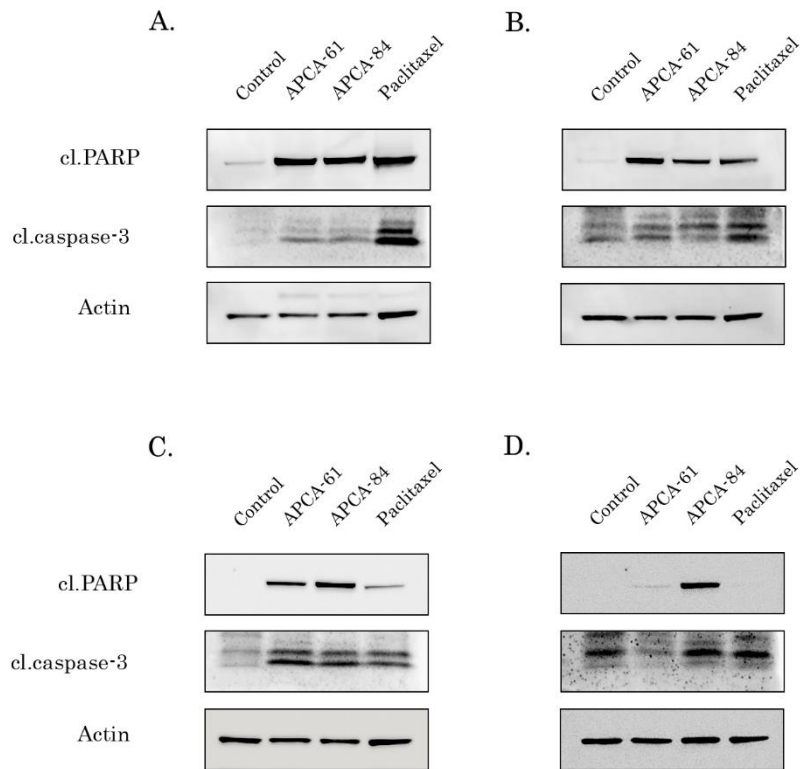
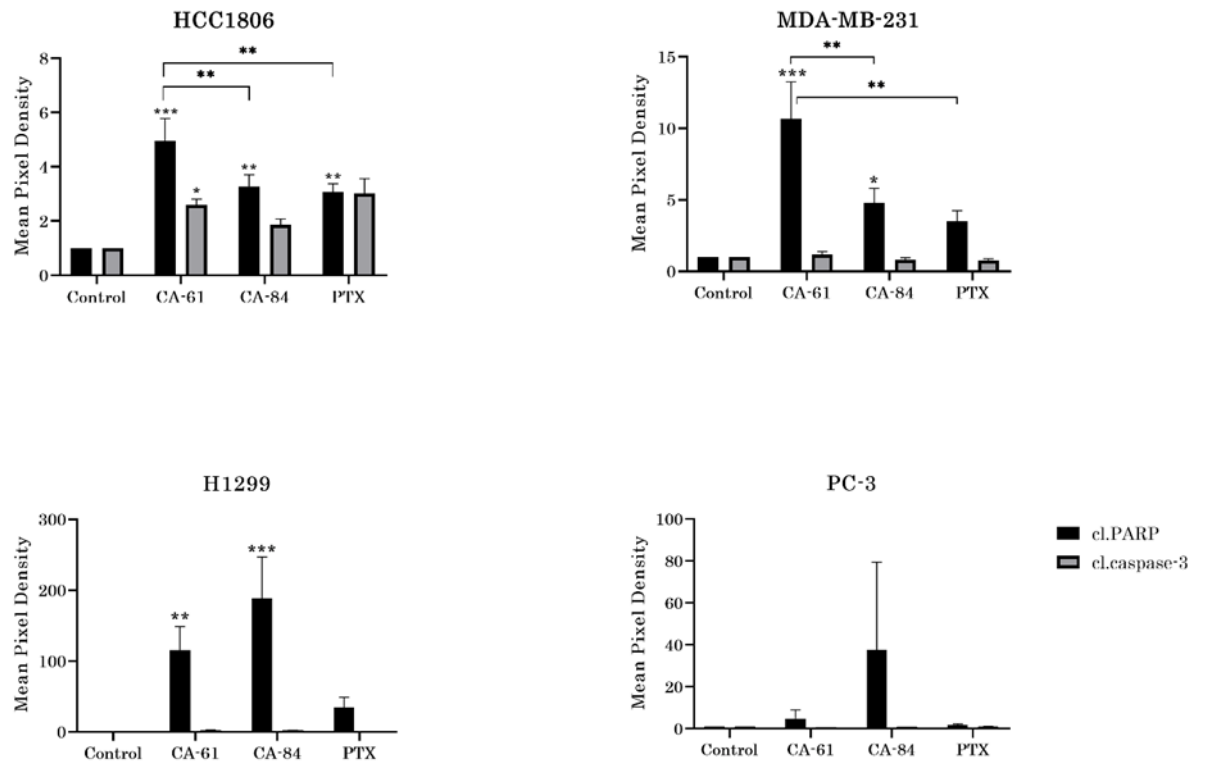


Supplementary Figure 1. Densitometry analysis of cleaved PARP and caspase-3 in cancer cell lines treated with CAs and Vin. bars, SD. * $p < 0.05$; ** $p < 0.01$.



