | 0.070 | HepG2 | Hepatoblastoma | Liver | Hepatoblastoma |
| 4 | 0.408 | 0.007 | 5637 | Urothelial bladder carcinoma | Urinary tract | Carcinoma |
| 5 | 0.391 | 0.093 | YAPC | Pancreatic carcinoma | Pancreas | Carcinoma |
| 6 | 0.352 | 0.030 | NCI-H661 | Lung carcinoma | Lung | Carcinoma |
| 7 | 0.348 | 0.006 | C8166 | Leukemic T-cells | Blood | Leukemia |
| 8 | 0.325 | 0.144 | SK-MES-1 | Squamous cell lung carcinoma | Lung | Carcinoma |
| 9 | 0.322 | 0.191 | SK-MEL-1 | Metastatic melanoma | Skin | Melanoma |
| 10 | 0.317 | 0.248 | SK-LU-1 | Adenocarcinoma | Lung | Carcinoma |

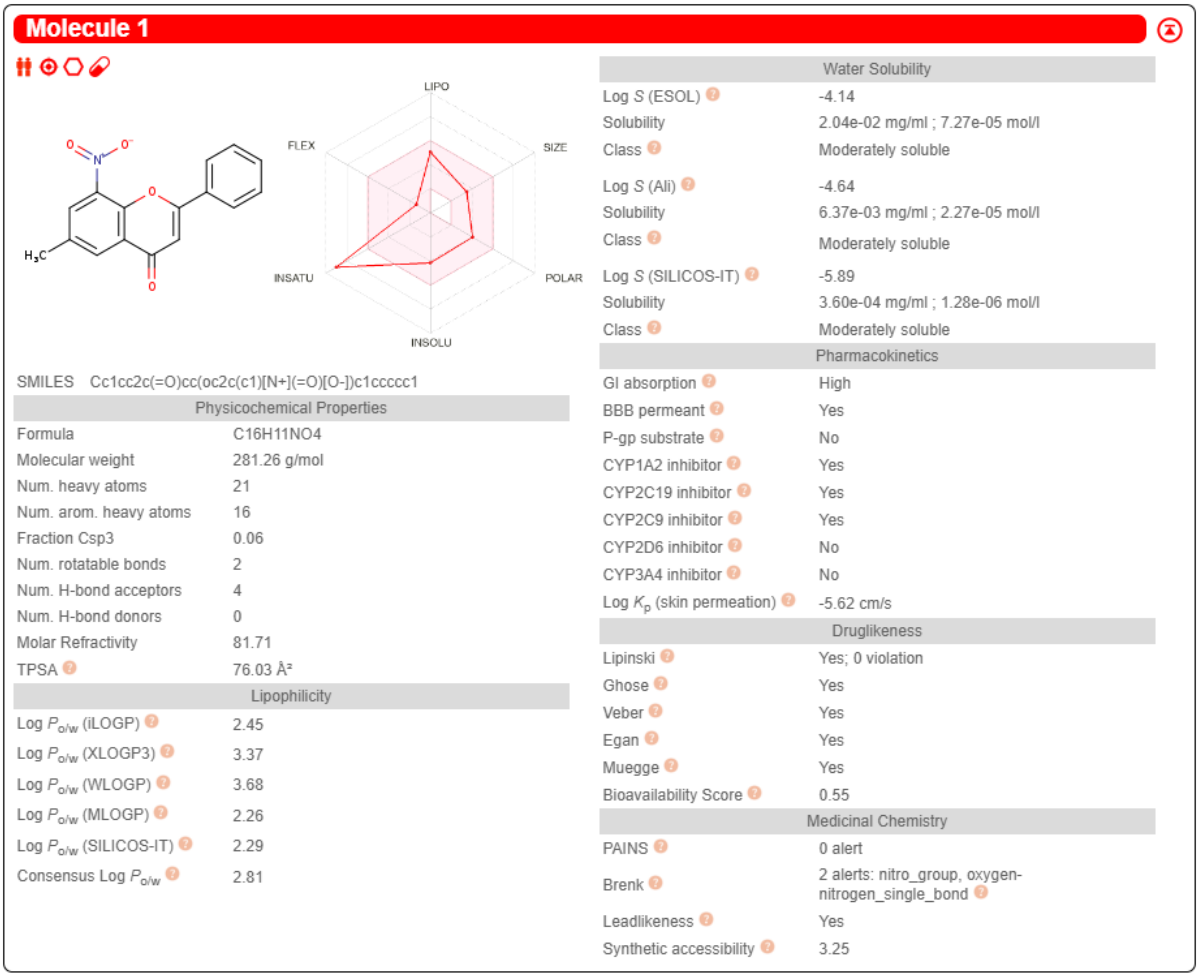



*Figure S 3. 6-Methyl-8-nitroflavone (**3**) activity prediction using SwissADME.*

Compound name: 3′-Bromo-5′-chloro-2′-hydroxychalcone
Symbol: **4**
Molecular Formula: $C_{15}H_{10}BrClO_2$
Formula Weight: 337.596
SMILE: Oc1c(cc(Cl)cc1Br)C(=O)/C=C/c1ccccc1

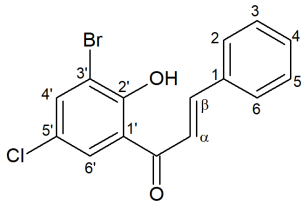



*Table S 4. 3′-Bromo-5′-chloro-2′-hydroxychalcone (**4**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.716 | 0.062 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.504 | 0.086 | MCF7 | Breast carcinoma | Breast | Carcinoma |
| 3 | 0.388 | 0.053 | K562 | Erythroleukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 4 | 0.386 | 0.054 | TK-10 | Renal carcinoma | Kidney | Carcinoma |
| 5 | 0.386 | 0.065 | SNU-475 | Hepatocellular carcinoma | Liver | Carcinoma |
| 6 | 0.360 | 0.031 | RCC4 | Clear cell renal cell carcinoma | Kidney | Carcinoma |
| 7 | 0.352 | 0.021 | RL | Non-Hodgkin's Lymphoma | Ascites | Lymphoma |
| 8 | 0.340 | 0.206 | DU-4475 | Breast Carcinoma | Breast | Carcinoma |
| 9 | 0.323 | 0.231 | SW48 | Colorectal Adenocarcinoma | Colon | Adenocarcinoma |
| 10 | 0.320 | 0.006 | KOPTK1 | Childhood T acute lymphoblastic leukemia | Blood | Leukemia |

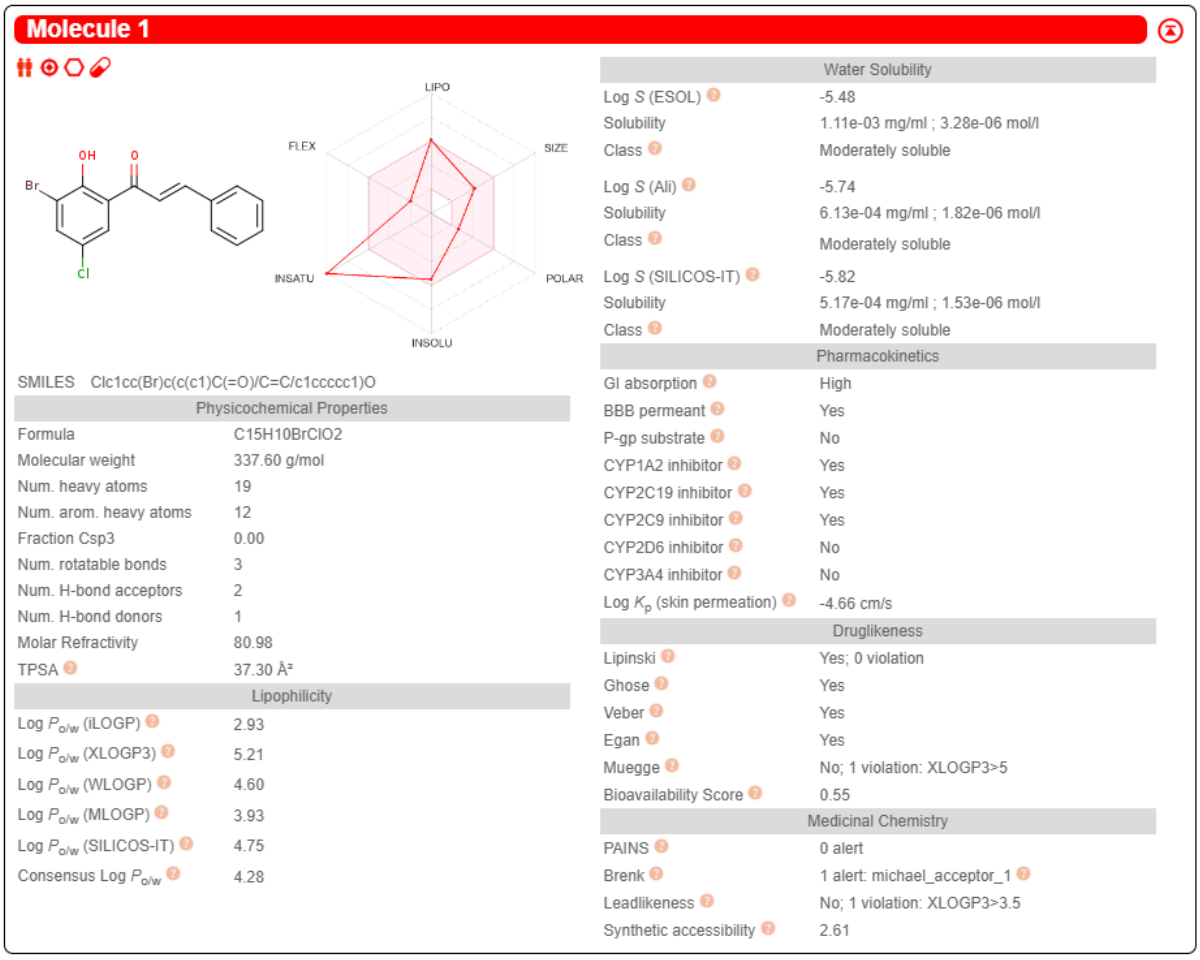



*Figure S 4. 3′-Bromo-5′-chloro-2′-hydroxychalcone (**4**) activity prediction using SwissADME.*

