# Supporting Information

# Efficient Calculation of Molecular Properties from Simulation using Kernel Molecular Dynamics

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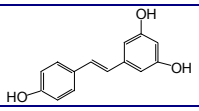
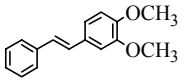
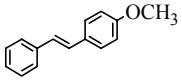
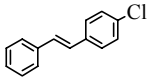
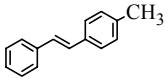
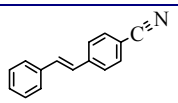
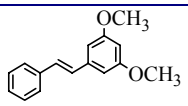
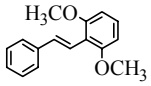
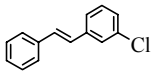
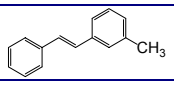
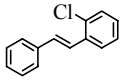
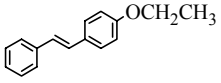
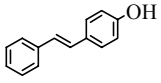
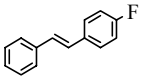
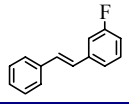
**Table 1.** Structures, activities, and some $IC_{50}$'s for resveratrol analogues. Activity is measured as percent inhibition of TNF-α induced activation of NF-κB at a 15μM concentration using the Panomics NF-κB stable reporter cell line 293/ NF-κB-luc. Compounds used for kMD training are marked as active/inactive.

| Analogue # | Structure | NFκB % of Control (15 μM) | NFκB $IC_{50}$ (μM) ± SD | kMD Training |
|---|---|---|---|---|
| Resveratrol |  | 58.2 | 20 ± 2.9 | Active |
| 1 |  | 86.5 | | Inactive |
| 2 |  | 18.5 | | |
| 3 |  | 19.3 | | |
| 4 |  | 13.1 | | Active |
| 5 |  | 55.1 | | |
| 6 |  | 63.9 | | |
| 7 |  | 75.6 | | |
| 8 |  | 26.4 | | |
| 9 |  | 24.5 | | |
| 10 |  | 31.7 | | |
| 11 |  | 6.0 | 0.33 ± 0.03 | Active |
| 12 |  | 45.6 | | |
| 13 |  | 34.3 | | |
| 14 |  | 45.2 | | |

| | | | | |
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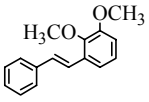
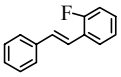
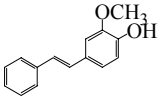
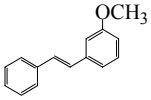
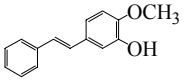
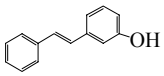
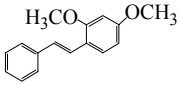
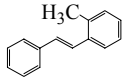
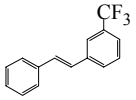
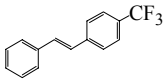
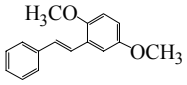
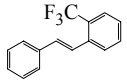
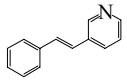
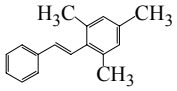
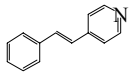
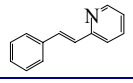
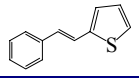
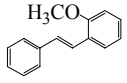
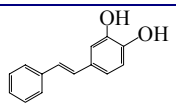
| 15 |  | 38.1 | | |
| 16 |  | 41.1 | | |
| 17 |  | 78.1 | | Inactive |
| 18 |  | 26.6 | | |
| 19 |  | 9.4 | | Active |
| 20 |  | 19.1 | | |
| 21 |  | 10.7 | | Active |
| 22 |  | 54.8 | | |
| 23 |  | 67.3 | | |
| 24 |  | 19.7 | | |
| 25 |  | 84.3 | | Inactive |
| 26 |  | 152.4 | | Inactive |
| 27 |  | 80.1 | | Inactive |
| 28 |  | 74.3 | | |
| 29 |  | 75.1 | | |
| 30 |  | 84.0 | | Inactive |
| 31 |  | 76.1 | | |
| 32 |  | 28.0 | | |
| 33 |  | 15.3 | | Active |

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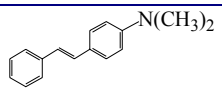
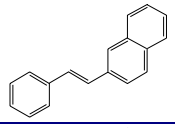
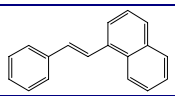
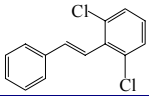
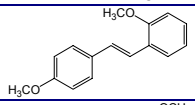
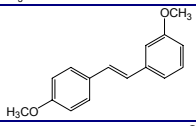
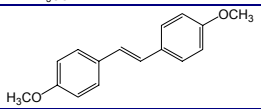
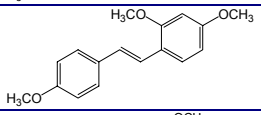
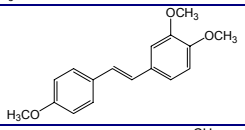
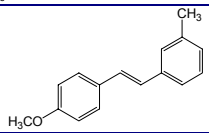
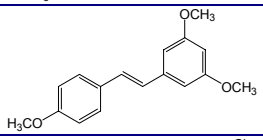
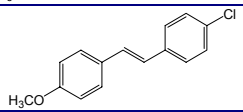
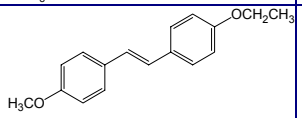
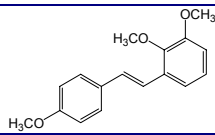
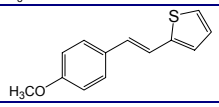
| 34 |  | 3.1 | 0.15 ± 0.07 | Active |
| 35 |  | 7.7 | 1.34 ± 0.3 | Active |
| 36 |  | 23.7 | | |
| 37 |  | 69.2 | | |
| 38 |  | 52.0 | | |
| 39 |  | 6.1 | 0.47 ± 0.14 | Active |
| 40 |  | 27.2 | | |
| 41 |  | 33.4 | | |
| 42 |  | 62.6 | | |
| 43 |  | 6.8 | 0.83 ± 0.2 | Active |
| 44 |  | 19.0 | | |
| 45 |  | 25.6 | | |
| 46 |  | 69.4 | | |
| 47 |  | 16.6 | | |
| 48 |  | 17.0 | | |

| | | | | |
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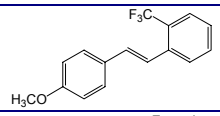
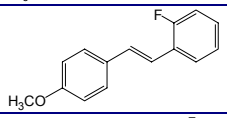
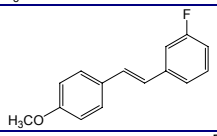
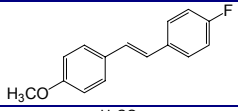
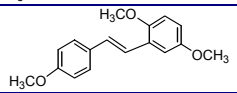
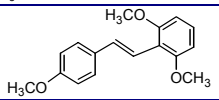
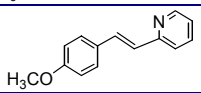
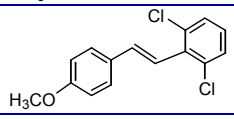
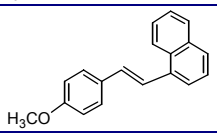
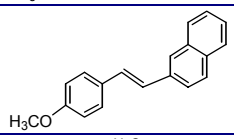
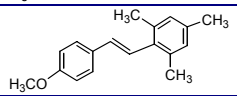
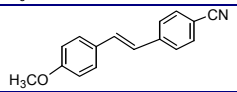
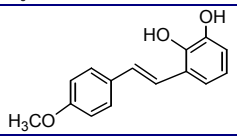
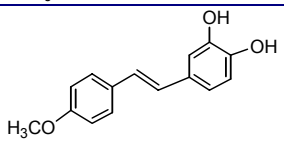
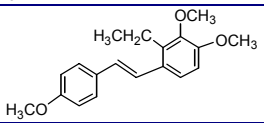
| 49 |  | 27.3 | | |
| 50 |  | 5.2 | 0.15 ± 0.1 | Active |
| 51 |  | 6.0 | 1.34 ± 0.3 | Active |
| 52 |  | 15.5 | | Active |
| 53 |  | 67.7 | | |
| 54 |  | 69.4 | | |
| 55 |  | 19.7 | | |
| 56 |  | 44.8 | | |
| 57 |  | 39.3 | | |
| 58 |  | 35.7 | | |
| 59 |  | 50.9 | | |
| 60 |  | 31.4 | | |
| 61 |  | 10.9 | 0.53 ± 0.3 | Active |
| 62 |  | 8.7 | 0.64 ± 0.4 | Active |
| 63 |  | 43.0 | | |

