Electronic supplementary materials

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Scavenging activity and mechanism study of ferulic acid against reactive carbonyl species acrolein

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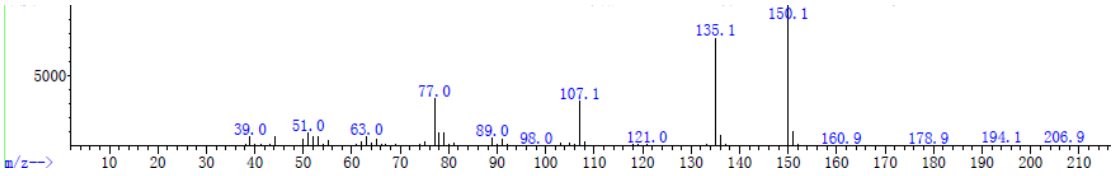
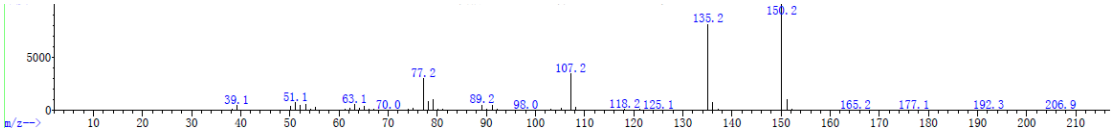


a



b

Figure S1. GC-MS of product **21**. (a) Isolated product **21** (retention time: 4.197 min);

(b) standard 2-methoxy-4-vinylphenol (retention time: 4.198 min).

