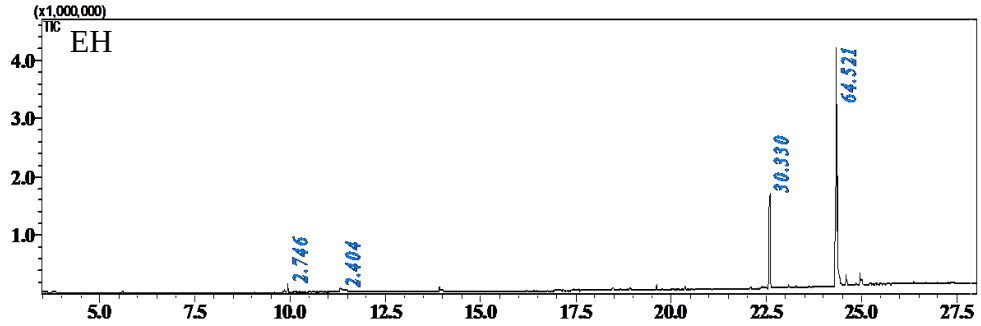
# Linking the Phytochemicals and the $\alpha$-Glucosidase and $\alpha$-Amylase Enzyme Inhibitory Effects of *Nigella Sativa* Seed Extracts

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## Supplementary Materials

a.




b.

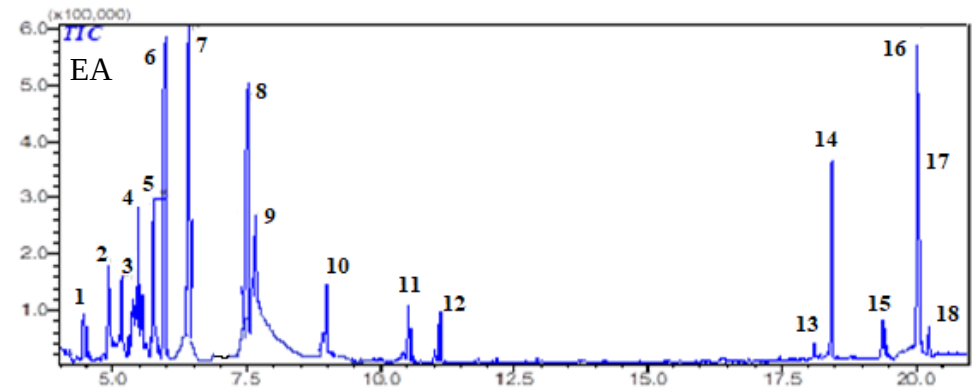



**Figure S1:** GC-MS chromatograms of **(a)** hexane extract (EH, x 1, 000, 000) and **(b)** acetone extract (EA, x 100, 000) of *N. sativa* seed. Details of compound identifications are provided in Table S1.