Supplementary Figure 2. CA-61 and 84 induce apoptosis of epithelial cancer cell lines. Immunoblot analysis for apoptosis markers (cleaved forms of PARP and caspase-3) in HCC1806 breast cancer (A), MDA-MB-231 breast cancer (B), H1299 lung cancer (C), and PC-3 prostate cancer (D) cells after treatment with DMSO (negative control), CA-61, -84 (10 μ M), and Paclitaxel (0.1 μ M) for 48 h. Actin stain is used as a loading control.



Supplementary Figure 3. Densitometry analysis of cleaved PARP and caspase-3 in cancer cell lines (as shown in Supplementary Figure 2) treated with CAs and PTX. bars, SD. ** p < 0.05; *** p < 0.01.

Ethyl 2-amino-1-(2-methyl-5-nitrophenyl)-4-oxo-5-(2-oxo-2-phenylethylidene)-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-33).

IR spectre, ν , cm^{-1} : 3304 (NH), 1697 (COOEt), 1648, 1600 (C=O, C=C). NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.10 t (3H, CMe), 2.24 s (3H, Me), 3.99 q (2H, CH₂), 5.40 s (1H, CH), 7.80 m (8H, Ar), 8.24 s (1H, NH), 8.32 s (1H, NH).

Ethyl 2-amino-1-(2-methyl-5-nitrophenyl)-4-oxo-5-(2-oxo-2-(p-tolyl)ethylidene)-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-208).

IR spectre, ν , cm^{-1} : 3303, 3168 (NH), 1672 (COOEt), 1646, 1608 (C=O, C=C). NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.09 t (3H, C-Me), 2.25 s (3H, Me), 2.28 s (3H, Me), 3.92 q (2H, CH₂), 5.34 s (1H, CH), 7.80 m (7H, Ar), 8.24 s (1H, NH), 8.34 s (1H, NH).

Ethyl 2-amino-5-(2-(4-chlorophenyl)-2-oxoethylidene)-1-(2-methyl-5-nitrophenyl)-4-oxo-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-59).

IR spectre, ν , cm^{-1} : 3296, 3172 (NH), 1670 (COOEt), 1650, 1596 (C=O, C=C). NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.16 t (3H, C-Me), 2.29 s (3H, Me), 4.00 q (2H, CH₂), 5.43 s (1H, CH), 7.80 m (7H, Ar), 8.34 s (1H, NH), 8.40 s (1H, NH).

Ethyl 2-amino-5-(2-(2,4-dimethylphenyl)-2-oxoethylidene)-1-(2-methyl-5-nitrophenyl)-4-oxo-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-166).

IR spectre, ν , cm^{-1} : 3296 (NH), 1676 (COOEt), 1650, 1612 (C=O, C=C). NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.16 t (3H, CMe), 2.26 s (3H, Me), 2.26 s (3H, Me), 2.26 s (3H, Me), 4.0 q (2H, CH₂), 5.43 s (1H, CH), 7.80 m (8H, Ar), 8.32 s (1H, NH), 8.40 s (1H, NH).

Ethyl 2-amino-1-(2-methyl-5-nitrophenyl)-5-(2-(naphthalen-1-yl)-2-oxoethylidene)-4-oxo-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-90).

IR spectre, ν , cm^{-1} : 3288, 3216 (NH), 1676 (COOEt), 1646, 1612 (C=O, C=C). NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.10 t (3H, C-Me), 2.31 s (3H, Me), 4.02 q (2H, CH₂), 5.71 s (1H, CH), 7.90 m (10H, Ar), 8.73 s (1H, NH), 8.80 s (1H, NH).

Ethyl 2-amino-1-(4-bromophenyl)-5-(3,3-dimethyl-2-oxobutyl)-4-oxo-5-(phenylthio)-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-1474I)

NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.80 s (9H, t-Bu), 1.17 t (3H, CH₂CH₃, J 7.0 Hz), 2.95 d (2H, CH₂, J 18.6 Hz), 3.18 d (2H, CH₂, J 18.6 Hz), 4.04 m (2H, CH₂CH₃), 7.46 m (9Har+1H, NH), 7.80 widened s (1H, NH).

Ethyl 2-amino-1-(4-bromophenyl)-5-((4-chlorophenyl)thio)-5-(3,3-dimethyl-2-oxobutyl)-4-oxo-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-1488I)

NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.80 s (9H, t-Bu), 1.17 t (3H, CH₂CH₃, J 7.0 Hz), 2.97 d (2H, CH₂, J 18.6 Hz), 3.19 d (2H, CH₂, J 18.6 Hz), 4.08 m (2H, CH₂CH₃), 7.48 m (8Har+1H, NH), 7.82 widened s (1H, NH).

2-amino-1-(4-bromophenyl)-5-((4-chlorophenyl)thio)-5-(3,3-dimethyl-2-oxobutyl)-4-oxo-4,5-dihydro-1H-pyrrole-3-carboxamide (CA-1489I)

NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.80 s (9H, t-Bu), 3.04 d (2H, CH₂, J 18.6 Hz), 3.22 d (2H, CH₂, J 18.6 Hz), 6.62 widened s (1H, NH), 7.12 widened s (1H, NH), 7.48 m (8Har), 7.83 widened s (1H, NH), 8.23 widened s (1H, NH).