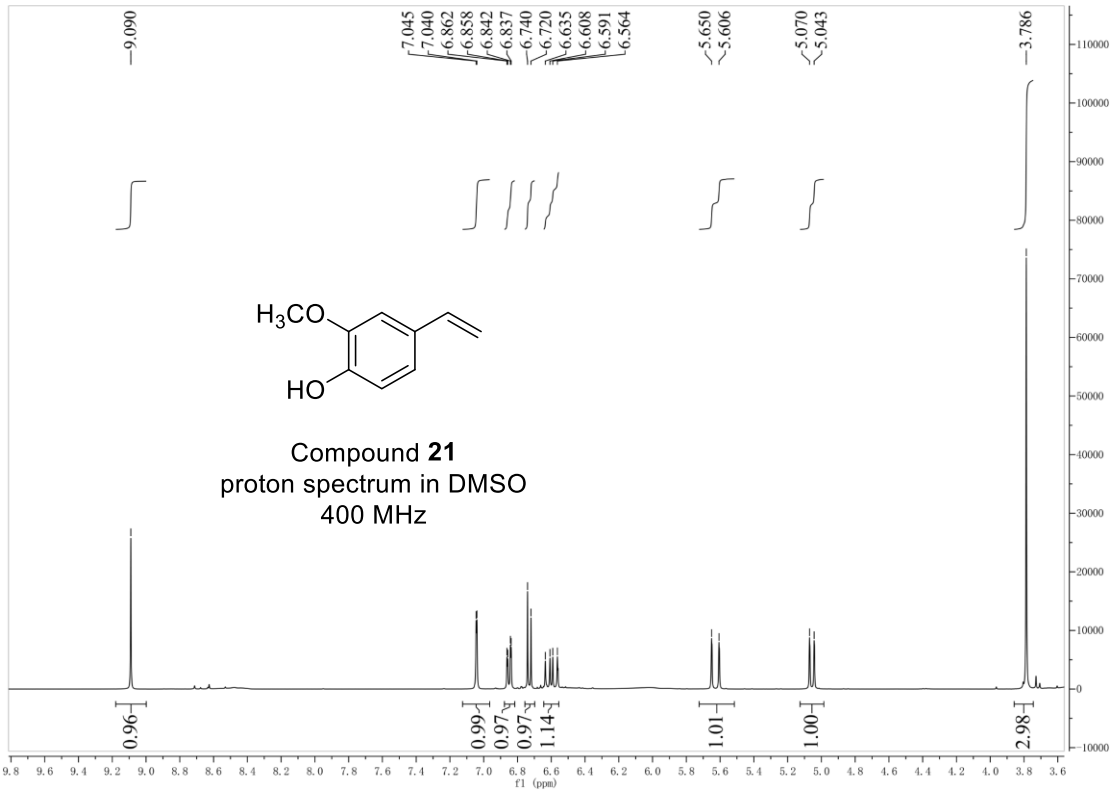
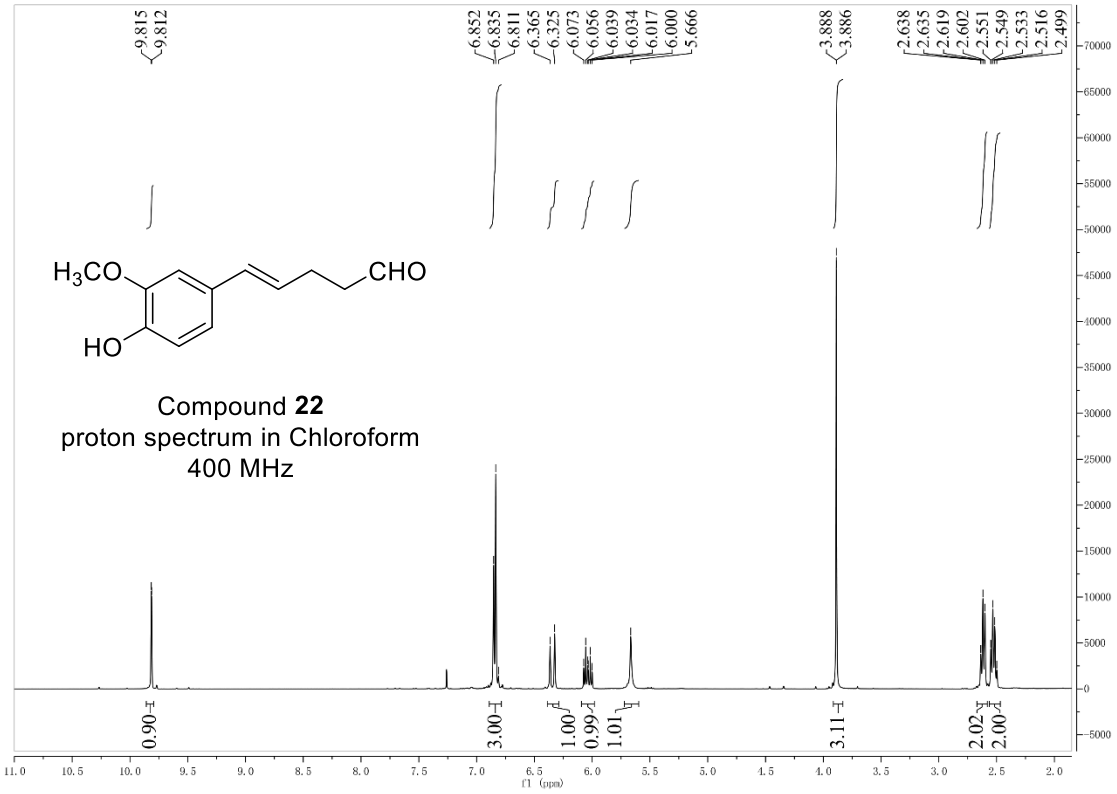
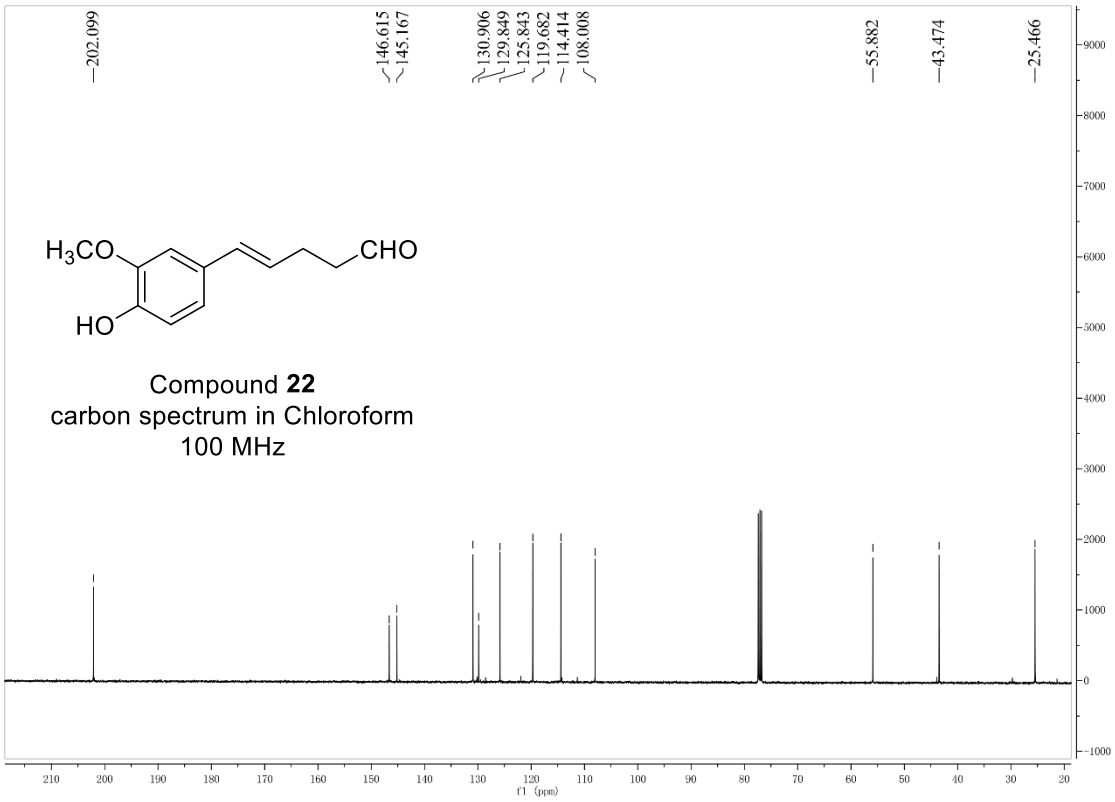