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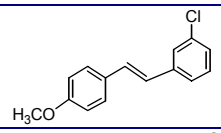
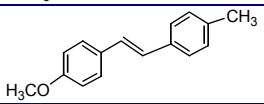
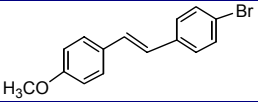
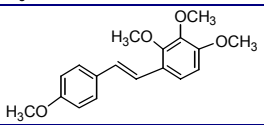
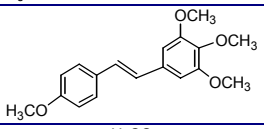
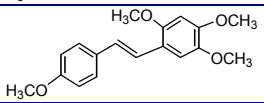
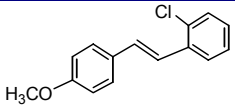
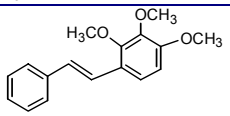
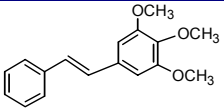
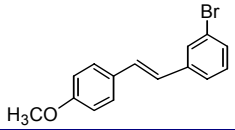
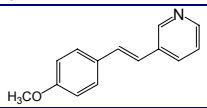
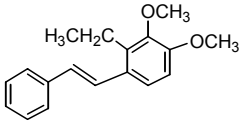
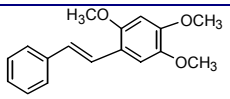
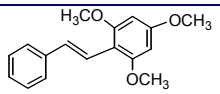
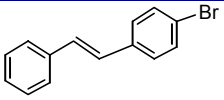
|---|---|---|---|---|
| 64 |  | 5.8 | 1.0 ± 0.07 | Active |
| 65 |  | 9.2 | 0.9 ± 0.1 | Active |
| 66 |  | 40.8 | | |
| 67 |  | 70.3 | | |
| 68 |  | 43.2 | | |
| 69 |  | 67.2 | | |
| 70 |  | 6.1 | 1.5 ± 0.03 | Active |
| 71 |  | 50.3 | | |
| 72 |  | 49.4 | | |
| 73 |  | 15.4 ± 0.4 | | Active |
| 74 |  | 49.1 | | |
| 75 |  | 96.2 | | Inactive |
| 76 |  | 70.5 ± 0.4 | | |
| 77 |  | 97.0 ± 14 | | Inactive |
| 78 |  | 21.0 ± 6.6 | | |

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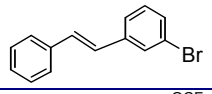
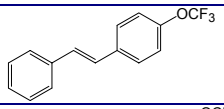
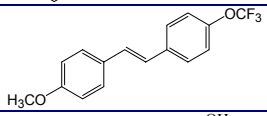
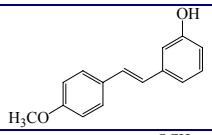
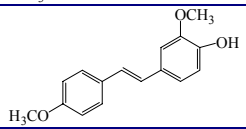
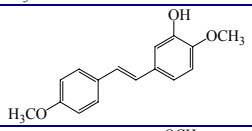
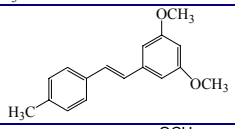
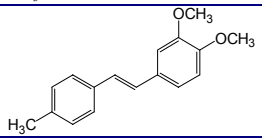
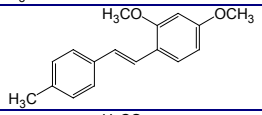
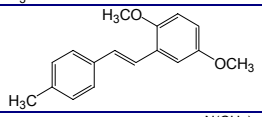
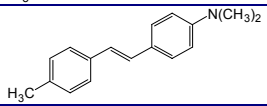
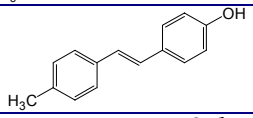
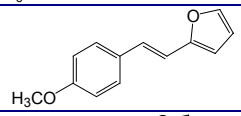
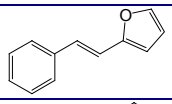
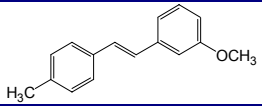
|---|---|---|---|---|
| 79 |  | 47.9 ± 1.2 | | |
| 80 |  | 16.8 ± 1.6 | | |
| 81 |  | 66.5 ± 7.3 | | |
| 82 |  | 35.6 ± 3.7 | | |
| 83 |  | 38.9 ± 2.2 | | |
| 84 |  | 32.3 ± 6.5 | | |
| 85 |  | 25.7 ± 1.8 | | |
| 86 |  | 56.1 ± 1.5 | | |
| 87 |  | 45.1 ± 7.3 | | |
| 88 |  | 108 ± 5.1 | | Inactive |
| 89 |  | 13.1 ± 2.2 | | Active |
| 90 |  | 29.0 ± 2.8 | | |
| 91 |  | 55.4 ± 1.1 | | |
| 92 |  | 101± 5.5 | | Inactive |
| 93 |  | 10.2 ± 0.3 | | Active |

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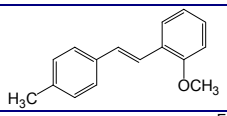
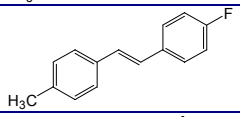
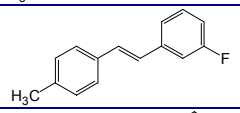
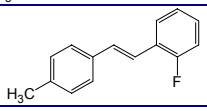
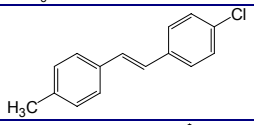
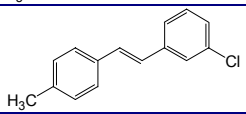
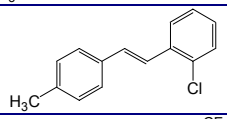
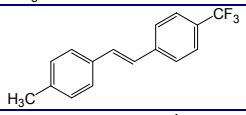
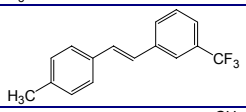
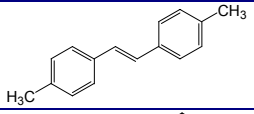
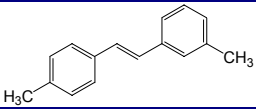
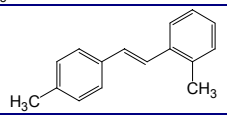
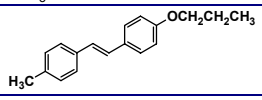
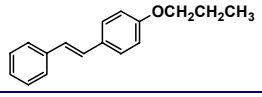
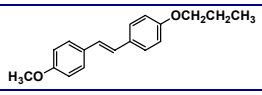
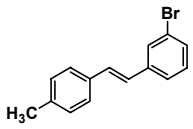
|---|---|---|---|---|
| 94 |  | 38.5 ± 2.4 | | |
| 95 |  | 20.4 ± 2.2 | | |
| 96 |  | 10.5 ± 0.9 | | Active |
| 97 |  | 6.8 ± 1.1 | | Active |
| 98 |  | 48.4 ± 17 | | |
| 99 |  | 21.6 ± 0.5 | | |
| 100 |  | 59.1 ± 5.3 | | |
| 101 |  | 73.2 ± 20 | | |
| 102 |  | 24.7 ± 2.8 | | |
| 103 |  | 24.7 ± 2.8 | | |
| 104 |  | 11.8 ± 0.6 | | Active |
| 105 |  | 16.6 ± 1.2 | | |
| 106 |  | 55 ± 0.04 | | |
| 107 |  | 12.6 ± 1.6 | | Active |
| 108 |  | 63.6 ± 23 | | |
| 109 |  | 23.0 ± 1.8 | | |

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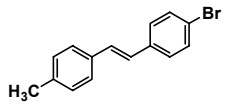
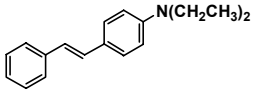
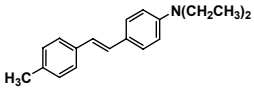
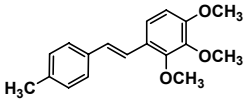
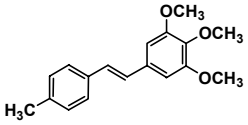
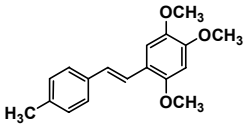
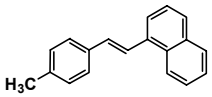
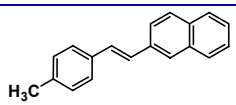
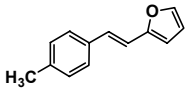
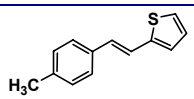
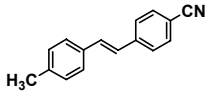
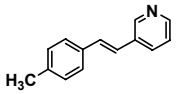
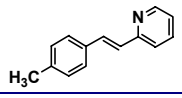
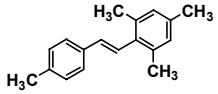
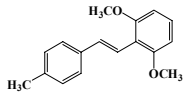
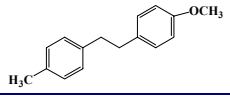
|---|---|---|---|---|
| 110 |  | 72.3 ± 9.8 | | |
| 111 |  | 16.7 ± 1.6 | | |
| 112 |  | 93.8 ± 34 | | Inactive |
| 113 |  | 53.8 ± 1.2 | | |
| 114 |  | 68.6 ± 13 | | |
| 115 |  | 68.3 ± 2.4 | | |
| 116 |  | 57.1 ± 0.5 | | |
| 117 |  | 49.8 ± 0.1 | | |
| 118 |  | 45.8 ± 5.2 | | |
| 119 |  | 34.1 ± 4.7 | | |
| 120 |  | 52.6 ± .44 | | |
| 121 |  | 48.1 ± 1.8 | | |
| 122 |  | 21.1 ± 2.6 | | |
| 123 |  | 76.1 ± 5.7 | | Inactive |
| 124 |  | 110 ± 9.1 | | Inactive |
| 125 |  | 101 ± 4.6 | | Inactive |