Ethyl 2-amino-1-(4-chlorophenyl)-5-(3,3-dimethyl-2-oxobutylidene)-4-oxo-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-1453I)

NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.06 s (9H, *t*-Bu), 1.21 t (3H, Me, J 7.1 Hz), 4.14 q (2H, CH_2 , J 7.1 Hz), 5.44 s (1H, CH), 7.45 d (2H_{ar}, J 8.4 Hz), 7.64 d (2H_{ar}, J 8.4 Hz), 8.09 widened s (1H, NH), 8.15 widened s (1H, NH).

Amino-1-benzamido-5-(3,3-dimethyl-2-oxobutylidene)-4-oxo-N-(p-tolyl)-4,5-dihydro-1H-pyrrole-3-carboxamide (CA-1265I)

NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.98 s (9H, *t*-Bu), 2.28 s (3H, Me), 6.51 s (1H, CH), 7.14 d (2H, ar., J 8.1 Hz), 7.50 d (2H, ar., J 8.1 Hz), 7.57 m (3H, ar.), 7.94 d (2H, ar., J 7.5 Hz), 8.77 widened s (1H, NH), 9.39 s (1H, NH), 9.99 s (1H, NH), 10.94 s (1H, NH).

Ethyl-2-amino-5-(3,3-dimethyl-2-oxobutylidene)-1-(2-hydroxybenzamido)-4-oxo-4,5-dihydro-1H-pyrrole-3-carboxylate (CA-1348I)

NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.93 s (9H, *t*-Bu), 1.24 t (3H, Me, J 7.1 Hz), 4.18 q (2H, CH_2 , J 7.1 Hz), 6.33 s (1H, CH), 7.36 m (4H, ar.), 8.38 widened s (1H, NH), 9.05 s (1H, NH), 10.65 s (1H, OH), 11.35 s (1H, NH).

2-Amino-5-(3,3-dimethyl-2-oxobutylidene)-1-(2,2-diphenylvinyl)-4-oxo-4,5-dihydro-1H-pyrrole-3-carbonitrile (CA-23)

NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.93 s (9H, *t*-Bu), 5.93 s (1H, CH), 7.51 m (7H_{ar}), 7.64 m (3H_{ar}), 8.73 widened s (1H, NH₂), 9.09 widened s (1H, NH₂).

CA-610I NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.91 s (*t*-Bu), 1.23 t (3H, CMe), 2.40 s (3H, Me), 4.21 q (2H, CH_2), 6.32 s (1H, CH), 7.32 d (2H, Ar), 7.83 d (2H, Ar), 8.44 s (1H, NH), 9.20 s (1H, NH), 10.86 s (1H, NH).

CA-1296I NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.83 s (9H, *t*-Bu), 1.23 t (3H, CH_2CH_3 , J 7.1 Hz), 2.74 d (2H, CH_2 , J 18.7 Hz), 3.11 d (2H, CH_2 , J 18.7 Hz), 4.14 q (2H, CH_2CH_3 , J 7.1 Hz), 7.52 m (8H_{ar}, 1H, NH), 7.83 widened s (1H, NH), 8.03 widened s (1H, NH), 9.60 d (1H, NH, J 5.0 Hz).

CA-1283I NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.82 s (9H, *t*-Bu), 1.25 t (3H, CH_2CH_3 , J 7.1 Hz), 2.62 d (2H, CH_2 , J 18.7 Hz), 3.05 d (2H, CH_2 , J 18.7 Hz), 3.16 s (3H, OCH₃), 4.15 q (2H, CH_2CH_3 , J 7.1 Hz), 7.06 d (2H_{ar}, J 8.6 Hz), 7.7 d (2H_{ar}, J 8.6 Hz), 8.17 widened s (1H, NH), 8.22 widened s (1H, NH).

CA -1282I NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.89 s (9H, *t*-Bu), 1.23 t (3H, CH_2CH_3 , J 7.0 Hz), 2.80 d (2H, CH_2 , J 18.7 Hz), 3.27 d (2H, CH_2 , J 18.7 Hz), 3.46 d (2H, CH_2 , J 14.4 Hz), 3.62 d (2H, CH_2 , J 14.4 Hz), 4.14 d (2H, CH_2CH_3 , J 7.0 Hz), 7.35 m (9H_{ar}), 7.94 widened s (2H, 2NH), 10.07 widened s (1H, NH)

CA -1288I NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.89 s (9H, *t*-Bu), 2.84 s (2H, CH_2 , J 18.6 Hz), 3.28 d (2H, CH_2 , J 18.6 Hz), 3.42 d (2H, CH_2 , J 14.4 Hz), 3.58 d (2H, CH_2 , J 14.4 Hz), 6.81 widened s (1H, NH), 7.38 m (9H_{ar}+1H, NH), 8.51 widened s (1H, NH), 7.88 widened s (1H, NH), 10.11 s (1H, NH)

CA -1519I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.22 t (3H, CH_2CH_3 , J 7.0 Hz), 4.16 q (2H, CH_2CH_3 , J 7.0 Hz), 6.75 s (CH), 7.35 m (12H_{ar}), 8.38 s (1H, NH), 9.09 widened s (1H, NH), 10.93 s (1H, NH),

CA -581I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.18 t (3H, CH_2CH_3 , J 7.1 Hz), 4.15 q (2H, CH_2CH_3 , J 7.1 Hz), 6.64 s (CH), 7.54 m (7H_{ar}), 8.48 s (1H, NH), 8.62 m (2H_{ar}), 9.20 s (1H, NH), 11.31 s (1H, NH).