Compound name: 8-Bromo-6-chloroflavanone

Symbol: **5**

Molecular Formula: $C_{15}H_{10}BrClO_2$

Formula Weight: 337.596

SMILE: Clc1cc(Br)c2OC(CC(=O)c2c1)c1ccccc1

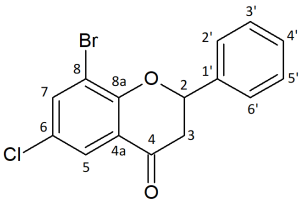



*Table S 5. 8-Bromo-6-chloroflavanone (**5**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.754 | 0.048 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.373 | 0.068 | SK-MES-1 | Squamous cell lung carcinoma | Lung | Carcinoma |
| 3 | 0.373 | 0.148 | DU-4475 | Breast Carcinoma | Breast | Carcinoma |
| 4 | 0.365 | 0.116 | SK-MEL-1 | Metastatic melanoma | Skin | Melanoma |
| 5 | 0.344 | 0.083 | NCI-H187 | Small cell lung carcinoma | Lung | Carcinoma |
| 6 | 0.335 | 0.021 | NALM-6 | Adult B acute lymphoblastic leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 7 | 0.302 | 0.294 | MONO-MAC-6 | Adult acute monocytic leukemia | Blood | Leukemia |
| 8 | 0.269 | 0.045 | SW1116 | Colorectal Adenocarcinoma | Colon | Adenocarcinoma |
| 9 | 0.257 | 0.031 | MDA-MB-435 | Amelanotic melanoma | Breast | Melanoma |
| 10 | 0.255 | 0.147 | MKN-74 | Gastric tubular adenocarcinoma | Stomach | Adenocarcinoma |

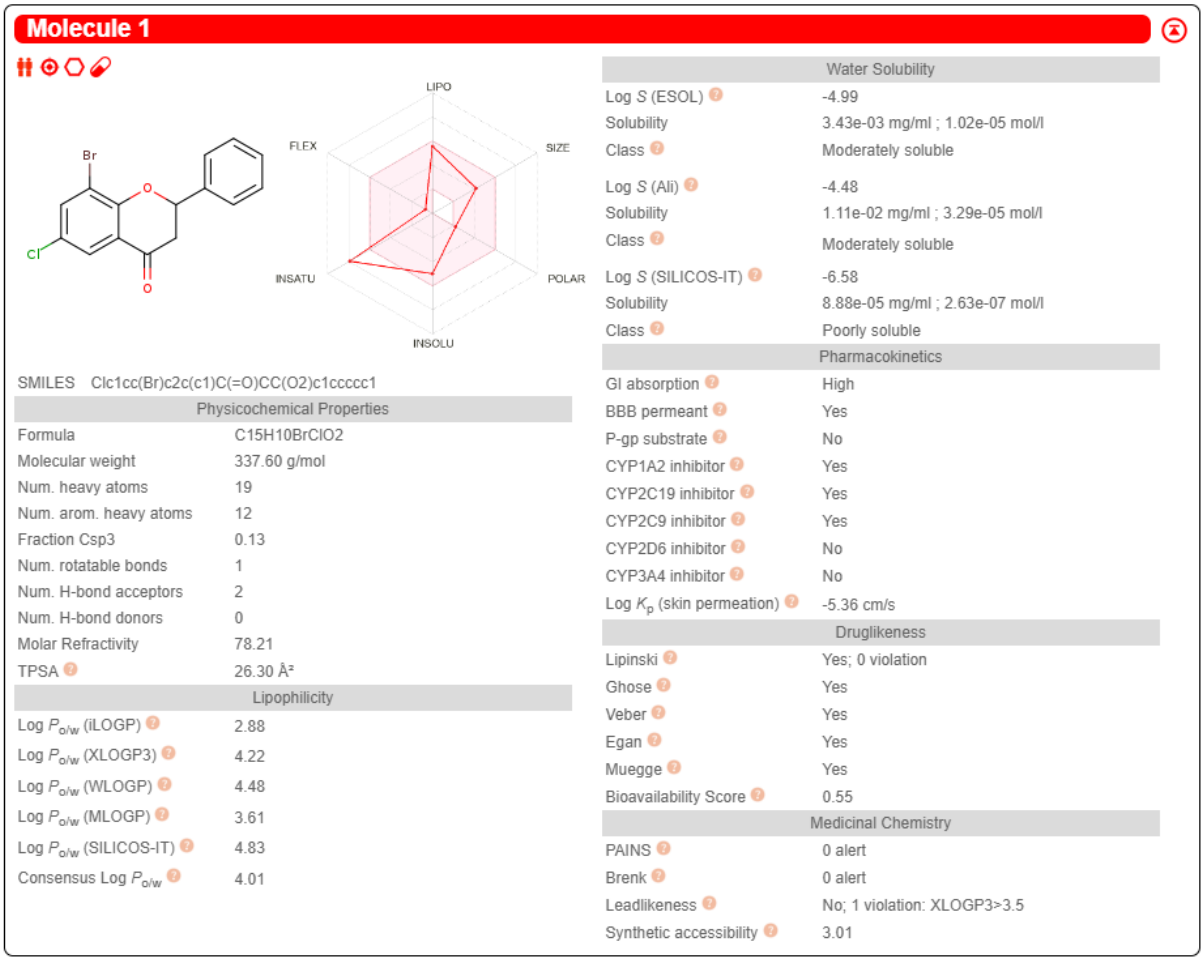



*Figure S 5. 8-Bromo-6-chloroflavanone (**5**) activity prediction using SwissADME.*

Compound name: 8-Bromo-6-chloroflavone
Symbol: **6**
Molecular Formula: $C_{15}H_8BrClO_2$
Formula Weight: 335.579
SMILE: Clc1cc(Br)c2OC(=CC(=O)c2c1)c1ccccc1

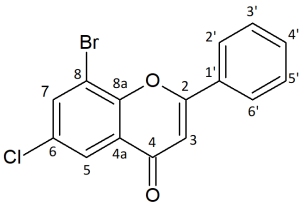



*Table S 6. 8-Bromo-6-chloroflavone (**6**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.609 | 0.107 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.426 | 0.050 | SK-MEL-1 | Metastatic melanoma | Skin | Melanoma |
| 3 | 0.381 | 0.058 | SK-MES-1 | Squamous cell lung carcinoma | Lung | Carcinoma |
| 4 | 0.374 | 0.147 | DU-4475 | Breast Carcinoma | Breast | Carcinoma |
| 5 | 0.354 | 0.204 | MONO-MAC-6 | Adult acute monocytic leukemia | Blood | Leukemia |
| 6 | 0.336 | 0.115 | COR-L23 | Lung large cell carcinoma | Lung | Carcinoma |
| 7 | 0.320 | 0.044 | NALM-6 | Adult B acute lymphoblastic leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 8 | 0.317 | 0.077 | NCI-H661 | Lung carcinoma | Lung | Carcinoma |
| 9 | 0.306 | 0.090 | HuP-T3 | Pancreatic adenocarcinoma | Pancreas | Adenocarcinoma |
| 10 | 0.287 | 0.281 | CA46 | Burkitts Lymphoma | Blood | Lymphoma |