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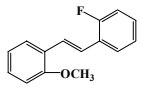
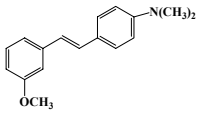
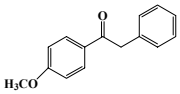
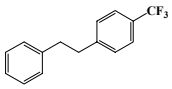
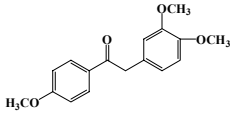
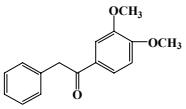
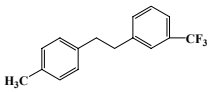
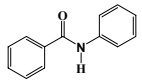
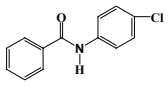
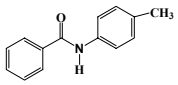
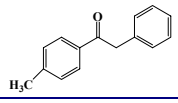
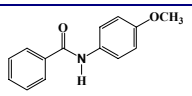
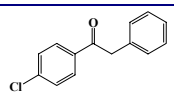
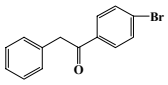
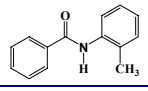
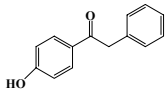
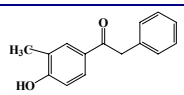
|---|---|---|---|---|
| 126 |  | 75.7 ± 7.2 | | |
| 127 |  | 3.5 ± 0.03 | 0.07 | Active |
| 128 |  | 51.2 ± 15 | | |
| 129 |  | 141 ± 28 | | Inactive |
| 130 |  | 116 ± 13 | | Inactive |
| 131 |  | 107 ± 23 | | Inactive |
| 132 |  | 89.7 ± 6.4 | | Inactive |
| 133 |  | 95.9 ± 13 | | Inactive |
| 134 |  | 83.8 ± 1.1 | | Inactive |
| 135 |  | 108 ± 9.3 | | Inactive |
| 136 |  | 110 ± 17 | | Inactive |
| 137 |  | 124 ± 3.3 | | Inactive |
| 138 |  | 105 ± 11 | | Inactive |
| 139 |  | 121 ± 1.2 | | Inactive |
| 140 |  | 124 ± 1.2 | | Inactive |
| 141 |  | 99 ± 25 | | Inactive |
| 142 |  | 101 ± 5.4 | | Inactive |

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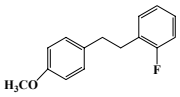
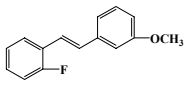
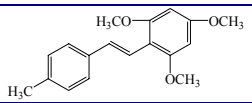
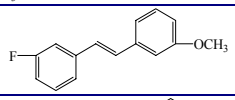
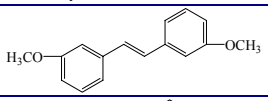
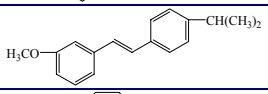
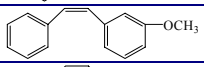
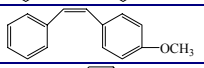
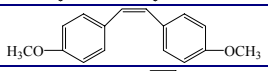
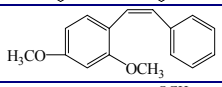
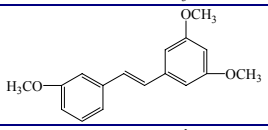
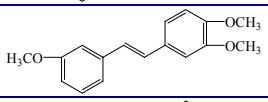
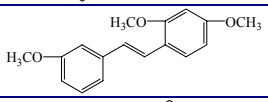
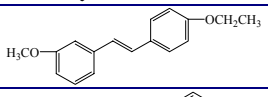
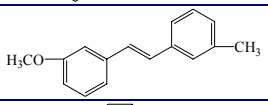
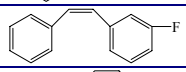
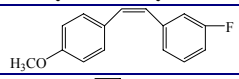
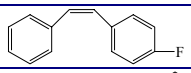
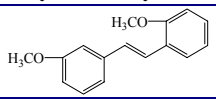
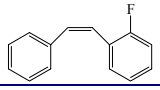
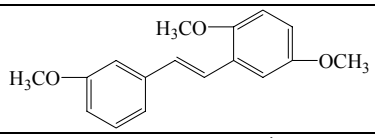
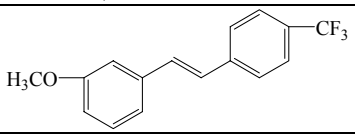
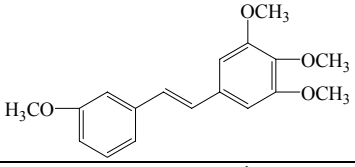
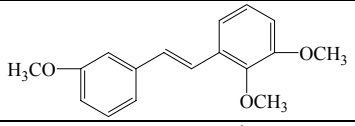
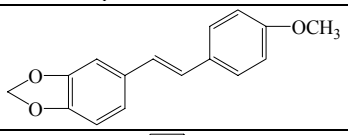
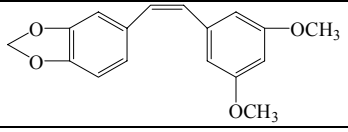
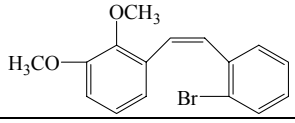
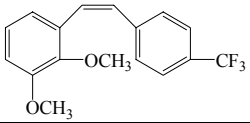
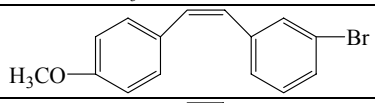
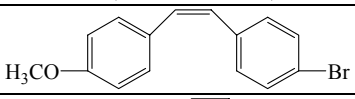
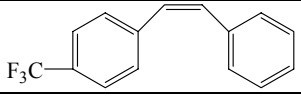
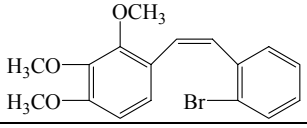
|---|---|---|---|---|
| 143 |  | 99.8 ± 23 | | Inactive |
| 144 |  | 23.1 ± 5.5 | | |
| 145 |  | 66.8 ± 7.8 | | |
| 146 |  | 27.8 ± 0.5 | | |
| 147 |  | 7.5 ± 0.8 | | Active |
| 148 |  | 3.8 ± 0.3 | 1.0 | Active |
| 149 |  | 25.6 ± 0.4 | | |
| 150 |  | 17.6 ± 2.5 | | |
| 151 |  | 31.2 ± 4.1 | | |
| 152 |  | 34.9 ± 9.2 | | |
| 153 |  | 23.1 ± 3.8 | | |
| 154 |  | 41.1 ± 3.1 | | |
| 155 |  | 26.2 ± 3.0 | | |
| 156 |  | 12.8 ± 0.9 | | Active |
| 157 |  | 25.3 ± 1.8 | | |
| 158 |  | 46.5 ± 9.9 | | |
| 159 |  | 14.4 ± 0.1 | | Active |
| 160 |  | 59.8 ± 17.1 | | |
| 161 |  | 48.1 ± 8.1 | | |
| 162 |  | 84.3 ± 2.9 | | Inactive |

**Table 2.** Structures and the resulting activities for the candidate resveratrol analogues.

| Analogue # | Structure | % of Control (15 μM) |
|---|---|---|
| 163 |  | 56 |
| 164 |  | 13 ± 0.7 |
| 165 |  | 39 ± 14 |
| 166 |  | 17 ± 1.8 |
| 167 |  | 4.5 ± 0.7 |
| 168 |  | 3.4 ± 0.07 |
| 169 |  | 74 ± 6.1 |
| 170 |  | 43 ± 5.6 |
| 171 |  | 57 ± 8.7 |
| 172 |  | 71 ± 10 |
| 173 |  | 67 ± 8.0 |
| 174 |  | 71 ± 12 |

