Supplementary Table 1. List of target protein abbreviations, full names, and functions corresponding to Figure 1C.

Note: Protein information is derived from the UniProt database *(*https://www.uniprot.org/*)*.

Abbreviation	Full Name	Function
CDK1	Cyclin-dependent kinase 1	Regulates G2/M transition, phosphorylates substrates for centrosome separation, Golgi dynamics, nuclear envelope breakdown, chromosome condensation; involved in oocyte maturation and follicle development.
MMP12	Matrix metallopeptidase 12	Degrades soluble and insoluble elastin; participates in extracellular matrix remodeling during ovulation and ovarian tissue remodeling.
DRD2	Dopamine receptor D2	G protein-coupled receptor; inhibits adenylate cyclase; involved in neuroendocrine regulation of hypothalamic-pituitary-ovarian axis.
EGFR	Epidermal growth factor receptor	Transmembrane protein; activates intracellular signaling promoting cell proliferation and survival; crucial for follicle development and granulosa cell proliferation.
CYP1B1	Cytochrome P450 family 1 subfamily B member 1	Endoplasmic reticulum enzyme; metabolizes polycyclic aromatic hydrocarbons and 17β-estradiol; involved in procarcinogen activation.
NR1I2	Nuclear receptor subfamily 1 group I member 2 (PXR)	Nuclear receptor; regulates expression of drug-metabolizing enzymes and transporters.
HDAC9	Histone deacetylase 9	Histone deacetylase; represses transcription by recruiting multi-protein complex to MEF2; regulates gene expression.
CXCR1	C-X-C motif chemokine receptor 1	G protein-coupled receptor; high-affinity receptor for IL-8; mediates chemotactic signals.
CNR1	Cannabinoid receptor 1	G protein-coupled receptor; involved in retrograde neural signaling.
MAOA	Monoamine oxidase A	Degrades neurotransmitters such as dopamine, norepinephrine, and serotonin.
CSK	C-terminal Src kinase	Negative regulator of Src family kinases; involved in cell signal transduction.
TOP1	DNA topoisomerase I	Regulates DNA supercoiling; relaxes supercoiled DNA during transcription and replication.

ESR2	Estrogen receptor 2 (ERβ)	Nuclear receptor; mediates physiological effects of estrogen.
MMP9	Matrix metalloproteinase 9	Degrades extracellular matrix components; involved in tissue remodeling during ovulation, corpus luteum formation and regression.
TOP2A	DNA topoisomerase II alpha	Regulates DNA topology; participates in DNA replication and chromosome segregation; affects cell proliferation.
FAS	Fas cell surface death receptor	Activates apoptotic signaling pathway; involved in follicular atresia and corpus luteum regression.
AGTR2	Angiotensin II receptor type 2	G protein-coupled receptor; regulates local ovarian blood flow and follicle development.
PTPRC	Protein tyrosine phosphatase receptor type C (CD45)	Leukocyte marker; regulates immune cell signaling.
KIT	KIT proto-oncogene, receptor tyrosine kinase	Expressed in oocytes and granulosa cells; regulates follicular initiation, recruitment, and development.
CCKAR	Cholecystokinin A receptor	G protein-coupled receptor; mediates cholecystokinin signaling.
DRD4	Dopamine receptor D4	G protein-coupled receptor; involved in neuroendocrine regulation.
ESR1	Estrogen receptor 1 (ERα)	Nuclear receptor; mediates main physiological effects of estrogen; highly expressed in endometrium and ovaries; regulates reproductive functions.
ERAP1	Endoplasmic reticulum aminopeptidase 1	Participates in antigen processing and peptide trimming for MHC class I presentation.
ADRB2	Adrenergic receptor beta 2	G protein-coupled receptor; mediates sympathetic nerve signals; affects ovarian blood flow and hormone secretion.
CCR5	C-C motif chemokine receptor 5	G protein-coupled receptor; involved in chemotaxis of inflammatory cells and immune regulation.
ERBB2	Erb-b2 receptor tyrosine kinase 2 (HER2)	Member of EGFR family; tyrosine kinase receptor; cooperates with EGFR to affect cell proliferation and differentiation.
STAT3	Signal transducer and activator of transcription 3	Mediates signaling of multiple cytokines; involved in cell proliferation, survival, and differentiation.