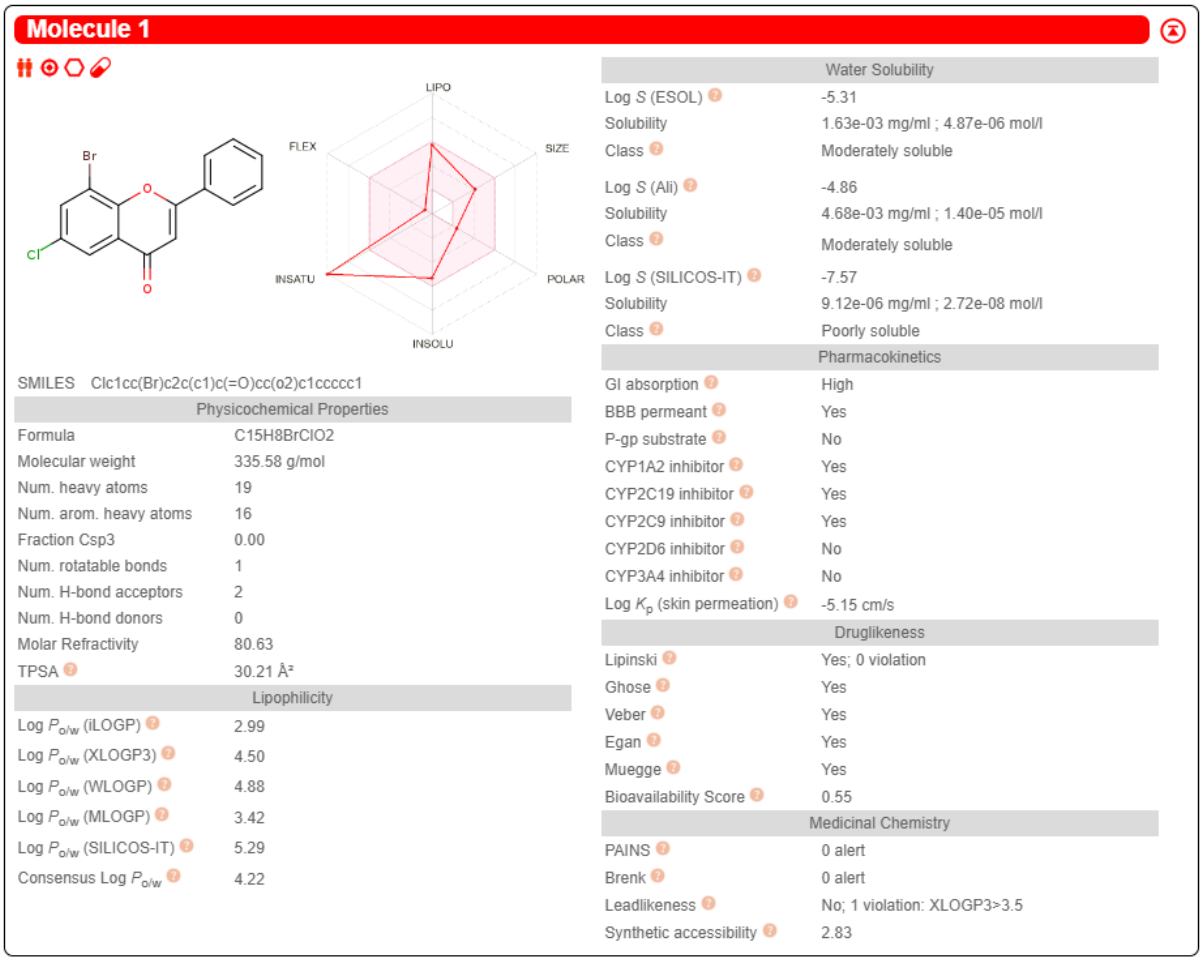



*Figure S 6. 8-Bromo-6-chloroflavone (**6**) activity prediction using SwissADME.*

Compound name: 8-Bromo-6-chloroflavone 4′-*O*-*β*-D-(4″-*O*-methyl)-glucopyranoside

Symbol: **6a**

Molecular Formula: $C_{22}H_{20}BrClO_8$

Formula Weight: 527.746

SMILE:

O=C1C=C(Oc2c1cc(Cl)cc2Br)c1ccc(cc1)O[C@@H]1OC(CO)[C@@H](OC)C(O)C1O

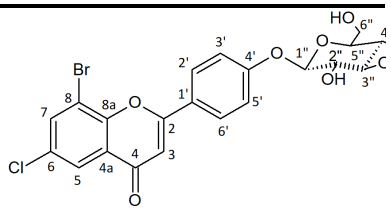



*Table S 7. 8-Bromo-6-chloroflavone 4′-O-β-D-(4″-O-methyl)-glucopyranoside (**6a**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.500 | 0.015 | MRC5 | Embryonic lung fibroblast | Lung | Normal |
| 2 | 0.497 | 0.020 | SK-MEL-1 | Metastatic melanoma | Skin | Melanoma |
| 3 | 0.489 | 0.036 | DU-4475 | Breast Carcinoma | Breast | Carcinoma |
| 4 | 0.488 | 0.044 | HL-60 | Promyeloblast leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 5 | 0.481 | 0.013 | SW1990 | Pancreatic adenocarcinoma | Pancreas | Adenocarcinoma |
| 6 | 0.458 | 0.013 | HEL299 | Fibroblasts | Lung | Normal |
| 7 | 0.447 | 0.014 | COR-L23 | Lung large cell carcinoma | Lung | Carcinoma |
| 8 | 0.411 | 0.158 | SK-LU-1 | Adenocarcinoma | Lung | Carcinoma |
| 9 | 0.384 | 0.027 | H9 | T-lymphoid | Haematopoietic and lymphoid tissue | Leukemia |
| 10 | 0.380 | 0.059 | SK-MES-1 | Squamous cell lung carcinoma | Lung | Carcinoma |

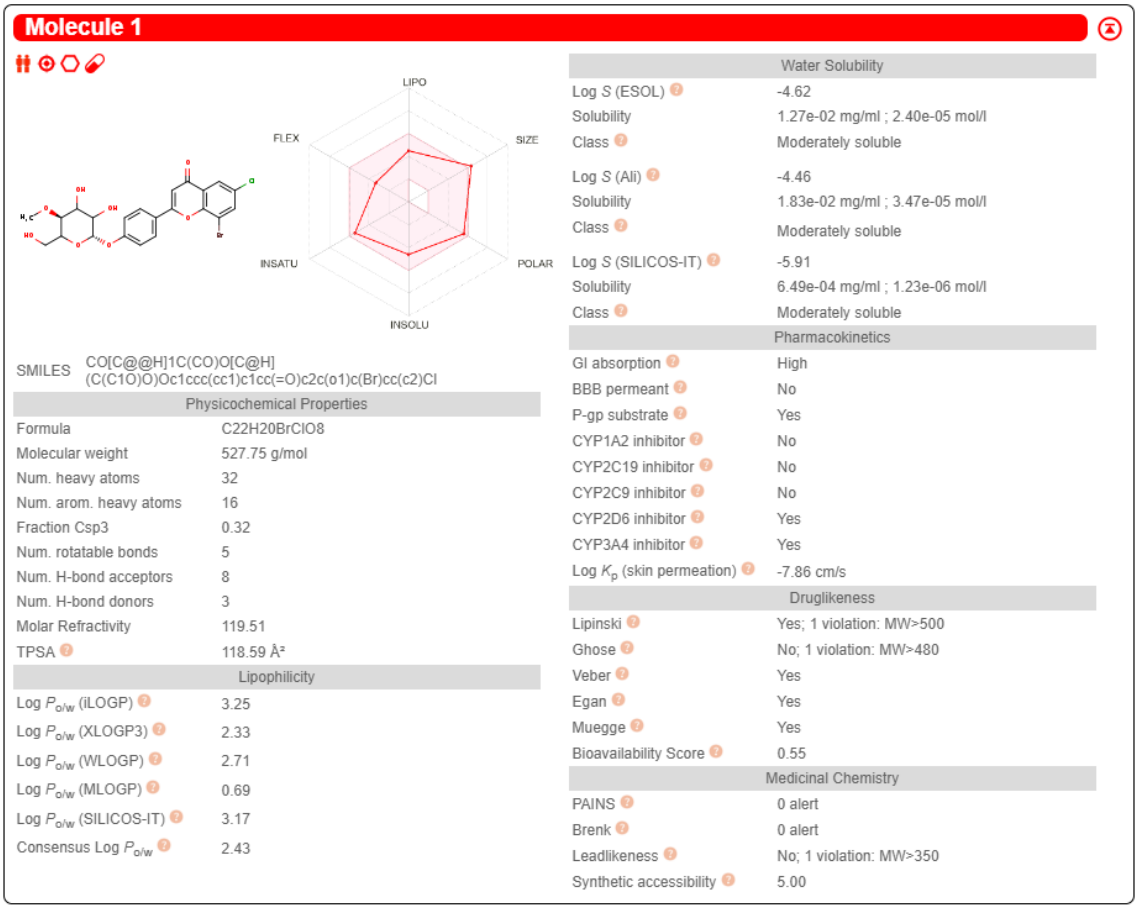



*Figure S 7. 8-Bromo-6-chloroflavone 4′-O-β-D-(4″-O-methyl)-glucopyranoside (**6a**) activity prediction using SwissADME.*

Compound name: 5′-Chloro-2′-hydroxy-3′-nitrochalcone
Symbol: **7**
Molecular Formula: $C_{15}H_{10}ClNO_4$
Formula Weight: 303.697
SMILE: O=[N+]([O-])c1cc(Cl)cc(c1O)C(=O)/C=C/c1ccccc1