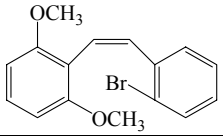
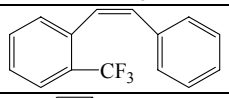
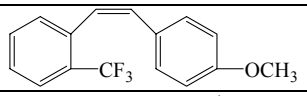
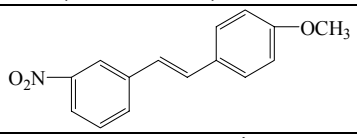
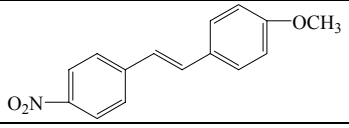
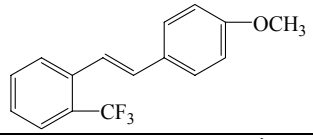
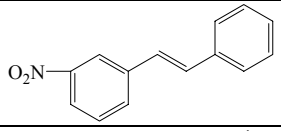
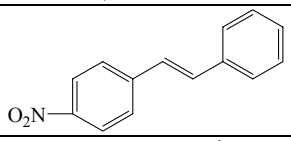
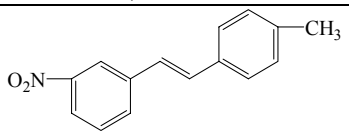
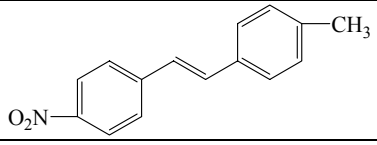
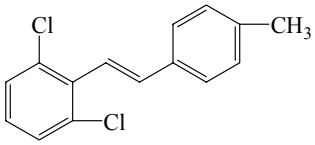
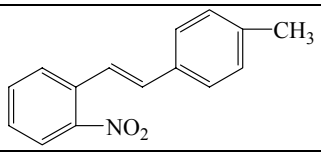
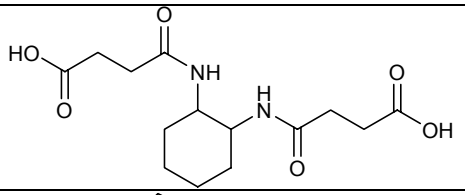
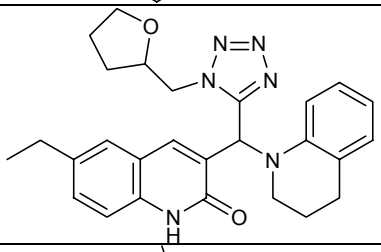
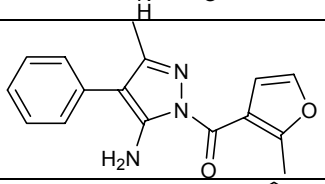
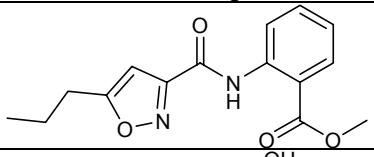
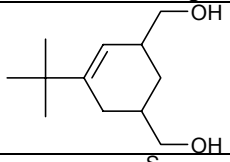
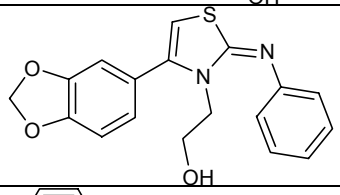
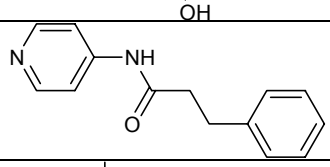
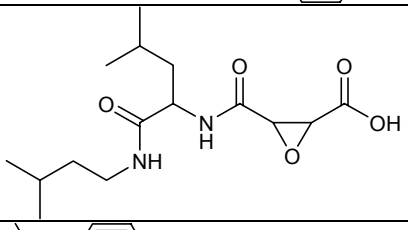
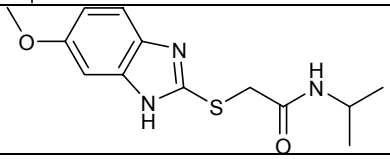
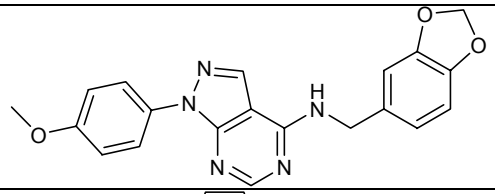
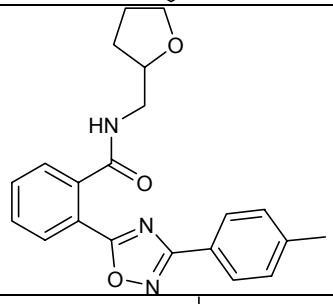
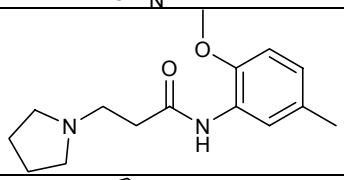
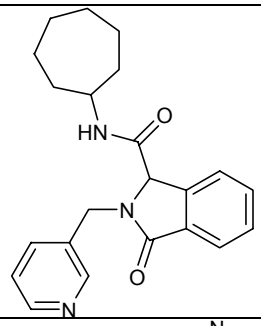
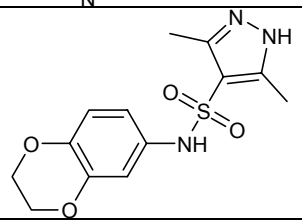
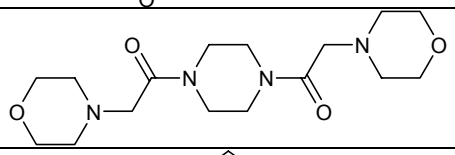
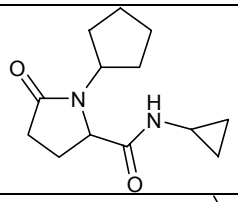
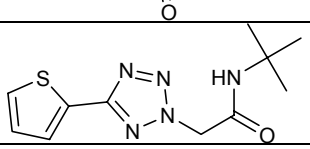
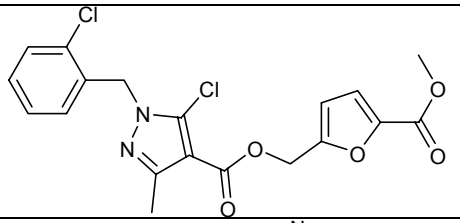
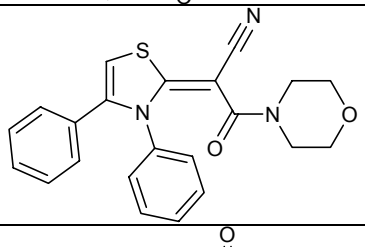
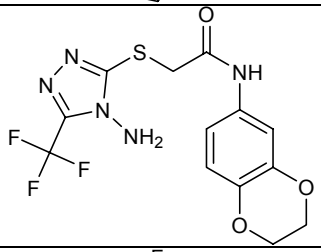
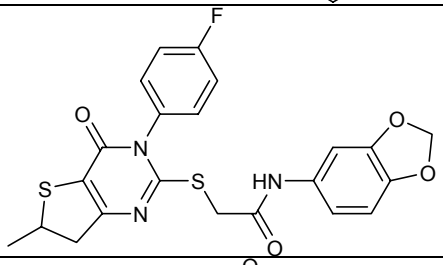
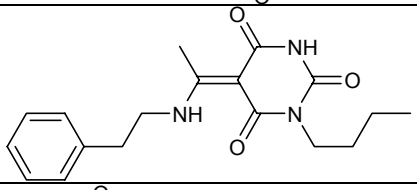
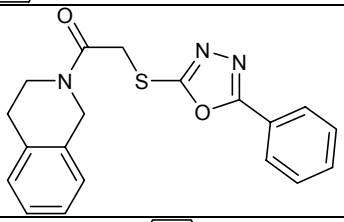
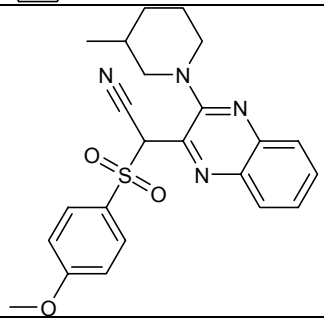
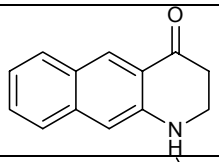
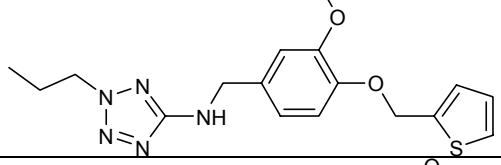
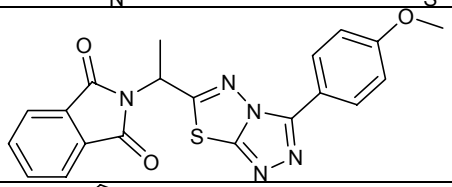
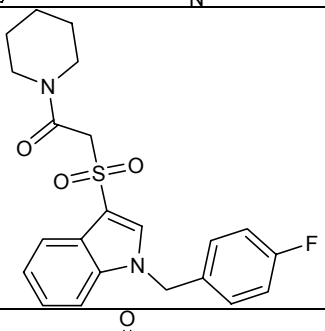
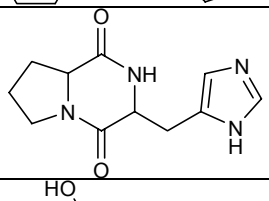
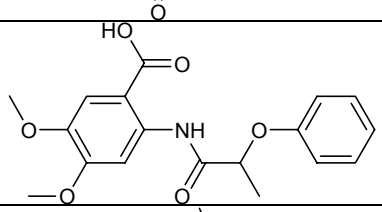
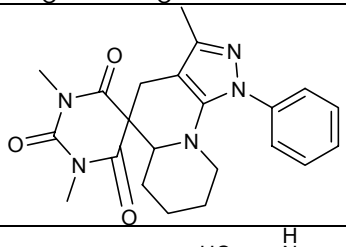
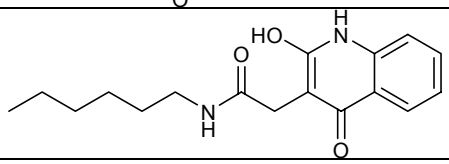
| | | |
|---|---|---|
| 175 |  | 97 ± 13 |
| 176 |  | 102 ± 2,8 |
| 177 |  | 67 ± 0.8 |
| 178 |  | 16 ± 4.0 |
| 179 |  | 21 ± 1.5 |
| 180 |  | 28 ± 2.5 |
| 181 |  | 55 ± 4.2 |
| 182 |  | 40 ± 0.2 |
| 183 |  | 14 ± 0.3 |
| 184 |  | 12 ± 0.9 |
| 185 |  | 57 ± 8.9 |
| 186 |  | 15 ± 4.8 |