EDNRA	Endothelin receptor type A	G protein-coupled receptor; regulates vascular contraction; affects ovarian blood flow.
MMP1	Matrix metallopeptidase 1	Degrades type I, II, and III collagen; involved in extracellular matrix remodeling.
CDC25C	Cell division cycle 25C	Phosphatase that activates CDK1; regulates G2/M transition.
AHR	Aryl hydrocarbon receptor	Transcription factor; mediates toxic effects of polycyclic aromatic hydrocarbons; regulates xenobiotic metabolism.
STAT1	Signal transducer and activator of transcription 1	Mediates interferon signaling; participates in immune regulation and apoptosis.
CCR2	C-C motif chemokine receptor 2	Receptor for monocyte chemoattractant protein-1 (MCP-1); involved in monocyte chemotaxis.
SMAD3	SMAD family member 3	Key signal transducer in transforming growth factor-β (TGF-β) pathway; regulates gene expression.
CYP1A2	Cytochrome P450 family 1 subfamily A member 2	Metabolizes polycyclic aromatic hydrocarbons, caffeine, and other xenobiotics; involved in drug metabolism.

Supplementary Table 2. List of target protein abbreviations, full names, and functions corresponding to Figure 1D.

Note: Protein information is derived from the UniProt database *(*https://www.uniprot.org/*)*.

Abbreviation	Full Name	Function
CDK1	Cyclin-dependent kinase 1	Regulates G2/M transition; phosphorylates substrates for centrosome separation, Golgi dynamics, nuclear envelope breakdown, and chromosome condensation; involved in oocyte maturation and follicle development.
STAT3	Signal transducer and activator of transcription 3	Mediates signaling of multiple cytokines; involved in cell proliferation, survival, and differentiation.
FAS	Fas cell surface death receptor	Activates apoptotic signaling pathway; involved in follicular atresia and corpus luteum regression.
DRD2	Dopamine receptor D2	G protein-coupled receptor; inhibits adenylate cyclase; involved in neuroendocrine regulation of

		hypothalamic-pituitary-ovarian axis.
EGFR	Epidermal growth factor receptor	Transmembrane protein; activates intracellular signaling promoting cell proliferation and survival; crucial for follicle development and granulosa cell proliferation.
CYP1B1	Cytochrome P450 family 1 subfamily B member 1	Endoplasmic reticulum enzyme; metabolizes polycyclic aromatic hydrocarbons and 17β-estradiol; involved in procarcinogen activation.
ZAP70	Zeta chain of T cell receptor associated protein kinase 70	Participates in T cell activation and signal transduction.
STAT1	Signal transducer and activator of transcription 1	Mediates interferon signaling; participates in immune regulation and apoptosis.
GRB2	Growth factor receptor bound protein 2	Adaptor protein; mediates receptor tyrosine kinase signaling.
ESR2	Estrogen receptor 2 (ERβ)	Nuclear receptor; mediates physiological effects of estrogen.
MMP9	Matrix metalloproteinase 9	Degrades extracellular matrix components; involved in tissue remodeling during ovulation, corpus luteum formation and regression.
ITK	IL2 inducible T cell kinase	Tec family non-receptor tyrosine kinase; involved in T cell signaling.
GSTP1	Glutathione S-transferase pi 1	Detoxification enzyme; catalyzes conjugation of electrophilic compounds with glutathione.
ADRB1	Adrenergic receptor beta 1	G protein-coupled receptor; mediates sympathetic nerve signals; affects cardiovascular function.
AGTR2	Angiotensin II receptor type 2	G protein-coupled receptor; regulates local ovarian blood flow and follicle development.
PTPRC	Protein tyrosine phosphatase receptor type C (CD45)	Leukocyte marker; regulates immune cell signaling.
TOP2A	DNA topoisomerase II alpha	Regulates DNA topology; participates in DNA replication and chromosome segregation; affects cell proliferation.
KCNA5	Potassium voltage-gated channel subfamily A member 5	Regulates cell membrane potential.