CA -1222I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.06 s (9H, *t*-Bu), 2.24 s (3H, Me), 5.54 s (1H, CH), 7.77 d (1H_{ar}, J 8.4 Hz), 8.18 widened s (1H, NH), 8.34 m (2H_{ar}), 8.96 widened s (1H, NH)

CA -26 NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.07 s (9H, *t*-Bu), 1.24 t (3H, CH_2CH_3 , J 7.0 Hz), 4.17 q (2H, CH_2CH_3 , J 7.0 Hz), 5.22 s (1H, CH), 7.70 m (4H_{ar}), 8.12 widened s (1H, NH), 8.26 s (1H, NH).

CA -46 NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.08 s (9H, *t*-Bu), 1.25 t (3H, Me, *J* 7.4 Hz), 4.05 q (2H, CH₂, *J* 7.4 Hz), 5.02 s (1H, CH), 7.23-8.12 m (6H, Ar+NH₂).

CA -20 NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.98 s (9H, *t*-Bu), 1.21 t (3H, Me, *J* 7.2 Hz), 4.03 q (2H, CH₂, *J* 7.2 Hz), 5.31 s (1H, CH), 7.49-7.85 m (3H_{ar}), 8.04 widened s (1H, NH), 8.26 widened s (1H, NH).

CA -28 NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.05 s (9H, *t*-Bu), 1.21 t (3H, Me, *J* 7.3 Hz), 4.09 q (2H, CH₂, *J* 7.3 Hz), 5.32 s (1H, CH), 7.42-8.28 m (5H, Ar+NH₂).

CA -631I NMR ^1H spectra (DMSO- d_6), δ , ppm: 0.99 s (9H, *t*-Bu), 1.16 t (3H, Me, *J* 7.3 Hz), 4.05 q (2H, CH₂, *J* 7.3 Hz), 5.31 s (1H, CH), 7.57-8.2 m (5H, Ar+NH₂).

CA -959I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.09 s (9H, *t*-Bu), 2.24 s (3H, Me), 5.69 s (1H, CH), 7.71 m (5H_{ar}), 8.46 s (1H, NH), 8.63 s (1H, NH), 11.21 s (1H, NH).

CA -915I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.15 s (9H, *t*-Bu), 5.79 s (1H, CH), 7.36 m (8H_{ar}), 8.10 widened s (1H, NH), 9.05 s (1H, NH), 11.45 s (1H, NH).

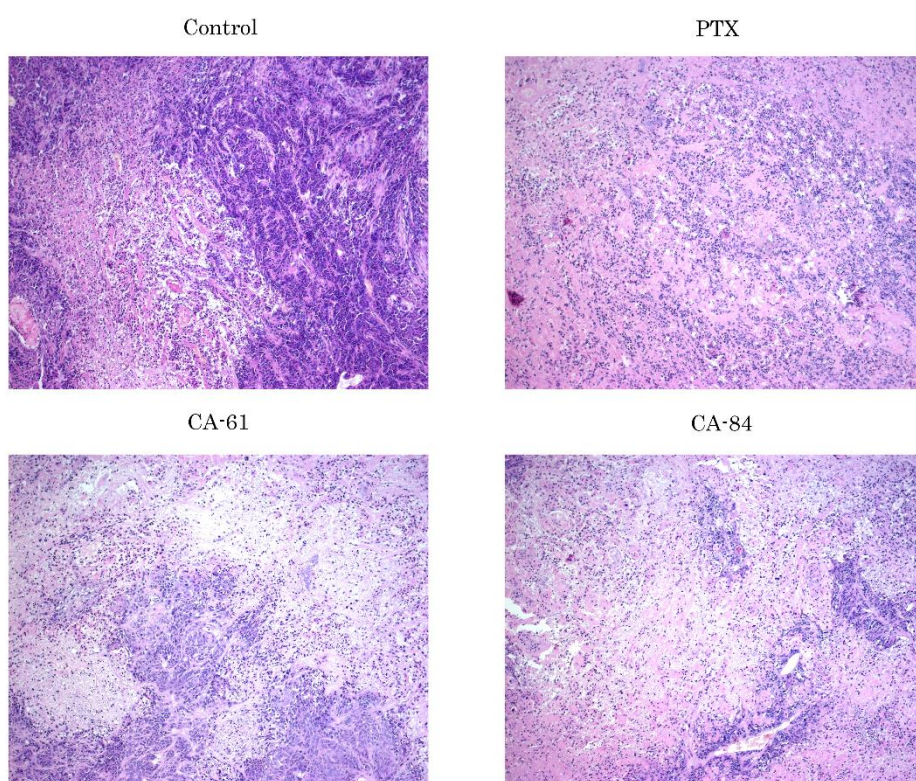
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CA -958I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.16 s (9H, *t*-Bu), 5.87 s (1H, CH), 7.23 m (8H_{ar}), 8.27 widened s (1H, NH), 11.24 s (1H, NH), 11.47 s (1H, NH).