**Table 3.** PubChem Compound IDs and Structures for inactive compounds used in additional models generated for the formylpeptide receptor assay.

| Group | PubChem CID | Structure |
|---|---|---|
| Group 1 | 2913415 |  |
| Group 1 | 645431 |  |
| Group 1 | 1263280 |  |
| Group 1 | 5308358 |  |
| Group 1 | 660718 |  |
| Group 1 | 6603372 |  |
| Group 1 | 814775 |  |
| Group 1 | 123664 |  |
| Group 1 | 2610597 |  |

| | | |
|---|---|---|
| Group 1 | 661116 |  |
| Group 1 | 665413 |  |
| Group 1 | 771481 |  |
| Group 1 | 3241679 |  |
| Group 1 | 866899 |  |
| Group 1 | 265941 |  |
| Group 1 | 3237546 |  |
| Group 1 | 1266316 |  |

| | | |
|---|---|---|
| Group 2 | 2571603 |  |
| Group 2 | 1972861 |  |
| Group 2 | 659582 |  |
| Group 2 | 4559027 |  |
| Group 2 | 5389543 |  |
| Group 2 | 2905400 |  |
| Group 2 | 664508 |  |

| | | |
|---|---|---|
| Group 2 | 607541 |  |
| Group 2 | 2084150 |  |
| Group 2 | 4246341 |  |
| Group 2 | 2053119 |  |
| Group 2 | 449094 |  |
| Group 2 | 2914913 |  |
| Group 2 | 2997534 |  |
| Group 2 | 657533 |  |

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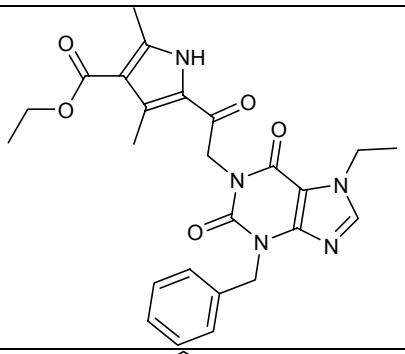
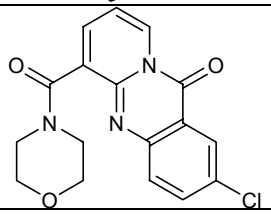
| Group 2 | 3000030 |  |
| Group 2 | 3243577 |  |

**Experimental Data.** Synthesis and verification resveratrol analogues.

All reagents were obtained from commercial sources and used without further purification. All compounds that were isolated were greater than 90% pure by $^{1}H$ and/or $^{13}C$ NMR. Column chromatographic separations were performed using EM Science type 60 silica gel (230-400 mesh). Preparative thin layer chromatography was performed using Analtech silica gel gf 2000 micron plates. Melting points were determined on a Thomas Hoover capillary melting point apparatus and are uncorrected. NMR spectra were recorded on a Bruker AC250 (250 MHz) NMR spectrometer in $CDCl_3$ unless otherwise noted. Chemical shifts are reported in ppm (δ) relative to $CHCl_3$ at 7.24 ppm for $^{1}H$ NMR and 77.0 for $^{13}C$ NMR. High resolution mass spectra were performed at the Mass Spectrometry Facility, University of New Mexico.

Compounds 1-73 were previously reported by Heynekamp et al.[1] Compounds 74-124, 126-127, 144-148, 153-157, 161, 163-167, 178-186 were synthesized using the method described by Heynekamp et al.[1] Compounds 128, 130-131, 136, 138-139, 141-142 were synthesized using a method described by Chhor[2] and Lubczyk.[3] Compounds 125, 129, 132, 134-135, 137, 140, 143 were synthesized by methods described by Cushman.[4] Compounds 149-152, 158-160, 162, 168, 170-173, 176-177 were synthesized using the method described by Bellucci et al.[5] Compounds 169, 174 and 175 were synthesized using the method described by Harrovwen et al.[6]

(E)-4'-Methoxy-3-stilbazole (74). mp 98-100 °C [lit[10] 99-100 °C].
(E)-2-Ethyl-3,4-dimethoxystilbene (75). mp 92-93 °C; $^{1}H$ NMR: δ 1.19 (t, 3H, $J$ = 7.75 Hz), 2.82 (q, 2H, $J$ = 7.55 Hz), 3.84 (s, 3H), 3.88 (s, 3H), 6.79 (d, 1H, $J$ = 8.54 Hz), 6.80 (d, 1H, $J$ = 16.28 Hz), 7.28 (d, 1H, $J$ = 16.09 Hz), 7.35 (m, 3H), 7.50 (d, 2H, $J$ = 7.15 Hz). Exact mass calcd for $C_{18}H_{20}O_2$: 268.1463, observed (M+H) 269.1543.
(E)-2,4,5-Trimethoxystilbene (76). mp 83-84 °C [lit[4] 81-82 °C].
(E)-2,4,6-Trimethoxystilbene (77). mp 59 °C [lit[4] 57-59 °C].
(E)-4-Bromostilbene (78). mp 138-139 °C [lit[15] 133-134 °C].
(E)-3-Bromostilbene (79). mp 90-90.5 °C [lit[16] 87-89 °C].
(E)-4-Trifluoromethoxystilbene (80). mp 110-111 °C; $^{1}H$ NMR: δ 7.07 (s, 2H), 7.17-7.38 (m, 3H), 7.48-7.53 (m, 6H). Exact mass calcd for $C_{15}H_{11}F_3O$: 264.0762, observed (M+) 264.0766.
(E)-4-Trifluoromethoxy-4'-methoxystilbene (81). mp 147-148 °C; $^{1}H$ NMR: δ 3.82 (s, 3H), 6.90 (d, 2H, $J$ = 8.74 Hz), 6.92 (d, 1H, $J$ = 16.48 Hz), 7.00 (d, 1H, J = 16.09 Hz), 7.16 (d, 2H, J = 8.14 Hz), 7.43 (d, 2H, $J$ = 9.33 Hz), 7.47 (d, 2H, $J$ = 9.14 Hz). Exact mass calcd for $C_{16}H_{13}F_3O_2$: 294.0868, observed (M+) 294.0871.
(E)-3-Hydroxy-4'-methoxystilbene (82). mp 160-162 °C [lit[11] 159-160 °C].
(E)-4-Hydroxy-3-methoxy-4'-methoxystilbene (83). mp 163-164 °C [lit[18] 163-166 °C].
(E)-3-Hydroxy-4-methoxy-4'-methoxystilbene (84). mp 201-202 °C [lit[19] 192-193 °C].
(E)-3,5-Dimethoxy-4'-methylstilbene (85). mp 62-63 °C [lit[20] 51 °C].
(E)-3,4-Dimethoxy-4'-methylstilbene (86). mp 165-166 °C [lit[20] 168 °C].
(E)-2,4-Dimethoxy-4'-methylstilbene (87). mp 72-73°C; $^{1}H$ NMR: δ 2.33 (s, 3H), 3.79 (s, 3H), 3.83 (s, 3H), 6.45 (m, 3H), 6.95 (d, 1H, $J$ = 16.49 Hz), 7.12 (d, 2H, $J$ = 7.95 Hz), 7.34 (d, 1H, $J$ = 16.49 Hz), 7.39 (d, 1H, $J$ = 7.94 Hz), 7.47 (d, 1H, $J$ = 8.35 Hz). Exact mass calcd for $C_{17}H_{18}O_2$: 254.1307, observed (M+) 254.1314.
(E)-2,5-Dimethoxy-4'-methylstilbene (88). mp 80-81 °C [lit[21] 78 °C].