ADRB2	Adrenergic receptor beta 2	G protein-coupled receptor; mediates sympathetic nerve signals; affects ovarian blood flow and hormone secretion.
CASP1	Caspase 1	Involved in inflammasome activation and pyroptosis.
ESR1	Estrogen receptor 1 (ERα)	Nuclear receptor; mediates main physiological effects of estrogen; highly expressed in endometrium and ovaries; regulates reproductive functions.
APEX1	APEX nuclease (multifunctional DNA repair enzyme) 1	Multifunctional DNA repair enzyme; involved in base excision repair.
HDAC9	Histone deacetylase 9	Histone deacetylase; represses transcription by recruiting multi-protein complex to MEF2; regulates gene expression.
LCK	LCK proto-oncogene, Src family tyrosine kinase	Involved in T cell activation and signaling.
CCR5	C-C motif chemokine receptor 5	G protein-coupled receptor; involved in chemotaxis of inflammatory cells and immune regulation.
ERBB2	Erb-b2 receptor tyrosine kinase 2 (HER2)	Member of EGFR family; tyrosine kinase receptor; cooperates with EGFR to affect cell proliferation and differentiation.
NTRK3	Neurotrophic receptor tyrosine kinase 3	Receptor tyrosine kinase; mediates neurotrophin signaling; involved in neuronal development and survival.
NFKB1	Nuclear factor kappa B subunit 1	Transcription factor; regulates inflammation and immune responses.
EDNRA	Endothelin receptor type A	G protein-coupled receptor; regulates vascular contraction; affects ovarian blood flow.
MMP1	Matrix metallopeptidase 1	Degrades type I, II, and III collagen; involved in extracellular matrix remodeling.
HPRT1	Hypoxanthine phosphoribosyltransferase 1	Participates in purine salvage synthesis pathway.
KCNH2	Potassium voltage-gated channel subfamily H member 2	Participates in cardiac action potential repolarization.
TLR8	Toll-like receptor 8	Recognizes viral single-stranded RNA; activates innate immunity.

MDM4	MDM4 regulator of p53	Inhibits p53 transcriptional activity; regulates cell cycle and apoptosis.
CXCR2	C-X-C motif chemokine receptor 2	Binds IL-8; mediates neutrophil chemotaxis.

Supplementary Table 3. Redocking validation results for the three target proteins

Protein	PDB ID	Co-crystallized	Redocking RMSD (Å)
BaP	EGFR	AQ4 (Erlotinib)	2.570
BaP	ESR1	29S (Bazedoxifene)	0.972
BaP	STAT3	KQV (SD36)	1.689

Supplementary Table 4. Grid parameters used for blind molecular docking of BaP with the three target proteins.

Protein	PDB ID	Grid Center (x, y, z)	Grid Points (npts)	Spacing (Å)	Physical Size (Å)
EGFR	1M17	(23.568, 9.824, 59.396)	126, 76, 62	0.986	124.2 × 74.9 × 61.1
ESR1	6PSJ	(16.112, -24.947, 22.318)	124, 112, 108	0.547	67.8 × 61.3 × 59.1
STAT3	6NJS	(-2.257, 19.470, 24.491)	80, 124, 102	0.917	73.4 × 113.7 × 93.5

Supplementary Table 5. The result of molecular docking

Ingredient	Target	Binding energy (kcal·mol-1)
BaP	EGFR	-7.33
BaP	ESR1	-9.12
BaP	STAT3	-6.44

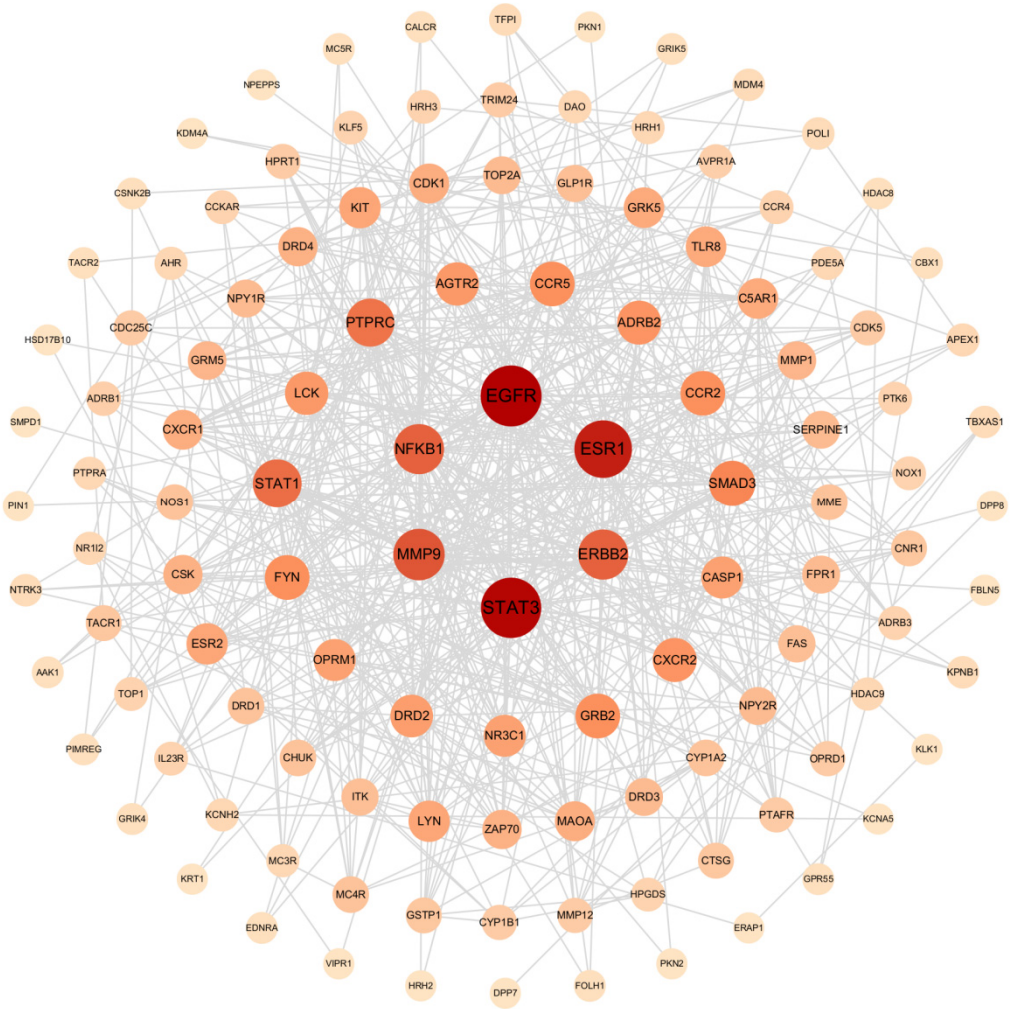
Supplementary Table 6. Primary antibody information