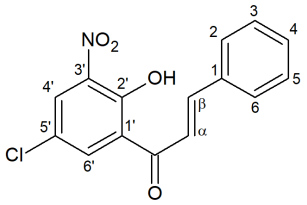



*Table S 8. 5′-Chloro-2′-hydroxy-3′-nitrochalcone (**7**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.647 | 0.091 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.484 | 0.030 | K562 | Erythroleukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 3 | 0.484 | 0.054 | HepG2 | Hepatoblastoma | Liver | Hepatoblastoma |
| 4 | 0.435 | 0.024 | HEK293 | Embryonic kidney fibroblast | Kidney | Normal |
| 5 | 0.373 | 0.072 | CAL-51 | Breast carcinoma | Breast | Carcinoma |
| 6 | 0.371 | 0.081 | SNU-475 | Hepatocellular carcinoma | Liver | Carcinoma |
| 7 | 0.365 | 0.126 | YAPC | Pancreatic carcinoma | Pancreas | Carcinoma |
| 8 | 0.347 | 0.023 | RL | Non-Hodgkin's Lymphoma | Ascites | Lymphoma |
| 9 | 0.334 | 0.041 | RCC4 | Clear cell renal cell carcinoma | Kidney | Carcinoma |
| 10 | 0.333 | 0.189 | NCI-H441 | Papillary adenocarcinoma | Lung | Adenocarcinoma |

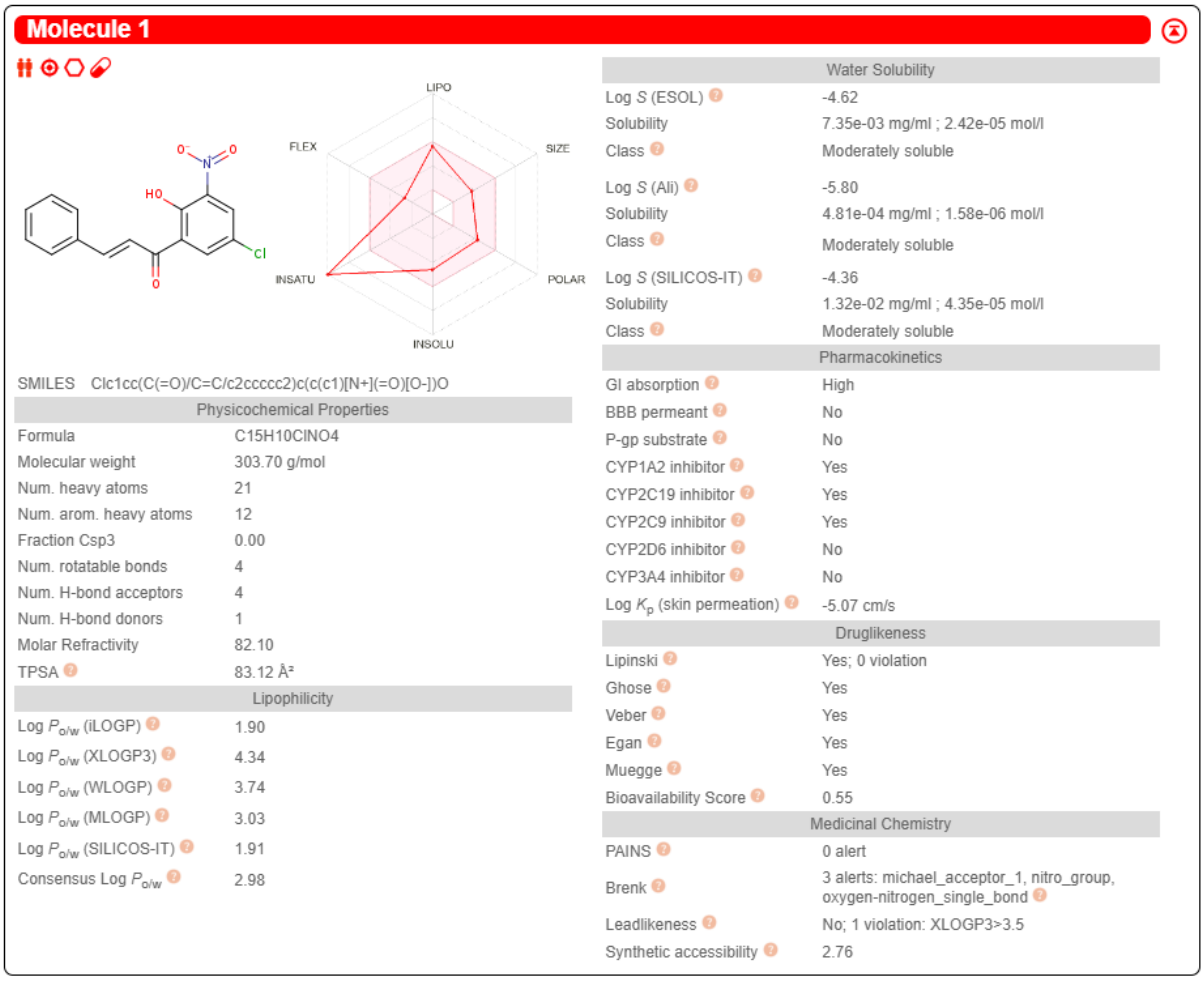



*Figure S 8. 5′-Chloro-2′-hydroxy-3′-nitrochalcone (**7**) activity prediction using SwissADME.*

Compound name: 6-Chloro-8-nitroflavanone

Symbol: **8**

Molecular Formula: $C_{15}H_{10}ClNO_4$

Formula Weight: 303.697

SMILE: [O-][N+](=O)c1cc(Cl)cc2c1OC(CC2=O)c1ccccc1

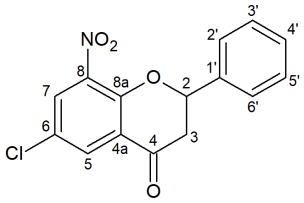



*Table S 9. 6-Chloro-8-nitroflavanone (**8**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.693 | 0.072 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.573 | 0.004 | MES-SA | Uterine corpus sarcoma | Uterus | Sarcoma |
| 3 | 0.358 | 0.069 | NCI-H187 | Small cell lung carcinoma | Lung | Carcinoma |
| 4 | 0.337 | 0.019 | NALM-6 | Adult B acute lymphoblastic leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 5 | 0.335 | 0.043 | 5637 | Urothelial bladder carcinoma | Urinary tract | Carcinoma |
| 6 | 0.319 | 0.101 | HCC1806 | Acantholytic Squamous Cell Carcinoma | Breast | Carcinoma |
| 7 | 0.302 | 0.211 | YAPC | Pancreatic carcinoma | Pancreas | Carcinoma |
| 8 | 0.290 | 0.066 | C8166 | Leukemic T-cells | Blood | Leukemia |
| 9 | 0.290 | 0.202 | SK-MES-1 | Squamous cell lung carcinoma | Lung | Carcinoma |
| 10 | 0.265 | 0.129 | MKN-74 | Gastric tubular adenocarcinoma | Stomach | Adenocarcinoma |