(E)- 4-N,N-Dimethylamino-4'-methylstilbene (89). mp 164-165 °C [lit[22] 163-165 °C].
(E)-4-Hydroxy-4'-methylstilbene (90). mp 212-213 °C [lit[15] 210-212 °C].
(E)-2-(4-Methoxylstyryl)furan (91). mp 73-74 °C [lit[23] 73-74 °C].
(E)-2-Styrylfuran (92). Mp 54-55° C [lit[24] 54-55 °C].
(E)-3-Methoxy-4'-methylstilbene (93). mp 77-78 °C [lit[25] 76 °C].
(E)-2-Methoxy-4'-methylstilbene (94). mp 78-79 °C [lit[25] 80 °C].
(E)-4-Fluoro-4'-methylstilbene (95). mp 157-158 °C [lit[26] 157.5-159 °C].
(E)-3-Fluoro-4'-methylstilbene (96). mp 104-105 °C [lit[27] 106 °C].
(E)-2-Fluoro-4'-methylstilbene (97). mp 77-78 °C [lit[27] 75 °C].
(E)-4-Chloro-4'-methylstilbene (98). mp 201-203 °C [lit[15] 206-207 °C].
(E)-3-Chloro-4'-methylstilbene (99). mp 117-118 °C [lit[25] 116 °C].
(E)-2-Chloro-4'-methylstilbene (100). mp 35-37 °C [lit[25] 36-39 °C].
(E)-4-Trifluoromethyl-4'-methylstilbene (101). mp 187-188 °C [lit[28] 187-189 °C].
(E)-3-Trifluoromethyl-4'-methylstilbene (102). mp 94-95 °C; $^1$H NMR: δ 2.36 (s, 3H), 7.04 (d, 1H, *J* = 16.49 Hz), 7.15 (d, 1H, *J* = 16.08 Hz), 7.17 (d, 2H, *J* = 7.94 Hz), 7.41 (d, 2H, *J* = 8.14 Hz), 7.44 (t, 1H, *J* = 8.34 Hz), 7.45 (d, 1H, *J* = 8.34 Hz), 7.64 (d, 1H, *J* = 6.75 Hz), 7.73 (s, 1H). Exact mass calcd for $C_{16}H_{13}F_3$: 262.0969, observed (M+) 262.0978.
(E)-4-Methyl-4'-methylstilbene (103). mp 178-180 °C [lit[15] 182-184 °C].
(E)-3-Methyl-4'-methylstilbene (104). mp 100-101 °C [lit[14] 101-102 °C].
(E)-2-Methyl-4'-methylstilbene (105). mp 50-51 °C [lit[30] 49-51 °C].
(E)-4-Methyl-4'-propoxystilbene (106). mp 150-151 °C; $^1$H NMR: δ 1.04 (t, 3H, *J* = 7.35 Hz), 1.81 (sex, 2H, *J* = 7.15 Hz), 2.35 (s, 3H), 3.93 (t, 2H, *J* = 6.56 Hz), 6.87 (d, 1H, *J* = 8.54 Hz), 6.93 (d, 1H, *J* = 16.08 Hz), 6.97 (d, 1H, *J* = 6.76 Hz), 7.03 (d, 1H, *J* = 15.89 Hz), 7.14 (d, 2H, *J* = 7.94 Hz), 7.38 (d, 2H, *J* = 9.53 Hz), 7.42 (d, 2H, *J* = 8.94 Hz). Exact mass calcd for $C_{18}H_{20}O$: 252.1514, observed (M+) 252.1522.
(E)-4-Propoxystilbene (107). mp 126-128 °C [lit[31]]; $^1$H NMR: δ 1.04 (t, 3H, *J* = 7.35 Hz), 1.81 (sex, 2H, *J* = 7.15 Hz), 3.93 (t, 2H, *J* = 6.56 Hz), 6.88 (d, 2H, *J* = 8.54 Hz), 6.92 (d, 1H, *J* = 15.90 Hz), 7.05 (d, 1H, *J* = 15.89 Hz), 7.23 (m, 1H), 7.31 (d, 1H, *J* = 7.75 Hz), 7.34 (d, 1H, *J* = 7.15Hz), 7.43 (d, 2H, *J* = 8.74Hz), 7.47 (d, 2H, *J* = 7.75 Hz).
(E)-4-Methoxy-4'-propoxystilbene (108). mp 177-178 °C [lit [32]]; $^1$H NMR: δ 1.04 (t, 3H, *J* = 7.15 Hz), 1.81 (sex, 2H, *J* = 7.15 Hz), 3.82 (s, 3H), 3.93 (t, 2H, *J* = 6.77 Hz), 6.88 (d, 4H, *J* = 7.35 Hz), 6.92 (s, 2H), 7.41 (dd, 4H, *J* = 8.74, 2.59 Hz).
(E)-3-Bromo-4'-methylstilbene (109). mp 115-117 °C [lit[33]]; $^1$H NMR: δ 2.35 (s, 3H), 6.93 (d, 1H, *J* = 16.49 Hz), 7.04 (d, 1H, *J* = 15.88 Hz), 7.15 (d, 2H, *J* = 8.14 Hz), 7.17 (t, 1H, *J* = 8.94 Hz), 7.34 (d, 1H, *J* = 9.73 Hz), 7.37 (d, 3H, *J* = 7.94 Hz), 7.62 (s, 1H).
(E)-4-Bromo-4'-methylstilbene (110). mp 213-214 °C [lit[28] 214-216 °C].
(E)-4-N,N-Dimethylaminostilbene (111). mp 96-97 °C [lit[34] 96 °C].
(E)-4-N,N-Diethylamino-4'-methylstilbene (112). mp 99-100 °C [lit [35]]; $^1$H NMR: δ 1.17 (t, 6H, *J* = 6.95 Hz), 2.34 (s, 3H), 3.37 (q, 4H, *J* = 6.95 Hz), 6.65 (d, 2H, *J* = 8.74 Hz), 6.85 (d, 1H, *J* = 16.88 Hz), 6.98 (d, 1H, *J* = 15.70 Hz), 7.12 (d, 2H, *J* = 7.95 Hz), 7.36 (d, 4H, *J* = 7.75 Hz).
(E)-2,3,4-Trimethoxy-4'-methylstilbene (113). mp 109-110 °C; $^1$H NMR: δ 2.34 (s, 3H), 3.87 (s, 3H), 3.89 (s, 3H), 6.68 (d, 1H, *J* = 8.74 Hz), 7.00 (d, 1H, *J* = 16.48 Hz), 7.14 (d, 2H, *J* = 7.94 Hz), 7.27 (d, 1H, *J* = 16.88 Hz), 7.29 (d, 1H, *J* = 8.73 Hz), 7.40 (d, 2H, *J* = 8.14 Hz). Exact mass calcd for $C_{18}H_{20}O_3$: 284.1412, observed (M+H) 285.1492.
(E)-3,4,5-Trimethoxy-4'-methylstilbene (114). mp 126-127 °C[lit[36] 125-127 °C].

(E)-2,4,5-Trimethoxy-4'-methylstilbene (115). mp 84-85 °C; $^1$H NMR: δ 2.34 (s, 3H), 3.85 (s, 3H), 3.90 (s, 6H), 6.52 (s, 1H), 6.94 (d, 1H, *J* = 16.48 Hz), 7.12 (d, 3H, *J* = 9.73 Hz), 7.36 (d, 1H, *J* = 16.29 Hz), 7.41 (d, 2H, *J* = 7.94 Hz). Exact mass calcd for $C_{18}H_{20}O_3$: 284.1412, observed (M+) 284.1422.

(E)-1-(4-Methylstyryl)naphthalene (116). mp 92-94 °C [lit[37] 86-87 °C].