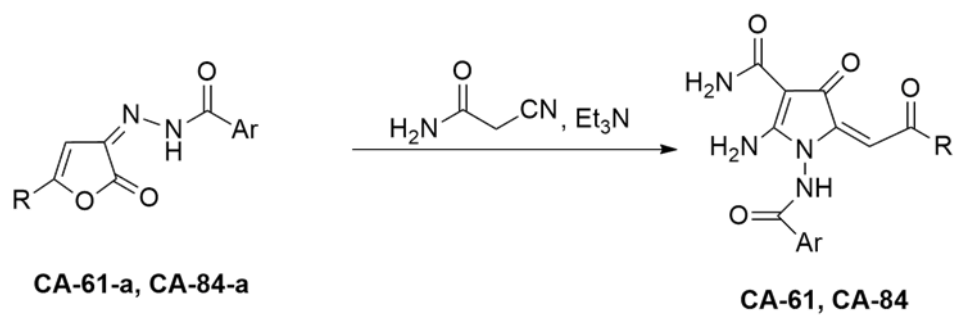
CA -974I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.07 s (9H, *t*-Bu), 5.72 s (1H, CH), 7.67 m (5H_{ar}), 8.53 s (1H, NH), 8.80 s (1H, NH), 11.33 widened s (1H, NH).

CA -1473I NMR ^1H spectra (DMSO- d_6), δ , ppm: 1.61 t (3H, Me, *J* 7.1 Hz), 4.23 q (2H, CH₂, *J* 7.1 Hz), 6.70 s (1H, CH), 7.62 m (7H_{ar}), 8.47 m (1H_{ar}), 8.73 m (1H_{ar}), 8.90 widened s (1H, NH), 9.16 widened s (1H, NH), 11.20 s (1H, NH).

Supplementary Figure 4. Spectra characteristics of CAs.



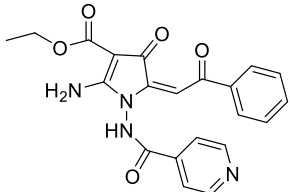
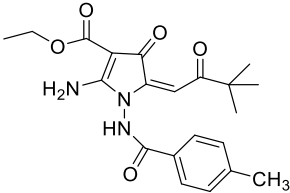
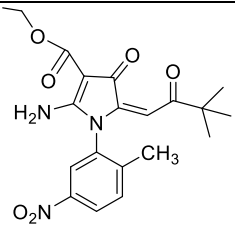
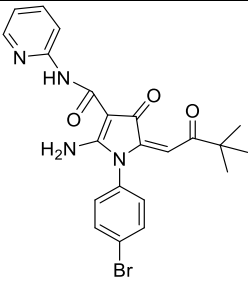
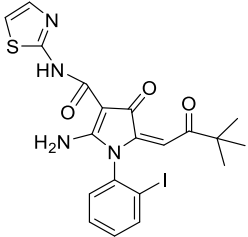
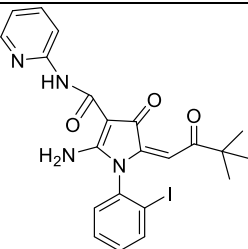
Supplementary Figure 5. Representative images of the HCC1806 xenografts treated with a solvent (control), paclitaxel (PTX), CA-61, and -84.

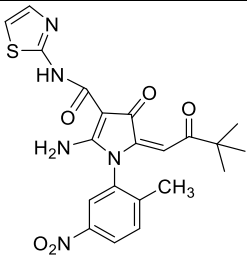
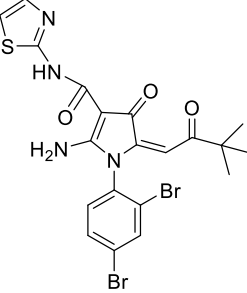
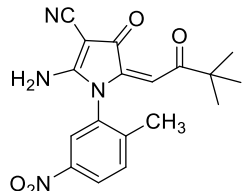
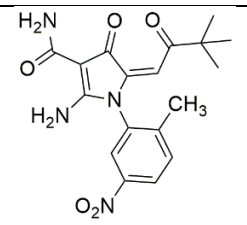
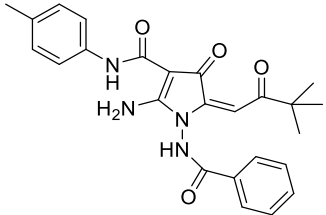
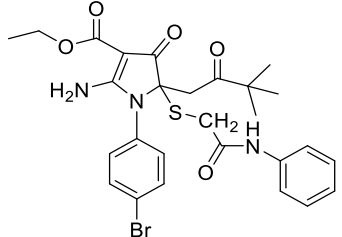