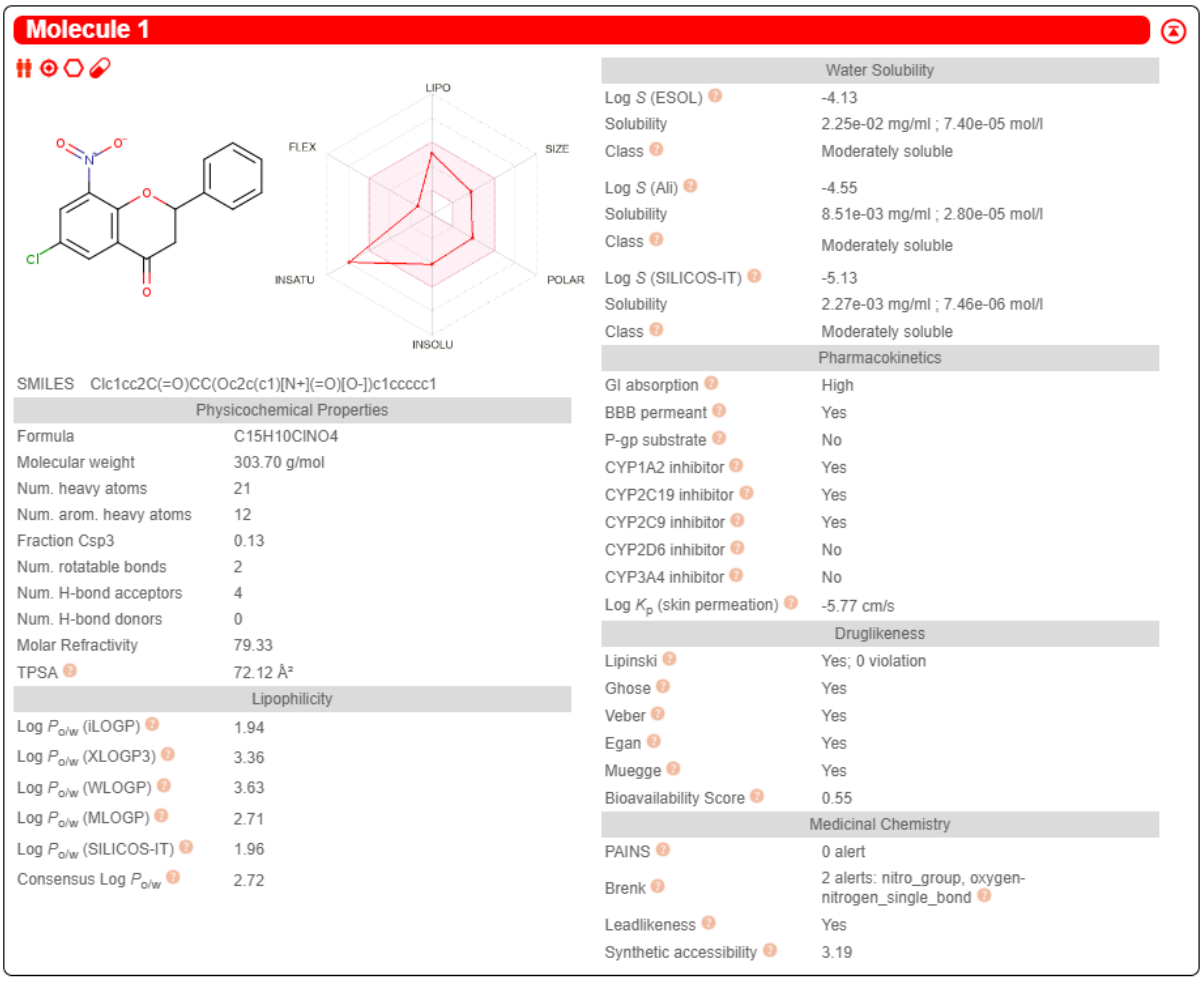



*Figure S 9. 6-Chloro-8-nitroflavanone (**8**) activity prediction using SwissADME.*

Compound name: 6-Chloro-8-nitroflavone
Symbol: **9**
Molecular Formula: $C_{15}H_8ClNO_4$
Formula Weight: 301.681
SMILE: [O-][N+](=O)c1cc(Cl)cc2c1OC(=CC2=O)c1ccccc1

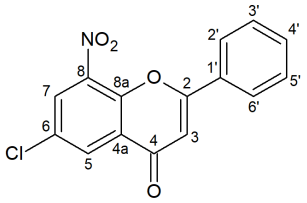



*Table S 10. 6-Chloro-8-nitroflavone (**9**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.704 | 0.003 | MES-SA | Uterine corpus sarcoma | Uterus | Sarcoma |
| 2 | 0.536 | 0.043 | HepG2 | Hepatoblastoma | Liver | Hepatoblastoma |
| 3 | 0.523 | 0.147 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 4 | 0.400 | 0.008 | 5637 | Urothelial bladder carcinoma | Urinary tract | Carcinoma |
| 5 | 0.346 | 0.218 | MONO-MAC-6 | Adult acute monocytic leukemia | Blood | Leukemia |
| 6 | 0.339 | 0.044 | NCI-H661 | Lung carcinoma | Lung | Carcinoma |
| 7 | 0.337 | 0.008 | C8166 | Leukemic T-cells | Blood | Leukemia |
| 8 | 0.324 | 0.035 | NALM-6 | Adult B acute lymphoblastic leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 9 | 0.318 | 0.192 | CA46 | Burkitts Lymphoma | Blood | Lymphoma |
| 10 | 0.305 | 0.134 | HCC1806 | Acantholytic Squamous Cell Carcinoma | Breast | Carcinoma |

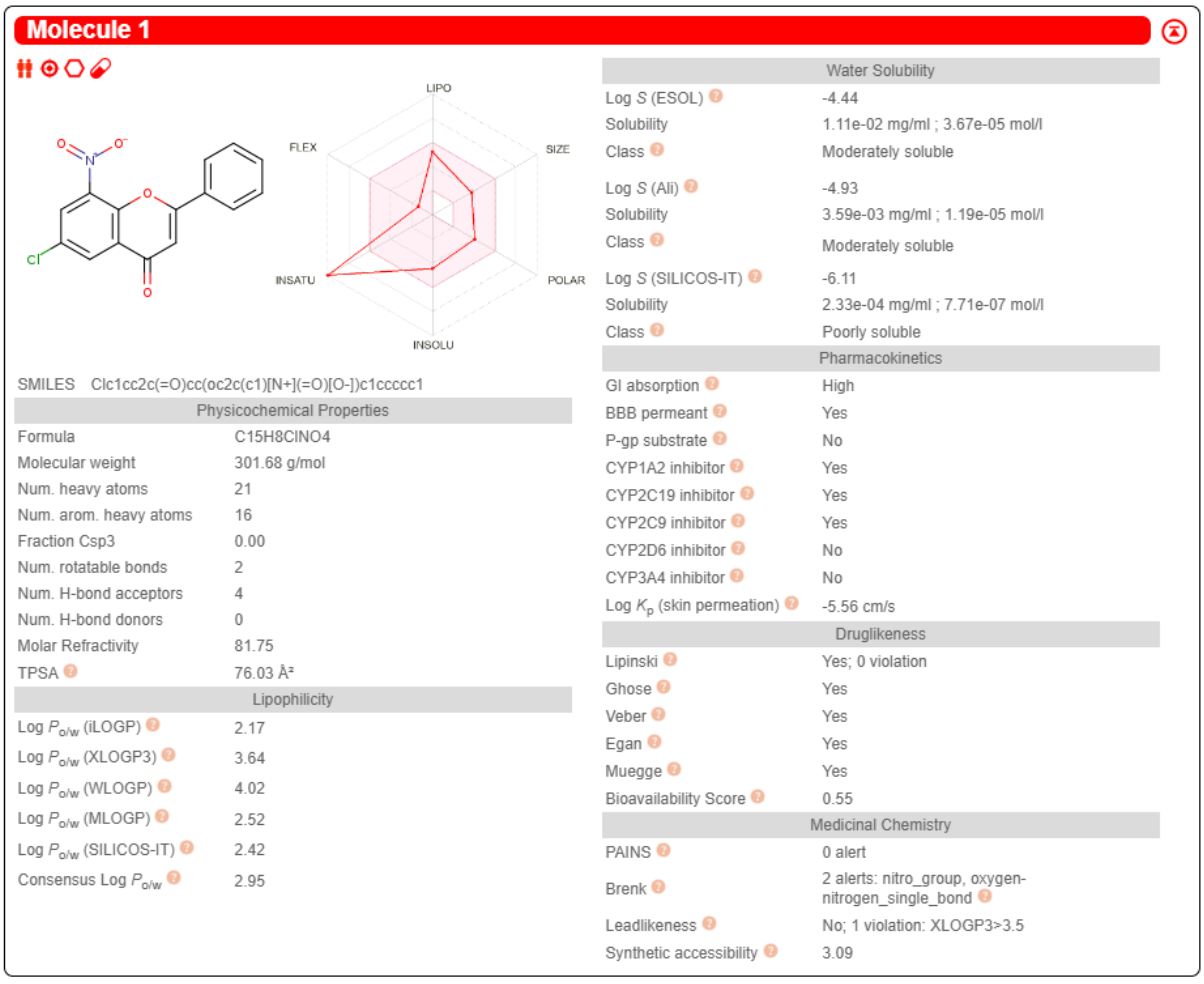



*Figure S 10. 6-Chloro-8-nitroflavone (**9**) activity prediction using SwissADME.*

Compound name: 5′-Bromo-2′-hydroxy-3′-nitrochalcone
Symbol: **10**
Molecular Formula: $C_{15}H_{10}BrNO_4$
Formula Weight: 348.148
SMILE: O=[N+]([O-])c1cc(Br)cc(c1O)C(=O)/C=C/c1ccccc1

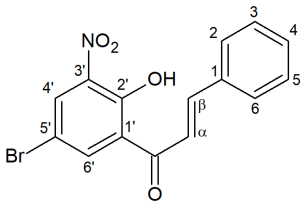



*Table S 11. 5′-Bromo-2′-hydroxy-3′-nitrochalcone (**10**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pi | Pa | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.647 | 0.091 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.503 | 0.026 | K562 | Erythroleukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 3 | 0.475 | 0.057 | HepG2 | Hepatoblastoma | Liver | Hepatoblastoma |
| 4 | 0.436 | 0.024 | HEK293 | Embryonic kidney fibroblast | Kidney | Normal |
| 5 | 0.435 | 0.120 | MCF7 | Breast carcinoma | Breast | Carcinoma |
| 6 | 0.371 | 0.081 | SNU-475 | Hepatocellular carcinoma | Liver | Carcinoma |
| 7 | 0.356 | 0.136 | YAPC | Pancreatic carcinoma | Pancreas | Carcinoma |
| 8 | 0.355 | 0.020 | RL | Non-Hodgkin's Lymphoma | Ascites | Lymphoma |
| 9 | 0.334 | 0.041 | RCC4 | Clear cell renal cell carcinoma | Kidney | Carcinoma |
| 10 | 0.330 | 0.149 | CAL-51 | Breast carcinoma | Breast | Carcinoma |