(E)-2-(4-Methylstyryl)naphthalene (117). mp 183-184 °C [lit[38] 189-190.5 °C].

(E)-4-Methylstyrylfuran (118). mp 74-75 °C [lit[39]]; $^1$H NMR: δ 2.37 (s, 3H), 6.34 (d, 1H, *J* = 3.18 Hz), 6.43 (m, 1H), 6.86 (d, 1H, *J* = 16.29 Hz), 7.04 (d, 1H, *J* = 15.89 Hz), 7.17 (d, 2H, *J* = 7.95 Hz), 7.38 (d, 3H, *J* = 8.34 Hz).

(E)-4-Methylstyrylthiophene (119). mp 116-117 °C [lit[22] 116 °C].

(E)-4-Cyano-4'-methylstilbene (120). mp 185-186 °C [lit[25] 182 °C].

(E)-4-Methyl-3-styrylpyridine (121). mp 109-110 °C [lit[40] 109.5-110 °C].

(E)-4-Methyl-2-styrylpyridine (122). mp 84-85 °C [lit[40] 84.5-85 °C].

(E)-4-Methyl-2',4',6'-trimethylstilbene (123). mp 48-50 °C [lit[41]]; $^1$H NMR: δ 2.28 (s, 3H), 2.33 (s, 6H), 2.36 (s, 3H), 6.54 (d, 1H, *J* = 16.68 Hz), 6.90 (s, 2H), 7.04 (d, 1H, *J* = 16.68 Hz), 7.17 (d, 2H, *J* = 7.94 Hz), 7.39 (d, 2H, *J* = 7.95 Hz).

(E)-2,6-Dimethoxy-4'-methylstilbene (124). mp 55-56 °C; $^1$H NMR: δ 2.29 (s, 3H), 3.82 (s, 6H), 6.52 (d, 2H, *J* = 8.54 Hz), 7.09 (m, 3H), 7.36 (d, 1H, *J* = 16.88 Hz), 7.38 (d, 2H, *J* = 6.75 Hz), 7.51 (d, 1H, *J* = 16.69 Hz). Exact mass calcd for $C_{17}H_{18}O_2$: 254.1307, observed (M+) 254.1315.

1-Methoxy-4-[2-(4-methylphenyl)ethyl]benzene (125). mp 59-60 °C [lit[42] 61-62.5 °C].

(E)-2-Fluoro-2'-methoxystilbene (126). mp 44-45 °C; $^1$H NMR: δ 3.73 (s, 3H), 7.28 (d, 1H, *J* = 16.88 Hz), 7.54 (d, 1H, *J* = 16.68 Hz), 6.88-7.29 (m, 6H), 7.60-7.69 (m, 2H). Exact mass calcd for $C_{15}H_{13}FO$: 228.0950, observed (M+) 228.0956.

(E)-4-N,N-Dimethylamino-3'-methoxystilbene (127). mp 93-94 °C [lit[43]]; $^1$H NMR: δ 2.97 (s, 6H), 3.83 (s, 3H), 6.70 (d, 2H, *J* = 8.94 Hz), 6.73 (dd, 1H, *J* = 8.94, 2.38 Hz), 6.87 (d, 1H, *J* = 16.29 Hz), 7.00 (s, 1H), 7.04 (d, 1H, *J* = 15.94 Hz), 7.05 (d, 1H, *J* = 8.15 Hz), 7.23 (t, 1H, *J* = 7.95 Hz), 7.39 (d, 2H, *J* = 8.93 Hz).

1-(4-Methoxyphenyl)-2-phenylethanone (128). mp 76-77 °C [lit[44] 77 °C].

1-(4-Trifluoromethylphenyl)-2-phenylethane (129). mp 40-42 °C[lit[45]].

1-(4-Methoxyphenyl)-2-(3,4-dimethoxyphenyl)ethanone (130). mp 137-138 °C [lit[46] 139 °C].

1-(3,4-Dimethoxyphenyl)-2-phenylethanone (131). mp 88-90 °C [lit[47] 86-88 °C].

1-(3-Trifluoromethylphenyl)-2-(4-methylphenyl)ethane (132). oil; $^1$H NMR: δ 2.32 (s, 3H), 2.91 (m, 4H), 7.04 (d, 2H, *J* = 8.34 Hz), 7.09 (d, 2H, *J* = 7.55 Hz), 7.30-7.45 (m, 4H). Exact mass calcd for $C_{16}H_{15}F_3$: 264.1126, observed (M+H) 265.1100.

N-Phenylbenzamide (133). mp 163-164 °C [lit[48] 164 °C].

N-(4-Chlorophenyl)benzamide (134). mp 193-194 °C [lit[49] 192-193 °C].

N-(4-Methylphenyl)benzamide (135). mp 157-158 °C [lit[49] 158-159 °C].

1-(4-Methylphenyl)-2-phenylethanone (136). mp 107-108 °C [lit [50] 106-108 °C].

N-(4-Methoxyphenyl)benzamide (137). mp 157-158 °C [lit[49] 157-158 °C].

1-(4-Chlorophenyl)-2-phenylethanone (138). mp 104-105 °C [lit[51] 105-105.5 °C].

1-(4-Bromophenyl)-2-phenylethanone (139). mp 111-112 °C [lit[52] 112-113 °C].

N-(2-Methylphenyl)benzamide (140). mp 142-143 °C [lit[53] 142-143 °C].

1-(4-Hydroxyphenyl)-2-phenylethanone (141). mp 149-150 °C [lit [2] 150 °C].

1-(3-Methylphenyl)-2-phenylethanone (142). mp 141-142 °C [lit [2] 143 °C].

1-(2-Fluorophenyl)-2-(3-methoxyphenyl)ethane (143). mp 39-40°C; $^1$H NMR: δ 2.90 (m, 4H), 3.76 (s, 3H), 6.72 (s, 1H), 6.73 (d, 1H, *J* = 6.95 Hz), 6.77 (d, 1H, *J* = 8.93Hz), 7.00 (t, 1H, *J* = 8.35 Hz), 7.02 (d, 1H, *J* = 7.55 Hz), 7.12 (t, 1H, *J* = 7.15 Hz), 7.14 (d, 1H, *J* = 7.85 Hz), 7.19 (t, 1H, *J* = 8.54 Hz).

(E)-2-Fluoro-3'-methoxystilbene (144). oil; $^1$H NMR: δ 3.84 (s, 3H), 6.83 (dd, 1H, *J* = 2.58, 8.14 Hz), 7.02-7.30 (m, 8H), 7.59 (t, 1H, *J* = 7.55 Hz). Exact mass calcd for $C_{15}H_{13}FO$: 228.0950, observed (M+) 228.0954.

(E)-2,4,6-Trimethoxy-4'-methylstilbene (145). mp 99-100 °C; $^1$H NMR: δ 2.33 (s, 3H), 3.82 (s, 3H), 3.87 (s, 6H), 6.16 (s, 2H), 7.10-7.30 (m, 2H), 7.36-7.42 (m, 4H). Exact mass calcd for $C_{18}H_{20}O_3$: 284.1412, observed (M+) 284.1422.

(E)-3-Fluoro-3'-methoxystilbene (146). oil; $^1$H NMR: δ 3.81 (s, 3H), 6.81 (dd, 1H, *J* = 8.14, 2.38 Hz), 7.03 (s, 2H), 6.89-7.29 (m, 7H). Exact mass calcd for $C_{15}H_{13}FO$: 228.0950, observed (M+) 228.0954.

(E)-3-Methoxy-3'-methoxystilbene (147). mp 98-99 °C [lit [60] 97 °C].

(E)-4-Isopropyl-3'-methoxystilbene (148). oil; $^1$H NMR: δ 1.26 (d, 6H, *J* = 6.75 Hz), 3.83 (s, 3H), 6.80 (d, 1H, *J* = Hz), 7.06 (d, 1H, *J* = Hz), 7.07 (s, 1H), 7.08 (d, 2H, *J* = 15.09 Hz), 7.21 (d, 2H, *J* = 7.75 Hz), 7.26 (t, 1H, *J* = 7.74 Hz), 7.44 (d, 2H, *J* = 8.14 Hz). Exact mass calcd for $C_{18}H_{20}O$: 252.1514, observed (M+) 252.1525.

(Z)-3-Methoxystilbene (149). oil [lit[61]].

(Z)-4-Methoxystilbene (150). oil [lit[62]].

(Z)-4-Methoxy-4'-methoxystilbene (151). oil [lit[5]].

(Z)-2,4-Dimethoxystilbene (152). oil [lit[9]].

(E)-3,5-Dimethoxy-3'-methoxystilbene (153). oil [lit[20]].