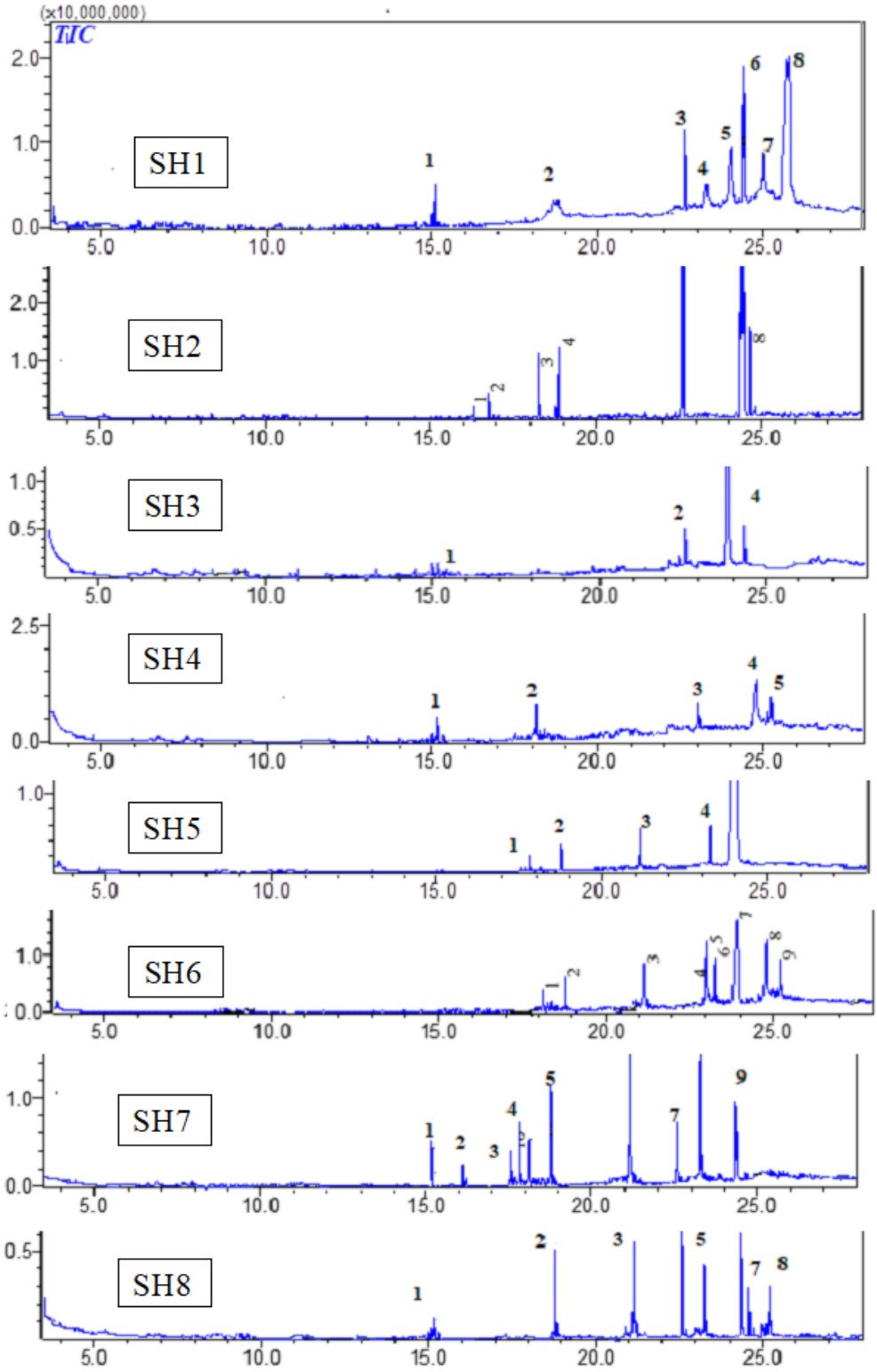



**Figure S2:** GC-MS chromatograms of the 8 hexane fractions (SH1 to SH8) resulting from the fractionation on silica gel column of the hexane extract (EH) from *N. sativa* seed. Details of compound identifications are provided in Table S1.