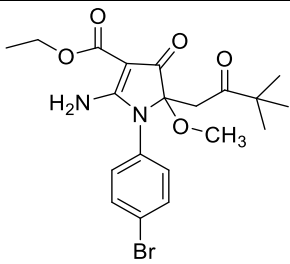
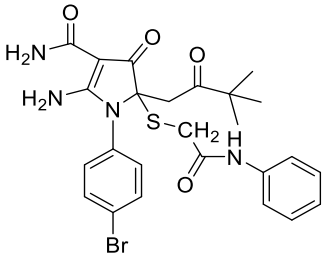
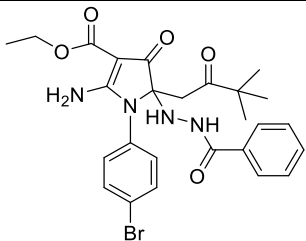
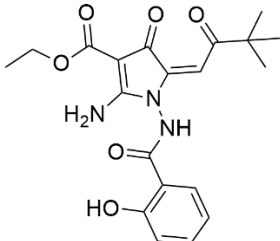
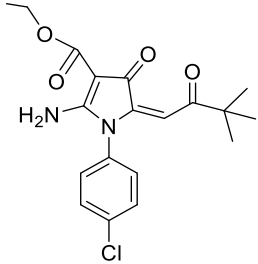
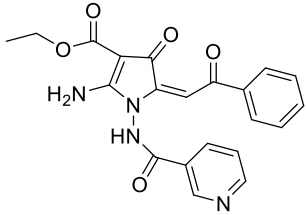
Ar = C₆H₅ (CA-61-a, CA-61), 2-C₆H₅NHC₆H₄ (CA-84-a, CA-84);
 R = naphthalen-2-yl (CA-61-a, CA-61), t-Bu (CA-84-a, CA-84)

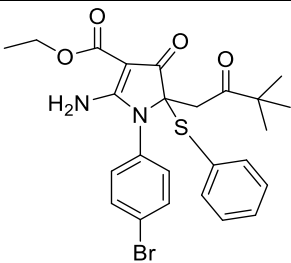
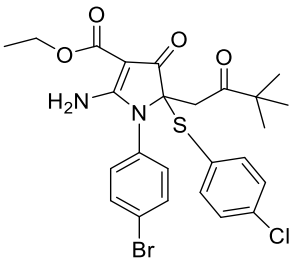
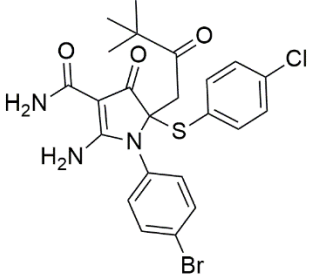
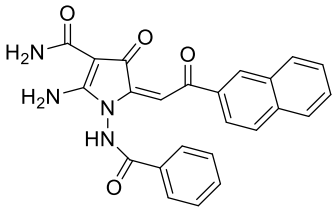
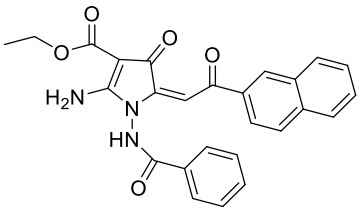
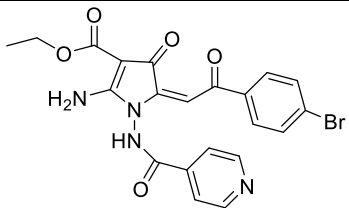
Supplementary Scheme 1. Synthetic pathway of the derivatives of 2-aminopyrrole

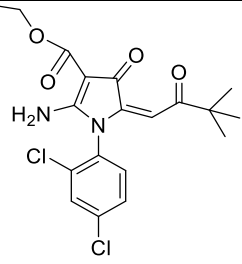
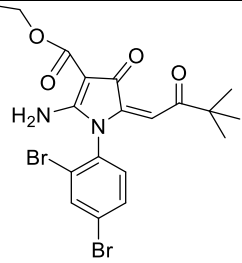
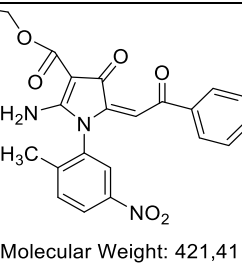
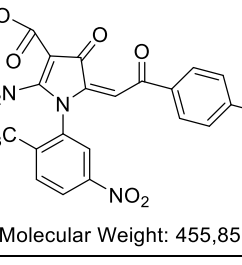
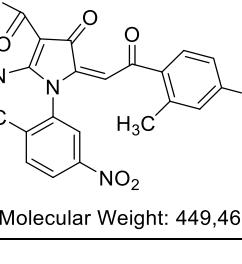
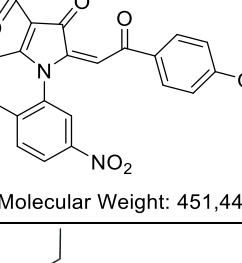
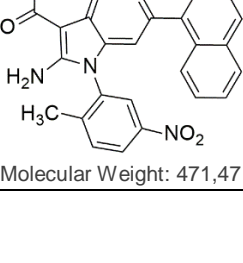
Supplementary Table 1. Characteristics of pyrrole-based compounds and IC₅₀ values in MDA-MB-231 breast cancer cell line