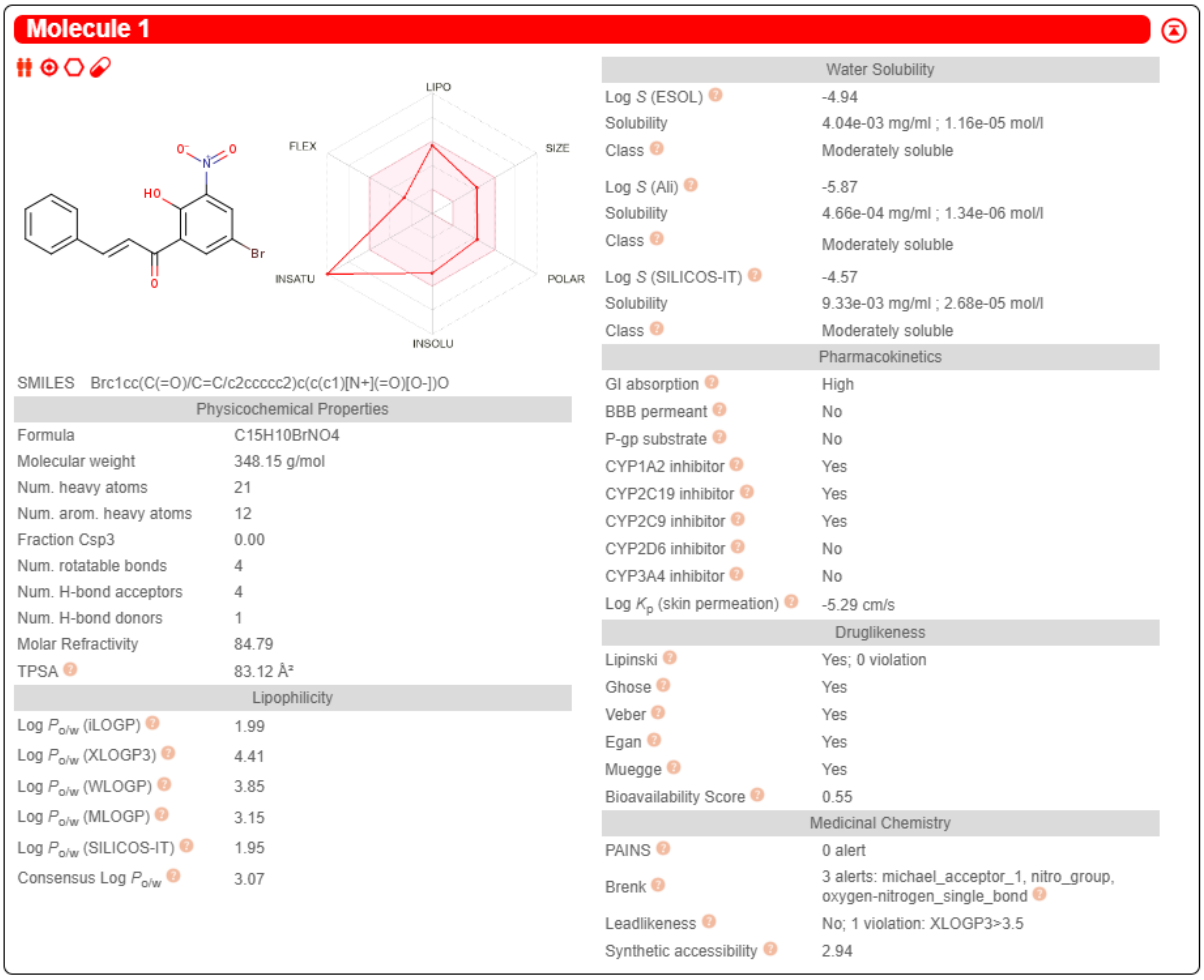



*Figure S 11. 5′-Bromo-2′-hydroxy-3′-nitrochalcone (**10**) activity prediction using SwissADME.*

Compound name: 6-Bromo-8-nitroflavanone
Symbol: **11**
Molecular Formula: $C_{15}H_{10}BrNO_4$
Formula Weight: 348.148
SMILE: [O-][N+](=O)c1cc(Br)cc2c1OC(CC2=O)c1ccccc1

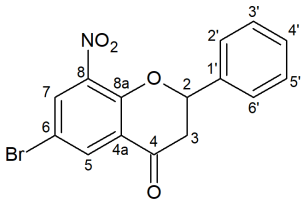



*Table S 12. 6-Bromo-8-nitroflavanone (**11**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.693 | 0.072 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 2 | 0.555 | 0.004 | MES-SA | Uterine corpus sarcoma | Uterus | Sarcoma |
| 3 | 0.343 | 0.084 | NCI-H187 | Small cell lung carcinoma | Lung | Carcinoma |
| 4 | 0.335 | 0.021 | NALM-6 | Adult B acute lymphoblastic leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 5 | 0.325 | 0.190 | MCF7 | Breast carcinoma | Breast | Carcinoma |
| 6 | 0.291 | 0.230 | YAPC | Pancreatic carcinoma | Pancreas | Carcinoma |
| 7 | 0.270 | 0.175 | 5637 | Urothelial bladder carcinoma | Urinary tract | Carcinoma |
| 8 | 0.268 | 0.130 | C8166 | Leukemic T-cells | Blood | Leukemia |
| 9 | 0.235 | 0.127 | NCI-H295R | Adrenal cortex carcinoma | Adrenal cortex | Carcinoma |
| 10 | 0.214 | 0.142 | SW1116 | Colorectal Adenocarcinoma | Colon | Adenocarcinoma |

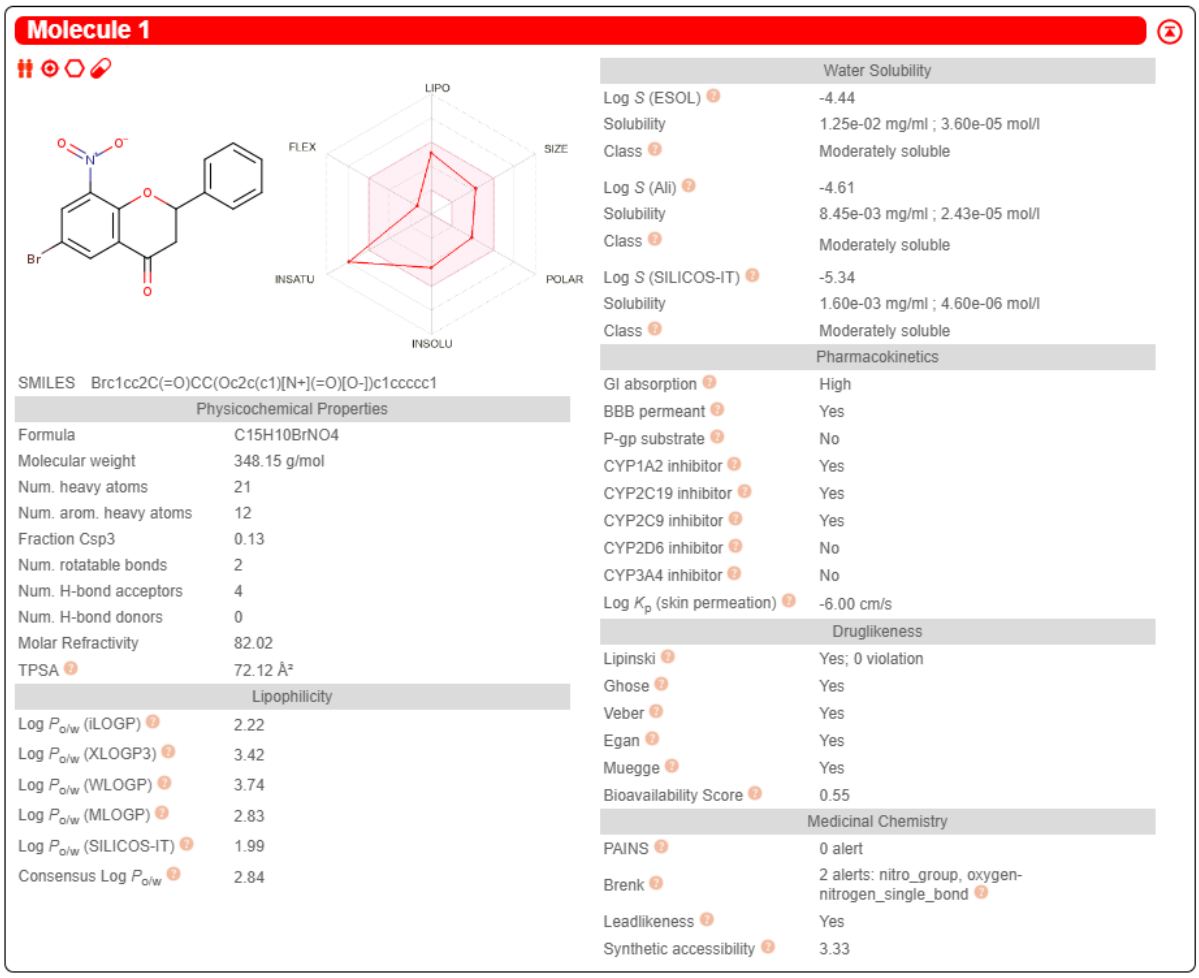



*Figure S 12. 6-Bromo-8-nitroflavanone (**11**) activity prediction using SwissADME.*