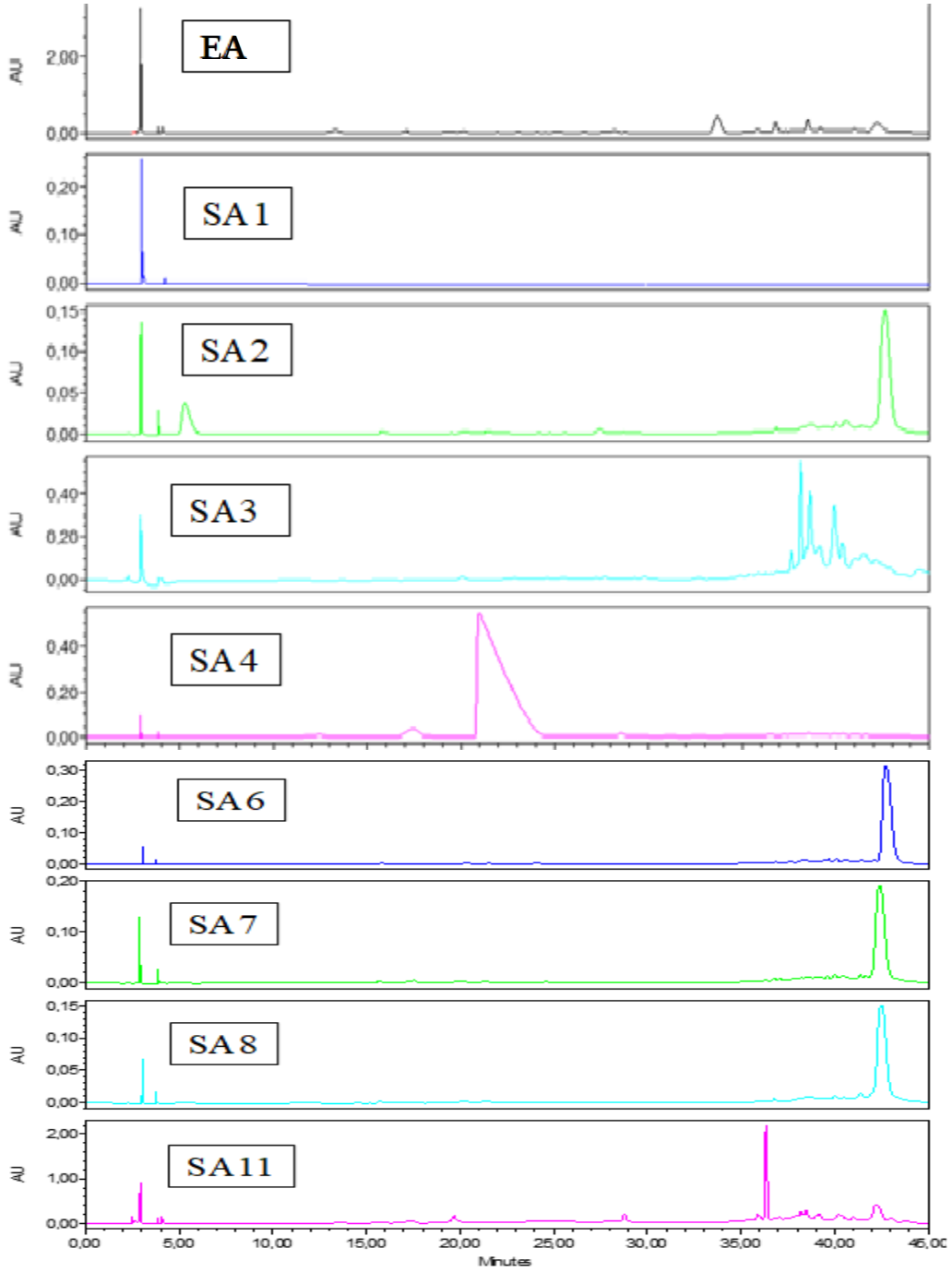



**Figure S3:** HPLC-DAD chromatograms of the acetone extract (EA) from *N. sativa* seed and its fractions (SA1-SA11) resulting from its fractionation on silica gel column. Details of compound identifications are provided in Table S1.