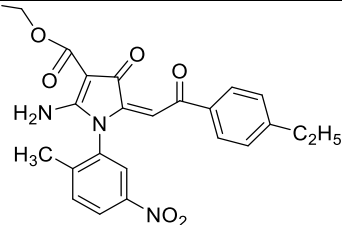
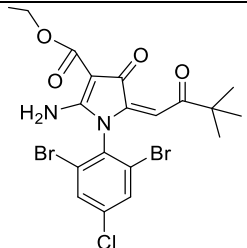
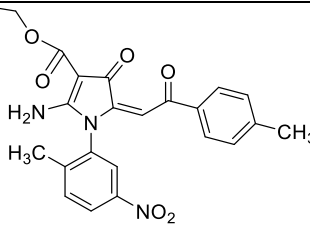
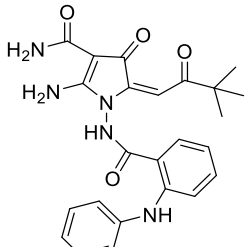
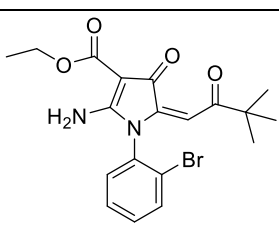
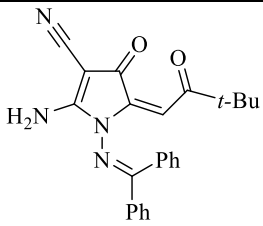
| Nº | Structure and molecule weight | Brutto formula | Abbreviation | IC ₅₀ (µM) |
|----|---|--|--------------|-----------------------|
| 1 |  <p>Molecular Weight: 406,40</p> | C ₂₁ H ₁₈ N ₄ O ₅ | CA-581I | >100 |
| 2 |  <p>Molecular Weight: 399,45</p> | C ₂₁ H ₂₅ N ₃ O ₅ | CA-610I | 66 ± 5.2 |
| 3 |  <p>Molecular Weight: 401,42</p> | C ₂₀ H ₂₃ N ₃ O ₆ | CA-631I | >100 |
| 4 |  <p>Molecular Weight: 469,34</p> | C ₂₂ H ₂₁ BrN ₄ O ₃ | CA-915I | >100 |
| 5 |  <p>Molecular Weight: 522,36</p> | C ₂₀ H ₁₉ IN ₄ O ₃ S | CA-957I | 76.7 ± 3.9 |
| 6 |  <p>Molecular Weight: 516,34</p> | C ₂₂ H ₂₁ IN ₄ O ₃ | CA-958I | >100 |

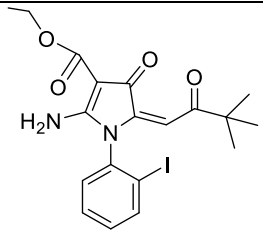
| | | | | |
|----|---|---------------------------|----------|-----------------|
| 7 |  <p>Molecular Weight: 455,49</p> | $C_{21}H_{21}N_5O_5S$ | CA-959I | >100 |
| 8 |  <p>Molecular Weight: 554,26</p> | $C_{20}H_{18}Br_2N_4O_3S$ | CA-974I | 82.9 ± 18.5 |
| 9 |  <p>Molecular Weight: 354,37</p> | $C_{18}H_{18}N_4O_4$ | CA-1222I | >100 |
| 10 |  <p>Molecular Weight: 372,38</p> | $C_{18}H_{20}N_4O_5$ | CA-1223I | >100 |
| 11 |  <p>Molecular Weight: 446,51</p> | $C_{25}H_{26}N_4O_4$ | CA-1265I | 40 ± 7.8 |
| 12 |  <p>Molecular Weight: 588,52</p> | $C_{27}H_{30}BrN_3O_5S$ | CA-1282I | >100 |

| | | | | |
|----|---|-------------------------|----------|----------------|
| 13 |  <p>Molecular Weight: 453,33</p> | $C_{20}H_{25}BrN_2O_5$ | CA-1283I | >100 |
| 14 |  <p>Molecular Weight: 559,48</p> | $C_{25}H_{27}BrN_4O_4S$ | CA-1288I | >100 |
| 15 |  <p>Molecular Weight: 557,45</p> | $C_{26}H_{29}BrN_4O_5$ | CA-1296I | >100 |
| 16 |  <p>Molecular Weight: 401,42</p> | $C_{20}H_{23}N_3O_6$ | CA-1348I | 21.3 ± 4 |
| 17 |  <p>Molecular Weight: 376,84</p> | $C_{19}H_{21}ClN_2O_4$ | CA-1453I | 58.7 ± 3.2 |
| 18 |  <p>Molecular Weight: 406,40</p> | $C_{21}H_{18}N_4O_5$ | CA-1473I | 87.3 ± 5.9 |

| | | | | |
|----|---|---------------------------|----------|----------------|
| 19 |  <p>Molecular Weight: 531,47</p> | $C_{25}H_{27}BrN_2O_4S$ | CA-1474I | 57.1 ± 6.6 |
| 20 |  <p>Molecular Weight: 565,91</p> | $C_{25}H_{26}BrClN_2O_4S$ | CA-1488I | 18.5 ± 0.5 |
| 21 |  <p>Molecular Weight: 536,87</p> | $C_{23}H_{23}BrClN_3O_3S$ | CA-1489I | 13 ± 0.4 |
| 22 |  <p>Molecular Weight: 426,43</p> | $C_{24}H_{18}N_4O_4$ | CA-61 | 3.2 ± 0.3 |
| 23 |  <p>Molecular Weight: 455,47</p> | $C_{26}H_{21}N_3O_5$ | CA-1519I | >100 |
| 24 |  <p>Molecular Weight: 485,29</p> | $C_{21}H_{17}BrN_4O_5$ | CA-1573I | >100 |