Figure S2. ^{1}H-NMR results of product **21**.

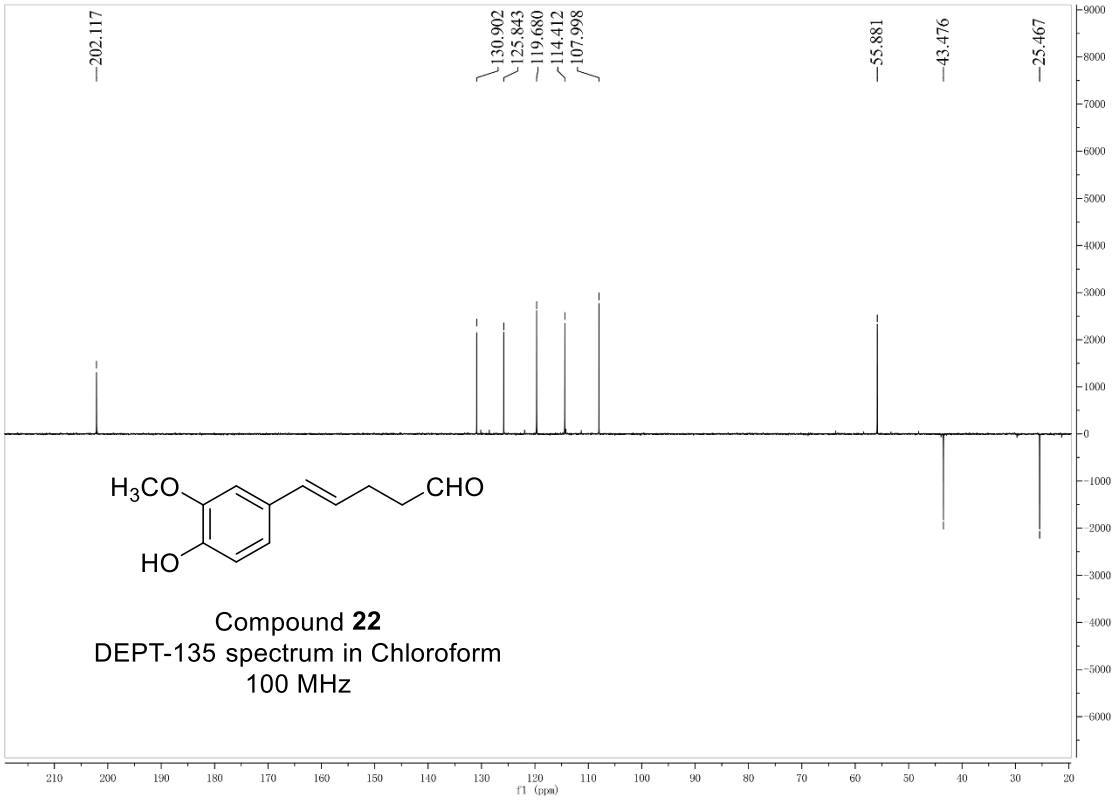
(a)