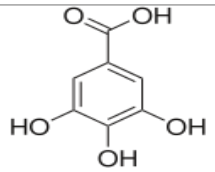
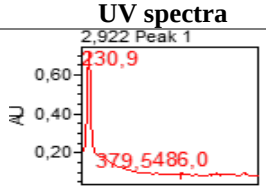
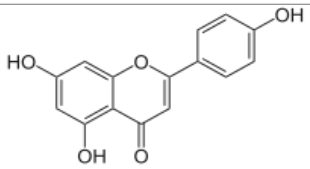
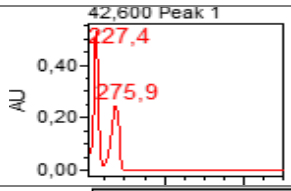
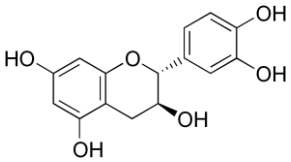
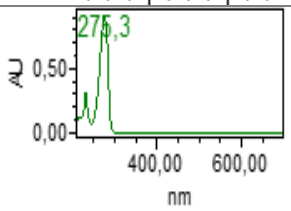
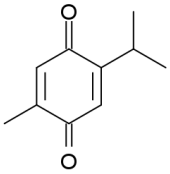
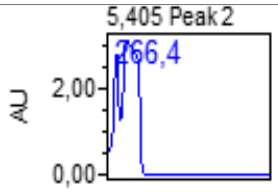
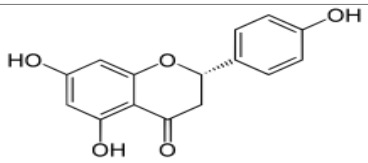
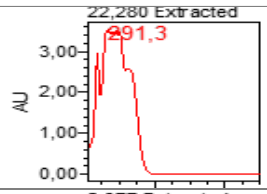
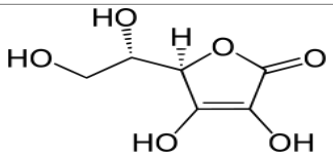
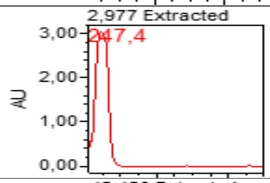
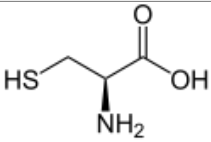
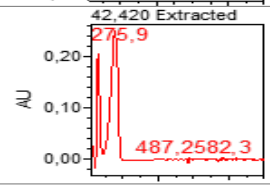
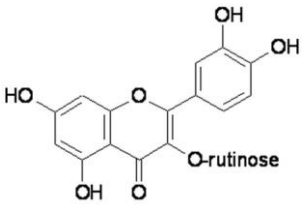
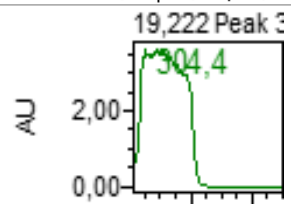
| Compound | Chemical structure | UV spectra |
|---|---|---|
| gallic Acid |  |   |
| apigenin |  |   |
| catechin |  |   |
| thymoquinone |  |   |
| naringenin |  |   |
| L-ascorbic acid |  |   |
| L-cysteine |  |   |
| rutin |  |   |

**Figure S4:** UV spectra of the compounds from acetone extract (EA) from *N. sativa* seed identified by HPLC-DAD analysis.

**Table S1:** Characteristics and relative abundance (% of TIC) of compounds from *N. sativa* hexane extract (EH) and its fractions (SH1-SH8) and acetone extract (EA) identified by GC-MS analysis.