Antibody	Concentration	Species	Manufacturer
EGFR	1:1000	Rabbit	CST
ESR1	1:1000	Rabbit	Proteintech
STAT3	1:1000	Rabbit	Proteintech
β-actin	1:3000	Mouse	Sigma

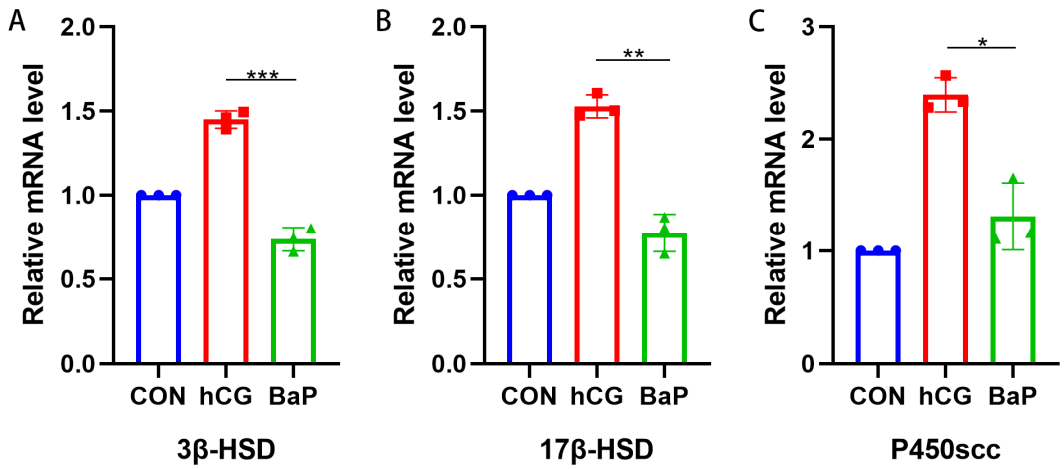
Supplementary Table 7. Primers sequence of genes

GENE	Forward	Reverse

3β-HSD	F:5' AGTACGTCCACTCTTCTGTCCA 3'	R:5' GTGCCGCCGTTTTTCAGATT 3'
17β-HSD	F:5' GGTGCTTGGCTTTCCAACTG 3'	R:5' GTCCTTGCTGGCTAACGAGT 3'
P450scc	F: 5' TGCCAGACCTTTCTGAGTGC 3'	R: 5' TACTGGTGATAGGCGACCCA 3'
β-actin	F:5' CCTCGCCTTTGCCGATCC 3'	R:5' GGATCTTCATGAGGTAGTCAGTC 3'



Supplementary Figure 1. PPI network diagram of BaP. Visualization of PPI network of BaP.



Supplementary Figure 2 A. PCR analysis of 3β-HSD; B. PCR analysis of 17β-HSD; C. PCR analysis of P450scc. Data are presented as mean ± SD. *: $p < 0.05$, **: $p < 0.01$, ***: $p < 0.001$ compared to control group.