9.815
9.812
6.852
6.835
6.811
6.365
6.325
6.073
6.056
6.039
6.034
6.017
6.000
5.666
3.888
3.886
2.638
2.635
2.619
2.602
2.551
2.549
2.533
2.516
2.499
H3CO
CHO
HO
Compound 22
proton spectrum in Chloroform
400 MHz
0.90
3.00
1.00
0.99
1.01
3.11
2.02
2.00
f1 (ppm)

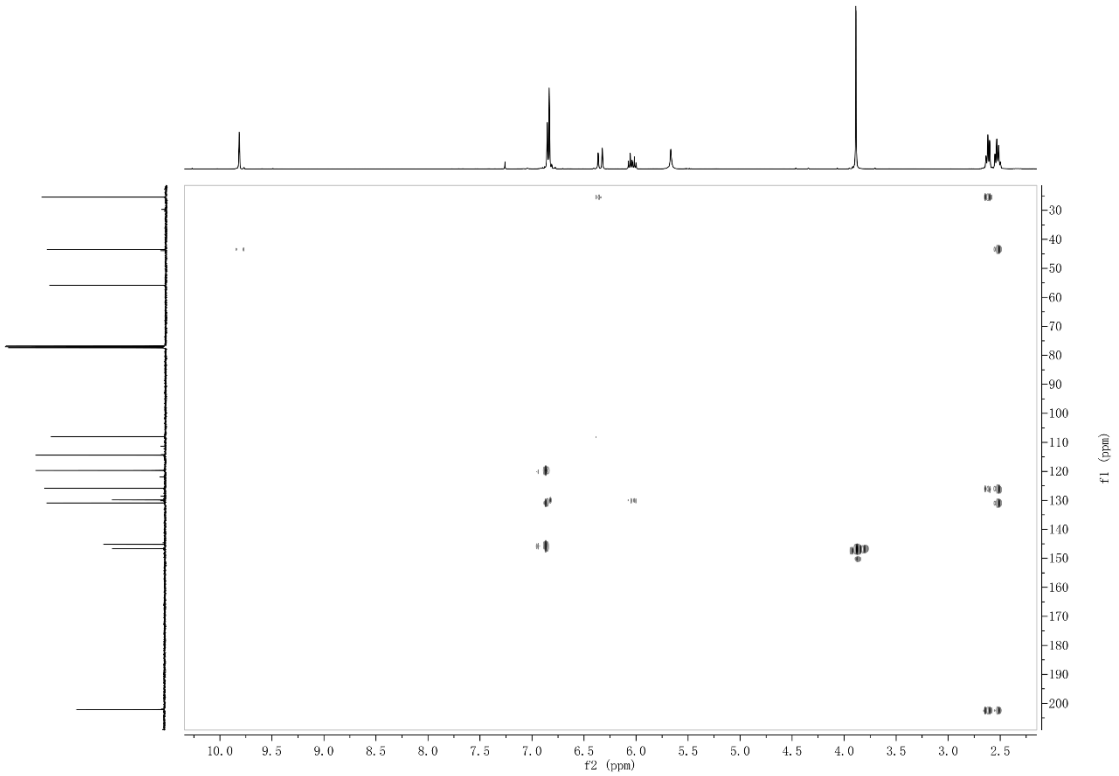
(b)

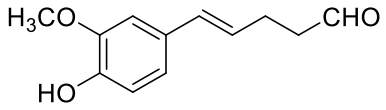

202.099
146.615
145.167
130.906
129.849
125.843
119.682
114.414
108.008
55.882
43.474
25.466
H3CO
CHO
HO
Compound 22
carbon spectrum in Chloroform
100 MHz
f1 (ppm)

(c)


202.117
130.902
125.843
119.680
114.412
107.998
55.881
43.476
25.467
H3CO
CHO
HO
Compound 22
DEPT-135 spectrum in Chloroform
100 MHz
f1 (ppm)