| Name of the compound | PubChem CID | Molecular formula | RT (min) | Relative quantity (%) | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | EH | SH1 | SH2 | SH3 | SH4 | SH5 | SH6 | SH7 | SH8 | EA |
| (1,3,+A2:J363-trimethylnonyl)benzene | 569261 | $C_{18}H_{30}$ | 5.95 | | | | | | | | | | 21.62 |
| (2,2-dimethyl-1,3-dioxolan-4-yl)methyl acetate | 252333 | $C_8H_{14}O_4$ | 7.66 | | | | | | | | | | 2.94 |
| (R)-solketal | 736056 | $C_6H_{12}O_3$ | 5.14 | | | | | | | | | | 3.28 |
| (Z)-9-tricosene | 5365075 | $C_{23}H_{46}$ | 23.28 | | | | | | 2.70 | 6.60 | 9.74 | | |
| 1,2-diacetin | 66021 | $C_7H_{12}O_5$ | 11.13 | | | | | | | | | | 1.88 |
| 17-pentatriacontene | 5365022 | $C_{35}H_{70}$ | 24.59 | | | | | 60.37 | | | | | |
| 1-monolinolein | 6436630 | $C_{21}H_{38}O_4$ | 20.03 | | | | | | | | | | 6.85 |
| 2,4-ditert-butylphenyl-5-hydroxypentanoate | 605777 | $C_{19}H_{30}O_3$ | 17.83 | | | | | | | | 3.87 | | |
| 2,6,11,15-tetramethylhexadecane | 136331 | $C_{20}H_{42}$ | 17.55 | | | | | | 0.29 | | 8.44 | | |
| 2,9-dimethyldecane | 517733 | $C_{12}H_{26}$ | 7.50 | | | | | | | | | | 17.31 |
| 2,4-decadienal | 5283349 | $C_{10}H_{16}O$ | 15.11 | | 4.95 | | 1.70 | | | | | 3.82 | |
| 2-methyl-3-methylene-1-hepten-5-yne | 569164 | $C_9H_{12}$ | 4.92 | | | | | | | | | | 4.56 |
| 2-methyl-heptadecane | 15265 | $C_{18}H_{38}$ | 18.13 | | | | | | | | 11.68 | | |
| 7,9-dimethylhexadecane | 545945 | $C_{18}H_{38}$ | 15.18 | | | | | 9.97 | | | 6.11 | | |
| 8-hydroxy-octanoic acid | 69820 | $C_8H_{16}O_3$ | 16.23 | | | 2.61 | | | | | | | |
| 8-methylhexadecane | 530042 | $C_{17}H_{36}$ | 15.18 | | | | | | | | 3.71 | | |
| 8-octadecenoic acid | 5282758 | $C_{18}H_{34}O_2$ | 24.43 | | | 1.25 | | | | | | | |
| 9-eicosene (E) | 5365037 | $C_{20}H_{40}$ | 18.78 | | | | | | 1.79 | | 16.82 | 16.53 | |
| 9-hexacosene | 5363630 | $C_{26}H_{52}$ | 24.24 | | | | | | | 3.95 | | 8.59 | |
| acetostearin | 314293 | $C_{23}H_{44}O_5$ | 11.31 | 2.40 | | | | | | | | | |
| azelaic acid | 2266 | $C_9H_{16}O_4$ | 18.26 | | | 9.44 | | | | | | | |
| beta-cymene | 10812 | $C_{10}H_{14}$ | 6.41 | | | | | | | | | | 15.76 |
| bromopropanoic acid | 11729 | $C_3H_5BrO_2$ | 23.26 | | 9.30 | | | | | | | | |
| butyl 12-acetoxyoctadecanoate | 222097 | $C_{24}H_{46}O_3$ | 25.79 | | 28.12 | | | | | | | | |
| cumene | 7406 | $C_9H_{12}$ | 5.46 | | | | | | | | | | 3.84 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| dodecanal dimethyl acetal | 84559 | $C_{14}H_{30}O_2$ | 18.89 | | | 12.14 | | | | | | | |
| dodecane | 8182 | $C_{12}H_{26}$ | 8.98 | | | | | | | | | | 3.56 |
| eicosane | 8222 | $C_{20}H_{42}$ | 18.13 | | | | | | | 2.19 | | | |
| heptadecanoic acid | 10465 | $C_{17}H_{34}O_2$ | 24.64 | | 11.02 | 16.35 | | | | | | | |
| heptadecyl dichloroacetate | 546049 | $C_{19}H_{36}Cl_2O_2$ | 18.77 | | | | | | | 9.20 | 6.42 | 16.84 | |
| heptyl valerate | 79544 | $C_{12}H_{24}O2$ | 4.47 | | | | | | | | | | 2.72 |
| hexadecane | 11006 | $C_{16}H_{34}$ | 18.13 | | | | | 10.84 | | | | | |
| l-(+)-ascorbic acid 2,6-dihexadecanoate | 54722209 | $C_{38}H_{68}O_8$ | 23.03 | | | | | | | 14.37 | | | |
| lauric acid | 3893 | $C_{12}H_{24}O_2$ | 18.68 | | 1.87 | | | | | | | | |
| lignocerol | 10472 | $C_{24}H_{50}O$ | 24.79 | | | | | 7.62 | | | | | |
| linoleic acid | 5280450 | $C_{18}H_{32}O_2$ | 24.36 | 64.52 | 18.29 | 17.10 | | | 92.54 | | 14.08 | | 1.12 |
| methyl 9-oxononanoate | 74732 | $C_{10}H_{18}O_3$ | 16.77 | | | 2.60 | | | | | | | |
| methyl oleate | 5364509 | $C_{19}H_{36}O_2$ | 24.39 | | | | | | | | | 5.57 | |
| methyl stearate | 8201 | $C_{19}H_{38}O_2$ | 24.62 | | | | | | | | | 10.49 | |
| methyl-10,14,18,22-tetramethyltricosanoate | 545641 | $C_{28}H_{56}O_2$ | 22.58 | | | | | 11.17 | | | | | |
| methyl-palmitate | 8181 | $C_{17}H_{34}O_2$ | 22.60 | | | | 5.65 | | 2.65 | | 18.89 | 24.91 | |
| nonadecanoic acid | 12591 | $C_{21}H_{42}O_2$ | 20.26 | | | | | | | | | | 0.98 |
| oleic acid | 445639 | $C_{18}H_{34}O_2$ | 24.34 | 2.74 | | | 5.31 | | | 12.34 | | | 0.56 |
| palmitic acid | 985 | $C_{16}H_{32}O_2$ | 22.61 | 30.33 | 8.64 | 40.98 | | | | 4.09 | | | 7.29 |
| Psi-cumene | 7247 | $C_9H_{12}$ | 5.73 | | | | | | | | | | 3.23 |
| stearic acid | 5281 | $C_{18}H_{36}O_2$ | 18.12 | | | | | | | | | | 0.73 |
| stearyl alcohol | 8221 | $C_{18}H_{38}O$ | 23.58 | | 17.79 | | 87.32 | | | 47.22 | | 13.23 | |
| thymol | 6989 | $C_4H_{14}O$ | 10.53 | | | | | | | | | | 1.84 |