Compound name: 6-Bromo-8-nitroflavone
Symbol: **12**
Molecular Formula: $C_{15}H_8BrNO_4$
Formula Weight: 346.132
SMILE: [O-][N+](=O)c1cc(Br)cc2c1OC(=CC2=O)c1ccccc1

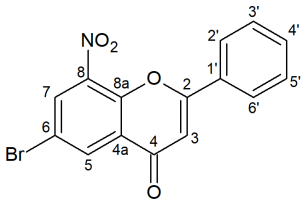



*Table S 13. 6-Bromo-8-nitroflavone (**12**) cytotoxicity prediction using Way2Drug CLC-pred.*

| Lp. | Pa | Pi | Cell-line | Description | Tissue/Organ | Type |
|---|---|---|---|---|---|---|
| 1 | 0.687 | 0.003 | MES-SA | Uterine corpus sarcoma | Uterus | Sarcoma |
| 2 | 0.606 | 0.031 | HepG2 | Hepatoblastoma | Liver | Hepatoblastoma |
| 3 | 0.523 | 0.147 | A2780cisR | Cisplatin-resistant ovarian carcinoma | Ovarium | Carcinoma |
| 4 | 0.368 | 0.161 | MCF7 | Breast carcinoma | Breast | Carcinoma |
| 5 | 0.362 | 0.020 | 5637 | Urothelial bladder carcinoma | Urinary tract | Carcinoma |
| 6 | 0.325 | 0.014 | C8166 | Leukemic T-cells | Blood | Leukemia |
| 7 | 0.321 | 0.041 | NALM-6 | Adult B acute lymphoblastic leukemia | Haematopoietic and lymphoid tissue | Leukemia |
| 8 | 0.320 | 0.072 | NCI-H661 | Lung carcinoma | Lung | Carcinoma |
| 9 | 0.306 | 0.225 | SK-MEL-1 | Metastatic melanoma | Skin | Melanoma |
| 10 | 0.280 | 0.039 | G-361 | Melanoma | Skin | Melanoma |

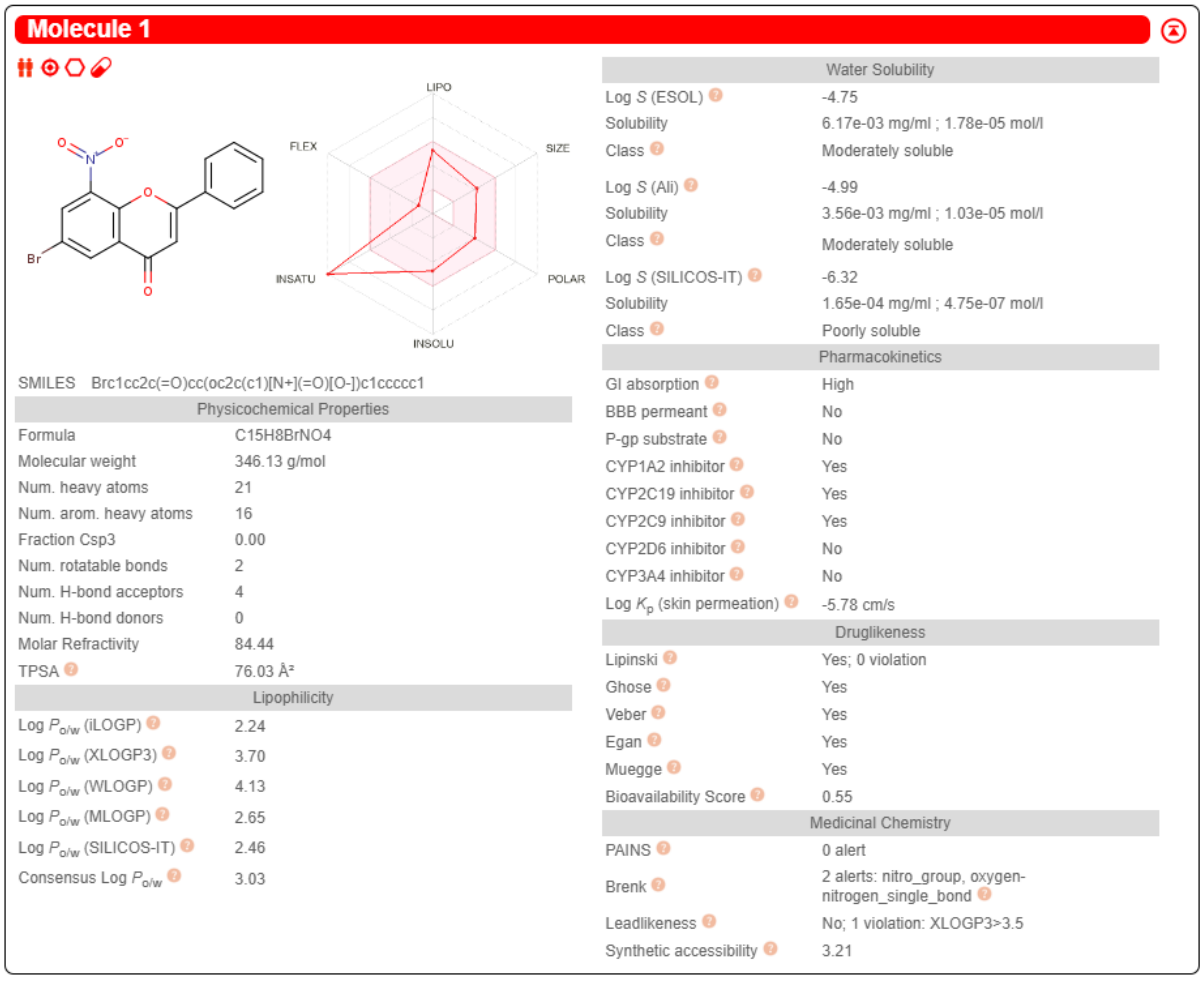



*Figure S 13. 6-Bromo-8-nitroflavone (**12**) activity prediction using SwissADME*

*Table S 14. Unequal variances t-test with Holm–Bonferroni correction for E. faecalis.*

| Probe | *E. faecalis* + DMSO | *E. faecalis* + (1) 0.1% | *E. faecalis* + (1) 0.05% | *E. faecalis* + (4) 0.1% | *E. faecalis* + (4) 0.05% | *E. faecalis* + (2) 0.1% | *E. faecalis* + (2) 0.05% | *E. faecalis* + (5) 0.1% | *E. faecalis* + (5) 0.05% | *E. faecalis* + (3) 0.1% | *E. faecalis* + (3) 0.05% | *E. faecalis* + (6) 0.1% | *E. faecalis* + (6) 0.05% | *E. faecalis* + (6a) 0.1% | *E. faecalis* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 0.026 | 0.019 | 0.040 | 0.000 | 0.047 | 0.002 | 0.001 | 0.001 | 0.001 | 0.000 | 0.045 | 0.044 | 0.029 | 0.022 | 0.041 |
| | * | * | * | *** | * | ** | *** | *** | *** | *** | * | * | * | * | * |

P-value <0.05 mark as significant.

*Table S 15. Unequal variances t-test with Holm–Bonferroni correction for S. aureus.*

| Probe | *S. aureus* + DMSO | *S. aureus* + (1) 0.1% | *S. aureus* + (1) 0.05% | *S. aureus* + (4) 0.1% | *S. aureus* + (4) 0.05% | *S. aureus* + (2) 0.1% | *S. aureus* + (2) 0.05% | *S. aureus* + (5) 0.1% | *S. aureus* + (5) 0.05% | *S. aureus* + (3) 0.1% | *S. aureus* + (3) 0.05% | *S. aureus* + (6) 0.1% | *S. aureus* + (6) 0.05% | *S. aureus* + (6a) 0.1% | *S. aureus* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 0.139 | 0.006 | 0.003 | 0.020 | 0.054 | 0.020 | 0.029 | 0.117 | 0.098 | 0.061 | 0.061 | 0.002 | 0.114 | 0.051 | 0.286 |
| | | ** | ** | * | | * | * | | | | | ** | | | |

P-value <0.05 mark as significant.

*Table S 16. Unequal variances t-test with Holm–Bonferroni correction for E. coli.*

| Probe | *E. coli* + DMSO | *E. coli* + (1) 0.1% | *E. coli* + (1) 0.05% | *E. coli* + (4) 0.1% | *E. coli* + (4) 0.05% | *E. coli* + (2) 0.1% | *E. coli* + (2) 0.05% | *E. coli* + (5) 0.1% | *E. coli* + (5) 0.05% | *E. coli* + (3) 0.1% | *E. coli* + (3) 0.05% | *E. coli* + (6) 0.1% | *E. coli* + (6) 0.05% | *E. coli* + (6a) 0.1% | *E. coli* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 0.401 | 0.001 | 0.111 | 0.002 | 0.003 | 0.000 | 0.068 | 0.377 | 0.242 | 0.188 | 0.115 | 0.008 | 0.001 | 0.930 | 0.625 |
| | | *** | | ** | ** | *** | | | | | | ** | *** | | |

P-value <0.05 mark as significant.