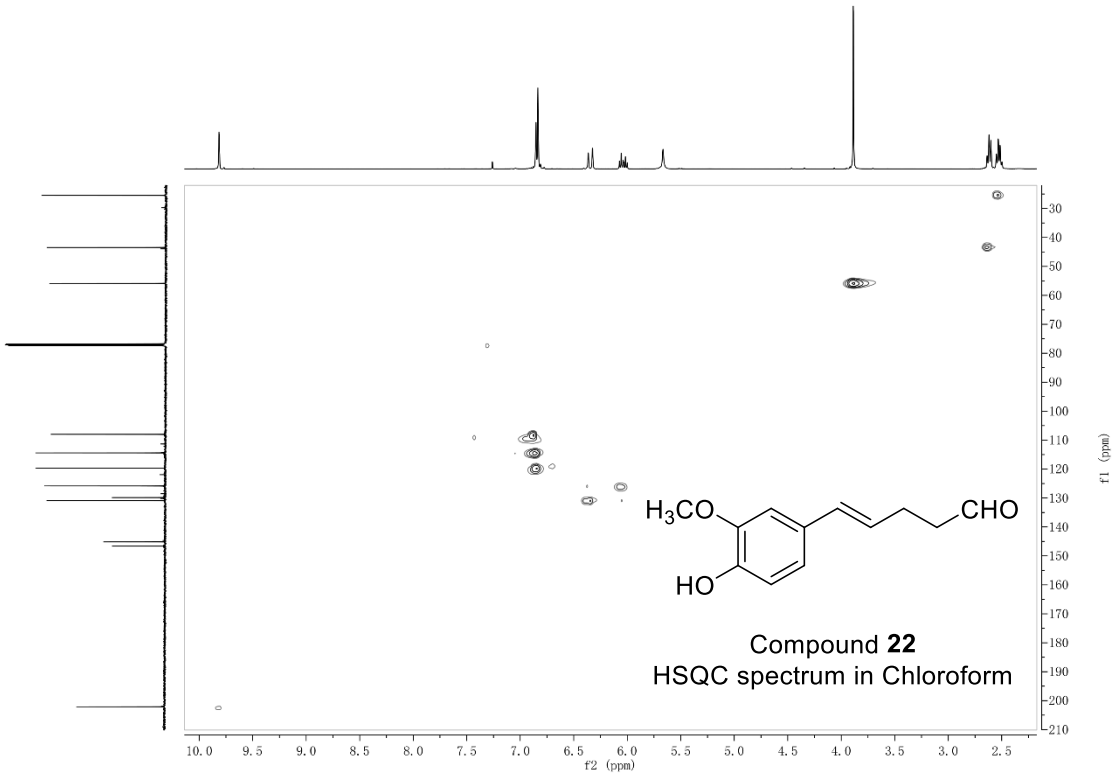
(d)





Compound **22**
HMBC spectrum in Chloroform

(e)


H3CO
CHO
HO
Compound 22
HSQC spectrum in Chloroform
f2 (ppm)
f1 (ppm)

(f)