**Table S2:** Characteristics and relative abundance (% of peaks relative area) of compounds from *N. sativa* acetone extract (EA) and its fractions (SA1-SA11) identified by HPLC-DAD analysis (by comparison with commercial standards).

| Name of the compound | PubChem CID | Molecular formula | RT (min) | λmax (nm) | Relative quantity (%) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | EA | SA1 | SA2 | SA3 | SA4 | SA6 | SA7 | SA8 | SA11 |
| apigenin | 5280443 | $C_{15}H_{10}O_5$ | 13.27 | 337 | 13.27 | | 73.50 | | | | | | |
| gallic acid | 370 | $C_7H_6O_5$ | 2.92 | 369 | 23.5 | 98.90 | 25.80 | 5.36 | | | | | |
| kaempferol | 5280863 | $C_{15}H_{10}O_6$ | 32.54 | 365 | 2.03 | | | | | | | | |
| l-ascorbic acid | 54670067 | $C_6H_8O_6$ | 2.97 | 295 | 2.03 | | | | | | 13.90 | | |
| l-cysteine | 5862 | $C_3H_7NO_2S$ | 42.42 | 320 | 13.2 | | | | | | 82.17 | | |
| l-histidine | 6274 | $C_6H_9N_3O_2$ | 42.24 | 300 | | | | | | | | | 12.30 |
| naringenin | 932 | $C_{15}H_{12}O_5$ | 22.28 | 292 | 8.45 | | | | 88.70 | | | | |
| catechin | 73160 | $C_{15}H_{14}O_6$ | 39.92 | 250 | | | | 79.83 | | | | | |
| quercetin | 5280343 | $C_{15}H_{10}O_7$ | 27.74 | 357 | 8.42 | | | | | | | | 7.65 |
| rutin | 5280805 | $C_{27}H_{30}O_{16}$ | 19.22 | 360 | 4.95 | | | | | | | | 4.80 |
| thymoquinone | 10281 | $C_{10}H_{14}O_2$ | 5.40 | 289 | 3.82 | | 12.30 | | | | | | |
| ND1 | - | - | 3.74 | 254 | 4.85 | | | | | 10.74 | | | |
| ND2 | - | - | 3.80 | 300 | 3.65 | | | | | | | 25.21 | |
| ND3 | - | - | 42.50 | 383 | 3.73 | | | | | | | 72.01 | |
| ND4 | - | - | 42.73 | 280 | 8.05 | | | | | 86.72 | | | |