| | | | | |
|----|---|--------------------------|-------|----------------|
| 25 |  <p>Molecular Weight: 411,28</p> | $C_{19}H_{20}Cl_2N_2O_4$ | CA-20 | >100 |
| 26 |  <p>Molecular Weight: 500,19</p> | $C_{19}H_{20}Br_2N_2O_4$ | CA-28 | >100 |
| 27 |  <p>Molecular Weight: 421,41</p> | $C_{22}H_{19}N_3O_6$ | CA-33 | 54.1 ± 5.1 |
| 28 |  <p>Molecular Weight: 455,85</p> | $C_{22}H_{18}ClN_3O_6$ | CA-59 | 6.2 ± 0.2 |
| 29 |  <p>Molecular Weight: 449,46</p> | $C_{24}H_{23}N_3O_6$ | CA-60 | 33 ± 3.7 |
| 30 |  <p>Molecular Weight: 451,44</p> | $C_{23}H_{21}N_3O_7$ | CA-68 | 80.7 ± 8.8 |
| 31 |  <p>Molecular Weight: 471,47</p> | $C_{26}H_{21}N_3O_6$ | CA-90 | 30.3 ± 2.7 |

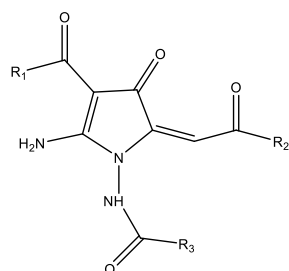
| | | | | |
|----|---|----------------------------|--------|----------------|
| 32 |  <p>Molecular Weight: 449,46</p> | $C_{24}H_{23}N_3O_6$ | CA-166 | 5.1 ± 0.7 |
| 33 |  <p>Molecular Weight: 534,63</p> | $C_{19}H_{19}Br_2ClN_2O_4$ | CA-174 | 83 ± 5.4 |
| 34 |  <p>Molecular Weight: 435,44</p> | $C_{23}H_{21}N_3O_6$ | CA-208 | 38.2 ± 4.8 |
| 35 |  <p>Molecular Weight: 447,50</p> | $C_{24}H_{25}N_5O_4$ | CA-84 | 4.8 ± 0.6 |
| 36 |  <p>Molecular Weight: 421,29</p> | $C_{19}H_{21}BrN_2O_4$ | CA-26 | >100 |
| 37 |  <p>Molecular Weight: 398,47</p> | $C_{24}H_{22}N_4O_2$ | CA-23 | 34.9 ± 7.2 |

| | | | | |
|----|---|-----------------------|-------|------|
| 38 |  <p data-bbox="414 392 678 425">Molecular Weight: 468,29</p> | $C_{19}H_{21}IN_2O_4$ | CA-46 | >100 |
|----|---|-----------------------|-------|------|

Supplementary Table 2. *Structure-activity relationship (SAR)-based analysis of the features of the molecules in the dataset with observed activities.*

Group I

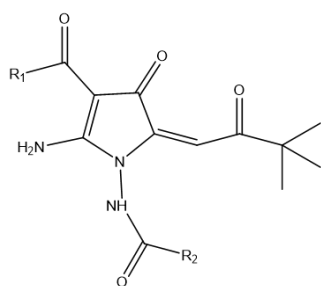
Core of structures



| Compound | R1 | R2 | R3 | IC ₅₀ |
|----------|----|----|----|------------------|
| CA-61 | | | | 3.2 |
| CA-1519I | | | | >100 |
| CA-1573I | | | | >100 |

Group II

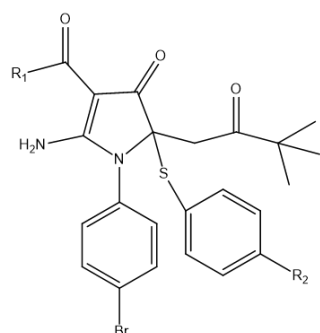
Core of structures



| Compound | R1 | R2 | IC ₅₀ |
|----------|----|----|------------------|
| CA-84 | | | 4.8 |
| CA-1348I | | | 21.3 |
| CA-610I | | | 66 |

Group III

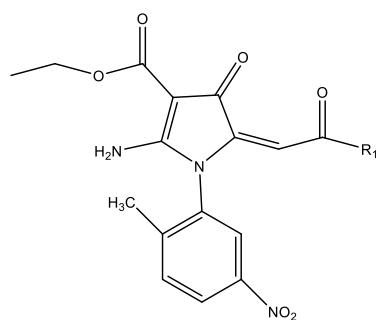
Core of structures



| Compound | R1 | R2 | IC ₅₀ |
|----------|----|----|------------------|
| CA-1489I | | | 13 |
| CA-1488I | | | 18.5 |
| CA-1474I | | | 57.1 |

Group IV

Core of structures



| Compound | R1 | IC ₅₀ |
|----------|----|------------------|
| CA-166 | | 5.1 |
| CA-59 | | 6.2 |
| CA-90 | | 30.3 |
| CA-60 | | 33.7 |
| CA-208 | | 38.2 |
| CA-33 | | 54.1 |
| CA-68 | | 80.7 |