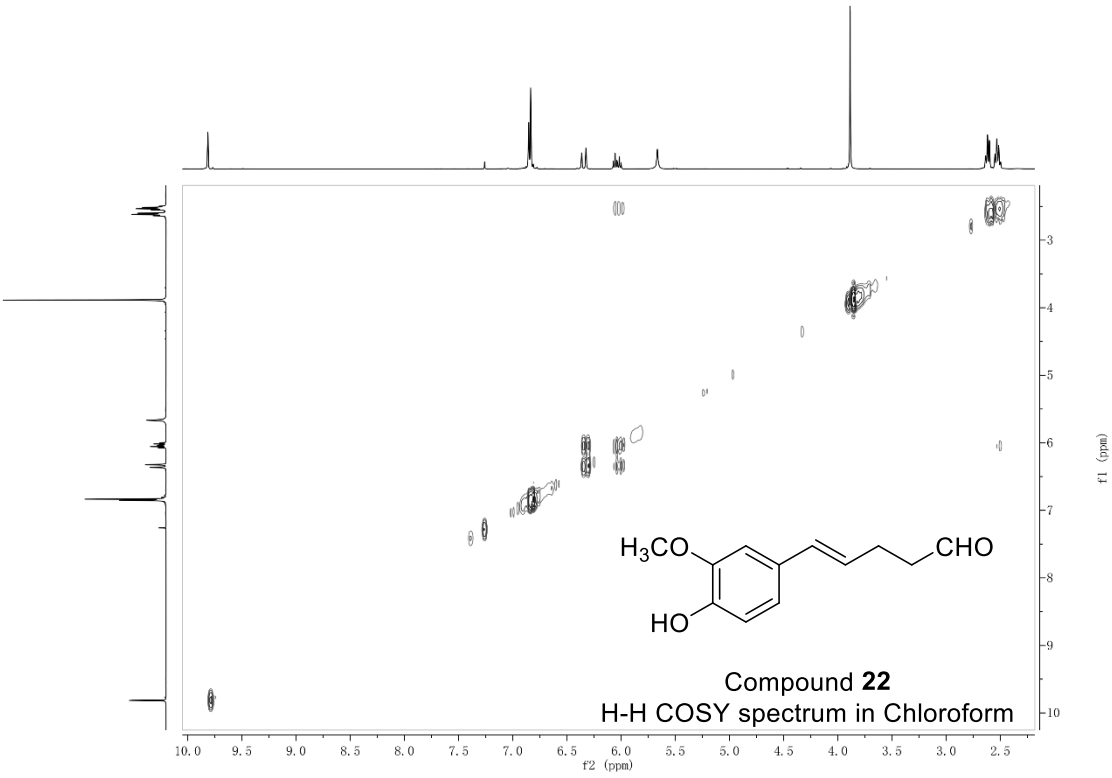


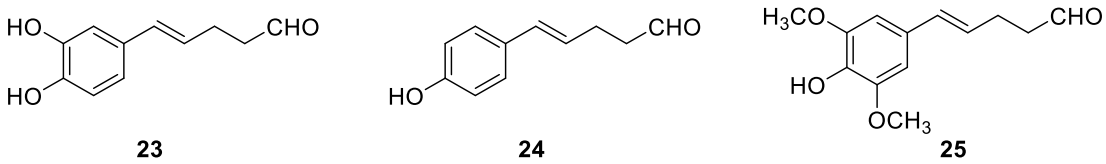
Figure S3. NMR results of product **22**. (a) ^{1}H-NMR, (b) ^{13}C-NMR, (c) DEPT-135 NMR, (d) HMBC-NMR, (e) HSQC-NMR, (f) H-H COSY-NMR.

^{1}H-NMR (400 MHz, $CDCl_3$) results of adducts caffeic acid, trans-4-coumaric acid or sinapic acid and acrolein:

Compound **23**: 9.81 (1H, s), 6.88 (1H, d, *J* = 2.0 Hz), 6.80-6.74 (2H, m), 6.29 (1H, d, *J* = 16.0 Hz), 6.00 (1H, dt, *J* = 6.8 Hz and 16.0 Hz), 5.65 (2H, s), 2.61 (2H, m), 2.51 (2H, m).

Compound **24**: 9.78 (1H, s), 7.17 (2H, d, *J* = 8.6 Hz), 6.78 (2H, d, *J* = 8.6 Hz), 6.55 (1H, s), 6.33 (1H, d, *J* = 16.0 Hz), 6.00 (1H, dt, *J* = 6.8 Hz and 16.0 Hz), 2.62 (2H, m), 2.51 (2H, m).

Compound **25**: 9.83 (1H, s), 6.57 (2H, s), 6.34 (1H, d, *J* = 15.6 Hz), 6.06 (1H, dt, *J* = 6.6 Hz and 15.6 Hz), 5.50 (1H, s), 3.90 (6H, s), 2.64 (2H, m), 2.54 (2H, m).



23 **24** **25**

Figure S4. Structures of compound **23**-**25**.

Table S1. Diseases proved to be related to acrolein.

Diseases	References
Alzheimer's	[4] Luo J et al., Neurochemistry International 2005
	[5] Lovell M A et al., Neurobiology of Aging 2001
Parkinson's	[6] Shamoto-Nagai M et al., Journal of Neural Transmission 2007
Diabetes	[7] Suzuki D et al., Internal Medicine 1999
Atherosclerosis	[8] Rom O et al., Archives of Toxicology 2017
	[9] Dejarnett N., Journal of the American Heart Association 2014