(E)-3,4-Dimethoxy-3'-methoxystilbene (154). mp 98-99 °C [lit[20] 145 °C]; $^1$H NMR: δ 3.84 (s, 3H), 3.89 (s, 3H), 3.94 (s, 3H), 6.79 (dd, 1H, *J* = 8.34, 2.18 Hz), 6.85 (d, 1H, *J* = 7.94 Hz), 6.94 (d, 1H, *J* = 16.68 Hz), 7.02-7.10 (m, 5H), 7.26 (t, 1H, *J* = 7.75 Hz).

(E)-2,4-Dimethoxy-3'-methoxystilbene (155). mp 54-55 °C; $^1$H NMR: δ 3.82 (s, 3H), 3.83 (s, 3H), 3.86 (s, 3H), 6.46 (d, 1H, *J* = 2.38 Hz), 6.51 (dd, 1H, *J* = 8.54, 2.39 Hz), 6.77 (dd, 1H, *J* = 7.15, 1.00 Hz), 6.97 (d, 1H, *J* = 16.48 Hz), 7.04 (d, 1H, *J* = 2.18 Hz), 7.10 (d, 1H, 8.70 Hz), 7.24 (t, 1H, *J* = 7.75 Hz), 7.38 (d, 1H, *J* = 16.28 Hz), 7.50 (d, 1H, *J* = 8.54 Hz). Exact mass calcd for $C_{17}H_{18}O_3$: 270.1256, observed (M+H) 271.1334.

(E)-4-Ethoxy-3'-methoxystilbene (156). mp 89-90 °C [lit[63] 86-87 °C].

(E)-3-Methoxy-3'-methylstilbene (157). mp 34°C; $^1$H NMR: δ 2.35 (s, 3H), 3.81 (s, 3H), 6.79 (dd, 1H), 7.05 (s, 2H), 7.03-7.09 (m, 3H), 7.24 (t, 1H), 7.25 (t, 1H), 7.29 (d, 1H, *J* = 5.75 Hz), 7.31 (s, 1H). Exact mass calcd for $C_{16}H_{16}O$: 224.1201, observed (M+) 224.1207.

(Z)-3-Fluorostilbene (158). oil [lit[64]].

(Z)-3-Fluoro-4'-methoxystilbene (159). oil; $^1$H NMR: δ 3.79 (s, 3H), 6.44 (d, 1H, *J* = 12.31 Hz), 6.57 (d, 1H, *J* = 12.11 Hz), 6.76 (d, 2H, *J* = 8.74 Hz), 6.81-7.08 (m, 3H), 7.16 (d, 2H, *J* = 8.94 Hz), 7.18 (t, 1H).

(Z)-4-Fluorostilbene (160). oil [lit [65]].

(E)-2-Methoxy-3'-methoxystilbene (161). mp 58-60 °C [lit [66]].

(Z)-2-Fluorostilbene (162). oil [lit[67]].

(E)-2,5-Dimethoxy-3'-methoxystilbene (163). mp 57-58°C; $^1$H NMR: δ 3.82 (s, 3H), 3.84 (s, 6H), 6.75-6.83 (m, 4H), 7.02 (d, 1H, *J* = 16.49 Hz), 7.02-7.30 (m, 4H), 7.46 (d, 1H, *J* = 16.48 Hz). Exact mass calcd for $C_{17}H_{18}O_3$: 270.1256, observed (M+H) 271.1339.

(E)-4-Trifluoromethyl-3'-methoxystilbene (164). mp 82-83 °C [lit [68]].

(E)-3,4,5-Trimethoxy-3'-methoxystilbene (165). mp 128-129 °C [lit[4] 123-125 °C].
(E)-2,3-Dimethoxy-3'-methoxystilbene (166). oil; $^1$H NMR: δ 3.85 (s, 6H), 3.87 (s, 3H), 6.82 (m, 3H), 7.04 (d, 1H, *J* = 16.08 Hz), 7.06 (d, 1H, *J* = 7.74 Hz), 7.14 (d, 1H, *J* = 7.55 Hz), 7.22 (d, 1H, *J* = 7.35 Hz), 7.28 (t, 1H, *J* = 7.54 Hz), 7.43 (d, 1H, *J* = 16.28 Hz). Exact mass calcd for $C_{17}H_{18}O_3$: 270.1256, observed (M+H) 271.1338.
(E)-1-(3,4-Methylenedioxyphenyl)-2-(4-methoxyphenyl)ethene (167). mp 143-144 °C [lit[70] 139-141 °C].
(Z)-1-(3,4-Methylenedioxyphenyl)-2-(3,5-dimethoxyphenyl)ethene (168). oil; $^1$H NMR: δ 3.67 (s, 6H), 5.88 (s, 2H), 6.32 (t, 1H, *J* = 2.18 Hz), 6.42 (s, 1H), 6.43 (s, 1H), 6.44 (s, 1H), 6.45 (s, 1H), 6.62-6.78 (m, 3H).
(Z)-2,3-Dimethoxy-2'-bromostilbene (169). mp 89-90 °C [lit[6] 88-92 °C].
(Z)-2,3-Dimethoxy-4'-trifluoromethylstilbene (170). mp 72-74 °C; $^1$H NMR: δ 3.87 (s, 3H), 3.89 (s, 3H), 6.84 (d, 1H, *J* = 8.25 Hz), 6.85 (d, 1H, *J* = 12.25 Hz), 7.07 (t, 1H, *J* = 7.75 Hz), 7.53 (d, 1H, *J* = 8.25 Hz), 7.60 (d, 2H, *J* = 7.25 Hz), 7.62 (d, 2H, *J* = 7.25 Hz).
(Z)-4-Methoxy-3'-bromostilbene (171). oil; $^1$H NMR: δ 3.74 (s, 3H), 6.37 (d, 1H, *J* = 12.31 Hz), 6.54 (d, 1H, *J* = 12.11 Hz), 6.73 (d, 2H, *J* = 8.74 Hz), 7.04 (t, 1H, *J* = 7.72 Hz), 7.27 (d, 1H), 7.15 (m, 3H), 7.40 (s, 1H). Exact mass calcd for $C_{15}H_{13}BrO$: 288.0150, observed (M+) 288.0156.
(Z)-4-Methoxy-4'-bromostilbene (172). oil [lit[71]].
(Z)-4-Trifluoromethylstilbene (173). oil [lit[5]].
(Z)-2,3,4-Trimethoxy-2'-bromostilbene (174). mp 78-79 °C [lit[72]].
(E)-2,6-Dimethoxy-2'-bromostilbene (175). mp 88-90 °C; $^1$H NMR: δ 3.91 (s, 6H), 6.59 (d, 2H, *J* = 8.34 Hz), 7.06 (t, 1H, *J* = 7.75 Hz), 7.17 (t, 1H, *J* = 8.34 Hz), 7.28 (t, 1H, *J* = 7.94 Hz), 7.39 (d, 1H, *J* = 16.48 Hz), 7.55 (d, 1H, *J* = 7.94 Hz), 7.72 (d, 1H, *J* = 7.94 Hz), 7.95 (d, 1H, *J* = 16.48 Hz). Exact mass calcd for $C_{16}H_{15}BrO_2$: 318.0255, observed (M+H) 319.0331.
(Z)-2-Trifluoromethylstilbene (176). oil [lit[57]].
(Z)-2-Trifluoromethyl-4'-methoxystilbene (177). oil [lit[29]]
(E)-4-Methoxy-3'-nitrostilbene (178). mp 92-93 °C [lit[62] 87.5-89 °C].
(E)-4-Methoxy-4'-nitrostilbene (179). mp 131-132 °C [lit[14] 133-134 °C].
(E)-2-Trifluoromethyl-3'-methoxystilbene (180). oil [lit[29]].
(E)-3-Nitrostilbene (181). mp 110-111 °C [lit[73] 102-105 °C].
(E)-4-Nitrostilbene (182). mp 156-157 °C [lit[74] 156-157 °C].
(E)-4-Methyl-3'-nitrostilbene (183). mp 98-99 °C [lit[75] 99-100 °C].
(E)-4-Methyl-4'-nitrostilbene (184). mp 147-148 °C [lit[14] 150 °C].
(E)-2,6-Dichloro-4'-methylstilbene (185). mp 69-70 °C; $^1$H NMR: δ 2.36 (s, 3H), 7.04 (d, 1H, *J* = 16.49 Hz), 7.06 (t, 1H, *J* = 7.75 Hz), 7.11 (s, 1H), 7.18 (d, 2H, *J* = 7.55 Hz), 7.32 (d, 2H, *J* = 8.14 Hz), 7.43 (d, 2H, *J* = 7.75 Hz). Exact mass calcd for $C_{15}H_{12}Cl_2$: 262.0316, observed (M+) 262.0311.
(E)-4-Methyl-2'-nitrostilbene (186). mp 29-30 °C [lit[27] 31 °C].

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