*Table S 17. Unequal variances t-test with Holm–Bonferroni correction for C. albicans.*

| Probe | *C. albicans* + DMSO | *C. albicans* + (1) 0.1% | *C. albicans* + (1) 0.05% | *C. albicans* + (4) 0.1% | *C. albicans* + (4) 0.05% | *C. albicans* + (2) 0.1% | *C. albicans* + (2) 0.05% | *C. albicans* + (5) 0.1% | *C. albicans* + (5) 0.05% | *C. albicans* + (3) 0.1% | *C. albicans* + (3) 0.05% | *C. albicans* + (6) 0.1% | *C. albicans* + (6) 0.05% | *C. albicans* + (6a) 0.1% | *C. albicans* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 0.074 | 0.007 | 0.105 | 0.000 | 0.117 | 0.000 | 0.265 | 0.075 | 0.174 | 0.003 | 0.025 | 0.068 | 0.508 | 0.328 | 0.008 |
| | | ** | | *** | | *** | | | | ** | * | | | | ** |

P-value <0.05 mark as significant.

*Table S 18. Unequal variances t-test with Holm–Bonferroni correction for L. acidophilus.*

| Probe | *L. acidophilus* + DMSO | *L. acidophilus* + (1) 0.1% | *L. acidophilus* + (1) 0.05% | *L. acidophilus* + (4) 0.1% | *L. acidophilus* + (4) 0.05% | *L. acidophilus* + (2) 0.1% | *L. acidophilus* + (2) 0.05% | *L. acidophilus* + (5) 0.1% | *L. acidophilus* + (5) 0.05% | *L. acidophilus* + (3) 0.1% | *L. acidophilus* + (3) 0.05% | *L. acidophilus* + (6) 0.1% | *L. acidophilus* + (6) 0.05% | *L. acidophilus* + (6a) 0.1% | *L. acidophilus* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 0.042 | 0.002 | 0.052 | 0.004 | 0.049 | 0.066 | 0.088 | 0.077 | 0.049 | 0.111 | 0.056 | 0.095 | 0.037 | 0.018 | 0.259 |
| | * | ** | | ** | * | | | | * | | | | * | * | |

P-value <0.05 mark as significant.

*Table S 19. Unequal variances t-test with Holm–Bonferroni correction for L. casei.*

| Probe | *L. casei* + DMSO | *L. casei* + (1) 0.1% | *L. casei* + (1) 0.05% | *L. casei* + (4) 0.1% | *L. casei* + (4) 0.05% | *L. casei* + (2) 0.1% | *L. casei* + (2) 0.05% | *L. casei* + (5) 0.1% | *L. casei* + (5) 0.05% | *L. casei* + (3) 0.1% | *L. casei* + (3) 0.05% | *L. casei* + (6) 0.1% | *L. casei* + (6) 0.05% | *L. casei* + (6a) 0.1% | *L. casei* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 1 | 0.840 | 1 | 0.039 | 0.819 | 0.844 | 1 | 0.868 | 1 | 0.564 | 0.979 | 0.767 | 1 | 0.527 | 0.463 |
| | | | | * | | | | | | | | | | | |

P-value <0.05 mark as significant.

*Table S 20. Unequal variances t-test with Holm–Bonferroni correction for L. plantarum.*

| Probe | *L. plantarum* + DMSO | *L. plantarum* + (1) 0.1% | *L. plantarum* + (1) 0.05% | *L. plantarum* + (4) 0.1% | *L. plantarum* + (4) 0.05% | *L. plantarum* + (2) 0.1% | *L. plantarum* + (2) 0.05% | *L. plantarum* + (5) 0.1% | *L. plantarum* + (5) 0.05% | *L. plantarum* + (3) 0.1% | *L. plantarum* + (3) 0.05% | *L. plantarum* + (6) 0.1% | *L. plantarum* + (6) 0.05% | *L. plantarum* + (6a) 0.1% | *L. plantarum* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 0.974 | 0.582 | 1 | 0.512 | 0.853 | 0.810 | 0.128 | 0.906 | 0.155 | 0.985 | 0.988 | 0.812 | 0.892 | 0.223 | 0.999 |
| | | | | | | | | | | | | | | | |

P-value <0.05 mark as significant.

*Table S 21. Unequal variances t-test with Holm–Bonferroni correction for P. pentosaceus.*

| Probe | *P. pentosaceus* + DMSO | *P. pentosaceus* + (1) 0.1% | *P. pentosaceus* + (1) 0.05% | *P. pentosaceus* + (4) 0.1% | *P. pentosaceus* + (4) 0.05% | *P. pentosaceus* + (2) 0.1% | *P. pentosaceus* + (2) 0.05% | *P. pentosaceus* + (5) 0.1% | *P. pentosaceus* + (5) 0.05% | *P. pentosaceus* + (3) 0.1% | *P. pentosaceus* + (3) 0.05% | *P. pentosaceus* + (6) 0.1% | *P. pentosaceus* + (6) 0.05% | *P. pentosaceus* + (6a) 0.1% | *P. pentosaceus* + (6a) 0.05% |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P-value | 0.109 | 0.984 | 1.553 | 0.125 | 0.553 | 1 | 0.768 | 0.790 | 1 | 0.902 | 1.642 | 0.314 | 0.351 | 1 | 1 |
| | | | | | | | | | | | | | | | |

P-value <0.05 mark as significant.

*Table S 22. One-sample Student's t-test with Holm–Bonferroni correction for digestion in vitro studies.*

| Compound | Origin of the intestinal microbiome* | Total numer of microorganisms | *Bifidobacterium* sp. | *Lactobacillus* sp. | Nonpathogenic *E.coli* | *Enterococcus* sp. | *Clostridium* sp. | *E.coli* | Proteolytic bacteria | Yeast-like fungi |
|---|---|---|---|---|---|---|---|---|---|---|
| (**3**) | 1M | 0.523 | 0.595 | 0.321 | 0.186 | 0.307 | 0.296 | 0.296 | 0.176 | absence |
| | 2M | 0.397 | 0.032 * | 0.276 | 0.023 * | 0.238 | 0.005 ** | 0.038 * | 0.010 ** | absence |
| | 3M | 0.980 | 0.392 | 0.675 | 0.601 | 0.617 | 1 | 0.668 | 0.072 | absence |
| | 4M | 1 | 1 | 1 | 0.868 | 0.852 | 1 | 1 | 0.929 | absence |
| | 5M | 0.575 | 0.730 | 0.089 | 0.096 | 0.475 | 0.000 *** | 0.063 | 1 | absence |
| (**6**) | 1M | 0.414 | 1 | 1 | 0.301 | 0.337 | 1 | 0.156 | 0.320 | absence |
| | 2M | 0.791 | 0.048 * | 0.642 | 0.557 | 0.004 ** | 0.126 | 0.546 | 0.288 | 1 |
| | 3M | 0.657 | 1 | 0.374 | 1 | 1 | 0.998 | 1 | absence | 0.015 * |
| | 4M | 0.505 | 0.972 | 1 | 0.576 | 0.598 | 0.520 | 0.277 | absence | absence |
| | 5M | 1 | 0.413 | 0.276 | 0.003 ** | 1 | 0.001 *** | 0.019 * | 0.446 | absence |
| (**9**) | 1M | 0.138 | 0.796 | 1 | 0.308 | 0.268 | 0.306 | 1 | 1 | absence |
| | 2M | 0.137 | 0.466 | 0.353 | 0.799 | 1 | 0.019 * | 0.052 | 0.140 | 0.207 |
| | 3M | 0.182 | 1 | 1 | 1 | 1 | 1 | 1 | absence | 1 |
| | 4M | 1 | 1 | 1 | 1 | 0.940 | 1 | 0.701 | absence | absence |
| | 5M | 0.594 | 0.799 | 0.557 | 1 | 0.537 | 0.416 | 0.277 | 0.822 | absence |
| (**12**) | 1M | 1 | 1 | 1 | 1 | 0.989 | 0.009 | 1 | 0.221 | absence |
| | 2M | 0.398 | 0.966 | 1 | 1 | 0.997 | 0.287 | 0.842 | 1 | 0.422 |
| | 3M | 1 | 1 | 0.064 | 1 | 1 | 1 | 1 | 0.756 | 0.244 |
| | 4M | 0.374 | 1 | 1 | 1 | 1 | 0.488 | 1 | 1 | 1 |
| | 5M | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | absence |

*1M - Microbiome of healthy people, 2M - Microbiome of people over 75 y.o., 3M - Microbiome of people after antibiotic therapy, 4M - Microbiome of people after chemotherapy, 5M - Microbiome of obese people. P-value <0.05 mark as significant.